

Combined Theoretical and Experimental Studies Unravel Multiple Pathways to Convergent Asymmetric Hydrogenation of Enamides.

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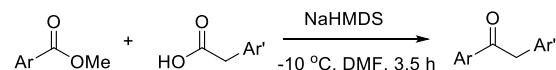
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1. General methods

All reactions were conducted under dry and inert atmosphere using magnetic stirring. CH_2Cl_2 , used in the hydrogenation, was freshly distilled from CaH_2 under nitrogen. THF was freshly distilled from sodium-benzophenone under nitrogen. All reagents were used as supplied commercially without further purification. Chromatographic separations were performed on Kiesel gel 60 H silica gel (particle size: 0.063-0.100 mm) or Brockmann I, activated. Thin layer chromatography (TLC) was performed on aluminum plates coated with Kieselgel 60 (0.20 mm, UV254) and visualized under ultraviolet light ($\nu = 254 \text{ nm}$). ^1H NMR spectra were recorded on a Bruker 400 or 500 at 400/500 MHz in CDCl_3 and referenced internally to the residual CHCl_3 peak (7.26 ppm). ^{13}C NMR spectra were recorded at 100 MHz in CDCl_3 and referenced to the central peak of CDCl_3 (77.16 ppm). Chemical shifts are reported in ppm (δ scale). Enantiomeric excesses were determined either using chiral HPLC, SFC or GC with a diode array detector at 220 and 254 nm. Racemic compounds were used for comparison. HRMS data were obtained using a Bruker MicroTOF-Q II instrument operation at ambient temperature. Optical rotations were recorded on an Autopol IV polarimeter from Rudolph Research Analytical, equipped with a sodium lamp (589 nm) and a 10 cm cell.

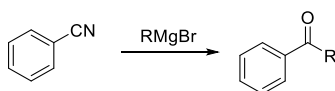
2. General procedure for substrates synthesis

2.1. General procedure for preparation of 1,2-diarylethan-1-one



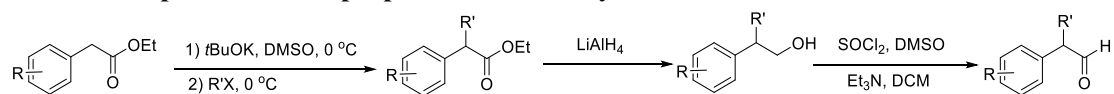
To a solution of aromatic acetic acid (10 mmol, 1.0 equiv.) and aromatic methyl ester (10 mmol, 1.0 equiv.) in DMF (30 mL) was added NaHMDS (2.0 M in THF) (20 mL, 40 mmol, 4.0 equiv.) at -10°C over 1 min. The resulting mixture was stirred at -10°C for 3.5 hours. To the resulting solution was then added saturated aqueous NH_4Cl solution. The resulting mixture was extracted with EtOAc (2x100 ml). The combined organic phase was washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by silica gel column chromatography.

2.2 General procedure for preparation α -Aryl-Alkyl ketones



Grignard reagent (15 mmol, 1.5 equiv.) was slowly added to a solution of cyano (-CN) (10 mmol, 1.0 equiv.) aromatic compounds in dry THF (30 mL) at 0°C . The reaction was allowed to stir at room temperature for 16 h. The reaction was quenched by addition of a saturated aqueous NH_4Cl solution, and 1M HCl was added and the mixture was stirred for 1 h. The mixture was extracted with Et_2O (3x100 ml). The combined organic phases were combined and washed brine and dried over Na_2SO_4 . The solvent was evaporated under reduced pressure to afford the crude products which then were purified by column chromatography on silica gel.

2.3 General procedure for preparation of aldehydes



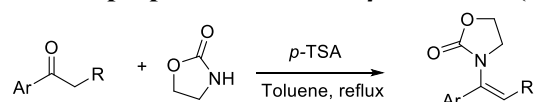
Potassium tert-butoxide (1 equiv.) was suspended in dry DMF (7 mL/10 mmol) at 0°C under nitrogen atmosphere and methyl phenylacetate (1 equiv.) was added in one portion, followed

by alkyl halide (1 equiv.) after 2 min. The reaction was allowed to warm up to room temperature and magnetic stirring was continued for 1 h. Water (10 mL) was added and the solution was extracted with CH₂Cl₂ (2 times). The organic layers were washed with 10 mL of a saturated, aqueous solution of NH₄Cl and 10 mL of water, and dried over Na₂SO₄. The solvent was evaporated and the crude product was purified by column chromatography.

LiAlH₄ (1.2 equiv.) was suspended in dry Et₂O (3 mL/10 mmol). Then, a solution of alkylated ester (1 equiv.) in 20 mL of Et₂O was added slowly while stirring. The reaction was monitored by TLC and after complete consumption of the ester the reaction was quenched by adding water. The layers were separated and the aqueous layer was extracted with CH₂Cl₂ (2 times). The combined organic layers were dried over Na₂SO₄. The solvent was evaporated and the product was obtained as colorless oil after purification by column chromatography.

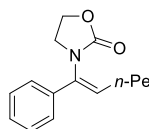
To a solution of oxalyl chloride (1.1 equiv.) in CH₂Cl₂ (13 mL/10 mmol) was added a solution of DMSO (2.4 equiv.) in CH₂Cl₂ (3 mL/10 mmol) at -78 °C. The solution was stirred for 10 min and alcohol (1 equiv.) in CH₂Cl₂ (20 mL/10 mmol) was added. After 15 min, Et₃N (7.5 mL/ 10 mmol of alcohol) was added, and the solution was allowed to warm up to room temperature and stirred for 1 h. Water was added to quench the reaction, the phases were separated, and the aqueous layer was extracted with CH₂Cl₂ (2 times). The organic phase was washed with water, dried over Na₂SO₄, and the solvent was evaporated. The corresponding aldehyde was obtained as colorless solid after silica-gel flash chromatography.

2.4. General procedure for the preparation of the α,β -enamides (*Z*-isomer)

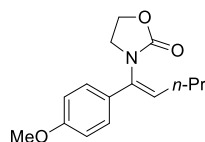


A solution of the ketone (10 mmol, 1.0 equiv.), 2-oxazolidinone (30 mmol, 2.610g, 3 equiv.), and 10 mol% of *p*-toluenesulfonic acid (1 mmol, 190 mg) in toluene (30 mL: 10 mmol ketone) was heated to reflux and the formed water was removed by azeotropic distillation over 36 h. After cooling the solution to room temperature, it was washed with a saturated, aqueous solution of NH₄Cl (10 mL) and water (10 mL), and the combined organic layers were dried over Na₂SO₄. After evaporation of the organic solvent and purification by silica-gel flash chromatography (pentane/ethyl acetate 80:20 to 70:30), the pure *Z*-isomers of the α,β -enamides were obtained.

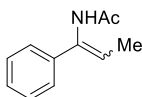
Characterization for the following compounds have been previously reported: **1a-1k**,¹ **2a-2c**,¹ **2f-2h**,¹ **4a**,² **4b**,³ **4c**,¹ **11c**,^{4,5} **11d**.⁶



(*Z*)-3-(1-phenylhept-1-en-1-yl)oxazolidin-2-one (*Z*-2d) White solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.27 (m, 5H), 6.01 (t, *J* = 7.2 Hz, 1H), 4.54 – 4.41 (m, 2H), 3.70 – 3.55 (m, 2H), 2.22 (q, *J* = 7.3 Hz, 2H), 1.58 – 1.44 (m, 2H), 1.44 – 1.31 (m, 4H), 0.91 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 156.6, 136.0, 133.8, 131.0, 128.8, 128.3, 126.0, 62.4, 45.8, 31.8, 28.7, 28.4, 22.6, 14.1. HRMS-ESI calcd for C₁₆H₂₁NO₂ [M+Na]⁺ : 282.1465, found: 282.1463.



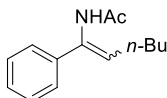
(Z)-3-(1-(4-methoxyphenyl)pent-1-en-1-yl)oxazolidin-2-one(Z-2e) Colorless oil. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.23 (m, 2H), 6.92 – 6.83 (m, 2H), 5.89 (t, *J* = 7.2 Hz, 1H), 4.53 – 4.41 (m, 2H), 3.81 (s, 3H), 3.68 – 3.60 (m, 2H), 2.18 (q, *J* = 7.3 Hz, 2H), 1.62 – 1.48 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 159.8, 156.6, 133.6, 128.9, 128.6, 127.3, 114.2, 62.4, 55.5, 45.9, 30.4, 22.4, 14.2. HRMS-ESI calcd for C₁₅H₁₉NO₃ [M+Na]⁺ : 284.1257, found: 284.1244.



(Z/E)-N-(1-phenylprop-1-en-1-yl)acetamide(11a)⁷ White solid. (*Z*)-*N*-Acetyl-1-phenylpropenamine (rotamers ratio 1.9:1): Major rotamer: ¹H NMR (400 MHz, CDCl₃): δ 7.23-7.45 (m, 5H), 6.57 (br, s, 1H), 5.97 (q, *J* = 6.9 Hz, 1H), 2.19 (s, 3H) 1.77 (d, *J* = 7.0 Hz, 3H). Minor rotamer: δ 7.23-7.45 (m, 5H), 6.58 (br, s, 1H), 6.05 (q, *J* = 7.0 Hz, 1H), 1.86 (d, *J* = 7.0 Hz, 3H), 1.82 (s, 3H).

(*Z*)-*N*-Acetyl-1-phenylpropenamine (rotamers are not splitted in DMSO): ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.10 (s, 1H), 7.21 - 7.40 (m, 5H), 5.90 (q, *J* = 6.8 Hz, 1H), 2.01 (s, 3H), 1.63 - 1.70(m, 3H).

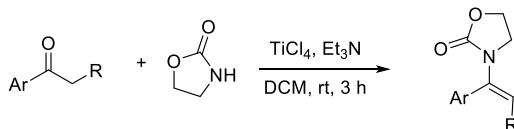
Isolated (*E*)- *N*-Acetyl-1-phenylpropenamine: ¹H NMR (400 MHz, CDCl₃): δ 7.30-7.40 (m, 5H), 6.62 (br, s, 1H), 6.33 (q, *J* = 6.42, 1H), 2.03-2.04 (m, 3H), 1.83-1.86 (m, 1H), 1.70 (d, *J* = 7.2 Hz, 3H). HRMS-ESI calcd for C₁₁H₁₃NO [M+Na]⁺ : 198.0889, found: 198.0895.



(Z/E)-N-(1-phenylhex-1-en-1-yl)acetamide(11b) White solid. (*Z*)-*N*-(1-phenylhex-1-en-1-yl)acetamide (rotamers ratio 1.6:1) Major rotamer: ¹H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.12 (m, 5H), 6.61 (br, s, 1H), 5.86 (t, *J* = 7.11 Hz, 1H), 2.21 – 2.11 (m, 5H), 1.52 – 1.33 (m, 4H), 0.93 (t, *J* = 7.20 Hz, 3H). Minor rotamer: ¹H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.20 (m, 5H), 6.61 (br, s, 1H), 5.94 (t, *J* = 7.42 Hz, 1H), 2.28 – 2.21 (m, 2H), 2.17 (s, 3H), 1.52 – 1.33 (m, 4H), 0.93 (t, *J* = 7.30 Hz, 3H).

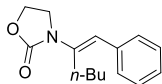
(*E*)-*N*-(1-phenylhex-1-en-1-yl)acetamide. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.22 (m, 5H), 6.52 (br, s, 1H), 6.30 (t, *J* = 7.79 Hz, 1H), 2.07 – 2.00 (m, 5H), 1.35 – 1.17 (m, 4H), 0.83 (t, *J* = 7.19 Hz, 3H). HRMS-ESI calcd for C₁₄H₁₉NO [M+Na]⁺ : 240.1359, found: 240.1346.

2.5. General procedure for the preparation of the α,β- enamides (*E*-isomer)

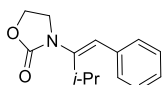


A nitrogen-flooded sealed vial containing corresponding ketones (1.1 equiv.) in dry CH₂Cl₂ was cooled down to 0°C before TiCl₄ (1M solution in CH₂Cl₂ or neat, 1.2 equiv.) was added dropwise. The resulting light yellow/orange solution was stirred at this temperature for 5 min and 0°C 2-oxazolidone (1 equiv.) pre-dissolved in CH₂Cl₂ (5 mL) was added slowly followed by dropwise addition of NEt₃ (5 equiv.). The color of the reaction mixture turned black upon addition of the base, a color change that did not occur when using most other bases. The reaction mixture was allowed to warm up to r.t. and was stirred over 3 h with regular monitoring using thin layer chromatography plates (eluent: ethyl acetate 1:2 pentane). The crude mixture was cooled to 0°C, quenched by water (4 equiv.) and diluted with CH₂Cl₂

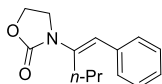
followed by portwise addition of silica. The mixture was filtered by celite. The filtrate was washed with water. The layers were separated and the organic phase was extracted with CH_2Cl_2 (3×50 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel (ethyl acetate/pentane, gradient from 1:4 to 1:2) to provide clean *E*-enamides.



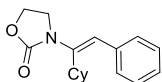
(E)-3-(1-phenylhex-1-en-2-yl)oxazolidin-2-one (E-3a) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.30 (m, 2H), 7.25 – 7.19 (m, 3H), 6.18 (s, 1H), 4.44 – 4.35 (m, 2H), 3.94 – 3.83 (m, 2H), 2.77 – 2.66 (m, 2H), 1.56 – 1.47 (m, 2H), 1.33 (h, $J = 7.3$ Hz, 2H), 0.87 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) 155.2, 140.1, 136.4, 129.0, 128.4, 126.7, 117.3, 61.5, 46.5, 30.8, 27.4, 22.6, 14.0, HRMS-ESI calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 268.1313, found: 268.1308.



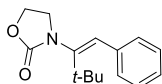
(E)-3-(3-methyl-1-phenylbut-1-en-2-yl)oxazolidin-2-one (E-3b) White solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.27 (m, 4H), 7.26 – 7.21 (m, 1H), 6.34 (s, 1H), 4.31 – 4.21 (m, 2H), 3.49 – 3.40 (m, 2H), 3.00 (heptd, $J = 6.8, 1.4$ Hz, 1H), 1.19 (d, $J = 6.9$ Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.8, 142.5, 135.6, 128.7, 128.0, 127.6, 123.0, 62.6, 46.0, 31.8, 20.8. HRMS-ESI calcd for $\text{C}_{14}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 254.1157, found: 254.1169.



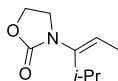
(E)-3-(1-phenylpent-1-en-2-yl)oxazolidin-2-one (E-3c) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.30 (m, 2H), 7.25 – 7.18 (m, 3H), 6.19 (s, 1H), 4.44 – 4.36 (m, 2H), 3.94 – 3.87 (m, 2H), 2.74 – 2.62 (m, 2H), 1.62 – 1.48 (m, 2H), 0.92 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.2, 139.9, 136.4, 129.0, 128.4, 126.7, 61.5, 46.5, 29.5, 21.9, 13.9, HRMS-ESI calcd for $\text{C}_{14}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 254.1157, found: 254.11538.



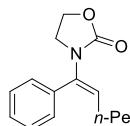
(E)-3-(1-cyclohexyl-2-phenylvinyl)oxazolidin-2-one (E-3d) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.26 (m, 4H), 7.25 – 7.20 (m, 1H), 6.30 (s, 1H), 4.31 – 4.20 (m, 2H), 3.49 – 3.34 (m, 2H), 2.61 (tdt, $J = 10.1, 3.0, 1.4$ Hz, 1H), 2.06 – 1.94 (m, 2H), 1.82 (dt, $J = 12.4, 3.0$ Hz, 2H), 1.77 – 1.69 (m, 1H), 1.45 – 1.09 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.9, 141.9, 135.7, 128.7, 128.1, 127.5, 123.5, 62.5, 46.2, 41.7, 31.5, 26.4, 26.4. HRMS-ESI calcd for $\text{C}_{17}\text{H}_{21}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 294.1470, found: 294.1479.



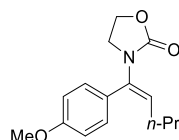
(E)-3-(3,3-dimethyl-1-phenylbut-1-en-2-yl)oxazolidin-2-one (E-3e) White solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.27 (m, 2H), 7.30 – 7.20 (m, 3H), 6.64 (s, 1H), 4.43 – 3.88 (m, 2H), 3.71 – 3.17 (m, 2H), 1.27 (d, $J = 1.0$ Hz, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.1, 145.4, 135.5, 128.8, 128.0, 127.7, 126.6, 62.3, 47.3, 38.8, 29.7, HRMS-ESI calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 268.1313, found: 268.1302.



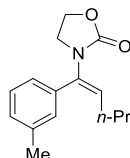
(E)-3-(4-methylpent-2-en-3-yl)oxazolidin-2-one(E-3f) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 5.50 (q, $J = 7.1$ Hz, 1H), 4.38 – 4.29 (m, 2H), 3.77 – 3.67 (m, 2H), 2.96 (p, $J = 7.0$ Hz, 1H), 1.72 (d, $J = 7.1$ Hz, 3H), 1.10 (d, $J = 7.0$ Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.1, 141.7, 123.6, 61.8, 49.7, 29.2, 20.8, 12.9, HRMS-ESI calcd for $\text{C}_9\text{H}_{15}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 192.1000, found: 192.0993.



(E)-3-(1-phenylhept-1-en-1-yl)oxazolidin-2-one(E-2d) White solid. ^1H NMR (500 MHz, Chloroform-*d*) δ 7.40 – 7.35 (m, 2H), 7.35 – 7.31 (m, 1H), 7.28 – 7.25 (m, 2H), 5.86 (t, $J = 7.8$ Hz, 1H), 4.36 – 4.23 (m, 2H), 3.59 – 3.44 (m, 2H), 2.10 (q, $J = 7.7$ Hz, 2H), 1.42 (p, $J = 7.3$ Hz, 2H), 1.30 – 1.20 (m, 4H), 0.86 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 156.6, 134.8, 134.4, 129.0, 128.5, 128.3, 126.0, 61.6, 46.2, 31.5, 29.7, 28.1, 22.6, 14.1. HRMS-ESI calcd for $\text{C}_{16}\text{H}_{21}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 282.1465, found: 282.1463.

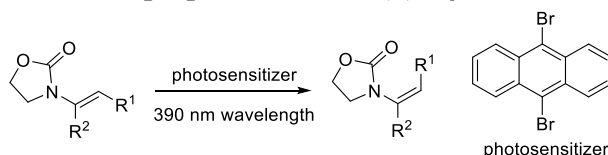


(E)-3-(1-(4-methoxyphenyl)pent-1-en-1-yl)oxazolidin-2-one(E-2e) White solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.21 (m, 2H), 6.90 – 6.82 (m, 2H), 5.88 (t, $J = 7.2$ Hz, 1H), 4.52 – 4.40 (m, 2H), 3.81 (s, 3H), 3.68 – 3.58 (m, 2H), 2.18 (q, $J = 7.3$ Hz, 2H), 1.60 – 1.46 (m, 2H), 0.97 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.8, 156.6, 133.6, 128.9, 128.6, 127.3, 114.2, 62.4, 55.5, 45.9, 30.4, 22.3, 14.2. HRMS-ESI calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_3$ $[\text{M}+\text{Na}]^+$: 284.1257, found: 284.1232.

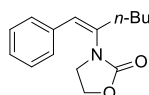


(E)-3-(1-(m-tolyl)pent-1-en-1-yl)oxazolidin-2-one(E-2g) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.23 (m, 1H), 7.14 (d, $J = 7.6$ Hz, 1H), 7.06 (d, $J = 7.4$ Hz, 2H), 5.84 (t, $J = 7.7$ Hz, 1H), 4.34 – 4.25 (m, 2H), 3.59 – 3.47 (m, 2H), 2.36 (s, 3H), 2.08 (q, $J = 7.6$ Hz, 2H), 1.44 (h, $J = 7.3$ Hz, 2H), 0.90 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.7, 138.2, 134.8, 134.7, 129.5, 129.1, 128.4, 126.2, 125.8, 61.6, 46.2, 30.2, 23.2, 21.6, 13.9. HRMS-ESI calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 268.1308, found: 268.1314.

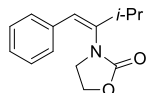
2.6. General procedure for the preparation of the (Z)- α,β -enamides from *E* isomer



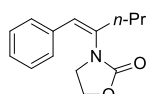
A solution of (*E*)- α,β -enamides (1.0 equiv.) and a catalytic amount (5 mol%) of photosensitizer in CH_2Cl_2 (2 mL/2 mmol enamides) was irradiated using 390 nm sodium lamp overnight. The solvent was removed under vacuum. After purification by silica-gel flash chromatography, the pure *Z*-enamides were obtained.



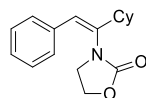
(Z)-3-(1-phenylhex-1-en-2-yl)oxazolidin-2-one(Z-3a) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.27 (m, 4H), 7.26 – 7.21 (m, 1H), 6.28 (s, 1H), 4.34 – 4.24 (m, 2H), 3.52 – 3.44 (m, 2H), 2.59 – 2.47 (m, 2H), 1.55 – 1.32 (m, 4H), 0.95 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.6, 137.1, 135.6, 128.7, 128.2, 127.6, 124.5, 62.7, 45.6, 33.9, 29.5, 22.5, 14.1, HRMS-ESI calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 268.1313, found: 268.1309.



(Z)-3-(3-methyl-1-phenylbut-1-en-2-yl)oxazolidin-2-one(Z-3b) White solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.28 (m, 2H), 7.27 – 7.20 (m, 3H), 6.47 (s, 1H), 4.41 – 4.31 (m, 2H), 3.85 (ddd, $J = 9.2, 6.7, 1.6$ Hz, 2H), 3.15 (pd, $J = 7.0, 1.5$ Hz, 1H), 1.13 (dt, $J = 7.0, 1.3$ Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.8, 143.7, 135.7, 128.9, 128.4, 128.4, 127.5, 61.9, 49.9, 30.2, 21.3. HRMS-ESI calcd for $\text{C}_{14}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 254.1157, found: 254.1154.

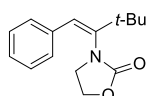


(Z)-3-(1-phenylpent-1-en-2-yl)oxazolidin-2-one(Z-3c) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.28 (m, 4H), 7.25 – 7.20 (m, 1H), 6.28 (s, 1H), 4.33 – 4.22 (m, 2H), 3.51 – 3.42 (m, 2H), 2.57 – 2.47 (m, 2H), 1.63 – 1.49 (m, 2H), 0.99 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.6, 136.9, 135.6, 128.7, 128.2, 127.6, 124.7, 62.7, 45.6, 36.3, 20.5, 13.8, HRMS-ESI calcd for $\text{C}_{14}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 254.1157, found: 254.1157.

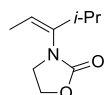


(Z)-3-(1-cyclohexyl-2-phenylvinyl)oxazolidin-2-one(Z-3d)

^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.32 (m, 2H), 7.31 – 7.21 (m, 3H), 6.49 (s, 1H), 4.44 – 4.35 (m, 2H), 3.92 – 3.83 (m, 2H), 2.81 (tt, $J = 12.1, 3.1$ Hz, 1H), 1.90 – 1.70 (m, 4H), 1.70 – 1.60 (m, 1H), 1.53 – 1.37 (m, 2H), 1.31 – 1.16 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.9, 143.2, 135.6, 129.2, 128.9, 128.5, 127.5, 61.9, 50.1, 41.1, 31.4, 26.2, 26.0. HRMS-ESI calcd for $\text{C}_{17}\text{H}_{21}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 294.1465, found: 294.1453.



(Z)-3-(3,3-dimethyl-1-phenylbut-1-en-2-yl)oxazolidin-2-one(Z-3e) White solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.28 (m, 2H), 7.28 – 7.21 (m, 3H), 6.68 (s, 1H), 4.44 – 4.36 (m, 2H), 3.93 – 3.85 (m, 2H), 1.08 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.1, 146.5, 136.9, 131.6, 128.7, 128.0, 127.1, 61.9, 50.8, 38.6, 30.7. HRMS-ESI calcd for $\text{C}_{15}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 268.1313, found: 268.1324.



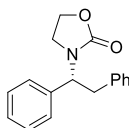
(Z)-3-(4-methylpent-2-en-3-yl)oxazolidin-2-one(Z-3f) Colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 5.48 (qd, $J = 6.8, 1.3$ Hz, 1H), 4.46 – 4.36 (m, 2H), 3.75 – 3.66 (m, 2H), 2.49 (ttt, $J = 6.8, 5.4, 1.5$ Hz, 1H), 1.61 (dd, $J = 6.9, 1.4$ Hz, 3H), 1.08 (s, 3H), 1.07 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.5, 140.8, 120.0, 62.3, 46.2, 31.6, 20.9, 13.0. HRMS-ESI calcd for $\text{C}_9\text{H}_{15}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 192.1000, found: 192.0992.

3. General procedure for asymmetric hydrogenation

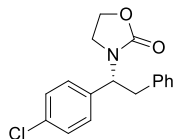
A vial was charged with substrate (0.015 mmol) and Ir-complex (1 mol%). Dry CH₂Cl₂ (1.5 mL) was added (so that the concentration of the substrate was 0.1 M) and the vial was placed in a high-pressure hydrogenation apparatus. The reactor was purged three times with Ar gas, then filled with H₂. The reaction was stirred at room temperature for 16 hours before the H₂ pressure was released and the solvent was removed *in vacuo*. The crude product was filtered through on a short plug of silica. Conversions were determined by ¹H NMR spectroscopy and *ee* values were determined by HPLC, SFC or GCMS using a chiral stationary phase.

Characterization for the following compounds have been previously reported: **12a**⁸, **12b**⁹, **12c**¹⁰, **12d**¹¹, **13a**¹².

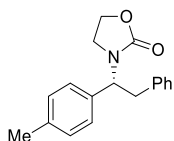
The characterization of the hydrogenated compounds:



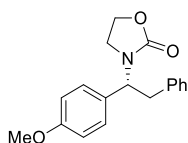
(R)-3-(1,2-diphenylethyl)oxazolidin-2-one(5a) White solid, 98% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.34 (m, 4H), 7.34 – 7.29 (m, 2H), 7.27 (tt, *J* = 3.5, 2.0 Hz, 3H), 7.24 – 7.18 (m, 1H), 5.35 (dd, *J* = 9.7, 6.7 Hz, 1H), 4.29 – 3.87 (m, 2H), 3.53 (td, *J* = 8.2, 6.9 Hz, 1H), 3.45 – 3.03 (m, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 138.4, 137.4, 128.8, 128.8, 128.7, 128.2, 127.7, 126.8, 61.9, 57.5, 40.9, 36.8, HRMS-ESI calcd for C₁₇H₁₇NO₂ [M+Na]⁺: 290.1151, found: 290.1157.



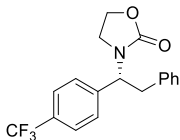
(R)-3-(1-(4-chlorophenyl)-2-phenylethyl)oxazolidin-2-one(5b) white solid, 92% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.34 (s, 4H), 7.32 – 7.27 (m, 2H), 7.25 – 7.19 (m, 3H), 5.31 (dd, *J* = 9.4, 7.1 Hz, 1H), 4.25 – 4.12 (m, 2H), 3.52 (td, *J* = 8.3, 6.7 Hz, 1H), 3.39 – 3.11 (m, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 137.1, 136.9, 134.1, 129.1, 129.1, 128.8, 128.8, 127.0, 62.0, 57.0, 41.0, 36.9, HRMS-ESI calcd for C₁₇H₁₆ClNO₂ [M+Na]⁺: 324.0762, found: 324.0757.



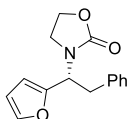
(R)-3-(2-phenyl-1-(p-tolyl)ethyl)oxazolidin-2-one(5c) White solid, 95% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.24 (m, 6H), 7.23 – 7.15 (m, 3H), 5.32 (dd, *J* = 9.6, 6.7 Hz, 1H), 4.18 – 4.10 (m, 2H), 3.52 (td, *J* = 8.2, 6.9 Hz, 1H), 3.36 – 3.20 (m, 3H), 2.35 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 138.0, 137.6, 135.4, 129.5, 128.9, 128.7, 127.6, 126.8, 61.9, 57.2, 40.8, 36.9, 21.2, HRMS-ESI calcd for C₁₈H₁₉NO₂ [M+Na]⁺: 304.1308, found: 304.1306.



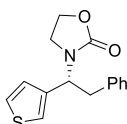
(R)-3-(1-(4-methoxyphenyl)-2-phenylethyl)oxazolidin-2-one(5d) white solid, 90% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.26 (m, 4H), 7.26 – 7.18 (m, 3H), 6.93 – 6.83 (m, 2H), 5.30 (dd, *J* = 9.5, 6.9 Hz, 1H), 4.18 – 4.12 (m, 2H), 3.80 (s, 3H), 3.51 (td, *J* = 8.2, 6.8 Hz, 1H), 3.35 – 3.18 (m, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 159.4, 158.0, 137.6, 130.5, 129.0, 128.9, 128.7, 126.8, 114.2, 61.9, 57.0, 55.4, 40.8, 37.1, HRMS-ESI calcd for C₁₈H₁₉NO₃ [M+Na]⁺: 320.1257, found: 320.1259.



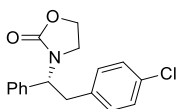
(R)-3-(2-phenyl-1-(4-(trifluoromethyl)phenyl)ethyl)oxazolidin-2-one(5e) White solid, 92% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 8.1 Hz, 2H), 7.53 (d, *J* = 8.1 Hz, 2H), 7.38 – 7.18 (m, 5H), 5.38 (dd, *J* = 9.3, 7.1 Hz, 1H), 4.30 – 4.10 (m, 2H), 3.56 (td, *J* = 8.3, 6.7 Hz, 1H), 3.39 – 3.14 (m, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 142.5, 136.8, 130.5 (q, *J* = 32.7 Hz), 128.9, 128.8, 128.1, 128.1, 127.1, 125.9 (q, *J* = 3.8 Hz), 122.7 (q, *J* = 272.2 Hz), 62.0, 57.2, 41.1, 36.8. ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -62.7. HRMS-ESI calcd for C₁₈H₁₆F₃NO₂ [M+Na]⁺: 358.1025, found: 358.1024.



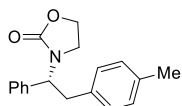
(R)-3-(1-(furan-2-yl)-2-phenylethyl)oxazolidin-2-one(5f) Colorless oil, 80% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.26 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.17 – 7.12 (m, 2H), 7.10 – 7.03 (m, 4H), 6.20 – 6.04 (m, 2H), 5.23 – 5.13 (m, 1H), 4.15 – 4.00 (m, 2H), 3.46 (td, *J* = 8.7, 6.1 Hz, 1H), 3.28 – 3.16 (m, 2H), 3.01 (dd, *J* = 14.1, 8.8 Hz, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 152.0, 142.5, 136.8, 128.9, 128.7, 127.0, 110.5, 108.5, 62.1, 52.0, 41.4, 36.6. HRMS-ESI calcd for C₁₅H₁₅NO₃ [M+Na]⁺: 280.0950, found: 280.0967.



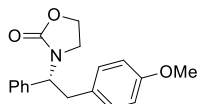
(R)-3-(2-phenyl-1-(thiophen-3-yl)ethyl)oxazolidin-2-one(5g) Colorless oil, 90% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.28 (m, 1H), 7.28 – 7.25 (m, 2H), 7.25 – 7.17 (m, 4H), 7.09 (dd, *J* = 5.0, 1.4 Hz, 1H), 5.39 (dd, *J* = 9.5, 6.4 Hz, 1H), 4.21 – 4.04 (m, 2H), 3.46 (dd, *J* = 8.7, 5.9 Hz, 1H), 3.34 (dd, *J* = 14.3, 6.3 Hz, 1H), 3.25 – 3.13 (m, 2H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 139.8, 137.2, 128.7, 128.7, 127.1, 126.9, 126.5, 122.6, 61.9, 53.3, 40.7, 37.7, HRMS-ESI calcd for C₁₅H₁₅NO₂S [M+Na]⁺: 296.0716, found: 296.0721.



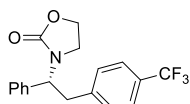
(R)-3-(2-(4-chlorophenyl)-1-phenylethyl)oxazolidin-2-one(5h) White solid, 98% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.34 (s, 4H), 7.31 – 7.27 (m, 2H), 7.25 – 7.19 (m, 3H), 5.31 (dd, *J* = 9.4, 7.1 Hz, 1H), 4.22 – 4.11 (m, 2H), 3.52 (td, *J* = 8.3, 6.7 Hz, 1H), 3.34 – 3.15 (m, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.0, 137.1, 136.9, 134.1, 129.1, 129.1, 128.8, 128.8, 127.0, 62.0, 57.0, 41.0, 36.9, HRMS-ESI calcd for C₁₇H₁₆ClNO₂ [M+Na]⁺: 324.0762, found: 324.0754.



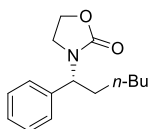
(R)-3-(1-phenyl-2-(p-tolyl)ethyl)oxazolidin-2-one(5i) White solid, 95% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.34 (m, 4H), 7.34 – 7.28 (m, 1H), 7.14 (d, J = 8.1 Hz, 2H), 7.09 (d, J = 7.9 Hz, 2H), 5.33 (dd, J = 9.8, 6.5 Hz, 1H), 4.20 – 4.09 (m, 2H), 3.53 (td, J = 8.3, 6.9 Hz, 1H), 3.37 – 3.18 (m, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.1, 138.6, 136.4, 134.3, 129.4, 128.9, 128.7, 128.2, 127.7, 61.9, 57.5, 40.8, 36.5, 21.2, HRMS-ESI calcd for $\text{C}_{18}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 304.1308, found: 304.1304.



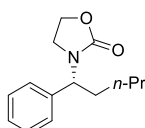
(R)-3-(2-(4-methoxyphenyl)-1-phenylethyl)oxazolidin-2-one(5j) Colorless oil, 98% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.28 (m, 5H), 7.19 – 7.14 (m, 2H), 6.85 – 6.80 (m, 2H), 5.29 (dd, J = 9.7, 6.6 Hz, 1H), 4.19 – 4.13 (m, 2H), 3.77 (s, 3H), 3.52 (td, J = 8.2, 7.0 Hz, 1H), 3.32 – 3.18 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.4, 158.1, 138.5, 129.8, 129.4, 128.9, 128.2, 127.7, 114.1, 61.9, 57.6, 55.3, 40.9, 36.0, HRMS-ESI calcd for $\text{C}_{18}\text{H}_{19}\text{NO}_3$ $[\text{M}+\text{Na}]^+$: 320.1257, found: 320.1242.



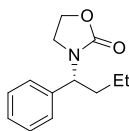
(R)-3-(1-phenyl-2-(4-(trifluoromethyl)phenyl)ethyl)oxazolidin-2-one(5k) White solid, 93% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, J = 8.0 Hz, 2H), 7.42 – 7.32 (m, 7H), 5.34 (dd, J = 8.6, 7.7 Hz, 1H), 4.18 (dd, J = 8.6, 7.4 Hz, 2H), 3.57 – 3.45 (m, 1H), 3.39 (d, J = 8.2 Hz, 2H), 3.24 (q, J = 8.3 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.0, 142.5, 136.8, 130.5 (q, J = 32.7 Hz), 128.9, 128.8, 128.1, 128.1, 127.1, 125.9 (q, J = 3.8 Hz), 122.7 (q, J = 272.2 Hz), 62.0, 57.2, 41.1, 36.8. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.5. HRMS-ESI calcd for $\text{C}_{18}\text{H}_{16}\text{F}_3\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 358.1025, found: 358.1028.



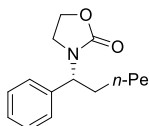
(R)-3-(1-phenylhexyl)oxazolidin-2-one(6a) Colorless oil, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.27 (m, 5H), 4.99 (dd, J = 8.6, 7.2 Hz, 1H), 4.35 – 4.15 (m, 2H), 3.54 – 3.39 (m, 1H), 3.25 – 3.11 (m, 1H), 2.02 – 1.85 (m, 2H), 1.40 – 1.26 (m, 6H), 0.89 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.3, 138.9, 128.8, 128.1, 127.8, 62.0, 56.6, 40.3, 31.7, 30.4, 26.2, 22.7, 14.1. HRMS-ESI calcd for $\text{C}_{15}\text{H}_{21}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 270.1465, found: 270.1479.



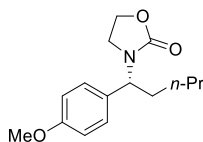
(R)-3-(1-phenylpentyl)oxazolidin-2-one(6b) Colorless oil, 92% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.27 (m, 5H), 4.98 (dd, J = 8.5, 7.3 Hz, 1H), 4.33 – 4.25 (m, 1H), 4.24 – 4.17 (m, 1H), 3.51 – 3.43 (m, 1H), 3.22 – 3.14 (m, 1H), 2.03 – 1.87 (m, 2H), 1.48 – 1.28 (m, 4H), 0.92 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.13, 138.74, 128.64, 127.87, 127.55, 61.82, 56.36, 40.09, 29.89, 28.48, 22.36, 13.92. HRMS-ESI calcd for $\text{C}_{14}\text{H}_{19}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 256.1308, found: 256.1313.



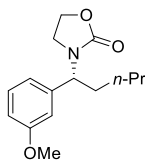
(R)-3-(1-phenylbutyl)oxazolidin-2-one(6c) Colorless oil, 93% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.27 (m, 5H), 5.00 (s, 1H), 4.33 – 4.14 (m, 2H), 3.52 – 3.40 (m, 1H), 3.24 – 3.14 (m, 1H), 1.99 – 1.88 (m, 2H), 1.46 – 1.32 (m, 2H), 0.99 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.3, 138.9, 128.8, 128.1, 127.7, 62.0, 56.2, 40.2, 32.5, 19.7, 13.9. HRMS-ESI calcd for $\text{C}_{13}\text{H}_{17}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 242.1151, found: 242.1165.



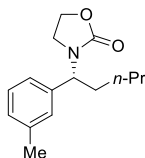
(R)-3-(1-phenylheptyl)oxazolidin-2-one(6d) Colorless oil, 93% yield. Colorless oil, 98% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.27 (m, 5H), δ 5.03 – 4.92 (m, 1H), 4.37 – 4.09 (m, 2H), 3.53 – 3.42 (m, 1H), 3.29 – 3.13 (m, 1H), 2.04 – 1.84 (m, 2H), 1.45 – 1.20 (m, 8H), 0.88 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.3, 138.9, 128.8, 128.1, 127.7, 62.0, 56.6, 40.3, 31.8, 30.4, 29.1, 26.5, 22.7, 14.2. HRMS-ESI calcd for $\text{C}_{16}\text{H}_{23}\text{NO}_2$ $[\text{M}+\text{Na}]^+$: 284.1621, found: 284.1641.



(R)-3-(1-(4-methoxyphenyl)pentyl)oxazolidin-2-one(6e) Colorless oil, 95% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.21 (m, 2H), 6.92 – 6.82 (m, 2H), 4.93 (t, $J = 7.9$ Hz, 1H), 4.33 – 4.14 (m, 2H), 3.44 (td, $J = 8.8, 6.1$ Hz, 1H), 3.23 – 3.09 (m, 1H), 1.98 – 1.84 (m, 3H), 1.47 – 1.23 (m, 5H), 0.91 (t, $J = 7.1$ Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.3, 158.3, 131.0, 128.9, 114.1, 62.0, 56.0, 55.4, 40.2, 30.3, 28.7, 22.5, 14.1. HRMS-ESI calcd for $\text{C}_{15}\text{H}_{21}\text{NO}_3$ $[\text{M}+\text{Na}]^+$: 286.1414, found: 286.1389.

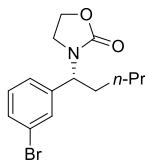


(R)-3-(1-(3-methoxyphenyl)pentyl)oxazolidin-2-one(6f) Colorless oil, 90% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.27 (t, $J = 7.9$ Hz, 1H), 6.93 – 6.81 (m, 3H), 4.95 (dd, $J = 8.7, 7.1$ Hz, 1H), 4.37 – 4.09 (m, 2H), 3.50 – 3.42 (m, 1H), 3.24 – 3.15 (m, 1H), 2.00 – 1.80 (m, 2H), 1.49 – 1.18 (m, 4H), 0.91 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.0, 158.3, 140.5, 129.8, 119.9, 113.8, 113.2, 62.0, 56.5, 55.4, 40.3, 30.1, 28.6, 22.6, 14.1. HRMS-ESI calcd for $\text{C}_{15}\text{H}_{21}\text{NO}_3$ $[\text{M}+\text{Na}]^+$: 286.1414, found: 286.1420.

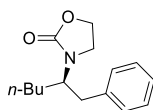


(R)-3-(1-(*m*-tolyl)pentyl)oxazolidin-2-one(6g) Colorless oil, 99% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.23 (t, $J = 7.5$ Hz, 1H), 7.16 – 7.07 (m, 3H), 4.94 (t, $J = 7.9$ Hz, 1H), 4.33 – 4.23 (m, 1H), 4.23 – 4.14 (m, 1H), 3.52 – 3.41 (m, 1H), 3.25 – 3.12 (m, 1H), 2.34 (s, 3H), 1.99 – 1.86 (m, 2H), 1.46 – 1.26 (m, 4H), 0.91 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.12, 138.63, 138.35, 128.59, 128.49, 128.42, 124.31, 61.79, 56.30, 40.05,

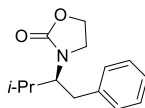
29.86, 28.48, 22.35, 21.40, 13.91. HRMS-ESI calcd for C₁₅H₂₁NO₂ [M+Na]⁺: 270.1465, found: 270.1467.



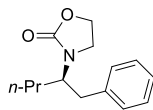
(R)-3-(1-(3-bromophenyl)pentyl)oxazolidin-2-one(6h) Colorless oil, 97% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.41 (m, 2H), 7.30 – 7.19 (m, 2H), 4.94 (t, *J* = 7.9 Hz, 1H), 4.35 – 4.18 (m, 2H), 3.47 (td, *J* = 8.8, 6.2 Hz, 1H), 3.25 – 3.15 (m, 1H), 1.91 (q, *J* = 8.4, 8.0 Hz, 1H), 1.46 – 1.24 (m, 4H), 0.92 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.05, 141.19, 131.05, 130.29, 126.32, 122.79, 61.87, 55.88, 40.04, 29.80, 28.38, 22.29, 13.89. HRMS-ESI calcd for C₁₄H₁₈BrNO₂ [M+Na]⁺: 334.0413, found: 334.0419.



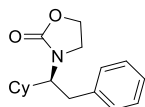
(R)-3-(1-phenylhexan-2-yl)oxazolidin-2-one(7a) Colorless oil, 99% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.26 (m, 2H), 7.24 – 7.17(m, 3H), 4.19 (dtd, *J* = 31.0, 8.7, 7.0 Hz, 2H), 4.09– 3.95(m, 1H), 3.45– 3.28 (m, 2H), 2.90 – 2.74 (m, 2H), 1.62 – 1.50 (m, 2H), 1.41– 1.20 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.2, 138.0, 129.0, 128.6, 126.7, 62.0, 54.7, 40.7, 39.2, 31.6, 28.6, 22.5, 14.1, HRMS-ESI calcd for C₁₅H₂₁NO₂ [M+Na]⁺: 270.1470, found: 270.1459.



(S)-3-(3-methyl-1-phenylbutan-2-yl)oxazolidin-2-one(7b) Colorless oil, 93% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.24 (m, 2H), 7.20 (dt, *J* = 5.9, 1.4 Hz, 3H), 4.19 – 4.09 (m, 1H), 4.05 – 3.91 (m, 1H), 3.80 – 3.67 (m, 1H), 3.41 – 3.21 (m, 2H), 3.12 (dd, *J* = 14.6, 4.4 Hz, 1H), 2.67 (dd, *J* = 14.6, 11.4 Hz, 1H), 1.97 – 1.79 (m, 1H), 1.08 (d, *J* = 6.7 Hz, 3H), 0.97 (d, *J* = 6.7 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.4, 138.2, 128.6, 126.6, 61.9, 60.5, 41.5, 36.1, 31.1, 20.2, 19.9. HRMS-ESI calcd for C₁₄H₁₉NO₂ [M+Na]⁺: 256.1313, found: 256.1308.

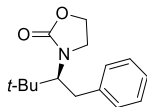


(R)-3-(1-phenylpentan-2-yl)oxazolidin-2-one(7c) Colorless oil, 92% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.26 (m, 2H), 7.23 – 7.18 (m, 3H), 4.26 – 4.02 (m, 3H), 3.43 – 3.29 (m, 2H), 2.87 – 2.76 (m, 2H), 1.63 – 1.46 (m, 2H), 1.42 – 1.24 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.2, 138.0, 129.0, 128.6, 126.7, 62.0, 54.4, 40.7, 39.2, 34.0, 19.7, 13.9, HRMS-ESI calcd for C₁₄H₁₉NO₂ [M+Na]⁺: 256.1313, found: 256.1317.



(S)-3-(1-cyclohexyl-2-phenylethyl)oxazolidin-2-one(7d) Colorless oil, 90% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.26 (m, 2H), 7.20 (s, 3H), 4.13 (ddd, *J* = 9.3, 8.4, 6.2 Hz, 1H), 4.03 – 3.95 (m, 1H), 3.78 (ddd, *J* = 11.4, 9.4, 4.5 Hz, 1H), 3.34 (ddd, *J* = 9.3, 8.3, 6.2 Hz, 1H), 3.29 – 3.20 (m, 1H), 3.13 (dd, *J* = 14.6, 4.5 Hz, 1H), 2.68 (dd, *J* = 14.6, 11.4 Hz,

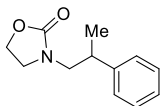
1H), 1.96 – 1.88 (m, 1H), 1.85 – 1.55 (m, 5H), 1.36 – 1.00 (m, 5H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 158.4, 138.4, 128.7, 128.7, 126.6, 61.9, 59.6, 42.0, 40.4, 35.8, 30.6, 30.1, 26.4, 26.1, 26.1, HRMS-ESI calcd for C₁₇H₂₃NO₂ [M+Na]⁺: 296.1626, found: 296.1615.



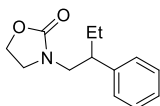
(S)-3-(3,3-dimethyl-1-phenylbutan-2-yl)oxazolidin-2-one(7e) Colorless oil, 93% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.26 (m, 2H), 7.23 – 7.16 (m, 3H), 4.26 – 4.00 (m, 2H), 3.97 – 3.74 (m, 1H), 3.70 – 3.52 (m, 1H), 3.51 – 3.40 (m, 1H), 3.17 – 3.00 (m, 1H), 2.87 – 2.60 (m, 1H), 1.08 (s, 9H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 159.2, 138.7, 128.8, 128.5, 126.7, 77.4, 62.0, 42.1, 35.9, 32.5, 27.7. HRMS-ESI calcd for C₁₅H₂₁NO₂ [M+Na]⁺: 270.1465, found: 270.1478.



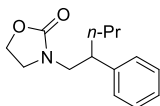
(S)-3-(2-methylpentan-3-yl)oxazolidin-2-one(7f) Colorless oil, 95% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 4.31 (dd, *J* = 8.4, 7.7 Hz, 2H), 3.41 (td, *J* = 7.8, 2.0 Hz, 2H), 3.33 (ddd, *J* = 11.4, 9.4, 3.7 Hz, 1H), 1.81 – 1.60 (m, 2H), 1.40 – 1.24 (m, 1H), 0.95 (d, *J* = 6.6 Hz, 3H), 0.91 – 0.83 (m, 6H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 159.1, 62.0, 61.2, 40.2, 31.0, 22.5, 20.0, 19.9, 11.0, HRMS-ESI calcd for C₉H₁₇NO₂ [M+Na]⁺: 194.1151, found: 194.1156.



3-(2-phenylpropyl)oxazolidin-2-one (8a) Colorless oil, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.27 (m, 2H), 7.27 – 7.19 (m, 3H), 4.14 (dd, *J* = 8.5, 7.6 Hz, 2H), 3.54 (dd, *J* = 13.9, 6.9 Hz, 1H), 3.35 – 3.21 (m, 2H), 3.18 – 3.00 (m, 2H), 1.28 (d, *J* = 7.0 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 158.5, 143.8, 128.6, 127.0, 126.7, 61.6, 51.2, 45.1, 38.6, 19.1. HRMS-ESI calcd for C₁₂H₁₅NO₂ [M+Na]⁺: 228.0995, found: 228.1000.

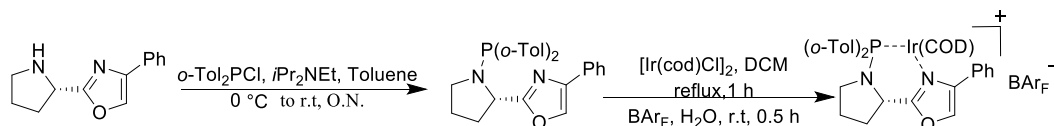


3-(2-phenylbutyl)oxazolidin-2-one (8b) Colorless oil, ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.27 (m, 2H), 7.27 – 7.19 (m, 3H), 4.14 (dd, *J* = 8.5, 7.6 Hz, 2H), 3.54 (dd, *J* = 13.9, 6.9 Hz, 1H), 3.35 – 3.21 (m, 2H), 3.18 – 3.00 (m, 2H), 1.60 – 1.50 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 158.5, 143.7, 128.5, 127.0, 126.7, 62.0, 54.4, 40.7, 39.2, 24.0, 21.2 HRMS-ESI calcd for C₁₃H₁₇NO₂ [M+Na]⁺: 242.1157, found: 242.1162.



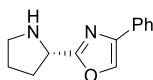
3-(2-phenylpentyl)oxazolidin-2-one (8c) Colorless oil, ¹H NMR (400 MHz, CDCl₃) δ 7.36 – 7.28 (m, 2H), 7.26 – 7.18 (m, 3H), 4.17 – 4.02 (m, 2H), 3.62 (dd, *J* = 13.9, 6.2 Hz, 1H), 3.31 – 3.17 (m, 2H), 3.07 – 2.97 (m, 1H), 2.90 (tt, *J* = 9.5, 5.8 Hz, 1H), 1.70 – 1.50 (m, 2H), 1.20 (h, *J* = 7.5 Hz, 2H), 0.85 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 158.5, 143.7, 128.5, 127.0, 126.7, 54.4, 46.0, 40.7, 39.2, 34.0, 19.9, 13.9. HRMS-ESI calcd for C₁₄H₁₉NO₂ [M+Na]⁺: 256.1313, found: 256.1307.

4. General procedure for the preparation of iridium complexes

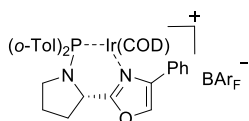


Amine (1 mmol) was co-evaporated with dry toluene (3 x 20 mL) and dissolved in dry toluene or THF (6 mL) under N₂. Freshly distilled di-*iso*-propylethylamine (3 mmol) was added and the solution was cooled to 0 °C in an ice-bath. Freshly distilled (prepared) suitable phosphine chloride (1.2 mmol) was dissolved in toluene (2 mL) and added dropwise to the reaction mixture and stirred at room temperature for 24 hours. After completion of the reaction, monitored by TLC, it was quenched with saturated NaHCO₃ solution and the reaction mixture was extracted in CH₂Cl₂ (3 x10 mL). The combined organic layers were dried over Na₂SO₄, filtered and concentrated under reduced pressure. The oily residual was quickly passed through a small pad of silica and used to make the Ir-complex without further characterization.

The synthesized oxazoline ligand was dissolved in CH₂Cl₂ (20 mL) and [Ir(COD)Cl]₂ (0.25 mmol) was added. The atmosphere in the flask was evacuated and replenished three times with N₂. The mixture was heated to reflux for 1 hour. After the solution was cooled to room temperature, distilled H₂O (20 mL) was added. Under vigorous stirring, NaBArF₄·xH₂O (0.6 mmol) was added to the biphasic solution in one portion. The mixture was stirred vigorously for 30 minutes and extracted with CH₂Cl₂ (3 x10 mL). Combined organic phase was dried over Na₂SO₄. After concentration in vacuum, the residue was purified on silica gel with CH₂Cl₂: pentane (1 : 1) as the eluent to afford the iridium complex as an orange solid.



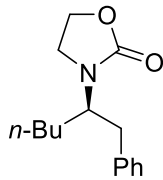
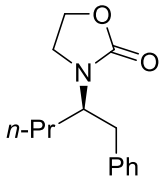
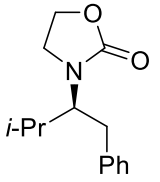
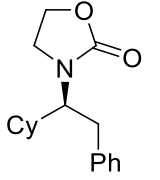
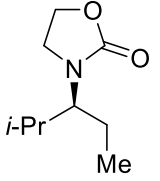
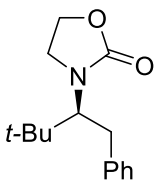
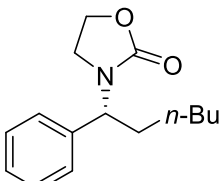
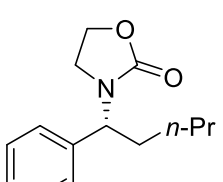
White solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (s, 1H), 7.77 – 7.68 (m, 2H), 7.42 – 7.33 (m, 2H), 7.33 – 7.26 (m, 1H), 4.39 (ddd, *J* = 7.6, 6.0, 1.2 Hz, 1H), 3.23 – 3.13 (m, 1H), 3.09 – 2.89 (m, 1H), 2.44 (s, 1H), 2.32 – 2.05 (m, 2H), 2.05 – 1.69 (m, 2H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.8, 140.6, 133.5, 131.2, 128.8, 128.03, 125.6, 55.74, 47.0, 31.0, 25.5. HRMS-EI calcd for C₁₃H₁₄NO[M+Na]⁺: 727.2425, found: 727.2445.

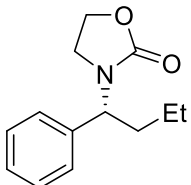
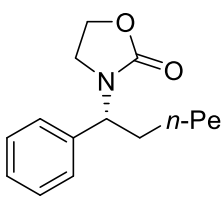
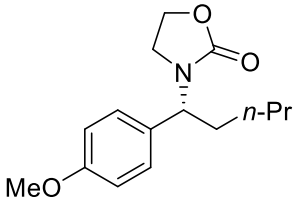
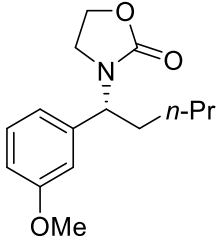
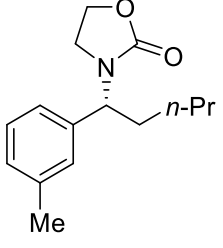
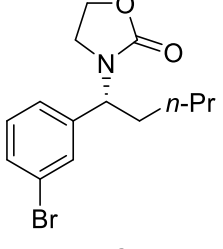
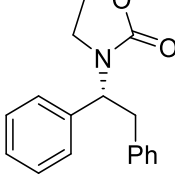
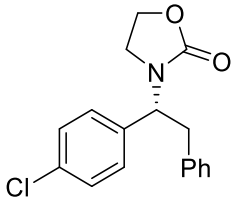


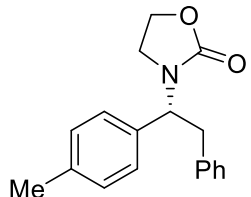
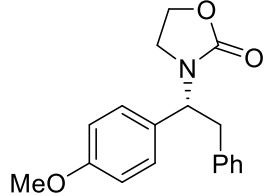
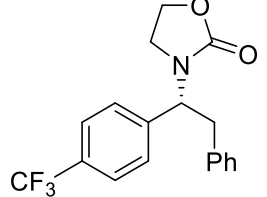
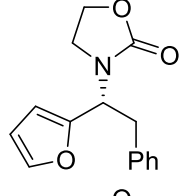
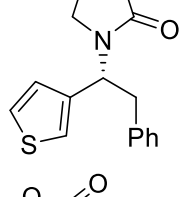
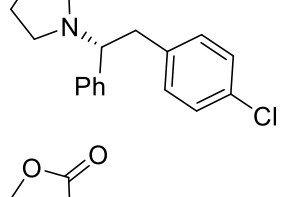
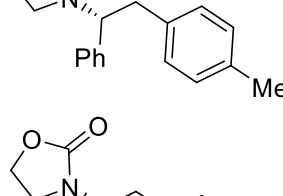
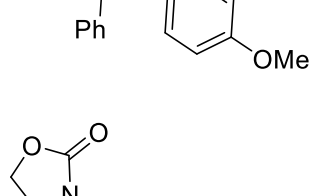
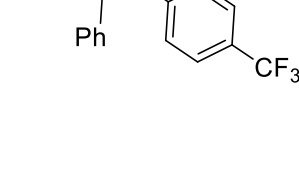
Orange solid. [α]_D^{25.0} = +51 (C= 0.10 in CHCl₃). ¹H NMR (400 MHz, Chloroform-*d*): δ 7.73 (p, *J* = 2.2 Hz, 8H), 7.62 (s, 1H), 7.52 (s, 5H), 7.43 (q, *J* = 8.4, 7.7 Hz, 4H), 7.32 (d, *J* = 7.7 Hz, 3H), 7.25 – 7.20 (m, 1H), 7.11 (dd, *J* = 12.7, 7.9 Hz, 2H), 6.98 (d, *J* = 7.6 Hz, 2H), 6.66 (t, *J* = 9.2 Hz, 1H), 5.22 (t, *J* = 7.1 Hz, 1H), 4.73 – 4.56 (m, 1H), 4.20 (s, 1H), 3.62 – 3.48 (m, 1H), 3.33 (t, *J* = 6.8 Hz, 1H), 3.07 (dd, *J* = 11.2, 5.4 Hz, 1H), 2.86 (s, 3H), 2.74 (s, 3H), 2.65 (td, *J* = 11.9, 10.0, 5.4 Hz, 2H), 2.49 (dd, *J* = 13.5, 6.9 Hz, 1H), 2.28 – 1.82 (m, 6H), 1.68 (d, *J* = 10.9 Hz, 1H), 1.41 (td, *J* = 9.8, 8.7, 4.7 Hz, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 165.6, 161.8 (ddd, *J* = 99.7, 49.8, 3.2 Hz), 141.9, 140.9 (dd, *J* = 105.7, 14.0 Hz), 136.1, 134.9, 133.3 – 132.2 (m), 131.8, 131.6 (d, *J* = 47.2 Hz), 130.7, 129.4, 129.1 (dt, *J* = 5.8, 3.1 Hz), 129.0 – 128.6 (m), 128.5 (d, *J* = 3.6 Hz), 128.0, 127.5 (d, *J* = 7.4 Hz), 126.9 (d, *J* = 10.1 Hz), 126.4, 126.0 (d, *J* = 2.2 Hz), 123.3 (d, *J* = 2.2 Hz), 121.8 (d, *J* = 62.7 Hz), 120.6, 117.6, 94.5 (d, *J* = 10.9 Hz), 86.9 (d, *J* = 14.0 Hz), 69.7, 68.0, 59.0 (d, *J* = 11.5 Hz), 47.8, 34.3, 31.0 (d, *J* = 170.9 Hz), 27.9 – 26.6 (m), 26.4, 25.1 (d, *J* = 6.3 Hz), 21.3 (d, *J* = 6.7 Hz). ³¹P NMR (162

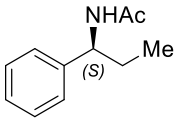
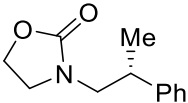
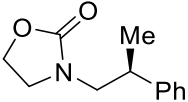
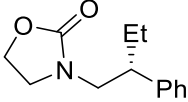
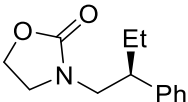
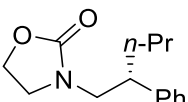
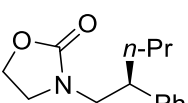
MHz, Chloroform-*d*) δ 51.1 (s). HRMS-EI calcd for C₃₅H₄₀IrN₂OP [M]⁺: 727.2425, found: 727.2445.

5. Separation method data and specific rotation of chiral compounds

| Entry | Product | Separation method | Optical rotation | <i>ee</i> (%) |
|-------|---|---|---|---------------|
| 1 |  | SFC, OZH column, 10% MeOH, 2 ml/min, $t_R = 7.4$ min (major)/8.2 (minor) | $[\alpha]_D^{25.0} = -18$ (C= 0.10 in CHCl ₃) | 95 |
| 2 |  | SFC, IF column, 15% MeOH, 2 ml/min, $t_R = 5.8$ min (minor)/6.1 (major) | $[\alpha]_D^{25.0} = -23$ (C= 0.10 in CHCl ₃) | 93 |
| 3 |  | SFC, ASH column, 15% MeOH, 2 ml/min, $t_R = 2.8$ min (minor)/2.9 (major) | $[\alpha]_D^{25.0} = -45$ (C= 0.10 in CHCl ₃) | 96 |
| 4 |  | SFC, OZH column, 15% MeOH, 2 ml/min, $t_R = 7.5$ min (major)/8.4 (minor) | $[\alpha]_D^{25.0} = -22$ (C= 0.10 in CHCl ₃) | 96 |
| 5 |  | GC-MS, Hydrodex β -3P, 50 °C to 175 °C, 1 degree/min, $t_R = 87.6$ min (minor)/88.7 (major) | $[\alpha]_D^{25.0} = -4$ (C= 0.10 in CHCl ₃) | 93 |
| 6 |  | SFC, IF column, 15% MeOH, 2 ml/min, $t_R = 5.3$ min (minor)/5.8 (major) | $[\alpha]_D^{25.0} = -12$ (C= 0.10 in CHCl ₃) | 99 |
| 7 |  | SFC, IF column, 15% MeOH, 2 ml/min, $t_R = 6.0$ min (major)/7.7 (minor) | $[\alpha]_D^{25.0} = +165$ (C= 0.73 in CHCl ₃) | 92 |
| 8 |  | SFC, IF column, 15% MeOH, 2 ml/min, $t_R = 5.5$ min (major)/6.3 (minor) | $[\alpha]_D^{25.0} = +106.8$ (C = 0.54 in CHCl ₃) | 89 |

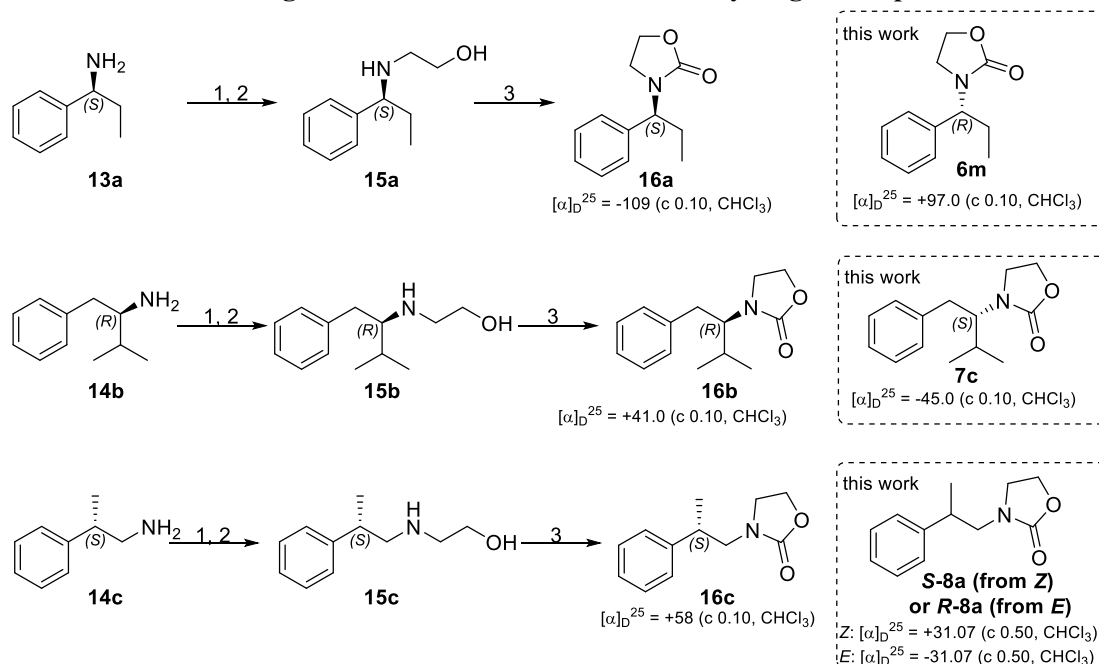
| | | | | |
|----|---|--|--|----|
| 9 |  | HPLC , ASH column, 25% <i>i</i> PrOH in hexane, 0.5 ml/min, $t_R = 30.5$ min (major)/40.8 min (minor) | $[\alpha]_D^{25.0} = +97$ (C= 0.10 in CHCl_3) | 88 |
| 10 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 6.1$ min (major)/7.1 min (minor) | $[\alpha]_D^{25.0} = +101$ (C= 0.10 in CHCl_3) | 93 |
| 11 |  | SFC , IF column, ASH column, 25% <i>i</i> PrOH in hexane, $t_R = 45.3$ min (major)/53.6 min (minor) | $[\alpha]_D^{25.0} = +180$ (C= 0.10 in CDCl_3) | 93 |
| 12 |  | SFC , IF column, 10% MeOH, 2 ml/min, $t_R = 11.0$ min (major)/13.7 min (minor) | $[\alpha]_D^{25.0} = +63$ (C= 0.10 in CHCl_3) | 93 |
| 13 |  | SFC , ASH column, 15% MeOH, 2 ml/min, $t_R = 3.2$ min (minor)/3.6 min (major) | $[\alpha]_D^{25.0} = +100.7$ (C= 0.77 in CHCl_3) | 95 |
| 14 |  | SFC , ASH column, 15% MeOH, 2 ml/min, $t_R = 4.4$ min (minor)/5.0 min (major) | $[\alpha]_D^{25.0} = +85.6$ (C= 0.73 in CHCl_3) | 91 |
| 15 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 12.2$ min (major) / 13.2 min (minor) | $[\alpha]_D^{25.0} = +82$ (C= 0.10 in CHCl_3) | 93 |
| 16 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 14.6$ min (minor)/ 14.9 min (major) | $[\alpha]_D^{25.0} = +67$ (C= 0.45 in CHCl_3) | 97 |

| | | | |
|----|---|--|---|
| 17 |  | SFC, OJH column, 15% MeOH, 2 ml/min, $t_R = 5.3$ min (major)/9.3(minor) | $[\alpha]_D^{25.0} = +82$ 92 (C= 0.10 in CHCl ₃) |
| 18 |  | SFC, OZH column, 10% MeOH, 2 ml/min, $t_R = 7.0$ min (minor)/7.8 (major) | $[\alpha]_D^{25.0} = +90$ (C= 94 0.10 in CHCl ₃) |
| 19 |  | SFC, OZH column, 15% MeOH, 2 ml/min, $t_R = 4.5$ min (minor)/5.0 (major) | $[\alpha]_D^{25.0} = +68$ (C= 95 0.10 in CHCl ₃) |
| 20 |  | SFC, ODH column, 15% MeOH, 2 ml/min, $t_R = 4.4$ min (major)/4.6 (minor) | $[\alpha]_D^{25.0} = +83$ (C= 99 0.10 in CHCl ₃) |
| 21 |  | SFC, IF column, 15% MeOH, 2 ml/min, $t_R = 16.5$ min (major)/ 18.0 (minor) | $[\alpha]_D^{25.0} = +78$ 88 (C= 0.10 in CHCl ₃) |
| 22 |  | SFC, ASH column, 15% MeOH, 2 ml/min, $t_R = 6.9$ min (minor)/9.3 (major) | $[\alpha]_D^{25.0} = +79$ 92 (C= 0.10 in CHCl ₃) |
| 23 |  | SFC, ASH column, 15% MeOH, 2 ml/min, $t_R = 6.1$ min (minor)/7.2 (major) | $[\alpha]_D^{25.0} = +37$ 92 (C= 0.10 in CHCl ₃) |
| 24 |  | SFC, ASH column, 15% MeOH, 2 ml/min, $t_R = 6.4$ min (minor)/7.5 (major) | $[\alpha]_D^{25.0} = +67$ 95 (C= 0.10 in CHCl ₃) |
| 25 |  | SFC, IF column, 15% MeOH, 2 ml/min, $t_R = 6.0$ min (minor)/6.6 (major) | $[\alpha]_D^{25.0} = +73$ 96 (C= 0.10 in CHCl ₃) |

| | | | | |
|----|---|---|--|----|
| 26 |  | SFC , ADH column, 15% MeOH, 2 ml/min, $t_R = 5.7$ min (minor)/6.6 (major) | $[\alpha]_D^{25.0} = -110.5$ (C= 0.20 in CHCl_3) | 98 |
| 27 |  | SFC , ASH column, 15% MeOH, 2 ml/min, 15min, $t_R = 4.7$ min (minor)/5.2 min (major) | $[\alpha]_D^{25.0} = -31$ (C= 0.1 in CHCl_3) | 97 |
| 28 |  | SFC , ASH column, 15% MeOH, 2 ml/min, 15min, $t_R = 4.7$ min (major)/5.2 min (minor) | $[\alpha]_D^{25.0} = 31$ (C= 0.1 in CHCl_3) | 97 |
| 29 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 5.1$ min (minor)/5.5 (major) | $[\alpha]_D^{25.0} = -22$ (C= 0.10 in CHCl_3) | 96 |
| 30 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 5.1$ min (minor)/5.5 (major) | $[\alpha]_D^{25.0} = 21$ (C= 0.10 in CHCl_3) | 93 |
| 31 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 5.4$ min (minor)/5.7 (major) | $[\alpha]_D^{25.0} = -25$ (C= 0.10 in CHCl_3) | 96 |
| 32 |  | SFC , IF column, 15% MeOH, 2 ml/min, $t_R = 5.4$ min (minor)/5.7 (major) | $[\alpha]_D^{25.0} = 22$ (C= 0.10 in CHCl_3) | 90 |

6. Absolute configuration determination

6.1 The absolute configuration of the different classes of hydrogenated products

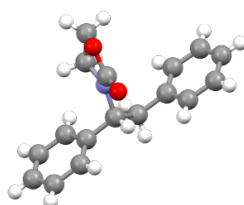


Reaction condition (1) ethyl 2-chloro-2-oxoacetate, NEt₃, CH₂Cl₂, r.t., 2 h. (2) LAH, THF, reflux. o.n. (3) triphosgene, NEt₃, rt. o.n.

The absolute configuration of the different classes of hydrogenated product was determined by transformation of known compounds **13a**, **14b**, **14c** into compound **15a-15c** and comparison with hydrogenated products **6m**, **7c**, **S-8a** and **Z-8a**. First, the amines **12a-12c** were treated with ethyl 2-chloro-2-oxoacetate to furnish compounds **13a**, **14b**, **14c**. Then a cyclization using triphosgene and NEt₃ afforded compound **15a-15c**, of which optical rotation were compared to hydrogenated products **6m**, **7c**, **S-8a** and **Z-8a**. The absolute configuration of the other products has been tentatively assigned by comparison of elution order from HPLC and SFC, using a chiral stationary phase and the optical rotation of products **6m**, **7c**, **S-8a** and **Z-8a**.

6.2 Di-aryl enamides by single crystal X-ray diffraction

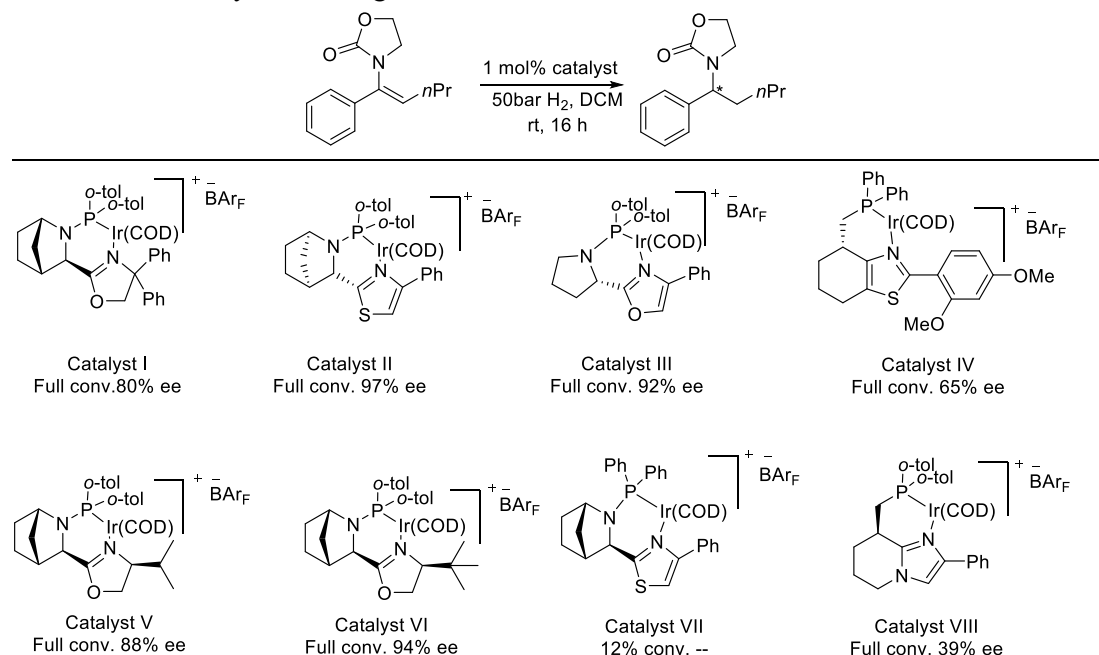
Single crystal of **5a** was grown by dissolving in pentane diethyl ether and slow evaporation at room temperature. Detailed information for this crystal is available in CCDC 1955080.



X-ray crystal structure of **5**.

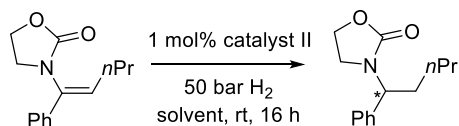
7. Conditions screening

Table S1 The catalyst screening ^a



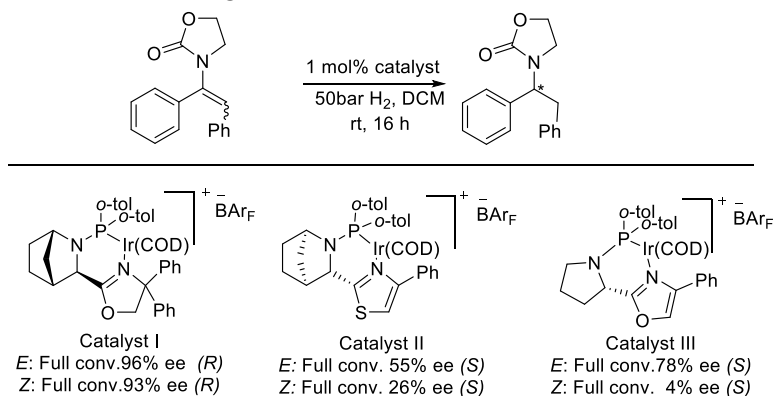
^a 0.05 mmol of substrates in 0.5 mL of DCM. Conversion was determined by ¹H NMR spectroscopy. Enantiomeric excess was determined by SFC analysis, using chiral stationary phases.

Table S2 The solvent screening ^a

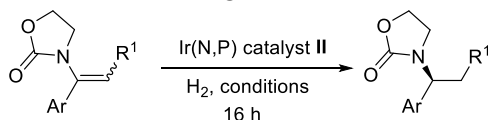


| Entry | Solvent | Conv.(%) | ee (%) |
|-------|-------------------|----------|--------|
| 1 | DCM | Full | 97 |
| 2 | Toluene | Full | 97 |
| 3 | PhCF ₃ | Full | 97 |
| 4 | Benzene | Full | 97 |
| 5 | DCE | Full | 97 |

^a 0.05 mmol of substrates in 0.5 mL of solvent. Conversion was determined by ¹H NMR spectroscopy. Enantiomeric excess was determined by SFC analysis, using chiral stationary phases.

Table S3 The condition screening of class 1

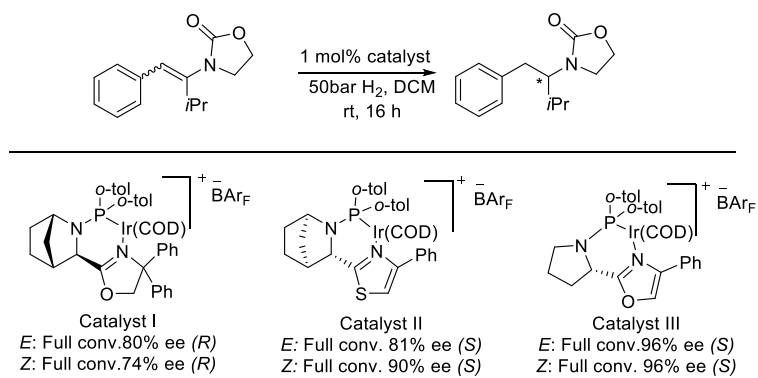
^a 0.05 mmol of substrates in 0.5 mL of DCM. Conversion was determined by ¹H NMR spectroscopy. Enantiomeric excess was determined by SFC analysis, using chiral stationary phase

Table S4 The additional condition screening of class 2 ^a

| Entry | Subs. | Solvent | Press.(bar) | Temp.(°C) | Conv.(%) | ee(%) |
|-------|----------------|---------|-------------|-----------|----------|----------------|
| 1 | <i>(E)</i> -2c | DCM | 50 | r.t | 99 | 43(<i>S</i>) |
| | <i>(Z)</i> -2c | DCM | 50 | r.t | 99 | 98(<i>R</i>) |
| 2 | <i>(E)</i> -2c | Toluene | 50 | 60 | 99 | 10(<i>R</i>) |
| | <i>(Z)</i> -2c | Toluene | 50 | 60 | 99 | 97(<i>R</i>) |
| 3 | <i>(E)</i> -2c | Toluene | 3 | 60 | 99 | 47(<i>R</i>) |
| | <i>(Z)</i> -2c | Toluene | 3 | 60 | 99 | 97(<i>R</i>) |
| 4 | <i>(E)</i> -2c | Toluene | 1 | 60 | 76 | 60(<i>R</i>) |
| | <i>(Z)</i> -2c | Toluene | 1 | 60 | 99 | 97(<i>R</i>) |
| 5 | <i>(E)</i> -2c | DCE | 1 | 60 | 99 | 63(<i>R</i>) |
| | <i>(Z)</i> -2c | DCE | 1 | 60 | 99 | 97(<i>R</i>) |
| 6 | <i>(E)</i> -2a | DCE | 1 | 60 | 99 | 80(<i>R</i>) |
| | <i>(Z)</i> -2a | DCE | 1 | 60 | 99 | 97(<i>R</i>) |

^a 0.05 mmol of substrates in 0.5 mL of solvent. Conversion was determined by ¹H NMR spectroscopy. Enantiomeric excess was determined by SFC analysis, using chiral stationary phase

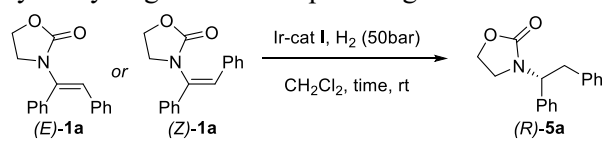
Table S5 The condition screening of class 3^a



^a 0.05 mmol of substrates in 0.5 mL of DCM. Conversion was determined by ¹H NMR spectroscopy. Enantiomeric excess was determined by SFC analysis, using chiral stationary phase

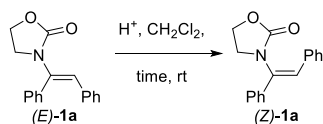
8. Mechanistic study

Table S6 Kinetic study on hydrogenation of separated geometric isomer

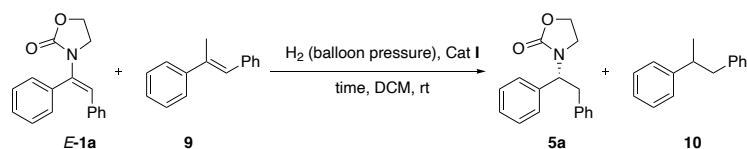


| Entry | Time (min) | E | | Z | |
|-------|------------|-------------|------------|-------------|------------|
| | | Z/E (ratio) | conv.to 5a | Z/E (ratio) | conv.to 5a |
| 1 | 5 | 1:1.1 | 22% | 5.8:1 | 10% |
| 2 | 15 | 1:1.1 | 31% | 5.9:1 | 27% |
| 3 | 30 | 5:1 | 51% | 6:1 | 31% |
| 4 | 60 | 6:1 | 69% | 6:1 | 40% |

Table S7 Acid catalyzed isomerization



| Entry | H ⁺ source | Z/E (ratio) | Time (days) |
|-------|-----------------------|-------------|-------------|
| 1 | AcOH (100 mol%) | 2:1 | 14 |
| 2 | TCA (100 mol%) | 6:1 | 7 |
| 3 | TCA (5 mol%) | 5:1 | 14 |
| 4 | Ir-H (5 mol%) | 6:1 | 8 |



Competition (Enamide Class 1 vs Stilbene)

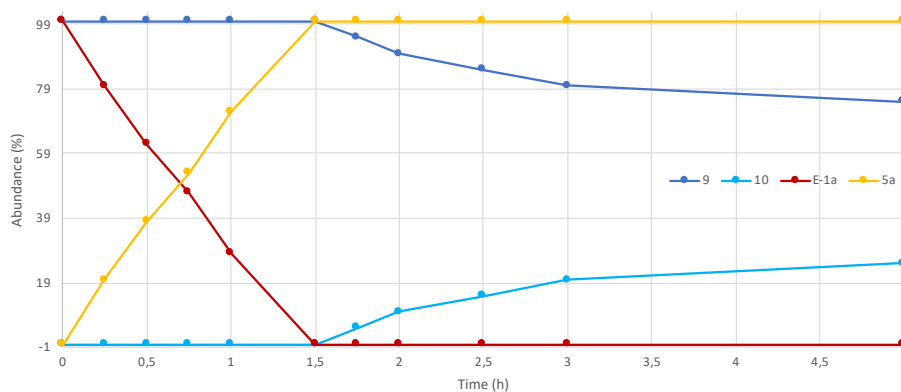


Figure S1 Competition experiments for class 1 enamide and trans methyl stilbene.

Labeling study

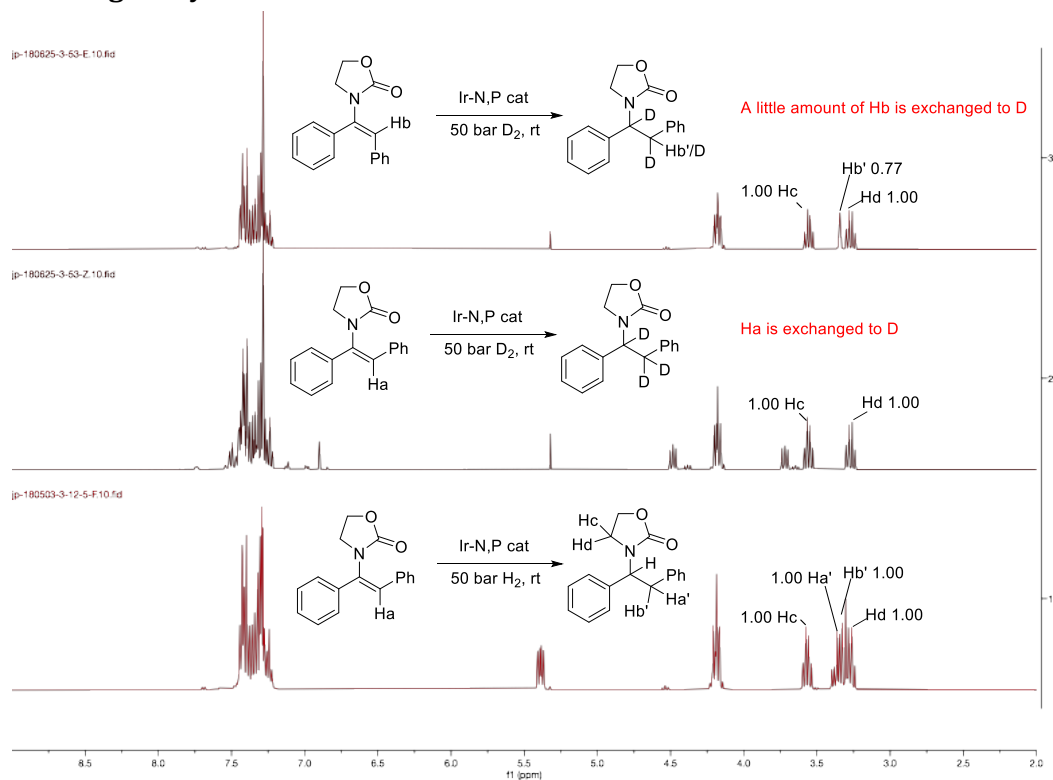


Figure S2 Deuterium study on 1a

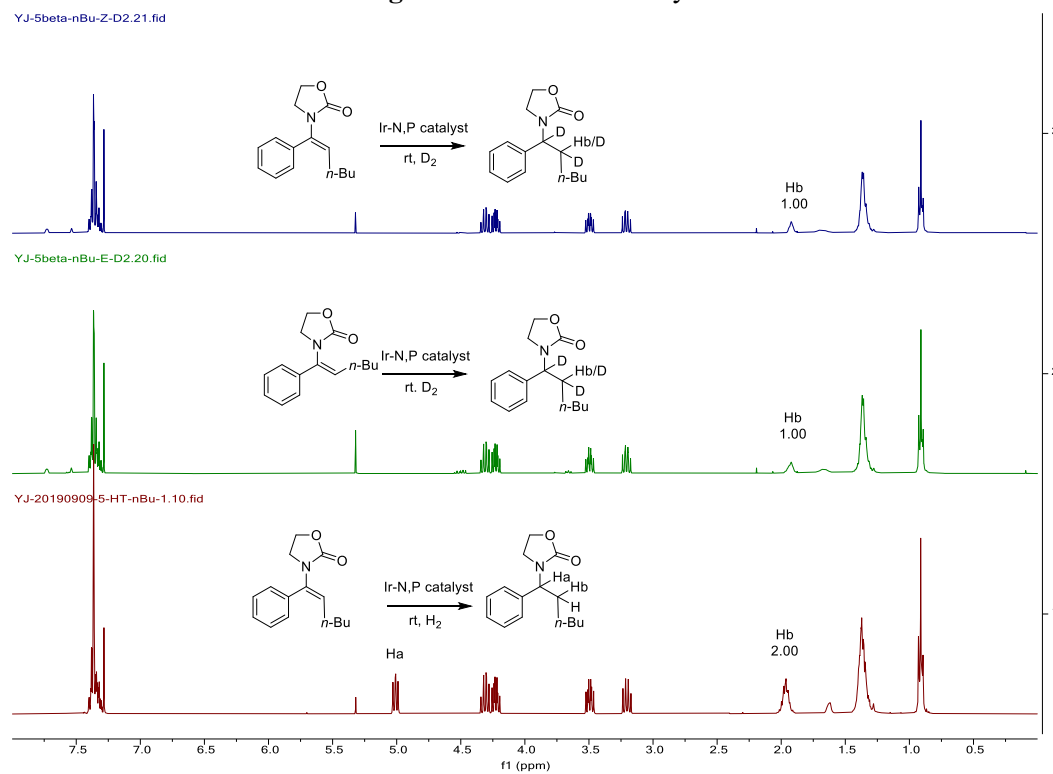


Figure S3 Deuterium study on 2a (rt, 50bar)

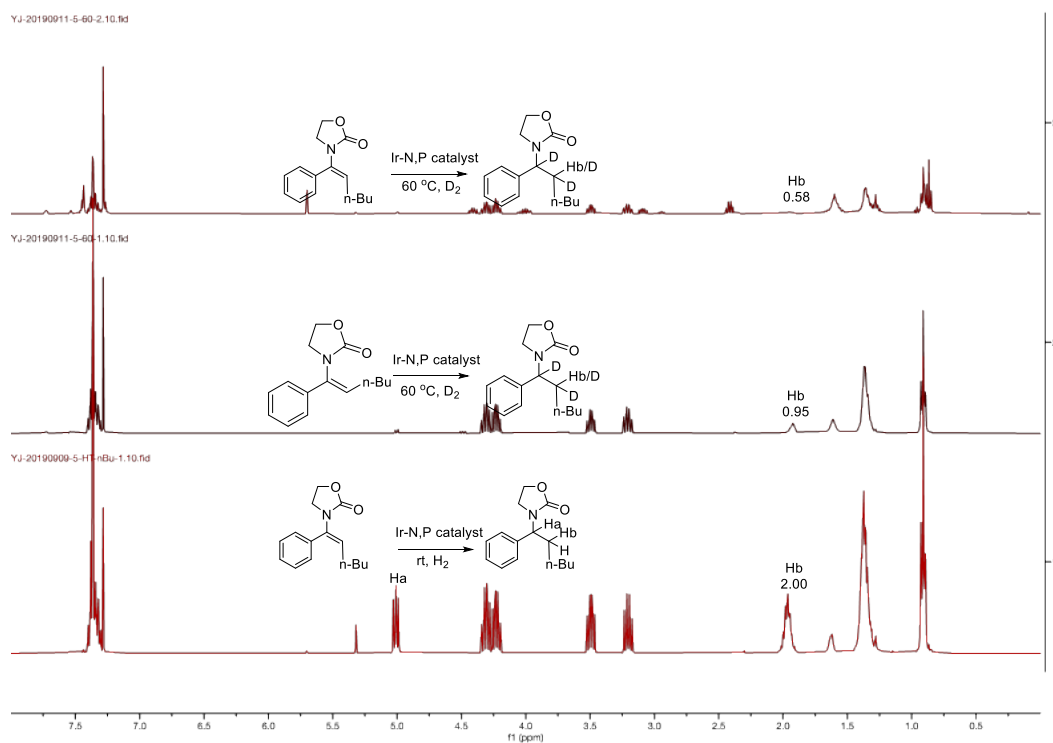


Figure S4 Deuterium study on **2a** (60 °C, 1 bar)

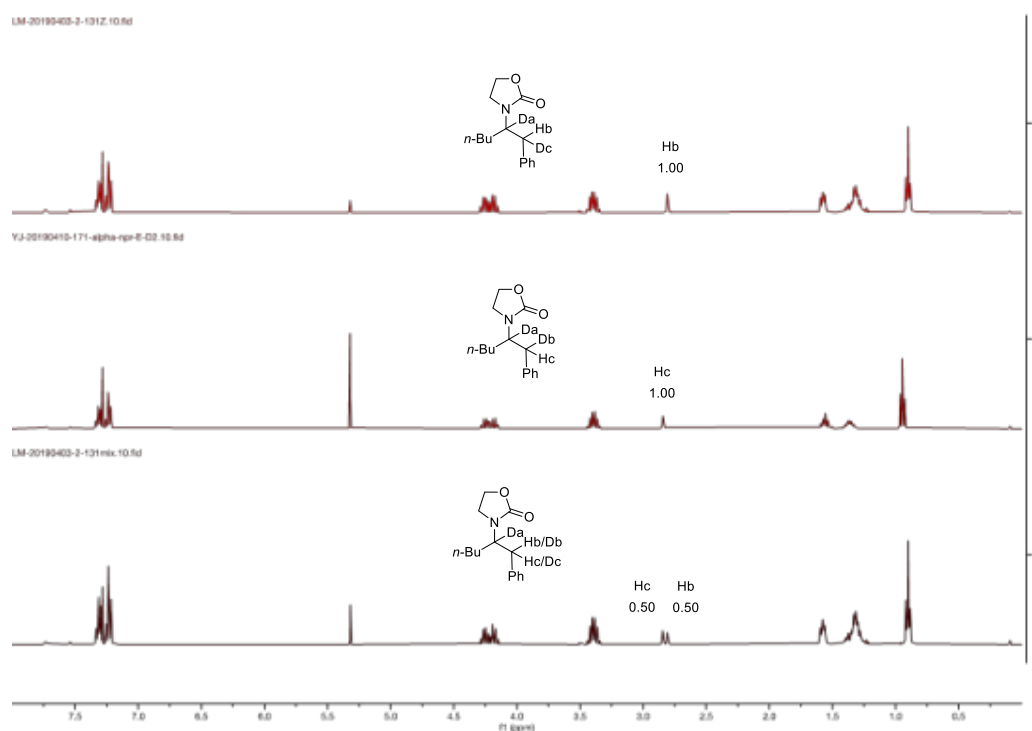


Figure S5 Deuterium study on **3a** (rt)

9. DTF computational details

Single point free energy with solvation (dichloromethane) were carried out with Jaguar¹³ (version 10.1) using the B3LYP-D3^{14,15} functional in combination with the psLACVP** basis set.¹⁶ The structures were first optimized in the gas phase. The transition states were characterized by one negative vibrational frequency and QRC¹⁷ (quick reaction coordinate) calculations. The solvent energies for the optimized structures were then calculated using the Poisson-Boltzmann solver with dichloromethane as the solvent. The energy that is depicted with the XYZ coordinates (listed below) was obtained from the optimized gas phase calculation. All computations were carried out using the computational cluster resources at the National Supercomputer Centre based at Linkoping University, Sweden and at the Center for High Performance Computing, South Africa.

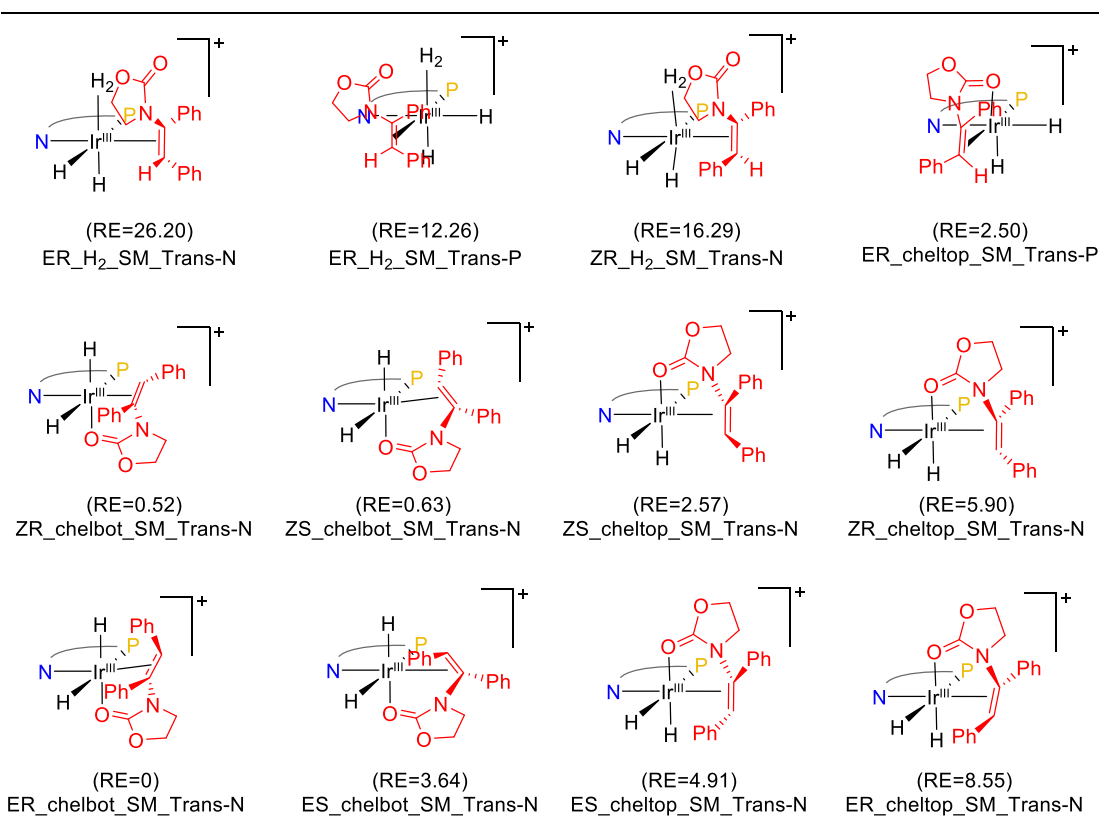


Figure S6 The substrate-catalyst complexes explored in this calculation. The P, N ligand is abbreviated as P and N; the relative energies are shown in parentheses.

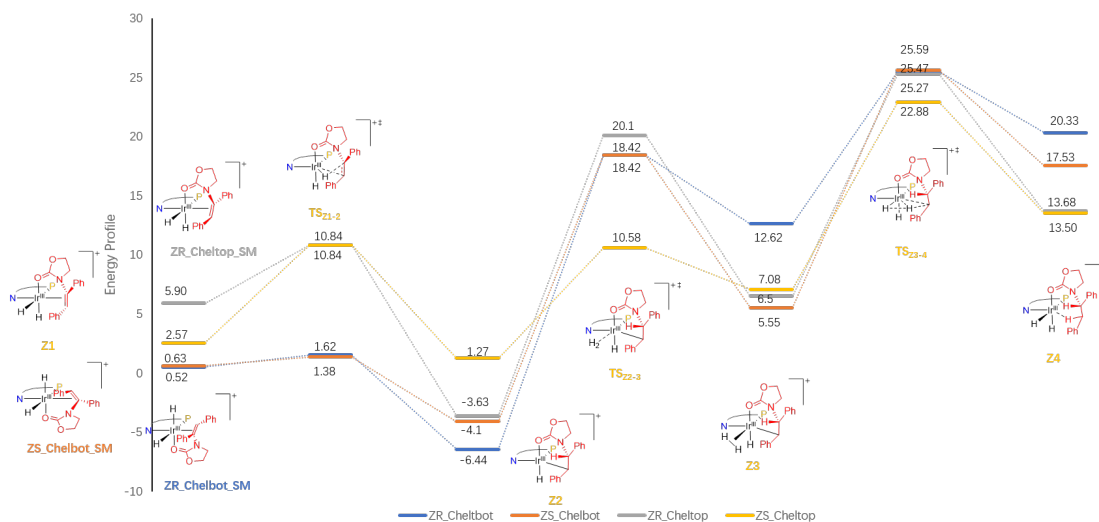


Figure S7 Free energy profile of hydrogenation for the Z isomer. ZS_cheltop is the most favored pathway.

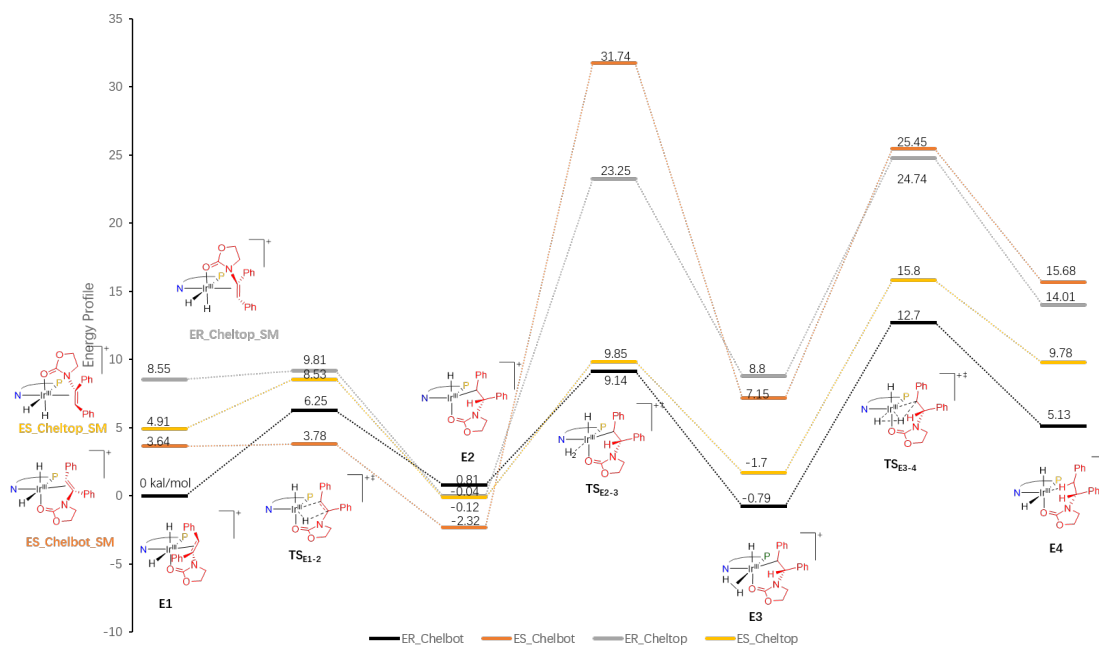


Figure S8 Free energy profile of hydrogenation for the E isomer. ER_Chelbot is the most favored pathway.

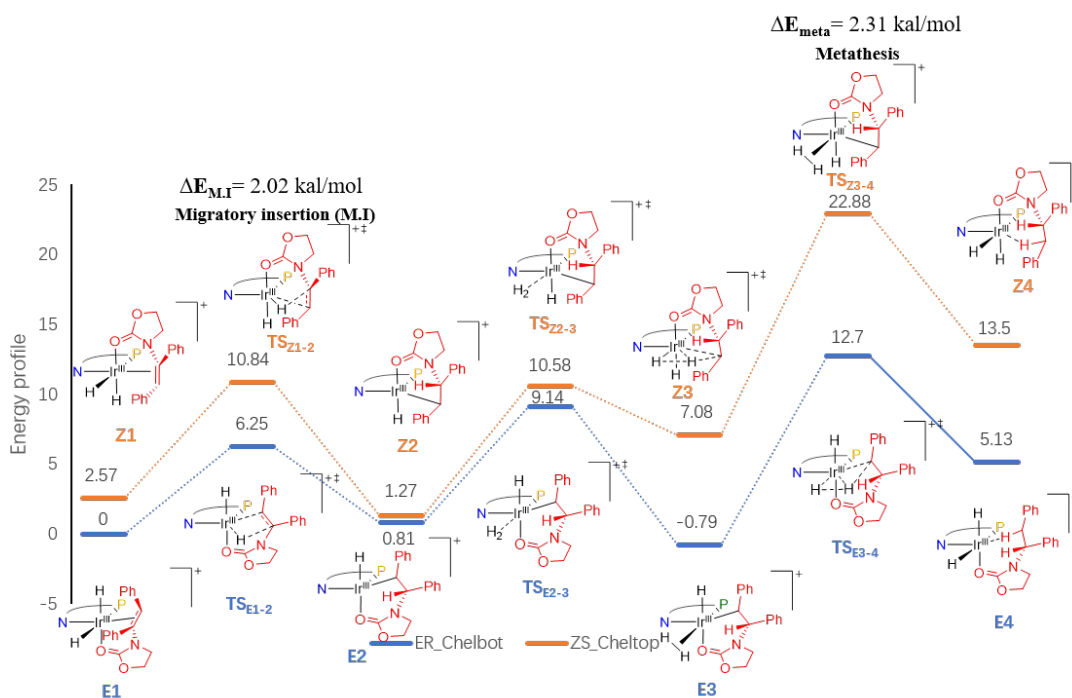


Figure S9 Energy comparison of the favored pathway for the hydrogenation of *Z*-isomer and *E*-isomer.

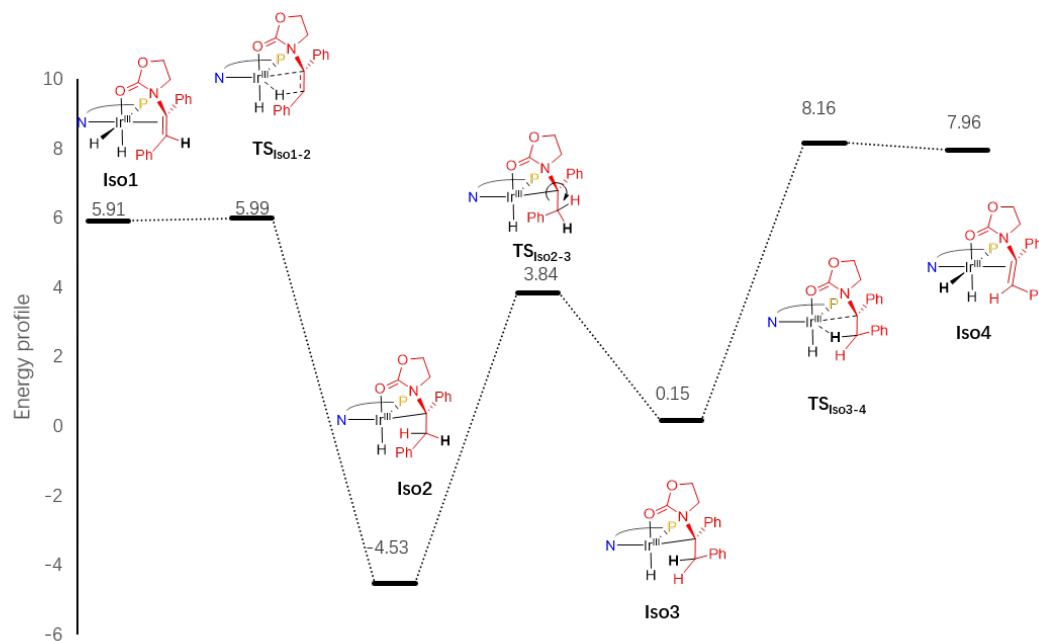


Figure S10 Free energy profile of *Z*-*E* isomerization.

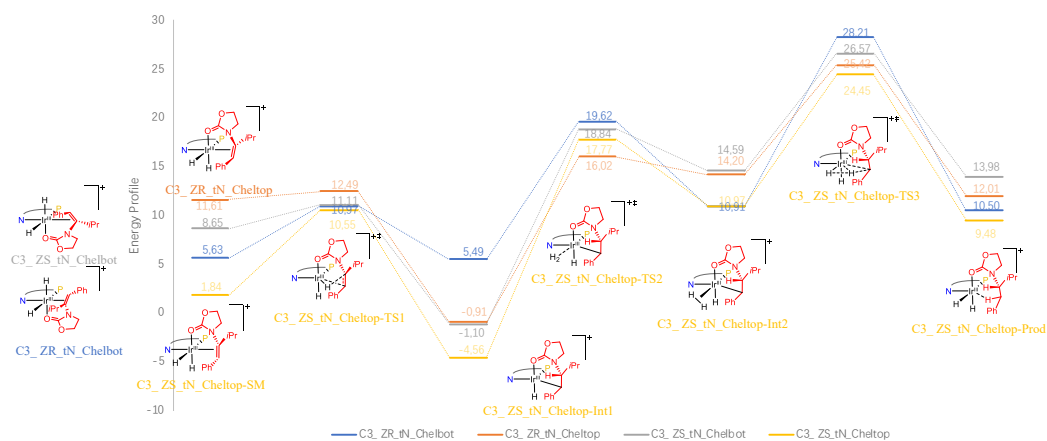


Figure S11 Free energy profile of hydrogenation for the Z isomer (class 3). ZS_Cheltop is the most favored pathway.

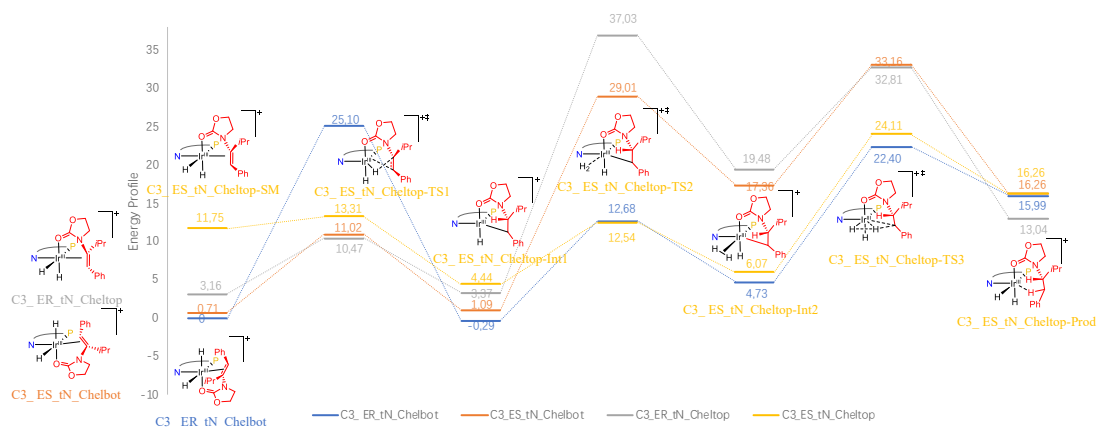
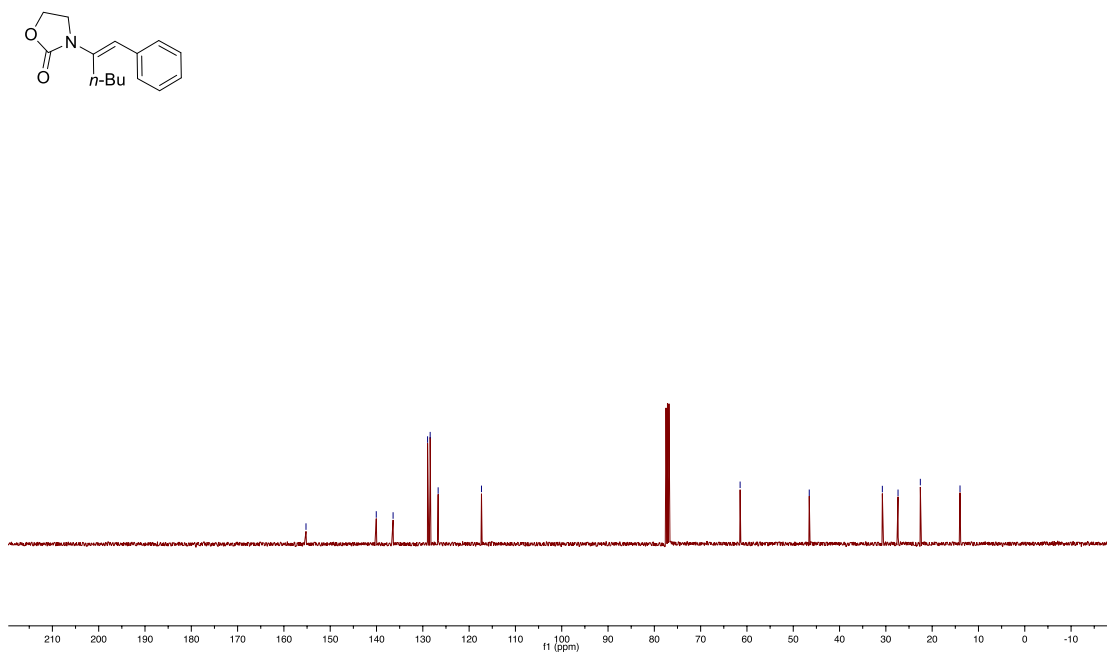
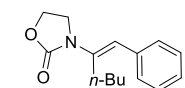
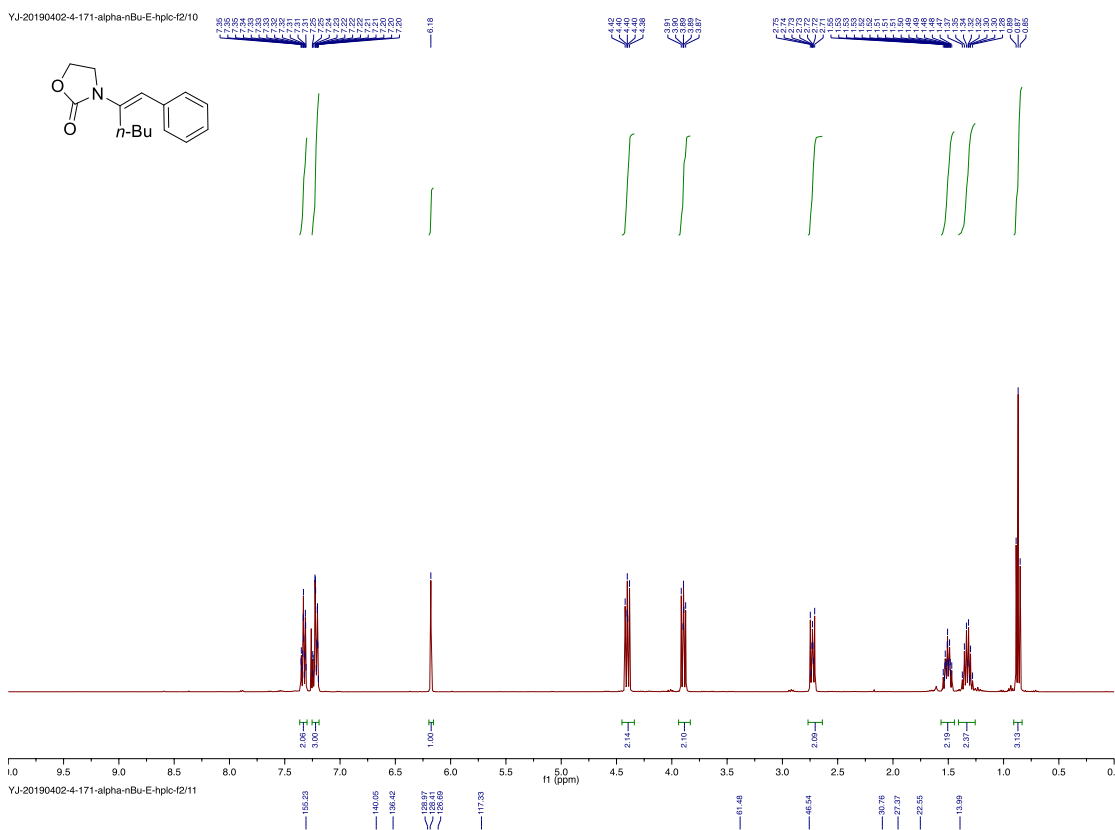
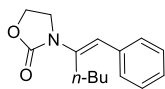


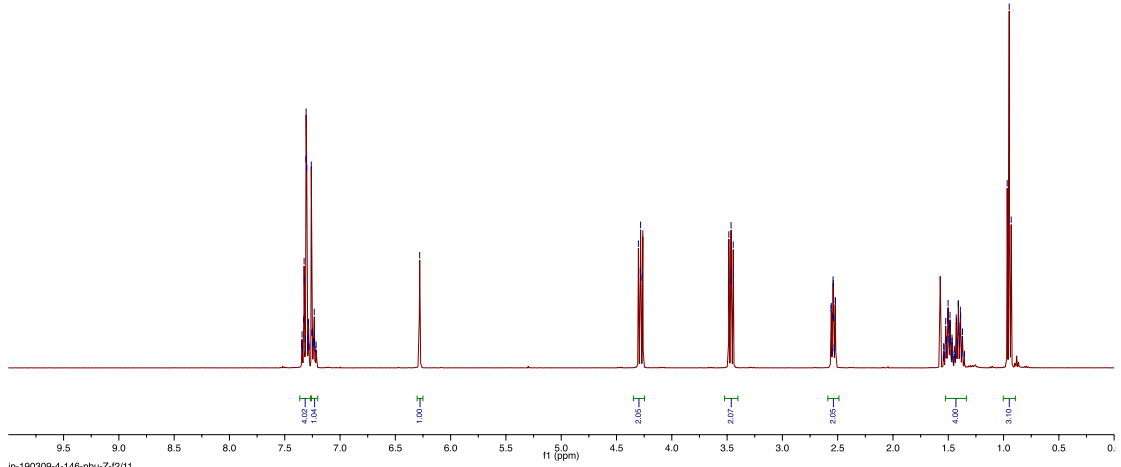
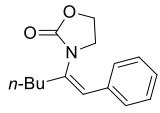
Figure S12 Free energy profile of hydrogenation for the E isomer (class 3). ES_Cheltop is the most favored pathway.

10. NMR spectra of new compounds

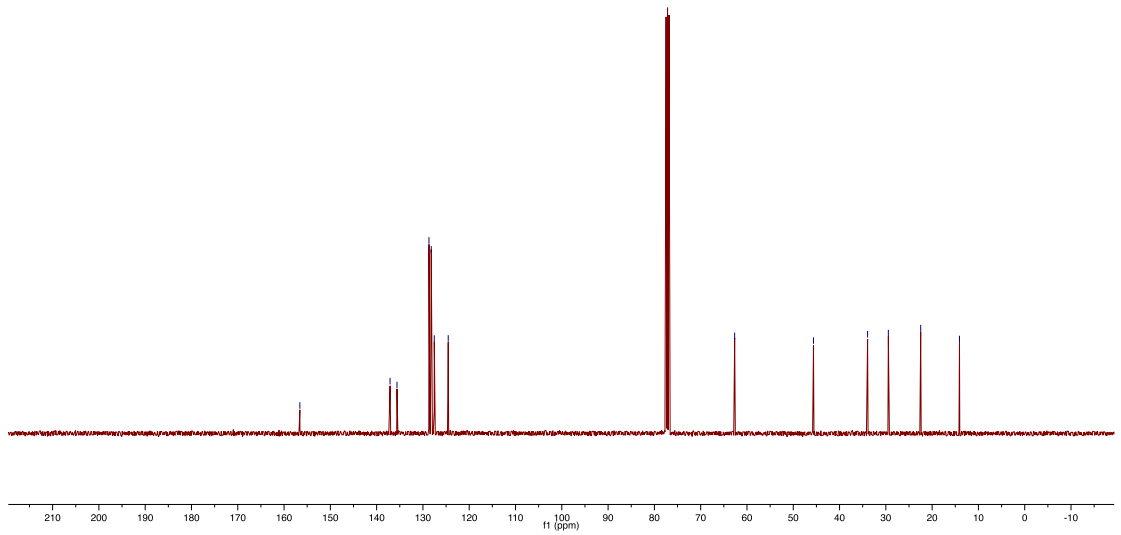
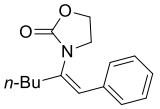
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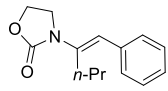
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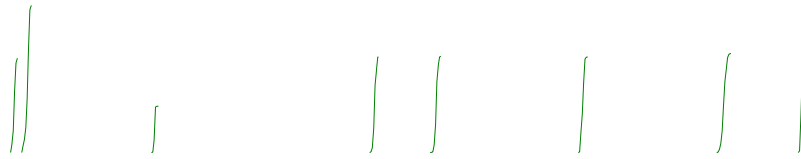
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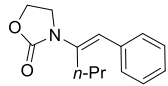
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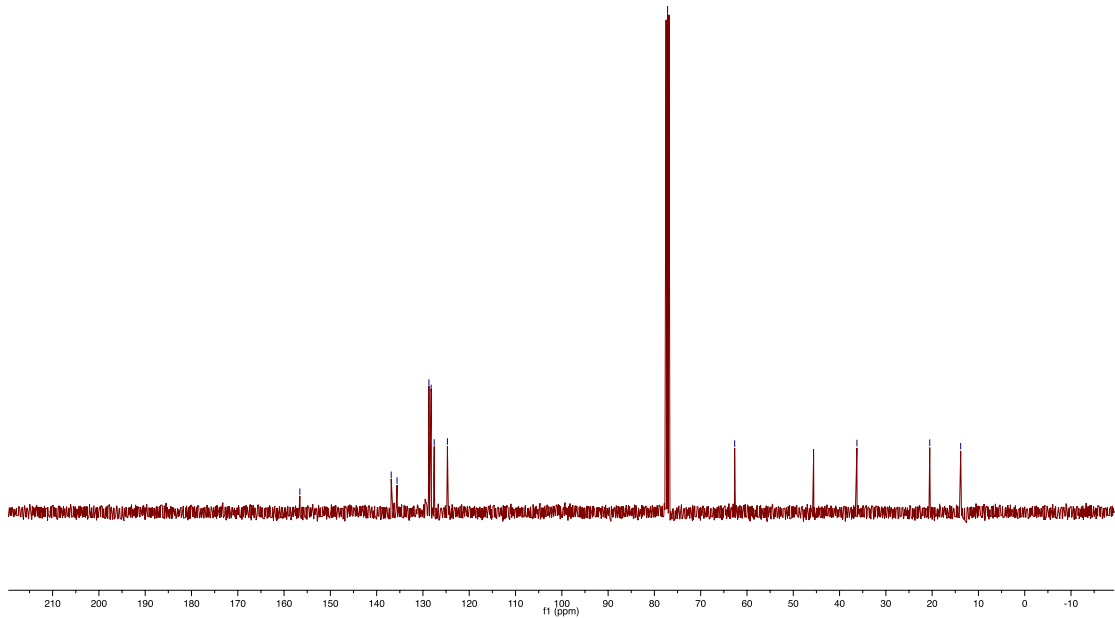
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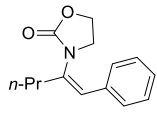
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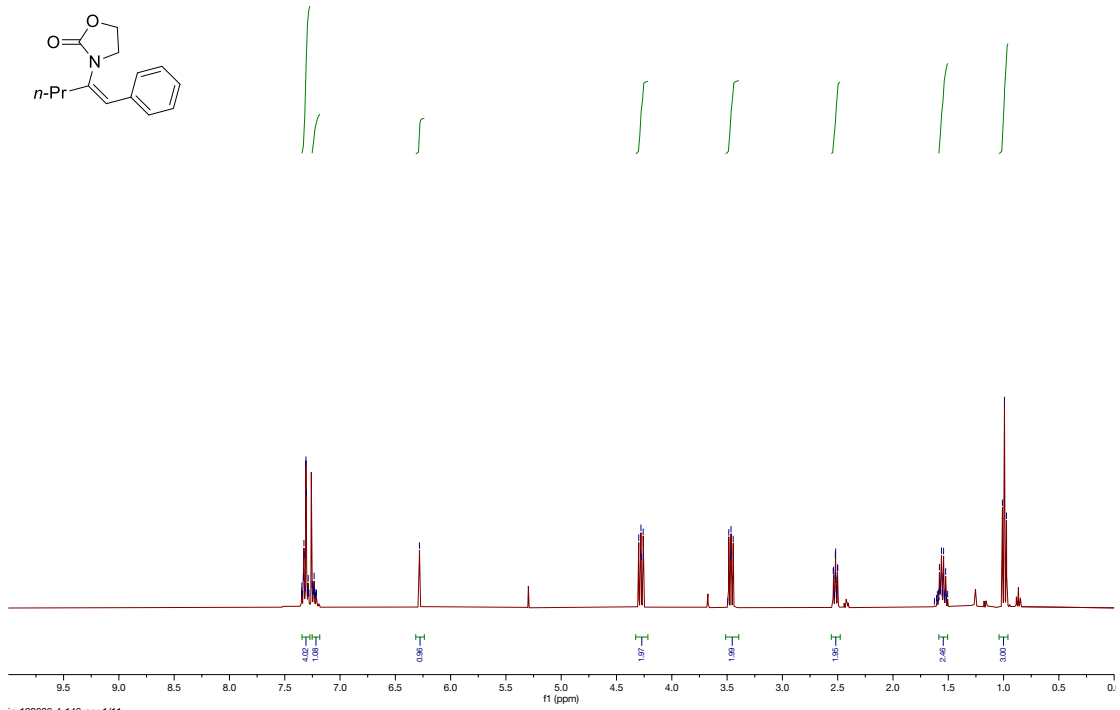


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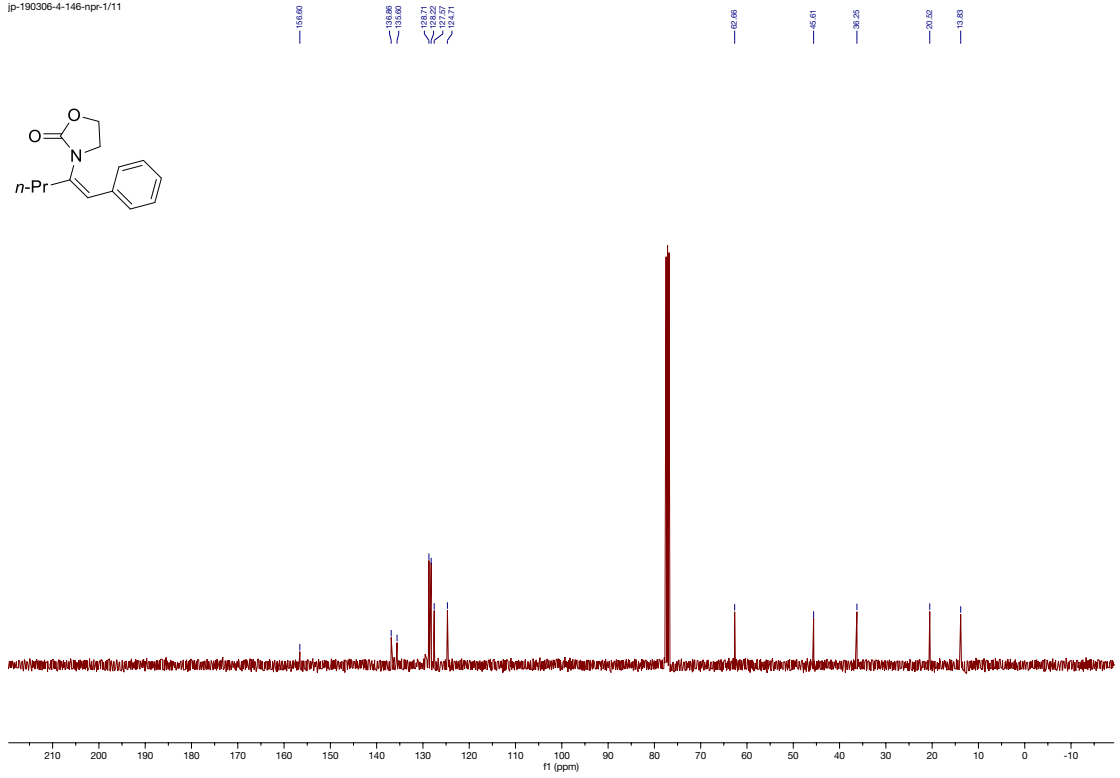
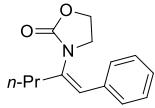
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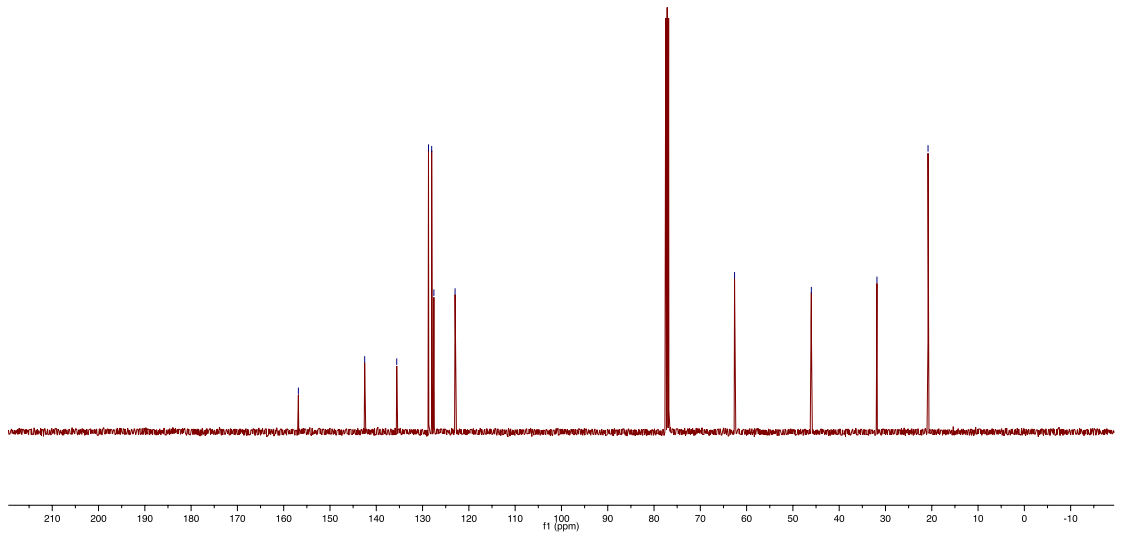
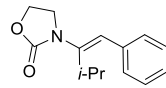
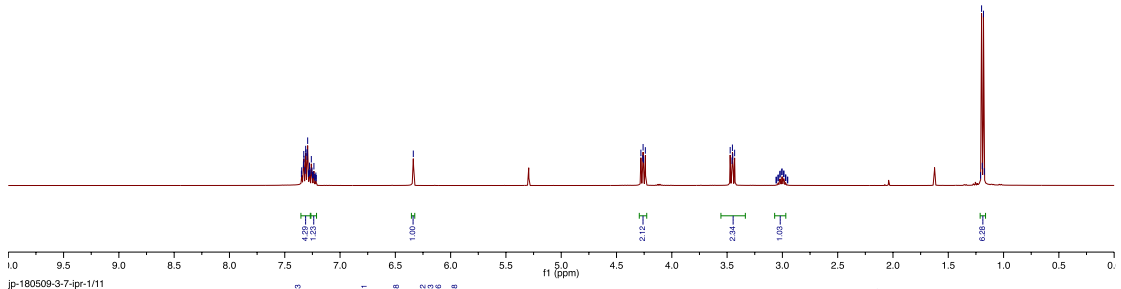
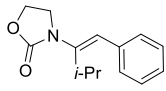
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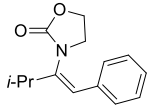
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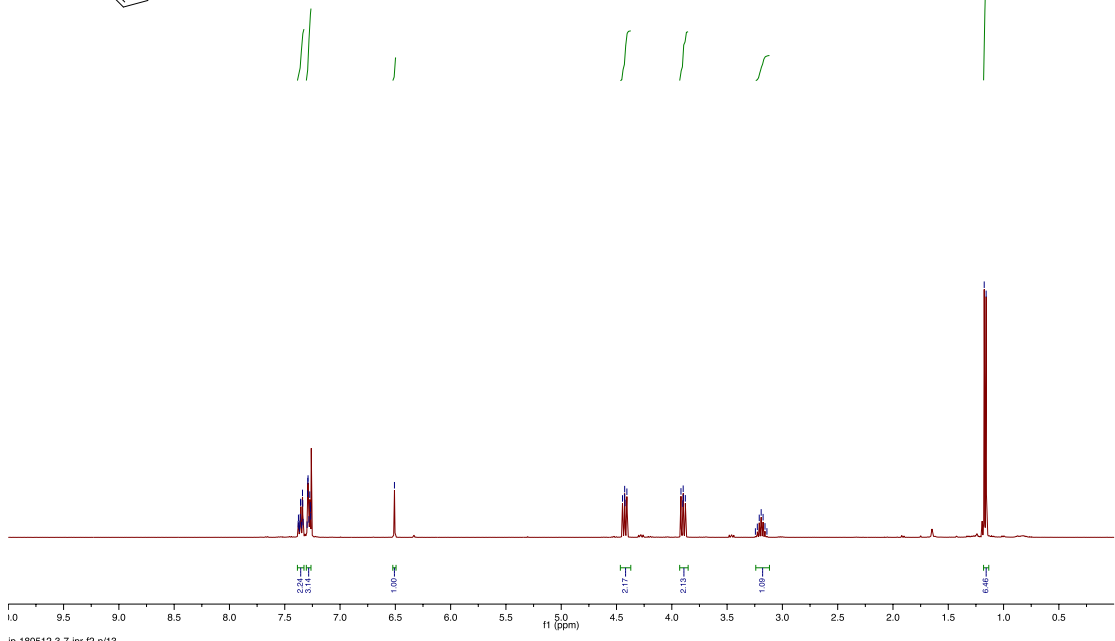
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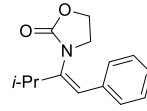
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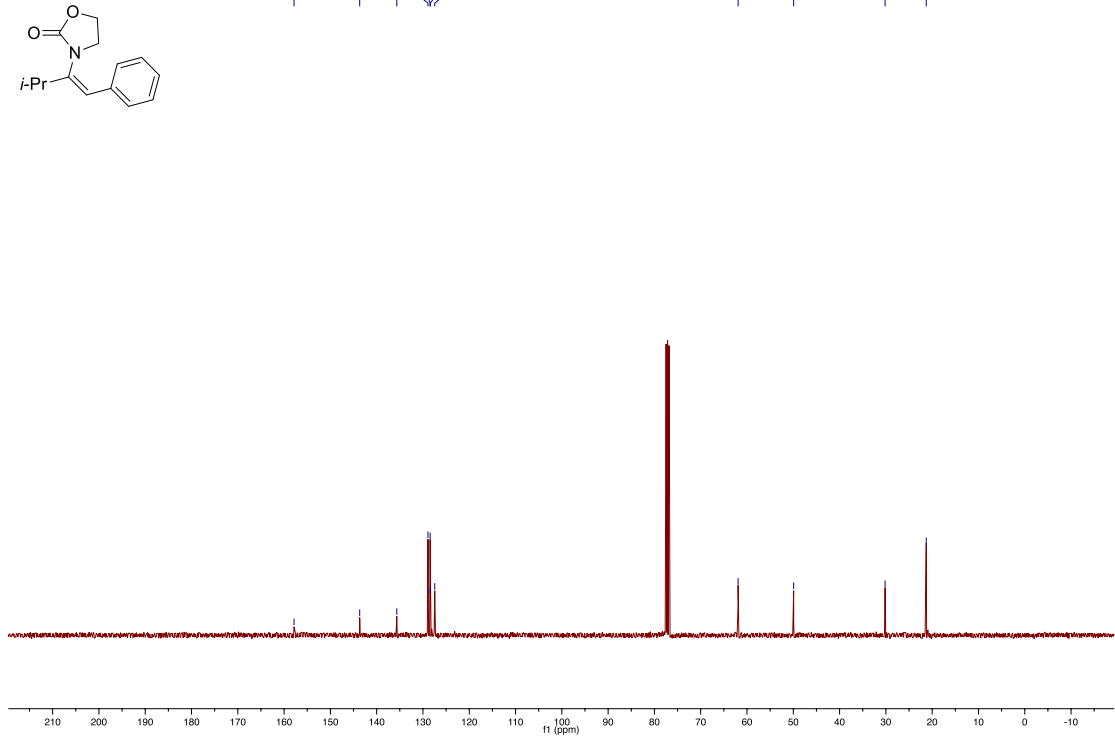
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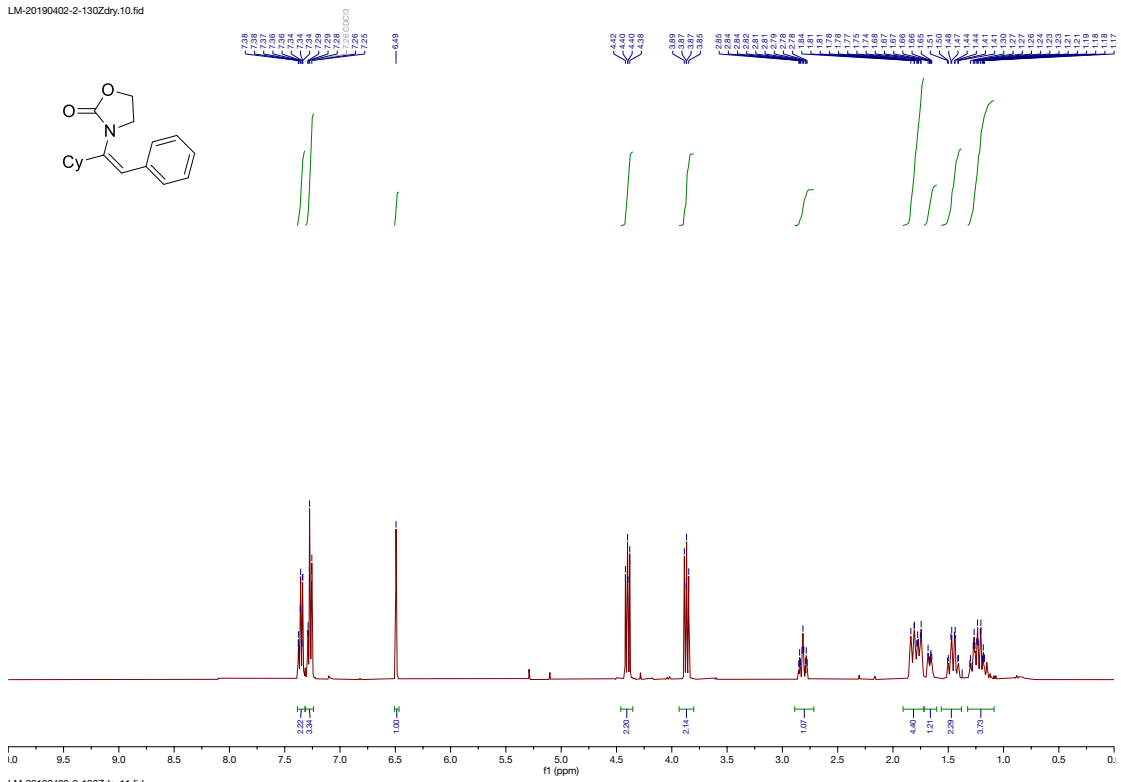
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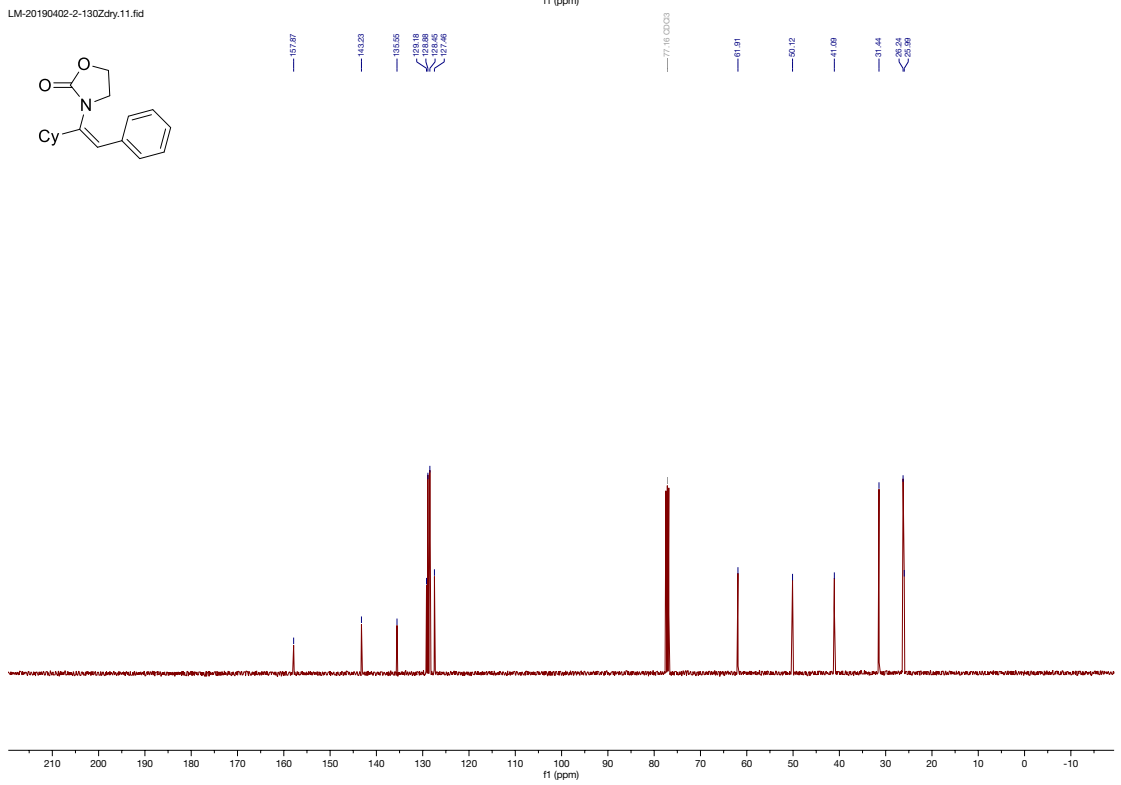
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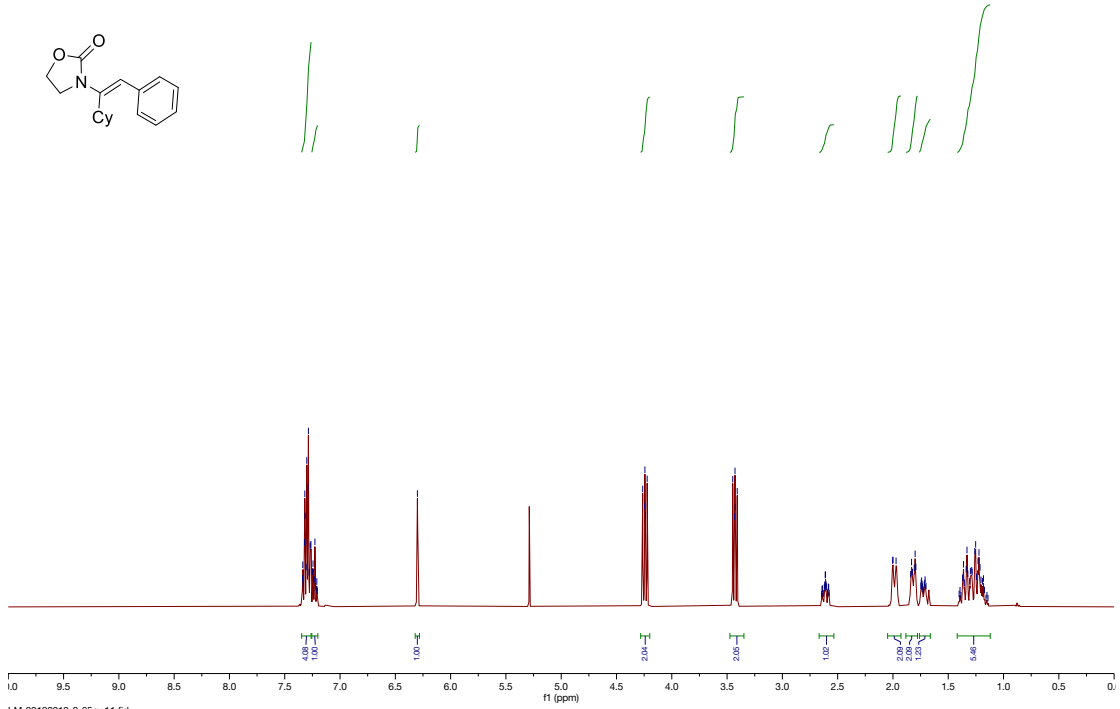
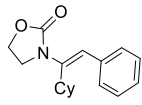
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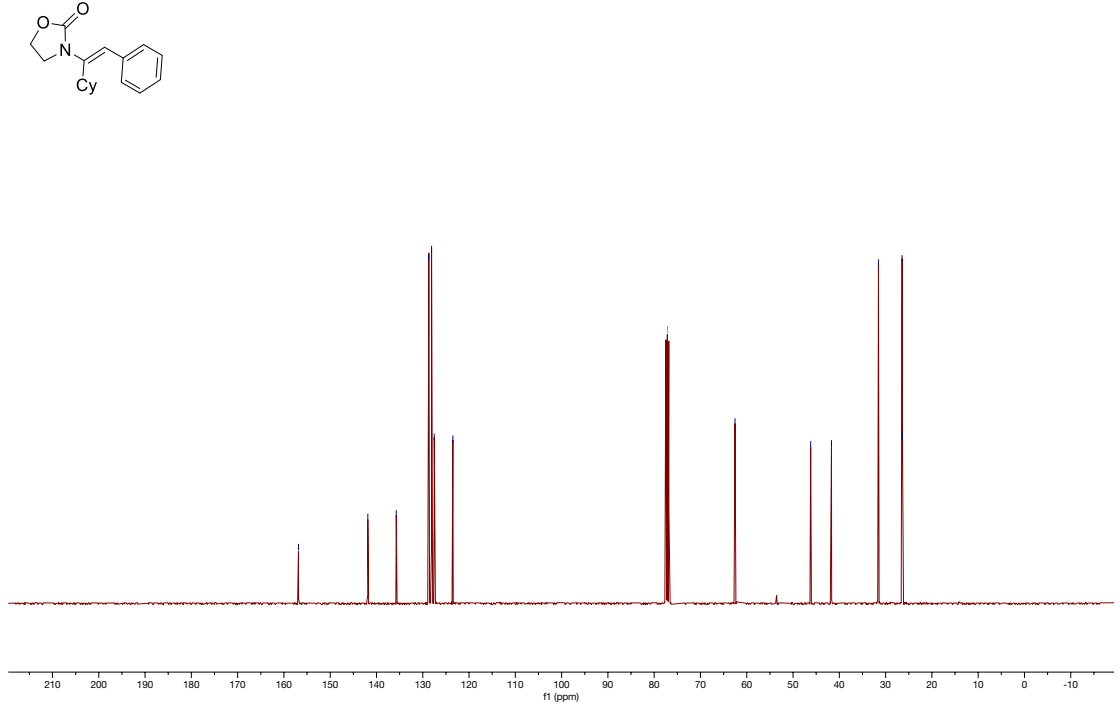
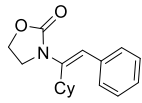
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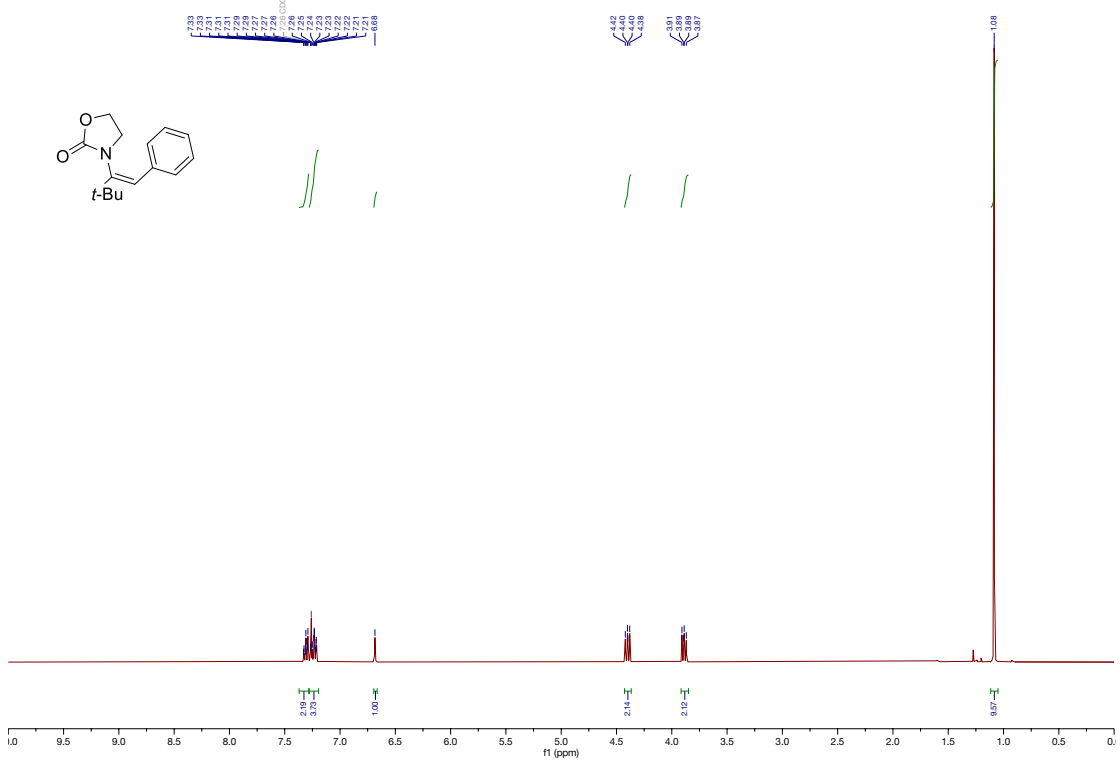
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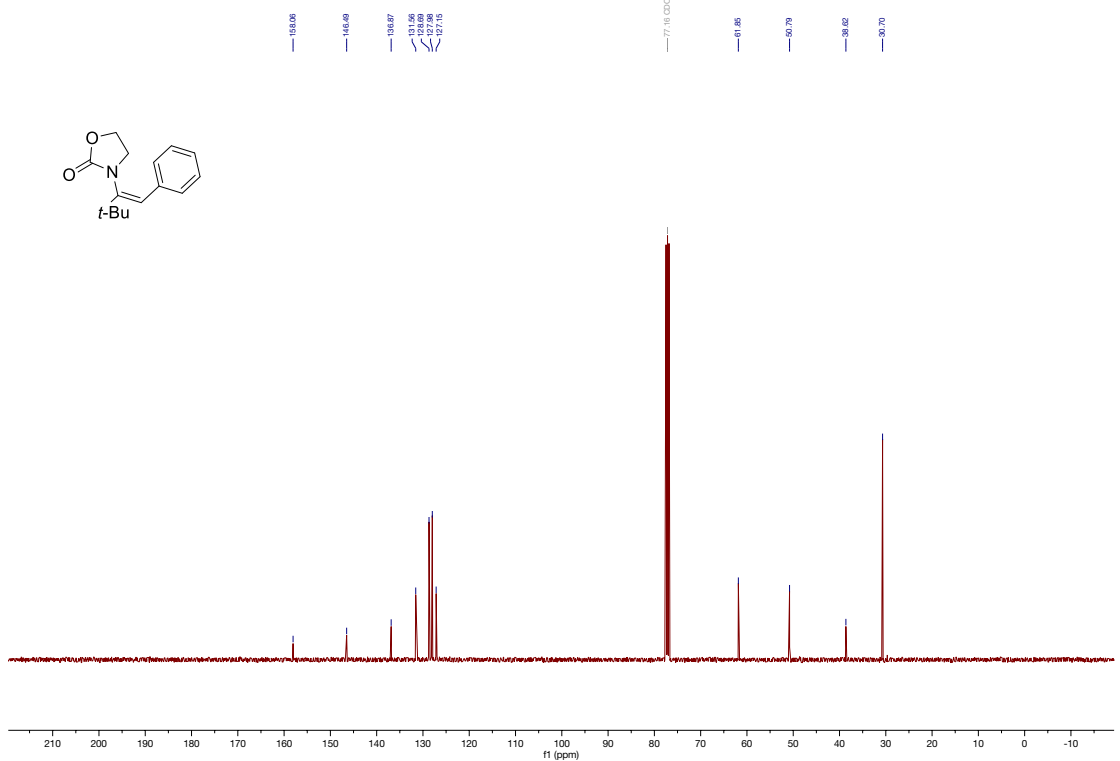
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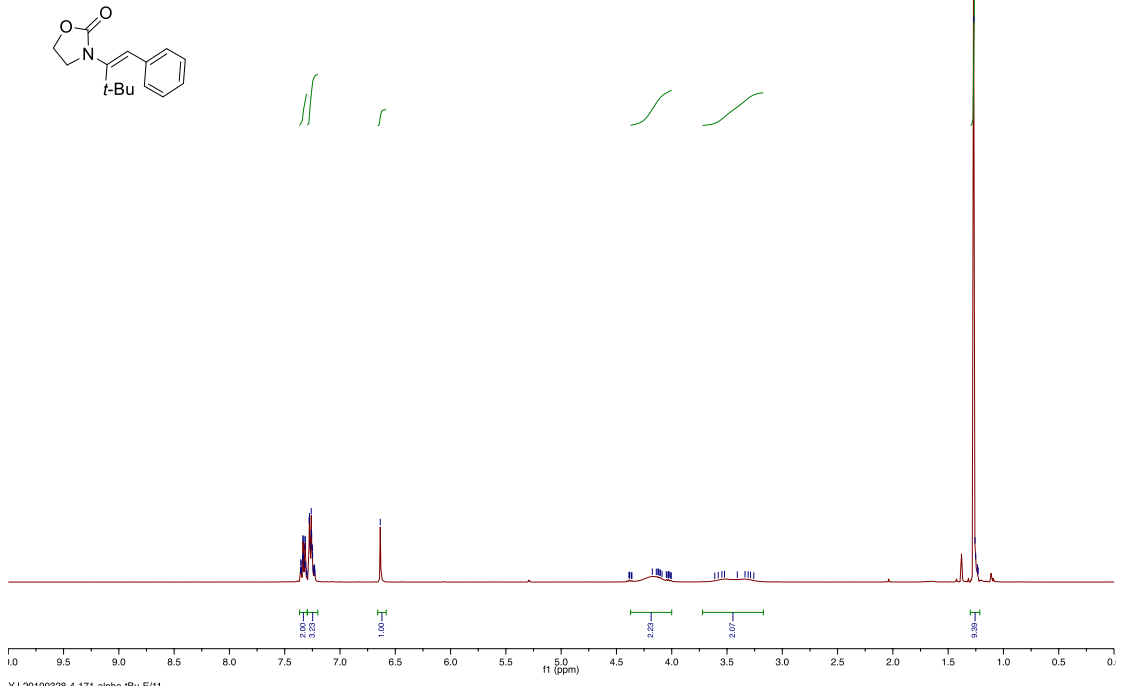
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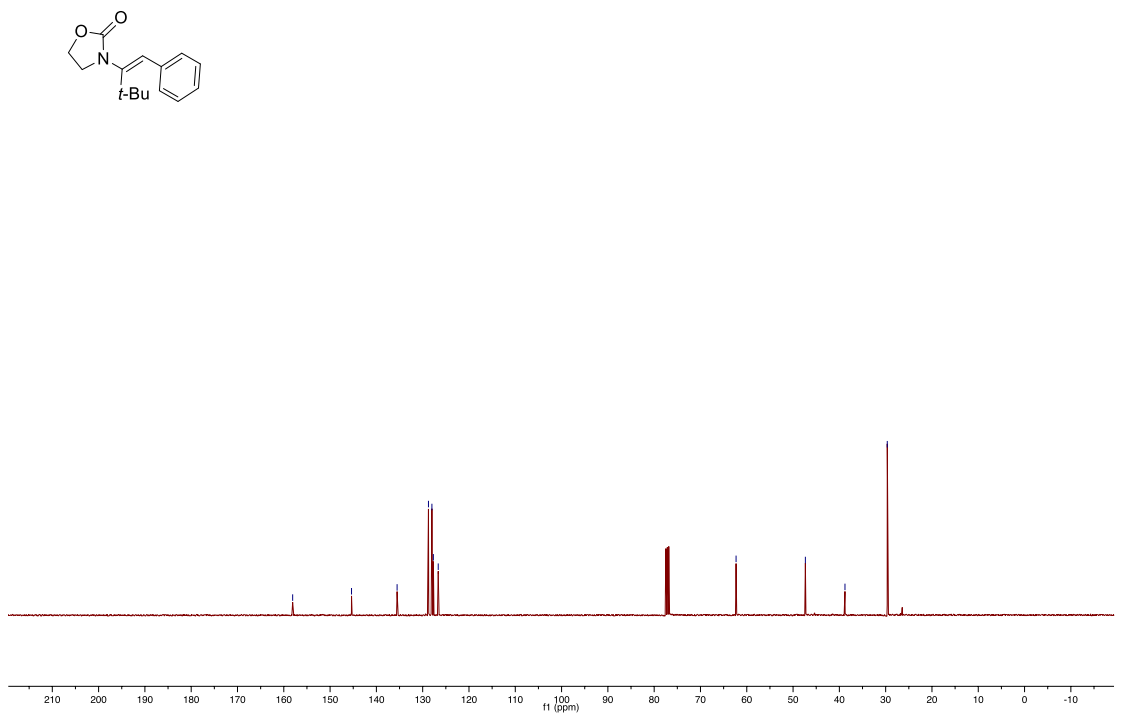
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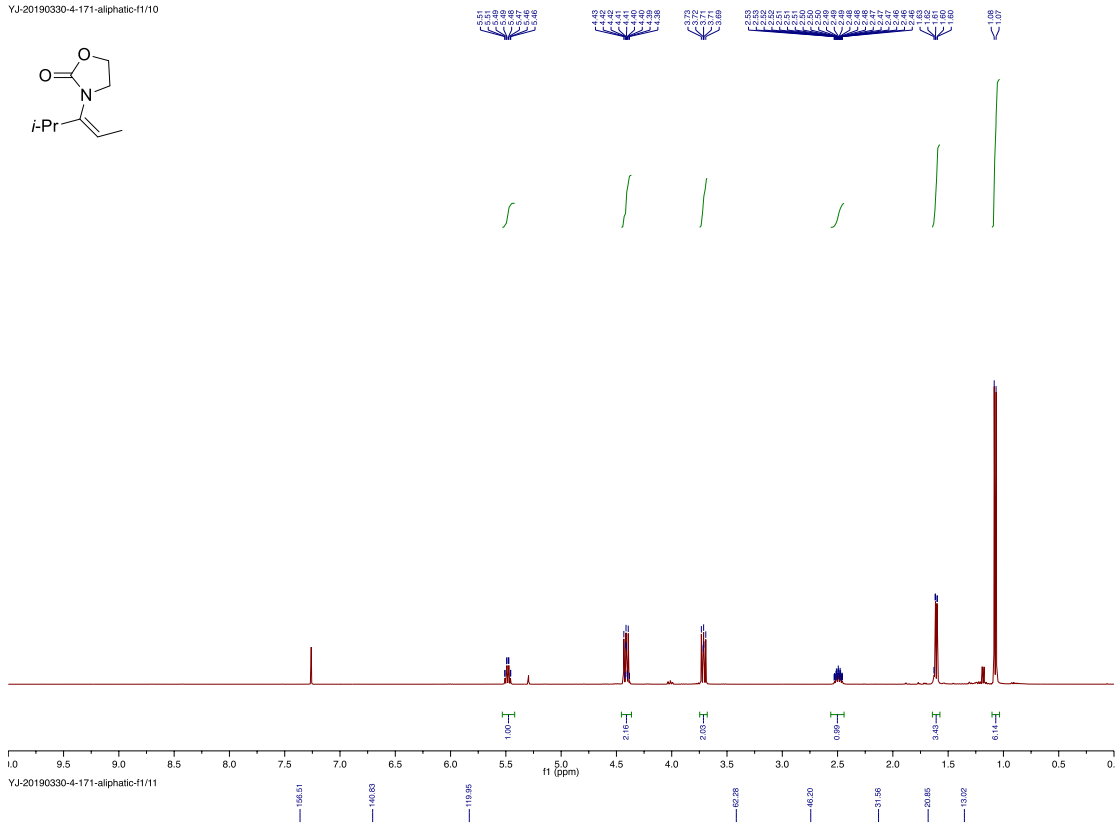
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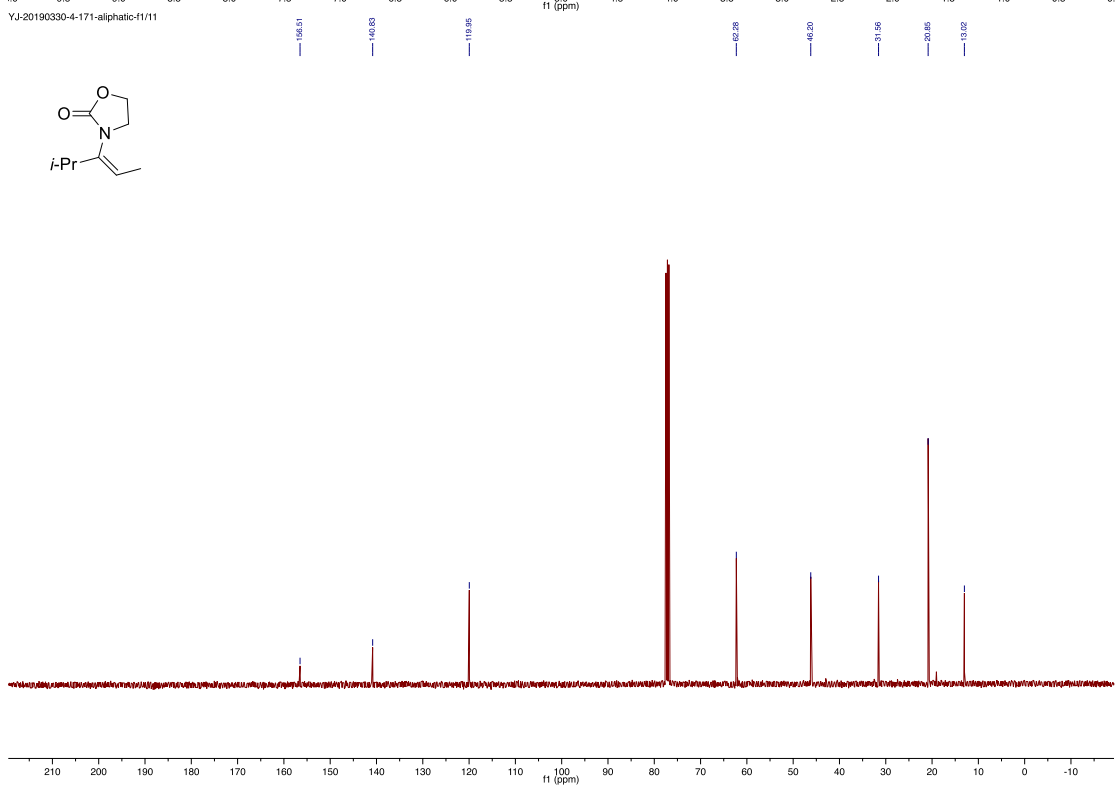
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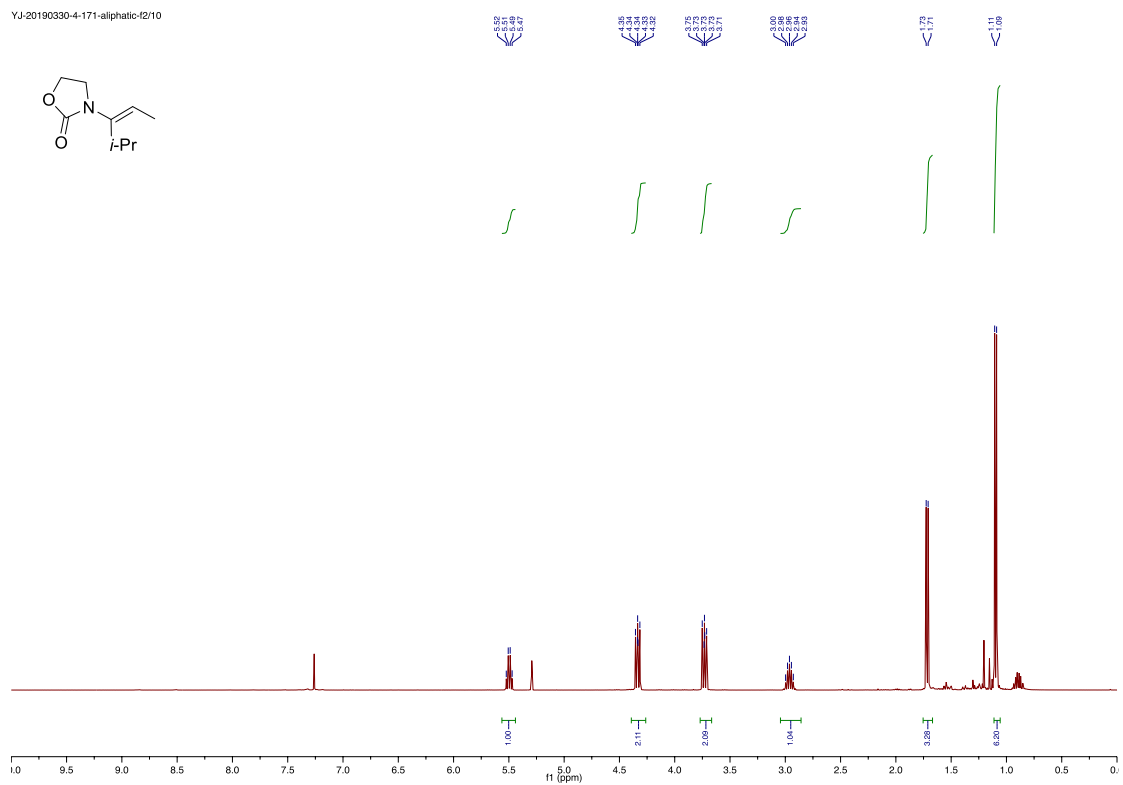
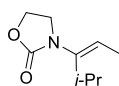
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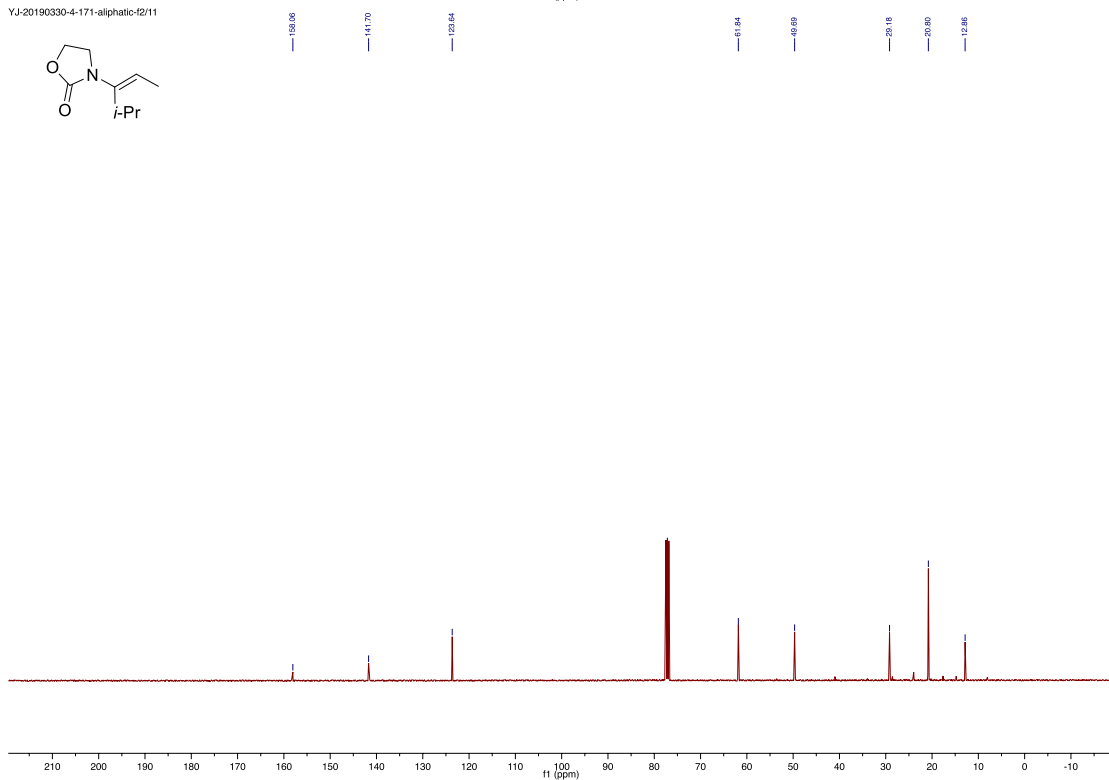
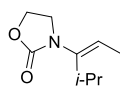
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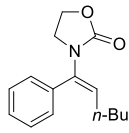
YJ-20190330-4-171-aliphatic-12/10



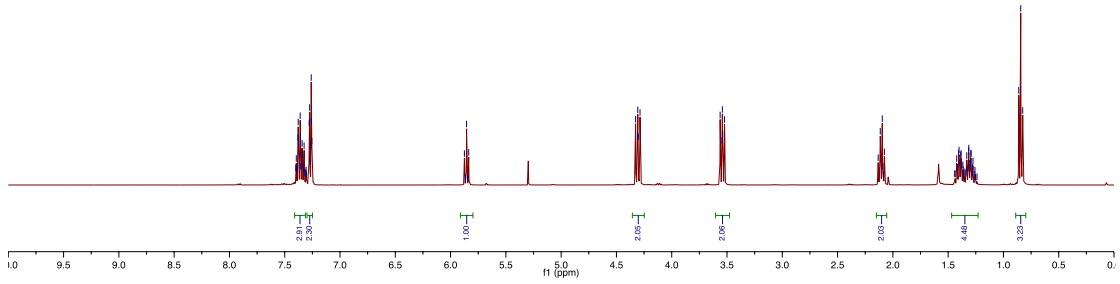
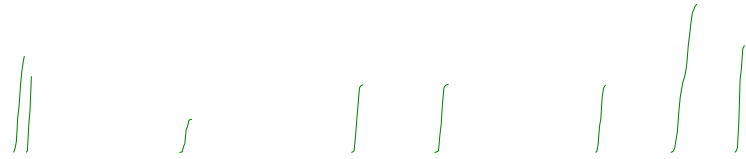
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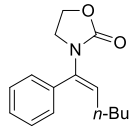
YJ-20190329-4-171-beta-nBu-E/10



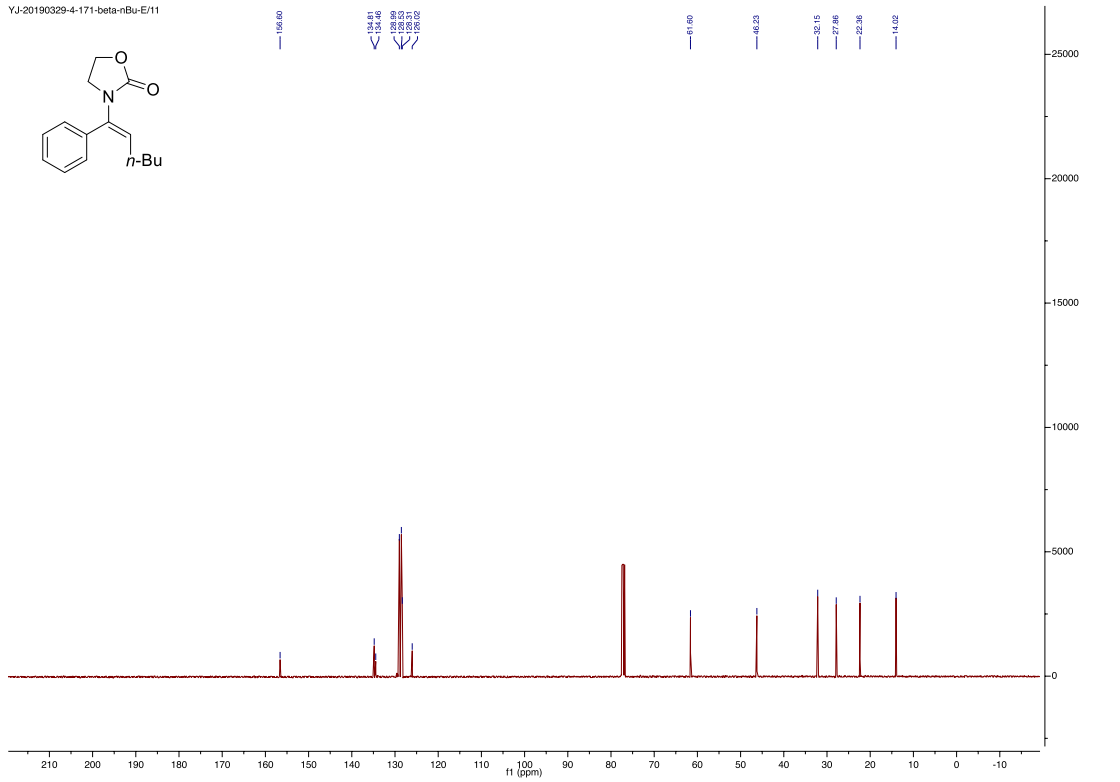
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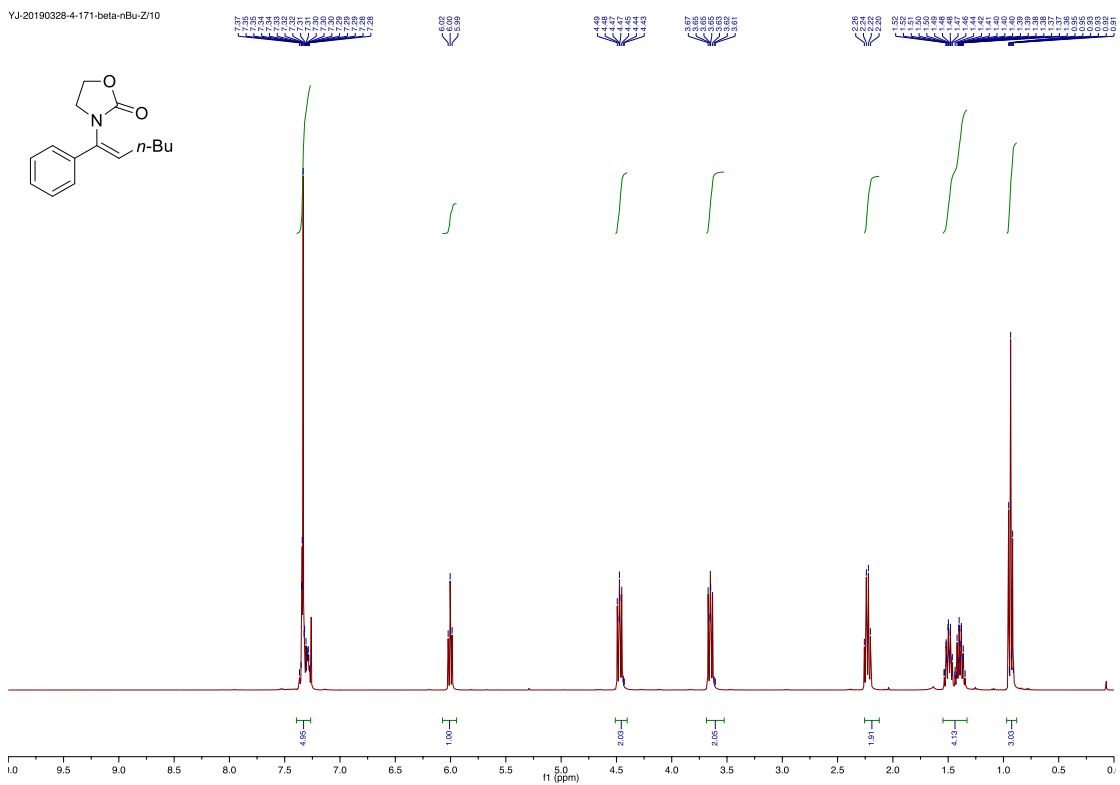
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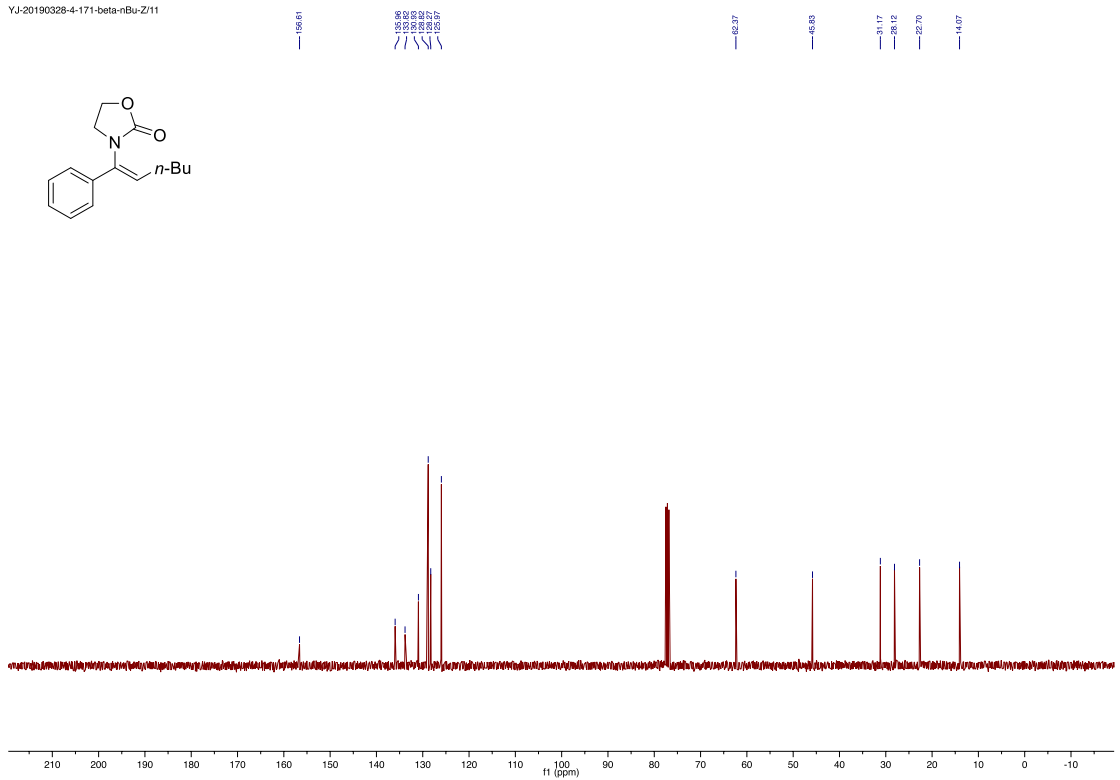
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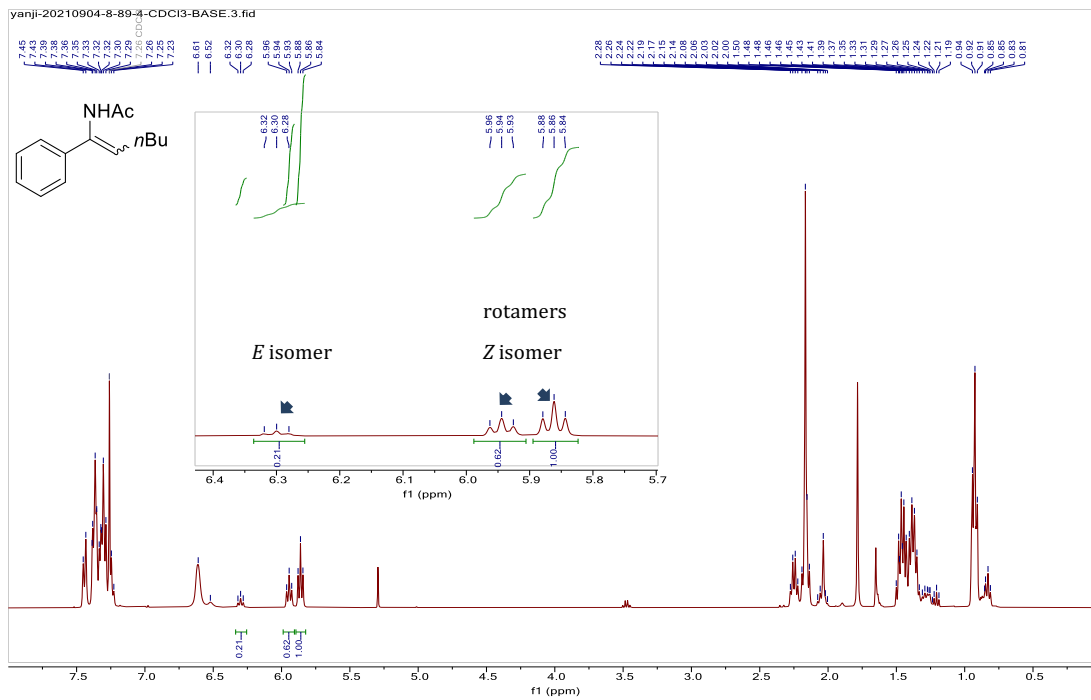


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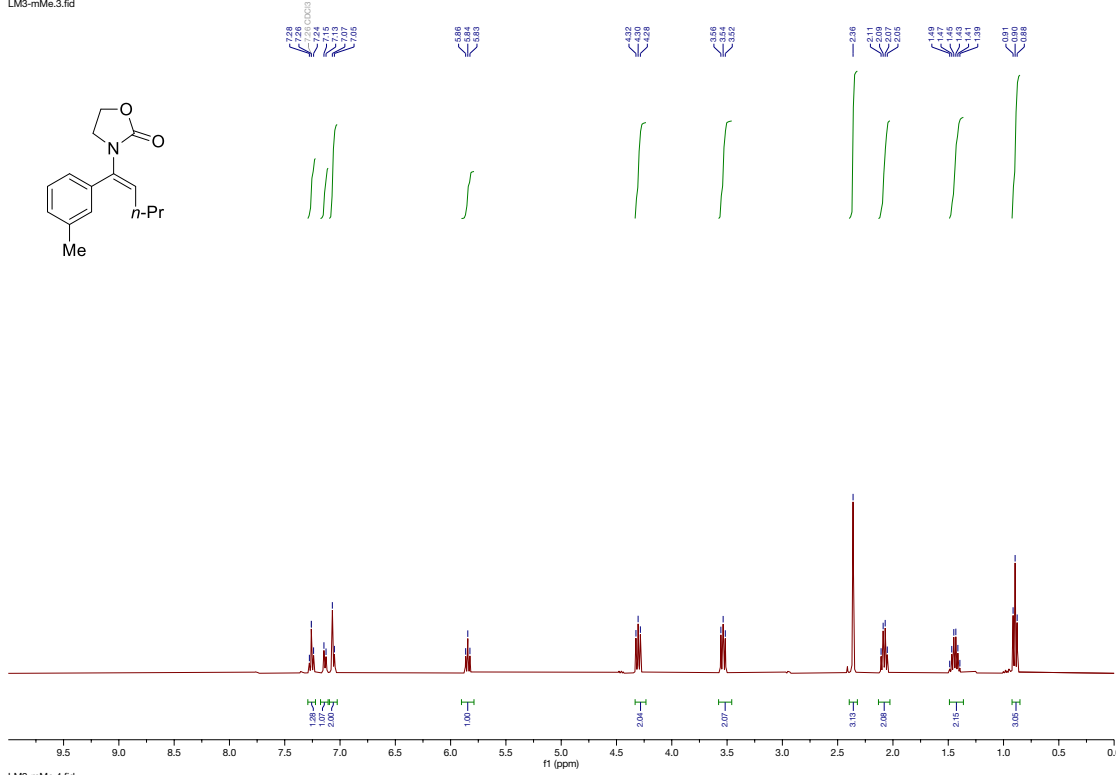
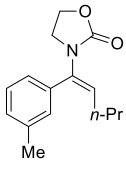


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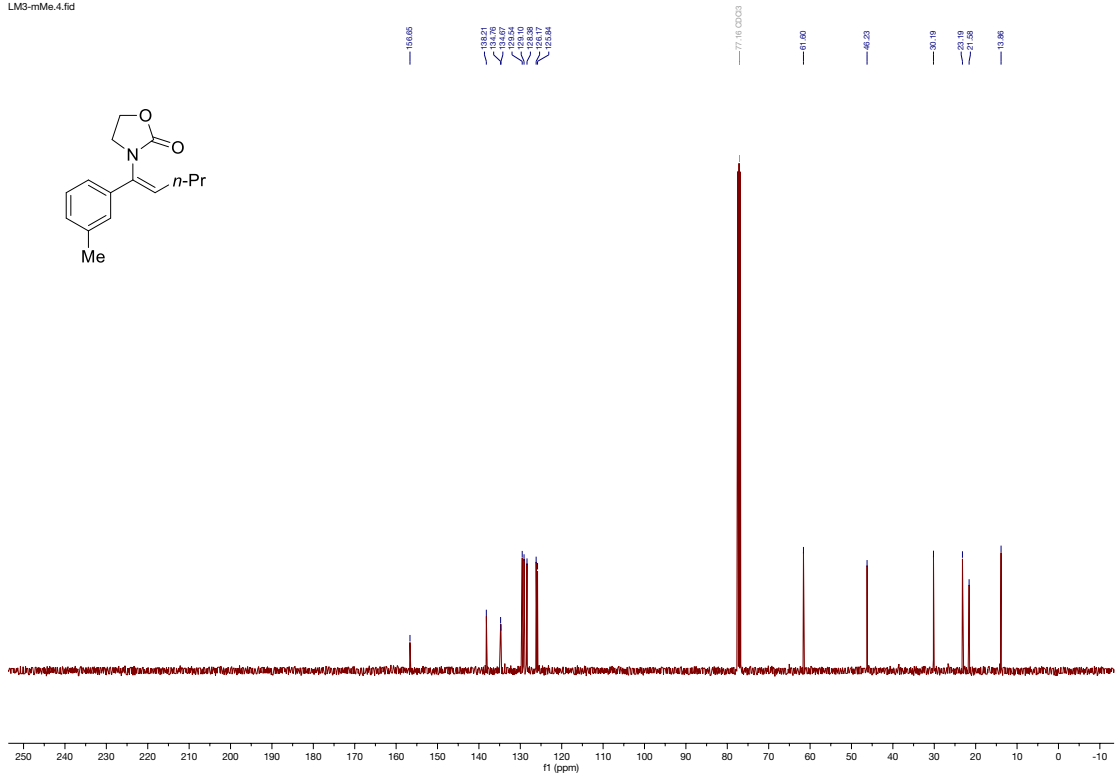
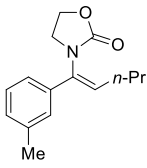




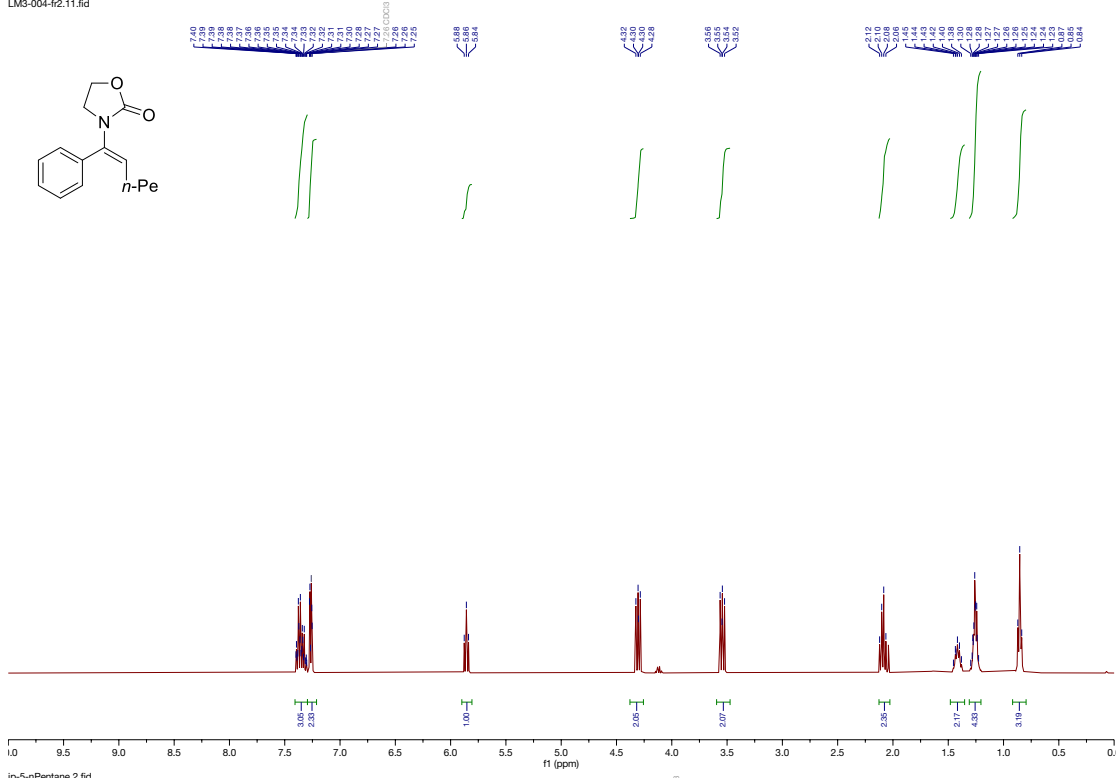
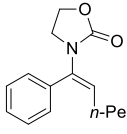
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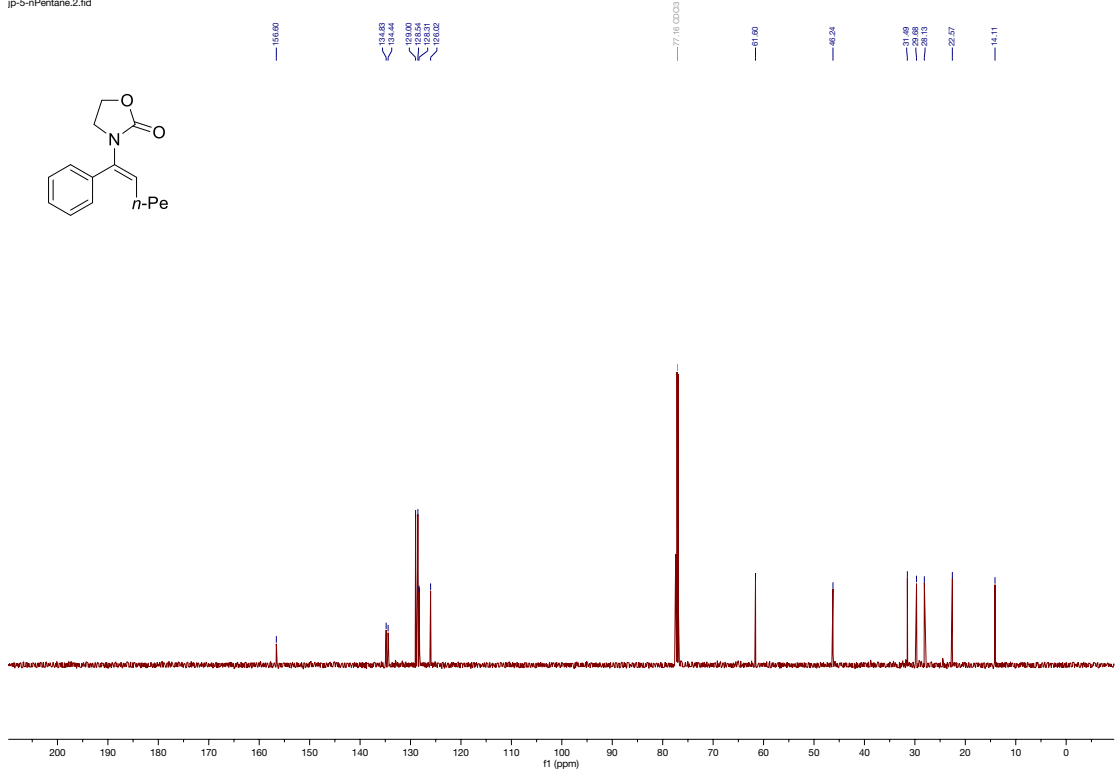
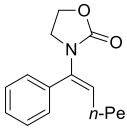
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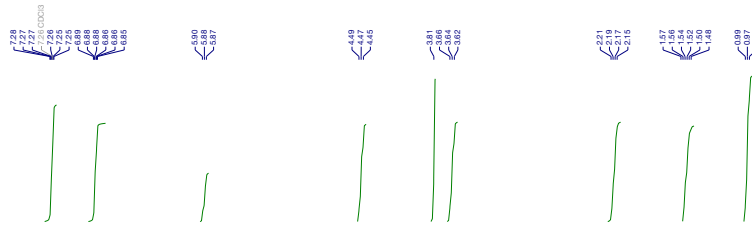
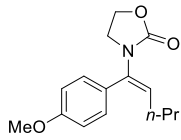
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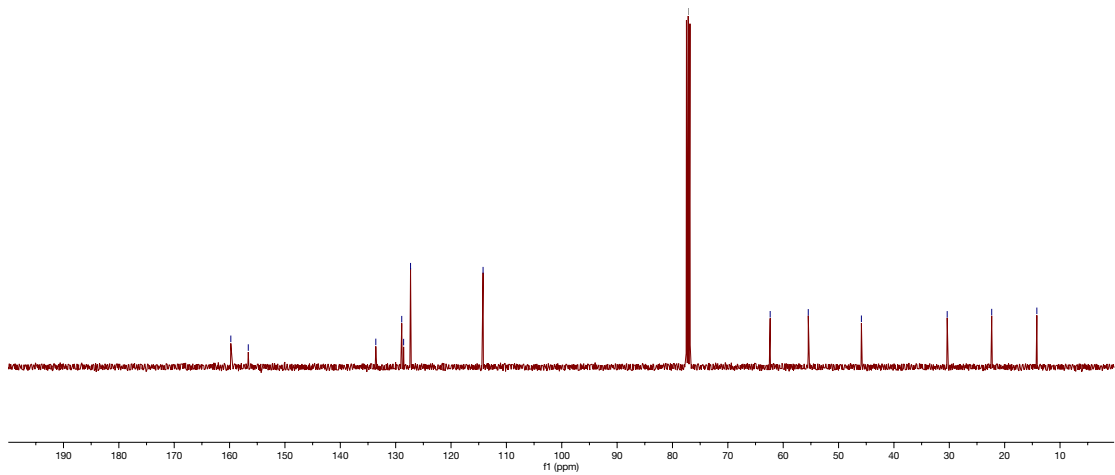
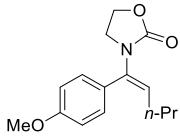
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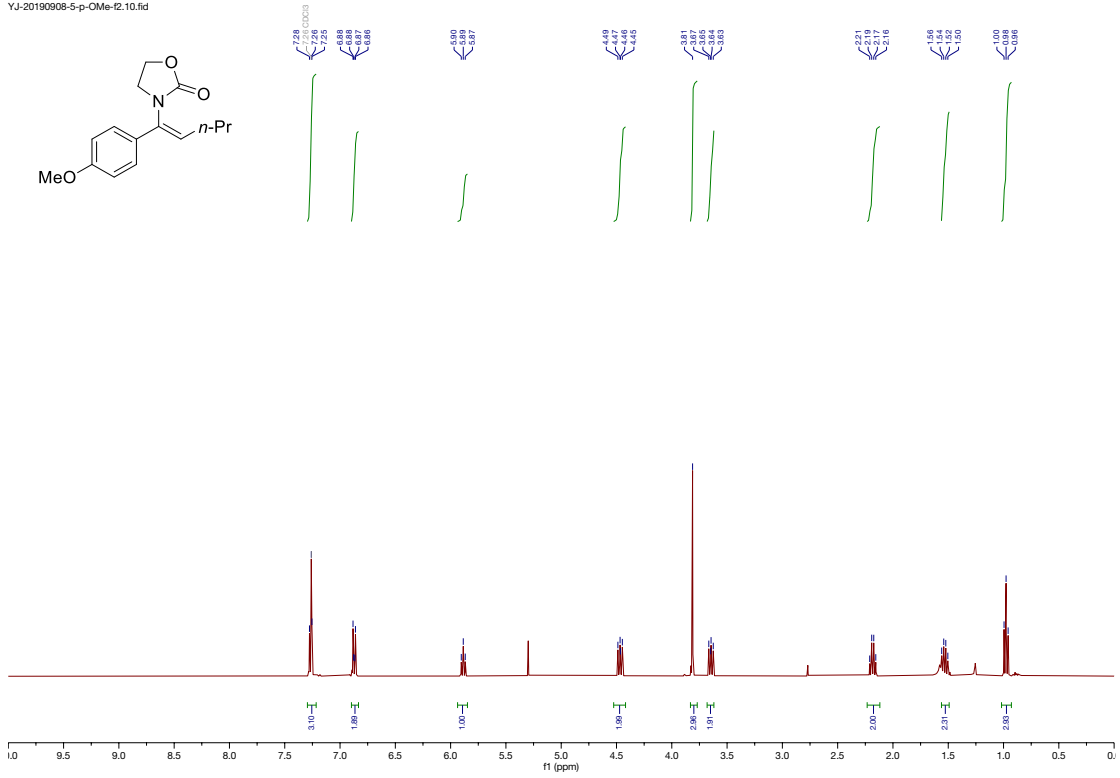
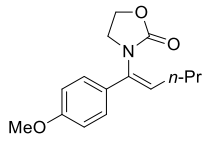
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 PROTON, SU CDCl3 /opt/nmrdata yangi 20



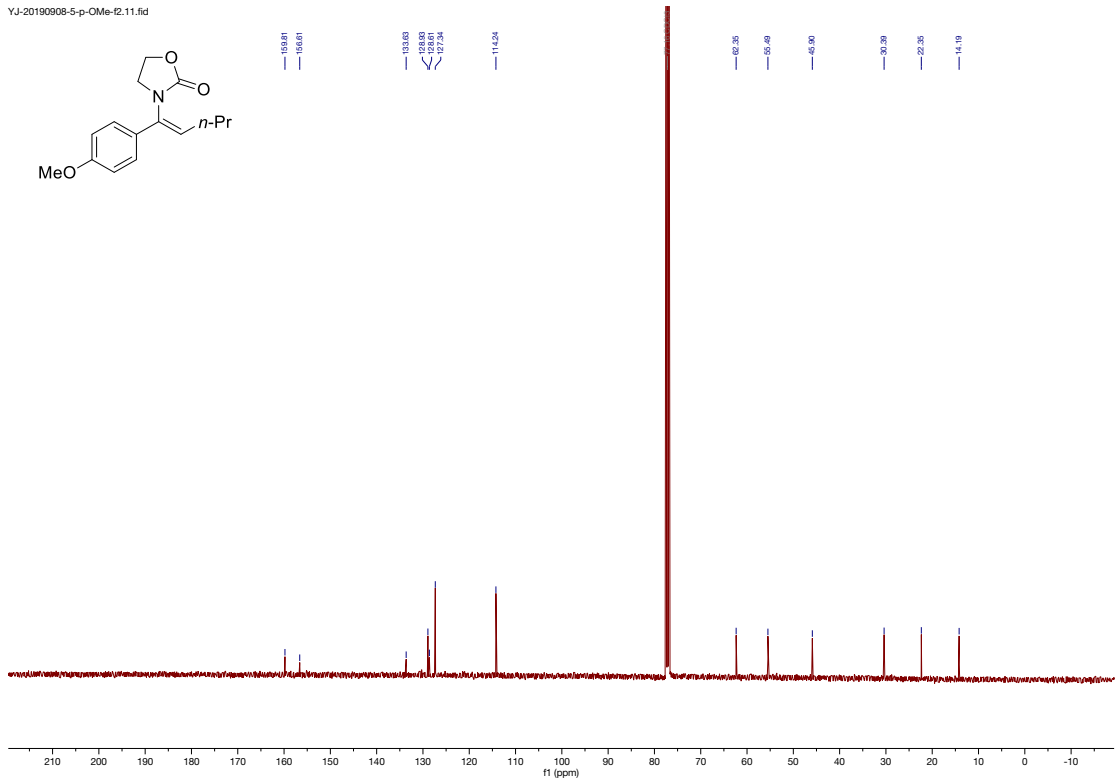
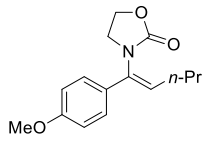
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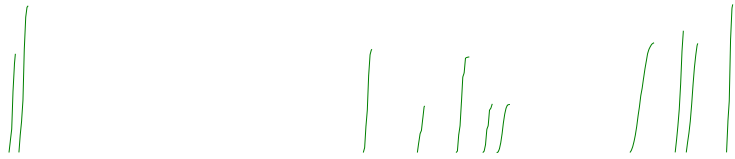
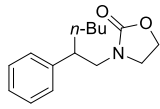
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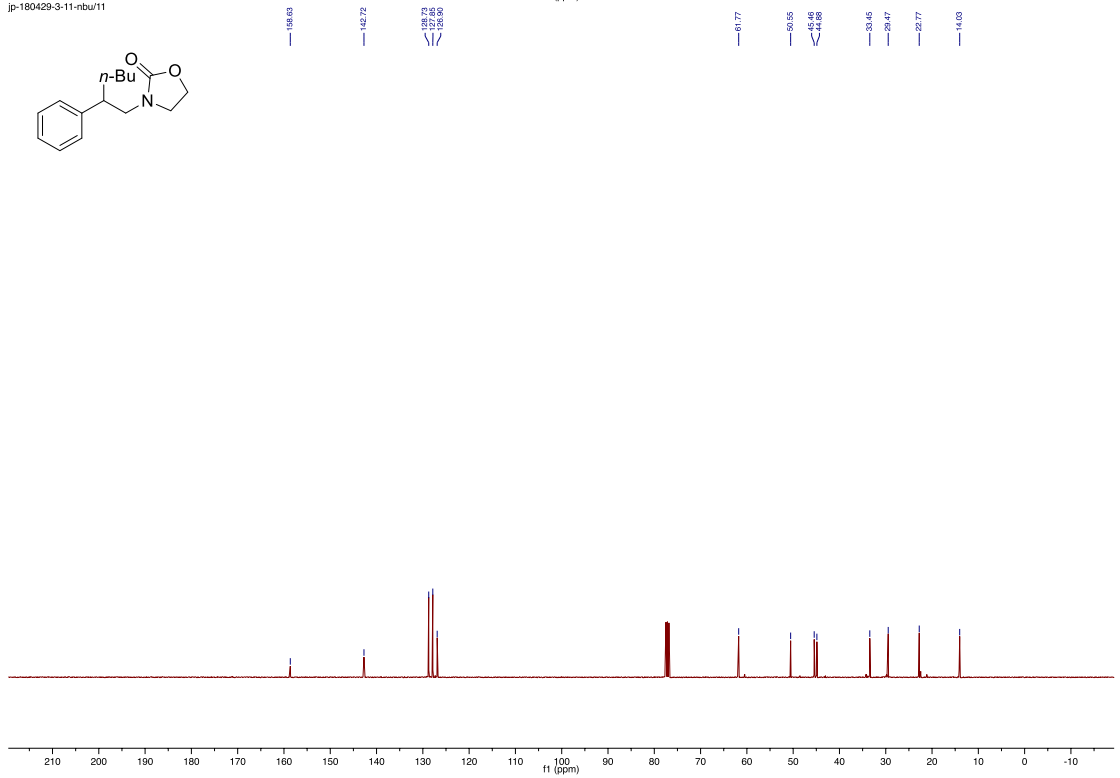
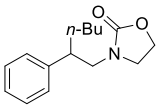
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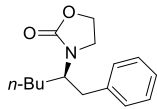
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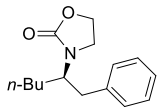
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LM-20190311-2-120J/10

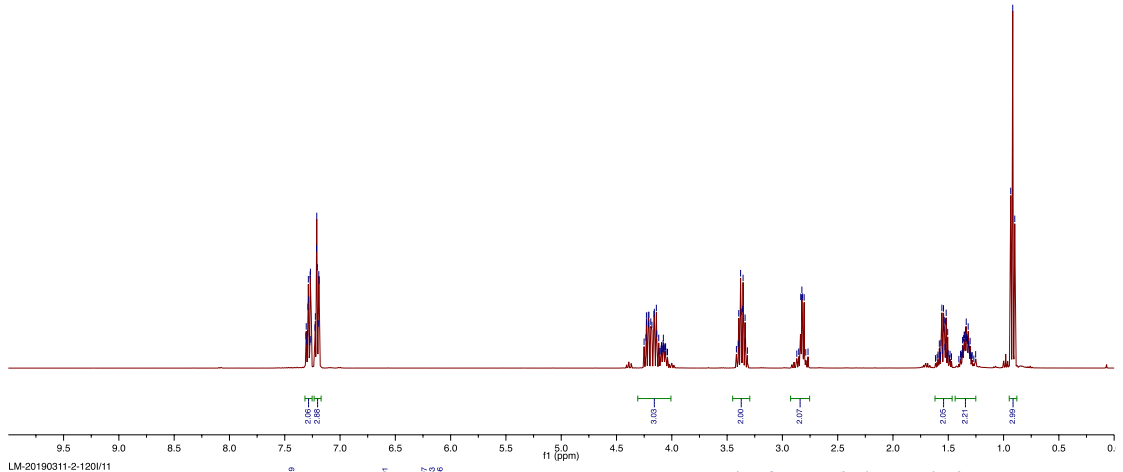
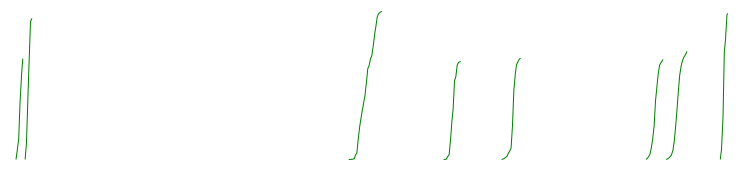
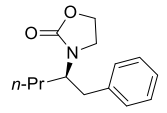


LM-20190311-2-120J/10



LM-20190311-2-1201/10

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LM-20190311-2-1201/11

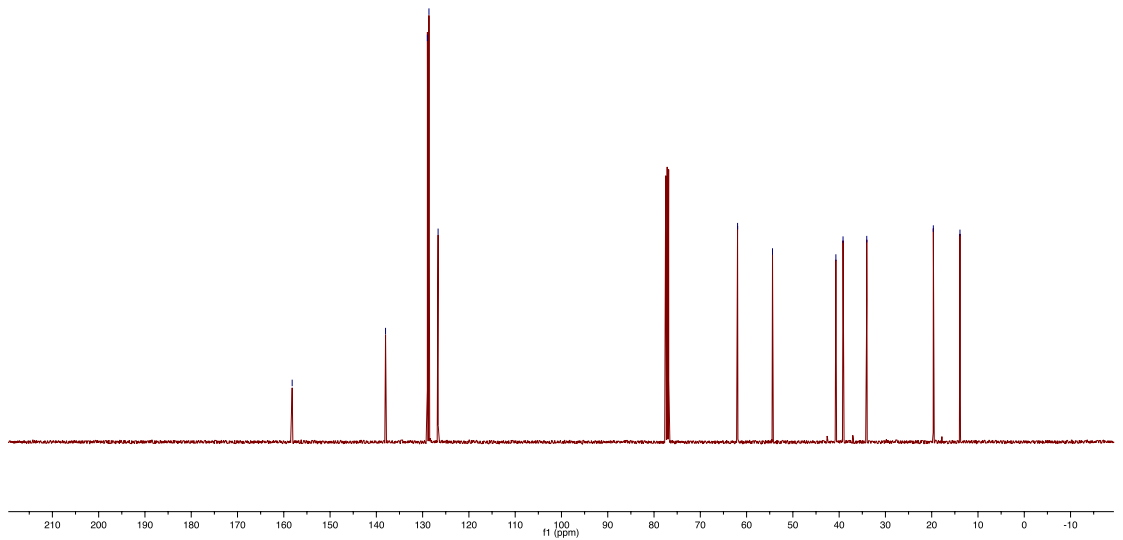
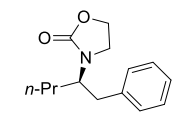
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138.01
138.87
138.86

51.95
54.40

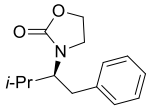
40.71
39.74

34.03

19.85
13.89

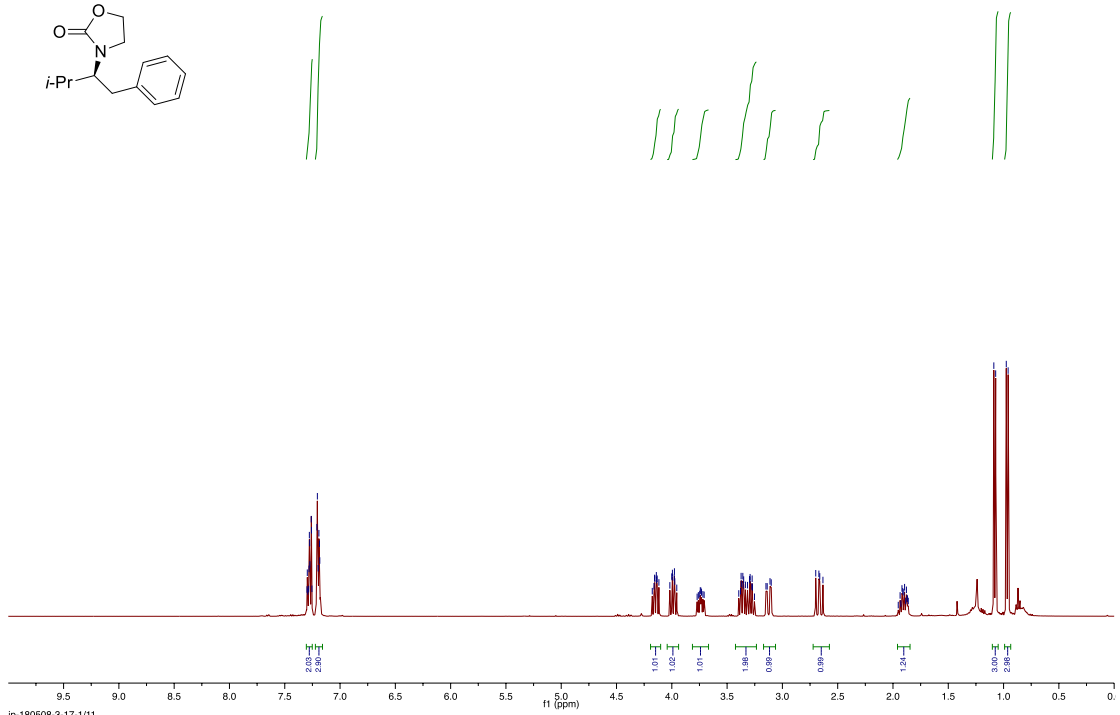


jp-180508-3-17-1/10

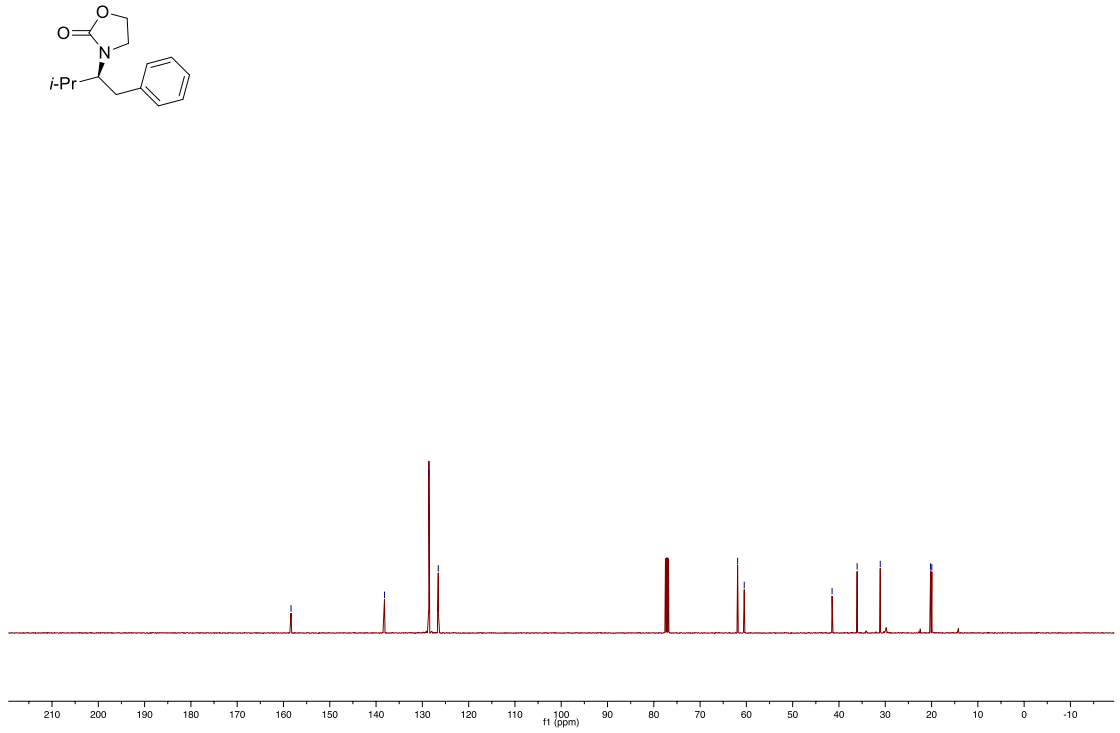
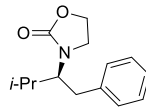


1H NMR (CDCl₃)

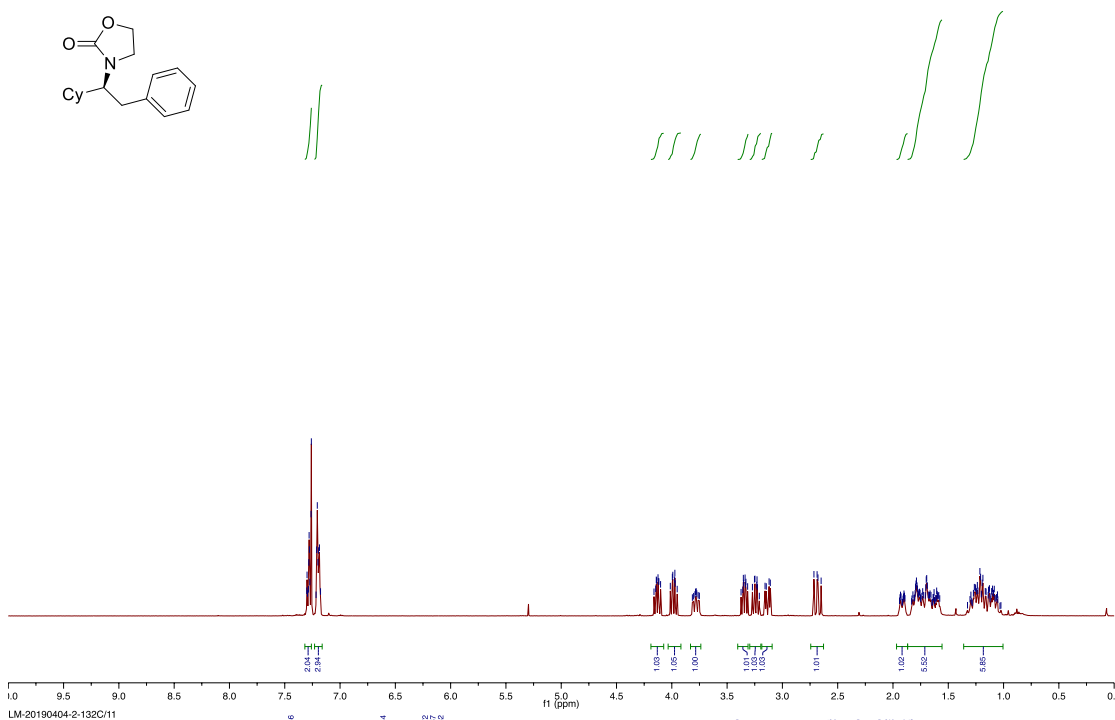
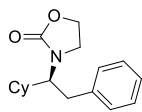
13C NMR (CDCl₃)



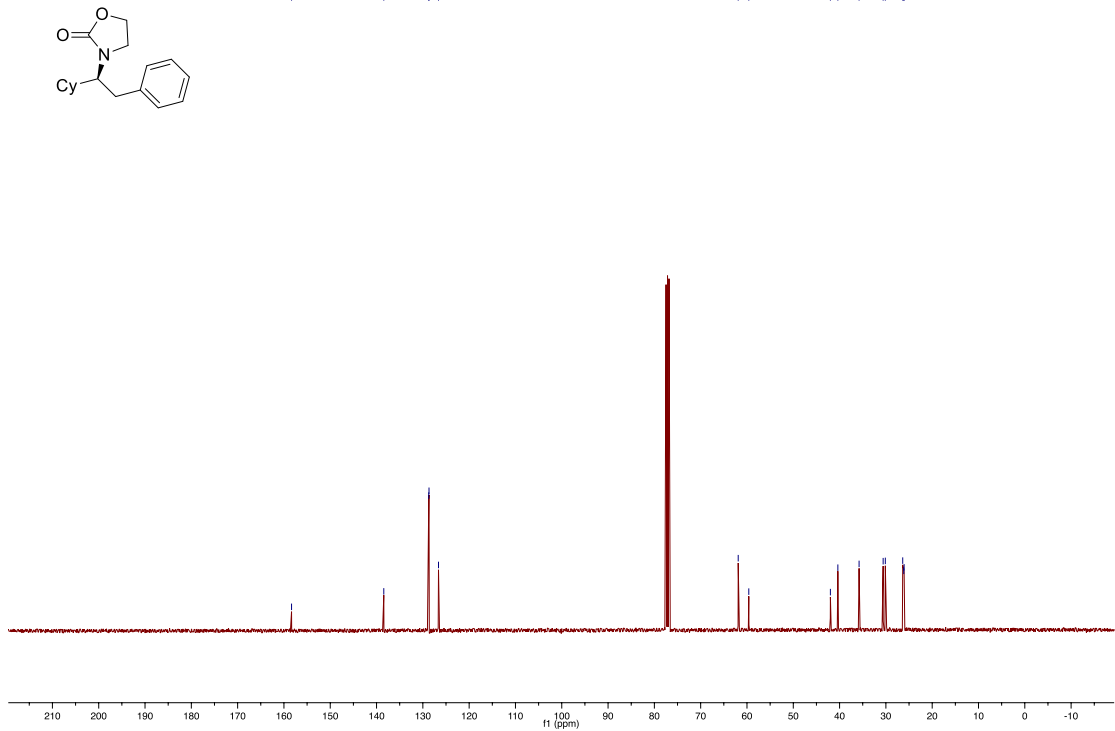
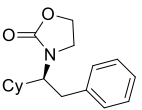
jp-180508-3-17-1/11

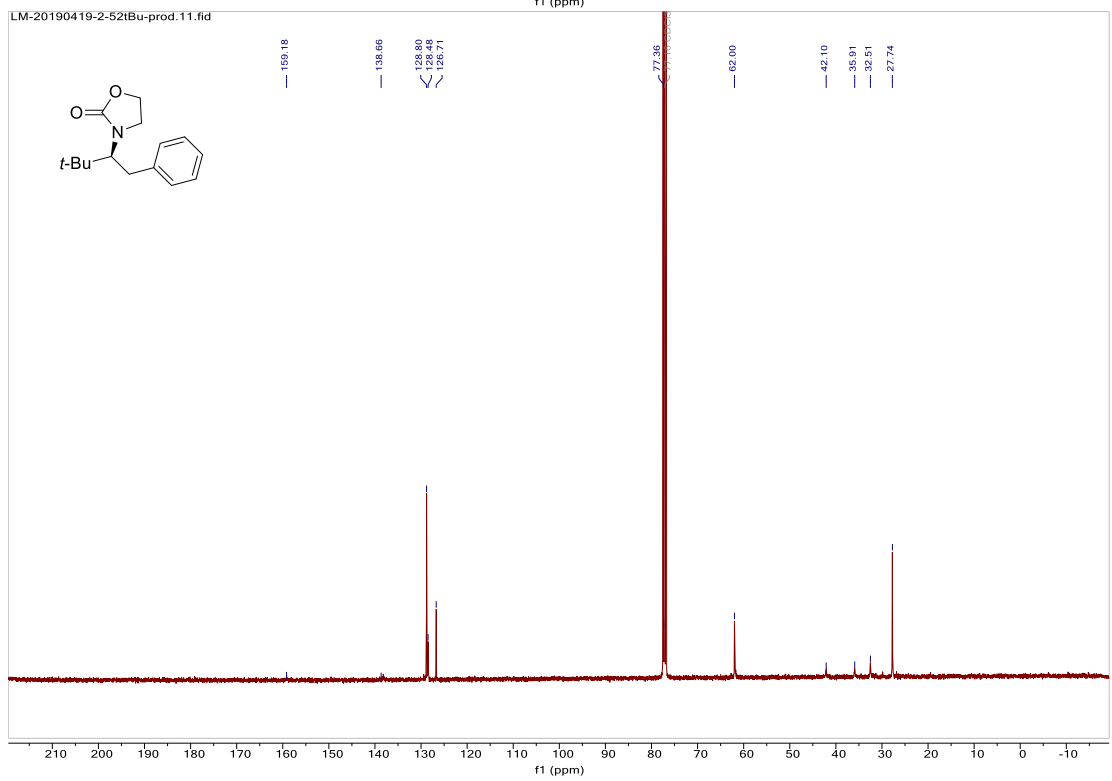
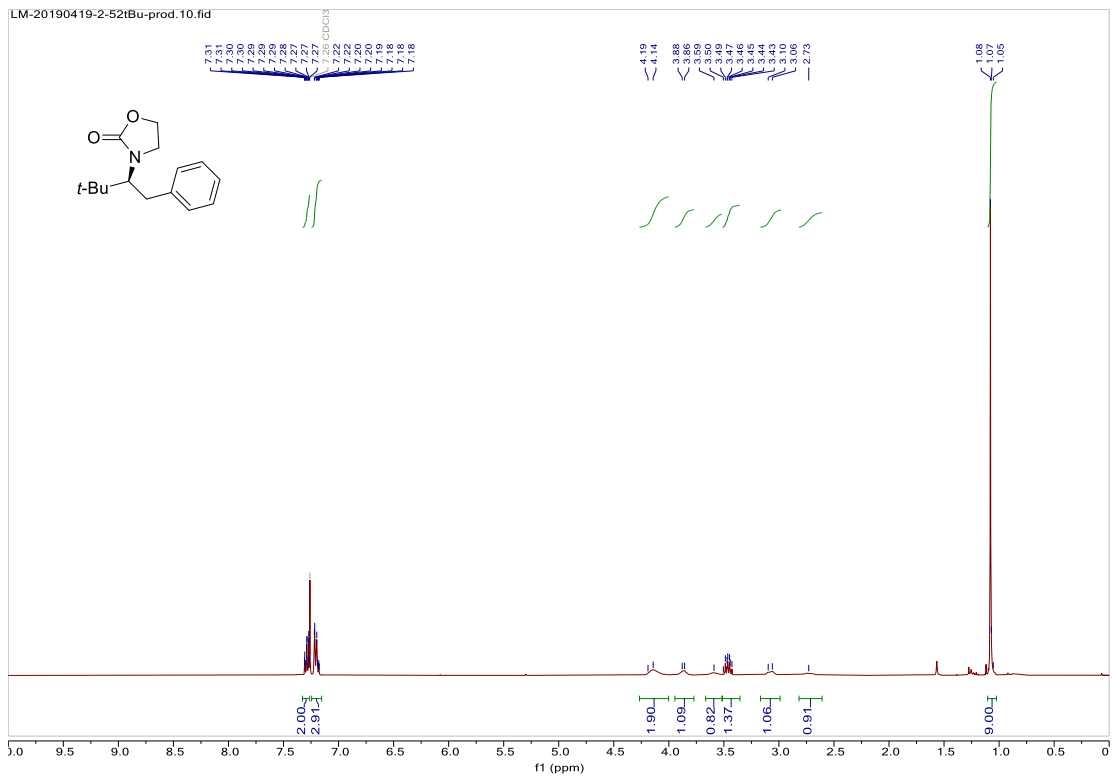


LM-20190404-2-132C/10

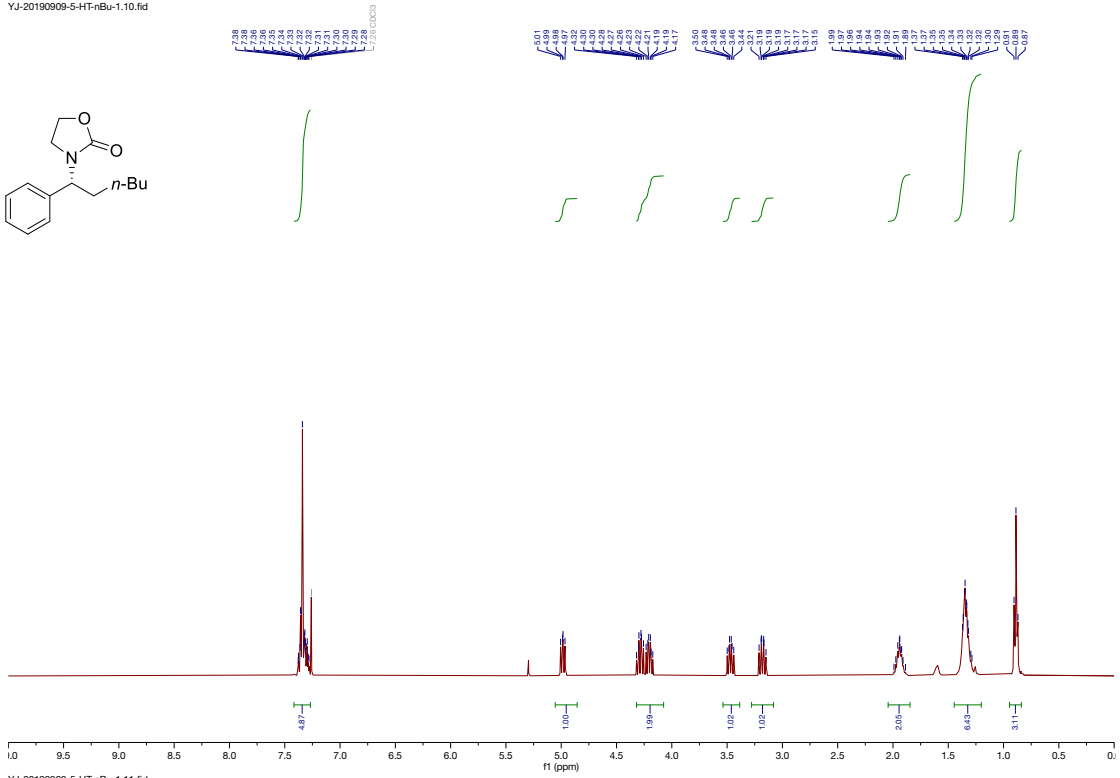
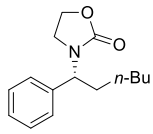


LM-20190404-2-132C/11

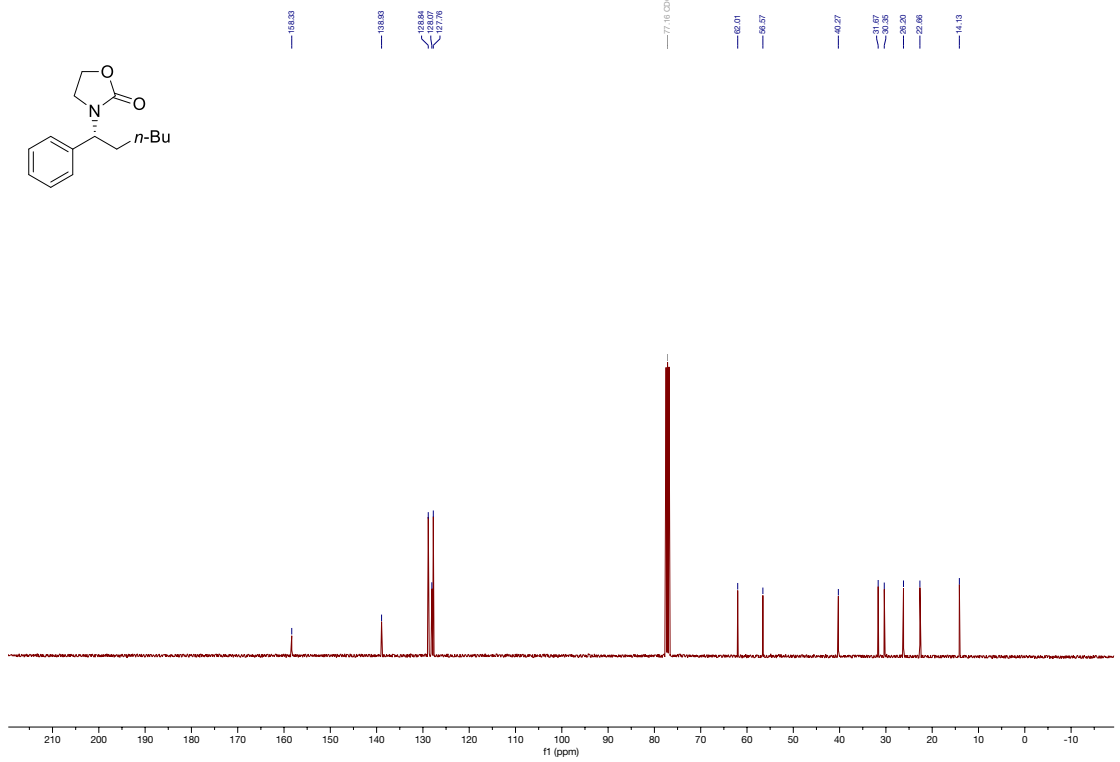
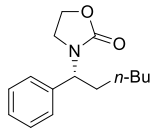




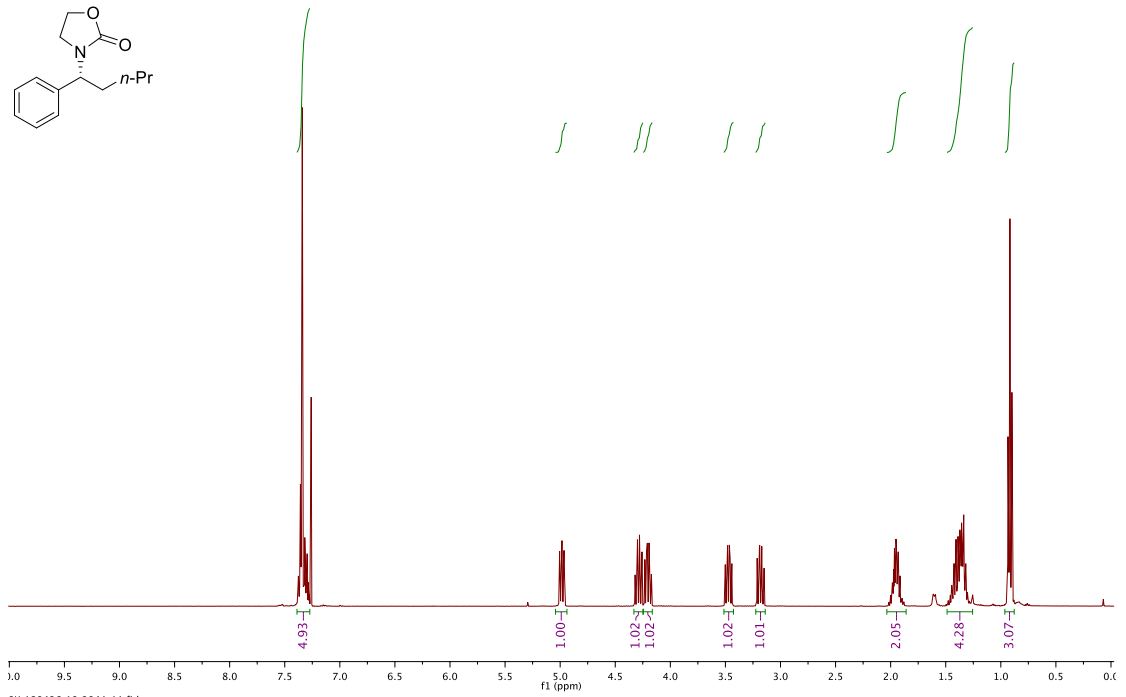
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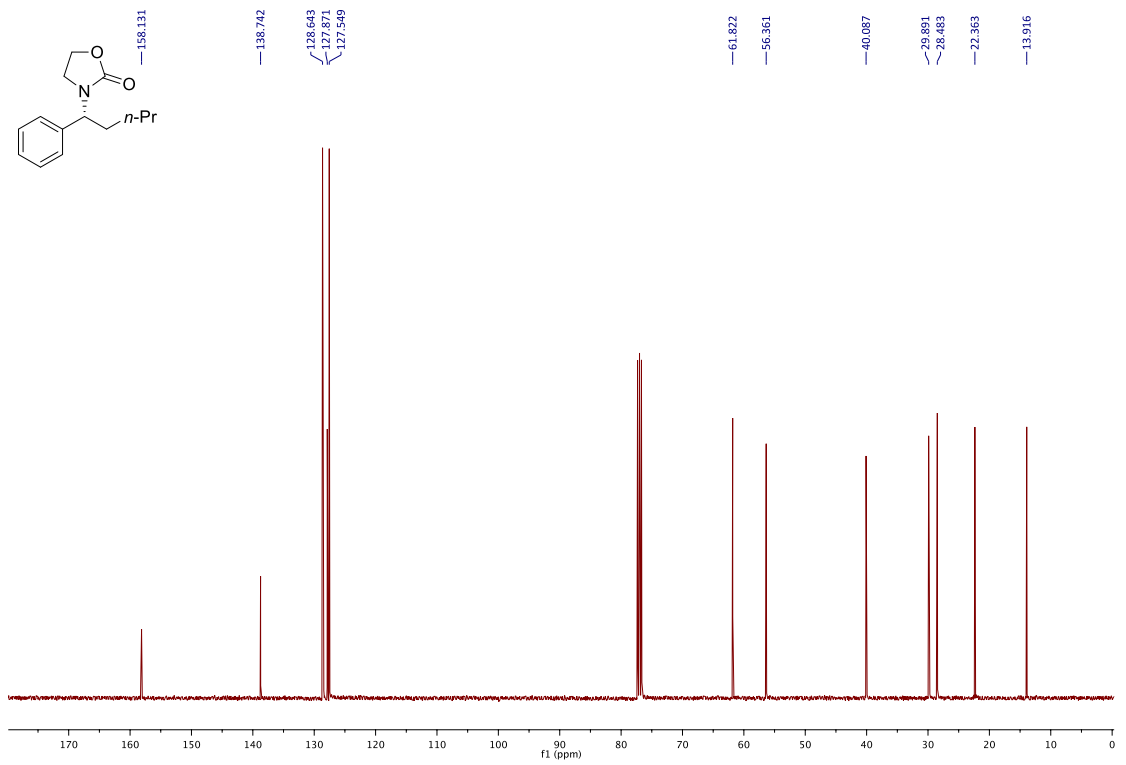
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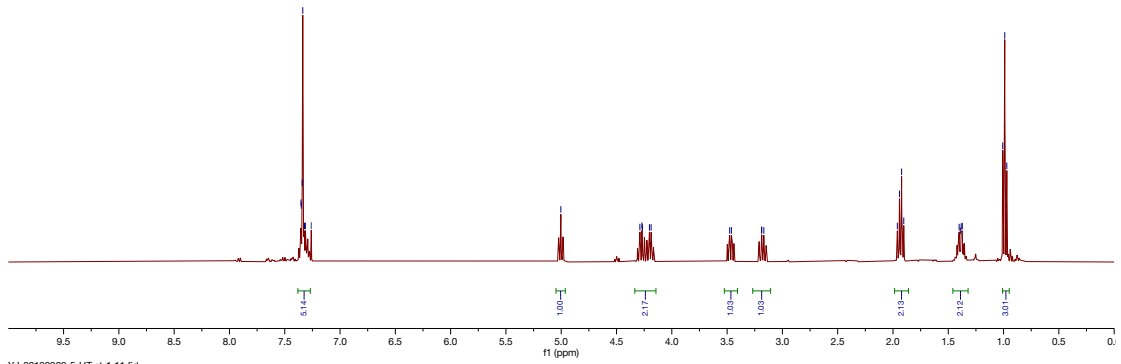
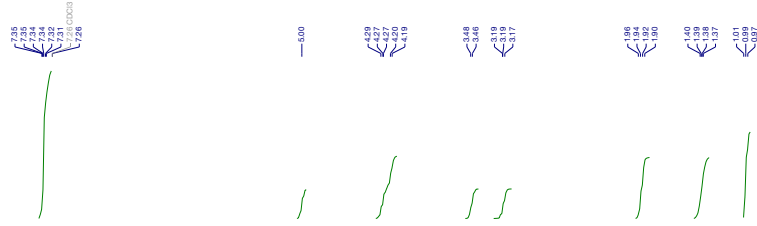
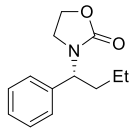
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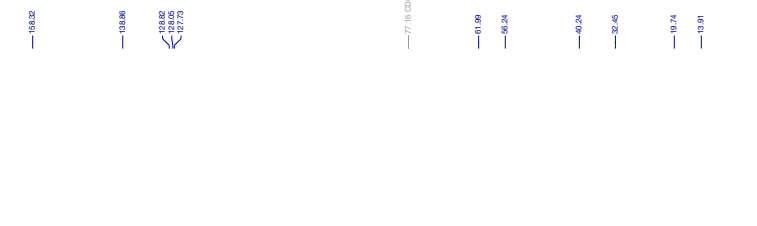
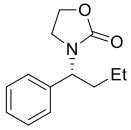
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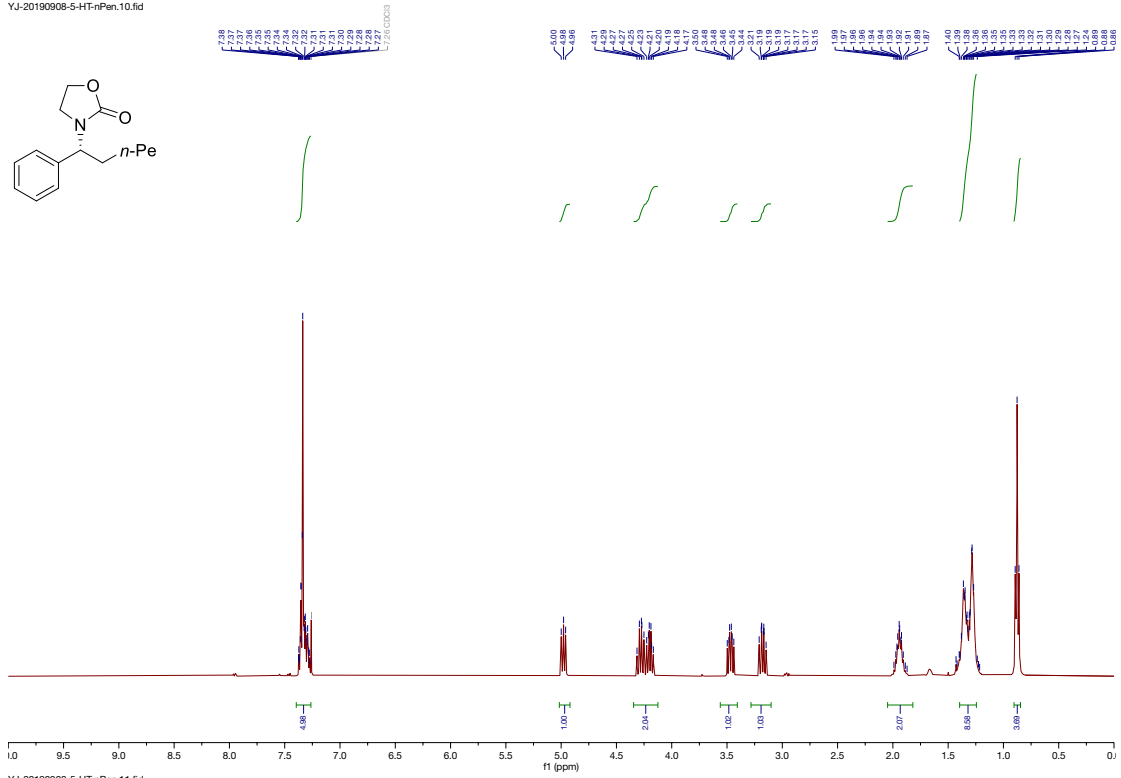
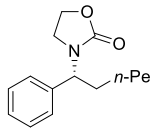
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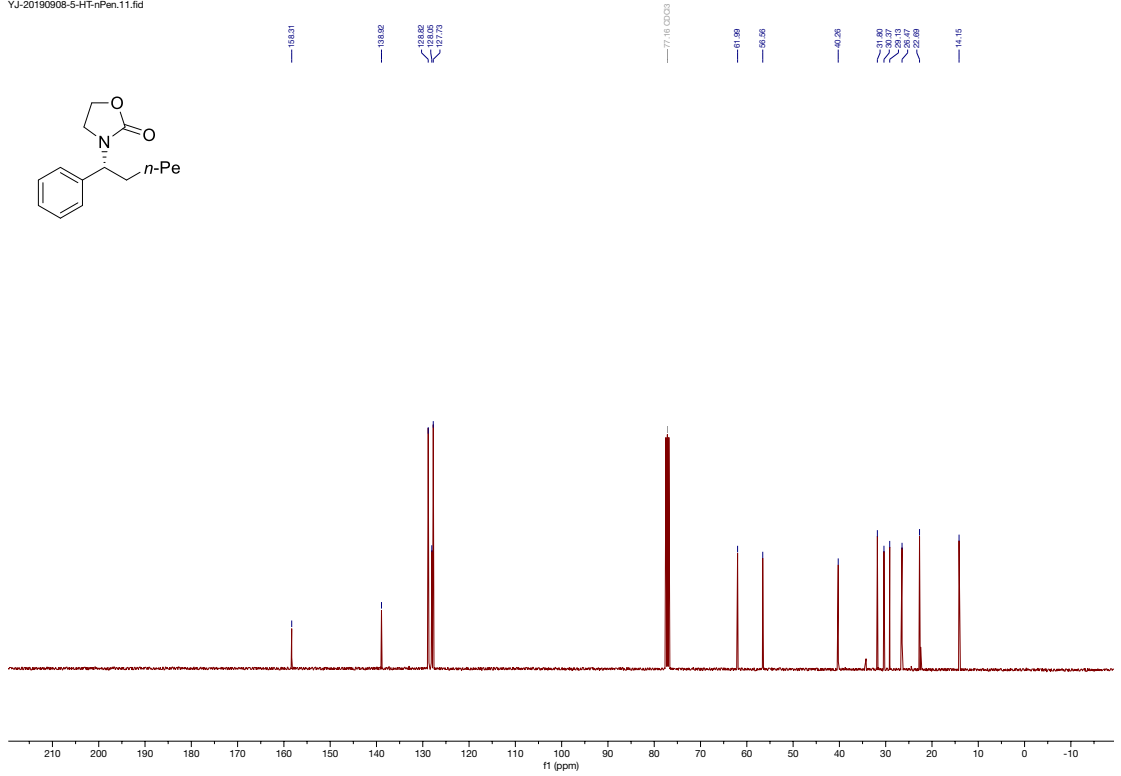
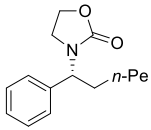
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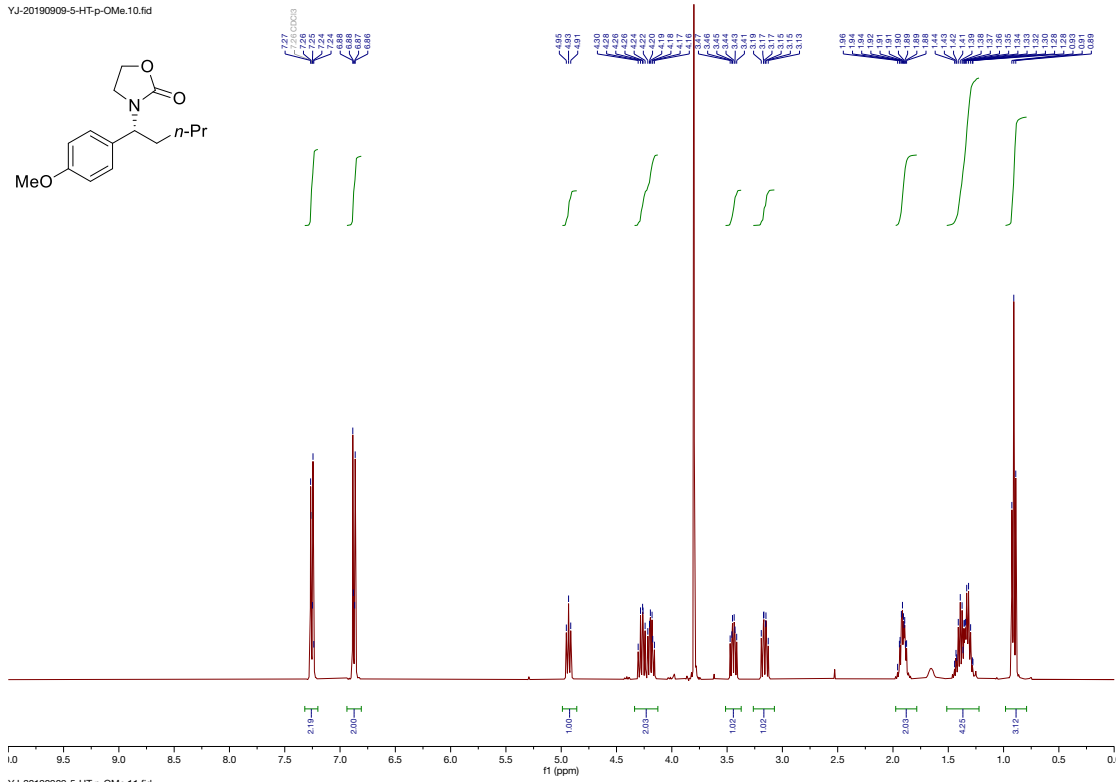
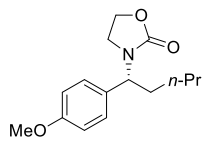
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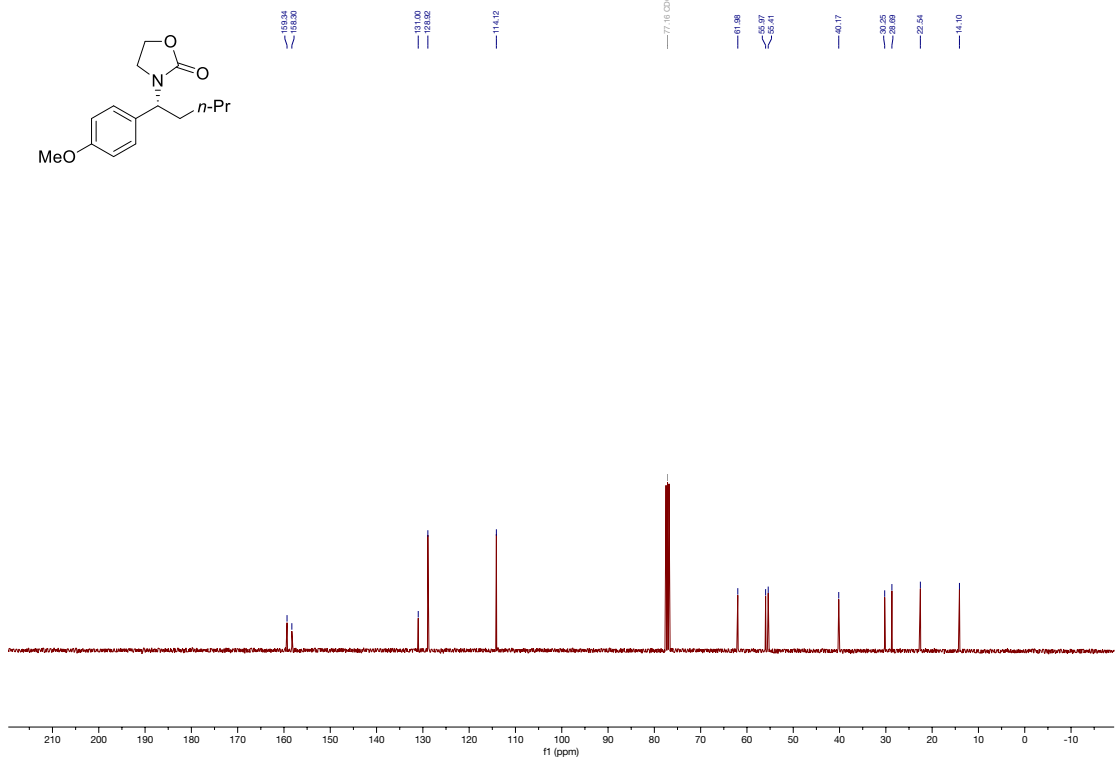
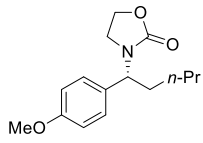
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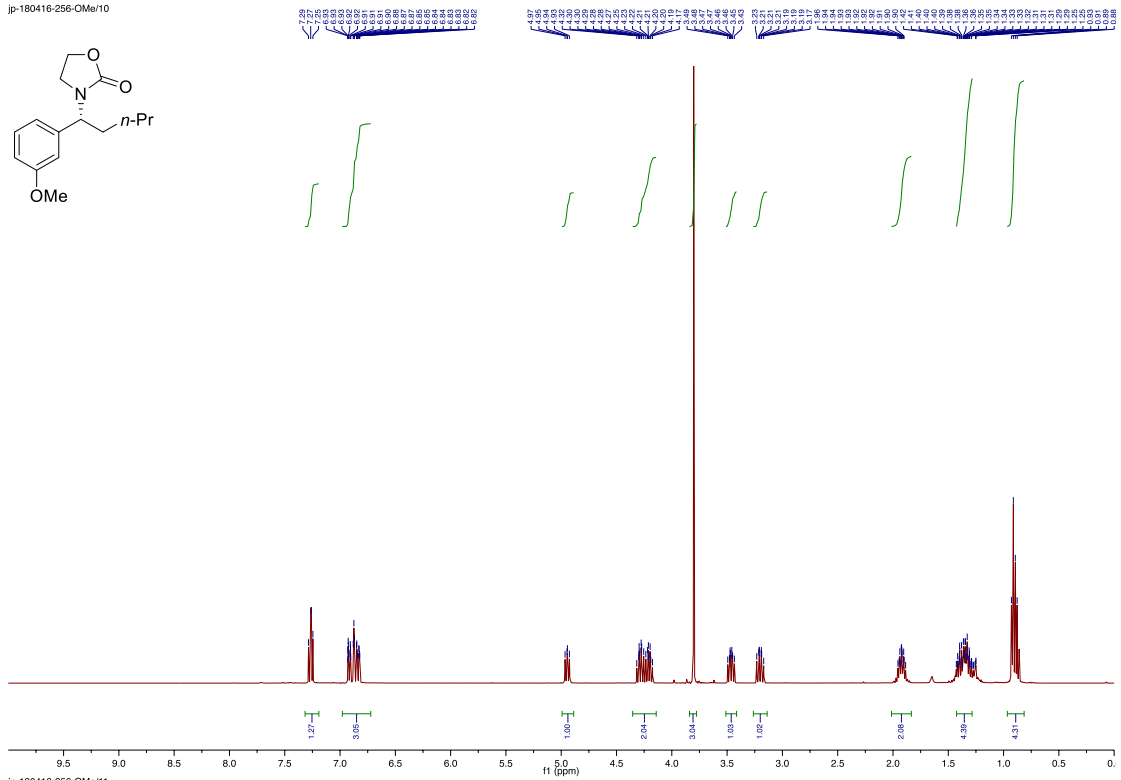
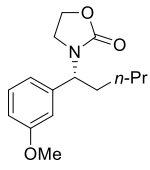
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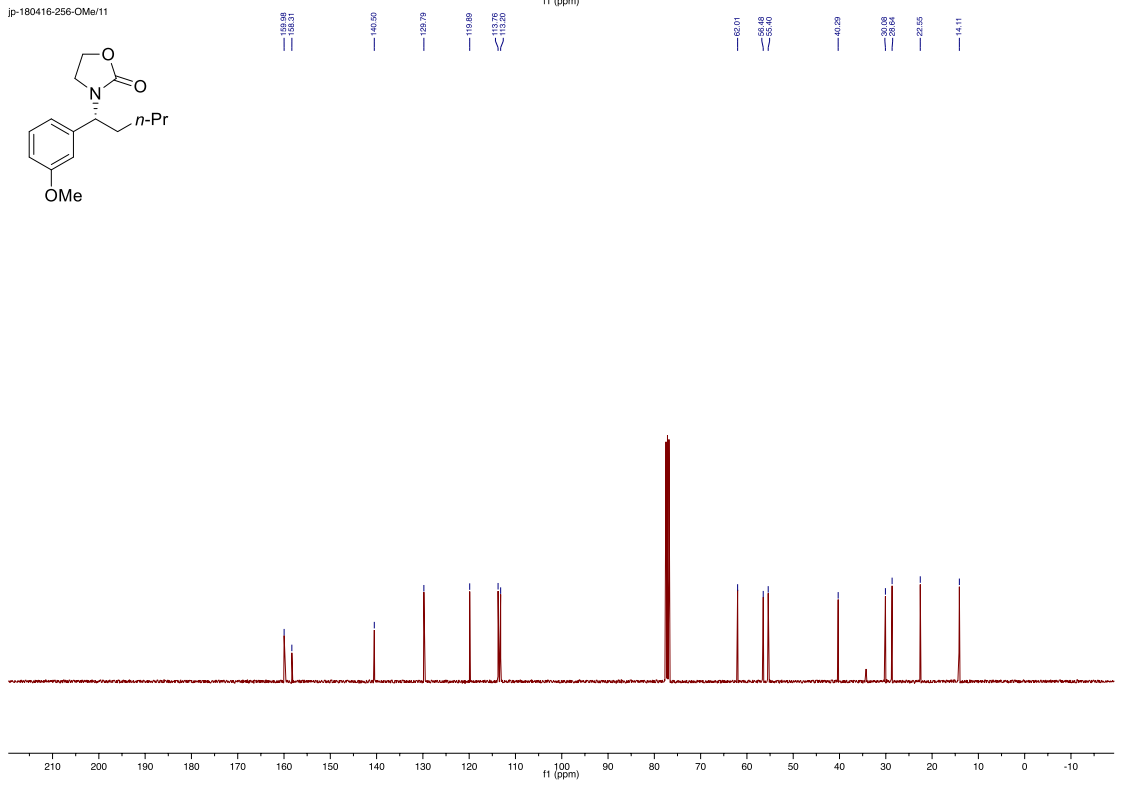
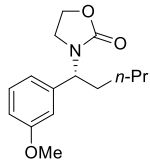
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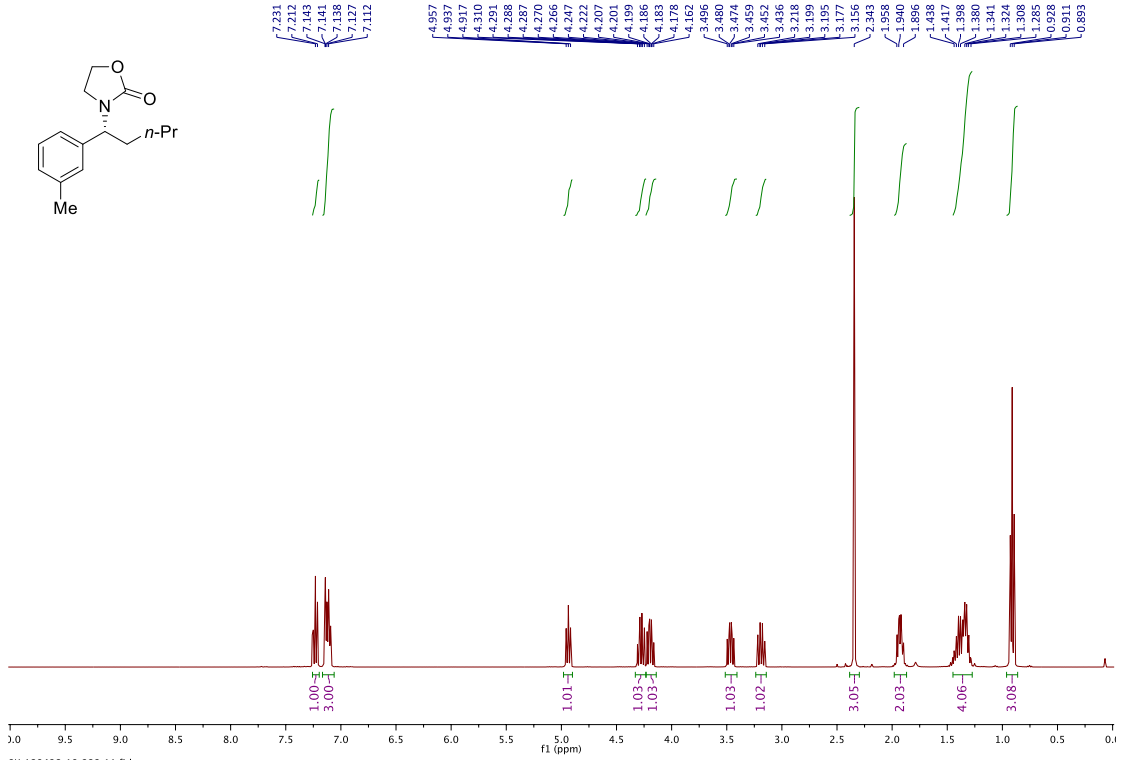
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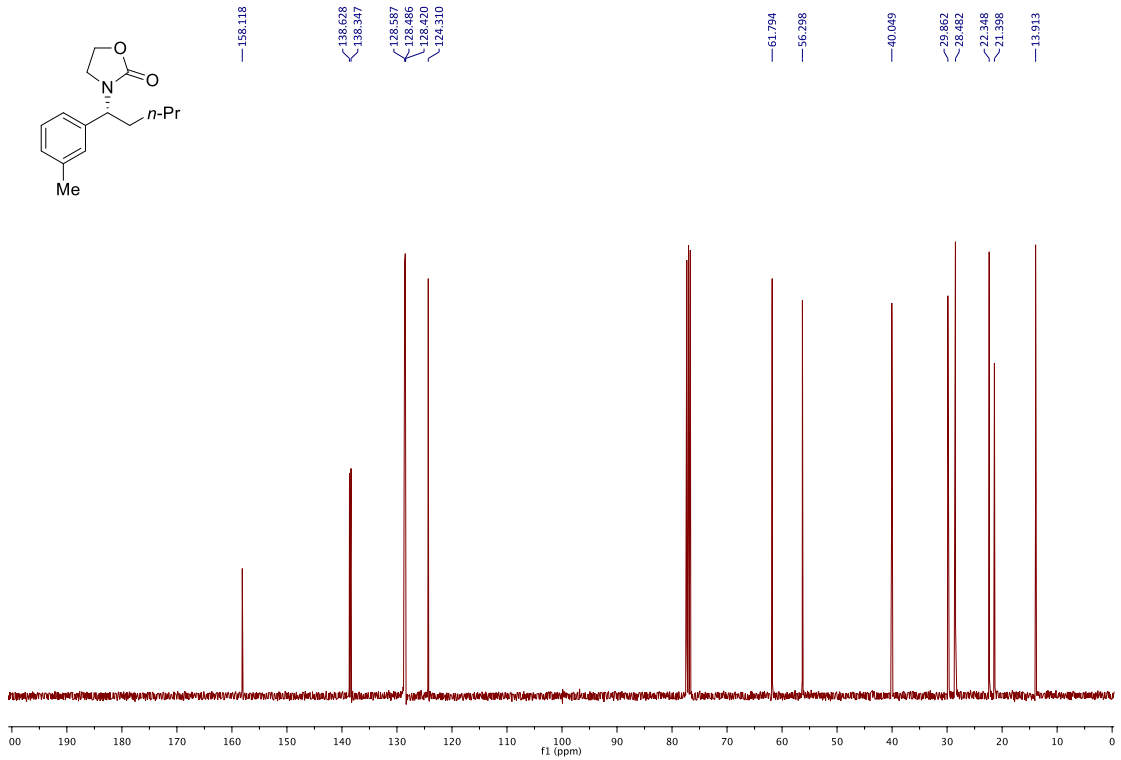
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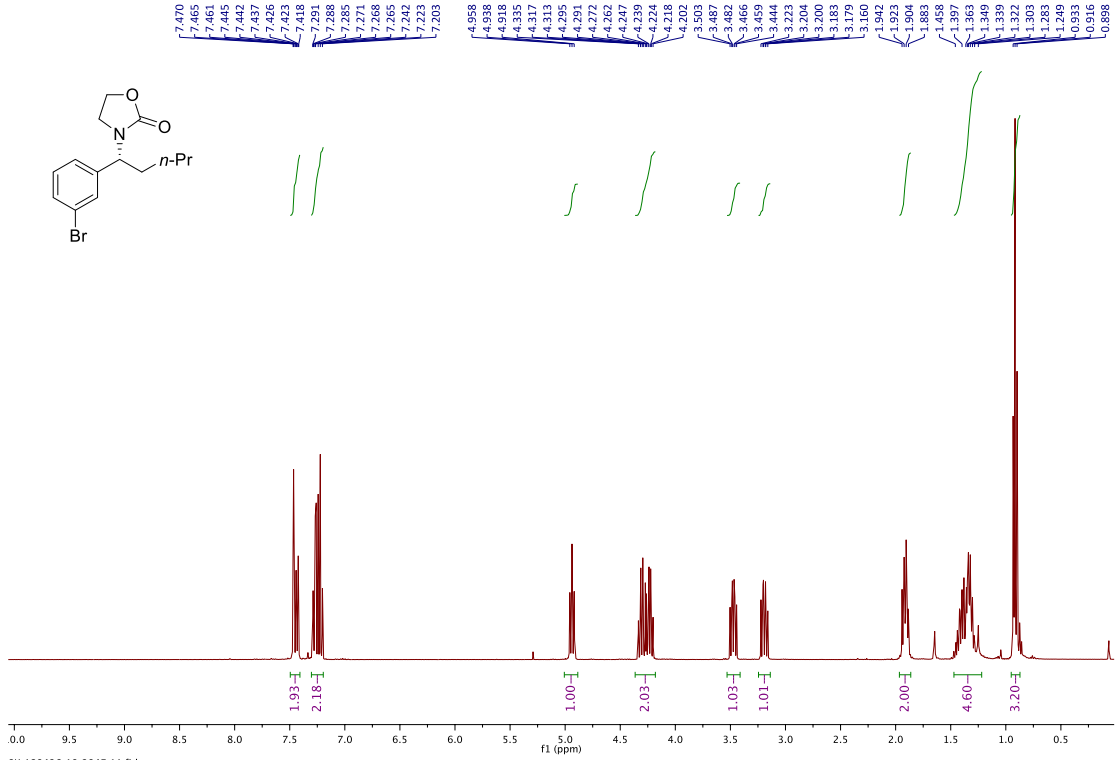
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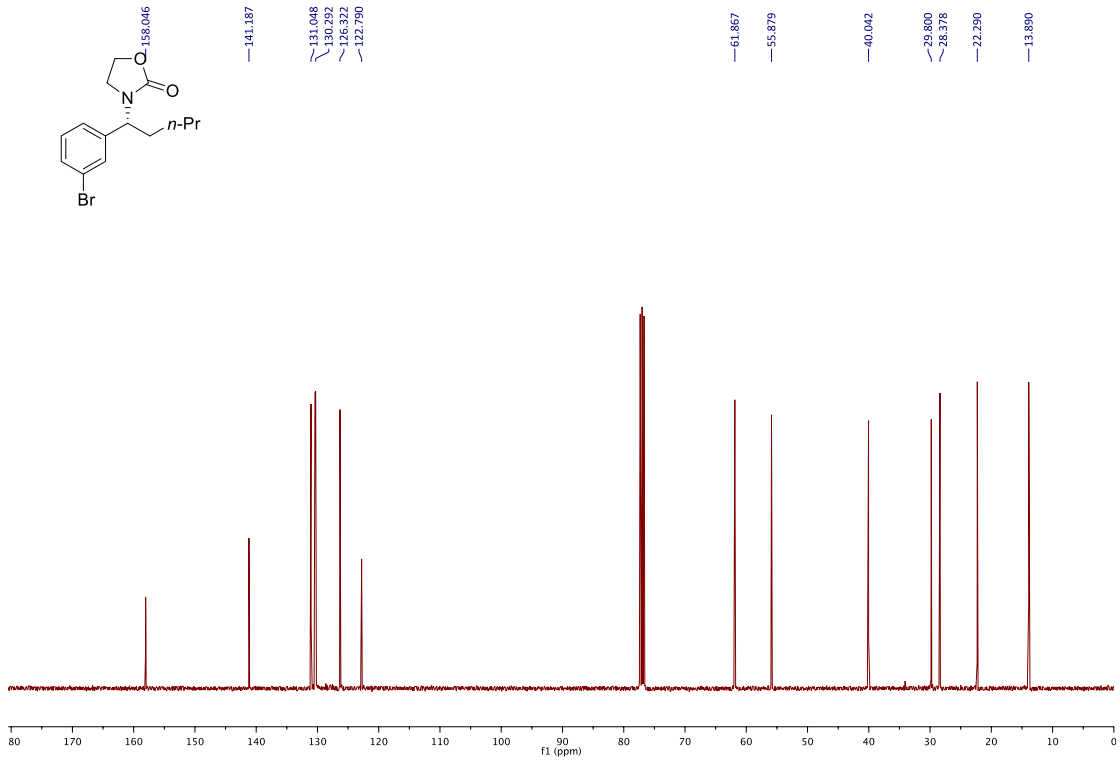
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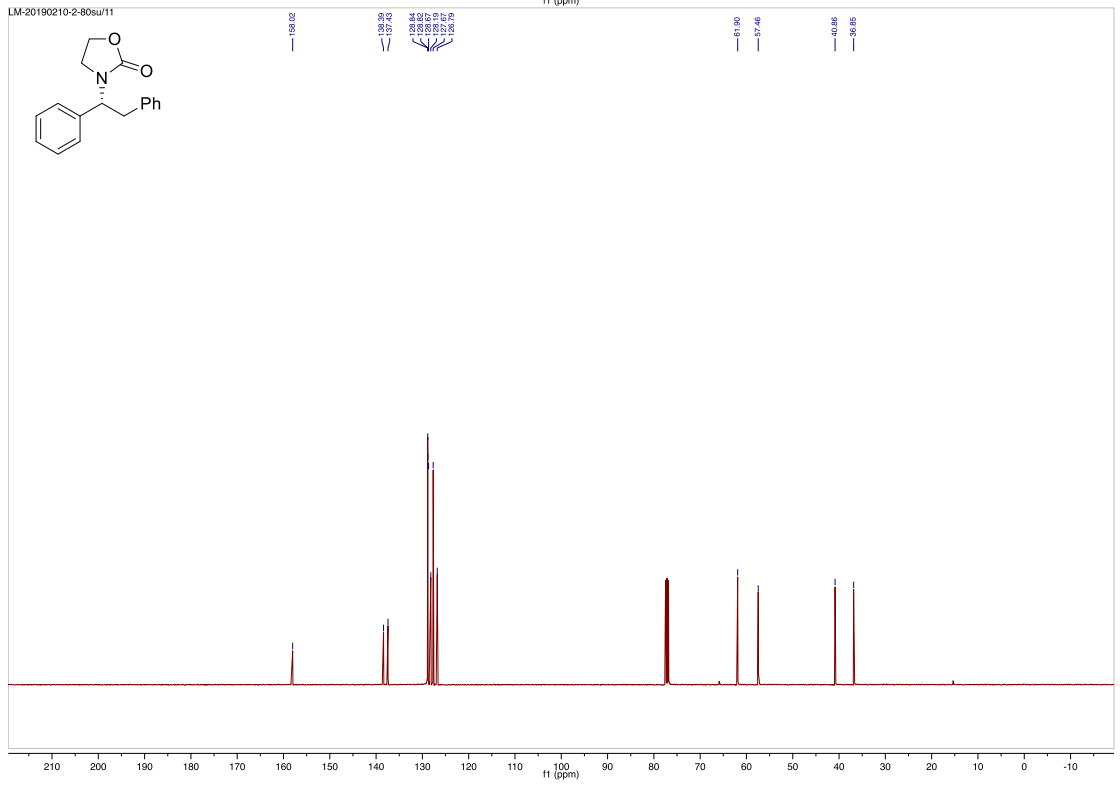
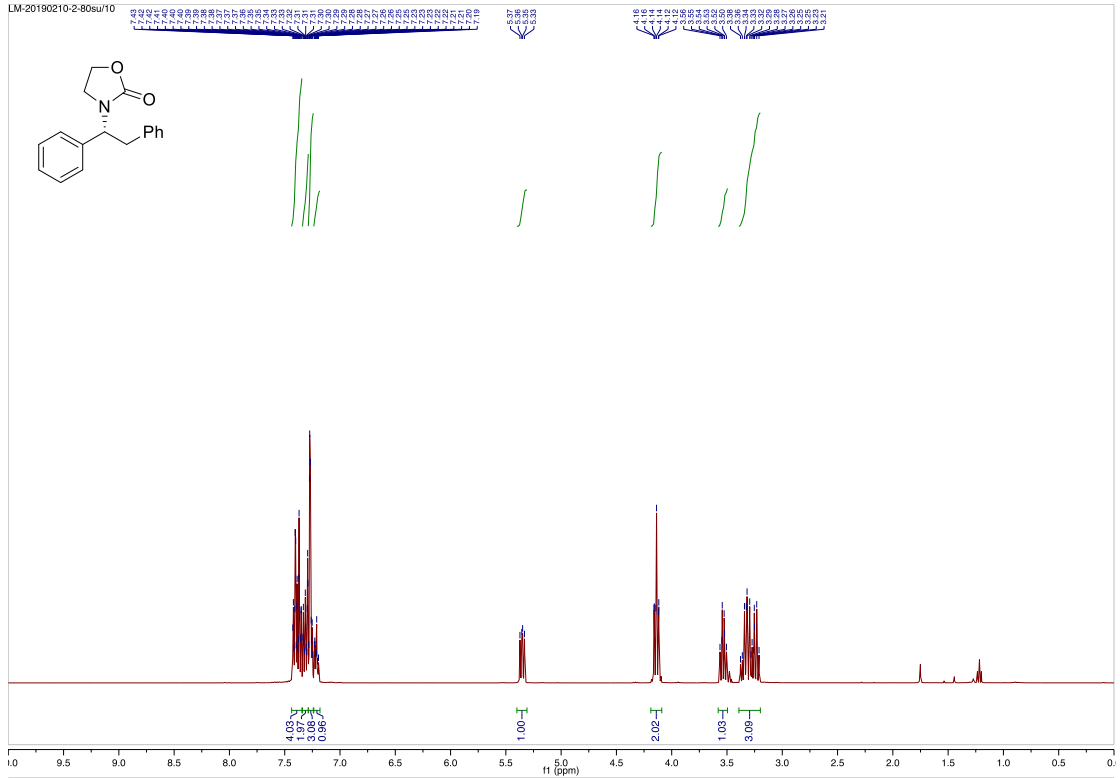


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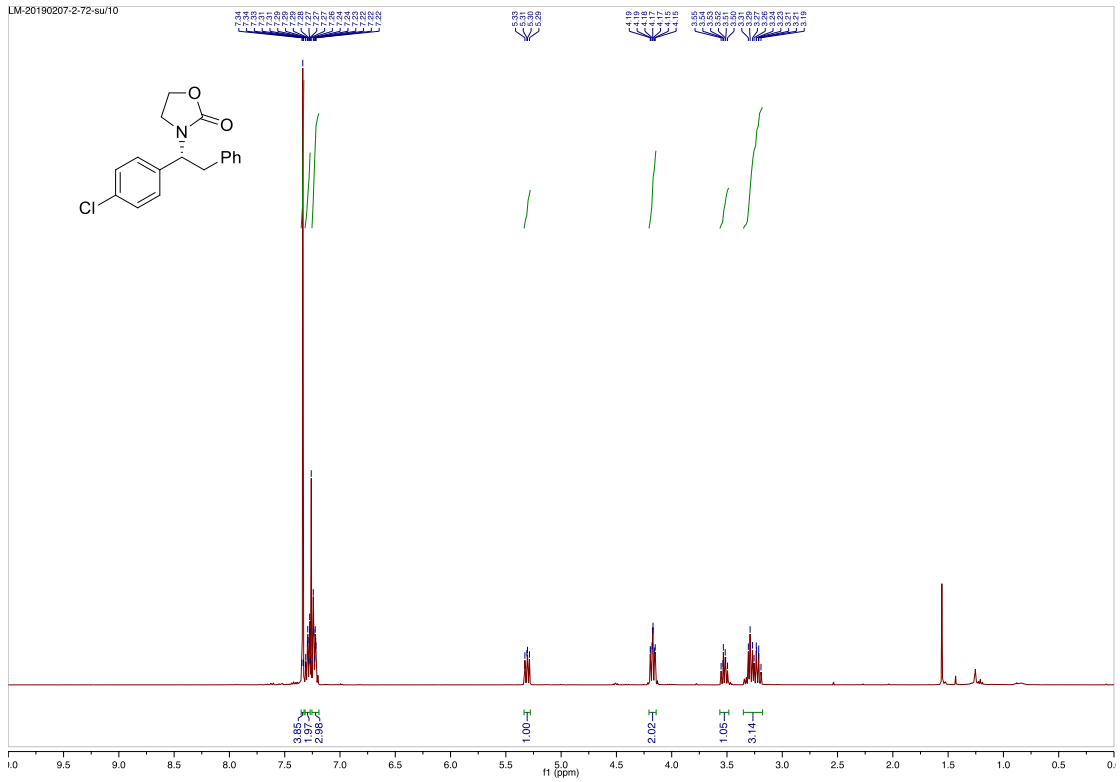


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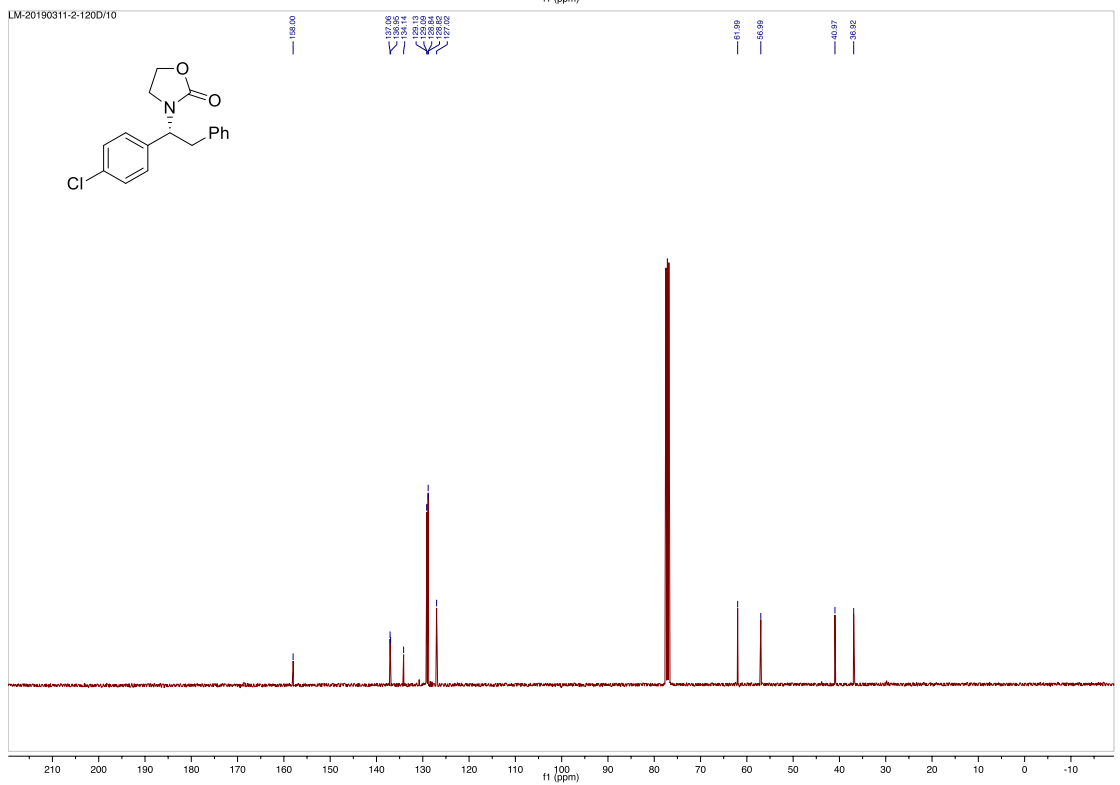




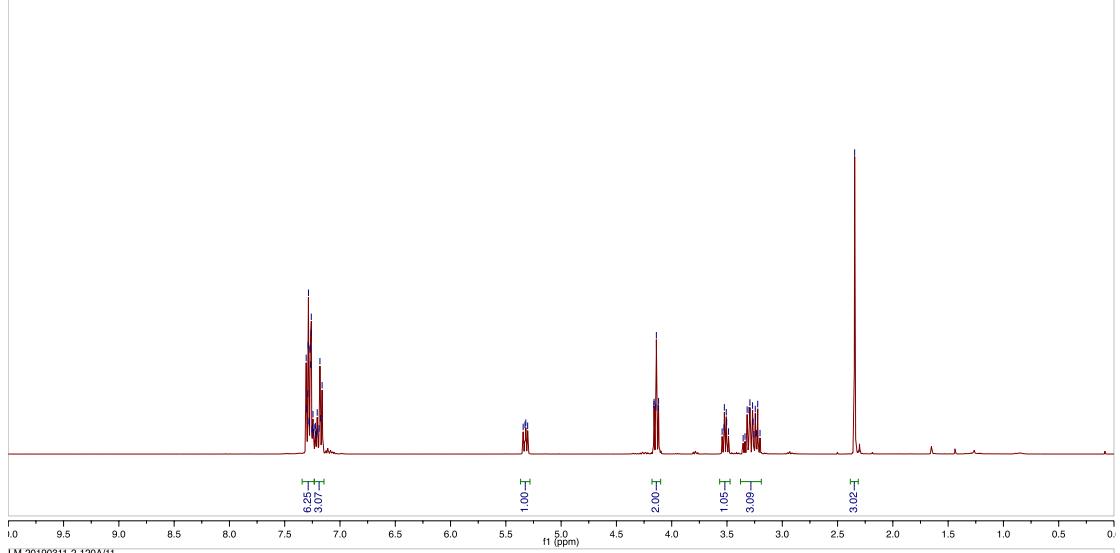
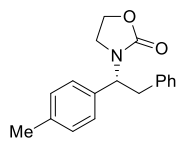
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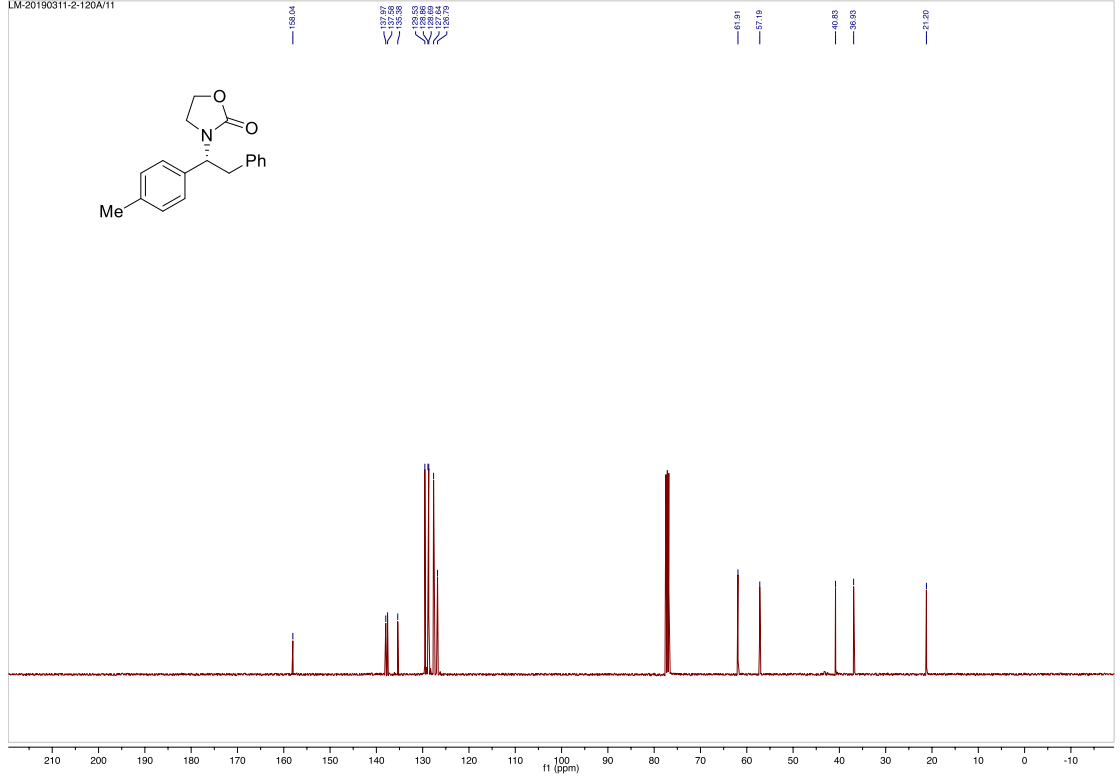
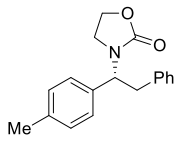
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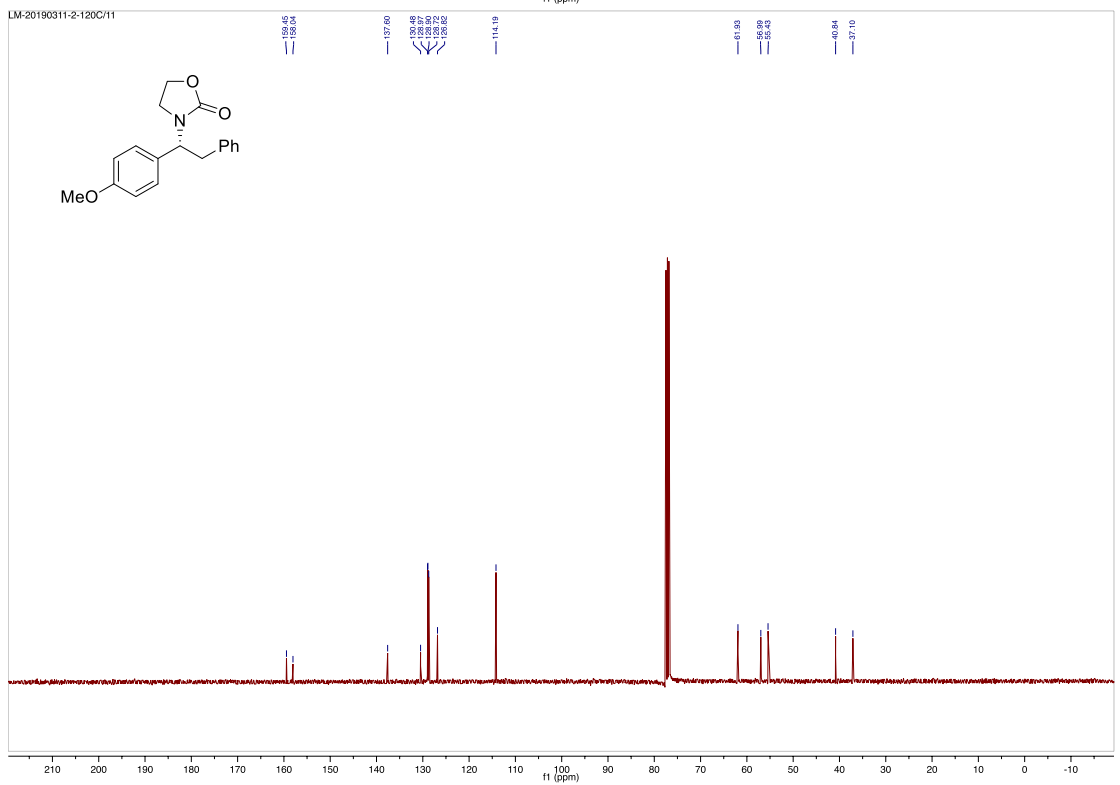
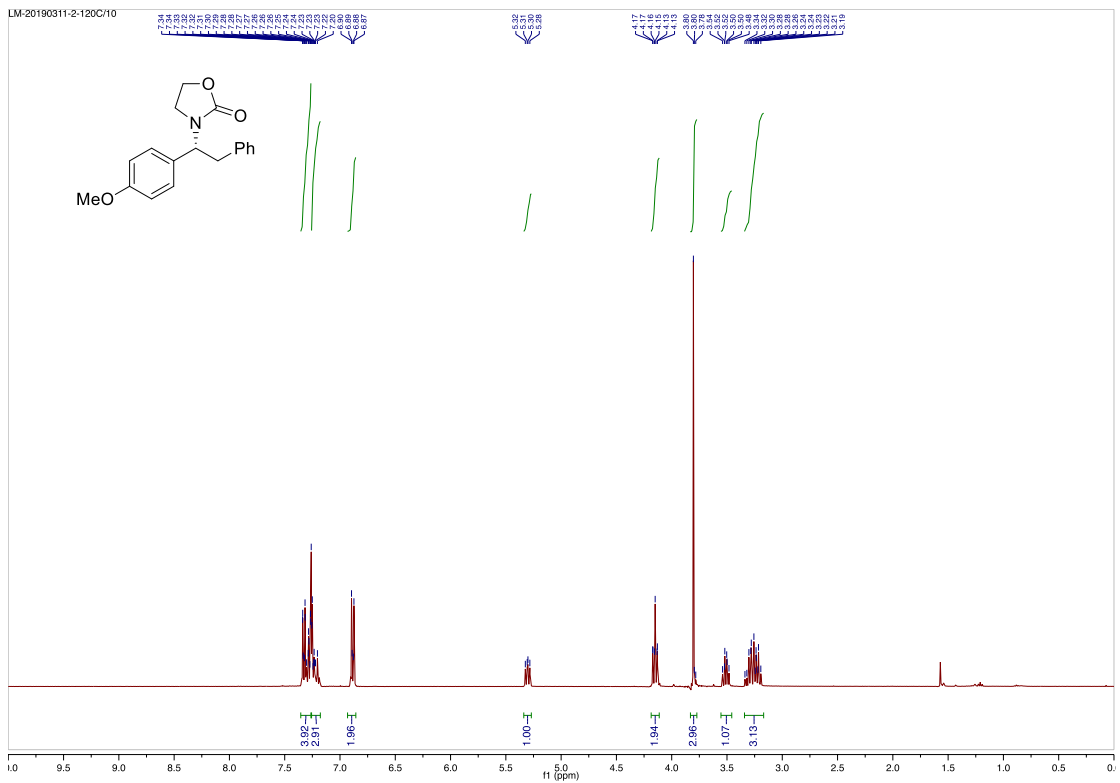


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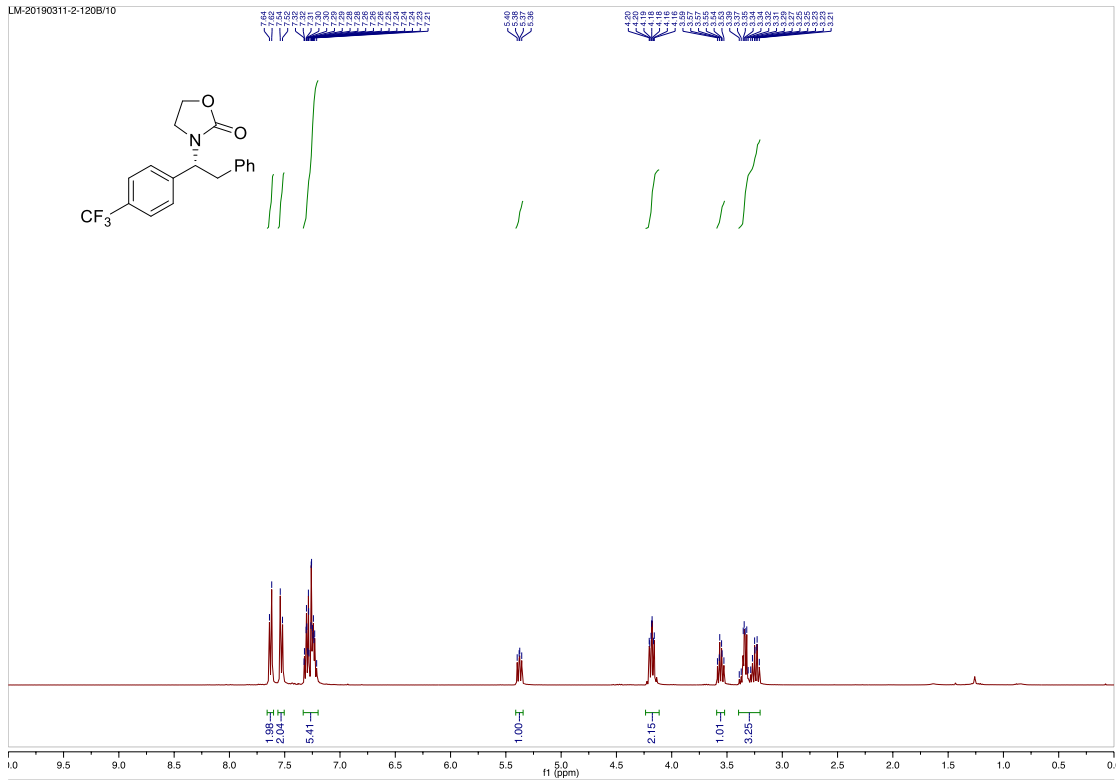


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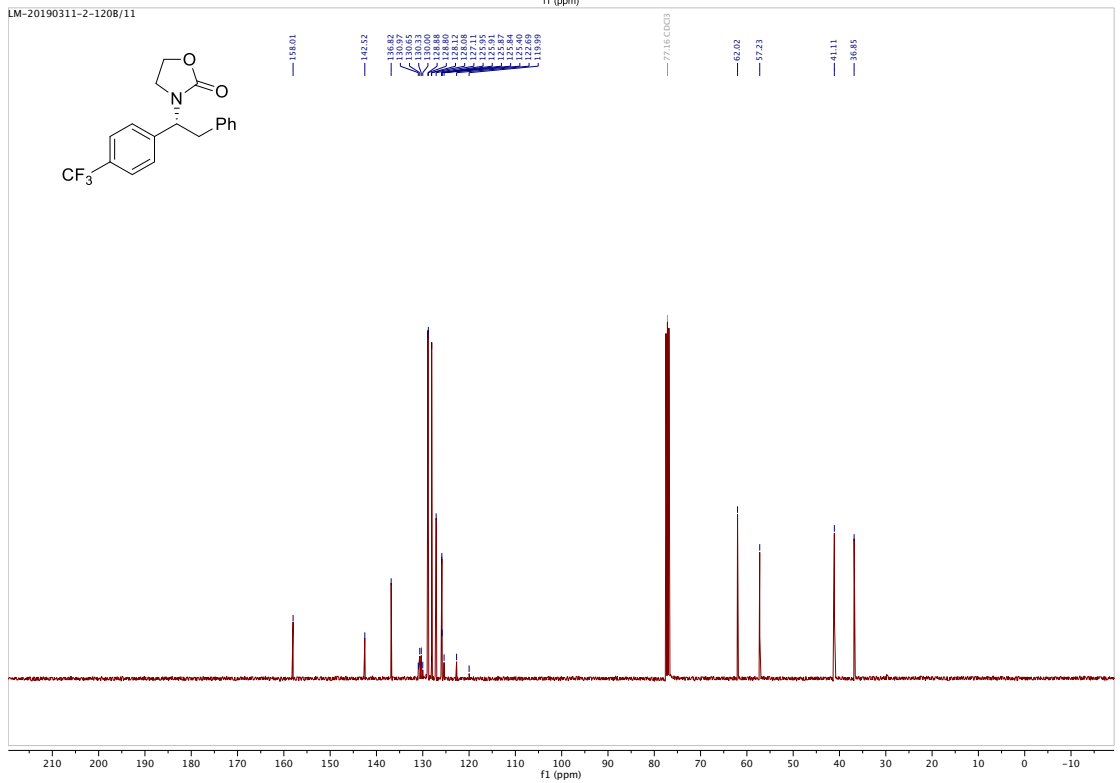




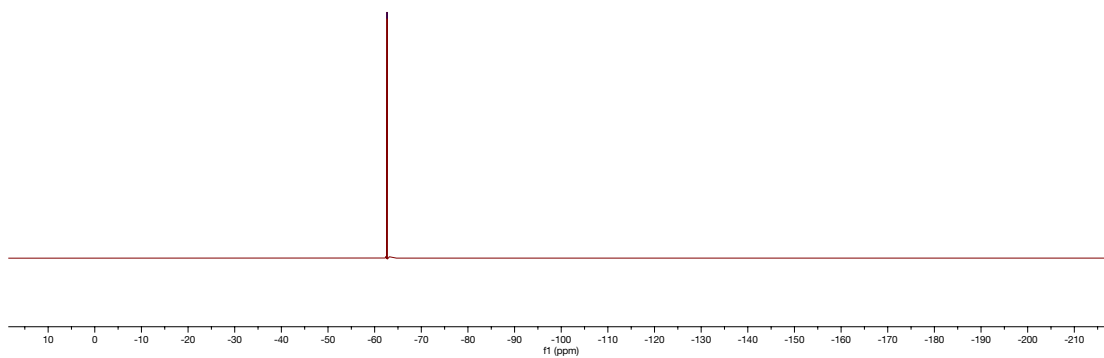
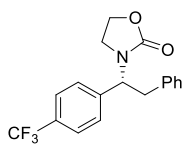
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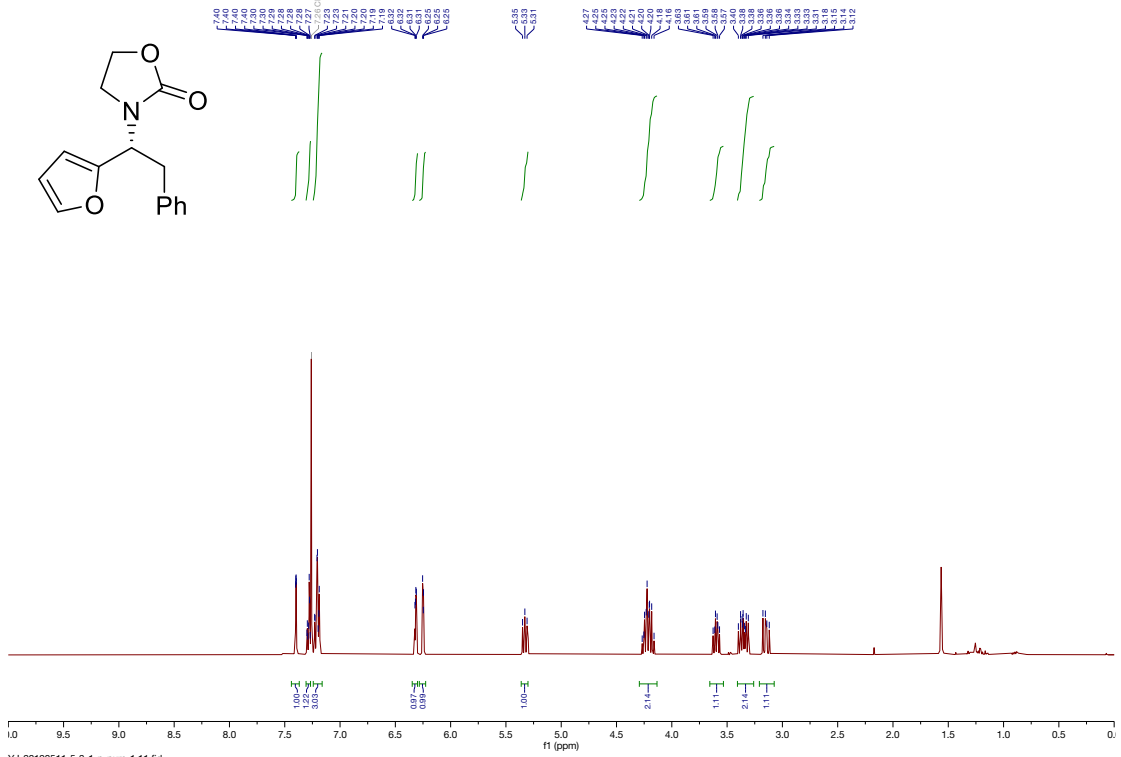
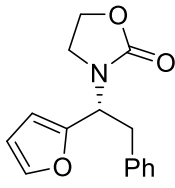
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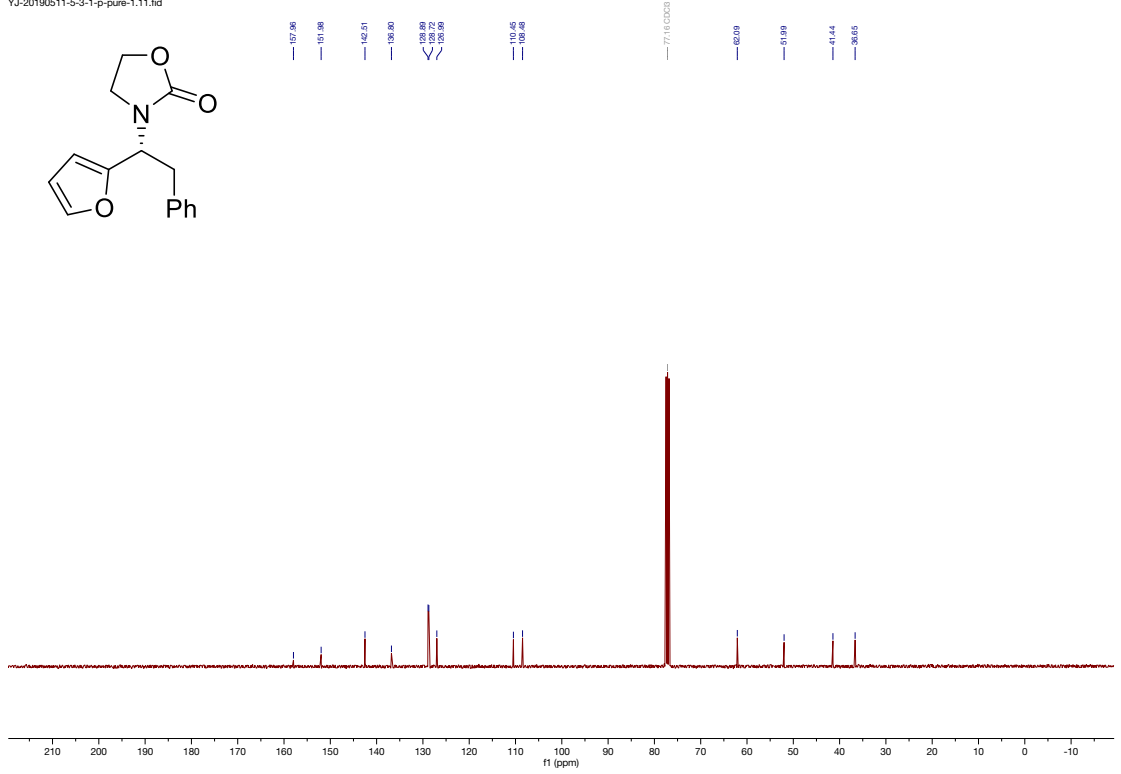
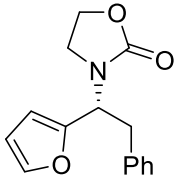
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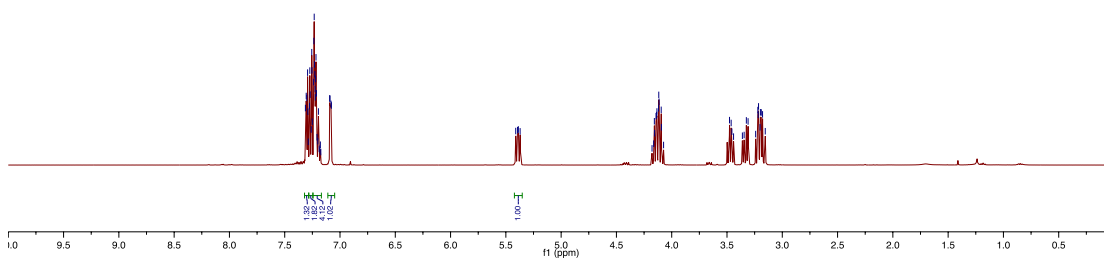
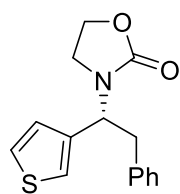
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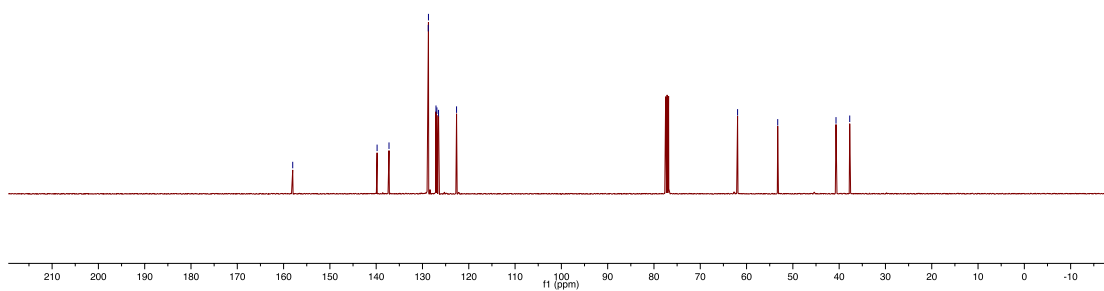
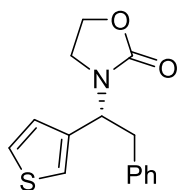
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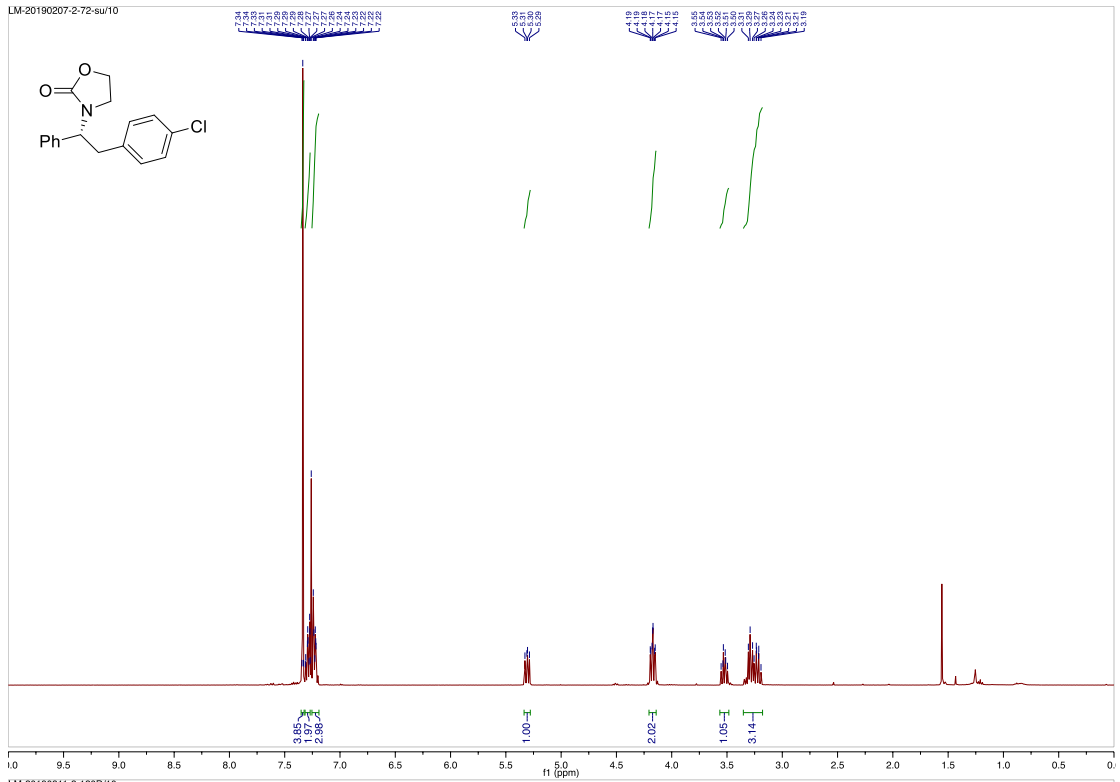
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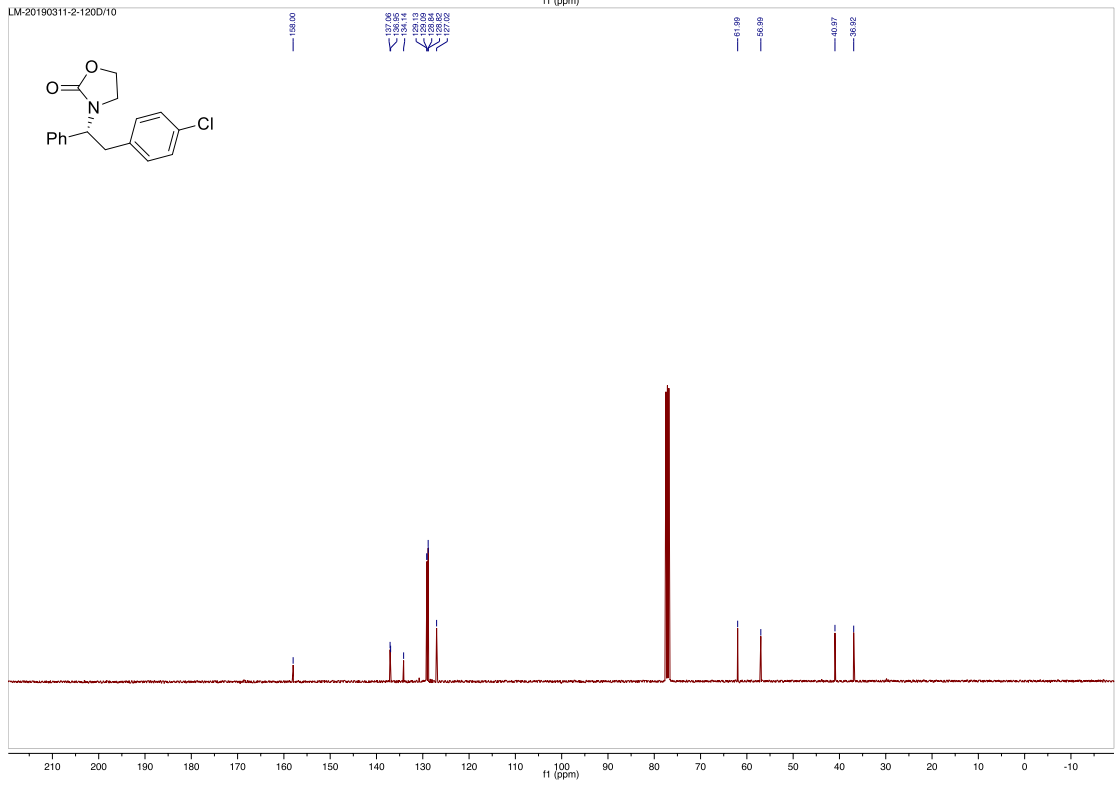
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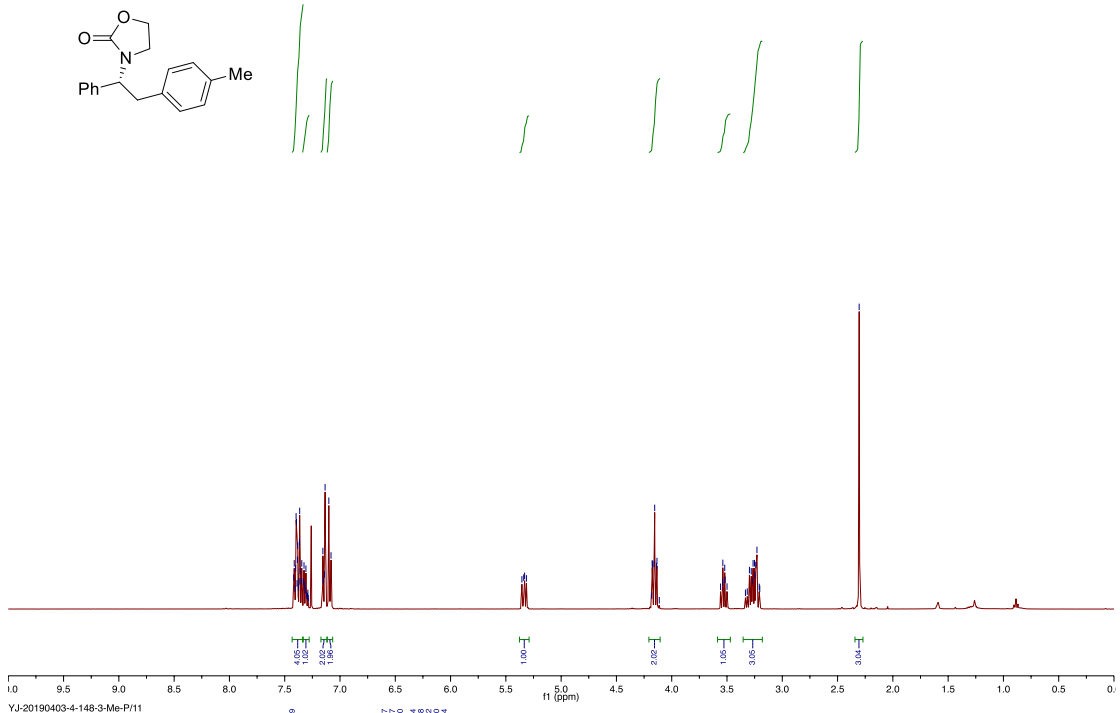
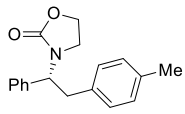
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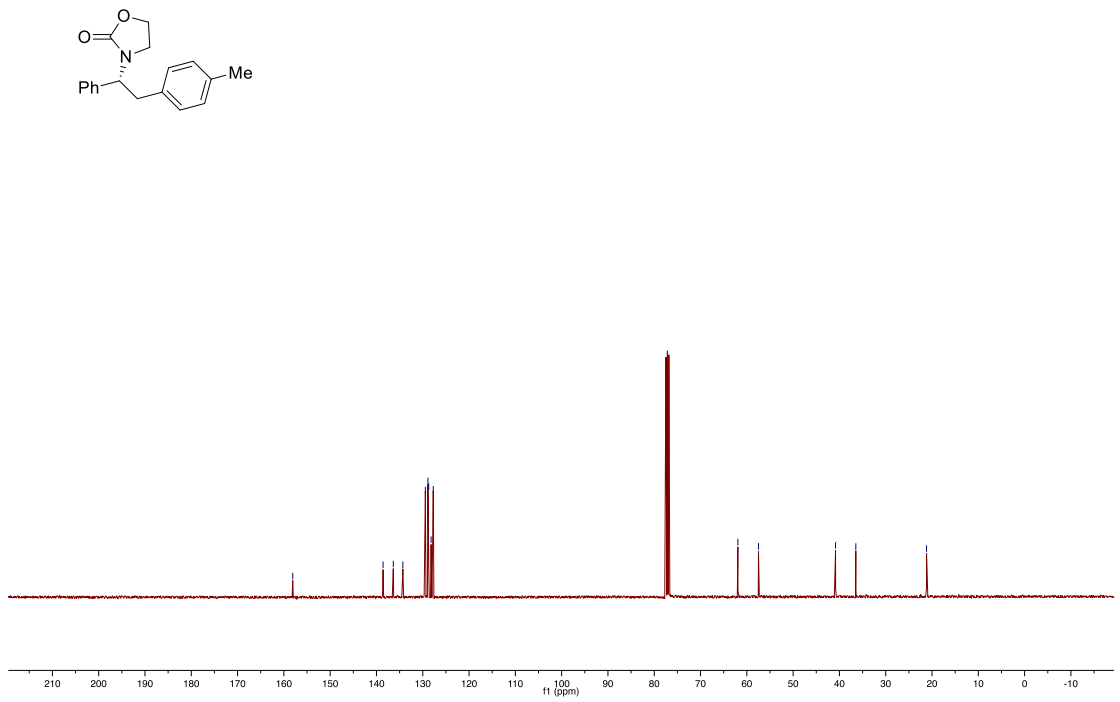
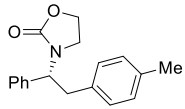
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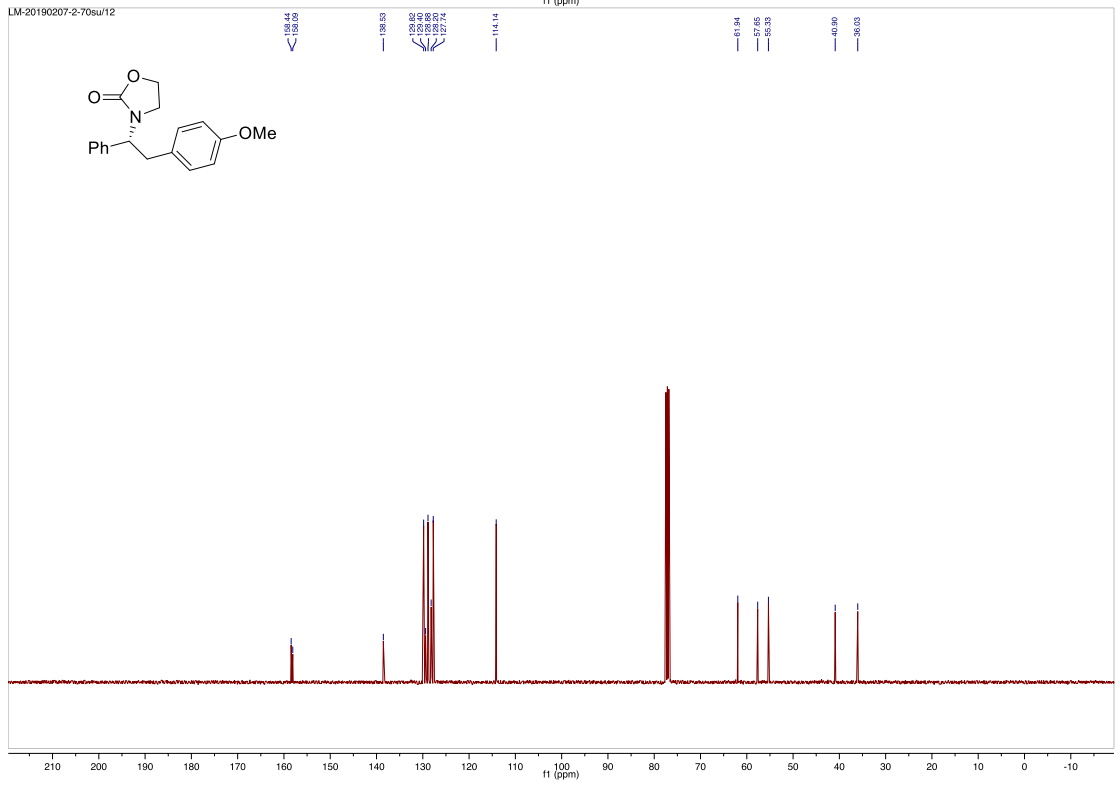
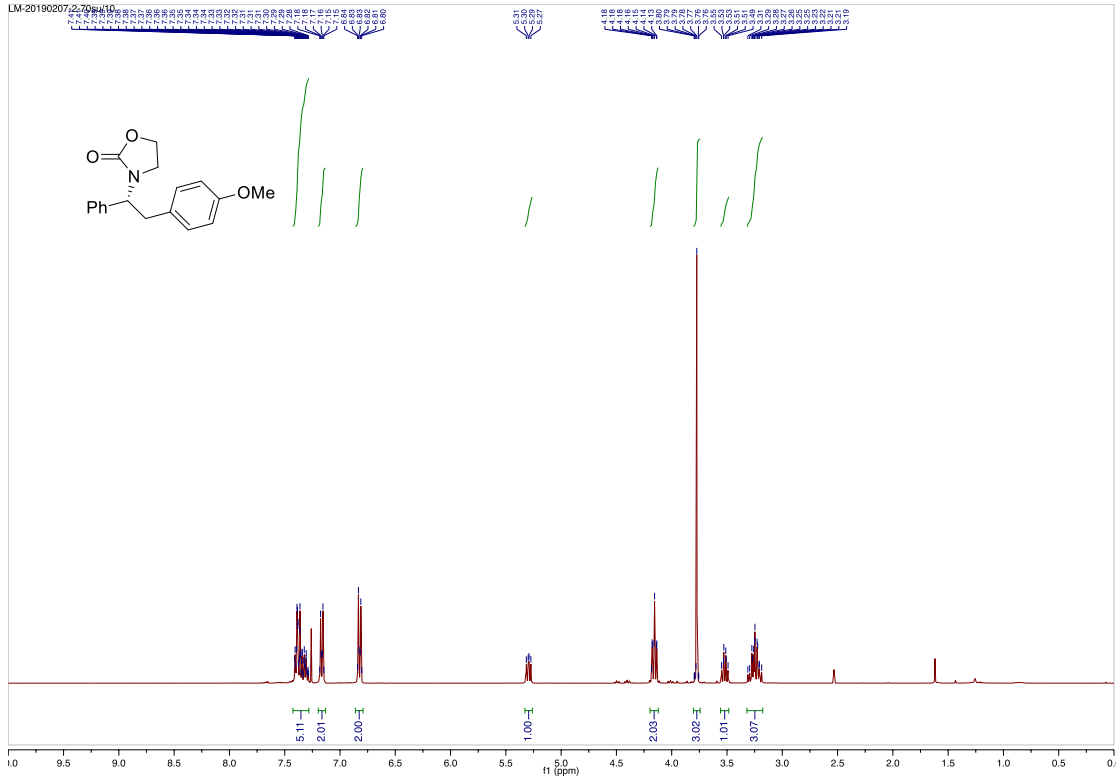


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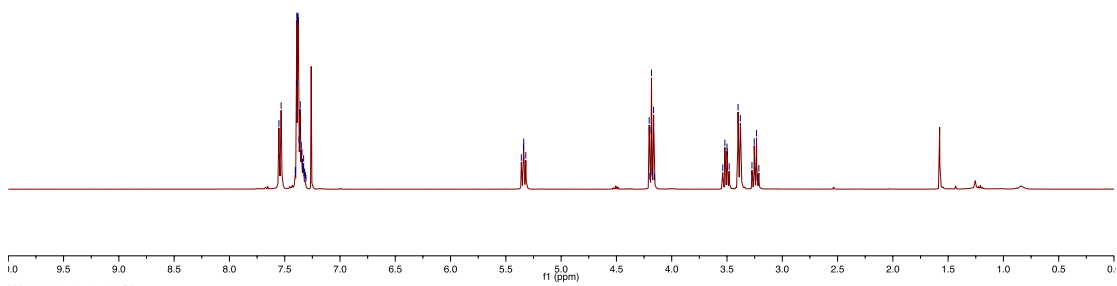
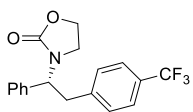


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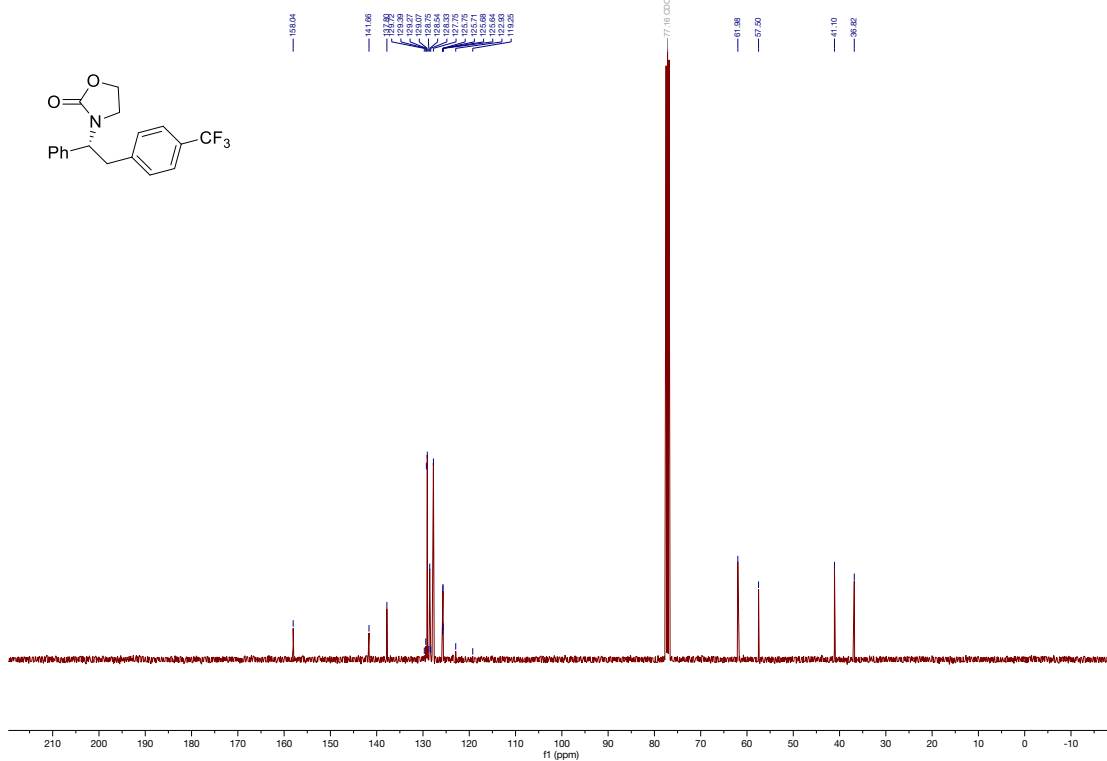
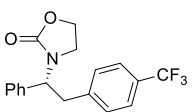


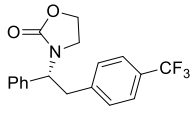


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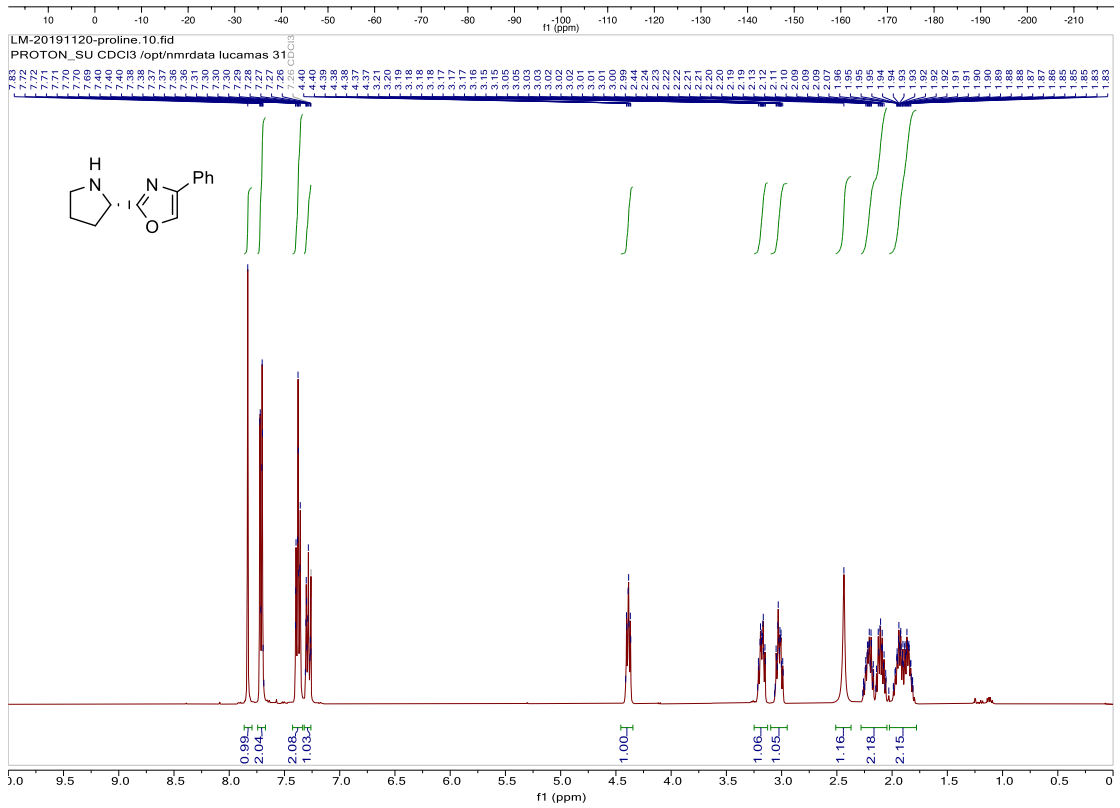
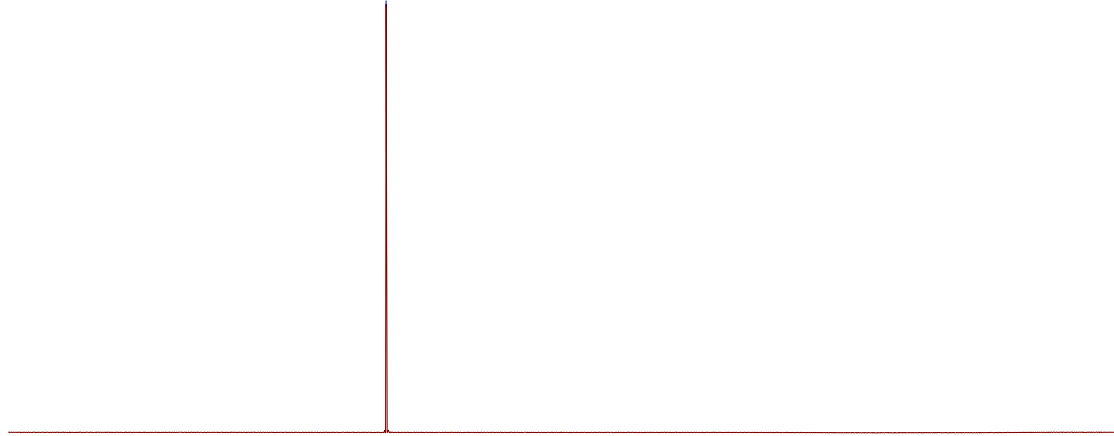


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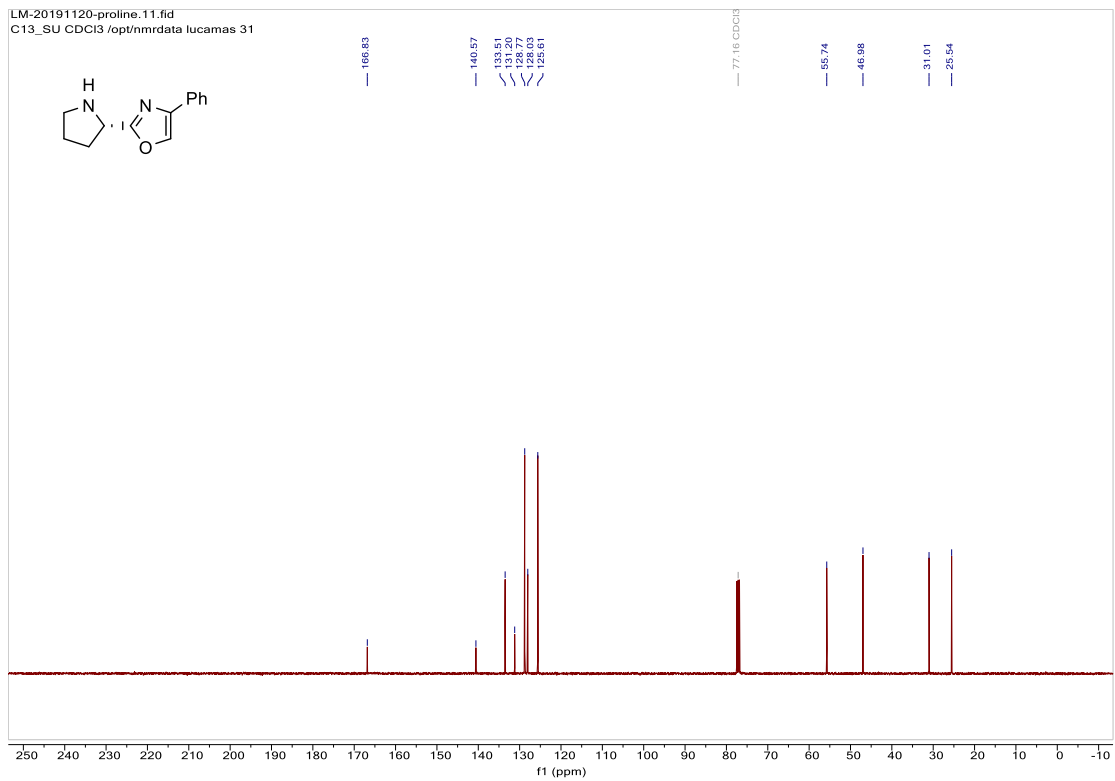




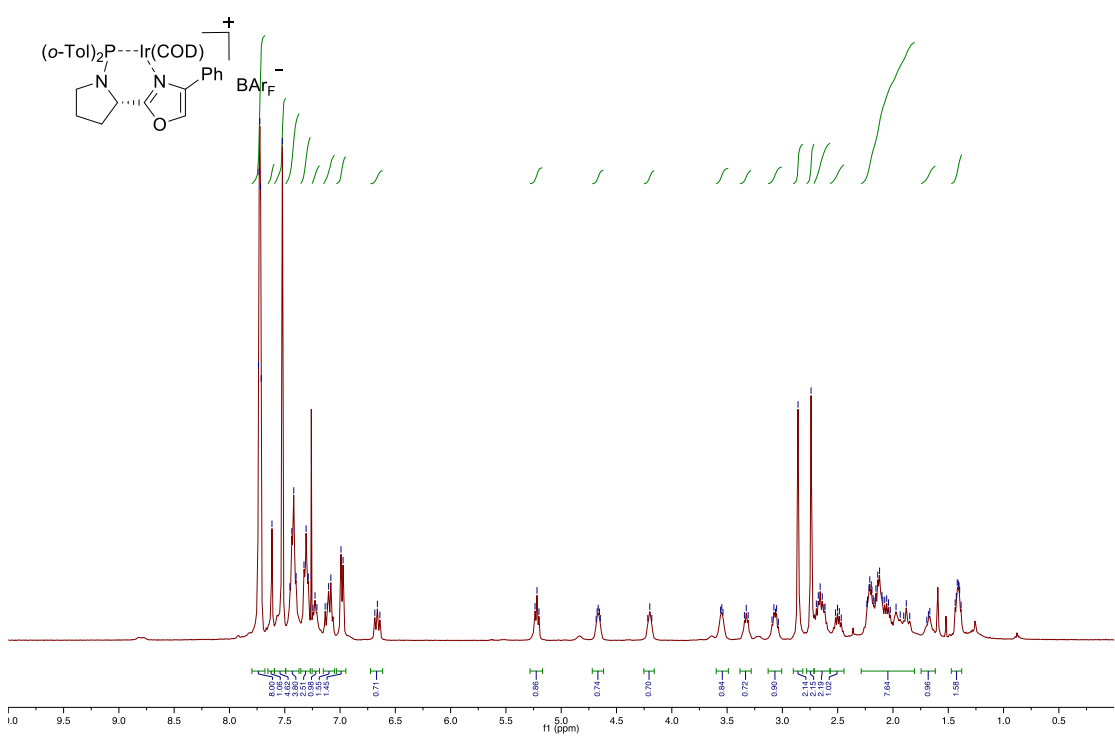
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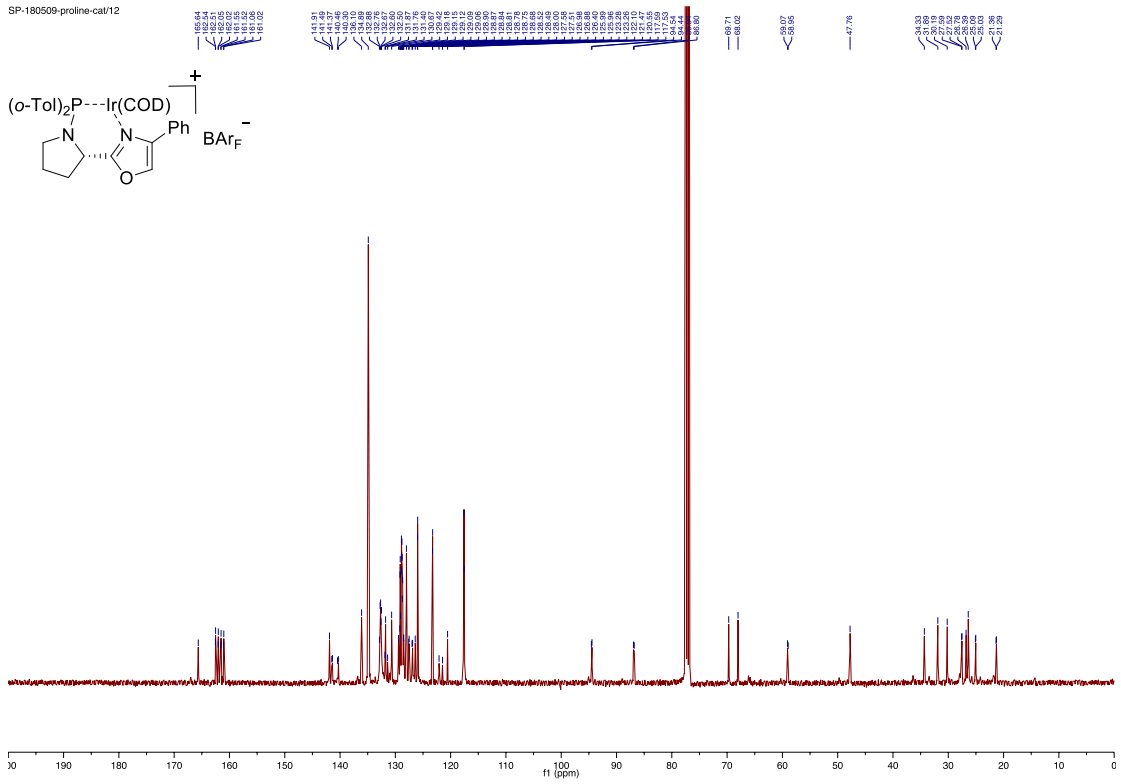
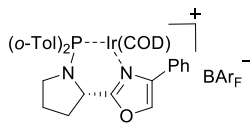
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C13_SU CDCl3 /opt/nmrdata lucamas 31



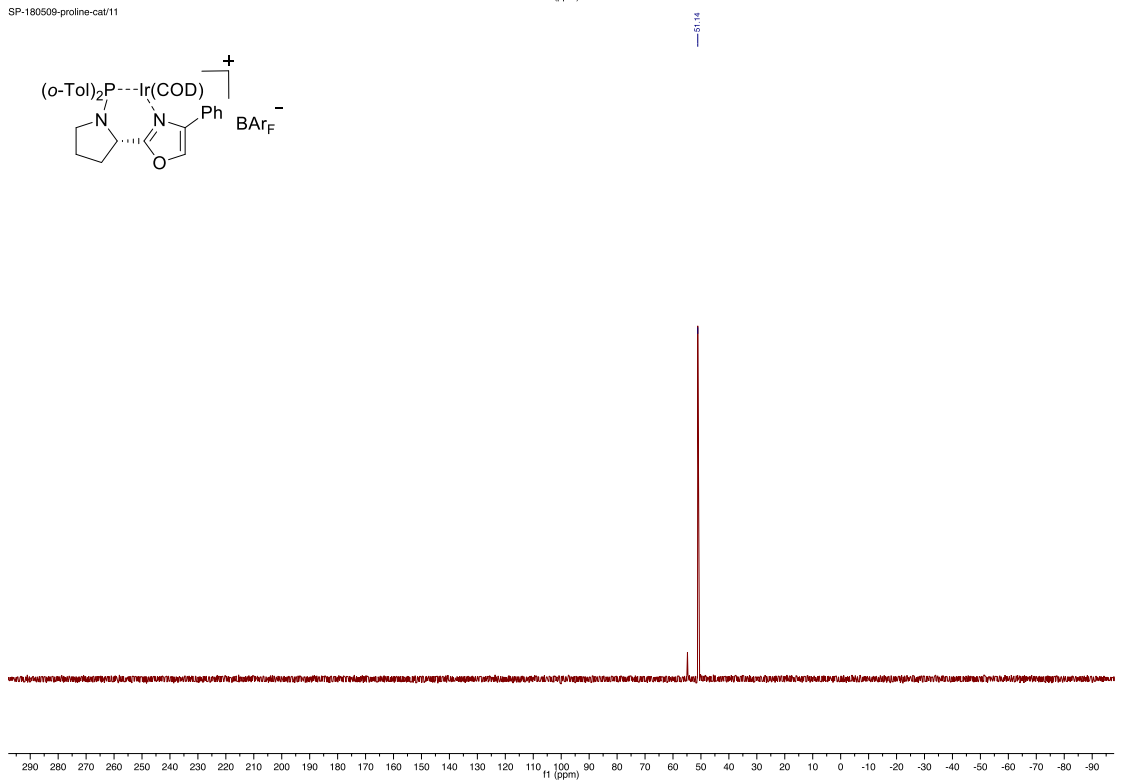
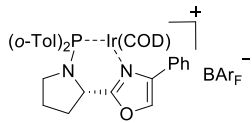
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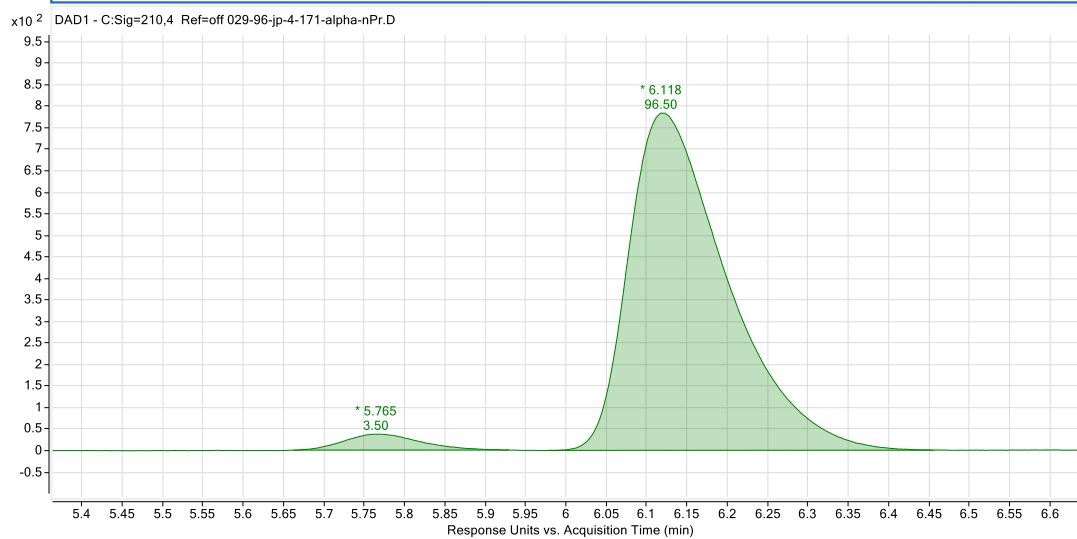
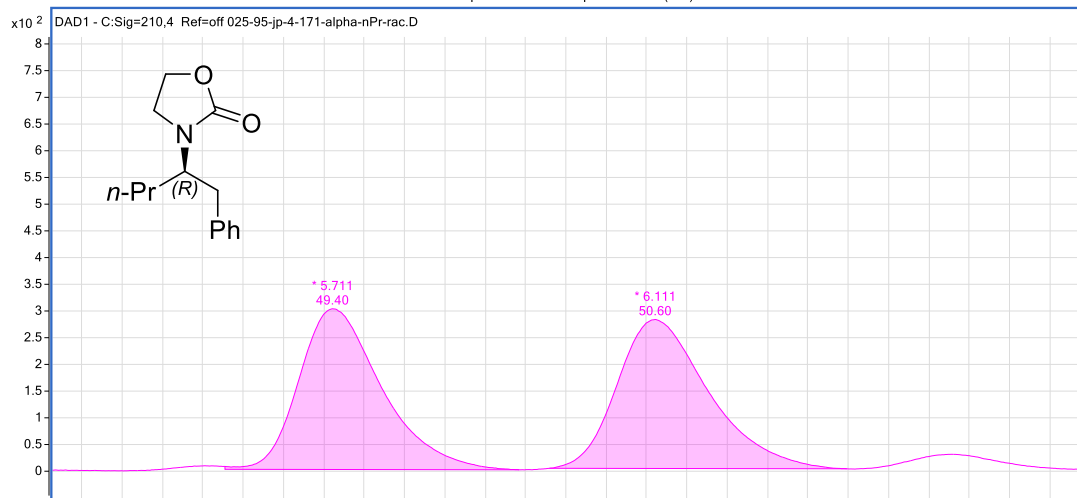
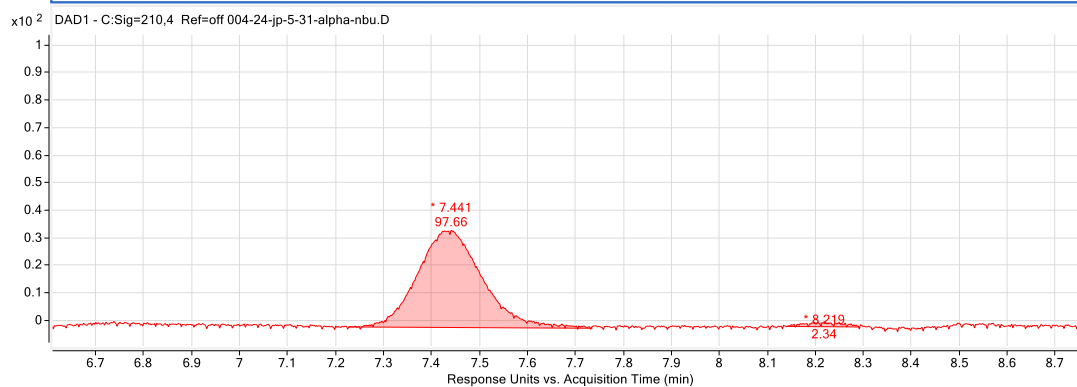
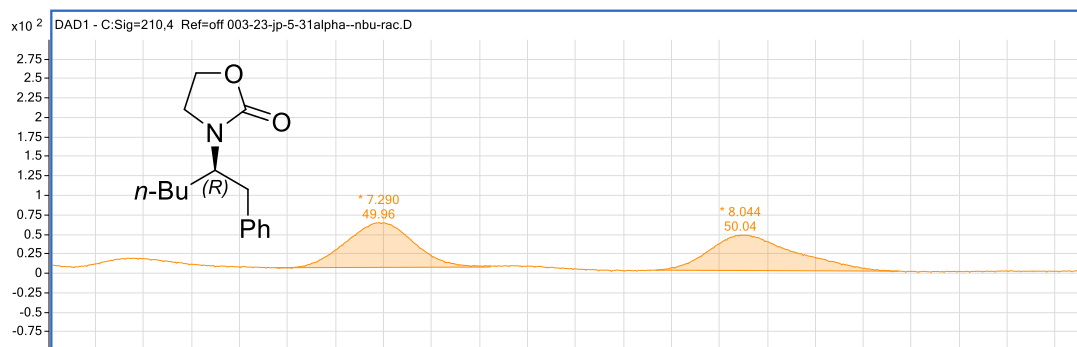
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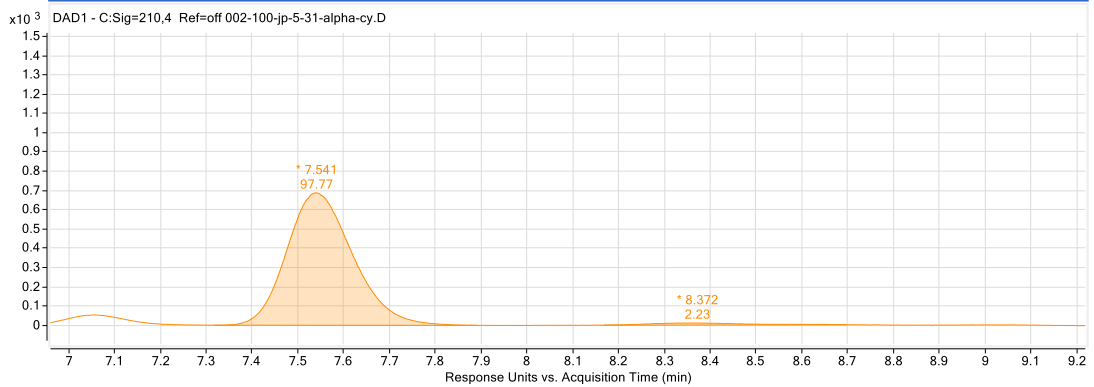
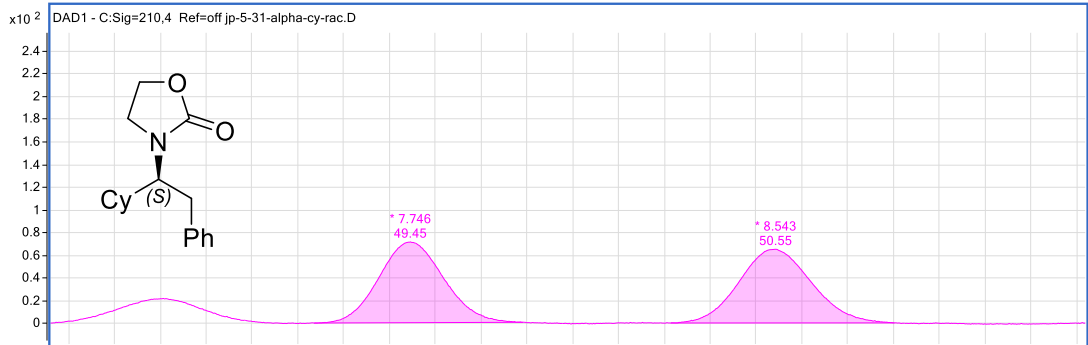
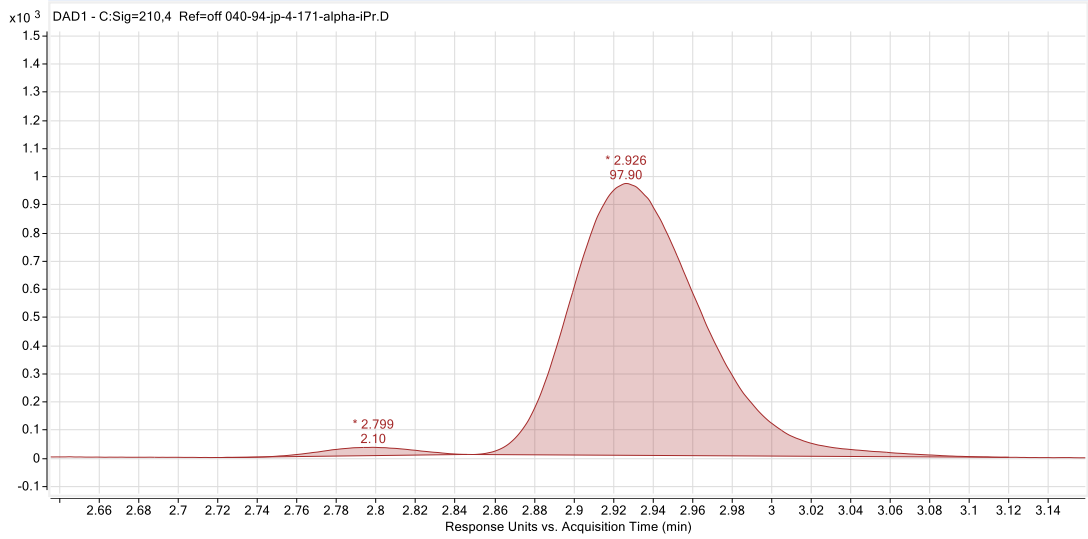
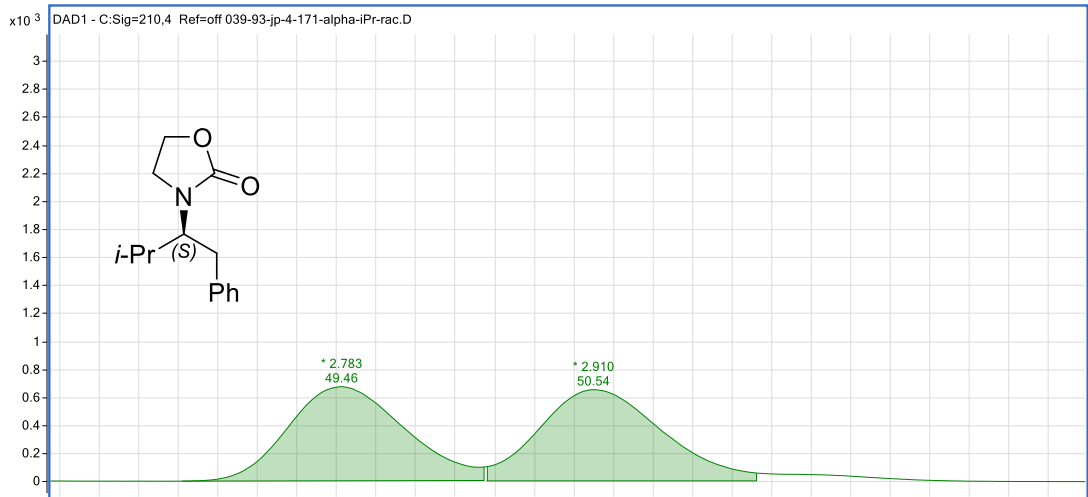


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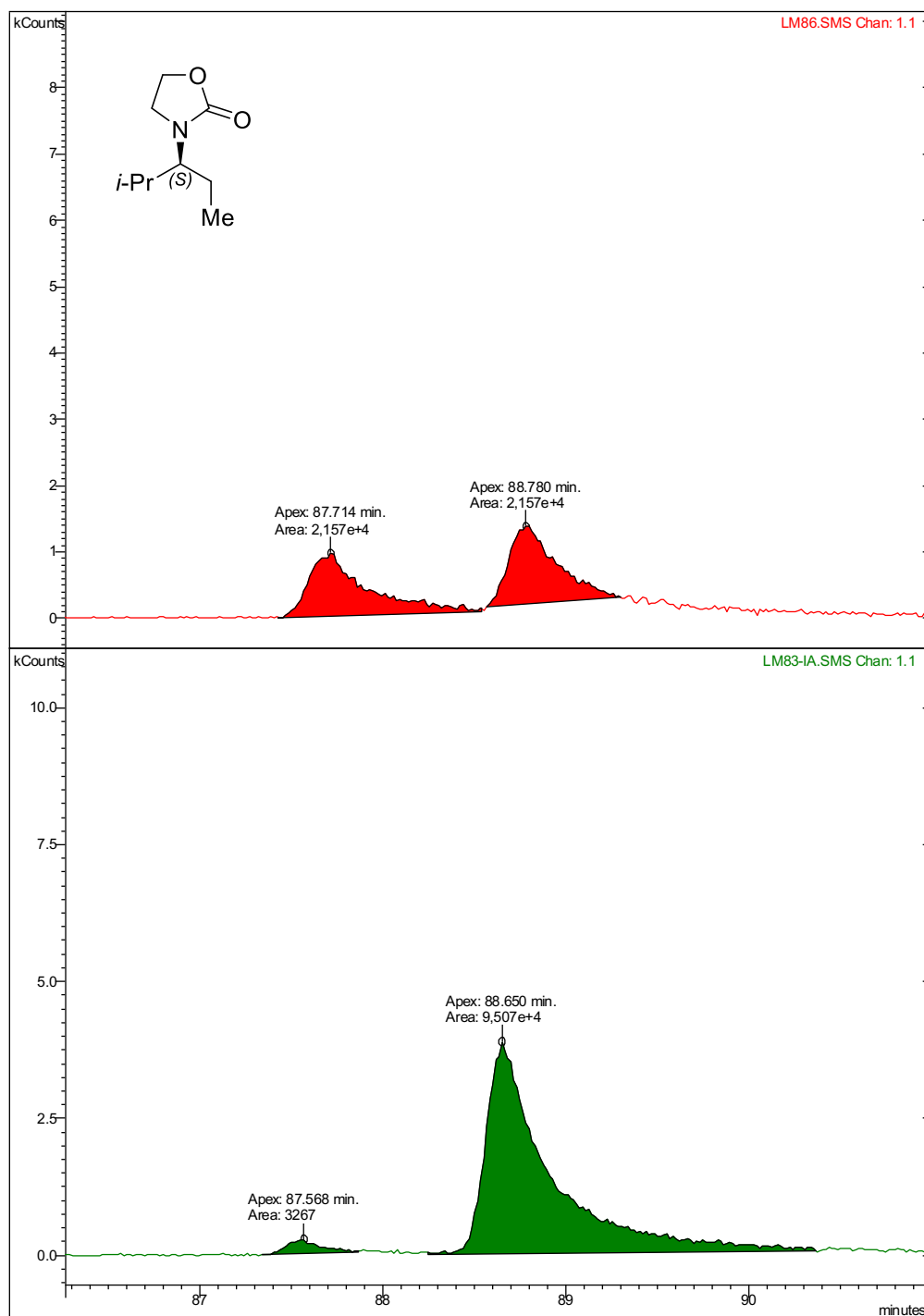


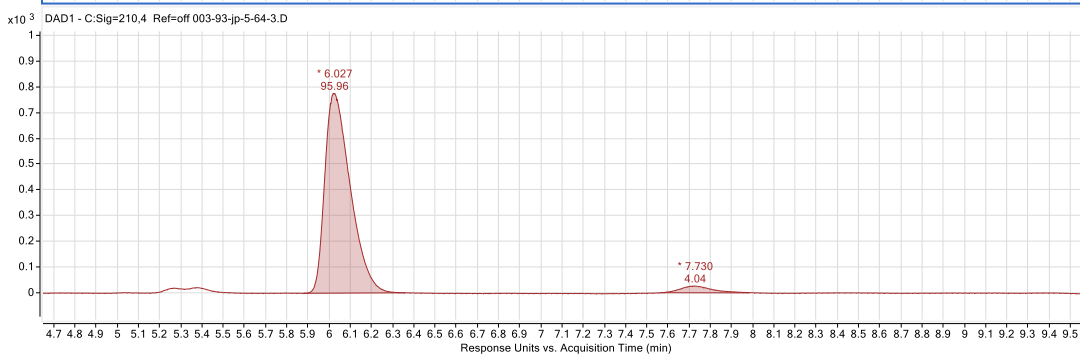
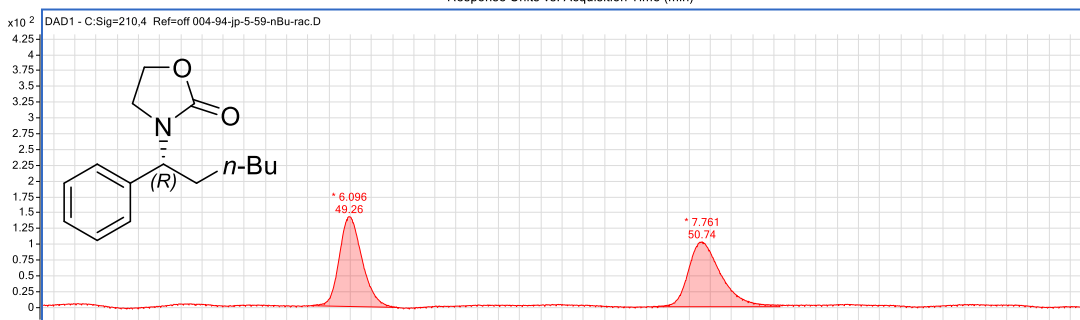
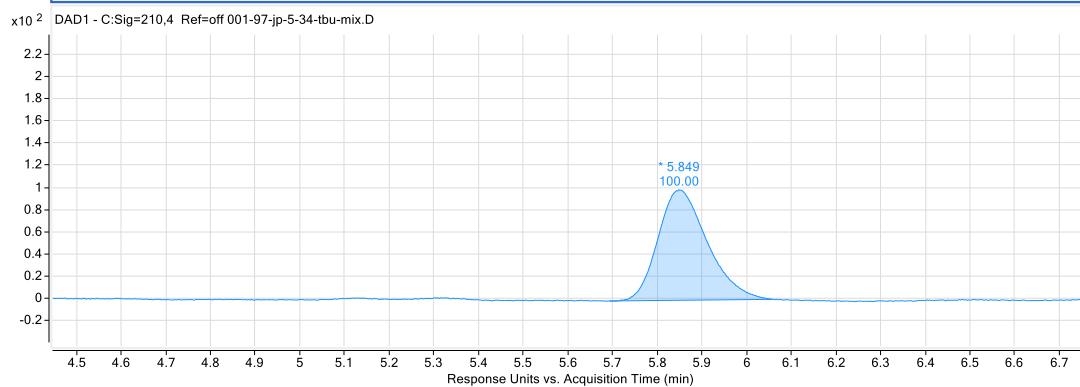
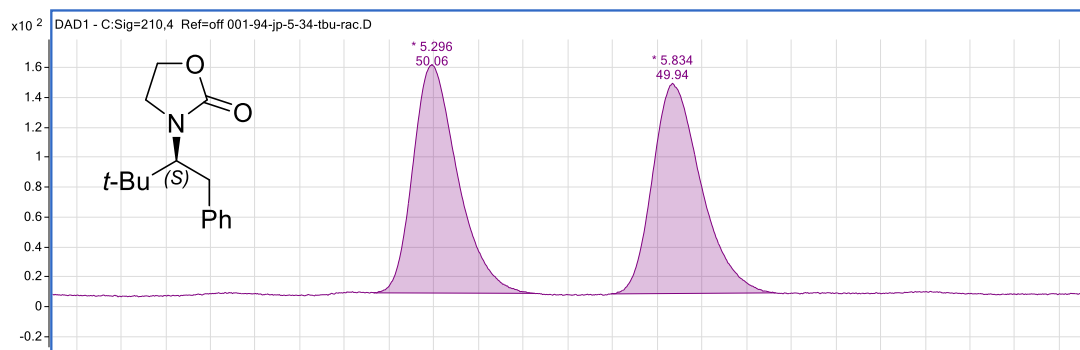
11. Chromatogram of chiral compounds

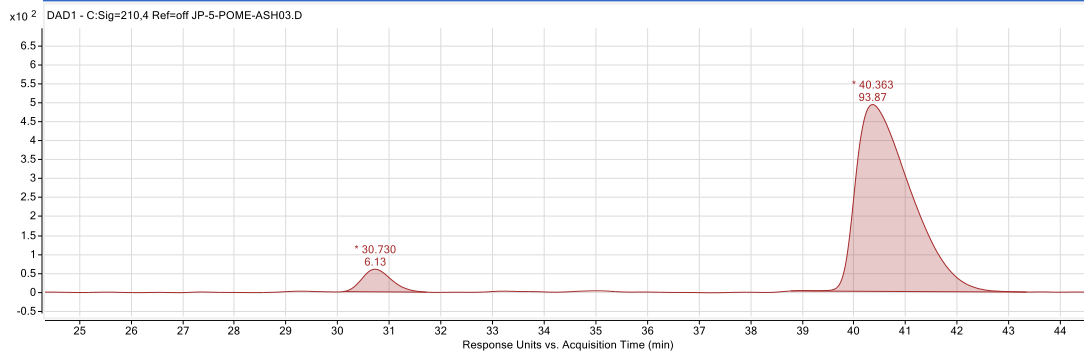
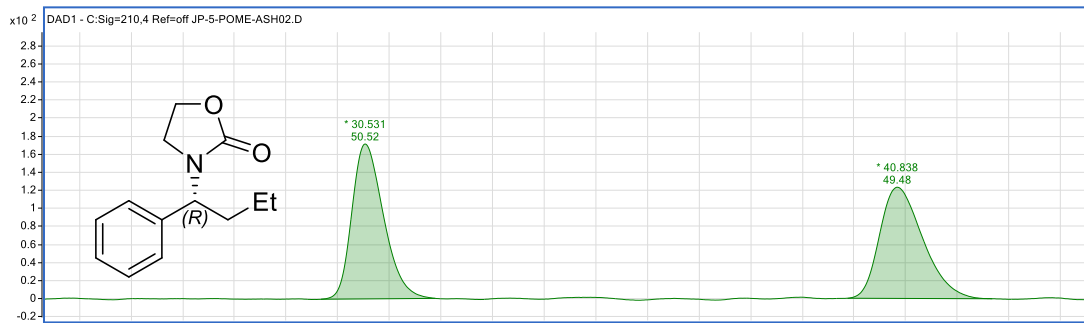
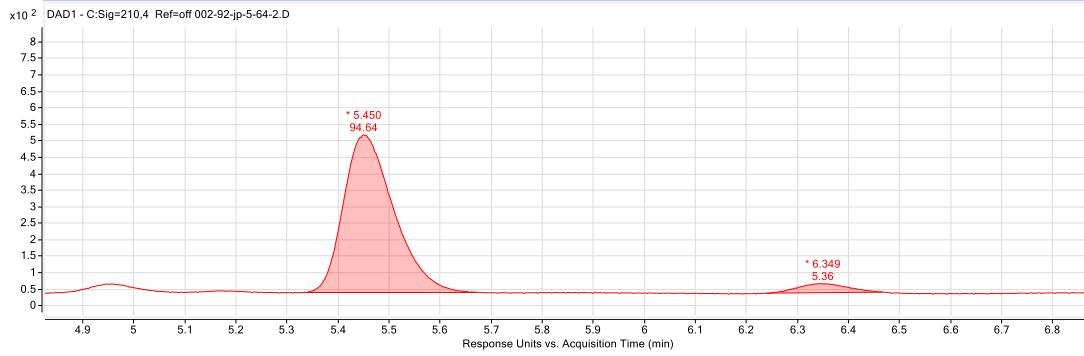
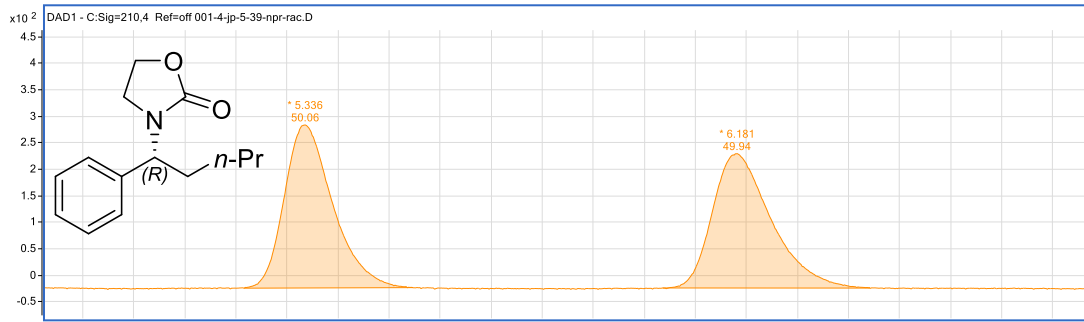


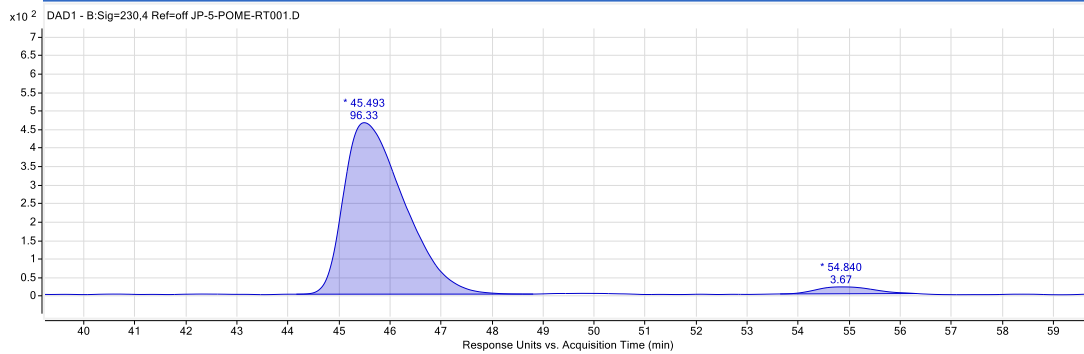
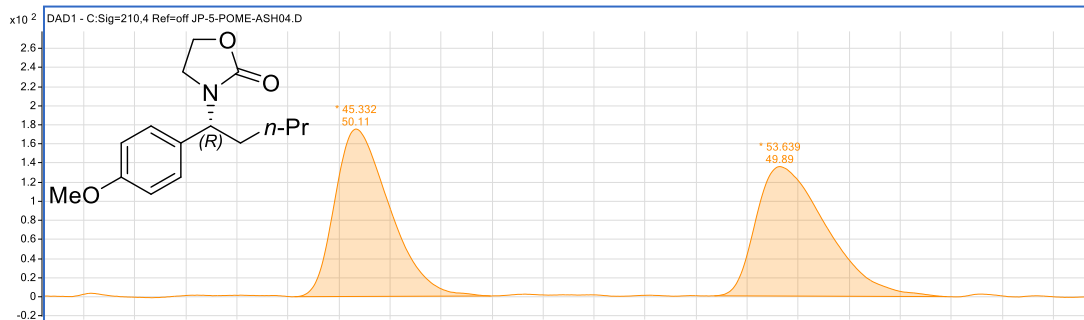
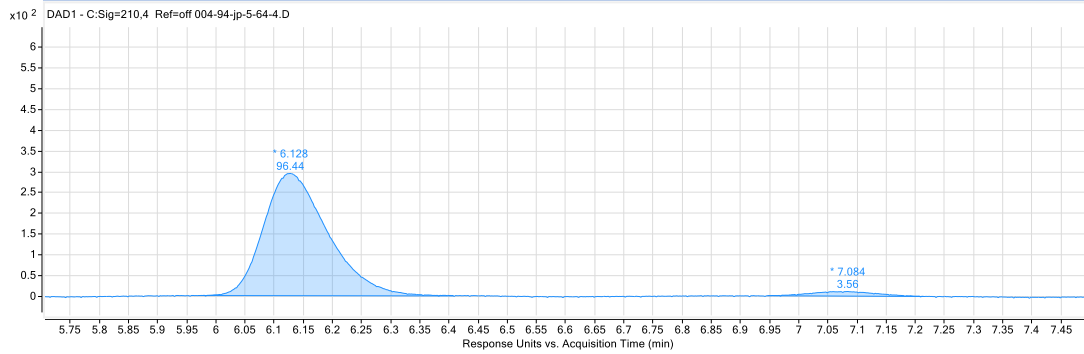
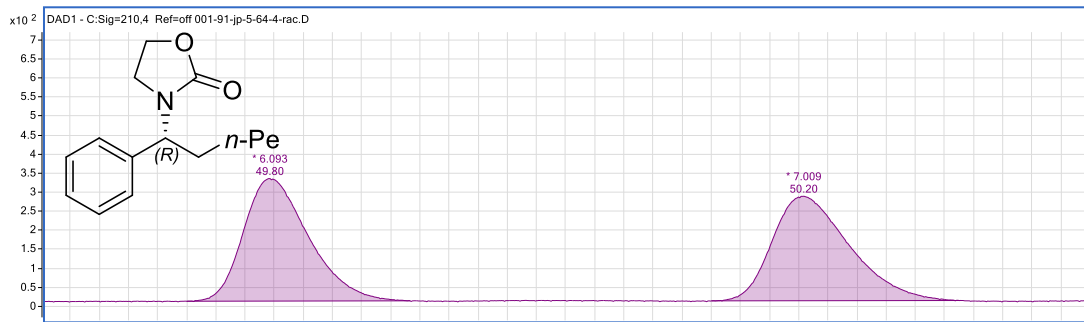


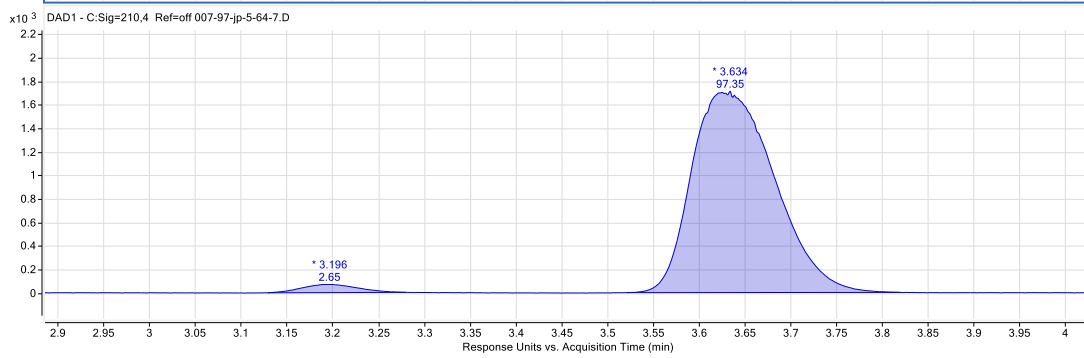
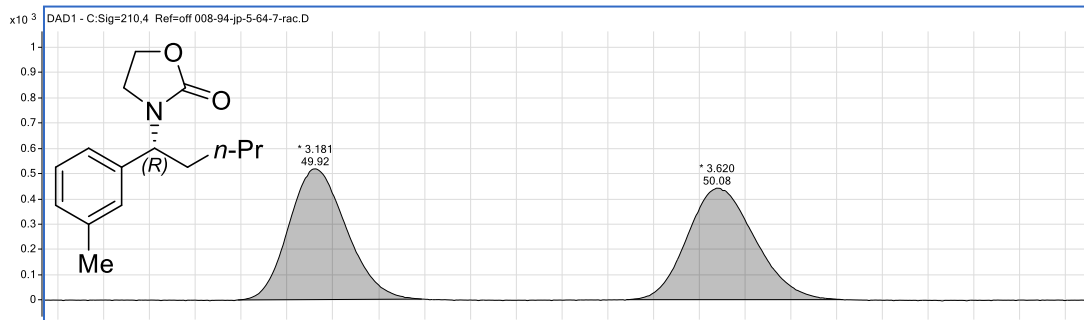
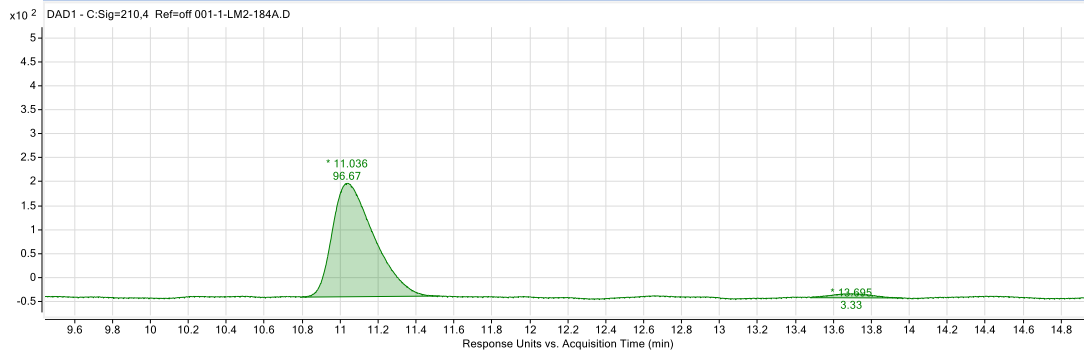
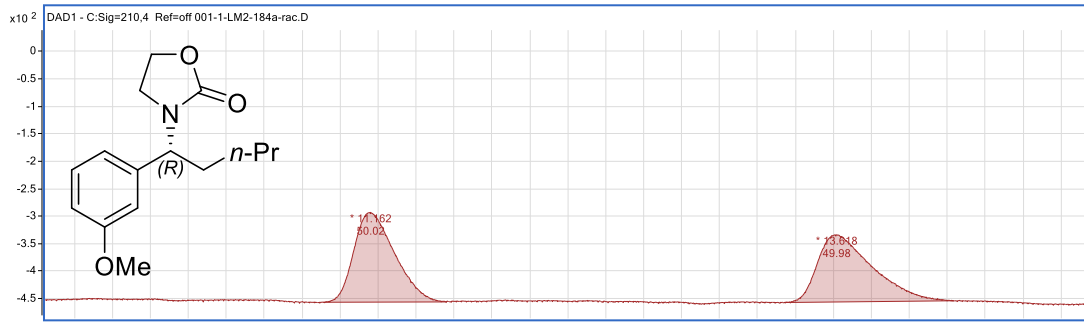
Chromatogram Plots

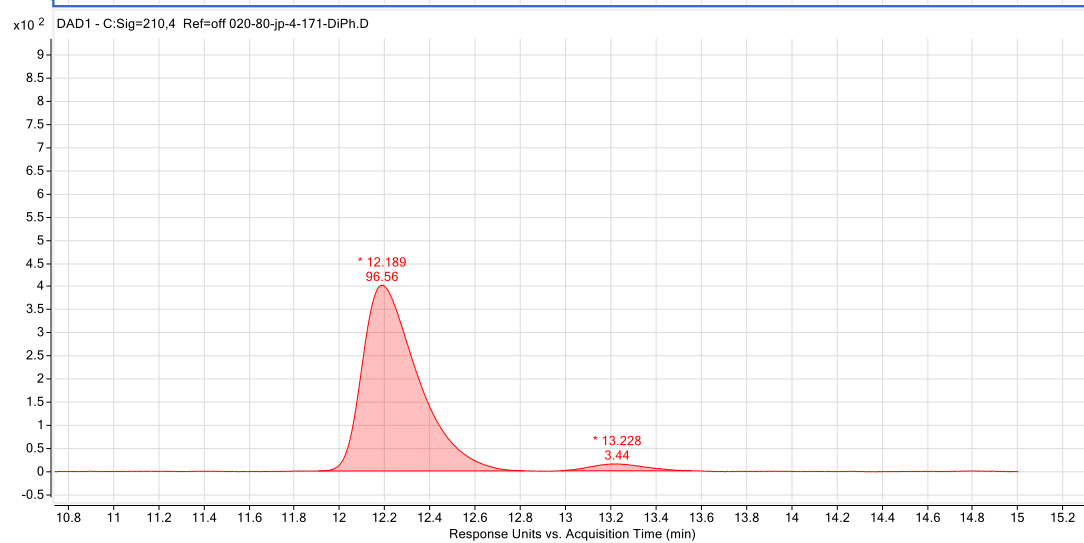
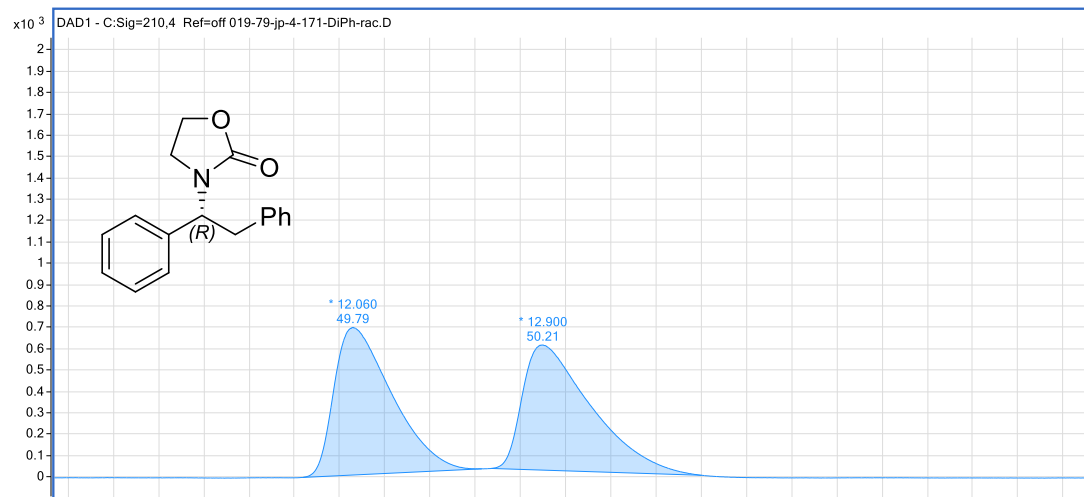
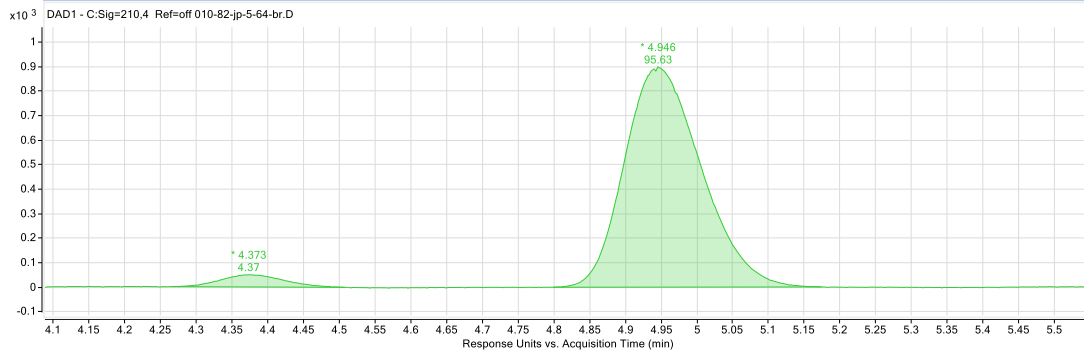
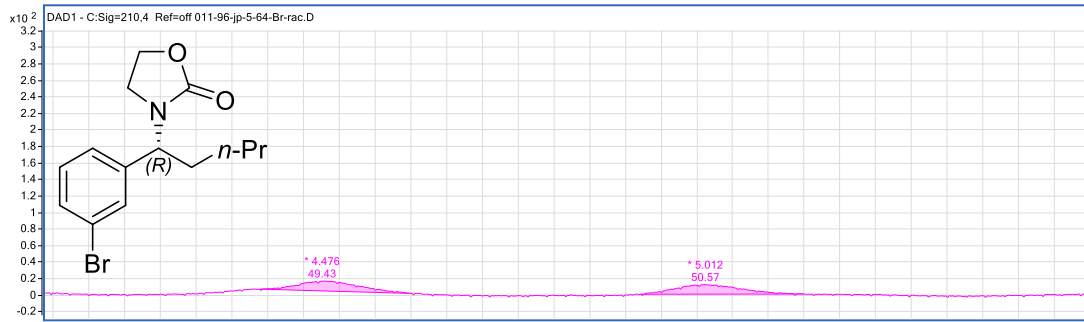


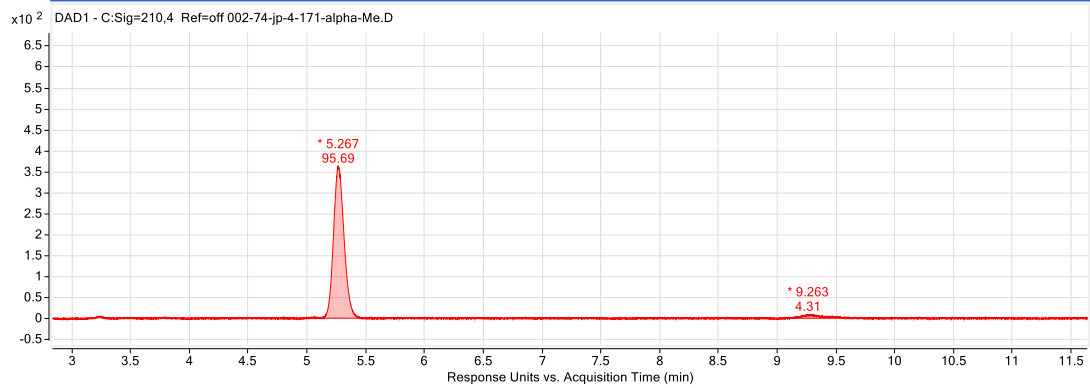
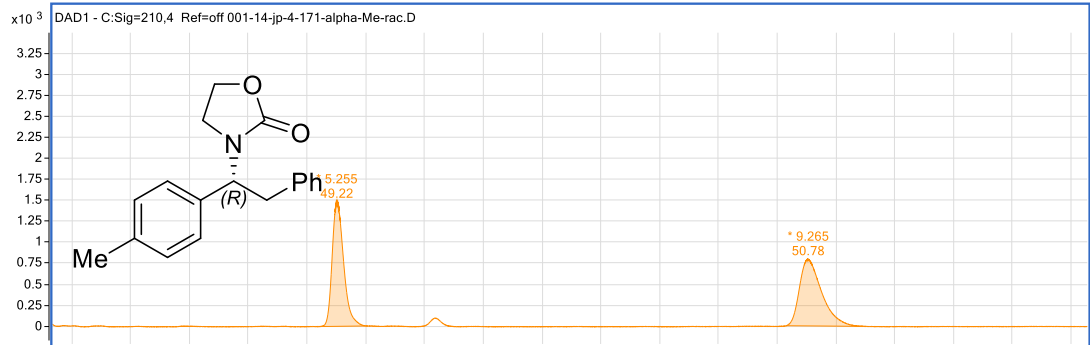
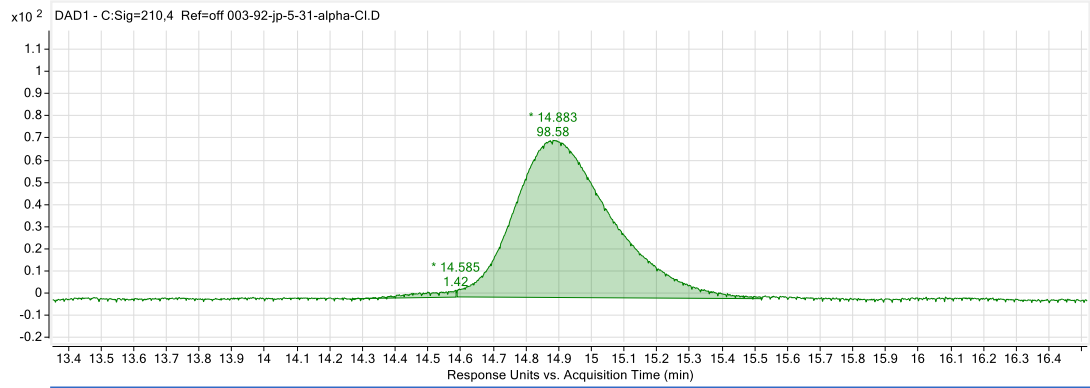
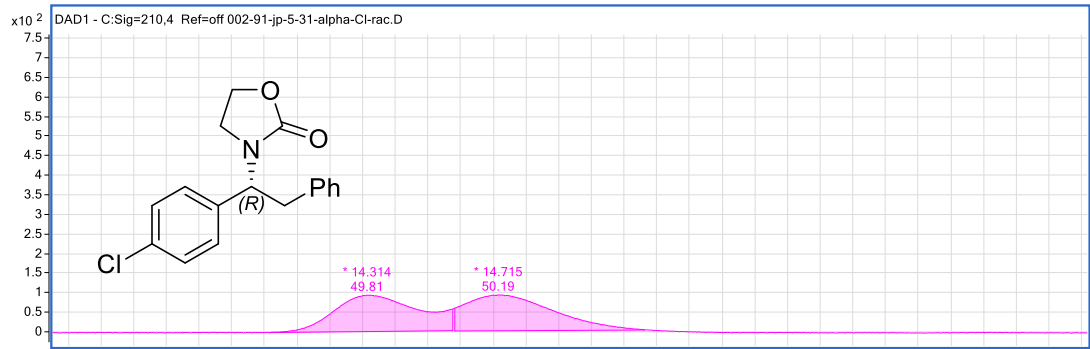


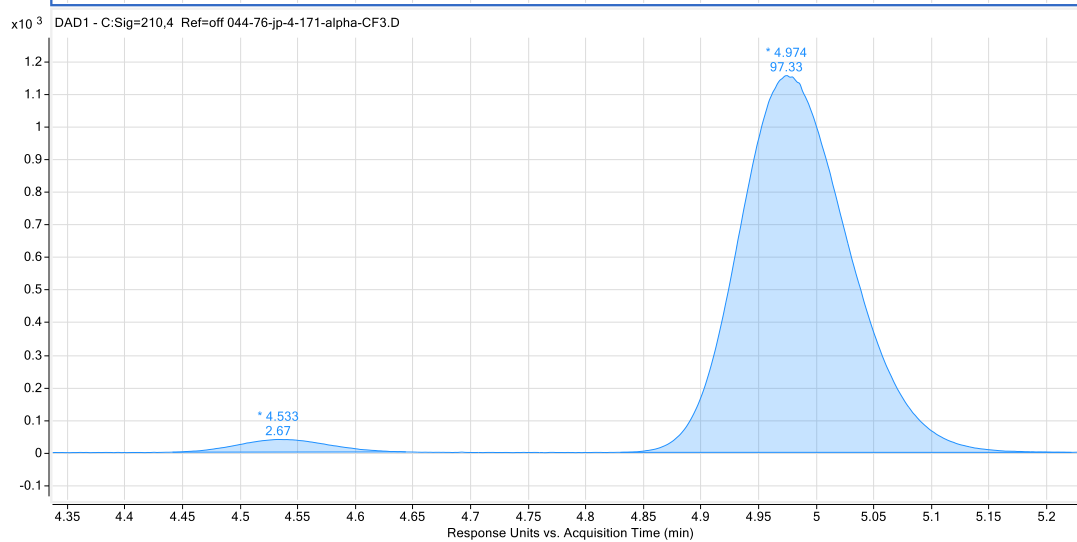
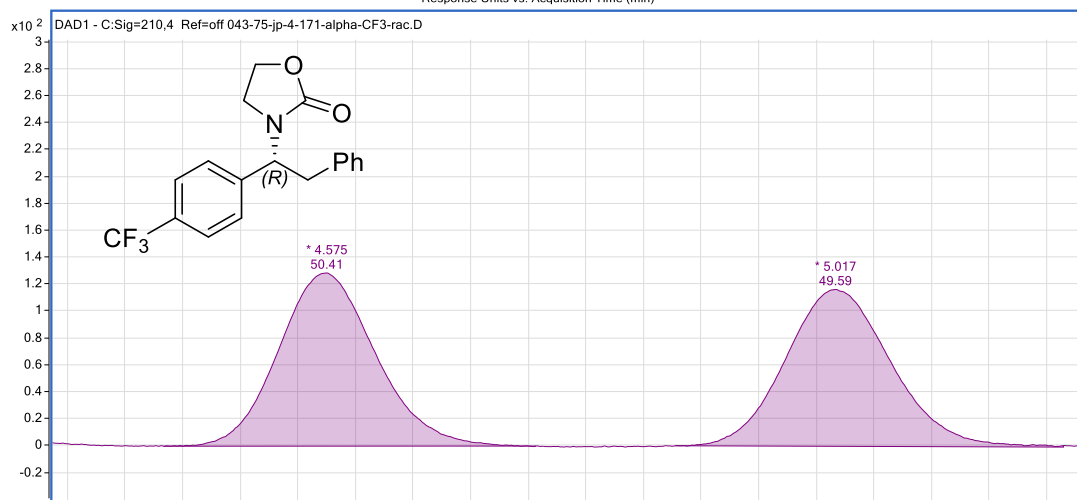
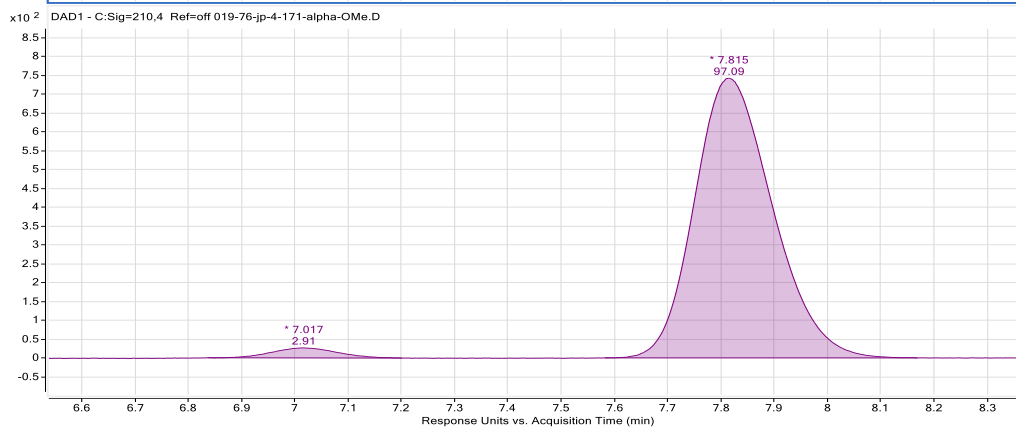
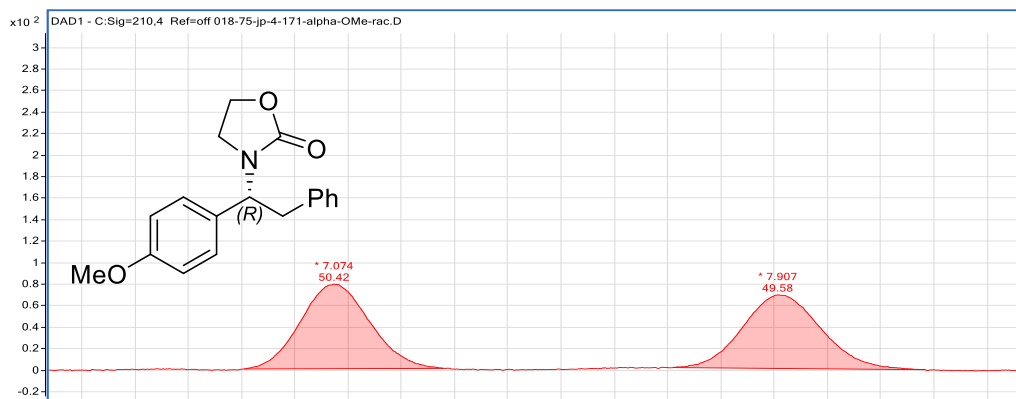


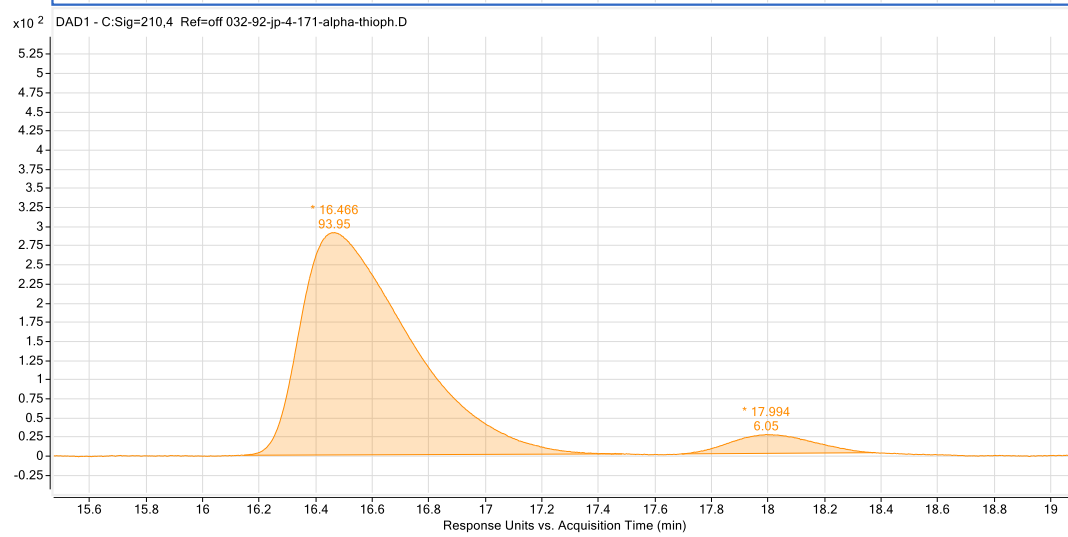
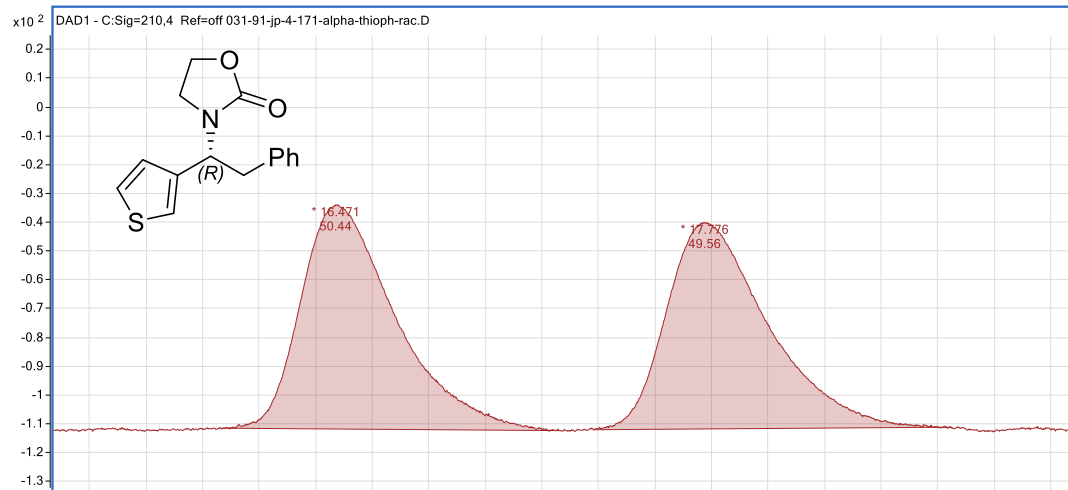
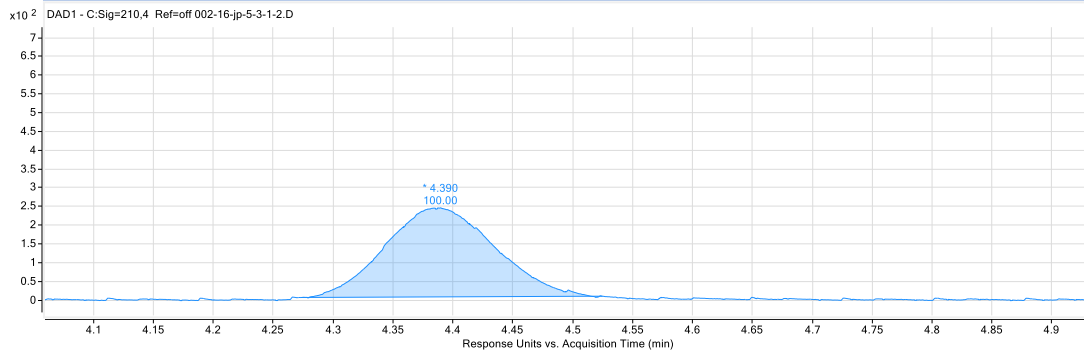
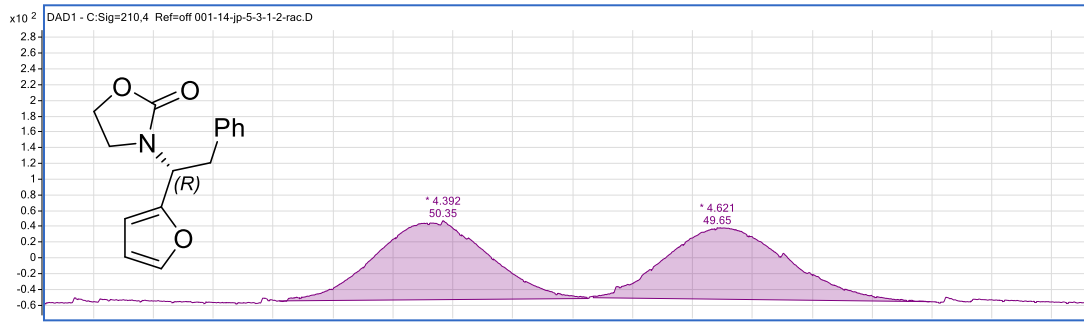


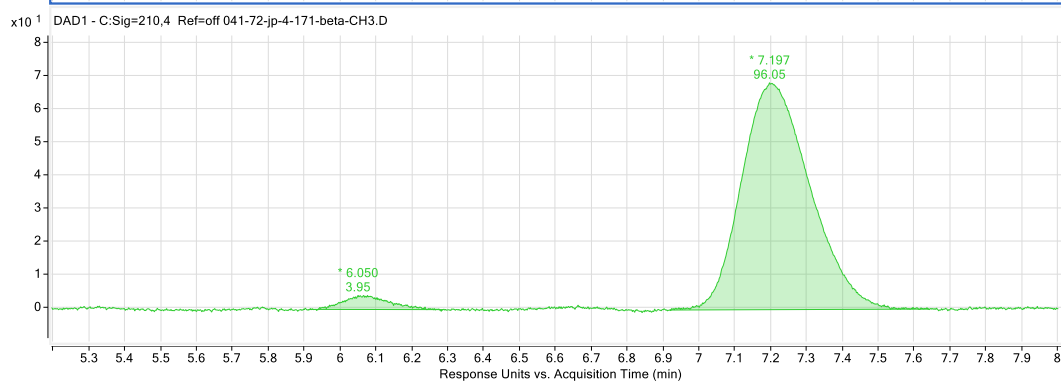
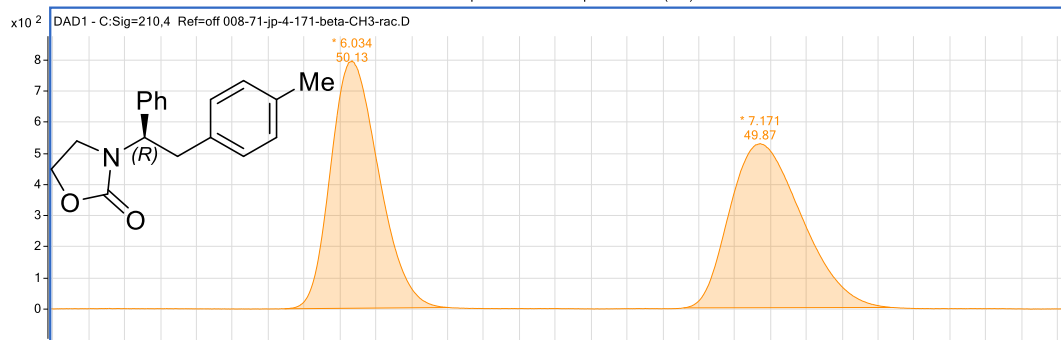
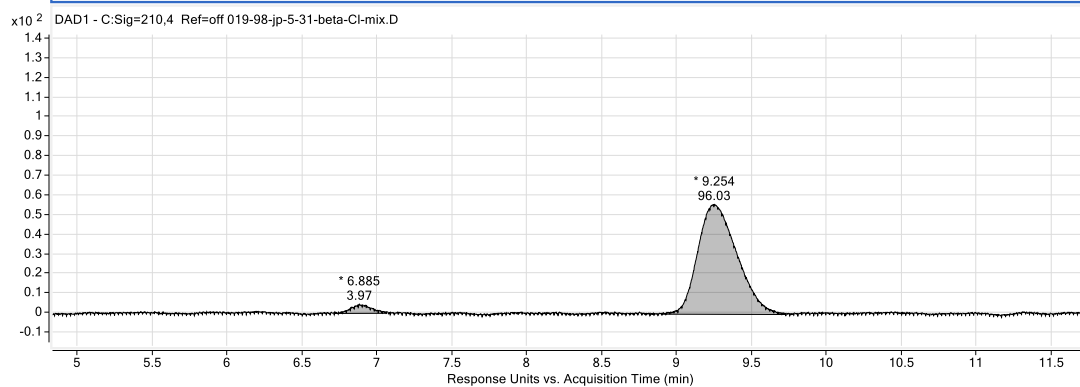
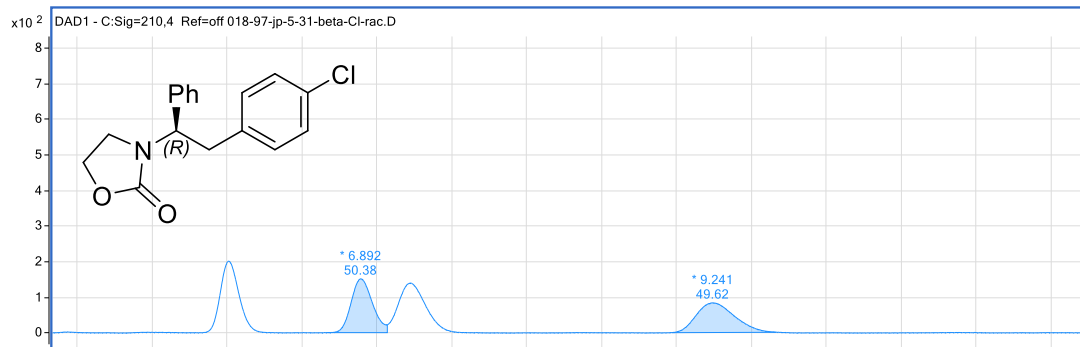


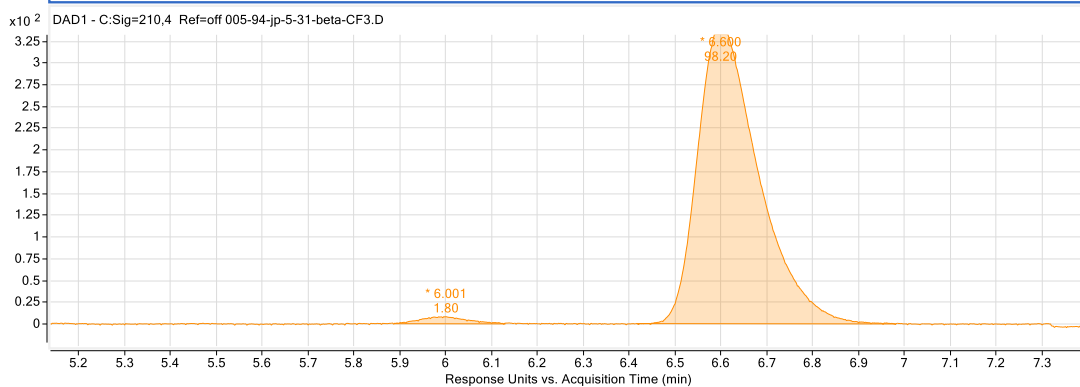
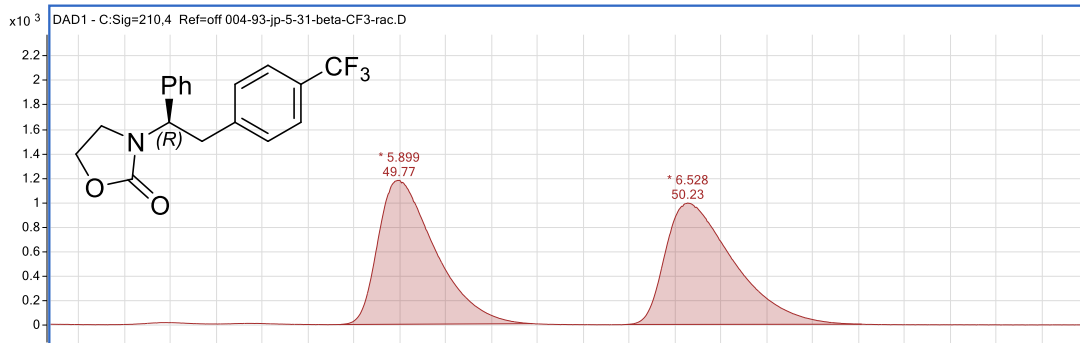
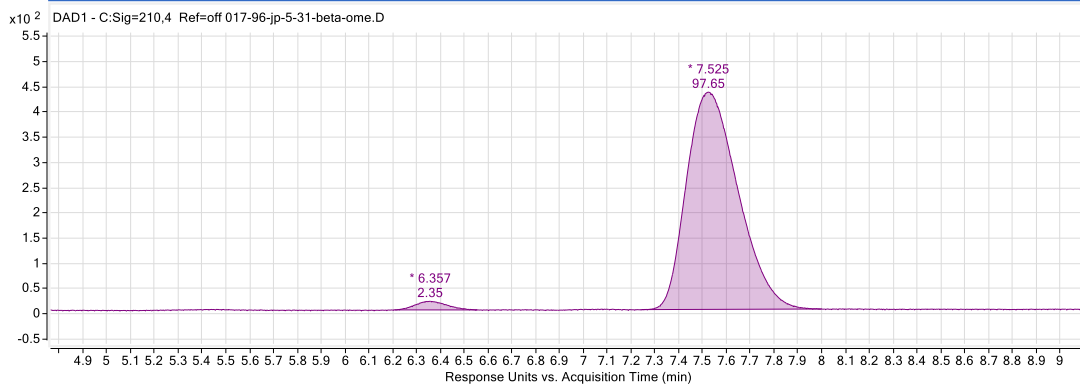
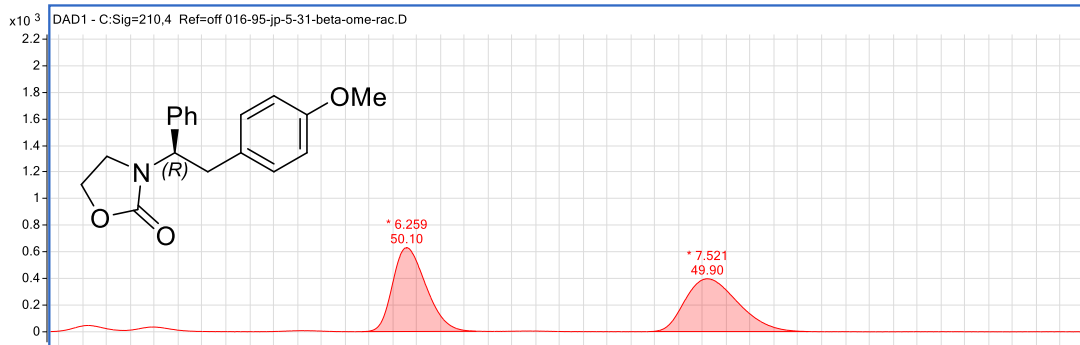


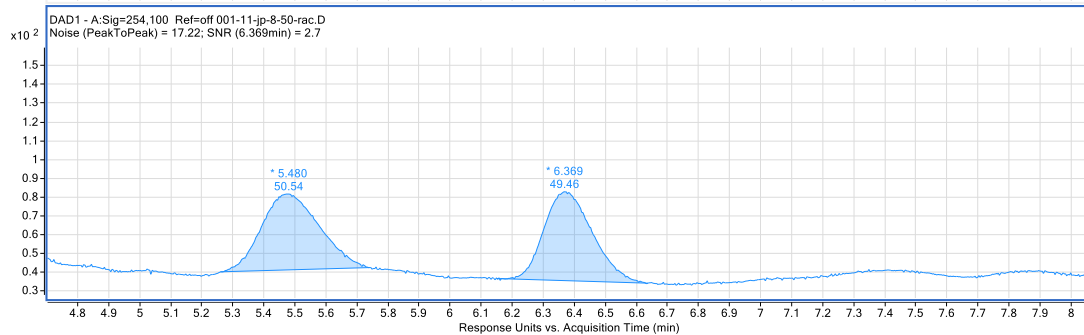
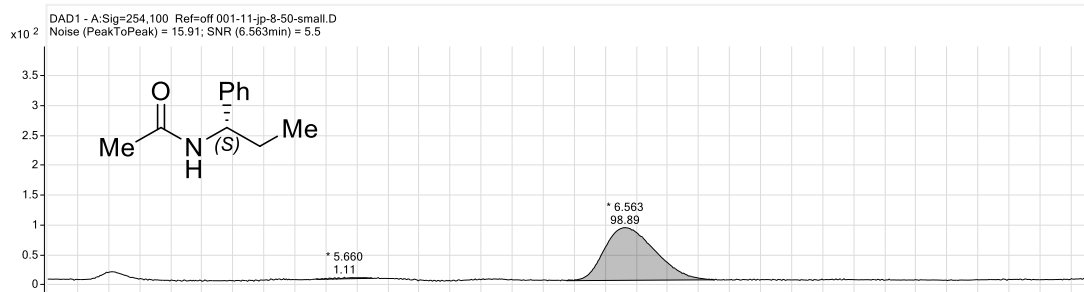
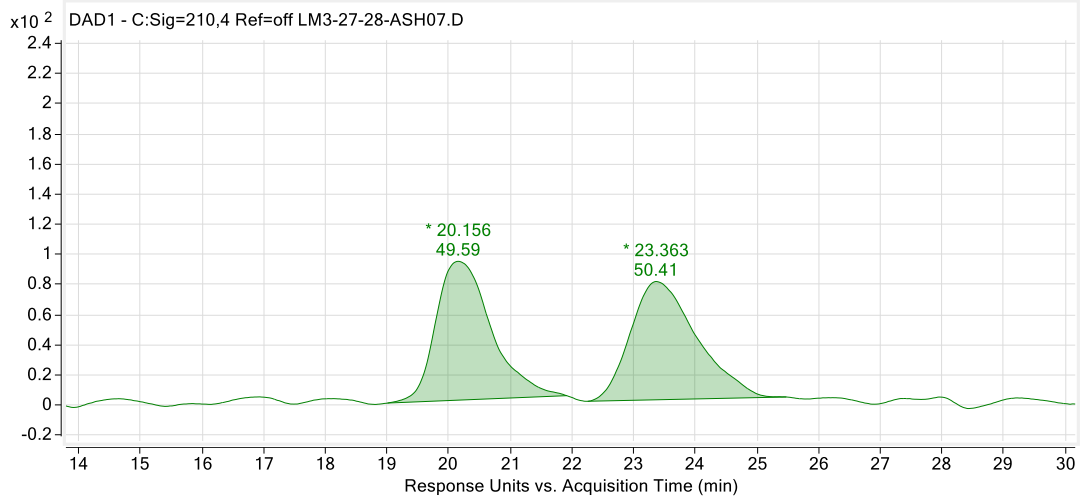
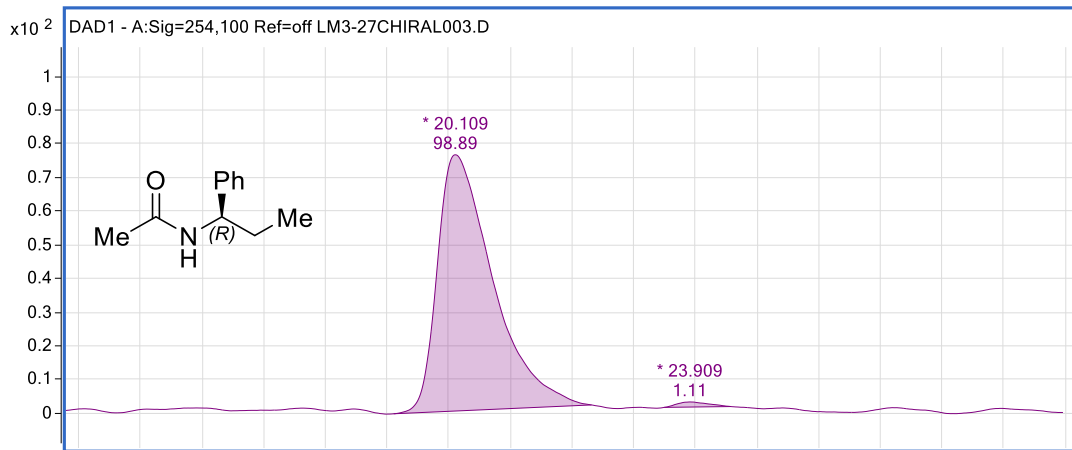


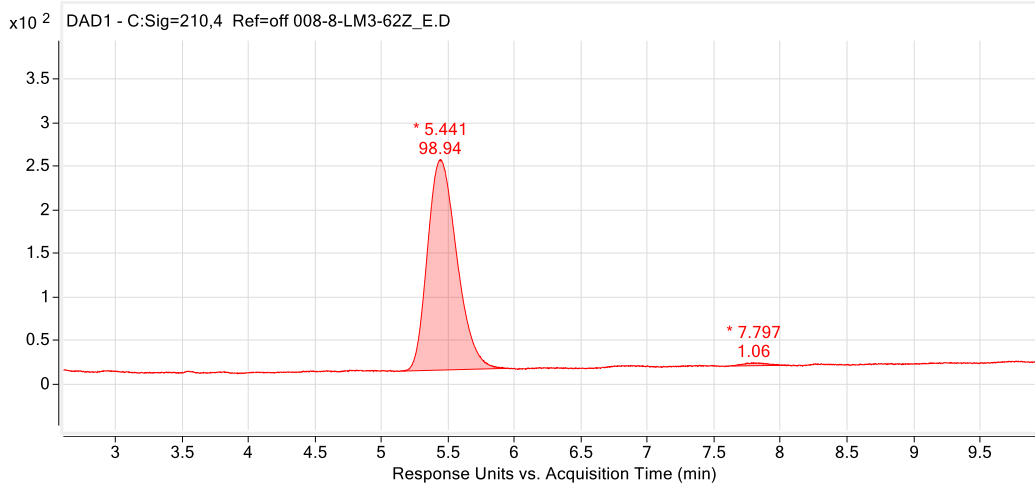
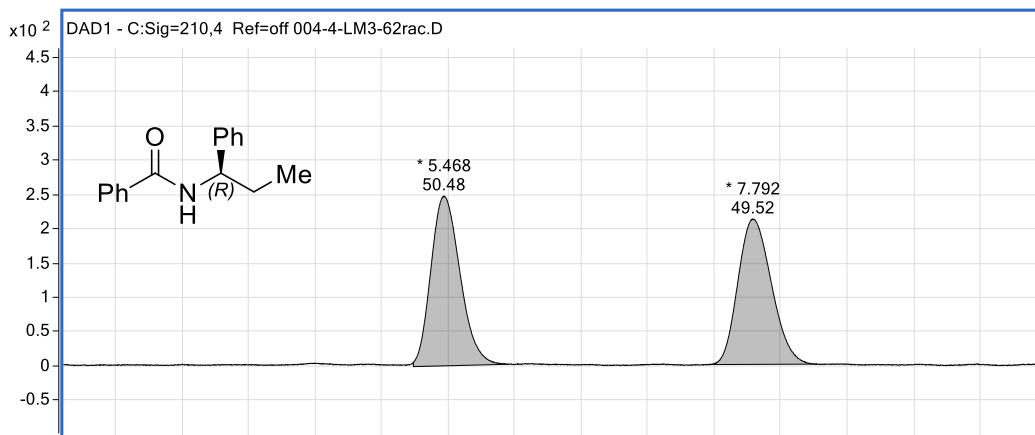
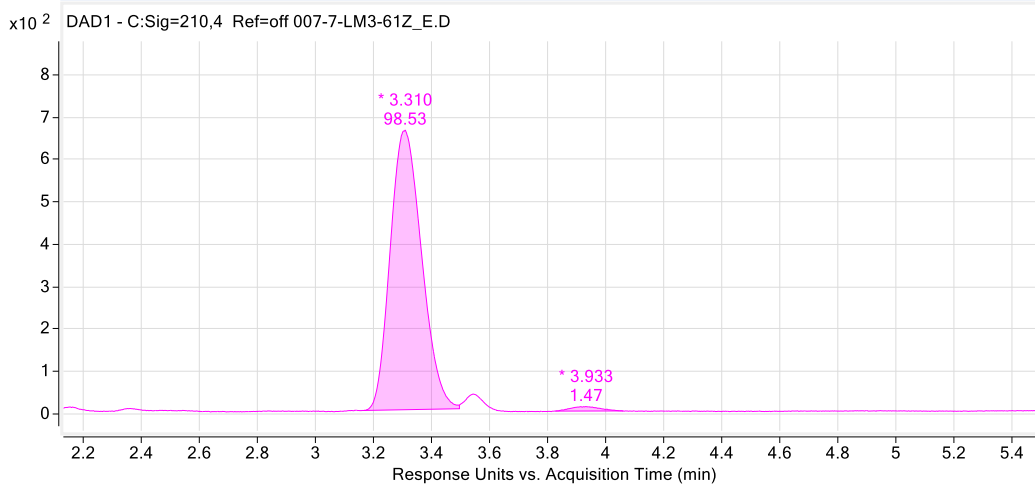
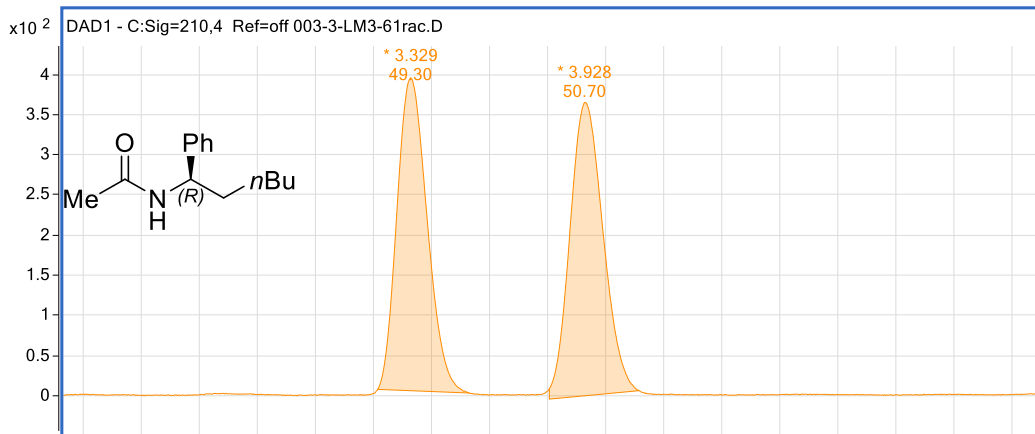


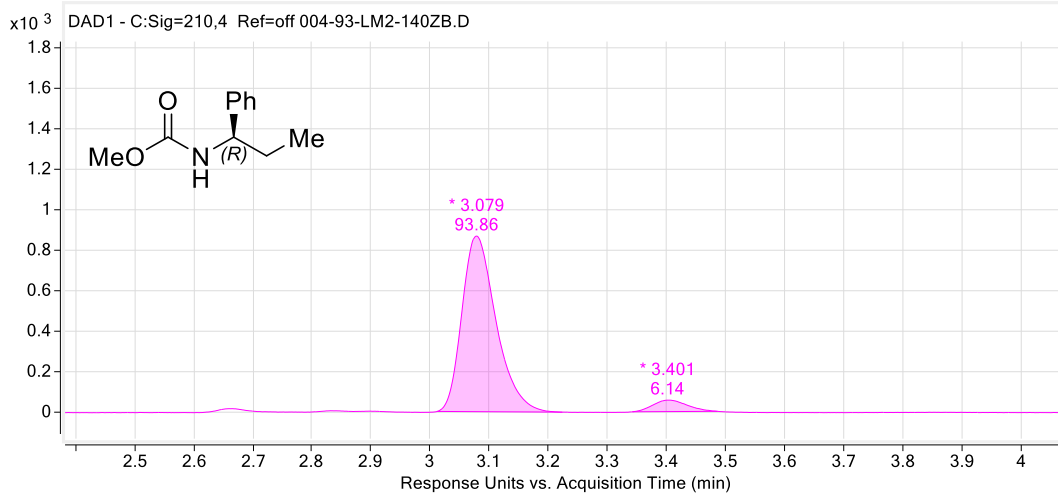
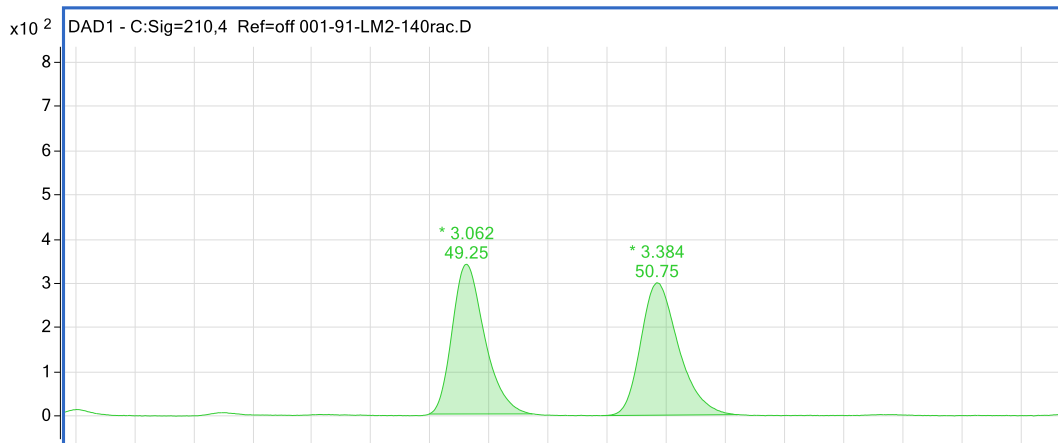












12. XYZ Coordinates

C1_E_R_tN_Chelbot

| <i>EI</i> | | | | TS_{E1-2} | | | |
|-----------|-----------|-----------|-----------|-------------|-----------|-----------|-----------|
| C1 | -4,217983 | -2,961081 | -0,742644 | C1 | -4,326353 | -3,069149 | -0,140508 |
| C2 | -2,146720 | -4,230141 | -1,006060 | C2 | -2,298479 | -4,317481 | -0,691570 |
| C3 | -3,448169 | -3,861797 | -1,767178 | C3 | -3,698641 | -3,965591 | -1,261091 |
| C4 | -3,244984 | -2,932842 | 0,457047 | C4 | -3,200364 | -3,040437 | 0,917641 |
| H5 | -5,174511 | -3,406053 | -0,449666 | H5 | -5,234702 | -3,516393 | 0,276092 |
| H6 | -3,242012 | -3,348974 | -2,711854 | H6 | -3,635005 | -3,454494 | -2,226967 |
| H7 | -3,666576 | -2,567680 | 1,394082 | H7 | -3,492970 | -2,686622 | 1,906936 |
| H8 | -4,416042 | -1,955037 | -1,117025 | H8 | -4,574771 | -2,062567 | -0,483851 |
| H9 | -1,599874 | -5,081628 | -1,411687 | H9 | -1,801689 | -5,158727 | -1,174628 |
| H10 | -4,011077 | -4,769262 | -2,002925 | H10 | -4,278898 | -4,880162 | -1,412470 |
| C11 | -2,661192 | -4,356709 | 0,444933 | C11 | -2,604801 | -4,455684 | 0,816870 |
| H12 | -1,867298 | -4,511814 | 1,181620 | H12 | -1,715398 | -4,594538 | 1,439202 |
| H13 | -3,420952 | -5,135101 | 0,558334 | H13 | -3,329531 | -5,246423 | 1,030452 |
| C14 | 0,136670 | -3,117726 | -0,470256 | C14 | 0,029577 | -3,170008 | -0,512794 |
| N15 | 0,945008 | -2,141631 | -0,217192 | N15 | 0,845228 | -2,194731 | -0,297325 |
| C16 | 2,285599 | -2,703712 | 0,189977 | C16 | 2,230390 | -2,744495 | -0,142560 |
| C17 | 1,961868 | -4,240930 | 0,205644 | C17 | 1,989389 | -4,264031 | -0,471878 |
| P18 | -1,642551 | -0,562963 | 0,482416 | P18 | -1,701858 | -0,619263 | 0,613492 |
| Ir19 | 0,507575 | -0,096073 | -0,642132 | Ir19 | 0,268037 | -0,103879 | -0,509097 |
| C20 | -1,584430 | -0,516713 | 2,312500 | C20 | -1,565712 | -0,388031 | 2,416768 |
| C21 | -1,306935 | -0,427523 | 5,105348 | C21 | -1,061501 | 0,028596 | 5,139894 |
| C22 | -1,562094 | -1,700793 | 3,064011 | C22 | -1,332524 | -1,477949 | 3,266335 |
| C23 | -1,444521 | 0,714030 | 2,976223 | C23 | -1,533391 | 0,915829 | 2,938951 |
| C24 | -1,308760 | 0,754856 | 4,362232 | C24 | -1,281444 | 1,118262 | 4,293713 |
| C25 | -1,429720 | -1,654058 | 4,452087 | C25 | -1,088141 | -1,267963 | 4,624533 |
| H26 | -1,439490 | 1,642076 | 2,420113 | H26 | -1,691820 | 1,772571 | 2,293468 |
| H27 | -1,199532 | 1,715866 | 4,856587 | H27 | -1,250387 | 2,131733 | 4,682901 |
| H28 | -1,412366 | -2,579102 | 5,021146 | H28 | -0,909408 | -2,118618 | 5,276163 |
| H29 | -1,202378 | -0,393318 | 6,186140 | H29 | -0,866253 | 0,190082 | 6,196336 |
| O30 | 0,601784 | -4,352360 | -0,305102 | O30 | 0,544130 | -4,397058 | -0,582575 |
| C31 | 2,708978 | -2,294362 | 1,598708 | C31 | 2,730609 | -2,593664 | 1,294562 |
| C32 | 1,873687 | -1,591198 | 2,467328 | C32 | 2,010779 | -1,902579 | 2,271580 |
| C33 | 3,947759 | -2,751317 | 2,078196 | C33 | 3,928071 | -3,226263 | 1,666424 |
| C34 | 2,279970 | -1,309031 | 3,773741 | C34 | 2,489850 | -1,814182 | 3,580310 |
| H35 | 0,902173 | -1,258948 | 2,138525 | H35 | 1,070139 | -1,435256 | 2,022996 |
| C36 | 4,352384 | -2,474159 | 3,381663 | C36 | 4,409299 | -3,136010 | 2,970557 |
| H37 | 4,605795 | -3,316608 | 1,423298 | H37 | 4,496541 | -3,788116 | 0,929360 |
| C38 | 3,521596 | -1,742162 | 4,233446 | C38 | 3,693234 | -2,421217 | 3,933232 |
| H39 | 1,609716 | -0,755633 | 4,424736 | H39 | 1,905697 | -1,272607 | 4,318942 |
| H40 | 5,318218 | -2,828055 | 3,730890 | H40 | 5,342112 | -3,626144 | 3,234479 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H41 | 3,839997 | -1,521054 | 5,248203 | H41 | 4,068228 | -2,349612 | 4,950148 |
| C42 | -3,105029 | 0,438837 | 0,002537 | C42 | -3,163881 | 0,345875 | 0,082363 |
| C43 | -3,991432 | 1,029815 | 0,910083 | C43 | -4,137639 | 0,818475 | 0,971414 |
| C44 | -3,335795 | 0,582522 | -1,377719 | C44 | -3,329497 | 0,547047 | -1,298585 |
| C45 | -5,083130 | 1,767663 | 0,444787 | C45 | -5,252463 | 1,503642 | 0,486761 |
| H46 | -3,836449 | 0,921464 | 1,978259 | H46 | -4,027051 | 0,662314 | 2,039464 |
| C47 | -4,427992 | 1,316089 | -1,836038 | C47 | -4,449318 | 1,223660 | -1,777266 |
| C48 | -5,302309 | 1,917454 | -0,924484 | C48 | -5,408674 | 1,709532 | -0,884080 |
| H49 | -5,763259 | 2,223892 | 1,158548 | H49 | -5,999182 | 1,875358 | 1,182631 |
| H50 | -4,598848 | 1,419094 | -2,903984 | H50 | -4,573866 | 1,376074 | -2,845695 |
| H51 | -6,151228 | 2,492966 | -1,281399 | H51 | -6,277328 | 2,244172 | -1,257524 |
| H52 | 1,217781 | 0,301025 | 0,671998 | H52 | 0,809250 | 0,302155 | 0,885602 |
| H53 | 1,966990 | -0,193766 | -1,251191 | H53 | 1,761691 | 0,324223 | -1,126202 |
| H54 | -1,621030 | -2,661793 | 2,566426 | H54 | -1,314295 | -2,485659 | 2,864748 |
| H55 | -2,659288 | 0,112099 | -2,087244 | H55 | -2,580808 | 0,172955 | -1,992892 |
| H56 | 2,613839 | -4,832065 | -0,438096 | H56 | 2,421554 | -4,567450 | -1,427849 |
| C57 | 5,054144 | -1,695549 | -3,004939 | C57 | 4,668804 | -0,975381 | -3,284282 |
| C58 | 3,980620 | -2,560454 | -3,230625 | C58 | 3,413773 | -1,524739 | -3,560180 |
| C59 | 3,115557 | -2,883708 | -2,188385 | C59 | 2,657527 | -2,085738 | -2,535536 |
| C60 | 3,300606 | -2,348532 | -0,905519 | C60 | 3,130491 | -2,104447 | -1,212755 |
| C61 | 4,362372 | -1,462754 | -0,696142 | C61 | 4,382883 | -1,545776 | -0,945475 |
| C62 | 5,240365 | -1,149591 | -1,736252 | C62 | 5,148338 | -0,991676 | -1,976867 |
| H63 | 5,737463 | -1,449884 | -3,812761 | H63 | 5,267369 | -0,543320 | -4,081299 |
| H64 | 3,820805 | -2,987374 | -4,216507 | H64 | 3,024195 | -1,526816 | -4,575128 |
| H65 | 2,278247 | -3,548897 | -2,386337 | H65 | 1,673687 | -2,485027 | -2,762653 |
| H66 | 4,505742 | -1,006868 | 0,275629 | H66 | 4,767213 | -1,526120 | 0,067613 |
| H67 | 6,066795 | -0,469186 | -1,549668 | H67 | 6,120499 | -0,563825 | -1,748669 |
| C68 | 3,267813 | 4,712826 | -1,323067 | C68 | 3,347349 | 4,696527 | -1,269022 |
| C69 | 2,107553 | 3,939122 | -1,346076 | C69 | 2,257195 | 3,863278 | -1,506913 |
| C70 | 2,182263 | 2,550650 | -1,537215 | C70 | 2,361124 | 2,483024 | -1,282835 |
| C71 | 3,434405 | 1,959059 | -1,735215 | C71 | 3,556407 | 1,952717 | -0,797408 |
| C72 | 4,592860 | 2,732861 | -1,711982 | C72 | 4,645917 | 2,789070 | -0,552133 |
| C73 | 4,514114 | 4,110933 | -1,499640 | C73 | 4,544937 | 4,159851 | -0,790562 |
| H74 | 3,196343 | 5,785120 | -1,164808 | H74 | 3,257307 | 5,765118 | -1,440894 |
| H75 | 1,142227 | 4,413318 | -1,204033 | H75 | 1,313108 | 4,283658 | -1,842150 |
| H76 | 3,500934 | 0,889610 | -1,896792 | H76 | 3,628938 | 0,889274 | -0,599538 |
| H77 | 5,558408 | 2,256440 | -1,857889 | H77 | 5,570902 | 2,368436 | -0,168303 |
| H78 | 5,418000 | 4,713050 | -1,475040 | H78 | 5,391708 | 4,811301 | -0,594551 |
| C79 | 0,902514 | 1,769095 | -1,664965 | C79 | 1,157428 | 1,631428 | -1,598407 |
| C80 | -0,237991 | 1,965231 | -0,820551 | C80 | -0,154618 | 1,918012 | -0,987593 |
| C81 | 0,558192 | 2,556093 | -4,091901 | C81 | 1,504788 | 2,137058 | -4,129043 |
| C82 | -0,096858 | 0,424383 | -3,470273 | C82 | 0,319956 | 0,254852 | -3,453272 |
| C83 | 0,155122 | 1,716382 | -5,317908 | C83 | 1,218739 | 1,194877 | -5,315228 |
| H84 | 1,530633 | 3,038250 | -4,202904 | H84 | 2,559418 | 2,405080 | -4,046797 |
| H85 | -0,187469 | 3,318441 | -3,830072 | H85 | 0,907966 | 3,057059 | -4,159715 |
| H86 | -0,575690 | 2,199179 | -5,967003 | H86 | 0,743135 | 1,685709 | -6,164536 |
| H87 | 1,022577 | 1,399900 | -5,904479 | H87 | 2,118496 | 0,667777 | -5,644443 |
| N88 | 0,599315 | 1,508777 | -3,069530 | N88 | 1,085669 | 1,282304 | -3,019554 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| O89 | -0,461746 | 0,520574 | -4,757112 | O89 | 0,291728 | 0,200603 | -4,792627 |
| O90 | -0,389742 | -0,552526 | -2,762735 | O90 | -0,283618 | -0,560806 | -2,738448 |
| H91 | 1,964421 | -4,648753 | 1,216712 | H91 | 2,324442 | -4,930267 | 0,322429 |
| N92 | -2,035846 | -2,150666 | 0,080105 | N92 | -2,054302 | -2,251580 | 0,395421 |
| C93 | -1,290393 | -2,942639 | -0,929703 | C93 | -1,458690 | -3,015969 | -0,725121 |
| H94 | -1,249303 | -2,439083 | -1,900732 | H94 | -1,574455 | -2,503202 | -1,689593 |
| H96 | -1,194468 | 1,932784 | -1,335777 | H96 | -0,962564 | 1,948410 | -1,718876 |
| C97 | -0,498673 | 4,443000 | 2,681663 | C97 | -0,985647 | 4,668138 | 2,219882 |
| C98 | -1,561021 | 4,344187 | 1,783534 | C98 | -1,913474 | 4,439515 | 1,203315 |
| C99 | -1,450823 | 3,527516 | 0,656440 | C99 | -1,611458 | 3,559742 | 0,162861 |
| C100 | -0,278246 | 2,796547 | 0,409463 | C100 | -0,382765 | 2,880911 | 0,123258 |
| C101 | 0,785585 | 2,902920 | 1,324251 | C101 | 0,536328 | 3,109490 | 1,162412 |
| C102 | 0,674778 | 3,719417 | 2,444452 | C102 | 0,241342 | 3,999650 | 2,190582 |
| H103 | -0,581478 | 5,077476 | 3,559638 | H103 | -1,215570 | 5,357422 | 3,027490 |
| H104 | -2,478782 | 4,898225 | 1,958897 | H104 | -2,875106 | 4,945002 | 1,217179 |
| H105 | -2,288299 | 3,445093 | -0,031522 | H105 | -2,347117 | 3,377852 | -0,616807 |
| H106 | 1,697500 | 2,343717 | 1,156198 | H106 | 1,481502 | 2,578997 | 1,172862 |
| H107 | 1,507146 | 3,789394 | 3,139051 | H107 | 0,969596 | 4,164491 | 2,980032 |

E2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,310252 | -2,924883 | -0,331866 |
| C2 | -2,335369 | -4,299957 | -0,749330 |
| C3 | -3,684718 | -3,888881 | -1,395958 |
| C4 | -3,240892 | -2,935730 | 0,783455 |
| H5 | -5,264549 | -3,303359 | 0,048446 |
| H6 | -3,547236 | -3,412233 | -2,371652 |
| H7 | -3,567149 | -2,543731 | 1,747216 |
| H8 | -4,477788 | -1,914490 | -0,711340 |
| H9 | -1,860365 | -5,177825 | -1,187676 |
| H10 | -4,309415 | -4,773470 | -1,548834 |
| C11 | -2,722906 | -4,384139 | 0,743944 |
| H12 | -1,875215 | -4,557498 | 1,414056 |
| H13 | -3,501852 | -5,127177 | 0,937118 |
| C14 | 0,048710 | -3,271948 | -0,515508 |
| N15 | 0,867103 | -2,323492 | -0,227775 |
| C16 | 2,230002 | -2,895045 | -0,033744 |
| C17 | 2,004946 | -4,364624 | -0,540303 |
| P18 | -1,598852 | -0,615465 | 0,580967 |
| Ir19 | 0,316723 | -0,213543 | -0,443297 |
| C20 | -1,518308 | -0,421521 | 2,390162 |
| C21 | -1,145881 | -0,071354 | 5,141192 |
| C22 | -1,456268 | -1,534034 | 3,239332 |
| C23 | -1,371556 | 0,870271 | 2,924533 |
| C24 | -1,187587 | 1,039322 | 4,293923 |
| C25 | -1,279222 | -1,355842 | 4,612617 |
| H26 | -1,385641 | 1,740031 | 2,276880 |
| H27 | -1,067555 | 2,041546 | 4,694532 |
| H28 | -1,234850 | -2,222899 | 5,265627 |

TS_{E2-3}

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,379163 | -2,466986 | -0,570456 |
| C2 | -2,518987 | -3,920038 | -1,199674 |
| C3 | -3,806656 | -3,278377 | -1,780971 |
| C4 | -3,337855 | -2,755309 | 0,533395 |
| H5 | -5,365366 | -2,833067 | -0,266676 |
| H6 | -3,596981 | -2,648985 | -2,651604 |
| H7 | -3,649388 | -2,501741 | 1,547016 |
| H8 | -4,466252 | -1,397555 | -0,770684 |
| H9 | -2,117193 | -4,753144 | -1,776493 |
| H10 | -4,500832 | -4,060062 | -2,102078 |
| C11 | -2,950066 | -4,217981 | 0,253925 |
| H12 | -2,138595 | -4,581238 | 0,892112 |
| H13 | -3,797556 | -4,906863 | 0,311831 |
| C14 | -0,068588 | -3,203272 | -0,720364 |
| N15 | 0,827096 | -2,417788 | -0,237825 |
| C16 | 2,125528 | -3,148807 | -0,159069 |
| C17 | 1,691392 | -4,589260 | -0,623258 |
| P18 | -1,485328 | -0,605602 | 0,761344 |
| Ir19 | 0,501156 | -0,238348 | -0,128020 |
| C20 | -1,427804 | -0,744901 | 2,576922 |
| C21 | -1,077195 | -0,936324 | 5,347086 |
| C22 | -1,467774 | -1,995812 | 3,207787 |
| C23 | -1,189389 | 0,411065 | 3,340824 |
| C24 | -1,018596 | 0,310591 | 4,718797 |
| C25 | -1,299789 | -2,087288 | 4,590690 |
| H26 | -1,118755 | 1,382259 | 2,864281 |
| H27 | -0,828851 | 1,209564 | 5,297719 |
| H28 | -1,333497 | -3,060084 | 5,072872 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H29 | -1,003119 | 0,064363 | 6,209590 | H29 | -0,942385 | -1,010820 | 6,422489 |
| O30 | 0,554934 | -4,501211 | -0,641230 | O30 | 0,297433 | -4,451438 | -1,025002 |
| C31 | 2,620530 | -2,888413 | 1,445135 | C31 | 2,659326 | -3,223281 | 1,265878 |
| C32 | 1,873682 | -2,208993 | 2,409726 | C32 | 1,942736 | -2,720863 | 2,353953 |
| C33 | 3,758114 | -3,602557 | 1,851339 | C33 | 3,859123 | -3,911626 | 1,502969 |
| C34 | 2,260830 | -2,229865 | 3,751081 | C34 | 2,430909 | -2,872573 | 3,653485 |
| H35 | 0,989240 | -1,660306 | 2,121231 | H35 | 1,005222 | -2,207361 | 2,194083 |
| C36 | 4,146315 | -3,622584 | 3,188999 | C36 | 4,345603 | -4,063904 | 2,799427 |
| H37 | 4,356600 | -4,135040 | 1,115902 | H37 | 4,421272 | -4,321764 | 0,667303 |
| C38 | 3,398394 | -2,931582 | 4,145199 | C38 | 3,634417 | -3,537851 | 3,880614 |
| H39 | 1,660076 | -1,695653 | 4,481712 | H39 | 1,857784 | -2,468659 | 4,483561 |
| H40 | 5,032614 | -4,177043 | 3,483833 | H40 | 5,279886 | -4,592790 | 2,964873 |
| H41 | 3,700777 | -2,946691 | 5,188376 | H41 | 4,015727 | -3,654000 | 4,891040 |
| C42 | -2,988850 | 0,424621 | 0,009737 | C42 | -2,791648 | 0,605202 | 0,352697 |
| C43 | -3,935209 | 0,975723 | 0,883932 | C43 | -3,664908 | 1,143449 | 1,305132 |
| C44 | -3,135409 | 0,608714 | -1,375971 | C44 | -2,959896 | 0,926050 | -1,006044 |
| C45 | -5,003560 | 1,718615 | 0,379234 | C45 | -4,685970 | 2,007268 | 0,904484 |
| H46 | -3,841287 | 0,835581 | 1,955323 | H46 | -3,555323 | 0,895374 | 2,355122 |
| C47 | -4,206658 | 1,346558 | -1,873335 | C47 | -3,979844 | 1,787782 | -1,398754 |
| C48 | -5,138986 | 1,908644 | -0,995517 | C48 | -4,841875 | 2,333960 | -0,441942 |
| H49 | -5,728862 | 2,149065 | 1,063737 | H49 | -5,357824 | 2,424673 | 1,648854 |
| H50 | -4,315444 | 1,487015 | -2,945073 | H50 | -4,103403 | 2,036957 | -2,448738 |
| H51 | -5,970279 | 2,489610 | -1,384446 | H51 | -5,635153 | 3,009527 | -0,748552 |
| H52 | 0,809053 | 0,157331 | 0,981979 | H52 | 0,968672 | -0,141924 | 1,352492 |
| H53 | 2,047387 | 0,863061 | -1,374622 | H53 | 2,266332 | 2,540376 | -0,831852 |
| H54 | -1,516365 | -2,536595 | 2,830006 | H54 | -1,601152 | -2,898364 | 2,621524 |
| H55 | -2,408008 | 0,175781 | -2,058066 | H55 | -2,285478 | 0,505054 | -1,748260 |
| H56 | 2,421253 | -4,542872 | -1,535173 | H56 | 2,255235 | -4,962075 | -1,479695 |
| C57 | 4,834744 | -0,651981 | -2,701715 | C57 | 4,696218 | -1,261266 | -3,114600 |
| C58 | 3,663794 | -1,251717 | -3,170682 | C58 | 3,509661 | -1,896637 | -3,490989 |
| C59 | 2,853897 | -1,975094 | -2,298984 | C59 | 2,708411 | -2,498927 | -2,525404 |
| C60 | 3,191436 | -2,109314 | -0,940943 | C60 | 3,076157 | -2,486679 | -1,170520 |
| C61 | 4,356489 | -1,491161 | -0,477299 | C61 | 4,253264 | -1,827376 | -0,799977 |
| C62 | 5,175415 | -0,774653 | -1,355161 | C62 | 5,060280 | -1,224668 | -1,769188 |
| H63 | 5,473597 | -0,092268 | -3,378792 | H63 | 5,336226 | -0,806461 | -3,866172 |
| H64 | 3,382810 | -1,163289 | -4,216768 | H64 | 3,206374 | -1,926867 | -4,533200 |
| H65 | 1,932889 | -2,413621 | -2,671358 | H65 | 1,780565 | -2,973331 | -2,832966 |
| H66 | 4,630280 | -1,561623 | 0,568838 | H66 | 4,546510 | -1,782760 | 0,241930 |
| H67 | 6,082135 | -0,309267 | -0,978912 | H67 | 5,976253 | -0,725560 | -1,465943 |
| C68 | 2,660470 | 5,313225 | -1,876282 | C68 | -0,752253 | 5,308402 | -2,843922 |
| C69 | 1,819634 | 4,204236 | -1,916397 | C69 | -0,260874 | 4,033248 | -2,573675 |
| C70 | 2,342395 | 2,916028 | -1,740419 | C70 | 0,831014 | 3,860769 | -1,713484 |
| C71 | 3,711113 | 2,753727 | -1,514358 | C71 | 1,422272 | 4,981887 | -1,127836 |
| C72 | 4,552174 | 3,867034 | -1,465784 | C72 | 0,926473 | 6,259920 | -1,391208 |
| C73 | 4,028538 | 5,146673 | -1,648049 | C73 | -0,160134 | 6,425780 | -2,249302 |
| H74 | 2,246482 | 6,308930 | -2,005749 | H74 | -1,599398 | 5,432459 | -3,512889 |
| H75 | 0,750667 | 4,338862 | -2,052288 | H75 | -0,731962 | 3,162429 | -3,025384 |
| H76 | 4,117708 | 1,756544 | -1,369740 | H76 | 2,256624 | 4,852811 | -0,442675 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H77 | 5,614189 | 3,734129 | -1,280425 | H77 | 1,387934 | 7,124467 | -0,922774 |
| H78 | 4,681263 | 6,013712 | -1,603976 | H78 | -0,546675 | 7,420000 | -2,454012 |
| C79 | 1,422904 | 1,711106 | -1,783340 | C79 | 1,299681 | 2,461003 | -1,338421 |
| C80 | 0,097319 | 1,789934 | -0,975761 | C80 | 0,252126 | 1,828277 | -0,369658 |
| C81 | 1,327522 | 2,153929 | -4,362892 | C81 | 2,379657 | 2,255228 | -3,635790 |
| C82 | 0,394676 | 0,227534 | -3,477145 | C82 | 0,942216 | 0,548706 | -2,997785 |
| C83 | 0,951166 | 1,156350 | -5,473193 | C83 | 2,261227 | 1,192754 | -4,746260 |
| H84 | 2,356316 | 2,509075 | -4,441496 | H84 | 3,408553 | 2,387213 | -3,286018 |
| H85 | 0,661688 | 3,024430 | -4,327564 | H85 | 1,986055 | 3,230554 | -3,935077 |
| H86 | 0,329850 | 1,584084 | -6,260358 | H86 | 1,932439 | 1,598781 | -5,704309 |
| H87 | 1,830817 | 0,678451 | -5,914814 | H87 | 3,183567 | 0,623382 | -4,881949 |
| N88 | 1,145242 | 1,309095 | -3,182027 | N88 | 1,549182 | 1,676539 | -2,574485 |
| O89 | 0,177093 | 0,125476 | -4,798603 | O89 | 1,245437 | 0,270825 | -4,276384 |
| O90 | -0,060548 | -0,614869 | -2,682659 | O90 | 0,194444 | -0,223518 | -2,367461 |
| H91 | 2,359818 | -5,120694 | 0,158207 | H91 | 1,727602 | -5,312094 | 0,193050 |
| N92 | -2,022513 | -2,224649 | 0,307754 | N92 | -2,049981 | -2,086587 | 0,189963 |
| C93 | -1,423224 | -3,048065 | -0,771947 | C93 | -1,490750 | -2,779336 | -0,995755 |
| H94 | -1,477038 | -2,548494 | -1,749471 | H94 | -1,447903 | -2,124893 | -1,876957 |
| H96 | -0,729762 | 1,934787 | -1,677822 | H96 | -0,704380 | 1,951594 | -0,883318 |
| C97 | -0,414768 | 4,575743 | 2,278842 | C97 | 0,021719 | 4,188704 | 3,252687 |
| C98 | -1,416475 | 4,395741 | 1,324955 | C98 | -1,028026 | 4,195892 | 2,333744 |
| C99 | -1,221674 | 3,512891 | 0,260294 | C99 | -0,939815 | 3,444468 | 1,160010 |
| C100 | -0,030623 | 2,781645 | 0,135076 | C100 | 0,188995 | 2,658177 | 0,889353 |
| C101 | 0,968399 | 2,972693 | 1,105483 | C101 | 1,239919 | 2,668108 | 1,819706 |
| C102 | 0,781599 | 3,861168 | 2,159571 | C102 | 1,161865 | 3,424918 | 2,986472 |
| H103 | -0,560455 | 5,266837 | 3,104342 | H103 | -0,043594 | 4,775173 | 4,164909 |
| H104 | -2,351666 | 4,943510 | 1,405705 | H104 | -1,916820 | 4,790886 | 2,526293 |
| H105 | -2,012523 | 3,372766 | -0,473041 | H105 | -1,756673 | 3,465031 | 0,443840 |
| H106 | 1,897454 | 2,415045 | 1,033031 | H106 | 2,114056 | 2,050170 | 1,636152 |
| H107 | 1,570145 | 3,995205 | 2,895200 | H107 | 1,986454 | 3,413178 | 3,694376 |
| | | | | H108 | 3,293888 | 0,440742 | -0,341385 |
| | | | | H109 | 3,385246 | 0,864873 | 0,262884 |

E3

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -4,355556 | -2,461423 | -0,796930 |
| C2 | -2,464517 | -3,925156 | -1,300068 |
| C3 | -3,708816 | -3,278811 | -1,965573 |
| C4 | -3,387604 | -2,750304 | 0,372202 |
| H5 | -5,361223 | -2,822084 | -0,557254 |
| H6 | -3,440042 | -2,652892 | -2,822424 |
| H7 | -3,760128 | -2,490877 | 1,363835 |
| H8 | -4,424135 | -1,392214 | -1,005325 |
| H9 | -2,031946 | -4,762519 | -1,847532 |
| H10 | -4,384329 | -4,058292 | -2,329190 |
| C11 | -2,991084 | -4,215905 | 0,123019 |
| H12 | -2,224535 | -4,581682 | 0,813192 |
| H13 | -3,844385 | -4,899983 | 0,127859 |
| C14 | -0,041523 | -3,216597 | -0,678653 |

TS_{E3-4}

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -4,413515 | -2,302062 | -0,638785 |
| C2 | -2,573687 | -3,727476 | -1,382061 |
| C3 | -3,831807 | -2,993428 | -1,917442 |
| C4 | -3,398989 | -2,726113 | 0,447706 |
| H5 | -5,411763 | -2,679139 | -0,393277 |
| H6 | -3,586142 | -2,279212 | -2,710042 |
| H7 | -3,723856 | -2,569196 | 1,476909 |
| H8 | -4,479944 | -1,216799 | -0,729393 |
| H9 | -2,182898 | -4,507789 | -2,035118 |
| H10 | -4,536185 | -3,717304 | -2,336824 |
| C11 | -3,042881 | -4,161916 | 0,025095 |
| H12 | -2,253650 | -4,608941 | 0,636961 |
| H13 | -3,907675 | -4,830721 | -0,005156 |
| C14 | -0,120623 | -3,128987 | -0,781702 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| N15 | 0,855807 | -2,435612 | -0,188945 | N15 | 0,842850 | -2,407734 | -0,317074 |
| C16 | 2,150333 | -3,183753 | -0,098660 | C16 | 2,093723 | -3,245358 | -0,251711 |
| C17 | 1,693364 | -4,631656 | -0,500993 | C17 | 1,513592 | -4,657923 | -0,600204 |
| P18 | -1,544302 | -0,606122 | 0,700196 | P18 | -1,514687 | -0,591532 | 0,806256 |
| Ir19 | 0,592166 | -0,231970 | -0,063785 | Ir19 | 0,759673 | -0,294219 | -0,009525 |
| C20 | -1,546094 | -0,756007 | 2,518475 | C20 | -1,527905 | -0,749885 | 2,623980 |
| C21 | -1,268381 | -0,974106 | 5,295448 | C21 | -1,192945 | -0,974831 | 5,402275 |
| C22 | -1,613054 | -2,010979 | 3,136475 | C22 | -1,582486 | -2,005246 | 3,244667 |
| C23 | -1,320531 | 0,390585 | 3,298644 | C23 | -1,289125 | 0,393669 | 3,406372 |
| C24 | -1,186329 | 0,277843 | 4,679770 | C24 | -1,127005 | 0,277702 | 4,785551 |
| C25 | -1,480049 | -2,116059 | 4,522682 | C25 | -1,420279 | -2,113807 | 4,628231 |
| H26 | -1,228715 | 1,365464 | 2,832543 | H26 | -1,211470 | 1,371615 | 2,941757 |
| H27 | -1,006549 | 1,170753 | 5,271393 | H27 | -0,939308 | 1,169871 | 5,376001 |
| H28 | -1,534139 | -3,092813 | 4,994983 | H28 | -1,468306 | -3,092136 | 5,098143 |
| H29 | -1,161769 | -1,058831 | 6,373224 | H29 | -1,062974 | -1,061784 | 6,476900 |
| O30 | 0,315250 | -4,477679 | -0,946080 | O30 | 0,153901 | -4,405804 | -1,055895 |
| C31 | 2,692002 | -3,204161 | 1,325974 | C31 | 2,656906 | -3,306900 | 1,165422 |
| C32 | 1,933285 | -2,734603 | 2,402212 | C32 | 1,851683 | -2,996121 | 2,267468 |
| C33 | 3,925829 | -3,819134 | 1,584584 | C33 | 3,933919 | -3,837038 | 1,392778 |
| C34 | 2,414434 | -2,841554 | 3,707916 | C34 | 2,332424 | -3,153284 | 3,566629 |
| H35 | 0,964536 | -2,285964 | 2,228755 | H35 | 0,845660 | -2,624832 | 2,118836 |
| C36 | 4,404621 | -3,928758 | 2,888826 | C36 | 4,412205 | -4,001835 | 2,692640 |
| H37 | 4,519070 | -4,210503 | 0,762383 | H37 | 4,562518 | -4,118616 | 0,553695 |
| C38 | 3,652706 | -3,432261 | 3,955601 | C38 | 3,617779 | -3,649556 | 3,784303 |
| H39 | 1,808509 | -2,464015 | 4,527096 | H39 | 1,692948 | -2,885840 | 4,403490 |
| H40 | 5,364893 | -4,402755 | 3,070793 | H40 | 5,408485 | -4,405297 | 2,849429 |
| H41 | 4,028208 | -3,514824 | 4,971468 | H41 | 3,995484 | -3,770533 | 4,795471 |
| C42 | -2,833127 | 0,613549 | 0,264873 | C42 | -2,782174 | 0,663567 | 0,374632 |
| C43 | -3,739434 | 1,151767 | 1,185436 | C43 | -3,678867 | 1,242747 | 1,280670 |
| C44 | -2,932165 | 0,965633 | -1,093502 | C44 | -2,844866 | 1,033951 | -0,982416 |
| C45 | -4,723273 | 2,044848 | 0,755652 | C45 | -4,605088 | 2,192258 | 0,842814 |
| H46 | -3,681164 | 0,882844 | 2,234835 | H46 | -3,651992 | 0,963920 | 2,329021 |
| C47 | -3,915922 | 1,855544 | -1,516099 | C47 | -3,771994 | 1,980211 | -1,415246 |
| C48 | -4,810581 | 2,400715 | -0,589921 | C48 | -4,650489 | 2,568971 | -0,500624 |
| H49 | -5,421157 | 2,461786 | 1,476048 | H49 | -5,292730 | 2,638111 | 1,555837 |
| H50 | -3,985367 | 2,127252 | -2,565685 | H50 | -3,805810 | 2,262920 | -2,463592 |
| H51 | -5,575048 | 3,098789 | -0,918751 | H51 | -5,368613 | 3,311869 | -0,834699 |
| H52 | 0,938347 | -0,159584 | 1,456331 | H52 | 1,201376 | -0,519862 | 1,467952 |
| H53 | 2,237083 | 2,572303 | -0,914469 | H53 | 2,235772 | 2,842658 | -0,820397 |
| H54 | -1,742447 | -2,906701 | 2,538588 | H54 | -1,725901 | -2,899988 | 2,647340 |
| H55 | -2,232119 | 0,545014 | -1,811352 | H55 | -2,159470 | 0,583233 | -1,697304 |
| H56 | 2,268557 | -5,060674 | -1,322576 | H56 | 2,053272 | -5,173120 | -1,394721 |
| C57 | 4,568871 | -1,291076 | -3,176957 | C57 | 4,634502 | -1,691483 | -3,416030 |
| C58 | 3,404767 | -1,992444 | -3,500726 | C58 | 3,491573 | -2,436607 | -3,713740 |
| C59 | 2,670007 | -2,620247 | -2,498426 | C59 | 2,705712 | -2,947164 | -2,683056 |
| C60 | 3,079091 | -2,565381 | -1,157038 | C60 | 3,042282 | -2,725863 | -1,340225 |
| C61 | 4,241555 | -1,853755 | -0,842254 | C61 | 4,169474 | -1,947620 | -1,053712 |
| C62 | 4,982539 | -1,223934 | -1,846404 | C62 | 4,964774 | -1,442494 | -2,083470 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H63 | 5,154549 | -0,811033 | -3,956473 | H63 | 5,265520 | -1,314213 | -4,216714 |
| H64 | 3,065233 | -2,051321 | -4,530629 | H64 | 3,211678 | -2,623443 | -4,746369 |
| H65 | 1,754383 | -3,139489 | -2,767786 | H65 | 1,809273 | -3,506118 | -2,938483 |
| H66 | 4,568313 | -1,776593 | 0,188657 | H66 | 4,426158 | -1,727026 | -0,024981 |
| H67 | 5,887109 | -0,682849 | -1,583338 | H67 | 5,845499 | -0,854931 | -1,839697 |
| C68 | -0,941122 | 5,302451 | -2,740422 | C68 | -1,239374 | 4,946582 | -2,928325 |
| C69 | -0,431422 | 4,033568 | -2,472621 | C69 | -0,551899 | 3,791548 | -2,561081 |
| C70 | 0,727766 | 3,879871 | -1,700349 | C70 | 0,578611 | 3,869342 | -1,737125 |
| C71 | 1,364559 | 5,016680 | -1,197934 | C71 | 1,010644 | 5,118463 | -1,287847 |
| C72 | 0,851294 | 6,289036 | -1,459581 | C72 | 0,321163 | 6,276717 | -1,653362 |
| C73 | -0,300712 | 6,436348 | -2,232445 | C73 | -0,804963 | 6,194623 | -2,473050 |
| H74 | -1,839673 | 5,408351 | -3,342105 | H74 | -2,114219 | 4,874586 | -3,568649 |
| H75 | -0,939400 | 3,152935 | -2,860069 | H75 | -0,897795 | 2,821789 | -2,911454 |
| H76 | 2,254152 | 4,906666 | -0,582773 | H76 | 1,878616 | 5,186070 | -0,636870 |
| H77 | 1,352876 | 7,164651 | -1,057594 | H77 | 0,664912 | 7,243025 | -1,295989 |
| H78 | -0,698665 | 7,425733 | -2,437694 | H78 | -1,340163 | 7,095563 | -2,757880 |
| C79 | 1,231840 | 2,485709 | -1,345623 | C79 | 1,274027 | 2,589293 | -1,281250 |
| C80 | 0,279531 | 1,841264 | -0,299986 | C80 | 0,372635 | 1,899074 | -0,228570 |
| C81 | 2,151619 | 2,261051 | -3,712667 | C81 | 2,400094 | 2,320958 | -3,538157 |
| C82 | 0,782285 | 0,546597 | -2,957598 | C82 | 1,014190 | 0,596770 | -2,844703 |
| C83 | 2,014814 | 1,157578 | -4,780137 | C83 | 2,468118 | 1,132737 | -4,513051 |
| H84 | 3,191369 | 2,438017 | -3,419097 | H84 | 3,385466 | 2,620698 | -3,168950 |
| H85 | 1,711908 | 3,213123 | -4,023323 | H85 | 1,902296 | 3,199144 | -3,963897 |
| H86 | 1,646053 | 1,522587 | -5,740083 | H86 | 2,285224 | 1,405084 | -5,553185 |
| H87 | 2,942325 | 0,598696 | -4,927832 | H87 | 3,403706 | 0,573880 | -4,427801 |
| N88 | 1,393658 | 1,692068 | -2,593554 | N88 | 1,591135 | 1,753662 | -2,455804 |
| O89 | 1,034454 | 0,235540 | -4,241015 | O89 | 1,400449 | 0,249112 | -4,082562 |
| O90 | 0,078574 | -0,220276 | -2,272604 | O90 | 0,219975 | -0,126608 | -2,215423 |
| H91 | 1,690070 | -5,312458 | 0,351887 | H91 | 1,447322 | -5,296437 | 0,281753 |
| N92 | -2,080084 | -2,087632 | 0,108145 | N92 | -2,087663 | -2,064249 | 0,206832 |
| C93 | -1,446616 | -2,787698 | -1,033627 | C93 | -1,525662 | -2,638929 | -1,042371 |
| H94 | -1,346212 | -2,138015 | -1,912527 | H94 | -1,450423 | -1,900535 | -1,850148 |
| H96 | -0,716715 | 1,933407 | -0,735762 | H96 | -0,597644 | 1,756589 | -0,693654 |
| C97 | 0,235005 | 4,156271 | 3,364446 | C97 | -0,236548 | 4,407980 | 3,247056 |
| C98 | -0,859212 | 4,173709 | 2,498619 | C98 | -1,216081 | 4,311537 | 2,257278 |
| C99 | -0,829433 | 3,439081 | 1,310489 | C99 | -1,010305 | 3,503095 | 1,138514 |
| C100 | 0,285664 | 2,660352 | 0,968642 | C100 | 0,175897 | 2,770876 | 0,994377 |
| C101 | 1,384234 | 2,665596 | 1,842038 | C101 | 1,155033 | 2,879072 | 1,991695 |
| C102 | 1,363454 | 3,404076 | 3,023469 | C102 | 0,954964 | 3,691472 | 3,106647 |
| H103 | 0,214639 | 4,726860 | 4,288540 | H103 | -0,398089 | 5,034912 | 4,119123 |
| H104 | -1,739287 | 4,762289 | 2,744004 | H104 | -2,146081 | 4,864790 | 2,353170 |
| H105 | -1,684065 | 3,464982 | 0,640713 | H105 | -1,775623 | 3,439963 | 0,371914 |
| H106 | 2,255799 | 2,060338 | 1,605442 | H106 | 2,075091 | 2,302378 | 1,912977 |
| H107 | 2,225188 | 3,385879 | 3,685470 | H107 | 1,724494 | 3,756468 | 3,870542 |
| H108 | 2,247137 | -0,082602 | -0,743504 | H108 | 1,441819 | 1,010523 | 0,528848 |
| H109 | 2,300523 | 0,156327 | 0,049631 | H109 | 2,296573 | -0,250062 | -0,468067 |

C1_E_S_tN_Chelbot

E4

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,387460 | -2,211852 | -0,807837 |
| C2 | -2,560348 | -3,673862 | -1,510030 |
| C3 | -3,781732 | -2,902100 | -2,076284 |
| C4 | -3,428396 | -2,686235 | 0,307894 |
| H5 | -5,407566 | -2,555375 | -0,607275 |
| H6 | -3,493339 | -2,185626 | -2,852141 |
| H7 | -3,790207 | -2,539275 | 1,326188 |
| H8 | -4,408994 | -1,122843 | -0,879941 |
| H9 | -2,163541 | -4,451804 | -2,162495 |
| H10 | -4,489920 | -3,603704 | -2,526086 |
| C11 | -3,091201 | -4,122596 | -0,128994 |
| H12 | -2,335354 | -4,599039 | 0,502410 |
| H13 | -3,969194 | -4,770443 | -0,204618 |
| C14 | -0,115842 | -3,133136 | -0,819463 |
| N15 | 0,855719 | -2,422475 | -0,344808 |
| C16 | 2,088143 | -3,287961 | -0,208621 |
| C17 | 1,496230 | -4,686332 | -0,596486 |
| P18 | -1,463684 | -0,638096 | 0,799795 |
| Ir19 | 0,764257 | -0,393387 | -0,081898 |
| C20 | -1,434252 | -0,882337 | 2,610002 |
| C21 | -1,050883 | -1,224185 | 5,370405 |
| C22 | -1,659851 | -2,128835 | 3,206427 |
| C23 | -1,001241 | 0,192121 | 3,407457 |
| C24 | -0,816415 | 0,020691 | 4,777355 |
| C25 | -1,471666 | -2,295649 | 4,581704 |
| H26 | -0,791768 | 1,158814 | 2,956523 |
| H27 | -0,479380 | 0,858597 | 5,381073 |
| H28 | -1,649047 | -3,267840 | 5,033054 |
| H29 | -0,902197 | -1,357017 | 6,438074 |
| O30 | 0,140693 | -4,417845 | -1,058913 |
| C31 | 2,575370 | -3,374404 | 1,235853 |
| C32 | 1,738916 | -3,034309 | 2,303963 |
| C33 | 3,818086 | -3,961689 | 1,513001 |
| C34 | 2,157313 | -3,219027 | 3,621350 |
| H35 | 0,757704 | -2,618897 | 2,117960 |
| C36 | 4,233500 | -4,153228 | 2,830433 |
| H37 | 4,468741 | -4,266833 | 0,698631 |
| C38 | 3,409275 | -3,771222 | 3,889778 |
| H39 | 1,494281 | -2,928672 | 4,431452 |
| H40 | 5,203891 | -4,600364 | 3,026734 |
| H41 | 3,738409 | -3,913053 | 4,915210 |
| C42 | -2,695400 | 0,694027 | 0,507896 |
| C43 | -3,510995 | 1,248321 | 1,502547 |
| C44 | -2,802919 | 1,173814 | -0,810901 |
| C45 | -4,405507 | 2,274103 | 1,188812 |
| H46 | -3,443706 | 0,891041 | 2,524994 |
| C47 | -3,698230 | 2,196855 | -1,119891 |

ES_Chelbot_SM

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,836737 | -3,471497 | -1,259336 |
| C2 | -1,575812 | -4,394314 | -1,183623 |
| C3 | -2,779710 | -4,212660 | -2,145241 |
| C4 | -3,076036 | -3,299379 | 0,073748 |
| H5 | -4,735065 | -4,078844 | -1,107657 |
| H6 | -2,506930 | -3,647510 | -3,042214 |
| H7 | -3,689116 | -3,013060 | 0,929069 |
| H8 | -4,148384 | -2,510838 | -1,671522 |
| H9 | -0,850984 | -5,148978 | -1,489145 |
| H10 | -3,146271 | -5,189082 | -2,473613 |
| C11 | -2,285763 | -4,615981 | 0,171169 |
| H12 | -1,602327 | -4,654871 | 1,024821 |
| H13 | -2,925090 | -5,503106 | 0,175121 |
| C14 | 0,397301 | -2,993957 | -0,274591 |
| N15 | 0,994784 | -1,926316 | 0,128865 |
| C16 | 2,361894 | -2,307373 | 0,663661 |
| C17 | 2,212405 | -3,860688 | 0,717650 |
| P18 | -1,887688 | -0,707420 | 0,306425 |
| Ir19 | 0,360292 | 0,089759 | -0,263447 |
| C20 | -2,135881 | -0,625658 | 2,115336 |
| C21 | -2,235048 | -0,404548 | 4,909137 |
| C22 | -2,068036 | -1,771869 | 2,918547 |
| C23 | -2,237870 | 0,635968 | 2,725764 |
| C24 | -2,290180 | 0,742376 | 4,113113 |
| C25 | -2,120844 | -1,658999 | 4,309610 |
| H26 | -2,264456 | 1,536426 | 2,124824 |
| H27 | -2,365927 | 1,725373 | 4,568829 |
| H28 | -2,065328 | -2,553441 | 4,923345 |
| H29 | -2,274006 | -0,319762 | 5,991346 |
| O30 | 1,019899 | -4,156116 | -0,068915 |
| C31 | 2,597816 | -1,790388 | 2,078822 |
| C32 | 1,526073 | -1,419158 | 2,897940 |
| C33 | 3,889310 | -1,804741 | 2,623743 |
| C34 | 1,743895 | -1,008563 | 4,212969 |
| H35 | 0,515500 | -1,440064 | 2,513029 |
| C36 | 4,107174 | -1,400935 | 3,940909 |
| H37 | 4,731903 | -2,119531 | 2,015629 |
| C38 | 3,036921 | -0,987775 | 4,735983 |
| H39 | 0,894925 | -0,707890 | 4,820268 |
| H40 | 5,116374 | -1,406836 | 4,342766 |
| H41 | 3,210579 | -0,663028 | 5,757954 |
| C42 | -3,389500 | 0,037719 | -0,447270 |
| C43 | -4,450416 | 0,582424 | 0,285180 |
| C44 | -3,453890 | 0,047937 | -1,852055 |
| C45 | -5,538757 | 1,159076 | -0,374869 |
| H46 | -4,431403 | 0,570788 | 1,369333 |
| C47 | -4,537761 | 0,627590 | -2,507199 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C48 | -4,498141 | 2,755788 | -0,118213 | C48 | -5,580224 | 1,198237 | -1,768330 |
| H49 | -5,029501 | 2,698374 | 1,970489 | H49 | -6,353853 | 1,580232 | 0,206638 |
| H50 | -3,761413 | 2,569191 | -2,137926 | H50 | -4,575811 | 0,622694 | -3,593265 |
| H51 | -5,189586 | 3,558702 | -0,356404 | H51 | -6,425218 | 1,652493 | -2,277076 |
| H52 | 1,334877 | -0,565343 | 1,349212 | H52 | 0,608897 | 0,404722 | 1,229184 |
| H53 | 2,149311 | 3,251278 | -1,021340 | H53 | 1,928447 | 0,164483 | -0,493086 |
| H54 | -1,951088 | -2,978885 | 2,598262 | H54 | -1,945313 | -2,749349 | 2,464864 |
| H55 | -2,173458 | 0,752234 | -1,591435 | H55 | -2,663078 | -0,416282 | -2,432207 |
| H56 | 2,038645 | -5,185579 | -1,399547 | H56 | 3,053669 | -4,399567 | 0,282697 |
| C57 | 4,834472 | -1,733562 | -3,191210 | C57 | 5,053766 | -0,914149 | -2,449808 |
| C58 | 3,691967 | -2,441800 | -3,568945 | C58 | 4,295305 | -2,073232 | -2,626408 |
| C59 | 2,840907 | -2,960146 | -2,595211 | C59 | 3,468129 | -2,530832 | -1,603228 |
| C60 | 3,111117 | -2,781081 | -1,232241 | C60 | 3,386346 | -1,846427 | -0,382129 |
| C61 | 4,239823 | -2,039708 | -0,864913 | C61 | 4,145640 | -0,679903 | -0,219943 |
| C62 | 5,100784 | -1,529550 | -1,836827 | C62 | 4,974457 | -0,219299 | -1,244106 |
| H63 | 5,514478 | -1,348777 | -3,946903 | H63 | 5,699427 | -0,556992 | -3,247079 |
| H64 | 3,463428 | -2,594027 | -4,619719 | H64 | 4,344835 | -2,619914 | -3,563588 |
| H65 | 1,944476 | -3,487728 | -2,911461 | H65 | 2,867147 | -3,419729 | -1,776360 |
| H66 | 4,442397 | -1,845599 | 0,181491 | H66 | 4,088834 | -0,114113 | 0,700613 |
| H67 | 5,980021 | -0,969166 | -1,531299 | H67 | 5,551694 | 0,688682 | -1,093785 |
| C68 | -1,619221 | 4,680817 | -3,163111 | C68 | -1,304366 | 4,199888 | 2,244393 |
| C69 | -0,772133 | 3,659344 | -2,735448 | C69 | -0,506681 | 3,450245 | 1,382024 |
| C70 | 0,327739 | 3,948895 | -1,918474 | C70 | -1,034630 | 2,920125 | 0,190256 |
| C71 | 0,564092 | 5,270574 | -1,531943 | C71 | -2,392371 | 3,156656 | -0,086778 |
| C72 | -0,288416 | 6,292483 | -1,953748 | C72 | -3,189872 | 3,900135 | 0,783879 |
| C73 | -1,381457 | 6,000909 | -2,770938 | C73 | -2,651271 | 4,432892 | 1,954603 |
| H74 | -2,465959 | 4,447639 | -3,802926 | H74 | -0,865607 | 4,601276 | 3,153717 |
| H75 | -0,972236 | 2,632587 | -3,030194 | H75 | 0,522738 | 3,272204 | 1,651035 |
| H76 | 1,407548 | 5,500227 | -0,885605 | H76 | -2,844845 | 2,726444 | -0,972318 |
| H77 | -0,096951 | 7,315657 | -1,643653 | H77 | -4,238464 | 4,049667 | 0,543237 |
| H78 | -2,042679 | 6,796158 | -3,102243 | H78 | -3,268447 | 5,017175 | 2,630616 |
| C79 | 1,213216 | 2,823567 | -1,397356 | C79 | -0,212417 | 2,109027 | -0,765035 |
| C80 | 0,505030 | 2,121767 | -0,211166 | C80 | 1,236053 | 1,998019 | -0,778653 |
| C81 | 2,505019 | 2,394979 | -3,524387 | C81 | -0,935934 | 3,245910 | -2,968553 |
| C82 | 1,012506 | 0,747479 | -2,861258 | C82 | -0,604715 | 0,968105 | -2,897709 |
| C83 | 2,672634 | 1,127555 | -4,376003 | C83 | -1,484582 | 2,573157 | -4,233728 |
| H84 | 3,449881 | 2,743866 | -3,097502 | H84 | 0,035666 | 3,732796 | -3,131542 |
| H85 | 2,035246 | 3,223588 | -4,068778 | H85 | -1,626170 | 3,968899 | -2,532463 |
| H86 | 2,639344 | 1,308128 | -5,450906 | H86 | -2,576900 | 2,505584 | -4,216071 |
| H87 | 3,572152 | 0,564111 | -4,113036 | H87 | -1,148363 | 3,022190 | -5,168140 |
| N88 | 1,608002 | 1,904113 | -2,475788 | N88 | -0,777338 | 2,062452 | -2,113428 |
| O89 | 1,530593 | 0,306335 | -4,018970 | O89 | -0,953693 | 1,217123 | -4,168339 |
| O90 | 0,105644 | 0,116493 | -2,294220 | O90 | -0,188645 | -0,141709 | -2,532029 |
| H91 | 1,418863 | -5,346297 | 0,268038 | H91 | 2,025618 | -4,212674 | 1,733630 |
| N92 | -2,097414 | -2,050395 | 0,126010 | N92 | -1,955636 | -2,335852 | -0,120541 |
| C93 | -1,503158 | -2,612989 | -1,115709 | C93 | -0,939826 | -2,999620 | -0,973852 |
| H94 | -1,388952 | -1,858094 | -1,903955 | H94 | -0,797152 | -2,470932 | -1,924990 |
| H96 | -0,467384 | 1,790031 | -0,549387 | H96 | 1,632593 | 1,919787 | -1,792671 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|----------|----------|-----------|
| C97 | 0,042285 | 4,614948 | 3,271978 | C97 | 4,106730 | 4,162268 | 1,598419 |
| C98 | -1,019338 | 4,449636 | 2,380960 | C98 | 3,600068 | 4,678341 | 0,404511 |
| C99 | -0,869644 | 3,643445 | 1,252427 | C99 | 2,670158 | 3,947225 | -0,332235 |
| C100 | 0,346525 | 2,995341 | 1,008341 | C100 | 2,223482 | 2,693929 | 0,112234 |
| C101 | 1,407988 | 3,162052 | 1,906104 | C101 | 2,742664 | 2,181849 | 1,308224 |
| C102 | 1,258170 | 3,969559 | 3,032783 | C102 | 3,675540 | 2,912540 | 2,044777 |
| H103 | -0,077135 | 5,240585 | 4,152132 | H103 | 4,833841 | 4,729271 | 2,172496 |
| H104 | -1,968753 | 4,944422 | 2,564869 | H104 | 3,929354 | 5,649145 | 0,044810 |
| H105 | -1,697485 | 3,515661 | 0,562448 | H105 | 2,279596 | 4,355741 | -1,261870 |
| H106 | 2,347995 | 2,641552 | 1,733005 | H106 | 2,412168 | 1,214930 | 1,667817 |
| H107 | 2,085266 | 4,089246 | 3,726858 | H107 | 4,065613 | 2,496102 | 2,969302 |
| H108 | 1,259546 | 1,308447 | 0,135352 | | | | |
| H109 | 2,294829 | -0,311753 | -0,568377 | | | | |

C1_ES_Chelbot_TS1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,890112 | -3,534552 | -1,110363 |
| C2 | -1,631229 | -4,463929 | -1,079330 |
| C3 | -2,860492 | -4,296359 | -2,010860 |
| C4 | -3,098485 | -3,354119 | 0,203868 |
| H5 | -4,791446 | -4,130297 | -0,932523 |
| H6 | -2,611115 | -3,749735 | -2,925971 |
| H7 | -3,692147 | -3,060030 | 1,070139 |
| H8 | -4,200129 | -2,574781 | -1,526957 |
| H9 | -0,912709 | -5,220574 | -1,394775 |
| H10 | -3,239313 | -5,277707 | -2,309765 |
| C11 | -2,305924 | -4,670014 | 0,295949 |
| H12 | -1,601790 | -4,695968 | 1,133361 |
| H13 | -2,943691 | -5,557847 | 0,326556 |
| C14 | 0,375664 | -3,038611 | -0,272659 |
| N15 | 0,964758 | -1,964872 | 0,122388 |
| C16 | 2,361157 | -2,312735 | 0,580526 |
| C17 | 2,287653 | -3,875147 | 0,555195 |
| P18 | -1,910208 | -0,754765 | 0,349199 |
| Ir19 | 0,258869 | 0,046517 | -0,229981 |
| C20 | -2,166115 | -0,608508 | 2,153143 |
| C21 | -2,285923 | -0,278419 | 4,932011 |
| C22 | -2,091489 | -1,722022 | 2,998906 |
| C23 | -2,282990 | 0,676374 | 2,709582 |
| C24 | -2,345880 | 0,836609 | 4,091358 |
| C25 | -2,155165 | -1,554879 | 4,384161 |
| H26 | -2,311218 | 1,552412 | 2,071727 |
| H27 | -2,433659 | 1,835787 | 4,508617 |
| H28 | -2,096141 | -2,423513 | 5,033743 |
| H29 | -2,334347 | -0,151092 | 6,009859 |
| O30 | 1,043765 | -4,187098 | -0,141976 |
| C31 | 2,620273 | -1,843382 | 2,009016 |
| C32 | 1,561546 | -1,505858 | 2,859452 |
| C33 | 3,923944 | -1,845388 | 2,524295 |

C1_ES_Chelbot_INT1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,922167 | -3,535557 | -0,845760 |
| C2 | -1,682248 | -4,505975 | -0,875384 |
| C3 | -2,953609 | -4,365892 | -1,753156 |
| C4 | -3,070026 | -3,317475 | 0,424945 |
| H5 | -4,830153 | -4,096773 | -0,602200 |
| H6 | -2,742784 | -3,875484 | -2,708887 |
| H7 | -3,621589 | -2,980046 | 1,302946 |
| H8 | -4,225582 | -2,587775 | -1,293789 |
| H9 | -0,986636 | -5,283712 | -1,190540 |
| H10 | -3,364253 | -5,354445 | -1,977010 |
| C11 | -2,293896 | -4,641574 | 0,537149 |
| H12 | -1,553521 | -4,641675 | 1,343164 |
| H13 | -2,942847 | -5,516412 | 0,634798 |
| C14 | 0,392823 | -3,057206 | -0,284548 |
| N15 | 0,973673 | -1,977302 | 0,101590 |
| C16 | 2,391639 | -2,285109 | 0,467499 |
| C17 | 2,451027 | -3,830399 | 0,178239 |
| P18 | -1,853245 | -0,733679 | 0,405834 |
| Ir19 | 0,162355 | 0,023971 | -0,226352 |
| C20 | -2,106193 | -0,495120 | 2,195510 |
| C21 | -2,224971 | -0,020267 | 4,948810 |
| C22 | -1,997456 | -1,560878 | 3,096608 |
| C23 | -2,252957 | 0,815868 | 2,679828 |
| C24 | -2,315188 | 1,047145 | 4,050899 |
| C25 | -2,063542 | -1,321142 | 4,470965 |
| H26 | -2,299480 | 1,654485 | 1,993543 |
| H27 | -2,425078 | 2,064209 | 4,415679 |
| H28 | -1,981091 | -2,151921 | 5,165988 |
| H29 | -2,273650 | 0,163365 | 6,018355 |
| O30 | 1,112447 | -4,180872 | -0,282738 |
| C31 | 2,653678 | -2,025228 | 1,948413 |
| C32 | 1,642403 | -1,613607 | 2,820671 |
| C33 | 3,933065 | -2,277612 | 2,466512 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C34 | 1,802708 | -1,114500 | 4,176428 | C34 | 1,912668 | -1,417012 | 4,176514 |
| H35 | 0,543045 | -1,534022 | 2,496000 | H35 | 0,641530 | -1,442598 | 2,449502 |
| C36 | 4,165740 | -1,459895 | 3,842702 | C36 | 4,202199 | -2,084241 | 3,819623 |
| H37 | 4,758040 | -2,132333 | 1,890729 | H37 | 4,726595 | -2,614502 | 1,803764 |
| C38 | 3,107118 | -1,078671 | 4,669629 | C38 | 3,192788 | -1,643410 | 4,678766 |
| H39 | 0,963357 | -0,837997 | 4,808594 | H39 | 1,110925 | -1,089531 | 4,832750 |
| H40 | 5,184133 | -1,453199 | 4,220924 | H40 | 5,200432 | -2,276392 | 4,202194 |
| H41 | 3,299200 | -0,767310 | 5,692646 | H41 | 3,404345 | -1,488175 | 5,732729 |
| C42 | -3,390656 | -0,008389 | -0,442763 | C42 | -3,313379 | -0,014336 | -0,432881 |
| C43 | -4,477904 | 0,520503 | 0,262061 | C43 | -4,424227 | 0,501728 | 0,245164 |
| C44 | -3,415408 | 0,004708 | -1,848767 | C44 | -3,327834 | -0,065129 | -1,838067 |
| C45 | -5,557299 | 1,080916 | -0,426530 | C45 | -5,521627 | 0,983296 | -0,472164 |
| H46 | -4,487374 | 0,507958 | 1,346507 | H46 | -4,441957 | 0,533224 | 1,328818 |
| C47 | -4,490757 | 0,567569 | -2,532213 | C47 | -4,422684 | 0,418417 | -2,548940 |
| C48 | -5,562904 | 1,118700 | -1,821105 | C48 | -5,520833 | 0,951413 | -1,865920 |
| H49 | -6,394213 | 1,489442 | 0,132900 | H49 | -6,378083 | 1,382686 | 0,063519 |
| H50 | -4,498692 | 0,566789 | -3,618943 | H50 | -4,425781 | 0,369922 | -3,634506 |
| H51 | -6,401826 | 1,559208 | -2,351904 | H51 | -6,375877 | 1,328324 | -2,419691 |
| H52 | 0,457604 | 0,364248 | 1,272720 | H52 | 0,358663 | 0,395830 | 1,270501 |
| H53 | 1,838351 | 0,335246 | -0,465687 | H53 | 1,871495 | 0,851245 | -0,692610 |
| H54 | -1,956438 | -2,714707 | 2,583102 | H54 | -1,834992 | -2,569632 | 2,732095 |
| H55 | -2,598603 | -0,440567 | -2,407009 | H55 | -2,488276 | -0,498212 | -2,371281 |
| H56 | 3,109171 | -4,345687 | 0,014995 | H56 | 3,155528 | -4,097031 | -0,611527 |
| C57 | 4,816541 | -0,608844 | -2,574212 | C57 | 4,704679 | 0,044809 | -2,381224 |
| C58 | 4,066745 | -1,766983 | -2,793793 | C58 | 3,824536 | -0,953112 | -2,809206 |
| C59 | 3,323707 | -2,326082 | -1,757026 | C59 | 3,120652 | -1,706632 | -1,874740 |
| C60 | 3,317342 | -1,747101 | -0,479742 | C60 | 3,283051 | -1,485582 | -0,496839 |
| C61 | 4,069059 | -0,583788 | -0,272697 | C61 | 4,162720 | -0,481686 | -0,080571 |
| C62 | 4,814453 | -0,020288 | -1,310833 | C62 | 4,868908 | 0,277489 | -1,017569 |
| H63 | 5,395670 | -0,171067 | -3,382532 | H63 | 5,255310 | 0,635584 | -3,107678 |
| H64 | 4,056111 | -2,231644 | -3,775444 | H64 | 3,681512 | -1,139944 | -3,869559 |
| H65 | 2,723676 | -3,209141 | -1,961149 | H65 | 2,414839 | -2,454559 | -2,226424 |
| H66 | 4,069425 | -0,096633 | 0,693143 | H66 | 4,291531 | -0,269082 | 0,972870 |
| H67 | 5,384835 | 0,885651 | -1,124589 | H67 | 5,537115 | 1,060542 | -0,671961 |
| C68 | -1,312077 | 4,269219 | 2,125774 | C68 | -1,293136 | 4,392223 | 1,919171 |
| C69 | -0,481794 | 3,501711 | 1,310432 | C69 | -0,432849 | 3,588225 | 1,170940 |
| C70 | -0,972984 | 2,923672 | 0,126520 | C70 | -0,869760 | 2,960597 | -0,006787 |
| C71 | -2,326072 | 3,134474 | -0,194809 | C71 | -2,211631 | 3,160841 | -0,386631 |
| C72 | -3,154931 | 3,896090 | 0,627310 | C72 | -3,072504 | 3,957567 | 0,367018 |
| C73 | -2,652283 | 4,473680 | 1,792664 | C73 | -2,618370 | 4,586561 | 1,527293 |
| H74 | -0,903382 | 4,708587 | 3,031712 | H74 | -0,917234 | 4,866891 | 2,821494 |
| H75 | 0,542235 | 3,349637 | 1,612343 | H75 | 0,574745 | 3,443768 | 1,527002 |
| H76 | -2,747985 | 2,667276 | -1,076987 | H76 | -2,602182 | 2,651659 | -1,260435 |
| H77 | -4,198644 | 4,025099 | 0,355404 | H77 | -4,104223 | 4,073485 | 0,046179 |
| H78 | -3,294276 | 5,071701 | 2,433071 | H78 | -3,283940 | 5,212161 | 2,114844 |
| C79 | -0,141191 | 2,059050 | -0,773661 | C79 | -0,035033 | 2,001046 | -0,815950 |
| C80 | 1,325181 | 1,901088 | -0,730143 | C80 | 1,528273 | 1,952514 | -0,804268 |
| C81 | -0,738153 | 3,220427 | -3,014941 | C81 | -0,493325 | 3,152482 | -3,120438 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C82 | -0,506030 | 0,928816 | -2,912554 | C82 | -0,366617 | 0,858869 | -2,949818 |
| C83 | -1,264999 | 2,554987 | -4,294921 | C83 | -0,967209 | 2,474263 | -4,416301 |
| H84 | 0,249749 | 3,682628 | -3,149341 | H84 | 0,511373 | 3,588726 | -3,211370 |
| H85 | -1,424039 | 3,962468 | -2,603526 | H85 | -1,180186 | 3,920758 | -2,762166 |
| H86 | -2,359110 | 2,534707 | -4,321333 | H86 | -2,056776 | 2,502854 | -4,517208 |
| H87 | -0,874589 | 2,979665 | -5,219596 | H87 | -0,498017 | 2,854180 | -5,323827 |
| N88 | -0,639548 | 2,040288 | -2,149315 | N88 | -0,472891 | 1,992406 | -2,224088 |
| O89 | -0,796713 | 1,177204 | -4,197871 | O89 | -0,573248 | 1,078384 | -4,255755 |
| O90 | -0,166263 | -0,196571 | -2,512724 | O90 | -0,111426 | -0,273208 | -2,497675 |
| H91 | 2,211398 | -4,293652 | 1,559984 | H91 | 2,653979 | -4,414920 | 1,075975 |
| N92 | -1,979476 | -2,397273 | -0,019156 | N92 | -1,941224 | -2,393571 | 0,121692 |
| C93 | -0,994454 | -3,064104 | -0,905874 | C93 | -1,024587 | -3,105439 | -0,800368 |
| H94 | -0,894851 | -2,547034 | -1,869506 | H94 | -0,992803 | -2,635734 | -1,793755 |
| H96 | 1,754188 | 1,850258 | -1,733389 | H96 | 1,890278 | 2,146172 | -1,819924 |
| C97 | 4,039952 | 4,049582 | 1,832525 | C97 | 3,962379 | 4,173220 | 1,975169 |
| C98 | 3,634125 | 4,563725 | 0,599762 | C98 | 3,602111 | 4,725439 | 0,744703 |
| C99 | 2,760803 | 3,835634 | -0,206261 | C99 | 2,815826 | 3,994281 | -0,145069 |
| C100 | 2,271669 | 2,589590 | 0,210919 | C100 | 2,375330 | 2,708806 | 0,187351 |
| C101 | 2,690171 | 2,076926 | 1,444958 | C101 | 2,746334 | 2,156933 | 1,419282 |
| C102 | 3,568065 | 2,804094 | 2,248849 | C102 | 3,533377 | 2,886670 | 2,309082 |
| H103 | 4,721350 | 4,615800 | 2,460738 | H103 | 4,577018 | 4,741068 | 2,667633 |
| H104 | 3,996747 | 5,531341 | 0,264487 | H104 | 3,934321 | 5,724264 | 0,476356 |
| H105 | 2,444894 | 4,242523 | -1,164574 | H105 | 2,536109 | 4,428420 | -1,102477 |
| H106 | 2,321234 | 1,115366 | 1,782109 | H106 | 2,409950 | 1,159499 | 1,684405 |
| H107 | 3,881413 | 2,389230 | 3,202543 | H107 | 3,813598 | 2,446717 | 3,262111 |

C1_ES_Chelbot_TS2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,650305 | -3,586452 | -1,241988 |
| C2 | -1,338706 | -4,369441 | -1,173943 |
| C3 | -2,561092 | -4,280839 | -2,125448 |
| C4 | -2,881591 | -3,320390 | 0,069718 |
| H5 | -4,498515 | -4,251430 | -1,048284 |
| H6 | -2,331831 | -3,717474 | -3,035668 |
| H7 | -3,499735 | -3,042241 | 0,923327 |
| H8 | -4,042814 | -2,667627 | -1,677501 |
| H9 | -0,576787 | -5,090752 | -1,467999 |
| H10 | -2,872577 | -5,283084 | -2,431975 |
| C11 | -2,018488 | -4,588765 | 0,194891 |
| H12 | -1,321679 | -4,571294 | 1,038206 |
| H13 | -2,612162 | -5,506219 | 0,234050 |
| C14 | 0,563521 | -2,848393 | -0,317652 |
| N15 | 1,066515 | -1,758079 | 0,145894 |
| C16 | 2,426403 | -2,073775 | 0,726181 |
| C17 | 2,525042 | -3,620846 | 0,452218 |
| P18 | -1,822959 | -0,694314 | 0,327291 |
| Ir19 | 0,140518 | 0,230819 | -0,282948 |
| C20 | -2,047449 | -0,716779 | 2,138345 |
| C21 | -2,265128 | -0,681916 | 4,931522 |

C1_ES_Chelbot_INT2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,667825 | -3,630981 | -1,228670 |
| C2 | -1,348608 | -4,386477 | -1,123571 |
| C3 | -2,561129 | -4,325891 | -2,089436 |
| C4 | -2,915992 | -3,337030 | 0,087052 |
| H5 | -4,510983 | -4,302555 | -1,035418 |
| H6 | -2,327993 | -3,774555 | -3,005954 |
| H7 | -3,547028 | -3,054098 | 0,929832 |
| H8 | -4,064352 | -2,722299 | -1,681437 |
| H9 | -0,576528 | -5,104267 | -1,399279 |
| H10 | -2,857415 | -5,336666 | -2,383267 |
| C11 | -2,041194 | -4,594271 | 0,240845 |
| H12 | -1,354692 | -4,556401 | 1,092076 |
| H13 | -2,623771 | -5,518616 | 0,285708 |
| C14 | 0,541263 | -2,842588 | -0,285806 |
| N15 | 1,050429 | -1,751769 | 0,170334 |
| C16 | 2,411576 | -2,050986 | 0,735784 |
| C17 | 2,521310 | -3,597967 | 0,457111 |
| P18 | -1,893270 | -0,690939 | 0,318551 |
| Ir19 | 0,193972 | 0,247753 | -0,286031 |
| C20 | -2,101447 | -0,686860 | 2,136290 |
| C21 | -2,305027 | -0,609038 | 4,931207 |

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|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C22 | -1,900591 | -1,901155 | 2,873567 | C22 | -1,967284 | -1,861006 | 2,888711 |
| C23 | -2,283428 | 0,488321 | 2,816920 | C23 | -2,313545 | 0,532084 | 2,798446 |
| C24 | -2,393678 | 0,503574 | 4,204604 | C24 | -2,416844 | 0,567976 | 4,186990 |
| C25 | -2,016462 | -1,881495 | 4,263482 | C25 | -2,074431 | -1,820493 | 4,279495 |
| H26 | -2,376489 | 1,415156 | 2,268935 | H26 | -2,391479 | 1,454238 | 2,238376 |
| H27 | -2,574237 | 1,445204 | 4,714993 | H27 | -2,580896 | 1,519488 | 4,684602 |
| H28 | -1,895201 | -2,803562 | 4,824371 | H28 | -1,964736 | -2,736621 | 4,852600 |
| H29 | -2,351672 | -0,670895 | 6,014354 | H29 | -2,388260 | -0,580602 | 6,013990 |
| O30 | 1,274375 | -3,969402 | -0,201321 | O30 | 1,264423 | -3,957179 | -0,179555 |
| C31 | 2,484549 | -1,818452 | 2,231097 | C31 | 2,484058 | -1,804271 | 2,241722 |
| C32 | 1,434164 | -1,267911 | 2,962645 | C32 | 1,429094 | -1,258855 | 2,972583 |
| C33 | 3,642894 | -2,220551 | 2,917874 | C33 | 3,641077 | -2,209107 | 2,927661 |
| C34 | 1,541047 | -1,102907 | 4,346600 | C34 | 1,532206 | -1,096807 | 4,356498 |
| H35 | 0,529187 | -0,965066 | 2,462850 | H35 | 0,519619 | -0,965553 | 2,473032 |
| C36 | 3,753482 | -2,052980 | 4,294891 | C36 | 3,745402 | -2,048587 | 4,306629 |
| H37 | 4,473781 | -2,654762 | 2,367637 | H37 | 4,472162 | -2,644142 | 2,377984 |
| C38 | 2,699365 | -1,488051 | 5,016939 | C38 | 2,689383 | -1,485091 | 5,027158 |
| H39 | 0,705529 | -0,673753 | 4,890985 | H39 | 0,693320 | -0,673756 | 4,900751 |
| H40 | 4,660942 | -2,365142 | 4,803848 | H40 | 4,650409 | -2,364096 | 4,817885 |
| H41 | 2,782321 | -1,357183 | 6,092093 | H41 | 2,770053 | -1,358941 | 6,103013 |
| C42 | -3,404295 | -0,073061 | -0,366221 | C42 | -3,494091 | -0,088258 | -0,358760 |
| C43 | -4,459636 | 0,406910 | 0,419526 | C43 | -4,543050 | 0,398174 | 0,430846 |
| C44 | -3,577133 | -0,170765 | -1,757214 | C44 | -3,682519 | -0,188532 | -1,748070 |
| C45 | -5,652237 | 0,815585 | -0,179074 | C45 | -5,740956 | 0,808633 | -0,158935 |
| H46 | -4,367942 | 0,458161 | 1,497162 | H46 | -4,438416 | 0,462273 | 1,507323 |
| C47 | -4,767950 | 0,238507 | -2,350571 | C47 | -4,877671 | 0,223313 | -2,333728 |
| C48 | -5,805962 | 0,745849 | -1,562382 | C48 | -5,909991 | 0,735923 | -1,540774 |
| H49 | -6,461904 | 1,185751 | 0,443037 | H49 | -6,543170 | 1,183473 | 0,470236 |
| H50 | -4,895209 | 0,141859 | -3,425338 | H50 | -5,012023 | 0,123501 | -3,407515 |
| H51 | -6,735729 | 1,064533 | -2,024556 | H51 | -6,842909 | 1,054844 | -1,995864 |
| H52 | 0,426716 | 0,674167 | 1,182408 | H52 | 0,365066 | 0,684781 | 1,203127 |
| H53 | 1,213594 | 2,719704 | -2,168545 | H53 | 1,258609 | 2,637417 | -2,208456 |
| H54 | -1,667540 | -2,831993 | 2,371920 | H54 | -1,750809 | -2,802608 | 2,399629 |
| H55 | -2,798473 | -0,608262 | -2,372083 | H55 | -2,908530 | -0,622366 | -2,371948 |
| H56 | 3,338924 | -3,887404 | -0,223646 | H56 | 3,328707 | -3,857095 | -0,229944 |
| C57 | 5,405154 | -0,025842 | -1,682206 | C57 | 5,315983 | 0,083749 | -1,708907 |
| C58 | 4,498827 | -0,919771 | -2,259289 | C58 | 4,382249 | -0,784697 | -2,283656 |
| C59 | 3,553345 | -1,560772 | -1,463797 | C59 | 3,473548 | -1,464851 | -1,476530 |
| C60 | 3,490666 | -1,322050 | -0,081959 | C60 | 3,461690 | -1,281469 | -0,083770 |
| C61 | 4,385196 | -0,408945 | 0,481979 | C61 | 4,380934 | -0,392404 | 0,479157 |
| C62 | 5,345118 | 0,224225 | -0,312992 | C62 | 5,314018 | 0,267262 | -0,327779 |
| H63 | 6,153177 | 0,467092 | -2,296485 | H63 | 6,036680 | 0,604917 | -2,331797 |
| H64 | 4,531409 | -1,118643 | -3,326671 | H64 | 4,367594 | -0,938371 | -3,358858 |
| H65 | 2,852872 | -2,249858 | -1,929367 | H65 | 2,753244 | -2,133499 | -1,941444 |
| H66 | 4,341616 | -0,185095 | 1,541302 | H66 | 4,380101 | -0,209390 | 1,547170 |
| H67 | 6,039158 | 0,922821 | 0,145341 | H67 | 6,039592 | 0,931012 | 0,132966 |
| C68 | -1,708231 | 3,874909 | 2,305937 | C68 | -1,604444 | 3,941757 | 2,271165 |
| C69 | -0,916093 | 3,206987 | 1,376789 | C69 | -0,817438 | 3,281424 | 1,331314 |

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|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C70 | -1,407634 | 2,855384 | 0,105601 | C70 | -1,340844 | 2,870040 | 0,089846 |
| C71 | -2,758770 | 3,122226 | -0,156161 | C71 | -2,709334 | 3,084892 | -0,130233 |
| C72 | -3,566779 | 3,765842 | 0,786400 | C72 | -3,508037 | 3,726256 | 0,822209 |
| C73 | -3,043264 | 4,168415 | 2,012511 | C73 | -2,960138 | 4,177228 | 2,021382 |
| H74 | -1,288139 | 4,140072 | 3,272666 | H74 | -1,158960 | 4,253618 | 3,212055 |
| H75 | 0,092987 | 2,923977 | 1,646266 | H75 | 0,214053 | 3,059932 | 1,571001 |
| H76 | -3,213191 | 2,784044 | -1,079480 | H76 | -3,181840 | 2,707015 | -1,028248 |
| H77 | -4,612733 | 3,944449 | 0,553383 | H77 | -4,566872 | 3,860000 | 0,619564 |
| H78 | -3,667794 | 4,681722 | 2,737979 | H78 | -3,577690 | 4,685303 | 2,756068 |
| C79 | -0,465556 | 2,198501 | -0,888494 | C79 | -0,423112 | 2,200669 | -0,920572 |
| C80 | 0,718068 | 3,195837 | -1,316237 | C80 | 0,763888 | 3,153339 | -1,375943 |
| C81 | -1,611294 | 3,016398 | -3,162003 | C81 | -1,611731 | 2,969333 | -3,176808 |
| C82 | -0,904734 | 0,853407 | -2,900058 | C82 | -0,947598 | 0,798387 | -2,876817 |
| C83 | -2,174247 | 2,123654 | -4,271265 | C83 | -2,228857 | 2,060141 | -4,243783 |
| H84 | -0,773607 | 3,624654 | -3,518881 | H84 | -0,771596 | 3,548628 | -3,574463 |
| H85 | -2,356904 | 3,674051 | -2,717172 | H85 | -2,329147 | 3,653815 | -2,725338 |
| H86 | -3,228900 | 1,882907 | -4,108992 | H86 | -3,282548 | 1,847043 | -4,041971 |
| H87 | -2,024690 | 2,511207 | -5,278865 | H87 | -2,101622 | 2,415230 | -5,266264 |
| N88 | -1,148301 | 1,983514 | -2,210043 | N88 | -1,143672 | 1,951993 | -2,212696 |
| O89 | -1,409715 | 0,889720 | -4,142304 | O89 | -1,488899 | 0,811922 | -4,103280 |
| O90 | -0,303024 | -0,157367 | -2,481060 | O90 | -0,362764 | -0,217232 | -2,446833 |
| H91 | 2,591048 | -4,205527 | 1,370044 | H91 | 2,605140 | -4,182761 | 1,373263 |
| N92 | -1,816098 | -2,298649 | -0,178865 | N92 | -1,862538 | -2,305979 | -0,162793 |
| C93 | -0,772948 | -2,937490 | -1,009045 | C93 | -0,800090 | -2,945069 | -0,972224 |
| H94 | -0,662468 | -2,435359 | -1,977645 | H94 | -0,687492 | -2,456342 | -1,947006 |
| H95 | 0,190929 | 4,070891 | -1,718362 | H95 | 0,289901 | 4,045841 | -1,802597 |
| C96 | 3,883141 | 4,849470 | 1,165850 | C96 | 3,813558 | 4,653363 | 1,312632 |
| C97 | 2,557910 | 5,228119 | 1,385219 | C97 | 2,584626 | 5,306426 | 1,201113 |
| C98 | 1,532960 | 4,702389 | 0,599380 | C98 | 1,608592 | 4,816989 | 0,336351 |
| C99 | 1,799578 | 3,768518 | -0,414107 | C99 | 1,825743 | 3,655514 | -0,421688 |
| C100 | 3,143746 | 3,445489 | -0,656257 | C100 | 3,083396 | 3,042333 | -0,337913 |
| C101 | 4,173660 | 3,968888 | 0,125231 | C101 | 4,063169 | 3,527855 | 0,529803 |
| H102 | 4,680124 | 5,258241 | 1,780604 | H102 | 4,577037 | 5,033683 | 1,985255 |
| H103 | 2,318096 | 5,944828 | 2,166170 | H103 | 2,389201 | 6,203623 | 1,781790 |
| H104 | 0,519347 | 5,049690 | 0,759873 | H104 | 0,658570 | 5,336595 | 0,251996 |
| H105 | 3,386092 | 2,823360 | -1,513493 | H105 | 3,327115 | 2,199766 | -0,978698 |
| H106 | 5,203097 | 3,696802 | -0,092055 | H106 | 5,028947 | 3,034393 | 0,576921 |
| H107 | 2,819279 | 1,196713 | -0,936483 | H107 | 1,766102 | 0,905772 | -0,108723 |
| H108 | 2,611383 | 0,899730 | -1,585830 | H108 | 1,749935 | 0,617851 | -0,922717 |

C1_ES_Chelbot_TS3

| | | | |
|----|-----------|-----------|-----------|
| C1 | -3,687428 | -3,668740 | -1,267620 |
| C2 | -1,367048 | -4,416472 | -1,152490 |
| C3 | -2,569987 | -4,344974 | -2,129406 |
| C4 | -2,953396 | -3,403422 | 0,065073 |
| H5 | -4,533364 | -4,344078 | -1,101193 |
| H6 | -2,330437 | -3,778407 | -3,034973 |
| H7 | -3,599036 | -3,143257 | 0,903864 |

C1_ES_Chelbot_PROD

| | | | |
|----|-----------|-----------|-----------|
| C1 | -3,668498 | -3,640196 | -1,327243 |
| C2 | -1,348884 | -4,392078 | -1,239709 |
| C3 | -2,547434 | -4,272620 | -2,216826 |
| C4 | -2,943162 | -3,449399 | 0,023486 |
| H5 | -4,518301 | -4,319846 | -1,204179 |
| H6 | -2,304050 | -3,661673 | -3,092115 |
| H7 | -3,598002 | -3,236830 | 0,868555 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H8 | -4,077587 | -2,749719 | -1,705134 | H8 | -4,051825 | -2,697125 | -1,717171 |
| H9 | -0,586433 | -5,122722 | -1,434761 | H9 | -0,565011 | -5,080350 | -1,555409 |
| H10 | -2,859116 | -5,352324 | -2,441811 | H10 | -2,834646 | -5,263213 | -2,580285 |
| C11 | -2,073377 | -4,659283 | 0,199984 | C11 | -2,060452 | -4,708192 | 0,096121 |
| H12 | -1,396594 | -4,634450 | 1,059333 | H12 | -1,389326 | -4,721618 | 0,960119 |
| H13 | -2,649001 | -5,589064 | 0,216555 | H13 | -2,630677 | -5,640763 | 0,059782 |
| C14 | 0,498407 | -2,865991 | -0,269807 | C14 | 0,512630 | -2,884525 | -0,283919 |
| N15 | 1,021788 | -1,763271 | 0,148763 | N15 | 1,065293 | -1,796807 | 0,148525 |
| C16 | 2,375599 | -2,056324 | 0,751744 | C16 | 2,412885 | -2,121786 | 0,764372 |
| C17 | 2,430662 | -3,620133 | 0,598191 | C17 | 2,411346 | -3,684804 | 0,620562 |
| P18 | -1,909134 | -0,750646 | 0,359581 | P18 | -1,891068 | -0,791254 | 0,407180 |
| Ir19 | 0,289021 | 0,185794 | -0,314224 | Ir19 | 0,317679 | 0,056497 | -0,228298 |
| C20 | -2,145908 | -0,768079 | 2,174071 | C20 | -2,134319 | -0,806354 | 2,220584 |
| C21 | -2,409055 | -0,684076 | 4,965811 | C21 | -2,389691 | -0,676820 | 5,010409 |
| C22 | -2,106517 | -1,950425 | 2,925569 | C22 | -2,230674 | -1,981153 | 2,976998 |
| C23 | -2,285759 | 0,459932 | 2,838697 | C23 | -2,135527 | 0,434892 | 2,878007 |
| C24 | -2,421918 | 0,499979 | 4,224633 | C24 | -2,269939 | 0,498120 | 4,262803 |
| C25 | -2,241255 | -1,906163 | 4,313784 | C25 | -2,359925 | -1,913828 | 4,365875 |
| H26 | -2,284737 | 1,386587 | 2,279902 | H26 | -2,023537 | 1,352449 | 2,310469 |
| H27 | -2,533279 | 1,459046 | 4,722523 | H27 | -2,273184 | 1,465273 | 4,757639 |
| H28 | -2,208107 | -2,829078 | 4,885816 | H28 | -2,432570 | -2,831010 | 4,943433 |
| H29 | -2,517665 | -0,653759 | 6,046309 | H29 | -2,493653 | -0,628324 | 6,090747 |
| O30 | 1,197551 | -3,982760 | -0,084106 | O30 | 1,190506 | -4,013289 | -0,103354 |
| C31 | 2,445341 | -1,718915 | 2,239428 | C31 | 2,482625 | -1,799706 | 2,256286 |
| C32 | 1,340549 | -1,280092 | 2,969060 | C32 | 1,345087 | -1,510966 | 3,011922 |
| C33 | 3,644548 | -1,977221 | 2,923686 | C33 | 3,710524 | -1,959292 | 2,917889 |
| C34 | 1,435188 | -1,069619 | 4,346941 | C34 | 1,434808 | -1,338281 | 4,394449 |
| H35 | 0,398415 | -1,102562 | 2,475472 | H35 | 0,382516 | -1,416484 | 2,533050 |
| C36 | 3,739142 | -1,772542 | 4,297889 | C36 | 3,799360 | -1,793770 | 4,298335 |
| H37 | 4,513646 | -2,333218 | 2,376924 | H37 | 4,603454 | -2,207111 | 2,350790 |
| C38 | 2,633118 | -1,310480 | 5,015445 | C38 | 2,661413 | -1,473352 | 5,041447 |
| H39 | 0,558631 | -0,726193 | 4,888061 | H39 | 0,535108 | -1,103628 | 4,955334 |
| H40 | 4,676864 | -1,974497 | 4,807791 | H40 | 4,759153 | -1,914711 | 4,792593 |
| H41 | 2,706881 | -1,149009 | 6,087142 | H41 | 2,732489 | -1,339730 | 6,117192 |
| C42 | -3,499164 | -0,108409 | -0,315476 | C42 | -3,477749 | -0,120284 | -0,248902 |
| C43 | -4,535405 | 0,417740 | 0,465720 | C43 | -4,510618 | 0,377337 | 0,554155 |
| C44 | -3,681914 | -0,199759 | -1,706441 | C44 | -3,652289 | -0,145407 | -1,643330 |
| C45 | -5,715443 | 0,868144 | -0,132166 | C45 | -5,690774 | 0,849856 | -0,025180 |
| H46 | -4,433417 | 0,480714 | 1,542902 | H46 | -4,402720 | 0,399512 | 1,633005 |
| C47 | -4,860414 | 0,248103 | -2,300759 | C47 | -4,831216 | 0,323598 | -2,219111 |
| C48 | -5,880446 | 0,795578 | -1,515028 | C48 | -5,853854 | 0,829238 | -1,409704 |
| H49 | -6,508393 | 1,271619 | 0,491200 | H49 | -6,486131 | 1,226850 | 0,611728 |
| H50 | -4,991284 | 0,149411 | -3,375210 | H50 | -4,962946 | 0,272057 | -3,296826 |
| H51 | -6,800611 | 1,142186 | -1,975961 | H51 | -6,775759 | 1,190249 | -1,856377 |
| H52 | 0,667863 | 0,606360 | 1,130818 | H52 | 0,721904 | 0,403421 | 1,226187 |
| H53 | 1,265819 | 3,002237 | -2,324231 | H53 | 1,221148 | 3,309406 | -2,484816 |
| H54 | -1,943914 | -2,904291 | 2,438959 | H54 | -2,177709 | -2,950241 | 2,494881 |
| H55 | -2,914979 | -0,652929 | -2,325382 | H55 | -2,879010 | -0,564988 | -2,278457 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H56 | 3,265684 | -3,970069 | -0,010106 | H56 | 3,257058 | -4,072403 | 0,052128 |
| C57 | 5,280433 | -0,101817 | -1,828584 | C57 | 5,348083 | -0,187807 | -1,780960 |
| C58 | 4,469260 | -1,134276 | -2,307325 | C58 | 4,627738 | -1,293994 | -2,234462 |
| C59 | 3,563824 | -1,761152 | -1,454977 | C59 | 3,710074 | -1,919866 | -1,393617 |
| C60 | 3,441363 | -1,368515 | -0,113453 | C60 | 3,494140 | -1,454267 | -0,090589 |
| C61 | 4,241259 | -0,320120 | 0,351824 | C61 | 4,199635 | -0,326858 | 0,345049 |
| C62 | 5,163601 | 0,296891 | -0,497722 | C62 | 5,128501 | 0,293470 | -0,490632 |
| H63 | 5,995917 | 0,383188 | -2,485903 | H63 | 6,071579 | 0,297345 | -2,429795 |
| H64 | 4,544111 | -1,453363 | -3,342841 | H64 | 4,781460 | -1,670725 | -3,241397 |
| H65 | 2,930343 | -2,551600 | -1,850974 | H65 | 3,142581 | -2,765997 | -1,773905 |
| H66 | 4,142959 | 0,026255 | 1,373942 | H66 | 4,015822 | 0,078323 | 1,332532 |
| H67 | 5,790719 | 1,096832 | -0,114917 | H67 | 5,679539 | 1,158640 | -0,133056 |
| C68 | -1,426527 | 3,845266 | 2,321838 | C68 | -1,519890 | 3,977947 | 2,221694 |
| C69 | -0,654603 | 3,239486 | 1,334035 | C69 | -0,710806 | 3,483084 | 1,201607 |
| C70 | -1,218045 | 2,870185 | 0,097983 | C70 | -1,265821 | 3,122624 | -0,037695 |
| C71 | -2,593665 | 3,068325 | -0,080613 | C71 | -2,652063 | 3,206724 | -0,204105 |
| C72 | -3,371042 | 3,660026 | 0,919706 | C72 | -3,461885 | 3,693104 | 0,824737 |
| C73 | -2,792040 | 4,069961 | 2,119339 | C73 | -2,899285 | 4,097625 | 2,033349 |
| H74 | -0,959115 | 4,126389 | 3,261507 | H74 | -1,070387 | 4,258004 | 3,170237 |
| H75 | 0,388940 | 3,031901 | 1,530275 | H75 | 0,350658 | 3,360152 | 1,375770 |
| H76 | -3,082050 | 2,722559 | -0,983313 | H76 | -3,120138 | 2,848431 | -1,113994 |
| H77 | -4,436968 | 3,786769 | 0,754053 | H77 | -4,536702 | 3,737216 | 0,678077 |
| H78 | -3,394630 | 4,539036 | 2,891450 | H78 | -3,529602 | 4,482315 | 2,830001 |
| C79 | -0,326110 | 2,322887 | -1,000298 | C79 | -0,340696 | 2,662307 | -1,155593 |
| C80 | 0,758272 | 3,412119 | -1,441227 | C80 | 0,720735 | 3,729703 | -1,604146 |
| C81 | -1,552076 | 3,017529 | -3,204018 | C81 | -1,590754 | 3,139172 | -3,347643 |
| C82 | -0,953385 | 0,815901 | -2,884879 | C82 | -0,937183 | 0,961525 | -2,908423 |
| C83 | -2,280964 | 2,105454 | -4,192807 | C83 | -2,305273 | 2,156577 | -4,278207 |
| H84 | -0,723859 | 3,552046 | -3,680956 | H84 | -0,784951 | 3,677468 | -3,858641 |
| H85 | -2,208418 | 3,739197 | -2,717253 | H85 | -2,265631 | 3,863031 | -2,887773 |
| H86 | -3,322510 | 1,936663 | -3,904859 | H86 | -3,343396 | 1,989618 | -3,976548 |
| H87 | -2,219895 | 2,430702 | -5,231181 | H87 | -2,253954 | 2,423932 | -5,333489 |
| N88 | -1,052446 | 2,007897 | -2,246997 | N88 | -1,048514 | 2,199818 | -2,351467 |
| O89 | -1,575309 | 0,838530 | -4,073795 | O89 | -1,579943 | 0,913007 | -4,089447 |
| O90 | -0,395683 | -0,213048 | -2,475731 | O90 | -0,369871 | -0,037953 | -2,459251 |
| H91 | 2,431416 | -4,128781 | 1,562492 | H91 | 2,354877 | -4,180806 | 1,589692 |
| N92 | -1,903346 | -2,362716 | -0,142698 | N92 | -1,892824 | -2,401175 | -0,112082 |
| C93 | -0,835088 | -2,972932 | -0,968819 | C93 | -0,825192 | -2,957234 | -0,980759 |
| H94 | -0,725099 | -2,461302 | -1,932216 | H94 | -0,724393 | -2,393324 | -1,916743 |
| H95 | 0,184935 | 4,284679 | -1,772032 | H95 | 0,165610 | 4,617095 | -1,927353 |
| C96 | 3,668142 | 4,769177 | 1,453715 | C96 | 3,635672 | 4,854472 | 1,373627 |
| C97 | 2,522566 | 5,524009 | 1,197068 | C97 | 2,617615 | 5,741429 | 1,021110 |
| C98 | 1,594238 | 5,083460 | 0,255529 | C98 | 1,682494 | 5,379280 | 0,051612 |
| C99 | 1,791114 | 3,884269 | -0,443335 | C99 | 1,755268 | 4,131695 | -0,580224 |
| C100 | 2,962528 | 3,153858 | -0,204520 | C100 | 2,794314 | 3,255678 | -0,237877 |
| C101 | 3,887137 | 3,587311 | 0,745375 | C101 | 3,721757 | 3,612871 | 0,739910 |
| H102 | 4,391328 | 5,107164 | 2,190549 | H102 | 4,361467 | 5,131902 | 2,132960 |
| H103 | 2,350569 | 6,454303 | 1,730972 | H103 | 2,548041 | 6,712422 | 1,503306 |

| | | | | | | | |
|------|----------|----------|-----------|------|----------|----------|-----------|
| H104 | 0,694699 | 5,665834 | 0,073543 | H104 | 0,879439 | 6,065666 | -0,205829 |
| H105 | 3,168962 | 2,246564 | -0,763404 | H105 | 2,873728 | 2,287398 | -0,722489 |
| H106 | 4,786797 | 3,005785 | 0,923994 | H106 | 4,515941 | 2,920998 | 1,004532 |
| H107 | 1,817888 | 0,469221 | -0,698205 | H107 | 1,811776 | 0,456909 | -0,605517 |
| H108 | 0,978495 | 1,530354 | -0,784155 | H108 | 0,357523 | 1,838784 | -0,797711 |

C1_E_R_tN_Cheltop

C1_ER_Cheltop_SM

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,302899 | -3,269123 | 0,477358 |
| C2 | -2,234129 | -4,424221 | -0,110304 |
| C3 | -3,701964 | -4,254214 | -0,579317 |
| C4 | -3,088001 | -2,998150 | 1,395876 |
| H5 | -5,110120 | -3,735254 | 1,051931 |
| H6 | -3,766758 | -3,866753 | -1,601135 |
| H7 | -3,316796 | -2,531709 | 2,354787 |
| H8 | -4,696438 | -2,354347 | 0,033750 |
| H9 | -1,714728 | -5,288447 | -0,523966 |
| H10 | -4,212548 | -5,221149 | -0,563506 |
| C11 | -2,389101 | -4,368486 | 1,426287 |
| H12 | -1,439335 | -4,356936 | 1,969424 |
| H13 | -3,024821 | -5,168384 | 1,815710 |
| C14 | -0,002198 | -3,133241 | -0,266159 |
| N15 | 0,766005 | -2,099433 | -0,226667 |
| C16 | 2,205075 | -2,573141 | -0,131995 |
| C17 | 1,991230 | -4,110631 | 0,068169 |
| P18 | -1,919840 | -0,525555 | 0,560710 |
| Ir19 | 0,164061 | -0,058183 | -0,624820 |
| C20 | -1,837053 | 0,029039 | 2,300580 |
| C21 | -1,361624 | 1,003374 | 4,893823 |
| C22 | -1,278160 | -0,801845 | 3,281893 |
| C23 | -2,164294 | 1,352567 | 2,636372 |
| C24 | -1,928352 | 1,833539 | 3,924106 |
| C25 | -1,044974 | -0,317082 | 4,569458 |
| H26 | -2,608373 | 2,005351 | 1,892753 |
| H27 | -2,194874 | 2,857350 | 4,172941 |
| H28 | -0,612812 | -0,973485 | 5,319492 |
| H29 | -1,174678 | 1,380491 | 5,894729 |
| O30 | 0,574234 | -4,332342 | -0,178612 |
| C31 | 2,905725 | -2,040141 | 1,112898 |
| C32 | 2,168997 | -1,569838 | 2,201171 |
| C33 | 4,297294 | -2,163935 | 1,242284 |
| C34 | 2,808335 | -1,170048 | 3,373585 |
| H35 | 1,094785 | -1,478376 | 2,124841 |
| C36 | 4,936465 | -1,774415 | 2,417961 |
| H37 | 4,887805 | -2,555183 | 0,419791 |
| C38 | 4,194339 | -1,265143 | 3,485196 |
| H39 | 2,215171 | -0,771340 | 4,191732 |
| H40 | 6,016173 | -1,864436 | 2,496214 |

C1_ER_Cheltop_TS1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,286837 | -3,352529 | 0,426943 |
| C2 | -2,199749 | -4,483993 | -0,140674 |
| C3 | -3,662853 | -4,325548 | -0,628286 |
| C4 | -3,090734 | -3,087898 | 1,372293 |
| H5 | -5,106897 | -3,824474 | 0,977817 |
| H6 | -3,718388 | -3,933490 | -1,648908 |
| H7 | -3,339635 | -2,637759 | 2,334084 |
| H8 | -4,669314 | -2,431553 | -0,014609 |
| H9 | -1,663649 | -5,335884 | -0,558576 |
| H10 | -4,164215 | -5,297420 | -0,623942 |
| C11 | -2,378708 | -4,451782 | 1,393717 |
| H12 | -1,437516 | -4,437401 | 1,951435 |
| H13 | -3,011708 | -5,263925 | 1,761569 |
| C14 | 0,018307 | -3,154722 | -0,270531 |
| N15 | 0,762321 | -2,105515 | -0,204842 |
| C16 | 2,207523 | -2,547578 | -0,132412 |
| C17 | 2,031791 | -4,093063 | 0,037113 |
| P18 | -1,923668 | -0,595165 | 0,600194 |
| Ir19 | 0,085291 | -0,060798 | -0,554580 |
| C20 | -1,860499 | -0,053368 | 2,343610 |
| C21 | -1,384675 | 0,922331 | 4,931644 |
| C22 | -1,308609 | -0,887565 | 3,325153 |
| C23 | -2,176064 | 1,274694 | 2,671821 |
| C24 | -1,939032 | 1,756883 | 3,958363 |
| C25 | -1,077303 | -0,401633 | 4,612871 |
| H26 | -2,614352 | 1,927322 | 1,923877 |
| H27 | -2,193318 | 2,784536 | 4,203230 |
| H28 | -0,653009 | -1,058844 | 5,366510 |
| H29 | -1,198058 | 1,300967 | 5,932005 |
| O30 | 0,622321 | -4,344541 | -0,225983 |
| C31 | 2,911195 | -2,017880 | 1,110460 |
| C32 | 2,182989 | -1,546120 | 2,203911 |
| C33 | 4,304674 | -2,136296 | 1,223507 |
| C34 | 2,834980 | -1,140024 | 3,367954 |
| H35 | 1,107083 | -1,457548 | 2,138739 |
| C36 | 4,955145 | -1,740646 | 2,390215 |
| H37 | 4,885545 | -2,524558 | 0,391915 |
| C38 | 4,222534 | -1,229909 | 3,463697 |
| H39 | 2,249768 | -0,740422 | 4,191342 |
| H40 | 6,035925 | -1,825643 | 2,457256 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H41 | 4,695087 | -0,948253 | 4,395547 | H41 | 4,732035 | -0,907610 | 4,367141 |
| C42 | -3,532178 | 0,052655 | -0,081620 | C42 | -3,510682 | 0,013018 | -0,067890 |
| C43 | -4,625225 | 0,333816 | 0,753062 | C43 | -4,625385 | 0,251716 | 0,750925 |
| C44 | -3,723611 | 0,000009 | -1,470139 | C44 | -3,652987 | 0,070750 | -1,462002 |
| C45 | -5,885661 | 0,564937 | 0,203069 | C45 | -5,860621 | 0,551748 | 0,179077 |
| H46 | -4,500499 | 0,359873 | 1,830830 | H46 | -4,533710 | 0,198026 | 1,831134 |
| C47 | -4,986797 | 0,224342 | -2,014354 | C47 | -4,890852 | 0,366154 | -2,028320 |
| C48 | -6,070883 | 0,506633 | -1,180224 | C48 | -5,995215 | 0,607268 | -1,209543 |
| H49 | -6,725485 | 0,781365 | 0,857342 | H49 | -6,719412 | 0,736629 | 0,817824 |
| H50 | -5,121517 | 0,192381 | -3,091235 | H50 | -4,988032 | 0,425016 | -3,107821 |
| H51 | -7,054671 | 0,682545 | -1,605206 | H51 | -6,959235 | 0,840868 | -1,652079 |
| H52 | -0,435034 | -0,548872 | -1,980053 | H52 | -0,539363 | -0,570115 | -1,890886 |
| H53 | 1,588385 | -0,151212 | -1,322466 | H53 | 1,512869 | 0,041373 | -1,323708 |
| H54 | -1,016799 | -1,825873 | 3,034088 | H54 | -1,050987 | -1,912725 | 3,076942 |
| H55 | -2,879198 | -0,201801 | -2,121573 | H55 | -2,790241 | -0,095418 | -2,098070 |
| H56 | 2,563314 | -4,730981 | -0,621481 | H56 | 2,625534 | -4,686835 | -0,657657 |
| C57 | 3,984224 | -1,592429 | -3,974116 | C57 | 3,945391 | -1,409283 | -3,949645 |
| C58 | 3,103811 | -2,668184 | -3,849196 | C58 | 3,121858 | -2,531247 | -3,850158 |
| C59 | 2,558973 | -2,985306 | -2,605396 | C59 | 2,585814 | -2,899702 | -2,616403 |
| C60 | 2,889343 | -2,243420 | -1,463048 | C60 | 2,871367 | -2,163345 | -1,458710 |
| C61 | 3,753906 | -1,148967 | -1,607112 | C61 | 3,679300 | -1,023084 | -1,576255 |
| C62 | 4,300792 | -0,830754 | -2,850506 | C62 | 4,216194 | -0,653660 | -2,810222 |
| H63 | 4,408542 | -1,341302 | -4,941800 | H63 | 4,360137 | -1,117816 | -4,909909 |
| H64 | 2,838430 | -3,260459 | -4,720246 | H64 | 2,893728 | -3,120702 | -4,733631 |
| H65 | 1,857482 | -3,813115 | -2,537239 | H65 | 1,928924 | -3,764611 | -2,567585 |
| H66 | 3,999304 | -0,537673 | -0,746867 | H66 | 3,897414 | -0,424724 | -0,698580 |
| H67 | 4,966835 | 0,022438 | -2,940336 | H67 | 4,839862 | 0,232782 | -2,880176 |
| C68 | -3,025228 | 2,780749 | -3,433654 | C68 | -2,969114 | 2,940590 | -3,459192 |
| C69 | -1,850460 | 2,287163 | -2,872265 | C69 | -1,797577 | 2,408809 | -2,923319 |
| C70 | -1,549668 | 2,521044 | -1,518909 | C70 | -1,506963 | 2,540585 | -1,555675 |
| C71 | -2,495310 | 3,218273 | -0,748858 | C71 | -2,459706 | 3,189512 | -0,749076 |
| C72 | -3,677904 | 3,696992 | -1,308849 | C72 | -3,635313 | 3,710292 | -1,283317 |
| C73 | -3,943075 | 3,493775 | -2,661013 | C73 | -3,892418 | 3,599989 | -2,648672 |
| H74 | -3,227502 | 2,596650 | -4,485181 | H74 | -3,159113 | 2,832804 | -4,523598 |
| H75 | -1,177508 | 1,710174 | -3,488962 | H75 | -1,119592 | 1,884817 | -3,579757 |
| H76 | -2,312078 | 3,378234 | 0,307451 | H76 | -2,280515 | 3,279639 | 0,316375 |
| H77 | -4,391239 | 4,225732 | -0,683172 | H77 | -4,351075 | 4,198500 | -0,628110 |
| H78 | -4,859258 | 3,872621 | -3,104347 | H78 | -4,803663 | 4,011542 | -3,072649 |
| C79 | -0,272201 | 2,065134 | -0,890670 | C79 | -0,248410 | 2,030883 | -0,917981 |
| C80 | 0,942489 | 1,720350 | -1,598378 | C80 | 0,987982 | 1,642943 | -1,615878 |
| C92 | 0,303878 | 4,150068 | 0,510510 | C92 | 0,356285 | 4,175216 | 0,399014 |
| C93 | 0,734094 | 2,050287 | 1,326804 | C93 | 0,723904 | 2,099485 | 1,317144 |
| C94 | 0,684668 | 4,208735 | 1,995722 | C94 | 0,711910 | 4,287502 | 1,888587 |
| H95 | -0,554609 | 4,774028 | 0,260227 | H95 | -0,497346 | 4,790361 | 0,111642 |
| H96 | 1,141261 | 4,415674 | -0,150291 | H96 | 1,204520 | 4,415047 | -0,258004 |
| H97 | 1,468415 | 4,928285 | 2,232671 | H97 | 1,508312 | 4,998152 | 2,109684 |
| H98 | -0,186864 | 4,375521 | 2,636899 | H98 | -0,167089 | 4,505497 | 2,503655 |
| N99 | -0,003521 | 2,716083 | 0,395521 | N99 | 0,044321 | 2,741296 | 0,331961 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| O100 | 1,196364 | 2,874938 | 2,274277 | O100 | 1,184783 | 2,955432 | 2,239114 |
| O101 | 0,989271 | 0,841848 | 1,310468 | O101 | 0,935149 | 0,882223 | 1,366944 |
| H102 | 2,191756 | -4,414172 | 1,096744 | H102 | 2,231816 | -4,409332 | 1,062147 |
| N103 | -2,052431 | -2,210710 | 0,669314 | N103 | -2,052378 | -2,280894 | 0,674570 |
| C104 | -1,503502 | -3,087580 | -0,393018 | C104 | -1,483954 | -3,134066 | -0,397517 |
| H105 | -1,730096 | -2,716589 | -1,402352 | H105 | -1,713814 | -2,752235 | -1,402398 |
| C107 | 1,629127 | 2,213194 | -5,816506 | C107 | 1,557874 | 1,984005 | -5,866112 |
| C108 | 1,455273 | 3,311866 | -4,971562 | C108 | 1,620856 | 3,100521 | -5,028592 |
| C109 | 1,225948 | 3,113663 | -3,612845 | C109 | 1,443288 | 2,950676 | -3,655794 |
| C110 | 1,159031 | 1,817117 | -3,077706 | C110 | 1,191868 | 1,686429 | -3,100905 |
| C111 | 1,349096 | 0,723662 | -3,925993 | C111 | 1,154129 | 0,571361 | -3,940716 |
| C112 | 1,581390 | 0,923648 | -5,288464 | C112 | 1,332593 | 0,722120 | -5,317075 |
| H113 | 1,801211 | 2,364751 | -6,878269 | H113 | 1,688588 | 2,099489 | -6,938266 |
| H114 | 1,490807 | 4,321282 | -5,371578 | H114 | 1,801026 | 4,087224 | -5,445576 |
| H115 | 1,071771 | 3,970131 | -2,960588 | H115 | 1,472931 | 3,824330 | -3,008669 |
| H116 | 1,316617 | -0,280810 | -3,521626 | H116 | 0,997732 | -0,413452 | -3,516012 |
| H117 | 1,726390 | 0,063636 | -5,936058 | H117 | 1,299815 | -0,153490 | -5,959196 |
| H107 | 1,843120 | 2,004118 | -1,049859 | H107 | 1,879356 | 1,990612 | -1,088375 |

C1_ER_Cheltop_INT1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,226375 | -3,382837 | 0,456156 |
| C2 | -2,132592 | -4,536453 | -0,041782 |
| C3 | -3,594362 | -4,407823 | -0,544119 |
| C4 | -3,041075 | -3,079813 | 1,402035 |
| H5 | -5,057226 | -3,822782 | 1,017287 |
| H6 | -3,646503 | -4,070964 | -1,584328 |
| H7 | -3,302762 | -2,590662 | 2,341002 |
| H8 | -4,595199 | -2,478438 | -0,030994 |
| H9 | -1,588617 | -5,402771 | -0,418041 |
| H10 | -4,093514 | -5,379433 | -0,489665 |
| C11 | -2,323620 | -4,438350 | 1,488466 |
| H12 | -1,387096 | -4,395063 | 2,052795 |
| H13 | -2,956543 | -5,236185 | 1,886949 |
| C14 | 0,083680 | -3,195037 | -0,253152 |
| N15 | 0,799178 | -2,128629 | -0,201023 |
| C16 | 2,245320 | -2,516010 | -0,094856 |
| C17 | 2,142921 | -4,084469 | -0,115820 |
| P18 | -1,853243 | -0,620424 | 0,592018 |
| Ir19 | 0,007333 | -0,096391 | -0,527968 |
| C20 | -1,735947 | -0,062844 | 2,326915 |
| C21 | -1,236858 | 0,919029 | 4,906301 |
| C22 | -1,272686 | -0,920661 | 3,332725 |
| C23 | -1,949935 | 1,292630 | 2,624820 |
| C24 | -1,701084 | 1,778379 | 3,907158 |
| C25 | -1,030395 | -0,430814 | 4,617350 |
| H26 | -2,315999 | 1,963335 | 1,854179 |
| H27 | -1,874559 | 2,827747 | 4,129868 |
| H28 | -0,677847 | -1,105909 | 5,391962 |

C1_ER_Cheltop_TS2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,086516 | -3,371088 | 1,275450 |
| C2 | -2,062815 | -4,535970 | 0,579430 |
| C3 | -3,588434 | -4,496900 | 0,312334 |
| C4 | -2,772404 | -2,906951 | 1,946211 |
| H5 | -4,765337 | -3,764769 | 2,039330 |
| H6 | -3,820306 | -4,284581 | -0,736405 |
| H7 | -2,900024 | -2,299575 | 2,841851 |
| H8 | -4,606441 | -2,565752 | 0,760769 |
| H9 | -1,557742 | -5,437680 | 0,235240 |
| H10 | -4,035975 | -5,464304 | 0,556944 |
| C11 | -2,001667 | -4,230710 | 2,093024 |
| H12 | -0,987339 | -4,099671 | 2,482127 |
| H13 | -2,534327 | -4,972525 | 2,694591 |
| C14 | 0,050340 | -3,236770 | -0,126110 |
| N15 | 0,785475 | -2,182928 | -0,244849 |
| C16 | 2,221748 | -2,650976 | -0,113575 |
| C17 | 2,051479 | -4,173112 | -0,394002 |
| P18 | -1,840601 | -0,570371 | 0,590710 |
| Ir19 | -0,112727 | -0,196721 | -0,777157 |
| C20 | -1,610779 | 0,254558 | 2,196185 |
| C21 | -1,097209 | 1,601797 | 4,597896 |
| C22 | -1,003467 | -0,416720 | 3,266910 |
| C23 | -1,958418 | 1,606926 | 2,339199 |
| C24 | -1,702117 | 2,274956 | 3,534605 |
| C25 | -0,755810 | 0,255565 | 4,462941 |
| H26 | -2,442721 | 2,127775 | 1,522918 |
| H27 | -1,986313 | 3,318300 | 3,641259 |
| H28 | -0,297668 | -0,276200 | 5,291839 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H29 | -1,042987 | 1,299594 | 5,904806 | H29 | -0,900285 | 2,122405 | 5,530456 |
| O30 | 0,718341 | -4,369738 | -0,229652 | O30 | 0,656356 | -4,424132 | -0,085279 |
| C31 | 2,847055 | -2,100297 | 1,247133 | C31 | 2,706219 | -2,461753 | 1,330983 |
| C32 | 2,046770 | -1,658930 | 2,299660 | C32 | 2,002541 | -1,677541 | 2,243954 |
| C33 | 4,221957 | -2,277174 | 1,464998 | C33 | 3,894877 | -3,081733 | 1,744446 |
| C34 | 2,608846 | -1,361891 | 3,541426 | C34 | 2,471465 | -1,515676 | 3,549404 |
| H35 | 0,988308 | -1,510971 | 2,143526 | H35 | 1,116219 | -1,151546 | 1,923350 |
| C36 | 4,782643 | -1,989958 | 2,707449 | C36 | 4,363162 | -2,921808 | 3,045829 |
| H37 | 4,857736 | -2,626854 | 0,655719 | H37 | 4,476273 | -3,669095 | 1,037738 |
| C38 | 3,976670 | -1,524529 | 3,749793 | C38 | 3,651818 | -2,134341 | 3,954752 |
| H39 | 1,969655 | -0,990476 | 4,337625 | H39 | 1,916856 | -0,884914 | 4,238223 |
| H40 | 5,849751 | -2,123661 | 2,860341 | H40 | 5,287411 | -3,405448 | 3,348342 |
| H41 | 4,416074 | -1,290547 | 4,715334 | H41 | 4,018843 | -2,006387 | 4,969012 |
| C42 | -3,440861 | 0,021971 | -0,039673 | C42 | -3,556290 | -0,253481 | 0,054074 |
| C43 | -4,508889 | 0,306159 | 0,826719 | C43 | -4,542293 | 0,178211 | 0,955420 |
| C44 | -3,645773 | 0,062573 | -1,426201 | C44 | -3,944806 | -0,770596 | -1,191245 |
| C45 | -5,761066 | 0,631086 | 0,307553 | C45 | -5,890441 | 0,101069 | 0,609063 |
| H46 | -4,370279 | 0,268264 | 1,902391 | H46 | -4,268916 | 0,547954 | 1,937097 |
| C47 | -4,899485 | 0,385540 | -1,937899 | C47 | -5,293693 | -0,860868 | -1,524527 |
| C48 | -5,958312 | 0,669473 | -1,073649 | C48 | -6,269090 | -0,421803 | -0,627677 |
| H49 | -6,582942 | 0,851412 | 0,982844 | H49 | -6,645064 | 0,439306 | 1,313209 |
| H50 | -5,044471 | 0,432229 | -3,012603 | H50 | -5,583049 | -1,261543 | -2,491659 |
| H51 | -6,934698 | 0,924609 | -1,475574 | H51 | -7,320696 | -0,489244 | -0,891041 |
| H52 | -0,694161 | -0,623209 | -1,828489 | H52 | -0,943801 | -0,903491 | -1,912028 |
| H53 | 1,543876 | 0,579390 | -1,588868 | H53 | -0,195438 | 1,338848 | -3,550153 |
| H54 | -1,092031 | -1,967195 | 3,109914 | H54 | -0,719257 | -1,457827 | 3,165609 |
| H55 | -2,819050 | -0,134374 | -2,099433 | H55 | -3,189954 | -1,106243 | -1,894402 |
| H56 | 2,653276 | -4,555840 | -0,956692 | H56 | 2,211773 | -4,446948 | -1,439700 |
| C57 | 4,124138 | -0,762351 | -3,604468 | C57 | 4,741670 | -0,694513 | -3,061633 |
| C58 | 3,372615 | -1,933947 | -3,713843 | C58 | 3,716524 | -1,554768 | -3,460454 |
| C59 | 2,787942 | -2,500832 | -2,581756 | C59 | 2,938817 | -2,210018 | -2,504191 |
| C60 | 2,959692 | -1,922758 | -1,315785 | C60 | 3,159794 | -2,008958 | -1,134274 |
| C61 | 3,701158 | -0,737633 | -1,218836 | C61 | 4,192534 | -1,146333 | -0,745495 |
| C62 | 4,278107 | -0,163361 | -2,354411 | C62 | 4,981618 | -0,502922 | -1,700266 |
| H63 | 4,571460 | -0,314523 | -4,486531 | H63 | 5,347446 | -0,183895 | -3,804429 |
| H64 | 3,231155 | -2,402424 | -4,683525 | H64 | 3,517878 | -1,715194 | -4,516311 |
| H65 | 2,181614 | -3,395386 | -2,697828 | H65 | 2,123046 | -2,844081 | -2,840505 |
| H66 | 3,827704 | -0,261101 | -0,252467 | H66 | 4,383437 | -0,968411 | 0,305593 |
| H67 | 4,850853 | 0,754814 | -2,257765 | H67 | 5,778139 | 0,160045 | -1,374722 |
| C68 | -2,934329 | 2,874876 | -3,497142 | C68 | -4,041492 | 1,826175 | -3,080540 |
| C69 | -1,750384 | 2,335358 | -2,993803 | C69 | -2,717920 | 1,518616 | -2,789386 |
| C70 | -1,389073 | 2,509781 | -1,647612 | C70 | -2,058827 | 2,085463 | -1,684199 |
| C71 | -2,293993 | 3,211893 | -0,828239 | C71 | -2,806502 | 2,937224 | -0,862484 |
| C72 | -3,484488 | 3,735605 | -1,326834 | C72 | -4,145195 | 3,229903 | -1,135430 |
| C73 | -3,810851 | 3,581138 | -2,673509 | C73 | -4,767875 | 2,688506 | -2,255317 |
| H74 | -3,172807 | 2,729878 | -4,547507 | H74 | -4,514529 | 1,380263 | -3,951085 |
| H75 | -1,119530 | 1,766732 | -3,660144 | H75 | -2,184662 | 0,827356 | -3,433121 |
| H76 | -2,070621 | 3,335492 | 0,225776 | H76 | -2,342625 | 3,396362 | 0,001890 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H77 | -4,158382 | 4,261209 | -0,656109 | H77 | -4,693736 | 3,893339 | -0,472280 |
| H78 | -4,732989 | 3,994595 | -3,070656 | H78 | -5,804364 | 2,922800 | -2,478209 |
| C79 | -0,147961 | 1,926460 | -1,025081 | C79 | -0,585175 | 1,798897 | -1,467293 |
| C80 | 1,166380 | 1,642484 | -1,823318 | C80 | 0,190079 | 2,051477 | -2,814758 |
| C92 | 0,575641 | 4,119874 | 0,206825 | C81 | 0,141036 | 4,157024 | -0,403737 |
| C93 | 0,915896 | 2,057502 | 1,155916 | C82 | 0,782446 | 2,172208 | 0,552999 |
| C94 | 1,020176 | 4,253510 | 1,671657 | C83 | 0,620462 | 4,368491 | 1,035163 |
| H95 | -0,274617 | 4,754495 | -0,045557 | H84 | -0,791063 | 4,667928 | -0,640373 |
| H96 | 1,391832 | 4,326682 | -0,500415 | H85 | 0,892005 | 4,461648 | -1,134928 |
| H97 | 1,855753 | 4,935486 | 1,830121 | H86 | 1,346085 | 5,173608 | 1,151424 |
| H98 | 0,187835 | 4,522773 | 2,329816 | H87 | -0,206006 | 4,503046 | 1,742125 |
| N99 | 0,219934 | 2,695003 | 0,184487 | N88 | -0,019093 | 2,683735 | -0,401437 |
| O100 | 1,458342 | 2,911360 | 2,032255 | O89 | 1,281759 | 3,113091 | 1,364387 |
| O101 | 1,072987 | 0,829018 | 1,231394 | O90 | 1,074585 | 0,967979 | 0,707416 |
| H102 | 2,490764 | -4,525281 | 0,818505 | H91 | 2,656972 | -4,804926 | 0,251933 |
| N103 | -1,998956 | -2,301271 | 0,677675 | N92 | -1,873660 | -2,220516 | 0,964777 |
| C104 | -1,422776 | -3,194926 | -0,357408 | C93 | -1,449944 | -3,241134 | -0,017432 |
| H105 | -1,663445 | -2,858762 | -1,376121 | H94 | -1,848542 | -3,050612 | -1,024395 |
| C107 | 1,317174 | 2,035884 | -6,107680 | C95 | 0,329240 | 6,067238 | -4,488217 |
| C108 | 1,459600 | 3,157008 | -5,287134 | C96 | -0,902931 | 5,430563 | -4,344037 |
| C109 | 1,419615 | 3,016250 | -3,901196 | C97 | -0,981904 | 4,140632 | -3,815542 |
| C110 | 1,231318 | 1,756128 | -3,321834 | C98 | 0,175851 | 3,459546 | -3,409518 |
| C111 | 1,104049 | 0,635701 | -4,146704 | C99 | 1,410084 | 4,108554 | -3,578877 |
| C112 | 1,143949 | 0,775108 | -5,533922 | C100 | 1,491742 | 5,396034 | -4,108651 |
| H113 | 1,344817 | 2,145131 | -7,187957 | H101 | 0,383605 | 7,071469 | -4,898940 |
| H114 | 1,598540 | 4,140442 | -5,726960 | H102 | -1,814790 | 5,937712 | -4,648186 |
| H115 | 1,518184 | 3,892782 | -3,264536 | H103 | -1,952981 | 3,671967 | -3,728041 |
| H116 | 0,974268 | -0,343535 | -3,696995 | H104 | 2,323731 | 3,596935 | -3,281781 |
| H117 | 1,043428 | -0,102177 | -6,166878 | H105 | 2,461211 | 5,872799 | -4,224903 |
| H107 | 1,977254 | 2,227550 | -1,373961 | H106 | 1,237121 | 1,793709 | -2,688421 |
| | | | | H107 | 2,418223 | 0,613369 | -1,428334 |
| | | | | H108 | 2,158133 | 0,188329 | -1,984950 |

C1_ER_Cheltop_INT2

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -4,137901 | -3,412395 | 1,327088 |
| C2 | -2,112310 | -4,596984 | 0,674184 |
| C3 | -3,636475 | -4,564864 | 0,397333 |
| C4 | -2,827482 | -2,936069 | 1,998049 |
| H5 | -4,826919 | -3,783078 | 2,093276 |
| H6 | -3,861024 | -4,381874 | -0,658446 |
| H7 | -2,964274 | -2,310099 | 2,879279 |
| H8 | -4,646105 | -2,615604 | 0,786356 |
| H9 | -1,602904 | -5,505572 | 0,353605 |
| H10 | -4,087041 | -5,524644 | 0,665742 |
| C11 | -2,059748 | -4,256894 | 2,180524 |
| H12 | -1,047597 | -4,117583 | 2,572355 |
| H13 | -2,596278 | -4,985283 | 2,795005 |
| C14 | -0,002780 | -3,313277 | -0,085491 |

C1_ER_Cheltop_TS3

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -4,146374 | -3,505526 | 1,373241 |
| C2 | -2,052622 | -4,634007 | 0,841155 |
| C3 | -3,566742 | -4,677968 | 0,514518 |
| C4 | -2,882256 | -2,965302 | 2,084887 |
| H5 | -4,870290 | -3,864226 | 2,112200 |
| H6 | -3,763242 | -4,556906 | -0,555628 |
| H7 | -3,071033 | -2,316211 | 2,940190 |
| H8 | -4,636904 | -2,737795 | 0,773902 |
| H9 | -1,494544 | -5,528703 | 0,566517 |
| H10 | -3,985302 | -5,642295 | 0,816320 |
| C11 | -2,068956 | -4,246649 | 2,336546 |
| H12 | -1,078198 | -4,051071 | 2,758071 |
| H13 | -2,594007 | -4,980111 | 2,954799 |
| C14 | 0,016324 | -3,276251 | 0,079785 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| N15 | 0,703751 | -2,255374 | -0,270126 | N15 | 0,692566 | -2,210951 | -0,194348 |
| C16 | 2,157032 | -2,655334 | -0,153609 | C16 | 2,167227 | -2,554129 | -0,087194 |
| C17 | 2,033550 | -4,192889 | -0,352305 | C17 | 2,088087 | -4,107803 | -0,111774 |
| P18 | -1,888504 | -0,613459 | 0,629171 | P18 | -1,975140 | -0,646416 | 0,682235 |
| Ir19 | -0,118743 | -0,285076 | -0,853649 | Ir19 | -0,153699 | -0,399017 | -0,962993 |
| C20 | -1,640841 | 0,215022 | 2,241394 | C20 | -1,746251 | 0,191378 | 2,298251 |
| C21 | -1,102763 | 1,580543 | 4,638277 | C21 | -1,198572 | 1,566444 | 4,688542 |
| C22 | -1,058253 | -0,455197 | 3,326019 | C22 | -1,102916 | -0,455931 | 3,362191 |
| C23 | -1,956523 | 1,576514 | 2,373807 | C23 | -2,126191 | 1,533891 | 2,455338 |
| C24 | -1,687339 | 2,252799 | 3,562827 | C24 | -1,853538 | 2,215658 | 3,640238 |
| C25 | -0,797118 | 0,224581 | 4,516414 | C25 | -0,832435 | 0,227938 | 4,547693 |
| H26 | -2,430018 | 2,101064 | 1,552918 | H26 | -2,667508 | 2,036673 | 1,663151 |
| H27 | -1,948164 | 3,303782 | 3,654420 | H27 | -2,169111 | 3,249803 | 3,752102 |
| H28 | -0,356542 | -0,311793 | 5,351984 | H28 | -0,340098 | -0,291456 | 5,365032 |
| H29 | -0,896840 | 2,106318 | 5,565608 | H29 | -0,987787 | 2,096359 | 5,612805 |
| O30 | 0,647170 | -4,476353 | 0,000232 | O30 | 0,706799 | -4,398478 | 0,258024 |
| C31 | 2,673939 | -2,376229 | 1,262950 | C31 | 2,728299 | -2,126074 | 1,274517 |
| C32 | 1,931708 | -1,669830 | 2,205889 | C32 | 1,962830 | -1,472422 | 2,234983 |
| C33 | 3,946116 | -2,850435 | 1,616263 | C33 | 4,065149 | -2,436976 | 1,567627 |
| C34 | 2,443984 | -1,442504 | 3,484676 | C34 | 2,519707 | -1,116123 | 3,464524 |
| H35 | 0,970290 | -1,265072 | 1,934442 | H35 | 0,942887 | -1,204115 | 2,012183 |
| C36 | 4,455656 | -2,630761 | 2,892779 | C36 | 4,621192 | -2,088614 | 2,794894 |
| H37 | 4,550971 | -3,379265 | 0,883488 | H37 | 4,680247 | -2,931702 | 0,820098 |
| C38 | 3,702520 | -1,924576 | 3,834734 | C38 | 3,847959 | -1,421411 | 3,749188 |
| H39 | 1,855045 | -0,873352 | 4,197719 | H39 | 1,909240 | -0,584816 | 4,188826 |
| H40 | 5,442028 | -3,005114 | 3,150796 | H40 | 5,659724 | -2,328750 | 3,003364 |
| H41 | 4,100749 | -1,748706 | 4,829759 | H41 | 4,283868 | -1,139795 | 4,703417 |
| C42 | -3,610511 | -0,254534 | 0,132577 | C42 | -3,704382 | -0,287209 | 0,197183 |
| C43 | -4,581679 | 0,171414 | 1,052952 | C43 | -4,703533 | 0,045067 | 1,124767 |
| C44 | -4,019422 | -0,708952 | -1,130099 | C44 | -4,066180 | -0,574675 | -1,126911 |
| C45 | -5,933108 | 0,145469 | 0,711257 | C45 | -6,039455 | 0,094302 | 0,729581 |
| H46 | -4,292580 | 0,502874 | 2,044230 | H46 | -4,445253 | 0,253354 | 2,158067 |
| C47 | -5,371790 | -0,746039 | -1,461623 | C47 | -5,403748 | -0,536164 | -1,515370 |
| C48 | -6,331650 | -0,320793 | -0,542262 | C48 | -6,392574 | -0,201516 | -0,588656 |
| H49 | -6,675241 | 0,477613 | 1,431557 | H49 | -6,806248 | 0,351959 | 1,454738 |
| H50 | -5,675557 | -1,097728 | -2,443199 | H50 | -5,672602 | -0,754662 | -2,544605 |
| H51 | -7,385797 | -0,350852 | -0,802215 | H51 | -7,435032 | -0,169670 | -0,892337 |
| H52 | -1,034947 | -0,968793 | -1,942098 | H52 | -1,000337 | -1,349643 | -1,898896 |
| H53 | 0,024973 | 1,335818 | -3,585450 | H53 | 0,069502 | 1,509152 | -3,728913 |
| H54 | -0,800788 | -1,504878 | 3,241999 | H54 | -0,810964 | -1,495565 | 3,263632 |
| H55 | -3,278482 | -1,032441 | -1,853531 | H55 | -3,297430 | -0,816919 | -1,853324 |
| H56 | 2,179671 | -4,524834 | -1,382743 | H56 | 2,258868 | -4,552800 | -1,093902 |
| C57 | 4,175405 | -0,333916 | -3,208758 | C57 | 4,146788 | -0,674479 | -3,457336 |
| C58 | 3,498777 | -1,505495 | -3,556312 | C58 | 3,420459 | -1,851951 | -3,640604 |
| C59 | 2,902963 | -2,292078 | -2,569283 | C59 | 2,817003 | -2,478713 | -2,551419 |
| C60 | 2,976698 | -1,926378 | -1,218510 | C60 | 2,935555 | -1,947801 | -1,260445 |
| C61 | 3,664423 | -0,752422 | -0,876753 | C61 | 3,658965 | -0,760229 | -1,088318 |
| C62 | 4,258995 | 0,035361 | -1,865034 | C62 | 4,260861 | -0,130294 | -2,177327 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H63 | 4,634765 | 0,280598 | -3,977228 | H63 | 4,618317 | -0,185339 | -4,304996 |
| H64 | 3,427479 | -1,805645 | -4,597709 | H64 | 3,317139 | -2,280990 | -4,632960 |
| H65 | 2,346538 | -3,172592 | -2,875519 | H65 | 2,221633 | -3,368432 | -2,732456 |
| H66 | 3,707811 | -0,436452 | 0,158803 | H66 | 3,729623 | -0,311905 | -0,104264 |
| H67 | 4,784431 | 0,942475 | -1,580128 | H67 | 4,820370 | 0,788493 | -2,022221 |
| C68 | -3,914812 | 1,790012 | -3,247800 | C68 | -3,914323 | 2,033685 | -3,378723 |
| C69 | -2,593128 | 1,500221 | -2,930502 | C69 | -2,592686 | 1,701803 | -3,100763 |
| C70 | -1,979443 | 2,035092 | -1,783357 | C70 | -1,988779 | 2,073807 | -1,887467 |
| C71 | -2,766840 | 2,839255 | -0,951609 | C71 | -2,776559 | 2,751736 | -0,952723 |
| C72 | -4,103235 | 3,114623 | -1,252926 | C72 | -4,107966 | 3,073880 | -1,220139 |
| C73 | -4,682421 | 2,603605 | -2,409629 | C73 | -4,681233 | 2,727828 | -2,439520 |
| H74 | -4,353308 | 1,369748 | -4,148838 | H74 | -4,349320 | 1,744723 | -4,331183 |
| H75 | -2,025231 | 0,847777 | -3,585194 | H75 | -2,026136 | 1,156075 | -3,849847 |
| H76 | -2,337484 | 3,269554 | -0,055119 | H76 | -2,350005 | 3,033418 | 0,000389 |
| H77 | -4,685082 | 3,739578 | -0,580963 | H77 | -4,693273 | 3,596660 | -0,469191 |
| H78 | -5,717546 | 2,823945 | -2,652161 | H78 | -5,714727 | 2,982104 | -2,653736 |
| C79 | -0,515606 | 1,746312 | -1,523617 | C79 | -0,523615 | 1,751958 | -1,643533 |
| C80 | 0,349331 | 2,033137 | -2,806166 | C80 | 0,401596 | 2,100262 | -2,867640 |
| C81 | 0,175431 | 4,059403 | -0,355579 | C81 | 0,105676 | 3,962135 | -0,297585 |
| C82 | 0,760649 | 2,041831 | 0,565052 | C82 | 0,784381 | 1,903066 | 0,459558 |
| C83 | 0,598437 | 4,222244 | 1,107423 | C83 | 0,557915 | 4,029752 | 1,163922 |
| H84 | -0,744295 | 4,583915 | -0,611564 | H84 | -0,836703 | 4,472180 | -0,491399 |
| H85 | 0,956446 | 4,380423 | -1,047307 | H85 | 0,860708 | 4,358991 | -0,976132 |
| H86 | 1,324053 | 5,017562 | 1,278003 | H86 | 1,256274 | 4,839564 | 1,374935 |
| H87 | -0,254822 | 4,339862 | 1,784476 | H87 | -0,279860 | 4,057787 | 1,868590 |
| N88 | 0,004380 | 2,588999 | -0,403900 | N88 | -0,020058 | 2,490850 | -0,448732 |
| O89 | 1,236923 | 2,951358 | 1,423841 | O89 | 1,253531 | 2,765727 | 1,364761 |
| O90 | 1,024765 | 0,829422 | 0,699560 | O90 | 1,079925 | 0,696271 | 0,495664 |
| H91 | 2,670577 | -4,767546 | 0,316595 | H91 | 2,735962 | -4,575720 | 0,626716 |
| N92 | -1,922931 | -2,268669 | 1,011402 | N92 | -1,981831 | -2,291878 | 1,106799 |
| C93 | -1,502605 | -3,315699 | 0,047759 | C93 | -1,485171 | -3,344450 | 0,190848 |
| H94 | -1,909820 | -3,145305 | -0,959594 | H94 | -1,874456 | -3,231130 | -0,831606 |
| C95 | 0,631385 | 6,053215 | -4,429762 | C95 | 0,924589 | 6,241306 | -4,045216 |
| C96 | -0,615476 | 5,432918 | -4,351029 | C96 | -0,354262 | 5,683724 | -4,044312 |
| C97 | -0,736068 | 4,140973 | -3,836629 | C97 | -0,546177 | 4,352229 | -3,674313 |
| C98 | 0,391772 | 3,443747 | -3,378748 | C98 | 0,539847 | 3,553939 | -3,285388 |
| C99 | 1,641494 | 4,075454 | -3,481263 | C99 | 1,822929 | 4,122143 | -3,308902 |
| C100 | 1,765480 | 5,364782 | -3,997758 | C100 | 2,017024 | 5,451983 | -3,683343 |
| H101 | 0,719551 | 7,058931 | -4,830736 | H101 | 1,069253 | 7,278626 | -4,333133 |
| H102 | -1,504255 | 5,954319 | -4,696466 | H102 | -1,209936 | 6,286157 | -4,337131 |
| H103 | -1,714804 | 3,681233 | -3,798038 | H103 | -1,547552 | 3,941233 | -3,689893 |
| H104 | 2,531739 | 3,546938 | -3,144689 | H104 | 2,679224 | 3,514079 | -3,024270 |
| H105 | 2,745370 | 5,829640 | -4,063542 | H105 | 3,019496 | 5,870697 | -3,692331 |
| H106 | 1,382225 | 1,762122 | -2,572066 | H106 | 1,390385 | 1,704516 | -2,618569 |
| H107 | 1,403385 | -0,105371 | -1,725533 | H107 | 1,025620 | -0,408231 | -2,044249 |
| H108 | 0,873670 | -0,454531 | -2,275755 | H108 | -0,572072 | 0,292056 | -2,344071 |

C1_E_S_tN_Cheltop

C1_ER_Cheltop_PROD

C1_ES_Cheltop_SM

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C1 | -4,108083 | -4,025846 | 0,538970 | C1 | -4,058318 | -3,565409 | 0,059551 |
| C2 | -1,876337 | -4,968475 | 0,274129 | C2 | -1,868330 | -4,632708 | -0,011502 |
| C3 | -3,307108 | -5,064570 | -0,315496 | C3 | -3,240745 | -4,638964 | -0,730987 |
| C4 | -3,034940 | -3,518627 | 1,532057 | C4 | -3,037534 | -3,090362 | 1,121744 |
| H5 | -4,936027 | -4,496837 | 1,078518 | H5 | -4,929764 | -4,005838 | 0,555172 |
| H6 | -3,330923 | -4,842357 | -1,387199 | H6 | -3,150955 | -4,400153 | -1,795681 |
| H7 | -3,426050 | -2,996903 | 2,405332 | H7 | -3,462096 | -2,527225 | 1,952839 |
| H8 | -4,520495 | -3,207605 | -0,054980 | H8 | -4,413431 | -2,749720 | -0,569850 |
| H9 | -1,208476 | -5,786929 | 0,004860 | H9 | -1,238193 | -5,499413 | -0,210410 |
| H10 | -3,697563 | -6,077595 | -0,182857 | H10 | -3,697880 | -5,629658 | -0,655333 |
| C11 | -2,177600 | -4,772932 | 1,777078 | C11 | -2,285822 | -4,390691 | 1,456776 |
| H12 | -1,290968 | -4,572712 | 2,385619 | H12 | -1,445218 | -4,238168 | 2,140065 |
| H13 | -2,739814 | -5,608083 | 2,204514 | H13 | -2,938041 | -5,178931 | 1,843028 |
| C14 | 0,161224 | -3,375687 | -0,015341 | C14 | 0,289342 | -3,206229 | -0,039854 |
| N15 | 0,765598 | -2,245585 | -0,196307 | N15 | 0,991342 | -2,124014 | -0,061005 |
| C16 | 2,223677 | -2,413628 | 0,196293 | C16 | 2,355600 | -2,450001 | 0,516288 |
| C17 | 2,316546 | -3,962328 | 0,124197 | C17 | 2,328384 | -4,005280 | 0,420952 |
| P18 | -2,038616 | -1,000412 | 0,569323 | P18 | -1,869994 | -0,672048 | 0,114232 |
| Ir19 | -0,116039 | -0,525259 | -0,805459 | Ir19 | 0,360007 | -0,203232 | -0,780506 |
| C20 | -2,099900 | -0,256912 | 2,242292 | C20 | -2,198309 | 0,188538 | 1,693561 |
| C21 | -2,022986 | 1,042067 | 4,731438 | C21 | -2,436837 | 1,663845 | 4,073781 |
| C22 | -1,844504 | -0,983150 | 3,412929 | C22 | -1,958259 | -0,419884 | 2,933816 |
| C23 | -2,296229 | 1,132088 | 2,328868 | C23 | -2,564655 | 1,544263 | 1,660659 |
| C24 | -2,258188 | 1,774030 | 3,564149 | C24 | -2,680997 | 2,275058 | 2,841930 |
| C25 | -1,816078 | -0,335412 | 4,650580 | C25 | -2,082498 | 0,314647 | 4,114505 |
| H26 | -2,485778 | 1,715506 | 1,432818 | H26 | -2,781135 | 2,024243 | 0,711493 |
| H27 | -2,414126 | 2,848066 | 3,612406 | H27 | -2,969282 | 3,321668 | 2,800132 |
| H28 | -1,625435 | -0,912015 | 5,551468 | H28 | -1,904638 | -0,172456 | 5,069230 |
| H29 | -1,997584 | 1,542293 | 5,694936 | H29 | -2,528359 | 2,233407 | 4,993652 |
| O30 | 0,936993 | -4,411064 | 0,298800 | O30 | 0,912404 | -4,326300 | 0,323634 |
| C31 | 2,449521 | -1,978151 | 1,650609 | C31 | 2,419714 | -2,075277 | 2,005020 |
| C32 | 1,456690 | -1,414826 | 2,448738 | C32 | 1,323560 | -1,571081 | 2,700566 |
| C33 | 3,722623 | -2,190418 | 2,203616 | C33 | 3,607148 | -2,329355 | 2,710048 |
| C34 | 1,728665 | -1,054800 | 3,770777 | C34 | 1,413503 | -1,294567 | 4,066304 |
| H35 | 0,472503 | -1,229012 | 2,045799 | H35 | 0,405599 | -1,362006 | 2,173449 |
| C36 | 3,993782 | -1,838665 | 3,521934 | C36 | 3,697237 | -2,059344 | 4,073128 |
| H37 | 4,513786 | -2,612347 | 1,589097 | H37 | 4,472926 | -2,724655 | 2,185070 |
| C38 | 2,994017 | -1,264613 | 4,311595 | C38 | 2,598091 | -1,533947 | 4,758681 |
| H39 | 0,941271 | -0,603588 | 4,366479 | H39 | 0,553126 | -0,874223 | 4,578375 |
| H40 | 4,986150 | -2,006081 | 3,930510 | H40 | 4,627776 | -2,254300 | 4,598509 |
| H41 | 3,205162 | -0,983289 | 5,339237 | H41 | 2,669848 | -1,314269 | 5,819743 |
| C42 | -3,667902 | -0,565728 | -0,170451 | C42 | -3,335599 | -0,372192 | -0,942283 |
| C43 | -4,778100 | -0,172600 | 0,590746 | C43 | -4,581505 | 0,022343 | -0,433700 |
| C44 | -3,812565 | -0,700021 | -1,562632 | C44 | -3,232178 | -0,748051 | -2,291199 |
| C45 | -5,999969 | 0,097119 | -0,027783 | C45 | -5,702863 | 0,043420 | -1,263300 |
| H46 | -4,688912 | -0,063927 | 1,667032 | H46 | -4,683579 | 0,302499 | 0,609740 |
| C47 | -5,036585 | -0,436730 | -2,178014 | C47 | -4,356932 | -0,733646 | -3,113581 |
| C48 | -6,133241 | -0,029785 | -1,412401 | C48 | -5,595286 | -0,338318 | -2,602300 |

| | | | | | | | |
|-----|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H49 | -6,849756 | 0,405528 | 0,574736 | H49 | -6,663079 | 0,352551 | -0,860252 |
| H50 | -5,133328 | -0,543575 | -3,254901 | H50 | -4,263008 | -1,014769 | -4,158277 |
| H51 | -7,085484 | 0,179528 | -1,890842 | H51 | -6,470526 | -0,323187 | -3,245139 |
| H52 | -0,743069 | -1,359252 | -1,966227 | H52 | -0,029588 | -0,825621 | -2,156933 |
| H53 | -1,673549 | 1,598960 | -3,371206 | H53 | 1,848624 | -0,275747 | -1,317886 |
| H54 | -1,639625 | -2,047044 | 3,360552 | H54 | -1,665664 | -1,463170 | 2,979884 |
| H55 | -2,958898 | -0,999712 | -2,164479 | H55 | -2,268398 | -1,033893 | -2,697402 |
| H56 | 2,657731 | -4,341792 | -0,841329 | H56 | 2,816179 | -4,409252 | -0,468605 |
| C57 | 4,612981 | -0,181652 | -2,650617 | C57 | 5,382240 | -0,565831 | -1,966770 |
| C58 | 4,060871 | -1,410630 | -3,014334 | C58 | 4,689876 | -1,687098 | -2,426679 |
| C59 | 3,319078 | -2,145595 | -2,091060 | C59 | 3,731871 | -2,297686 | -1,618760 |
| C60 | 3,129309 | -1,673263 | -0,786880 | C60 | 3,460367 | -1,814206 | -0,330529 |
| C61 | 3,679038 | -0,434115 | -0,434076 | C61 | 4,148599 | -0,677413 | 0,113064 |
| C62 | 4,413801 | 0,305722 | -1,358810 | C62 | 5,101091 | -0,060508 | -0,697951 |
| H63 | 5,193584 | 0,389499 | -3,369849 | H63 | 6,127337 | -0,087427 | -2,595723 |
| H64 | 4,201311 | -1,796091 | -4,019970 | H64 | 4,888096 | -2,083469 | -3,418514 |
| H65 | 2,862793 | -3,075593 | -2,416078 | H65 | 3,176876 | -3,140338 | -2,019790 |
| H66 | 3,511150 | -0,030488 | 0,556826 | H66 | 3,932633 | -0,267179 | 1,092956 |
| H67 | 4,830743 | 1,264470 | -1,062513 | H67 | 5,628753 | 0,816533 | -0,332897 |
| C68 | -4,159253 | 3,354906 | -0,659299 | C68 | 1,860865 | 3,456766 | -4,799203 |
| C69 | -3,104192 | 2,679817 | -1,266512 | C69 | 1,291795 | 3,152012 | -3,564777 |
| C70 | -1,774684 | 2,988935 | -0,943379 | C70 | 1,585962 | 1,937533 | -2,923334 |
| C71 | -1,527086 | 3,983033 | 0,008623 | C71 | 2,460105 | 1,037998 | -3,537376 |
| C72 | -2,584371 | 4,671582 | 0,606901 | C72 | 3,027297 | 1,342565 | -4,775486 |
| C73 | -3,902422 | 4,359567 | 0,276805 | C73 | 2,728899 | 2,548995 | -5,409944 |
| H74 | -5,179671 | 3,084214 | -0,911429 | H74 | 1,618229 | 4,395663 | -5,288653 |
| H75 | -3,325310 | 1,892757 | -1,978033 | H75 | 0,595267 | 3,845785 | -3,102977 |
| H76 | -0,511231 | 4,221835 | 0,302356 | H76 | 2,685790 | 0,095998 | -3,052421 |
| H77 | -2,373476 | 5,448067 | 1,336586 | H77 | 3,699967 | 0,630757 | -5,246011 |
| H78 | -4,724043 | 4,889157 | 0,749881 | H78 | 3,165593 | 2,780374 | -6,377513 |
| C79 | -0,648162 | 2,187287 | -1,592308 | C79 | 0,989849 | 1,719253 | -1,559443 |
| C80 | -0,710005 | 2,061233 | -3,135593 | C80 | -0,423190 | 1,797097 | -1,310796 |
| C81 | 1,421467 | 3,745750 | -1,564667 | C92 | 2,509508 | 3,580016 | -0,575297 |
| C82 | 1,267776 | 2,010721 | -0,014321 | C93 | 1,780771 | 1,825754 | 0,751351 |
| C83 | 2,352841 | 3,982307 | -0,362194 | C94 | 3,224552 | 3,570785 | 0,789922 |
| H84 | 0,760743 | 4,590049 | -1,769651 | H95 | 1,769041 | 4,385811 | -0,663939 |
| H85 | 1,967404 | 3,506937 | -2,480342 | H96 | 3,200759 | 3,645014 | -1,417234 |
| H86 | 3,385152 | 4,189743 | -0,644966 | H97 | 4,260433 | 3,228188 | 0,706647 |
| H87 | 1,989907 | 4,771637 | 0,304174 | H98 | 3,191474 | 4,526096 | 1,314229 |
| N88 | 0,667051 | 2,574422 | -1,096476 | N99 | 1,854224 | 2,272999 | -0,520568 |
| O89 | 2,332286 | 2,730892 | 0,373459 | O100 | 2,496866 | 2,592059 | 1,586792 |
| O90 | 0,946351 | 0,972057 | 0,569397 | O101 | 1,146441 | 0,829601 | 1,122806 |
| H91 | 2,910626 | -4,391873 | 0,927894 | H102 | 2,722379 | -4,489422 | 1,312457 |
| N92 | -2,034951 | -2,677397 | 0,820548 | N103 | -1,920954 | -2,326405 | 0,491559 |
| C93 | -1,326036 | -3,576744 | -0,129100 | C104 | -1,178031 | -3,289805 | -0,362172 |
| H94 | -1,579832 | -3,356304 | -1,175408 | H105 | -1,280921 | -3,067156 | -1,433986 |
| C95 | -0,159791 | 5,680951 | -5,448716 | C107 | -3,381279 | 2,529983 | -4,341602 |
| C96 | -1,266154 | 5,558527 | -4,606731 | C108 | -3,501692 | 3,083403 | -3,068010 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|----------|-----------|
| C97 | -1,457781 | 4,396612 | -3,858972 | C109 | -2,537109 | 2,815543 | -2,097277 |
| C98 | -0,538049 | 3,340068 | -3,932057 | C110 | -1,444398 | 1,980092 | -2,371756 |
| C99 | 0,561193 | 3,469812 | -4,791863 | C111 | -1,345484 | 1,416693 | -3,654692 |
| C100 | 0,751396 | 4,628775 | -5,544846 | C112 | -2,295819 | 1,699106 | -4,629750 |
| H101 | -0,014721 | 6,585607 | -6,032154 | H113 | -4,127328 | 2,740447 | -5,102555 |
| H102 | -1,988539 | 6,367045 | -4,536203 | H114 | -4,342083 | 3,728740 | -2,828799 |
| H103 | -2,330244 | 4,314555 | -3,220968 | H115 | -2,626239 | 3,277433 | -1,116801 |
| H104 | 1,274077 | 2,651777 | -4,873712 | H116 | -0,520271 | 0,754438 | -3,885867 |
| H105 | 1,608235 | 4,708023 | -6,207924 | H117 | -2,194238 | 1,260044 | -5,618562 |
| H106 | 0,054285 | 1,332848 | -3,417752 | H107 | -0,690930 | 2,271203 | -0,366928 |
| H107 | 1,102180 | -0,314064 | -1,831597 | | | | |
| H108 | -0,890966 | 1,139564 | -1,213599 | | | | |

C1_ES_Cheltop_TS1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,026752 | -3,759265 | 0,025393 |
| C2 | -1,807645 | -4,773433 | 0,022319 |
| C3 | -3,163969 | -4,825659 | -0,727846 |
| C4 | -3,051042 | -3,262224 | 1,117920 |
| H5 | -4,913263 | -4,206915 | 0,486361 |
| H6 | -3,056941 | -4,606043 | -1,794963 |
| H7 | -3,513456 | -2,707796 | 1,934797 |
| H8 | -4,362837 | -2,945323 | -0,619038 |
| H9 | -1,147652 | -5,622171 | -0,155863 |
| H10 | -3,598929 | -5,825482 | -0,641729 |
| C11 | -2,270461 | -4,538438 | 1,478183 |
| H12 | -1,452506 | -4,356539 | 2,181538 |
| H13 | -2,907943 | -5,344600 | 1,851997 |
| C14 | 0,313774 | -3,269555 | -0,002880 |
| N15 | 0,969328 | -2,159626 | -0,031176 |
| C16 | 2,348363 | -2,428026 | 0,514782 |
| C17 | 2,389545 | -3,986227 | 0,432649 |
| P18 | -1,903817 | -0,816213 | 0,172941 |
| Ir19 | 0,176472 | -0,244997 | -0,705693 |
| C20 | -2,184660 | 0,023858 | 1,767467 |
| C21 | -2,406447 | 1,465068 | 4,160683 |
| C22 | -2,013464 | -0,621301 | 2,998441 |
| C23 | -2,461278 | 1,400700 | 1,745528 |
| C24 | -2,571493 | 2,115293 | 2,935269 |
| C25 | -2,131425 | 0,098130 | 4,189095 |
| H26 | -2,603968 | 1,909546 | 0,796176 |
| H27 | -2,790565 | 3,179026 | 2,907897 |
| H28 | -2,008282 | -0,413212 | 5,139826 |
| H29 | -2,494978 | 2,022634 | 5,088552 |
| O30 | 0,987883 | -4,368593 | 0,345093 |
| C31 | 2,427819 | -2,033160 | 1,996418 |
| C32 | 1,326685 | -1,558584 | 2,705633 |
| C33 | 3,640243 | -2,226325 | 2,677317 |
| C34 | 1,435801 | -1,252576 | 4,063289 |

C1_ES_Cheltop_INT1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,236530 | -3,496566 | 0,109269 |
| C2 | -2,154753 | -4,671755 | 0,595512 |
| C3 | -3,432607 | -4,783393 | -0,276097 |
| C4 | -3,319204 | -2,843704 | 1,169685 |
| H5 | -5,208465 | -3,742612 | 0,548955 |
| H6 | -3,201833 | -4,834686 | -1,344954 |
| H7 | -3,790027 | -2,074813 | 1,782508 |
| H8 | -4,412890 | -2,830017 | -0,736778 |
| H9 | -1,574338 | -5,589957 | 0,688158 |
| H10 | -3,983226 | -5,692102 | -0,016767 |
| C11 | -2,722539 | -4,061643 | 1,896217 |
| H12 | -1,960304 | -3,790996 | 2,633362 |
| H13 | -3,478162 | -4,699038 | 2,363917 |
| C14 | 0,117265 | -3,413369 | 0,460217 |
| N15 | 0,806376 | -2,331031 | 0,427287 |
| C16 | 2,171229 | -2,615017 | 0,961806 |
| C17 | 2,167200 | -4,177844 | 0,913184 |
| P18 | -1,835972 | -0,740733 | -0,032032 |
| Ir19 | 0,252906 | -0,525898 | -0,678026 |
| C20 | -2,108180 | 0,330749 | 1,417023 |
| C21 | -2,276153 | 2,062747 | 3,615447 |
| C22 | -2,001991 | -0,170725 | 2,721889 |
| C23 | -2,284159 | 1,710908 | 1,221379 |
| C24 | -2,370496 | 2,568761 | 2,315647 |
| C25 | -2,092382 | 0,693176 | 3,814449 |
| H26 | -2,360309 | 2,112427 | 0,214866 |
| H27 | -2,513764 | 3,633442 | 2,154849 |
| H28 | -2,018181 | 0,293115 | 4,821685 |
| H29 | -2,345449 | 2,733214 | 4,466864 |
| O30 | 0,749560 | -4,528580 | 0,837682 |
| C31 | 2,289397 | -2,107729 | 2,402599 |
| C32 | 1,359973 | -1,218749 | 2,948065 |
| C33 | 3,354237 | -2,541153 | 3,206120 |
| C34 | 1,494478 | -0,766378 | 4,260917 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H35 | 0,388139 | -1,397231 | 2,197933 | H35 | 0,538453 | -0,859953 | 2,346253 |
| C36 | 3,749161 | -1,928024 | 4,032454 | C36 | 3,491425 | -2,087173 | 4,517503 |
| H37 | 4,508942 | -2,595981 | 2,138460 | H37 | 4,096419 | -3,227013 | 2,804494 |
| C38 | 2,644209 | -1,433273 | 4,730545 | C38 | 2,559945 | -1,194529 | 5,051890 |
| H39 | 0,570776 | -0,856944 | 4,587198 | H39 | 0,760531 | -0,069345 | 4,656177 |
| H40 | 4,696835 | -2,076370 | 4,542142 | H40 | 4,326936 | -2,431931 | 5,119840 |
| H41 | 2,730023 | -1,191021 | 5,785891 | H41 | 2,665880 | -0,839622 | 6,072703 |
| C42 | -3,379567 | -0,427293 | -0,832560 | C42 | -3,195709 | -0,406639 | -1,197071 |
| C43 | -4,597641 | -0,039200 | -0,253156 | C43 | -4,384565 | 0,215741 | -0,787043 |
| C44 | -3,317844 | -0,652276 | -2,215963 | C44 | -3,111253 | -0,947208 | -2,489952 |
| C45 | -5,730119 | 0,128573 | -1,049135 | C45 | -5,464748 | 0,307450 | -1,665451 |
| H46 | -4,666979 | 0,131628 | 0,816375 | H46 | -4,477263 | 0,622673 | 0,214140 |
| C47 | -4,452266 | -0,485645 | -3,006366 | C47 | -4,191787 | -0,853882 | -3,360914 |
| C48 | -5,659591 | -0,093918 | -2,425160 | C48 | -5,370345 | -0,225033 | -2,950990 |
| H49 | -6,667896 | 0,432379 | -0,592380 | H49 | -6,380632 | 0,793236 | -1,341296 |
| H50 | -4,387142 | -0,641848 | -4,078493 | H50 | -4,107395 | -1,254919 | -4,365968 |
| H51 | -6,542481 | 0,042371 | -3,043236 | H51 | -6,211614 | -0,148483 | -3,633877 |
| H52 | -0,230137 | -0,919524 | -2,052003 | H52 | -0,250375 | -1,412071 | -1,866816 |
| H53 | 1,642090 | 0,147778 | -1,401239 | H53 | 1,925585 | 1,117744 | -2,875022 |
| H54 | -1,775983 | -1,679299 | 3,030751 | H54 | -1,834204 | -1,230337 | 2,882616 |
| H55 | -2,376687 | -0,931660 | -2,675942 | H55 | -2,190635 | -1,411962 | -2,823041 |
| H56 | 2,890705 | -4,377735 | -0,455010 | H56 | 2,650197 | -4,571650 | 0,013693 |
| C57 | 5,289439 | -0,436039 | -1,992737 | C57 | 4,911375 | -0,820029 | -1,904028 |
| C58 | 4,671404 | -1,609231 | -2,428285 | C58 | 3,819963 | -1,579157 | -2,330983 |
| C59 | 3,724379 | -2,242784 | -1,624599 | C59 | 2,973109 | -2,170369 | -1,392913 |
| C60 | 3,399517 | -1,738107 | -0,357331 | C60 | 3,187719 | -1,996755 | -0,012385 |
| C61 | 4,010230 | -0,547637 | 0,059296 | C61 | 4,277392 | -1,227273 | 0,402542 |
| C62 | 4,944382 | 0,097546 | -0,752038 | C62 | 5,137608 | -0,654016 | -0,537894 |
| H63 | 6,023804 | 0,060734 | -2,619843 | H63 | 5,582517 | -0,370810 | -2,630904 |
| H64 | 4,917159 | -2,027869 | -3,400112 | H64 | 3,632994 | -1,724065 | -3,391346 |
| H65 | 3,230906 | -3,130785 | -2,007206 | H65 | 2,137415 | -2,770589 | -1,739678 |
| H66 | 3,762609 | -0,130714 | 1,029014 | H66 | 4,446498 | -1,048812 | 1,457539 |
| H67 | 5,413468 | 1,014846 | -0,405614 | H67 | 5,985676 | -0,067933 | -0,194278 |
| C68 | 2,065579 | 3,392295 | -4,763384 | C68 | 0,674376 | 5,515007 | -2,762253 |
| C69 | 1,512088 | 3,101018 | -3,519468 | C69 | 0,939545 | 4,304360 | -2,125669 |
| C70 | 1,731941 | 1,848539 | -2,925207 | C70 | 1,290273 | 3,171416 | -2,870900 |
| C71 | 2,490867 | 0,891460 | -3,596382 | C71 | 1,379420 | 3,271304 | -4,260625 |
| C72 | 3,038800 | 1,182103 | -4,846583 | C72 | 1,106764 | 4,481095 | -4,900785 |
| C73 | 2,829025 | 2,431190 | -5,430724 | C73 | 0,752124 | 5,604384 | -4,154125 |
| H74 | 1,884977 | 4,360764 | -5,220610 | H74 | 0,401351 | 6,387615 | -2,175121 |
| H75 | 0,881080 | 3,830891 | -3,021486 | H75 | 0,868577 | 4,232107 | -1,042638 |
| H76 | 2,637661 | -0,084617 | -3,147564 | H76 | 1,631510 | 2,392401 | -4,847458 |
| H77 | 3,622887 | 0,427614 | -5,365610 | H77 | 1,166985 | 4,543791 | -5,983584 |
| H78 | 3,248246 | 2,653965 | -6,407687 | H78 | 0,537030 | 6,545301 | -4,652562 |
| C79 | 1,116157 | 1,605328 | -1,572825 | C79 | 1,466707 | 1,827277 | -2,172568 |
| C80 | -0,340749 | 1,713569 | -1,383165 | C80 | 0,059565 | 1,287973 | -1,727192 |
| C92 | 2,689443 | 3,420946 | -0,562317 | C92 | 3,718276 | 2,642193 | -1,259829 |
| C93 | 1,687283 | 1,817259 | 0,791545 | C93 | 2,340261 | 1,487518 | 0,186670 |

| | | | | | | | |
|-------------------|-----------|-----------|-----------|--------------------|-----------|-----------|-----------|
| C94 | 3,251552 | 3,459270 | 0,874037 | C94 | 4,177869 | 2,826490 | 0,193662 |
| H95 | 2,049246 | 4,282163 | -0,790233 | H95 | 3,611564 | 3,587728 | -1,793709 |
| H96 | 3,470797 | 3,354222 | -1,321456 | H96 | 4,372968 | 1,974377 | -1,832310 |
| H97 | 4,267560 | 3,057461 | 0,928581 | H97 | 5,227264 | 2,581196 | 0,360332 |
| H98 | 3,221548 | 4,448715 | 1,331044 | H98 | 3,966818 | 3,830810 | 0,573717 |
| N99 | 1,907108 | 2,188945 | -0,492585 | N99 | 2,413534 | 2,005931 | -1,053818 |
| O100 | 2,386183 | 2,579115 | 1,645086 | O100 | 3,373213 | 1,883084 | 0,948665 |
| O101 | 0,960452 | 0,887150 | 1,157636 | O101 | 1,486310 | 0,719863 | 0,665301 |
| H102 | 2,808714 | -4,445266 | 1,326166 | H102 | 2,577948 | -4,650626 | 1,803012 |
| N103 | -1,944695 | -2,472467 | 0,509032 | N103 | -2,081141 | -2,319603 | 0,523147 |
| C104 | -1,152276 | -3,411789 | -0,325411 | C104 | -1,323240 | -3,490878 | 0,029357 |
| H105 | -1,254276 | -3,199388 | -1,399464 | H105 | -1,300870 | -3,537355 | -1,070525 |
| C107 | -3,175575 | 2,396908 | -4,548633 | C107 | -2,433211 | 1,481414 | -5,258193 |
| C108 | -3,331045 | 2,993715 | -3,298652 | C108 | -2,703069 | 2,296030 | -4,159063 |
| C109 | -2,397218 | 2,754981 | -2,291275 | C109 | -1,906565 | 2,217683 | -3,017088 |
| C110 | -1,299814 | 1,907351 | -2,502464 | C110 | -0,838693 | 1,315391 | -2,937578 |
| C111 | -1,167473 | 1,294427 | -3,761210 | C111 | -0,587364 | 0,493972 | -4,047258 |
| C112 | -2,089010 | 1,547397 | -4,773052 | C112 | -1,369002 | 0,578415 | -5,197462 |
| H113 | -3,896103 | 2,586057 | -5,339253 | H113 | -3,045260 | 1,548319 | -6,153354 |
| H114 | -4,176260 | 3,648591 | -3,106121 | H114 | -3,529202 | 3,001140 | -4,192874 |
| H115 | -2,520468 | 3,237733 | -1,323814 | H115 | -2,102779 | 2,884706 | -2,180884 |
| H116 | -0,342147 | 0,616604 | -3,945697 | H116 | 0,230020 | -0,222274 | -4,000589 |
| H117 | -1,962775 | 1,072715 | -5,742507 | H117 | -1,150730 | -0,061957 | -6,048448 |
| H107 | -0,605482 | 2,315601 | -0,512655 | H107 | -0,313217 | 2,030575 | -1,008705 |
| C1_ES_Cheltop_TS2 | | | | C1_ES_Cheltop_INT2 | | | |
| C1 | -4,270611 | -3,334181 | 0,391654 | C1 | -4,284394 | -3,315052 | 0,401414 |
| C2 | -2,197265 | -4,561846 | 0,760893 | C2 | -2,221698 | -4,565507 | 0,750002 |
| C3 | -3,535809 | -4,654367 | -0,014407 | C3 | -3,558142 | -4,631278 | -0,031672 |
| C4 | -3,259085 | -2,680708 | 1,363016 | C4 | -3,270202 | -2,689578 | 1,389504 |
| H5 | -5,212097 | -3,537685 | 0,912211 | H5 | -5,228525 | -3,523474 | 0,915211 |
| H6 | -3,383710 | -4,738425 | -1,095097 | H6 | -3,403050 | -4,692145 | -1,113629 |
| H7 | -3,660975 | -1,881134 | 1,985466 | H7 | -3,669331 | -1,901107 | 2,027871 |
| H8 | -4,495254 | -2,689444 | -0,458966 | H8 | -4,502768 | -2,651283 | -0,435964 |
| H9 | -1,643496 | -5,496912 | 0,842171 | H9 | -1,675084 | -5,506373 | 0,812358 |
| H10 | -4,093285 | -5,538606 | 0,307457 | H10 | -4,123172 | -5,518561 | 0,268003 |
| C11 | -2,649951 | -3,897644 | 2,080542 | C11 | -2,673588 | -3,926818 | 2,082395 |
| H12 | -1,828602 | -3,632566 | 2,753238 | H12 | -1,851756 | -3,683603 | 2,762510 |
| H13 | -3,390500 | -4,495283 | 2,619450 | H13 | -3,420330 | -4,530604 | 2,605637 |
| C14 | 0,096471 | -3,389849 | 0,460621 | C14 | 0,082356 | -3,405084 | 0,478186 |
| N15 | 0,865908 | -2,378601 | 0,260947 | N15 | 0,862755 | -2,404869 | 0,270551 |
| C16 | 2,199445 | -2,697368 | 0,881588 | C16 | 2,190204 | -2,722838 | 0,905151 |
| C17 | 2,077814 | -4,244128 | 1,039371 | C17 | 2,056360 | -4,265123 | 1,082713 |
| P18 | -1,824999 | -0,694376 | -0,082670 | P18 | -1,826299 | -0,684601 | -0,026825 |
| Ir19 | 0,236056 | -0,559728 | -0,859118 | Ir19 | 0,290779 | -0,602884 | -0,908234 |
| C20 | -2,084959 | 0,497509 | 1,271939 | C20 | -2,068451 | 0,505354 | 1,336931 |
| C21 | -2,226919 | 2,416779 | 3,308323 | C21 | -2,198114 | 2,425606 | 3,381282 |
| C22 | -1,896915 | 0,123948 | 2,609850 | C22 | -1,894127 | 0,128603 | 2,675438 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C23 | -2,353553 | 1,841687 | 0,964297 | C23 | -2,314294 | 1,855004 | 1,032772 |
| C24 | -2,420865 | 2,794458 | 1,977579 | C24 | -2,375411 | 2,806811 | 2,048745 |
| C25 | -1,973480 | 1,080882 | 3,621945 | C25 | -1,964516 | 1,084622 | 3,690158 |
| H26 | -2,523263 | 2,142083 | -0,064254 | H26 | -2,476531 | 2,161554 | 0,004224 |
| H27 | -2,631503 | 3,830524 | 1,728353 | H27 | -2,570916 | 3,845823 | 1,799027 |
| H28 | -1,836113 | 0,780624 | 4,656952 | H28 | -1,839532 | 0,777567 | 4,724818 |
| H29 | -2,282029 | 3,160120 | 4,098355 | H29 | -2,250083 | 3,167201 | 4,172801 |
| O30 | 0,641724 | -4,482760 | 1,005016 | O30 | 0,617049 | -4,495101 | 1,039013 |
| C31 | 2,308524 | -2,075141 | 2,280275 | C31 | 2,298954 | -2,074210 | 2,291472 |
| C32 | 1,320527 | -1,250367 | 2,812633 | C32 | 1,300584 | -1,257340 | 2,817166 |
| C33 | 3,440156 | -2,367598 | 3,057120 | C33 | 3,435304 | -2,342590 | 3,070194 |
| C34 | 1,459985 | -0,713869 | 4,093988 | C34 | 1,433107 | -0,707105 | 4,093958 |
| H35 | 0,458170 | -0,996558 | 2,216348 | H35 | 0,432579 | -1,023216 | 2,221257 |
| C36 | 3,580091 | -1,835507 | 4,335874 | C36 | 3,566831 | -1,798518 | 4,345432 |
| H37 | 4,228411 | -2,995874 | 2,648334 | H37 | 4,230409 | -2,966781 | 2,667999 |
| C38 | 2,587367 | -1,002407 | 4,858891 | C38 | 2,563092 | -0,974446 | 4,863718 |
| H39 | 0,686438 | -0,056312 | 4,480808 | H39 | 0,649709 | -0,057141 | 4,473294 |
| H40 | 4,465340 | -2,065226 | 4,921885 | H40 | 4,454885 | -2,013548 | 4,932838 |
| H41 | 2,697921 | -0,581277 | 5,854073 | H41 | 2,667245 | -0,545515 | 5,855964 |
| C42 | -3,210043 | -0,449196 | -1,247607 | C42 | -3,224192 | -0,409461 | -1,173183 |
| C43 | -4,421750 | 0,117257 | -0,820831 | C43 | -4,428471 | 0,164547 | -0,735699 |
| C44 | -3,120075 | -0,991417 | -2,538353 | C44 | -3,147525 | -0,938432 | -2,470778 |
| C45 | -5,518856 | 0,151437 | -1,680650 | C45 | -5,529848 | 0,218861 | -1,589255 |
| H46 | -4,518632 | 0,525051 | 0,179847 | H46 | -4,513945 | 0,566009 | 0,268841 |
| C47 | -4,218927 | -0,954936 | -3,391579 | C47 | -4,251325 | -0,885782 | -3,317873 |
| C48 | -5,419161 | -0,382179 | -2,965790 | C48 | -5,443317 | -0,305435 | -2,879870 |
| H49 | -6,451402 | 0,594920 | -1,343448 | H49 | -6,456037 | 0,668890 | -1,243264 |
| H50 | -4,130626 | -1,356378 | -4,396163 | H50 | -4,171658 | -1,277735 | -4,327008 |
| H51 | -6,273815 | -0,348704 | -3,635399 | H51 | -6,301924 | -0,258240 | -3,543636 |
| H52 | -0,285583 | -1,454994 | -2,033056 | H52 | -0,294534 | -1,521870 | -2,040990 |
| H53 | 1,706015 | 1,610778 | -2,985633 | H53 | 1,763996 | 1,590537 | -2,943609 |
| H54 | -1,682918 | -0,909433 | 2,860323 | H54 | -1,695967 | -0,908064 | 2,926061 |
| H55 | -2,182111 | -1,408102 | -2,885373 | H55 | -2,215490 | -1,358526 | -2,829946 |
| H56 | 2,523408 | -4,812612 | 0,219737 | H56 | 2,506177 | -4,847656 | 0,274816 |
| C57 | 5,322285 | -1,381730 | -1,837350 | C57 | 5,085677 | -1,290685 | -1,989207 |
| C58 | 4,550563 | -2,505095 | -2,141787 | C58 | 4,365455 | -2,462661 | -2,232934 |
| C59 | 3,558603 | -2,933160 | -1,260793 | C59 | 3,478177 | -2,950750 | -1,274716 |
| C60 | 3,325844 | -2,255549 | -0,056020 | C60 | 3,296110 | -2,283494 | -0,055463 |
| C61 | 4,089838 | -1,115445 | 0,229904 | C61 | 4,018649 | -1,106223 | 0,178612 |
| C62 | 5,083010 | -0,686396 | -0,652575 | C62 | 4,908890 | -0,617425 | -0,780203 |
| H63 | 6,101058 | -1,053006 | -2,519618 | H63 | 5,779530 | -0,910950 | -2,733818 |
| H64 | 4,719279 | -3,048248 | -3,067044 | H64 | 4,491000 | -2,994848 | -3,171472 |
| H65 | 2,950531 | -3,789222 | -1,536703 | H65 | 2,897527 | -3,838370 | -1,507120 |
| H66 | 3,907818 | -0,555762 | 1,139656 | H66 | 3,871881 | -0,555842 | 1,100738 |
| H67 | 5,673313 | 0,192458 | -0,406019 | H67 | 5,470335 | 0,290381 | -0,574921 |
| C68 | 0,056245 | 5,720461 | -1,875603 | C68 | -0,007559 | 5,679008 | -1,921578 |
| C69 | 0,451845 | 4,430427 | -1,527431 | C69 | 0,402257 | 4,399047 | -1,553533 |
| C70 | 0,859849 | 3,522664 | -2,513347 | C70 | 0,868320 | 3,497423 | -2,519195 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C71 | 0,867548 | 3,925583 | -3,850280 | C71 | 0,919291 | 3,896545 | -3,856210 |
| C72 | 0,466656 | 5,215663 | -4,201249 | C72 | 0,503957 | 5,176289 | -4,227463 |
| C73 | 0,060692 | 6,115170 | -3,215827 | C73 | 0,040349 | 6,069650 | -3,262004 |
| H74 | -0,257728 | 6,418251 | -1,104072 | H74 | -0,367381 | 6,371656 | -1,165596 |
| H75 | 0,438038 | 4,120882 | -0,484364 | H75 | 0,352360 | 4,091932 | -0,510894 |
| H76 | 1,159995 | 3,218602 | -4,622255 | H76 | 1,257146 | 3,194005 | -4,613583 |
| H77 | 0,467710 | 5,515538 | -5,245243 | H77 | 0,539133 | 5,473071 | -5,271747 |
| H78 | -0,251885 | 7,119000 | -3,488865 | H78 | -0,283347 | 7,065526 | -3,550919 |
| C79 | 1,208645 | 2,088125 | -2,132571 | C79 | 1,220196 | 2,069598 | -2,119000 |
| C80 | -0,106432 | 1,303807 | -1,804859 | C80 | -0,087803 | 1,265586 | -1,841775 |
| C81 | 3,457737 | 2,838283 | -1,164236 | C81 | 3,406461 | 2,860647 | -1,044793 |
| C82 | 2,084958 | 1,572292 | 0,197177 | C82 | 1,983023 | 1,586924 | 0,259823 |
| C83 | 3,843637 | 3,012860 | 0,311323 | C83 | 3,717419 | 3,049666 | 0,446996 |
| H84 | 3,315333 | 3,789740 | -1,680429 | H84 | 3,268576 | 3,807599 | -1,570635 |
| H85 | 4,175844 | 2,225938 | -1,724570 | H85 | 4,163832 | 2,264574 | -1,568998 |
| H86 | 4,901370 | 2,850268 | 0,519921 | H86 | 4,765716 | 2,902755 | 0,708502 |
| H87 | 3,531753 | 3,983902 | 0,708714 | H87 | 3,374942 | 4,019817 | 0,820717 |
| N88 | 2,187114 | 2,121613 | -1,028658 | N88 | 2,146509 | 2,117464 | -0,968749 |
| O89 | 3,087374 | 1,980393 | 0,999836 | O89 | 2,941710 | 2,013081 | 1,106138 |
| O90 | 1,249433 | 0,756181 | 0,617528 | O90 | 1,128129 | 0,776668 | 0,650839 |
| H91 | 2,455710 | -4,608715 | 1,992641 | H91 | 2,422879 | -4,619229 | 2,044333 |
| N92 | -2,049495 | -2,214234 | 0,622235 | N92 | -2,055513 | -2,213198 | 0,665236 |
| C93 | -1,367268 | -3,426609 | 0,105935 | C93 | -1,382088 | -3,422757 | 0,122587 |
| H94 | -1,416899 | -3,494665 | -0,990914 | H94 | -1,431564 | -3,465963 | -0,975108 |
| C95 | -2,496480 | 1,482293 | -5,406655 | C95 | -2,423782 | 1,440246 | -5,479051 |
| C96 | -2,839568 | 2,252882 | -4,295885 | C96 | -2,783083 | 2,205633 | -4,369748 |
| C97 | -2,070604 | 2,186262 | -3,135093 | C97 | -2,030378 | 2,134208 | -3,199113 |
| C98 | -0,961685 | 1,335117 | -3,047745 | C98 | -0,916780 | 1,289464 | -3,101544 |
| C99 | -0,623095 | 0,573673 | -4,175502 | C99 | -0,565161 | 0,529594 | -4,225935 |
| C100 | -1,379427 | 0,645499 | -5,344056 | C100 | -1,307354 | 0,603594 | -5,403896 |
| H101 | -3,090263 | 1,535550 | -6,314909 | H101 | -3,005541 | 1,495559 | -6,395040 |
| H102 | -3,701741 | 2,913017 | -4,334669 | H102 | -3,647464 | 2,862370 | -4,416209 |
| H103 | -2,322783 | 2,821537 | -2,289726 | H103 | -2,300711 | 2,757683 | -2,350660 |
| H104 | 0,231913 | -0,096415 | -4,122521 | H104 | 0,289632 | -0,140033 | -4,167529 |
| H105 | -1,100943 | 0,045596 | -6,206661 | H105 | -1,017951 | 0,005467 | -6,264103 |
| H106 | -0,597482 | 1,920986 | -1,045311 | H106 | -0,615783 | 1,854357 | -1,085278 |
| H107 | 2,532304 | -0,352007 | -1,755555 | H107 | 2,027015 | -0,529438 | -1,430504 |
| H108 | 2,514286 | -0,506386 | -2,487906 | H108 | 1,606264 | -0,798939 | -2,085190 |

C1_ES_Cheltop_TS3

| | | | |
|----|-----------|-----------|-----------|
| C1 | -4,312000 | -3,322437 | 0,506855 |
| C2 | -2,228695 | -4,536352 | 0,867410 |
| C3 | -3,570544 | -4,638056 | 0,098770 |
| C4 | -3,294897 | -2,656585 | 1,464824 |
| H5 | -5,246358 | -3,532051 | 1,037909 |
| H6 | -3,422934 | -4,722414 | -0,982623 |
| H7 | -3,695770 | -1,854008 | 2,084342 |
| H8 | -4,550559 | -2,683811 | -0,344254 |

C1_ES_Cheltop_PROD

| | | | |
|----|-----------|-----------|-----------|
| C1 | -4,286520 | -3,433255 | 0,557377 |
| C2 | -2,187377 | -4,581184 | 1,034519 |
| C3 | -3,508585 | -4,754013 | 0,241444 |
| C4 | -3,314131 | -2,702360 | 1,513435 |
| H5 | -5,238264 | -3,633237 | 1,060540 |
| H6 | -3,334590 | -4,898461 | -0,829603 |
| H7 | -3,750533 | -1,881319 | 2,082874 |
| H8 | -4,499326 | -2,836608 | -0,331551 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H9 | -1,671929 | -5,469413 | 0,950086 | H9 | -1,611043 | -5,495292 | 1,176370 |
| H10 | -4,120002 | -5,526019 | 0,424192 | H10 | -4,048363 | -5,632590 | 0,606416 |
| C11 | -2,676873 | -3,866879 | 2,186180 | C11 | -2,686442 | -3,861136 | 2,307694 |
| H12 | -1,852297 | -3,595053 | 2,851985 | H12 | -1,885748 | -3,536658 | 2,978804 |
| H13 | -3,410744 | -4,465824 | 2,732755 | H13 | -3,419062 | -4,452393 | 2,864468 |
| C14 | 0,052693 | -3,345789 | 0,563420 | C14 | 0,072331 | -3,345417 | 0,700789 |
| N15 | 0,844791 | -2,353677 | 0,325540 | N15 | 0,866858 | -2,381923 | 0,356428 |
| C16 | 2,161971 | -2,643977 | 1,012910 | C16 | 2,183249 | -2,573539 | 1,092725 |
| C17 | 2,011777 | -4,172752 | 1,260762 | C17 | 2,035995 | -4,068791 | 1,495299 |
| P18 | -1,863207 | -0,693989 | -0,053029 | P18 | -1,851121 | -0,775982 | -0,038358 |
| Ir19 | 0,402377 | -0,702897 | -0,978802 | Ir19 | 0,389529 | -0,865133 | -0,935307 |
| C20 | -2,148262 | 0,551585 | 1,251311 | C20 | -2,152066 | 0,511704 | 1,226906 |
| C21 | -2,299444 | 2,580513 | 3,186648 | C21 | -2,357452 | 2,602339 | 3,092542 |
| C22 | -1,972204 | 0,251648 | 2,609521 | C22 | -2,056612 | 0,249776 | 2,600108 |
| C23 | -2,408299 | 1,880569 | 0,875739 | C23 | -2,353195 | 1,835586 | 0,800672 |
| C24 | -2,477294 | 2,887660 | 1,836430 | C24 | -2,447932 | 2,873197 | 1,725296 |
| C25 | -2,055969 | 1,260839 | 3,569479 | C25 | -2,169428 | 1,289336 | 3,525454 |
| H26 | -2,588091 | 2,124018 | -0,165777 | H26 | -2,468080 | 2,053697 | -0,256712 |
| H27 | -2,682228 | 3,909477 | 1,529525 | H27 | -2,605738 | 3,890634 | 1,377624 |
| H28 | -1,933705 | 1,012924 | 4,620263 | H28 | -2,109447 | 1,070034 | 4,588038 |
| H29 | -2,360386 | 3,363316 | 3,937030 | H29 | -2,440473 | 3,408565 | 3,815740 |
| O30 | 0,573706 | -4,398031 | 1,190802 | O30 | 0,599225 | -4,306768 | 1,456946 |
| C31 | 2,218164 | -1,937711 | 2,374916 | C31 | 2,215711 | -1,731852 | 2,374649 |
| C32 | 1,211768 | -1,085321 | 2,823121 | C32 | 1,189879 | -0,864957 | 2,743461 |
| C33 | 3,312842 | -2,192426 | 3,215421 | C33 | 3,308338 | -1,893796 | 3,241824 |
| C34 | 1,299150 | -0,483021 | 4,079589 | C34 | 1,256822 | -0,157227 | 3,944959 |
| H35 | 0,371162 | -0,864556 | 2,184224 | H35 | 0,344884 | -0,715349 | 2,089839 |
| C36 | 3,400845 | -1,595141 | 4,469450 | C36 | 3,375585 | -1,191504 | 4,441489 |
| H37 | 4,113106 | -2,845885 | 2,877271 | H37 | 4,121090 | -2,561750 | 2,966345 |
| C38 | 2,391752 | -0,732827 | 4,905694 | C38 | 2,346653 | -0,315376 | 4,796618 |
| H39 | 0,511703 | 0,193761 | 4,398184 | H39 | 0,452293 | 0,525520 | 4,200986 |
| H40 | 4,259135 | -1,797705 | 5,103492 | H40 | 4,231366 | -1,325717 | 5,096986 |
| H41 | 2,461736 | -0,260851 | 5,881514 | H41 | 2,398520 | 0,236985 | 5,730655 |
| C42 | -3,257445 | -0,480523 | -1,219502 | C42 | -3,218802 | -0,524706 | -1,233028 |
| C43 | -4,490595 | 0,061757 | -0,824146 | C43 | -4,468126 | -0,011273 | -0,846436 |
| C44 | -3,124688 | -1,010665 | -2,511487 | C44 | -3,028362 | -0,929162 | -2,562703 |
| C45 | -5,565868 | 0,080777 | -1,711153 | C45 | -5,501289 | 0,098967 | -1,774729 |
| H46 | -4,615026 | 0,469342 | 0,174215 | H46 | -4,632543 | 0,310626 | 0,177587 |
| C47 | -4,202763 | -0,993441 | -3,393732 | C47 | -4,064628 | -0,819468 | -3,489327 |
| C48 | -5,423972 | -0,446724 | -2,996077 | C48 | -5,300511 | -0,304041 | -3,097447 |
| H49 | -6,515332 | 0,505397 | -1,397252 | H49 | -6,462844 | 0,500076 | -1,466574 |
| H50 | -4,083037 | -1,390586 | -4,397037 | H50 | -3,898226 | -1,116038 | -4,520379 |
| H51 | -6,262784 | -0,428759 | -3,686038 | H51 | -6,105841 | -0,211355 | -3,820714 |
| H52 | -0,120143 | -1,747571 | -2,020912 | H52 | -0,045028 | -1,974537 | -1,943550 |
| H53 | 1,705924 | 1,797545 | -3,103234 | H53 | 1,637235 | 2,100797 | -3,373237 |
| H54 | -1,764667 | -0,767448 | 2,918045 | H54 | -1,881583 | -0,762643 | 2,948867 |
| H55 | -2,169271 | -1,409881 | -2,833806 | H55 | -2,061142 | -1,308618 | -2,876142 |
| H56 | 2,477237 | -4,795680 | 0,493493 | H56 | 2,499788 | -4,761899 | 0,789564 |

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|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C57 | 5,328281 | -1,524135 | -1,731502 | C57 | 5,398528 | -1,813733 | -1,714134 |
| C58 | 4,529719 | -2,639708 | -1,991381 | C58 | 4,541385 | -2,901847 | -1,893010 |
| C59 | 3,539230 | -3,015127 | -1,086898 | C59 | 3,530358 | -3,151417 | -0,969517 |
| C60 | 3,331218 | -2,289797 | 0,094669 | C60 | 3,358892 | -2,326012 | 0,150235 |
| C61 | 4,131181 | -1,169197 | 0,343319 | C61 | 4,212202 | -1,231545 | 0,315276 |
| C62 | 5,122561 | -0,791264 | -0,563076 | C62 | 5,227107 | -0,980674 | -0,609655 |
| H63 | 6,103613 | -1,232088 | -2,434233 | H63 | 6,192095 | -1,620250 | -2,430599 |
| H64 | 4,673179 | -3,214017 | -2,901951 | H64 | 4,655580 | -3,551625 | -2,755808 |
| H65 | 2,898854 | -3,856806 | -1,334187 | H65 | 2,844935 | -3,973751 | -1,153281 |
| H66 | 3,969086 | -0,572690 | 1,232134 | H66 | 4,076826 | -0,558155 | 1,151787 |
| H67 | 5,739420 | 0,077740 | -0,348227 | H67 | 5,891424 | -0,133400 | -0,458319 |
| C68 | -0,068364 | 5,672034 | -1,450077 | C68 | -0,218971 | 5,476803 | -0,903713 |
| C69 | 0,398999 | 4,371235 | -1,272778 | C69 | 0,258692 | 4,173788 | -1,022535 |
| C70 | 0,811268 | 3,612060 | -2,375447 | C70 | 0,731629 | 3,705884 | -2,257196 |
| C71 | 0,754237 | 4,171296 | -3,653329 | C71 | 0,721064 | 4,555210 | -3,364454 |
| C72 | 0,284924 | 5,473545 | -3,832018 | C72 | 0,242057 | 5,861763 | -3,244811 |
| C73 | -0,128190 | 6,224991 | -2,731954 | C73 | -0,228814 | 6,323424 | -2,016294 |
| H74 | -0,387405 | 6,255175 | -0,590556 | H74 | -0,583701 | 5,833480 | 0,055783 |
| H75 | 0,434376 | 3,938545 | -0,275232 | H75 | 0,251277 | 3,516648 | -0,155635 |
| H76 | 1,054214 | 3,578804 | -4,513925 | H76 | 1,070741 | 4,190695 | -4,327226 |
| H77 | 0,238452 | 5,898302 | -4,830549 | H77 | 0,235075 | 6,515816 | -4,111856 |
| H78 | -0,495151 | 7,237846 | -2,870978 | H78 | -0,602093 | 7,339284 | -1,923378 |
| C79 | 1,234331 | 2,160616 | -2,180669 | C79 | 1,202844 | 2,260438 | -2,380135 |
| C80 | -0,028667 | 1,299995 | -1,888564 | C80 | -0,023708 | 1,324928 | -2,245622 |
| C81 | 3,535771 | 2,779196 | -1,281010 | C81 | 3,589418 | 2,629000 | -1,625785 |
| C82 | 2,163181 | 1,512559 | 0,089121 | C82 | 2,171248 | 1,509691 | -0,161698 |
| C83 | 3,981630 | 2,883763 | 0,185494 | C83 | 4,134573 | 2,679300 | -0,186041 |
| H84 | 3,400429 | 3,756041 | -1,751579 | H84 | 3,475853 | 3,625654 | -2,062515 |
| H85 | 4,215492 | 2,172963 | -1,892436 | H85 | 4,201226 | 2,010446 | -2,292167 |
| H86 | 5,037977 | 2,666304 | 0,345386 | H86 | 5,156227 | 2,309536 | -0,093192 |
| H87 | 3,731636 | 3,853531 | 0,627148 | H87 | 4,061088 | 3,676941 | 0,256763 |
| N88 | 2,252544 | 2,093131 | -1,124848 | N88 | 2,282584 | 2,003428 | -1,416785 |
| O89 | 3,205303 | 1,864740 | 0,868029 | O89 | 3,268966 | 1,791633 | 0,564729 |
| O90 | 1,293346 | 0,744768 | 0,522096 | O90 | 1,234611 | 0,872205 | 0,334947 |
| H91 | 2,350490 | -4,481807 | 2,247540 | H91 | 2,381899 | -4,274971 | 2,506027 |
| N92 | -2,095817 | -2,186579 | 0,714740 | N92 | -2,112337 | -2,240940 | 0,768604 |
| C93 | -1,409533 | -3,399006 | 0,201883 | C93 | -1,384040 | -3,457603 | 0,327998 |
| H94 | -1,459573 | -3,478009 | -0,893623 | H94 | -1,414827 | -3,590080 | -0,762850 |
| C95 | -2,728348 | 1,712190 | -5,232967 | C95 | -2,760058 | 1,970142 | -5,510160 |
| C96 | -2,942639 | 2,430669 | -4,056686 | C96 | -2,965818 | 2,608997 | -4,286439 |
| C97 | -2,073366 | 2,278924 | -2,979099 | C97 | -2,085697 | 2,390993 | -3,229156 |
| C98 | -0,988349 | 1,395038 | -3,047184 | C98 | -0,996605 | 1,526163 | -3,381610 |
| C99 | -0,782374 | 0,681325 | -4,234254 | C99 | -0,791615 | 0,892765 | -4,611354 |
| C100 | -1,641106 | 0,840875 | -5,320824 | C100 | -1,669485 | 1,113286 | -5,672393 |
| H101 | -3,404243 | 1,828893 | -6,075306 | H101 | -3,447105 | 2,139060 | -6,334508 |
| H102 | -3,782996 | 3,114304 | -3,978144 | H102 | -3,811668 | 3,277507 | -4,154591 |
| H103 | -2,218713 | 2,879667 | -2,086619 | H103 | -2,232506 | 2,911938 | -2,287743 |
| H104 | 0,042985 | -0,024426 | -4,302397 | H104 | 0,050277 | 0,213973 | -4,734993 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H105 | -1,467376 | 0,277014 | -6,233173 | H105 | -1,505450 | 0,613999 | -6,623100 |
| H106 | -0,488911 | 1,729658 | -0,998898 | H106 | -0,507002 | 1,525374 | -1,295915 |
| H107 | 1,900232 | -0,915987 | -1,512540 | H107 | 1,854834 | -1,015969 | -1,578418 |
| H108 | 0,778736 | -0,055882 | -2,351456 | H108 | 0,372212 | 0,246418 | -2,390326 |

C1_Z_S_tN_Chelbot

C1_ZS_Chelbot_SM

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,834726 | -3,440265 | -1,131187 |
| C2 | -1,572816 | -4,361917 | -1,123160 |
| C3 | -2,812893 | -4,200243 | -2,041485 |
| C4 | -3,021692 | -3,235666 | 0,165912 |
| H5 | -4,724173 | -4,045921 | -0,928194 |
| H6 | -2,575031 | -3,653776 | -2,959722 |
| H7 | -3,602548 | -2,928361 | 1,036048 |
| H8 | -4,166707 | -2,490636 | -1,552410 |
| H9 | -0,861328 | -5,124834 | -1,439320 |
| H10 | -3,191657 | -5,183073 | -2,335190 |
| C11 | -2,229218 | -4,551012 | 0,263373 |
| H12 | -1,512414 | -4,571388 | 1,089879 |
| H13 | -2,868602 | -5,436774 | 0,313151 |
| C14 | 0,434905 | -2,948415 | -0,321957 |
| N15 | 1,051812 | -1,877563 | 0,044736 |
| C16 | 2,422087 | -2,262006 | 0,566694 |
| C17 | 2,271672 | -3,816161 | 0,630724 |
| P18 | -1,808214 | -0,647503 | 0,317043 |
| Ir19 | 0,421412 | 0,131843 | -0,397577 |
| C20 | -1,965545 | -0,540345 | 2,136538 |
| C21 | -2,002193 | -0,281379 | 4,929058 |
| C22 | -1,928253 | -1,677905 | 2,953141 |
| C23 | -2,000260 | 0,731780 | 2,732831 |
| C24 | -2,023294 | 0,857373 | 4,119459 |
| C25 | -1,948875 | -1,546283 | 4,343295 |
| H26 | -2,004269 | 1,625138 | 2,120603 |
| H27 | -2,051464 | 1,847789 | 4,564783 |
| H28 | -1,917082 | -2,434786 | 4,967306 |
| H29 | -2,019406 | -0,182267 | 6,010711 |
| O30 | 1,053825 | -4,111652 | -0,113937 |
| C31 | 2,677903 | -1,750921 | 1,979388 |
| C32 | 1,626172 | -1,347827 | 2,807157 |
| C33 | 3,971263 | -1,819684 | 2,517085 |
| C34 | 1,865360 | -0,967490 | 4,128013 |
| H35 | 0,614971 | -1,322988 | 2,426435 |
| C36 | 4,210325 | -1,444381 | 3,838607 |
| H37 | 4,798944 | -2,155090 | 1,899054 |
| C38 | 3,159461 | -1,005775 | 4,646024 |
| H39 | 1,030845 | -0,645326 | 4,744237 |
| H40 | 5,220649 | -1,492080 | 4,234845 |
| H41 | 3,349343 | -0,704970 | 5,672467 |

C1_ZS_Chelbot_TS1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,839587 | -3,515745 | -1,066689 |
| C2 | -1,575933 | -4,433007 | -1,087895 |
| C3 | -2,829196 | -4,276061 | -1,989470 |
| C4 | -3,013826 | -3,318454 | 0,223940 |
| H5 | -4,729740 | -4,118214 | -0,857936 |
| H6 | -2,605583 | -3,731558 | -2,912478 |
| H7 | -3,587875 | -3,018608 | 1,101266 |
| H8 | -4,171427 | -2,562988 | -1,481519 |
| H9 | -0,863987 | -5,190538 | -1,415702 |
| H10 | -3,210727 | -5,260226 | -2,275194 |
| C11 | -2,214637 | -4,630962 | 0,305835 |
| H12 | -1,488869 | -4,648383 | 1,124608 |
| H13 | -2,848735 | -5,520335 | 0,359032 |
| C14 | 0,444761 | -2,993733 | -0,339298 |
| N15 | 1,042912 | -1,913942 | 0,029475 |
| C16 | 2,428546 | -2,265621 | 0,510805 |
| C17 | 2,340385 | -3,828621 | 0,520510 |
| P18 | -1,807734 | -0,724541 | 0,353267 |
| Ir19 | 0,315968 | 0,087960 | -0,358562 |
| C20 | -1,961349 | -0,571470 | 2,168046 |
| C21 | -1,982061 | -0,221112 | 4,945809 |
| C22 | -1,950994 | -1,683645 | 3,017349 |
| C23 | -1,960295 | 0,721821 | 2,719103 |
| C24 | -1,975636 | 0,892298 | 4,100488 |
| C25 | -1,964036 | -1,505812 | 4,402952 |
| H26 | -1,936613 | 1,594132 | 2,074645 |
| H27 | -1,974690 | 1,896473 | 4,514620 |
| H28 | -1,953283 | -2,373454 | 5,056256 |
| H29 | -1,991991 | -0,086167 | 6,023621 |
| O30 | 1,105194 | -4,144028 | -0,186793 |
| C31 | 2,692664 | -1,795814 | 1,938142 |
| C32 | 1,649040 | -1,420832 | 2,788501 |
| C33 | 3,993903 | -1,870573 | 2,455769 |
| C34 | 1,904650 | -1,072818 | 4,115443 |
| H35 | 0,632755 | -1,394040 | 2,420868 |
| C36 | 4,248527 | -1,530636 | 3,783406 |
| H37 | 4,814654 | -2,182067 | 1,815950 |
| C38 | 3,205636 | -1,118599 | 4,614962 |
| H39 | 1,077311 | -0,770098 | 4,750946 |
| H40 | 5,264009 | -1,583484 | 4,165411 |
| H41 | 3,407305 | -0,844242 | 5,646437 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C42 | -3,362171 | 0,083848 | -0,344786 | C42 | -3,342526 | 0,019026 | -0,328493 |
| C43 | -4,366195 | 0,644260 | 0,453989 | C43 | -4,345788 | 0,597627 | 0,457650 |
| C44 | -3,536228 | 0,060501 | -1,739925 | C44 | -3,502392 | -0,017791 | -1,725030 |
| C45 | -5,505322 | 1,202015 | -0,132190 | C45 | -5,478335 | 1,151405 | -0,143700 |
| H46 | -4,264363 | 0,659166 | 1,533363 | H46 | -4,249346 | 0,626495 | 1,537248 |
| C47 | -4,670570 | 0,622039 | -2,322033 | C47 | -4,629942 | 0,540329 | -2,321803 |
| C48 | -5,655535 | 1,207577 | -1,518702 | C48 | -5,619089 | 1,134090 | -1,530653 |
| H49 | -6,275271 | 1,633349 | 0,501262 | H49 | -6,250610 | 1,596775 | 0,476966 |
| H50 | -4,793466 | 0,590078 | -3,401353 | H50 | -4,744319 | 0,500418 | -3,401749 |
| H51 | -6,540186 | 1,646208 | -1,970806 | H51 | -6,499687 | 1,569145 | -1,994428 |
| H52 | 0,808324 | 0,517362 | 1,054024 | H52 | 0,654856 | 0,462048 | 1,110068 |
| H53 | 1,980098 | 0,209429 | -0,675304 | H53 | 1,879183 | 0,443791 | -0,659854 |
| H54 | -1,853471 | -2,665274 | 2,511439 | H54 | -1,902489 | -2,685759 | 2,605304 |
| H55 | -2,793125 | -0,417423 | -2,369373 | H55 | -2,752396 | -0,500417 | -2,342400 |
| H56 | 3,097424 | -4,358712 | 0,171070 | H56 | 3,166532 | -4,322317 | 0,009072 |
| C57 | 5,131769 | -0,895235 | -2,541755 | C57 | 5,106027 | -0,719182 | -2,541423 |
| C58 | 4,366425 | -2,048685 | -2,720289 | C58 | 4,360659 | -1,876818 | -2,768696 |
| C59 | 3,527259 | -2,496641 | -1,700877 | C59 | 3,519888 | -2,373741 | -1,773715 |
| C60 | 3,442335 | -1,807318 | -0,483315 | C60 | 3,415804 | -1,730493 | -0,532612 |
| C61 | 4,201725 | -0,639806 | -0,323560 | C61 | 4,145923 | -0,552070 | -0,327148 |
| C62 | 5,043052 | -0,191348 | -1,341975 | C62 | 4,989452 | -0,055144 | -1,321605 |
| H63 | 5,782992 | -0,541604 | -3,335702 | H63 | 5,760323 | -0,328944 | -3,315256 |
| H64 | 4,419302 | -2,599898 | -3,654736 | H64 | 4,431878 | -2,394229 | -3,721179 |
| H65 | 2,921882 | -3,383012 | -1,873017 | H65 | 2,932837 | -3,265241 | -1,979851 |
| H66 | 4,131118 | -0,070845 | 0,595712 | H66 | 4,061018 | -0,022215 | 0,614939 |
| H67 | 5,619348 | 0,718048 | -1,198826 | H67 | 5,547850 | 0,859183 | -1,143519 |
| C68 | -1,038242 | 4,284989 | 2,059129 | C68 | -0,997895 | 4,388338 | 1,966126 |
| C69 | -0,328236 | 3,512750 | 1,144220 | C69 | -0,275695 | 3,589226 | 1,083006 |
| C70 | -0,968516 | 2,947614 | 0,025963 | C70 | -0,905394 | 2,964960 | -0,006302 |
| C71 | -2,342387 | 3,181662 | -0,135903 | C71 | -2,283569 | 3,173987 | -0,178956 |
| C72 | -3,053196 | 3,953527 | 0,784255 | C72 | -3,005924 | 3,974075 | 0,705983 |
| C73 | -2,406683 | 4,511475 | 1,885187 | C73 | -2,368563 | 4,586817 | 1,783752 |
| H74 | -0,519827 | 4,711517 | 2,913202 | H74 | -0,484962 | 4,860748 | 2,799164 |
| H75 | 0,727512 | 3,342432 | 1,318330 | H75 | 0,784620 | 3,447288 | 1,262401 |
| H76 | -2,871526 | 2,731724 | -0,967181 | H76 | -2,804020 | 2,679889 | -0,991040 |
| H77 | -4,118696 | 4,105315 | 0,638271 | H77 | -4,073110 | 4,105740 | 0,552366 |
| H78 | -2,958164 | 5,115122 | 2,600003 | H78 | -2,928829 | 5,212893 | 2,471882 |
| C79 | -0,214418 | 2,117247 | -0,965847 | C79 | -0,161051 | 2,072606 | -0,951256 |
| C80 | 1,228678 | 2,056915 | -0,985404 | C80 | 1,305669 | 1,972765 | -0,937986 |
| H81 | 1,732139 | 2,471968 | -0,118569 | H81 | 1,785944 | 2,397967 | -0,061938 |
| C82 | 2,004538 | 2,282510 | -2,252542 | C82 | 2,089233 | 2,223535 | -2,193803 |
| C83 | 2,363752 | 3,616100 | -2,516649 | C83 | 2,526959 | 3,542133 | -2,398084 |
| C84 | 2,366656 | 1,294030 | -3,171265 | C84 | 2,355981 | 1,259032 | -3,167415 |
| C85 | 3,043921 | 3,954199 | -3,685337 | C85 | 3,196148 | 3,891980 | -3,569282 |
| H86 | 2,099964 | 4,391750 | -1,800550 | H86 | 2,332324 | 4,296180 | -1,638479 |
| C87 | 3,046943 | 1,634824 | -4,343199 | C87 | 3,021141 | 1,612678 | -4,342848 |
| H88 | 2,122759 | 0,258243 | -2,969180 | H88 | 2,055327 | 0,231377 | -3,000767 |
| C89 | 3,382493 | 2,961741 | -4,609626 | C89 | 3,437333 | 2,926892 | -4,550783 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H90 | 3,310174 | 4,990809 | -3,872581 | H90 | 3,528618 | 4,915853 | -3,715551 |
| H91 | 3,318514 | 0,852444 | -5,045966 | H91 | 3,220341 | 0,852245 | -5,092339 |
| H92 | 3,910057 | 3,222872 | -5,522271 | H92 | 3,954929 | 3,199227 | -5,466134 |
| C93 | -1,125803 | 3,157944 | -3,157111 | C93 | -0,989990 | 3,153900 | -3,169383 |
| C94 | -0,747045 | 0,882959 | -3,005556 | C94 | -0,710500 | 0,865578 | -3,000873 |
| C95 | -1,743835 | 2,412567 | -4,349893 | C95 | -1,623077 | 2,426759 | -4,366593 |
| H96 | -0,194523 | 3,674919 | -3,412413 | H96 | -0,040547 | 3,639187 | -3,417788 |
| H97 | -1,816589 | 3,862358 | -2,692558 | H97 | -1,660992 | 3,883060 | -2,712641 |
| H98 | -2,832711 | 2,338941 | -4,267697 | H98 | -2,715191 | 2,398751 | -4,299517 |
| H99 | -1,464594 | 2,816339 | -5,322827 | H99 | -1,314991 | 2,812743 | -5,338104 |
| N100 | -0,848723 | 2,017238 | -2,271389 | N100 | -0,759634 | 2,007861 | -2,278074 |
| O101 | -1,202356 | 1,062326 | -4,251434 | O101 | -1,140133 | 1,054879 | -4,254258 |
| O102 | -0,319315 | -0,213301 | -2,608826 | O102 | -0,338831 | -0,247097 | -2,588449 |
| H103 | 2,118656 | -4,163603 | 1,653599 | H103 | 2,242713 | -4,219143 | 1,534474 |
| N104 | -1,909566 | -2,277621 | -0,095536 | N104 | -1,905234 | -2,358794 | -0,037298 |
| C105 | -0,927416 | -2,963677 | -0,971016 | C105 | -0,938625 | -3,029816 | -0,943366 |
| H106 | -0,822518 | -2,457924 | -1,938426 | H106 | -0,869127 | -2,520223 | -1,912415 |

C1_ZS_Chelbot_INT1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,837347 | -3,522150 | -0,960991 |
| C2 | -1,577798 | -4,444827 | -0,996165 |
| C3 | -2,846078 | -4,311452 | -1,879954 |
| C4 | -2,994721 | -3,304616 | 0,315783 |
| H5 | -4,730618 | -4,111033 | -0,728504 |
| H6 | -2,638445 | -3,794510 | -2,822435 |
| H7 | -3,558584 | -2,991075 | 1,194818 |
| H8 | -4,166186 | -2,575666 | -1,392669 |
| H9 | -0,867489 | -5,205364 | -1,320568 |
| H10 | -3,235218 | -5,302323 | -2,130114 |
| C11 | -2,194007 | -4,615715 | 0,410416 |
| H12 | -1,456471 | -4,615400 | 1,218924 |
| H13 | -2,826998 | -5,503814 | 0,490653 |
| C14 | 0,469288 | -2,972915 | -0,364508 |
| N15 | 1,035737 | -1,884271 | 0,018868 |
| C16 | 2,457731 | -2,171467 | 0,385715 |
| C17 | 2,494496 | -3,734084 | 0,232243 |
| P18 | -1,802125 | -0,710518 | 0,394982 |
| Ir19 | 0,167131 | 0,087492 | -0,298276 |
| C20 | -1,975078 | -0,523245 | 2,198599 |
| C21 | -2,013227 | -0,122602 | 4,966202 |
| C22 | -1,937078 | -1,619906 | 3,066637 |
| C23 | -2,007600 | 0,781062 | 2,723329 |
| C24 | -2,032739 | 0,975654 | 4,100855 |
| C25 | -1,960534 | -1,416572 | 4,448488 |
| H26 | -1,991213 | 1,640252 | 2,059728 |
| H27 | -2,056371 | 1,986385 | 4,497870 |
| H28 | -1,928516 | -2,271166 | 5,118102 |
| H29 | -2,029689 | 0,032236 | 6,041196 |

C1_ZS_Chelbot_TS2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,837789 | -3,593314 | -0,714641 |
| C2 | -1,564852 | -4,485327 | -0,782117 |
| C3 | -2,865712 | -4,414655 | -1,625164 |
| C4 | -2,938812 | -3,254563 | 0,493634 |
| H5 | -4,691368 | -4,196052 | -0,386981 |
| H6 | -2,698177 | -3,943045 | -2,598883 |
| H7 | -3,459616 | -2,871908 | 1,371848 |
| H8 | -4,230519 | -2,698194 | -1,196010 |
| H9 | -0,868271 | -5,270108 | -1,076028 |
| H10 | -3,246983 | -5,422190 | -1,812515 |
| C11 | -2,123785 | -4,549971 | 0,656300 |
| H12 | -1,353407 | -4,492479 | 1,430922 |
| H13 | -2,750074 | -5,429238 | 0,830697 |
| C14 | 0,474126 | -3,004590 | -0,224180 |
| N15 | 1,082707 | -1,910842 | 0,081487 |
| C16 | 2,461772 | -2,270252 | 0,585263 |
| C17 | 2,387306 | -3,843960 | 0,585499 |
| P18 | -1,767841 | -0,663363 | 0,356286 |
| Ir19 | 0,175377 | 0,074241 | -0,508614 |
| C20 | -1,830650 | -0,432306 | 2,165414 |
| C21 | -1,721250 | -0,005526 | 4,934029 |
| C22 | -1,634747 | -1,510546 | 3,038478 |
| C23 | -1,963092 | 0,863515 | 2,689047 |
| C24 | -1,909497 | 1,072634 | 4,064739 |
| C25 | -1,586712 | -1,295306 | 4,417061 |
| H26 | -2,095532 | 1,710303 | 2,029405 |
| H27 | -2,009507 | 2,081840 | 4,453808 |
| H28 | -1,428657 | -2,136741 | 5,085210 |
| H29 | -1,678418 | 0,158901 | 6,006819 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| O30 | 1,199418 | -4,091119 | -0,336952 | O30 | 1,112646 | -4,159262 | -0,031778 |
| C31 | 2,759205 | -1,807739 | 1,835646 | C31 | 2,716199 | -1,806941 | 2,015858 |
| C32 | 1,745117 | -1,476803 | 2,737663 | C32 | 1,754528 | -1,134707 | 2,769821 |
| C33 | 4,077543 | -1,911777 | 2,302589 | C33 | 3,925082 | -2,169038 | 2,633272 |
| C34 | 2,047419 | -1,211038 | 4,074211 | C34 | 2,003562 | -0,797606 | 4,102323 |
| H35 | 0,718739 | -1,415311 | 2,402083 | H35 | 0,809241 | -0,869664 | 2,323173 |
| C36 | 4,378189 | -1,652038 | 3,637941 | C36 | 4,176749 | -1,827097 | 3,959325 |
| H37 | 4,875053 | -2,180279 | 1,614597 | H37 | 4,676836 | -2,718833 | 2,072729 |
| C38 | 3,363473 | -1,291093 | 4,527004 | C38 | 3,216779 | -1,132773 | 4,699304 |
| H39 | 1,244250 | -0,941931 | 4,754652 | H39 | 1,237158 | -0,272820 | 4,664622 |
| H40 | 5,405907 | -1,726610 | 3,981615 | H40 | 5,122155 | -2,106682 | 4,415400 |
| H41 | 3,600024 | -1,079900 | 5,565818 | H41 | 3,413805 | -0,864970 | 5,733297 |
| C42 | -3,315511 | 0,019933 | -0,342815 | C42 | -3,371443 | -0,056801 | -0,297562 |
| C43 | -4,334176 | 0,617176 | 0,409333 | C43 | -4,370444 | 0,507813 | 0,504961 |
| C44 | -3,449595 | -0,058037 | -1,740609 | C44 | -3,635932 | -0,286621 | -1,658530 |
| C45 | -5,456940 | 1,149547 | -0,228269 | C45 | -5,599769 | 0,865253 | -0,051648 |
| H46 | -4,259051 | 0,675075 | 1,489335 | H46 | -4,202633 | 0,671441 | 1,562513 |
| C47 | -4,566524 | 0,481233 | -2,372733 | C47 | -4,861131 | 0,075653 | -2,210954 |
| C48 | -5,571391 | 1,093592 | -1,616330 | C48 | -5,844630 | 0,662930 | -1,408792 |
| H49 | -6,242012 | 1,609147 | 0,365332 | H49 | -6,366699 | 1,301083 | 0,581988 |
| H50 | -4,661563 | 0,410963 | -3,452989 | H50 | -5,058169 | -0,122308 | -3,261030 |
| H51 | -6,444508 | 1,512722 | -2,108110 | H51 | -6,802655 | 0,942046 | -1,837729 |
| H52 | 0,462729 | 0,495796 | 1,179312 | H52 | 0,578113 | 0,656845 | 0,883632 |
| H53 | 1,861260 | 1,043524 | -0,849721 | H53 | 1,465355 | 2,075189 | -2,364341 |
| H54 | -1,859291 | -2,627244 | 2,672564 | H54 | -1,487478 | -2,510454 | 2,646801 |
| H55 | -2,687822 | -0,556120 | -2,330672 | H55 | -2,902092 | -0,790054 | -2,277264 |
| H56 | 3,272865 | -4,094156 | -0,441231 | H56 | 3,175801 | -4,311039 | -0,006108 |
| C57 | 4,847820 | -0,136681 | -2,624073 | C57 | 5,267274 | -0,907435 | -2,443701 |
| C58 | 4,124017 | -1,286590 | -2,943968 | C58 | 4,188968 | -1,732908 | -2,772732 |
| C59 | 3,371984 | -1,933191 | -1,965124 | C59 | 3,322853 | -2,176948 | -1,776615 |
| C60 | 3,340941 | -1,455107 | -0,646628 | C60 | 3,503959 | -1,796062 | -0,438524 |
| C61 | 4,048334 | -0,284893 | -0,343871 | C61 | 4,581429 | -0,963909 | -0,121026 |
| C62 | 4,798190 | 0,366815 | -1,325495 | C62 | 5,461628 | -0,532064 | -1,116492 |
| H63 | 5,428347 | 0,374294 | -3,386314 | H63 | 5,947351 | -0,562061 | -3,216918 |
| H64 | 4,139309 | -1,677536 | -3,957445 | H64 | 4,023807 | -2,032829 | -3,803722 |
| H65 | 2,794487 | -2,811871 | -2,241629 | H65 | 2,487064 | -2,813848 | -2,053946 |
| H66 | 4,019274 | 0,119438 | 0,661801 | H66 | 4,736720 | -0,632155 | 0,898209 |
| H67 | 5,339541 | 1,273895 | -1,072915 | H67 | 6,292305 | 0,115175 | -0,850086 |
| C68 | -1,026272 | 4,593725 | 1,768782 | C68 | -1,314100 | 4,197665 | 1,693451 |
| C69 | -0,279187 | 3,743541 | 0,954655 | C69 | -0,606850 | 3,392347 | 0,806064 |
| C70 | -0,879905 | 3,029475 | -0,094707 | C70 | -1,229477 | 2,809279 | -0,315883 |
| C71 | -2,261880 | 3,204115 | -0,292602 | C71 | -2,603208 | 3,028650 | -0,474750 |
| C72 | -3,009120 | 4,052891 | 0,521691 | C72 | -3,320320 | 3,827433 | 0,422175 |
| C73 | -2,396205 | 4,756068 | 1,558492 | C73 | -2,681938 | 4,428811 | 1,504484 |
| H74 | -0,530829 | 5,133590 | 2,570976 | H74 | -0,796551 | 4,642900 | 2,538761 |
| H75 | 0,778932 | 3,633701 | 1,164900 | H75 | 0,447262 | 3,211035 | 0,986698 |
| H76 | -2,766475 | 2,640968 | -1,069049 | H76 | -3,136556 | 2,553772 | -1,288661 |
| H77 | -4,076519 | 4,153406 | 0,346039 | H77 | -4,385770 | 3,971783 | 0,266144 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H78 | -2,975224 | 5,421042 | 2,192414 | H78 | -3,235574 | 5,059853 | 2,193189 |
| C79 | -0,131449 | 2,037913 | -0,939082 | C79 | -0,394436 | 1,990400 | -1,282199 |
| C80 | 1,424826 | 2,098392 | -0,954156 | C80 | 0,934290 | 2,735010 | -1,674333 |
| H81 | 1,798529 | 2,597557 | -0,063360 | H81 | 1,560934 | 2,824439 | -0,782346 |
| C82 | 2,047455 | 2,666508 | -2,203486 | C82 | 0,844499 | 4,086833 | -2,375551 |
| C83 | 2,314811 | 4,039939 | -2,263699 | C83 | 0,235109 | 5,222153 | -1,821270 |
| C84 | 2,263533 | 1,875691 | -3,336354 | C84 | 1,438762 | 4,210551 | -3,642040 |
| C85 | 2,771663 | 4,617833 | -3,448737 | C85 | 0,198061 | 6,426272 | -2,526458 |
| H86 | 2,144928 | 4,660199 | -1,386808 | H86 | -0,212363 | 5,177098 | -0,836828 |
| C87 | 2,713921 | 2,454788 | -4,523295 | C87 | 1,404929 | 5,413390 | -4,347262 |
| H88 | 2,085275 | 0,805420 | -3,285343 | H88 | 1,932688 | 3,347332 | -4,084370 |
| C89 | 2,963191 | 3,827524 | -4,584490 | C89 | 0,774121 | 6,527383 | -3,792593 |
| H90 | 2,972542 | 5,684834 | -3,486763 | H90 | -0,282879 | 7,291651 | -2,078320 |
| H91 | 2,872768 | 1,832768 | -5,399818 | H91 | 1,871124 | 5,479253 | -5,326564 |
| H92 | 3,311619 | 4,278928 | -5,509081 | H92 | 0,741127 | 7,466706 | -4,337170 |
| C93 | -0,969772 | 3,055675 | -3,238207 | C93 | -1,651536 | 2,657425 | -3,558339 |
| C94 | -0,636837 | 0,786582 | -2,964264 | C94 | -1,028250 | 0,492696 | -3,106771 |
| C95 | -1,555897 | 2,257489 | -4,416109 | C95 | -2,345253 | 1,675259 | -4,510162 |
| H96 | -0,049273 | 3,582428 | -3,503153 | H96 | -0,836664 | 3,198725 | -4,041751 |
| H97 | -1,681185 | 3,764965 | -2,813170 | H97 | -2,331122 | 3,382785 | -3,112007 |
| H98 | -2,648590 | 2,207397 | -4,381222 | H98 | -3,394344 | 1,509787 | -4,247119 |
| H99 | -1,226570 | 2,605738 | -5,394899 | H99 | -2,258212 | 1,940228 | -5,563937 |
| N100 | -0,688826 | 1,955960 | -2,300165 | N100 | -1,125197 | 1,709717 | -2,550687 |
| O101 | -1,050853 | 0,899475 | -4,229916 | O101 | -1,633195 | 0,417315 | -4,300755 |
| O102 | -0,265761 | -0,306320 | -2,481778 | O102 | -0,461024 | -0,508073 | -2,612405 |
| H103 | 2,577112 | -4,235153 | 1,197212 | H103 | 2,376630 | -4,258659 | 1,594686 |
| N104 | -1,883906 | -2,352752 | 0,030123 | N104 | -1,853878 | -2,317861 | 0,066305 |
| C105 | -0,943369 | -3,036259 | -0,894683 | C105 | -0,920298 | -3,077369 | -0,796788 |
| H106 | -0,914962 | -2,548025 | -1,877255 | H106 | -0,876581 | -2,664619 | -1,811035 |
| | | | | H107 | 2,798605 | 0,792432 | -0,891140 |
| | | | | H108 | 2,635385 | 0,542488 | -1,580453 |

C1_ZS_Chelbot_INT2

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -3,895545 | -3,652880 | -0,713507 |
| C2 | -1,626151 | -4,552766 | -0,715590 |
| C3 | -2,910565 | -4,501680 | -1,584023 |
| C4 | -3,018669 | -3,288625 | 0,504401 |
| H5 | -4,759287 | -4,242718 | -0,389050 |
| H6 | -2,723553 | -4,057338 | -2,566894 |
| H7 | -3,557316 | -2,885563 | 1,362508 |
| H8 | -4,271790 | -2,766874 | -1,224608 |
| H9 | -0,924434 | -5,344510 | -0,977513 |
| H10 | -3,291585 | -5,513052 | -1,750435 |
| C11 | -2,211161 | -4,581963 | 0,713693 |
| H12 | -1,454279 | -4,507913 | 1,500501 |
| H13 | -2,842023 | -5,456069 | 0,897304 |
| C14 | 0,413430 | -3,064571 | -0,181271 |
| N15 | 1,010237 | -1,961689 | 0,102655 |

C1_ZS_Chelbot_TS3

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -3,902284 | -3,697218 | -0,835905 |
| C2 | -1,624458 | -4,577357 | -0,792315 |
| C3 | -2,881691 | -4,511628 | -1,699288 |
| C4 | -3,070342 | -3,369664 | 0,423870 |
| H5 | -4,775422 | -4,300515 | -0,566125 |
| H6 | -2,668128 | -4,037709 | -2,662749 |
| H7 | -3,641581 | -2,999325 | 1,275670 |
| H8 | -4,260816 | -2,792942 | -1,328562 |
| H9 | -0,905126 | -5,352117 | -1,057781 |
| H10 | -3,247251 | -5,521263 | -1,906217 |
| C11 | -2,254824 | -4,660853 | 0,616068 |
| H12 | -1,523755 | -4,603135 | 1,428160 |
| H13 | -2,878810 | -5,548893 | 0,750006 |
| C14 | 0,373186 | -3,070636 | -0,150979 |
| N15 | 0,971173 | -1,964390 | 0,137861 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C16 | 2,407627 | -2,272591 | 0,569457 | C16 | 2,368904 | -2,278364 | 0,625623 |
| C17 | 2,376714 | -3,843388 | 0,580535 | C17 | 2,272664 | -3,832500 | 0,768619 |
| P18 | -1,850054 | -0,697769 | 0,340132 | P18 | -1,872667 | -0,768230 | 0,391167 |
| Ir19 | 0,230695 | 0,027190 | -0,502825 | Ir19 | 0,310792 | -0,037404 | -0,464531 |
| C20 | -1,933083 | -0,449981 | 2,151729 | C20 | -1,963254 | -0,568273 | 2,207142 |
| C21 | -1,837496 | 0,010991 | 4,919394 | C21 | -1,829772 | -0,135324 | 4,978274 |
| C22 | -1,757045 | -1,517716 | 3,041778 | C22 | -1,880591 | -1,653008 | 3,089354 |
| C23 | -2,053569 | 0,852434 | 2,660388 | C23 | -1,969117 | 0,736699 | 2,725344 |
| C24 | -2,007009 | 1,078762 | 4,033933 | C24 | -1,907562 | 0,950008 | 4,100482 |
| C25 | -1,715042 | -1,285940 | 4,418401 | C25 | -1,816000 | -1,434337 | 4,467795 |
| H26 | -2,175141 | 1,692178 | 1,990550 | H26 | -2,006775 | 1,588260 | 2,057528 |
| H27 | -2,097807 | 2,094599 | 4,407569 | H27 | -1,910422 | 1,966837 | 4,482954 |
| H28 | -1,572515 | -2,121796 | 5,097229 | H28 | -1,745190 | -2,283084 | 5,141876 |
| H29 | -1,800681 | 0,188472 | 5,990252 | H29 | -1,776786 | 0,030755 | 6,050238 |
| O30 | 1,085315 | -4,201461 | 0,010998 | O30 | 1,033922 | -4,201704 | 0,095424 |
| C31 | 2,677509 | -1,767254 | 1,982263 | C31 | 2,666172 | -1,686209 | 1,997037 |
| C32 | 1,685643 | -1,180173 | 2,768317 | C32 | 1,655712 | -1,175713 | 2,815815 |
| C33 | 3,944974 | -1,984719 | 2,545124 | C33 | 3,970070 | -1,772112 | 2,506936 |
| C34 | 1,960057 | -0,780987 | 4,077975 | C34 | 1,948423 | -0,712697 | 4,099759 |
| H35 | 0,694774 | -1,033296 | 2,367365 | H35 | 0,637161 | -1,132140 | 2,458594 |
| C36 | 4,219400 | -1,590081 | 3,852437 | C36 | 4,260951 | -1,317594 | 3,791865 |
| H37 | 4,727371 | -2,451534 | 1,952592 | H37 | 4,766454 | -2,180831 | 1,891798 |
| C38 | 3,227659 | -0,977410 | 4,622285 | C38 | 3,251877 | -0,775092 | 4,589844 |
| H39 | 1,169792 | -0,322655 | 4,665187 | H39 | 1,145800 | -0,309440 | 4,710056 |
| H40 | 5,208737 | -1,758474 | 4,268057 | H40 | 5,278593 | -1,382693 | 4,166079 |
| H41 | 3,443466 | -0,664020 | 5,639669 | H41 | 3,481499 | -0,411723 | 5,587442 |
| C42 | -3,456961 | -0,102161 | -0,324571 | C42 | -3,458720 | -0,105878 | -0,260876 |
| C43 | -4,461872 | 0,469654 | 0,464540 | C43 | -4,439501 | 0,508904 | 0,524130 |
| C44 | -3,702352 | -0,323572 | -1,690841 | C44 | -3,692014 | -0,279853 | -1,636389 |
| C45 | -5,680596 | 0,838815 | -0,108637 | C45 | -5,625991 | 0,960424 | -0,059281 |
| H46 | -4,306063 | 0,629092 | 1,525177 | H46 | -4,286294 | 0,640900 | 1,589498 |
| C47 | -4,917030 | 0,051141 | -2,259664 | C47 | -4,874612 | 0,173497 | -2,215858 |
| C48 | -5,908408 | 0,640941 | -1,469522 | C48 | -5,844096 | 0,802114 | -1,427234 |
| H49 | -6,453393 | 1,278745 | 0,515101 | H49 | -6,381889 | 1,433181 | 0,561281 |
| H50 | -5,097872 | -0,137720 | -3,314384 | H50 | -5,048751 | 0,018469 | -3,277422 |
| H51 | -6,858174 | 0,928404 | -1,911057 | H51 | -6,768783 | 1,152952 | -1,876328 |
| H52 | 0,549595 | 0,583644 | 0,923200 | H52 | 0,769510 | 0,510379 | 0,914300 |
| H53 | 1,642442 | 2,071860 | -2,289987 | H53 | 1,824742 | 2,359993 | -2,342432 |
| H54 | -1,619531 | -2,524785 | 2,665738 | H54 | -1,831826 | -2,666321 | 2,707266 |
| H55 | -2,959913 | -0,821968 | -2,303915 | H55 | -2,961431 | -0,796678 | -2,249286 |
| H56 | 3,154592 | -4,299422 | -0,033262 | H56 | 3,093835 | -4,369551 | 0,294082 |
| C57 | 4,912859 | -0,644450 | -2,583132 | C57 | 4,921648 | -1,009112 | -2,650457 |
| C58 | 4,045626 | -1,711795 | -2,831034 | C58 | 4,141257 | -2,161741 | -2,758407 |
| C59 | 3,283857 | -2,245157 | -1,793961 | C59 | 3,356239 | -2,575939 | -1,684429 |
| C60 | 3,372675 | -1,727830 | -0,493333 | C60 | 3,336841 | -1,850973 | -0,484847 |
| C61 | 4,241099 | -0,656987 | -0,255385 | C61 | 4,112208 | -0,688712 | -0,392000 |
| C62 | 5,008311 | -0,121859 | -1,293914 | C62 | 4,903685 | -0,275128 | -1,465020 |
| H63 | 5,508097 | -0,225779 | -3,389467 | H63 | 5,538606 | -0,687116 | -3,484605 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H64 | 3,959906 | -2,125754 | -3,831595 | H64 | 4,143235 | -2,738437 | -3,678837 |
| H65 | 2,595913 | -3,058738 | -2,011280 | H65 | 2,739464 | -3,464016 | -1,798671 |
| H66 | 4,314751 | -0,226163 | 0,736530 | H66 | 4,091517 | -0,096501 | 0,515549 |
| H67 | 5,678123 | 0,708887 | -1,090726 | H67 | 5,504456 | 0,625312 | -1,371579 |
| C68 | -1,188624 | 4,134686 | 1,750431 | C68 | -1,125948 | 4,053193 | 1,738528 |
| C69 | -0,478259 | 3,349420 | 0,847963 | C69 | -0,383698 | 3,313117 | 0,823553 |
| C70 | -1,098358 | 2,781603 | -0,283206 | C70 | -0,979974 | 2,780156 | -0,335914 |
| C71 | -2,475114 | 2,991253 | -0,432705 | C71 | -2,356381 | 2,964756 | -0,508322 |
| C72 | -3,195723 | 3,770062 | 0,479378 | C72 | -3,103664 | 3,701497 | 0,415835 |
| C73 | -2,558234 | 4,360044 | 1,568702 | C73 | -2,494798 | 4,264208 | 1,535379 |
| H74 | -0,672280 | 4,567114 | 2,602948 | H74 | -0,634122 | 4,461959 | 2,616689 |
| H75 | 0,577330 | 3,173251 | 1,025213 | H75 | 0,670434 | 3,143767 | 1,015188 |
| H76 | -3,006968 | 2,523965 | -1,252136 | H76 | -2,862287 | 2,518227 | -1,355206 |
| H77 | -4,263141 | 3,906525 | 0,329946 | H77 | -4,169641 | 3,826377 | 0,250844 |
| H78 | -3,114799 | 4,975627 | 2,268852 | H78 | -3,073863 | 4,847961 | 2,244311 |
| C79 | -0,261928 | 1,982961 | -1,267334 | C79 | -0,117395 | 2,087879 | -1,373971 |
| C80 | 1,066715 | 2,737411 | -1,639757 | C80 | 1,158127 | 2,970867 | -1,720780 |
| H81 | 1,657667 | 2,849603 | -0,724864 | H81 | 1,697544 | 3,127270 | -0,782101 |
| C82 | 0,979396 | 4,079841 | -2,351848 | C82 | 0,953839 | 4,298715 | -2,428380 |
| C83 | 0,356910 | 5,212611 | -1,806403 | C83 | 0,199081 | 5,350603 | -1,888879 |
| C84 | 1,571383 | 4,199504 | -3,619230 | C84 | 1,576133 | 4,495239 | -3,670693 |
| C85 | 0,307690 | 6,411315 | -2,519822 | C85 | 0,054727 | 6,550326 | -2,587596 |
| H86 | -0,091959 | 5,167363 | -0,821936 | H86 | -0,274443 | 5,242720 | -0,921057 |
| C87 | 1,525846 | 5,396901 | -4,332983 | C87 | 1,435896 | 5,695081 | -4,367427 |
| H88 | 2,070755 | 3,336558 | -4,056117 | H88 | 2,176342 | 3,695152 | -4,099608 |
| C89 | 0,885166 | 6,509085 | -3,785940 | C89 | 0,667352 | 6,727353 | -3,828538 |
| H90 | -0,182826 | 7,275014 | -2,078934 | H90 | -0,535117 | 7,353264 | -2,154006 |
| H91 | 1,990505 | 5,460564 | -5,313162 | H91 | 1,928189 | 5,823484 | -5,327369 |
| H92 | 0,843245 | 7,444087 | -4,337341 | H92 | 0,553233 | 7,663768 | -4,367105 |
| C93 | -1,528772 | 2,680757 | -3,518840 | C93 | -1,341858 | 2,681314 | -3,628340 |
| C94 | -1,014776 | 0,484801 | -3,066485 | C94 | -0,932904 | 0,472894 | -3,080181 |
| C95 | -2,321423 | 1,732242 | -4,424867 | C95 | -2,225823 | 1,738818 | -4,447768 |
| H96 | -0,708413 | 3,170032 | -4,046193 | H96 | -0,516773 | 3,087644 | -4,215855 |
| H97 | -2,142492 | 3,447702 | -3,046605 | H97 | -1,882605 | 3,510921 | -3,173386 |
| H98 | -3,363627 | 1,624807 | -4,108139 | H98 | -3,256016 | 1,704722 | -4,078956 |
| H99 | -2,272265 | 1,981692 | -5,484804 | H99 | -2,213992 | 1,936920 | -5,519546 |
| N100 | -1,010084 | 1,713204 | -2,526117 | N100 | -0,842162 | 1,737788 | -2,604328 |
| O101 | -1,670572 | 0,439441 | -4,235244 | O101 | -1,633299 | 0,426785 | -4,224314 |
| O102 | -0,516313 | -0,551943 | -2,574121 | O102 | -0,478751 | -0,564211 | -2,569995 |
| H103 | 2,412300 | -4,247834 | 1,593029 | H103 | 2,178844 | -4,136949 | 1,812087 |
| N104 | -1,926512 | -2,362183 | 0,077006 | N104 | -1,981827 | -2,418072 | 0,059691 |
| C105 | -0,981312 | -3,145705 | -0,753144 | C105 | -1,001148 | -3,160780 | -0,767315 |
| H106 | -0,922814 | -2,756209 | -1,776906 | H106 | -0,920236 | -2,739986 | -1,776791 |
| H107 | 1,884302 | 0,518632 | -0,527380 | H107 | 1,844101 | 0,190167 | -0,909082 |
| H108 | 1,756145 | 0,220554 | -1,314889 | H108 | 1,016851 | 1,141453 | -1,252165 |

C1_Z_R_tN_Chelbot

C1_ZS_Chelbot_PROD

C1_ZR_Chelbot_SM

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C1 | -3,895922 | -3,761888 | -0,807289 | C1 | -3,911023 | -3,442904 | -0,965329 |
| C2 | -1,611516 | -4,628001 | -0,814296 | C2 | -1,654917 | -4,372785 | -1,080668 |
| C3 | -2,879615 | -4,544402 | -1,704816 | C3 | -2,937462 | -4,192420 | -1,935271 |
| C4 | -3,056682 | -3,478251 | 0,458669 | C4 | -3,035457 | -3,261598 | 0,294444 |
| H5 | -4,768217 | -4,374019 | -0,555182 | H5 | -4,791402 | -4,049259 | -0,728091 |
| H6 | -2,680477 | -4,042137 | -2,656970 | H6 | -2,742000 | -3,632442 | -2,855544 |
| H7 | -3,625711 | -3,144465 | 1,326852 | H7 | -3,571256 | -2,967028 | 1,197291 |
| H8 | -4,255978 | -2,839789 | -1,265641 | H8 | -4,260560 | -2,487612 | -1,358033 |
| H9 | -0,887972 | -5,386720 | -1,112821 | H9 | -0,962714 | -5,132937 | -1,442878 |
| H10 | -3,240886 | -5,550362 | -1,935843 | H10 | -3,334149 | -5,169111 | -2,225796 |
| C11 | -2,227490 | -4,766916 | 0,597420 | C11 | -2,244867 | -4,580882 | 0,332946 |
| H12 | -1,490650 | -4,726185 | 1,405041 | H12 | -1,490737 | -4,614585 | 1,124972 |
| H13 | -2,839974 | -5,666642 | 0,704666 | H13 | -2,884962 | -5,464971 | 0,399432 |
| C14 | 0,379637 | -3,118052 | -0,154831 | C14 | 0,390990 | -2,971424 | -0,353773 |
| N15 | 1,009889 | -2,014295 | 0,088871 | N15 | 1,022528 | -1,909009 | 0,013916 |
| C16 | 2,406287 | -2,342350 | 0,597189 | C16 | 2,407443 | -2,307558 | 0,479052 |
| C17 | 2,238712 | -3,874569 | 0,846809 | C17 | 2,261580 | -3,864107 | 0,505018 |
| P18 | -1,884586 | -0,848083 | 0,416895 | P18 | -1,838355 | -0,660972 | 0,350615 |
| Ir19 | 0,301293 | -0,167029 | -0,395677 | Ir19 | 0,382327 | 0,114335 | -0,361366 |
| C20 | -2,006830 | -0,593820 | 2,221393 | C20 | -1,997047 | -0,498259 | 2,163913 |
| C21 | -1,965504 | -0,049291 | 4,970549 | C21 | -1,988179 | -0,148502 | 4,943616 |
| C22 | -1,993666 | -1,643067 | 3,147286 | C22 | -1,869959 | -1,604093 | 3,013718 |
| C23 | -1,976377 | 0,732811 | 2,683147 | C23 | -2,104079 | 0,789101 | 2,717042 |
| C24 | -1,962631 | 1,001893 | 4,048719 | C24 | -2,102112 | 0,958920 | 4,099060 |
| C25 | -1,974665 | -1,368628 | 4,517379 | C25 | -1,869399 | -1,427157 | 4,398861 |
| H26 | -1,950887 | 1,556347 | 1,976973 | H26 | -2,181556 | 1,659302 | 2,075570 |
| H27 | -1,939915 | 2,032487 | 4,391844 | H27 | -2,183760 | 1,959649 | 4,513403 |
| H28 | -1,962148 | -2,188561 | 5,229816 | H28 | -1,769541 | -2,290276 | 5,050508 |
| H29 | -1,951166 | 0,160294 | 6,036375 | H29 | -1,985690 | -0,013659 | 6,021385 |
| O30 | 1,016120 | -4,249661 | 0,145983 | O30 | 1,016107 | -4,139259 | -0,198722 |
| C31 | 2,719210 | -1,696690 | 1,942185 | C31 | 2,706913 | -1,836703 | 1,896549 |
| C32 | 1,687964 | -1,343276 | 2,821944 | C32 | 1,686681 | -1,425759 | 2,759101 |
| C33 | 4,043923 | -1,614331 | 2,390364 | C33 | 4,010630 | -1,953214 | 2,400467 |
| C34 | 1,975249 | -0,857107 | 4,096288 | C34 | 1,968943 | -1,081671 | 4,081188 |
| H35 | 0,654114 | -1,438278 | 2,515764 | H35 | 0,666868 | -1,367783 | 2,404916 |
| C36 | 4,330796 | -1,136369 | 3,669555 | C36 | 4,292062 | -1,615249 | 3,723370 |
| H37 | 4,857998 | -1,919662 | 1,740737 | H37 | 4,813358 | -2,297232 | 1,754612 |
| C38 | 3,299247 | -0,743910 | 4,522226 | C38 | 3,273673 | -1,166387 | 4,565712 |
| H39 | 1,156348 | -0,571742 | 4,750527 | H39 | 1,159050 | -0,751167 | 4,725345 |
| H40 | 5,364684 | -1,070759 | 3,996312 | H40 | 5,309927 | -1,699832 | 4,093027 |
| H41 | 3,526146 | -0,363505 | 5,514109 | H41 | 3,496627 | -0,894002 | 5,593210 |
| C42 | -3,466202 | -0,190101 | -0,258407 | C42 | -3,386154 | 0,036679 | -0,351752 |
| C43 | -4,478542 | 0,383015 | 0,519570 | C43 | -4,437412 | 0,550272 | 0,415747 |
| C44 | -3,656243 | -0,309531 | -1,646717 | C44 | -3,513005 | 0,003555 | -1,751945 |
| C45 | -5,654466 | 0,840743 | -0,080383 | C45 | -5,583539 | 1,049693 | -0,206959 |
| H46 | -4,356063 | 0,477679 | 1,593200 | H46 | -4,367779 | 0,571412 | 1,497470 |
| C47 | -4,828453 | 0,150374 | -2,243062 | C47 | -4,654560 | 0,507128 | -2,370444 |
| C48 | -5,830807 | 0,732526 | -1,459732 | C48 | -5,691209 | 1,040649 | -1,597060 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H49 | -6,435376 | 1,278214 | 0,535531 | H49 | -6,392840 | 1,446364 | 0,399296 |
| H50 | -4,968018 | 0,036990 | -3,314963 | H50 | -4,742459 | 0,471032 | -3,453101 |
| H51 | -6,747229 | 1,088094 | -1,921989 | H51 | -6,582448 | 1,434197 | -2,077303 |
| H52 | 0,768505 | 0,254352 | 1,017848 | H52 | 0,738871 | 0,482595 | 1,102281 |
| H53 | 1,724053 | 2,564102 | -2,332798 | H53 | 1,947942 | 0,211072 | -0,596350 |
| H54 | -1,970052 | -2,672660 | 2,806899 | H54 | -1,742559 | -2,598109 | 2,598445 |
| H55 | -2,895684 | -0,783385 | -2,258687 | H55 | -2,728184 | -0,439748 | -2,355317 |
| H56 | 3,059862 | -4,475110 | 0,457501 | H56 | 3,068590 | -4,391006 | -0,003620 |
| C57 | 4,991660 | -1,403990 | -2,761781 | C57 | 5,092901 | -0,927283 | -2,646196 |
| C58 | 4,256115 | -2,589353 | -2,740235 | C58 | 4,269375 | -2,035193 | -2,851029 |
| C59 | 3,455715 | -2,894935 | -1,640725 | C59 | 3,429223 | -2,479230 | -1,831037 |
| C60 | 3,377565 | -2,026672 | -0,543052 | C60 | 3,401087 | -1,830790 | -0,588050 |
| C61 | 4,102149 | -0,828965 | -0,586424 | C61 | 4,211959 | -0,702676 | -0,404312 |
| C62 | 4,909951 | -0,525254 | -1,682057 | C62 | 5,055295 | -0,259453 | -1,423603 |
| H63 | 5,621101 | -1,166851 | -3,614760 | H63 | 5,748754 | -0,579033 | -3,438674 |
| H64 | 4,304155 | -3,277726 | -3,578967 | H64 | 4,279660 | -2,555028 | -3,804731 |
| H65 | 2,875290 | -3,813680 | -1,659638 | H65 | 2,782162 | -3,332403 | -2,019582 |
| H66 | 4,028270 | -0,125036 | 0,233279 | H66 | 4,183688 | -0,163721 | 0,535666 |
| H67 | 5,471954 | 0,404514 | -1,691203 | H67 | 5,674687 | 0,617815 | -1,262399 |
| C68 | -1,402244 | 4,278878 | 1,708394 | C68 | -1,258348 | 4,359429 | 1,974947 |
| C69 | -0,582999 | 3,674960 | 0,757209 | C69 | -0,494232 | 3,571748 | 1,117336 |
| C70 | -1,131351 | 3,080542 | -0,390773 | C70 | -1,072780 | 2,945900 | -0,000629 |
| C71 | -2,522014 | 3,068860 | -0,537507 | C71 | -2,444334 | 3,144234 | -0,226629 |
| C72 | -3,343085 | 3,676067 | 0,416119 | C72 | -3,209369 | 3,933587 | 0,633692 |
| C73 | -2,790032 | 4,292247 | 1,537199 | C73 | -2,623732 | 4,546338 | 1,740727 |
| H74 | -0,954303 | 4,739342 | 2,584305 | H74 | -0,782168 | 4,831908 | 2,829406 |
| H75 | 0,490097 | 3,667517 | 0,917340 | H75 | 0,559887 | 3,440894 | 1,335398 |
| H76 | -2,979220 | 2,560615 | -1,379011 | H76 | -2,927555 | 2,657604 | -1,065294 |
| H77 | -4,419607 | 3,649942 | 0,279652 | H77 | -4,270045 | 4,057061 | 0,435296 |
| H78 | -3,428908 | 4,769492 | 2,274167 | H78 | -3,217025 | 5,163940 | 2,408168 |
| C79 | -0,205978 | 2,450869 | -1,423057 | C79 | -0,259672 | 2,105563 | -0,938625 |
| C80 | 1,099436 | 3,244404 | -1,745554 | C80 | 1,183331 | 2,057881 | -0,890153 |
| H81 | 1,628893 | 3,388465 | -0,798352 | H81 | 1,640315 | 2,470704 | 0,003330 |
| C82 | 0,958265 | 4,564407 | -2,477095 | C82 | 2,017395 | 2,295927 | -2,116026 |
| C83 | 0,269826 | 5,658769 | -1,934677 | C83 | 2,420158 | 3,625387 | -2,330373 |
| C84 | 1,559312 | 4,710447 | -3,735968 | C84 | 2,388708 | 1,320183 | -3,045345 |
| C85 | 0,169959 | 6,856313 | -2,643929 | C85 | 3,153505 | 3,973944 | -3,462733 |
| H86 | -0,186952 | 5,583352 | -0,954823 | H86 | 2,149118 | 4,389477 | -1,604886 |
| C87 | 1,463297 | 5,908410 | -4,444405 | C87 | 3,120243 | 1,672015 | -4,181764 |
| H88 | 2,109587 | 3,875735 | -4,165320 | H88 | 2,119311 | 0,284205 | -2,876634 |
| C89 | 0,761165 | 6,984962 | -3,901313 | C89 | 3,499620 | 2,995596 | -4,398317 |
| H90 | -0,367228 | 7,693980 | -2,207789 | H90 | 3,455805 | 5,006587 | -3,613165 |
| H91 | 1,938853 | 6,000545 | -5,416795 | H91 | 3,400783 | 0,900464 | -4,892908 |
| H92 | 0,683352 | 7,919529 | -4,449309 | H92 | 4,069419 | 3,265086 | -5,283021 |
| C93 | -1,440324 | 2,931061 | -3,643066 | C93 | -1,052933 | 3,149969 | -3,170443 |
| C94 | -0,959587 | 0,726682 | -3,089247 | C94 | -0,699927 | 0,871607 | -3,004040 |
| C95 | -2,302487 | 1,959610 | -4,451759 | C95 | -1,608374 | 2,412051 | -4,399016 |
| H96 | -0,635059 | 3,368874 | -4,236449 | H96 | -0,106583 | 3,663042 | -3,372847 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H97 | -2,007170 | 3,738898 | -3,178476 | H97 | -1,764476 | 3,857272 | -2,741883 |
| H98 | -3,328601 | 1,898876 | -4,074182 | H98 | -2,701184 | 2,352893 | -4,384631 |
| H99 | -2,305464 | 2,156233 | -5,523808 | H99 | -1,266011 | 2,813458 | -5,352711 |
| N100 | -0,898764 | 2,007069 | -2,628628 | N100 | -0,828599 | 2,005139 | -2,274738 |
| O101 | -1,671851 | 0,669221 | -4,230032 | O101 | -1,091024 | 1,055182 | -4,271082 |
| O102 | -0,486221 | -0,299965 | -2,592687 | O102 | -0,298411 | -0,227067 | -2,588307 |
| H103 | 2,081190 | -4,093352 | 1,904450 | H103 | 2,150079 | -4,241970 | 1,522430 |
| N104 | -1,977605 | -2,508617 | 0,128879 | N104 | -1,928044 | -2,307721 | 0,003075 |
| C105 | -1,005052 | -3,204737 | -0,750252 | C105 | -0,998812 | -2,978426 | -0,939137 |
| H106 | -0,951399 | -2,745269 | -1,746428 | H106 | -0,941017 | -2,458745 | -1,903402 |
| H107 | 1,792663 | 0,188149 | -0,856433 | | | | |
| H108 | 0,332760 | 1,550416 | -0,984123 | | | | |

C1_ZR_Chelbot_TS1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,864759 | -3,516923 | -1,067888 |
| C2 | -1,600828 | -4,431882 | -1,089187 |
| C3 | -2,854837 | -4,278750 | -1,989746 |
| C4 | -3,039585 | -3,319404 | 0,223327 |
| H5 | -4,755778 | -4,118286 | -0,859452 |
| H6 | -2,633169 | -3,736841 | -2,914779 |
| H7 | -3,614560 | -3,021147 | 1,100525 |
| H8 | -4,195639 | -2,564345 | -1,483698 |
| H9 | -0,887309 | -5,187953 | -1,417097 |
| H10 | -3,235561 | -5,264266 | -2,271972 |
| C11 | -2,238363 | -4,630723 | 0,304979 |
| H12 | -1,512358 | -4,646825 | 1,123588 |
| H13 | -2,871083 | -5,521105 | 0,358469 |
| C14 | 0,418433 | -2,990358 | -0,344426 |
| N15 | 1,017392 | -1,909778 | 0,019982 |
| C16 | 2,403520 | -2,259484 | 0,500815 |
| C17 | 2,321688 | -3,823667 | 0,501877 |
| P18 | -1,840371 | -0,721124 | 0,345760 |
| Ir19 | 0,287431 | 0,092211 | -0,357916 |
| C20 | -1,999137 | -0,560474 | 2,157947 |
| C21 | -2,024060 | -0,198613 | 4,935738 |
| C22 | -1,988501 | -1,668839 | 3,012759 |
| C23 | -2,001892 | 0,734789 | 2,704783 |
| C24 | -2,018990 | 0,910976 | 4,085486 |
| C25 | -2,003735 | -1,485359 | 4,397808 |
| H26 | -1,979577 | 1,604742 | 2,057421 |
| H27 | -2,020633 | 1,917032 | 4,495065 |
| H28 | -1,992779 | -2,350452 | 5,054541 |
| H29 | -2,035222 | -0,059195 | 6,012991 |
| O30 | 1,079275 | -4,140173 | -0,191907 |
| C31 | 2,661574 | -1,796163 | 1,931509 |
| C32 | 1,612886 | -1,432147 | 2,780458 |
| C33 | 3,960813 | -1,870081 | 2,454397 |
| C34 | 1,861288 | -1,094446 | 4,111329 |

C1_ZR_Chelbot_INT1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,907882 | -3,536817 | -0,962417 |
| C2 | -1,664930 | -4,499785 | -0,956801 |
| C3 | -2,921843 | -4,361916 | -1,855378 |
| C4 | -3,074916 | -3,310526 | 0,318844 |
| H5 | -4,814509 | -4,104491 | -0,728611 |
| H6 | -2,696241 | -3,868595 | -2,806159 |
| H7 | -3,642533 | -2,971044 | 1,185743 |
| H8 | -4,213623 | -2,592149 | -1,414809 |
| H9 | -0,965170 | -5,279244 | -1,258447 |
| H10 | -3,325877 | -5,351089 | -2,088262 |
| C11 | -2,298196 | -4,633339 | 0,446644 |
| H12 | -1,568846 | -4,631249 | 1,262586 |
| H13 | -2,947156 | -5,508962 | 0,536972 |
| C14 | 0,396178 | -3,060515 | -0,312579 |
| N15 | 0,983531 | -1,977408 | 0,055406 |
| C16 | 2,379121 | -2,301557 | 0,494194 |
| C17 | 2,363393 | -3,868664 | 0,400799 |
| P18 | -1,828624 | -0,739123 | 0,373067 |
| Ir19 | 0,167751 | 0,014471 | -0,322023 |
| C20 | -2,002419 | -0,533823 | 2,177854 |
| C21 | -2,058397 | -0,113456 | 4,944521 |
| C22 | -2,016855 | -1,624699 | 3,054456 |
| C23 | -1,992600 | 0,773519 | 2,695643 |
| C24 | -2,025358 | 0,978352 | 4,071684 |
| C25 | -2,049241 | -1,411643 | 4,434894 |
| H26 | -1,941128 | 1,627695 | 2,028393 |
| H27 | -2,015420 | 1,992319 | 4,460903 |
| H28 | -2,057770 | -2,262793 | 5,109657 |
| H29 | -2,082024 | 0,048871 | 6,018357 |
| O30 | 1,086804 | -4,200282 | -0,220805 |
| C31 | 2,638638 | -1,904851 | 1,944521 |
| C32 | 1,599236 | -1,544732 | 2,805097 |
| C33 | 3,937840 | -2,021226 | 2,460233 |
| C34 | 1,857026 | -1,261635 | 4,147457 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H35 | 0,598045 | -1,405448 | 2,408868 | H35 | 0,586751 | -1,475410 | 2,432622 |
| C36 | 4,208285 | -1,539470 | 3,785712 | C36 | 4,194305 | -1,745099 | 3,801673 |
| H37 | 4,785743 | -2,174077 | 1,816353 | H37 | 4,755284 | -2,313681 | 1,806563 |
| C38 | 3,160205 | -1,139032 | 4,616179 | C38 | 3,154611 | -1,354681 | 4,648461 |
| H39 | 1,030150 | -0,799896 | 4,745698 | H39 | 1,033963 | -0,970065 | 4,793890 |
| H40 | 5,222331 | -1,591504 | 4,171615 | H40 | 5,207649 | -1,830791 | 4,183464 |
| H41 | 3,356319 | -0,872528 | 5,650769 | H41 | 3,357226 | -1,131538 | 5,692032 |
| C42 | -3,376310 | 0,015579 | -0,341393 | C42 | -3,329952 | 0,015568 | -0,362756 |
| C43 | -4,386627 | 0,582865 | 0,444082 | C43 | -4,341373 | 0,618623 | 0,394769 |
| C44 | -3,533888 | -0,020954 | -1,738013 | C44 | -3,468612 | -0,059094 | -1,759878 |
| C45 | -5,524547 | 1,124844 | -0,157832 | C45 | -5,464259 | 1,157167 | -0,237127 |
| H46 | -4,291642 | 0,611643 | 1,523803 | H46 | -4,261148 | 0,674214 | 1,474579 |
| C47 | -4,666591 | 0,525989 | -2,335582 | C47 | -4,586227 | 0,486031 | -2,386269 |
| C48 | -5,663649 | 1,107125 | -1,545062 | C48 | -5,585451 | 1,101433 | -1,624833 |
| H49 | -6,302475 | 1,560747 | 0,462581 | H49 | -6,244482 | 1,619913 | 0,360472 |
| H50 | -4,778785 | 0,486388 | -3,415759 | H50 | -4,685660 | 0,418113 | -3,466218 |
| H51 | -6,548757 | 1,532405 | -2,009430 | H51 | -6,459502 | 1,523607 | -2,112357 |
| H52 | 0,626889 | 0,460564 | 1,112018 | H52 | 0,467885 | 0,413201 | 1,153718 |
| H53 | 1,852467 | 0,443352 | -0,648809 | H53 | 1,877691 | 0,879817 | -0,787723 |
| H54 | -1,936881 | -2,672771 | 2,605577 | H54 | -1,971385 | -2,637384 | 2,669513 |
| H55 | -2,778672 | -0,495492 | -2,354946 | H55 | -2,710435 | -0,559092 | -2,352973 |
| H56 | 3,143119 | -4,310474 | -0,023792 | H56 | 3,162040 | -4,284680 | -0,213991 |
| C57 | 5,093236 | -0,702864 | -2,536596 | C57 | 4,968388 | -0,444405 | -2,462052 |
| C58 | 4,339454 | -1,852997 | -2,773952 | C58 | 4,245945 | -1,597677 | -2,771766 |
| C59 | 3,493654 | -2,351350 | -1,784179 | C59 | 3,428778 | -2,189766 | -1,810405 |
| C60 | 3,392427 | -1,717475 | -0,537950 | C60 | 3,329812 | -1,651331 | -0,519367 |
| C61 | 4,129472 | -0,544932 | -0,323087 | C61 | 4,036636 | -0,477562 | -0,228499 |
| C62 | 4,978448 | -0,046620 | -1,312524 | C62 | 4,852481 | 0,118460 | -1,192204 |
| H63 | 5,751918 | -0,311848 | -3,306256 | H63 | 5,600883 | 0,022483 | -3,211021 |
| H64 | 4,408031 | -2,363266 | -3,730465 | H64 | 4,314195 | -2,035279 | -3,763716 |
| H65 | 2,900697 | -3,237236 | -1,997937 | H65 | 2,855710 | -3,073592 | -2,079709 |
| H66 | 4,045526 | -0,020054 | 0,621909 | H66 | 3,957107 | -0,029321 | 0,755770 |
| H67 | 5,542323 | 0,862867 | -1,126899 | H67 | 5,393680 | 1,028120 | -0,948713 |
| C68 | -1,018546 | 4,399570 | 1,971311 | C68 | -0,860448 | 4,488106 | 1,817789 |
| C69 | -0,294585 | 3,603150 | 1,086653 | C69 | -0,142710 | 3,641548 | 0,973494 |
| C70 | -0,925015 | 2,973972 | 0,000843 | C70 | -0,772418 | 2,969592 | -0,085844 |
| C71 | -2,304763 | 3,176522 | -0,168261 | C71 | -2,151909 | 3,181903 | -0,264534 |
| C72 | -3,028405 | 3,973632 | 0,717655 | C72 | -2,869800 | 4,026042 | 0,580158 |
| C73 | -2,390716 | 4,590415 | 1,793004 | C73 | -2,228626 | 4,687129 | 1,628035 |
| H74 | -0,505783 | 4,875888 | 2,802251 | H74 | -0,343671 | 4,994852 | 2,628131 |
| H75 | 0,767356 | 3,467625 | 1,261818 | H75 | 0,914481 | 3,499336 | 1,169473 |
| H76 | -2,824680 | 2,679595 | -0,978842 | H76 | -2,677011 | 2,648398 | -1,048554 |
| H77 | -4,096673 | 4,100017 | 0,567126 | H77 | -3,936643 | 4,155340 | 0,420760 |
| H78 | -2,952219 | 5,214076 | 2,482271 | H78 | -2,784978 | 5,347762 | 2,286392 |
| C79 | -0,182349 | 2,081541 | -0,945151 | C79 | -0,063987 | 1,974434 | -0,959600 |
| C80 | 1,283682 | 1,971606 | -0,934368 | C80 | 1,491258 | 1,952635 | -0,971161 |
| H81 | 1,769847 | 2,396435 | -0,061141 | H81 | 1,895851 | 2,481755 | -0,110271 |
| C82 | 2,063191 | 2,209391 | -2,195562 | C82 | 2,165732 | 2,387421 | -2,246967 |

| | | | | | | | |
|-------------------|-----------|-----------|-----------|--------------------|-----------|-----------|-----------|
| C83 | 2,503305 | 3,524422 | -2,416308 | C83 | 2,552612 | 3,726008 | -2,389767 |
| C84 | 2,322208 | 1,233306 | -3,160021 | C84 | 2,348640 | 1,502999 | -3,314159 |
| C85 | 3,168371 | 3,859371 | -3,594266 | C85 | 3,097648 | 4,177344 | -3,592193 |
| H86 | 2,313641 | 4,287365 | -1,664301 | H86 | 2,414463 | 4,417475 | -1,561678 |
| C87 | 2,983193 | 1,572368 | -4,342021 | C87 | 2,886986 | 1,956389 | -4,518997 |
| H88 | 2,019283 | 0,207858 | -2,981141 | H88 | 2,079360 | 0,457401 | -3,196619 |
| C89 | 3,402531 | 2,882899 | -4,566045 | C89 | 3,258731 | 3,294329 | -4,662679 |
| H90 | 3,503197 | 4,880574 | -3,753224 | H90 | 3,394057 | 5,217541 | -3,693830 |
| H91 | 3,176953 | 0,803356 | -5,084104 | H91 | 3,021086 | 1,261541 | -5,343245 |
| H92 | 3,916947 | 3,143612 | -5,486523 | H92 | 3,678367 | 3,647114 | -5,600420 |
| C93 | -1,010792 | 3,172859 | -3,158726 | C93 | -0,860106 | 3,074323 | -3,222287 |
| C94 | -0,751064 | 0,881822 | -2,993883 | C94 | -0,641907 | 0,785407 | -3,004086 |
| C95 | -1,660842 | 2,452266 | -4,351066 | C95 | -1,508255 | 2,335988 | -4,405981 |
| H96 | -0,059061 | 3,650487 | -3,415649 | H96 | 0,088668 | 3,549379 | -3,488266 |
| H97 | -1,671709 | 3,906852 | -2,694850 | H97 | -1,521969 | 3,815820 | -2,772391 |
| H98 | -2,752608 | 2,434966 | -4,275335 | H98 | -2,601267 | 2,338919 | -4,347608 |
| H99 | -1,356996 | 2,836020 | -5,324804 | H99 | -1,183279 | 2,691472 | -5,383603 |
| N100 | -0,782210 | 2,023887 | -2,271215 | N100 | -0,633035 | 1,941099 | -2,312165 |
| O101 | -1,190225 | 1,075696 | -4,243615 | O101 | -1,066275 | 0,952252 | -4,261755 |
| O102 | -0,384354 | -0,233173 | -2,584822 | O102 | -0,313698 | -0,332843 | -2,558744 |
| H103 | 2,239179 | -4,221656 | 1,514152 | H103 | 2,375905 | -4,332420 | 1,387800 |
| N104 | -1,931401 | -2,358329 | -0,035909 | N104 | -1,945580 | -2,383268 | 0,025971 |
| C105 | -0,966151 | -3,027444 | -0,945347 | C105 | -1,005525 | -3,100915 | -0,873520 |
| H106 | -0,899334 | -2,517034 | -1,914169 | H106 | -0,951887 | -2,629077 | -1,863264 |
| C1_ZR_Chelbot_TS2 | | | | C1_ZR_Chelbot_INT2 | | | |
| C1 | -4,265594 | -2,911447 | 0,903202 | C1 | -4,350695 | -2,897125 | 0,679996 |
| C2 | -2,396518 | -4,291031 | 0,165889 | C2 | -2,435451 | -4,275968 | 0,077365 |
| C3 | -3,898367 | -4,035131 | -0,120366 | C3 | -3,911982 | -4,018420 | -0,316786 |
| C4 | -2,917310 | -2,661695 | 1,617148 | C4 | -3,055677 | -2,647477 | 1,487462 |
| H5 | -5,011552 | -3,251399 | 1,629273 | H5 | -5,143350 | -3,240323 | 1,353281 |
| H6 | -4,075305 | -3,733867 | -1,157684 | H6 | -4,014260 | -3,714519 | -1,363519 |
| H7 | -2,982646 | -2,098612 | 2,545761 | H7 | -3,189140 | -2,087283 | 2,410874 |
| H8 | -4,654698 | -2,013698 | 0,423532 | H8 | -4,710281 | -2,001195 | 0,176063 |
| H9 | -2,006614 | -5,230070 | -0,225639 | H9 | -2,020161 | -5,214869 | -0,287350 |
| H10 | -4,474875 | -4,946764 | 0,060265 | H10 | -4,499997 | -4,930582 | -0,180516 |
| C11 | -2,326206 | -4,078948 | 1,693140 | C11 | -2,476944 | -4,067165 | 1,604947 |
| H12 | -1,311902 | -4,097489 | 2,103589 | H12 | -1,495429 | -4,089749 | 2,088350 |
| H13 | -2,960318 | -4,777223 | 2,246747 | H13 | -3,152024 | -4,764194 | 2,109684 |
| C14 | -0,121802 | -3,250116 | -0,470988 | C14 | -0,121439 | -3,245725 | -0,430460 |
| N15 | 0,759980 | -2,320511 | -0,391729 | N15 | 0,775480 | -2,331484 | -0,330880 |
| C16 | 2,114756 | -2,922675 | -0,616041 | C16 | 2,119214 | -2,954018 | -0,597479 |
| C17 | 1,758373 | -4,447585 | -0,738622 | C17 | 1,743215 | -4,473308 | -0,677998 |
| P18 | -1,704937 | -0,396317 | 0,284150 | P18 | -1,772386 | -0,376043 | 0,245233 |
| Ir19 | 0,414820 | -0,129807 | -0,293349 | Ir19 | 0,492499 | -0,117294 | -0,203332 |
| C20 | -2,153345 | 0,511328 | 1,792027 | C20 | -2,264261 | 0,509633 | 1,759838 |
| C21 | -2,628221 | 1,934978 | 4,154547 | C21 | -2,825968 | 1,892088 | 4,135498 |
| C22 | -1,647200 | 0,042319 | 3,016967 | C22 | -1,815056 | 0,012627 | 2,995650 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C23 | -2,855496 | 1,722228 | 1,754785 | C23 | -2,957587 | 1,725415 | 1,722722 |
| C24 | -3,096422 | 2,424091 | 2,937023 | C24 | -3,240208 | 2,406704 | 2,908567 |
| C25 | -1,894255 | 0,744713 | 4,191699 | C25 | -2,103228 | 0,694946 | 4,174363 |
| H26 | -3,190591 | 2,141036 | 0,814286 | H26 | -3,254808 | 2,165057 | 0,778921 |
| H27 | -3,637962 | 3,364273 | 2,894569 | H27 | -3,774664 | 3,350875 | 2,861401 |
| H28 | -1,508953 | 0,370069 | 5,135530 | H28 | -1,760463 | 0,295188 | 5,124404 |
| H29 | -2,819112 | 2,483928 | 5,072179 | H29 | -3,049933 | 2,423756 | 5,055574 |
| O30 | 0,305350 | -4,492009 | -0,736667 | O30 | 0,291449 | -4,493476 | -0,696141 |
| C31 | 3,013919 | -2,741220 | 0,604716 | C31 | 3,082186 | -2,756101 | 0,568552 |
| C32 | 2,486431 | -2,362827 | 1,843855 | C32 | 2,636806 | -2,310285 | 1,817822 |
| C33 | 4,371621 | -3,082155 | 0,524347 | C33 | 4,422356 | -3,147379 | 0,429557 |
| C34 | 3,312138 | -2,267381 | 2,964965 | C34 | 3,524897 | -2,205613 | 2,890021 |
| H35 | 1,432463 | -2,126057 | 1,927854 | H35 | 1,596985 | -2,037029 | 1,950500 |
| C36 | 5,194641 | -2,991378 | 1,645861 | C36 | 5,306179 | -3,049492 | 1,502664 |
| H37 | 4,793178 | -3,409481 | -0,421897 | H37 | 4,780048 | -3,522362 | -0,525416 |
| C38 | 4,669799 | -2,570908 | 2,868809 | C38 | 4,862554 | -2,566443 | 2,735042 |
| H39 | 2,889564 | -1,955903 | 3,916297 | H39 | 3,164857 | -1,844209 | 3,849244 |
| H40 | 6,246843 | -3,247737 | 1,562029 | H40 | 6,342390 | -3,348501 | 1,373983 |
| H41 | 5,312287 | -2,491767 | 3,740816 | H41 | 5,553018 | -2,481575 | 3,569021 |
| C42 | -2,973783 | -0,087851 | -1,007621 | C42 | -3,032918 | -0,069026 | -1,053153 |
| C43 | -4,295991 | 0,248800 | -0,671824 | C43 | -4,361120 | 0,277140 | -0,755436 |
| C44 | -2,661149 | -0,369479 | -2,347382 | C44 | -2,689244 | -0,366205 | -2,382935 |
| C45 | -5,272282 | 0,340194 | -1,661981 | C45 | -5,313326 | 0,358437 | -1,769687 |
| H46 | -4,574170 | 0,436366 | 0,358944 | H46 | -4,662587 | 0,478847 | 0,266223 |
| C47 | -3,646470 | -0,285959 | -3,331568 | C47 | -3,649617 | -0,292760 | -3,392860 |
| C48 | -4,950611 | 0,077146 | -2,994703 | C48 | -4,960820 | 0,076072 | -3,091107 |
| H49 | -6,286984 | 0,614535 | -1,388165 | H49 | -6,334094 | 0,637972 | -1,524827 |
| H50 | -3,388687 | -0,498364 | -4,365255 | H50 | -3,367659 | -0,518296 | -4,417493 |
| H51 | -5,714413 | 0,149897 | -3,763393 | H51 | -5,706445 | 0,139150 | -3,878501 |
| H52 | 0,606833 | -0,127122 | 1,257815 | H52 | 0,533159 | -0,112644 | 1,364152 |
| H53 | 2,634819 | 1,945031 | -0,943192 | H53 | 2,684589 | 2,064176 | -0,876188 |
| H54 | -1,050745 | -0,865083 | 3,043481 | H54 | -1,235837 | -0,905682 | 3,030013 |
| H55 | -1,643052 | -0,612305 | -2,629515 | H55 | -1,664799 | -0,614881 | -2,636296 |
| H56 | 2,119295 | -4,912752 | -1,656913 | H56 | 2,107254 | -4,969371 | -1,578426 |
| C57 | 3,511446 | -1,200657 | -4,357973 | C57 | 3,350259 | -1,387115 | -4,467707 |
| C58 | 2,474400 | -2,135331 | -4,340007 | C58 | 2,293432 | -2,292249 | -4,358928 |
| C59 | 2,052283 | -2,686615 | -3,134034 | C59 | 1,927199 | -2,791158 | -3,112388 |
| C60 | 2,663359 | -2,329325 | -1,923427 | C60 | 2,612117 | -2,410442 | -1,949155 |
| C61 | 3,691820 | -1,380250 | -1,952144 | C61 | 3,660718 | -1,490777 | -2,069358 |
| C62 | 4,113054 | -0,819165 | -3,160500 | C62 | 4,027226 | -0,983295 | -3,318984 |
| H63 | 3,843884 | -0,773419 | -5,299945 | H63 | 3,639856 | -1,000653 | -5,440788 |
| H64 | 1,986066 | -2,424813 | -5,265524 | H64 | 1,747070 | -2,601439 | -5,244831 |
| H65 | 1,223660 | -3,390285 | -3,137938 | H65 | 1,085129 | -3,475511 | -3,047752 |
| H66 | 4,179450 | -1,089097 | -1,029604 | H66 | 4,215498 | -1,179199 | -1,191809 |
| H67 | 4,925727 | -0,097317 | -3,160090 | H67 | 4,857071 | -0,284759 | -3,389187 |
| C68 | 1,343299 | 6,233598 | -1,654507 | C68 | 1,198887 | 6,248088 | -1,818479 |
| C69 | 1,152961 | 4,867377 | -1,850035 | C69 | 1,072993 | 4,865594 | -1,937354 |
| C70 | 1,945659 | 3,934266 | -1,166486 | C70 | 1,895505 | 4,006316 | -1,194044 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C71 | 2,925684 | 4,397748 | -0,283650 | C71 | 2,843583 | 4,564459 | -0,331596 |
| C72 | 3,110953 | 5,766193 | -0,079721 | C72 | 2,965641 | 5,949964 | -0,204699 |
| C73 | 2,320715 | 6,687526 | -0,766586 | C73 | 2,144353 | 6,797086 | -0,949106 |
| H74 | 0,718517 | 6,944692 | -2,187600 | H74 | 0,549215 | 6,897440 | -2,398688 |
| H75 | 0,368533 | 4,520631 | -2,515903 | H75 | 0,314634 | 4,448413 | -2,592111 |
| H76 | 3,546461 | 3,683638 | 0,253600 | H76 | 3,491200 | 3,911784 | 0,250496 |
| H77 | 3,875136 | 6,110952 | 0,611055 | H77 | 3,706982 | 6,365945 | 0,471504 |
| H78 | 2,464311 | 7,753070 | -0,611529 | H78 | 2,239627 | 7,874800 | -0,854434 |
| C79 | 1,714698 | 2,434511 | -1,284130 | C79 | 1,737191 | 2,490357 | -1,233232 |
| C80 | 0,545071 | 1,985334 | -0,320043 | C80 | 0,605102 | 2,015829 | -0,242737 |
| H81 | 0,942294 | 2,258358 | 0,664124 | H81 | 1,015116 | 2,301070 | 0,731798 |
| C82 | -0,690208 | 2,826273 | -0,538697 | C82 | -0,653959 | 2,824311 | -0,436937 |
| C83 | -1,526114 | 2,661356 | -1,652311 | C83 | -1,499662 | 2,647572 | -1,541205 |
| C84 | -0,996731 | 3,859736 | 0,360279 | C84 | -0,959783 | 3,860860 | 0,458732 |
| C85 | -2,640039 | 3,477883 | -1,849368 | C85 | -2,619370 | 3,456782 | -1,735135 |
| H86 | -1,321245 | 1,867815 | -2,358688 | H86 | -1,294833 | 1,854915 | -2,247392 |
| C87 | -2,100389 | 4,688124 | 0,163844 | C87 | -2,066832 | 4,684801 | 0,263435 |
| H88 | -0,352781 | 4,019057 | 1,221034 | H88 | -0,308817 | 4,031783 | 1,312063 |
| C89 | -2,932126 | 4,497760 | -0,941536 | C89 | -2,907136 | 4,483349 | -0,833900 |
| H90 | -3,282961 | 3,309496 | -2,709210 | H90 | -3,268798 | 3,277223 | -2,587854 |
| H91 | -2,310313 | 5,483549 | 0,874007 | H91 | -2,274331 | 5,484553 | 0,969317 |
| H92 | -3,796525 | 5,137996 | -1,094649 | H92 | -3,774612 | 5,119832 | -0,985318 |
| C93 | 2,391051 | 2,611983 | -3,766876 | C93 | 2,423898 | 2,556477 | -3,713159 |
| C94 | 0,975105 | 0,915680 | -3,159240 | C94 | 0,963038 | 0,910143 | -3,070061 |
| C95 | 1,705344 | 2,022441 | -5,001092 | C95 | 1,715806 | 1,967326 | -4,934575 |
| H96 | 3,422897 | 2,255237 | -3,646798 | H96 | 3,446740 | 2,174282 | -3,594589 |
| H97 | 2,388376 | 3,700905 | -3,756395 | H97 | 2,448771 | 3,645321 | -3,718143 |
| H98 | 0,929669 | 2,684612 | -5,399548 | H98 | 0,959177 | 2,645886 | -5,342335 |
| H99 | 2,390499 | 1,729226 | -5,796980 | H99 | 2,388717 | 1,639762 | -5,727673 |
| N100 | 1,538125 | 2,056308 | -2,703999 | N100 | 1,565199 | 2,040366 | -2,634777 |
| O101 | 1,061658 | 0,823442 | -4,497743 | O101 | 1,038656 | 0,798095 | -4,408679 |
| O102 | 0,424807 | 0,003379 | -2,523802 | O102 | 0,379081 | 0,024021 | -2,428622 |
| H103 | 2,105455 | -5,015496 | 0,125902 | H103 | 2,071683 | -5,020397 | 0,207144 |
| N104 | -1,926185 | -2,036466 | 0,685811 | N104 | -1,986555 | -2,025764 | 0,644742 |
| C105 | -1,611257 | -3,054354 | -0,345297 | C105 | -1,613213 | -3,037865 | -0,370724 |
| H106 | -1,976861 | -2,762982 | -1,342890 | H106 | -1,917141 | -2,742822 | -1,388324 |
| H107 | 3,184696 | 0,236705 | 0,010217 | H107 | 2,235104 | -0,062561 | -0,578998 |
| H108 | 3,035165 | 0,236918 | 0,740057 | H108 | 2,180693 | -0,027832 | 0,254869 |

C1_ZR_Chelbot_TS3

| | | | |
|----|-----------|-----------|-----------|
| C1 | -4,378606 | -3,027690 | 0,449091 |
| C2 | -2,399283 | -4,287599 | -0,212623 |
| C3 | -3,873445 | -4,043290 | -0,626116 |
| C4 | -3,113888 | -2,807595 | 1,310806 |
| H5 | -5,176735 | -3,454033 | 1,066162 |
| H6 | -3,958454 | -3,653164 | -1,645464 |
| H7 | -3,289096 | -2,328297 | 2,273199 |
| H8 | -4,755086 | -2,102015 | 0,015707 |

C1_ZR_Chelbot_PROD

| | | | |
|----|-----------|-----------|-----------|
| C1 | -4,378606 | -3,027690 | 0,449091 |
| C2 | -2,399283 | -4,287599 | -0,212623 |
| C3 | -3,873445 | -4,043290 | -0,626116 |
| C4 | -3,113888 | -2,807595 | 1,310806 |
| H5 | -5,176735 | -3,454033 | 1,066162 |
| H6 | -3,958454 | -3,653164 | -1,645464 |
| H7 | -3,289096 | -2,328297 | 2,273199 |
| H8 | -4,755086 | -2,102015 | 0,015707 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H9 | -1,945859 | -5,179554 | -0,643236 | H9 | -1,945859 | -5,179554 | -0,643236 |
| H10 | -4,431990 | -4,982843 | -0,586428 | H10 | -4,431990 | -4,982843 | -0,586428 |
| C11 | -2,489473 | -4,213635 | 1,326896 | C11 | -2,489473 | -4,213635 | 1,326896 |
| H12 | -1,520946 | -4,245842 | 1,835469 | H12 | -1,520946 | -4,245842 | 1,835469 |
| H13 | -3,152278 | -4,974493 | 1,748723 | H13 | -3,152278 | -4,974493 | 1,748723 |
| C14 | -0,106290 | -3,144510 | -0,569121 | C14 | -0,106290 | -3,144510 | -0,569121 |
| N15 | 0,777196 | -2,219449 | -0,410801 | N15 | 0,777196 | -2,219449 | -0,410801 |
| C16 | 2,151192 | -2,817823 | -0,582275 | C16 | 2,151192 | -2,817823 | -0,582275 |
| C17 | 1,795730 | -4,331617 | -0,776587 | C17 | 1,795730 | -4,331617 | -0,776587 |
| P18 | -1,884972 | -0,401510 | 0,276436 | P18 | -1,884972 | -0,401510 | 0,276436 |
| Ir19 | 0,516610 | -0,091166 | -0,174670 | Ir19 | 0,516610 | -0,091166 | -0,174670 |
| C20 | -2,254069 | 0,359488 | 1,891262 | C20 | -2,254069 | 0,359488 | 1,891262 |
| C21 | -2,491479 | 1,645197 | 4,370627 | C21 | -2,491479 | 1,645197 | 4,370627 |
| C22 | -1,798057 | -0,267141 | 3,062846 | C22 | -1,798057 | -0,267141 | 3,062846 |
| C23 | -2,801552 | 1,647029 | 1,970346 | C23 | -2,801552 | 1,647029 | 1,970346 |
| C24 | -2,920912 | 2,282236 | 3,207318 | C24 | -2,920912 | 2,282236 | 3,207318 |
| C25 | -1,925921 | 0,369488 | 4,294891 | C25 | -1,925921 | 0,369488 | 4,294891 |
| H26 | -3,114960 | 2,168770 | 1,073816 | H26 | -3,114960 | 2,168770 | 1,073816 |
| H27 | -3,344445 | 3,281438 | 3,254547 | H27 | -3,344445 | 3,281438 | 3,254547 |
| H28 | -1,579811 | -0,127462 | 5,196822 | H28 | -1,579811 | -0,127462 | 5,196822 |
| H29 | -2,587528 | 2,141654 | 5,331994 | H29 | -2,587528 | 2,141654 | 5,331994 |
| O30 | 0,344110 | -4,370816 | -0,844640 | O30 | 0,344110 | -4,370816 | -0,844640 |
| C31 | 2,985822 | -2,697162 | 0,692122 | C31 | 2,985822 | -2,697162 | 0,692122 |
| C32 | 2,380252 | -2,471807 | 1,932871 | C32 | 2,380252 | -2,471807 | 1,932871 |
| C33 | 4,361191 | -2,970373 | 0,649928 | C33 | 4,361191 | -2,970373 | 0,649928 |
| C34 | 3,141876 | -2,459749 | 3,101307 | C34 | 3,141876 | -2,459749 | 3,101307 |
| H35 | 1,311520 | -2,300800 | 1,986672 | H35 | 1,311520 | -2,300800 | 1,986672 |
| C36 | 5,120158 | -2,964980 | 1,819660 | C36 | 5,120158 | -2,964980 | 1,819660 |
| H37 | 4,844079 | -3,184622 | -0,298603 | H37 | 4,844079 | -3,184622 | -0,298603 |
| C38 | 4,515376 | -2,696982 | 3,048172 | C38 | 4,515376 | -2,696982 | 3,048172 |
| H39 | 2,657789 | -2,268118 | 4,054873 | H39 | 2,657789 | -2,268118 | 4,054873 |
| H40 | 6,185759 | -3,169420 | 1,768577 | H40 | 6,185759 | -3,169420 | 1,768577 |
| H41 | 5,108889 | -2,684373 | 3,957697 | H41 | 5,108889 | -2,684373 | 3,957697 |
| C42 | -3,269587 | 0,017680 | -0,861700 | C42 | -3,269587 | 0,017680 | -0,861700 |
| C43 | -4,551839 | 0,398706 | -0,437945 | C43 | -4,551839 | 0,398706 | -0,437945 |
| C44 | -3,039119 | -0,187254 | -2,233093 | C44 | -3,039119 | -0,187254 | -2,233093 |
| C45 | -5,572120 | 0,598045 | -1,367679 | C45 | -5,572120 | 0,598045 | -1,367679 |
| H46 | -4,760450 | 0,538173 | 0,617685 | H46 | -4,760450 | 0,538173 | 0,617685 |
| C47 | -4,066751 | -0,000257 | -3,159052 | C47 | -4,066751 | -0,000257 | -3,159052 |
| C48 | -5,333664 | 0,401748 | -2,730334 | C48 | -5,333664 | 0,401748 | -2,730334 |
| H49 | -6,557223 | 0,902835 | -1,025546 | H49 | -6,557223 | 0,902835 | -1,025546 |
| H50 | -3,874253 | -0,158979 | -4,216495 | H50 | -3,874253 | -0,158979 | -4,216495 |
| H51 | -6,131488 | 0,556649 | -3,450720 | H51 | -6,131488 | 0,556649 | -3,450720 |
| H52 | 0,562366 | -0,390766 | 1,365799 | H52 | 0,562366 | -0,390766 | 1,365799 |
| H53 | 2,685002 | 1,971802 | -1,117626 | H53 | 2,685002 | 1,971802 | -1,117626 |
| H54 | -1,333226 | -1,247151 | 3,005697 | H54 | -1,333226 | -1,247151 | 3,005697 |
| H55 | -2,045266 | -0,458891 | -2,578724 | H55 | -2,045266 | -0,458891 | -2,578724 |
| H56 | 2,195709 | -4,769962 | -1,691014 | H56 | 2,195709 | -4,769962 | -1,691014 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C57 | 3,858221 | -1,042968 | -4,169130 | C57 | 3,858221 | -1,042968 | -4,169130 |
| C58 | 2,867649 | -2,021125 | -4,258645 | C58 | 2,867649 | -2,021125 | -4,258645 |
| C59 | 2,336077 | -2,583068 | -3,099465 | C59 | 2,336077 | -2,583068 | -3,099465 |
| C60 | 2,790417 | -2,194554 | -1,832636 | C60 | 2,790417 | -2,194554 | -1,832636 |
| C61 | 3,760650 | -1,185846 | -1,754136 | C61 | 3,760650 | -1,185846 | -1,754136 |
| C62 | 4,292003 | -0,617820 | -2,912825 | C62 | 4,292003 | -0,617820 | -2,912825 |
| H63 | 4,289609 | -0,616598 | -5,071041 | H63 | 4,289609 | -0,616598 | -5,071041 |
| H64 | 2,501754 | -2,342710 | -5,228881 | H64 | 2,501754 | -2,342710 | -5,228881 |
| H65 | 1,544020 | -3,321161 | -3,193693 | H65 | 1,544020 | -3,321161 | -3,193693 |
| H66 | 4,113765 | -0,848815 | -0,787401 | H66 | 4,113765 | -0,848815 | -0,787401 |
| H67 | 5,061072 | 0,145725 | -2,829192 | H67 | 5,061072 | 0,145725 | -2,829192 |
| C68 | 1,267425 | 6,168859 | -2,182380 | C68 | 1,267425 | 6,168859 | -2,182380 |
| C69 | 1,089014 | 4,787794 | -2,213848 | C69 | 1,089014 | 4,787794 | -2,213848 |
| C70 | 1,966483 | 3,943095 | -1,519425 | C70 | 1,966483 | 3,943095 | -1,519425 |
| C71 | 3,020425 | 4,506718 | -0,794617 | C71 | 3,020425 | 4,506718 | -0,794617 |
| C72 | 3,195776 | 5,891311 | -0,756804 | C72 | 3,195776 | 5,891311 | -0,756804 |
| C73 | 2,319642 | 6,724788 | -1,451321 | C73 | 2,319642 | 6,724788 | -1,451321 |
| H74 | 0,578686 | 6,812693 | -2,722001 | H74 | 0,578686 | 6,812693 | -2,722001 |
| H75 | 0,255430 | 4,360912 | -2,762851 | H75 | 0,255430 | 4,360912 | -2,762851 |
| H76 | 3,710018 | 3,860502 | -0,255127 | H76 | 3,710018 | 3,860502 | -0,255127 |
| H77 | 4,019319 | 6,316482 | -0,190399 | H77 | 4,019319 | 6,316482 | -0,190399 |
| H78 | 2,455740 | 7,802153 | -1,425316 | H78 | 2,455740 | 7,802153 | -1,425316 |
| C79 | 1,750251 | 2,436729 | -1,455192 | C79 | 1,750251 | 2,436729 | -1,455192 |
| C80 | 0,673460 | 2,128733 | -0,360302 | C80 | 0,673460 | 2,128733 | -0,360302 |
| H81 | 1,143442 | 2,615515 | 0,503572 | H81 | 1,143442 | 2,615515 | 0,503572 |
| C82 | -0,636732 | 2,856515 | -0,521587 | C82 | -0,636732 | 2,856515 | -0,521587 |
| C83 | -1,526536 | 2,597372 | -1,571205 | C83 | -1,526536 | 2,597372 | -1,571205 |
| C84 | -0,945937 | 3,899458 | 0,364781 | C84 | -0,945937 | 3,899458 | 0,364781 |
| C85 | -2,694719 | 3,342192 | -1,723735 | C85 | -2,694719 | 3,342192 | -1,723735 |
| H86 | -1,318852 | 1,790119 | -2,258489 | H86 | -1,318852 | 1,790119 | -2,258489 |
| C87 | -2,106949 | 4,655056 | 0,211602 | C87 | -2,106949 | 4,655056 | 0,211602 |
| H88 | -0,262408 | 4,128945 | 1,178352 | H88 | -0,262408 | 4,128945 | 1,178352 |
| C89 | -2,989624 | 4,376662 | -0,833697 | C89 | -2,989624 | 4,376662 | -0,833697 |
| H90 | -3,381904 | 3,098187 | -2,528898 | H90 | -3,381904 | 3,098187 | -2,528898 |
| H91 | -2,321268 | 5,460701 | 0,908448 | H91 | -2,321268 | 5,460701 | 0,908448 |
| H92 | -3,899068 | 4,958890 | -0,952251 | H92 | -3,899068 | 4,958890 | -0,952251 |
| C93 | 2,301501 | 2,339536 | -3,949388 | C93 | 2,301501 | 2,339536 | -3,949388 |
| C94 | 0,873166 | 0,744320 | -3,122369 | C94 | 0,873166 | 0,744320 | -3,122369 |
| C95 | 1,598722 | 1,605072 | -5,095028 | C95 | 1,598722 | 1,605072 | -5,095028 |
| H96 | 3,335848 | 2,002917 | -3,805729 | H96 | 3,335848 | 2,002917 | -3,805729 |
| H97 | 2,289182 | 3,422271 | -4,068268 | H97 | 2,289182 | 3,422271 | -4,068268 |
| H98 | 0,843021 | 2,225603 | -5,586954 | H98 | 0,843021 | 2,225603 | -5,586954 |
| H99 | 2,279890 | 1,187310 | -5,836870 | H99 | 2,279890 | 1,187310 | -5,836870 |
| N100 | 1,474473 | 1,913520 | -2,808324 | N100 | 1,474473 | 1,913520 | -2,808324 |
| O101 | 0,919527 | 0,503331 | -4,441405 | O101 | 0,919527 | 0,503331 | -4,441405 |
| O102 | 0,289191 | -0,064390 | -2,385866 | O102 | 0,289191 | -0,064390 | -2,385866 |
| H103 | 2,097937 | -4,931829 | 0,082197 | H103 | 2,097937 | -4,931829 | 0,082197 |
| N104 | -2,045885 | -2,084187 | 0,558289 | N104 | -2,045885 | -2,084187 | 0,558289 |

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|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C105 | -1,610030 | -2,987370 | -0,532290 | C105 | -1,610030 | -2,987370 | -0,532290 |
| H106 | -1,900084 | -2,619624 | -1,528870 | H106 | -1,900084 | -2,619624 | -1,528870 |
| H107 | 2,062945 | 0,012316 | -0,199976 | H107 | 2,062945 | 0,012316 | -0,199976 |
| H108 | 1,172634 | 1,006051 | 0,770765 | H108 | 1,172634 | 1,006051 | 0,770765 |

C1_Z_R_tN_Cheltop

C1_ZR_Cheltop_SM

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,163822 | -3,413246 | 0,500286 |
| C2 | -2,022887 | -4,484285 | 0,029911 |
| C3 | -3,482708 | -4,418509 | -0,485656 |
| C4 | -2,990179 | -3,023927 | 1,429779 |
| H5 | -4,960655 | -3,890715 | 1,080214 |
| H6 | -3,537678 | -4,090098 | -1,528487 |
| H7 | -3,266325 | -2,517402 | 2,355083 |
| H8 | -4,593539 | -2,548370 | -0,004974 |
| H9 | -1,449989 | -5,341411 | -0,322379 |
| H10 | -3,942435 | -5,409219 | -0,430607 |
| C11 | -2,222742 | -4,350826 | 1,555913 |
| H12 | -1,291846 | -4,256405 | 2,123303 |
| H13 | -2,827439 | -5,159721 | 1,975102 |
| C14 | 0,151678 | -3,109060 | -0,165865 |
| N15 | 0,893574 | -2,055927 | -0,124078 |
| C16 | 2,348581 | -2,500516 | -0,199586 |
| C17 | 2,186909 | -4,027765 | 0,061654 |
| P18 | -1,924114 | -0,542219 | 0,464727 |
| Ir19 | 0,274759 | -0,006737 | -0,426515 |
| C20 | -2,162716 | 0,089448 | 2,164020 |
| C21 | -2,175954 | 1,166236 | 4,755891 |
| C22 | -1,462221 | -0,543592 | 3,203525 |
| C23 | -2,866203 | 1,270886 | 2,439398 |
| C24 | -2,872043 | 1,804441 | 3,729486 |
| C25 | -1,474891 | -0,012104 | 4,489994 |
| H26 | -3,422200 | 1,770175 | 1,654765 |
| H27 | -3,430909 | 2,714014 | 3,931950 |
| H28 | -0,929103 | -0,512075 | 5,284699 |
| H29 | -2,180416 | 1,582866 | 5,758834 |
| O30 | 0,770845 | -4,292897 | -0,146065 |
| C31 | 3,198648 | -1,909446 | 0,917743 |
| C32 | 2,602939 | -1,431603 | 2,087810 |
| C33 | 4,598555 | -1,958000 | 0,841655 |
| C34 | 3,385224 | -0,937864 | 3,131366 |
| H35 | 1,525079 | -1,409146 | 2,174545 |
| C36 | 5,380990 | -1,479057 | 1,891304 |
| H37 | 5,081246 | -2,358149 | -0,044546 |
| C38 | 4,776182 | -0,952864 | 3,034442 |
| H39 | 2,900404 | -0,533988 | 4,015167 |
| H40 | 6,463771 | -1,512751 | 1,811564 |
| H41 | 5,386241 | -0,565986 | 3,845709 |

C1_ZR_Cheltop_TS1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,985440 | -3,688238 | -0,507837 |
| C2 | -1,734715 | -4,631017 | -0,543501 |
| C3 | -3,047673 | -4,600110 | -1,368599 |
| C4 | -3,087472 | -3,351155 | 0,705208 |
| H5 | -4,883957 | -4,222408 | -0,182525 |
| H6 | -2,892273 | -4,214193 | -2,381196 |
| H7 | -3,608539 | -2,947615 | 1,573525 |
| H8 | -4,305188 | -2,784063 | -1,030201 |
| H9 | -1,034948 | -5,420752 | -0,816730 |
| H10 | -3,451332 | -5,612221 | -1,462982 |
| C11 | -2,280997 | -4,646727 | 0,901562 |
| H12 | -1,506873 | -4,558960 | 1,669698 |
| H13 | -2,906425 | -5,520161 | 1,106645 |
| C14 | 0,326072 | -3,079454 | -0,205062 |
| N15 | 0,939385 | -1,957501 | -0,044093 |
| C16 | 2,312987 | -2,246486 | 0,502841 |
| C17 | 2,395602 | -3,792228 | 0,269504 |
| P18 | -1,959485 | -0,752685 | 0,333158 |
| Ir19 | 0,057576 | -0,027395 | -0,574160 |
| C20 | -2,264643 | -0,340436 | 2,085234 |
| C21 | -2,578878 | 0,396040 | 4,770759 |
| C22 | -2,042342 | -1,275781 | 3,105793 |
| C23 | -2,636043 | 0,971563 | 2,422520 |
| C24 | -2,786680 | 1,335525 | 3,758526 |
| C25 | -2,207644 | -0,908526 | 4,441686 |
| H26 | -2,813548 | 1,707959 | 1,646633 |
| H27 | -3,069697 | 2,354762 | 4,005273 |
| H28 | -2,040677 | -1,643151 | 5,224339 |
| H29 | -2,703695 | 0,679968 | 5,811790 |
| O30 | 1,018348 | -4,196436 | 0,026023 |
| C31 | 2,383891 | -1,973353 | 2,009128 |
| C32 | 1,328318 | -1,423166 | 2,731866 |
| C33 | 3,556796 | -2,332258 | 2,692828 |
| C34 | 1,440773 | -1,218145 | 4,108391 |
| H35 | 0,423527 | -1,125694 | 2,225214 |
| C36 | 3,671468 | -2,130130 | 4,065202 |
| H37 | 4,395118 | -2,753869 | 2,142682 |
| C38 | 2,610036 | -1,567748 | 4,779095 |
| H39 | 0,606278 | -0,778066 | 4,646106 |
| H40 | 4,589323 | -2,406990 | 4,575872 |
| H41 | 2,698798 | -1,404638 | 5,849405 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C42 | -3,402936 | -0,059681 | -0,500964 | C42 | -3,461673 | -0,149575 | -0,545760 |
| C43 | -4,683414 | 0,031264 | 0,073048 | C43 | -4,679724 | 0,053980 | 0,121837 |
| C44 | -3,265983 | 0,099566 | -1,887507 | C44 | -3,424286 | -0,001169 | -1,942236 |
| C45 | -5,795759 | 0,294955 | -0,724477 | C45 | -5,823651 | 0,422240 | -0,587352 |
| H46 | -4,815878 | -0,109619 | 1,141559 | H46 | -4,740781 | -0,068436 | 1,198095 |
| C47 | -4,382791 | 0,355496 | -2,682549 | C47 | -4,570765 | 0,359940 | -2,649149 |
| C48 | -5,648482 | 0,457646 | -2,104662 | C48 | -5,773174 | 0,580210 | -1,972919 |
| H49 | -6,778963 | 0,367892 | -0,268299 | H49 | -6,755678 | 0,583359 | -0,053295 |
| H50 | -4,258583 | 0,492985 | -3,752287 | H50 | -4,523722 | 0,472884 | -3,728586 |
| H51 | -6,516452 | 0,664815 | -2,723537 | H51 | -6,664589 | 0,867691 | -2,522395 |
| H52 | -0,118265 | -0,426696 | -1,876820 | H52 | -0,510252 | -0,644608 | -1,887817 |
| H53 | 1,756879 | -0,019484 | -0,994288 | H53 | 1,397277 | 0,442583 | -1,474525 |
| H54 | -0,898290 | -1,447363 | 2,994827 | H54 | -1,721794 | -2,282353 | 2,859900 |
| H55 | -2,280543 | 0,049830 | -2,337724 | H55 | -2,495843 | -0,169604 | -2,477892 |
| H56 | 2,759819 | -4,655219 | -0,620771 | H56 | 2,982088 | -4,077008 | -0,606850 |
| C57 | 3,440060 | -1,516173 | -4,289974 | C57 | 5,278874 | -0,073434 | -1,818180 |
| C58 | 2,651651 | -2,634007 | -4,010154 | C58 | 4,545152 | -1,111458 | -2,396651 |
| C59 | 2,347692 | -2,964294 | -2,691094 | C59 | 3,583240 | -1,788578 | -1,648684 |
| C60 | 2,827657 | -2,190005 | -1,625024 | C60 | 3,359116 | -1,467652 | -0,302456 |
| C61 | 3,616145 | -1,069096 | -1,919436 | C61 | 4,079120 | -0,405985 | 0,259426 |
| C62 | 3,920989 | -0,736308 | -3,239883 | C62 | 5,028943 | 0,286194 | -0,493901 |
| H63 | 3,677595 | -1,258404 | -5,318104 | H63 | 6,032949 | 0,452262 | -2,397083 |
| H64 | 2,270926 | -3,249316 | -4,820205 | H64 | 4,715479 | -1,390389 | -3,432589 |
| H65 | 1,711277 | -3,824846 | -2,502155 | H65 | 2,999655 | -2,568986 | -2,128895 |
| H66 | 3,992277 | -0,439695 | -1,123062 | H66 | 3,898699 | -0,116723 | 1,287815 |
| H67 | 4,533014 | 0,138668 | -3,440284 | H67 | 5,587728 | 1,096835 | -0,033233 |
| C68 | -2,453897 | 3,302128 | -3,398380 | C68 | 0,931160 | 3,343253 | -5,053464 |
| C69 | -1,343744 | 2,760440 | -2,754242 | C69 | 0,511598 | 3,021901 | -3,761657 |
| C70 | -1,295880 | 2,674830 | -1,354769 | C70 | 1,250817 | 2,119419 | -2,987345 |
| C71 | -2,394101 | 3,159978 | -0,628321 | C71 | 2,416733 | 1,552185 | -3,512369 |
| C72 | -3,505105 | 3,700735 | -1,270648 | C72 | 2,833070 | 1,873488 | -4,801413 |
| C73 | -3,541160 | 3,774906 | -2,662024 | C73 | 2,089144 | 2,768352 | -5,575929 |
| H74 | -2,464601 | 3,362781 | -4,483077 | H74 | 0,352978 | 4,044331 | -5,648205 |
| H75 | -0,513075 | 2,408586 | -3,356781 | H75 | -0,378273 | 3,487901 | -3,348754 |
| H76 | -2,371831 | 3,109198 | 0,453696 | H76 | 2,989997 | 0,854594 | -2,910692 |
| H77 | -4,342910 | 4,062848 | -0,681596 | H77 | 3,735000 | 1,422223 | -5,204906 |
| H78 | -4,403005 | 4,199897 | -3,167737 | H78 | 2,411881 | 3,015712 | -6,583039 |
| C79 | -0,105718 | 2,135046 | -0,625453 | C79 | 0,832097 | 1,869472 | -1,562285 |
| C80 | 1,125894 | 1,794340 | -1,301997 | C80 | -0,606508 | 1,880847 | -1,238592 |
| H81 | 1,049895 | 1,681344 | -2,378278 | H81 | -1,193797 | 1,718687 | -2,138942 |
| C82 | 2,448627 | 2,374831 | -0,891429 | C82 | -1,284687 | 2,908453 | -0,388149 |
| C83 | 3,258886 | 1,897898 | 0,145576 | C83 | -2,452759 | 3,484804 | -0,923395 |
| C84 | 2,869544 | 3,501593 | -1,616833 | C84 | -0,870269 | 3,344976 | 0,882602 |
| C85 | 4,457747 | 2,542401 | 0,457150 | C85 | -3,160040 | 4,470630 | -0,238679 |
| H86 | 2,963486 | 1,017598 | 0,704094 | H86 | -2,818511 | 3,139636 | -1,887186 |
| C87 | 4,065072 | 4,145460 | -1,302243 | C87 | -1,566655 | 4,346704 | 1,559318 |
| H88 | 2,252098 | 3,875455 | -2,430776 | H88 | -0,052512 | 2,862983 | 1,396188 |
| C89 | 4,863186 | 3,667668 | -0,260299 | C89 | -2,711491 | 4,918294 | 1,004833 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H90 | 5,074813 | 2,151098 | 1,260956 | H90 | -4,061421 | 4,888643 | -0,678137 |
| H91 | 4,375024 | 5,015702 | -1,874073 | H91 | -1,221336 | 4,661866 | 2,540376 |
| H92 | 5,797544 | 4,165669 | -0,017714 | H92 | -3,254796 | 5,691960 | 1,539509 |
| C93 | 0,253719 | 4,152200 | 0,963127 | C93 | 2,382860 | 3,788424 | -0,767224 |
| C94 | 0,565857 | 1,992161 | 1,718499 | C94 | 1,894209 | 1,996902 | 0,636393 |
| C95 | 0,396116 | 4,111600 | 2,494225 | C95 | 3,297123 | 3,777524 | 0,475681 |
| H96 | -0,600665 | 4,744427 | 0,631138 | H96 | 1,629901 | 4,584521 | -0,736266 |
| H97 | 1,160012 | 4,506365 | 0,458763 | H97 | 2,941272 | 3,854964 | -1,702679 |
| H98 | 1,140008 | 4,802905 | 2,890317 | H98 | 4,319853 | 3,477591 | 0,230771 |
| H99 | -0,562381 | 4,255793 | 3,002762 | H99 | 3,305754 | 4,720004 | 1,023389 |
| N100 | 0,050859 | 2,720383 | 0,699010 | N100 | 1,746671 | 2,480445 | -0,618967 |
| O101 | 0,845388 | 2,755521 | 2,780340 | O101 | 2,735547 | 2,756401 | 1,350476 |
| O102 | 0,775563 | 0,772568 | 1,698640 | O102 | 1,327054 | 1,001924 | 1,100646 |
| H103 | 2,418786 | -4,287215 | 1,096734 | H103 | 2,750948 | -4,333692 | 1,144298 |
| N104 | -1,976677 | -2,223764 | 0,684957 | N104 | -1,989625 | -2,441503 | 0,280211 |
| C105 | -1,350842 | -3,127565 | -0,305465 | C105 | -1,113954 | -3,213520 | -0,634717 |
| H106 | -1,566896 | -2,828804 | -1,342630 | H106 | -1,162456 | -2,841813 | -1,667793 |

C1_ZR_Cheltop_INT1

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,965371 | -3,603242 | 0,894195 |
| C2 | -1,807226 | -4,586670 | 0,328842 |
| C3 | -3,308515 | -4,668443 | -0,044655 |
| C4 | -2,746872 | -3,064935 | 1,680435 |
| H5 | -4,688654 | -4,056746 | 1,579988 |
| H6 | -3,482983 | -4,463705 | -1,105671 |
| H7 | -2,981112 | -2,496035 | 2,580074 |
| H8 | -4,477660 | -2,811469 | 0,345697 |
| H9 | -1,203606 | -5,431669 | -0,001192 |
| H10 | -3,688950 | -5,672947 | 0,161330 |
| C11 | -1,878268 | -4,322733 | 1,849076 |
| H12 | -0,909819 | -4,114419 | 2,314479 |
| H13 | -2,383090 | -5,125848 | 2,393340 |
| C14 | 0,233641 | -3,113761 | -0,248708 |
| N15 | 0,898406 | -2,015381 | -0,211861 |
| C16 | 2,362284 | -2,337685 | -0,304198 |
| C17 | 2,306569 | -3,856450 | -0,681605 |
| P18 | -1,877231 | -0,606696 | 0,489458 |
| Ir19 | 0,052281 | -0,009391 | -0,441195 |
| C20 | -2,044303 | 0,117001 | 2,161606 |
| C21 | -1,972406 | 1,380194 | 4,668642 |
| C22 | -1,302231 | -0,436064 | 3,217533 |
| C23 | -2,746097 | 1,312634 | 2,375558 |
| C24 | -2,710630 | 1,937755 | 3,623393 |
| C25 | -1,273186 | 0,188122 | 4,462641 |
| H26 | -3,332616 | 1,749932 | 1,575627 |
| H27 | -3,270119 | 2,856042 | 3,779407 |
| H28 | -0,697809 | -0,251712 | 5,271768 |
| H29 | -1,945254 | 1,867889 | 5,638509 |

C1_ZR_Cheltop_TS2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -4,124279 | -3,124928 | 0,159666 |
| C2 | -2,071143 | -4,280357 | -0,462415 |
| C3 | -3,526487 | -4,057611 | -0,943572 |
| C4 | -2,921098 | -2,931449 | 1,113872 |
| H5 | -4,943845 | -3,611002 | 0,699304 |
| H6 | -3,568062 | -3,608201 | -1,940951 |
| H7 | -3,164399 | -2,523652 | 2,094954 |
| H8 | -4,504241 | -2,184666 | -0,236744 |
| H9 | -1,558463 | -5,125849 | -0,919556 |
| H10 | -4,054480 | -5,014082 | -0,992957 |
| C11 | -2,250662 | -4,315372 | 1,071898 |
| H12 | -1,311238 | -4,357489 | 1,631160 |
| H13 | -2,911579 | -5,122046 | 1,401071 |
| C14 | 0,190230 | -3,038574 | -0,521293 |
| N15 | 0,982463 | -2,039426 | -0,338734 |
| C16 | 2,375695 | -2,606747 | -0,134967 |
| C17 | 2,158346 | -4,105806 | -0,527743 |
| P18 | -1,691060 | -0,440560 | 0,483200 |
| Ir19 | 0,241647 | 0,088237 | -0,520707 |
| C20 | -1,692013 | -0,024819 | 2,259580 |
| C21 | -1,509535 | 0,659845 | 4,970534 |
| C22 | -1,219419 | -0,956484 | 3,195247 |
| C23 | -2,068589 | 1,255335 | 2,694128 |
| C24 | -1,982942 | 1,590901 | 4,044238 |
| C25 | -1,131467 | -0,613943 | 4,543471 |
| H26 | -2,443652 | 1,980147 | 1,982429 |
| H27 | -2,296176 | 2,577192 | 4,375737 |
| H28 | -0,771434 | -1,345983 | 5,260452 |
| H29 | -1,442334 | 0,923942 | 6,021850 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| O30 | 0,926436 | -4,244285 | -0,422043 | O30 | 0,717182 | -4,262340 | -0,571687 |
| C31 | 3,041728 | -2,165921 | 1,055857 | C31 | 2,773039 | -2,551243 | 1,345502 |
| C32 | 2,350929 | -1,707868 | 2,178550 | C32 | 1,977616 | -1,946896 | 2,314873 |
| C33 | 4,394523 | -2,519961 | 1,188266 | C33 | 3,973539 | -3,163827 | 1,740280 |
| C34 | 3,003761 | -1,578190 | 3,406301 | C34 | 2,375367 | -1,932983 | 3,653712 |
| H35 | 1,311543 | -1,426684 | 2,093481 | H35 | 1,063006 | -1,456726 | 2,025763 |
| C36 | 5,043550 | -2,395515 | 2,413868 | C36 | 4,369878 | -3,155506 | 3,074522 |
| H37 | 4,947073 | -2,880981 | 0,324681 | H37 | 4,612916 | -3,631150 | 0,994762 |
| C38 | 4,349258 | -1,917785 | 3,528417 | C38 | 3,571038 | -2,533467 | 4,038366 |
| H39 | 2,453574 | -1,203494 | 4,265085 | H39 | 1,747252 | -1,436035 | 4,387808 |
| H40 | 6,091784 | -2,667457 | 2,498531 | H40 | 5,305137 | -3,627295 | 3,361900 |
| H41 | 4,856531 | -1,814740 | 4,483423 | H41 | 3,883834 | -2,518877 | 5,078564 |
| C42 | -3,410829 | -0,181838 | -0,416465 | C42 | -3,280746 | 0,135662 | -0,205942 |
| C43 | -4,651108 | -0,192902 | 0,248425 | C43 | -4,388259 | 0,383808 | 0,621354 |
| C44 | -3,379940 | 0,066275 | -1,795605 | C44 | -3,470630 | 0,020260 | -1,590665 |
| C45 | -5,829808 | 0,047598 | -0,455155 | C45 | -5,658406 | 0,530328 | 0,066376 |
| H46 | -4,698822 | -0,384023 | 1,316619 | H46 | -4,273720 | 0,436284 | 1,697996 |
| C47 | -4,563028 | 0,303476 | -2,495379 | C47 | -4,744342 | 0,154177 | -2,137193 |
| C48 | -5,788971 | 0,296108 | -1,829957 | C48 | -5,840110 | 0,412826 | -1,312053 |
| H49 | -6,780164 | 0,040644 | 0,070752 | H49 | -6,507920 | 0,722742 | 0,715304 |
| H50 | -4,519784 | 0,512808 | -3,559690 | H50 | -4,878716 | 0,069294 | -3,211426 |
| H51 | -6,708399 | 0,486914 | -2,375627 | H51 | -6,831837 | 0,519912 | -1,741657 |
| H52 | -0,499029 | -0,476815 | -1,835112 | H52 | -0,460208 | -0,276032 | -1,881130 |
| H53 | 1,689038 | 0,816110 | -1,337113 | H53 | 2,059941 | 2,372488 | -1,299922 |
| H54 | -0,742926 | -1,352240 | 3,058460 | H54 | -0,920574 | -1,946289 | 2,868888 |
| H55 | -2,429294 | 0,107492 | -2,313095 | H55 | -2,621805 | -0,170656 | -2,237499 |
| H56 | 2,511863 | -4,048623 | -1,737491 | H56 | 2,549328 | -4,370108 | -1,511811 |
| C57 | 3,867317 | 0,164987 | -3,532433 | C57 | 5,158228 | -0,529783 | -2,743216 |
| C58 | 2,847442 | -0,765338 | -3,753614 | C58 | 4,260433 | -1,461032 | -3,267941 |
| C59 | 2,403420 | -1,577635 | -2,712860 | C59 | 3,389585 | -2,146684 | -2,422345 |
| C60 | 2,966512 | -1,483406 | -1,428689 | C60 | 3,404316 | -1,924236 | -1,038340 |
| C61 | 3,984541 | -0,547275 | -1,219068 | C61 | 4,302632 | -0,980139 | -0,522822 |
| C62 | 4,432934 | 0,267083 | -2,263058 | C62 | 5,168410 | -0,284895 | -1,369847 |
| H63 | 4,211869 | 0,804624 | -4,339553 | H63 | 5,836225 | 0,007455 | -3,399813 |
| H64 | 2,392485 | -0,854220 | -4,736138 | H64 | 4,232658 | -1,650516 | -4,337007 |
| H65 | 1,582436 | -2,265987 | -2,893925 | H65 | 2,667664 | -2,827673 | -2,863763 |
| H66 | 4,420072 | -0,429997 | -0,234874 | H66 | 4,336193 | -0,793349 | 0,544504 |
| H67 | 5,210415 | 0,999553 | -2,068916 | H67 | 5,865262 | 0,434807 | -0,949454 |
| C68 | -2,424056 | 3,268821 | -3,607780 | C68 | -2,906270 | 2,929868 | -3,091969 |
| C69 | -1,309563 | 2,726601 | -2,966457 | C69 | -1,709520 | 2,469765 | -2,556167 |
| C70 | -1,245890 | 2,651581 | -1,567599 | C70 | -1,389169 | 2,663024 | -1,199533 |
| C71 | -2,346575 | 3,139198 | -0,840517 | C71 | -2,349622 | 3,290150 | -0,398445 |
| C72 | -3,458254 | 3,682495 | -1,477034 | C72 | -3,562865 | 3,738518 | -0,927104 |
| C73 | -3,503651 | 3,752468 | -2,869559 | C73 | -3,842072 | 3,577863 | -2,280280 |
| H74 | -2,442109 | 3,318209 | -4,693081 | H74 | -3,113906 | 2,776989 | -4,147555 |
| H75 | -0,493242 | 2,358373 | -3,578541 | H75 | -1,007090 | 1,952684 | -3,201373 |
| H76 | -2,329196 | 3,075794 | 0,241464 | H76 | -2,158260 | 3,439189 | 0,656797 |
| H77 | -4,292745 | 4,045800 | -0,883513 | H77 | -4,285481 | 4,219204 | -0,273454 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H78 | -4,366815 | 4,178710 | -3,372117 | H78 | -4,778638 | 3,936459 | -2,696539 |
| C79 | -0,093832 | 2,039747 | -0,824433 | C79 | -0,029569 | 2,227352 | -0,697608 |
| C80 | 1,247613 | 1,836162 | -1,588043 | C80 | 1,102930 | 2,767369 | -1,644807 |
| H81 | 1,072242 | 1,759075 | -2,657857 | H81 | 0,950791 | 2,328878 | -2,635364 |
| C82 | 2,347522 | 2,822712 | -1,288230 | C82 | 1,273868 | 4,275258 | -1,797267 |
| C83 | 3,198653 | 2,659181 | -0,188976 | C83 | 2,518075 | 4,834894 | -1,463912 |
| C84 | 2,472330 | 3,966178 | -2,085879 | C84 | 0,272066 | 5,136045 | -2,269301 |
| C85 | 4,147058 | 3,634875 | 0,119601 | C85 | 2,751471 | 6,205992 | -1,570353 |
| H86 | 3,118931 | 1,765432 | 0,423230 | H86 | 3,314955 | 4,184711 | -1,107691 |
| C87 | 3,425807 | 4,938979 | -1,781682 | C87 | 0,502362 | 6,508558 | -2,373769 |
| H88 | 1,810970 | 4,100688 | -2,938456 | H88 | -0,693117 | 4,744111 | -2,560874 |
| C89 | 4,261765 | 4,778211 | -0,674464 | C89 | 1,737337 | 7,052208 | -2,020228 |
| H90 | 4,798463 | 3,500396 | 0,978552 | H90 | 3,723183 | 6,611196 | -1,301455 |
| H91 | 3,513367 | 5,823056 | -2,406983 | H91 | -0,291972 | 7,154971 | -2,737452 |
| H92 | 5,001354 | 5,537014 | -0,435650 | H92 | 1,909433 | 8,121722 | -2,100760 |
| C93 | 0,229008 | 4,166322 | 0,734180 | C93 | 0,342734 | 4,149922 | 1,149049 |
| C94 | 0,650785 | 2,029694 | 1,487534 | C94 | 0,928539 | 1,965472 | 1,537772 |
| C95 | 0,431488 | 4,137670 | 2,259971 | C95 | 0,635785 | 3,913148 | 2,635092 |
| H96 | -0,672629 | 4,704801 | 0,439315 | H96 | -0,575311 | 4,708366 | 0,971136 |
| H97 | 1,088431 | 4,585541 | 0,203589 | H97 | 1,161814 | 4,666400 | 0,646886 |
| H98 | 1,163227 | 4,859632 | 2,622522 | H98 | 1,326996 | 4,634651 | 3,071246 |
| H99 | -0,509794 | 4,245409 | 2,808366 | H99 | -0,273279 | 3,849496 | 3,241941 |
| N100 | 0,105592 | 2,723211 | 0,469756 | N100 | 0,240239 | 2,745849 | 0,681762 |
| O101 | 0,944106 | 2,800521 | 2,536980 | O101 | 1,272573 | 2,604302 | 2,661610 |
| O102 | 0,884939 | 0,805960 | 1,470536 | O102 | 1,244135 | 0,773003 | 1,350070 |
| H103 | 2,950629 | -4,473271 | -0,057339 | H103 | 2,544312 | -4,797287 | 0,219226 |
| N104 | -1,859897 | -2,275589 | 0,778054 | N104 | -1,842443 | -2,125764 | 0,460872 |
| C105 | -1,271037 | -3,225788 | -0,192738 | C105 | -1,307514 | -2,942947 | -0,651962 |
| H106 | -1,623720 | -3,044151 | -1,220328 | H106 | -1,522293 | -2,504147 | -1,636701 |
| | | | | H107 | 2,650155 | 0,421250 | -1,775188 |
| | | | | H108 | 2,146376 | 0,370561 | -2,334344 |

C1_ZR_Cheltop_INT2

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -4,167331 | -3,142396 | 0,230583 |
| C2 | -2,120207 | -4,319958 | -0,368700 |
| C3 | -3,574095 | -4,097924 | -0,855289 |
| C4 | -2,963069 | -2,937606 | 1,181343 |
| H5 | -4,990534 | -3,613905 | 0,777507 |
| H6 | -3,611611 | -3,666187 | -1,860660 |
| H7 | -3,206608 | -2,511553 | 2,154529 |
| H8 | -4,540155 | -2,206299 | -0,182838 |
| H9 | -1,610507 | -5,175872 | -0,810352 |
| H10 | -4,108041 | -5,051783 | -0,888602 |
| C11 | -2,300112 | -4,325805 | 1,165775 |
| H12 | -1,360844 | -4,361659 | 1,726012 |
| H13 | -2,964177 | -5,123839 | 1,509209 |
| C14 | 0,146935 | -3,089053 | -0,471259 |
| N15 | 0,931379 | -2,083208 | -0,313602 |

C1_ZR_Cheltop_TS3

| | | | |
|-----|-----------|-----------|-----------|
| C1 | -4,121495 | -3,584966 | -0,338868 |
| C2 | -1,920310 | -4,598277 | -0,615310 |
| C3 | -3,301718 | -4,495156 | -1,312578 |
| C4 | -3,098773 | -3,308374 | 0,787814 |
| H5 | -4,995754 | -4,106900 | 0,063850 |
| H6 | -3,225791 | -4,076935 | -2,321620 |
| H7 | -3,524812 | -2,913053 | 1,709774 |
| H8 | -4,470339 | -2,661805 | -0,804314 |
| H9 | -1,279640 | -5,402957 | -0,975753 |
| H10 | -3,748720 | -5,489164 | -1,404042 |
| C11 | -2,328372 | -4,637079 | 0,874493 |
| H12 | -1,483219 | -4,599438 | 1,568575 |
| H13 | -2,964832 | -5,493754 | 1,113631 |
| C14 | 0,224093 | -3,145207 | -0,445415 |
| N15 | 0,903229 | -2,061157 | -0,268789 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C16 | 2,333920 | -2,614577 | -0,131000 | C16 | 2,318326 | -2,448174 | 0,115215 |
| C17 | 2,142515 | -4,106971 | -0,551656 | C17 | 2,318386 | -3,934280 | -0,344257 |
| P18 | -1,721689 | -0,457490 | 0,521379 | P18 | -1,929437 | -0,728332 | 0,358471 |
| Ir19 | 0,295014 | 0,053284 | -0,531703 | Ir19 | 0,197622 | -0,117626 | -0,671197 |
| C20 | -1,727228 | -0,025904 | 2,298803 | C20 | -2,113877 | -0,352477 | 2,140993 |
| C21 | -1,544160 | 0,697333 | 5,002364 | C21 | -2,191517 | 0,348189 | 4,859360 |
| C22 | -1,260312 | -0,944768 | 3,249369 | C22 | -1,860449 | -1,313139 | 3,130245 |
| C23 | -2,102608 | 1,259967 | 2,717323 | C23 | -2,399041 | 0,965678 | 2,530260 |
| C24 | -2,015790 | 1,615021 | 4,062524 | C24 | -2,436957 | 1,311914 | 3,879492 |
| C25 | -1,170112 | -0,582833 | 4,592883 | C25 | -1,905859 | -0,963457 | 4,480273 |
| H26 | -2,477884 | 1,976285 | 1,996279 | H26 | -2,602078 | 1,721886 | 1,780870 |
| H27 | -2,327062 | 2,606661 | 4,379640 | H27 | -2,665016 | 2,335394 | 4,165094 |
| H28 | -0,811567 | -1,305714 | 5,320036 | H28 | -1,719882 | -1,721085 | 5,236513 |
| H29 | -1,475801 | 0,976409 | 6,049642 | H29 | -2,225268 | 0,617060 | 5,911184 |
| O30 | 0,699674 | -4,302332 | -0,537972 | O30 | 0,902961 | -4,288804 | -0,397266 |
| C31 | 2,754898 | -2,555384 | 1,338414 | C31 | 2,479782 | -2,420228 | 1,641431 |
| C32 | 1,952259 | -1,988914 | 2,325148 | C32 | 1,442956 | -2,078213 | 2,506262 |
| C33 | 3,985499 | -3,121324 | 1,706841 | C33 | 3,711068 | -2,818651 | 2,184372 |
| C34 | 2,372220 | -1,968822 | 3,656748 | C34 | 1,631994 | -2,113368 | 3,888960 |
| H35 | 1,014189 | -1,532347 | 2,055051 | H35 | 0,494635 | -1,752053 | 2,108016 |
| C36 | 4,403314 | -3,108147 | 3,034566 | C36 | 3,900250 | -2,859391 | 3,562842 |
| H37 | 4,629938 | -3,556707 | 0,946893 | H37 | 4,532873 | -3,079900 | 1,522528 |
| C38 | 3,596164 | -2,527025 | 4,016744 | C38 | 2,857824 | -2,502975 | 4,422623 |
| H39 | 1,737722 | -1,501584 | 4,404695 | H39 | 0,814851 | -1,820907 | 4,541739 |
| H40 | 5,361152 | -3,544804 | 3,302191 | H40 | 4,861921 | -3,164119 | 3,965751 |
| H41 | 3,925081 | -2,509685 | 5,051782 | H41 | 3,005324 | -2,528356 | 5,498579 |
| C42 | -3,314848 | 0,127499 | -0,159162 | C42 | -3,482109 | -0,140448 | -0,431548 |
| C43 | -4,431264 | 0,370387 | 0,657377 | C43 | -4,631542 | 0,244516 | 0,270053 |
| C44 | -3,491909 | 0,044539 | -1,548380 | C44 | -3,529677 | -0,192304 | -1,835494 |
| C45 | -5,694622 | 0,537279 | 0,091236 | C45 | -5,795953 | 0,592205 | -0,418428 |
| H46 | -4,327489 | 0,408672 | 1,736023 | H46 | -4,625522 | 0,278216 | 1,354455 |
| C47 | -4,758606 | 0,199519 | -2,108092 | C47 | -4,697992 | 0,135933 | -2,520128 |
| C48 | -5,864683 | 0,444709 | -1,291441 | C48 | -5,835227 | 0,538207 | -1,812428 |
| H49 | -6,549065 | 0,725545 | 0,735021 | H49 | -6,676834 | 0,897612 | 0,139357 |
| H50 | -4,879460 | 0,140351 | -3,185676 | H50 | -4,720024 | 0,087414 | -3,605367 |
| H51 | -6,851077 | 0,565263 | -1,729275 | H51 | -6,744892 | 0,801923 | -2,344130 |
| H52 | -0,430829 | -0,307752 | -1,884546 | H52 | -0,275949 | -0,697879 | -2,058817 |
| H53 | 2,163318 | 2,376647 | -1,207793 | H53 | 1,571784 | 2,111698 | -2,462171 |
| H54 | -0,964553 | -1,940735 | 2,938582 | H54 | -1,616013 | -2,331718 | 2,850557 |
| H55 | -2,636712 | -0,129670 | -2,192239 | H55 | -2,641774 | -0,480784 | -2,392231 |
| H56 | 2,497371 | -4,332806 | -1,559657 | H56 | 2,728151 | -4,094984 | -1,343810 |
| C57 | 4,691268 | -0,156526 | -2,812719 | C57 | 4,957007 | 0,270457 | -2,004644 |
| C58 | 3,812398 | -1,117050 | -3,320125 | C58 | 4,357674 | -0,795060 | -2,679566 |
| C59 | 3,107298 | -1,947570 | -2,450606 | C59 | 3,547137 | -1,696520 | -1,989789 |
| C60 | 3,266918 | -1,836901 | -1,061985 | C60 | 3,327256 | -1,558162 | -0,613528 |
| C61 | 4,148770 | -0,870997 | -0,562625 | C61 | 3,933787 | -0,486633 | 0,054649 |
| C62 | 4,858022 | -0,039053 | -1,433118 | C62 | 4,740374 | 0,418702 | -0,633485 |
| H63 | 5,238483 | 0,494492 | -3,488241 | H63 | 5,590123 | 0,971869 | -2,540912 |

| | | | | | | | |
|--------------------|-----------|-----------|-----------|-------------------|-----------|-----------|-----------|
| H64 | 3,671094 | -1,214816 | -4,392620 | H64 | 4,513341 | -0,921663 | -3,747117 |
| H65 | 2,394357 | -2,654043 | -2,866361 | H65 | 3,055847 | -2,485134 | -2,551775 |
| H66 | 4,267262 | -0,749384 | 0,507867 | H66 | 3,752957 | -0,340661 | 1,112220 |
| H67 | 5,536867 | 0,705619 | -1,027192 | H67 | 5,201233 | 1,241011 | -0,092441 |
| C68 | -2,747438 | 2,847795 | -3,230580 | C68 | -3,543250 | 3,354554 | -1,335046 |
| C69 | -1,556215 | 2,420189 | -2,655721 | C69 | -2,310112 | 2,748477 | -1,546375 |
| C70 | -1,290833 | 2,613972 | -1,287574 | C70 | -1,268525 | 2,875854 | -0,614451 |
| C71 | -2,298593 | 3,204708 | -0,517348 | C71 | -1,510962 | 3,619170 | 0,546282 |
| C72 | -3,504173 | 3,622573 | -1,085748 | C72 | -2,745277 | 4,238194 | 0,757875 |
| C73 | -3,730178 | 3,462897 | -2,448791 | C73 | -3,765526 | 4,110895 | -0,181821 |
| H74 | -2,913282 | 2,696410 | -4,293750 | H74 | -4,335918 | 3,220443 | -2,063647 |
| H75 | -0,815526 | 1,930092 | -3,279253 | H75 | -2,164493 | 2,160094 | -2,446379 |
| H76 | -2,150677 | 3,344787 | 0,545501 | H76 | -0,746648 | 3,707611 | 1,308161 |
| H77 | -4,263516 | 4,076283 | -0,454953 | H77 | -2,905462 | 4,815646 | 1,664108 |
| H78 | -4,661596 | 3,796784 | -2,895926 | H78 | -4,727147 | 4,587120 | -0,015909 |
| C79 | 0,055921 | 2,204535 | -0,732279 | C79 | 0,089119 | 2,258797 | -0,920868 |
| C80 | 1,227284 | 2,759930 | -1,624911 | C80 | 0,661459 | 2,696300 | -2,315090 |
| H81 | 1,133091 | 2,307975 | -2,617502 | H81 | -0,043760 | 2,347956 | -3,077034 |
| C82 | 1,395878 | 4,267404 | -1,771264 | C82 | 0,953046 | 4,168194 | -2,547633 |
| C83 | 2,617232 | 4,838930 | -1,379540 | C83 | 2,268305 | 4,555980 | -2,841512 |
| C84 | 0,407507 | 5,120230 | -2,285922 | C84 | -0,042096 | 5,156735 | -2,520278 |
| C85 | 2,840169 | 6,213120 | -1,469608 | C85 | 2,591093 | 5,892927 | -3,072396 |
| H86 | 3,403347 | 4,196109 | -0,987705 | H86 | 3,048730 | 3,798748 | -2,885772 |
| C87 | 0,626489 | 6,495883 | -2,373016 | C87 | 0,279931 | 6,495558 | -2,746363 |
| H88 | -0,539970 | 4,718861 | -2,620267 | H88 | -1,073121 | 4,887400 | -2,324982 |
| C89 | 1,838077 | 7,050499 | -1,960721 | C89 | 1,596621 | 6,869900 | -3,016898 |
| H90 | 3,793895 | 6,628250 | -1,155230 | H90 | 3,617028 | 6,170474 | -3,297258 |
| H91 | -0,157221 | 7,136479 | -2,768593 | H91 | -0,504199 | 7,247092 | -2,717130 |
| H92 | 2,002243 | 8,122265 | -2,027678 | H92 | 1,843324 | 7,912928 | -3,192971 |
| C93 | 0,323720 | 4,117108 | 1,133968 | C93 | 1,734702 | 3,873847 | 0,336456 |
| C94 | 0,874088 | 1,931409 | 1,562927 | C94 | 1,402777 | 1,734554 | 1,145503 |
| C95 | 0,528788 | 3,883566 | 2,635121 | C95 | 2,124845 | 3,768592 | 1,818127 |
| H96 | -0,582740 | 4,674733 | 0,900810 | H96 | 1,066762 | 4,708503 | 0,123653 |
| H97 | 1,170022 | 4,634125 | 0,681580 | H97 | 2,604297 | 3,953271 | -0,317753 |
| H98 | 1,195492 | 4,604109 | 3,109300 | H98 | 3,114541 | 4,167232 | 2,042286 |
| H99 | -0,413627 | 3,823642 | 3,188553 | H99 | 1,385450 | 4,225748 | 2,484651 |
| N100 | 0,249495 | 2,714356 | 0,662047 | N100 | 1,063341 | 2,571666 | 0,143243 |
| O101 | 1,158301 | 2,572558 | 2,701524 | O101 | 2,142175 | 2,339305 | 2,082120 |
| O102 | 1,175888 | 0,731286 | 1,406825 | O102 | 1,116572 | 0,532517 | 1,225294 |
| H103 | 2,579859 | -4,805299 | 0,159903 | H103 | 2,802108 | -4,598458 | 0,369136 |
| N104 | -1,880640 | -2,147989 | 0,518467 | N104 | -2,006714 | -2,424261 | 0,292122 |
| C105 | -1,352098 | -2,989662 | -0,581753 | C105 | -1,257369 | -3,200046 | -0,724320 |
| H106 | -1,570160 | -2,567614 | -1,573579 | H106 | -1,387310 | -2,797159 | -1,739490 |
| H107 | 1,956990 | 0,305012 | -1,078480 | H107 | 1,588143 | 0,144206 | -1,404078 |
| H108 | 1,512272 | 0,162463 | -1,775920 | H108 | -0,370591 | 1,038500 | -1,603213 |
| C1_ZR_Cheltop_PROD | | | | C1_Z_S_tN_Cheltop | | | |
| C1 | | | | C1 | | | |
| | -4,025728 | -3,711207 | -0,533282 | | -3,899940 | -3,462945 | -0,928246 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C2 | -1,807264 | -4,712122 | -0,673039 | C2 | -1,668150 | -4,447952 | -0,847333 |
| C3 | -3,148361 | -4,630704 | -1,446877 | C3 | -2,908687 | -4,333484 | -1,771731 |
| C4 | -3,078959 | -3,432975 | 0,658050 | C4 | -3,090599 | -3,210004 | 0,365116 |
| H5 | -4,930521 | -4,223701 | -0,190831 | H5 | -4,823053 | -4,005966 | -0,701228 |
| H6 | -3,021104 | -4,229752 | -2,457491 | H6 | -2,664269 | -3,882194 | -2,738946 |
| H7 | -3,565364 | -3,043351 | 1,552091 | H7 | -3,666474 | -2,842694 | 1,214719 |
| H8 | -4,332845 | -2,784916 | -1,023194 | H8 | -4,174585 | -2,527456 | -1,418895 |
| H9 | -1,136493 | -5,509633 | -0,992897 | H9 | -0,964753 | -5,237641 | -1,112651 |
| H10 | -3,583097 | -5,629721 | -1,543812 | H10 | -3,318084 | -5,328024 | -1,970189 |
| C11 | -2,301168 | -4,754309 | 0,790645 | C11 | -2,327892 | -4,533824 | 0,546328 |
| H12 | -1,498472 | -4,705996 | 1,532418 | H12 | -1,614970 | -4,513656 | 1,375746 |
| H13 | -2,940741 | -5,618219 | 0,993068 | H13 | -2,986109 | -5,401193 | 0,648800 |
| C14 | 0,301125 | -3,214794 | -0,406079 | C14 | 0,370360 | -2,969254 | -0,211017 |
| N15 | 0,965741 | -2,110595 | -0,284999 | N15 | 0,988499 | -1,863789 | 0,036766 |
| C16 | 2,355818 | -2,442367 | 0,238217 | C16 | 2,304697 | -2,178942 | 0,710469 |
| C17 | 2,393949 | -3,956947 | -0,111306 | C17 | 2,329803 | -3,740657 | 0,563276 |
| P18 | -1,886818 | -0,845470 | 0,285838 | P18 | -1,899614 | -0,617089 | 0,268061 |
| Ir19 | 0,248955 | -0,248985 | -0,656488 | Ir19 | 0,309386 | 0,048477 | -0,606920 |
| C20 | -2,140431 | -0,418736 | 2,045887 | C20 | -2,310644 | -0,370818 | 2,034744 |
| C21 | -2,350192 | 0,392929 | 4,722770 | C21 | -2,684252 | 0,073870 | 4,785902 |
| C22 | -2,029939 | -1,356699 | 3,080893 | C22 | -2,077025 | -1,398318 | 2,962364 |
| C23 | -2,338958 | 0,934464 | 2,366200 | C23 | -2,726802 | 0,886496 | 2,504566 |
| C24 | -2,442645 | 1,335066 | 3,695343 | C24 | -2,909102 | 1,103280 | 3,869272 |
| C25 | -2,143725 | -0,951072 | 4,412294 | C25 | -2,269806 | -1,177798 | 4,326294 |
| H26 | -2,421185 | 1,676513 | 1,579077 | H26 | -2,910648 | 1,699578 | 1,813308 |
| H27 | -2,597511 | 2,385252 | 3,926506 | H27 | -3,225406 | 2,084042 | 4,212163 |
| H28 | -2,066162 | -1,688867 | 5,206264 | H28 | -2,084218 | -1,984585 | 5,029492 |
| H29 | -2,435405 | 0,705233 | 5,759706 | H29 | -2,829001 | 0,245551 | 5,848438 |
| O30 | 0,987451 | -4,337825 | -0,205646 | O30 | 0,993913 | -4,099585 | 0,103606 |
| C31 | 2,409873 | -2,302231 | 1,765189 | C31 | 2,289491 | -1,814237 | 2,197503 |
| C32 | 1,329469 | -1,879714 | 2,535930 | C32 | 1,248064 | -1,117821 | 2,806107 |
| C33 | 3,599331 | -2,673048 | 2,413392 | C33 | 3,371952 | -2,231393 | 2,988953 |
| C34 | 1,435093 | -1,810941 | 3,926933 | C34 | 1,282491 | -0,836438 | 4,173890 |
| H35 | 0,406172 | -1,579376 | 2,063881 | H35 | 0,412056 | -0,769021 | 2,219705 |
| C36 | 3,704490 | -2,611083 | 3,799256 | C36 | 3,410757 | -1,949644 | 4,351999 |
| H37 | 4,455477 | -2,994767 | 1,826034 | H37 | 4,203187 | -2,763099 | 2,531884 |
| C38 | 2,618625 | -2,175109 | 4,563199 | C38 | 2,361902 | -1,247629 | 4,952731 |
| H39 | 0,583589 | -1,462166 | 4,503088 | H39 | 0,454965 | -0,293642 | 4,620360 |
| H40 | 4,634190 | -2,898258 | 4,282096 | H40 | 4,261564 | -2,275693 | 4,943400 |
| H41 | 2,699680 | -2,120353 | 5,645068 | H41 | 2,390688 | -1,025775 | 6,015430 |
| C42 | -3,401752 | -0,207894 | -0,543923 | C42 | -3,345893 | 0,023878 | -0,679990 |
| C43 | -4,597138 | 0,050606 | 0,141999 | C43 | -4,582329 | 0,324457 | -0,092610 |
| C44 | -3,365291 | -0,036256 | -1,937711 | C44 | -3,225158 | 0,105335 | -2,079509 |
| C45 | -5,727357 | 0,489291 | -0,549415 | C45 | -5,661634 | 0,727949 | -0,882137 |
| H46 | -4,645541 | -0,076188 | 1,218955 | H46 | -4,712070 | 0,246973 | 0,981260 |
| C47 | -4,497072 | 0,399416 | -2,627799 | C47 | -4,305171 | 0,503342 | -2,865420 |
| C48 | -5,680581 | 0,669962 | -1,933964 | C48 | -5,527331 | 0,824184 | -2,267477 |
| H49 | -6,645849 | 0,689646 | -0,004745 | H49 | -6,610820 | 0,963565 | -0,409445 |

| | | | | | | | |
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| H50 | -4,454895 | 0,533685 | -3,705100 | H50 | -4,191816 | 0,563227 | -3,944302 |
| H51 | -6,561052 | 1,012675 | -2,469670 | H51 | -6,368294 | 1,139251 | -2,878042 |
| H52 | -0,197633 | -0,791208 | -2,051810 | H52 | -0,265516 | -0,559521 | -1,919076 |
| H53 | 1,328472 | 2,542302 | -2,714972 | H53 | 1,715643 | -0,015333 | -1,341261 |
| H54 | -1,831776 | -2,398739 | 2,854276 | H54 | -1,721178 | -2,364000 | 2,620082 |
| H55 | -2,441941 | -0,231626 | -2,477157 | H55 | -2,282625 | -0,144566 | -2,558524 |
| H56 | 2,853002 | -4,180348 | -1,076569 | H56 | 3,041120 | -4,098945 | -0,183341 |
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| C58 | 4,596081 | -1,006562 | -2,516046 | C58 | 4,614325 | -1,227355 | -2,185385 |
| C59 | 3,716546 | -1,840461 | -1,827851 | C59 | 3,657574 | -1,876826 | -1,408726 |
| C60 | 3,408994 | -1,603773 | -0,482614 | C60 | 3,437291 | -1,505394 | -0,074208 |
| C61 | 3,985906 | -0,497108 | 0,153203 | C61 | 4,191208 | -0,457844 | 0,463037 |
| C62 | 4,861156 | 0,341000 | -0,535144 | C62 | 5,148282 | 0,197153 | -0,314396 |
| H63 | 5,863398 | 0,734940 | -2,406074 | H63 | 6,117034 | 0,320482 | -2,239194 |
| H64 | 4,823435 | -1,208339 | -3,558751 | H64 | 4,768641 | -1,531178 | -3,216852 |
| H65 | 3,246060 | -2,655854 | -2,368622 | H65 | 3,054294 | -2,657610 | -1,865254 |
| H66 | 3,733298 | -0,272324 | 1,181879 | H66 | 4,014980 | -0,130184 | 1,479628 |
| H67 | 5,301348 | 1,191386 | -0,020742 | H67 | 5,725647 | 1,006967 | 0,123274 |
| C68 | -3,474147 | 3,527540 | -0,366109 | C68 | 0,130934 | 2,435432 | -5,297935 |
| C69 | -2,297175 | 3,008367 | -0,897531 | C69 | -0,107627 | 2,425524 | -3,922096 |
| C70 | -1,064058 | 3,251792 | -0,278975 | C70 | 0,879381 | 1,976976 | -3,035478 |
| C71 | -1,029942 | 4,029798 | 0,881576 | C71 | 2,118938 | 1,564644 | -3,547949 |
| C72 | -2,207908 | 4,563477 | 1,409366 | C72 | 2,358885 | 1,587203 | -4,918048 |
| C73 | -3,431838 | 4,312299 | 0,790325 | C73 | 1,361903 | 2,016342 | -5,799828 |
| H74 | -4,421530 | 3,300699 | -0,844668 | H74 | -0,643063 | 2,786226 | -5,974650 |
| H75 | -2,345121 | 2,386749 | -1,785047 | H75 | -1,057181 | 2,791352 | -3,544137 |
| H76 | -0,089614 | 4,220703 | 1,387102 | H76 | 2,884404 | 1,204904 | -2,865238 |
| H77 | -2,165753 | 5,170683 | 2,309172 | H77 | 3,321380 | 1,261014 | -5,302301 |
| H78 | -4,348133 | 4,718486 | 1,208553 | H78 | 1,548152 | 2,028794 | -6,869894 |
| C79 | 0,195135 | 2,675298 | -0,901786 | C79 | 0,645922 | 1,978365 | -1,553598 |
| C80 | 0,483066 | 3,137736 | -2,357131 | C80 | -0,679448 | 1,986896 | -1,018926 |
| H81 | -0,385474 | 2,828300 | -2,948148 | H81 | -1,426494 | 1,761687 | -1,768261 |
| C82 | 0,745800 | 4,616374 | -2,571059 | C82 | -1,250093 | 2,870914 | 0,034383 |
| C83 | 1,985200 | 5,034546 | -3,073480 | C83 | -2,503414 | 3,439309 | -0,268464 |
| C84 | -0,230265 | 5,588154 | -2,303258 | C84 | -0,664684 | 3,196604 | 1,269417 |
| C85 | 2,256213 | 6,387370 | -3,280946 | C85 | -3,130471 | 4,321406 | 0,609194 |
| H86 | 2,745917 | 4,292210 | -3,306367 | H86 | -2,995079 | 3,176174 | -1,201554 |
| C87 | 0,041564 | 6,941422 | -2,503585 | C87 | -1,288367 | 4,089290 | 2,141216 |
| H88 | -1,207800 | 5,291057 | -1,941767 | H88 | 0,235253 | 2,701757 | 1,598506 |
| C89 | 1,286262 | 7,346520 | -2,987740 | C89 | -2,519754 | 4,661096 | 1,818717 |
| H90 | 3,222597 | 6,691134 | -3,673151 | H90 | -4,097111 | 4,741884 | 0,346709 |
| H91 | -0,725201 | 7,680073 | -2,287223 | H91 | -0,814224 | 4,318097 | 3,091567 |
| H92 | 1,494627 | 8,400956 | -3,144402 | H92 | -3,002538 | 5,352045 | 2,503443 |
| C93 | 2,308075 | 3,895438 | -0,002084 | C93 | 2,278112 | 3,933621 | -1,094251 |
| C94 | 1,618688 | 1,894630 | 0,974436 | C94 | 2,127988 | 2,147301 | 0,383256 |
| C95 | 2,931424 | 3,705319 | 1,392575 | C95 | 3,448174 | 3,931379 | -0,091131 |
| H96 | 1,801672 | 4,855115 | -0,112208 | H96 | 1,538700 | 4,717168 | -0,889796 |
| H97 | 3,039883 | 3,797663 | -0,808085 | H97 | 2,609428 | 4,010113 | -2,132018 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H98 | 4,015912 | 3,817263 | 1,405341 | H98 | 4,384992 | 3,607142 | -0,554384 |
| H99 | 2,486390 | 4,365538 | 2,144087 | H99 | 3,594003 | 4,881060 | 0,423496 |
| N100 | 1,357144 | 2,775736 | -0,028851 | N100 | 1,715003 | 2,612258 | -0,815776 |
| O101 | 2,616095 | 2,337024 | 1,756080 | O101 | 3,081656 | 2,931881 | 0,905300 |
| O102 | 1,071150 | 0,811152 | 1,188685 | O102 | 1,685716 | 1,144473 | 0,960867 |
| H103 | 2,850827 | -4,561010 | 0,669708 | H103 | 2,497492 | -4,249692 | 1,510825 |
| N104 | -1,969066 | -2,539188 | 0,230697 | N104 | -1,950436 | -2,298604 | 0,069645 |
| C105 | -1,161648 | -3,304292 | -0,753602 | C105 | -1,012849 | -3,045795 | -0,801422 |
| H106 | -1,254334 | -2,898491 | -1,771112 | H106 | -0,946036 | -2,619786 | -1,811643 |
| H107 | 1,640099 | 0,070385 | -1,392492 | | | | |
| H108 | -0,005514 | 1,573306 | -1,104460 | | | | |

TS_{Z1-2}

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,985439 | -3,688239 | -0,507839 |
| C2 | -1,734714 | -4,631018 | -0,543502 |
| C3 | -3,047672 | -4,600110 | -1,368600 |
| C4 | -3,087472 | -3,351156 | 0,705207 |
| H5 | -4,883956 | -4,222408 | -0,182527 |
| H6 | -2,892271 | -4,214192 | -2,381197 |
| H7 | -3,608538 | -2,947617 | 1,573524 |
| H8 | -4,305187 | -2,784063 | -1,030202 |
| H9 | -1,034947 | -5,420752 | -0,816732 |
| H10 | -3,451331 | -5,612221 | -1,462984 |
| C11 | -2,280996 | -4,646728 | 0,901560 |
| H12 | -1,506873 | -4,558962 | 1,669697 |
| H13 | -2,906425 | -5,520162 | 1,106643 |
| C14 | 0,326072 | -3,079454 | -0,205062 |
| N15 | 0,939385 | -1,957501 | -0,044093 |
| C16 | 2,312987 | -2,246486 | 0,502841 |
| C17 | 2,395602 | -3,792227 | 0,269505 |
| P18 | -1,959484 | -0,752686 | 0,333158 |
| Ir19 | 0,057576 | -0,027396 | -0,574160 |
| C20 | -2,264643 | -0,340436 | 2,085234 |
| C21 | -2,578879 | 0,396040 | 4,770758 |
| C22 | -2,042342 | -1,275782 | 3,105793 |
| C23 | -2,636043 | 0,971562 | 2,422520 |
| C24 | -2,786681 | 1,335525 | 3,758525 |
| C25 | -2,207645 | -0,908526 | 4,441686 |
| H26 | -2,813547 | 1,707959 | 1,646632 |
| H27 | -3,069698 | 2,354762 | 4,005272 |
| H28 | -2,040678 | -1,643151 | 5,224340 |
| H29 | -2,703697 | 0,679968 | 5,811790 |
| O30 | 1,018349 | -4,196435 | 0,026023 |
| C31 | 2,383889 | -1,973352 | 2,009129 |
| C32 | 1,328316 | -1,423165 | 2,731866 |
| C33 | 3,556794 | -2,332257 | 2,692830 |
| C34 | 1,440769 | -1,218143 | 4,108391 |
| H35 | 0,423525 | -1,125693 | 2,225213 |

E2

| | | | |
|------|-----------|-----------|-----------|
| C1 | -3,953441 | -3,737875 | -0,490279 |
| C2 | -1,738154 | -4,720753 | -0,164229 |
| C3 | -2,974412 | -4,797818 | -1,099743 |
| C4 | -3,138153 | -3,203440 | 0,708846 |
| H5 | -4,887552 | -4,196450 | -0,149715 |
| H6 | -2,718083 | -4,588487 | -2,143136 |
| H7 | -3,699464 | -2,631179 | 1,447934 |
| H8 | -4,208213 | -2,935662 | -1,186266 |
| H9 | -1,054985 | -5,567017 | -0,232123 |
| H10 | -3,403487 | -5,803143 | -1,065182 |
| C11 | -2,403616 | -4,460701 | 1,204462 |
| H12 | -1,695799 | -4,257593 | 2,013833 |
| H13 | -3,080965 | -5,265083 | 1,504614 |
| C14 | 0,352381 | -3,208348 | 0,132350 |
| N15 | 0,938930 | -2,084612 | 0,353717 |
| C16 | 2,312079 | -2,357608 | 0,896507 |
| C17 | 2,399386 | -3,912739 | 0,712715 |
| P18 | -1,888703 | -0,737937 | 0,044494 |
| Ir19 | 0,187428 | -0,161789 | -0,454795 |
| C20 | -2,299889 | -0,139517 | 1,721759 |
| C21 | -2,717579 | 0,786808 | 4,333224 |
| C22 | -1,938307 | -0,932229 | 2,824504 |
| C23 | -2,851515 | 1,132469 | 1,941525 |
| C24 | -3,062560 | 1,586152 | 3,242312 |
| C25 | -2,151059 | -0,472729 | 4,122167 |
| H26 | -3,111424 | 1,772299 | 1,106948 |
| H27 | -3,489709 | 2,572316 | 3,397605 |
| H28 | -1,870762 | -1,096577 | 4,965992 |
| H29 | -2,885693 | 1,144881 | 5,345105 |
| O30 | 1,044412 | -4,324334 | 0,372189 |
| C31 | 2,380339 | -1,948186 | 2,370590 |
| C32 | 1,487057 | -1,022863 | 2,919123 |
| C33 | 3,378638 | -2,482996 | 3,198089 |
| C34 | 1,580104 | -0,650105 | 4,259946 |
| H35 | 0,710247 | -0,587287 | 2,305693 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C36 | 3,671464 | -2,130128 | 4,065205 | C36 | 3,477552 | -2,106914 | 4,536833 |
| H37 | 4,395116 | -2,753868 | 2,142685 | H37 | 4,105214 | -3,184048 | 2,796142 |
| C38 | 2,610031 | -1,567746 | 4,779096 | C38 | 2,575112 | -1,188640 | 5,074459 |
| H39 | 0,606274 | -0,778064 | 4,646105 | H39 | 0,865005 | 0,061946 | 4,662431 |
| H40 | 4,589318 | -2,406988 | 4,575876 | H40 | 4,261272 | -2,531691 | 5,157336 |
| H41 | 2,698792 | -1,404636 | 5,849406 | H41 | 2,648653 | -0,897423 | 6,118272 |
| C42 | -3,461673 | -0,149576 | -0,545760 | C42 | -3,261470 | -0,210928 | -1,045786 |
| C43 | -4,679724 | 0,053978 | 0,121837 | C43 | -4,553910 | 0,010705 | -0,542540 |
| C44 | -3,424286 | -0,001170 | -1,942236 | C44 | -3,050097 | -0,132183 | -2,431178 |
| C45 | -5,823651 | 0,422238 | -0,587352 | C45 | -5,601979 | 0,333179 | -1,404339 |
| H46 | -4,740781 | -0,068438 | 1,198095 | H46 | -4,746681 | -0,060747 | 0,522902 |
| C47 | -4,570765 | 0,359940 | -2,649149 | C47 | -4,100752 | 0,187547 | -3,290547 |
| C48 | -5,773174 | 0,580210 | -1,972919 | C48 | -5,378494 | 0,428415 | -2,779273 |
| H49 | -6,755678 | 0,583357 | -0,053294 | H49 | -6,593981 | 0,509800 | -0,998717 |
| H50 | -4,523722 | 0,472884 | -3,728585 | H50 | -3,920001 | 0,253308 | -4,359546 |
| H51 | -6,664589 | 0,867691 | -2,522395 | H51 | -6,194848 | 0,684656 | -3,447917 |
| H52 | -0,510252 | -0,644608 | -1,887816 | H52 | -0,210303 | -0,892075 | -1,766382 |
| H53 | 1,397277 | 0,442584 | -1,474526 | H53 | 1,502939 | 1,415293 | -2,584303 |
| H54 | -1,721795 | -2,282353 | 2,859900 | H54 | -1,482651 | -1,902800 | 2,663060 |
| H55 | -2,495843 | -0,169605 | -2,477892 | H55 | -2,060850 | -0,315823 | -2,838128 |
| H56 | 2,982090 | -4,077008 | -0,606848 | H56 | 3,048340 | -4,200828 | -0,118019 |
| C57 | 5,278873 | -0,073433 | -1,818179 | C57 | 5,095729 | -0,261516 | -1,699143 |
| C58 | 4,545151 | -1,111456 | -2,396650 | C58 | 4,071229 | -1,048389 | -2,231162 |
| C59 | 3,583240 | -1,788577 | -1,648683 | C59 | 3,210425 | -1,737586 | -1,379360 |
| C60 | 3,359116 | -1,467651 | -0,302455 | C60 | 3,347437 | -1,643033 | 0,013897 |
| C61 | 4,079121 | -0,405985 | 0,259428 | C61 | 4,380192 | -0,862303 | 0,536560 |
| C62 | 5,028944 | 0,286194 | -0,493899 | C62 | 5,250693 | -0,179801 | -0,315432 |
| H63 | 6,032949 | 0,452263 | -2,397081 | H63 | 5,771836 | 0,274035 | -2,359980 |
| H64 | 4,715477 | -1,390387 | -3,432588 | H64 | 3,945300 | -1,129814 | -3,307375 |
| H65 | 2,999654 | -2,568983 | -2,128895 | H65 | 2,406824 | -2,333045 | -1,803902 |
| H66 | 3,898700 | -0,116724 | 1,287817 | H66 | 4,489380 | -0,752496 | 1,608837 |
| H67 | 5,587729 | 1,096834 | -0,033231 | H67 | 6,046153 | 0,425585 | 0,110067 |
| C68 | 0,931158 | 3,343255 | -5,053463 | C68 | -0,096490 | 5,541896 | -3,622395 |
| C69 | 0,511597 | 3,021903 | -3,761656 | C69 | 0,233323 | 4,590673 | -2,658792 |
| C70 | 1,250815 | 2,119419 | -2,987346 | C70 | 0,752785 | 3,342021 | -3,038055 |
| C71 | 2,416730 | 1,552183 | -3,512371 | C71 | 0,922666 | 3,071713 | -4,400955 |
| C72 | 2,833066 | 1,873487 | -4,801416 | C72 | 0,584494 | 4,021052 | -5,366442 |
| C73 | 2,089140 | 2,768352 | -5,575930 | C73 | 0,075345 | 5,260200 | -4,978737 |
| H74 | 0,352975 | 4,044333 | -5,648204 | H74 | -0,497683 | 6,502327 | -3,311211 |
| H75 | -0,378273 | 3,487903 | -3,348752 | H75 | 0,067290 | 4,815320 | -1,611076 |
| H76 | 2,989994 | 0,854591 | -2,910695 | H76 | 1,321711 | 2,108200 | -4,710440 |
| H77 | 3,734994 | 1,422221 | -5,204911 | H77 | 0,723160 | 3,793130 | -6,419343 |
| H78 | 2,411876 | 3,015713 | -6,583040 | H78 | -0,186907 | 6,002171 | -5,727390 |
| C79 | 0,832097 | 1,869472 | -1,562286 | C79 | 1,044248 | 2,245448 | -2,031076 |
| C80 | -0,606508 | 1,880847 | -1,238591 | C80 | -0,265587 | 1,673943 | -1,389529 |
| H81 | -1,193798 | 1,718687 | -2,138941 | C82 | -1,024984 | 2,666259 | -0,543314 |
| C82 | -1,284687 | 2,908453 | -0,388148 | C83 | -2,245642 | 3,184831 | -1,009500 |
| C83 | -2,452759 | 3,484804 | -0,923393 | C84 | -0,556433 | 3,127941 | 0,700680 |

| | | | | | | | |
|--------------------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C84 | -0,870267 | 3,344976 | 0,882603 | C85 | -2,957773 | 4,137519 | -0,279817 |
| C85 | -3,160040 | 4,470629 | -0,238676 | H86 | -2,636470 | 2,837610 | -1,961654 |
| H86 | -2,818511 | 3,139636 | -1,887184 | C87 | -1,254269 | 4,095756 | 1,422746 |
| C87 | -1,566653 | 4,346704 | 1,559319 | H88 | 0,337837 | 2,698355 | 1,137423 |
| H88 | -0,052510 | 2,862983 | 1,396188 | C89 | -2,457290 | 4,609929 | 0,935008 |
| C89 | -2,711489 | 4,918293 | 1,004836 | H90 | -3,898704 | 4,518811 | -0,667116 |
| H90 | -4,061420 | 4,888642 | -0,678134 | H91 | -0,866349 | 4,434102 | 2,379931 |
| H91 | -1,221333 | 4,661866 | 2,540377 | H92 | -3,002307 | 5,361779 | 1,498799 |
| H92 | -3,254794 | 5,691960 | 1,539512 | C93 | 2,819586 | 3,935730 | -1,053641 |
| C93 | 2,382863 | 3,788423 | -0,767227 | C94 | 2,402990 | 1,940863 | 0,020020 |
| C94 | 1,894211 | 1,996902 | 0,636392 | C95 | 3,929974 | 3,603574 | -0,043900 |
| C95 | 3,297126 | 3,777523 | 0,475678 | H96 | 2,187015 | 4,765531 | -0,724590 |
| H96 | 1,629906 | 4,584521 | -0,736269 | H97 | 3,201241 | 4,162454 | -2,050567 |
| H97 | 2,941275 | 3,854960 | -1,702682 | H98 | 4,844259 | 3,248017 | -0,529630 |
| H98 | 4,319856 | 3,477588 | 0,230767 | H99 | 4,163537 | 4,417729 | 0,642112 |
| H99 | 3,305758 | 4,720002 | 1,023385 | N100 | 2,062432 | 2,677108 | -1,043492 |
| N100 | 1,746671 | 2,480445 | -0,618968 | O101 | 3,390188 | 2,498530 | 0,733012 |
| O101 | 2,735550 | 2,756400 | 1,350474 | O102 | 1,912842 | 0,853126 | 0,391025 |
| O102 | 1,327056 | 1,001924 | 1,100645 | H103 | 2,684994 | -4,448523 | 1,616242 |
| H103 | 2,750948 | -4,333692 | 1,144300 | N104 | -1,982215 | -2,416679 | 0,197585 |
| N104 | -1,989624 | -2,441503 | 0,280211 | C105 | -1,042152 | -3,360401 | -0,435020 |
| C105 | -1,113953 | -3,213521 | -0,634717 | H106 | -0,945914 | -3,193184 | -1,518434 |
| H106 | -1,162455 | -2,841813 | -1,667793 | H107 | -0,880113 | 1,465577 | -2,269023 |
| TS _{Z2-3} | | | | Z3 | | | |
| C1 | -3,784872 | -3,856984 | -0,824496 | C1 | -3,856889 | -3,856465 | -0,553987 |
| C2 | -1,569341 | -4,766921 | -0,344530 | C2 | -1,628280 | -4,774443 | -0,179079 |
| C3 | -2,715698 | -4,853284 | -1,386188 | C3 | -2,833221 | -4,880180 | -1,148429 |
| C4 | -3,098714 | -3,339821 | 0,460695 | C4 | -3,096015 | -3,315245 | 0,679386 |
| H5 | -4,723555 | -4,364540 | -0,579080 | H5 | -4,786109 | -4,345424 | -0,243383 |
| H6 | -2,380221 | -4,590021 | -2,394433 | H6 | -2,554541 | -4,649644 | -2,181748 |
| H7 | -3,746237 | -2,822051 | 1,168502 | H7 | -3,703007 | -2,779465 | 1,409012 |
| H8 | -4,016533 | -3,041789 | -1,512317 | H8 | -4,117588 | -3,057258 | -1,249608 |
| H9 | -0,848680 | -5,583639 | -0,382257 | H9 | -0,913511 | -5,595105 | -0,238761 |
| H10 | -3,103853 | -5,874842 | -1,428056 | H10 | -3,232298 | -5,898465 | -1,137363 |
| C11 | -2,358647 | -4,587910 | 0,970445 | C11 | -2,337480 | -4,557487 | 1,175392 |
| H12 | -1,730163 | -4,390773 | 1,843949 | H12 | -1,658438 | -4,344296 | 2,006428 |
| H13 | -3,026571 | -5,427764 | 1,181450 | H13 | -2,997146 | -5,387381 | 1,443955 |
| C14 | 0,408191 | -3,184663 | 0,211601 | C14 | 0,394613 | -3,204907 | 0,200224 |
| N15 | 0,963961 | -2,043648 | 0,424959 | N15 | 0,964978 | -2,064246 | 0,360772 |
| C16 | 2,234757 | -2,277792 | 1,195318 | C16 | 2,270616 | -2,287010 | 1,077682 |
| C17 | 2,317787 | -3,844050 | 1,185816 | C17 | 2,390061 | -3,844310 | 0,996259 |
| P18 | -1,927185 | -0,803073 | -0,036520 | P18 | -1,951647 | -0,790950 | 0,060752 |
| Ir19 | 0,150558 | -0,146561 | -0,464542 | Ir19 | 0,181004 | -0,192588 | -0,581390 |
| C20 | -2,562811 | -0,283833 | 1,596689 | C20 | -2,560999 | -0,235709 | 1,694978 |
| C21 | -3,378933 | 0,513153 | 4,155455 | C21 | -3,334231 | 0,660460 | 4,243187 |
| C22 | -2,260265 | -1,074369 | 2,718773 | C22 | -2,235254 | -0,978315 | 2,842144 |
| C23 | -3,275373 | 0,911749 | 1,770899 | C23 | -3,291242 | 0,952905 | 1,839028 |

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|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C24 | -3,682050 | 1,302050 | 3,045624 | C24 | -3,670455 | 1,396542 | 3,106302 |
| C25 | -2,666817 | -0,677168 | 3,990146 | C25 | -2,619812 | -0,532462 | 4,105728 |
| H26 | -3,514773 | 1,540266 | 0,922877 | H26 | -3,568347 | 1,535444 | 0,969954 |
| H27 | -4,231236 | 2,231075 | 3,165647 | H27 | -4,230128 | 2,322998 | 3,197845 |
| H28 | -2,428892 | -1,298223 | 4,848976 | H28 | -2,362485 | -1,121331 | 4,981692 |
| H29 | -3,698175 | 0,822053 | 5,146911 | H29 | -3,633378 | 1,007546 | 5,228153 |
| O30 | 1,037374 | -4,277720 | 0,649649 | O30 | 1,063457 | -4,291504 | 0,594409 |
| C31 | 2,121461 | -1,783421 | 2,639149 | C31 | 2,186846 | -1,851379 | 2,542679 |
| C32 | 1,055323 | -1,009538 | 3,093943 | C32 | 1,109868 | -1,131274 | 3,053083 |
| C33 | 3,146234 | -2,119910 | 3,536720 | C33 | 3,247294 | -2,184252 | 3,400119 |
| C34 | 0,999821 | -0,591463 | 4,425336 | C34 | 1,081330 | -0,753876 | 4,397088 |
| H35 | 0,275396 | -0,709005 | 2,410679 | H35 | 0,304162 | -0,834685 | 2,401377 |
| C36 | 3,096714 | -1,698859 | 4,862403 | C36 | 3,222430 | -1,807167 | 4,740292 |
| H37 | 4,000595 | -2,697652 | 3,190527 | H37 | 4,109551 | -2,722997 | 3,012661 |
| C38 | 2,017347 | -0,934197 | 5,312969 | C38 | 2,134379 | -1,089355 | 5,244731 |
| H39 | 0,156362 | 0,007346 | 4,757301 | H39 | 0,230522 | -0,190280 | 4,769109 |
| H40 | 3,900508 | -1,964860 | 5,542748 | H40 | 4,053200 | -2,068959 | 5,389546 |
| H41 | 1,976513 | -0,606295 | 6,347806 | H41 | 2,114510 | -0,793096 | 6,289748 |
| C42 | -3,227567 | -0,375815 | -1,264093 | C42 | -3,294248 | -0,407222 | -1,132691 |
| C43 | -4,579077 | -0,300979 | -0,885696 | C43 | -4,637592 | -0,359212 | -0,724268 |
| C44 | -2,902639 | -0,282369 | -2,626649 | C44 | -3,002002 | -0,307137 | -2,501511 |
| C45 | -5,573284 | -0,101766 | -1,843873 | C45 | -5,657091 | -0,185109 | -1,659605 |
| H46 | -4,864270 | -0,396829 | 0,156077 | H46 | -4,896745 | -0,455904 | 0,324835 |
| C47 | -3,899580 | -0,085494 | -3,582593 | C47 | -4,024330 | -0,141085 | -3,435431 |
| C48 | -5,237705 | 0,012566 | -3,194218 | C48 | -5,355083 | -0,071617 | -3,017851 |
| H49 | -6,612007 | -0,037879 | -1,532655 | H49 | -6,689294 | -0,140942 | -1,323859 |
| H50 | -3,630380 | -0,005726 | -4,631850 | H50 | -3,778913 | -0,057252 | -4,490425 |
| H51 | -6,013455 | 0,171711 | -3,937445 | H51 | -6,150555 | 0,065958 | -3,744228 |
| H52 | -0,178846 | -0,932762 | -1,773420 | H52 | -0,253707 | -1,007853 | -1,852492 |
| H53 | 1,417830 | 1,999250 | -2,474531 | H53 | 1,625402 | 2,047717 | -2,297429 |
| H54 | -1,708400 | -1,999381 | 2,594531 | H54 | -1,683996 | -1,907067 | 2,746089 |
| H55 | -1,867634 | -0,358005 | -2,940213 | H55 | -1,971226 | -0,343954 | -2,835865 |
| H56 | 3,099690 | -4,243234 | 0,537836 | H56 | 3,098841 | -4,196180 | 0,243070 |
| C57 | 5,417760 | -0,357543 | -1,055047 | C57 | 5,156417 | -0,021172 | -1,243785 |
| C58 | 4,844092 | -1,543879 | -1,516524 | C58 | 4,640071 | -1,221891 | -1,738922 |
| C59 | 3,834855 | -2,162917 | -0,781265 | C59 | 3,753152 | -1,972233 | -0,967909 |
| C60 | 3,393807 | -1,621641 | 0,434641 | C60 | 3,368536 | -1,542072 | 0,310287 |
| C61 | 3,966722 | -0,427242 | 0,884233 | C61 | 3,889611 | -0,337266 | 0,797647 |
| C62 | 4,968039 | 0,202075 | 0,141254 | C62 | 4,777490 | 0,415551 | 0,025862 |
| H63 | 6,206043 | 0,125908 | -1,625169 | H63 | 5,850697 | 0,563039 | -1,841451 |
| H64 | 5,174593 | -1,982062 | -2,453705 | H64 | 4,925614 | -1,572297 | -2,726731 |
| H65 | 3,375076 | -3,062201 | -1,182077 | H65 | 3,332514 | -2,880566 | -1,390911 |
| H66 | 3,621842 | 0,025615 | 1,805281 | H66 | 3,585446 | 0,030906 | 1,769956 |
| H67 | 5,403709 | 1,125267 | 0,513258 | H67 | 5,177826 | 1,342755 | 0,427841 |
| C68 | -0,338272 | 6,178271 | -2,151870 | C68 | -0,140097 | 6,219147 | -2,100726 |
| C69 | 0,171865 | 5,024770 | -1,559865 | C69 | 0,269783 | 5,044523 | -1,473087 |
| C70 | 0,438801 | 3,886833 | -2,331875 | C70 | 0,626590 | 3,920436 | -2,228875 |
| C71 | 0,194030 | 3,930504 | -3,707664 | C71 | 0,575491 | 4,000906 | -3,624296 |

| | | | | | | | |
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| C72 | -0,322333 | 5,082803 | -4,301545 | C72 | 0,160622 | 5,174091 | -4,255184 |
| C73 | -0,591723 | 6,209518 | -3,523887 | C73 | -0,200388 | 6,286549 | -3,493775 |
| H74 | -0,549836 | 7,049373 | -1,538059 | H74 | -0,422835 | 7,079149 | -1,499705 |
| H75 | 0,329234 | 4,994483 | -0,486377 | H75 | 0,280368 | 4,988785 | -0,389596 |
| H76 | 0,399072 | 3,053353 | -4,318272 | H76 | 0,854391 | 3,135934 | -4,223399 |
| H77 | -0,512062 | 5,101426 | -5,370994 | H77 | 0,122779 | 5,220915 | -5,340168 |
| H78 | -0,995834 | 7,106847 | -3,983804 | H78 | -0,525082 | 7,200919 | -3,982182 |
| C79 | 0,870885 | 2,564541 | -1,709824 | C79 | 0,965065 | 2,576034 | -1,596113 |
| C80 | -0,390125 | 1,708108 | -1,328323 | C80 | -0,327551 | 1,699787 | -1,427245 |
| C81 | -1,408711 | 2,547235 | -0,578130 | C81 | -1,440174 | 2,517312 | -0,793926 |
| C82 | -2,579322 | 2,950786 | -1,242120 | C82 | -2,542237 | 2,888274 | -1,583666 |
| C83 | -1,203460 | 3,036118 | 0,724127 | C83 | -1,378260 | 3,046641 | 0,507188 |
| C84 | -3,489703 | 3,825094 | -0,650110 | C84 | -3,527117 | 3,753223 | -1,109837 |
| H85 | -2,770196 | 2,586363 | -2,247004 | H85 | -2,620601 | 2,502516 | -2,595805 |
| C86 | -2,098210 | 3,931876 | 1,311315 | C86 | -2,340355 | 3,943435 | 0,973046 |
| H87 | -0,355370 | 2,695743 | 1,303006 | H87 | -0,592788 | 2,741910 | 1,183003 |
| C88 | -3,241657 | 4,339313 | 0,623696 | C88 | -3,421465 | 4,303193 | 0,169464 |
| H89 | -4,382814 | 4,120691 | -1,193890 | H89 | -4,366036 | 4,014228 | -1,749664 |
| H90 | -1,906032 | 4,299293 | 2,316058 | H90 | -2,253981 | 4,340675 | 1,981251 |
| H91 | -3,938105 | 5,037612 | 1,079725 | H91 | -4,174299 | 4,996558 | 0,534567 |
| C92 | 3,006057 | 3,660722 | -0,798582 | C92 | 2,953821 | 3,607009 | -0,345477 |
| C93 | 1,950171 | 2,118464 | 0,541939 | C93 | 1,689001 | 2,052610 | 0,790714 |
| C94 | 3,485129 | 3,790304 | 0,649468 | C94 | 3,208088 | 3,704574 | 1,160966 |
| H95 | 2,737245 | 4,617234 | -1,247008 | H95 | 2,766177 | 4,575036 | -0,810113 |
| H96 | 3,734115 | 3,152568 | -1,444263 | H96 | 3,766242 | 3,100081 | -0,882699 |
| H97 | 4,568776 | 3,784792 | 0,767737 | H97 | 4,261043 | 3,685333 | 1,442886 |
| H98 | 3,059328 | 4,665816 | 1,150360 | H98 | 2,719879 | 4,576847 | 1,607869 |
| N99 | 1,822127 | 2,809784 | -0,608577 | N99 | 1,746854 | 2,768046 | -0,354989 |
| O100 | 2,955222 | 2,601043 | 1,294723 | O100 | 2,577639 | 2,510518 | 1,694860 |
| O101 | 1,300125 | 1,141541 | 0,955497 | O101 | 0,964152 | 1,087891 | 1,086083 |
| H102 | 2,416310 | -4,267053 | 2,184523 | H102 | 2,615897 | -4,303519 | 1,957208 |
| N103 | -1,932908 | -2,488360 | 0,088996 | N103 | -1,945661 | -2,478546 | 0,233283 |
| C104 | -0,909328 | -3,373464 | -0,503324 | C104 | -0,972728 | -3,388514 | -0,411890 |
| H105 | -0,725668 | -3,150942 | -1,563692 | H105 | -0,861804 | -3,188748 | -1,487319 |
| H106 | -0,822903 | 1,508685 | -2,312001 | H106 | -0,627785 | 1,522449 | -2,464089 |
| H107 | 2,625373 | 0,300477 | -1,375021 | H107 | 1,939844 | 0,093834 | -0,980810 |
| H108 | 2,220954 | 0,038109 | -1,947079 | H108 | 1,579833 | -0,115056 | -1,684124 |
| TS _{Z3-4} | | | | Z4 | | | |
| C1 | -3,825379 | -3,978950 | -0,556223 | C1 | -3,724188 | -4,145535 | -0,601233 |
| C2 | -1,576345 | -4,798897 | -0,085304 | C2 | -1,431953 | -4,908094 | -0,254999 |
| C3 | -2,744638 | -4,978256 | -1,089017 | C3 | -2,624689 | -5,062497 | -1,234931 |
| C4 | -3,128953 | -3,382549 | 0,689612 | C4 | -3,018518 | -3,624586 | 0,673326 |
| H5 | -4,748573 | -4,493732 | -0,270380 | H5 | -4,623784 | -4,712282 | -0,340194 |
| H6 | -2,441784 | -4,767119 | -2,119629 | H6 | -2,363736 | -4,769768 | -2,257076 |
| H7 | -3,781483 | -2,856239 | 1,385886 | H7 | -3,675693 | -3,181735 | 1,421898 |
| H8 | -4,085984 | -3,202514 | -1,277820 | H8 | -4,025449 | -3,322328 | -1,252660 |
| H9 | -0,826793 | -5,589871 | -0,103490 | H9 | -0,651200 | -5,662247 | -0,355034 |

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|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H10 | -3,104497 | -6,010701 | -1,059569 | H10 | -2,945925 | -6,107585 | -1,266573 |
| C11 | -2,339022 | -4,582128 | 1,239238 | C11 | -2,162442 | -4,828263 | 1,104139 |
| H12 | -1,697124 | -4,324657 | 2,086894 | H12 | -1,504510 | -4,606817 | 1,949678 |
| H13 | -2,972779 | -5,433253 | 1,504184 | H13 | -2,750512 | -5,725124 | 1,319190 |
| C14 | 0,368465 | -3,124441 | 0,292926 | C14 | 0,455248 | -3,163681 | 0,156530 |
| N15 | 0,940273 | -1,967862 | 0,366923 | N15 | 0,995364 | -1,988681 | 0,220941 |
| C16 | 2,224506 | -2,122128 | 1,152780 | C16 | 2,303748 | -2,096125 | 0,978172 |
| C17 | 2,351690 | -3,680109 | 1,176471 | C17 | 2,491733 | -3,646664 | 0,958792 |
| P18 | -2,029434 | -0,819072 | 0,075898 | P18 | -2,006428 | -0,987823 | 0,159494 |
| Ir19 | 0,234097 | -0,237977 | -0,717338 | Ir19 | 0,176343 | -0,294797 | -0,592589 |
| C20 | -2,704035 | -0,284353 | 1,693296 | C20 | -2,580001 | -0,432357 | 1,804169 |
| C21 | -3,611371 | 0,585711 | 4,204250 | C21 | -3,269108 | 0,564140 | 4,339074 |
| C22 | -2,417799 | -1,024897 | 2,851873 | C22 | -2,444862 | -1,237277 | 2,944719 |
| C23 | -3,447714 | 0,898084 | 1,810267 | C23 | -3,050131 | 0,881667 | 1,949782 |
| C24 | -3,896438 | 1,328246 | 3,058224 | C24 | -3,391119 | 1,374245 | 3,207159 |
| C25 | -2,870377 | -0,592937 | 4,097316 | C25 | -2,796029 | -0,742295 | 4,202257 |
| H26 | -3,681044 | 1,485676 | 0,930558 | H26 | -3,158460 | 1,520852 | 1,082310 |
| H27 | -4,469102 | 2,248508 | 3,129380 | H27 | -3,752669 | 2,394561 | 3,297321 |
| H28 | -2,644592 | -1,180420 | 4,982800 | H28 | -2,692055 | -1,380042 | 5,075851 |
| H29 | -3,966761 | 0,920605 | 5,174686 | H29 | -3,540048 | 0,947236 | 5,318632 |
| O30 | 1,027842 | -4,160221 | 0,804419 | O30 | 1,170030 | -4,174026 | 0,646572 |
| C31 | 2,052798 | -1,611318 | 2,586572 | C31 | 2,134933 | -1,627453 | 2,426105 |
| C32 | 0,919375 | -0,925262 | 3,018126 | C32 | 0,958853 | -1,060130 | 2,911785 |
| C33 | 3,071951 | -1,877513 | 3,514847 | C33 | 3,205847 | -1,825326 | 3,314232 |
| C34 | 0,801191 | -0,508870 | 4,345291 | C34 | 0,854210 | -0,678978 | 4,251352 |
| H35 | 0,128679 | -0,692624 | 2,322030 | H35 | 0,119707 | -0,893153 | 2,255043 |
| C36 | 2,959711 | -1,459072 | 4,838030 | C36 | 3,103441 | -1,446772 | 4,649307 |
| H37 | 3,971421 | -2,399270 | 3,195803 | H37 | 4,133812 | -2,262880 | 2,953144 |
| C38 | 1,819162 | -0,771136 | 5,259057 | C38 | 1,923176 | -0,866953 | 5,122816 |
| H39 | -0,095297 | 0,020811 | 4,654131 | H39 | -0,072961 | -0,234544 | 4,600040 |
| H40 | 3,762356 | -1,669459 | 5,538986 | H40 | 3,944292 | -1,603281 | 5,319026 |
| H41 | 1,728416 | -0,445221 | 6,291344 | H41 | 1,841782 | -0,568693 | 6,164165 |
| C42 | -3,385106 | -0,460426 | -1,120661 | C42 | -3,396488 | -0,592776 | -0,978443 |
| C43 | -4,736926 | -0,485769 | -0,738734 | C43 | -4,716497 | -0,401762 | -0,545497 |
| C44 | -3,075320 | -0,278911 | -2,477171 | C44 | -3,119902 | -0,563499 | -2,355554 |
| C45 | -5,746566 | -0,310151 | -1,684454 | C45 | -5,734605 | -0,167900 | -1,469867 |
| H46 | -5,007744 | -0,637126 | 0,301230 | H46 | -4,951345 | -0,424557 | 0,513704 |
| C47 | -4,086245 | -0,107751 | -3,423553 | C47 | -4,140777 | -0,338903 | -3,278760 |
| C48 | -5,425625 | -0,116949 | -3,029855 | C48 | -5,449801 | -0,134676 | -2,836335 |
| H49 | -6,785848 | -0,327174 | -1,368527 | H49 | -6,752623 | -0,015893 | -1,122323 |
| H50 | -3,826509 | 0,035619 | -4,468699 | H50 | -3,915097 | -0,319656 | -4,341367 |
| H51 | -6,213194 | 0,020297 | -3,764815 | H51 | -6,245267 | 0,045668 | -3,553756 |
| H52 | -0,210499 | -1,255857 | -1,826913 | H52 | 0,024073 | -1,144867 | -1,892784 |
| H53 | 1,555422 | 2,119155 | -2,491652 | H53 | 1,525102 | 2,075720 | -2,241352 |
| H54 | -1,840819 | -1,940154 | 2,779619 | H54 | -2,044189 | -2,241678 | 2,856304 |
| H55 | -2,038607 | -0,271529 | -2,795138 | H55 | -2,101054 | -0,713552 | -2,701930 |
| H56 | 3,059101 | -4,070821 | 0,441499 | H56 | 3,173124 | -3,991654 | 0,177702 |
| C57 | 5,423022 | -0,256283 | -1,114905 | C57 | 5,396341 | -0,049999 | -1,280131 |

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| C58 | 4,690083 | -1,317715 | -1,652307 | C58 | 4,692204 | -1,119556 | -1,838605 |
| C59 | 3,679599 | -1,914083 | -0,903705 | C59 | 3,713598 | -1,771950 | -1,095099 |
| C60 | 3,382766 | -1,469006 | 0,393169 | C60 | 3,416362 | -1,372721 | 0,216041 |
| C61 | 4,115293 | -0,403166 | 0,919624 | C61 | 4,109796 | -0,288863 | 0,760279 |
| C62 | 5,129488 | 0,197410 | 0,169748 | C62 | 5,099276 | 0,361251 | 0,018187 |
| H63 | 6,217297 | 0,207245 | -1,693505 | H63 | 6,170940 | 0,453099 | -1,852148 |
| H64 | 4,902721 | -1,676915 | -2,655068 | H64 | 4,904792 | -1,443622 | -2,853274 |
| H65 | 3,092411 | -2,711368 | -1,351616 | H65 | 3,149595 | -2,576766 | -1,558513 |
| H66 | 3,884092 | -0,017208 | 1,903865 | H66 | 3,874899 | 0,061389 | 1,757652 |
| H67 | 5,695080 | 1,019084 | 0,601448 | H67 | 5,650083 | 1,184497 | 0,466205 |
| C68 | -0,154047 | 6,292520 | -1,925787 | C68 | 0,564137 | 6,521623 | -2,256494 |
| C69 | 0,293322 | 5,082247 | -1,399706 | C69 | 0,665451 | 5,306467 | -1,579982 |
| C70 | 0,592160 | 4,009622 | -2,248211 | C70 | 0,902002 | 4,121891 | -2,286465 |
| C71 | 0,443625 | 4,171401 | -3,629110 | C71 | 1,041090 | 4,175192 | -3,678027 |
| C72 | -0,010282 | 5,380510 | -4,156680 | C72 | 0,932811 | 5,388999 | -4,356417 |
| C73 | -0,311338 | 6,443592 | -3,304867 | C73 | 0,692384 | 6,565482 | -3,645707 |
| H74 | -0,389179 | 7,115755 | -1,257266 | H74 | 0,379615 | 7,434674 | -1,697721 |
| H75 | 0,384427 | 4,958186 | -0,325385 | H75 | 0,557109 | 5,278825 | -0,500936 |
| H76 | 0,680619 | 3,345609 | -4,297449 | H76 | 1,237158 | 3,261106 | -4,235424 |
| H77 | -0,123623 | 5,493128 | -5,231051 | H77 | 1,042281 | 5,416194 | -5,436682 |
| H78 | -0,664460 | 7,386026 | -3,713399 | H78 | 0,609390 | 7,512461 | -4,171029 |
| C79 | 0,973034 | 2,633749 | -1,715121 | C79 | 0,938567 | 2,753291 | -1,609507 |
| C80 | -0,324363 | 1,790153 | -1,491813 | C80 | -0,500876 | 2,188391 | -1,621974 |
| C81 | -1,376192 | 2,505756 | -0,653054 | C81 | -1,623274 | 2,876605 | -0,877962 |
| C82 | -2,535834 | 2,947807 | -1,312657 | C82 | -2,905501 | 2,807284 | -1,446959 |
| C83 | -1,200065 | 2,901029 | 0,683563 | C83 | -1,467679 | 3,592655 | 0,316400 |
| C84 | -3,458783 | 3,783652 | -0,684941 | C84 | -3,999342 | 3,421390 | -0,840359 |
| H85 | -2,709510 | 2,648571 | -2,342312 | H85 | -3,053510 | 2,253419 | -2,369557 |
| C86 | -2,106987 | 3,761109 | 1,303069 | C86 | -2,557452 | 4,229488 | 0,912564 |
| H87 | -0,370707 | 2,522211 | 1,260981 | H87 | -0,500497 | 3,666445 | 0,791389 |
| C88 | -3,237602 | 4,215998 | 0,623966 | C88 | -3,829085 | 4,142116 | 0,343774 |
| H89 | -4,340851 | 4,110186 | -1,228383 | H89 | -4,980951 | 3,336620 | -1,296630 |
| H90 | -1,935223 | 4,057254 | 2,334134 | H90 | -2,409163 | 4,788470 | 1,832243 |
| H91 | -3,940728 | 4,886962 | 1,108887 | H91 | -4,675937 | 4,633481 | 0,813899 |
| C92 | 3,095934 | 3,541071 | -0,638378 | C92 | 3,010360 | 3,358518 | -0,302808 |
| C93 | 1,900929 | 1,977082 | 0,553064 | C93 | 1,445737 | 2,065438 | 0,790836 |
| C94 | 3,520453 | 3,549604 | 0,833087 | C94 | 3,298930 | 3,327357 | 1,199419 |
| H95 | 2,905675 | 4,539019 | -1,034557 | H95 | 3,057612 | 4,362133 | -0,726572 |
| H96 | 3,818289 | 3,024534 | -1,283904 | H96 | 3,669594 | 2,688389 | -0,870052 |
| H97 | 4,595278 | 3,454299 | 0,988146 | H97 | 4,321216 | 3,043962 | 1,450322 |
| H98 | 3,140975 | 4,424625 | 1,370450 | H98 | 3,041025 | 4,269817 | 1,693501 |
| N99 | 1,855376 | 2,758419 | -0,547637 | N99 | 1,636308 | 2,834913 | -0,315855 |
| O100 | 2,881273 | 2,369690 | 1,385141 | O100 | 2,410085 | 2,297530 | 1,700432 |
| O101 | 1,171547 | 1,028199 | 0,875838 | O101 | 0,523274 | 1,282289 | 1,044818 |
| H102 | 2,581328 | -4,076257 | 2,163749 | H102 | 2,791400 | -4,051417 | 1,923361 |
| N103 | -2,002558 | -2,508662 | 0,260001 | N103 | -1,938419 | -2,675849 | 0,295397 |
| C104 | -0,977166 | -3,389805 | -0,337436 | C104 | -0,905285 | -3,459454 | -0,422409 |
| H105 | -0,850098 | -3,221421 | -1,416639 | H105 | -0,846076 | -3,196765 | -1,488015 |

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| H106 | -0,761489 | 1,776629 | -2,495548 | H106 | -0,756238 | 2,197980 | -2,687412 |
| H107 | 1,679775 | -0,119202 | -1,392547 | H107 | 1,628191 | 0,057484 | -1,189735 |
| H108 | 0,236253 | 0,431305 | -2,148581 | H108 | -0,616550 | 1,043242 | -1,516089 |

Isomerization

| Iso1 | | | | TS _{Iso1-2} | | | |
|------|-----------|-----------|-----------|----------------------|-----------|-----------|-----------|
| C1 | -4,163957 | -3,413621 | 0,495949 | C1 | 4,346353 | 3,217037 | 0,263892 |
| C2 | -2,022982 | -4,485459 | 0,026619 | C2 | 2,259239 | 4,384293 | -0,227178 |
| C3 | -3,482403 | -4,418747 | -0,490090 | C3 | 3,701615 | 4,202789 | -0,765849 |
| C4 | -2,991128 | -3,026092 | 1,427059 | C4 | 3,176618 | 2,961192 | 1,243615 |
| H5 | -4,961675 | -3,891034 | 1,074636 | H5 | 5,189183 | 3,675193 | 0,791983 |
| H6 | -3,536093 | -4,089495 | -1,532711 | H6 | 3,714378 | 3,813073 | -1,788864 |
| H7 | -3,267742 | -2,520272 | 2,352589 | H7 | 3,447576 | 2,499120 | 2,193547 |
| H8 | -4,592510 | -2,548004 | -0,008998 | H8 | 4,704699 | 2,294690 | -0,194802 |
| H9 | -1,449996 | -5,342382 | -0,325984 | H9 | 1,725944 | 5,248340 | -0,622460 |
| H10 | -3,942675 | -5,409269 | -0,436314 | H10 | 4,218791 | 5,166392 | -0,777937 |
| C11 | -2,224355 | -4,353581 | 1,552521 | C11 | 2,489743 | 4,336607 | 1,299949 |
| H12 | -1,293876 | -4,260150 | 2,120793 | H12 | 1,569152 | 4,334075 | 1,891728 |
| H13 | -2,829643 | -5,162804 | 1,970202 | H13 | 3,149606 | 5,133868 | 1,653067 |
| C14 | 0,152012 | -3,110362 | -0,165796 | C14 | 0,007517 | 3,108169 | -0,317945 |
| N15 | 0,893885 | -2,057120 | -0,123457 | N15 | -0,776244 | 2,091120 | -0,209954 |
| C16 | 2,348877 | -2,501544 | -0,197728 | C16 | -2,208721 | 2,585513 | -0,307392 |
| C17 | 2,186916 | -4,028465 | 0,065158 | C17 | -1,986872 | 4,122475 | -0,162750 |
| P18 | -1,924278 | -0,543643 | 0,464644 | P18 | 1,940575 | 0,495614 | 0,482512 |
| Ir19 | 0,274502 | -0,008131 | -0,426442 | Ir19 | -0,226986 | -0,002426 | -0,404242 |
| C20 | -2,161935 | 0,087161 | 2,164131 | C20 | 2,094370 | -0,042618 | 2,218503 |
| C21 | -2,171526 | 1,163910 | 4,755967 | C21 | 1,929672 | -0,988937 | 4,852181 |
| C22 | -1,463363 | -0,548212 | 3,203504 | C22 | 1,506843 | 0,743900 | 3,220487 |
| C23 | -2,861686 | 1,270604 | 2,439483 | C23 | 2,591663 | -1,312005 | 2,548385 |
| C24 | -2,865622 | 1,804291 | 3,729439 | C24 | 2,509920 | -1,780063 | 3,860198 |
| C25 | -1,474395 | -0,016881 | 4,490101 | C25 | 1,432581 | 0,275533 | 4,529763 |
| H26 | -3,416156 | 1,771534 | 1,654956 | H26 | 3,047757 | -1,933487 | 1,786119 |
| H27 | -3,421403 | 2,715740 | 3,931945 | H27 | 2,908258 | -2,760313 | 4,107698 |
| H28 | -0,930393 | -0,518863 | 5,284880 | H28 | 0,978728 | 0,894090 | 5,298525 |
| H29 | -2,174407 | 1,580659 | 5,758915 | H29 | 1,865129 | -1,355148 | 5,872519 |
| O30 | 0,771150 | -4,294209 | -0,144853 | O30 | -0,561993 | 4,315914 | -0,381884 |
| C31 | 3,198321 | -1,908942 | 0,919348 | C31 | -3,068113 | 2,107681 | 0,855317 |
| C32 | 2,602482 | -1,431515 | 2,089597 | C32 | -2,482060 | 1,634149 | 2,031931 |
| C33 | 4,598267 | -1,955256 | 0,842561 | C33 | -4,462657 | 2,248537 | 0,800891 |
| C34 | 3,384829 | -0,936438 | 3,132724 | C34 | -3,275588 | 1,242064 | 3,110371 |
| H35 | 1,524467 | -1,410267 | 2,176880 | H35 | -1,406851 | 1,537510 | 2,100836 |
| C36 | 5,380638 | -1,474994 | 1,891534 | C36 | -5,254385 | 1,872044 | 1,884198 |
| H37 | 5,081068 | -2,354774 | -0,043770 | H37 | -4,933773 | 2,640566 | -0,095448 |
| C38 | 4,775849 | -0,949494 | 3,034920 | C38 | -4,663589 | 1,353918 | 3,038720 |
| H39 | 2,899988 | -0,532960 | 4,016736 | H39 | -2,801210 | 0,841484 | 4,001305 |
| H40 | 6,463394 | -1,507060 | 1,811104 | H40 | -6,333562 | 1,978923 | 1,822859 |
| H41 | 5,385885 | -0,561588 | 3,845728 | H41 | -5,282228 | 1,048285 | 3,877653 |
| C42 | -3,402865 | -0,059708 | -0,500188 | C42 | 3,400544 | -0,148548 | -0,410044 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C43 | -4,682540 | 0,032883 | 0,074487 | C43 | 4,637022 | -0,363737 | 0,220583 |
| C44 | -3,266370 | 0,099402 | -1,886597 | C44 | 3,305935 | -0,287794 | -1,802633 |
| C45 | -5,794990 | 0,298304 | -0,722171 | C45 | 5,753766 | -0,723571 | -0,531561 |
| H46 | -4,814556 | -0,107826 | 1,142984 | H46 | 4,733825 | -0,242250 | 1,294890 |
| C47 | -4,383129 | 0,357195 | -2,681144 | C47 | 4,427149 | -0,640176 | -2,551205 |
| C48 | -5,648418 | 0,461097 | -2,102500 | C48 | 5,650327 | -0,861592 | -1,917425 |
| H49 | -6,777827 | 0,372730 | -0,265463 | H49 | 6,706050 | -0,890578 | -0,036308 |
| H50 | -4,259303 | 0,494953 | -3,750946 | H50 | 4,340139 | -0,759443 | -3,626752 |
| H51 | -6,516448 | 0,669770 | -2,720887 | H51 | 6,522661 | -1,141944 | -2,500838 |
| H52 | -0,118809 | -0,428638 | -1,876377 | H52 | 0,213168 | 0,348314 | -1,859339 |
| H53 | 1,756460 | -0,020859 | -0,994801 | H53 | -1,709866 | -0,069468 | -1,031224 |
| H54 | -0,902186 | -1,453808 | 2,994702 | H54 | 1,095098 | 1,715715 | 2,965622 |
| H55 | -2,281344 | 0,048333 | -2,337410 | H55 | 2,348110 | -0,150459 | -2,292681 |
| H56 | 2,761357 | -4,656663 | -0,615218 | H56 | -2,534652 | 4,718544 | -0,892680 |
| C57 | 3,441736 | -1,519157 | -4,288053 | C57 | -3,380542 | 1,313445 | -4,294481 |
| C58 | 2,656782 | -2,639437 | -4,007968 | C58 | -2,534468 | 2,409817 | -4,114400 |
| C59 | 2,351987 | -2,968942 | -2,688848 | C59 | -2,204142 | 2,835734 | -2,829575 |
| C60 | 2,828100 | -2,191625 | -1,623160 | C60 | -2,714522 | 2,181545 | -1,699572 |
| C61 | 3,612994 | -1,068426 | -1,918028 | C61 | -3,563190 | 1,083499 | -1,893208 |
| C62 | 3,918381 | -0,736228 | -3,238228 | C62 | -3,893035 | 0,652750 | -3,179390 |
| H63 | 3,679810 | -1,262062 | -5,316241 | H63 | -3,638810 | 0,981313 | -5,295981 |
| H64 | 2,279453 | -3,257252 | -4,817746 | H64 | -2,129848 | 2,933481 | -4,975774 |
| H65 | 1,718127 | -3,831351 | -2,499850 | H65 | -1,524674 | 3,676047 | -2,716567 |
| H66 | 3,986116 | -0,436856 | -1,122065 | H66 | -3,969731 | 0,549772 | -1,043602 |
| H67 | 4,527618 | 0,140556 | -3,439156 | H67 | -4,550803 | -0,203286 | -3,301388 |
| C68 | -2,454159 | 3,304004 | -3,397543 | C68 | 2,183042 | -3,383957 | -3,440746 |
| C69 | -1,344000 | 2,761373 | -2,754102 | C69 | 1,118782 | -2,796816 | -2,759807 |
| C70 | -1,296252 | 2,673925 | -1,354775 | C70 | 1,101550 | -2,745230 | -1,357878 |
| C71 | -2,394445 | 3,157909 | -0,627800 | C71 | 2,189606 | -3,303290 | -0,668332 |
| C72 | -3,505325 | 3,699669 | -1,269321 | C72 | 3,255000 | -3,889432 | -1,347517 |
| C73 | -3,541384 | 3,775807 | -2,660551 | C73 | 3,257004 | -3,935284 | -2,740328 |
| H74 | -2,464845 | 3,366183 | -4,482193 | H74 | 2,169500 | -3,414206 | -4,526705 |
| H75 | -0,513264 | 2,410466 | -3,357111 | H75 | 0,302662 | -2,375385 | -3,337364 |
| H76 | -2,372119 | 3,105654 | 0,454095 | H76 | 2,202863 | -3,265504 | 0,415075 |
| H77 | -4,343115 | 4,061073 | -0,679835 | H77 | 4,086985 | -4,303722 | -0,785321 |
| H78 | -4,403228 | 4,201513 | -3,165751 | H78 | 4,084166 | -4,393350 | -3,274316 |
| C79 | -0,106033 | 2,133807 | -0,626018 | C79 | -0,029502 | -2,139255 | -0,585748 |
| C80 | 1,125307 | 1,792608 | -1,303040 | C80 | -1,278532 | -1,740727 | -1,230887 |
| H81 | 1,048777 | 1,679271 | -2,379219 | H81 | -1,234841 | -1,675966 | -2,313437 |
| C82 | 2,448229 | 2,373226 | -0,893344 | C82 | -2,608088 | -2,259811 | -0,762282 |
| C83 | 3,259374 | 1,896668 | 0,143166 | C83 | -3,366989 | -1,707009 | 0,274847 |
| C84 | 2,868132 | 3,500193 | -1,619064 | C84 | -3,090482 | -3,398122 | -1,427581 |
| C85 | 4,457768 | 2,542121 | 0,454324 | C85 | -4,579246 | -2,290845 | 0,647646 |
| H86 | 2,964816 | 1,016009 | 0,701672 | H86 | -3,018353 | -0,817984 | 0,787117 |
| C87 | 4,063310 | 4,144893 | -1,304865 | C87 | -4,299106 | -3,981243 | -1,051220 |
| H88 | 2,250148 | 3,873636 | -2,432802 | H88 | -2,512526 | -3,827686 | -2,243129 |
| C89 | 4,862027 | 3,667689 | -0,263125 | C89 | -5,046992 | -3,429131 | -0,008597 |
| H90 | 5,075384 | 2,151381 | 1,257963 | H90 | -5,156448 | -1,843327 | 1,451478 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H91 | 4,372375 | 5,015353 | -1,876865 | H91 | -4,658645 | -4,861684 | -1,576393 |
| H92 | 5,795992 | 4,166521 | -0,020807 | H92 | -5,991259 | -3,880471 | 0,281643 |
| C93 | 0,254094 | 4,151686 | 0,961488 | C93 | -0,441600 | -4,136937 | 1,023317 |
| C94 | 0,565770 | 1,991957 | 1,718085 | C94 | -0,644979 | -1,957904 | 1,764513 |
| C95 | 0,397076 | 4,111983 | 2,492557 | C95 | -0,572213 | -4,076367 | 2,555191 |
| H96 | -0,600219 | 4,743908 | 0,629460 | H96 | 0,381277 | -4,771882 | 0,690919 |
| H97 | 1,160255 | 4,505547 | 0,456694 | H97 | -1,366196 | -4,460016 | 0,531103 |
| H98 | 1,141533 | 4,803136 | 2,887851 | H98 | -1,344412 | -4,730195 | 2,960863 |
| H99 | -0,561121 | 4,257198 | 3,001336 | H99 | 0,380953 | -4,266026 | 3,059316 |
| N100 | 0,050990 | 2,719689 | 0,698213 | N100 | -0,181224 | -2,718297 | 0,742361 |
| O101 | 0,845583 | 2,755845 | 2,779472 | O101 | -0,953012 | -2,700218 | 2,833473 |
| O102 | 0,775321 | 0,772262 | 1,698901 | O102 | -0,798476 | -0,729771 | 1,735516 |
| H103 | 2,416940 | -4,286348 | 1,101050 | H103 | -2,213139 | 4,468237 | 0,848174 |
| N104 | -1,976927 | -2,225396 | 0,683726 | N104 | 2,103820 | 2,178035 | 0,571835 |
| C105 | -1,350348 | -3,128567 | -0,306966 | C105 | 1,508408 | 3,047827 | -0,464122 |
| H106 | -1,565209 | -2,828735 | -1,344085 | H106 | 1,696789 | 2,674951 | -1,483108 |

| Iso2 | | | | TS _{Iso2-3} | | | |
|------|-----------|-----------|-----------|----------------------|-----------|-----------|-----------|
| C1 | 4,843561 | 2,498820 | -0,482967 | C1 | -4,338247 | 2,694784 | -1,634939 |
| C2 | 2,981888 | 3,839251 | -1,315714 | C2 | -4,312143 | 0,407061 | -2,480902 |
| C3 | 4,382473 | 3,321595 | -1,731988 | C3 | -4,451374 | 1,874037 | -2,962482 |
| C4 | 3,642901 | 2,666109 | 0,476882 | C4 | -4,170576 | 1,580282 | -0,575436 |
| H5 | 5,750371 | 2,916876 | -0,033693 | H5 | -5,246363 | 3,273413 | -1,436174 |
| H6 | 4,346168 | 2,720039 | -2,645717 | H6 | -3,682692 | 2,143279 | -3,693827 |
| H7 | 3,829001 | 2,398250 | 1,517273 | H7 | -4,339121 | 1,887039 | 0,457034 |
| H8 | 5,037176 | 1,448989 | -0,709024 | H8 | -3,495340 | 3,388306 | -1,629491 |
| H9 | 2,595418 | 4,660659 | -1,918503 | H9 | -4,629488 | -0,349141 | -3,199008 |
| H10 | 5,049894 | 4,166554 | -1,923308 | H10 | -5,423860 | 2,018465 | -3,441791 |
| C11 | 3,185366 | 4,106635 | 0,191923 | C11 | -5,059647 | 0,454014 | -1,129735 |
| H12 | 2,270165 | 4,379259 | 0,726734 | H12 | -4,993582 | -0,470937 | -0,548078 |
| H13 | 3,960976 | 4,852394 | 0,387020 | H13 | -6,108235 | 0,745263 | -1,238163 |
| C14 | 0,555778 | 2,940029 | -1,236661 | C14 | -2,381232 | -1,207984 | -1,850879 |
| N15 | -0,358347 | 2,145518 | -0,806548 | N15 | -1,396209 | -1,553909 | -1,104642 |
| C16 | -1,690595 | 2,816668 | -0,959944 | C16 | -1,238082 | -3,038369 | -1,168230 |
| C17 | -1,289397 | 4,113461 | -1,748727 | C17 | -2,186359 | -3,381344 | -2,366780 |
| P18 | 1,991962 | 0,342789 | 0,307287 | P18 | -1,414846 | 1,349289 | 0,095074 |
| Ir19 | -0,073215 | -0,003165 | -0,435216 | Ir19 | 0,106655 | -0,202197 | -0,291685 |
| C20 | 2,018273 | 0,280332 | 2,128194 | C20 | -1,889612 | 1,357047 | 1,852694 |
| C21 | 1,641370 | 0,120230 | 4,900222 | C21 | -2,380294 | 1,086581 | 4,597613 |
| C22 | 1,608052 | 1,408195 | 2,854719 | C22 | -2,881016 | 0,477863 | 2,311952 |
| C23 | 2,239199 | -0,929057 | 2,804339 | C23 | -1,142188 | 2,098289 | 2,782086 |
| C24 | 2,052507 | -1,005522 | 4,184384 | C24 | -1,391777 | 1,964028 | 4,147019 |
| C25 | 1,426065 | 1,327932 | 4,233494 | C25 | -3,126111 | 0,348046 | 3,677748 |
| H26 | 2,568168 | -1,805532 | 2,256557 | H26 | -0,369203 | 2,777857 | 2,439124 |
| H27 | 2,234305 | -1,943571 | 4,701675 | H27 | -0,819442 | 2,550926 | 4,860545 |
| H28 | 1,109658 | 2,207252 | 4,787112 | H28 | -3,898394 | -0,332829 | 4,024012 |
| H29 | 1,491790 | 0,057316 | 5,974100 | H29 | -2,570066 | 0,981790 | 5,661885 |
| O30 | 0,167030 | 4,115478 | -1,737839 | O30 | -2,980892 | -2,171094 | -2,556556 |

| | | | | | | | |
|-----|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| C31 | -2,278706 | 3,197707 | 0,396966 | C31 | -1,758951 | -3,693655 | 0,112502 |
| C32 | -1,658360 | 2,861172 | 1,599704 | C32 | -2,139546 | -2,948186 | 1,228139 |
| C33 | -3,466153 | 3,945586 | 0,429776 | C33 | -1,858315 | -5,092088 | 0,161802 |
| C34 | -2,227680 | 3,239694 | 2,817435 | C34 | -2,611304 | -3,586560 | 2,376801 |
| H35 | -0,746941 | 2,282426 | 1,593911 | H35 | -2,044052 | -1,872766 | 1,215750 |
| C36 | -4,031252 | 4,327533 | 1,643615 | C36 | -2,331096 | -5,728997 | 1,306237 |
| H37 | -3,960194 | 4,215570 | -0,500960 | H37 | -1,544776 | -5,687768 | -0,693003 |
| C38 | -3,413882 | 3,969676 | 2,845044 | C38 | -2,710158 | -4,975562 | 2,420491 |
| H39 | -1,739223 | 2,951131 | 3,744044 | H39 | -2,890739 | -2,988564 | 3,240044 |
| H40 | -4,954625 | 4,899653 | 1,651929 | H40 | -2,400185 | -6,812753 | 1,330297 |
| H41 | -3,857450 | 4,261052 | 3,792803 | H41 | -3,076130 | -5,472077 | 3,314604 |
| C42 | 3,311368 | -0,776198 | -0,282387 | C42 | -1,043174 | 3,074582 | -0,369582 |
| C43 | 4,489556 | -0,947278 | 0,465789 | C43 | -1,601144 | 4,154602 | 0,334706 |
| C44 | 3,213191 | -1,370297 | -1,548818 | C44 | -0,346045 | 3,316340 | -1,562379 |
| C45 | 5,541302 | -1,707847 | -0,042925 | C45 | -1,450888 | 5,454781 | -0,145483 |
| H46 | 4,589032 | -0,488319 | 1,444955 | H46 | -2,162357 | 3,988169 | 1,248218 |
| C47 | 4,270648 | -2,125073 | -2,054765 | C47 | -0,204075 | 4,616890 | -2,038597 |
| C48 | 5,434979 | -2,298252 | -1,304711 | C48 | -0,755164 | 5,687715 | -1,332579 |
| H49 | 6,444348 | -1,837384 | 0,546767 | H49 | -1,883394 | 6,284576 | 0,406479 |
| H50 | 4,173041 | -2,595672 | -3,028103 | H50 | 0,353092 | 4,795075 | -2,953047 |
| H51 | 6,254528 | -2,892943 | -1,697183 | H51 | -0,639272 | 6,701928 | -1,704031 |
| H52 | 0,512792 | -0,095084 | -1,888116 | H52 | 0,264459 | 0,385997 | -1,737970 |
| H53 | -1,908184 | -0,614304 | -1,123946 | H53 | 2,453381 | -1,490840 | 0,680694 |
| H54 | 1,421649 | 2,343264 | 2,336171 | H54 | -3,450937 | -0,110971 | 1,600720 |
| H55 | 2,297886 | -1,271168 | -2,120767 | H55 | 0,111077 | 2,491977 | -2,097377 |
| H56 | -1,613290 | 4,105252 | -2,791941 | H56 | -1,658086 | -3,582087 | -3,302155 |
| C57 | -4,049059 | 0,075552 | -3,372072 | C57 | 2,992897 | -3,673457 | -1,945403 |
| C58 | -2,848751 | 0,607543 | -3,850578 | C58 | 2,176119 | -3,067224 | -2,902874 |
| C59 | -2,124452 | 1,504140 | -3,070110 | C59 | 0,817147 | -2,890511 | -2,650107 |
| C60 | -2,581430 | 1,889875 | -1,798802 | C60 | 0,245390 | -3,325960 | -1,442849 |
| C61 | -3,779899 | 1,345487 | -1,327514 | C61 | 1,076485 | -3,917714 | -0,483601 |
| C62 | -4,509387 | 0,447392 | -2,111173 | C62 | 2,438960 | -4,092721 | -0,736746 |
| H63 | -4,614752 | -0,628902 | -3,974851 | H63 | 4,054442 | -3,800782 | -2,134572 |
| H64 | -2,475100 | 0,320525 | -4,829484 | H64 | 2,598442 | -2,725899 | -3,843795 |
| H65 | -1,176175 | 1,882766 | -3,442187 | H65 | 0,203778 | -2,386686 | -3,392295 |
| H66 | -4,142737 | 1,605442 | -0,340817 | H66 | 0,662461 | -4,237491 | 0,465926 |
| H67 | -5,428105 | 0,022187 | -1,719355 | H67 | 3,069105 | -4,552585 | 0,019190 |
| C68 | 1,381926 | -4,589811 | -2,459505 | C68 | 3,252546 | 3,348508 | -1,799379 |
| C69 | 0,469924 | -3,614166 | -2,053382 | C69 | 2,858619 | 2,099851 | -1,326414 |
| C70 | 0,486154 | -3,110351 | -0,745354 | C70 | 2,338287 | 1,939718 | -0,033293 |
| C71 | 1,460406 | -3,617419 | 0,133444 | C71 | 2,172664 | 3,099609 | 0,741889 |
| C72 | 2,367854 | -4,592608 | -0,266440 | C72 | 2,556656 | 4,353692 | 0,269307 |
| C73 | 2,331801 | -5,089302 | -1,569700 | C73 | 3,117462 | 4,484516 | -0,999096 |
| H74 | 1,340046 | -4,967045 | -3,477565 | H74 | 3,663822 | 3,434227 | -2,801634 |
| H75 | -0,255023 | -3,255223 | -2,776100 | H75 | 2,934463 | 1,242648 | -1,980858 |
| H76 | 1,506444 | -3,226956 | 1,144191 | H76 | 1,711460 | 3,031246 | 1,720527 |
| H77 | 3,109519 | -4,957749 | 0,438523 | H77 | 2,407258 | 5,229278 | 0,895075 |
| H78 | 3,034275 | -5,854302 | -1,886850 | H78 | 3,427578 | 5,458307 | -1,366766 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C79 | -0,455128 | -2,050446 | -0,249052 | C79 | 1,900289 | 0,594367 | 0,463107 |
| C80 | -1,724319 | -1,738381 | -1,097761 | C80 | 2,677043 | -0,691837 | -0,032987 |
| H81 | -1,551770 | -1,976878 | -2,144944 | H81 | 2,236952 | -1,030630 | -0,992783 |
| C82 | -3,023016 | -2,335138 | -0,614414 | C82 | 4,182318 | -0,672268 | -0,244258 |
| C83 | -3,793648 | -1,707996 | 0,371142 | C83 | 5,051211 | -0,878796 | 0,834740 |
| C84 | -3,430210 | -3,576776 | -1,115837 | C84 | 4,740418 | -0,529958 | -1,520965 |
| C85 | -4,947932 | -2,321437 | 0,859073 | C85 | 6,434129 | -0,885105 | 0,656417 |
| H86 | -3,491226 | -0,735734 | 0,750028 | H86 | 4,643803 | -1,076527 | 1,822409 |
| C87 | -4,587886 | -4,187742 | -0,632244 | C87 | 6,122422 | -0,536553 | -1,707448 |
| H88 | -2,831370 | -4,071392 | -1,876943 | H88 | 4,087903 | -0,435125 | -2,384391 |
| C89 | -5,347332 | -3,563095 | 0,359302 | C89 | 6,975628 | -0,704329 | -0,616525 |
| H90 | -5,538025 | -1,827586 | 1,626036 | H90 | 7,087177 | -1,047014 | 1,509564 |
| H91 | -4,895104 | -5,151805 | -1,027957 | H91 | 6,531464 | -0,418820 | -2,707065 |
| H92 | -6,247557 | -4,039725 | 0,736492 | H92 | 8,052357 | -0,709386 | -0,759101 |
| C93 | -1,250301 | -3,555380 | 1,783132 | C93 | 2,821267 | 0,923180 | 2,940787 |
| C94 | -1,114377 | -1,255243 | 1,953235 | C94 | 0,961978 | -0,352135 | 2,470866 |
| C95 | -1,457783 | -3,084619 | 3,235876 | C95 | 2,104312 | 0,481807 | 4,228532 |
| H96 | -0,497522 | -4,340545 | 1,699009 | H96 | 3,053016 | 1,987921 | 2,930821 |
| H97 | -2,176498 | -3,896790 | 1,314752 | H97 | 3,750056 | 0,375376 | 2,765908 |
| H98 | -2,367533 | -3,470552 | 3,696385 | H98 | 2,759294 | 0,017511 | 4,966488 |
| H99 | -0,595346 | -3,301705 | 3,873754 | H99 | 1,545903 | 1,300918 | 4,692902 |
| N100 | -0,787489 | -2,300227 | 1,168516 | N100 | 1,798829 | 0,566746 | 1,941505 |
| O101 | -1,580779 | -1,635455 | 3,146055 | O101 | 1,139593 | -0,512747 | 3,786849 |
| O102 | -1,023991 | -0,058569 | 1,623522 | O102 | 0,128047 | -1,013839 | 1,825621 |
| H103 | -1,626603 | 5,026165 | -1,259088 | H103 | -2,872777 | -4,197104 | -2,146128 |
| N104 | 2,462291 | 1,926124 | -0,051385 | N104 | -2,836648 | 0,931216 | -0,722518 |
| C105 | 2,028368 | 2,615268 | -1,285238 | C105 | -2,843037 | 0,216407 | -2,018754 |
| H106 | 2,171109 | 1,994454 | -2,183379 | H106 | -2,153691 | 0,670207 | -2,748212 |

Iso3

| | | | |
|-----|-----------|-----------|-----------|
| C1 | 0,752502 | -4,421648 | -2,686798 |
| C2 | 2,233990 | -2,621454 | -3,403070 |
| C3 | 1,197550 | -3,629712 | -3,961557 |
| C4 | 1,624601 | -3,779605 | -1,582144 |
| H5 | 0,975938 | -5,489776 | -2,773877 |
| H6 | 0,362918 | -3,130510 | -4,463699 |
| H7 | 1,692563 | -4,347080 | -0,653879 |
| H8 | -0,312051 | -4,321303 | -2,467938 |
| H9 | 2,868743 | -2,146360 | -4,150831 |
| H10 | 1,674306 | -4,286817 | -4,694343 |
| C11 | 2,938163 | -3,472267 | -2,322073 |
| H12 | 3,654048 | -2,914746 | -1,710427 |
| H13 | 3,420670 | -4,361940 | -2,736115 |
| C14 | 2,181002 | -0,324762 | -2,190834 |
| N15 | 1,821642 | 0,469845 | -1,246896 |
| C16 | 2,856950 | 1,553201 | -1,125031 |
| C17 | 3,621835 | 1,367451 | -2,472698 |
| P18 | 0,044718 | -1,886140 | -0,156067 |

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| | | | |
|-----|-----------|-----------|-----------|
| C1 | -2,811440 | -3,038130 | -3,146331 |
| C2 | -0,422953 | -2,999946 | -3,658226 |
| C3 | -1,805447 | -2,708276 | -4,299074 |
| C4 | -1,862659 | -3,459388 | -2,000405 |
| H5 | -3,473487 | -3,868878 | -3,411446 |
| H6 | -1,888101 | -1,674101 | -4,648384 |
| H7 | -2,337359 | -3,973386 | -1,163952 |
| H8 | -3,437549 | -2,189735 | -2,866396 |
| H9 | 0,398516 | -3,118128 | -4,364443 |
| H10 | -1,959646 | -3,358154 | -5,164907 |
| C11 | -0,749461 | -4,209618 | -2,753001 |
| H12 | 0,078246 | -4,516938 | -2,106781 |
| H13 | -1,114975 | -5,072785 | -3,315899 |
| C14 | 1,238004 | -1,797616 | -2,070486 |
| N15 | 1,583019 | -1,104094 | -1,041237 |
| C16 | 3,069013 | -1,264845 | -0,826640 |
| C17 | 3,419875 | -2,311481 | -1,941339 |
| P18 | -1,488143 | -1,209507 | -0,280571 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| Ir19 | -0,074724 | 0,341953 | -0,157424 | Ir19 | 0,309495 | 0,332786 | -0,010396 |
| C20 | 0,682992 | -2,523155 | 1,434225 | C20 | -1,698765 | -2,253244 | 1,199683 |
| C21 | 1,639218 | -3,226468 | 3,978610 | C21 | -1,741791 | -3,673678 | 3,616442 |
| C22 | 2,039424 | -2,816486 | 1,624770 | C22 | -1,053890 | -3,492444 | 1,303526 |
| C23 | -0,192584 | -2,592966 | 2,529981 | C23 | -2,370524 | -1,733691 | 2,317915 |
| C24 | 0,284490 | -2,939047 | 3,792915 | C24 | -2,389612 | -2,440332 | 3,518308 |
| C25 | 2,510866 | -3,172251 | 2,890131 | C25 | -1,079542 | -4,199287 | 2,506598 |
| H26 | -1,248236 | -2,389593 | 2,388334 | H26 | -2,875000 | -0,775287 | 2,248834 |
| H27 | -0,403611 | -2,995231 | 4,631866 | H27 | -2,913151 | -2,031021 | 4,377922 |
| H28 | 3,562927 | -3,407277 | 3,023701 | H28 | -0,578278 | -5,160402 | 2,575778 |
| H29 | 2,009899 | -3,499342 | 4,962152 | H29 | -1,755886 | -4,222692 | 4,553195 |
| O30 | 3,255391 | 0,021584 | -2,906000 | O30 | 2,190533 | -2,487053 | -2,699188 |
| C31 | 3,816903 | 1,266225 | 0,035096 | C31 | 3,384238 | -1,902589 | 0,523235 |
| C32 | 3,659372 | 0,175601 | 0,886411 | C32 | 2,396300 | -2,534812 | 1,277849 |
| C33 | 4,904755 | 2,130254 | 0,232025 | C33 | 4,718005 | -1,975879 | 0,952909 |
| C34 | 4,559130 | -0,044223 | 1,931082 | C34 | 2,722366 | -3,200069 | 2,459501 |
| H35 | 2,816625 | -0,484733 | 0,759355 | H35 | 1,363858 | -2,488442 | 0,963637 |
| C36 | 5,806121 | 1,909509 | 1,269906 | C36 | 5,045839 | -2,648684 | 2,128015 |
| H37 | 5,031990 | 2,994164 | -0,416312 | H37 | 5,501197 | -1,496122 | 0,372534 |
| C38 | 5,632652 | 0,819755 | 2,127614 | C38 | 4,046318 | -3,259604 | 2,889181 |
| H39 | 4,402513 | -0,887934 | 2,596876 | H39 | 1,930472 | -3,661023 | 3,042925 |
| H40 | 6,638287 | 2,591598 | 1,415486 | H40 | 6,081928 | -2,691728 | 2,451024 |
| H41 | 6,329608 | 0,652230 | 2,943749 | H41 | 4,302200 | -3,776494 | 3,809525 |
| C42 | -1,497643 | -2,815638 | -0,457087 | C42 | -3,148968 | -0,577093 | -0,700174 |
| C43 | -1,671097 | -4,107415 | 0,066948 | C43 | -4,329557 | -1,188110 | -0,253027 |
| C44 | -2,452213 | -2,299453 | -1,344980 | C44 | -3,219881 | 0,447134 | -1,656942 |
| C45 | -2,784695 | -4,864564 | -0,290885 | C45 | -5,563565 | -0,774846 | -0,755278 |
| H46 | -0,939110 | -4,526214 | 0,750063 | H46 | -4,290618 | -1,992333 | 0,474240 |
| C47 | -3,564097 | -3,061113 | -1,697823 | C47 | -4,453222 | 0,849289 | -2,161579 |
| C48 | -3,732155 | -4,343415 | -1,173619 | C48 | -5,626629 | 0,240377 | -1,710553 |
| H49 | -2,911220 | -5,862219 | 0,119389 | H49 | -6,474366 | -1,252133 | -0,405164 |
| H50 | -4,307574 | -2,644960 | -2,370480 | H50 | -4,500632 | 1,650091 | -2,892728 |
| H51 | -4,601242 | -4,934202 | -1,448395 | H51 | -6,588719 | 0,558342 | -2,101597 |
| H52 | -0,831413 | 0,233738 | -1,530023 | H52 | -0,012877 | 0,952030 | -1,406386 |
| H53 | -1,147446 | 2,917124 | 1,330328 | H53 | 1,347700 | 2,264984 | 1,677842 |
| H54 | 2,729667 | -2,758143 | 0,790274 | H54 | -0,519949 | -3,896714 | 0,449707 |
| H55 | -2,337525 | -1,295229 | -1,735696 | H55 | -2,310870 | 0,938235 | -1,988788 |
| H56 | 3,315367 | 2,061206 | -3,258926 | H56 | 4,204264 | -1,988179 | -2,625661 |
| C57 | 0,589788 | 5,230008 | -0,684315 | C57 | 4,790170 | 2,664396 | -1,511134 |
| C58 | 0,661250 | 4,590010 | -1,922130 | C58 | 4,415431 | 1,858109 | -2,586533 |
| C59 | 1,416480 | 3,427944 | -2,066560 | C59 | 3,881329 | 0,590448 | -2,358162 |
| C60 | 2,129181 | 2,892781 | -0,983609 | C60 | 3,726878 | 0,099275 | -1,054940 |
| C61 | 2,041888 | 3,536775 | 0,257661 | C61 | 4,085367 | 0,926790 | 0,018399 |
| C62 | 1,279490 | 4,697307 | 0,403694 | C62 | 4,616218 | 2,197451 | -0,209049 |
| H63 | -0,009204 | 6,128293 | -0,568648 | H63 | 5,200456 | 3,654195 | -1,686624 |
| H64 | 0,108745 | 4,982971 | -2,769577 | H64 | 4,533613 | 2,217026 | -3,604795 |
| H65 | 1,419355 | 2,922980 | -3,027940 | H65 | 3,572990 | -0,008711 | -3,211000 |
| H66 | 2,553748 | 3,121326 | 1,117332 | H66 | 3,951473 | 0,575039 | 1,035530 |

| | | | | | | | |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H67 | 1,225812 | 5,183365 | 1,373764 | H67 | 4,889726 | 2,823672 | 0,635193 |
| C68 | -5,187056 | -0,203434 | -0,391292 | C68 | -3,273770 | 3,931915 | -0,739652 |
| C69 | -3,969106 | 0,464308 | -0,270602 | C69 | -2,050629 | 3,369276 | -0,379862 |
| C70 | -3,097531 | 0,197801 | 0,797671 | C70 | -1,964398 | 2,458589 | 0,685894 |
| C71 | -3,491735 | -0,799949 | 1,709194 | C71 | -3,158808 | 2,104656 | 1,338148 |
| C72 | -4,699831 | -1,480005 | 1,580278 | C72 | -4,382114 | 2,658216 | 0,969973 |
| C73 | -5,565984 | -1,176555 | 0,531856 | C73 | -4,445391 | 3,589508 | -0,064515 |
| H74 | -5,840730 | 0,039617 | -1,224591 | H74 | -3,307485 | 4,643123 | -1,560350 |
| H75 | -3,703388 | 1,186518 | -1,026165 | H75 | -1,167554 | 3,640644 | -0,940228 |
| H76 | -2,833402 | -1,059756 | 2,529947 | H76 | -3,133806 | 1,373037 | 2,138029 |
| H77 | -4,960665 | -2,249343 | 2,301584 | H77 | -5,285620 | 2,354049 | 1,490350 |
| H78 | -6,513874 | -1,696850 | 0,430651 | H78 | -5,395651 | 4,030484 | -0,350528 |
| C79 | -1,754181 | 0,855415 | 0,975294 | C79 | -0,674308 | 1,848670 | 1,142784 |
| C80 | -1,433311 | 2,303456 | 0,470158 | C80 | 0,677078 | 2,333190 | 0,817837 |
| H81 | -0,442221 | 2,301483 | -0,111507 | H81 | 1,674286 | 1,210019 | 0,023134 |
| C82 | -2,397498 | 3,068608 | -0,396509 | C82 | 1,002453 | 3,541341 | -0,010799 |
| C83 | -3,443430 | 3,769730 | 0,212006 | C83 | 0,849930 | 4,786776 | 0,616974 |
| C84 | -2,284835 | 3,080946 | -1,789627 | C84 | 1,461723 | 3,495144 | -1,328820 |
| C85 | -4,374479 | 4,461708 | -0,561081 | C85 | 1,131741 | 5,965214 | -0,068793 |
| H86 | -3,539360 | 3,760263 | 1,295517 | H86 | 0,489269 | 4,830366 | 1,642118 |
| C87 | -3,216017 | 3,771514 | -2,564848 | C87 | 1,744624 | 4,677226 | -2,015476 |
| H88 | -1,470901 | 2,536644 | -2,259117 | H88 | 1,604079 | 2,535368 | -1,811644 |
| C89 | -4,264283 | 4,461779 | -1,952618 | C89 | 1,576531 | 5,913232 | -1,392087 |
| H90 | -5,187530 | 4,995948 | -0,078129 | H90 | 1,000739 | 6,922706 | 0,426909 |
| H91 | -3,124619 | 3,770741 | -3,647405 | H91 | 2,103075 | 4,627843 | -3,039582 |
| H92 | -4,991317 | 4,997147 | -2,556197 | H92 | 1,792903 | 6,831451 | -1,930231 |
| C93 | -2,069338 | 1,373048 | 3,527580 | C93 | -0,988452 | 2,236675 | 3,683775 |
| C94 | -0,020531 | 0,780498 | 2,680540 | C94 | 0,043969 | 0,333235 | 2,908198 |
| C95 | -1,068001 | 1,085416 | 4,656564 | C95 | -0,792624 | 1,216578 | 4,814844 |
| H96 | -3,040047 | 0,901017 | 3,681966 | H96 | -1,985230 | 2,678622 | 3,668672 |
| H97 | -2,223220 | 2,449446 | 3,365771 | H97 | -0,244580 | 3,045726 | 3,712420 |
| H98 | -1,006403 | 1,863886 | 5,416919 | H98 | -0,321846 | 1,622484 | 5,710269 |
| H99 | -1,250712 | 0,114678 | 5,128533 | H99 | -1,728991 | 0,715662 | 5,081658 |
| N100 | -1,343287 | 0,778175 | 2,396599 | N100 | -0,754382 | 1,364552 | 2,524922 |
| O101 | 0,219484 | 1,014942 | 3,976008 | O101 | 0,102043 | 0,222485 | 4,242407 |
| O102 | 0,887860 | 0,618303 | 1,848544 | O102 | 0,675679 | -0,406576 | 2,144371 |
| H103 | 4,703366 | 1,395318 | -2,353093 | H103 | 3,681303 | -3,280425 | -1,514458 |
| N104 | 1,169658 | -2,386403 | -1,314869 | N104 | -1,085086 | -2,285135 | -1,519589 |
| C105 | 1,451136 | -1,597058 | -2,540445 | C105 | -0,166208 | -1,887841 | -2,610269 |
| H106 | 0,528312 | -1,287902 | -3,053367 | H106 | -0,410488 | -0,899243 | -3,024358 |

Iso4

| | | | |
|----|-----------|-----------|-----------|
| C1 | -2,836136 | -2,994277 | -3,124542 |
| C2 | -0,450569 | -2,963668 | -3,644260 |
| C3 | -1,833267 | -2,668976 | -4,280964 |
| C4 | -1,884882 | -3,414609 | -1,979532 |
| H5 | -3,498509 | -3,826252 | -3,385556 |
| H6 | -1,914933 | -1,635029 | -4,631322 |

| | | | |
|------|-----------|-----------|-----------|
| H7 | -2,356025 | -3,925955 | -1,139378 |
| H8 | -3,462063 | -2,145142 | -2,849296 |
| H9 | 0,367323 | -3,086668 | -4,353920 |
| H10 | -1,991487 | -3,320158 | -5,145221 |
| C11 | -0,777723 | -4,170020 | -2,735348 |
| H12 | 0,050888 | -4,480338 | -2,091780 |
| H13 | -1,149393 | -5,032159 | -3,296011 |
| C14 | 1,222434 | -1,798046 | -2,055600 |
| N15 | 1,591139 | -1,119294 | -1,023561 |
| C16 | 3,085163 | -1,303914 | -0,838600 |
| C17 | 3,374985 | -2,412577 | -1,903151 |
| P18 | -1,512349 | -1,146720 | -0,278427 |
| Ir19 | 0,385131 | 0,355230 | 0,015098 |
| C20 | -1,759174 | -2,193443 | 1,195869 |
| C21 | -1,842191 | -3,619662 | 3,609432 |
| C22 | -1,065253 | -3,403670 | 1,328428 |
| C23 | -2,501900 | -1,707756 | 2,283579 |
| C24 | -2,542070 | -2,418204 | 3,481844 |
| C25 | -1,109920 | -4,112866 | 2,528905 |
| H26 | -3,053803 | -0,778735 | 2,189890 |
| H27 | -3,125487 | -2,037096 | 4,315687 |
| H28 | -0,569820 | -5,051091 | 2,619469 |
| H29 | -1,871682 | -4,170441 | 4,544929 |
| O30 | 2,153004 | -2,516198 | -2,685065 |
| C31 | 3,431866 | -1,877448 | 0,529428 |
| C32 | 2,462520 | -2,502201 | 1,315113 |
| C33 | 4,771822 | -1,921453 | 0,943624 |
| C34 | 2,809266 | -3,108498 | 2,521850 |
| H35 | 1,426669 | -2,489493 | 1,007157 |
| C36 | 5,120455 | -2,537190 | 2,144093 |
| H37 | 5,544465 | -1,464235 | 0,332374 |
| C38 | 4,137412 | -3,124466 | 2,943437 |
| H39 | 2,030365 | -3,556081 | 3,132705 |
| H40 | 6,160572 | -2,552496 | 2,456912 |
| H41 | 4,408855 | -3,592054 | 3,885554 |
| C42 | -3,161180 | -0,518910 | -0,748129 |
| C43 | -4,351369 | -1,160134 | -0,373554 |
| C44 | -3,199992 | 0,509402 | -1,701321 |
| C45 | -5,563476 | -0,769334 | -0,941032 |
| H46 | -4,335220 | -1,970438 | 0,347993 |
| C47 | -4,412078 | 0,890008 | -2,271523 |
| C48 | -5,594989 | 0,251682 | -1,892604 |
| H49 | -6,481759 | -1,269867 | -0,647230 |
| H50 | -4,435678 | 1,693868 | -3,000905 |
| H51 | -6,540056 | 0,550150 | -2,337131 |
| H52 | 0,123999 | 1,014749 | -1,373579 |
| H53 | 1,300700 | 2,218456 | 1,738425 |
| H54 | -0,481667 | -3,783790 | 0,495881 |

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|------|-----------|-----------|-----------|
| H55 | -2,282803 | 1,017716 | -1,982130 |
| H56 | 4,198267 | -2,176342 | -2,576931 |
| C57 | 4,861690 | 2,526948 | -1,860351 |
| C58 | 4,381949 | 1,675848 | -2,856953 |
| C59 | 3,832401 | 0,440389 | -2,516553 |
| C60 | 3,762625 | 0,027138 | -1,179094 |
| C61 | 4,225034 | 0,901022 | -0,185296 |
| C62 | 4,774442 | 2,138128 | -0,524585 |
| H63 | 5,287987 | 3,490745 | -2,122616 |
| H64 | 4,433255 | 1,973200 | -3,900497 |
| H65 | 3,444393 | -0,196141 | -3,307995 |
| H66 | 4,154411 | 0,615915 | 0,858308 |
| H67 | 5,126530 | 2,801523 | 0,259915 |
| C68 | -3,333282 | 3,848014 | -0,699825 |
| C69 | -2,107575 | 3,292534 | -0,340852 |
| C70 | -2,012999 | 2,397543 | 0,737557 |
| C71 | -3,201390 | 2,047870 | 1,401614 |
| C72 | -4,428979 | 2,592048 | 1,032392 |
| C73 | -4,500033 | 3,509328 | -0,013789 |
| H74 | -3,374321 | 4,547696 | -1,530091 |
| H75 | -1,227523 | 3,554685 | -0,910090 |
| H76 | -3,167602 | 1,330507 | 2,213504 |
| H77 | -5,328838 | 2,292690 | 1,562047 |
| H78 | -5,453296 | 3,943468 | -0,300625 |
| C79 | -0,713307 | 1,823017 | 1,205902 |
| C80 | 0,610364 | 2,326599 | 0,899325 |
| H81 | 1,825470 | 1,026720 | -0,007609 |
| C82 | 0,941900 | 3,540869 | 0,082884 |
| C83 | 0,641554 | 4,784539 | 0,661890 |
| C84 | 1,567600 | 3,509123 | -1,166016 |
| C85 | 0,940059 | 5,970062 | -0,004644 |
| H86 | 0,147672 | 4,818704 | 1,630193 |
| C87 | 1,869364 | 4,698634 | -1,832049 |
| H88 | 1,824146 | 2,556698 | -1,613793 |
| C89 | 1,551966 | 5,929622 | -1,259931 |
| H90 | 0,688676 | 6,923681 | 0,450897 |
| H91 | 2,356015 | 4,656683 | -2,802375 |
| H92 | 1,779603 | 6,852897 | -1,785106 |
| C93 | -1,034213 | 2,138634 | 3,742234 |
| C94 | 0,008614 | 0,257199 | 2,933546 |
| C95 | -0,849707 | 1,095411 | 4,852201 |
| H96 | -2,028107 | 2,587372 | 3,732191 |
| H97 | -0,282415 | 2,939368 | 3,785461 |
| H98 | -0,387717 | 1,481131 | 5,761044 |
| H99 | -1,787233 | 0,584716 | 5,094972 |
| N100 | -0,804562 | 1,285238 | 2,566529 |
| O101 | 0,054176 | 0,117640 | 4,265373 |
| O102 | 0,656841 | -0,458017 | 2,163041 |

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|------|-----------|-----------|-----------|
| H103 | 3,544406 | -3,383175 | -1,435082 |
| N104 | -1,099178 | -2,242343 | -1,501082 |
| C105 | -0,182291 | -1,853139 | -2,597381 |
| H106 | -0,411950 | -0,859171 | -3,006370 |

C3_ES_Cheltop

C3_ES_Cheltop_SM

| | | | |
|------|---------|----------|----------|
| C1 | -4.0724 | -3.51299 | 0.036369 |
| C2 | -1.8955 | -4.6104 | -0.0578 |
| C3 | -3.2708 | -4.58461 | -0.77373 |
| C4 | -3.0409 | -3.0685 | 1.099679 |
| H5 | -4.9481 | -3.95009 | 0.527236 |
| H6 | -3.1799 | -4.33063 | -1.83487 |
| H7 | -3.4541 | -2.50923 | 1.939156 |
| H8 | -4.4174 | -2.68016 | -0.57691 |
| H9 | -1.2803 | -5.48425 | -0.27085 |
| H10 | -3.7418 | -5.56971 | -0.7131 |
| C11 | -2.3053 | -4.38271 | 1.41487 |
| H12 | -1.4597 | -4.25058 | 2.09635 |
| H13 | -2.9662 | -5.16734 | 1.793514 |
| C14 | 0.2855 | -3.21475 | -0.07198 |
| N15 | 1.00283 | -2.14212 | -0.06856 |
| C16 | 2.36915 | -2.50715 | 0.481172 |
| C17 | 2.31978 | -4.05556 | 0.332861 |
| P18 | -1.8319 | -0.65359 | 0.136554 |
| Ir19 | 0.39762 | -0.21244 | -0.78742 |
| C20 | -2.0534 | 0.18371 | 1.747998 |
| C21 | -2.1596 | 1.602723 | 4.171654 |
| C22 | -1.8664 | -0.47916 | 2.967765 |
| C23 | -2.2946 | 1.568215 | 1.757012 |
| C24 | -2.3451 | 2.270794 | 2.959086 |
| C25 | -1.926 | 0.227567 | 4.170467 |
| H26 | -2.4684 | 2.096825 | 0.823661 |
| H27 | -2.5383 | 3.339764 | 2.949911 |
| H28 | -1.7927 | -0.3024 | 5.109459 |
| H29 | -2.2026 | 2.149461 | 5.108652 |
| O30 | 0.89751 | -4.35409 | 0.249968 |
| C31 | 2.45183 | -2.17837 | 1.977896 |
| C32 | 1.37517 | -1.6637 | 2.695179 |
| C33 | 3.64318 | -2.47288 | 2.659895 |
| C34 | 1.48863 | -1.41958 | 4.065322 |
| H35 | 0.45567 | -1.42313 | 2.184695 |
| C36 | 3.75582 | -2.23582 | 4.02645 |
| H37 | 4.49366 | -2.87101 | 2.112608 |
| C38 | 2.67593 | -1.70178 | 4.734896 |

C3_ES_Cheltop_INT2

| | | | |
|------|---------|----------|----------|
| C1 | -4.296 | -3.09198 | 0.982633 |
| C2 | -2.2841 | -4.45618 | 0.821148 |
| C3 | -3.7472 | -4.39582 | 0.316365 |
| C4 | -3.0709 | -2.59069 | 1.783265 |
| H5 | -5.1262 | -3.30296 | 1.664684 |
| H6 | -3.8076 | -4.36995 | -0.77618 |
| H7 | -3.2878 | -1.83811 | 2.541337 |
| H8 | -4.643 | -2.35523 | 0.258351 |
| H9 | -1.7969 | -5.42435 | 0.710107 |
| H10 | -4.2955 | -5.27988 | 0.653826 |
| C11 | -2.4264 | -3.90436 | 2.257373 |
| H12 | -1.4743 | -3.75305 | 2.775052 |
| H13 | -3.0917 | -4.51103 | 2.877991 |
| C14 | -0.0022 | -3.40527 | 0.212148 |
| N15 | 0.80884 | -2.43403 | -0.01197 |
| C16 | 2.19654 | -2.90991 | 0.332237 |
| C17 | 1.97075 | -4.45157 | 0.379789 |
| P18 | -1.7918 | -0.5564 | 0.233929 |
| Ir19 | 0.20783 | -0.45887 | -0.85362 |
| C20 | -1.8784 | 0.533078 | 1.699952 |
| C21 | -1.8774 | 2.251068 | 3.918953 |
| C22 | -1.4465 | 0.075739 | 2.953735 |
| C23 | -2.2857 | 1.870496 | 1.564177 |
| C24 | -2.2954 | 2.718936 | 2.671326 |
| C25 | -1.4459 | 0.930976 | 4.054683 |
| H26 | -2.6228 | 2.244792 | 0.602152 |
| H27 | -2.6435 | 3.742448 | 2.560719 |
| H28 | -1.1148 | 0.561978 | 5.020978 |
| H29 | -1.8942 | 2.910789 | 4.781901 |
| O30 | 0.52926 | -4.58752 | 0.54402 |
| C31 | 2.5885 | -2.42971 | 1.733473 |
| C32 | 1.70798 | -1.71826 | 2.546477 |
| C33 | 3.85136 | -2.7709 | 2.239724 |
| C34 | 2.08722 | -1.32248 | 3.829412 |
| H35 | 0.74018 | -1.43794 | 2.161025 |
| C36 | 4.22961 | -2.38392 | 3.522989 |
| H37 | 4.55006 | -3.32621 | 1.618962 |
| C38 | 3.34796 | -1.6513 | 4.322025 |

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|-----|---------|----------|----------|-----|---------|----------|----------|
| H39 | 0.64488 | -0.9919 | 4.598414 | H39 | 1.3961 | -0.74054 | 4.43307 |
| H40 | 4.6875 | -2.46151 | 4.537066 | H40 | 5.21459 | -2.64833 | 3.896729 |
| H41 | 2.76496 | -1.50769 | 5.799832 | H41 | 3.64663 | -1.34047 | 5.31905 |
| C42 | -3.3366 | -0.25293 | -0.82492 | C42 | -3.2935 | -0.16732 | -0.74574 |
| C43 | -4.5077 | 0.269182 | -0.25842 | C43 | -4.4733 | 0.284508 | -0.1253 |
| C44 | -3.3393 | -0.64039 | -2.17425 | C44 | -3.3284 | -0.48705 | -2.11096 |
| C45 | -5.6562 | 0.415519 | -1.03712 | C45 | -5.65 | 0.423664 | -0.85889 |
| H46 | -4.5322 | 0.553861 | 0.788137 | H46 | -4.4811 | 0.521324 | 0.933909 |
| C47 | -4.4888 | -0.49943 | -2.94592 | C47 | -4.5108 | -0.35291 | -2.84015 |
| C48 | -5.6489 | 0.03278 | -2.37867 | C48 | -5.6736 | 0.103163 | -2.21927 |
| H49 | -6.5594 | 0.822749 | -0.59161 | H49 | -6.5505 | 0.778504 | -0.36569 |
| H50 | -4.4744 | -0.78734 | -3.99244 | H50 | -4.5122 | -0.59018 | -3.89972 |
| H51 | -6.5449 | 0.148404 | -2.98167 | H51 | -6.5919 | 0.212335 | -2.78858 |
| H52 | 0.07278 | -0.86118 | -2.16901 | H52 | -0.555 | -1.17989 | -2.01873 |
| H53 | 1.90809 | -0.24684 | -1.26165 | H53 | 1.88357 | 2.066437 | -1.50151 |
| H54 | -1.6612 | -1.54403 | 2.982211 | H54 | -1.1179 | -0.95091 | 3.070574 |
| H55 | -2.4339 | -1.03695 | -2.62163 | H55 | -2.426 | -0.81333 | -2.61379 |
| H56 | 2.78496 | -4.43454 | -0.57938 | H56 | 2.24879 | -4.9714 | -0.54017 |
| C57 | 5.36018 | -0.5051 | -1.9464 | C57 | 4.5597 | -1.35704 | -2.95078 |
| C58 | 4.70474 | -1.63696 | -2.43238 | C58 | 3.69354 | -2.43533 | -3.14809 |
| C59 | 3.76353 | -2.29444 | -1.64176 | C59 | 2.98925 | -2.97099 | -2.07109 |
| C60 | 3.47169 | -1.84552 | -0.34648 | C60 | 3.1384 | -2.44621 | -0.77945 |
| C61 | 4.12651 | -0.70015 | 0.126049 | C61 | 4.00547 | -1.36318 | -0.59212 |
| C62 | 5.06208 | -0.03638 | -0.66684 | C62 | 4.71354 | -0.82563 | -1.67003 |
| H63 | 6.0927 | 0.008702 | -2.56228 | H63 | 5.10793 | -0.93597 | -3.78865 |
| H64 | 4.91611 | -2.00276 | -3.43288 | H64 | 3.55946 | -2.85438 | -4.14125 |
| H65 | 3.23529 | -3.14309 | -2.06502 | H65 | 2.285 | -3.77627 | -2.25852 |
| H66 | 3.89157 | -0.31695 | 1.112322 | H66 | 4.10684 | -0.91681 | 0.390129 |
| H67 | 5.561 | 0.848177 | -0.28036 | H67 | 5.38169 | 0.01528 | -1.50583 |
| C68 | 1.93349 | 1.965337 | -2.77994 | C68 | 0.9006 | 3.912055 | -1.96872 |
| C69 | 1.02357 | 1.732293 | -1.54504 | C69 | 0.90492 | 2.510067 | -1.28081 |
| C70 | -0.4129 | 1.716096 | -1.49386 | C70 | -0.2166 | 1.493179 | -1.67255 |
| C71 | 1.90531 | 3.837858 | -0.31361 | C71 | 0.55144 | 3.929205 | 0.961451 |
| C72 | 1.45963 | 1.912349 | 0.873904 | C72 | 1.18452 | 1.720334 | 1.055645 |
| C73 | 2.40814 | 3.951041 | 1.136305 | C73 | 1.12996 | 3.581632 | 2.342373 |
| H74 | 0.98897 | 4.416642 | -0.49282 | H74 | -0.5337 | 4.064278 | 0.998729 |
| H75 | 2.6623 | 4.142064 | -1.03811 | H75 | 1.00409 | 4.828546 | 0.544802 |
| H76 | 3.498 | 3.875966 | 1.199972 | H76 | 2.12813 | 4.004117 | 2.496873 |
| H77 | 2.06841 | 4.848112 | 1.654792 | H77 | 0.47448 | 3.857779 | 3.168377 |
| N78 | 1.62659 | 2.398673 | -0.37843 | N78 | 0.89963 | 2.719439 | 0.201999 |
| O79 | 1.83816 | 2.795953 | 1.808198 | O79 | 1.24665 | 2.1386 | 2.331739 |
| O80 | 1.01104 | 0.796259 | 1.159321 | O80 | 1.38949 | 0.52762 | 0.782372 |
| H81 | 2.7232 | -4.57591 | 1.19933 | H81 | 2.4523 | -4.92467 | 1.233927 |
| N82 | -1.9205 | -2.31229 | 0.468105 | N82 | -1.9946 | -2.11531 | 0.864439 |
| C83 | -1.185 | -3.27418 | -0.39165 | C83 | -1.5052 | -3.30924 | 0.124773 |

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|------|---------|----------|----------|------|---------|----------|----------|
| H84 | -1.2822 | -3.03959 | -1.46126 | H84 | -1.7551 | -3.26332 | -0.94538 |
| C85 | -3.1362 | 2.229675 | -4.78445 | C85 | -1.0422 | 1.173228 | -5.92307 |
| C86 | -3.2778 | 2.951964 | -3.60017 | C86 | -2.0173 | 1.621529 | -5.03434 |
| C87 | -2.3899 | 2.744747 | -2.54629 | C87 | -1.7262 | 1.734964 | -3.67359 |
| C88 | -1.3477 | 1.809618 | -2.64569 | C88 | -0.466 | 1.395222 | -3.15998 |
| C89 | -1.243 | 1.06398 | -3.829 | C89 | 0.50628 | 0.953458 | -4.07494 |
| C90 | -2.1161 | 1.282377 | -4.89112 | C90 | 0.22617 | 0.846751 | -5.43443 |
| H91 | -3.8223 | 2.392279 | -5.61051 | H91 | -1.262 | 1.084877 | -6.98299 |
| H92 | -4.0785 | 3.678302 | -3.49481 | H92 | -3.0067 | 1.889193 | -5.39599 |
| H93 | -2.5044 | 3.321872 | -1.63128 | H93 | -2.4964 | 2.08598 | -2.99232 |
| H94 | -0.4953 | 0.287295 | -3.90029 | H94 | 1.50704 | 0.712717 | -3.72822 |
| H95 | -2.0095 | 0.697646 | -5.80077 | H95 | 1.00176 | 0.511658 | -6.11771 |
| H96 | -0.8069 | 2.234557 | -0.62012 | H96 | -1.1348 | 1.888391 | -1.22404 |
| C97 | 2.18427 | 0.805459 | -3.75435 | C97 | 1.54501 | 3.922157 | -3.36618 |
| H98 | 3.00212 | 1.089173 | -4.42542 | H98 | 1.74703 | 4.957562 | -3.66039 |
| H99 | 2.47506 | -0.10467 | -3.2305 | H99 | 2.49809 | 3.38187 | -3.37756 |
| H100 | 1.31774 | 0.591059 | -4.37995 | H100 | 0.89757 | 3.481589 | -4.12383 |
| C101 | 1.49124 | 3.221134 | -3.56327 | C101 | -0.4781 | 4.590549 | -2.02084 |
| H102 | 2.28103 | 3.519195 | -4.25978 | H102 | -0.3691 | 5.637388 | -2.32172 |
| H103 | 0.58888 | 3.020677 | -4.14375 | H103 | -1.1172 | 4.100269 | -2.75763 |
| H104 | 1.27717 | 4.075145 | -2.91508 | H104 | -1.0058 | 4.576261 | -1.06305 |
| H105 | 2.91225 | 2.168069 | -2.32793 | H105 | 1.56698 | 4.527413 | -1.35049 |
| X | 0.28333 | 1.758175 | -1.43512 | H106 | 1.87986 | -0.2998 | -1.55546 |
| | | | | H107 | 1.43672 | -0.66616 | -2.13286 |

C3_ES_Cheltop_TS1

| | | | |
|------|---------|----------|----------|
| C1 | -3.9716 | -3.84047 | -0.22732 |
| C2 | -1.7434 | -4.82485 | -0.09421 |
| C3 | -3.0499 | -4.89436 | -0.927 |
| C4 | -3.0726 | -3.33449 | 0.924586 |
| H5 | -4.8806 | -4.29993 | 0.174117 |
| H6 | -2.8789 | -4.67259 | -1.98543 |
| H7 | -3.5945 | -2.78729 | 1.709782 |
| H8 | -4.2737 | -3.02599 | -0.88813 |
| H9 | -1.061 | -5.66305 | -0.23328 |
| H10 | -3.476 | -5.89997 | -0.86912 |
| C11 | -2.2984 | -4.60056 | 1.330739 |
| H12 | -1.5272 | -4.40965 | 2.08309 |
| H13 | -2.9452 | -5.41734 | 1.663052 |
| C14 | 0.35836 | -3.29588 | -0.00243 |
| N15 | 0.99191 | -2.17409 | 0.02348 |
| C16 | 2.36691 | -2.43008 | 0.588551 |
| C17 | 2.43741 | -3.98411 | 0.464518 |
| P18 | -1.8699 | -0.85554 | 0.159474 |
| Ir19 | 0.21484 | -0.29456 | -0.75023 |
| C20 | -2.0886 | -0.11032 | 1.817309 |

C3_ES_Cheltop_TS3

| | | | |
|------|---------|----------|----------|
| C1 | -4.2969 | -3.17722 | 0.770562 |
| C2 | -2.2627 | -4.5163 | 0.671137 |
| C3 | -3.697 | -4.45095 | 0.088825 |
| C4 | -3.1256 | -2.69894 | 1.662421 |
| H5 | -5.1655 | -3.42072 | 1.391329 |
| H6 | -3.6985 | -4.38606 | -1.00388 |
| H7 | -3.3927 | -1.97884 | 2.436389 |
| H8 | -4.6052 | -2.41508 | 0.054253 |
| H9 | -1.7576 | -5.47402 | 0.548636 |
| H10 | -4.2524 | -5.35222 | 0.363885 |
| C11 | -2.4933 | -4.02561 | 2.118346 |
| H12 | -1.5739 | -3.88736 | 2.694892 |
| H13 | -3.1851 | -4.66536 | 2.673612 |
| C14 | 0.02766 | -3.39217 | 0.223953 |
| N15 | 0.84302 | -2.41704 | 0.001216 |
| C16 | 2.22063 | -2.85388 | 0.451641 |
| C17 | 2.00124 | -4.39214 | 0.574999 |
| P18 | -1.7776 | -0.60947 | 0.230384 |
| Ir19 | 0.34883 | -0.55441 | -0.93573 |

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|-----|---------|----------|----------|-----|---------|----------|----------|
| C21 | -2.2847 | 1.161643 | 4.311486 | C20 | -1.8999 | 0.466114 | 1.704466 |
| C22 | -2.0581 | -0.86154 | 2.998594 | C21 | -1.8669 | 2.193601 | 3.921646 |
| C23 | -2.1996 | 1.287729 | 1.898078 | C22 | -1.5333 | -0.00759 | 2.973085 |
| C24 | -2.2986 | 1.917674 | 3.136015 | C23 | -2.2446 | 1.821271 | 1.560673 |
| C25 | -2.1624 | -0.22611 | 4.23858 | C24 | -2.2346 | 2.675238 | 2.663863 |
| H26 | -2.2171 | 1.88275 | 0.988634 | C25 | -1.5161 | 0.851101 | 4.071213 |
| H27 | -2.3876 | 2.999155 | 3.18524 | H26 | -2.5574 | 2.206711 | 0.594505 |
| H28 | -2.1467 | -0.82065 | 5.147644 | H27 | -2.532 | 3.713673 | 2.542584 |
| H29 | -2.3653 | 1.652995 | 5.276446 | H28 | -1.2386 | 0.466128 | 5.048259 |
| O30 | 1.04446 | -4.39188 | 0.329487 | H29 | -1.8676 | 2.856944 | 4.781884 |
| C31 | 2.41909 | -2.05501 | 2.073619 | O30 | 0.55416 | -4.53716 | 0.655517 |
| C32 | 1.32909 | -1.51875 | 2.755174 | C31 | 2.52175 | -2.30706 | 1.853458 |
| C33 | 3.60457 | -2.30859 | 2.782131 | C32 | 1.59517 | -1.56411 | 2.580919 |
| C34 | 1.42384 | -1.21525 | 4.115006 | C33 | 3.75018 | -2.62674 | 2.450624 |
| H35 | 0.41065 | -1.31082 | 2.228522 | C34 | 1.8934 | -1.1173 | 3.868419 |
| C36 | 3.69923 | -2.01125 | 4.138392 | H35 | 0.65276 | -1.29968 | 2.128198 |
| H37 | 4.4656 | -2.72241 | 2.262148 | C36 | 4.048 | -2.19009 | 3.738933 |
| C38 | 2.60593 | -1.45684 | 4.809953 | H37 | 4.48606 | -3.20322 | 1.89611 |
| H39 | 0.56648 | -0.77921 | 4.61894 | C38 | 3.11953 | -1.42693 | 4.45214 |
| H40 | 4.62609 | -2.20695 | 4.669889 | H39 | 1.16707 | -0.51052 | 4.401548 |
| H41 | 2.67987 | -1.21718 | 5.866859 | H40 | 5.00748 | -2.4393 | 4.183255 |
| C42 | -3.3695 | -0.37018 | -0.76992 | H41 | 3.35581 | -1.07727 | 5.453192 |
| C43 | -4.4969 | 0.209728 | -0.17081 | C42 | -3.254 | -0.20105 | -0.77829 |
| C44 | -3.4003 | -0.67598 | -2.13931 | C43 | -4.4454 | 0.282086 | -0.20825 |
| C45 | -5.6279 | 0.493786 | -0.93698 | C44 | -3.2433 | -0.55299 | -2.1366 |
| H46 | -4.4984 | 0.441256 | 0.888989 | C45 | -5.5944 | 0.415703 | -0.98481 |
| C47 | -4.5328 | -0.39683 | -2.89852 | H46 | -4.483 | 0.544322 | 0.84443 |
| C48 | -5.6469 | 0.194288 | -2.29907 | C47 | -4.3996 | -0.43135 | -2.90712 |
| H49 | -6.4953 | 0.947555 | -0.46613 | C48 | -5.5748 | 0.054631 | -2.33502 |
| H50 | -4.5371 | -0.61909 | -3.96082 | H49 | -6.5082 | 0.792762 | -0.53406 |
| H51 | -6.5271 | 0.421404 | -2.89347 | H50 | -4.3718 | -0.69657 | -3.95962 |
| H52 | -0.1712 | -1.04069 | -2.06716 | H51 | -6.4736 | 0.15507 | -2.93688 |
| H53 | 1.70962 | 0.029888 | -1.39183 | H52 | -0.3351 | -1.35333 | -2.08891 |
| H54 | -1.9303 | -1.9377 | 2.957132 | H53 | 1.9093 | 2.047066 | -1.57735 |
| H55 | -2.5286 | -1.11529 | -2.61208 | H54 | -1.2634 | -1.04978 | 3.102968 |
| H56 | 2.96926 | -4.33648 | -0.42227 | H55 | -2.3254 | -0.90007 | -2.59754 |
| C57 | 5.22545 | -0.28049 | -1.87891 | H56 | 2.33884 | -4.96377 | -0.2917 |
| C58 | 4.58167 | -1.41767 | -2.37027 | C57 | 4.9915 | -1.65554 | -2.66098 |
| C59 | 3.67651 | -2.11074 | -1.5688 | C58 | 4.11707 | -2.72466 | -2.86615 |
| C60 | 3.41081 | -1.69616 | -0.25613 | C59 | 3.25457 | -3.12462 | -1.84803 |
| C61 | 4.04682 | -0.54245 | 0.219896 | C60 | 3.25447 | -2.47267 | -0.60679 |
| C62 | 4.94723 | 0.157656 | -0.58433 | C61 | 4.12044 | -1.38986 | -0.41773 |
| H63 | 5.93625 | 0.256804 | -2.50039 | C62 | 4.98543 | -0.98797 | -1.43605 |
| H64 | 4.77694 | -1.76097 | -3.38186 | H63 | 5.66776 | -1.34363 | -3.452 |
| H65 | 3.15795 | -2.9677 | -1.98837 | H64 | 4.10185 | -3.24424 | -3.81998 |

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|--------------------|---------|----------|----------|--------------------|---------|----------|----------|
| H66 | 3.83825 | -0.18886 | 1.223246 | H65 | 2.55447 | -3.93056 | -2.04795 |
| H67 | 5.44019 | 1.043113 | -0.19106 | H66 | 4.10263 | -0.84298 | 0.517314 |
| C68 | 2.0338 | 1.6051 | -3.00445 | H67 | 5.65427 | -0.14781 | -1.27046 |
| C69 | 1.18782 | 1.494998 | -1.70724 | C68 | 1.04971 | 3.919447 | -2.09962 |
| C70 | -0.2759 | 1.612147 | -1.58891 | C69 | 0.96041 | 2.551368 | -1.36479 |
| C71 | 2.47026 | 3.511606 | -0.65039 | C70 | -0.21 | 1.553455 | -1.70808 |
| C72 | 1.61071 | 1.840935 | 0.690614 | C71 | 0.56876 | 3.95237 | 0.859355 |
| C73 | 2.9891 | 3.632853 | 0.791963 | C72 | 1.26956 | 1.753956 | 0.95501 |
| H74 | 1.70199 | 4.260161 | -0.8841 | C73 | 1.13553 | 3.612246 | 2.248243 |
| H75 | 3.27423 | 3.584578 | -1.38389 | H74 | -0.5221 | 4.051729 | 0.878148 |
| H76 | 4.03148 | 3.311369 | 0.880791 | H75 | 1.00098 | 4.867278 | 0.452636 |
| H77 | 2.86862 | 4.626473 | 1.224117 | H76 | 2.11767 | 4.06476 | 2.418486 |
| N78 | 1.88932 | 2.165835 | -0.59849 | H77 | 0.45931 | 3.863606 | 3.065402 |
| O79 | 2.16814 | 2.705323 | 1.549753 | N78 | 0.9749 | 2.762593 | 0.104361 |
| O80 | 0.93699 | 0.876355 | 1.067473 | O79 | 1.29638 | 2.173504 | 2.233194 |
| H81 | 2.84166 | -4.46317 | 1.354248 | O80 | 1.50393 | 0.574799 | 0.668829 |
| N82 | -1.9461 | -2.52795 | 0.378479 | H81 | 2.43029 | -4.80858 | 1.484463 |
| C83 | -1.0877 | -3.45325 | -0.40004 | N82 | -2.0064 | -2.17609 | 0.828351 |
| H84 | -1.1262 | -3.24292 | -1.47882 | C83 | -1.4686 | -3.33114 | 0.061657 |
| C85 | -3.0469 | 2.291296 | -4.82306 | H84 | -1.667 | -3.24417 | -1.01618 |
| C86 | -3.0363 | 3.103206 | -3.68948 | C85 | -2.1183 | 1.710536 | -5.59002 |
| C87 | -2.1341 | 2.851538 | -2.65689 | C86 | -2.7241 | 2.279431 | -4.47034 |
| C88 | -1.2321 | 1.777746 | -2.72055 | C87 | -2.0957 | 2.21098 | -3.22749 |
| C89 | -1.2909 | 0.943001 | -3.84653 | C88 | -0.8467 | 1.593212 | -3.0773 |
| C90 | -2.1698 | 1.207523 | -4.8938 | C89 | -0.2611 | 1.004428 | -4.2079 |
| H91 | -3.7395 | 2.491665 | -5.63531 | C90 | -0.8853 | 1.067274 | -5.4524 |
| H92 | -3.7251 | 3.939541 | -3.61036 | H91 | -2.6066 | 1.754475 | -6.55948 |
| H93 | -2.124 | 3.50449 | -1.78674 | H92 | -3.694 | 2.760861 | -4.55748 |
| H94 | -0.6633 | 0.062566 | -3.88473 | H93 | -2.5906 | 2.632302 | -2.35614 |
| H95 | -2.1837 | 0.551273 | -5.76007 | H94 | 0.68585 | 0.478613 | -4.11404 |
| H96 | -0.547 | 2.28378 | -0.77153 | H95 | -0.4125 | 0.606637 | -6.31516 |
| C97 | 2.01109 | 0.40436 | -3.96409 | H96 | -0.9951 | 1.774794 | -0.98674 |
| H98 | 2.89172 | 0.458274 | -4.6119 | C97 | 1.64794 | 3.774623 | -3.50914 |
| H99 | 2.04447 | -0.54517 | -3.42681 | H98 | 1.86282 | 4.76653 | -3.91949 |
| H100 | 1.13408 | 0.415496 | -4.61069 | H99 | 2.58708 | 3.210564 | -3.49326 |
| C101 | 1.70977 | 2.89827 | -3.78073 | H100 | 0.96012 | 3.274521 | -4.19256 |
| H102 | 2.44062 | 3.03112 | -4.58456 | C101 | -0.2393 | 4.758856 | -2.15478 |
| H103 | 0.71803 | 2.837916 | -4.2325 | H102 | 0.01023 | 5.798225 | -2.39101 |
| H104 | 1.73472 | 3.796926 | -3.15982 | H103 | -0.907 | 4.395999 | -2.93674 |
| H105 | 3.0639 | 1.659055 | -2.63114 | H104 | -0.8024 | 4.760881 | -1.21759 |
| X | 0.28333 | 1.758175 | -1.43512 | H105 | 1.79522 | 4.478239 | -1.51703 |
| | | | | H106 | 1.73418 | -0.76873 | -1.72083 |
| | | | | H107 | 0.80616 | 0.406179 | -2.08986 |
| C3_ES_Cheltop_INT1 | | | | C3_ES_Cheltop_PROD | | | |
| C1 | -4.2887 | -3.09818 | 0.869072 | | | | |
| C2 | -2.2605 | -4.44892 | 0.851244 | | | | |

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|------|---------|----------|----------|------|---------|----------|----------|
| C3 | -3.712 | -4.44089 | 0.309091 | C1 | -4.2226 | -3.44318 | 0.909874 |
| C4 | -3.0956 | -2.54123 | 1.682443 | C2 | -2.1136 | -4.6673 | 0.87345 |
| H5 | -5.1478 | -3.26836 | 1.526023 | C3 | -3.5567 | -4.72665 | 0.312056 |
| H6 | -3.747 | -4.49469 | -0.78348 | C4 | -3.0717 | -2.83842 | 1.747925 |
| H7 | -3.3427 | -1.74932 | 2.389882 | H5 | -5.0735 | -3.68934 | 1.553586 |
| H8 | -4.6024 | -2.4071 | 0.084879 | H6 | -3.5755 | -4.74437 | -0.78215 |
| H9 | -1.7538 | -5.41309 | 0.805324 | H7 | -3.3704 | -2.08059 | 2.473023 |
| H10 | -4.2598 | -5.30432 | 0.697088 | H8 | -4.5737 | -2.74775 | 0.145653 |
| C11 | -2.449 | -3.81708 | 2.248336 | H9 | -1.5561 | -5.60142 | 0.810693 |
| H12 | -1.5144 | -3.6214 | 2.783 | H10 | -4.0542 | -5.63543 | 0.662617 |
| H13 | -3.1238 | -4.39762 | 2.883751 | C11 | -2.3546 | -4.08876 | 2.286179 |
| C14 | 0.01735 | -3.40518 | 0.187164 | H12 | -1.4374 | -3.85433 | 2.834697 |
| N15 | 0.78625 | -2.38156 | 0.11211 | H13 | -2.9979 | -4.72758 | 2.897866 |
| C16 | 2.19563 | -2.82656 | 0.311455 | C14 | 0.10437 | -3.45875 | 0.31115 |
| C17 | 2.03718 | -4.35243 | 0.033904 | N15 | 0.88217 | -2.47209 | -0.00108 |
| P18 | -1.7689 | -0.56058 | 0.109939 | C16 | 2.27999 | -2.80503 | 0.503924 |
| Ir19 | 0.24654 | -0.46169 | -0.72223 | C17 | 2.13293 | -4.34277 | 0.657935 |
| C20 | -1.8838 | 0.589153 | 1.525037 | P18 | -1.83 | -0.7752 | 0.167791 |
| C21 | -1.7337 | 2.453166 | 3.618267 | Ir19 | 0.29932 | -0.75864 | -0.95688 |
| C22 | -1.4461 | 0.194344 | 2.797795 | C20 | -1.9933 | 0.383525 | 1.579379 |
| C23 | -2.2315 | 1.933685 | 1.30663 | C21 | -1.9587 | 2.28838 | 3.649577 |
| C24 | -2.1616 | 2.856345 | 2.350502 | C22 | -1.6122 | 0.019712 | 2.878895 |
| C25 | -1.3769 | 1.121446 | 3.836931 | C23 | -2.361 | 1.718558 | 1.332848 |
| H26 | -2.5721 | 2.256652 | 0.327216 | C24 | -2.3421 | 2.662481 | 2.359841 |
| H27 | -2.4539 | 3.888127 | 2.174886 | C25 | -1.5981 | 0.964542 | 3.9045 |
| H28 | -1.042 | 0.802343 | 4.819226 | H26 | -2.702 | 2.014873 | 0.344499 |
| H29 | -1.687 | 3.170824 | 4.43206 | H27 | -2.6506 | 3.684987 | 2.156997 |
| O30 | 0.61293 | -4.60071 | 0.276796 | H28 | -1.3116 | 0.662647 | 4.907954 |
| C31 | 2.60818 | -2.59932 | 1.768861 | H29 | -1.9563 | 3.019468 | 4.453202 |
| C32 | 1.80981 | -1.87379 | 2.655348 | O30 | 0.69735 | -4.54033 | 0.816277 |
| C33 | 3.81001 | -3.1499 | 2.234439 | C31 | 2.50009 | -2.2213 | 1.90987 |
| C34 | 2.20688 | -1.69649 | 3.981142 | C32 | 1.50297 | -1.55338 | 2.616415 |
| H35 | 0.89452 | -1.4226 | 2.300153 | C33 | 3.73739 | -2.44 | 2.535502 |
| C36 | 4.20715 | -2.97452 | 3.558416 | C34 | 1.73943 | -1.08023 | 3.908242 |
| H37 | 4.45031 | -3.70844 | 1.555879 | H35 | 0.55062 | -1.3664 | 2.145425 |
| C38 | 3.4042 | -2.24514 | 4.43809 | C36 | 3.97275 | -1.97796 | 3.82831 |
| H39 | 1.57863 | -1.11935 | 4.65434 | H37 | 4.5284 | -2.95766 | 1.998687 |
| H40 | 5.14249 | -3.40626 | 3.902484 | C38 | 2.97322 | -1.28851 | 4.520964 |
| H41 | 3.7122 | -2.10717 | 5.470548 | H39 | 0.9562 | -0.53256 | 4.424139 |
| C42 | -3.1978 | -0.20304 | -0.96946 | H40 | 4.93981 | -2.15053 | 4.292156 |
| C43 | -4.4048 | 0.27124 | -0.42185 | H41 | 3.15949 | -0.91898 | 5.525171 |
| C44 | -3.1535 | -0.55379 | -2.327 | C42 | -3.3052 | -0.38891 | -0.85908 |
| C45 | -5.5367 | 0.399286 | -1.22337 | C43 | -4.5464 | -0.05935 | -0.28438 |
| H46 | -4.4654 | 0.534278 | 0.629909 | C44 | -3.2055 | -0.47118 | -2.25575 |
| C47 | -4.2928 | -0.43061 | -3.12122 | C45 | -5.6569 | 0.180191 | -1.09075 |

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|-----|---------|----------|----------|-----|---------|----------|----------|
| C48 | -5.4827 | 0.046799 | -2.57403 | H46 | -4.6427 | 0.018874 | 0.795126 |
| H49 | -6.4615 | 0.771322 | -0.79202 | C47 | -4.3191 | -0.22718 | -3.06176 |
| H50 | -4.2379 | -0.68898 | -4.17406 | C48 | -5.5456 | 0.097778 | -2.48289 |
| H51 | -6.3667 | 0.148412 | -3.19657 | H49 | -6.6094 | 0.434081 | -0.63393 |
| H52 | -0.4056 | -1.18071 | -1.94516 | H50 | -4.218 | -0.27412 | -4.14182 |
| H53 | 2.19711 | 1.507362 | -1.53638 | H51 | -6.4115 | 0.291187 | -3.10932 |
| H54 | -1.1575 | -0.8371 | 2.972243 | H52 | -0.2991 | -1.64707 | -2.0953 |
| H55 | -2.2247 | -0.89347 | -2.77046 | H53 | 1.95181 | 1.709941 | -1.61163 |
| H56 | 2.24539 | -4.62643 | -1.00474 | H54 | -1.328 | -1.00509 | 3.091615 |
| C57 | 4.3878 | -0.50862 | -2.6467 | H55 | -2.2516 | -0.70747 | -2.71474 |
| C58 | 3.36216 | -1.3746 | -3.03228 | H56 | 2.44209 | -4.91357 | -0.22007 |
| C59 | 2.69127 | -2.13721 | -2.07366 | C57 | 5.1334 | -1.47704 | -2.47679 |
| C60 | 3.048 | -2.06419 | -0.71456 | C58 | 4.38666 | -2.63666 | -2.68828 |
| C61 | 4.07857 | -1.19608 | -0.34102 | C59 | 3.49146 | -3.07853 | -1.71592 |
| C62 | 4.7426 | -0.42741 | -1.29907 | C60 | 3.33395 | -2.37774 | -0.51358 |
| H63 | 4.9086 | 0.087731 | -3.39016 | C61 | 4.07319 | -1.2048 | -0.3196 |
| H64 | 3.08076 | -1.45922 | -4.07807 | C62 | 4.96857 | -0.76072 | -1.29114 |
| H65 | 1.87816 | -2.78446 | -2.3892 | H63 | 5.83474 | -1.1336 | -3.23214 |
| H66 | 4.34905 | -1.0986 | 0.703146 | H64 | 4.4957 | -3.19625 | -3.61283 |
| H67 | 5.53877 | 0.24223 | -0.98656 | H65 | 2.89333 | -3.95946 | -1.92725 |
| C68 | 1.73891 | 3.446856 | -2.29745 | H66 | 3.93053 | -0.62396 | 0.583503 |
| C69 | 1.35772 | 2.207514 | -1.42684 | H67 | 5.53817 | 0.148754 | -1.12023 |
| C70 | 0.01132 | 1.44765 | -1.67268 | C68 | 1.55821 | 3.682572 | -2.30062 |
| C71 | 0.95755 | 3.875681 | 0.593364 | C69 | 1.13433 | 2.426881 | -1.49399 |
| C72 | 1.47698 | 1.674373 | 0.972223 | C70 | -0.1853 | 1.64719 | -1.86493 |
| C73 | 1.35276 | 3.65142 | 2.06242 | C71 | 0.69355 | 3.935947 | 0.633225 |
| H74 | -0.1254 | 4.004701 | 0.475823 | C72 | 1.22131 | 1.698357 | 0.854679 |
| H75 | 1.46985 | 4.731639 | 0.152773 | C73 | 1.10604 | 3.605285 | 2.078696 |
| H76 | 2.34374 | 4.054454 | 2.292877 | H74 | -0.3903 | 4.084448 | 0.539147 |
| H77 | 0.61816 | 4.025331 | 2.77545 | H75 | 1.20954 | 4.816931 | 0.248842 |
| N78 | 1.39728 | 2.605518 | 0.006932 | H76 | 2.09882 | 3.995537 | 2.324011 |
| O79 | 1.40956 | 2.207839 | 2.201961 | H77 | 0.37937 | 3.927256 | 2.824517 |
| O80 | 1.60127 | 0.446749 | 0.812955 | N78 | 1.11838 | 2.709479 | -0.04458 |
| H81 | 2.60273 | -4.98606 | 0.713875 | O79 | 1.16556 | 2.158513 | 2.116751 |
| N82 | -2.0016 | -2.10573 | 0.765805 | O80 | 1.35567 | 0.496284 | 0.615768 |
| C83 | -1.4853 | -3.33066 | 0.103218 | H81 | 2.62519 | -4.72899 | 1.54824 |
| H84 | -1.7293 | -3.35541 | -0.97057 | N82 | -2.0041 | -2.31227 | 0.855074 |
| C85 | -1.2722 | 0.973297 | -5.78468 | C83 | -1.3976 | -3.48474 | 0.168485 |
| C86 | -2.0209 | 1.737683 | -4.8916 | H84 | -1.609 | -3.48841 | -0.91022 |
| C87 | -1.5912 | 1.89701 | -3.57252 | C85 | -2.7345 | 2.650835 | -5.19567 |
| C88 | -0.4063 | 1.305098 | -3.1136 | C86 | -3.0151 | 3.136699 | -3.91728 |
| C89 | 0.33495 | 0.538516 | -4.0288 | C87 | -2.1807 | 2.810211 | -2.85106 |
| C90 | -0.0884 | 0.37327 | -5.34475 | C88 | -1.0497 | 2.00881 | -3.04858 |
| H91 | -1.603 | 0.846689 | -6.81145 | C89 | -0.7881 | 1.506574 | -4.32832 |
| H92 | -2.9452 | 2.208055 | -5.21639 | C90 | -1.6225 | 1.830979 | -5.39815 |

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|-------------------|---------|----------|----------|------|---------|----------|----------|
| H93 | -2.1925 | 2.484682 | -2.88235 | H91 | -3.3856 | 2.901023 | -6.02817 |
| H94 | 1.2536 | 0.067191 | -3.69478 | H92 | -3.8886 | 3.759775 | -3.749 |
| H95 | 0.50584 | -0.22291 | -6.03247 | H93 | -2.4071 | 3.183842 | -1.85502 |
| H96 | -0.7573 | 2.050167 | -1.1726 | H94 | 0.06227 | 0.846359 | -4.48388 |
| C97 | 2.46702 | 3.049723 | -3.59239 | H95 | -1.4087 | 1.437376 | -6.38757 |
| H98 | 2.88561 | 3.942112 | -4.06913 | H96 | -0.8217 | 1.674974 | -0.98522 |
| H99 | 3.2926 | 2.357658 | -3.39165 | C97 | 2.19618 | 3.280483 | -3.64076 |
| H100 | 1.79227 | 2.575037 | -4.30616 | H98 | 2.59896 | 4.166252 | -4.14209 |
| C101 | 0.58469 | 4.413211 | -2.61118 | H99 | 3.01717 | 2.568907 | -3.50215 |
| H102 | 0.98401 | 5.348959 | -3.01587 | H100 | 1.46075 | 2.830635 | -4.31243 |
| H103 | -0.085 | 3.986989 | -3.35987 | C101 | 0.48917 | 4.767987 | -2.52982 |
| H104 | -0.0208 | 4.664822 | -1.73582 | H102 | 0.9802 | 5.715454 | -2.77394 |
| H105 | 2.48301 | 3.98452 | -1.69237 | H103 | -0.1631 | 4.511255 | -3.36524 |
| X | 0.28333 | 1.758175 | -1.43512 | H104 | -0.1515 | 4.942863 | -1.66137 |
| C3_ES_Cheltop_TS2 | | | | H105 | 2.3607 | 4.120634 | -1.69076 |
| C1 | -4.297 | -3.13353 | 0.572658 | H106 | 1.66898 | -0.82986 | -1.79182 |
| C2 | -2.261 | -4.47681 | 0.547246 | H107 | 0.1548 | 0.579674 | -2.16827 |
| C3 | -3.6737 | -4.40787 | -0.08718 | | | | |
| C4 | -3.1563 | -2.65575 | 1.502212 | | | | |
| H5 | -5.185 | -3.37673 | 1.165185 | | | | |
| H6 | -3.6346 | -4.34135 | -1.17904 | | | | |
| H7 | -3.4472 | -1.93238 | 2.264404 | | | | |
| H8 | -4.5822 | -2.37148 | -0.15352 | | | | |
| H9 | -1.7548 | -5.43618 | 0.445561 | | | | |
| H10 | -4.2411 | -5.30804 | 0.16545 | | | | |
| C11 | -2.5422 | -3.98184 | 1.983488 | | | | |
| H12 | -1.6435 | -3.84445 | 2.592057 | | | | |
| H13 | -3.255 | -4.61759 | 2.516006 | | | | |
| C14 | 0.05239 | -3.3602 | 0.183945 | | | | |
| N15 | 0.85883 | -2.37189 | 0.013934 | | | | |
| C16 | 2.22965 | -2.81867 | 0.447998 | | | | |
| C17 | 2.01637 | -4.36618 | 0.561849 | | | | |
| P18 | -1.7687 | -0.5562 | 0.167501 | | | | |
| Ir19 | 0.19377 | -0.39543 | -0.80124 | | | | |
| C20 | -1.8301 | 0.451363 | 1.692376 | | | | |
| C21 | -1.7448 | 2.039978 | 4.003726 | | | | |
| C22 | -1.4901 | -0.11299 | 2.9305 | | | | |
| C23 | -2.1173 | 1.824591 | 1.622403 | | | | |
| C24 | -2.0839 | 2.60993 | 2.773907 | | | | |
| C25 | -1.4456 | 0.678874 | 4.077815 | | | | |
| H26 | -2.3883 | 2.278589 | 0.674003 | | | | |
| H27 | -2.3342 | 3.665761 | 2.712956 | | | | |
| H28 | -1.186 | 0.228186 | 5.031213 | | | | |
| H29 | -1.7241 | 2.652354 | 4.900684 | | | | |

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|-----|---------|----------|----------|
| O30 | 0.56974 | -4.52575 | 0.58197 |
| C31 | 2.56953 | -2.26758 | 1.835551 |
| C32 | 1.70509 | -1.43373 | 2.541956 |
| C33 | 3.76833 | -2.66539 | 2.446553 |
| C34 | 2.03512 | -0.98152 | 3.819648 |
| H35 | 0.78722 | -1.10609 | 2.079702 |
| C36 | 4.1 | -2.21866 | 3.723263 |
| H37 | 4.45691 | -3.31544 | 1.912834 |
| C38 | 3.23308 | -1.3695 | 4.415003 |
| H39 | 1.35517 | -0.3098 | 4.335723 |
| H40 | 5.03709 | -2.53026 | 4.17544 |
| H41 | 3.49434 | -1.01483 | 5.407901 |
| C42 | -3.2653 | -0.1181 | -0.79062 |
| C43 | -4.3998 | 0.435964 | -0.17241 |
| C44 | -3.3588 | -0.55733 | -2.12047 |
| C45 | -5.5955 | 0.559855 | -0.87831 |
| H46 | -4.3631 | 0.756535 | 0.863112 |
| C47 | -4.5608 | -0.44506 | -2.81636 |
| C48 | -5.6797 | 0.115874 | -2.19942 |
| H49 | -6.4639 | 0.994379 | -0.39157 |
| H50 | -4.6142 | -0.77857 | -3.84815 |
| H51 | -6.6143 | 0.208069 | -2.74506 |
| H52 | -0.5612 | -1.11977 | -1.95976 |
| H53 | 1.80926 | 2.099095 | -1.7609 |
| H54 | -1.2572 | -1.17014 | 2.995755 |
| H55 | -2.4877 | -0.96664 | -2.61967 |
| H56 | 2.39973 | -4.92418 | -0.29542 |
| C57 | 4.98382 | -1.82318 | -2.75871 |
| C58 | 3.9189 | -2.70024 | -2.97358 |
| C59 | 3.05283 | -3.0113 | -1.92794 |
| C60 | 3.23588 | -2.46174 | -0.65006 |
| C61 | 4.29033 | -1.56665 | -0.4507 |
| C62 | 5.16064 | -1.25425 | -1.49855 |
| H63 | 5.66373 | -1.57985 | -3.57007 |
| H64 | 3.76037 | -3.1391 | -3.95453 |
| H65 | 2.21237 | -3.67303 | -2.12049 |
| H66 | 4.42853 | -1.09801 | 0.516123 |
| H67 | 5.97765 | -0.55952 | -1.32523 |
| C68 | 0.78369 | 3.955274 | -2.06348 |
| C69 | 0.87697 | 2.545255 | -1.39924 |
| C70 | -0.2934 | 1.53335 | -1.63383 |
| C71 | 0.69693 | 3.853125 | 0.91878 |
| C72 | 1.51243 | 1.702277 | 0.82215 |
| C73 | 1.35373 | 3.450031 | 2.253027 |
| H74 | -0.391 | 3.921546 | 1.006419 |

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|------|---------|----------|----------|
| H75 | 1.07967 | 4.802444 | 0.54149 |
| H76 | 2.30549 | 3.961607 | 2.424164 |
| H77 | 0.69712 | 3.582201 | 3.113323 |
| N78 | 1.08365 | 2.723545 | 0.066815 |
| O79 | 1.62542 | 2.031423 | 2.117594 |
| O80 | 1.79616 | 0.553856 | 0.426818 |
| H81 | 2.41173 | -4.78414 | 1.486162 |
| N82 | -2.0089 | -2.14095 | 0.698381 |
| C83 | -1.4385 | -3.29801 | -0.03524 |
| H84 | -1.5934 | -3.21741 | -1.12069 |
| C85 | -1.5106 | 1.146554 | -5.77937 |
| C86 | -2.3822 | 1.674082 | -4.82801 |
| C87 | -1.9754 | 1.801174 | -3.49897 |
| C88 | -0.6949 | 1.406252 | -3.08397 |
| C89 | 0.17208 | 0.883495 | -4.05963 |
| C90 | -0.2274 | 0.754202 | -5.3873 |
| H91 | -1.8225 | 1.047378 | -6.81503 |
| H92 | -3.3822 | 1.987475 | -5.11574 |
| H93 | -2.6708 | 2.201501 | -2.76591 |
| H94 | 1.17878 | 0.601135 | -3.77538 |
| H95 | 0.46648 | 0.353698 | -6.12133 |
| H96 | -1.1522 | 1.964551 | -1.10668 |
| C97 | 1.25282 | 3.966439 | -3.52888 |
| H98 | 1.3788 | 5.002295 | -3.86099 |
| H99 | 2.21559 | 3.458305 | -3.64978 |
| H100 | 0.5326 | 3.488679 | -4.19355 |
| C101 | -0.5917 | 4.633716 | -1.95204 |
| H102 | -0.5142 | 5.683457 | -2.25243 |
| H103 | -1.3102 | 4.153623 | -2.6188 |
| H104 | -1.0104 | 4.612424 | -0.94203 |
| H105 | 1.51639 | 4.567496 | -1.51991 |
| H106 | 2.68306 | -0.01544 | -1.97187 |
| H107 | 2.31957 | -0.39918 | -2.49978 |

C3_ES_Chelbot

| | | | |
|-------------------------|----------|----------|----------|
| C3_ES_Chelbot_SM | | | |
| C1 | -3.92334 | -3.52563 | -0.95247 |
| C2 | -1.6669 | -4.46398 | -0.96739 |
| C3 | -2.92551 | -4.31793 | -1.86331 |
| C4 | -3.09225 | -3.32181 | 0.333851 |
| H5 | -4.82519 | -4.10781 | -0.73666 |
| H6 | -2.70519 | -3.79957 | -2.80185 |
| H7 | -3.65581 | -3.0096 | 1.213869 |
| H8 | -4.23468 | -2.57194 | -1.38269 |
| H9 | -0.95787 | -5.22735 | -1.2881 |
| H10 | -3.31721 | -5.30626 | -2.1198 |

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|---------------------------|----------|----------|----------|
| C3_ES_Chelbot_int2 | | | |
| C1 | -3.64301 | -3.342 | -1.96871 |
| C2 | -1.38485 | -4.21093 | -1.64029 |
| C3 | -2.43784 | -3.95995 | -2.75276 |
| C4 | -3.07706 | -3.23895 | -0.53632 |
| H5 | -4.51478 | -4.00482 | -1.97916 |
| H6 | -2.05735 | -3.29438 | -3.53389 |
| H7 | -3.81167 | -3.02735 | 0.241043 |
| H8 | -3.95996 | -2.37275 | -2.3521 |
| H9 | -0.60686 | -4.92936 | -1.89761 |
| H10 | -2.71222 | -4.90405 | -3.23129 |

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|------|----------|----------|----------|------|----------|----------|----------|
| C11 | -2.3003 | -4.63802 | 0.430447 | C11 | -2.27591 | -4.5511 | -0.42848 |
| H12 | -1.57272 | -4.65033 | 1.247961 | H12 | -1.71426 | -4.66434 | 0.503192 |
| H13 | -2.94055 | -5.52192 | 0.499462 | H13 | -2.89355 | -5.43976 | -0.58551 |
| C14 | 0.369131 | -3.00871 | -0.27084 | C14 | 0.404818 | -2.89054 | -0.32633 |
| N15 | 0.92404 | -1.93078 | 0.158627 | N15 | 0.87795 | -1.88895 | 0.332738 |
| C16 | 2.347562 | -2.22891 | 0.526082 | C16 | 2.162049 | -2.31954 | 0.997783 |
| C17 | 2.388381 | -3.78733 | 0.327028 | C17 | 2.190737 | -3.85033 | 0.634477 |
| P18 | -1.92296 | -0.72309 | 0.399554 | P18 | -1.9584 | -0.74854 | 0.288742 |
| Ir19 | 0.099792 | 0.075575 | -0.19174 | Ir19 | 0.164935 | 0.204216 | -0.13281 |
| C20 | -2.18718 | -0.6099 | 2.204439 | C20 | -2.10105 | -1.0866 | 2.091348 |
| C21 | -2.3016 | -0.37148 | 4.996218 | C21 | -2.24105 | -1.58468 | 4.852575 |
| C22 | -1.91962 | -1.71597 | 3.022034 | C22 | -2.1699 | -2.39773 | 2.575872 |
| C23 | -2.50669 | 0.621292 | 2.800085 | C23 | -2.08061 | -0.02465 | 3.011334 |
| C24 | -2.5647 | 0.73708 | 4.187008 | C24 | -2.16112 | -0.27208 | 4.379964 |
| C25 | -1.97939 | -1.59624 | 4.41165 | C25 | -2.23653 | -2.64456 | 3.948152 |
| H26 | -2.70141 | 1.493899 | 2.185441 | H26 | -1.98644 | 0.998335 | 2.665624 |
| H27 | -2.81177 | 1.69432 | 4.636825 | H27 | -2.14932 | 0.56071 | 5.077464 |
| H28 | -1.76902 | -2.46078 | 5.0347 | H28 | -2.2776 | -3.66877 | 4.307221 |
| H29 | -2.34532 | -0.27826 | 6.077518 | H29 | -2.29267 | -1.77798 | 5.92009 |
| O30 | 1.098317 | -4.12724 | -0.26138 | O30 | 1.068448 | -4.04604 | -0.26674 |
| C31 | 2.640009 | -1.88956 | 1.983252 | C31 | 2.173263 | -2.16289 | 2.516515 |
| C32 | 1.638424 | -1.45846 | 2.857001 | C32 | 1.238365 | -1.41497 | 3.228407 |
| C33 | 3.931119 | -2.10161 | 2.490286 | C33 | 3.20723 | -2.80017 | 3.223892 |
| C34 | 1.926937 | -1.20446 | 4.199261 | C34 | 1.337898 | -1.29482 | 4.618064 |
| H35 | 0.630036 | -1.3172 | 2.495765 | H35 | 0.430534 | -0.92738 | 2.707074 |
| C36 | 4.219535 | -1.84991 | 3.830055 | C36 | 3.303741 | -2.68547 | 4.607849 |
| H37 | 4.720206 | -2.45339 | 1.831239 | H37 | 3.960922 | -3.37007 | 2.684816 |
| C38 | 3.21848 | -1.39083 | 4.689012 | C38 | 2.367035 | -1.92532 | 5.313566 |
| H39 | 1.130455 | -0.86488 | 4.855716 | H39 | 0.59684 | -0.70666 | 5.149342 |
| H40 | 5.226995 | -2.01201 | 4.202302 | H40 | 4.114522 | -3.18221 | 5.133048 |
| H41 | 3.444835 | -1.19092 | 5.732406 | H41 | 2.44303 | -1.82865 | 6.392534 |
| C42 | -3.41981 | -0.01954 | -0.39514 | C42 | -3.59498 | -0.03835 | -0.16662 |
| C43 | -4.58916 | 0.304597 | 0.305617 | C43 | -4.55131 | 0.333242 | 0.787611 |
| C44 | -3.4058 | 0.096919 | -1.79534 | C44 | -3.9035 | 0.107644 | -1.52884 |
| C45 | -5.71257 | 0.771721 | -0.38099 | C45 | -5.78061 | 0.861629 | 0.388538 |
| H46 | -4.63462 | 0.193591 | 1.383547 | H46 | -4.34809 | 0.212828 | 1.845716 |
| C47 | -4.53065 | 0.555811 | -2.47584 | C47 | -5.13497 | 0.626976 | -1.92358 |
| C48 | -5.68554 | 0.905913 | -1.76893 | C48 | -6.07584 | 1.015932 | -0.96532 |
| H49 | -6.61134 | 1.024906 | 0.17397 | H49 | -6.5099 | 1.144413 | 1.142094 |
| H50 | -4.51022 | 0.635703 | -3.55923 | H50 | -5.37182 | 0.709254 | -2.98109 |
| H51 | -6.56144 | 1.268497 | -2.29858 | H51 | -7.03563 | 1.419723 | -1.2735 |
| H52 | 0.269764 | 0.481403 | 1.299186 | H52 | 0.247393 | 0.567546 | 1.376663 |
| H53 | 1.855511 | 0.762868 | -0.591 | H53 | 1.342812 | 2.041705 | -2.28691 |
| H54 | -1.64145 | -2.66388 | 2.574681 | H54 | -2.14988 | -3.23434 | 1.891416 |
| H55 | -2.52153 | -0.1967 | -2.34931 | H55 | -3.19864 | -0.22024 | -2.28441 |

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|------|----------|----------|----------|------|----------|----------|----------|
| H56 | 3.168344 | -4.11754 | -0.36028 | H56 | 3.098247 | -4.15753 | 0.113064 |
| C57 | 4.670766 | -0.13685 | -2.49537 | C57 | 5.450083 | -0.28326 | -0.98842 |
| C58 | 3.784599 | -1.16014 | -2.84473 | C58 | 4.573699 | -1.10012 | -1.70844 |
| C59 | 3.074856 | -1.83394 | -1.85571 | C59 | 3.523591 | -1.74052 | -1.05405 |
| C60 | 3.235688 | -1.50546 | -0.49948 | C60 | 3.325286 | -1.57287 | 0.325557 |
| C61 | 4.123618 | -0.47986 | -0.16227 | C61 | 4.185331 | -0.72515 | 1.030878 |
| C62 | 4.83581 | 0.2 | -1.15369 | C62 | 5.248825 | -0.09694 | 0.377753 |
| H63 | 5.226377 | 0.390975 | -3.26526 | H63 | 6.277528 | 0.207292 | -1.49292 |
| H64 | 3.643591 | -1.43026 | -3.88732 | H64 | 4.713525 | -1.24508 | -2.77584 |
| H65 | 2.372592 | -2.60977 | -2.14909 | H65 | 2.854014 | -2.37803 | -1.62674 |
| H66 | 4.254274 | -0.18689 | 0.870528 | H66 | 4.041203 | -0.56239 | 2.091621 |
| H67 | 5.510014 | 1.002074 | -0.86793 | H67 | 5.918106 | 0.542018 | 0.945789 |
| C68 | -0.62429 | 3.259812 | -0.19303 | C68 | -0.8588 | 3.214511 | 0.184472 |
| C69 | 0.024602 | 2.032898 | -0.8655 | C69 | -0.25795 | 2.195762 | -0.81744 |
| C70 | 1.579927 | 1.862547 | -0.82691 | C70 | 0.991321 | 2.808932 | -1.5869 |
| C71 | -0.28766 | 3.105033 | -3.24037 | C71 | -1.87967 | 3.005975 | -2.76986 |
| C72 | -0.29748 | 0.824549 | -2.96531 | C72 | -0.99679 | 0.882997 | -2.71721 |
| C73 | -0.71953 | 2.395815 | -4.53505 | C73 | -2.39057 | 2.167577 | -3.95803 |
| H74 | 0.742489 | 3.48602 | -3.28762 | H74 | -1.17039 | 3.779501 | -3.08386 |
| H75 | -0.95366 | 3.926479 | -2.97187 | H75 | -2.69378 | 3.484488 | -2.22395 |
| H76 | -1.7962 | 2.485915 | -4.71018 | H76 | -3.44511 | 1.904876 | -3.85014 |
| H77 | -0.17106 | 2.706907 | -5.42425 | H77 | -2.21992 | 2.628417 | -4.9315 |
| N78 | -0.38344 | 1.990335 | -2.29227 | N78 | -1.21933 | 1.971741 | -1.95805 |
| O79 | -0.4233 | 0.990938 | -4.28982 | O79 | -1.61939 | 0.93375 | -3.9033 |
| O80 | -0.12168 | -0.29793 | -2.45422 | O80 | -0.3115 | -0.10484 | -2.38448 |
| H81 | 2.470472 | -4.32189 | 1.274348 | H81 | 2.024153 | -4.48548 | 1.505407 |
| N82 | -1.97825 | -2.37383 | 0.054894 | N82 | -1.97523 | -2.22442 | -0.52942 |
| C83 | -1.02543 | -3.05957 | -0.84711 | C83 | -0.81266 | -2.83566 | -1.22049 |
| H84 | -0.96204 | -2.57133 | -1.82906 | H84 | -0.52645 | -2.2433 | -2.09527 |
| H85 | 1.981595 | 1.925169 | -1.84452 | H85 | 0.593505 | 3.619824 | -2.20985 |
| C86 | 4.055047 | 4.211489 | 1.8045 | C86 | 4.451846 | 4.573964 | 0.330182 |
| C87 | 3.697967 | 4.693083 | 0.543954 | C87 | 3.261144 | 5.295305 | 0.214795 |
| C88 | 2.898972 | 3.919948 | -0.29866 | C88 | 2.150006 | 4.714793 | -0.38973 |
| C89 | 2.439582 | 2.664388 | 0.113423 | C89 | 2.189726 | 3.397545 | -0.87533 |
| C90 | 2.805336 | 2.185018 | 1.376311 | C90 | 3.399925 | 2.698549 | -0.77949 |
| C91 | 3.608374 | 2.954134 | 2.216858 | C91 | 4.51859 | 3.278304 | -0.1774 |
| H92 | 4.680635 | 4.811273 | 2.459089 | H92 | 5.323446 | 5.027757 | 0.793108 |
| H93 | 4.04499 | 5.668248 | 0.21427 | H93 | 3.203195 | 6.315 | 0.585274 |
| H94 | 2.629798 | 4.295591 | -1.28377 | H94 | 1.234519 | 5.292507 | -0.48808 |
| H95 | 2.446525 | 1.215099 | 1.706133 | H95 | 3.493864 | 1.705805 | -1.21118 |
| H96 | 3.884096 | 2.569337 | 3.194691 | H96 | 5.447337 | 2.718932 | -0.12652 |
| C97 | -0.36298 | 3.398097 | 1.316545 | C97 | -0.06893 | 3.303609 | 1.506533 |
| H98 | -0.61659 | 2.47241 | 1.839296 | H98 | -0.32646 | 2.465495 | 2.160047 |
| H99 | 0.670866 | 3.642688 | 1.55095 | H99 | 1.010091 | 3.286186 | 1.365043 |
| H100 | -0.99114 | 4.200457 | 1.718792 | H100 | -0.32412 | 4.229422 | 2.033062 |

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|------|----------|----------|----------|------|----------|----------|----------|
| C101 | -2.14562 | 3.273673 | -0.42767 | C101 | -2.33603 | 2.996794 | 0.536178 |
| H102 | -2.43258 | 3.138174 | -1.47336 | H102 | -2.99866 | 2.905767 | -0.32561 |
| H103 | -2.62218 | 2.465125 | 0.129834 | H103 | -2.46209 | 2.087424 | 1.120759 |
| H104 | -2.57044 | 4.220022 | -0.07832 | H104 | -2.6946 | 3.829948 | 1.149624 |
| H105 | -0.19455 | 4.154821 | -0.67461 | H105 | -0.79168 | 4.200818 | -0.30435 |
| X | 0.511818 | 2.053523 | -0.77184 | H106 | 1.739713 | 0.822751 | 0.183774 |
| | | | | H107 | 1.806645 | 0.475789 | -0.59764 |

C3_ES_Chelbot_TS1

| | | | |
|------|----------|----------|----------|
| C1 | -3.93912 | -3.46052 | -0.95048 |
| C2 | -1.68073 | -4.389 | -1.04942 |
| C3 | -2.95225 | -4.19683 | -1.91795 |
| C4 | -3.08363 | -3.30895 | 0.328034 |
| H5 | -4.82802 | -4.0651 | -0.74251 |
| H6 | -2.74585 | -3.62404 | -2.82787 |
| H7 | -3.63021 | -3.03743 | 1.231817 |
| H8 | -4.274 | -2.49489 | -1.3317 |
| H9 | -0.97927 | -5.13821 | -1.41719 |
| H10 | -3.34461 | -5.16992 | -2.22635 |
| C11 | -2.29073 | -4.62743 | 0.349901 |
| H12 | -1.54949 | -4.6759 | 1.153507 |
| H13 | -2.93011 | -5.51374 | 0.388837 |
| C14 | 0.353981 | -2.98157 | -0.28065 |
| N15 | 0.943549 | -1.91756 | 0.139939 |
| C16 | 2.349481 | -2.27218 | 0.560244 |
| C17 | 2.313694 | -3.83328 | 0.416056 |
| P18 | -1.94784 | -0.68812 | 0.391717 |
| Ir19 | 0.239724 | 0.115333 | -0.21513 |
| C20 | -2.21427 | -0.56727 | 2.200572 |
| C21 | -2.29716 | -0.30982 | 4.999506 |
| C22 | -1.90103 | -1.65609 | 3.025823 |
| C23 | -2.57703 | 0.652043 | 2.795097 |
| C24 | -2.61699 | 0.778198 | 4.182915 |
| C25 | -1.9442 | -1.52758 | 4.415856 |
| H26 | -2.82507 | 1.510643 | 2.180522 |
| H27 | -2.89632 | 1.729658 | 4.626431 |
| H28 | -1.69671 | -2.38114 | 5.040668 |
| H29 | -2.32663 | -0.20886 | 6.080452 |
| O30 | 1.029682 | -4.129 | -0.20866 |
| C31 | 2.621108 | -1.90086 | 2.014627 |
| C32 | 1.604092 | -1.46639 | 2.867621 |
| C33 | 3.910489 | -2.07663 | 2.538807 |
| C34 | 1.875217 | -1.16388 | 4.202957 |
| H35 | 0.596151 | -1.35583 | 2.495609 |
| C36 | 4.181858 | -1.78024 | 3.873324 |
| H37 | 4.712657 | -2.43006 | 1.896988 |

C3_ES_Chelbot_TS3

| | | | |
|------|----------|----------|----------|
| C1 | -3.70265 | -3.39788 | -1.93728 |
| C2 | -1.41948 | -4.22001 | -1.6525 |
| C3 | -2.49522 | -3.98019 | -2.74619 |
| C4 | -3.11803 | -3.30314 | -0.51145 |
| H5 | -4.56159 | -4.07722 | -1.94773 |
| H6 | -2.1408 | -3.29882 | -3.52618 |
| H7 | -3.84532 | -3.11669 | 0.279092 |
| H8 | -4.04179 | -2.42755 | -2.30007 |
| H9 | -0.62895 | -4.9167 | -1.93069 |
| H10 | -2.75553 | -4.92527 | -3.23072 |
| C11 | -2.2856 | -4.59739 | -0.4326 |
| H12 | -1.70877 | -4.70864 | 0.489979 |
| H13 | -2.88261 | -5.49938 | -0.59397 |
| C14 | 0.349895 | -2.86209 | -0.34533 |
| N15 | 0.825786 | -1.85013 | 0.302742 |
| C16 | 2.117715 | -2.27304 | 0.971746 |
| C17 | 2.138079 | -3.80774 | 0.630135 |
| P18 | -2.01136 | -0.79277 | 0.319203 |
| Ir19 | 0.218239 | 0.201783 | -0.11591 |
| C20 | -2.17321 | -1.15057 | 2.117368 |
| C21 | -2.3223 | -1.65812 | 4.87935 |
| C22 | -2.21903 | -2.46333 | 2.600717 |
| C23 | -2.17818 | -0.0919 | 3.041904 |
| C24 | -2.26471 | -0.34359 | 4.409907 |
| C25 | -2.28987 | -2.71509 | 3.97166 |
| H26 | -2.09856 | 0.934774 | 2.701866 |
| H27 | -2.27583 | 0.487615 | 5.109484 |
| H28 | -2.31622 | -3.74083 | 4.327993 |
| H29 | -2.37884 | -1.85488 | 5.946002 |
| O30 | 1.01236 | -4.01344 | -0.26408 |
| C31 | 2.122689 | -2.10584 | 2.489756 |
| C32 | 1.16943 | -1.38156 | 3.203055 |
| C33 | 3.168383 | -2.72118 | 3.200545 |
| C34 | 1.266119 | -1.25701 | 4.592397 |
| H35 | 0.341678 | -0.92258 | 2.686928 |
| C36 | 3.260986 | -2.60397 | 4.584802 |

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| C38 | 3.165914 | -1.31024 | 4.708664 | H37 | 3.933107 | -3.27802 | 2.663294 |
| H39 | 1.066866 | -0.8164 | 4.840453 | C38 | 2.309129 | -1.8621 | 5.289641 |
| H40 | 5.189204 | -1.9116 | 4.258047 | H39 | 0.508499 | -0.68862 | 5.122132 |
| H41 | 3.380371 | -1.07008 | 5.746084 | H40 | 4.080878 | -3.08492 | 5.110691 |
| C42 | -3.47249 | -0.03508 | -0.39704 | H41 | 2.381956 | -1.76347 | 6.368644 |
| C43 | -4.66907 | 0.188969 | 0.296533 | C42 | -3.64008 | -0.06587 | -0.14136 |
| C44 | -3.45054 | 0.125701 | -1.79218 | C43 | -4.60816 | 0.318435 | 0.794268 |
| C45 | -5.81378 | 0.599273 | -0.39078 | C44 | -3.91598 | 0.092109 | -1.50976 |
| H46 | -4.71571 | 0.047969 | 1.371117 | C45 | -5.82072 | 0.866333 | 0.371135 |
| C47 | -4.59679 | 0.525205 | -2.47563 | H46 | -4.42836 | 0.188418 | 1.855508 |
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| H50 | -4.56919 | 0.637667 | -3.55623 | H49 | -6.56228 | 1.158335 | 1.10906 |
| H51 | -6.6744 | 1.089229 | -2.30586 | H50 | -5.34782 | 0.716476 | -2.99094 |
| H52 | 0.440795 | 0.470646 | 1.277764 | H51 | -7.03318 | 1.44295 | -1.31421 |
| H53 | 1.827948 | 0.267238 | -0.41732 | H52 | 0.404685 | 0.542426 | 1.380155 |
| H54 | -1.60126 | -2.59925 | 2.581476 | H53 | 1.381403 | 2.223882 | -2.38209 |
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| H56 | 3.09997 | -4.23074 | -0.22647 | H55 | -3.19568 | -0.2427 | -2.24929 |
| C57 | 4.811202 | -0.34089 | -2.45531 | H56 | 3.042282 | -4.12477 | 0.109227 |
| C58 | 3.973102 | -1.41001 | -2.7855 | C57 | 5.415678 | -0.30581 | -1.062 |
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| C60 | 3.298979 | -1.62224 | -0.45796 | C59 | 3.468644 | -1.73484 | -1.09447 |
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| H64 | 3.898705 | -1.74818 | -3.81509 | H63 | 6.246651 | 0.165637 | -1.57884 |
| H65 | 2.554201 | -2.84802 | -2.07919 | H64 | 4.649095 | -1.27736 | -2.83165 |
| H66 | 4.201935 | -0.18647 | 0.877702 | H65 | 2.782203 | -2.36479 | -1.65513 |
| H67 | 5.526882 | 0.923674 | -0.86101 | H66 | 4.028656 | -0.52938 | 2.032488 |
| C68 | -0.77662 | 3.269234 | -0.11252 | H67 | 5.917714 | 0.526824 | 0.861312 |
| C69 | -0.05998 | 2.129942 | -0.85972 | C68 | -0.78431 | 3.197684 | 0.206473 |
| C70 | 1.387426 | 1.900124 | -0.77461 | C69 | -0.15936 | 2.199771 | -0.81446 |
| C71 | -0.47046 | 3.197312 | -3.18824 | C70 | 1.036423 | 2.955678 | -1.64312 |
| C72 | -0.37428 | 0.911093 | -2.96299 | C71 | -1.8223 | 2.945431 | -2.73113 |
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| H74 | 0.548165 | 3.605702 | -3.25223 | C73 | -2.33998 | 2.100282 | -3.91093 |
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| H77 | -0.41388 | 2.85718 | -5.38276 | H76 | -3.38517 | 1.813991 | -3.78079 |
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| H81 | 2.329541 | -4.33606 | 1.38428 | O80 | -0.16315 | -0.12451 | -2.4048 |
| N82 | -1.97318 | -2.34877 | 0.07771 | H81 | 1.971845 | -4.43048 | 1.509982 |

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|--------------------|----------|----------|----------|--------------------|----------|----------|----------|
| C83 | -1.03473 | -2.99457 | -0.87061 | N82 | -2.04307 | -2.26408 | -0.50943 |
| H84 | -0.9708 | -2.4579 | -1.8265 | C83 | -0.87777 | -2.83401 | -1.22635 |
| H85 | 1.855524 | 1.751697 | -1.75075 | H84 | -0.61562 | -2.22713 | -2.09898 |
| C86 | 4.155679 | 4.045976 | 1.72781 | H85 | 0.548282 | 3.770826 | -2.18092 |
| C87 | 3.755381 | 4.539545 | 0.484603 | C86 | 4.450712 | 4.65706 | 0.382524 |
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| C89 | 2.332918 | 2.595239 | 0.158598 | C88 | 2.189689 | 4.854968 | -0.44238 |
| C90 | 2.743471 | 2.105408 | 1.403216 | C89 | 2.227351 | 3.537071 | -0.92249 |
| C91 | 3.648534 | 2.82725 | 2.181093 | C90 | 3.403644 | 2.79506 | -0.75472 |
| H92 | 4.859471 | 4.607171 | 2.335643 | C91 | 4.506287 | 3.35222 | -0.10558 |
| H93 | 4.145381 | 5.485777 | 0.120094 | H92 | 5.311831 | 5.090509 | 0.882878 |
| H94 | 2.550732 | 4.201207 | -1.2661 | H93 | 3.24188 | 6.433397 | 0.571413 |
| H95 | 2.350579 | 1.162868 | 1.765479 | H94 | 1.292342 | 5.452421 | -0.58505 |
| H96 | 3.955959 | 2.431117 | 3.144755 | H95 | 3.469052 | 1.783275 | -1.14562 |
| C97 | -0.46543 | 3.355589 | 1.389859 | H96 | 5.411688 | 2.764719 | 0.006815 |
| H98 | -0.66727 | 2.403298 | 1.885921 | C97 | 0.017014 | 3.294268 | 1.521415 |
| H99 | 0.570257 | 3.624309 | 1.587866 | H98 | -0.20496 | 2.438105 | 2.164083 |
| H100 | -1.10109 | 4.121628 | 1.846742 | H99 | 1.095802 | 3.323015 | 1.370755 |
| C101 | -2.29977 | 3.232371 | -0.3164 | H100 | -0.26978 | 4.204365 | 2.057732 |
| H102 | -2.59912 | 3.142018 | -1.36368 | C101 | -2.24939 | 2.922729 | 0.565286 |
| H103 | -2.74336 | 2.384278 | 0.206604 | H102 | -2.92111 | 2.838773 | -0.28938 |
| H104 | -2.74903 | 4.146284 | 0.085089 | H103 | -2.33625 | 1.991034 | 1.119844 |
| H105 | -0.40041 | 4.201564 | -0.56716 | H104 | -2.62221 | 3.725831 | 1.209351 |
| X | 0.511818 | 2.053523 | -0.77184 | H105 | -0.74317 | 4.184796 | -0.27785 |
| C3_ES_Chelbot_intl | | | | H106 | 1.765166 | 0.539234 | -0.26164 |
| C1 | -3.91123 | -3.50203 | -0.99682 | H107 | 0.924033 | 1.60068 | -0.38607 |
| C2 | -1.6571 | -4.44651 | -1.00624 | C3_ES_Chelbot_PROD | | | |
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| C4 | -3.08915 | -3.31582 | 0.298042 | C2 | -1.43563 | -4.35964 | -1.54081 |
| H5 | -4.81524 | -4.08571 | -0.79452 | C3 | -2.57349 | -4.13509 | -2.57037 |
| H6 | -2.67865 | -3.75283 | -2.83965 | C4 | -3.08564 | -3.49382 | -0.29419 |
| H7 | -3.65869 | -3.01239 | 1.177278 | H5 | -4.5989 | -4.22958 | -1.67685 |
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| H10 | -3.30062 | -5.26744 | -2.1847 | H8 | -4.08259 | -2.57843 | -2.02384 |
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| H12 | -1.58123 | -4.66096 | 1.207046 | H10 | -2.85425 | -5.08605 | -3.03158 |
| H13 | -2.94635 | -5.51823 | 0.436763 | C11 | -2.22811 | -4.77192 | -0.27856 |
| C14 | 0.377909 | -3.00157 | -0.27548 | H12 | -1.60789 | -4.87147 | 0.617247 |
| N15 | 0.930582 | -1.9249 | 0.160199 | H13 | -2.80946 | -5.68654 | -0.42582 |
| C16 | 2.3488 | -2.226 | 0.544272 | C14 | 0.390649 | -2.97744 | -0.35521 |
| C17 | 2.389129 | -3.7848 | 0.344292 | N15 | 0.939 | -1.93696 | 0.185548 |
| P18 | -1.91029 | -0.72241 | 0.40241 | C16 | 2.262718 | -2.33553 | 0.814969 |
| Ir19 | 0.105397 | 0.081757 | -0.20228 | C17 | 2.174123 | -3.89096 | 0.658129 |

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|-----|----------|----------|----------|------|----------|----------|----------|
| C20 | -2.16375 | -0.61926 | 2.209298 | P18 | -1.98692 | -0.92546 | 0.430301 |
| C21 | -2.28074 | -0.39528 | 5.001425 | Ir19 | 0.230896 | -0.04724 | -0.0847 |
| C22 | -1.92687 | -1.73676 | 3.019722 | C20 | -2.24544 | -1.14402 | 2.231037 |
| C23 | -2.45175 | 0.616348 | 2.811423 | C21 | -2.52222 | -1.34378 | 5.01738 |
| C24 | -2.51167 | 0.724981 | 4.198476 | C22 | -2.46055 | -2.38951 | 2.834967 |
| C25 | -1.98902 | -1.62416 | 4.409958 | C23 | -2.13315 | -0.00302 | 3.043886 |
| H26 | -2.62093 | 1.497405 | 2.201372 | C24 | -2.28226 | -0.10047 | 4.425595 |
| H27 | -2.73448 | 1.685718 | 4.653539 | C25 | -2.597 | -2.48663 | 4.221317 |
| H28 | -1.80183 | -2.49729 | 5.028376 | H26 | -1.91215 | 0.962815 | 2.597492 |
| H29 | -2.32698 | -0.30802 | 6.083131 | H27 | -2.19833 | 0.790215 | 5.0417 |
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| C31 | 2.62649 | -1.88796 | 2.004646 | H29 | -2.63444 | -1.42148 | 6.09497 |
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| C34 | 1.896373 | -1.18626 | 4.209149 | C32 | 1.197574 | -1.80554 | 3.075817 |
| H35 | 0.615538 | -1.29965 | 2.493191 | C33 | 3.574476 | -2.19037 | 2.964853 |
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| H37 | 4.704512 | -2.46476 | 1.873983 | H35 | 0.231104 | -1.72666 | 2.599794 |
| C38 | 3.181969 | -1.37881 | 4.711978 | C36 | 3.662466 | -2.05701 | 4.349477 |
| H39 | 1.095943 | -0.83796 | 4.856143 | H37 | 4.471219 | -2.40478 | 2.391472 |
| H40 | 5.191433 | -2.01514 | 4.24805 | C38 | 2.51962 | -1.78261 | 5.102208 |
| H41 | 3.399846 | -1.17427 | 5.756247 | H39 | 0.384658 | -1.46636 | 5.031168 |
| C42 | -3.41111 | -0.01333 | -0.37431 | H40 | 4.626095 | -2.1675 | 4.838564 |
| C43 | -4.5685 | 0.319822 | 0.340854 | H41 | 2.590025 | -1.67212 | 6.180605 |
| C44 | -3.4101 | 0.100601 | -1.77453 | C42 | -3.54673 | -0.14124 | -0.15392 |
| C45 | -5.69601 | 0.792948 | -0.33354 | C43 | -4.53415 | 0.366815 | 0.699986 |
| H46 | -4.60122 | 0.211096 | 1.419419 | C44 | -3.72948 | -0.04193 | -1.54383 |
| C47 | -4.53867 | 0.5666 | -2.44254 | C45 | -5.67703 | 0.973485 | 0.173825 |
| C48 | -5.68176 | 0.924306 | -1.72127 | H46 | -4.41996 | 0.289834 | 1.776223 |
| H49 | -6.58731 | 1.054037 | 0.229721 | C47 | -4.87707 | 0.551679 | -2.06492 |
| H50 | -4.53133 | 0.645626 | -3.52623 | C48 | -5.85196 | 1.068253 | -1.20608 |
| H51 | -6.56117 | 1.292364 | -2.24175 | H49 | -6.43606 | 1.361468 | 0.847098 |
| H52 | 0.28258 | 0.492499 | 1.285983 | H50 | -5.02023 | 0.593205 | -3.14155 |
| H53 | 1.856497 | 0.773653 | -0.62434 | H51 | -6.74763 | 1.529717 | -1.61172 |
| H54 | -1.6708 | -2.68836 | 2.567142 | H52 | 0.630508 | 0.168779 | 1.395744 |
| H55 | -2.53356 | -0.20047 | -2.33694 | H53 | 1.563305 | 2.443327 | -2.10695 |
| H56 | 3.175331 | -4.11568 | -0.33556 | H54 | -2.49564 | -3.29131 | 2.235925 |
| C57 | 4.690465 | -0.11278 | -2.44757 | H55 | -2.98453 | -0.45057 | -2.21861 |
| C58 | 3.809906 | -1.1367 | -2.80935 | H56 | 3.05816 | -4.3361 | 0.202291 |
| C59 | 3.096032 | -1.81886 | -1.82894 | C57 | 5.30449 | -0.535 | -1.70109 |
| C60 | 3.247305 | -1.49875 | -0.46958 | C58 | 4.584077 | -1.64689 | -2.13996 |
| C61 | 4.130568 | -0.47307 | -0.1195 | C59 | 3.629363 | -2.23129 | -1.30987 |
| C62 | 4.846672 | 0.215223 | -1.10265 | C60 | 3.379142 | -1.7182 | -0.03067 |
| H63 | 5.24829 | 0.422733 | -3.21059 | C61 | 4.089945 | -0.589 | 0.39049 |
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|-------------------|----------|----------|----------|------|----------|----------|----------|
| H65 | 2.397125 | -2.59413 | -2.13176 | H63 | 6.053466 | -0.08075 | -2.34334 |
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| C68 | -0.63392 | 3.263257 | -0.21128 | H66 | 3.882648 | -0.15165 | 1.360277 |
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| C72 | -0.31878 | 0.82166 | -2.97616 | C70 | 1.171292 | 3.269402 | -1.50383 |
| C73 | -0.77425 | 2.385102 | -4.54425 | C71 | -1.5966 | 3.402589 | -2.94597 |
| H74 | 0.693534 | 3.494035 | -3.31968 | C72 | -0.99733 | 1.182798 | -2.67897 |
| H75 | -1.00284 | 3.916639 | -2.98185 | C73 | -2.37106 | 2.506183 | -3.91871 |
| H76 | -1.85384 | 2.466057 | -4.70556 | H74 | -0.80377 | 3.969588 | -3.44755 |
| H77 | -0.24025 | 2.698467 | -5.44141 | H75 | -2.24378 | 4.099869 | -2.41104 |
| N78 | -0.40244 | 1.988372 | -2.30547 | H76 | -3.40764 | 2.363013 | -3.6015 |
| O79 | -0.46358 | 0.98327 | -4.29933 | H77 | -2.33329 | 2.83839 | -4.95617 |
| O80 | -0.13061 | -0.2982 | -2.46338 | N78 | -1.03461 | 2.387237 | -2.04415 |
| H81 | 2.459064 | -4.32137 | 1.291749 | O79 | -1.69796 | 1.224172 | -3.82733 |
| N82 | -1.96971 | -2.36842 | 0.039461 | O80 | -0.45393 | 0.136854 | -2.31161 |
| C83 | -1.01199 | -3.04607 | -0.86404 | H81 | 1.958406 | -4.37788 | 1.609781 |
| H84 | -0.94098 | -2.54627 | -1.83945 | N82 | -2.0151 | -2.45713 | -0.2842 |
| H85 | 1.96699 | 1.939305 | -1.87608 | C83 | -0.9046 | -2.96258 | -1.13197 |
| C86 | 4.076681 | 4.215674 | 1.755303 | H84 | -0.74158 | -2.32223 | -2.00847 |
| C87 | 3.727275 | 4.689898 | 0.489913 | H85 | 0.916737 | 4.079286 | -2.19702 |
| C88 | 2.917367 | 3.919772 | -0.34499 | C86 | 4.232804 | 4.722049 | 1.173748 |
| C89 | 2.440812 | 2.675027 | 0.079826 | C87 | 3.426933 | 5.621739 | 0.474416 |
| C90 | 2.797315 | 2.203229 | 1.348203 | C88 | 2.440704 | 5.147983 | -0.39185 |
| C91 | 3.610594 | 2.969734 | 2.181086 | C89 | 2.242928 | 3.772572 | -0.56617 |
| H92 | 4.711037 | 4.812732 | 2.403844 | C90 | 3.065972 | 2.877833 | 0.12773 |
| H93 | 4.088653 | 5.656452 | 0.15044 | C91 | 4.050319 | 3.349026 | 0.994673 |
| H94 | 2.654171 | 4.28865 | -1.33432 | H92 | 5.001354 | 5.089317 | 1.847873 |
| H95 | 2.424397 | 1.240989 | 1.686402 | H93 | 3.568295 | 6.691586 | 0.599562 |
| H96 | 3.880096 | 2.591899 | 3.163317 | H94 | 1.817575 | 5.855286 | -0.93549 |
| C97 | -0.35325 | 3.419922 | 1.292897 | H95 | 2.925945 | 1.812569 | -0.0083 |
| H98 | -0.57019 | 2.491204 | 1.826491 | H96 | 4.677653 | 2.642074 | 1.531606 |
| H99 | 0.67641 | 3.697727 | 1.508352 | C97 | -0.20241 | 3.694756 | 1.466703 |
| H100 | -0.99846 | 4.206449 | 1.699437 | H98 | -0.14149 | 2.676294 | 1.870312 |
| C101 | -2.15877 | 3.262884 | -0.42543 | H99 | 0.806861 | 4.098821 | 1.423916 |
| H102 | -2.45913 | 3.098405 | -1.46323 | H100 | -0.78145 | 4.30264 | 2.168627 |
| H103 | -2.62534 | 2.467864 | 0.159801 | C101 | -2.36666 | 3.232732 | 0.314484 |
| H104 | -2.58328 | 4.216327 | -0.09539 | H102 | -2.97543 | 3.221295 | -0.59205 |
| H105 | -0.2192 | 4.157279 | -0.70763 | H103 | -2.39219 | 2.219123 | 0.722088 |
| X | 0.511818 | 2.053523 | -0.77184 | H104 | -2.8542 | 3.894846 | 1.036267 |
| C3_ES_Chelbot_TS2 | | | | H105 | -0.89449 | 4.692923 | -0.31959 |
| C1 | -3.68141 | -3.36122 | -1.85634 | H106 | 1.728182 | 0.357927 | -0.43177 |
| | | | | H107 | 0.063298 | 1.836492 | -0.30471 |

| | | | |
|------|----------|----------|----------|
| C2 | -1.41707 | -4.24234 | -1.59908 |
| C3 | -2.50391 | -3.98486 | -2.67772 |
| C4 | -3.07329 | -3.26947 | -0.44108 |
| H5 | -4.55861 | -4.01679 | -1.84497 |
| H6 | -2.1444 | -3.32141 | -3.47057 |
| H7 | -3.78195 | -3.05939 | 0.360619 |
| H8 | -4.00132 | -2.38679 | -2.22501 |
| H9 | -0.64903 | -4.96182 | -1.88241 |
| H10 | -2.79846 | -4.92719 | -3.14771 |
| C11 | -2.27231 | -4.58392 | -0.36166 |
| H12 | -1.68488 | -4.69972 | 0.553866 |
| H13 | -2.89671 | -5.47054 | -0.50296 |
| C14 | 0.417925 | -2.91322 | -0.34543 |
| N15 | 0.88584 | -1.91264 | 0.319402 |
| C16 | 2.202731 | -2.31759 | 0.923178 |
| C17 | 2.265812 | -3.84063 | 0.520313 |
| P18 | -1.92274 | -0.78408 | 0.343949 |
| Ir19 | 0.062728 | 0.156356 | -0.04692 |
| C20 | -2.09303 | -1.09834 | 2.144596 |
| C21 | -2.22985 | -1.55747 | 4.910269 |
| C22 | -2.1031 | -2.4036 | 2.648373 |
| C23 | -2.13109 | -0.02038 | 3.045761 |
| C24 | -2.20773 | -0.24941 | 4.417352 |
| C25 | -2.17082 | -2.63091 | 4.023895 |
| H26 | -2.08073 | 0.999683 | 2.681054 |
| H27 | -2.23929 | 0.593437 | 5.101976 |
| H28 | -2.16779 | -3.64974 | 4.400145 |
| H29 | -2.28068 | -1.7358 | 5.980529 |
| O30 | 1.117307 | -4.04767 | -0.3441 |
| C31 | 2.242126 | -2.18526 | 2.443986 |
| C32 | 1.334746 | -1.41439 | 3.171472 |
| C33 | 3.246284 | -2.87534 | 3.144246 |
| C34 | 1.433469 | -1.32327 | 4.562303 |
| H35 | 0.54057 | -0.89224 | 2.660654 |
| C36 | 3.34523 | -2.78597 | 4.531214 |
| H37 | 3.973017 | -3.47598 | 2.601628 |
| C38 | 2.437504 | -2.00343 | 5.24913 |
| H39 | 0.708485 | -0.72254 | 5.102736 |
| H40 | 4.133416 | -3.32533 | 5.048895 |
| H41 | 2.513279 | -1.93085 | 6.330108 |
| C42 | -3.50423 | -0.0196 | -0.17477 |
| C43 | -4.49135 | 0.388088 | 0.731878 |
| C44 | -3.74422 | 0.107368 | -1.55295 |
| C45 | -5.6883 | 0.93533 | 0.267541 |
| H46 | -4.33865 | 0.277159 | 1.799394 |

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|-----|----------|----------|----------|
| C47 | -4.94123 | 0.650187 | -2.01233 |
| C48 | -5.91373 | 1.073702 | -1.1015 |
| H49 | -6.44729 | 1.245734 | 0.979713 |
| H50 | -5.12692 | 0.723636 | -3.08054 |
| H51 | -6.84898 | 1.494518 | -1.45941 |
| H52 | 0.090123 | 0.535517 | 1.452153 |
| H53 | 1.68063 | 1.536088 | -1.6961 |
| H54 | -2.03461 | -3.24846 | 1.97655 |
| H55 | -3.01304 | -0.2551 | -2.26649 |
| H56 | 3.161687 | -4.09909 | -0.0458 |
| C57 | 5.401829 | -0.27969 | -1.21734 |
| C58 | 4.309498 | -0.81866 | -1.90057 |
| C59 | 3.285492 | -1.44798 | -1.19439 |
| C60 | 3.33006 | -1.54892 | 0.205333 |
| C61 | 4.4192 | -0.98926 | 0.882717 |
| C62 | 5.448519 | -0.36409 | 0.174061 |
| H63 | 6.202386 | 0.209305 | -1.76485 |
| H64 | 4.25387 | -0.75116 | -2.98344 |
| H65 | 2.443864 | -1.85735 | -1.74516 |
| H66 | 4.469037 | -1.02971 | 1.963985 |
| H67 | 6.287324 | 0.062078 | 0.71722 |
| C68 | -0.80057 | 3.225367 | 0.180761 |
| C69 | -0.2314 | 2.124171 | -0.73929 |
| C70 | 1.201209 | 2.479946 | -1.3985 |
| C71 | -1.61469 | 3.077921 | -2.7763 |
| C72 | -0.87481 | 0.902571 | -2.72411 |
| C73 | -2.13317 | 2.292979 | -3.99522 |
| H74 | -0.81385 | 3.782326 | -3.03905 |
| H75 | -2.40718 | 3.630749 | -2.27011 |
| H76 | -3.2028 | 2.081635 | -3.91684 |
| H77 | -1.91529 | 2.76275 | -4.95474 |
| N78 | -1.10288 | 1.981173 | -1.94733 |
| O79 | -1.42365 | 1.022016 | -3.94354 |
| O80 | -0.24517 | -0.11477 | -2.37816 |
| H81 | 2.152202 | -4.50693 | 1.376643 |
| N82 | -1.96406 | -2.26436 | -0.45809 |
| C83 | -0.82963 | -2.86834 | -1.19528 |
| H84 | -0.57715 | -2.27286 | -2.07913 |
| H85 | 0.958414 | 2.95414 | -2.35696 |
| C86 | 4.296773 | 5.040328 | 0.219116 |
| C87 | 3.053652 | 5.574235 | -0.1285 |
| C88 | 2.051378 | 4.746211 | -0.62778 |
| C89 | 2.255968 | 3.364185 | -0.7693 |
| C90 | 3.520911 | 2.852047 | -0.45424 |
| C91 | 4.529693 | 3.677104 | 0.043164 |

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|------|----------|----------|----------|
| H92 | 5.080128 | 5.685813 | 0.605966 |
| H93 | 2.868958 | 6.639488 | -0.02132 |
| H94 | 1.09917 | 5.18237 | -0.91658 |
| H95 | 3.735915 | 1.800817 | -0.61713 |
| H96 | 5.500404 | 3.250865 | 0.28218 |
| C97 | -0.04282 | 3.345864 | 1.516131 |
| H98 | -0.30181 | 2.511761 | 2.175149 |
| H99 | 1.039649 | 3.351101 | 1.394268 |
| H100 | -0.32492 | 4.274808 | 2.022359 |
| C101 | -2.29557 | 3.067988 | 0.491871 |
| H102 | -2.92452 | 2.922411 | -0.38873 |
| H103 | -2.46053 | 2.204492 | 1.135819 |
| H104 | -2.65844 | 3.95187 | 1.026783 |
| H105 | -0.68006 | 4.182286 | -0.3507 |
| H106 | 1.991109 | 1.051144 | 1.195641 |
| H107 | 2.467578 | 0.840205 | 0.659932 |

C3_ER_Cheltop

C3_ER_Cheltop_SM

| | | | |
|------|----------|----------|----------|
| C1 | -4.24858 | -3.40287 | 0.876158 |
| C2 | -2.19851 | -4.54636 | 0.222072 |
| C3 | -3.70397 | -4.46459 | -0.13559 |
| C4 | -2.98079 | -3.03809 | 1.685035 |
| H5 | -5.00531 | -3.82988 | 1.54224 |
| H6 | -3.86632 | -4.17636 | -1.17917 |
| H7 | -3.16654 | -2.51518 | 2.623062 |
| H8 | -4.69005 | -2.53279 | 0.388719 |
| H9 | -1.67552 | -5.41833 | -0.17013 |
| H10 | -4.17723 | -5.4395 | 0.011934 |
| C11 | -2.23552 | -4.38247 | 1.758077 |
| H12 | -1.24827 | -4.30122 | 2.222813 |
| H13 | -2.81224 | -5.17038 | 2.250566 |
| C14 | -0.04929 | -3.19441 | -0.3028 |
| N15 | 0.663073 | -2.12554 | -0.36302 |
| C16 | 2.108723 | -2.53303 | -0.27201 |
| C17 | 1.994708 | -4.06112 | -0.5708 |
| P18 | -1.92685 | -0.59942 | 0.626944 |
| Ir19 | -0.12601 | -0.07979 | -0.60076 |
| C20 | -1.77477 | 0.092013 | 2.312401 |
| C21 | -1.26204 | 1.281777 | 4.802089 |
| C22 | -1.28723 | -0.67666 | 3.377904 |
| C23 | -1.99657 | 1.465526 | 2.503436 |
| C24 | -1.74324 | 2.053451 | 3.741555 |
| C25 | -1.03854 | -0.08306 | 4.616192 |
| H26 | -2.35908 | 2.076643 | 1.684825 |

C3_ER_Cheltop_int2

| | | | |
|------|----------|----------|----------|
| C1 | -3.64301 | -3.342 | -1.96871 |
| C2 | -1.38485 | -4.21093 | -1.64029 |
| C3 | -2.43784 | -3.95995 | -2.75276 |
| C4 | -3.07706 | -3.23895 | -0.53632 |
| H5 | -4.51478 | -4.00482 | -1.97916 |
| H6 | -2.05735 | -3.29438 | -3.53389 |
| H7 | -3.81167 | -3.02735 | 0.241043 |
| H8 | -3.95996 | -2.37275 | -2.3521 |
| H9 | -0.60686 | -4.92936 | -1.89761 |
| H10 | -2.71222 | -4.90405 | -3.23129 |
| C11 | -2.27591 | -4.5511 | -0.42848 |
| H12 | -1.71426 | -4.66434 | 0.503192 |
| H13 | -2.89355 | -5.43976 | -0.58551 |
| C14 | 0.404818 | -2.89054 | -0.32633 |
| N15 | 0.87795 | -1.88895 | 0.332738 |
| C16 | 2.162049 | -2.31954 | 0.997783 |
| C17 | 2.190737 | -3.85033 | 0.634477 |
| P18 | -1.9584 | -0.74854 | 0.288742 |
| Ir19 | 0.164935 | 0.204216 | -0.13281 |
| C20 | -2.10105 | -1.0866 | 2.091348 |
| C21 | -2.24105 | -1.58468 | 4.852575 |
| C22 | -2.1699 | -2.39773 | 2.575872 |
| C23 | -2.08061 | -0.02465 | 3.011334 |
| C24 | -2.16112 | -0.27208 | 4.379964 |
| C25 | -2.23653 | -2.64456 | 3.948152 |
| H26 | -1.98644 | 0.998335 | 2.665624 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| H27 | -1.92598 | 3.115739 | 3.879585 | H27 | -2.14932 | 0.56071 | 5.077464 |
| H28 | -0.66799 | -0.69078 | 5.436761 | H28 | -2.2776 | -3.66877 | 4.307221 |
| H29 | -1.06391 | 1.741177 | 5.765789 | H29 | -2.29267 | -1.77798 | 5.92009 |
| O30 | 0.59354 | -4.36538 | -0.31403 | O30 | 1.068448 | -4.04604 | -0.26674 |
| C31 | 2.622259 | -2.35892 | 1.16244 | C31 | 2.173263 | -2.16289 | 2.516515 |
| C32 | 1.812878 | -1.89252 | 2.195652 | C32 | 1.238365 | -1.41497 | 3.228407 |
| C33 | 3.940743 | -2.74288 | 1.453906 | C33 | 3.20723 | -2.80017 | 3.223892 |
| C34 | 2.312431 | -1.78603 | 3.495098 | C34 | 1.337898 | -1.29482 | 4.618064 |
| H35 | 0.80116 | -1.58235 | 1.985305 | H35 | 0.430534 | -0.92738 | 2.707074 |
| C36 | 4.438046 | -2.64467 | 2.750236 | C36 | 3.303741 | -2.68547 | 4.607849 |
| H37 | 4.586342 | -3.10323 | 0.656334 | H37 | 3.960922 | -3.37007 | 2.684816 |
| C38 | 3.623435 | -2.16002 | 3.777756 | C38 | 2.367035 | -1.92532 | 5.313566 |
| H39 | 1.670324 | -1.39544 | 4.279544 | H39 | 0.59684 | -0.70666 | 5.149342 |
| H40 | 5.462377 | -2.94024 | 2.95835 | H40 | 4.114522 | -3.18221 | 5.133048 |
| H41 | 4.013202 | -2.07532 | 4.788103 | H41 | 2.44303 | -1.82865 | 6.392534 |
| C42 | -3.58158 | -0.12243 | 0.003396 | C42 | -3.59498 | -0.03835 | -0.16662 |
| C43 | -4.60661 | 0.330204 | 0.847351 | C43 | -4.55131 | 0.333242 | 0.787611 |
| C44 | -3.87987 | -0.40833 | -1.33952 | C44 | -3.9035 | 0.107644 | -1.52884 |
| C45 | -5.89822 | 0.513382 | 0.348975 | C45 | -5.78061 | 0.861629 | 0.388538 |
| H46 | -4.40612 | 0.53439 | 1.893808 | H46 | -4.34809 | 0.212828 | 1.845716 |
| C47 | -5.1718 | -0.23345 | -1.83025 | C47 | -5.13497 | 0.626976 | -1.92358 |
| C48 | -6.18519 | 0.232727 | -0.98783 | C48 | -6.07584 | 1.015932 | -0.96532 |
| H49 | -6.68165 | 0.870797 | 1.010891 | H49 | -6.5099 | 1.144413 | 1.142094 |
| H50 | -5.38639 | -0.45527 | -2.87162 | H50 | -5.37182 | 0.709254 | -2.98109 |
| H51 | -7.19122 | 0.373969 | -1.37124 | H51 | -7.03563 | 1.419723 | -1.2735 |
| H52 | -0.8981 | -0.54383 | -1.88353 | H52 | 0.247393 | 0.567546 | 1.376663 |
| H53 | 1.409335 | 0.461057 | -1.67983 | H53 | 1.342812 | 2.041705 | -2.28691 |
| H54 | -1.08557 | -1.7332 | 3.239491 | H54 | -2.14988 | -3.23434 | 1.891416 |
| H55 | -3.09717 | -0.76644 | -2.00083 | H55 | -3.19864 | -0.22024 | -2.28441 |
| H56 | 2.204227 | -4.33156 | -1.60787 | H56 | 3.098247 | -4.15753 | 0.113064 |
| C57 | 4.364205 | -0.28039 | -3.22523 | C57 | 5.450083 | -0.28326 | -0.98842 |
| C58 | 3.541895 | -1.33511 | -3.62218 | C58 | 4.573699 | -1.10012 | -1.70844 |
| C59 | 2.824133 | -2.05997 | -2.67248 | C59 | 3.523591 | -1.74052 | -1.05405 |
| C60 | 2.929988 | -1.76078 | -1.30622 | C60 | 3.325286 | -1.57287 | 0.325557 |
| C61 | 3.744627 | -0.68763 | -0.92082 | C61 | 4.185331 | -0.72515 | 1.030878 |
| C62 | 4.455947 | 0.044947 | -1.87256 | C62 | 5.248825 | -0.09694 | 0.377753 |
| H63 | 4.916825 | 0.289559 | -3.96607 | H63 | 6.277528 | 0.207292 | -1.49292 |
| H64 | 3.444642 | -1.58297 | -4.67476 | H64 | 4.713525 | -1.24508 | -2.77584 |
| H65 | 2.163517 | -2.85163 | -3.01334 | H65 | 2.854014 | -2.37803 | -1.62674 |
| H66 | 3.819095 | -0.4187 | 0.126063 | H66 | 4.041203 | -0.56239 | 2.091621 |
| H67 | 5.086296 | 0.869622 | -1.55136 | H67 | 5.918106 | 0.542018 | 0.945789 |
| C68 | -1.24031 | 2.787857 | -1.78502 | C68 | -0.8588 | 3.214511 | 0.184472 |
| C69 | -0.16018 | 1.953707 | -1.06278 | C69 | -0.25795 | 2.195762 | -0.81744 |
| C70 | 1.14421 | 1.571587 | -1.84497 | C70 | 0.991321 | 2.808932 | -1.5869 |
| C71 | 0.681335 | 4.089993 | 0.21131 | C71 | -1.87967 | 3.005975 | -2.76986 |

| | | | | | | | |
|-------------------|----------|----------|----------|-------------------|----------|----------|----------|
| C72 | 0.933303 | 1.996982 | 1.109036 | C72 | -0.99679 | 0.882997 | -2.71721 |
| C73 | 1.157755 | 4.170013 | 1.670497 | C73 | -2.39057 | 2.167577 | -3.95803 |
| H74 | -0.13753 | 4.77855 | -0.00167 | H74 | -1.17039 | 3.779501 | -3.08386 |
| H75 | 1.493071 | 4.27488 | -0.50732 | H75 | -2.69378 | 3.484488 | -2.22395 |
| H76 | 2.027916 | 4.807761 | 1.826996 | H76 | -3.44511 | 1.904876 | -3.85014 |
| H77 | 0.350068 | 4.465143 | 2.347887 | H77 | -2.21992 | 2.628417 | -4.9315 |
| N78 | 0.255094 | 2.685692 | 0.162502 | N78 | -1.21933 | 1.971741 | -1.95805 |
| O79 | 1.534553 | 2.802234 | 1.994194 | O79 | -1.61939 | 0.93375 | -3.9033 |
| O80 | 1.03332 | 0.760221 | 1.157098 | O80 | -0.3115 | -0.10484 | -2.38448 |
| H81 | 2.598643 | -4.67009 | 0.098754 | H81 | 2.024153 | -4.48548 | 1.505407 |
| N82 | -2.01218 | -2.27816 | 0.841469 | N82 | -1.97523 | -2.22442 | -0.52942 |
| C83 | -1.55239 | -3.20774 | -0.2213 | C83 | -0.81266 | -2.83566 | -1.22049 |
| H84 | -1.91945 | -2.91651 | -1.21669 | H84 | -0.52645 | -2.2433 | -2.09527 |
| C85 | 1.429962 | 2.168658 | -6.10242 | H85 | 0.593505 | 3.619824 | -2.20985 |
| C86 | 1.67575 | 3.221285 | -5.21928 | C86 | 4.451846 | 4.573964 | 0.330182 |
| C87 | 1.583128 | 3.014114 | -3.84295 | C87 | 3.261144 | 5.295305 | 0.214795 |
| C88 | 1.236783 | 1.756973 | -3.33585 | C88 | 2.150006 | 4.714793 | -0.38973 |
| C89 | 0.999274 | 0.705823 | -4.22574 | C89 | 2.189726 | 3.397545 | -0.87533 |
| C90 | 1.094105 | 0.909324 | -5.60132 | C90 | 3.399925 | 2.698549 | -0.77949 |
| H91 | 1.5033 | 2.328487 | -7.17422 | C91 | 4.51859 | 3.278304 | -0.1774 |
| H92 | 1.942904 | 4.202407 | -5.60153 | H92 | 5.323446 | 5.027757 | 0.793108 |
| H93 | 1.782758 | 3.835665 | -3.15807 | H93 | 3.203195 | 6.315 | 0.585274 |
| H94 | 0.732758 | -0.26941 | -3.83108 | H94 | 1.234519 | 5.292507 | -0.48808 |
| H95 | 0.90559 | 0.08489 | -6.28344 | H95 | 3.493864 | 1.705805 | -1.21118 |
| H96 | 2.008898 | 2.037484 | -1.36006 | H96 | 5.447337 | 2.718932 | -0.12652 |
| C97 | -2.37539 | 3.202775 | -0.8314 | C97 | -0.06893 | 3.303609 | 1.506533 |
| H98 | -2.0229 | 3.684175 | 0.084488 | H98 | -0.32646 | 2.465495 | 2.160047 |
| H99 | -3.04764 | 3.903648 | -1.33642 | H99 | 1.010091 | 3.286186 | 1.365043 |
| H100 | -2.96752 | 2.33007 | -0.54796 | H100 | -0.32412 | 4.229422 | 2.033062 |
| C101 | -1.87503 | 2.125358 | -3.01609 | C101 | -2.33603 | 2.996794 | 0.536178 |
| H102 | -1.16726 | 1.954688 | -3.82284 | H102 | -2.99866 | 2.905767 | -0.32561 |
| H103 | -2.32138 | 1.170245 | -2.73907 | H103 | -2.46209 | 2.087424 | 1.120759 |
| H104 | -2.6719 | 2.769437 | -3.40286 | H104 | -2.6946 | 3.829948 | 1.149624 |
| H105 | -0.74097 | 3.706022 | -2.13749 | H105 | -0.79168 | 4.200818 | -0.30435 |
| X | 0.335144 | 1.892742 | -1.24452 | H106 | 1.739713 | 0.822751 | 0.183774 |
| | | | | H107 | 1.806645 | 0.475789 | -0.59764 |
| C3_ER_Cheltop_TS1 | | | | C3_ER_Cheltop_TS3 | | | |
| C1 | -4.23697 | -3.40379 | 1.037604 | C1 | -4.17391 | -3.53776 | 1.247801 |
| C2 | -2.21525 | -4.53811 | 0.282813 | C2 | -2.1636 | -4.5345 | 0.299761 |
| C3 | -3.7345 | -4.45052 | -0.01029 | C3 | -3.70167 | -4.50714 | 0.116194 |
| C4 | -2.93366 | -3.03925 | 1.788053 | C4 | -2.83619 | -3.12007 | 1.903142 |
| H5 | -4.95871 | -3.84224 | 1.734542 | H5 | -4.79723 | -4.0525 | 1.986577 |
| H6 | -3.93999 | -4.14694 | -1.04179 | H6 | -3.99192 | -4.16217 | -0.88136 |
| H7 | -3.07343 | -2.52002 | 2.736178 | H7 | -2.93018 | -2.64016 | 2.876748 |
| H8 | -4.7069 | -2.53277 | 0.579937 | | | | |

| | | | | | | | |
|------|----------|----------|----------|------|----------|----------|----------|
| H9 | -1.71352 | -5.40991 | -0.13599 | H8 | -4.74112 | -2.68715 | 0.873269 |
| H10 | -4.20183 | -5.42745 | 0.142464 | H9 | -1.65632 | -5.36863 | -0.18411 |
| C11 | -2.18494 | -4.38295 | 1.82002 | H10 | -4.11283 | -5.51197 | 0.248048 |
| H12 | -1.17844 | -4.30363 | 2.241419 | C11 | -2.02579 | -4.42616 | 1.835053 |
| H13 | -2.73946 | -5.17339 | 2.333472 | H12 | -0.99492 | -4.31405 | 2.184016 |
| C14 | -0.0814 | -3.18831 | -0.30531 | H13 | -2.504 | -5.25724 | 2.360976 |
| N15 | 0.643368 | -2.13224 | -0.43258 | C14 | -0.12996 | -3.08624 | -0.34417 |
| C16 | 2.090921 | -2.55746 | -0.38447 | N15 | 0.558306 | -2.00326 | -0.46557 |
| C17 | 1.950272 | -4.10526 | -0.55063 | C16 | 2.024689 | -2.37885 | -0.45344 |
| P18 | -1.9657 | -0.60077 | 0.636026 | C17 | 1.92601 | -3.9284 | -0.65016 |
| Ir19 | -0.0877 | -0.05098 | -0.60624 | P18 | -2.08363 | -0.59104 | 0.763588 |
| C20 | -1.87383 | 0.132562 | 2.307403 | Ir19 | -0.20852 | 0.007456 | -0.70942 |
| C21 | -1.42639 | 1.390446 | 4.773565 | C20 | -1.93811 | 0.058438 | 2.469403 |
| C22 | -1.25744 | -0.56303 | 3.357272 | C21 | -1.52665 | 1.140584 | 5.028787 |
| C23 | -2.24852 | 1.47126 | 2.500243 | C22 | -1.2344 | -0.66373 | 3.445348 |
| C24 | -2.02879 | 2.093043 | 3.728476 | C23 | -2.42027 | 1.338387 | 2.786728 |
| C25 | -1.04127 | 0.06256 | 4.584289 | C24 | -2.22747 | 1.866176 | 4.063956 |
| H26 | -2.71134 | 2.029504 | 1.695049 | C25 | -1.02797 | -0.12369 | 4.713677 |
| H27 | -2.33575 | 3.125749 | 3.871008 | H26 | -2.95392 | 1.92142 | 2.043852 |
| H28 | -0.57086 | -0.48897 | 5.393277 | H27 | -2.63462 | 2.843955 | 4.308701 |
| H29 | -1.25641 | 1.875971 | 5.73006 | H28 | -0.48389 | -0.69688 | 5.458863 |
| O30 | 0.546699 | -4.3669 | -0.27301 | H29 | -1.37429 | 1.556237 | 6.020518 |
| C31 | 2.680056 | -2.28384 | 1.00556 | O30 | 0.535733 | -4.23937 | -0.35949 |
| C32 | 1.884968 | -1.89087 | 2.080368 | C31 | 2.623819 | -2.12287 | 0.936338 |
| C33 | 4.045358 | -2.53309 | 1.224749 | C32 | 1.853023 | -1.683 | 2.01034 |
| C34 | 2.441624 | -1.71512 | 3.348114 | C33 | 3.970043 | -2.45173 | 1.167851 |
| H35 | 0.835585 | -1.68915 | 1.925743 | C34 | 2.415396 | -1.52924 | 3.278408 |
| C36 | 4.59977 | -2.36339 | 2.490416 | H35 | 0.814834 | -1.43705 | 1.859354 |
| H37 | 4.676775 | -2.84811 | 0.398189 | C36 | 4.532551 | -2.30494 | 2.433098 |
| C38 | 3.798395 | -1.9465 | 3.557258 | H37 | 4.586802 | -2.81657 | 0.350896 |
| H39 | 1.808562 | -1.38029 | 4.165074 | C38 | 3.756133 | -1.83469 | 3.49549 |
| H40 | 5.658517 | -2.55141 | 2.643984 | H39 | 1.796188 | -1.15936 | 4.090675 |
| H41 | 4.233734 | -1.80462 | 4.542261 | H40 | 5.57764 | -2.55715 | 2.588886 |
| C42 | -3.61124 | -0.15826 | -0.03348 | H41 | 4.195968 | -1.71371 | 4.481261 |
| C43 | -4.69075 | 0.199727 | 0.789577 | C42 | -3.81763 | -0.28998 | 0.234054 |
| C44 | -3.83181 | -0.34322 | -1.40733 | C43 | -4.86586 | -0.00383 | 1.121163 |
| C45 | -5.95668 | 0.400633 | 0.239718 | C44 | -4.11651 | -0.55465 | -1.11309 |
| H46 | -4.54959 | 0.319936 | 1.858643 | C45 | -6.18303 | 0.038101 | 0.661658 |
| C47 | -5.10061 | -0.15226 | -1.95152 | H46 | -4.66377 | 0.176963 | 2.171543 |
| C48 | -6.16365 | 0.228655 | -1.13025 | C47 | -5.4346 | -0.52498 | -1.56506 |
| H49 | -6.7827 | 0.688323 | 0.883795 | C48 | -6.47248 | -0.22529 | -0.67875 |
| H50 | -5.25682 | -0.29101 | -3.01734 | H49 | -6.98544 | 0.266988 | 1.357191 |
| H51 | -7.15035 | 0.387963 | -1.55524 | H50 | -5.65058 | -0.72894 | -2.6098 |
| H52 | -0.80705 | -0.47018 | -1.92904 | H51 | -7.49947 | -0.19702 | -1.0302 |
| H53 | 1.251525 | 0.226844 | -1.45559 | H52 | -1.02025 | -0.54962 | -1.92828 |

| | | | | | | | |
|-----|----------|----------|----------|-----|----------|----------|----------|
| H54 | -0.94196 | -1.591 | 3.215367 | H53 | 1.72159 | 2.527477 | -1.16878 |
| H55 | -3.00516 | -0.62808 | -2.05025 | H54 | -0.8435 | -1.64797 | 3.21409 |
| H56 | 2.159778 | -4.47268 | -1.55661 | H55 | -3.31237 | -0.77063 | -1.81049 |
| C57 | 4.265378 | -0.62228 | -3.61509 | H56 | 2.134075 | -4.25923 | -1.66958 |
| C58 | 3.4549 | -1.72636 | -3.87634 | C57 | 4.141677 | -0.59936 | -3.80512 |
| C59 | 2.752238 | -2.34205 | -2.84157 | C58 | 3.091771 | -1.49604 | -4.01554 |
| C60 | 2.868658 | -1.88696 | -1.52082 | C59 | 2.413107 | -2.04204 | -2.92887 |
| C61 | 3.663171 | -0.75735 | -1.27609 | C60 | 2.772866 | -1.71436 | -1.6126 |
| C62 | 4.35317 | -0.13035 | -2.31377 | C61 | 3.78943 | -0.77264 | -1.41492 |
| H63 | 4.805531 | -0.13706 | -4.42229 | C62 | 4.474126 | -0.22692 | -2.50331 |
| H64 | 3.356692 | -2.10313 | -4.89021 | H63 | 4.681405 | -0.17975 | -4.64905 |
| H65 | 2.103388 | -3.1785 | -3.08312 | H64 | 2.801152 | -1.77137 | -5.02519 |
| H66 | 3.744371 | -0.36799 | -0.26724 | H65 | 1.584362 | -2.72014 | -3.1136 |
| H67 | 4.965157 | 0.741514 | -2.10039 | H66 | 4.057208 | -0.46601 | -0.41082 |
| C68 | -1.21423 | 2.858865 | -1.70985 | H67 | 5.26941 | 0.491987 | -2.32837 |
| C69 | -0.14824 | 2.030781 | -0.9646 | C68 | -1.74472 | 2.884943 | -1.57412 |
| C70 | 1.110848 | 1.5549 | -1.65304 | C69 | -0.4359 | 2.338554 | -0.955 |
| C71 | 0.58543 | 4.109454 | 0.445775 | C70 | 0.844195 | 2.987513 | -1.63784 |
| C72 | 0.819649 | 1.980157 | 1.269154 | C71 | -0.27929 | 4.129116 | 0.97043 |
| C73 | 0.942734 | 4.131703 | 1.940644 | C72 | 0.509064 | 1.992303 | 1.285203 |
| H74 | -0.23169 | 4.789703 | 0.200734 | C73 | 0.183688 | 3.918564 | 2.421509 |
| H75 | 1.445765 | 4.342036 | -0.19867 | H74 | -1.2642 | 4.59254 | 0.909279 |
| H76 | 1.78012 | 4.781681 | 2.19478 | H75 | 0.429755 | 4.743695 | 0.406546 |
| H77 | 0.075272 | 4.374053 | 2.562758 | H76 | 0.887585 | 4.673435 | 2.773308 |
| N78 | 0.196579 | 2.700948 | 0.305887 | H77 | -0.65339 | 3.831909 | 3.117806 |
| O79 | 1.329242 | 2.759828 | 2.232073 | N78 | -0.29775 | 2.733756 | 0.483452 |
| O80 | 0.947665 | 0.747029 | 1.2716 | O79 | 0.867881 | 2.639222 | 2.398083 |
| H81 | 2.544921 | -4.65831 | 0.174872 | O80 | 0.894917 | 0.838256 | 1.051822 |
| N82 | -2.00716 | -2.27384 | 0.904676 | H81 | 2.546666 | -4.48105 | 0.053274 |
| C83 | -1.58403 | -3.19817 | -0.17796 | N82 | -2.01352 | -2.27862 | 0.981213 |
| H84 | -1.98428 | -2.90141 | -1.1587 | C83 | -1.62168 | -3.15344 | -0.15296 |
| C85 | 1.726606 | 2.093438 | -5.87365 | H84 | -2.08381 | -2.84674 | -1.10204 |
| C86 | 1.975347 | 3.128744 | -4.96989 | C85 | 1.207018 | 2.861139 | -5.95217 |
| C87 | 1.782523 | 2.922795 | -3.60511 | C86 | 0.571408 | 3.93651 | -5.3266 |
| C88 | 1.334152 | 1.682992 | -3.13131 | C87 | 0.469592 | 3.978625 | -3.93687 |
| C89 | 1.094321 | 0.649345 | -4.03786 | C88 | 0.990167 | 2.945631 | -3.14357 |
| C90 | 1.290546 | 0.85443 | -5.40304 | C89 | 1.654616 | 1.889966 | -3.78082 |
| H91 | 1.87403 | 2.252987 | -6.93777 | C90 | 1.757587 | 1.84405 | -5.17149 |
| H92 | 2.317142 | 4.095709 | -5.32771 | H91 | 1.286373 | 2.827794 | -7.03479 |
| H93 | 1.975725 | 3.730972 | -2.90259 | H92 | 0.158827 | 4.746536 | -5.9215 |
| H94 | 0.757907 | -0.31303 | -3.66846 | H93 | -0.02145 | 4.824981 | -3.46217 |
| H95 | 1.101824 | 0.043332 | -6.10058 | H94 | 2.117976 | 1.108381 | -3.19184 |
| H96 | 2.01225 | 1.837107 | -1.10037 | H95 | 2.280251 | 1.014164 | -5.6382 |
| C97 | -2.41007 | 3.197392 | -0.8025 | H96 | 0.845648 | 4.043328 | -1.34881 |
| H98 | -2.11585 | 3.624467 | 0.159458 | C97 | -2.951 | 2.928912 | -0.6296 |

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|--------------------|----------|----------|----------|--------------------|----------|----------|----------|
| H99 | -3.06351 | 3.91886 | -1.3027 | H98 | -2.79653 | 3.555426 | 0.251551 |
| H100 | -3.00106 | 2.299935 | -0.60673 | H99 | -3.81787 | 3.329763 | -1.16489 |
| C101 | -1.75216 | 2.244487 | -3.0099 | H100 | -3.21708 | 1.929716 | -0.2924 |
| H102 | -0.99658 | 2.161507 | -3.78665 | C101 | -2.14769 | 2.146223 | -2.86327 |
| H103 | -2.15892 | 1.250364 | -2.8201 | H102 | -1.30106 | 1.94138 | -3.51701 |
| H104 | -2.5623 | 2.872087 | -3.39539 | H103 | -2.61038 | 1.190749 | -2.60853 |
| H105 | -0.72062 | 3.806319 | -1.98683 | H104 | -2.87584 | 2.741054 | -3.42328 |
| X | 0.335144 | 1.892742 | -1.24452 | H105 | -1.51825 | 3.926135 | -1.85453 |
| | | | | H106 | 1.104133 | 0.10416 | -1.60944 |
| | | | | H107 | 0.114904 | 1.046027 | -1.83155 |
| C3_ER_Cheltop_int1 | | | | | | | |
| C1 | -4.24811 | -3.40733 | 0.803086 | | | | |
| C2 | -2.18985 | -4.55236 | 0.175567 | | | | |
| C3 | -3.68894 | -4.4622 | -0.208 | C3_ER_Cheltop_PROD | | | |
| C4 | -2.99282 | -3.05031 | 1.633905 | C1 | -4.26675 | -3.67258 | 0.615979 |
| H5 | -5.01504 | -3.83888 | 1.454416 | C2 | -2.1218 | -4.62818 | -0.05525 |
| H6 | -3.83165 | -4.16453 | -1.25186 | C3 | -3.61261 | -4.57791 | -0.48109 |
| H7 | -3.19331 | -2.5321 | 2.571516 | C4 | -3.05703 | -3.32986 | 1.516942 |
| H8 | -4.68157 | -2.53295 | 0.316267 | H5 | -5.0251 | -4.21571 | 1.18934 |
| H9 | -1.6633 | -5.42391 | -0.21309 | H6 | -3.74165 | -4.17818 | -1.49199 |
| H10 | -4.16831 | -5.43652 | -0.07767 | H7 | -3.30099 | -2.91577 | 2.496103 |
| C11 | -2.25264 | -4.39728 | 1.711644 | H8 | -4.73625 | -2.77643 | 0.207913 |
| H12 | -1.27282 | -4.32177 | 2.192787 | H9 | -1.53944 | -5.42995 | -0.50896 |
| H13 | -2.83988 | -5.18627 | 2.189713 | H10 | -4.03503 | -5.58662 | -0.47236 |
| C14 | -0.0273 | -3.2004 | -0.30039 | C11 | -2.24177 | -4.63387 | 1.484689 |
| N15 | 0.679364 | -2.12709 | -0.33716 | H12 | -1.28254 | -4.55527 | 2.005016 |
| C16 | 2.124962 | -2.5263 | -0.21621 | H13 | -2.79388 | -5.49923 | 1.862213 |
| C17 | 2.026636 | -4.04805 | -0.54646 | C14 | -0.02563 | -3.12019 | -0.26549 |
| P18 | -1.90389 | -0.60785 | 0.624448 | N15 | 0.652759 | -2.01852 | -0.29784 |
| Ir19 | -0.11649 | -0.09114 | -0.62362 | C16 | 2.133951 | -2.34172 | -0.23135 |
| C20 | -1.72672 | 0.063225 | 2.315852 | C17 | 2.081967 | -3.90841 | -0.16193 |
| C21 | -1.21879 | 1.218265 | 4.822343 | P18 | -2.09326 | -0.73994 | 0.729234 |
| C22 | -1.29919 | -0.73137 | 3.387349 | Ir19 | -0.13178 | -0.14897 | -0.56584 |
| C23 | -1.89023 | 1.444918 | 2.508807 | C20 | -1.94911 | -0.22305 | 2.478863 |
| C24 | -1.63879 | 2.015544 | 3.75474 | C21 | -1.38944 | 0.705265 | 5.073425 |
| C25 | -1.05324 | -0.15435 | 4.634624 | C22 | -1.35148 | -1.06792 | 3.424222 |
| H26 | -2.20453 | 2.074789 | 1.683938 | C23 | -2.26196 | 1.096297 | 2.84868 |
| H27 | -1.77441 | 3.084683 | 3.893851 | C24 | -1.98592 | 1.552634 | 4.136944 |
| H28 | -0.72933 | -0.78174 | 5.46021 | C25 | -1.07609 | -0.60577 | 4.712407 |
| H29 | -1.02328 | 1.664189 | 5.792851 | H26 | -2.72181 | 1.768936 | 2.129723 |
| O30 | 0.623376 | -4.367 | -0.31047 | H27 | -2.24339 | 2.571478 | 4.4144 |
| C31 | 2.605647 | -2.37186 | 1.23196 | H28 | -0.61547 | -1.27446 | 5.434251 |
| C32 | 1.788996 | -1.8707 | 2.242788 | H29 | -1.1736 | 1.063146 | 6.075562 |
| C33 | 3.906854 | -2.78757 | 1.554141 | O30 | 0.667528 | -4.25132 | -0.18437 |
| C34 | 2.263792 | -1.76778 | 3.551829 | C31 | 2.76164 | -1.83765 | 1.06586 |
| H35 | 0.792442 | -1.53115 | 2.007884 | C32 | 1.992218 | -1.36108 | 2.127628 |
| | | | | C33 | 4.145165 | -1.99225 | 1.2508 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| C36 | 4.379958 | -2.69146 | 2.859351 | C34 | 2.592126 | -1.00091 | 3.3353 |
| H37 | 4.560612 | -3.16998 | 0.774192 | H35 | 0.923606 | -1.24532 | 2.019398 |
| C38 | 3.557648 | -2.17623 | 3.865234 | C36 | 4.742825 | -1.64162 | 2.458466 |
| H39 | 1.616536 | -1.35218 | 4.318873 | H37 | 4.758846 | -2.38191 | 0.443134 |
| H40 | 5.391548 | -3.01213 | 3.090809 | C38 | 3.967723 | -1.13605 | 3.504888 |
| H41 | 3.928305 | -2.09351 | 4.882891 | H39 | 1.971375 | -0.6093 | 4.136293 |
| C42 | -3.56426 | -0.10201 | 0.03967 | H40 | 5.815419 | -1.76112 | 2.580891 |
| C43 | -4.55538 | 0.380686 | 0.905932 | H41 | 4.435676 | -0.8554 | 4.443988 |
| C44 | -3.89771 | -0.38602 | -1.29464 | C42 | -3.77867 | -0.23573 | 0.204778 |
| C45 | -5.85131 | 0.598784 | 0.435092 | C43 | -4.83242 | 0.015874 | 1.095695 |
| H46 | -4.32536 | 0.583035 | 1.946516 | C44 | -4.03445 | -0.23328 | -1.17659 |
| C47 | -5.19309 | -0.1737 | -1.75821 | C45 | -6.11396 | 0.278878 | 0.61055 |
| C48 | -6.17205 | 0.324665 | -0.89443 | H46 | -4.65618 | 0.004359 | 2.166855 |
| H49 | -6.61094 | 0.97954 | 1.111632 | C47 | -5.31793 | 0.021617 | -1.65779 |
| H50 | -5.43809 | -0.39142 | -2.79371 | C48 | -6.36071 | 0.281649 | -0.76438 |
| H51 | -7.1814 | 0.495517 | -1.25717 | H49 | -6.92261 | 0.474954 | 1.308859 |
| H52 | -0.90346 | -0.58102 | -1.88882 | H50 | -5.50311 | 0.022905 | -2.72808 |
| H53 | 1.393004 | 0.43891 | -1.77407 | H51 | -7.36032 | 0.483987 | -1.13711 |
| H54 | -1.13969 | -1.79503 | 3.247921 | H52 | -0.70661 | -0.74134 | -1.88963 |
| H55 | -3.14004 | -0.77127 | -1.96974 | H53 | 1.664342 | 2.510185 | -1.33961 |
| H56 | 2.248036 | -4.29336 | -1.58771 | H54 | -1.08698 | -2.08362 | 3.147017 |
| C57 | 4.348209 | -0.15448 | -3.09485 | H55 | -3.22166 | -0.4323 | -1.87047 |
| C58 | 3.518542 | -1.19073 | -3.52488 | H56 | 2.559862 | -4.40029 | -1.01002 |
| C59 | 2.821912 | -1.96063 | -2.59579 | C57 | 3.806147 | -0.8761 | -3.96026 |
| C60 | 2.953724 | -1.723 | -1.2193 | C58 | 2.943297 | -1.97246 | -3.94563 |
| C61 | 3.776654 | -0.67029 | -0.79885 | C59 | 2.442104 | -2.44879 | -2.73539 |
| C62 | 4.469797 | 0.105197 | -1.73047 | C60 | 2.793261 | -1.8431 | -1.52201 |
| H63 | 4.883622 | 0.451519 | -3.81952 | C61 | 3.643716 | -0.73188 | -1.54973 |
| H64 | 3.397339 | -1.38608 | -4.58587 | C62 | 4.151593 | -0.25747 | -2.75944 |
| H65 | 2.151145 | -2.73462 | -2.9574 | H63 | 4.197514 | -0.50036 | -4.90097 |
| H66 | 3.868504 | -0.44745 | 0.257741 | H64 | 2.657998 | -2.4563 | -4.87534 |
| H67 | 5.107519 | 0.913973 | -1.38428 | H65 | 1.747777 | -3.28578 | -2.74901 |
| C68 | -1.25734 | 2.752592 | -1.83533 | H66 | 3.898903 | -0.22157 | -0.62877 |
| C69 | -0.15888 | 1.934141 | -1.12312 | H67 | 4.810748 | 0.605876 | -2.76218 |
| C70 | 1.135685 | 1.550476 | -1.92553 | C68 | -1.77011 | 3.35101 | -1.52363 |
| C71 | 0.701422 | 4.091289 | 0.102896 | C69 | -0.43466 | 2.744915 | -1.01147 |
| C72 | 0.967784 | 2.013326 | 1.030969 | C70 | 0.859572 | 3.090628 | -1.80201 |
| C73 | 1.201786 | 4.195465 | 1.55248 | C71 | -0.07164 | 4.481822 | 0.846769 |
| H74 | -0.12109 | 4.7761 | -0.10829 | C72 | 0.429445 | 2.271054 | 1.29545 |
| H75 | 1.501354 | 4.264344 | -0.6316 | C73 | 0.17306 | 4.264663 | 2.344684 |
| H76 | 2.074722 | 4.835085 | 1.683988 | H74 | -0.97448 | 5.060878 | 0.646022 |
| H77 | 0.405683 | 4.503034 | 2.238068 | H75 | 0.778801 | 4.973861 | 0.360319 |
| N78 | 0.274806 | 2.686389 | 0.084182 | H76 | 0.873541 | 4.972524 | 2.788078 |
| O79 | 1.583139 | 2.832843 | 1.893129 | H77 | -0.75983 | 4.251474 | 2.91802 |
| O80 | 1.06656 | 0.777357 | 1.098932 | N78 | -0.20625 | 3.086009 | 0.40329 |

| | | | | | | | |
|-------------------|----------|----------|----------|------|----------|----------|----------|
| H81 | 2.626367 | -4.66822 | 0.116959 | O79 | 0.756296 | 2.941839 | 2.412915 |
| N82 | -2.0094 | -2.2882 | 0.80949 | O80 | 0.683466 | 1.072865 | 1.180199 |
| C83 | -1.53143 | -3.21418 | -0.24843 | H81 | 2.496237 | -4.28957 | 0.77115 |
| H84 | -1.87774 | -2.91657 | -1.24924 | N82 | -2.11476 | -2.43393 | 0.794299 |
| C85 | 1.348045 | 2.218715 | -6.1783 | C83 | -1.52831 | -3.22106 | -0.31676 |
| C86 | 1.604241 | 3.257122 | -5.28135 | H84 | -1.83197 | -2.8464 | -1.30422 |
| C87 | 1.536953 | 3.025198 | -3.90749 | C85 | 0.886794 | 2.58168 | -6.09768 |
| C88 | 1.206226 | 1.757836 | -3.41625 | C86 | 0.67256 | 3.84214 | -5.53559 |
| C89 | 0.956684 | 0.721235 | -4.31988 | C87 | 0.675388 | 3.998196 | -4.14913 |
| C90 | 1.026147 | 0.949045 | -5.6934 | C88 | 0.880588 | 2.900135 | -3.30224 |
| H91 | 1.400754 | 2.397733 | -7.24837 | C89 | 1.118418 | 1.644244 | -3.87493 |
| H92 | 1.858882 | 4.246408 | -5.65104 | C90 | 1.118048 | 1.48763 | -5.26127 |
| H93 | 1.743873 | 3.836097 | -3.21228 | H91 | 0.885641 | 2.457743 | -7.17661 |
| H94 | 0.697361 | -0.26078 | -3.93705 | H92 | 0.506847 | 4.704498 | -6.17526 |
| H95 | 0.826798 | 0.136676 | -6.38686 | H93 | 0.507897 | 4.984302 | -3.71995 |
| H96 | 2.007019 | 2.011555 | -1.4491 | H94 | 1.300421 | 0.786941 | -3.23694 |
| C97 | -2.37398 | 3.176806 | -0.86352 | H95 | 1.307383 | 0.504988 | -5.6846 |
| H98 | -2.00478 | 3.684591 | 0.031543 | H96 | 1.064601 | 4.147302 | -1.59497 |
| H99 | -3.06606 | 3.858927 | -1.36764 | C97 | -2.88915 | 3.263644 | -0.47365 |
| H100 | -2.94945 | 2.305824 | -0.54335 | H98 | -2.65602 | 3.77273 | 0.464138 |
| C101 | -1.91004 | 2.065256 | -3.04328 | H99 | -3.80506 | 3.707949 | -0.87328 |
| H102 | -1.2186 | 1.905675 | -3.86645 | H100 | -3.11079 | 2.219078 | -0.2425 |
| H103 | -2.32568 | 1.101075 | -2.75047 | C101 | -2.25545 | 2.666225 | -2.81468 |
| H104 | -2.73147 | 2.687567 | -3.41416 | H102 | -1.56994 | 2.79278 | -3.64878 |
| H105 | -0.77086 | 3.668125 | -2.21289 | H103 | -2.38958 | 1.593542 | -2.64225 |
| X | 0.335144 | 1.892742 | -1.24452 | H104 | -3.22617 | 3.080232 | -3.10374 |
| | | | | H105 | -1.5626 | 4.408594 | -1.74717 |
| | | | | H106 | 1.192192 | 0.157971 | -1.38755 |
| | | | | H107 | -0.63743 | 1.627002 | -1.08584 |
| C3_ER_Cheltop_TS2 | | | | | | | |
| C1 | -4.17685 | -3.43818 | 1.005979 | | | | |
| C2 | -2.15991 | -4.48112 | 0.118916 | | | | |
| C3 | -3.6871 | -4.39428 | -0.12836 | | | | |
| C4 | -2.8513 | -3.05527 | 1.705867 | | | | |
| H5 | -4.82221 | -3.95886 | 1.721568 | | | | |
| H6 | -3.92205 | -4.01206 | -1.12693 | | | | |
| H7 | -2.96074 | -2.57438 | 2.677412 | | | | |
| H8 | -4.72994 | -2.57901 | 0.631905 | | | | |
| H9 | -1.66751 | -5.33303 | -0.34795 | | | | |
| H10 | -4.13797 | -5.38696 | -0.04308 | | | | |
| C11 | -2.08036 | -4.38612 | 1.659261 | | | | |
| H12 | -1.06114 | -4.31292 | 2.049305 | | | | |
| H13 | -2.60798 | -5.2015 | 2.161882 | | | | |
| C14 | -0.03018 | -3.112 | -0.34897 | | | | |
| N15 | 0.715403 | -2.06246 | -0.38933 | | | | |
| C16 | 2.157765 | -2.55361 | -0.25169 | | | | |
| C17 | 1.976885 | -4.10576 | -0.38143 | | | | |

| | | | |
|------|----------|----------|----------|
| P18 | -1.99026 | -0.55544 | 0.60646 |
| Ir19 | -0.24064 | 0.065871 | -0.61511 |
| C20 | -1.84075 | 0.08007 | 2.310682 |
| C21 | -1.35336 | 1.111739 | 4.873133 |
| C22 | -1.14716 | -0.68124 | 3.265106 |
| C23 | -2.27699 | 1.370396 | 2.650242 |
| C24 | -2.04371 | 1.874605 | 3.929493 |
| C25 | -0.90585 | -0.16673 | 4.537233 |
| H26 | -2.79629 | 1.981349 | 1.922895 |
| H27 | -2.40764 | 2.864528 | 4.19122 |
| H28 | -0.37013 | -0.76799 | 5.2659 |
| H29 | -1.16665 | 1.511102 | 5.865641 |
| O30 | 0.550552 | -4.31232 | -0.28136 |
| C31 | 2.722904 | -2.25972 | 1.140182 |
| C32 | 2.009082 | -1.5838 | 2.124021 |
| C33 | 3.995174 | -2.76635 | 1.456795 |
| C34 | 2.555674 | -1.39353 | 3.395513 |
| H35 | 1.037492 | -1.18172 | 1.895534 |
| C36 | 4.538567 | -2.58591 | 2.724671 |
| H37 | 4.570688 | -3.29353 | 0.699942 |
| C38 | 3.817545 | -1.89464 | 3.702247 |
| H39 | 1.986355 | -0.84284 | 4.138932 |
| H40 | 5.52529 | -2.98114 | 2.948464 |
| H41 | 4.243022 | -1.74731 | 4.690678 |
| C42 | -3.70514 | -0.26474 | 0.03704 |
| C43 | -4.74078 | 0.055213 | 0.928994 |
| C44 | -4.02662 | -0.63668 | -1.27832 |
| C45 | -6.06848 | 0.031734 | 0.500598 |
| H46 | -4.52296 | 0.307521 | 1.960444 |
| C47 | -5.35519 | -0.67096 | -1.69708 |
| C48 | -6.3809 | -0.33388 | -0.80978 |
| H49 | -6.8599 | 0.287311 | 1.199168 |
| H50 | -5.58921 | -0.9589 | -2.71772 |
| H51 | -7.41589 | -0.35881 | -1.13691 |
| H52 | -1.0512 | -0.40472 | -1.87381 |
| H53 | 1.604243 | 2.033348 | -1.52451 |
| H54 | -0.78821 | -1.67173 | 3.009966 |
| H55 | -3.23699 | -0.89639 | -1.97592 |
| H56 | 2.309284 | -4.51035 | -1.33881 |
| C57 | 4.48604 | -1.02211 | -3.57563 |
| C58 | 3.458785 | -1.94488 | -3.78727 |
| C59 | 2.731169 | -2.43399 | -2.70657 |
| C60 | 3.013447 | -2.01625 | -1.39696 |
| C61 | 4.037932 | -1.08542 | -1.19331 |
| C62 | 4.769951 | -0.59389 | -2.27905 |

| | | | |
|------|----------|----------|----------|
| H63 | 5.059169 | -0.6403 | -4.41547 |
| H64 | 3.221603 | -2.27858 | -4.79336 |
| H65 | 1.912368 | -3.12271 | -2.89632 |
| H66 | 4.261384 | -0.73194 | -0.19328 |
| H67 | 5.563427 | 0.127526 | -2.10657 |
| C68 | -1.82594 | 2.795402 | -1.51803 |
| C69 | -0.53954 | 2.174965 | -0.91833 |
| C70 | 0.751081 | 2.677219 | -1.75756 |
| C71 | -0.26387 | 4.184056 | 0.813806 |
| C72 | 0.603967 | 2.104505 | 1.225311 |
| C73 | 0.337841 | 4.105342 | 2.22836 |
| H74 | -1.26054 | 4.62477 | 0.810426 |
| H75 | 0.369017 | 4.759736 | 0.126776 |
| H76 | 1.049192 | 4.90012 | 2.454355 |
| H77 | -0.43221 | 4.058668 | 3.003167 |
| N78 | -0.28636 | 2.757303 | 0.449865 |
| O79 | 1.053171 | 2.840366 | 2.245915 |
| O80 | 0.996956 | 0.938144 | 1.03372 |
| H81 | 2.451591 | -4.6524 | 0.432234 |
| N82 | -1.97116 | -2.23799 | 0.808409 |
| C83 | -1.53666 | -3.12285 | -0.29666 |
| H84 | -1.91212 | -2.79755 | -1.27613 |
| C85 | 0.471733 | 3.547247 | -6.00807 |
| C86 | -0.00924 | 4.447917 | -5.05685 |
| C87 | 0.108751 | 4.159079 | -3.69936 |
| C88 | 0.682333 | 2.95683 | -3.25118 |
| C89 | 1.217507 | 2.095345 | -4.2194 |
| C90 | 1.107863 | 2.382773 | -5.58083 |
| H91 | 0.378717 | 3.766584 | -7.06782 |
| H92 | -0.46774 | 5.381375 | -5.37106 |
| H93 | -0.24445 | 4.888598 | -2.97533 |
| H94 | 1.782586 | 1.229931 | -3.9066 |
| H95 | 1.535918 | 1.697509 | -6.30753 |
| H96 | 1.016175 | 3.636175 | -1.30036 |
| C97 | -3.02773 | 2.95987 | -0.57784 |
| H98 | -2.80676 | 3.540735 | 0.320343 |
| H99 | -3.82688 | 3.486256 | -1.11082 |
| H100 | -3.43455 | 2.001417 | -0.26957 |
| C101 | -2.28892 | 2.070368 | -2.79435 |
| H102 | -1.45954 | 1.758878 | -3.42805 |
| H103 | -2.86086 | 1.181097 | -2.5311 |
| H104 | -2.93719 | 2.726273 | -3.3846 |
| H105 | -1.54777 | 3.815605 | -1.8139 |
| H106 | 2.170064 | 0.082601 | -2.28846 |
| H107 | 1.522537 | 0.013901 | -2.64664 |

C3_ER_Chelbot

C3_ER_Chelbot_SM

| | | | |
|------|----------|----------|----------|
| C1 | -4.16247 | -2.95873 | -0.95958 |
| C2 | -2.08426 | -4.23421 | -1.11606 |
| C3 | -3.34145 | -3.85776 | -1.94525 |
| C4 | -3.25484 | -2.93737 | 0.290598 |
| H5 | -5.13432 | -3.40233 | -0.71983 |
| H6 | -3.0825 | -3.34128 | -2.87486 |
| H7 | -3.72516 | -2.57343 | 1.204659 |
| H8 | -4.33844 | -1.95088 | -1.34004 |
| H9 | -1.51971 | -5.08643 | -1.49506 |
| H10 | -3.89434 | -4.76162 | -2.21589 |
| C11 | -2.67699 | -4.36381 | 0.304223 |
| H12 | -1.92464 | -4.5257 | 1.081746 |
| H13 | -3.44503 | -5.13927 | 0.372556 |
| C14 | 0.172051 | -3.1261 | -0.46 |
| N15 | 0.971339 | -2.14999 | -0.17699 |
| C16 | 2.297827 | -2.71908 | 0.275285 |
| C17 | 1.936137 | -4.23983 | 0.36871 |
| P18 | -1.63417 | -0.58196 | 0.429118 |
| Ir19 | 0.558135 | -0.10417 | -0.60809 |
| C20 | -1.64813 | -0.55929 | 2.259773 |
| C21 | -1.48251 | -0.50155 | 5.062194 |
| C22 | -1.68372 | -1.75012 | 2.999481 |
| C23 | -1.50772 | 0.66191 | 2.940944 |
| C24 | -1.42883 | 0.687585 | 4.331736 |
| C25 | -1.6058 | -1.71889 | 4.392288 |
| H26 | -1.45714 | 1.594778 | 2.394279 |
| H27 | -1.31979 | 1.641329 | 4.839939 |
| H28 | -1.63404 | -2.64903 | 4.952397 |
| H29 | -1.42187 | -0.47965 | 6.146553 |
| O30 | 0.624701 | -4.36086 | -0.25733 |
| C31 | 2.715175 | -2.24987 | 1.666948 |
| C32 | 1.824404 | -1.61469 | 2.534679 |
| C33 | 3.990506 | -2.59299 | 2.14188 |
| C34 | 2.21117 | -1.28088 | 3.833846 |
| H35 | 0.824429 | -1.37546 | 2.207525 |
| C36 | 4.37565 | -2.26491 | 3.440322 |
| H37 | 4.691361 | -3.10652 | 1.489818 |
| C38 | 3.489776 | -1.59735 | 4.288616 |
| H39 | 1.499661 | -0.77923 | 4.483244 |
| H40 | 5.370464 | -2.52895 | 3.78748 |
| H41 | 3.794257 | -1.33591 | 5.298047 |
| C42 | -3.07062 | 0.438329 | -0.08711 |
| C43 | -3.95768 | 1.062592 | 0.79685 |

jag_C3_ER_Chelbot_int2

| | | | |
|------|----------|----------|----------|
| C1 | -3.98064 | -2.87851 | -1.56255 |
| C2 | -1.97142 | -4.23452 | -1.30007 |
| C3 | -3.05847 | -3.87029 | -2.3449 |
| C4 | -3.26549 | -2.77463 | -0.19825 |
| H5 | -4.98754 | -3.28614 | -1.42376 |
| H6 | -2.62646 | -3.42486 | -3.24667 |
| H7 | -3.85739 | -2.31033 | 0.590348 |
| H8 | -4.08311 | -1.9052 | -2.04289 |
| H9 | -1.4068 | -5.13951 | -1.52113 |
| H10 | -3.60406 | -4.76731 | -2.65063 |
| C11 | -2.77689 | -4.21882 | 0.017655 |
| H12 | -2.15703 | -4.34498 | 0.910738 |
| H13 | -3.5883 | -4.95192 | 0.028658 |
| C14 | 0.257452 | -3.24788 | -0.43211 |
| N15 | 1.022963 | -2.3415 | 0.066027 |
| C16 | 2.257395 | -3.00326 | 0.613071 |
| C17 | 2.066254 | -4.4705 | 0.096664 |
| P18 | -1.50175 | -0.57464 | 0.241258 |
| Ir19 | 0.680155 | -0.17332 | -0.31493 |
| C20 | -1.71208 | -0.57676 | 2.065442 |
| C21 | -1.95621 | -0.48352 | 4.85948 |
| C22 | -2.23479 | -1.66955 | 2.767177 |
| C23 | -1.27847 | 0.552572 | 2.78231 |
| C24 | -1.40865 | 0.600596 | 4.168017 |
| C25 | -2.35613 | -1.6202 | 4.157772 |
| H26 | -0.81499 | 1.386821 | 2.264213 |
| H27 | -1.06759 | 1.479826 | 4.70711 |
| H28 | -2.75594 | -2.4779 | 4.690881 |
| H29 | -2.05426 | -0.44758 | 5.94084 |
| O30 | 0.701515 | -4.50792 | -0.41095 |
| C31 | 2.282337 | -2.98186 | 2.141578 |
| C32 | 1.357362 | -2.26918 | 2.904046 |
| C33 | 3.274915 | -3.72335 | 2.802345 |
| C34 | 1.422823 | -2.29068 | 4.300564 |
| H35 | 0.585658 | -1.69267 | 2.416964 |
| C36 | 3.34062 | -3.74553 | 4.193463 |
| H37 | 4.014735 | -4.27235 | 2.223557 |
| C38 | 2.412151 | -3.02551 | 4.950792 |
| H39 | 0.689475 | -1.72865 | 4.870658 |
| H40 | 4.118305 | -4.32238 | 4.68585 |
| H41 | 2.462754 | -3.04148 | 6.035533 |
| C42 | -2.77663 | 0.601839 | -0.36746 |
| C43 | -3.37323 | 1.576111 | 0.445117 |

| | | | | | | | |
|-----|----------|----------|----------|-----|----------|----------|----------|
| C44 | -3.27062 | 0.572715 | -1.47319 | C44 | -3.11386 | 0.55392 | -1.72933 |
| C45 | -5.02089 | 1.822292 | 0.302518 | C45 | -4.28165 | 2.488439 | -0.09659 |
| H46 | -3.82823 | 0.960116 | 1.868777 | H46 | -3.14435 | 1.624374 | 1.50374 |
| C47 | -4.33383 | 1.328102 | -1.96066 | C47 | -4.03466 | 1.455684 | -2.2618 |
| C48 | -5.20864 | 1.9607 | -1.07174 | C48 | -4.61615 | 2.433425 | -1.44947 |
| H49 | -5.70428 | 2.302611 | 0.997054 | H49 | -4.7353 | 3.236489 | 0.547224 |
| H50 | -4.48375 | 1.421335 | -3.03268 | H50 | -4.30573 | 1.392572 | -3.31253 |
| H51 | -6.03671 | 2.552356 | -1.45113 | H51 | -5.33058 | 3.13748 | -1.86538 |
| H52 | 1.232255 | 0.274951 | 0.732036 | H52 | 0.856304 | 0.196388 | 1.185598 |
| H53 | 2.041136 | -0.16673 | -1.16949 | H53 | 1.930231 | 1.627962 | -2.38154 |
| H54 | -1.74936 | -2.70472 | 2.490644 | H54 | -2.52309 | -2.57397 | 2.248344 |
| H55 | -2.59798 | 0.071916 | -2.16408 | H55 | -2.66155 | -0.19391 | -2.37265 |
| H56 | 2.630441 | -4.89079 | -0.16234 | H56 | 2.733184 | -4.73308 | -0.72775 |
| C57 | 5.062536 | -1.846 | -2.95821 | C57 | 5.431445 | -0.75467 | -1.31211 |
| C58 | 4.068543 | -2.81416 | -3.11075 | C58 | 4.54984 | -1.53859 | -2.06276 |
| C59 | 3.205649 | -3.09994 | -2.05468 | C59 | 3.576191 | -2.30318 | -1.42243 |
| C60 | 3.318497 | -2.42618 | -0.83091 | C60 | 3.463142 | -2.30316 | -0.02382 |
| C61 | 4.299605 | -1.43691 | -0.69808 | C61 | 4.353574 | -1.5225 | 0.719839 |
| C62 | 5.172486 | -1.1582 | -1.75044 | C62 | 5.332017 | -0.75605 | 0.079408 |
| H63 | 5.742194 | -1.62677 | -3.77658 | H63 | 6.190154 | -0.15619 | -1.80788 |
| H64 | 3.966549 | -3.34929 | -4.05037 | H64 | 4.614804 | -1.54867 | -3.14709 |
| H65 | 2.427861 | -3.84595 | -2.19968 | H65 | 2.866354 | -2.86177 | -2.02652 |
| H66 | 4.38079 | -0.87566 | 0.22538 | H66 | 4.27611 | -1.49198 | 1.800532 |
| H67 | 5.933391 | -0.39309 | -1.62567 | H67 | 6.013393 | -0.15515 | 0.674918 |
| C68 | 2.309309 | 2.455737 | -1.49248 | C68 | 1.267965 | 3.624811 | -2.61702 |
| C69 | 0.934827 | 1.780133 | -1.62323 | C69 | 0.966953 | 2.140863 | -2.27297 |
| C70 | -0.15309 | 1.9816 | -0.71704 | C70 | 0.39377 | 1.879605 | -0.8438 |
| C71 | 0.175032 | 2.689067 | -3.91877 | C71 | -0.9903 | 2.103963 | -4.05254 |
| C72 | -0.168 | 0.472023 | -3.38791 | C72 | -0.07348 | 0.143384 | -3.27566 |
| C73 | -0.34023 | 1.903016 | -5.13678 | C73 | -1.43782 | 0.916168 | -4.91742 |
| H74 | 1.050246 | 3.290774 | -4.16111 | H74 | -0.62476 | 2.928618 | -4.66089 |
| H75 | -0.58792 | 3.336661 | -3.46649 | H75 | -1.78481 | 2.467628 | -3.39287 |
| H76 | -1.20814 | 2.351157 | -5.62132 | H76 | -2.51871 | 0.847872 | -5.04619 |
| H77 | 0.447452 | 1.725379 | -5.87479 | H77 | -0.94685 | 0.904423 | -5.89517 |
| N78 | 0.50486 | 1.583079 | -3.01121 | N78 | 0.085507 | 1.479657 | -3.27198 |
| O79 | -0.74132 | 0.616614 | -4.59082 | O79 | -0.99701 | -0.25243 | -4.17831 |
| O80 | -0.29765 | -0.5654 | -2.72174 | O80 | 0.498928 | -0.7007 | -2.56511 |
| H81 | 1.831765 | -4.56827 | 1.403657 | H81 | 2.144535 | -5.21322 | 0.888689 |
| N82 | -2.02534 | -2.1575 | -0.01944 | N82 | -1.95835 | -2.07174 | -0.37376 |
| C83 | -1.22942 | -2.95015 | -0.99106 | C83 | -1.06262 | -2.99079 | -1.12609 |
| H84 | -1.13974 | -2.44407 | -1.95665 | H84 | -0.79183 | -2.56127 | -2.09773 |
| H85 | -1.128 | 1.97256 | -1.19895 | H85 | -0.67982 | 2.081642 | -0.91194 |
| C86 | -0.39296 | 4.457059 | 2.795261 | C86 | 1.91942 | 4.359174 | 2.367505 |
| C87 | -1.42421 | 4.414711 | 1.856955 | C87 | 0.548644 | 4.250401 | 2.136297 |
| C88 | -1.31236 | 3.597593 | 0.731763 | C88 | 0.074549 | 3.472479 | 1.077767 |

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|-------------------|----------|----------|----------|-----------------------|----------|----------|----------|
| C89 | -0.16923 | 2.807728 | 0.518994 | C89 | 0.951682 | 2.769932 | 0.2371 |
| C90 | 0.857271 | 2.854749 | 1.478022 | C90 | 2.330434 | 2.903611 | 0.477478 |
| C91 | 0.747029 | 3.672669 | 2.598791 | C91 | 2.808725 | 3.687861 | 1.524393 |
| H92 | -0.47652 | 5.091213 | 3.673177 | H92 | 2.2933 | 4.965252 | 3.187525 |
| H93 | -2.31939 | 5.013105 | 2.000562 | H93 | -0.15486 | 4.780433 | 2.773226 |
| H94 | -2.12809 | 3.558954 | 0.01425 | H94 | -0.99649 | 3.408295 | 0.893141 |
| H95 | 1.732368 | 2.227258 | 1.365247 | H95 | 3.042701 | 2.385335 | -0.16082 |
| H96 | 1.551994 | 3.690129 | 3.328051 | H96 | 3.880038 | 3.774795 | 1.685741 |
| C97 | 3.320351 | 1.927417 | -2.51739 | C97 | 1.965817 | 3.776531 | -3.97815 |
| H98 | 3.403517 | 0.838951 | -2.47912 | H98 | 2.836915 | 3.116051 | -4.05248 |
| H99 | 3.044847 | 2.20957 | -3.53925 | H99 | 1.309334 | 3.549225 | -4.82434 |
| H100 | 4.308763 | 2.35267 | -2.3169 | H100 | 2.316021 | 4.805328 | -4.10944 |
| C101 | 2.210186 | 3.995759 | -1.5534 | C101 | 0.106503 | 4.618155 | -2.43587 |
| H102 | 1.489046 | 4.385324 | -0.83206 | H102 | -0.38832 | 4.485015 | -1.47103 |
| H103 | 3.185816 | 4.434558 | -1.32159 | H103 | 0.500016 | 5.639279 | -2.4627 |
| H104 | 1.926762 | 4.355938 | -2.54702 | H104 | -0.6512 | 4.55254 | -3.22049 |
| H105 | 2.680801 | 2.195098 | -0.49962 | H105 | 2.010597 | 3.901652 | -1.86166 |
| X | 0.332262 | 1.867163 | -1.24276 | H107 | 2.413561 | 0.218992 | -0.11672 |
| C3_ER_Chelbot_TS1 | | | | H108 | 2.386856 | 0.00773 | -0.9041 |
| C1 | -4.04644 | -3.46425 | -0.71608 | | | | |
| C2 | -1.84423 | -4.39029 | -1.23333 | jag_C3_ER_Chelbot_TS3 | | | |
| C3 | -3.22304 | -4.103 | -1.88623 | C1 | -4.012 | -2.73533 | -1.59376 |
| C4 | -3.03158 | -3.4971 | 0.449095 | C2 | -2.00349 | -4.11457 | -1.44359 |
| H5 | -4.93318 | -4.05787 | -0.47131 | C3 | -3.08622 | -3.65558 | -2.45668 |
| H6 | -3.14036 | -3.44356 | -2.7556 | C4 | -3.29984 | -2.75221 | -0.22349 |
| H7 | -3.45343 | -3.34172 | 1.442844 | H5 | -5.02015 | -3.15218 | -1.49745 |
| H8 | -4.37348 | -2.44348 | -0.9267 | H6 | -2.6488 | -3.13192 | -3.31303 |
| H9 | -1.21016 | -5.08718 | -1.78164 | H7 | -3.889 | -2.35529 | 0.603053 |
| H10 | -3.67512 | -5.03915 | -2.22582 | H8 | -4.10901 | -1.72254 | -1.98651 |
| C11 | -2.2647 | -4.8066 | 0.194982 | H9 | -1.4424 | -4.99995 | -1.7408 |
| H12 | -1.42352 | -4.95549 | 0.877228 | H10 | -3.63093 | -4.52097 | -2.84431 |
| H13 | -2.90782 | -5.69123 | 0.202801 | C11 | -2.81339 | -4.20937 | -0.13028 |
| C14 | 0.283957 | -3.02344 | -0.59805 | H12 | -2.19671 | -4.40831 | 0.751455 |
| N15 | 1.008106 | -1.9833 | -0.32666 | H13 | -3.62492 | -4.94066 | -0.18328 |
| C16 | 2.367552 | -2.47742 | 0.128748 | C14 | 0.203929 | -3.19711 | -0.44986 |
| C17 | 2.162501 | -4.04193 | 0.083344 | N15 | 1.02082 | -2.31578 | 0.022021 |
| P18 | -1.75216 | -0.93888 | 0.700363 | C16 | 2.225764 | -3.02071 | 0.599144 |
| Ir19 | 0.055377 | 0.062793 | -0.42751 | C17 | 1.877203 | -4.51748 | 0.271715 |
| C20 | -1.59505 | -0.98887 | 2.515724 | P18 | -1.51434 | -0.55741 | 0.284461 |
| C21 | -1.25069 | -0.94337 | 5.292134 | Ir19 | 0.829392 | -0.20234 | -0.28619 |
| C22 | -1.47975 | -2.18672 | 3.229712 | C20 | -1.72257 | -0.57271 | 2.103038 |
| C23 | -1.50547 | 0.236699 | 3.197202 | C21 | -1.92291 | -0.4747 | 4.897485 |
| C24 | -1.34008 | 0.256823 | 4.579812 | C22 | -2.25907 | -1.65484 | 2.810322 |
| C25 | -1.31213 | -2.16101 | 4.615524 | C23 | -1.25206 | 0.54711 | 2.811072 |
| H26 | -1.55713 | 1.172607 | 2.645753 | C24 | -1.36218 | 0.598399 | 4.198833 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| H27 | -1.27669 | 1.207668 | 5.101256 | C25 | -2.35799 | -1.60341 | 4.202486 |
| H28 | -1.22247 | -3.09378 | 5.164715 | H26 | -0.78612 | 1.373166 | 2.280057 |
| H29 | -1.12206 | -0.92646 | 6.37057 | H27 | -0.99728 | 1.470149 | 4.734617 |
| O30 | 0.83295 | -4.22812 | -0.45184 | H28 | -2.7695 | -2.45088 | 4.743136 |
| C31 | 2.721528 | -2.11291 | 1.573256 | H29 | -2.00439 | -0.43686 | 5.980206 |
| C32 | 1.889365 | -1.37885 | 2.416814 | O30 | 0.557571 | -4.4761 | -0.34142 |
| C33 | 3.890286 | -2.67283 | 2.123425 | C31 | 2.329028 | -2.86367 | 2.116258 |
| C34 | 2.231406 | -1.15705 | 3.753509 | C32 | 1.382276 | -2.18322 | 2.880503 |
| H35 | 0.957843 | -0.98718 | 2.047808 | C33 | 3.383851 | -3.51564 | 2.776771 |
| C36 | 4.235015 | -2.4537 | 3.454174 | C34 | 1.500326 | -2.12396 | 4.27244 |
| H37 | 4.538278 | -3.28983 | 1.506754 | H35 | 0.547223 | -1.69623 | 2.402275 |
| C38 | 3.408695 | -1.68371 | 4.275987 | C36 | 3.500066 | -3.46115 | 4.163565 |
| H39 | 1.554254 | -0.58413 | 4.379656 | H37 | 4.127556 | -4.05868 | 2.19862 |
| H40 | 5.147404 | -2.89056 | 3.849953 | C38 | 2.559122 | -2.75657 | 4.919818 |
| H41 | 3.677117 | -1.51216 | 5.314395 | H39 | 0.750725 | -1.58211 | 4.840562 |
| C42 | -3.33643 | -0.06356 | 0.411673 | H40 | 4.327353 | -3.96725 | 4.652911 |
| C43 | -4.32139 | 0.056699 | 1.400843 | H41 | 2.651062 | -2.7099 | 6.001003 |
| C44 | -3.58471 | 0.434204 | -0.87886 | C42 | -2.79119 | 0.638453 | -0.29319 |
| C45 | -5.53502 | 0.679203 | 1.106524 | C43 | -3.47381 | 1.517243 | 0.558723 |
| H46 | -4.14198 | -0.32458 | 2.401333 | C44 | -3.05118 | 0.689139 | -1.673 |
| C47 | -4.80159 | 1.048281 | -1.1677 | C45 | -4.39512 | 2.430211 | 0.040389 |
| C48 | -5.77534 | 1.177384 | -0.17379 | H46 | -3.29772 | 1.490354 | 1.628361 |
| H49 | -6.29104 | 0.776213 | 1.880369 | C47 | -3.98149 | 1.592618 | -2.18467 |
| H50 | -4.99094 | 1.428366 | -2.16763 | C48 | -4.65161 | 2.471601 | -1.32948 |
| H51 | -6.72051 | 1.662925 | -0.3987 | H49 | -4.91974 | 3.102484 | 0.713386 |
| H52 | 0.636068 | 0.434376 | 0.953909 | H50 | -4.19359 | 1.60617 | -3.25081 |
| H53 | -0.93457 | 1.286653 | -0.21567 | H51 | -5.37493 | 3.176802 | -1.7285 |
| H54 | -1.49954 | -3.1365 | 2.705756 | H52 | 1.090456 | 0.062014 | 1.219535 |
| H55 | -2.82974 | 0.326939 | -1.6542 | H53 | 1.957465 | 1.769654 | -2.35906 |
| H56 | 2.867565 | -4.5479 | -0.5771 | H54 | -2.57446 | -2.5512 | 2.290208 |
| C57 | 5.406552 | -1.8087 | -2.90378 | H55 | -2.5413 | 0.005935 | -2.3454 |
| C58 | 4.148684 | -2.31692 | -3.2376 | H56 | 2.561175 | -4.97728 | -0.44335 |
| C59 | 3.174041 | -2.46572 | -2.25514 | C57 | 5.606568 | -1.5839 | -1.71472 |
| C60 | 3.429426 | -2.10857 | -0.92062 | C58 | 4.586871 | -2.32435 | -2.31716 |
| C61 | 4.677613 | -1.56359 | -0.6064 | C59 | 3.525699 | -2.79807 | -1.55079 |
| C62 | 5.661625 | -1.42692 | -1.58939 | C60 | 3.462658 | -2.54538 | -0.17281 |
| H63 | 6.174769 | -1.70448 | -3.66429 | C61 | 4.478439 | -1.78808 | 0.418355 |
| H64 | 3.92989 | -2.60628 | -4.26159 | C62 | 5.546635 | -1.3167 | -0.34773 |
| H65 | 2.205963 | -2.87581 | -2.52923 | H63 | 6.43932 | -1.21709 | -2.30816 |
| H66 | 4.895028 | -1.24102 | 0.404317 | H64 | 4.616846 | -2.5298 | -3.38345 |
| H67 | 6.628604 | -1.0113 | -1.32046 | H65 | 2.724047 | -3.34304 | -2.04325 |
| C68 | 2.693942 | 1.977072 | -1.32243 | H66 | 4.436322 | -1.5527 | 1.475356 |
| C69 | 1.23654 | 1.559297 | -1.58239 | H67 | 6.331087 | -0.73593 | 0.129284 |
| C70 | 0.104461 | 2.231961 | -0.93567 | C68 | 1.273816 | 3.764729 | -2.5825 |
| C71 | 1.106622 | 2.255408 | -4.09628 | C69 | 0.989798 | 2.274564 | -2.26464 |

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|--------------------|----------|----------|----------|------------------------|----------|----------|----------|
| C72 | -0.01579 | 0.400865 | -3.34079 | C70 | 0.419159 | 1.988379 | -0.82771 |
| C73 | 0.556625 | 1.430962 | -5.26994 | C71 | -0.93907 | 2.217706 | -4.06158 |
| H74 | 2.149033 | 2.534687 | -4.24074 | C72 | -0.01035 | 0.25541 | -3.27669 |
| H75 | 0.520301 | 3.163592 | -3.89854 | C73 | -1.36959 | 1.026064 | -4.93044 |
| H76 | -0.02043 | 2.00709 | -5.99355 | H74 | -0.56567 | 3.040042 | -4.66864 |
| H77 | 1.344869 | 0.870208 | -5.78158 | H75 | -1.74474 | 2.584788 | -3.41666 |
| N78 | 0.941108 | 1.29127 | -2.99689 | H76 | -2.4488 | 0.950207 | -5.07022 |
| O79 | -0.33879 | 0.473228 | -4.63902 | H77 | -0.86999 | 1.02057 | -5.90393 |
| O80 | -0.59216 | -0.39249 | -2.57561 | N78 | 0.127588 | 1.600881 | -3.26381 |
| H81 | 2.182525 | -4.49436 | 1.075773 | O79 | -0.9275 | -0.1385 | -4.1894 |
| N82 | -1.94802 | -2.51809 | 0.175222 | O80 | 0.561049 | -0.58487 | -2.57159 |
| C83 | -1.17343 | -3.01343 | -0.99311 | H81 | 1.803675 | -5.13306 | 1.1677 |
| H84 | -1.28225 | -2.36842 | -1.86839 | N82 | -1.99369 | -2.04192 | -0.33925 |
| H85 | -0.69008 | 2.503883 | -1.63444 | C83 | -1.09558 | -2.89226 | -1.16295 |
| C86 | 0.244302 | 5.197605 | 2.18891 | H84 | -0.80905 | -2.38757 | -2.0928 |
| C87 | -0.55738 | 5.368053 | 1.061697 | H85 | -0.65963 | 1.897418 | -0.93612 |
| C88 | -0.58648 | 4.385569 | 0.071624 | C86 | 1.109505 | 4.83202 | 2.358038 |
| C89 | 0.187105 | 3.222924 | 0.18807 | C87 | -0.18355 | 4.56797 | 1.908414 |
| C90 | 0.980556 | 3.055529 | 1.334278 | C88 | -0.39302 | 3.657404 | 0.870292 |
| C91 | 1.011848 | 4.037161 | 2.320338 | C89 | 0.684591 | 2.993707 | 0.268484 |
| H92 | 0.267521 | 5.958906 | 2.963118 | C90 | 1.979735 | 3.259025 | 0.740673 |
| H93 | -1.16455 | 6.261773 | 0.951622 | C91 | 2.192437 | 4.174557 | 1.768149 |
| H94 | -1.21725 | 4.527285 | -0.80332 | H92 | 1.274816 | 5.539511 | 3.16545 |
| H95 | 1.570436 | 2.154562 | 1.457466 | H93 | -1.03254 | 5.070532 | 2.363713 |
| H96 | 1.636014 | 3.893162 | 3.197695 | H94 | -1.40454 | 3.455354 | 0.525116 |
| C97 | 3.668859 | 1.187585 | -2.20236 | H95 | 2.830257 | 2.730565 | 0.313457 |
| H98 | 3.399218 | 0.136489 | -2.24905 | H96 | 3.202706 | 4.367472 | 2.117795 |
| H99 | 3.695625 | 1.573259 | -3.22677 | C97 | 2.047816 | 3.925021 | -3.90062 |
| H100 | 4.68378 | 1.267871 | -1.80703 | H98 | 2.957111 | 3.314592 | -3.90723 |
| C101 | 2.951455 | 3.492084 | -1.4894 | H99 | 1.452758 | 3.639791 | -4.77452 |
| H102 | 2.32968 | 4.101127 | -0.83208 | H100 | 2.344649 | 4.969682 | -4.03695 |
| H103 | 3.999097 | 3.71216 | -1.25778 | C101 | 0.082584 | 4.73904 | -2.49807 |
| H104 | 2.773769 | 3.822388 | -2.51849 | H102 | -0.56064 | 4.535265 | -1.63971 |
| H105 | 2.90378 | 1.717739 | -0.28057 | H103 | 0.462826 | 5.758671 | -2.38302 |
| X | 0.332262 | 1.867163 | -1.24276 | H104 | -0.5366 | 4.737145 | -3.39835 |
| | | | | H105 | 1.960288 | 4.055384 | -1.77973 |
| C3_ER_Chelbot_INT1 | | | | H107 | 1.632158 | 1.140709 | -0.40673 |
| C1 | -4.09098 | -2.80674 | -1.48151 | H108 | 2.416745 | -0.2278 | -0.52064 |
| C2 | -2.12993 | -4.23952 | -1.26557 | | | | |
| C3 | -3.22642 | -3.83432 | -2.28533 | jag_C3_ER_Chelbot_PROD | | | |
| C4 | -3.3638 | -2.75963 | -0.11992 | C1 | -4.01655 | -2.80759 | -1.58036 |
| H5 | -5.11855 | -3.1598 | -1.34587 | C2 | -1.97983 | -4.15199 | -1.50539 |
| H6 | -2.80042 | -3.40824 | -3.19907 | C3 | -3.08118 | -3.67378 | -2.48845 |
| H7 | -3.93375 | -2.29583 | 0.685279 | C4 | -3.3011 | -2.88207 | -0.21324 |
| H8 | -4.13848 | -1.82023 | -1.94491 | H5 | -5.02029 | -3.23891 | -1.50526 |

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|------|----------|----------|----------|------|----------|----------|----------|
| H9 | -1.58913 | -5.15454 | -1.50817 | H6 | -2.66377 | -3.10957 | -3.32869 |
| H10 | -3.81373 | -4.71033 | -2.57443 | H7 | -3.89626 | -2.54299 | 0.634902 |
| C11 | -2.91759 | -4.22244 | 0.062781 | H8 | -4.12292 | -1.77723 | -1.92283 |
| H12 | -2.29281 | -4.38237 | 0.94697 | H9 | -1.39944 | -5.00867 | -1.84734 |
| H13 | -3.75078 | -4.93091 | 0.071166 | H10 | -3.61274 | -4.53445 | -2.90385 |
| C14 | 0.148229 | -3.28522 | -0.45041 | C11 | -2.78144 | -4.33048 | -0.19538 |
| N15 | 0.856372 | -2.36121 | 0.088198 | H12 | -2.15765 | -4.5573 | 0.67442 |
| C16 | 2.188286 | -2.90165 | 0.458431 | H13 | -3.57539 | -5.07763 | -0.28302 |
| C17 | 1.999161 | -4.41818 | 0.131104 | C14 | 0.204752 | -3.2235 | -0.47408 |
| P18 | -1.56489 | -0.59349 | 0.311555 | N15 | 1.022059 | -2.34155 | 0.004248 |
| Ir19 | 0.531074 | -0.24443 | -0.25293 | C16 | 2.253178 | -3.04554 | 0.54285 |
| C20 | -1.80218 | -0.5906 | 2.129078 | C17 | 1.780557 | -4.53247 | 0.447995 |
| C21 | -2.03512 | -0.50326 | 4.922381 | P18 | -1.56107 | -0.64539 | 0.335218 |
| C22 | -2.26282 | -1.70839 | 2.83525 | Ir19 | 0.768721 | -0.31138 | -0.16947 |
| C23 | -1.42929 | 0.564898 | 2.839112 | C20 | -1.80969 | -0.67278 | 2.147238 |
| C24 | -1.55353 | 0.608315 | 4.224745 | C21 | -1.97619 | -0.62124 | 4.945992 |
| C25 | -2.38051 | -1.66099 | 4.226677 | C22 | -2.27343 | -1.79223 | 2.847977 |
| H26 | -1.01668 | 1.421771 | 2.315286 | C23 | -1.39751 | 0.464654 | 2.864902 |
| H27 | -1.25964 | 1.506968 | 4.759502 | C24 | -1.49138 | 0.492725 | 4.253827 |
| H28 | -2.73571 | -2.53517 | 4.76457 | C25 | -2.35595 | -1.76397 | 4.242504 |
| H29 | -2.12908 | -0.469 | 6.004052 | H26 | -0.98525 | 1.3223 | 2.33779 |
| O30 | 0.692243 | -4.50457 | -0.52298 | H27 | -1.17233 | 1.377509 | 4.797186 |
| C31 | 2.48147 | -2.70372 | 1.940532 | H28 | -2.71368 | -2.63917 | 4.777156 |
| C32 | 1.485854 | -2.298 | 2.832866 | H29 | -2.04366 | -0.60126 | 6.029945 |
| C33 | 3.7669 | -2.97856 | 2.424167 | O30 | 0.565422 | -4.50135 | -0.35517 |
| C34 | 1.77495 | -2.15452 | 4.190815 | C31 | 2.503357 | -2.74057 | 2.017661 |
| H35 | 0.490595 | -2.07474 | 2.47052 | C32 | 1.459045 | -2.31605 | 2.847911 |
| C36 | 4.052005 | -2.84364 | 3.781567 | C33 | 3.738379 | -3.05404 | 2.601702 |
| H37 | 4.550717 | -3.28242 | 1.734228 | C34 | 1.659815 | -2.14632 | 4.217649 |
| C38 | 3.056581 | -2.42613 | 4.668356 | H35 | 0.482347 | -2.10901 | 2.430973 |
| H39 | 0.991949 | -1.82441 | 4.867687 | C36 | 3.937299 | -2.89117 | 3.973622 |
| H40 | 5.052784 | -3.05692 | 4.145871 | H37 | 4.552453 | -3.42311 | 1.985632 |
| H41 | 3.282378 | -2.31266 | 5.724755 | C38 | 2.903492 | -2.42406 | 4.786586 |
| C42 | -2.79216 | 0.587897 | -0.35958 | H39 | 0.835388 | -1.797 | 4.83251 |
| C43 | -3.49569 | 1.510278 | 0.424831 | H40 | 4.905362 | -3.13063 | 4.404523 |
| C44 | -2.98341 | 0.581275 | -1.75178 | H41 | 3.063437 | -2.29017 | 5.852456 |
| C45 | -4.37367 | 2.415717 | -0.1759 | C42 | -2.81568 | 0.557488 | -0.28286 |
| H46 | -3.3726 | 1.522838 | 1.502177 | C43 | -3.5405 | 1.432196 | 0.537752 |
| C47 | -3.86656 | 1.480007 | -2.34424 | C44 | -2.99022 | 0.631781 | -1.676 |
| C48 | -4.55982 | 2.404905 | -1.55718 | C45 | -4.4163 | 2.365186 | -0.02349 |
| H49 | -4.91762 | 3.124557 | 0.441674 | H46 | -3.43204 | 1.387163 | 1.616037 |
| H50 | -4.0251 | 1.455748 | -3.41917 | C47 | -3.87502 | 1.554587 | -2.23119 |
| H51 | -5.24833 | 3.106257 | -2.01939 | C48 | -4.5862 | 2.43048 | -1.40592 |
| H52 | 0.721199 | 0.121231 | 1.243231 | H49 | -4.975 | 3.033297 | 0.625838 |
| H53 | 2.103883 | 1.376409 | -2.05265 | H50 | -4.02312 | 1.582476 | -3.30757 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| H54 | -2.50772 | -2.62648 | 2.317034 | H51 | -5.27479 | 3.150635 | -1.83803 |
| H55 | -2.44797 | -0.13379 | -2.36902 | H52 | 1.0547 | -0.16117 | 1.347757 |
| H56 | 2.744611 | -4.83927 | -0.54387 | H53 | 2.010871 | 1.676168 | -2.08355 |
| C57 | 4.567235 | -0.44255 | -2.20631 | H54 | -2.54582 | -2.6977 | 2.318115 |
| C58 | 4.182349 | -1.72133 | -2.60795 | H55 | -2.45155 | -0.04981 | -2.32654 |
| C59 | 3.470527 | -2.55073 | -1.73927 | H56 | 2.498866 | -5.19209 | -0.03787 |
| C60 | 3.148923 | -2.12076 | -0.4505 | C57 | 5.371148 | -2.05573 | -2.30999 |
| C61 | 3.536357 | -0.82716 | -0.04841 | C58 | 4.396291 | -3.00495 | -2.61979 |
| C62 | 4.243195 | 0.002164 | -0.92413 | C59 | 3.421106 | -3.33457 | -1.68081 |
| H63 | 5.124034 | 0.198646 | -2.88347 | C60 | 3.402687 | -2.72744 | -0.41785 |
| H64 | 4.428535 | -2.07556 | -3.60465 | C61 | 4.369372 | -1.75807 | -0.12746 |
| H65 | 3.14682 | -3.52358 | -2.09586 | C62 | 5.351851 | -1.43259 | -1.06262 |
| H66 | 3.326659 | -0.4919 | 0.962639 | H63 | 6.13783 | -1.80272 | -3.03687 |
| H67 | 4.559419 | 0.987672 | -0.59455 | H64 | 4.394166 | -3.48996 | -3.59167 |
| C68 | 1.71383 | 3.425077 | -2.40923 | H65 | 2.657997 | -4.05899 | -1.95391 |
| C69 | 1.199236 | 1.996283 | -2.09428 | H66 | 4.349612 | -1.24524 | 0.826149 |
| C70 | 0.380633 | 1.81254 | -0.77585 | H67 | 6.100426 | -0.68541 | -0.81421 |
| C71 | -0.58963 | 2.09958 | -4.02803 | C68 | 1.698653 | 3.739191 | -2.44813 |
| C72 | 0.164015 | 0.082816 | -3.2251 | C69 | 1.140419 | 2.338497 | -2.09593 |
| C73 | -1.07184 | 0.946048 | -4.9214 | C70 | 0.447678 | 2.189351 | -0.69207 |
| H74 | -0.14683 | 2.903677 | -4.61395 | C71 | -0.74088 | 2.475152 | -3.92716 |
| H75 | -1.38901 | 2.508786 | -3.39938 | C72 | 0.033522 | 0.424001 | -3.19935 |
| H76 | -2.1477 | 0.945805 | -5.1006 | C73 | -1.19851 | 1.354391 | -4.87189 |
| H77 | -0.53776 | 0.907919 | -5.87553 | H74 | -0.30708 | 3.307234 | -4.47719 |
| N78 | 0.412098 | 1.406074 | -3.20895 | H75 | -1.54993 | 2.848212 | -3.28684 |
| O79 | -0.73898 | -0.25133 | -4.17128 | H76 | -2.27132 | 1.351674 | -5.06746 |
| O80 | 0.645034 | -0.79081 | -2.48201 | H77 | -0.64983 | 1.36396 | -5.81869 |
| H81 | 1.949805 | -5.01838 | 1.040343 | N78 | 0.266298 | 1.760406 | -3.13554 |
| N82 | -2.03512 | -2.09888 | -0.28789 | O79 | -0.86446 | 0.133398 | -4.16755 |
| C83 | -1.19038 | -3.01988 | -1.09569 | O80 | 0.504733 | -0.47538 | -2.49857 |
| H84 | -0.9444 | -2.57786 | -2.07002 | H81 | 1.509126 | -4.93085 | 1.426538 |
| H85 | -0.6559 | 2.065792 | -1.02365 | N82 | -2.01174 | -2.14202 | -0.28888 |
| C86 | 1.476662 | 4.231194 | 2.652851 | C83 | -1.10216 | -2.9203 | -1.17341 |
| C87 | 0.16842 | 4.22948 | 2.167538 | H84 | -0.84028 | -2.36011 | -2.07808 |
| C88 | -0.16548 | 3.471683 | 1.042057 | H85 | -0.59485 | 1.923004 | -0.84061 |
| C89 | 0.791993 | 2.685588 | 0.38009 | C86 | 0.586994 | 5.297269 | 2.297997 |
| C90 | 2.105478 | 2.705188 | 0.880277 | C87 | -0.62895 | 4.926494 | 1.723177 |
| C91 | 2.445538 | 3.466707 | 1.99628 | C88 | -0.66714 | 3.92555 | 0.75099 |
| H92 | 1.740926 | 4.823509 | 3.523761 | C89 | 0.513209 | 3.292641 | 0.340802 |
| H93 | -0.5953 | 4.827294 | 2.6587 | C90 | 1.727017 | 3.652649 | 0.941362 |
| H94 | -1.18818 | 3.483388 | 0.668918 | C91 | 1.764922 | 4.655474 | 1.90776 |
| H95 | 2.86392 | 2.097948 | 0.394857 | H92 | 0.617492 | 6.076494 | 3.054031 |
| H96 | 3.470063 | 3.462017 | 2.359131 | H93 | -1.54902 | 5.414802 | 2.031659 |
| C97 | 2.570356 | 3.447136 | -3.68442 | H94 | -1.61675 | 3.633261 | 0.308345 |
| H98 | 3.36074 | 2.689028 | -3.64489 | H95 | 2.641646 | 3.133371 | 0.663655 |

| | | | | | | | |
|-----------------------|----------|----------|----------|------|----------|----------|----------|
| H99 | 1.980768 | 3.257212 | -4.58784 | H96 | 2.71147 | 4.929833 | 2.364379 |
| H100 | 3.047819 | 4.424405 | -3.80649 | C97 | 2.541071 | 3.679928 | -3.73269 |
| C101 | 0.662947 | 4.548641 | -2.39246 | H98 | 3.326913 | 2.919992 | -3.6655 |
| H102 | 0.039299 | 4.502636 | -1.49687 | H99 | 1.930905 | 3.4468 | -4.61215 |
| H103 | 1.171706 | 5.517842 | -2.38749 | H100 | 3.02155 | 4.646226 | -3.91418 |
| H104 | 0.007682 | 4.542803 | -3.26724 | C101 | 0.703813 | 4.915921 | -2.48409 |
| H105 | 2.387238 | 3.635049 | -1.57062 | H102 | -0.01253 | 4.886058 | -1.66145 |
| X | 0.332262 | 1.867163 | -1.24276 | H103 | 1.259911 | 5.854216 | -2.39663 |
| jag_C3_ER_Chelbot_TS2 | | | | H104 | 0.14614 | 4.972166 | -3.42212 |
| C1 | -3.93835 | -2.71353 | -1.61154 | H105 | 2.38753 | 3.946443 | -1.62141 |
| C2 | -1.94822 | -4.11256 | -1.40996 | H107 | 1.095206 | 1.412215 | -0.10894 |
| C3 | -3.01803 | -3.66788 | -2.44291 | H108 | 2.353954 | -0.16609 | -0.38121 |
| C4 | -3.23306 | -2.69667 | -0.23871 | | | | |
| H5 | -4.95068 | -3.11741 | -1.50608 | | | | |
| H6 | -2.56753 | -3.17168 | -3.30865 | | | | |
| H7 | -3.81893 | -2.26952 | 0.575367 | | | | |
| H8 | -4.02504 | -1.71236 | -2.03494 | | | | |
| H9 | -1.39594 | -5.01285 | -1.67749 | | | | |
| H10 | -3.57076 | -4.53602 | -2.81215 | | | | |
| C11 | -2.76658 | -4.1583 | -0.10134 | | | | |
| H12 | -2.15694 | -4.34639 | 0.787458 | | | | |
| H13 | -3.5901 | -4.8769 | -0.13766 | | | | |
| C14 | 0.271274 | -3.1912 | -0.43425 | | | | |
| N15 | 1.046664 | -2.29268 | 0.064292 | | | | |
| C16 | 2.255605 | -2.9703 | 0.643295 | | | | |
| C17 | 2.007553 | -4.4593 | 0.200706 | | | | |
| P18 | -1.44647 | -0.53418 | 0.292733 | | | | |
| Ir19 | 0.630642 | -0.13472 | -0.34062 | | | | |
| C20 | -1.6352 | -0.61003 | 2.116049 | | | | |
| C21 | -1.87272 | -0.63973 | 4.913751 | | | | |
| C22 | -2.09244 | -1.75669 | 2.776128 | | | | |
| C23 | -1.2641 | 0.514683 | 2.874361 | | | | |
| C24 | -1.39146 | 0.499953 | 4.261742 | | | | |
| C25 | -2.21082 | -1.76842 | 4.167921 | | | | |
| H26 | -0.85565 | 1.394848 | 2.385931 | | | | |
| H27 | -1.10118 | 1.376694 | 4.833601 | | | | |
| H28 | -2.55878 | -2.6678 | 4.667472 | | | | |
| H29 | -1.96804 | -0.65154 | 5.99545 | | | | |
| O30 | 0.665949 | -4.46322 | -0.36379 | | | | |
| C31 | 2.306781 | -2.87324 | 2.167851 | | | | |
| C32 | 1.490874 | -2.01426 | 2.903449 | | | | |
| C33 | 3.218629 | -3.68889 | 2.858258 | | | | |
| C34 | 1.580194 | -1.96806 | 4.297551 | | | | |
| H35 | 0.784096 | -1.37792 | 2.395775 | | | | |

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|-----|----------|----------|----------|
| C36 | 3.311017 | -3.64122 | 4.247275 |
| H37 | 3.879437 | -4.352 | 2.304102 |
| C38 | 2.488365 | -2.77803 | 4.975652 |
| H39 | 0.928893 | -1.29321 | 4.843372 |
| H40 | 4.02731 | -4.27707 | 4.759521 |
| H41 | 2.558141 | -2.74074 | 6.058642 |
| C42 | -2.74423 | 0.635362 | -0.26987 |
| C43 | -3.44738 | 1.489025 | 0.589122 |
| C44 | -3.01244 | 0.674544 | -1.64846 |
| C45 | -4.40055 | 2.370801 | 0.074995 |
| H46 | -3.26736 | 1.464508 | 1.657804 |
| C47 | -3.97115 | 1.548411 | -2.15469 |
| C48 | -4.66391 | 2.403703 | -1.29288 |
| H49 | -4.943 | 3.026041 | 0.750013 |
| H50 | -4.18637 | 1.560633 | -3.22004 |
| H51 | -5.41117 | 3.085739 | -1.68726 |
| H52 | 0.832294 | 0.290297 | 1.136683 |
| H53 | 1.991924 | 1.703458 | -2.30892 |
| H54 | -2.33147 | -2.65384 | 2.219396 |
| H55 | -2.47454 | 0.011494 | -2.31992 |
| H56 | 2.693958 | -4.79274 | -0.58062 |
| C57 | 5.69995 | -1.33801 | -1.44137 |
| C58 | 4.629551 | -1.89549 | -2.14518 |
| C59 | 3.538269 | -2.4169 | -1.4548 |
| C60 | 3.496933 | -2.39373 | -0.05219 |
| C61 | 4.566038 | -1.822 | 0.643636 |
| C62 | 5.661984 | -1.30081 | -0.04912 |
| H63 | 6.55383 | -0.93292 | -1.97651 |
| H64 | 4.642854 | -1.92181 | -3.23109 |
| H65 | 2.698177 | -2.81598 | -2.01678 |
| H66 | 4.549257 | -1.77651 | 1.7263 |
| H67 | 6.485744 | -0.86281 | 0.50701 |
| C68 | 1.248223 | 3.664067 | -2.62831 |
| C69 | 1.0011 | 2.171349 | -2.2773 |
| C70 | 0.333892 | 1.903567 | -0.89098 |
| C71 | -0.88843 | 1.991412 | -4.11181 |
| C72 | 0.146961 | 0.108107 | -3.28964 |
| C73 | -1.29296 | 0.749917 | -4.92372 |
| H74 | -0.56405 | 2.806314 | -4.75729 |
| H75 | -1.69095 | 2.34937 | -3.45922 |
| H76 | -2.3715 | 0.619157 | -5.02249 |
| H77 | -0.82587 | 0.727932 | -5.91262 |
| N78 | 0.221717 | 1.450154 | -3.31815 |
| O79 | -0.77211 | -0.36784 | -4.1565 |
| O80 | 0.792387 | -0.67613 | -2.56799 |

| | | | |
|------|----------|----------|----------|
| H81 | 2.01526 | -5.16092 | 1.033633 |
| N82 | -1.91532 | -2.00493 | -0.37435 |
| C83 | -1.02277 | -2.89758 | -1.15789 |
| H84 | -0.72636 | -2.42906 | -2.10386 |
| H85 | -0.73382 | 2.091403 | -1.0369 |
| C86 | 1.583404 | 4.379187 | 2.436092 |
| C87 | 0.231317 | 4.214188 | 2.133408 |
| C88 | -0.15291 | 3.441708 | 1.036759 |
| C89 | 0.798423 | 2.802731 | 0.224756 |
| C90 | 2.155806 | 2.997413 | 0.531949 |
| C91 | 2.543951 | 3.774395 | 1.622061 |
| H92 | 1.886444 | 4.981967 | 3.287193 |
| H93 | -0.52658 | 4.696749 | 2.745363 |
| H94 | -1.2093 | 3.328009 | 0.800711 |
| H95 | 2.91436 | 2.53783 | -0.09359 |
| H96 | 3.600763 | 3.90925 | 1.836453 |
| C97 | 1.991623 | 3.828135 | -3.96315 |
| H98 | 2.892933 | 3.206213 | -3.99487 |
| H99 | 1.376276 | 3.559339 | -4.82801 |
| H100 | 2.30001 | 4.869712 | -4.0981 |
| C101 | 0.032529 | 4.601154 | -2.51609 |
| H102 | -0.49233 | 4.468025 | -1.56709 |
| H103 | 0.375315 | 5.639957 | -2.55593 |
| H104 | -0.6892 | 4.477899 | -3.32748 |
| H105 | 1.942313 | 3.987905 | -1.84608 |
| H107 | 3.310868 | 0.471611 | -0.37389 |
| H108 | 3.287537 | 0.320133 | -1.10657 |

C3_ZS_Cheltop

C3_ZS_Cheltop_SM

| | | | |
|-----|---------|----------|----------|
| C1 | -3.9825 | -3.39713 | -0.74319 |
| C2 | -1.7632 | -4.41248 | -0.77251 |
| C3 | -3.0528 | -4.29503 | -1.62635 |
| C4 | -3.0978 | -3.13606 | 0.497881 |
| H5 | -4.8983 | -3.92313 | -0.45436 |
| H6 | -2.8584 | -3.86286 | -2.61329 |
| H7 | -3.6204 | -2.74861 | 1.372277 |
| H8 | -4.273 | -2.466 | -1.23281 |
| H9 | -1.0871 | -5.21641 | -1.06389 |
| H10 | -3.486 | -5.28678 | -1.78401 |
| C11 | -2.3435 | -4.46683 | 0.658105 |
| H12 | -1.5851 | -4.44182 | 1.44604 |
| H13 | -3.0059 | -5.32316 | 0.813004 |
| C14 | 0.32964 | -2.96266 | -0.27405 |
| N15 | 0.98401 | -1.87155 | -0.05726 |

C3_ZS_Cheltop_INT2

| | | | |
|-----|---------|----------|----------|
| C1 | -3.7376 | -4.15979 | -0.76753 |
| C2 | -1.432 | -4.92519 | -0.55026 |
| C3 | -2.6547 | -5.02208 | -1.49666 |
| C4 | -2.9794 | -3.68937 | 0.496529 |
| H5 | -4.6097 | -4.75812 | -0.48455 |
| H6 | -2.4282 | -4.65487 | -2.50254 |
| H7 | -3.5991 | -3.28239 | 1.295316 |
| H8 | -4.0903 | -3.32031 | -1.36709 |
| H9 | -0.6593 | -5.67511 | -0.71646 |
| H10 | -2.9689 | -6.06521 | -1.59248 |
| C11 | -2.1124 | -4.91296 | 0.8363 |
| H12 | -1.4262 | -4.73742 | 1.67059 |
| H13 | -2.6975 | -5.81664 | 1.028415 |
| C14 | 0.47108 | -3.26417 | -0.02371 |
| N15 | 0.93988 | -2.12147 | 0.334915 |

| | | | | | | | |
|------|---------|----------|----------|------|---------|----------|----------|
| C16 | 2.32103 | -2.22668 | 0.558691 | C16 | 2.30778 | -2.35072 | 0.940872 |
| C17 | 2.32208 | -3.77854 | 0.351499 | C17 | 2.52132 | -3.87585 | 0.654105 |
| P18 | -1.8892 | -0.56048 | 0.26754 | P18 | -2.0564 | -1.03234 | 0.131689 |
| Ir19 | 0.31609 | 0.07191 | -0.64967 | Ir19 | 0.03653 | -0.19328 | -0.42745 |
| C20 | -2.2825 | -0.27233 | 2.032207 | C20 | -2.5999 | -0.70382 | 1.859106 |
| C21 | -2.7077 | 0.214137 | 4.76517 | C21 | -3.2091 | -0.1671 | 4.556167 |
| C22 | -2.0092 | -1.26689 | 2.984809 | C22 | -2.1183 | -1.53418 | 2.882844 |
| C23 | -2.765 | 0.972762 | 2.468162 | C23 | -3.4236 | 0.379044 | 2.206667 |
| C24 | -2.973 | 1.211003 | 3.825363 | C24 | -3.7209 | 0.644946 | 3.543337 |
| C25 | -2.2257 | -1.02519 | 4.340898 | C25 | -2.4164 | -1.26529 | 4.218784 |
| H26 | -2.9872 | 1.757406 | 1.755898 | H26 | -3.8595 | 1.000343 | 1.435235 |
| H27 | -3.3438 | 2.180879 | 4.143893 | H27 | -4.3655 | 1.483966 | 3.790869 |
| H28 | -2.0117 | -1.80622 | 5.064843 | H28 | -2.0284 | -1.91936 | 4.99442 |
| H29 | -2.8743 | 0.401608 | 5.822092 | H29 | -3.4402 | 0.042843 | 5.59625 |
| O30 | 0.9477 | -4.10796 | -0.00103 | O30 | 1.24134 | -4.34086 | 0.147558 |
| C31 | 2.35088 | -1.93246 | 2.061578 | C31 | 2.32196 | -2.11945 | 2.453381 |
| C32 | 1.31717 | -1.28778 | 2.735512 | C32 | 1.23682 | -1.59399 | 3.147793 |
| C33 | 3.46863 | -2.36598 | 2.792426 | C33 | 3.48614 | -2.45099 | 3.16584 |
| C34 | 1.39442 | -1.07034 | 4.112693 | C34 | 1.30573 | -1.39205 | 4.528236 |
| H35 | 0.45896 | -0.92485 | 2.191456 | H35 | 0.352 | -1.30103 | 2.610501 |
| C36 | 3.54931 | -2.14905 | 4.164828 | C36 | 3.55548 | -2.25661 | 4.542703 |
| H37 | 4.29237 | -2.85675 | 2.278972 | H37 | 4.35258 | -2.8435 | 2.638747 |
| C38 | 2.50845 | -1.4971 | 4.831146 | C38 | 2.46192 | -1.72291 | 5.230427 |
| H39 | 0.57602 | -0.56196 | 4.613712 | H39 | 0.44988 | -0.96321 | 5.042171 |
| H40 | 4.4252 | -2.48433 | 4.71274 | H40 | 4.4648 | -2.51418 | 5.078011 |
| H41 | 2.57059 | -1.3238 | 5.901709 | H41 | 2.5182 | -1.5645 | 6.303616 |
| C42 | -3.3552 | 0.064711 | -0.66294 | C42 | -3.5059 | -0.69772 | -0.93287 |
| C43 | -4.6009 | 0.297382 | -0.06158 | C43 | -4.8176 | -0.83564 | -0.44913 |
| C44 | -3.2508 | 0.177469 | -2.06033 | C44 | -3.3001 | -0.54858 | -2.31151 |
| C45 | -5.7027 | 0.670074 | -0.83362 | C45 | -5.8984 | -0.81198 | -1.32918 |
| H46 | -4.7213 | 0.189345 | 1.010628 | H46 | -5.0013 | -0.97959 | 0.610312 |
| C47 | -4.3536 | 0.545513 | -2.83013 | C47 | -4.384 | -0.53364 | -3.18825 |
| C48 | -5.5832 | 0.802022 | -2.2176 | C48 | -5.6855 | -0.66581 | -2.7015 |
| H49 | -6.6575 | 0.852884 | -0.34896 | H49 | -6.9075 | -0.91888 | -0.94148 |
| H50 | -4.2526 | 0.631355 | -3.90841 | H50 | -4.2102 | -0.40952 | -4.253 |
| H51 | -6.4418 | 1.093309 | -2.81522 | H51 | -6.5283 | -0.65375 | -3.38593 |
| H52 | -0.278 | -0.51192 | -1.96569 | H52 | -0.2656 | -0.82386 | -1.8367 |
| H53 | 1.72312 | 0.018467 | -1.38447 | H53 | 1.4913 | 2.42071 | -0.29219 |
| H54 | -1.6123 | -2.22501 | 2.667749 | H54 | -1.5102 | -2.39589 | 2.631909 |
| H55 | -2.304 | -0.02859 | -2.54969 | H55 | -2.2917 | -0.43277 | -2.6936 |
| H56 | 2.96013 | -4.11436 | -0.46819 | H56 | 3.2779 | -4.08512 | -0.10448 |
| C57 | 5.38909 | -0.18815 | -1.74243 | C57 | 4.83632 | 0.391301 | -1.26731 |
| C58 | 4.64442 | -1.2223 | -2.31284 | C58 | 4.39103 | -0.79103 | -1.86378 |
| C59 | 3.67557 | -1.88073 | -1.55887 | C59 | 3.62799 | -1.69943 | -1.13127 |
| C60 | 3.44125 | -1.53001 | -0.22158 | C60 | 3.30143 | -1.44583 | 0.207408 |

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|------|---------|----------|----------|------|---------|----------|----------|
| C61 | 4.18192 | -0.48283 | 0.336297 | C61 | 3.75252 | -0.25864 | 0.797945 |
| C62 | 5.14882 | 0.182018 | -0.4195 | C62 | 4.51625 | 0.652745 | 0.064992 |
| H63 | 6.14786 | 0.324595 | -2.32684 | H63 | 5.43075 | 1.099959 | -1.83643 |
| H64 | 4.81325 | -1.51227 | -3.34587 | H64 | 4.63402 | -1.00395 | -2.90052 |
| H65 | 3.08002 | -2.65579 | -2.03404 | H65 | 3.25573 | -2.59104 | -1.62821 |
| H66 | 3.99335 | -0.17132 | 1.356091 | H66 | 3.48854 | -0.0352 | 1.825336 |
| H67 | 5.71955 | 0.98767 | 0.034945 | H67 | 4.85908 | 1.56821 | 0.539122 |
| C68 | 1.09976 | 2.184765 | -2.9974 | C68 | 0.61954 | 4.232777 | -0.98429 |
| C69 | 0.72311 | 2.029038 | -1.51524 | C69 | 0.47036 | 2.815358 | -0.36949 |
| C70 | -0.6365 | 2.027849 | -1.07288 | C70 | -0.3684 | 1.781021 | -1.19394 |
| H71 | -1.3414 | 1.839404 | -1.8711 | H71 | 0.12005 | 1.751331 | -2.17207 |
| C72 | -1.2567 | 2.891685 | -0.02846 | C72 | -1.7801 | 2.237385 | -1.43712 |
| C73 | -2.494 | 3.467449 | -0.37839 | C73 | -2.2329 | 2.490674 | -2.74035 |
| C74 | -0.7233 | 3.206348 | 1.233934 | C74 | -2.6927 | 2.435501 | -0.39206 |
| C75 | -3.1499 | 4.352326 | 0.474519 | C75 | -3.5329 | 2.932917 | -2.98667 |
| H76 | -2.9489 | 3.20921 | -1.33088 | H76 | -1.5608 | 2.32184 | -3.57856 |
| C77 | -1.3723 | 4.106141 | 2.07915 | C77 | -3.9919 | 2.880278 | -0.62724 |
| H78 | 0.15165 | 2.699014 | 1.609064 | H78 | -2.3883 | 2.202501 | 0.618987 |
| C79 | -2.5826 | 4.68962 | 1.704875 | C79 | -4.4205 | 3.134903 | -1.93038 |
| H80 | -4.1035 | 4.778263 | 0.176008 | H80 | -3.8544 | 3.114044 | -4.00859 |
| H81 | -0.9381 | 4.327624 | 3.050099 | H81 | -4.6761 | 3.017064 | 0.20715 |
| H82 | -3.0865 | 5.385187 | 2.369746 | H82 | -5.4339 | 3.475646 | -2.12008 |
| C83 | 2.16468 | 4.04194 | -0.72817 | C83 | -0.7229 | 4.060095 | 1.656579 |
| C84 | 2.03844 | 2.114143 | 0.546573 | C84 | -0.0161 | 1.865865 | 1.84657 |
| C85 | 3.2258 | 4.039402 | 0.390344 | C85 | -0.8247 | 3.565468 | 3.114851 |
| H86 | 1.33201 | 4.726794 | -0.5272 | H86 | -1.7007 | 4.203193 | 1.188538 |
| H87 | 2.59721 | 4.272823 | -1.70367 | H87 | -0.1655 | 4.994315 | 1.586522 |
| H88 | 4.23325 | 3.865243 | 0.001162 | H88 | -0.0809 | 4.031958 | 3.767636 |
| H89 | 3.21596 | 4.936214 | 1.010168 | H89 | -1.8188 | 3.68607 | 3.547654 |
| N90 | 1.71021 | 2.651726 | -0.64702 | N90 | -0.0034 | 2.938811 | 1.035855 |
| O91 | 2.87277 | 2.906447 | 1.232989 | O91 | -0.5383 | 2.144989 | 3.051984 |
| O92 | 1.60677 | 1.047171 | 1.004686 | O92 | 0.38397 | 0.719762 | 1.585328 |
| H93 | 2.56858 | -4.32406 | 1.260484 | H93 | 2.74333 | -4.44132 | 1.557728 |
| N94 | -1.9616 | -2.24698 | 0.126793 | N94 | -1.9113 | -2.72187 | 0.117564 |
| C95 | -1.0863 | -3.01881 | -0.78487 | C95 | -0.8895 | -3.47394 | -0.6391 |
| H96 | -1.0701 | -2.60576 | -1.80287 | H96 | -0.8168 | -3.14834 | -1.68664 |
| C97 | 2.51758 | 1.68591 | -3.30861 | C97 | 1.7652 | 4.996274 | -0.28963 |
| H98 | 2.82564 | 2.021413 | -4.30402 | H98 | 1.7662 | 6.048927 | -0.58843 |
| H99 | 3.25446 | 2.04314 | -2.58374 | H99 | 1.72078 | 4.95623 | 0.802357 |
| H100 | 2.55352 | 0.593142 | -3.28845 | H100 | 2.73041 | 4.567942 | -0.58464 |
| C101 | 0.09302 | 1.580093 | -3.98267 | C101 | 0.90929 | 4.189731 | -2.49148 |
| H102 | 0.03463 | 0.495229 | -3.85661 | H102 | 1.76381 | 3.537814 | -2.71031 |
| H103 | -0.9119 | 1.998579 | -3.87343 | H103 | 0.05217 | 3.843484 | -3.06905 |
| H104 | 0.4195 | 1.785086 | -5.00638 | H104 | 1.16325 | 5.193263 | -2.84652 |
| H105 | 1.08242 | 3.275146 | -3.16346 | H105 | -0.3265 | 4.771469 | -0.84293 |

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|-------------------|---------|----------|----------|-------------------|---------|----------|----------|
| | | | | H106 | 1.73351 | 0.347158 | -0.61627 |
| C3_ZS_Cheltop_TS1 | | | | H107 | 1.51709 | 0.051438 | -1.35887 |
| C1 | -3.91 | -3.63089 | -0.75081 | | | | |
| C2 | -1.6608 | -4.58155 | -0.77398 | C3_ZS_Cheltop_TS3 | | | |
| C3 | -2.9491 | -4.49655 | -1.63398 | C1 | -3.7035 | -4.30885 | -0.77303 |
| C4 | -3.0448 | -3.3646 | 0.502611 | C2 | -1.3634 | -4.96963 | -0.53593 |
| H5 | -4.8186 | -4.1791 | -0.48216 | C3 | -2.5698 | -5.10392 | -1.50255 |
| H6 | -2.7627 | -4.05438 | -2.61798 | C4 | -2.9828 | -3.82418 | 0.505637 |
| H7 | -3.5858 | -3.00428 | 1.377872 | H5 | -4.5503 | -4.95318 | -0.51435 |
| H8 | -4.212 | -2.69729 | -1.23025 | H6 | -2.348 | -4.70777 | -2.49872 |
| H9 | -0.9576 | -5.36003 | -1.06979 | H7 | -3.6313 | -3.45583 | 1.300976 |
| H10 | -3.3528 | -5.49962 | -1.79807 | H8 | -4.088 | -3.47261 | -1.35855 |
| C11 | -2.2494 | -4.67313 | 0.651305 | H9 | -0.5572 | -5.68285 | -0.7048 |
| H12 | -1.497 | -4.63363 | 1.444612 | H10 | -2.8339 | -6.15837 | -1.62245 |
| H13 | -2.8844 | -5.55259 | 0.790649 | C11 | -2.0631 | -5.01059 | 0.840208 |
| C14 | 0.39179 | -3.06336 | -0.2698 | H12 | -1.3946 | -4.8156 | 1.684245 |
| N15 | 1.00515 | -1.95275 | -0.04248 | H13 | -2.6064 | -5.94408 | 1.011308 |
| C16 | 2.36602 | -2.26487 | 0.520077 | C14 | 0.45449 | -3.21383 | 0.034232 |
| C17 | 2.41361 | -3.82331 | 0.335154 | N15 | 0.92178 | -2.04434 | 0.323096 |
| P18 | -1.8945 | -0.75864 | 0.333207 | C16 | 2.28042 | -2.22378 | 0.978105 |
| Ir19 | 0.14087 | -0.0026 | -0.53731 | C17 | 2.52015 | -3.7501 | 0.736559 |
| C20 | -2.2189 | -0.49817 | 2.114683 | P18 | -2.1402 | -1.11693 | 0.162751 |
| C21 | -2.5651 | -0.02649 | 4.858484 | Ir19 | 0.07188 | -0.24591 | -0.52912 |
| C22 | -1.9696 | -1.51598 | 3.046768 | C20 | -2.6946 | -0.81578 | 1.892165 |
| C23 | -2.6428 | 0.760085 | 2.572792 | C21 | -3.3157 | -0.28866 | 4.588139 |
| C24 | -2.8099 | 0.992894 | 3.936373 | C22 | -2.2649 | -1.67949 | 2.910715 |
| C25 | -2.1467 | -1.28027 | 4.410581 | C23 | -3.4647 | 0.30364 | 2.246915 |
| H26 | -2.8472 | 1.557901 | 1.868008 | C24 | -3.7645 | 0.568593 | 3.582774 |
| H27 | -3.1364 | 1.971798 | 4.275951 | C25 | -2.5749 | -1.42012 | 4.245445 |
| H28 | -1.9523 | -2.07779 | 5.121962 | H26 | -3.865 | 0.950268 | 1.477098 |
| H29 | -2.6998 | 0.155421 | 5.920827 | H27 | -4.366 | 1.437612 | 3.836093 |
| O30 | 1.05944 | -4.19522 | -0.04456 | H28 | -2.2374 | -2.10738 | 5.016287 |
| C31 | 2.45415 | -1.95778 | 2.018061 | H29 | -3.5545 | -0.08546 | 5.628127 |
| C32 | 1.38484 | -1.44976 | 2.750322 | O30 | 1.23277 | -4.26168 | 0.29257 |
| C33 | 3.6483 | -2.26713 | 2.688585 | C31 | 2.23057 | -1.97755 | 2.489511 |
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| H37 | 4.49383 | -2.66225 | 2.130435 | H35 | 0.18925 | -1.34272 | 2.597543 |
| C38 | 2.69696 | -1.52368 | 4.781013 | C36 | 3.41016 | -2.03416 | 4.613355 |
| H39 | 0.65927 | -0.82146 | 4.669488 | H37 | 4.30485 | -2.53728 | 2.727935 |
| H40 | 4.7055 | -2.28414 | 4.55893 | C38 | 2.25672 | -1.59818 | 5.272162 |
| H41 | 2.79342 | -1.34691 | 5.848429 | H39 | 0.19289 | -1.01307 | 5.030254 |
| C42 | -3.3921 | -0.08984 | -0.50653 | H40 | 4.32185 | -2.22224 | 5.173285 |
| C43 | -4.6165 | 0.062927 | 0.162903 | H41 | 2.26884 | -1.44323 | 6.347447 |

| | | | | | | | |
|-----|---------|----------|----------|-----|---------|----------|----------|
| C44 | -3.3451 | 0.156321 | -1.88887 | C42 | -3.6231 | -0.77465 | -0.86957 |
| C45 | -5.7548 | 0.481733 | -0.52705 | C43 | -4.9328 | -0.91727 | -0.3837 |
| H46 | -4.6896 | -0.14178 | 1.225516 | C44 | -3.4315 | -0.51578 | -2.23415 |
| C47 | -4.4852 | 0.56886 | -2.57693 | C45 | -6.0228 | -0.79361 | -1.2447 |
| C48 | -5.6932 | 0.740943 | -1.89669 | H46 | -5.1058 | -1.12888 | 0.666886 |
| H49 | -6.6916 | 0.602089 | 0.009444 | C47 | -4.5223 | -0.39665 | -3.09451 |
| H50 | -4.43 | 0.757688 | -3.64538 | C48 | -5.8215 | -0.53534 | -2.60279 |
| H51 | -6.5798 | 1.068543 | -2.43125 | H49 | -7.0306 | -0.90637 | -0.85479 |
| H52 | -0.4406 | -0.58929 | -1.8569 | H50 | -4.3569 | -0.19028 | -4.14788 |
| H53 | 1.50773 | 0.4522 | -1.39359 | H51 | -6.6716 | -0.44394 | -3.27239 |
| H54 | -1.6195 | -2.48555 | 2.709389 | H52 | 0.05352 | -1.07572 | -1.85972 |
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| H56 | 3.08423 | -4.15662 | -0.4589 | H54 | -1.6863 | -2.5606 | 2.658095 |
| C57 | 5.4102 | -0.25761 | -1.8489 | H55 | -2.4253 | -0.40569 | -2.62573 |
| C58 | 4.68722 | -1.32584 | -2.38282 | H56 | 3.2502 | -3.97119 | -0.04415 |
| C59 | 3.70013 | -1.95102 | -1.62236 | C57 | 4.92059 | 0.446754 | -1.18575 |
| C60 | 3.43373 | -1.54002 | -0.30877 | C58 | 4.49951 | -0.75059 | -1.76711 |
| C61 | 4.13543 | -0.4406 | 0.201231 | C59 | 3.68733 | -1.62597 | -1.04982 |
| C62 | 5.11759 | 0.192437 | -0.56215 | C60 | 3.28881 | -1.32665 | 0.258959 |
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| H64 | 4.89042 | -1.67322 | -3.39174 | C62 | 4.5211 | 0.758276 | 0.114417 |
| H65 | 3.13399 | -2.76498 | -2.06745 | H63 | 5.55488 | 1.130635 | -1.74286 |
| H66 | 3.92273 | -0.08528 | 1.202473 | H64 | 4.79645 | -1 | -2.78167 |
| H67 | 5.6645 | 1.031587 | -0.14036 | H65 | 3.33399 | -2.52828 | -1.54088 |
| C68 | 1.37409 | 2.091291 | -2.95459 | H66 | 3.38424 | 0.140654 | 1.831515 |
| C69 | 0.90983 | 1.88153 | -1.49978 | H67 | 4.84277 | 1.688568 | 0.575181 |
| C70 | -0.5246 | 1.916966 | -1.16603 | C68 | 0.79136 | 4.242575 | -1.01953 |
| H71 | -1.1501 | 1.804603 | -2.04546 | C69 | 0.58921 | 2.812254 | -0.43721 |
| C72 | -1.1164 | 2.97213 | -0.27627 | C70 | -0.3231 | 1.908398 | -1.32692 |
| C73 | -1.943 | 3.926776 | -0.89593 | H71 | 0.14077 | 1.970092 | -2.31207 |
| C74 | -0.9013 | 3.091127 | 1.105744 | C72 | -1.7577 | 2.366717 | -1.44575 |
| C75 | -2.5104 | 4.973689 | -0.173 | C73 | -2.2796 | 2.718212 | -2.69791 |
| H76 | -2.1423 | 3.843322 | -1.96179 | C74 | -2.6197 | 2.400693 | -0.34261 |
| C77 | -1.4602 | 4.14685 | 1.829348 | C75 | -3.6116 | 3.109815 | -2.83893 |
| H78 | -0.3438 | 2.331837 | 1.637202 | H76 | -1.6446 | 2.665475 | -3.57881 |
| C79 | -2.2616 | 5.095292 | 1.195486 | C77 | -3.9469 | 2.802609 | -0.47586 |
| H80 | -3.1475 | 5.694178 | -0.67819 | H78 | -2.2617 | 2.067475 | 0.62235 |
| H81 | -1.2784 | 4.211956 | 2.898904 | C79 | -4.4506 | 3.15924 | -1.72683 |
| H82 | -2.6998 | 5.912006 | 1.761771 | H80 | -3.9961 | 3.366094 | -3.82179 |
| C83 | 2.14994 | 3.949141 | -0.57458 | H81 | -4.598 | 2.817878 | 0.394356 |
| C84 | 1.88702 | 2.056346 | 0.731206 | H82 | -5.4896 | 3.455396 | -1.83458 |
| C85 | 3.00501 | 4.031088 | 0.704255 | C83 | -0.5756 | 4.053318 | 1.594783 |
| H86 | 1.24854 | 4.571071 | -0.52483 | C84 | 0.08366 | 1.84138 | 1.761543 |
| H87 | 2.7194 | 4.201694 | -1.47095 | C85 | -0.6308 | 3.562215 | 3.055282 |
| H88 | 4.0711 | 3.899721 | 0.497033 | H86 | -1.5688 | 4.197218 | 1.158361 |

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|--------------------|---------|----------|----------|--------------------|---------|----------|----------|
| H89 | 2.8458 | 4.941639 | 1.281978 | H87 | -0.0169 | 4.984954 | 1.505753 |
| N90 | 1.78969 | 2.528226 | -0.53809 | H88 | 0.16253 | 3.996259 | 3.671123 |
| O91 | 2.565 | 2.904304 | 1.513238 | H89 | -1.5977 | 3.722531 | 3.533734 |
| O92 | 1.41138 | 0.995151 | 1.152714 | N90 | 0.1204 | 2.924472 | 0.959146 |
| H93 | 2.65266 | -4.34421 | 1.261074 | O91 | -0.4073 | 2.131447 | 2.976296 |
| N94 | -1.9365 | -2.43773 | 0.149965 | O92 | 0.42694 | 0.688309 | 1.476885 |
| C95 | -1.0294 | -3.16641 | -0.76805 | H93 | 2.78602 | -4.27954 | 1.649801 |
| H96 | -1.0343 | -2.74172 | -1.7813 | N94 | -1.9627 | -2.80318 | 0.145774 |
| C97 | 2.85395 | 1.750256 | -3.15634 | C95 | -0.8905 | -3.49354 | -0.59803 |
| H98 | 3.17849 | 2.053686 | -4.15606 | H96 | -0.8179 | -3.15922 | -1.64275 |
| H99 | 3.50629 | 2.232909 | -2.42473 | C97 | 1.97797 | 4.926278 | -0.31328 |
| H100 | 3.01056 | 0.671739 | -3.06306 | H98 | 2.02045 | 5.987636 | -0.57608 |
| C101 | 0.51847 | 1.334646 | -3.97813 | H99 | 1.93787 | 4.849801 | 0.776792 |
| H102 | 0.57625 | 0.256293 | -3.79968 | H100 | 2.91896 | 4.465253 | -0.63377 |
| H103 | -0.5332 | 1.631349 | -3.95598 | C101 | 1.04546 | 4.257512 | -2.5347 |
| H104 | 0.89425 | 1.534529 | -4.98554 | H102 | 1.85864 | 3.5762 | -2.81122 |
| H105 | 1.22566 | 3.169104 | -3.12834 | H103 | 0.15662 | 3.993632 | -3.11055 |
| X | 0 | 0 | 0 | H104 | 1.34124 | 5.264822 | -2.84392 |
| | | | | H105 | -0.1275 | 4.815356 | -0.83933 |
| | | | | H106 | 1.53035 | 0.14181 | -1.03154 |
| | | | | H107 | -0.5987 | 0.498669 | -1.74381 |
| C3_ZS_Cheltop_INT1 | | | | | | | |
| C1 | -3.775 | -3.59274 | -1.4966 | | | | |
| C2 | -1.6 | -4.576 | -0.94604 | | | | |
| C3 | -2.641 | -4.49469 | -2.09664 | | | | |
| C4 | -3.2128 | -3.26743 | -0.09513 | C3_ZS_Cheltop_PROD | | | |
| H5 | -4.7247 | -4.13207 | -1.42037 | C1 | -3.6213 | -4.5574 | -0.57437 |
| H6 | -2.211 | -4.08094 | -3.01426 | C2 | -1.2541 | -5.14108 | -0.46282 |
| H7 | -3.9209 | -2.84378 | 0.618627 | C3 | -2.5077 | -5.33251 | -1.35532 |
| H8 | -3.9495 | -2.68055 | -2.07191 | C4 | -2.853 | -4.05082 | 0.668342 |
| H9 | -0.8793 | -5.39021 | -1.03086 | H5 | -4.4425 | -5.21751 | -0.2763 |
| H10 | -3.012 | -5.49581 | -2.33324 | H6 | -2.3564 | -4.95179 | -2.3703 |
| C11 | -2.5173 | -4.58368 | 0.296334 | H7 | -3.4746 | -3.70869 | 1.495984 |
| H12 | -1.9747 | -4.53444 | 1.243917 | H8 | -4.0484 | -3.729 | -1.14314 |
| H13 | -3.1988 | -5.43891 | 0.312738 | H9 | -0.4299 | -5.82252 | -0.67284 |
| C14 | 0.27475 | -3.07158 | 0.064446 | H10 | -2.7451 | -6.397 | -1.43767 |
| N15 | 0.8996 | -1.96467 | 0.258982 | C11 | -1.8718 | -5.20119 | 0.952056 |
| C16 | 2.07136 | -2.2253 | 1.156048 | H12 | -1.1652 | -4.97539 | 1.756313 |
| C17 | 1.72484 | -3.6687 | 1.659285 | H13 | -2.3679 | -6.15464 | 1.15455 |
| P18 | -1.9343 | -0.71875 | 0.014156 | C14 | 0.52596 | -3.30366 | -0.04938 |
| Ir19 | 0.15034 | -0.01561 | -0.45145 | N15 | 0.98376 | -2.10547 | 0.120783 |
| C20 | -2.2917 | -0.51682 | 1.80394 | C16 | 2.35118 | -2.20387 | 0.777918 |
| C21 | -2.5102 | -0.16175 | 4.582705 | C17 | 2.65831 | -3.70554 | 0.512692 |
| C22 | -2.1097 | -1.59938 | 2.677713 | P18 | -2.0959 | -1.31184 | 0.254542 |
| C23 | -2.5765 | 0.749392 | 2.339839 | Ir19 | 0.03309 | -0.39534 | -0.46867 |
| C24 | -2.6882 | 0.92145 | 3.719272 | C20 | -2.6864 | -0.96114 | 1.957182 |
| C25 | -2.2219 | -1.42242 | 4.056431 | C21 | -3.3987 | -0.27784 | 4.590768 |
| | | | | C22 | -2.3166 | -1.78124 | 3.032876 |

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|-----|---------|----------|----------|-----|---------|----------|----------|
| H26 | -2.7006 | 1.605836 | 1.688882 | C23 | -3.4293 | 0.201321 | 2.220871 |
| H27 | -2.9045 | 1.909789 | 4.114076 | C24 | -3.7756 | 0.543068 | 3.526847 |
| H28 | -2.0788 | -2.27013 | 4.720446 | C25 | -2.6769 | -1.44454 | 4.338001 |
| H29 | -2.5918 | -0.02442 | 5.656941 | H26 | -3.7712 | 0.823301 | 1.400316 |
| O30 | 0.70572 | -4.14987 | 0.73142 | H27 | -4.3557 | 1.443168 | 3.712431 |
| C31 | 2.12061 | -1.27102 | 2.341874 | H28 | -2.3931 | -2.09873 | 5.157753 |
| C32 | 1.16527 | -0.27809 | 2.565047 | H29 | -3.6751 | -0.01601 | 5.607998 |
| C33 | 3.13745 | -1.43815 | 3.294206 | O30 | 1.35264 | -4.30169 | 0.257148 |
| C34 | 1.2251 | 0.547175 | 3.688947 | C31 | 2.25292 | -1.98992 | 2.29345 |
| H35 | 0.31467 | -0.16436 | 1.897435 | C32 | 1.06243 | -1.68253 | 2.94527 |
| C36 | 3.20038 | -0.62263 | 4.421713 | C33 | 3.42015 | -2.152 | 3.057466 |
| H37 | 3.89711 | -2.19951 | 3.138383 | C34 | 1.03307 | -1.51975 | 4.332137 |
| C38 | 2.24575 | 0.377936 | 4.621669 | H35 | 0.15917 | -1.53189 | 2.376346 |
| H39 | 0.45631 | 1.29976 | 3.8319 | C36 | 3.39236 | -1.99753 | 4.440049 |
| H40 | 3.99918 | -0.76617 | 5.143647 | H37 | 4.3615 | -2.37824 | 2.56322 |
| H41 | 2.29524 | 1.011754 | 5.502392 | C38 | 2.19407 | -1.67621 | 5.083893 |
| C42 | -3.3393 | 0.034811 | -0.8805 | H39 | 0.09528 | -1.25791 | 4.812808 |
| C43 | -4.556 | 0.352476 | -0.26127 | H40 | 4.30622 | -2.12084 | 5.014128 |
| C44 | -3.2016 | 0.24118 | -2.26412 | H41 | 2.17192 | -1.54749 | 6.162318 |
| C45 | -5.6077 | 0.885682 | -1.00978 | C42 | -3.5577 | -0.89683 | -0.78122 |
| H46 | -4.687 | 0.191005 | 0.803678 | C43 | -4.8734 | -1.12257 | -0.33984 |
| C47 | -4.2536 | 0.771408 | -3.00772 | C44 | -3.3566 | -0.36561 | -2.06368 |
| C48 | -5.459 | 1.100967 | -2.38035 | C45 | -5.9573 | -0.80904 | -1.15753 |
| H49 | -6.5441 | 1.132345 | -0.51785 | H46 | -5.0523 | -1.53001 | 0.651097 |
| H50 | -4.1318 | 0.932844 | -4.0749 | C47 | -4.4431 | -0.04813 | -2.87993 |
| H51 | -6.2772 | 1.519921 | -2.95851 | C48 | -5.7451 | -0.2659 | -2.42841 |
| H52 | -0.0822 | -0.42782 | -1.91848 | H49 | -6.9686 | -0.98557 | -0.80179 |
| H53 | 0.91132 | 1.784722 | -2.73638 | H50 | -4.2701 | 0.382785 | -3.86154 |
| H54 | -1.8654 | -2.57814 | 2.279956 | H51 | -6.5917 | -0.01386 | -3.06032 |
| H55 | -2.2654 | -0.00863 | -2.75545 | H52 | -0.1584 | -1.05495 | -1.86805 |
| H56 | 2.5682 | -4.35782 | 1.627458 | H53 | 1.34781 | 2.234774 | -0.39873 |
| C57 | 5.61452 | -2.25936 | -1.36428 | H54 | -1.7434 | -2.68413 | 2.852234 |
| C58 | 4.64914 | -3.2619 | -1.47285 | H55 | -2.3465 | -0.18672 | -2.41827 |
| C59 | 3.52544 | -3.23837 | -0.65018 | H56 | 3.27379 | -3.88478 | -0.37115 |
| C60 | 3.34572 | -2.21711 | 0.294636 | C57 | 4.93522 | 0.651001 | -1.21606 |
| C61 | 4.31147 | -1.21164 | 0.38589 | C58 | 4.60069 | -0.54924 | -1.84499 |
| C62 | 5.439 | -1.23556 | -0.43504 | C59 | 3.79966 | -1.48257 | -1.1896 |
| H63 | 6.49461 | -2.27763 | -2.00082 | C60 | 3.32752 | -1.23865 | 0.105945 |
| H64 | 4.77224 | -4.06417 | -2.19482 | C61 | 3.65757 | -0.02607 | 0.723652 |
| H65 | 2.78407 | -4.0268 | -0.75387 | C62 | 4.45732 | 0.909963 | 0.068982 |
| H66 | 4.18081 | -0.39236 | 1.080457 | H63 | 5.56281 | 1.377733 | -1.7244 |
| H67 | 6.17878 | -0.44483 | -0.34753 | H64 | 4.95785 | -0.75778 | -2.8493 |
| C68 | 0.24467 | 3.811325 | -2.79744 | H65 | 3.51775 | -2.38689 | -1.72037 |
| C69 | 0.64965 | 2.549386 | -1.99459 | H66 | 3.26816 | 0.198287 | 1.709534 |
| C70 | -0.4359 | 1.924864 | -1.06901 | H67 | 4.70763 | 1.843067 | 0.566961 |

| | | | | | | | |
|-------------------|---------|----------|----------|------|---------|----------|----------|
| H71 | -1.3187 | 1.829074 | -1.69939 | C68 | 0.87419 | 4.214919 | -1.05562 |
| C72 | -0.8148 | 2.793762 | 0.11024 | C69 | 0.44656 | 2.849626 | -0.47657 |
| C73 | -2.0258 | 3.50798 | 0.11357 | C70 | -0.5474 | 2.055606 | -1.36904 |
| C74 | -0.0114 | 2.888425 | 1.263902 | H71 | -0.0648 | 1.780351 | -2.30429 |
| C75 | -2.4148 | 4.282545 | 1.209213 | C72 | -1.9007 | 2.688943 | -1.6101 |
| H76 | -2.6869 | 3.435027 | -0.74554 | C73 | -2.225 | 3.273979 | -2.83797 |
| C77 | -0.3935 | 3.663187 | 2.359049 | C74 | -2.8715 | 2.662637 | -0.59931 |
| H78 | 0.91795 | 2.330142 | 1.329558 | C75 | -3.4831 | 3.847623 | -3.03709 |
| C79 | -1.6007 | 4.365574 | 2.34082 | H76 | -1.5019 | 3.272745 | -3.64835 |
| H80 | -3.3595 | 4.818627 | 1.178883 | C77 | -4.1279 | 3.22718 | -0.7953 |
| H81 | 0.25245 | 3.711555 | 3.231972 | H78 | -2.6421 | 2.16818 | 0.338948 |
| H82 | -1.9 | 4.969362 | 3.192456 | C79 | -4.4356 | 3.82767 | -2.01835 |
| C83 | 2.38703 | 4.097468 | -0.71774 | H80 | -3.7209 | 4.301139 | -3.99495 |
| C84 | 2.53266 | 1.807914 | -0.61935 | H81 | -4.8714 | 3.184382 | -0.00421 |
| C85 | 3.74365 | 3.656882 | -0.1421 | H82 | -5.4163 | 4.265217 | -2.17993 |
| H86 | 1.70413 | 4.476919 | 0.049998 | C83 | -0.7744 | 4.114747 | 1.496899 |
| H87 | 2.49937 | 4.848359 | -1.49948 | C84 | -0.0349 | 1.923297 | 1.754138 |
| H88 | 4.56114 | 3.785301 | -0.8585 | C85 | -0.7938 | 3.685413 | 2.978016 |
| H89 | 3.99967 | 4.132581 | 0.804692 | H86 | -1.7763 | 4.220352 | 1.071959 |
| N90 | 1.90339 | 2.813137 | -1.24497 | H87 | -0.2386 | 5.05419 | 1.353575 |
| O91 | 3.58266 | 2.230963 | 0.10227 | H88 | -0.003 | 4.167413 | 3.56121 |
| O92 | 2.22367 | 0.598981 | -0.63056 | H89 | -1.7566 | 3.844177 | 3.465583 |
| H93 | 1.27842 | -3.65946 | 2.656875 | N90 | -0.0616 | 2.978957 | 0.900925 |
| N94 | -2.0344 | -2.37767 | -0.26651 | O91 | -0.5332 | 2.259895 | 2.958356 |
| C95 | -0.9318 | -3.18544 | -0.83842 | O92 | 0.36848 | 0.780295 | 1.524938 |
| H96 | -0.6232 | -2.81404 | -1.82383 | H93 | 3.0907 | -4.20746 | 1.375865 |
| C97 | 1.30797 | 4.137455 | -3.86368 | N94 | -1.8889 | -2.99336 | 0.264407 |
| H98 | 1.09238 | 5.09622 | -4.34492 | C95 | -0.8489 | -3.64742 | -0.56643 |
| H99 | 2.32526 | 4.183004 | -3.46521 | H96 | -0.8774 | -3.30971 | -1.61198 |
| H100 | 1.30525 | 3.366674 | -4.64332 | C97 | 2.01826 | 4.811874 | -0.21628 |
| C101 | -1.1118 | 3.628601 | -3.49809 | H98 | 2.26559 | 5.817725 | -0.56815 |
| H102 | -1.1178 | 2.713879 | -4.10384 | H99 | 1.78557 | 4.878083 | 0.849715 |
| H103 | -1.9466 | 3.574113 | -2.79782 | H100 | 2.91691 | 4.19181 | -0.31401 |
| H104 | -1.2995 | 4.470655 | -4.17154 | C101 | 1.34846 | 4.074443 | -2.51218 |
| H105 | 0.14957 | 4.653262 | -2.09788 | H102 | 2.12025 | 3.300162 | -2.59753 |
| | | | | H103 | 0.53734 | 3.8253 | -3.19878 |
| C3_ZS_Cheltop_TS2 | | | | H104 | 1.78436 | 5.017481 | -2.85527 |
| C1 | -3.7143 | -4.14033 | -0.8828 | H105 | 0.00858 | 4.891409 | -1.03911 |
| C2 | -1.4083 | -4.90543 | -0.6499 | H106 | 1.4367 | 0.080955 | -1.06961 |
| C3 | -2.6176 | -4.98212 | -1.61608 | H107 | -0.9092 | 1.117059 | -0.8077 |
| C4 | -2.9741 | -3.69225 | 0.399187 | | | | |
| H5 | -4.5862 | -4.7492 | -0.62197 | | | | |
| H6 | -2.3775 | -4.58913 | -2.60899 | | | | |
| H7 | -3.6053 | -3.30213 | 1.197983 | | | | |
| H8 | -4.0649 | -3.29063 | -1.46945 | | | | |

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|------|---------|----------|----------|
| H9 | -0.6332 | -5.65227 | -0.81928 |
| H10 | -2.9281 | -6.02304 | -1.74268 |
| C11 | -2.1078 | -4.92027 | 0.726849 |
| H12 | -1.4328 | -4.7599 | 1.573234 |
| H13 | -2.6939 | -5.82809 | 0.894533 |
| C14 | 0.47555 | -3.24371 | -0.04475 |
| N15 | 0.93222 | -2.0996 | 0.326698 |
| C16 | 2.28836 | -2.32164 | 0.953298 |
| C17 | 2.48668 | -3.86376 | 0.73203 |
| P18 | -2.036 | -1.02985 | 0.090818 |
| Ir19 | -0.0368 | -0.18229 | -0.38279 |
| C20 | -2.5787 | -0.729 | 1.819034 |
| C21 | -3.1834 | -0.25152 | 4.521759 |
| C22 | -2.1051 | -1.58941 | 2.821706 |
| C23 | -3.3872 | 0.358137 | 2.189081 |
| C24 | -3.6831 | 0.594244 | 3.530743 |
| C25 | -2.4021 | -1.34987 | 4.162232 |
| H26 | -3.8101 | 1.003853 | 1.430901 |
| H27 | -4.3162 | 1.434914 | 3.800715 |
| H28 | -2.0214 | -2.02446 | 4.923506 |
| H29 | -3.413 | -0.06428 | 5.56669 |
| O30 | 1.23696 | -4.32155 | 0.152152 |
| C31 | 2.30125 | -2.04126 | 2.456965 |
| C32 | 1.20836 | -1.52504 | 3.144915 |
| C33 | 3.47157 | -2.34201 | 3.173528 |
| C34 | 1.27524 | -1.30307 | 4.522412 |
| H35 | 0.31551 | -1.2609 | 2.605322 |
| C36 | 3.53868 | -2.12984 | 4.5474 |
| H37 | 4.34295 | -2.72754 | 2.64948 |
| C38 | 2.43541 | -1.60842 | 5.22911 |
| H39 | 0.41213 | -0.88345 | 5.031633 |
| H40 | 4.4525 | -2.36569 | 5.085033 |
| H41 | 2.48798 | -1.43655 | 6.300413 |
| C42 | -3.4697 | -0.67781 | -0.98697 |
| C43 | -4.7832 | -0.7922 | -0.4999 |
| C44 | -3.2634 | -0.57599 | -2.37032 |
| C45 | -5.8636 | -0.79377 | -1.38131 |
| H46 | -4.9704 | -0.90249 | 0.562553 |
| C47 | -4.3468 | -0.5885 | -3.24704 |
| C48 | -5.6495 | -0.69661 | -2.7572 |
| H49 | -6.8729 | -0.88165 | -0.98963 |
| H50 | -4.172 | -0.50401 | -4.31545 |
| H51 | -6.4918 | -0.70494 | -3.44229 |
| H52 | -0.2787 | -0.78902 | -1.81011 |
| H53 | 1.43881 | 2.429561 | -0.32464 |

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|-----|---------|----------|----------|
| H54 | -1.5043 | -2.44942 | 2.549775 |
| H55 | -2.2541 | -0.48025 | -2.75561 |
| H56 | 3.2919 | -4.11465 | 0.039888 |
| C57 | 5.1019 | 0.120271 | -1.27686 |
| C58 | 4.59336 | -1.05562 | -1.83196 |
| C59 | 3.69896 | -1.84001 | -1.10602 |
| C60 | 3.31089 | -1.47431 | 0.190012 |
| C61 | 3.81533 | -0.28716 | 0.733946 |
| C62 | 4.70408 | 0.505296 | 0.003513 |
| H63 | 5.79996 | 0.732486 | -1.84023 |
| H64 | 4.88896 | -1.35984 | -2.83171 |
| H65 | 3.28978 | -2.73349 | -1.57 |
| H66 | 3.50683 | 0.02292 | 1.725967 |
| H67 | 5.08999 | 1.421237 | 0.442275 |
| C68 | 0.54595 | 4.22739 | -1.02625 |
| C69 | 0.41615 | 2.821715 | -0.3813 |
| C70 | -0.4489 | 1.773788 | -1.16305 |
| H71 | 0.03277 | 1.7035 | -2.14425 |
| C72 | -1.8553 | 2.249838 | -1.40081 |
| C73 | -2.3329 | 2.471906 | -2.70036 |
| C74 | -2.7402 | 2.497692 | -0.34239 |
| C75 | -3.6312 | 2.928917 | -2.92976 |
| H76 | -1.6837 | 2.265369 | -3.54805 |
| C77 | -4.0373 | 2.956311 | -0.56005 |
| H78 | -2.4124 | 2.288285 | 0.66623 |
| C79 | -4.4913 | 3.177453 | -1.86091 |
| H80 | -3.9738 | 3.083971 | -3.94904 |
| H81 | -4.6989 | 3.129918 | 0.28563 |
| H82 | -5.5029 | 3.529795 | -2.03864 |
| C83 | -0.7053 | 4.072239 | 1.694843 |
| C84 | 0.07568 | 1.899275 | 1.852638 |
| C85 | -0.7141 | 3.576553 | 3.158937 |
| H86 | -1.7099 | 4.204066 | 1.283988 |
| H87 | -0.165 | 5.013656 | 1.591363 |
| H88 | 0.04773 | 4.06749 | 3.771345 |
| H89 | -1.6877 | 3.666554 | 3.642613 |
| N90 | -0.0067 | 2.960858 | 1.036051 |
| O91 | -0.3848 | 2.164354 | 3.085363 |
| O92 | 0.51692 | 0.773671 | 1.563023 |
| H93 | 2.6297 | -4.40009 | 1.669535 |
| N94 | -1.9021 | -2.71692 | 0.047217 |
| C95 | -0.8653 | -3.45327 | -0.70251 |
| H96 | -0.7697 | -3.10747 | -1.74133 |
| C97 | 1.70015 | 5.011922 | -0.37121 |
| H98 | 1.6917 | 6.056384 | -0.69739 |

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|------|---------|----------|----------|
| H99 | 1.67375 | 5.001517 | 0.721877 |
| H100 | 2.66208 | 4.579516 | -0.67072 |
| C101 | 0.80414 | 4.155383 | -2.53824 |
| H102 | 1.65702 | 3.502998 | -2.76106 |
| H103 | -0.0633 | 3.793635 | -3.09019 |
| H104 | 1.04567 | 5.152635 | -2.91877 |
| H105 | -0.4016 | 4.761621 | -0.87492 |
| H106 | 2.24919 | 0.591353 | -1.18911 |
| H107 | 1.9958 | 0.311567 | -1.83756 |

C3_ZR_Cheltop

C3_ZR_Cheltop_SM

| | | | |
|------|----------|----------|----------|
| C1 | -3.42767 | -4.99928 | 0.479053 |
| C2 | -1.07632 | -5.06677 | -0.16005 |
| C3 | -2.47179 | -5.55021 | -0.62902 |
| C4 | -2.44773 | -4.25965 | 1.419601 |
| H5 | -3.92578 | -5.80825 | 1.023599 |
| H6 | -2.72446 | -5.17828 | -1.6271 |
| H7 | -2.84639 | -4.00546 | 2.401367 |
| H8 | -4.2017 | -4.34184 | 0.084042 |
| H9 | -0.23432 | -5.58061 | -0.62223 |
| H10 | -2.49288 | -6.64278 | -0.67149 |
| C11 | -1.20833 | -5.16983 | 1.375254 |
| H12 | -0.35672 | -4.76126 | 1.92764 |
| H13 | -1.41156 | -6.18957 | 1.714036 |
| C14 | 0.343637 | -2.90881 | -0.32145 |
| N15 | 0.617797 | -1.65944 | -0.16291 |
| C16 | 2.110915 | -1.46655 | -0.38425 |
| C17 | 2.587364 | -2.95173 | -0.44308 |
| P18 | -2.54607 | -1.49083 | 0.626891 |
| Ir19 | -0.74214 | 0.008598 | -0.05545 |
| C20 | -3.15637 | -1.11929 | 2.307915 |
| C21 | -3.81411 | -0.25983 | 4.904451 |
| C22 | -2.39589 | -1.53501 | 3.413806 |
| C23 | -4.24099 | -0.25313 | 2.520374 |
| C24 | -4.56959 | 0.166839 | 3.81054 |
| C25 | -2.7274 | -1.1138 | 4.700168 |
| H26 | -4.83341 | 0.102073 | 1.683925 |
| H27 | -5.42115 | 0.825411 | 3.95831 |
| H28 | -2.12771 | -1.44353 | 5.543398 |
| H29 | -4.07096 | 0.067071 | 5.907833 |
| O30 | 1.367497 | -3.73463 | -0.55405 |
| C31 | 2.786102 | -0.80053 | 0.808679 |
| C32 | 2.180973 | -0.81334 | 2.068814 |
| C33 | 4.088303 | -0.29117 | 0.687809 |

C3_ZR_Cheltop_INT2

| | | | |
|------|----------|----------|----------|
| C1 | -4.04825 | -3.70792 | 1.012992 |
| C2 | -1.9792 | -4.72145 | 0.235016 |
| C3 | -3.50205 | -4.72514 | -0.04046 |
| C4 | -2.76 | -3.26768 | 1.751572 |
| H5 | -4.73054 | -4.18775 | 1.722404 |
| H6 | -3.73764 | -4.43444 | -1.06916 |
| H7 | -2.92599 | -2.76692 | 2.70453 |
| H8 | -4.57931 | -2.87114 | 0.561246 |
| H9 | -1.42924 | -5.55957 | -0.19259 |
| H10 | -3.90919 | -5.72776 | 0.118339 |
| C11 | -1.93794 | -4.56798 | 1.771924 |
| H12 | -0.93228 | -4.43476 | 2.181759 |
| H13 | -2.44246 | -5.38834 | 2.290096 |
| C14 | 0.068039 | -3.27072 | -0.36372 |
| N15 | 0.725981 | -2.17015 | -0.4416 |
| C16 | 2.191876 | -2.51519 | -0.31192 |
| C17 | 2.14716 | -4.02739 | -0.67101 |
| P18 | -1.95202 | -0.75675 | 0.642316 |
| Ir19 | -0.13697 | -0.13893 | -0.6763 |
| C20 | -1.93831 | -0.0852 | 2.3461 |
| C21 | -1.7045 | 1.084397 | 4.891056 |
| C22 | -1.29752 | -0.77028 | 3.389358 |
| C23 | -2.46 | 1.194817 | 2.593705 |
| C24 | -2.34871 | 1.77067 | 3.858899 |
| C25 | -1.1837 | -0.18811 | 4.651593 |
| H26 | -2.95836 | 1.740253 | 1.800765 |
| H27 | -2.77457 | 2.754057 | 4.039657 |
| H28 | -0.68912 | -0.73362 | 5.450106 |
| H29 | -1.61662 | 1.534331 | 5.875428 |
| O30 | 0.770934 | -4.407 | -0.37184 |
| C31 | 2.638369 | -2.38495 | 1.151956 |
| C32 | 1.760272 | -2.02653 | 2.171628 |
| C33 | 3.968007 | -2.69164 | 1.478231 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| C34 | 2.831787 | -0.26469 | 3.174009 | C34 | 2.199799 | -1.95382 | 3.494336 |
| H35 | 1.186292 | -1.22162 | 2.187385 | H35 | 0.741626 | -1.77114 | 1.927233 |
| C36 | 4.743273 | 0.244827 | 1.795902 | C36 | 4.406276 | -2.62908 | 2.798097 |
| H37 | 4.590628 | -0.3026 | -0.27381 | H37 | 4.668203 | -2.96374 | 0.692386 |
| C38 | 4.112107 | 0.272108 | 3.041183 | C38 | 3.52112 | -2.25554 | 3.813298 |
| H39 | 2.330197 | -0.25528 | 4.13737 | H39 | 1.505488 | -1.6454 | 4.270714 |
| H40 | 5.747219 | 0.644208 | 1.68376 | H40 | 5.43973 | -2.86558 | 3.034388 |
| H41 | 4.619502 | 0.699724 | 3.901403 | H41 | 3.864698 | -2.1986 | 4.842115 |
| C42 | -4.02203 | -1.64208 | -0.45836 | C42 | -3.64214 | -0.4778 | -0.01453 |
| C43 | -5.29444 | -2.01298 | 0.008349 | C43 | -4.74183 | -0.23665 | 0.822926 |
| C44 | -3.81647 | -1.51141 | -1.841 | C44 | -3.86232 | -0.69748 | -1.38419 |
| C45 | -6.33915 | -2.22659 | -0.89005 | C45 | -6.03139 | -0.18926 | 0.293165 |
| H46 | -5.47045 | -2.14381 | 1.071482 | H46 | -4.60221 | -0.09367 | 1.888864 |
| C47 | -4.86112 | -1.73847 | -2.73778 | C47 | -5.1529 | -0.66211 | -1.90685 |
| C48 | -6.12624 | -2.09063 | -2.26467 | C48 | -6.24053 | -0.40201 | -1.07004 |
| H49 | -7.32008 | -2.50596 | -0.5161 | H49 | -6.87389 | 0.007151 | 0.949963 |
| H50 | -4.68747 | -1.63125 | -3.80473 | H50 | -5.30811 | -0.82795 | -2.96891 |
| H51 | -6.94214 | -2.25963 | -2.96111 | H51 | -7.24611 | -0.36635 | -1.47853 |
| H52 | -0.9641 | -0.20249 | -1.58421 | H52 | -1.02533 | -0.56929 | -1.89993 |
| H53 | 0.603721 | 0.70044 | -0.51552 | H53 | 1.82407 | 1.934043 | -1.0084 |
| H54 | -1.52663 | -2.16616 | 3.26072 | H54 | -0.88531 | -1.75781 | 3.218586 |
| H55 | -2.83929 | -1.21677 | -2.21048 | H55 | -3.02059 | -0.87606 | -2.0449 |
| H56 | 3.22176 | -3.17837 | -1.29987 | H56 | 2.320471 | -4.24483 | -1.72748 |
| C57 | 2.321582 | 0.587778 | -4.21352 | C57 | 4.2689 | 0.170129 | -3.02006 |
| C58 | 2.014686 | -0.77314 | -4.14429 | C58 | 3.673177 | -0.99382 | -3.51075 |
| C59 | 1.991402 | -1.42516 | -2.91217 | C59 | 3.050436 | -1.8898 | -2.63963 |
| C60 | 2.276879 | -0.73721 | -1.72451 | C60 | 3.017315 | -1.6454 | -1.26051 |
| C61 | 2.575563 | 0.630247 | -1.80541 | C61 | 3.620658 | -0.47315 | -0.77729 |
| C62 | 2.601756 | 1.284365 | -3.03829 | C62 | 4.241509 | 0.424243 | -1.64805 |
| H63 | 2.343903 | 1.096566 | -5.17272 | H63 | 4.749803 | 0.86802 | -3.6988 |
| H64 | 1.793317 | -1.32933 | -5.0507 | H64 | 3.687318 | -1.20558 | -4.57593 |
| H65 | 1.727386 | -2.47966 | -2.88384 | H65 | 2.564479 | -2.76438 | -3.06046 |
| H66 | 2.779374 | 1.200601 | -0.90674 | H66 | 3.573091 | -0.24459 | 0.280608 |
| H67 | 2.838969 | 2.344021 | -3.07225 | H67 | 4.693874 | 1.328521 | -1.25091 |
| C68 | -3.37037 | 1.810127 | -0.49846 | C68 | -1.53135 | 2.731533 | -1.54233 |
| C69 | -1.99558 | 1.794022 | 0.208331 | C69 | -0.35681 | 2.037547 | -0.81149 |
| C70 | -0.78518 | 2.165951 | -0.47248 | C70 | 1.018176 | 2.528895 | -1.44575 |
| H71 | -0.86157 | 2.263781 | -1.55008 | H71 | 1.004688 | 2.293321 | -2.5135 |
| C72 | 0.237111 | 3.104047 | 0.106612 | C72 | 1.400541 | 3.97954 | -1.24622 |
| C73 | 1.243911 | 2.754967 | 1.014981 | C73 | 2.261755 | 4.32726 | -0.1933 |
| C74 | 0.141255 | 4.441415 | -0.31288 | C74 | 0.934449 | 5.003921 | -2.08309 |
| C75 | 2.120615 | 3.724479 | 1.50613 | C75 | 2.607977 | 5.657297 | 0.048605 |
| H76 | 1.355637 | 1.725691 | 1.333058 | H76 | 2.665509 | 3.542453 | 0.443958 |
| C77 | 1.016515 | 5.408282 | 0.179155 | C77 | 1.277677 | 6.336352 | -1.845 |
| H78 | -0.62742 | 4.723938 | -1.02925 | H78 | 0.306494 | 4.75673 | -2.9353 |

| | | | | | | | |
|------|----------|----------|----------|------|----------|----------|----------|
| C79 | 2.00888 | 5.052267 | 1.095543 | C79 | 2.10584 | 6.670413 | -0.77131 |
| H80 | 2.896732 | 3.427687 | 2.205952 | H80 | 3.277641 | 5.901939 | 0.868949 |
| H81 | 0.926633 | 6.437406 | -0.15734 | H81 | 0.902927 | 7.114462 | -2.50418 |
| H82 | 2.693689 | 5.804302 | 1.476796 | H82 | 2.372863 | 7.706937 | -0.58776 |
| C83 | -2.26456 | 3.417386 | 2.256212 | C83 | -0.58832 | 3.745983 | 1.265506 |
| C84 | -1.16508 | 1.414925 | 2.476444 | C84 | 0.53149 | 1.732297 | 1.411706 |
| C85 | -2.01 | 3.089677 | 3.732503 | C85 | 0.326214 | 3.700887 | 2.512399 |
| H86 | -3.28111 | 3.76281 | 2.094297 | H86 | -1.64203 | 3.80595 | 1.54916 |
| H87 | -1.56032 | 4.155563 | 1.857353 | H87 | -0.34771 | 4.578185 | 0.604267 |
| H88 | -1.53896 | 3.897483 | 4.293031 | H88 | 1.166075 | 4.395125 | 2.439018 |
| H89 | -2.91812 | 2.750595 | 4.240893 | H89 | -0.21444 | 3.858501 | 3.44654 |
| N90 | -2.01116 | 2.090075 | 1.649971 | N90 | -0.29666 | 2.44947 | 0.634061 |
| O91 | -1.08719 | 1.971033 | 3.688848 | O91 | 0.867303 | 2.349787 | 2.546083 |
| O92 | -0.50664 | 0.407783 | 2.185037 | O92 | 0.966781 | 0.59557 | 1.128987 |
| H93 | 3.084848 | -3.25259 | 0.480306 | H93 | 2.805421 | -4.63385 | -0.05179 |
| N94 | -1.87492 | -3.04733 | 0.762315 | N94 | -1.87523 | -2.44395 | 0.869288 |
| C95 | -1.03227 | -3.52829 | -0.359 | C95 | -1.42839 | -3.34704 | -0.22671 |
| H96 | -1.45464 | -3.26274 | -1.34117 | H96 | -1.85503 | -3.06363 | -1.20001 |
| C97 | -3.25087 | 1.834973 | -2.02974 | C97 | -2.8909 | 2.719906 | -0.8342 |
| H98 | -2.56416 | 1.075944 | -2.40638 | H98 | -2.87489 | 3.229021 | 0.131039 |
| H99 | -4.23217 | 1.644289 | -2.47331 | H99 | -3.6279 | 3.24399 | -1.4519 |
| H100 | -2.91182 | 2.814856 | -2.38537 | H100 | -3.25767 | 1.708994 | -0.68442 |
| C101 | -4.30004 | 2.959375 | -0.06328 | C101 | -1.70994 | 2.189399 | -2.97052 |
| H102 | -4.6357 | 2.846688 | 0.970915 | H102 | -0.77746 | 2.178565 | -3.54159 |
| H103 | -3.82318 | 3.939212 | -0.18037 | H103 | -2.09496 | 1.166793 | -2.94353 |
| H104 | -5.19623 | 2.954035 | -0.69179 | H104 | -2.42572 | 2.808119 | -3.52152 |
| H105 | -3.88348 | 0.884143 | -0.22924 | H105 | -1.25057 | 3.790536 | -1.63366 |
| X | -1.52878 | 1.835509 | -0.4773 | H106 | 1.39454 | 0.10461 | -1.54425 |
| | | | | H107 | 0.813622 | 0.006655 | -2.13567 |

C3_ZR_Cheltop_TS1

| | | | |
|-----|----------|----------|----------|
| C1 | -3.33943 | -5.09715 | 0.414086 |
| C2 | -0.97801 | -5.11036 | -0.19421 |
| C3 | -2.35639 | -5.62371 | -0.6825 |
| C4 | -2.38775 | -4.34241 | 1.371528 |
| H5 | -3.83085 | -5.91819 | 0.946416 |
| H6 | -2.60298 | -5.25479 | -1.68321 |
| H7 | -2.80471 | -4.10025 | 2.348941 |
| H8 | -4.11906 | -4.44978 | 0.011861 |
| H9 | -0.11802 | -5.60225 | -0.64709 |
| H10 | -2.35363 | -6.71632 | -0.72803 |
| C11 | -1.12682 | -5.2235 | 1.338969 |
| H12 | -0.29169 | -4.79687 | 1.902811 |
| H13 | -1.30882 | -6.24949 | 1.670621 |
| C14 | 0.392069 | -2.91542 | -0.32938 |
| N15 | 0.620199 | -1.65852 | -0.17185 |

C3_ZR_Cheltop_TS3

| | | | |
|-----|----------|----------|----------|
| C1 | -4.09624 | -3.79857 | 0.772442 |
| C2 | -1.96725 | -4.7499 | 0.07422 |
| C3 | -3.46996 | -4.74996 | -0.29848 |
| C4 | -2.86148 | -3.38455 | 1.610061 |
| H5 | -4.81353 | -4.32526 | 1.410508 |
| H6 | -3.6418 | -4.40382 | -1.32286 |
| H7 | -3.08931 | -2.93089 | 2.574517 |
| H8 | -4.6113 | -2.94377 | 0.335428 |
| H9 | -1.38322 | -5.56176 | -0.35878 |
| H10 | -3.8749 | -5.7632 | -0.22387 |
| C11 | -2.02593 | -4.67589 | 1.616452 |
| H12 | -1.04964 | -4.55571 | 2.095247 |
| H13 | -2.55171 | -5.52689 | 2.058451 |
| C14 | 0.100802 | -3.2539 | -0.32013 |

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|------|----------|----------|----------|------|----------|----------|----------|
| C16 | 2.106337 | -1.41687 | -0.33658 | N15 | 0.753395 | -2.15026 | -0.39112 |
| C17 | 2.638021 | -2.88274 | -0.48067 | C16 | 2.222503 | -2.46804 | -0.2396 |
| P18 | -2.51562 | -1.5642 | 0.630303 | C17 | 2.203716 | -4.01353 | -0.46457 |
| Ir19 | -0.84634 | -0.04572 | -0.08317 | P18 | -2.03999 | -0.81503 | 0.677837 |
| C20 | -3.04679 | -1.20148 | 2.336987 | Ir19 | -0.07992 | -0.10995 | -0.65665 |
| C21 | -3.60158 | -0.35085 | 4.95183 | C20 | -2.00301 | -0.20454 | 2.39839 |
| C22 | -2.27038 | -1.65748 | 3.414224 | C21 | -1.74116 | 0.878128 | 4.971821 |
| C23 | -4.08611 | -0.29066 | 2.58215 | C22 | -1.42157 | -0.95701 | 3.427685 |
| C24 | -4.36473 | 0.125249 | 3.884773 | C23 | -2.4485 | 1.099873 | 2.66954 |
| C25 | -2.55362 | -1.24221 | 4.712948 | C24 | -2.32114 | 1.633641 | 3.950836 |
| H26 | -4.68164 | 0.094648 | 1.760244 | C25 | -1.2949 | -0.41688 | 4.707381 |
| H27 | -5.18248 | 0.817671 | 4.064607 | H26 | -2.90121 | 1.694396 | 1.882905 |
| H28 | -1.94784 | -1.60474 | 5.538057 | H27 | -2.68393 | 2.637625 | 4.154425 |
| H29 | -3.81954 | -0.02665 | 5.96526 | H28 | -0.84917 | -1.01204 | 5.499112 |
| O30 | 1.44439 | -3.71097 | -0.5451 | H29 | -1.64175 | 1.295621 | 5.969482 |
| C31 | 2.727112 | -0.79952 | 0.912217 | O30 | 0.808812 | -4.38499 | -0.26402 |
| C32 | 2.070743 | -0.8553 | 2.144522 | C31 | 2.677047 | -2.21286 | 1.204081 |
| C33 | 4.030926 | -0.28323 | 0.861857 | C32 | 1.764975 | -1.96687 | 2.22875 |
| C34 | 2.675384 | -0.34096 | 3.292568 | C33 | 4.038554 | -2.33413 | 1.526464 |
| H35 | 1.072257 | -1.26702 | 2.206602 | C34 | 2.197608 | -1.80383 | 3.545229 |
| C36 | 4.638924 | 0.219522 | 2.010642 | H35 | 0.715997 | -1.86567 | 1.995816 |
| H37 | 4.570297 | -0.26218 | -0.08042 | C36 | 4.471342 | -2.17987 | 2.841513 |
| C38 | 3.957027 | 0.20395 | 3.229476 | H37 | 4.764671 | -2.5359 | 0.744174 |
| H39 | 2.135542 | -0.36345 | 4.234653 | C38 | 3.550915 | -1.90602 | 3.857046 |
| H40 | 5.64438 | 0.626389 | 1.951287 | H39 | 1.470341 | -1.57954 | 4.320438 |
| H41 | 4.427151 | 0.605615 | 4.122642 | H40 | 5.529069 | -2.26697 | 3.073453 |
| C42 | -4.05985 | -1.67954 | -0.35768 | H41 | 3.89043 | -1.77369 | 4.880508 |
| C43 | -5.27456 | -2.11585 | 0.200088 | C42 | -3.74492 | -0.49473 | 0.072961 |
| C44 | -3.99523 | -1.42923 | -1.73666 | C43 | -4.82354 | -0.25152 | 0.935842 |
| C45 | -6.3991 | -2.28454 | -0.60591 | C44 | -3.99094 | -0.64374 | -1.30171 |
| H46 | -5.34384 | -2.32261 | 1.263816 | C45 | -6.11778 | -0.13451 | 0.42735 |
| C47 | -5.12146 | -1.60705 | -2.5414 | H46 | -4.66272 | -0.15479 | 2.004265 |
| C48 | -6.32521 | -2.03358 | -1.97873 | C47 | -5.28506 | -0.53818 | -1.80477 |
| H49 | -7.33316 | -2.6165 | -0.16186 | C48 | -6.3516 | -0.27665 | -0.94084 |
| H50 | -5.05835 | -1.40615 | -3.60696 | H49 | -6.94456 | 0.063959 | 1.103522 |
| H51 | -7.20326 | -2.16649 | -2.60351 | H50 | -5.46076 | -0.64755 | -2.87088 |
| H52 | -1.10952 | -0.32876 | -1.59764 | H51 | -7.36006 | -0.1832 | -1.33324 |
| H53 | 0.335167 | 0.868692 | -0.62722 | H52 | -1.08873 | -0.56604 | -1.78024 |
| H54 | -1.43134 | -2.32036 | 3.228584 | H53 | 1.891189 | 1.968537 | -1.04992 |
| H55 | -3.06421 | -1.08337 | -2.17291 | H54 | -1.06356 | -1.9611 | 3.230689 |
| H56 | 3.221172 | -3.05305 | -1.38629 | H55 | -3.1656 | -0.82112 | -1.98465 |
| C57 | 2.269449 | 0.878293 | -4.02202 | H56 | 2.484442 | -4.32665 | -1.47214 |
| C58 | 1.967556 | -0.48551 | -4.03701 | C57 | 4.260118 | -0.1143 | -3.27425 |
| C59 | 1.967269 | -1.21442 | -2.85008 | C58 | 3.575202 | -1.27978 | -3.62474 |
| C60 | 2.27396 | -0.6028 | -1.62601 | C59 | 2.956635 | -2.05534 | -2.64309 |

| | | | | | | | |
|------|----------|----------|----------|------|----------|----------|----------|
| C61 | 2.571226 | 0.765302 | -1.62362 | C60 | 3.017476 | -1.69142 | -1.29193 |
| C62 | 2.570839 | 1.499309 | -2.81154 | C61 | 3.697581 | -0.51202 | -0.95278 |
| H63 | 2.268936 | 1.448597 | -4.9465 | C62 | 4.315758 | 0.266239 | -1.93279 |
| H64 | 1.727816 | -0.98071 | -4.97356 | H63 | 4.743556 | 0.488675 | -4.03726 |
| H65 | 1.698283 | -2.26755 | -2.88231 | H64 | 3.519535 | -1.58789 | -4.6649 |
| H66 | 2.78857 | 1.276851 | -0.69506 | H65 | 2.403319 | -2.93669 | -2.95337 |
| H67 | 2.80055 | 2.560747 | -2.78018 | H66 | 3.728581 | -0.18839 | 0.08063 |
| C68 | -3.28177 | 1.908127 | -0.69198 | H67 | 4.835855 | 1.175244 | -1.6435 |
| C69 | -1.93526 | 1.80131 | 0.064831 | C68 | -1.47732 | 2.720463 | -1.55914 |
| C70 | -0.65601 | 2.111446 | -0.59181 | C69 | -0.28132 | 2.062959 | -0.8288 |
| H71 | -0.71565 | 2.212906 | -1.67131 | C70 | 1.078998 | 2.56529 | -1.47042 |
| C72 | 0.341703 | 3.069449 | 0.001052 | H71 | 1.05324 | 2.326705 | -2.53699 |
| C73 | 1.28685 | 2.730358 | 0.975421 | C72 | 1.454195 | 4.016416 | -1.26366 |
| C74 | 0.287484 | 4.392216 | -0.4644 | C73 | 2.341045 | 4.345526 | -0.22618 |
| C75 | 2.153678 | 3.699991 | 1.483453 | C74 | 0.951858 | 5.057448 | -2.05817 |
| H76 | 1.358014 | 1.708212 | 1.329438 | C75 | 2.677745 | 5.671707 | 0.045382 |
| C77 | 1.149419 | 5.360203 | 0.048422 | H76 | 2.771569 | 3.546708 | 0.375214 |
| H78 | -0.43687 | 4.662928 | -1.22956 | C77 | 1.282564 | 6.387146 | -1.7884 |
| C79 | 2.085218 | 5.016228 | 1.027137 | H78 | 0.303506 | 4.827783 | -2.89978 |
| H80 | 2.886499 | 3.414159 | 2.23254 | C79 | 2.136663 | 6.699753 | -0.72912 |
| H81 | 1.094581 | 6.380506 | -0.3206 | H80 | 3.367145 | 5.90235 | 0.853432 |
| H82 | 2.760796 | 5.769357 | 1.422225 | H81 | 0.877345 | 7.180761 | -2.41004 |
| C83 | -2.2004 | 3.519579 | 2.058818 | H82 | 2.391449 | 7.734615 | -0.51921 |
| C84 | -1.18666 | 1.485621 | 2.36388 | C83 | -0.53115 | 3.793354 | 1.238435 |
| C85 | -1.98614 | 3.228868 | 3.549703 | C84 | 0.456759 | 1.726906 | 1.458604 |
| H86 | -3.20001 | 3.897031 | 1.867719 | C85 | 0.357897 | 3.727406 | 2.499569 |
| H87 | -1.46327 | 4.221609 | 1.655202 | H86 | -1.59067 | 3.865638 | 1.499945 |
| H88 | -1.49412 | 4.035386 | 4.093909 | H87 | -0.26562 | 4.623769 | 0.584586 |
| H89 | -2.91608 | 2.943834 | 4.05209 | H88 | 1.266215 | 4.325873 | 2.398713 |
| N90 | -1.98398 | 2.165674 | 1.495123 | H89 | -0.16837 | 3.989395 | 3.418094 |
| O91 | -1.10817 | 2.074036 | 3.560048 | N90 | -0.24742 | 2.489803 | 0.614725 |
| O92 | -0.55897 | 0.446862 | 2.115617 | O91 | 0.757395 | 2.329573 | 2.607475 |
| H93 | 3.208414 | -3.19737 | 0.394493 | O92 | 0.814764 | 0.546596 | 1.230735 |
| N94 | -1.83826 | -3.11703 | 0.723071 | H93 | 2.801491 | -4.55052 | 0.27019 |
| C95 | -0.96755 | -3.57092 | -0.38788 | N94 | -1.93989 | -2.50692 | 0.822906 |
| H96 | -1.38236 | -3.30885 | -1.37408 | C95 | -1.40234 | -3.35031 | -0.28064 |
| C97 | -3.10726 | 1.888518 | -2.21924 | H96 | -1.76522 | -3.02458 | -1.26597 |
| H98 | -2.44655 | 1.087631 | -2.55661 | C97 | -2.82108 | 2.670843 | -0.8252 |
| H99 | -4.08111 | 1.739719 | -2.69468 | H98 | -2.81168 | 3.213121 | 0.122037 |
| H100 | -2.70713 | 2.84206 | -2.58372 | H99 | -3.59913 | 3.130954 | -1.44322 |
| C101 | -4.15499 | 3.123543 | -0.32364 | H100 | -3.12812 | 1.648139 | -0.63032 |
| H102 | -4.54282 | 3.057081 | 0.696048 | C101 | -1.66111 | 2.16241 | -2.9805 |
| H103 | -3.61416 | 4.069987 | -0.43916 | H102 | -0.73353 | 2.156427 | -3.55945 |
| H104 | -5.02275 | 3.159889 | -0.99003 | H103 | -2.03567 | 1.135729 | -2.94205 |
| H105 | -3.85779 | 1.018983 | -0.41679 | H104 | -2.39001 | 2.766065 | -3.53089 |

| | | | | | | | |
|--------------------|----------|----------|----------|--------------------|----------|----------|----------|
| X | -1.52878 | 1.835509 | -0.4773 | H105 | -1.22423 | 3.785339 | -1.66326 |
| | | | | H106 | 1.373267 | 0.154683 | -1.24307 |
| | | | | H107 | 0.360374 | -0.09257 | -2.17009 |
| C3_ZR_Cheltop_INT1 | | | | C3_ZR_Cheltop_PROD | | | |
| C1 | -4.16881 | -3.50899 | 0.506112 | C1 | -4.09679 | -4.04262 | 0.439749 |
| C2 | -2.03965 | -4.58626 | 0.001888 | C2 | -1.88516 | -4.92213 | -0.08026 |
| C3 | -3.51107 | -4.52878 | -0.48183 | C3 | -3.34824 | -4.951 | -0.59184 |
| C4 | -2.9837 | -3.1361 | 1.427926 | C4 | -2.96634 | -3.66201 | 1.426152 |
| H5 | -4.96996 | -3.97141 | 1.091729 | H5 | -4.88842 | -4.58965 | 0.961883 |
| H6 | -3.59065 | -4.21593 | -1.52784 | H6 | -3.43607 | -4.5877 | -1.62081 |
| H7 | -3.25526 | -2.6401 | 2.359979 | H7 | -3.307 | -3.26592 | 2.382567 |
| H8 | -4.58635 | -2.63467 | 0.004602 | H8 | -4.54804 | -3.15841 | -0.01427 |
| H9 | -1.46428 | -5.43527 | -0.3664 | H9 | -1.23401 | -5.69158 | -0.49552 |
| H10 | -3.96976 | -5.51827 | -0.40083 | H10 | -3.72954 | -5.97602 | -0.57337 |
| C11 | -2.21201 | -4.46334 | 1.532112 | C11 | -2.09654 | -4.93151 | 1.450527 |
| H12 | -1.27078 | -4.37058 | 2.082655 | H12 | -1.17529 | -4.80856 | 2.027391 |
| H13 | -2.80734 | -5.27735 | 1.954972 | H13 | -2.63319 | -5.82057 | 1.793913 |
| C14 | 0.114089 | -3.1731 | -0.29997 | C14 | 0.13068 | -3.28926 | -0.27381 |
| N15 | 0.804969 | -2.09257 | -0.21828 | N15 | 0.723453 | -2.1401 | -0.32536 |
| C16 | 2.259598 | -2.46234 | -0.18792 | C16 | 2.205187 | -2.35396 | -0.05016 |
| C17 | 2.188668 | -3.99546 | -0.51573 | C17 | 2.289334 | -3.87585 | -0.35086 |
| P18 | -1.90602 | -0.64746 | 0.535682 | P18 | -2.03108 | -1.0282 | 0.755381 |
| Ir19 | 0.002896 | -0.04179 | -0.45029 | Ir19 | -0.18 | -0.35528 | -0.65146 |
| C20 | -1.90991 | -0.03114 | 2.248604 | C20 | -1.9677 | -0.52344 | 2.517177 |
| C21 | -1.52752 | 1.058013 | 4.799838 | C21 | -1.71841 | 0.420869 | 5.153291 |
| C22 | -1.39165 | -0.82106 | 3.283906 | C22 | -1.65892 | -1.40505 | 3.560874 |
| C23 | -2.22585 | 1.314009 | 2.498288 | C23 | -2.13341 | 0.84145 | 2.807367 |
| C24 | -2.03754 | 1.85158 | 3.770072 | C24 | -2.00812 | 1.308713 | 4.113448 |
| C25 | -1.2085 | -0.27796 | 4.555018 | C25 | -1.54512 | -0.93422 | 4.871653 |
| H26 | -2.60555 | 1.942061 | 1.69866 | H26 | -2.36517 | 1.539226 | 2.006855 |
| H27 | -2.28875 | 2.891798 | 3.958427 | H27 | -2.14244 | 2.366324 | 4.323716 |
| H28 | -0.80947 | -0.89826 | 5.352441 | H28 | -1.31461 | -1.63188 | 5.67206 |
| H29 | -1.37646 | 1.481025 | 5.788596 | H29 | -1.62629 | 0.783657 | 6.172535 |
| O30 | 0.776185 | -4.32882 | -0.39754 | O30 | 0.922281 | -4.35298 | -0.15835 |
| C31 | 2.838274 | -2.26456 | 1.212629 | C31 | 2.51758 | -2.1429 | 1.43766 |
| C32 | 2.074336 | -1.77405 | 2.271891 | C32 | 1.560097 | -1.77272 | 2.378275 |
| C33 | 4.164632 | -2.6538 | 1.459255 | C33 | 3.831013 | -2.38841 | 1.869086 |
| C34 | 2.633082 | -1.63801 | 3.5445 | C34 | 1.906213 | -1.63164 | 3.724124 |
| H35 | 1.049782 | -1.47556 | 2.10786 | H35 | 0.546193 | -1.56853 | 2.070045 |
| C36 | 4.72069 | -2.52427 | 2.728843 | C36 | 4.176078 | -2.25611 | 3.210286 |
| H37 | 4.771542 | -3.05021 | 0.649063 | H37 | 4.592584 | -2.66627 | 1.145068 |
| C38 | 3.955718 | -2.00739 | 3.777933 | C38 | 3.210949 | -1.87235 | 4.145106 |
| H39 | 2.02495 | -1.2334 | 4.348859 | H39 | 1.146275 | -1.32352 | 4.435216 |
| H40 | 5.750873 | -2.82431 | 2.898472 | H40 | 5.198119 | -2.447 | 3.524688 |
| H41 | 4.390405 | -1.89956 | 4.767593 | | | | |
| C42 | -3.50326 | -0.16208 | -0.21818 | | | | |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| C43 | -4.6144 | 0.201497 | 0.557499 | H41 | 3.478973 | -1.76225 | 5.191988 |
| C44 | -3.65872 | -0.32131 | -1.60454 | C42 | -3.71906 | -0.54524 | 0.21562 |
| C45 | -5.85035 | 0.428996 | -0.05031 | C43 | -4.77097 | -0.28861 | 1.106341 |
| H46 | -4.52313 | 0.305212 | 1.63355 | C44 | -3.96823 | -0.5138 | -1.16766 |
| C47 | -4.89591 | -0.10075 | -2.20576 | C45 | -6.04644 | 0.003278 | 0.621363 |
| C48 | -5.99448 | 0.282053 | -1.43087 | H46 | -4.59633 | -0.31121 | 2.177546 |
| H49 | -6.70158 | 0.718329 | 0.559175 | C47 | -5.24536 | -0.23031 | -1.64818 |
| H50 | -5.0018 | -0.2207 | -3.27995 | C48 | -6.28587 | 0.032158 | -0.75356 |
| H51 | -6.95711 | 0.461151 | -1.90019 | H49 | -6.85447 | 0.204884 | 1.318821 |
| H52 | -0.58754 | -0.49503 | -1.83036 | H50 | -5.42729 | -0.2059 | -2.71886 |
| H53 | 1.675255 | 0.601349 | -1.35197 | H51 | -7.28015 | 0.258969 | -1.12724 |
| H54 | -1.11229 | -1.85157 | 3.090307 | H52 | -0.86383 | -1.01244 | -1.89314 |
| H55 | -2.80604 | -0.60918 | -2.21116 | H53 | 1.478939 | 1.962218 | -1.61077 |
| H56 | 2.501406 | -4.23505 | -1.53463 | H54 | -1.47995 | -2.4542 | 3.352447 |
| C57 | 4.143622 | -0.2551 | -3.42499 | H55 | -3.15469 | -0.70044 | -1.86338 |
| C58 | 3.070523 | -1.118 | -3.66719 | H56 | 2.568873 | -4.11303 | -1.37944 |
| C59 | 2.495079 | -1.82451 | -2.61526 | C57 | 4.424899 | 0.287389 | -2.67331 |
| C60 | 2.97756 | -1.6885 | -1.30213 | C58 | 3.884776 | -0.89819 | -3.17246 |
| C61 | 4.041405 | -0.81267 | -1.07016 | C59 | 3.200133 | -1.76794 | -2.32446 |
| C62 | 4.621998 | -0.10402 | -2.12598 | C60 | 3.053602 | -1.47419 | -0.96366 |
| H63 | 4.594497 | 0.300216 | -4.24235 | C61 | 3.591133 | -0.27628 | -0.4736 |
| H64 | 2.681303 | -1.2375 | -4.67444 | C62 | 4.272543 | 0.595594 | -1.32093 |
| H65 | 1.642499 | -2.46835 | -2.81413 | H63 | 4.958236 | 0.96553 | -3.33336 |
| H66 | 4.414964 | -0.66412 | -0.06431 | H64 | 3.989563 | -1.1454 | -4.22489 |
| H67 | 5.436121 | 0.584429 | -1.92117 | H65 | 2.753445 | -2.66026 | -2.75184 |
| C68 | -1.01604 | 2.82103 | -1.72386 | H66 | 3.450251 | -0.01176 | 0.567471 |
| C69 | -0.02291 | 2.00203 | -0.87771 | H67 | 4.68554 | 1.518601 | -0.92273 |
| C70 | 1.318599 | 1.65783 | -1.6137 | C68 | -1.80027 | 3.235484 | -1.45325 |
| H71 | 1.136887 | 1.583456 | -2.68374 | C69 | -0.50647 | 2.514691 | -1.00054 |
| C72 | 2.512067 | 2.537494 | -1.33726 | C70 | 0.738614 | 2.70347 | -1.91536 |
| C73 | 3.324749 | 2.357653 | -0.21103 | H71 | 0.461773 | 2.451004 | -2.94153 |
| C74 | 2.790397 | 3.592198 | -2.21555 | C72 | 1.350897 | 4.082673 | -1.82073 |
| C75 | 4.384307 | 3.229528 | 0.041538 | C73 | 2.456756 | 4.284062 | -0.981 |
| H76 | 3.137375 | 1.524494 | 0.459169 | C74 | 0.829999 | 5.184268 | -2.51402 |
| C77 | 3.853701 | 4.461202 | -1.96623 | C75 | 3.009661 | 5.55478 | -0.81321 |
| H78 | 2.172065 | 3.732702 | -3.09915 | H76 | 2.889179 | 3.431682 | -0.46099 |
| C79 | 4.650993 | 4.284722 | -0.83369 | C77 | 1.379298 | 6.457215 | -2.34733 |
| H80 | 5.006951 | 3.078553 | 0.918941 | H78 | -0.00819 | 5.046799 | -3.19259 |
| H81 | 4.060031 | 5.273383 | -2.65765 | C79 | 2.464709 | 6.649083 | -1.48897 |
| H82 | 5.479195 | 4.960122 | -0.63971 | H80 | 3.869309 | 5.689592 | -0.16219 |
| C83 | 0.480585 | 4.164482 | 0.573524 | H81 | 0.961828 | 7.299659 | -2.89164 |
| C84 | 0.758787 | 2.039441 | 1.422353 | H82 | 2.891054 | 7.639549 | -1.36026 |
| C85 | 0.794052 | 4.199421 | 2.083073 | C83 | -0.26741 | 4.174904 | 0.982672 |
| H86 | -0.39661 | 4.76341 | 0.322686 | C84 | 0.605711 | 2.021948 | 1.168595 |
| H87 | 1.325616 | 4.49353 | -0.03774 | C85 | 0.79025 | 4.090237 | 2.099288 |

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|-------------------|----------|----------|----------|------|----------|----------|----------|
| H88 | 1.633957 | 4.845304 | 2.340257 | H86 | -1.27227 | 4.357446 | 1.375741 |
| H89 | -0.07985 | 4.466603 | 2.685019 | H87 | -0.02351 | 4.947676 | 0.253114 |
| N90 | 0.231728 | 2.725134 | 0.389567 | H88 | 1.719449 | 4.59329 | 1.819108 |
| O91 | 1.159077 | 2.832748 | 2.420673 | H89 | 0.438881 | 4.461446 | 3.062747 |
| O92 | 0.8975 | 0.8037 | 1.461012 | N90 | -0.17477 | 2.827715 | 0.395331 |
| H93 | 2.738228 | -4.60739 | 0.197615 | O91 | 1.070829 | 2.674793 | 2.242359 |
| N94 | -1.9751 | -2.33218 | 0.679515 | O92 | 0.872883 | 0.8321 | 0.983386 |
| C95 | -1.39066 | -3.22158 | -0.34925 | H93 | 2.930423 | -4.41182 | 0.345737 |
| H96 | -1.66917 | -2.9188 | -1.37052 | N94 | -2.0068 | -2.72545 | 0.77891 |
| C97 | -2.323 | 3.110926 | -0.96829 | C95 | -1.36021 | -3.4839 | -0.32501 |
| H98 | -2.15067 | 3.540773 | 0.022244 | H96 | -1.67734 | -3.1263 | -1.31475 |
| H99 | -2.93944 | 3.816733 | -1.53388 | C97 | -2.97824 | 2.982361 | -0.50003 |
| H100 | -2.90118 | 2.195754 | -0.83766 | H98 | -2.77829 | 3.300267 | 0.525364 |
| C101 | -1.34254 | 2.196347 | -3.08706 | H99 | -3.86118 | 3.529027 | -0.84466 |
| H102 | -0.47022 | 2.11717 | -3.74207 | H100 | -3.23716 | 1.921439 | -0.47961 |
| H103 | -1.76226 | 1.196931 | -2.96091 | C101 | -2.19623 | 2.812016 | -2.87673 |
| H104 | -2.08101 | 2.81295 | -3.60907 | H102 | -1.45467 | 3.09252 | -3.62815 |
| H105 | -0.52391 | 3.788502 | -1.92576 | H103 | -2.34028 | 1.726081 | -2.92971 |
| | | | | H104 | -3.14167 | 3.286554 | -3.15381 |
| C3_ZR_Cheltop_TS2 | | | | H105 | -1.57166 | 4.309596 | -1.46331 |
| C1 | -3.98524 | -3.88293 | 0.681175 | H106 | 0.992971 | -0.06361 | -1.69198 |
| C2 | -1.82005 | -4.74932 | -0.02122 | H107 | -0.83815 | 1.420418 | -1.05735 |
| C3 | -3.3232 | -4.8089 | -0.39123 | | | | |
| C4 | -2.7683 | -3.42863 | 1.522743 | | | | |
| H5 | -4.6862 | -4.43561 | 1.315278 | | | | |
| H6 | -3.51052 | -4.4698 | -1.41511 | | | | |
| H7 | -3.01474 | -2.98963 | 2.489112 | | | | |
| H8 | -4.52662 | -3.04274 | 0.246129 | | | | |
| H9 | -1.20364 | -5.53391 | -0.45951 | | | | |
| H10 | -3.68798 | -5.83713 | -0.31507 | | | | |
| C11 | -1.88052 | -4.68561 | 1.521458 | | | | |
| H12 | -0.90958 | -4.52668 | 1.999985 | | | | |
| H13 | -2.37033 | -5.55995 | 1.95921 | | | | |
| C14 | 0.175 | -3.14618 | -0.42073 | | | | |
| N15 | 0.765578 | -2.00379 | -0.43106 | | | | |
| C16 | 2.246123 | -2.26439 | -0.28724 | | | | |
| C17 | 2.302232 | -3.77706 | -0.65444 | | | | |
| P18 | -1.99793 | -0.82781 | 0.61814 | | | | |
| Ir19 | -0.2979 | -0.05879 | -0.57307 | | | | |
| C20 | -1.95251 | -0.23698 | 2.348416 | | | | |
| C21 | -1.69324 | 0.804446 | 4.942641 | | | | |
| C22 | -1.4005 | -1.01699 | 3.374571 | | | | |
| C23 | -2.37294 | 1.072138 | 2.635272 | | | | |
| C24 | -2.24414 | 1.586359 | 3.924692 | | | | |
| C25 | -1.27835 | -0.4987 | 4.66369 | | | | |

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|-----|----------|----------|----------|
| H26 | -2.80139 | 1.687366 | 1.853224 |
| H27 | -2.58187 | 2.597354 | 4.136319 |
| H28 | -0.85857 | -1.11707 | 5.451935 |
| H29 | -1.59414 | 1.205529 | 5.94688 |
| O30 | 0.941475 | -4.2396 | -0.42589 |
| C31 | 2.671494 | -2.11982 | 1.183345 |
| C32 | 1.763252 | -1.84751 | 2.202437 |
| C33 | 4.019419 | -2.3261 | 1.513892 |
| C34 | 2.188264 | -1.76501 | 3.52969 |
| H35 | 0.729173 | -1.66417 | 1.957088 |
| C36 | 4.444329 | -2.25442 | 2.837342 |
| H37 | 4.743527 | -2.52666 | 0.728473 |
| C38 | 3.526832 | -1.97033 | 3.853138 |
| H39 | 1.466881 | -1.52427 | 4.305264 |
| H40 | 5.492016 | -2.41361 | 3.076061 |
| H41 | 3.858807 | -1.90612 | 4.885489 |
| C42 | -3.70002 | -0.53486 | 0.010257 |
| C43 | -4.77059 | -0.32988 | 0.893557 |
| C44 | -3.96232 | -0.71209 | -1.35778 |
| C45 | -6.07831 | -0.28245 | 0.409657 |
| H46 | -4.5925 | -0.21141 | 1.956965 |
| C47 | -5.26985 | -0.66989 | -1.83469 |
| C48 | -6.33075 | -0.45134 | -0.952 |
| H49 | -6.90031 | -0.11705 | 1.100133 |
| H50 | -5.46091 | -0.80292 | -2.89552 |
| H51 | -7.3501 | -0.41443 | -1.32497 |
| H52 | -1.10979 | -0.50009 | -1.8372 |
| H53 | 1.415467 | 1.300055 | -1.44288 |
| H54 | -1.05717 | -2.02433 | 3.16864 |
| H55 | -3.14081 | -0.87414 | -2.04749 |
| H56 | 2.535195 | -3.98084 | -1.70101 |
| C57 | 4.543432 | 0.405966 | -2.84612 |
| C58 | 4.103117 | -0.82021 | -3.34333 |
| C59 | 3.368501 | -1.68763 | -2.53262 |
| C60 | 3.065855 | -1.35363 | -1.20625 |
| C61 | 3.505494 | -0.11196 | -0.71989 |
| C62 | 4.239351 | 0.755673 | -1.52985 |
| H63 | 5.1188 | 1.079638 | -3.47411 |
| H64 | 4.327171 | -1.10655 | -4.36673 |
| H65 | 3.022674 | -2.61895 | -2.96748 |
| H66 | 3.271265 | 0.16915 | 0.301459 |
| H67 | 4.57267 | 1.708972 | -1.13297 |
| C68 | -1.78142 | 2.761061 | -1.44996 |
| C69 | -0.60596 | 2.015559 | -0.77901 |
| C70 | 0.724671 | 2.149384 | -1.62794 |

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|------|----------|----------|----------|
| H71 | 0.473431 | 2.0746 | -2.68425 |
| C72 | 1.521492 | 3.412556 | -1.39065 |
| C73 | 2.506844 | 3.479488 | -0.39616 |
| C74 | 1.252689 | 4.560191 | -2.14852 |
| C75 | 3.191692 | 4.67018 | -0.14842 |
| H76 | 2.737284 | 2.595234 | 0.189754 |
| C77 | 1.931075 | 5.754048 | -1.8984 |
| H78 | 0.507909 | 4.518517 | -2.93948 |
| C79 | 2.898816 | 5.814408 | -0.8934 |
| H80 | 3.954184 | 4.703267 | 0.625474 |
| H81 | 1.707035 | 6.636 | -2.49188 |
| H82 | 3.428477 | 6.742956 | -0.70081 |
| C83 | -0.48701 | 3.973941 | 1.050756 |
| C84 | 0.474633 | 1.9 | 1.384183 |
| C85 | 0.457112 | 3.979658 | 2.278704 |
| H86 | -1.51942 | 4.19798 | 1.330276 |
| H87 | -0.16425 | 4.682079 | 0.285696 |
| H88 | 1.347587 | 4.589296 | 2.114738 |
| H89 | -0.03979 | 4.278499 | 3.203258 |
| N90 | -0.35932 | 2.584515 | 0.582028 |
| O91 | 0.89237 | 2.60116 | 2.43921 |
| O92 | 0.856548 | 0.731041 | 1.173597 |
| H93 | 2.967122 | -4.34739 | -0.00836 |
| N94 | -1.88249 | -2.51579 | 0.737858 |
| C95 | -1.31906 | -3.32493 | -0.37369 |
| H96 | -1.70418 | -3.00863 | -1.35402 |
| C97 | -3.07624 | 2.807662 | -0.62511 |
| H98 | -2.94988 | 3.266606 | 0.357284 |
| H99 | -3.8269 | 3.402774 | -1.15538 |
| H100 | -3.48933 | 1.810269 | -0.48733 |
| C101 | -2.12221 | 2.211609 | -2.84551 |
| H102 | -1.26434 | 2.178554 | -3.52152 |
| H103 | -2.52067 | 1.198036 | -2.76657 |
| H104 | -2.88443 | 2.840375 | -3.31654 |
| H105 | -1.4441 | 3.80245 | -1.58497 |
| H106 | 1.195932 | -0.30113 | -2.95842 |
| H107 | 0.503769 | -0.27478 | -3.22418 |

C3_ZS_Chelbot

C3_ZS_Chelbot_SM

| | | | |
|----|----------|----------|----------|
| C1 | -3.79966 | -3.44435 | -1.29761 |
| C2 | -1.52645 | -4.33553 | -1.22873 |
| C3 | -2.73555 | -4.17059 | -2.18718 |
| C4 | -3.03668 | -3.26023 | 0.032425 |
| H5 | -4.68885 | -4.06414 | -1.14223 |

C3_ZS_Chelbot_INT2

| | | | |
|----|----------|----------|----------|
| C1 | -3.75023 | -3.44428 | -1.46494 |
| C2 | -1.54938 | -4.41945 | -1.07503 |
| C3 | -2.63794 | -4.28781 | -2.17153 |
| C4 | -3.12083 | -3.16724 | -0.08256 |
| H5 | -4.67708 | -4.01518 | -1.34578 |

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|------|----------|----------|----------|------|----------|----------|----------|
| H6 | -2.47343 | -3.60082 | -3.08425 | H6 | -2.25319 | -3.80744 | -3.07646 |
| H7 | -3.65228 | -2.98187 | 0.888381 | H7 | -3.81307 | -2.78556 | 0.667985 |
| H8 | -4.12598 | -2.48768 | -1.70743 | H8 | -3.99517 | -2.52087 | -1.98952 |
| H9 | -0.79217 | -5.08004 | -1.5367 | H9 | -0.82705 | -5.21896 | -1.23754 |
| H10 | -3.08999 | -5.15188 | -2.51454 | H10 | -3.00602 | -5.2772 | -2.45676 |
| C11 | -2.22916 | -4.56731 | 0.12707 | C11 | -2.4007 | -4.49747 | 0.209719 |
| H12 | -1.54074 | -4.60091 | 0.976913 | H12 | -1.80518 | -4.48976 | 1.127558 |
| H13 | -2.85777 | -5.46209 | 0.13285 | H13 | -3.07607 | -5.35746 | 0.222241 |
| C14 | 0.429156 | -2.90221 | -0.32813 | C14 | 0.40533 | -3.02 | -0.12743 |
| N15 | 1.006666 | -1.82654 | 0.087315 | N15 | 0.976495 | -1.95737 | 0.323075 |
| C16 | 2.382772 | -2.19424 | 0.605014 | C16 | 2.326165 | -2.34275 | 0.877168 |
| C17 | 2.252397 | -3.74862 | 0.660058 | C17 | 2.245159 | -3.90668 | 0.801315 |
| P18 | -1.85716 | -0.67337 | 0.334943 | P18 | -1.80935 | -0.66996 | 0.317875 |
| Ir19 | 0.318295 | 0.191319 | -0.35401 | Ir19 | 0.314328 | 0.092851 | -0.31879 |
| C20 | -1.9784 | -0.686 | 2.165398 | C20 | -1.90806 | -0.69876 | 2.158825 |
| C21 | -1.94525 | -0.63074 | 4.973078 | C21 | -2.01122 | -0.70538 | 4.969021 |
| C22 | -1.93619 | -1.87835 | 2.898717 | C22 | -2.17422 | -1.88145 | 2.860367 |
| C23 | -1.98453 | 0.53702 | 2.856947 | C23 | -1.6704 | 0.478994 | 2.888631 |
| C24 | -1.97527 | 0.564489 | 4.249356 | C24 | -1.73211 | 0.477651 | 4.280151 |
| C25 | -1.92072 | -1.84861 | 4.294778 | C25 | -2.22212 | -1.8839 | 4.255745 |
| H26 | -1.98471 | 1.472943 | 2.310057 | H26 | -1.41112 | 1.397334 | 2.376082 |
| H27 | -1.98145 | 1.518352 | 4.769131 | H27 | -1.54895 | 1.399083 | 4.825708 |
| H28 | -1.88041 | -2.78044 | 4.851275 | H28 | -2.41967 | -2.81246 | 4.783222 |
| H29 | -1.93194 | -0.61044 | 6.059004 | H29 | -2.0512 | -0.70879 | 6.054379 |
| O30 | 1.074409 | -4.0559 | -0.14127 | O30 | 1.038862 | -4.18381 | 0.036874 |
| C31 | 2.655773 | -1.69109 | 2.017398 | C31 | 2.528845 | -1.92101 | 2.325928 |
| C32 | 1.6288 | -1.24947 | 2.855021 | C32 | 1.548041 | -1.26219 | 3.066561 |
| C33 | 3.954181 | -1.80284 | 2.536884 | C33 | 3.73355 | -2.27556 | 2.954 |
| C34 | 1.901031 | -0.8774 | 4.172624 | C34 | 1.777551 | -0.9341 | 4.405302 |
| H35 | 0.614761 | -1.19208 | 2.485765 | H35 | 0.605436 | -1.0052 | 2.6071 |
| C36 | 4.224577 | -1.43668 | 3.853796 | C36 | 3.96001 | -1.95231 | 4.289045 |
| H37 | 4.761611 | -2.1623 | 1.905247 | H37 | 4.505735 | -2.79076 | 2.38764 |
| C38 | 3.199328 | -0.96198 | 4.673913 | C38 | 2.98186 | -1.27209 | 5.018489 |
| H39 | 1.088104 | -0.52599 | 4.801205 | H39 | 1.002038 | -0.41729 | 4.962063 |
| H40 | 5.238032 | -1.51866 | 4.236188 | H40 | 4.900877 | -2.22628 | 4.757479 |
| H41 | 3.412523 | -0.66801 | 5.69766 | H41 | 3.159503 | -1.0134 | 6.058333 |
| C42 | -3.44751 | 0.039784 | -0.2504 | C42 | -3.40543 | 0.058362 | -0.21252 |
| C43 | -4.46565 | 0.475696 | 0.606205 | C43 | -4.33169 | 0.597357 | 0.688167 |
| C44 | -3.64125 | 0.120185 | -1.64015 | C44 | -3.70044 | 0.057905 | -1.58535 |
| C45 | -5.64458 | 1.011407 | 0.08193 | C45 | -5.52688 | 1.146238 | 0.219557 |
| H46 | -4.34485 | 0.405498 | 1.68225 | H46 | -4.12565 | 0.597948 | 1.753294 |
| C47 | -4.81904 | 0.65364 | -2.15844 | C47 | -4.89102 | 0.611 | -2.0492 |
| C48 | -5.82201 | 1.111316 | -1.29771 | C48 | -5.80573 | 1.161888 | -1.14651 |
| H49 | -6.42561 | 1.347793 | 0.757728 | H49 | -6.23999 | 1.56058 | 0.926271 |
| H50 | -4.95977 | 0.702468 | -3.23495 | H50 | -5.1137 | 0.59828 | -3.11266 |

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| H51 | -6.7394 | 1.529389 | -1.70103 | H51 | -6.73607 | 1.590768 | -1.50727 |
| H52 | 0.681668 | 0.604731 | 1.095665 | H52 | 0.478218 | 0.637759 | 1.132868 |
| H53 | 1.888502 | 0.314765 | -0.58516 | H53 | 1.740688 | 1.53362 | -2.432 |
| H54 | -1.88573 | -2.83159 | 2.386372 | H54 | -2.32342 | -2.8123 | 2.33072 |
| H55 | -2.88234 | -0.26333 | -2.31376 | H55 | -3.015 | -0.39849 | -2.29029 |
| H56 | 3.105699 | -4.27993 | 0.239506 | H56 | 3.088112 | -4.36283 | 0.280835 |
| C57 | 5.176147 | -0.84002 | -2.43866 | C57 | 5.103771 | -0.63532 | -1.99461 |
| C58 | 4.417824 | -1.99494 | -2.6342 | C58 | 4.229922 | -1.66129 | -2.36313 |
| C59 | 3.535797 | -2.42883 | -1.64562 | C59 | 3.377613 | -2.2242 | -1.41579 |
| C60 | 3.40223 | -1.72374 | -0.441 | C60 | 3.381477 | -1.77737 | -0.086 |
| C61 | 4.150038 | -0.55054 | -0.26708 | C61 | 4.261064 | -0.75014 | 0.27381 |
| C62 | 5.033246 | -0.11605 | -1.25624 | C62 | 5.117552 | -0.18517 | -0.67488 |
| H63 | 5.86251 | -0.49929 | -3.2081 | H63 | 5.767466 | -0.19218 | -2.73129 |
| H64 | 4.512195 | -2.56065 | -3.55678 | H64 | 4.208969 | -2.01977 | -3.38817 |
| H65 | 2.944355 | -3.3225 | -1.8274 | H65 | 2.688606 | -3.00576 | -1.72633 |
| H66 | 4.047576 | 0.023866 | 0.6469 | H66 | 4.271966 | -0.37579 | 1.29113 |
| H67 | 5.603498 | 0.795479 | -1.10267 | H67 | 5.793021 | 0.612209 | -0.37823 |
| C68 | -0.80095 | 3.322061 | -0.21356 | C68 | -0.60698 | 3.202018 | -0.44636 |
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| C70 | 1.275227 | 2.022899 | -1.04517 | C70 | 1.342016 | 2.422099 | -1.93156 |
| H71 | 1.793935 | 2.471395 | -0.20294 | H71 | 2.053138 | 2.679734 | -1.14228 |
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| C74 | 2.34916 | 1.040213 | -3.16987 | C74 | 1.226392 | 3.198004 | -4.32664 |
| C75 | 3.197021 | 3.607598 | -3.8687 | C75 | 1.240151 | 5.879053 | -3.58657 |
| H76 | 2.306077 | 4.235423 | -2.01247 | H76 | 1.412897 | 5.166858 | -1.56605 |
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| H78 | 2.044007 | 0.038347 | -2.89284 | H78 | 1.243198 | 2.150261 | -4.62124 |
| C79 | 3.457856 | 2.53292 | -4.72286 | C79 | 1.141979 | 5.535113 | -4.93594 |
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| H82 | 3.993504 | 2.694653 | -5.65396 | H82 | 1.079644 | 6.310373 | -5.69403 |
| C83 | -1.05436 | 3.145787 | -3.27797 | C83 | -1.79824 | 2.566101 | -3.20811 |
| C84 | -0.75856 | 0.872557 | -3.01119 | C84 | -0.81093 | 0.489663 | -2.97785 |
| C85 | -1.67341 | 2.363948 | -4.45001 | C85 | -1.92035 | 1.74246 | -4.50668 |
| H86 | -0.11481 | 3.643055 | -3.54466 | H86 | -1.328 | 3.533783 | -3.38013 |
| H87 | -1.7477 | 3.878216 | -2.86046 | H87 | -2.76776 | 2.711045 | -2.72285 |
| H88 | -2.76653 | 2.347837 | -4.40039 | H88 | -2.94451 | 1.646894 | -4.86941 |
| H89 | -1.34867 | 2.705584 | -5.43283 | H89 | -1.27524 | 2.125835 | -5.30091 |
| N90 | -0.80047 | 2.043621 | -2.34093 | N90 | -0.94748 | 1.685285 | -2.39385 |
| O91 | -1.20215 | 0.99882 | -4.26874 | O91 | -1.44774 | 0.406953 | -4.15569 |
| O92 | -0.38622 | -0.22136 | -2.55253 | O92 | -0.1978 | -0.48891 | -2.49687 |
| H93 | 2.055625 | -4.09861 | 1.674906 | H93 | 2.121578 | -4.35855 | 1.786948 |
| N94 | -1.93371 | -2.27836 | -0.17242 | N94 | -1.95159 | -2.25 | -0.25528 |
| C95 | -0.9095 | -2.93138 | -1.02311 | C95 | -0.87997 | -3.03157 | -0.91791 |

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| H96 | -0.78175 | -2.40568 | -1.97583 | H96 | -0.63211 | -2.59868 | -1.89385 |
| C97 | -2.32249 | 3.207897 | -0.06731 | C97 | -2.04015 | 3.026089 | 0.065809 |
| H98 | -2.73955 | 4.16126 | 0.272268 | H98 | -2.4106 | 3.976503 | 0.464536 |
| H99 | -2.81861 | 2.928824 | -0.99974 | H99 | -2.74107 | 2.693379 | -0.69944 |
| H100 | -2.59257 | 2.449973 | 0.667636 | H100 | -2.08602 | 2.298072 | 0.873769 |
| C101 | -0.14497 | 3.542552 | 1.157206 | C101 | 0.297069 | 3.608859 | 0.729321 |
| H102 | -0.1797 | 2.63138 | 1.760199 | H102 | 0.372138 | 2.797583 | 1.459782 |
| H103 | 0.901073 | 3.851691 | 1.078523 | H103 | 1.3133 | 3.867137 | 0.420768 |
| H104 | -0.67448 | 4.33462 | 1.69576 | H104 | -0.12079 | 4.484773 | 1.2363 |
| H105 | -0.59912 | 4.231462 | -0.80532 | H105 | -0.63061 | 4.057682 | -1.13745 |
| | | | | H106 | 1.951417 | 0.617822 | -0.12919 |
| | | | | H107 | 1.959393 | 0.244907 | -0.88899 |
| C3_ZS_Chelbot_TS1 | | | | C3_ZS_Chelbot_TS3 | | | |
| C1 | -3.77593 | -3.44484 | -1.26031 | C1 | -3.77689 | -3.40923 | -1.57868 |
| C2 | -1.5019 | -4.33488 | -1.20938 | C2 | -1.54655 | -4.33801 | -1.24718 |
| C3 | -2.71883 | -4.17131 | -2.15817 | C3 | -2.64318 | -4.17961 | -2.3324 |
| C4 | -3.00516 | -3.26653 | 0.066385 | C4 | -3.15265 | -3.19663 | -0.18206 |
| H5 | -4.66613 | -4.06245 | -1.10207 | H5 | -4.68829 | -4.01069 | -1.49532 |
| H6 | -2.46469 | -3.60233 | -3.05806 | H6 | -2.27607 | -3.64159 | -3.212 |
| H7 | -3.61664 | -2.99287 | 0.926887 | H7 | -3.857 | -2.87853 | 0.586339 |
| H8 | -4.10198 | -2.48611 | -1.66566 | H8 | -4.04644 | -2.46216 | -2.04688 |
| H9 | -0.76757 | -5.07637 | -1.52462 | H9 | -0.80095 | -5.10392 | -1.45772 |
| H10 | -3.07566 | -5.15308 | -2.48159 | H10 | -2.9829 | -5.16312 | -2.66896 |
| C11 | -2.19464 | -4.57252 | 0.150817 | C11 | -2.39106 | -4.51746 | 0.033093 |
| H12 | -1.50074 | -4.60588 | 0.996243 | H12 | -1.79479 | -4.53897 | 0.950432 |
| H13 | -2.82113 | -5.46882 | 0.157723 | H13 | -3.03571 | -5.4002 | -0.00406 |
| C14 | 0.460238 | -2.89096 | -0.33058 | C14 | 0.371836 | -2.93321 | -0.23554 |
| N15 | 1.032018 | -1.81046 | 0.078378 | N15 | 0.964548 | -1.88976 | 0.244537 |
| C16 | 2.412682 | -2.16388 | 0.584943 | C16 | 2.316257 | -2.30677 | 0.78952 |
| C17 | 2.304591 | -3.72148 | 0.630678 | C17 | 2.181037 | -3.86222 | 0.717324 |
| P18 | -1.82859 | -0.67719 | 0.359109 | P18 | -1.88087 | -0.68643 | 0.362552 |
| Ir19 | 0.295375 | 0.204808 | -0.33683 | Ir19 | 0.395203 | 0.137373 | -0.14334 |
| C20 | -1.95857 | -0.67384 | 2.187404 | C20 | -2.03336 | -0.81458 | 2.195006 |
| C21 | -1.9475 | -0.58476 | 4.992918 | C21 | -2.17754 | -0.90494 | 5.002916 |
| C22 | -1.91885 | -1.85762 | 2.933964 | C22 | -2.35749 | -2.00737 | 2.854848 |
| C23 | -1.97444 | 0.557584 | 2.863304 | C23 | -1.75809 | 0.327954 | 2.967044 |
| C24 | -1.97574 | 0.601872 | 4.254811 | C24 | -1.84026 | 0.286663 | 4.357014 |
| C25 | -1.91439 | -1.8108 | 4.329935 | C25 | -2.42462 | -2.05148 | 4.249183 |
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| H27 | -1.98916 | 1.561986 | 4.762684 | H27 | -1.62682 | 1.180954 | 4.935196 |
| H28 | -1.87625 | -2.73582 | 4.897817 | H28 | -2.66867 | -2.98665 | 4.744448 |
| H29 | -1.94314 | -0.55119 | 6.078527 | H29 | -2.23406 | -0.94122 | 6.086888 |
| O30 | 1.118829 | -4.03966 | -0.15521 | O30 | 0.997021 | -4.10239 | -0.09336 |
| C31 | 2.685456 | -1.66526 | 1.999358 | C31 | 2.524558 | -1.92089 | 2.248036 |
| C32 | 1.654782 | -1.24309 | 2.842306 | | | | |
| C33 | 3.987049 | -1.7573 | 2.514198 | | | | |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| C34 | 1.924951 | -0.86891 | 4.159549 | C32 | 1.466731 | -1.5155 | 3.065612 |
| H35 | 0.63883 | -1.20224 | 2.477049 | C33 | 3.788612 | -2.12129 | 2.822963 |
| C36 | 4.255941 | -1.38918 | 3.831148 | C34 | 1.678897 | -1.26471 | 4.422554 |
| H37 | 4.798068 | -2.10235 | 1.879161 | H35 | 0.474389 | -1.39793 | 2.652879 |
| C38 | 3.226255 | -0.93255 | 4.6558 | C36 | 3.997223 | -1.87866 | 4.178948 |
| H39 | 1.108374 | -0.53182 | 4.791164 | H37 | 4.616444 | -2.45785 | 2.20537 |
| H40 | 5.271858 | -1.45527 | 4.209905 | C38 | 2.943621 | -1.43916 | 4.981867 |
| H41 | 3.438614 | -0.63632 | 5.679054 | H39 | 0.844543 | -0.93895 | 5.035806 |
| C42 | -3.41032 | 0.038384 | -0.23961 | H40 | 4.984328 | -2.03053 | 4.605884 |
| C43 | -4.43564 | 0.473967 | 0.608031 | H41 | 3.108472 | -1.24264 | 6.037221 |
| C44 | -3.59048 | 0.113428 | -1.6311 | C42 | -3.46927 | 0.0808 | -0.15047 |
| C45 | -5.61177 | 1.002787 | 0.071908 | C43 | -4.3863 | 0.631768 | 0.752266 |
| H46 | -4.32327 | 0.407783 | 1.685137 | C44 | -3.74779 | 0.134363 | -1.52675 |
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| C48 | -5.77627 | 1.094626 | -1.3093 | H46 | -4.19301 | 0.59574 | 1.819355 |
| H49 | -6.40047 | 1.339805 | 0.738397 | C47 | -4.91729 | 0.733314 | -1.98831 |
| H50 | -4.89781 | 0.685605 | -3.23884 | C48 | -5.82415 | 1.290076 | -1.08105 |
| H51 | -6.6923 | 1.50704 | -1.72212 | H49 | -6.26242 | 1.655924 | 0.996329 |
| H52 | 0.642254 | 0.609789 | 1.120284 | H50 | -5.13007 | 0.755736 | -3.05387 |
| H53 | 1.868241 | 0.456635 | -0.59671 | H51 | -6.73715 | 1.756229 | -1.43946 |
| H54 | -1.8615 | -2.81661 | 2.432401 | H52 | 0.580581 | 0.432393 | 1.372975 |
| H55 | -2.82335 | -0.26894 | -2.29558 | H53 | 1.849203 | 1.619074 | -2.21304 |
| H56 | 3.158594 | -4.2386 | 0.193976 | H54 | -2.53914 | -2.91435 | 2.293976 |
| C57 | 5.180103 | -0.7539 | -2.4572 | H55 | -3.05992 | -0.31141 | -2.23841 |
| C58 | 4.434668 | -1.91629 | -2.65882 | H56 | 3.028658 | -4.35404 | 0.240233 |
| C59 | 3.5577 | -2.36532 | -1.67225 | C57 | 5.115569 | -0.7084 | -2.12005 |
| C60 | 3.417479 | -1.66875 | -0.46345 | C58 | 4.299215 | -1.79601 | -2.43515 |
| C61 | 4.148255 | -0.48595 | -0.28559 | C59 | 3.436059 | -2.32024 | -1.47598 |
| C62 | 5.026589 | -0.03638 | -1.27236 | C60 | 3.370422 | -1.77035 | -0.18772 |
| H63 | 5.863049 | -0.40174 | -3.22454 | C61 | 4.183094 | -0.67166 | 0.113809 |
| H64 | 4.535412 | -2.47617 | -3.58431 | C62 | 5.054868 | -0.15031 | -0.84355 |
| H65 | 2.976911 | -3.26522 | -1.85772 | H63 | 5.792312 | -0.29973 | -2.86501 |
| H66 | 4.040197 | 0.082083 | 0.631589 | H64 | 4.333439 | -2.236 | -3.42774 |
| H67 | 5.584847 | 0.881854 | -1.11539 | H65 | 2.793969 | -3.15347 | -1.7506 |
| C68 | -0.7413 | 3.3491 | -0.2103 | H66 | 4.127431 | -0.20959 | 1.092653 |
| C69 | -0.12148 | 2.190382 | -1.01012 | H67 | 5.682385 | 0.699322 | -0.58963 |
| C70 | 1.336222 | 2.019712 | -1.01909 | C68 | -0.63834 | 3.387669 | -0.48266 |
| H71 | 1.846072 | 2.47554 | -0.17493 | C69 | 0.019565 | 2.201782 | -1.22763 |
| C72 | 2.120305 | 2.126307 | -2.29581 | C70 | 1.40046 | 2.560668 | -1.88662 |
| C73 | 2.57817 | 3.410662 | -2.63444 | H71 | 2.067763 | 2.954448 | -1.11581 |
| C74 | 2.372827 | 1.065707 | -3.16872 | C72 | 1.318417 | 3.502348 | -3.06558 |
| C75 | 3.248028 | 3.632044 | -3.83629 | C73 | 1.227805 | 4.891823 | -2.90059 |
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| C79 | 3.472481 | 2.570098 | -4.71626 | C77 | 1.176178 | 3.822383 | -5.47513 |
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| H81 | 3.227448 | 0.454255 | -5.04269 | C79 | 1.060894 | 5.202096 | -5.29467 |
| H82 | 3.990281 | 2.741291 | -5.65573 | H80 | 1.026451 | 6.809065 | -3.85796 |
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| C84 | -0.71761 | 0.903716 | -3.00525 | H82 | 0.958866 | 5.858981 | -6.15344 |
| C85 | -1.59256 | 2.411345 | -4.45059 | C83 | -1.76305 | 2.530114 | -3.14681 |
| H86 | -0.01581 | 3.662545 | -3.538 | C84 | -0.63927 | 0.515022 | -2.86962 |
| H87 | -1.64728 | 3.926838 | -2.862 | C85 | -1.86743 | 1.647426 | -4.40919 |
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| H89 | -1.25675 | 2.746474 | -5.43196 | H87 | -2.73137 | 2.666554 | -2.65871 |
| N90 | -0.73599 | 2.075341 | -2.33643 | H88 | -2.89482 | 1.465449 | -4.72718 |
| O91 | -1.14743 | 1.037674 | -4.26664 | H89 | -1.28052 | 2.045974 | -5.23946 |
| O92 | -0.37166 | -0.19787 | -2.54223 | N90 | -0.8741 | 1.713204 | -2.3013 |
| H93 | 2.126582 | -4.08144 | 1.645976 | O91 | -1.28752 | 0.365022 | -4.03144 |
| N94 | -1.90335 | -2.28457 | -0.13769 | O92 | 0.055702 | -0.38931 | -2.37921 |
| C95 | -0.8881 | -2.92884 | -1.00624 | H93 | 1.997117 | -4.2991 | 1.699956 |
| H96 | -0.77787 | -2.39927 | -1.95928 | N94 | -2.01528 | -2.23595 | -0.29798 |
| C97 | -2.26693 | 3.247506 | -0.08707 | C95 | -0.92349 | -2.93723 | -1.01507 |
| H98 | -2.68165 | 4.197051 | 0.266401 | H96 | -0.69478 | -2.44519 | -1.96666 |
| H99 | -2.7539 | 2.991144 | -1.03161 | C97 | -2.01468 | 3.06898 | 0.108839 |
| H100 | -2.55132 | 2.475331 | 0.627562 | H98 | -2.46609 | 3.981009 | 0.512012 |
| C101 | -0.10304 | 3.564337 | 1.169217 | H99 | -2.71183 | 2.640358 | -0.6099 |
| H102 | -0.16186 | 2.657314 | 1.776455 | H100 | -1.91963 | 2.354753 | 0.927808 |
| H103 | 0.94902 | 3.856939 | 1.105457 | C101 | 0.260634 | 3.965516 | 0.622817 |
| H104 | -0.62716 | 4.367748 | 1.69631 | H102 | 0.455637 | 3.214637 | 1.398234 |
| H105 | -0.52106 | 4.255593 | -0.79979 | H103 | 1.223812 | 4.326736 | 0.254673 |
| X | 0 | 0 | 0 | H104 | -0.24304 | 4.810252 | 1.101654 |
| C3_ZS_Chelbot_INT1 | | | | H105 | -0.76909 | 4.173234 | -1.24021 |
| C1 | -3.86714 | -3.49565 | -1.04459 | H106 | 0.780395 | 1.650332 | 0.028914 |
| C2 | -1.61234 | -4.43598 | -1.02658 | H107 | 1.946964 | 0.42717 | -0.30181 |
| C3 | -2.85772 | -4.28916 | -1.94076 | C3_ZS_Chelbot_PROD | | | |
| C4 | -3.05305 | -3.28624 | 0.250898 | C1 | -3.86701 | -3.58765 | -1.17036 |
| H5 | -4.77059 | -4.0783 | -0.83687 | C2 | -1.5816 | -4.4505 | -1.13453 |
| H6 | -2.62283 | -3.77081 | -2.87571 | C3 | -2.79723 | -4.27619 | -2.08318 |
| H7 | -3.63099 | -2.96776 | 1.119241 | C4 | -3.10609 | -3.44363 | 0.166522 |
| H8 | -4.17533 | -2.54332 | -1.4796 | H5 | -4.75298 | -4.21764 | -1.03894 |
| H9 | -0.90169 | -5.20335 | -1.334 | H6 | -2.54725 | -3.68191 | -2.96789 |
| H10 | -3.24739 | -5.27674 | -2.20297 | H7 | -3.72708 | -3.20586 | 1.030753 |
| C11 | -2.26477 | -4.6039 | 0.363186 | H8 | -4.19831 | -2.61889 | -1.54778 |
| H12 | -1.54562 | -4.61598 | 1.188101 | H9 | -0.83626 | -5.17194 | -1.46941 |
| H13 | -2.90762 | -5.48628 | 0.427405 | H10 | -3.13998 | -5.25406 | -2.43292 |
| C14 | 0.415709 | -2.98534 | -0.2993 | C11 | -2.2784 | -4.7406 | 0.214365 |
| N15 | 0.980825 | -1.90046 | 0.100692 | H12 | -1.58987 | -4.78885 | 1.06337 |

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|------|----------|----------|----------|------|----------|----------|----------|
| C16 | 2.377932 | -2.21969 | 0.548556 | H13 | -2.89048 | -5.64665 | 0.188429 |
| C17 | 2.35054 | -3.78656 | 0.494668 | C14 | 0.363243 | -3.0087 | -0.21871 |
| P18 | -1.83208 | -0.71421 | 0.405865 | N15 | 0.966965 | -1.93913 | 0.192842 |
| Ir19 | 0.139123 | 0.090396 | -0.3147 | C16 | 2.360533 | -2.31106 | 0.673789 |
| C20 | -1.97328 | -0.63626 | 2.22913 | C17 | 2.212608 | -3.86311 | 0.720786 |
| C21 | -1.97906 | -0.44791 | 5.027153 | P18 | -1.92986 | -0.83339 | 0.502179 |
| C22 | -1.88074 | -1.79024 | 3.016284 | Ir19 | 0.278946 | -0.04765 | -0.10712 |
| C23 | -2.0522 | 0.617186 | 2.858553 | C20 | -2.13695 | -0.8426 | 2.322886 |
| C24 | -2.05986 | 0.709558 | 4.24747 | C21 | -2.20493 | -0.76308 | 5.130964 |
| C25 | -1.88657 | -1.69446 | 4.409505 | C22 | -2.12806 | -2.02872 | 3.068356 |
| H26 | -2.09381 | 1.523687 | 2.264679 | C23 | -2.15204 | 0.385691 | 3.004961 |
| H27 | -2.12058 | 1.684662 | 4.722174 | C24 | -2.19434 | 0.425532 | 4.396168 |
| H28 | -1.8081 | -2.59598 | 5.010153 | C25 | -2.16403 | -1.98706 | 4.464212 |
| H29 | -1.98127 | -0.37518 | 6.110938 | H26 | -2.11449 | 1.317931 | 2.449578 |
| O30 | 1.112609 | -4.12084 | -0.1991 | H27 | -2.20877 | 1.383538 | 4.908106 |
| C31 | 2.66203 | -1.79038 | 1.984137 | H28 | -2.15492 | -2.91473 | 5.029326 |
| C32 | 1.653657 | -1.34966 | 2.842342 | H29 | -2.2345 | -0.73282 | 6.216288 |
| C33 | 3.961568 | -1.95047 | 2.48882 | O30 | 1.013468 | -4.1601 | -0.05447 |
| C34 | 1.942751 | -1.0351 | 4.171837 | C31 | 2.640181 | -1.83203 | 2.093611 |
| H35 | 0.641896 | -1.24608 | 2.47918 | C32 | 1.585716 | -1.58563 | 2.981542 |
| C36 | 4.249259 | -1.64165 | 3.816396 | C33 | 3.953766 | -1.80069 | 2.578841 |
| H37 | 4.756401 | -2.30056 | 1.835396 | C34 | 1.840589 | -1.255 | 4.31119 |
| C38 | 3.240354 | -1.17377 | 4.661463 | H35 | 0.5601 | -1.64196 | 2.639156 |
| H39 | 1.142969 | -0.6849 | 4.818129 | C36 | 4.207909 | -1.47559 | 3.911659 |
| H40 | 5.262631 | -1.76211 | 4.188751 | H37 | 4.783882 | -2.02526 | 1.916519 |
| H41 | 3.467139 | -0.92536 | 5.694334 | C38 | 3.153717 | -1.19014 | 4.779153 |
| C42 | -3.3743 | 0.030086 | -0.24789 | H39 | 1.005595 | -1.05061 | 4.975417 |
| C43 | -4.41622 | 0.494077 | 0.564297 | H40 | 5.233289 | -1.4452 | 4.268874 |
| C44 | -3.51483 | 0.080107 | -1.64491 | H41 | 3.354825 | -0.92865 | 5.814113 |
| C45 | -5.56853 | 1.030857 | -0.0136 | C42 | -3.45071 | -0.04473 | -0.1665 |
| H46 | -4.3382 | 0.440625 | 1.64477 | C43 | -4.46546 | 0.526575 | 0.60919 |
| C47 | -4.66598 | 0.61467 | -2.21616 | C44 | -3.5543 | -0.00019 | -1.56804 |
| C48 | -5.69203 | 1.101374 | -1.40024 | C45 | -5.55571 | 1.147785 | -0.00622 |
| H49 | -6.37013 | 1.391474 | 0.624526 | H46 | -4.41415 | 0.48849 | 1.692413 |
| H50 | -4.76878 | 0.643885 | -3.29755 | C47 | -4.64395 | 0.614729 | -2.17917 |
| H51 | -6.5892 | 1.521431 | -1.84562 | C48 | -5.6462 | 1.198214 | -1.39677 |
| H52 | 0.435022 | 0.538428 | 1.146957 | H49 | -6.33868 | 1.586177 | 0.605956 |
| H53 | 1.885237 | 0.859331 | -0.83792 | H50 | -4.71823 | 0.62748 | -3.26343 |
| H54 | -1.77295 | -2.7615 | 2.548031 | H51 | -6.49757 | 1.678605 | -1.87015 |
| H55 | -2.7336 | -0.32413 | -2.27922 | H52 | 0.61502 | 0.261026 | 1.3761 |
| H56 | 3.182676 | -4.22662 | -0.05501 | H53 | 1.825206 | 1.824707 | -1.88888 |
| C57 | 5.035773 | -0.50388 | -2.43298 | H54 | -2.06599 | -2.98757 | 2.566751 |
| C58 | 4.301522 | -1.65702 | -2.71372 | H55 | -2.79178 | -0.47098 | -2.18052 |
| C59 | 3.455256 | -2.1993 | -1.7482 | H56 | 3.051804 | -4.39836 | 0.278028 |
| C60 | 3.338706 | -1.60964 | -0.48118 | C57 | 4.944933 | -0.91295 | -2.52291 |

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|------|----------|----------|----------|------|----------|----------|----------|
| C61 | 4.057912 | -0.43642 | -0.22029 | C58 | 4.215272 | -2.09404 | -2.66263 |
| C62 | 4.902289 | 0.109842 | -1.18875 | C59 | 3.420192 | -2.55165 | -1.61329 |
| H63 | 5.692529 | -0.07716 | -3.18504 | C60 | 3.340271 | -1.84195 | -0.40713 |
| H64 | 4.385148 | -2.13472 | -3.68582 | C61 | 4.062559 | -0.64861 | -0.28532 |
| H65 | 2.878189 | -3.08742 | -1.9935 | C62 | 4.864911 | -0.19274 | -1.33118 |
| H66 | 3.968688 | 0.047935 | 0.745925 | H63 | 5.569651 | -0.557 | -3.33728 |
| H67 | 5.453635 | 1.019337 | -0.96855 | H64 | 4.263794 | -2.66103 | -3.58787 |
| C68 | -0.60136 | 3.274113 | -0.35147 | H65 | 2.843711 | -3.46175 | -1.75697 |
| C69 | -0.03452 | 2.021722 | -1.04687 | H66 | 3.988995 | -0.06486 | 0.62388 |
| C70 | 1.529001 | 1.932435 | -1.05798 | H67 | 5.423434 | 0.731641 | -1.2137 |
| H71 | 1.933054 | 2.481155 | -0.20942 | C68 | -0.81401 | 3.701828 | -0.505 |
| C72 | 2.232673 | 2.306457 | -2.3369 | C69 | -0.08695 | 2.539966 | -1.22669 |
| C73 | 2.672248 | 3.625836 | -2.50938 | C70 | 1.389494 | 2.792707 | -1.63657 |
| C74 | 2.405643 | 1.388517 | -3.37741 | H71 | 1.940335 | 3.157269 | -0.76743 |
| C75 | 3.255218 | 4.025057 | -3.71285 | C72 | 1.518563 | 3.722145 | -2.82183 |
| H76 | 2.554476 | 4.342686 | -1.69975 | C73 | 1.457674 | 5.115937 | -2.68981 |
| C77 | 2.982809 | 1.788823 | -4.58285 | C74 | 1.662478 | 3.17602 | -4.10601 |
| H78 | 2.105192 | 0.355274 | -3.23533 | C75 | 1.517981 | 5.941272 | -3.81406 |
| C79 | 3.404328 | 3.108323 | -4.75628 | H76 | 1.368116 | 5.561673 | -1.70277 |
| H80 | 3.593483 | 5.050254 | -3.83501 | C77 | 1.723561 | 3.997791 | -5.23203 |
| H81 | 3.110853 | 1.06578 | -5.38348 | H78 | 1.736649 | 2.096384 | -4.22031 |
| H82 | 3.855612 | 3.419447 | -5.6941 | C79 | 1.644021 | 5.384453 | -5.08842 |
| C83 | -0.76816 | 3.018391 | -3.38751 | H80 | 1.470842 | 7.020032 | -3.69505 |
| C84 | -0.58674 | 0.744452 | -3.04942 | H81 | 1.842849 | 3.557459 | -6.21834 |
| C85 | -1.3351 | 2.229259 | -4.58362 | H82 | 1.692033 | 6.027634 | -5.96232 |
| H86 | 0.188196 | 3.499327 | -3.6132 | C83 | -1.61103 | 2.930912 | -3.28985 |
| H87 | -1.47133 | 3.76869 | -3.02159 | C84 | -0.72394 | 0.811556 | -2.9017 |
| H88 | -2.42782 | 2.268696 | -4.62675 | C85 | -1.65682 | 2.062898 | -4.55989 |
| H89 | -0.91383 | 2.524147 | -5.5448 | H86 | -1.08735 | 3.871379 | -3.4657 |
| N90 | -0.58457 | 1.92995 | -2.41557 | H87 | -2.60821 | 3.134676 | -2.8878 |
| O91 | -0.9543 | 0.845944 | -4.33161 | H88 | -2.64513 | 2.010224 | -5.01773 |
| O92 | -0.295 | -0.35483 | -2.53377 | H89 | -0.91528 | 2.379946 | -5.29769 |
| H93 | 2.292542 | -4.22237 | 1.493268 | N90 | -0.85687 | 2.057529 | -2.37682 |
| N94 | -1.93674 | -2.33879 | -0.02316 | O91 | -1.30065 | 0.728737 | -4.11167 |
| C95 | -0.96692 | -3.03385 | -0.90477 | O92 | -0.20406 | -0.18001 | -2.37881 |
| H96 | -0.89162 | -2.54792 | -1.88494 | H93 | 2.034033 | -4.21746 | 1.737162 |
| C97 | -2.13619 | 3.249847 | -0.28306 | N94 | -2.01572 | -2.44415 | 0.006624 |
| H98 | -2.51976 | 4.229475 | 0.020031 | C95 | -0.99204 | -3.03968 | -0.88623 |
| H99 | -2.6053 | 2.976742 | -1.23168 | H96 | -0.88857 | -2.47969 | -1.8243 |
| H100 | -2.47531 | 2.51655 | 0.450319 | C97 | -2.21275 | 3.276718 | -0.03532 |
| C101 | -0.03006 | 3.523597 | 1.052677 | H98 | -2.75881 | 4.137632 | 0.3601 |
| H102 | -0.17111 | 2.649043 | 1.693684 | H99 | -2.81929 | 2.817391 | -0.81702 |
| H103 | 1.036951 | 3.764362 | 1.045764 | H100 | -2.1243 | 2.539558 | 0.767939 |
| H104 | -0.54287 | 4.3741 | 1.513299 | C101 | -0.00053 | 4.203792 | 0.698554 |
| H105 | -0.30504 | 4.138053 | -0.97136 | H102 | 0.234439 | 3.375776 | 1.378808 |

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|-------------------|----------|----------|----------|------|----------|----------|----------|
| | | | | H103 | 0.939601 | 4.679982 | 0.411199 |
| | | | | H104 | -0.58485 | 4.940577 | 1.257282 |
| | | | | H105 | -0.90428 | 4.521882 | -1.22915 |
| | | | | H106 | -0.1176 | 1.763073 | -0.38246 |
| | | | | H107 | 1.792077 | 0.372584 | -0.36784 |
| C3_ZS_Chelbot_TS2 | | | | | | | |
| C1 | -3.76072 | -3.46184 | -1.38819 | | | | |
| C2 | -1.5185 | -4.39179 | -1.11872 | | | | |
| C3 | -2.65125 | -4.24252 | -2.16953 | | | | |
| C4 | -3.08706 | -3.22574 | -0.01968 | | | | |
| H5 | -4.66694 | -4.06347 | -1.26187 | | | | |
| H6 | -2.31234 | -3.71298 | -3.06551 | | | | |
| H7 | -3.75462 | -2.89488 | 0.776458 | | | | |
| H8 | -4.04801 | -2.52295 | -1.86263 | | | | |
| H9 | -0.78202 | -5.16381 | -1.34114 | | | | |
| H10 | -3.00297 | -5.22849 | -2.48555 | | | | |
| C11 | -2.32138 | -4.54678 | 0.189609 | | | | |
| H12 | -1.69383 | -4.56253 | 1.085699 | | | | |
| H13 | -2.97442 | -5.42398 | 0.189927 | | | | |
| C14 | 0.429822 | -2.95281 | -0.18358 | | | | |
| N15 | 0.964612 | -1.87664 | 0.279781 | | | | |
| C16 | 2.375102 | -2.1909 | 0.6919 | | | | |
| C17 | 2.372391 | -3.75723 | 0.591887 | | | | |
| P18 | -1.84293 | -0.69913 | 0.389213 | | | | |
| Ir19 | 0.136313 | 0.151505 | -0.16543 | | | | |
| C20 | -1.97499 | -0.76774 | 2.220683 | | | | |
| C21 | -2.02304 | -0.84252 | 5.026898 | | | | |
| C22 | -2.01928 | -1.99166 | 2.898022 | | | | |
| C23 | -1.93737 | 0.42253 | 2.967949 | | | | |
| C24 | -1.96981 | 0.38485 | 4.359226 | | | | |
| C25 | -2.04291 | -2.02736 | 4.293841 | | | | |
| H26 | -1.85774 | 1.37998 | 2.465257 | | | | |
| H27 | -1.94223 | 1.313178 | 4.922533 | | | | |
| H28 | -2.06809 | -2.98524 | 4.805106 | | | | |
| H29 | -2.04018 | -0.87191 | 6.112462 | | | | |
| O30 | 1.144115 | -4.07949 | -0.12057 | | | | |
| C31 | 2.667406 | -1.77214 | 2.127318 | | | | |
| C32 | 1.698162 | -1.17666 | 2.939993 | | | | |
| C33 | 3.917862 | -2.07684 | 2.687451 | | | | |
| C34 | 1.98836 | -0.8442 | 4.264757 | | | | |
| H35 | 0.712323 | -0.9745 | 2.546968 | | | | |
| C36 | 4.206059 | -1.74915 | 4.011496 | | | | |
| H37 | 4.677225 | -2.56727 | 2.08387 | | | | |
| C38 | 3.244496 | -1.11889 | 4.804785 | | | | |
| H39 | 1.216731 | -0.379 | 4.871711 | | | | |
| H40 | 5.183724 | -1.98598 | 4.421331 | | | | |
| H41 | 3.47107 | -0.85819 | 5.834324 | | | | |
| C42 | -3.40844 | 0.030915 | -0.20636 | | | | |
| C43 | -4.39476 | 0.537434 | 0.647701 | | | | |

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|-----|----------|----------|----------|
| C44 | -3.61933 | 0.049476 | -1.59529 |
| C45 | -5.56814 | 1.07663 | 0.117483 |
| H46 | -4.2545 | 0.515212 | 1.723094 |
| C47 | -4.7881 | 0.593928 | -2.11983 |
| C48 | -5.76294 | 1.114958 | -1.26269 |
| H49 | -6.33029 | 1.4652 | 0.786554 |
| H50 | -4.94767 | 0.598479 | -3.19457 |
| H51 | -6.67652 | 1.537166 | -1.67106 |
| H52 | 0.188189 | 0.675502 | 1.296074 |
| H53 | 1.883042 | 1.376416 | -1.68324 |
| H54 | -2.00914 | -2.92233 | 2.346688 |
| H55 | -2.88353 | -0.38639 | -2.26243 |
| H56 | 3.208629 | -4.15562 | 0.016549 |
| C57 | 4.842256 | -0.46862 | -2.47046 |
| C58 | 3.774796 | -1.31875 | -2.7651 |
| C59 | 3.01536 | -1.86861 | -1.7355 |
| C60 | 3.297827 | -1.58153 | -0.38924 |
| C61 | 4.378388 | -0.73796 | -0.10706 |
| C62 | 5.141977 | -0.18608 | -1.13908 |
| H63 | 5.43215 | -0.03149 | -3.27082 |
| H64 | 3.527486 | -1.55193 | -3.79695 |
| H65 | 2.184129 | -2.51512 | -1.99702 |
| H66 | 4.615931 | -0.48111 | 0.918181 |
| H67 | 5.969269 | 0.474137 | -0.8952 |
| C68 | -0.76158 | 3.271041 | -0.33962 |
| C69 | -0.14525 | 2.04535 | -1.05148 |
| C70 | 1.364898 | 2.323674 | -1.47201 |
| H71 | 1.888592 | 2.765671 | -0.62555 |
| C72 | 1.539736 | 3.195363 | -2.69524 |
| C73 | 1.501474 | 4.593953 | -2.60338 |
| C74 | 1.715453 | 2.611246 | -3.9576 |
| C75 | 1.602621 | 5.386473 | -3.74769 |
| H76 | 1.397225 | 5.066006 | -1.62989 |
| C77 | 1.820095 | 3.401316 | -5.10366 |
| H78 | 1.779374 | 1.528026 | -4.03912 |
| C79 | 1.753466 | 4.792303 | -5.0025 |
| H80 | 1.56912 | 6.468813 | -3.65919 |
| H81 | 1.961614 | 2.931824 | -6.07359 |
| H82 | 1.83318 | 5.409682 | -5.89259 |
| C83 | -1.59266 | 2.695411 | -3.21356 |
| C84 | -0.66544 | 0.595891 | -2.92555 |
| C85 | -1.60795 | 1.888447 | -4.53217 |
| H86 | -1.05034 | 3.635653 | -3.32305 |
| H87 | -2.60008 | 2.89961 | -2.83892 |
| H88 | -2.59893 | 1.804737 | -4.98097 |

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|------|----------|----------|----------|
| H89 | -0.89645 | 2.280298 | -5.26194 |
| N90 | -0.89047 | 1.767844 | -2.31625 |
| O91 | -1.17067 | 0.546725 | -4.16633 |
| O92 | -0.07694 | -0.38136 | -2.41539 |
| H93 | 2.321379 | -4.23419 | 1.572748 |
| N94 | -1.94764 | -2.27404 | -0.19804 |
| C95 | -0.8815 | -2.9939 | -0.92706 |
| H96 | -0.67773 | -2.51887 | -1.89464 |
| C97 | -2.23853 | 3.097608 | 0.031933 |
| H98 | -2.66606 | 4.057841 | 0.338182 |
| H99 | -2.84834 | 2.700195 | -0.77951 |
| H100 | -2.34359 | 2.409499 | 0.87104 |
| C101 | 0.015307 | 3.693025 | 0.91923 |
| H102 | 0.073087 | 2.864703 | 1.632952 |
| H103 | 1.035089 | 4.025827 | 0.708418 |
| H104 | -0.49866 | 4.526103 | 1.409487 |
| H105 | -0.70235 | 4.11117 | -1.04903 |
| H106 | 2.116397 | 1.057975 | 0.892576 |
| H107 | 2.528315 | 0.737021 | 0.356272 |

C3_ZR_Chelbot

C3_ZR_Chelbot_SM

| | | | |
|------|----------|----------|----------|
| C1 | -4.21652 | -2.94392 | 1.121838 |
| C2 | -2.20859 | -4.24784 | 0.653239 |
| C3 | -3.71566 | -4.17308 | 0.294898 |
| C4 | -2.92291 | -2.47574 | 1.826573 |
| H5 | -4.965 | -3.23304 | 1.867033 |
| H6 | -3.88076 | -4.0532 | -0.78058 |
| H7 | -3.06798 | -1.78553 | 2.656694 |
| H8 | -4.65393 | -2.16417 | 0.49822 |
| H9 | -1.7287 | -5.19659 | 0.416817 |
| H10 | -4.21713 | -5.09487 | 0.603061 |
| C11 | -2.21911 | -3.80897 | 2.133135 |
| H12 | -1.22462 | -3.67605 | 2.569894 |
| H13 | -2.81392 | -4.47316 | 2.766494 |
| C14 | -0.0145 | -3.11205 | -0.13523 |
| N15 | 0.818947 | -2.13676 | -0.27555 |
| C16 | 2.19706 | -2.7214 | -0.52892 |
| C17 | 1.931055 | -4.23502 | -0.25357 |
| P18 | -1.86464 | -0.34886 | 0.181523 |
| Ir19 | 0.44357 | -0.02243 | -0.46204 |
| C20 | -2.27295 | 0.737486 | 1.586155 |
| C21 | -2.59362 | 2.490097 | 3.752764 |
| C22 | -1.65536 | 0.466598 | 2.819937 |
| C23 | -3.03022 | 1.908058 | 1.443134 |

C3_ZR_Chelbot_INT2

| | | | |
|------|----------|----------|----------|
| C1 | -4.25596 | -3.0884 | -0.67751 |
| C2 | -2.13637 | -4.28408 | -0.8835 |
| C3 | -3.45882 | -4.01753 | -1.65133 |
| C4 | -3.25246 | -2.90055 | 0.484326 |
| H5 | -5.16212 | -3.57841 | -0.30566 |
| H6 | -3.28095 | -3.55056 | -2.62581 |
| H7 | -3.66835 | -2.47324 | 1.396806 |
| H8 | -4.55504 | -2.14431 | -1.13124 |
| H9 | -1.57071 | -5.14953 | -1.22844 |
| H10 | -3.98581 | -4.95868 | -1.83195 |
| C11 | -2.61962 | -4.2996 | 0.583735 |
| H12 | -1.81021 | -4.35776 | 1.317605 |
| H13 | -3.35145 | -5.08779 | 0.781659 |
| C14 | 0.121669 | -3.09627 | -0.46512 |
| N15 | 0.863027 | -2.10455 | -0.12261 |
| C16 | 2.247223 | -2.61782 | 0.155324 |
| C17 | 2.017945 | -4.16898 | 0.068319 |
| P18 | -1.86832 | -0.43784 | 0.074375 |
| Ir19 | 0.34326 | 0.040969 | -0.47435 |
| C20 | -2.1679 | 0.019014 | 1.814285 |
| C21 | -2.2944 | 0.781642 | 4.509212 |
| C22 | -1.88101 | -0.90905 | 2.826608 |
| C23 | -2.50089 | 1.337005 | 2.160346 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| C24 | -3.18929 | 2.776458 | 2.525611 | C24 | -2.5662 | 1.710614 | 3.50258 |
| C25 | -1.82268 | 1.333004 | 3.896662 | C25 | -1.9502 | -0.5285 | 4.166677 |
| H26 | -3.47646 | 2.164658 | 0.489931 | H26 | -2.69178 | 2.07892 | 1.394317 |
| H27 | -3.77836 | 3.680672 | 2.40186 | H27 | -2.82312 | 2.734972 | 3.756681 |
| H28 | -1.34774 | 1.109049 | 4.847558 | H28 | -1.73344 | -1.25679 | 4.943246 |
| H29 | -2.72138 | 3.167164 | 4.592386 | H29 | -2.34502 | 1.076862 | 5.553151 |
| O30 | 0.485638 | -4.35054 | -0.17942 | O30 | 0.669656 | -4.31628 | -0.45745 |
| C31 | 3.234277 | -2.24123 | 0.481078 | C31 | 2.710993 | -2.25974 | 1.563376 |
| C32 | 2.854172 | -1.676 | 1.703655 | C32 | 1.863741 | -1.6419 | 2.488062 |
| C33 | 4.591622 | -2.50687 | 0.253476 | C33 | 3.988474 | -2.6619 | 1.983926 |
| C34 | 3.815251 | -1.33001 | 2.653322 | C34 | 2.298258 | -1.39241 | 3.79185 |
| H35 | 1.806321 | -1.49302 | 1.907831 | H35 | 0.863304 | -1.35212 | 2.19556 |
| C36 | 5.551677 | -2.1659 | 1.205929 | C36 | 4.420004 | -2.41658 | 3.286376 |
| H37 | 4.903563 | -2.97576 | -0.67493 | H37 | 4.65333 | -3.16365 | 1.285236 |
| C38 | 5.167863 | -1.56497 | 2.404798 | C38 | 3.578297 | -1.77067 | 4.195523 |
| H39 | 3.503743 | -0.87827 | 3.591077 | H39 | 1.624244 | -0.90329 | 4.489972 |
| H40 | 6.599813 | -2.3707 | 1.007933 | H40 | 5.414825 | -2.73006 | 3.589815 |
| H41 | 5.915892 | -1.29208 | 3.143433 | H41 | 3.915965 | -1.57506 | 5.208938 |
| C42 | -3.20959 | -0.25349 | -1.05862 | C42 | -3.30086 | 0.161913 | -0.8979 |
| C43 | -4.54327 | 0.067682 | -0.76053 | C43 | -4.47754 | 0.663323 | -0.33006 |
| C44 | -2.87983 | -0.67835 | -2.3567 | C44 | -3.25706 | -0.07164 | -2.28197 |
| C45 | -5.52074 | -0.0068 | -1.75127 | C45 | -5.57299 | 0.969147 | -1.13973 |
| H46 | -4.82557 | 0.367744 | 0.243336 | H46 | -4.55187 | 0.817346 | 0.739841 |
| C47 | -3.86568 | -0.76988 | -3.33934 | C47 | -4.34966 | 0.23566 | -3.0881 |
| C48 | -5.18449 | -0.4262 | -3.04034 | C48 | -5.51062 | 0.767915 | -2.51856 |
| H49 | -6.54772 | 0.256163 | -1.5142 | H49 | -6.47849 | 1.363797 | -0.68791 |
| H50 | -3.59978 | -1.09725 | -4.34043 | H50 | -4.30176 | 0.042447 | -4.15664 |
| H51 | -5.95071 | -0.48618 | -3.80787 | H51 | -6.36559 | 1.008494 | -3.144 |
| H52 | 0.645051 | 0.162578 | 1.066484 | H52 | 0.40047 | 0.499997 | 1.018 |
| H53 | 2.029701 | -0.07706 | -0.56749 | H53 | 1.741568 | 1.732302 | -2.53119 |
| H54 | -1.0371 | -0.41977 | 2.928618 | H54 | -1.59116 | -1.92159 | 2.564402 |
| H55 | -1.84619 | -0.90565 | -2.60519 | H55 | -2.38266 | -0.52378 | -2.73059 |
| H56 | 2.291223 | -4.89514 | -1.04279 | H56 | 2.704944 | -4.67379 | -0.61167 |
| C57 | 2.925968 | -1.86614 | -4.72741 | C57 | 4.652468 | -1.18439 | -3.17684 |
| C58 | 2.016611 | -2.85214 | -4.34397 | C58 | 3.587322 | -2.06522 | -3.3792 |
| C59 | 1.821273 | -3.13479 | -2.99424 | C59 | 2.850208 | -2.52866 | -2.29296 |
| C60 | 2.529178 | -2.44322 | -2.00169 | C60 | 3.158877 | -2.12842 | -0.9837 |
| C61 | 3.432877 | -1.45123 | -2.39764 | C61 | 4.226327 | -1.24425 | -0.79198 |
| C62 | 3.632812 | -1.16865 | -3.74923 | C62 | 4.968436 | -0.7775 | -1.88071 |
| H63 | 3.079416 | -1.64383 | -5.77936 | H63 | 5.231688 | -0.82208 | -4.02158 |
| H64 | 1.455038 | -3.39893 | -5.09574 | H64 | 3.327569 | -2.38864 | -4.38331 |
| H65 | 1.089616 | -3.89076 | -2.71921 | H65 | 2.010625 | -3.19252 | -2.47653 |
| H66 | 3.98487 | -0.89125 | -1.6546 | H66 | 4.480217 | -0.90707 | 0.206828 |
| H67 | 4.349505 | -0.4027 | -4.03442 | H67 | 5.796261 | -0.09496 | -1.70967 |
| C68 | 2.465488 | 2.507405 | -0.24266 | C68 | 1.096119 | 3.716227 | -2.94917 |

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|-------------------|----------|----------|----------|-------------------|----------|----------|----------|
| C69 | 1.24798 | 1.918139 | -0.97523 | C69 | 0.784658 | 2.269143 | -2.47878 |
| C70 | -0.09223 | 2.12739 | -0.51047 | C70 | 0.282515 | 2.115589 | -1.01348 |
| H71 | -0.15605 | 2.423168 | 0.531472 | H71 | 1.120146 | 2.50071 | -0.42457 |
| C72 | -1.18225 | 2.76164 | -1.31438 | C72 | -0.89232 | 2.972601 | -0.63121 |
| C73 | -1.67947 | 2.307169 | -2.54349 | C73 | -2.09278 | 3.023884 | -1.35195 |
| C74 | -1.71754 | 3.953567 | -0.79016 | C74 | -0.7834 | 3.803626 | 0.499431 |
| C75 | -2.66696 | 3.018931 | -3.22605 | C75 | -3.13428 | 3.871763 | -0.97255 |
| H76 | -1.34206 | 1.366479 | -2.95007 | H76 | -2.23762 | 2.3676 | -2.19763 |
| C77 | -2.69767 | 4.669481 | -1.47441 | C77 | -1.81709 | 4.655448 | 0.882858 |
| H78 | -1.359 | 4.319016 | 0.168784 | H78 | 0.132241 | 3.776108 | 1.085686 |
| C79 | -3.17889 | 4.205291 | -2.70081 | C79 | -3.0015 | 4.696713 | 0.143579 |
| H80 | -3.0477 | 2.627984 | -4.16532 | H80 | -4.05472 | 3.876092 | -1.54967 |
| H81 | -3.08882 | 5.588119 | -1.04591 | H81 | -1.69577 | 5.290324 | 1.756429 |
| H82 | -3.94928 | 4.755927 | -3.2323 | H82 | -3.80896 | 5.361862 | 0.435384 |
| C83 | 1.720448 | 3.081158 | -3.23612 | C83 | -0.90954 | 2.188204 | -4.54136 |
| C84 | 0.956708 | 0.892903 | -3.18789 | C84 | -0.22711 | 0.251538 | -3.49323 |
| C85 | 1.785861 | 2.433048 | -4.63325 | C85 | -1.16733 | 0.964369 | -5.43454 |
| H86 | 2.665167 | 3.551617 | -2.9552 | H86 | -0.39264 | 2.981787 | -5.07809 |
| H87 | 0.907032 | 3.80994 | -3.14045 | H87 | -1.83183 | 2.599505 | -4.12041 |
| H88 | 1.293496 | 3.015814 | -5.41215 | H88 | -2.1927 | 0.897763 | -5.79991 |
| H89 | 2.812113 | 2.200903 | -4.93325 | H89 | -0.46981 | 0.904613 | -6.27589 |
| N90 | 1.439524 | 1.897542 | -2.41911 | N90 | -0.07643 | 1.587629 | -3.48821 |
| O91 | 1.070252 | 1.176013 | -4.49251 | O91 | -0.92393 | -0.17411 | -4.56839 |
| O92 | 0.433237 | -0.15187 | -2.77618 | O92 | 0.160346 | -0.57302 | -2.64768 |
| H93 | 2.334705 | -4.55032 | 0.709856 | H93 | 2.043936 | -4.6438 | 1.05041 |
| N94 | -1.94463 | -1.91462 | 0.849378 | N94 | -2.05932 | -2.1208 | 0.037119 |
| C95 | -1.51783 | -3.02952 | -0.02075 | C95 | -1.31193 | -2.9743 | -0.91562 |
| H96 | -1.88903 | -2.92365 | -1.05365 | H96 | -1.27868 | -2.55232 | -1.92929 |
| C97 | 2.345648 | 2.526671 | 1.286042 | C97 | 1.8095 | 4.539395 | -1.86541 |
| H98 | 3.217197 | 3.034777 | 1.709588 | H98 | 2.129699 | 5.498464 | -2.28432 |
| H99 | 1.456433 | 3.056842 | 1.637901 | H99 | 1.165163 | 4.749512 | -1.011 |
| H100 | 2.321386 | 1.507047 | 1.680008 | H100 | 2.708296 | 4.022617 | -1.5068 |
| C101 | 3.795623 | 1.857814 | -0.65106 | C101 | 1.987428 | 3.694447 | -4.20726 |
| H102 | 3.876284 | 1.718789 | -1.73315 | H102 | 1.635111 | 3.0129 | -4.987 |
| H103 | 4.634022 | 2.480297 | -0.32331 | H103 | 2.066199 | 4.694221 | -4.6451 |
| H104 | 3.900941 | 0.878071 | -0.17477 | H104 | 3.000023 | 3.37071 | -3.93912 |
| H105 | 2.487743 | 3.558994 | -0.57544 | H105 | 0.144199 | 4.217668 | -3.16782 |
| | | | | H106 | 2.015286 | 0.395229 | -0.12616 |
| | | | | H107 | 2.053062 | 0.219239 | -0.94206 |
| C3_ZR_Chelbot_TS1 | | | | C3_ZR_Chelbot_TS3 | | | |
| C1 | -4.25737 | -3.20512 | 0.941546 | C1 | -4.21821 | -3.17512 | -0.93054 |
| C2 | -2.16515 | -4.42446 | 0.664067 | C2 | -2.04941 | -4.28667 | -1.09864 |
| C3 | -3.63754 | -4.42084 | 0.177519 | C3 | -3.35532 | -4.04691 | -1.90187 |
| C4 | -3.0567 | -2.6892 | 1.769711 | C4 | -3.25904 | -2.98074 | 0.265129 |
| H5 | -5.06679 | -3.51558 | 1.610456 | | | | |
| H6 | -3.71546 | -4.31998 | -0.90975 | | | | |

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|------|----------|----------|----------|------|----------|----------|----------|
| H7 | -3.3129 | -2.01096 | 2.582884 | H5 | -5.11768 | -3.70714 | -0.60266 |
| H8 | -4.65643 | -2.44209 | 0.272758 | H6 | -3.1615 | -3.54818 | -2.85721 |
| H9 | -1.62062 | -5.34793 | 0.470834 | H7 | -3.71957 | -2.58887 | 1.172405 |
| H10 | -4.12492 | -5.35967 | 0.455664 | H8 | -4.53367 | -2.22718 | -1.366 |
| C11 | -2.3281 | -3.9935 | 2.137783 | H9 | -1.44348 | -5.12371 | -1.44501 |
| H12 | -1.38441 | -3.81974 | 2.663165 | H10 | -3.8405 | -5.00135 | -2.12458 |
| H13 | -2.94906 | -4.68675 | 2.712257 | C11 | -2.57671 | -4.35688 | 0.352688 |
| C14 | 0.026798 | -3.1879 | -0.01965 | H12 | -1.78688 | -4.40336 | 1.108745 |
| N15 | 0.801081 | -2.1729 | -0.19728 | H13 | -3.28185 | -5.17798 | 0.509525 |
| C16 | 2.197439 | -2.68214 | -0.46835 | C14 | 0.144111 | -3.04461 | -0.55803 |
| C17 | 2.033372 | -4.19587 | -0.12132 | N15 | 0.871926 | -2.04637 | -0.19501 |
| P18 | -1.93497 | -0.51394 | 0.240788 | C16 | 2.226116 | -2.56166 | 0.22966 |
| Ir19 | 0.258475 | -0.07233 | -0.37705 | C17 | 1.996385 | -4.11063 | 0.137179 |
| C20 | -2.40698 | 0.607713 | 1.594656 | P18 | -1.90974 | -0.46773 | 0.011619 |
| C21 | -2.79473 | 2.475528 | 3.646149 | Ir19 | 0.454693 | 0.04955 | -0.54822 |
| C22 | -1.98906 | 0.319317 | 2.903142 | C20 | -2.11103 | -0.11136 | 1.794885 |
| C23 | -2.99303 | 1.851853 | 1.316486 | C21 | -2.10907 | 0.533643 | 4.521472 |
| C24 | -3.18639 | 2.778056 | 2.341953 | C22 | -1.95877 | -1.11663 | 2.757623 |
| C25 | -2.19296 | 1.245478 | 3.924055 | C23 | -2.24926 | 1.223978 | 2.206708 |
| H26 | -3.27943 | 2.112503 | 0.30332 | C24 | -2.25015 | 1.540685 | 3.563277 |
| H27 | -3.63868 | 3.739113 | 2.115024 | C25 | -1.96312 | -0.79354 | 4.116114 |
| H28 | -1.87581 | 1.010421 | 4.936043 | H26 | -2.34572 | 2.018284 | 1.474655 |
| H29 | -2.94888 | 3.197717 | 4.442678 | H27 | -2.35568 | 2.577593 | 3.870036 |
| O30 | 0.596865 | -4.4001 | -0.02778 | H28 | -1.84738 | -1.58076 | 4.855955 |
| C31 | 3.239056 | -2.08122 | 0.470459 | H29 | -2.10879 | 0.783551 | 5.57871 |
| C32 | 2.868406 | -1.49583 | 1.686712 | O30 | 0.685769 | -4.26144 | -0.47481 |
| C33 | 4.604169 | -2.23127 | 0.187076 | C31 | 2.535408 | -2.21277 | 1.68208 |
| C34 | 3.83706 | -1.01513 | 2.569233 | C32 | 1.558459 | -1.70073 | 2.53986 |
| H35 | 1.819095 | -1.40269 | 1.938961 | C33 | 3.79377 | -2.53756 | 2.211125 |
| C36 | 5.572462 | -1.75368 | 1.0708 | C34 | 1.842999 | -1.47187 | 3.886172 |
| H37 | 4.915924 | -2.7155 | -0.73346 | H35 | 0.570031 | -1.47861 | 2.163541 |
| C38 | 5.193181 | -1.1294 | 2.260267 | C36 | 4.076495 | -2.31586 | 3.558023 |
| H39 | 3.526928 | -0.54918 | 3.500409 | H37 | 4.560371 | -2.95831 | 1.565734 |
| H40 | 6.624166 | -1.87045 | 0.825668 | C38 | 3.103518 | -1.77299 | 4.39974 |
| H41 | 5.946393 | -0.74999 | 2.944195 | H39 | 1.068529 | -1.06001 | 4.527265 |
| C42 | -3.24447 | -0.40871 | -1.03571 | H40 | 5.058968 | -2.56626 | 3.948349 |
| C43 | -4.57276 | -0.06002 | -0.74178 | H41 | 3.327463 | -1.59434 | 5.447508 |
| C44 | -2.91247 | -0.8109 | -2.3398 | C42 | -3.43373 | 0.20279 | -0.78308 |
| C45 | -5.54441 | -0.09161 | -1.74061 | C43 | -4.52733 | 0.717987 | -0.07919 |
| H46 | -4.85128 | 0.237681 | 0.264261 | C44 | -3.52165 | 0.081659 | -2.1802 |
| C47 | -3.89233 | -0.85292 | -3.33245 | C45 | -5.672 | 1.137746 | -0.7622 |
| C48 | -5.20644 | -0.48812 | -3.03645 | H46 | -4.49372 | 0.803494 | 1.001341 |
| H49 | -6.56637 | 0.192606 | -1.50606 | C47 | -4.66253 | 0.501895 | -2.85983 |
| H50 | -3.62472 | -1.15842 | -4.33994 | C48 | -5.74228 | 1.041792 | -2.15217 |
| H51 | -5.96648 | -0.5106 | -3.81216 | H49 | -6.51116 | 1.540105 | -0.20152 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| H52 | 0.440278 | 0.084173 | 1.15842 | H50 | -4.71835 | 0.395272 | -3.94027 |
| H53 | 1.86831 | 0.317359 | -0.59038 | H51 | -6.63332 | 1.370401 | -2.67919 |
| H54 | -1.48816 | -0.62062 | 3.11586 | H52 | 0.552303 | 0.305987 | 0.983879 |
| H55 | -1.88336 | -1.0529 | -2.58854 | H53 | 1.679679 | 1.687643 | -2.7629 |
| H56 | 2.427902 | -4.86776 | -0.88403 | H54 | -1.8147 | -2.14695 | 2.449804 |
| C57 | 2.646714 | -1.93252 | -4.72961 | H55 | -2.70771 | -0.36344 | -2.7414 |
| C58 | 1.828242 | -2.96208 | -4.26297 | H56 | 2.726918 | -4.62508 | -0.48802 |
| C59 | 1.729582 | -3.21262 | -2.89671 | C57 | 4.977717 | -1.12396 | -2.80688 |
| C60 | 2.44214 | -2.44207 | -1.96579 | C58 | 4.004234 | -2.07769 | -3.11107 |
| C61 | 3.250958 | -1.40684 | -2.44542 | C59 | 3.152354 | -2.5462 | -2.11466 |
| C62 | 3.359358 | -1.15984 | -3.81522 | C60 | 3.255556 | -2.07561 | -0.79839 |
| H63 | 2.7241 | -1.73536 | -5.79478 | C61 | 4.22422 | -1.10845 | -0.50632 |
| H64 | 1.262636 | -3.56919 | -4.9638 | C62 | 5.083358 | -0.64131 | -1.50318 |
| H65 | 1.068933 | -4.00697 | -2.55841 | H63 | 5.648752 | -0.76185 | -3.5807 |
| H66 | 3.801898 | -0.78563 | -1.7538 | H64 | 3.907707 | -2.45608 | -4.1247 |
| H67 | 4.005807 | -0.35811 | -4.1637 | H65 | 2.383864 | -3.26901 | -2.37668 |
| C68 | 2.636455 | 2.404166 | -0.24224 | H66 | 4.303286 | -0.70481 | 0.496472 |
| C69 | 1.403406 | 1.777333 | -0.92357 | H67 | 5.834712 | 0.103466 | -1.25572 |
| C70 | 0.04975 | 2.0483 | -0.41573 | C68 | 1.039768 | 3.673031 | -3.2634 |
| H71 | 0.051917 | 2.388221 | 0.616187 | C69 | 0.747901 | 2.260826 | -2.67778 |
| C72 | -0.94932 | 2.844561 | -1.20218 | C70 | 0.395602 | 2.242903 | -1.16787 |
| C73 | -1.67241 | 2.371555 | -2.30493 | H71 | 1.260483 | 2.778225 | -0.75432 |
| C74 | -1.18439 | 4.165213 | -0.77771 | C72 | -0.7762 | 3.03963 | -0.66912 |
| C75 | -2.59381 | 3.188057 | -2.96344 | C73 | -2.04293 | 3.010194 | -1.26079 |
| H76 | -1.55306 | 1.348178 | -2.62764 | C74 | -0.58329 | 3.895835 | 0.429095 |
| C77 | -2.10011 | 4.983943 | -1.43506 | C75 | -3.08025 | 3.81288 | -0.78578 |
| H78 | -0.6468 | 4.547701 | 0.086935 | H76 | -2.23755 | 2.328797 | -2.07415 |
| C79 | -2.8108 | 4.497206 | -2.53482 | C77 | -1.61664 | 4.69502 | 0.913426 |
| H80 | -3.15444 | 2.786827 | -3.80329 | H78 | 0.391565 | 3.933043 | 0.910699 |
| H81 | -2.26417 | 5.999429 | -1.08482 | C79 | -2.87337 | 4.659738 | 0.303576 |
| H82 | -3.53256 | 5.129998 | -3.04338 | H80 | -4.05549 | 3.757743 | -1.26027 |
| C83 | 1.814573 | 2.950593 | -3.17802 | H81 | -1.439 | 5.349374 | 1.762585 |
| C84 | 0.852302 | 0.841652 | -3.12521 | H82 | -3.68052 | 5.284499 | 0.675284 |
| C85 | 1.688353 | 2.357505 | -4.59428 | C83 | -1.17082 | 2.129644 | -4.51806 |
| H86 | 2.815866 | 3.339299 | -2.98163 | C84 | -0.3312 | 0.214372 | -3.52983 |
| H87 | 1.072394 | 3.731576 | -2.97612 | C85 | -1.52262 | 0.882243 | -5.34711 |
| H88 | 1.178002 | 3.013168 | -5.30016 | H86 | -0.71943 | 2.907113 | -5.13298 |
| H89 | 2.655878 | 2.049462 | -5.00165 | H87 | -2.04173 | 2.554141 | -4.00933 |
| N90 | 1.526683 | 1.756236 | -2.37603 | H88 | -2.58539 | 0.796242 | -5.57621 |
| O91 | 0.878655 | 1.164276 | -4.42359 | H89 | -0.93868 | 0.815159 | -6.27021 |
| O92 | 0.265918 | -0.16019 | -2.70061 | N90 | -0.21973 | 1.556713 | -3.55384 |
| H93 | 2.464844 | -4.43919 | 0.851179 | O91 | -1.15234 | -0.23728 | -4.50137 |
| N94 | -2.01016 | -2.0818 | 0.896864 | O92 | 0.197393 | -0.58005 | -2.74061 |
| C95 | -1.48334 | -3.17327 | 0.044746 | H93 | 1.952306 | -4.57746 | 1.122408 |
| H96 | -1.8062 | -3.06981 | -1.00516 | N94 | -2.09074 | -2.14402 | -0.13494 |

| | | | |
|------|----------|----------|----------|
| C97 | 2.543235 | 2.408693 | 1.28839 |
| H98 | 3.458512 | 2.838192 | 1.705893 |
| H99 | 1.703017 | 2.999955 | 1.65984 |
| H100 | 2.44498 | 1.386924 | 1.665381 |
| C101 | 3.959994 | 1.762522 | -0.68229 |
| H102 | 4.022308 | 1.634758 | -1.76704 |
| H103 | 4.803351 | 2.382578 | -0.36436 |
| H104 | 4.080044 | 0.77977 | -0.21293 |
| H105 | 2.621023 | 3.452434 | -0.58052 |
| X | 0 | 0 | 0 |

C3_ZR_Chelbot_INT1

| | | | |
|------|----------|----------|----------|
| C1 | -4.23933 | -3.19229 | 0.91985 |
| C2 | -2.16468 | -4.43755 | 0.641566 |
| C3 | -3.63943 | -4.42341 | 0.164499 |
| C4 | -3.03039 | -2.68661 | 1.742571 |
| H5 | -5.05267 | -3.48444 | 1.592062 |
| H6 | -3.72271 | -4.33334 | -0.92322 |
| H7 | -3.27931 | -2.00419 | 2.553573 |
| H8 | -4.62666 | -2.42831 | 0.244808 |
| H9 | -1.62824 | -5.36659 | 0.450766 |
| H10 | -4.13595 | -5.35324 | 0.456259 |
| C11 | -2.31317 | -3.9957 | 2.11338 |
| H12 | -1.36462 | -3.82758 | 2.631808 |
| H13 | -2.93778 | -4.67874 | 2.696137 |
| C14 | 0.035695 | -3.23848 | -0.07425 |
| N15 | 0.804372 | -2.2197 | -0.22512 |
| C16 | 2.199635 | -2.70115 | -0.50777 |
| C17 | 2.038988 | -4.23977 | -0.26109 |
| P18 | -1.88672 | -0.51556 | 0.223606 |
| Ir19 | 0.208571 | -0.1153 | -0.33082 |
| C20 | -2.44956 | 0.61371 | 1.52999 |
| C21 | -2.95049 | 2.529793 | 3.507231 |
| C22 | -2.10456 | 0.357168 | 2.865851 |
| C23 | -3.01412 | 1.851881 | 1.186159 |
| C24 | -3.26503 | 2.802092 | 2.175773 |
| C25 | -2.36685 | 1.307219 | 3.850134 |
| H26 | -3.23346 | 2.090952 | 0.151195 |
| H27 | -3.69703 | 3.759378 | 1.899225 |
| H28 | -2.10588 | 1.098896 | 4.88366 |
| H29 | -3.14694 | 3.272217 | 4.275355 |
| O30 | 0.603607 | -4.45178 | -0.14037 |
| C31 | 3.219542 | -2.14032 | 0.481007 |
| C32 | 2.826242 | -1.53009 | 1.677327 |
| C33 | 4.588608 | -2.33483 | 0.243158 |

| | | | |
|------|----------|----------|----------|
| C95 | -1.27158 | -2.94799 | -1.07346 |
| H96 | -1.21088 | -2.5 | -2.07307 |
| C97 | 1.851326 | 4.563928 | -2.30989 |
| H98 | 2.131374 | 5.488303 | -2.82456 |
| H99 | 1.285708 | 4.845583 | -1.41888 |
| H100 | 2.780693 | 4.07165 | -1.99783 |
| C101 | 1.807454 | 3.544827 | -4.59325 |
| H102 | 1.360359 | 2.828352 | -5.28879 |
| H103 | 1.869291 | 4.512615 | -5.1001 |
| H104 | 2.831701 | 3.205036 | -4.40073 |
| H105 | 0.078188 | 4.175526 | -3.43089 |
| H106 | 2.032027 | 0.121197 | -0.7808 |
| H107 | 1.298462 | 1.321552 | -0.23247 |

C3_ZR_Chelbot_PROD

| | | | |
|------|----------|----------|----------|
| C1 | -3.99134 | -3.54621 | -1.33026 |
| C2 | -1.73604 | -4.48176 | -1.32272 |
| C3 | -2.97647 | -4.31617 | -2.23979 |
| C4 | -3.18068 | -3.35633 | -0.02853 |
| H5 | -4.88974 | -4.14067 | -1.13331 |
| H6 | -2.73711 | -3.7761 | -3.16145 |
| H7 | -3.7664 | -3.05314 | 0.839581 |
| H8 | -4.30949 | -2.59064 | -1.74923 |
| H9 | -1.02682 | -5.24493 | -1.64293 |
| H10 | -3.36239 | -5.2982 | -2.52774 |
| C11 | -2.39438 | -4.67637 | 0.062637 |
| H12 | -1.67961 | -4.69983 | 0.89091 |
| H13 | -3.03558 | -5.56141 | 0.106135 |
| C14 | 0.291581 | -3.06843 | -0.56376 |
| N15 | 0.945595 | -2.01167 | -0.20298 |
| C16 | 2.332989 | -2.42151 | 0.260229 |
| C17 | 2.161978 | -3.97397 | 0.291795 |
| P18 | -1.92075 | -0.77208 | 0.118369 |
| Ir19 | 0.333539 | -0.08013 | -0.47957 |
| C20 | -2.1105 | -0.62058 | 1.930281 |
| C21 | -2.14445 | -0.26058 | 4.711994 |
| C22 | -2.18217 | -1.72664 | 2.784985 |
| C23 | -2.0294 | 0.669285 | 2.483886 |
| C24 | -2.05476 | 0.847568 | 3.864429 |
| C25 | -2.20118 | -1.54457 | 4.170565 |
| H26 | -1.92804 | 1.534962 | 1.833762 |
| H27 | -1.99215 | 1.849252 | 4.28011 |
| H28 | -2.25492 | -2.40984 | 4.825172 |
| H29 | -2.15889 | -0.12172 | 5.7892 |
| O30 | 0.910885 | -4.2378 | -0.40569 |

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|-----|----------|----------|----------|-----|----------|----------|----------|
| C34 | 3.781917 | -1.07018 | 2.587292 | C31 | 2.623803 | -1.96193 | 1.685595 |
| H35 | 1.77328 | -1.40601 | 1.897237 | C32 | 1.57535 | -1.6764 | 2.568752 |
| C36 | 5.541296 | -1.88296 | 1.155359 | C33 | 3.933915 | -1.9893 | 2.180517 |
| H37 | 4.913466 | -2.82945 | -0.66799 | C34 | 1.83522 | -1.36173 | 3.901231 |
| C38 | 5.142222 | -1.2349 | 2.326809 | H35 | 0.550121 | -1.68813 | 2.220784 |
| H39 | 3.45615 | -0.58707 | 3.504339 | C36 | 4.193266 | -1.68187 | 3.516459 |
| H40 | 6.596569 | -2.03553 | 0.947828 | H37 | 4.758276 | -2.2468 | 1.523363 |
| H41 | 5.884451 | -0.87507 | 3.033118 | C38 | 3.146483 | -1.35471 | 4.378354 |
| C42 | -3.1109 | -0.43864 | -1.14043 | H39 | 1.005239 | -1.12321 | 4.560472 |
| C43 | -4.45739 | -0.11283 | -0.90371 | H40 | 5.216766 | -1.69785 | 3.880155 |
| C44 | -2.71855 | -0.83709 | -2.42916 | H41 | 3.351584 | -1.1062 | 5.415706 |
| C45 | -5.3854 | -0.1633 | -1.94251 | C42 | -3.42831 | 0.021433 | -0.58895 |
| H46 | -4.78507 | 0.183131 | 0.087578 | C43 | -4.38016 | 0.734165 | 0.150913 |
| C47 | -3.65541 | -0.8937 | -3.46174 | C44 | -3.57191 | -0.05625 | -1.98544 |
| C48 | -4.98712 | -0.55296 | -3.22287 | C45 | -5.43996 | 1.37692 | -0.49661 |
| H49 | -6.42086 | 0.103158 | -1.75056 | H46 | -4.30014 | 0.79741 | 1.230978 |
| H50 | -3.33885 | -1.19472 | -4.45633 | C47 | -4.62928 | 0.584017 | -2.62758 |
| H51 | -5.713 | -0.58912 | -4.0301 | C48 | -5.56364 | 1.31437 | -1.8851 |
| H52 | 0.33306 | 0.011689 | 1.218594 | H49 | -6.17158 | 1.924796 | 0.090945 |
| H53 | 2.07818 | 0.822325 | -0.78257 | H50 | -4.73189 | 0.502498 | -3.70643 |
| H54 | -1.60763 | -0.57193 | 3.129201 | H51 | -6.38805 | 1.815833 | -2.38363 |
| H55 | -1.67867 | -1.0629 | -2.63848 | H52 | 0.639647 | 0.251027 | 1.002766 |
| H56 | 2.409456 | -4.85871 | -1.07898 | H53 | 1.512485 | 1.472658 | -2.55182 |
| C57 | 2.776642 | -1.65677 | -4.69703 | H54 | -2.19433 | -2.73193 | 2.378809 |
| C58 | 1.9412 | -2.71292 | -4.32605 | H55 | -2.86002 | -0.62562 | -2.57253 |
| C59 | 1.797564 | -3.05569 | -2.98395 | H56 | 2.960265 | -4.51435 | -0.21635 |
| C60 | 2.483593 | -2.35656 | -1.97995 | C57 | 4.937644 | -1.06502 | -2.93959 |
| C61 | 3.310043 | -1.29458 | -2.36193 | C58 | 4.129558 | -2.19106 | -3.10355 |
| C62 | 3.461828 | -0.95275 | -3.70812 | C59 | 3.328035 | -2.63284 | -2.0526 |
| H63 | 2.890478 | -1.39009 | -5.74357 | C60 | 3.31831 | -1.96333 | -0.82127 |
| H64 | 1.396407 | -3.26815 | -5.08405 | C61 | 4.116745 | -0.82268 | -0.67512 |
| H65 | 1.12255 | -3.86598 | -2.71945 | C62 | 4.926774 | -0.3832 | -1.72279 |
| H66 | 3.843897 | -0.72484 | -1.61186 | H63 | 5.57 | -0.72299 | -3.75422 |
| H67 | 4.119865 | -0.13051 | -3.97717 | H64 | 4.121972 | -2.72656 | -4.04868 |
| C68 | 2.806322 | 2.784248 | -0.59527 | H65 | 2.688167 | -3.49688 | -2.21352 |
| C69 | 1.663286 | 1.847357 | -1.06117 | H66 | 4.09771 | -0.26551 | 0.253682 |
| C70 | 0.266099 | 1.975282 | -0.40227 | H67 | 5.54809 | 0.497628 | -1.58558 |
| H71 | 0.383889 | 2.329021 | 0.622428 | C68 | 1.467396 | 3.498842 | -3.20628 |
| C72 | -0.70713 | 2.894172 | -1.09493 | C69 | 0.770785 | 2.275493 | -2.57005 |
| C73 | -1.54045 | 2.49056 | -2.14944 | C70 | 0.300309 | 2.475579 | -1.10183 |
| C74 | -0.78622 | 4.235682 | -0.68102 | H71 | 1.163351 | 2.611197 | -0.45348 |
| C75 | -2.40844 | 3.389112 | -2.77283 | C72 | -0.723 | 3.570935 | -0.87106 |
| H76 | -1.53549 | 1.457843 | -2.46948 | C73 | -2.09269 | 3.3045 | -0.98899 |
| C77 | -1.65106 | 5.138394 | -1.30095 | C74 | -0.31137 | 4.871754 | -0.55349 |
| H78 | -0.16249 | 4.57261 | 0.144264 | C75 | -3.03334 | 4.319689 | -0.81939 |

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|-------------------|----------|----------|----------|------|----------|----------|----------|
| C79 | -2.4666 | 4.719773 | -2.35539 | H76 | -2.42789 | 2.296241 | -1.20717 |
| H80 | -3.0479 | 3.040087 | -3.57938 | C77 | -1.25112 | 5.890238 | -0.39174 |
| H81 | -1.69028 | 6.169093 | -0.95853 | H78 | 0.743735 | 5.093433 | -0.42716 |
| H82 | -3.14322 | 5.419645 | -2.83716 | C79 | -2.61348 | 5.618255 | -0.52743 |
| C83 | 1.665454 | 2.975128 | -3.41518 | H80 | -4.0902 | 4.086523 | -0.90826 |
| C84 | 0.838254 | 0.839741 | -3.1359 | H81 | -0.91682 | 6.895188 | -0.15029 |
| C85 | 1.395239 | 2.302421 | -4.77273 | H82 | -3.34281 | 6.411961 | -0.39433 |
| H86 | 2.653252 | 3.43726 | -3.37564 | C83 | -1.30862 | 2.517154 | -4.18624 |
| H87 | 0.905237 | 3.718551 | -3.15387 | C84 | -0.5824 | 0.434411 | -3.47316 |
| H88 | 0.772574 | 2.896591 | -5.44178 | C85 | -1.82441 | 1.407239 | -5.11703 |
| H89 | 2.318584 | 2.008474 | -5.28137 | H86 | -0.85292 | 3.341977 | -4.73533 |
| N90 | 1.568928 | 1.80769 | -2.53055 | H87 | -2.09209 | 2.917636 | -3.53665 |
| O91 | 0.666246 | 1.090574 | -4.43992 | H88 | -2.90171 | 1.440895 | -5.28079 |
| O92 | 0.351514 | -0.16335 | -2.5946 | H89 | -1.30136 | 1.387806 | -6.07833 |
| H93 | 2.498858 | -4.54959 | 0.6788 | N90 | -0.32008 | 1.76041 | -3.40947 |
| N94 | -1.98268 | -2.09191 | 0.859294 | O91 | -1.51684 | 0.173423 | -4.41296 |
| C95 | -1.47365 | -3.19896 | 0.009547 | O92 | -0.09676 | -0.46804 | -2.78078 |
| H96 | -1.80595 | -3.09347 | -1.03729 | H93 | 2.047658 | -4.3456 | 1.311009 |
| C97 | 2.910491 | 2.818103 | 0.936414 | N94 | -2.06095 | -2.40592 | -0.27029 |
| H98 | 3.799162 | 3.382356 | 1.23436 | C95 | -1.09204 | -3.08081 | -1.17018 |
| H99 | 2.044626 | 3.291226 | 1.405032 | H96 | -1.00652 | -2.57196 | -2.13756 |
| H100 | 3.006251 | 1.803011 | 1.341203 | C97 | 2.691787 | 3.911714 | -2.37023 |
| C101 | 4.156678 | 2.349424 | -1.19196 | H98 | 3.219997 | 4.734543 | -2.86075 |
| H102 | 4.117726 | 2.199149 | -2.27456 | H99 | 2.435086 | 4.244929 | -1.36277 |
| H103 | 4.927471 | 3.096919 | -0.98149 | H100 | 3.393293 | 3.073802 | -2.27682 |
| H104 | 4.483128 | 1.405018 | -0.7393 | C101 | 1.941228 | 3.169391 | -4.6343 |
| H105 | 2.554848 | 3.794708 | -0.94768 | H102 | 1.132958 | 2.863775 | -5.30351 |
| | | | | H103 | 2.427895 | 4.041086 | -5.08155 |
| | | | | H104 | 2.672459 | 2.352965 | -4.61289 |
| C3_ZR_Chelbot_TS2 | | | | H105 | 0.761002 | 4.339507 | -3.23558 |
| C1 | -4.20889 | -3.12099 | -0.45781 | H106 | 1.870265 | 0.27823 | -0.71043 |
| C2 | -2.10398 | -4.32199 | -0.75642 | H107 | -0.3393 | 1.577574 | -0.74075 |
| C3 | -3.46948 | -4.0765 | -1.45166 | | | | |
| C4 | -3.14849 | -2.91973 | 0.648492 | | | | |
| H5 | -5.10037 | -3.59331 | -0.03187 | | | | |
| H6 | -3.35074 | -3.63722 | -2.44748 | | | | |
| H7 | -3.52047 | -2.48004 | 1.573576 | | | | |
| H8 | -4.51946 | -2.1808 | -0.91349 | | | | |
| H9 | -1.5519 | -5.18988 | -1.11685 | | | | |
| H10 | -4.00487 | -5.02223 | -1.57324 | | | | |
| C11 | -2.50487 | -4.31455 | 0.735745 | | | | |
| H12 | -1.65604 | -4.35664 | 1.425054 | | | | |
| H13 | -3.22103 | -5.10206 | 0.986596 | | | | |
| C14 | 0.167897 | -3.1041 | -0.50403 | | | | |
| N15 | 0.897243 | -2.08954 | -0.20541 | | | | |
| C16 | 2.282591 | -2.56733 | 0.097778 | | | | |

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|------|----------|----------|----------|
| C17 | 2.141688 | -4.11496 | -0.16697 |
| P18 | -1.76925 | -0.46762 | 0.162986 |
| Ir19 | 0.270487 | 0.016136 | -0.56511 |
| C20 | -1.99038 | -0.00409 | 1.910211 |
| C21 | -2.03481 | 0.78258 | 4.594724 |
| C22 | -1.73025 | -0.93887 | 2.922789 |
| C23 | -2.25248 | 1.332272 | 2.249153 |
| C24 | -2.27872 | 1.718582 | 3.587382 |
| C25 | -1.75874 | -0.54451 | 4.260562 |
| H26 | -2.41511 | 2.075462 | 1.477666 |
| H27 | -2.48309 | 2.754758 | 3.840775 |
| H28 | -1.56162 | -1.27467 | 5.040322 |
| H29 | -2.05384 | 1.087934 | 5.636978 |
| O30 | 0.742211 | -4.3078 | -0.51606 |
| C31 | 2.637079 | -2.32664 | 1.565644 |
| C32 | 1.772667 | -1.65921 | 2.437713 |
| C33 | 3.825306 | -2.86739 | 2.081412 |
| C34 | 2.103501 | -1.50024 | 3.784645 |
| H35 | 0.838606 | -1.26041 | 2.069817 |
| C36 | 4.157187 | -2.70748 | 3.425119 |
| H37 | 4.50058 | -3.41457 | 1.428297 |
| C38 | 3.299087 | -2.01502 | 4.281963 |
| H39 | 1.414338 | -0.97378 | 4.439588 |
| H40 | 5.085284 | -3.12664 | 3.802666 |
| H41 | 3.558475 | -1.88942 | 5.329078 |
| C42 | -3.21604 | 0.149191 | -0.76931 |
| C43 | -4.35307 | 0.698841 | -0.16601 |
| C44 | -3.23966 | -0.13806 | -2.14483 |
| C45 | -5.4817 | 0.989378 | -0.93542 |
| H46 | -4.3728 | 0.898673 | 0.898684 |
| C47 | -4.36484 | 0.155491 | -2.90872 |
| C48 | -5.48944 | 0.727952 | -2.30524 |
| H49 | -6.35702 | 1.420363 | -0.45828 |
| H50 | -4.36881 | -0.0755 | -3.9705 |
| H51 | -6.37072 | 0.955871 | -2.89787 |
| H52 | 0.506534 | 0.478395 | 0.902394 |
| H53 | 1.710037 | 1.589955 | -2.53459 |
| H54 | -1.48562 | -1.96425 | 2.666476 |
| H55 | -2.38691 | -0.60952 | -2.61639 |
| H56 | 2.746324 | -4.46048 | -1.00777 |
| C57 | 4.857778 | -0.75288 | -2.90473 |
| C58 | 3.661022 | -1.37934 | -3.25823 |
| C59 | 2.865116 | -1.96667 | -2.27748 |
| C60 | 3.241758 | -1.93305 | -0.92523 |
| C61 | 4.43959 | -1.30007 | -0.5809 |

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|------|----------|----------|----------|
| C62 | 5.243615 | -0.71936 | -1.56488 |
| H63 | 5.483401 | -0.29608 | -3.66625 |
| H64 | 3.344274 | -1.41114 | -4.29693 |
| H65 | 1.92336 | -2.42025 | -2.56808 |
| H66 | 4.742775 | -1.2303 | 0.45688 |
| H67 | 6.169677 | -0.23022 | -1.27658 |
| C68 | 1.252289 | 3.624233 | -2.96111 |
| C69 | 0.798328 | 2.205177 | -2.52408 |
| C70 | 0.19877 | 2.078314 | -1.09327 |
| H71 | 1.01039 | 2.436468 | -0.45151 |
| C72 | -0.96827 | 2.978197 | -0.78647 |
| C73 | -2.1548 | 3.005133 | -1.53346 |
| C74 | -0.87646 | 3.860325 | 0.306133 |
| C75 | -3.19501 | 3.879935 | -1.21824 |
| H76 | -2.29389 | 2.301844 | -2.34227 |
| C77 | -1.91347 | 4.733877 | 0.63054 |
| H78 | 0.024989 | 3.853163 | 0.91467 |
| C79 | -3.08057 | 4.752087 | -0.13601 |
| H80 | -4.10413 | 3.863717 | -1.81298 |
| H81 | -1.80674 | 5.405149 | 1.478548 |
| H82 | -3.88932 | 5.434266 | 0.109593 |
| C83 | -0.84306 | 2.29292 | -4.61829 |
| C84 | -0.3063 | 0.287301 | -3.59884 |
| C85 | -1.27968 | 1.097398 | -5.48646 |
| H86 | -0.23974 | 3.002965 | -5.18356 |
| H87 | -1.68844 | 2.832203 | -4.18187 |
| H88 | -2.33044 | 1.131039 | -5.77701 |
| H89 | -0.65535 | 0.976095 | -6.37662 |
| N90 | -0.06213 | 1.607128 | -3.57949 |
| O91 | -1.084 | -0.06732 | -4.64158 |
| O92 | 0.078425 | -0.57131 | -2.78415 |
| H93 | 2.347715 | -4.71606 | 0.71895 |
| N94 | -1.9804 | -2.14594 | 0.126764 |
| C95 | -1.2918 | -3.00803 | -0.86222 |
| H96 | -1.33228 | -2.59979 | -1.88146 |
| C97 | 1.977854 | 4.37744 | -1.83597 |
| H98 | 2.395184 | 5.310049 | -2.2282 |
| H99 | 1.310213 | 4.634868 | -1.01275 |
| H100 | 2.811512 | 3.78615 | -1.43867 |
| C101 | 2.188216 | 3.536146 | -4.18202 |
| H102 | 1.799453 | 2.905834 | -4.98741 |
| H103 | 2.380186 | 4.530503 | -4.59647 |
| H104 | 3.152754 | 3.110031 | -3.88171 |
| H105 | 0.355333 | 4.203061 | -3.21728 |
| H106 | 2.609021 | 0.994144 | -0.01636 |

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