Supporting Information

Experimental and Computational Study of the (*Z*)-Selective Formation of Trisubstituted Olefins and Benzo-Fused Oxacycles from the Ruthenium-Catalyzed Dehydrative C–H Coupling of Phenols with Ketones

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1. General Information

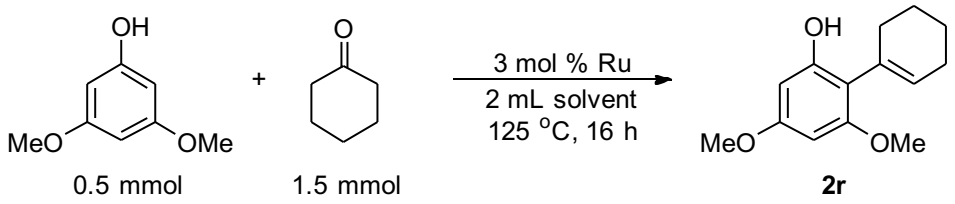
All operations were carried out in a nitrogen-filled glove box or by using standard high vacuum and Schlenk techniques unless otherwise noted. Solvents were freshly distilled over appropriate drying reagents. Benzene, toluene, and hexanes were distilled from purple solutions of sodium and benzophenone, and dichloromethane was dried over calcium hydride prior to use. All organic substrates were received from commercial sources and were used without further purification. Column chromatography was performed on Dynamic Absorbents silica gel 60A (32-63 μm particle size), and thin layer chromatography was performed on Agela glass back TLC plates pre-coated with silica gel MF254. The ^{1}H, ^{2}H, ^{13}C, ^{19}F and ^{31}P NMR spectra were recorded on a Varian 300 or 400 MHz FT-NMR spectrometer, and the data are reported in parts per million (ppm) relative to TMS, with the residual solvent peak as an internal reference. Multiplicities are reported as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad; coupling constant(s) in Hz. Mass spectra were recorded from Agilent 6850 GC-MS spectrometer with a HP-5 (5% phenylmethylpolysiloxane) column (30 m, 0.32 mm, 0.25 μm). High resolution mass spectra (HRMS) were obtained at the Mass Spectrometry/ICP Lab, Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, Milwaukee, WI. Elemental analyses were performed at the Midwest Microlab, Indianapolis, IN.

2. Experimental Procedure

General Procedure for the Catalytic C-H Coupling Reaction of Phenols with Ketones. In a glove box, a phenol (0.5 mmol), a ketone (1.0-1.5 mmol), and complex **1** (9 mg, 3 mol %) were dissolved in 1,2-dichloroethane (2 mL) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and was stirred in an oil bath preset at 125-140 °C for 16-72 h. The reaction tube was taken out of the oil bath, and was cooled to room temperature. After the tube was open to air, the solution was filtered through a short silica gel column by eluting with CH_2Cl_2 (10 mL), and the filtrate was analyzed by GC-MS. Analytically pure product was isolated by column chromatography on silica gel (230-460 mesh, hexanes/EtOAc). The product was completely characterized by NMR and GC-MS spectroscopic methods.

Catalyst Screening. In a glove box, 3,5-dimethoxyphenol (77 mg, 0.5 mmol), cyclohexanone (147 mg, 1.5 mmol), and a catalyst (3 mol % Ru) were dissolved in asolvent (2 mL) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and was stirred in an oil bath at 125 °C for 16 h. The product yield was determined by ^{1}H NMR using methylsulfonylmethane as an internal standard. The results are summarized in Table S1.

Table S1. Catalyst Screening for the Coupling Reaction of 3,5-Dimethoxyphenol with Cyclohexanone[a]



entry	catalyst	solvent	yield[b] (%)
1	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	1,2-DCE	92
2	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	chlorobenzene	72
3	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	toluene	90
4	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	benzene	87
5	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	*n*-hexane	55
6	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	1,4-dioxane	24
7	$[(C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ (**1**)	*t*-amyl alcohol	< 3
8	$[(PCy_3)(CO)RuH]_4(\mu\text{-}O)(\mu\text{-}OH)_2$	1,2-DCE	52
9	$[(PCy_3)(CO)RuH]_4(\mu\text{-}O)(\mu\text{-}OH)_2/HBF_4{\cdot}OEt_2$	1,2-DCE	< 3
10	$[RuCl_2(p\text{-cymene})]_2$	1,2-DCE	14
11	$[Ru(COD)Cl_2]_n$	1,2-DCE	< 3
12	$[(PCy_3)(CH_3CN)(CO)RuH]^+BF_4^-$	1,2-DCE	< 3
13	$RuCl_2(PPh_3)_3$	1,2-DCE	11
14	$RuHCl(CO)(PCy_3)_2$	1,2-DCE	< 3
15	$RuH_2(CO)(PPh_3)_3$	1,2-DCE	18
16	$RuCl_3{\cdot}3H_2O$	1,2-DCE	6
17	$Ru_3(CO)_{12}$	1,2-DCE	15
18	$HBF_4{\cdot}OEt_2$	1,2-DCE	< 3

[a] Reaction conditions: catalyst (3 mol % Ru), phenol (0.5 mmol), cyclohexanone (1.5 mmol), solvent (2 mL), 125 °C, 16 h. [b] The product yield of **2r** was determined by ^{1}H NMR using methylsulfonylmethane as an internal standard.

3. Deuterium Labeling Study. In a glove box, 3,5-dimethoxyphenol (77 mg, 0.5 mmol), cyclohexanone-2,2,6,6-d_4 (93 % D, 1.5 mmol), and complex **1** (3 mol %) were dissolved in 1,2-dichloroethane (2 mL) in a 25 mL Schlenk tube equipped with a Teflon screw cap stopcock and a stirring bar. The tube was brought out of the box, and immersed in an oil bath preset at 125 °C for 16 h. The reaction tube was taken out of the oil bath, and was cooled to room temperature. After the tube was open to air, the solution was filtered through a short silica gel column by eluting with CH_2Cl_2 (10 mL), and the filtrate was analyzed by GC-MS. Analytically pure product was isolated by column chromatography on silica gel (230-460 mesh, hexanes/EtOAc = 100:1 to 10:1), and it was completely characterized by ^{1}H, ^{2}H NMR and GC-MS spectroscopic methods. The ^{1}H and ^{2}H NMR spectra of the product **2r**-*d* are shown in Figure S1.

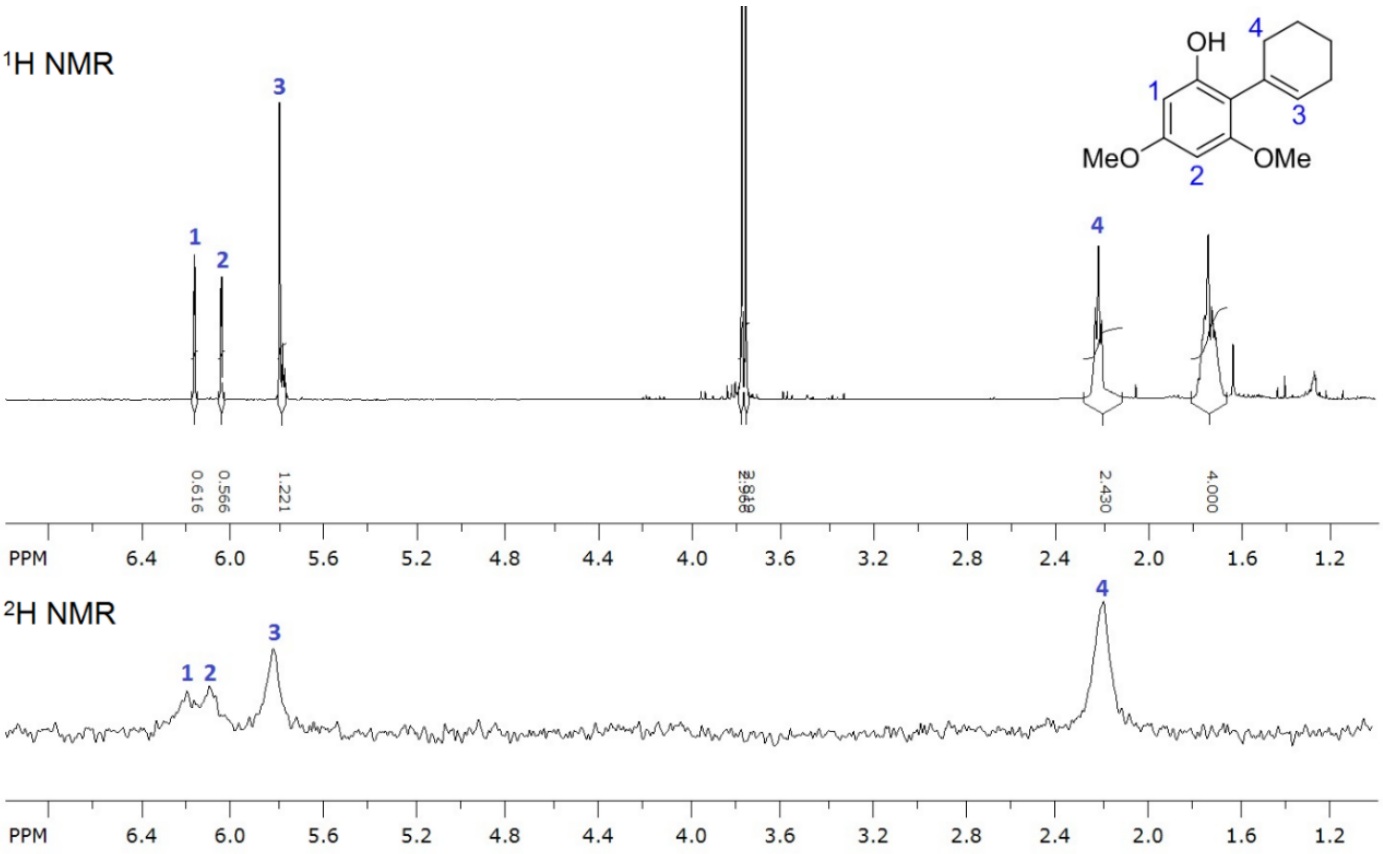
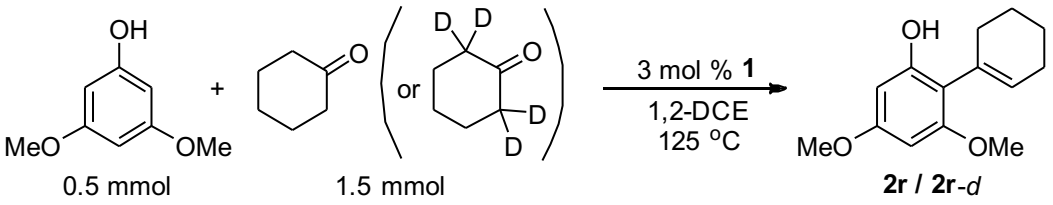


Figure S1. ^{1}H and ^{2}H NMR Spectra of the Product **2r**-*d* Isolated from the Reaction of 3,5-Methoxyphenol with Cyclohexanone-2,2,6,6-d_4.



4. Deuterium Isotope Effect Study. In a glove box, 3,5-methoxyphenol (0.5 mmol), cyclohexanone-2,2,6,6-d_4 (1.5 mmol), and complex **1** (9 mg, 3 mol %) were dissolved in 1,2-dichloroethane (2 mL) in a 25 mL Schlenk tube equipped with a Teflon screw cap stopcock and a magnetic stirring bar. The tube was brought out of the box, and immersed in an oil bath preset at 125 °C. The reaction rate was measured by monitoring the appearance of the product signals on ^{1}H NMR, which were normalized against the internal standard methylsulfonylmethane in 20-60 min intervals for 300 min of the reaction time. The experiment was repeated by using cyclohexanone. The k_{obs} was determined from a first-order plot of -*ln*[(3,5-dimethoxyphenol)$_t$/(3,5-dimethoxyphenol)$_0$] vs time (Figure S2).

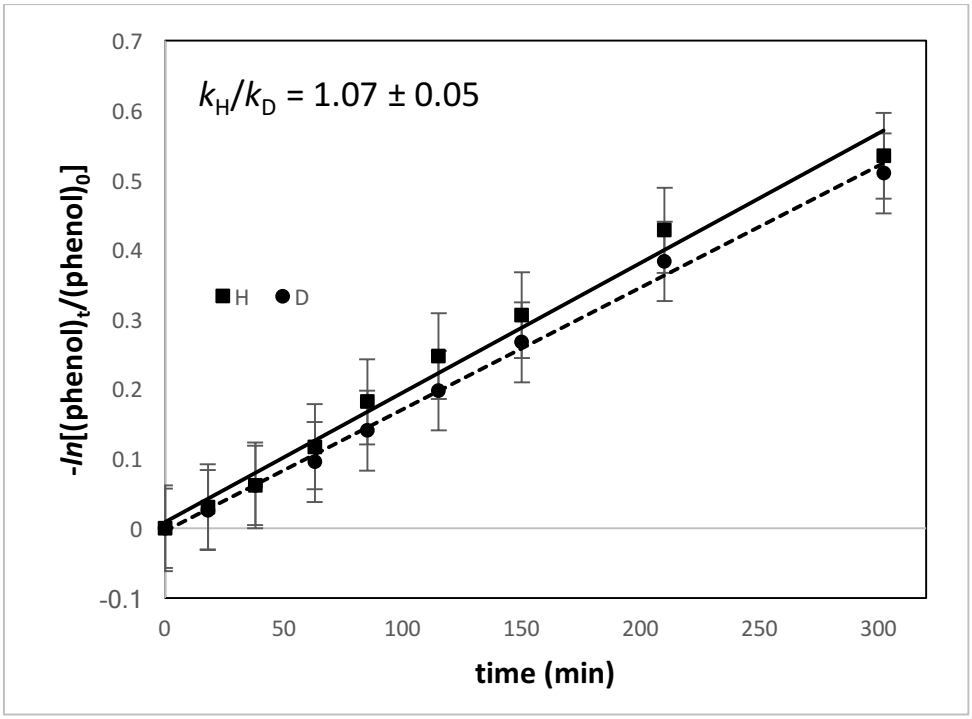


Figure S2. The Pseudo-First Order Plots for the Reaction of 3,5-Dimethoxyphenol with Cyclohexanone and with Cyclohexanone-2,2,6,6-d_4.

5. Carbon Isotope Effect Study. In a glove box, 3,5-dimethoxyphenol (0.5 mmol), propiophenone (1.0 mmol), and complex **1** (9 mg, 3 mol %) were dissolved in 1,2-dichloroethane (2 mL) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and was stirred in an oil bath preset at 125 °C for 16 h (high conversion). After the reaction, conversion was determined by GC-MS and NMR spectroscopy of a small sample of the crude mixture. The analytically pure product (*Z*)-**2a** was isolated by a column chromatography on silica gel. For low conversion samples, the reaction was repeated in three separate Schlenk tubes, each contains 3,5-dimethoxyphenol (1.0 mmol), propiophenone (2.0 mmol), and complex **1** (17 mg, 3 mol %) in 1,2-dichloroethane (3.5 mL). The tubes were stirred in an oil bath at 125 °C for 2 h. After the reaction, tubes were recombined into one reactor, and the conversion of combined sample was determined by GC-MS and NMR spectroscopy. The analytically pure product **2a** was isolated by a column chromatography on silica gel.

The $^{13}C\{^1H\}$ NMR analysis of the isolated product (*Z*)-**2a** was performed by following Singleton's NMR method (ref. 17 in the main text). The sample was prepared identically by dissolving 110 mg of the isolated (*Z*)-**2a** in $CDCl_3$ (0.4 mL) in a 5 mm high precision NMR tube. The $^{13}C\{^1H\}$ NMR spectra were recorded with H-decoupling and 45 degree pulses. A 120 s delay between pulses was imposed to minimize T1 variations (d1 = 120, at = 5.0, nt = 512). The data are summarized in Table S2.

Table S2. Average ^{13}C Intergration of the Product (*Z*)-**2a** at High Conversion (R_0; avg 96 % conversion of two samples), at Low Conversion (R; avg 19 % conversion of three samples), and the Calculated R_0/R.

carbon no.	high conversion, R_0	low conversion, R	R_0/R
1	1.0266	1.0249	1.0016
2	1.0017	0.9829	**1.0191**
3	0.9925	0.9917	1.0008
4 (ref)	1.0000	1.0000	1.0000

6. X-Ray Crystallographic Determination of (*Z*)-2a and 12.

For (*Z*)-**2a**: Colorless prisms of (*Z*)-**2a** were grown in CH_2Cl_2 at room temperature. A suitable crystal with the dimension of 0.51 × 0.5 × 0.45 mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 16395 reflection data were collected by using MoKα (λ = 0.71073) radiation while the crystal sample was cooled at 100.0 K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the

XL refinement package using Least Squares minimization. The molecular structure and crystal data of (*Z*)-**2a** are shown in Figure S3 and Table S3, respectively.

For **12**: Colorless flat needles of **12** were grown in CH_2Cl_2 at room temperature. A suitable crystal with the dimension of 0.58 × 0.24 × 0.10 mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 11890 reflection data were collected by using CuKα (λ = 1.54184) radiation while the crystal sample was cooled at 100.0 K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the XL refinement package using Least Squares minimization. The molecular structure and crystal data of **12** are shown in Figure S4 and Table S4, respectively.

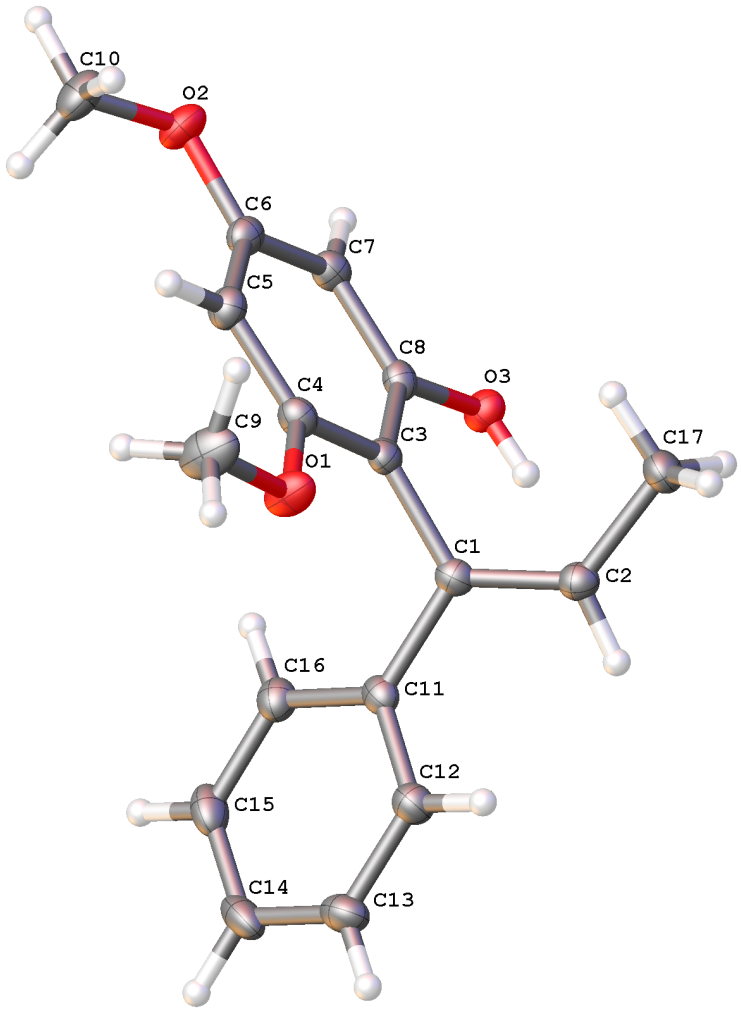


Figure S3. Molecular Structure of (*Z*)-**2a**.

Table S3. Crystal Data and Structure Refinement for (*Z*)-**2a**.

Identification code	yi3j
Empirical formula	$C_{17}H_{18}O_3$
Formula weight	270.31
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.9036(2)
b/Å	9.5634(2)
c/Å	15.2192(4)
α/°	90.00
β/°	93.961(2)
γ/°	90.00
Volume/Å^3	1438.01(6)
Z	4
ϱ_{calc}g/cm^3	1.249
μ/mm^{-1}	0.085
F(000)	576.0
Crystal size/mm^3	0.51 × 0.5 × 0.45
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.62 to 59.1
Index ranges	$-13 \le h \le 13$, $-12 \le k \le 13$, $-20 \le l \le 20$
Reflections collected	16395
Independent reflections	3669 [R_{int} = 0.0346, R_{sigma} = 0.0323]
Data/restraints/parameters	3669/0/185
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0444, wR_2 = 0.1001
Final R indexes [all data]	R_1 = 0.0628, wR_2 = 0.1117
Largest diff. peak/hole / e Å^{-3}	0.31/-0.26

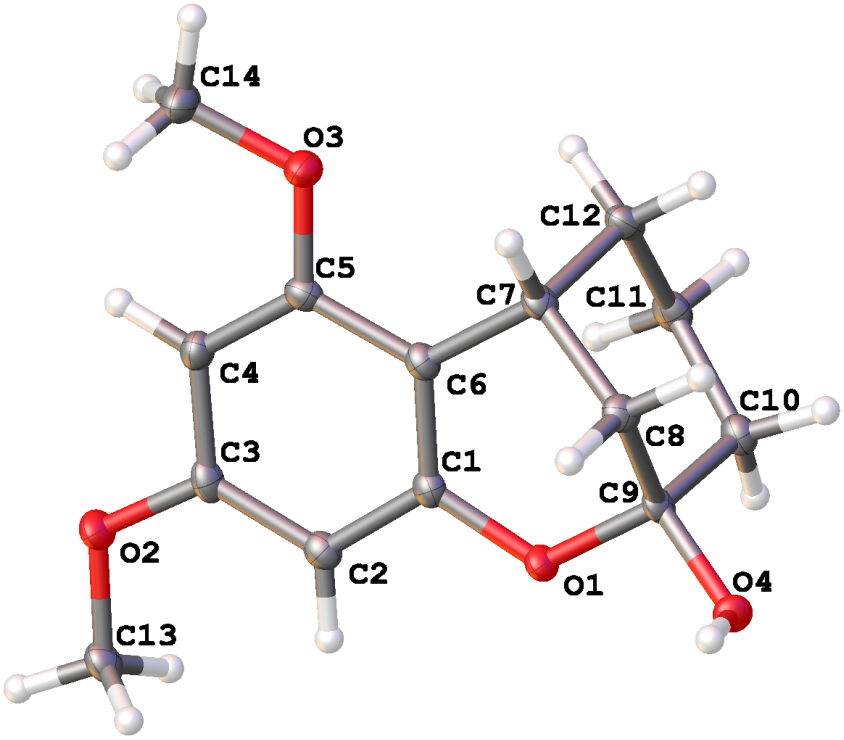
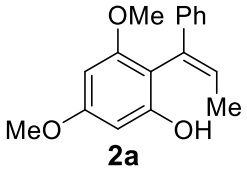


Figure S4. Molecular Structure of **12**.

Table S4. Crystal Data and Structure Refinement for **12**.

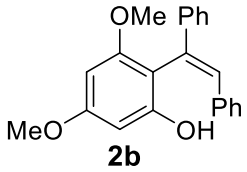
Identification code	yi3i
Empirical formula	$C_{14}H_{18}O_4$
Formula weight	250.28
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.53828(6)
b/Å	24.4737(4)
c/Å	8.98955(14)
α/°	90.00
β/°	91.2110(12)
γ/°	90.00
Volume/Å^3	1218.19(3)
Z	4
ρ_{calc}g/cm^3	1.365
μ/mm^{-1}	0.816
F(000)	536.0
Crystal size/mm^3	0.576 × 0.2375 × 0.1009
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.22 to 147.84
Index ranges	$-6 \le h \le 6$, $-29 \le k \le 29$, $-11 \le l \le 10$
Reflections collected	11890
Independent reflections	4642 [R_{int} = 0.0312, R_{sigma} = 0.0317]
Data/restraints/parameters	4642/1/338
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0372, wR_2 = 0.0971
Final R indexes [all data]	R_1 = 0.0399, wR_2 = 0.1010
Largest diff. peak/hole / e Å^{-3}	0.19/-0.25
Flack parameter	0.0(5)

7. Characterization Data of the Products.



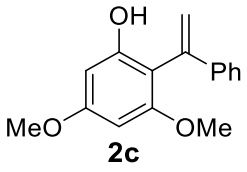
2a

Data for (*Z*)-**2a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.19 (m, 5H), 6.56 (q, *J* = 6.9 Hz, 1H), 6.25 (d, *J* = 2.3 Hz, 1H), 6.15 (d, *J* = 2.3 Hz, 1H), 5.22 (s, 1H), 3.83 (s, 3H), 3.63 (s, 3H), 1.72 (d, *J* = 6.9 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 161.03, 158.51, 154.20, 140.30, 132.97, 128.73, 128.32, 127.14, 125.70, 106.52, 92.27, 91.64, 55.71, 55.27, 15.51 ppm; GC-MS *m/z* = 270 (M^+); HRMS Calcd for $C_{17}H_{18}O_3$ ($[M+H]^+$): 271.1329, Found: 271.1304.



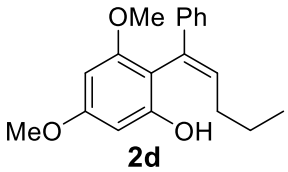
2b

Data for (*Z*)-**2b**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.39 (m, 2H), 7.36-7.27 (m, 4H), 7.24-7.15 (m, 5H), 6.19 (d, *J* = 2.3 Hz, 1H), 6.17 (d, *J* = 2.3 Hz, 1H), 5.27 (s, 1H), 3.83 (s, 3H), 3.57 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 161.35, 158.86, 153.81, 141.47, 136.41, 132.76, 131.47, 128.46, 128.33, 128.26, 127.67, 127.65, 126.05, 107.46, 92.77, 92.07, 55.64, 55.17 ppm; GC-MS *m/z* = 332 (M^+); HRMS Calcd for $C_{22}H_{20}O_3$ ($[M-H]^-$): 331.1340, Found: 331.1343.



2c

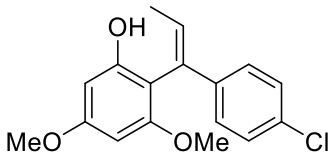
Data for **2c**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.33 (m, 2H), 7.33-7.27 (m, 3H), 6.26 (d, *J* = 2.3 Hz, 1H), 6.12 (d, *J* = 2.3 Hz, 1H), 6.08 (d, *J* = 1.4 Hz, 1H), 5.62 (s, 1H), 5.38 (d, *J* = 1.4 Hz, 1H), 3.83 (s, 3H), 3.59 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 160.97, 158.46, 154.55, 141.38, 139.43, 128.30, 128.06, 126.00, 117.55, 109.12, 92.46, 91.59, 55.70, 55.32 ppm; GC-MS *m/z* = 256 (M^+); HRMS Calcd for $C_{16}H_{16}O_3$ ($[M-H]^-$): 255.1027, Found: 255.1029.



2d

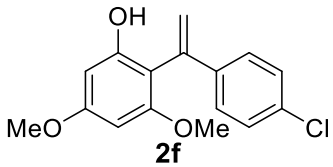
Data for (*Z*)-**2d**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.20 (m, 5H), 6.51 (t, *J* = 7.3 Hz, 1H), 6.26 (d, *J* = 2.3 Hz, 1H), 6.16 (d, *J* = 2.3 Hz, 1H), 5.26 (s, 1H), 3.83 (s, 3H), 3.64 (s, 3H), 2.07-1.99 (m, 2H), 1.49 (sextet, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 160.91, 158.47, 154.09, 140.19,

134.47, 131.75, 128.29, 127.13, 125.75, 106.95, 92.19, 91.52, 55.58, 55.21, 31.95, 22.35, 13.81 ppm; GC-MS *m/z* = 298 (M^+); HRMS Calcd for $C_{19}H_{22}O_3$ ($[M+H]^+$): 299.1642, Found: 299.1631.



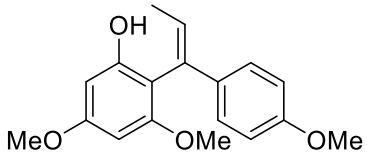
2e

Data for (*Z*)-**2e**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.18 (m, 4H), 6.52 (q, *J* = 6.9 Hz, 1H), 6.23 (d, *J* = 2.3 Hz, 1H), 6.14 (d, *J* = 2.3 Hz, 1H), 5.18 (s, 1H), 3.82 (s, 3H), 3.62 (s, 3H), 1.70 (s, *J* = 6.9 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 161.19, 158.46, 154.16, 138.96, 132.77, 132.13, 129.07, 128.39, 127.00, 106.03, 92.38, 91.70, 55.69, 55.29, 15.53 ppm; GC-MS *m/z* = 304 (M^+); HRMS Calcd for $C_{17}H_{17}O_3Cl$ ($[M+H]^+$): 305.0939, Found: 305.0937.



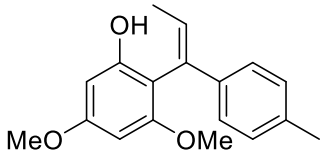
2f

Data for **2f**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.23 (m, 4H), 6.24 (d, *J* = 2.3 Hz, 1H), 6.09 (d, *J* = 2.3 Hz, 1H), 6.03 (d, *J* = 1.3 Hz, 1H), 5.58 (s, 1H), 5.37 (d, *J* = 1.3 Hz, 1H), 3.82 (s, 3H), 3.58 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 161.15, 158.39, 154.54, 140.51, 138.10, 133.82, 128.43, 127.35, 117.79, 108.59, 92.54, 91.61, 55.68, 55.35 ppm; GC-MS *m/z* = 290 (M^+); HRMS Calcd for $C_{16}H_{15}O_3Cl$ ($[M-H]^-$): 289.0637, Found: 289.0642.



2g

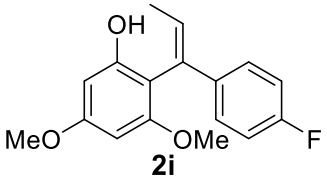
Data for (*Z*)-**2g**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.20 (m, 2H), 6.82-6.78 (m, 2H), 6.45 (q, *J* = 6.8 Hz, 1H), 6.24 (d, *J* = 2.3 Hz, 1H), 6.15 (d, *J* = 2.3 Hz, 1H), 5.25 (s, 1H), 3.82 (s, 3H), 3.78 (s, 3H), 3.65 (s, 3H), 1.68 (d, *J* = 6.8 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 160.94, 158.86, 158.47, 154.16, 132.82, 132.25, 126.80, 126.64, 113.67, 106.69, 92.27, 91.60, 55.72, 55.25, 55.15, 15.38 ppm; GC-MS *m/z* = 300 (M^+); HRMS Calcd for $C_{18}H_{20}O_4$ ($[M-H]^-$): 299.1289, Found: 299.1294.



2h

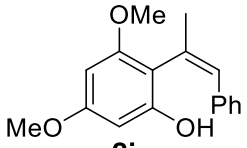
Data for (*Z*)-**2h**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.17 (m, 2H), 7.10-7.06 (m, 2H), 6.53 (q, *J* = 6.9 Hz, 1H), 6.25 (d, *J* = 2.3 Hz, 1H), 6.16 (d, *J* = 2.3 Hz, 1H), 5.23 (s, 1H), 3.83 (s, 3H), 3.65 (s, 3H), 2.33 (s, 3H), 1.71 (d,

J = 6.9 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 160.93, 158.48, 154.16, 137.36, 136.87, 132.70, 129.04, 127.72, 125.54, 106.63, 92.21, 91.59, 55.71, 55.25, 21.02, 15.42 ppm; GC-MS *m/z* = 284 (M^+); HRMS Calcd for $C_{18}H_{20}O_3$ ($[M+H]^+$): 285.1485, Found: 285.1478.



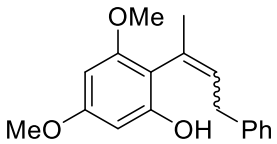
2i

Data for (*Z*)-**2i**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.21 (m, 2H), 6.98-6.91 (m, 2H), 6.47 (q, *J* = 6.8 Hz, 1H), 6.23 (d, *J* = 2.3 Hz, 1H), 6.14 (d, *J* = 2.3 Hz, 1H), 5.18 (s, 1H), 3.82 (s, 3H), 3.63 (s, 3H), 1.69 (d, *J* = 6.8 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 163.36, 161.16, 160.92, 158.47, 154.14, 136.54, 136.50, 132.13, 128.39, 128.38, 127.32, 127.24, 115.22, 115.00, 106.35, 92.35, 91.72, 55.72, 55.31, 15.49 ppm; GC-MS *m/z* = 288 (M^+); HRMS Calcd for $C_{17}H_{17}O_3F$ ($[M+H]^+$): 289.1234, Found: 289.1228.



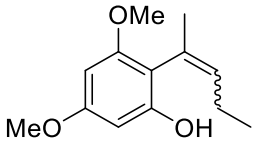
2j

Data for (*Z*)-**2j**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18-7.10 (m, 3H), 7.10-7.05 (m, 2H), 6.76-6.74 (m, 1H), 6.17 (d, *J* = 2.3 Hz, 1H), 6.09 (d, *J* = 2.3 Hz, 1H), 5.27 (s, 1H), 3.82 (s, 3H), 3.79 (s, 3H), 2.14 (d, *J* = 1.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 160.78, 158.28, 152.14, 136.23, 131.22, 130.74, 128.28, 127.80, 127.21, 109.06, 92.67, 91.75, 55.71, 55.28, 25.41 ppm; GC-MS *m/z* = 270 (M^+); HRMS Calcd for $C_{17}H_{18}O_3$ ($[M-H]^-$): 269.1183, Found: 269.1186.



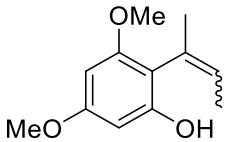
2k

Data for (*Z*)-**2k**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.14 (m, 5H), 6.23 (d, *J* = 2.3 Hz, 1H), 6.15 (d, *J* = 2.3 Hz, 1H), 5.98 (ddq, *J* = 7.9, 6.8, 1.4 Hz, 1H), 5.33 (s, 1H), 3.82 (s, 3H), 3.81 (s, 3H), 3.25 (dd, *J* = 15.1, 7.9 Hz, 1H), 3.15 (dd, *J* = 15.1, 6.8 Hz, 1H), 2.00 (d, *J* = 1.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 160.56, 158.04, 152.98, 140.35, 131.38, 129.60, 128.38, 128.36, 125.89, 108.25, 92.13, 91.42, 55.47, 55.26, 35.63, 23.59 ppm. Data for (*E*)-**2k**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.14 (m, 5H), 6.18 (d, *J* = 2.3 Hz, 1H), 6.10 (d, *J* = 2.3 Hz, 1H), 5.74 (tq, *J* = 7.4, 1.4 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.62 (d, *J* = 7.4 Hz, 2H), 2.06 (d, *J* = 1.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 160.09, 158.09, 153.28, 140.46, 131.24, 130.82, 128.65, 128.16, 126.09, 112.37, 92.21, 91.21, 55.54, 55.25, 34.50, 17.42 ppm; GC-MS *m/z* = 284 (M^+); HRMS Calcd for $C_{18}H_{20}O_3$ ($[M+H]^+$): 285.1485, Found: 285.1458.



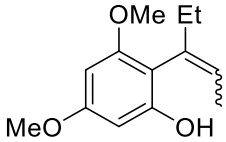
2l

Data for (*Z*)-**2l**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.09 (d, *J* = 2.3 Hz, 1H), 5.79 (tq, *J* = 7.2, 1.4 Hz, 1H), 5.34 (s, 1H), 3.78 (s, 3H), 3.77 (s, 3H), 1.94-1.93 (m, 3H), 1.88-1.79 (m, 2H), 0.92 (t, *J* = 7.5 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.36, 157.96, 152.83, 134.55, 128.11, 108.58, 91.95, 91.34, 55.55, 55.23, 23.46, 22.57, 13.91 ppm. Data for (*E*)-**2l**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.06 (d, *J* = 2.3 Hz, 1H), 5.81 (s, 1H), 5.49 (tq, *J* = 7.0, 1.4 Hz, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 2.29-2.21 (m, 2H), 1.90-1.89 (m, 3H), 1.07 (t, *J* = 7.5 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.96, 158.08, 153.25, 134.52, 129.39, 112.62, 92.12, 91.18, 55.53, 55.25, 21.51, 17.12, 14.09 ppm; GC-MS *m/z* = 222 (M^+); HRMS Calcd for $C_{13}H_{18}O_3$ ([M+H]$^+$): 223.1329, Found: 223.1323.



2m

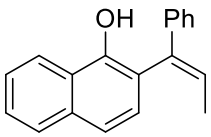
Data for (*Z*)-**2m**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.18 (d, *J* = 2.3 Hz, 1H), 6.10 (d, *J* = 2.3 Hz, 1H), 5.87 (qq, *J* = 6.7, 1.5 Hz, 1H), 5.37 (s, 1H), 3.79 (s, 3H), 3.77 (s, 3H), 1.95 (quintet, *J* = 1.5 Hz, 3H), 1.50 (dq, *J* = 6.7, 1.5 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.40, 157.96, 152.83, 129.89, 126.84, 108.16, 91.96, 91.33, 55.56, 55.20, 23.38, 14.60 ppm. Data for (*E*)-**2m**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.06 (d, *J* = 2.3 Hz, 1H), 5.78 (s, 1H), 5.57 (qq, *J* = 6.7, 1.5 Hz, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 1.91-1.89 (m, 3H), 1.84-1.81 (m, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.94, 158.00, 153.30, 130.79, 126.75, 112.68, 92.09, 91.09, 55.49, 55.20, 16.96, 13.86 ppm; GC-MS *m/z* = 208 (M^+); HRMS Calcd for $C_{12}H_{16}O_3$ ([M+H]$^+$): 209.1172, Found: 209.1171.



2n

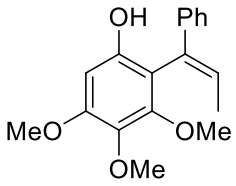
Data for (*Z*)-**2n**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.18 (d, *J* = 2.3 Hz, 1H), 6.10 (d, *J* = 2.3 Hz, 1H), 5.87 (qt, *J* = 6.7, 1,4 Hz, 1H), 5.33 (s, 1H), 3.79 (s, 3H), 3.75 (s, 3H), 2.36-2.27 (m, 2H), 1.51 (dt, *J* = 6.7, 1.3 Hz, 3H), 0.95 (t, *J* = 7.5 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.41, 157.94, 153.46, 136.13, 125.19, 107.25, 91.87, 91.31, 55.51, 55.17, 30.13, 14.43, 12.87 ppm. Data for (*E*)-**2n**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.05 (d, *J* = 2.3 Hz, 1H), 5.73 (s, 1H), 5.53 (q, *J* = 6.7 Hz, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 2.36-2.27 (m, 2H), 1.83 (d, *J* = 6.7 Hz, 3H), 0.88 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ

160.00, 157.98, 154.17, 137.28, 126.20, 111.05, 92.00, 91.02, 55.44, 55.17, 23.76, 13.51, 12.82 ppm; GC-MS *m/z* = 222 (M^+); HRMS Calcd for $C_{13}H_{18}O_3$ ($[M+H]^+$): 223.1329, Found: 223.1327.



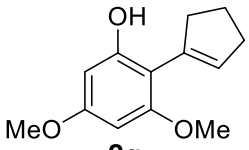
2o

Data for (*Z*)-**2o**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32-8.26 (m, 1H), 7.85-7.80 (m, 1H), 7.55-7.49 (m, 2H), 7.44 (d, *J* = 8.4 Hz, 1H), 7.30-7.24 (m, 5H), 7.10 (d, *J* = 8.4 Hz, 1H), 6.57 (q, *J* = 7.0 Hz, 1H), 5.62 (s, 1H), 1.77 (d, *J* = 7.0 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 148.21, 140.51, 136.93, 134.22, 128.50, 127.80, 127.75, 127.56, 127.47, 126.74, 126.39, 125.32, 123.96, 122.48, 120.04, 118.37, 15.70 ppm; GC-MS *m/z* = 260 (M^+); HRMS Calcd for $C_{19}H_{16}O$ ($[M-H]^-$): 259.1128, Found: 259.1125.



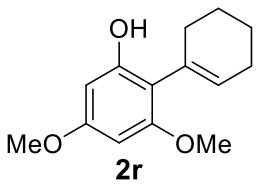
2p

Data for (*Z*)-**2p**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.20 (m, 5H), 6.50 (q, *J* = 6.9 Hz, 1H), 6.40 (s, 1H), 5.10 (s, 1H), 3.87 (s, 3H), 3.79 (s, 3H), 3.49 (s, 3H), 1.74 (d, *J* = 6.9 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 153.77, 151.46, 148.90, 140.92, 136.03, 133.60, 128.47, 128.34, 127.29, 125.96, 111.27, 94.59, 60.97, 60.50, 55.80, 15.66 ppm; GC-MS *m/z* = 300 (M^+); HRMS Calcd for $C_{18}H_{20}O_4$ ($[M-H]^-$): 299.1289, Found: 299.1294.



2q

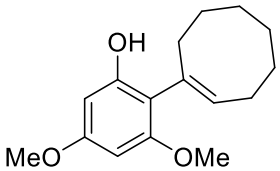
Data for **2q**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.18 (d, *J* = 2.4 Hz, 1H), 6.05 (d, *J* = 2.4 Hz, 1H), 5.86 (s, 1H), 5.85-5.82 (m, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 2.67-2.60 (m, 2H), 2.58-2.52 (m, 2H), 2.05-1.96 (m, 2H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 160.36, 158.53, 153.85, 138.58, 130.73, 106.14, 92.20, 91.18, 55.52, 55.29, 35.80, 32.92, 23.44 ppm; GC-MS *m/z* = 220 (M^+); HRMS Calcd for $C_{13}H_{16}O_3$ ($[M+H]^+$): 221.1172, Found: 221.1162.



2r

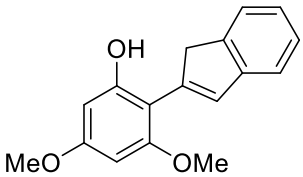
Data for **2r**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.05 (d, *J* = 2.3 Hz, 1H), 5.79 (s, 1H), 5.79-5.76 (m, 1H), 3.77 (s, 3H), 3.76 (s, 3H), 2.26-2.18 (m, 4H), 1.78-1.67 (m, 4H) ppm; $^{13}C\{^1H\}$ NMR (100

MHz, $CDCl_3$) δ 160.06, 158.13, 153.43, 133.09, 129.31, 111.50, 92.10, 91.18, 55.59, 55.28, 28.81, 25.50, 22.86, 22.02 ppm; GC-MS *m/z* = 234 (M^+); HRMS Calcd for $C_{14}H_{18}O_3$ ($[M+H]^+$): 235.1329, Found: 235.1311.



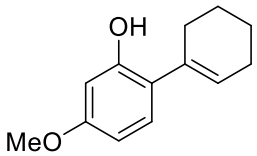
2s

Data for **2s**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.16 (d, *J* = 2.3 Hz, 1H), 6.06 (d, *J* = 2.3 Hz, 1H), 5.84 (s, 1H), 5.73 (t, *J* = 8.1 Hz, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 2.48-2.41 (m, 2H), 2.37-2.29 (m, 2H), 1.70-1.48 (m, 8H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.95, 158.06, 153.86, 136.28, 132.17, 112.18, 92.10, 91.21, 55.44, 55.27, 30.76, 29.66, 28.86, 26.88, 26.70, 26.52 ppm; GC-MS *m/z* = 262 (M^+); HRMS Calcd for $C_{16}H_{22}O_3$ ($[M+H]^+$): 263.1642, Found: 263.1631.



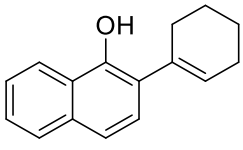
2t

Data for **2t**: ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.26 (t, *J* = 7.4 Hz, 1H), 6.98 (s, 1H), 6.28 (d, *J* = 2.4 Hz, 1H), 6.17 (d, *J* = 2.4 Hz, 1H), 5.90 (s, 1H), 3.88 (s, 2H), 3.84 (s, 3H), 3.80 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 160.79, 158.54, 154.38, 144.24, 144.10, 141.34, 130.93, 126.26, 124.80, 123.46, 120.89, 105.47, 92.62, 91.38, 55.48, 55.30, 42.20 ppm; GC-MS *m/z* = 268 (M^+); HRMS Calcd for $C_{17}H_{16}O_3$ ($[M-H]^-$): 267.1027, Found: 267.1028.



2u

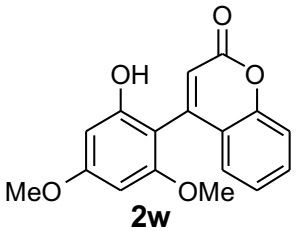
Data for **2u**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.99 (d, *J* = 8.4 Hz, 1H), 6.51 (d, *J* = 2.5 Hz, 1H), 6.46 (dd, *J* = 8.4, 2.5 Hz, 1H), 5.85-5.81 (m, 1H), 5.79 (s, 1H), 3.78 (s, 3H), 2.28-2.17 (m, 4H), 1.82-1.65 (m, 4H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.46, 152.98, 134.64, 128.44, 127.43, 122.37, 106.17, 100.55, 55.22, 29.96, 25.40, 22.96, 21.86 ppm; GC-MS *m/z* = 204 (M^+); HRMS Calcd for $C_{13}H_{16}O_2$ ($[M-H]^-$): 203.1078, Found: 203.1065..



2v

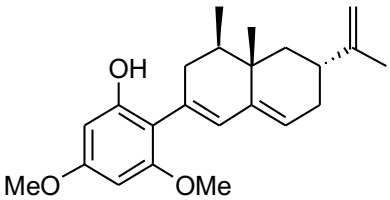
Data for **2v**: ^1H NMR (400 MHz, $CDCl_3$) δ 8.26-8.22 (m, 1H), 7.79-7.74 (m, 1H), 7.50-7.43 (m, 2H), 7.38 (d, *J* = 8.5 Hz, 1H), 7.21 (d, *J* = 8.5 Hz, 1H), 6.30 (s, 1H), 6.01-5.98 (m, 1H), 2.37-2.24 (m, 4H), 1.88-1.72 (m, 4H)

ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 147.08, 135.33, 133.45, 128.39, 127.33, 126.03, 125.53, 125.23, 123.98, 122.90, 122.53, 119.37, 29.82, 25.49, 23.00, 21.96 ppm; GC-MS *m/z* = 224 (M^+); HRMS Calcd for $C_{16}H_{16}O$ ([M-H]$^-$): 223.1128, Found: 223.1110.



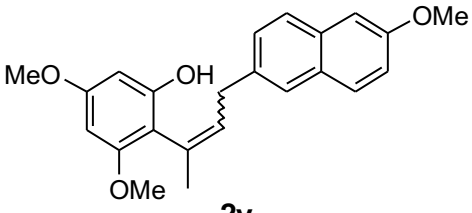
2w

Data for **2w**: ^1H NMR (400 MHz, DMSO-d_6) δ 9.75 (s, 1H), 7.59 (ddd, *J* = 8.3, 7.3, 1.6 Hz, 1H), 7.43 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.25 (ddd, *J* = 7.9, 7.3, 1.2 Hz, 1H), 7.12 (dd, *J* = 7.9, 1.6 Hz, 1H), 6.27 (s, 1H), 6.24 (d, *J* = 2.2 Hz, 1H), 6.21 (d, *J* = 2.2 Hz, 1H), 3.78 (s, 3H), 3.64 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6) δ 161.67, 160.09, 158.19, 156.06, 153.20, 150.70, 131.73, 126.91, 124.27, 119.70, 117.31, 116.48, 103.04, 93.91, 90.15, 55.70, 55.21 ppm; GC-MS *m/z* = 298 (M^+); HRMS Calcd for $C_{17}H_{14}O_5$ ([M+H]$^-$): 297.0768, Found: 297.0777.



2x

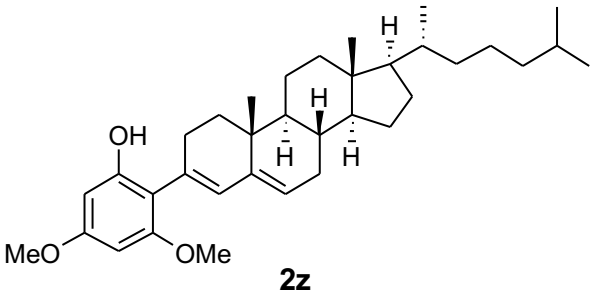
Data for **2x**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.06 (d, *J* = 2.3 Hz, 1H), 6.03 (br s, 1H), 5.65 (s, 1H), 5.55-5.51 (m, 1H), 4.79-4.75 (m, 2H), 3.78 (s, 3H), 3.75 (s, 3H), 2.53-2.44 (m, 1H), 2.33-2.14 (m, 3H), 2.06-1.95 (m, 1H), 1.83-1.66 (m, 2H), 1.78 (s, 3H), 1.24 (t, *J* = 12.7 Hz, 1H), 1.02 (s, 3H), 0.93 (d, *J* = 6.8 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 160.23, 158.44, 153.50, 150.08, 141.45, 130.88, 130.16, 124.81, 110.58, 108.74, 92.19, 91.28, 55.63, 55.29, 39.96, 38.99, 37.21, 35.73, 35.56, 31.21, 20.67, 17.65, 14.57 ppm; GC-MS *m/z* = 354 (M^+); HRMS Calcd for $C_{23}H_{30}O_3$ ([M+H]$^+$): 355.2268, Found: 355.2237.



2y

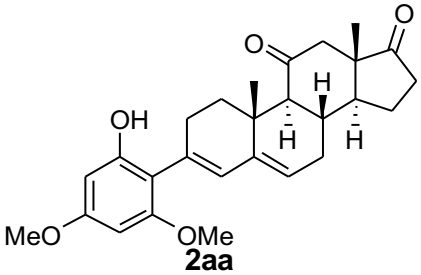
Data for (*Z*)-**2y**: ^1H NMR (400 MHz, $CDCl_3$) δ 7.74-7.63 (m, 2H), 7.52 (s, 1H), 7.27-7.23 (m, 1H), 7.18-7.10 (m, 2H), 6.25 (d, *J* = 2.3 Hz, 1H), 6.16 (d, *J* = 2.3 Hz, 1H), 6.07-6.02 (m, 1H), 5.38 (s, 1H), 3.92 (s, 3H), 3.82 (s, 3H), 3.82 (s, 3H), 3.36 (dd, *J* = 15.1, 8.0 Hz, 1H), 3.26 (dd, *J* = 15.1, 6.7 Hz, 1H), 2.02 (d, *J* = 1.3 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 160.59, 158.07, 157.09, 153.03, 135.50, 132.97, 131.41, 129.70, 129.04, 128.89, 127.75, 126.77, 126.23, 118.60, 108.32, 105.51, 92.17, 91.43, 55.49, 55.28, 55.19, 35.54, 23.64

ppm. Data for (*E*)-**2y**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.63 (m, 3H), 7.37 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.18-7.10 (m, 2H), 6.18 (d, *J* = 2.3 Hz, 1H), 6.10 (d, *J* = 2.3 Hz, 1H), 5.84-5.78 (m, 1H), 5.74 (s, 1H), 3.93 (s, 3H), 3.82 (s, 3H), 3.79 (s, 3H), 3.73 (d, *J* = 7.4 Hz, 2H), 2.10-2.08 (m, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.11, 158.11, 157.21, 153.31, 133.05, 131.29, 130.93, 129.11, 127.35, 127.18, 126.13, 118.80, 112.42, 105.56, 92.23, 91.22, 55.57, 55.26, 55.22, 34.43, 17.49 ppm (two carbon signals obscured or overlapping); GC-MS *m/z* = 364 (M^+); HRMS Calcd for $C_{23}H_{24}O_4$ ([M+H]$^+$): 365.1747, Found: 365.1741.



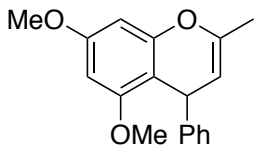
2z

Data for **2z**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (d, *J* = 2.3 Hz, 1H), 6.05 (d, *J* = 2.3 Hz, 1H), 5.99 (br s, 1H), 5.66 (s, 1H), 5.50-5.46 (m, 1H), 3.78 (s, 3H), 3.74 (s, 3H), 2.46-2.14 (m, 2H), 208-2.01 (m, 1H), 1.93-1.79 (m, 2H), 1.75-1.25 (m, 12H), 1.24-0.97 (m, 9H), 1.05 (s, 3H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.87 (d, *J* = 6.6 Hz, 6H), 0.72 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 160.23, 158.53, 153.58, 140.96, 130.55, 130.07, 125.39, 110.87, 92.21, 91.32, 56.93, 56.11, 55.65, 55.32, 48.26, 42.46, 39.76, 39.50, 36.17, 35.78, 34.68, 34.07, 31.92, 31.80, 28.23, 28.01, 26.58, 24.17, 23.80, 22.82, 22.56, 21.06, 19.18, 18.70, 12.00 ppm; GC-MS *m/z* = 520 (M^+); HRMS Calcd for $C_{35}H_{52}O_3$ ([M+H]$^+$): 521.3989, Found: 521.3950.



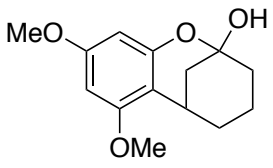
2aa

Data for **2aa**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.15 (d, *J* = 2.3 Hz, 1H), 6.04 (d, *J* = 2.3 Hz, 1H), 5.96 (br s, 1H), 5.61 (s, 1H), 5.47-5.42 (m, 1H), 3.76 (s, 3H), 3.73 (s, 3H), 2.68-2.42 (m, 5H), 2.38-1.89 (m, 8H), 1.76-1.64 (m, 1H), 1.31-1.22 (m, 1H), 1.25 (s, 3H), 0.88 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 217.55, 208.76, 160.37, 158.49, 153.46, 141.57, 132.20, 129.45, 122.41, 110.49, 92.29, 91.34, 59.34, 55.66, 55.33, 50.50, 50.48, 50.22, 36.16, 34.96, 33.05, 32.63, 31.50, 26.47, 21.70, 18.76, 14.74 ppm; GC-MS *m/z* = 436 (M^+); HRMS Calcd for $C_{27}H_{32}O_5$ ([M+H]$^+$): 437.2323, Found: 437.2309.



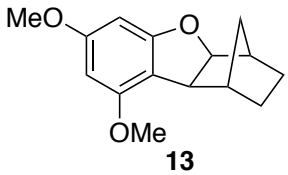
11

Data for **11**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.23 (m, 4H), 7.21-7.17 (m, 1H), 6.24 (d, *J* = 2.4 Hz, 1H), 6.14 (d, *J* = 2.4 Hz, 1H), 4.90 (d, *J* = 4.8 Hz, 1H), 4.63 (d, *J* = 4.8 Hz, 1H), 3.81 (s, 3H), 3.61 (s, 3H), 1.97 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.62, 158.26, 152.70, 147.35, 146.20, 127.99, 127.62, 125.73, 105.10, 101.79, 93.88, 92.61, 55.33, 55.22, 36.27, 19.12 ppm; GC-MS *m/z* = 282 (M^+); HRMS Calcd for $C_{18}H_{18}O_3$ ($[M+H]^+$): 283.1329, Found: 283.1349.



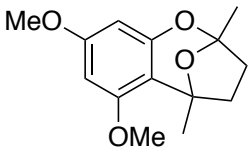
12

Data for **12**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.02 (d, *J* = 2.3 Hz, 1H), 6.00 (d, *J* = 2.3 Hz, 1H), 3.74 (s, 3H), 3.72 (s, 3H), 3.71-3.68 (br s, 1H), 3.43-3.38 (m, 1H), 2.09-2.01 (m, 1H), 1.96 (dd, *J* = 12.4, 2.9 Hz, 1H), 1.87-1.80 (m, 1H), 1.77-1.63 (m, 2H), 1.59-1.45 (m, 2H), 1.44-1.29 (m, 1H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.43, 156.90, 156.67, 106.08, 98.64, 92.12, 90.74, 55.24, 55.10, 38.69, 36.36, 29.51, 28.10, 19.13 ppm; GC-MS *m/z* = 250 (M^+); HRMS Calcd for $C_{14}H_{18}O_4$ ($[M+H]^+$): 251.1278, Found: 251.1271.



13

Data for **13**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.06 (d, *J* = 2.0 Hz, 1H), 6.03 (d, *J* = 2.0 Hz, 1H), 4.43-4.39 (m, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 2.38-2.25 (m, 2H), 1.93-1.90 (m, 2H), 1.81-1.69 (m, 1H), 1.60-1.54 (m, 1H), 1.48-1.41 (m, 1H), 1.35-1.24 (m, 2H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.84, 161.49, 157.40, 109.13, 94.09, 91.25, 89.24, 56.53, 55.44, 55.20, 41.83, 38.96, 37.49, 27.85, 27.37 ppm; GC-MS *m/z* = 246 (M^+); HRMS Calcd for $C_{15}H_{18}O_3$ ($[M+H]^+$): 247.1329, Found: 247.1328.



14

Data for **14**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.00 (d, *J* = 2.4 Hz, 1H), 5.96 (d, *J* = 2.4 Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 2.35-2.21 (m, 2H), 2.10-2.01 (m, 1H), 1.95-1.85 (m, 1H), 1.81 (s, 3H), 1.67 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.91, 156.62, 153.24, 110.33, 106.81, 93.10, 91.51, 83.21, 55.14, 55.05, 42.74, 38.37, 24.10, 23.10 ppm; GC-MS *m/z* = 250 (M^+); HRMS Calcd for $C_{14}H_{18}O_4$ ($[M+H]^+$): 251.1278, Found: 251.1274.

8. Computational Study

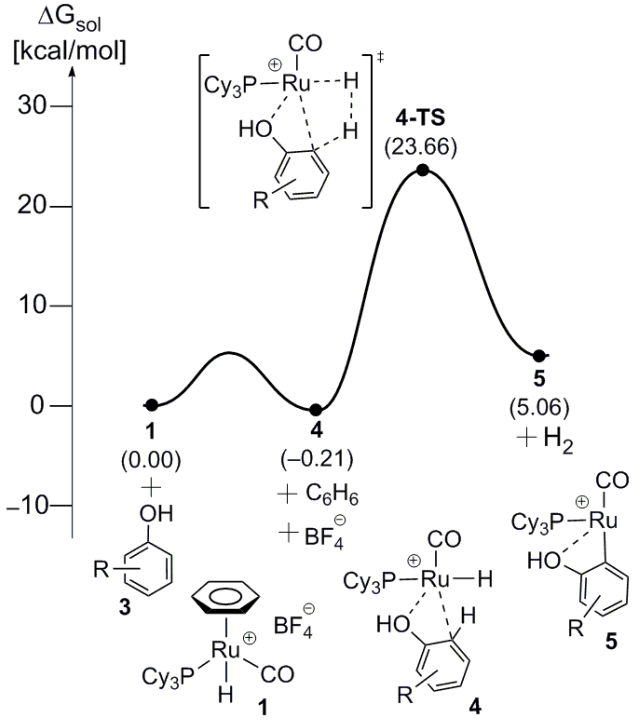


Figure S5: The free energy profile for the formation of the active catalyst **5**.

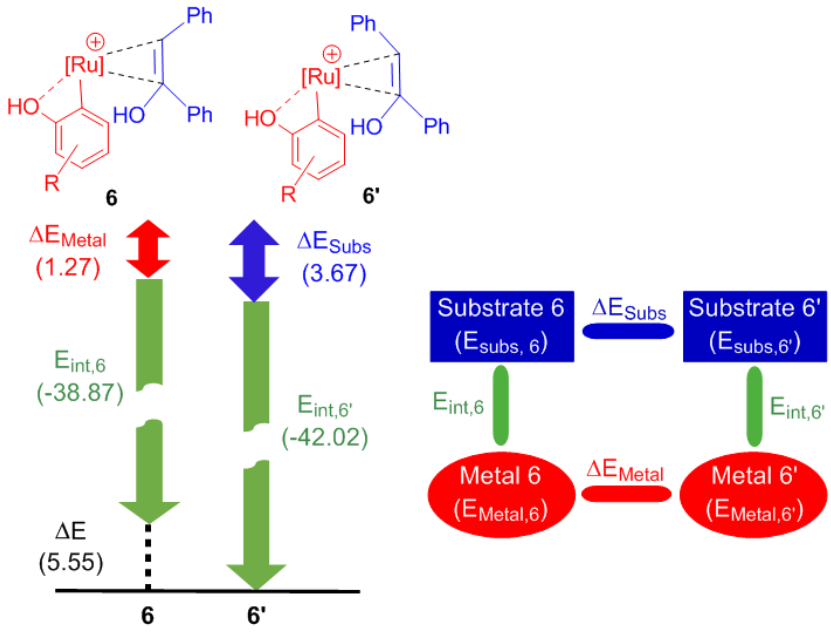


Figure S6. Graph of interaction energies for intermediates **6** and **6′**. The energy for structural changes and the metal-substrate interactions are indicated by bidirectional and unidirectional arrows, respectively. Dotted lines represent the difference between the two intermediates. Red, metal fragment; blue, substrate fragment; green, the interaction between the two fragments.

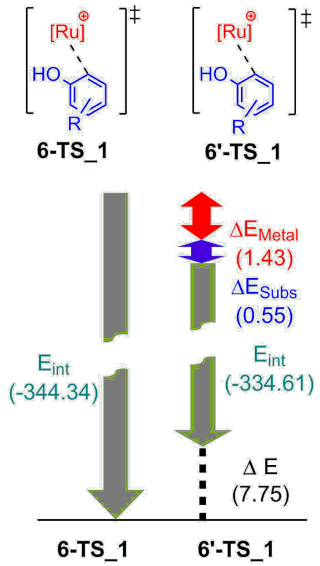


Figure S7. The metal fragment interaction energies for the transition states **6-TS** and **6′-TS**.

Table S5. Computed Energy Components for Optimized Structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol)	G(solv)/(kcal/mol)
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
1	-52039.055	392.05	212.940	-17.98
3	-14604.767	106.75	99.934	-10.05
4	-48761.843	424.46	214.865	-37.87
4-TS	-48760.581	420.48	222.168	-36.95
5	-48728.556	412.42	214.092	-45.06
5-TS	-65495.831	551.48	270.990	-36.46
6	-65496.025	551.68	277.161	-36.15
6-TS	-65494.840	551.04	272.598	-39.61
7	-65494.990	552.20	270.607	-42.42
7-TS	-65494.950	552.31	272.755	-40.46
8	-65495.937	553.54	269.539	-38.52
8-TS	-65495.023	551.64	272.955	-39.76
9	-65496.218	552.15	270.304	-36.15
10	-50809.714	428.95	219.086	-43.23
10-TS	-50808.783	426.17	221.519	-46.14
2b	-29290.580	229.49	161.172	-12.51

10	-80101.353	661.87	318.343	-38.54
10-TS	-80100.176	657.30	323.358	-40.35
11	-80101.704	660.48	323.718	-39.02
5'-TS	-65495.824	550.74	276.236	-39.08
6'	-65496.266	552.14	274.352	-39.07
6'-TS	-65494.663	550.65	273.63	-39.83
7'	-65495.014	552.13	268.896	-40.72
7'-TS	-65494.790	551.13	278.866	-38.66
8'	-65495.798	552.94	269.528	-39.89
8'-TS	-65495.121	551.53	269.548	-40.40
9'	-65495.976	552.94	269.528	-39.89
2b'	-29290.455	229.30	161.902	-12.87
10'	-80101.110	659.96	319.601	-39.99
10'-TS	-80099.894	656.64	323.603	-42.79
11'	-80101.498	659.68	328.522	-42.79
Ketone	-16766.273	137.22	107.198	-7.12
Z-enol	-16766.198	138.24	110.374	-7.77
E-enol	-16766.092	138.12	110.229	-7.69

Table S6. Cartesian Coordinates of the Optimized Geometries.

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1

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Ru	4.332017714	4.068157256	11.718217029
H	2.831323655	4.316104266	11.328771999
P	4.411073498	6.403507685	11.724025871
O	4.794142871	4.188450767	8.744302552
C	5.645699220	2.043607433	12.235727223
C	6.176562687	2.984169040	13.146651284
H	7.237083445	3.211355329	13.120013241
C	5.299780035	3.679575605	13.999256073
H	5.695150926	4.444966195	14.658622071
C	3.910379950	3.396879819	14.006556701
H	3.242677706	3.934974301	14.669741329
C	3.399973301	2.395929477	13.146214801
H	2.339346269	2.169189730	13.148304937
C	4.264673139	1.722987767	12.254102414
H	3.868043942	0.979436730	11.571653914
C	4.654193196	4.145304361	9.889963486
C	6.127997027	7.138255686	11.567459960
H	6.008229509	8.203219283	11.811513107
C	6.712756900	7.039605361	10.140665015
H	6.049443929	7.516661304	9.409939947
H	6.825764143	5.986380159	9.871611181

C	8.093779930	7.718725787	10.085652412
H	8.494440561	7.632728659	9.068819522
H	7.976136575	8.794542851	10.290249128
C	9.068583189	7.099417116	11.096756658
H	10.027425899	7.631553180	11.067178802
H	9.272385541	6.060698817	10.819362565
C	8.491099377	7.145264904	12.519619202
H	8.432028408	8.189410911	12.863955191
H	9.154600833	6.609949151	13.206902065
C	7.096424146	6.500138472	12.584352953
H	7.210863332	5.444808362	12.340409220
H	6.697728511	6.578304267	13.605648003
C	3.783816995	6.984828574	13.400293041
H	4.287233288	6.281391733	14.075559643
C	4.182401576	8.400678101	13.869188722
H	5.262516759	8.550300154	13.782038394
H	3.702491354	9.156891815	13.238002845
C	3.753717767	8.609087236	15.334142757
H	4.323106538	7.917544570	15.972259452
H	4.021240912	9.622034724	15.656563306
C	2.250816736	8.361459623	15.534227706
H	1.982753488	8.479514723	16.590580932
H	1.682875292	9.121275854	14.978361493
C	1.843802867	6.968610203	15.029877162
H	0.761772408	6.822697716	15.131190818
H	2.324475985	6.200341582	15.654672118
C	2.265427224	6.766096393	13.565974023
H	1.727326881	7.489428889	12.940552731
H	1.980373085	5.768613719	13.214593209
C	3.454069252	7.237500566	10.340578782
H	4.062508971	6.967845899	9.466578684
C	3.434334933	8.779347167	10.440624169
H	4.437266643	9.175946270	10.627545612
H	2.807810132	9.075654318	11.291765663
C	2.857994764	9.406414463	9.159456362
H	2.838902917	10.498231193	9.259819252
H	3.526657113	9.178994481	8.317322660
C	1.453228729	8.866148852	8.857856172
H	0.765643545	9.185702729	9.654757305
H	1.071745608	9.294529373	7.923596698
C	1.460107940	7.332355775	8.781250007
H	2.066958281	7.014266091	7.921663455
H	0.446524571	6.952325438	8.606677160
C	2.034920755	6.698410897	10.061024413
H	2.056502337	5.610510362	9.957561169
H	1.371382118	6.924748164	10.903715248
F	8.872751588	3.911975510	12.241125388
F	9.570630554	3.736232698	10.057609640
F	7.329360502	3.965153263	10.536353460
F	8.389556827	2.000164518	11.053226307
B	8.575956008	3.388908301	10.947075322
H	6.329403516	1.589126555	11.526311477

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3

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O	1.180719380	2.635873568	11.518811416
H	0.271649538	2.323103699	11.607103822
C	1.978162364	1.964099790	12.403660725
C	1.454053001	0.989511678	13.269268004
C	3.328023518	2.290098455	12.412763526
C	2.323451387	0.345387814	14.152130503
C	4.181124009	1.625857800	13.304868934
C	3.691516677	0.653704099	14.178816089
H	0.393755901	0.765351974	13.248954823
H	4.318661302	0.123769673	14.882404283
O	5.489169088	2.007374296	13.243111243
C	6.413403993	1.381595251	14.119059969

H	6.158372059	1.558904862	15.172364200
H	6.470325320	0.299047561	13.943311455
H	7.384330027	1.831631952	13.904121123
O	1.935722438	-0.614018317	15.044153478
C	0.568176491	-0.986145097	15.083860040
H	0.230797956	-1.399840897	14.123772109
H	0.485992969	-1.756243670	15.853108231
H	-0.076569781	-0.138659152	15.354099541
H	3.720310397	3.042422648	11.740452026

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4

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Ru	3.655598577	4.240755458	12.425499178
H	4.977377917	3.909169145	11.687564824
P	3.846443114	6.395719157	11.570415228
O	5.382370226	4.946985726	14.759404844
C	4.708716707	4.679766868	13.855152664
C	5.430923358	6.752646524	10.654407043
H	5.344672869	7.784932276	10.288341593
C	5.606775778	5.817332706	9.436284863
H	4.756070076	5.899134263	8.750710354
H	5.632510007	4.776835149	9.786552007
C	6.909798358	6.131126287	8.681460824
H	7.018201500	5.438174785	7.839621297
H	6.843692945	7.140639795	8.251641315
C	8.128796681	6.050136315	9.610685536
H	9.042392772	6.303966452	9.062304390
H	8.248758885	5.015332882	9.961912359
C	7.957586499	6.979157916	10.820552573
H	7.936146546	8.023670498	10.479321159
H	8.811382053	6.888766675	11.501113868
C	6.659836225	6.671731242	11.587723537
H	6.720472313	5.661366207	12.012470192
H	6.558979378	7.367077098	12.428409262
C	3.725233947	7.696410432	12.905049932
H	4.666978742	7.533486969	13.448746956
C	3.708698379	9.161707319	12.423064017
H	4.513761503	9.350973991	11.704794094
H	2.762180693	9.362207149	11.905475408
C	3.839270578	10.118582601	13.622313405
H	4.824521651	9.975550202	14.087679867
H	3.806023347	11.155558966	13.270357772
C	2.738663273	9.868212706	14.664413535
H	2.876107121	10.529790756	15.526482832
H	1.762579186	10.121736206	14.226496464
C	2.721007009	8.400418652	15.118746878
H	1.900026049	8.226620287	15.823715078
H	3.651400149	8.169027763	15.655825089
C	2.585885584	7.445399786	13.919865928
H	1.615457379	7.611234278	13.437422300
H	2.595790213	6.404728024	14.266643677
C	2.480650887	6.557745411	10.297733467
H	2.646505433	5.656432019	9.687273281
C	2.540649884	7.770104242	9.342121786
H	3.533240488	7.871622002	8.893443880
H	2.350215715	8.691062718	9.904582382
C	1.483103883	7.615598617	8.232458976
H	1.513172311	8.489200752	7.572372205
H	1.741826547	6.745757334	7.612079277
C	0.070055083	7.431909699	8.807630354
H	-0.233169350	8.353095810	9.324392941
H	-0.651843747	7.274069458	7.999351089
C	0.013547553	6.264830715	9.806550423
H	0.199131272	5.319506022	9.271646148
H	-0.986443734	6.186913198	10.248893652
C	1.067700123	6.442625027	10.911889952
H	1.014465724	5.622307810	11.641232173

H	0.842157754	7.357471344	11.472277453
O	2.168584433	3.015476131	11.012218767
H	1.335018458	3.424201988	10.731202896
C	2.074843249	2.555491011	12.326710822
C	1.015529069	2.956521145	13.155089231
C	3.188952507	1.836456307	12.785685498
C	1.056875587	2.540357495	14.499752774
C	3.185777379	1.430751762	14.157457117
C	2.136993271	1.786310015	14.999077599
H	0.195084244	3.536512233	12.753318388
H	3.916418808	1.414962077	12.102726199
H	2.105143650	1.499229654	16.041231593
O	0.107260004	2.835458615	15.400732904
C	-1.042079942	3.583940566	14.994905174
H	-0.756058038	4.579880780	14.635098814
H	-1.605771238	3.052737972	14.219202245
H	-1.658509404	3.683602570	15.887783943
O	4.248163856	0.701334055	14.518022484
C	4.358045280	0.251205349	15.875814896
H	4.398182344	1.101287873	16.565890943
H	3.521779334	-0.406006846	16.138228684
H	5.292837108	-0.306004928	15.923806550

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Ru	3.575891474	4.381766479	12.605036122
H	4.633843819	3.365810050	11.964481523
P	3.837722343	6.520032251	11.601054947
O	5.628370173	5.081582964	14.662980705
C	4.840066956	4.807843284	13.861540988
C	5.407836332	6.794963722	10.636089310
H	5.339435637	7.805061325	10.209553348
C	5.521465938	5.774729308	9.480070543
H	4.657778094	5.843535987	8.809270332
H	5.515430173	4.761280193	9.904568521
C	6.815306967	5.988379040	8.676257474
H	6.879431856	5.234952829	7.883251364
H	6.771758905	6.966811159	8.177308946
C	8.054164863	5.930780543	9.580528752
H	8.961010313	6.117057315	8.995108834
H	8.151184484	4.918800517	9.998846413
C	7.942674612	6.944527686	10.727740941
H	7.944896190	7.963858055	10.316859555
H	8.809981773	6.872415947	11.393127092
C	6.655706907	6.731620542	11.543959945
H	6.695064746	5.748020944	12.029824817
H	6.598593758	7.481699696	12.340580462
C	3.765476140	7.863476591	12.894458707
H	4.717054491	7.704672911	13.422665866
C	3.752352330	9.314502802	12.373848071
H	4.546674647	9.475018486	11.636489231
H	2.798900791	9.508286722	11.866573436
C	3.908835860	10.302577741	13.544237435
H	4.901127530	10.166883029	13.996617992
H	3.874515183	11.329805935	13.165022298
C	2.824851010	10.086275678	14.611701419
H	2.979216629	10.771328966	15.452194771
H	1.842156757	10.330540121	14.183577605
C	2.810359915	8.632446988	15.110090564
H	2.002151056	8.482472169	15.834586084
H	3.750490827	8.412847150	15.634878168
C	2.647538520	7.645950279	13.940776856
H	1.665987875	7.797713758	13.478120081
H	2.664229579	6.614158503	14.320997988
C	2.437474017	6.660799236	10.362444417
H	2.571549367	5.736890259	9.778930066
C	2.492170155	7.841943589	9.369220261

H	3.472009116	7.902932824	8.885663753
H	2.346016454	8.784022740	9.909395276
C	1.392323948	7.687066887	8.302057143
H	1.419717359	8.543492385	7.619741045
H	1.605770801	6.795954432	7.694888979
C	-0.001549054	7.552299608	8.934796764
H	-0.259864238	8.487771625	9.450145747
H	-0.758361426	7.404566342	8.156977396
C	-0.048338336	6.397457681	9.948409255
H	0.106349905	5.443200338	9.419806852
H	-1.034851414	6.342099585	10.422810244
C	1.041411996	6.579049771	11.019874695
H	0.993338664	5.771969982	11.766024183
H	0.843857581	7.507179474	11.568379806
O	1.733418259	3.162325244	11.327045605
H	0.918939268	3.578615484	11.007482381
C	1.525618448	2.536437603	12.562097162
C	0.266080106	2.309474896	13.089166809
C	2.739132456	2.323743811	13.229834023
C	0.244351432	1.749248816	14.383313649
C	2.679048747	1.760431888	14.528627623
C	1.432760699	1.488987129	15.092391025
H	-0.632961955	2.511110240	12.521637517
H	3.846406561	2.485101810	12.476535391
H	1.330400143	1.052790847	16.077299795
O	-0.882403808	1.423216162	15.040459786
C	-2.147968152	1.622183231	14.406792311
H	-2.319254019	2.682970482	14.187183396
H	-2.225901594	1.033375162	13.485171064
H	-2.893529525	1.275692973	15.122174008
O	3.861331199	1.538653555	15.126856217
C	3.875265455	1.004498197	16.455979898
H	3.361193564	1.674668939	17.154489831
H	3.413117993	0.011451946	16.484869352
H	4.927081421	0.926296740	16.729519331

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Ru	1.047291610	4.728104912	11.365818556
P	2.656111080	6.122086761	12.248791068
O	1.182532003	6.095999568	8.702663675
C	1.137763666	5.567452029	9.729754585
C	4.364161393	6.030861990	11.513056160
H	4.919887014	6.826955783	12.030999951
C	4.379299686	6.333269306	9.998259982
H	3.914648825	7.301762299	9.783402369
H	3.797712790	5.566123289	9.477547230
C	5.819086708	6.321303702	9.455976496
H	5.801314795	6.522080787	8.378941251
H	6.392383503	7.137042660	9.918361413
C	6.509913050	4.981570790	9.745944357
H	7.539335807	4.993527456	9.371813124
H	5.983591477	4.181232464	9.206294284
C	6.491066659	4.670266269	11.248816303
H	7.094656296	5.416648345	11.784281004
H	6.949806898	3.695172797	11.447466513
C	5.057025476	4.680309283	11.805830128
H	4.479354044	3.877534437	11.336701245
H	5.077998074	4.468445434	12.879652680
C	2.827405201	5.669333218	14.052333152
H	3.016758128	4.588597278	13.995314831
C	4.008496033	6.319859254	14.810810558
H	4.949606074	6.194075263	14.267566153
H	3.838646477	7.397584566	14.907253031
C	4.132747660	5.695691650	16.213603015
H	4.396157464	4.633589065	16.109473292
H	4.959216980	6.172294475	16.752160922

C	2.826441843	5.824471459	17.011505065
H	2.928599177	5.337058396	17.987020168
H	2.627845488	6.886898548	17.210860408
C	1.638554680	5.228514221	16.240899840
H	0.706246397	5.375574534	16.797574411
H	1.776500921	4.143328852	16.130896922
C	1.513439405	5.857418970	14.843235106
H	1.302090863	6.928531580	14.949679349
H	0.663203085	5.416317242	14.307672663
C	2.058857434	7.873577011	12.004539324
H	2.260389700	8.035177225	10.936230995
C	2.808255993	8.962437528	12.800408348
H	3.891885636	8.873506084	12.664287641
H	2.605656669	8.831878128	13.870472945
C	2.330909936	10.361101511	12.367819275
H	2.854748573	11.123526776	12.954662235
H	2.607601817	10.526579026	11.317392305
C	0.810065657	10.509148063	12.528782704
H	0.551561488	10.450232727	13.595562269
H	0.486949517	11.496670563	12.182698462
C	0.055586916	9.409406852	11.765032960
H	0.224604823	9.527291826	10.685834943
H	-1.024041608	9.498842441	11.927394643
C	0.529335326	8.010676046	12.197126132
H	-0.009415769	7.246832931	11.612640010
H	0.268604962	7.848111900	13.248657687
O	1.211517347	3.022504653	13.041823575
H	0.512876879	2.505156669	13.468810231
C	1.831170500	2.282381456	12.001339673
C	2.200297456	0.950306319	12.099281966
C	2.049462874	3.095405882	10.896447855
C	2.859887275	0.420510304	10.973852169
C	2.744203440	2.552372844	9.795269195
C	3.136320388	1.214707369	9.841775860
H	2.002622567	0.370321374	12.991743614
H	3.653823997	0.736642581	9.019996877
O	2.975923892	3.392854870	8.758750994
C	3.627452838	2.885600720	7.591435257
H	4.639917352	2.535009657	7.823887796
H	3.049718110	2.071155980	7.140022570
H	3.681844826	3.724091075	6.897019255
O	3.286928645	-0.856333751	10.881397978
C	3.043960881	-1.751651505	11.965839798
H	1.969263283	-1.865897973	12.153499230
H	3.461438538	-2.710222291	11.657630058
H	3.545426603	-1.413981608	12.881172865

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Ru	1.051735872	4.840003307	11.373239217
P	2.722491295	6.100781813	12.312000790
O	1.361699038	6.070359684	8.662369032
C	1.270427443	5.612169657	9.720793656
C	4.436993268	6.053596381	11.581012213
H	4.982425486	6.842461269	12.120638441
C	4.453416752	6.394667499	10.074597959
H	3.966656652	7.356952825	9.880409833
H	3.891926652	5.626497899	9.533579730
C	5.894247559	6.426463381	9.535280805
H	5.874569662	6.655670168	8.463848617
H	6.451451096	7.239972922	10.020670034
C	6.608943573	5.091990086	9.790375228
H	7.640242532	5.133505294	9.422983871
H	6.100079728	4.298894437	9.224026175
C	6.586048593	4.736148105	11.283550825
H	7.172823247	5.477392121	11.844258062
H	7.061630573	3.764150878	11.456167362

C	5.148491676	4.703728284	11.830908875
H	4.587093832	3.910505071	11.328787510
H	5.164927392	4.451615405	12.895728333
C	2.895617524	5.600754466	14.103394781
H	3.063400560	4.518542042	14.016245405
C	4.091294529	6.210152042	14.873500199
H	5.026770989	6.099693727	14.317909923
H	3.932577751	7.284846005	15.016146326
C	4.223250158	5.525594228	16.246959190
H	4.468347776	4.464833935	16.092783467
H	5.063719345	5.964964161	16.796220087
C	2.927828337	5.640008952	17.065871257
H	3.032795914	5.104546022	18.015816000
H	2.753952814	6.695794971	17.318578861
C	1.717750237	5.106098200	16.282766560
H	0.794987482	5.253891534	16.856256014
H	1.823551636	4.023374207	16.124268639
C	1.592297466	5.792051666	14.912395105
H	1.412530591	6.864344912	15.063039719
H	0.728106482	5.388845505	14.374439516
C	2.109191083	7.856214213	12.138894718
H	2.327301282	8.076979267	11.084378757
C	2.804741596	8.927258393	13.001982513
H	3.892520611	8.883492619	12.875286494
H	2.596072139	8.732405053	14.061052258
C	2.280824531	10.329031183	12.637443261
H	2.764524716	11.078868435	13.273026797
H	2.566485608	10.561988722	11.602167589
C	0.752430269	10.411329350	12.778803432
H	0.478903083	10.279845140	13.835442505
H	0.397164804	11.404892781	12.484681281
C	0.051988579	9.331037042	11.938854199
H	0.238043690	9.515267166	10.871810656
H	-1.033405810	9.374408687	12.083080036
C	0.570765499	7.929540535	12.304035872
H	0.072927680	7.181462668	11.661056116
H	0.293078735	7.695686942	13.337472468
O	1.048494248	3.190201780	13.105148453
H	0.230803873	2.746223302	13.393570648
C	1.757772544	2.408692746	12.164744704
C	2.079180119	1.068358310	12.336532455
C	2.078681250	3.168478901	11.051411027
C	2.796081969	0.478101833	11.282041267
C	2.803183280	2.559338749	10.013282086
C	3.162072344	1.215535196	10.138563177
H	1.788498557	0.530723668	13.230049859
H	3.711546984	0.690587845	9.367754780
O	3.078616478	3.335195997	8.932863598
C	3.721201763	2.734541228	7.808094382
H	4.727438719	2.383875869	8.063551033
H	3.130992507	1.899083724	7.416359525
H	3.791383662	3.517220694	7.053720902
O	3.179574828	-0.823524735	11.259233374
C	2.895945045	-1.640080102	12.392987140
H	1.814038957	-1.737810740	12.555651853
H	3.317173364	-2.621351330	12.168651097
H	3.367789300	-1.241111281	13.300148899
H	-1.275294673	4.034634130	7.353869713
O	-1.684474003	4.425636130	8.138163430
C	-1.609063020	3.539253538	9.175934909
C	-1.877956057	4.079374069	10.398175953
C	-1.311259145	2.144381909	8.772668756
H	-2.060899652	5.151937114	10.349840597
C	-1.996034988	3.510277579	11.744466743
C	-0.349188300	1.353386050	9.416380857
C	-1.973746582	1.627547269	7.643952157
C	-0.058685434	0.073909826	8.946491902
H	0.178280456	1.743488245	10.274332060

C	-1.687931063	0.345056325	7.183108028
H	-2.732699911	2.224859726	7.146355378
C	-0.727525947	-0.433765140	7.831328395
H	0.701798026	-0.517665126	9.446657708
H	-2.216435565	-0.046025158	6.319468367
H	-0.500605447	-1.431166805	7.466956660
C	-2.051986045	2.137971258	12.057782629
C	-2.030694653	4.427765695	12.821720383
C	-2.091143751	1.709786912	13.385432829
H	-2.068936092	1.402540933	11.263922307
C	-2.071160232	3.998737613	14.146425717
H	-2.025656481	5.494203158	12.605291514
C	-2.088821942	2.631734604	14.439985861
H	-2.134960043	0.645009247	13.597638402
H	-2.092709683	4.729976372	14.949534697
H	-2.122617714	2.289423906	15.469701302

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Ru	0.919682562	4.709784630	11.334013212
P	2.639571206	6.053926611	12.165170054
O	1.393226193	5.713606631	8.555901009
C	1.208711703	5.340471341	9.637124192
C	4.386493246	5.858054922	11.539947995
H	4.924528521	6.725133090	11.950605673
C	4.471414401	5.925935363	9.999511052
H	4.014609912	6.846620479	9.619722707
H	3.912160682	5.086725804	9.574095141
C	5.934306832	5.847102984	9.529157495
H	5.965887590	5.875124825	8.433808993
H	6.480487598	6.733636712	9.881476411
C	6.623545144	4.580994027	10.057665016
H	7.670817693	4.553608616	9.736720200
H	6.135444306	3.696727881	9.623440678
C	6.529223743	4.500749066	11.587903772
H	7.098634460	5.329656574	12.032326643
H	6.986277537	3.574236950	11.953809372
C	5.068054572	4.572309673	12.064721466
H	4.523244620	3.698133251	11.695404506
H	5.036761232	4.523115449	13.157497977
C	2.744982522	5.871816584	14.021487047
H	2.923571773	4.793954314	14.128057337
C	3.904469365	6.619898148	14.719892551
H	4.862051755	6.427622472	14.227283132
H	3.734589534	7.700918097	14.668659643
C	3.986587687	6.187842227	16.196485399
H	4.246532199	5.120459882	16.241471131
H	4.800118000	6.729755589	16.692147061
C	2.658172327	6.423473670	16.932162248
H	2.728516714	6.066620310	17.965775573
H	2.463858510	7.504263185	16.986144161
C	1.487174149	5.739511924	16.209088923
H	0.540485685	5.965361157	16.713627097
H	1.614300187	4.648146336	16.244733420
C	1.410620195	6.178852824	14.737237539
H	1.216252623	7.258309887	14.696735111
H	0.571925601	5.677565241	14.241157305
C	2.112644818	7.781110668	11.676209973
H	2.325208454	7.785318385	10.597448754
C	2.878967689	8.958476154	12.309836734
H	3.961511960	8.823117280	12.208042021
H	2.659113169	8.998442809	13.383849474
C	2.445830314	10.285748601	11.659961064
H	2.983608500	11.117924336	12.127822230
H	2.736647252	10.278702453	10.600042623
C	0.927596581	10.496125761	11.774210161
H	0.657789665	10.610449237	12.833878272

H	0.634319011	11.425769415	11.274447314
C	0.148942022	9.309765513	11.181978323
H	0.327894119	9.254338371	10.099129516
H	-0.929243580	9.451288214	11.317781580
C	0.585693085	7.984582474	11.829912090
H	0.029421190	7.152787986	11.364339638
H	0.314801796	7.991165622	12.891169162
O	1.108775754	3.358187354	13.288450627
H	0.318826324	2.879229824	13.601149341
C	1.869612194	2.494034139	12.459354840
C	2.412928416	1.290389732	12.891101048
C	2.029629245	3.043755886	11.201504184
C	3.189520772	0.600315253	11.947017143
C	2.825241656	2.346655770	10.279376202
C	3.393180777	1.125246128	10.655678631
H	2.246295544	0.934725658	13.899854753
H	4.009931926	0.545468216	9.980418975
O	2.996426058	2.928453235	9.054220142
C	3.815764695	2.267923418	8.092064185
H	4.842351963	2.144071639	8.456619247
H	3.406894669	1.284691096	7.828538255
H	3.818003754	2.911956161	7.211733708
O	3.802088483	-0.588908471	12.182342409
C	3.672296284	-1.176303257	13.472213312
H	2.623872611	-1.403094548	13.707313576
H	4.242393669	-2.105557937	13.437430521
H	4.086603360	-0.525639403	14.253486998
H	-1.262199937	4.173316812	7.934590362
O	-1.404445037	4.564655004	8.809238232
C	-1.347811323	3.591206123	9.755653416
C	-1.562979085	3.997723315	11.052934077
C	-1.122972268	2.223604138	9.235078541
H	-1.900340171	5.033248020	11.129148233
C	-1.782350363	3.193879491	12.273355090
C	-2.068956791	1.208751550	9.440056922
C	0.010800068	1.973896244	8.444454199
C	-1.869488266	-0.050175628	8.876188592
H	-2.950406934	1.409184454	10.041178833
C	0.208987191	0.707732210	7.894167857
H	0.755914578	2.751060107	8.304797142
C	-0.727924346	-0.304709841	8.110028355
H	-2.607100466	-0.832148132	9.031230534
H	1.095742888	0.511025710	7.297815267
H	-0.573522517	-1.289482616	7.677306407
C	-1.322908950	1.871671052	12.467025780
C	-2.434737300	3.823648674	13.354277837
C	-1.522251767	1.215809562	13.684893241
H	-0.772608173	1.367677385	11.681141467
C	-2.633863733	3.164939207	14.569105709
H	-2.793216195	4.844580231	13.235339494
C	-2.177535868	1.855386662	14.745866317
H	-1.151171388	0.200221822	13.804047124
H	-3.144730458	3.679567710	15.379634864
H	-2.328195426	1.341057940	15.691022565

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Ru	0.194056815	4.831697090	10.089732482
P	1.862614306	5.713415928	11.599418726
O	0.879145915	6.928403789	8.096932366
C	0.639483497	6.082903349	8.857396176
C	3.662537610	5.531951260	11.110988955
H	4.265786776	5.990355483	11.905875376
C	3.956907297	6.265663678	9.783607415
H	3.758798227	7.338489111	9.880772843
H	3.283802589	5.883018990	9.006385017
C	5.411411112	6.056707998	9.330367708

H	5.571247204	6.568879404	8.374279961
H	6.090050615	6.527806923	10.055252037
C	5.752211106	4.565987357	9.211128079
H	6.794345382	4.434355447	8.899207096
H	5.126530293	4.109756132	8.429865338
C	5.492189876	3.841316263	10.537565215
H	6.180704741	4.224731352	11.303893500
H	5.697018778	2.768487425	10.436718511
C	4.041604954	4.039038530	11.002994386
H	3.372778585	3.561376309	10.285077428
H	3.889483010	3.530303826	11.961779497
C	1.725951867	4.828024757	13.247503773
H	1.771486008	3.776755817	12.927241690
C	2.857857276	5.057901059	14.271262780
H	3.841020038	4.893889835	13.818992553
H	2.837999587	6.098270263	14.615083368
C	2.683514729	4.120316213	15.480508753
H	2.810901267	3.079881626	15.146375152
H	3.477201711	4.311069255	16.211871110
C	1.301572429	4.281090916	16.132595927
H	1.189799572	3.576096014	16.964092953
H	1.222710401	5.289240448	16.563669759
C	0.173588583	4.087282968	15.107041956
H	-0.804833176	4.252702307	15.572867250
H	0.177570331	3.047119257	14.747069315
C	0.345262765	5.033209401	13.907546478
H	0.263568095	6.068444069	14.261228254
H	-0.466050091	4.877944151	13.186388898
C	1.610968528	7.560850442	11.772183251
H	1.893643539	7.908413829	10.767980941
C	2.508843252	8.283740599	12.794780539
H	3.560710524	8.007899814	12.660967831
H	2.222915681	7.973959950	13.807990093
C	2.345149227	9.809072977	12.672476309
H	2.972878198	10.309323087	13.418712126
H	2.712732229	10.129708430	11.687250922
C	0.877694375	10.234062110	12.833451168
H	0.550130536	10.013602608	13.859805063
H	0.779592987	11.317115694	12.700428954
C	-0.031378632	9.491120513	11.842117779
H	0.217797570	9.798307636	10.816518658
H	-1.080291280	9.764858665	12.005684985
C	0.132544048	7.966908587	11.963757842
H	-0.503349647	7.461439051	11.224957444
H	-0.221145766	7.643049764	12.949406745
O	0.468731351	2.334685892	11.148275281
H	0.608508576	1.628933340	11.793546767
C	1.243050741	2.171619427	10.028328650
C	2.175450080	1.149367441	9.921634863
C	1.027722699	3.181356407	9.067252691
C	3.009975215	1.151279832	8.792683975
C	1.986995804	3.205750798	8.011610891
C	2.930840166	2.189940924	7.850009023
H	2.253339512	0.392114879	10.693039531
H	3.632449204	2.174423165	7.026580355
O	1.879376869	4.251763574	7.163057915
C	2.770896453	4.368749038	6.053466939
H	3.813545145	4.419229836	6.386879324
H	2.650312093	3.531372458	5.355238177
H	2.498146800	5.301622948	5.560242043
O	3.940618097	0.209388842	8.535932329
C	4.039283311	-0.922710096	9.400912304
H	3.080081888	-1.449622803	9.475288706
H	4.782464211	-1.578913602	8.947851114
H	4.375846221	-0.629312047	10.402730462
H	-0.319080501	2.873081263	6.493693720
O	-0.784279314	3.545883280	7.010434358
C	-0.990791745	3.102084393	8.276996577

C	-1.624384530	4.136871876	9.049084864
C	-1.309556974	1.634919780	8.349758305
C	-2.254362736	4.180168100	10.373917465
C	-0.424079557	0.673907501	7.836758620
C	-2.579484387	1.231936168	8.784066740
C	-0.790657043	-0.668070600	7.795034731
H	0.555222326	0.971861889	7.478226901
C	-2.940426007	-0.115170645	8.746122374
H	-3.296640022	1.969215066	9.123888299
C	-2.046508239	-1.068427233	8.259669743
H	-0.096194214	-1.402890815	7.398766332
H	-3.926830706	-0.413740674	9.088513752
H	-2.329019021	-2.116644107	8.234302938
C	-2.723284051	5.462900857	10.775956253
C	-2.334511202	3.137770285	11.329197227
C	-3.245871660	5.683217150	12.049650316
H	-2.700816346	6.278636050	10.057684235
C	-2.864161838	3.367907690	12.594841787
H	-1.975941372	2.151812270	11.074873863
C	-3.324842010	4.635380735	12.966138787
H	-3.600185458	6.674252672	12.317408075
H	-2.921155494	2.545238578	13.302220445
H	-3.735848494	4.800979327	13.957257985
H	-1.892243219	4.975638355	8.410862794

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Ru	0.752239103	4.482754861	9.718584620
P	2.445519876	5.163360050	11.380445407
O	2.000237905	6.382173799	7.803560000
C	1.527507594	5.625923787	8.552451046
C	4.227491880	4.679149476	11.033247472
H	4.851050296	5.276420523	11.712789791
C	4.615856473	5.025046923	9.578536899
H	4.431163817	6.081811621	9.357849038
H	3.972893197	4.444598840	8.903840654
C	6.085507711	4.679916319	9.288481765
H	6.320872817	4.925774833	8.246055282
H	6.737487735	5.307183993	9.912019422
C	6.374836101	3.198702234	9.571941588
H	7.434769938	2.977027441	9.404262757
H	5.806721589	2.573962028	8.868773260
C	5.973659359	2.829673348	11.007675227
H	6.619668530	3.365419956	11.717090249
H	6.138282530	1.760127062	11.189774637
C	4.504947770	3.186130041	11.299531498
H	3.850168748	2.594936138	10.652180136
H	4.261066326	2.911988463	12.330366876
C	2.031473085	4.423789904	13.054351707
H	1.947352797	3.354489724	12.798064626
C	3.049023609	4.539212949	14.210294753
H	4.055573430	4.247073510	13.895482308
H	3.115807641	5.580209222	14.539321619
C	2.587096446	3.671415635	15.396700028
H	2.584597883	2.614159021	15.092244864
H	3.306046104	3.756942078	16.219328807
C	1.180617366	4.071651199	15.872948654
H	0.854996092	3.417768637	16.689751180
H	1.219232762	5.090468494	16.283595057
C	0.163827336	4.037427118	14.720781453
H	-0.816919932	4.390364528	15.060935440
H	0.022238401	2.998474537	14.385448018
C	0.638375185	4.884091142	13.529663353
H	0.691756378	5.937248370	13.834908536
H	-0.088165209	4.830307701	12.714562846
C	2.569267789	7.041531861	11.501986321
H	3.162043853	7.284903977	10.607892442
C	3.323475357	7.590748844	12.730873560

H	4.288275399	7.089307040	12.864480496
H	2.730271778	7.389534895	13.631256972
C	3.527606934	9.112211089	12.614031009
H	4.063621345	9.479719619	13.496454244
H	4.165135784	9.327423074	11.744895332
C	2.183933813	9.839398586	12.457563976
H	1.589730204	9.700381189	13.372395147
H	2.342500771	10.917843167	12.347384061
C	1.401372425	9.288589761	11.257316132
H	1.941139595	9.526348812	10.329626264
H	0.420566051	9.773460810	11.180292901
C	1.215075283	7.764528571	11.347175388
H	0.697538618	7.407731436	10.454335018
H	0.566469167	7.521644711	12.198156780
O	0.242538177	1.925437064	10.547479881
H	0.495339318	1.400324748	11.320001374
C	1.162895521	1.817118186	9.550658510
C	2.275445247	0.997878023	9.673358270
C	0.866732311	2.630420347	8.404037979
C	3.219146846	1.012249355	8.636362047
C	1.955248376	2.690075671	7.438129227
C	3.075166133	1.887928546	7.541383790
H	2.417991967	0.405550774	10.568816452
H	3.872378339	1.907236948	6.811236542
O	1.790288633	3.591997312	6.450815404
C	2.831952354	3.793465150	5.483752925
H	3.759290538	4.094950703	5.980958123
H	2.993309954	2.887844816	4.890145765
H	2.479335069	4.600693531	4.843368097
O	4.340237242	0.279626296	8.627917195
C	4.594774409	-0.641875025	9.695935094
H	3.797882992	-1.390443053	9.764820118
H	5.535448393	-1.129414357	9.442769014
H	4.701053817	-0.114424916	10.650179590
H	-0.113891363	3.524181043	6.179603411
O	-0.729449012	2.846501353	6.496949471
C	-0.662694589	2.787674824	7.906741883
C	-1.019483513	4.146707842	8.511434844
C	-1.546787221	1.583501541	8.224888837
C	-1.630384876	4.555738329	9.763170952
C	-1.040195149	0.281550968	8.156611719
C	-2.921848194	1.765847741	8.395116134
C	-1.882415419	-0.816899582	8.321486191
H	0.014684190	0.117208175	7.957939458
C	-3.768512921	0.668371994	8.556615223
H	-3.335166725	2.769375046	8.397964839
C	-3.249467344	-0.626173409	8.531627584
H	-1.474211928	-1.822441486	8.270297017
H	-4.834195679	0.826629602	8.694074766
H	-3.906596592	-1.481412921	8.659710386
C	-2.113096725	3.705091903	10.803093979
C	-1.565962637	5.957816273	10.051986480
C	-2.589266695	4.242180277	11.989208363
H	-2.155868699	2.638615804	10.636964000
C	-2.039691752	6.477379517	11.266616340
H	-1.270484201	6.640621798	9.260767817
C	-2.562055642	5.627837354	12.232672500
H	-2.990506148	3.573521855	12.745802374
H	-2.007530229	7.549494142	11.433210371
H	-2.946418729	6.024972114	13.166857160
H	-1.059470364	4.908468975	7.733910240

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Ru	1.219740981	3.454271660	12.751253728
P	2.249120393	5.544739840	12.605267062
O	3.177793508	2.202797347	10.899079048
C	2.461073341	2.718118728	11.655593916

C	3.636222938	5.946218990	11.418713623
H	3.875089093	6.997529608	11.630389656
C	3.148761795	5.838789219	9.959974178
H	2.248793332	6.441848378	9.802849606
H	2.864040449	4.799102088	9.764154223
C	4.246552057	6.254111477	8.968215252
H	3.872790575	6.138545361	7.944204637
H	4.474142456	7.321462055	9.101319949
C	5.522200233	5.426675474	9.178450367
H	6.306110780	5.747409308	8.483598141
H	5.311398823	4.371496276	8.953721911
C	6.014961564	5.547838819	10.627340460
H	6.309872266	6.588014140	10.825990768
H	6.908259607	4.933074736	10.784618069
C	4.929644286	5.129659156	11.637894919
H	4.726389986	4.060386461	11.518932662
H	5.314571531	5.276002784	12.652610929
C	3.067365295	5.560203854	14.301586825
H	3.965247319	4.949986808	14.142649240
C	3.521802030	6.941697839	14.812943130
H	4.170415980	7.426217627	14.074115781
H	2.648021201	7.590459538	14.944241250
C	4.251441150	6.817039104	16.161728504
H	5.180800496	6.247399258	16.022469030
H	4.542769468	7.812261242	16.514952862
C	3.370419707	6.112390640	17.204095038
H	3.902174610	6.023292041	18.157461874
H	2.475863704	6.722198397	17.396739747
C	2.941966697	4.723456860	16.708156499
H	2.290558117	4.233934683	17.443253722
H	3.830417433	4.086120086	16.600239997
C	2.217540439	4.811556785	15.354708599
H	1.244871539	5.296379704	15.488762519
H	2.011480588	3.783673649	15.003368231
C	1.021956860	6.944199962	12.447544150
H	0.493358602	6.665919634	11.530329007
C	1.592693940	8.362843618	12.227067396
H	2.277426808	8.374682350	11.373311136
H	2.164226404	8.691459577	13.102269528
C	0.442275497	9.353323004	11.965070395
H	0.852940613	10.359047257	11.821558756
H	-0.056106953	9.076867889	11.025508962
C	-0.583047889	9.348711961	13.108759631
H	-0.100008203	9.703594365	14.030511078
H	-1.396611943	10.049924095	12.891956979
C	-1.143438766	7.937478327	13.340311358
H	-1.715120516	7.626262494	12.456787629
H	-1.837119803	7.927607417	14.189388690
C	-0.016237426	6.922215970	13.593001283
H	-0.444046303	5.919158797	13.711556884
H	0.473830781	7.174349016	14.541636212
O	0.193944079	1.988850615	14.311931678
H	0.631523405	1.797223330	15.153401312
C	-0.857237518	2.874513317	14.503682248
C	-1.047319115	3.383079768	15.793545925
C	-1.624807247	3.242667194	13.376399830
C	-2.065401077	4.308995082	16.006909530
C	-2.656321750	4.194697991	13.655948746
C	-2.865002382	4.714043919	14.930122067
H	-0.402383352	3.044433887	16.596043985
H	-3.647411153	5.433147556	15.129263480
O	-3.419881800	4.568151005	12.605581855
C	-4.550794374	5.415711876	12.799668680
H	-5.265211911	4.966960083	13.498688399
H	-4.249214098	6.406242807	13.161214454
H	-5.010448329	5.508918811	11.815609273
O	-2.348818286	4.883377509	17.194124859
C	-1.607940340	4.481551939	18.344892246

H	-0.539880896	4.708238721	18.229155394
H	-2.011877140	5.059192684	19.177100240
H	-1.736862197	3.410855191	18.547674905
H	-1.162201361	0.671472233	11.561033699
O	-0.930430741	1.236941151	12.310515638
C	-1.413755074	2.559552759	11.977354700
C	-0.245653727	3.249229583	11.197202293
C	-2.717014712	2.336026416	11.196516603
C	-0.447136113	4.441067011	10.329790498
C	-3.776289562	1.722839168	11.886054821
C	-2.852436190	2.563656000	9.824415357
C	-4.958086051	1.393478536	11.231570381
H	-3.668554738	1.514623686	12.946712561
C	-4.038905272	2.226232635	9.165109867
H	-2.050054051	3.010699446	9.252682343
C	-5.096870870	1.650989094	9.863904116
H	-5.771174228	0.932661609	11.785415724
H	-4.127916584	2.417312245	8.099272828
H	-6.019139957	1.396069108	9.349545499
C	0.244584985	4.474884795	9.102159596
C	-1.335452280	5.492141432	10.605996544
C	0.058497892	5.510127895	8.191299556
H	0.927714873	3.664236627	8.859728973
C	-1.531820719	6.526352719	9.690837765
H	-1.902278141	5.482421810	11.522637472
C	-0.834868621	6.545677091	8.481561260
H	0.602302204	5.505065806	7.250718780
H	-2.238909217	7.318516682	9.923423861
H	-0.993579536	7.349004816	7.768260697
H	0.163255699	2.456360738	10.565497786

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Ru	0.982346673	3.615954767	12.502822818
P	2.258879220	5.600312437	12.694755195
O	3.130433187	2.122150118	11.062285573
C	2.346173942	2.746061821	11.650534101
C	3.839483039	5.774461588	11.706626146
H	4.179468207	6.799939019	11.896494425
C	3.541888852	5.640822858	10.197155472
H	2.758921366	6.342830955	9.892035389
H	3.149381547	4.637731995	9.997377797
C	4.808108604	5.858522215	9.354477558
H	4.568520476	5.723904301	8.293216637
H	5.150044626	6.896969925	9.470337594
C	5.926132407	4.899487726	9.784879751
H	6.829321933	5.073265216	9.189522017
H	5.611323967	3.864693958	9.588845326
C	6.236936484	5.060529122	11.279305478
H	6.628711821	6.071226797	11.462187646
H	7.020642421	4.359745495	11.588110795
C	4.985783249	4.839163652	12.150398120
H	4.679969143	3.791356757	12.072946702
H	5.245093935	5.021840177	13.198834603
C	2.838792013	5.620535817	14.480538683
H	3.615095650	4.843175800	14.468456256
C	3.496048267	6.929555181	14.960834724
H	4.279163408	7.244038678	14.261783664
H	2.746093708	7.730097665	14.979344415
C	4.083983772	6.758804896	16.372890279
H	4.902289054	6.025947124	16.335984683
H	4.524538074	7.704759069	16.706517737
C	3.015788515	6.281610459	17.368476981
H	3.455805571	6.141231718	18.361596003
H	2.244477462	7.058407174	17.473100734
C	2.359724892	4.976331806	16.894313878
H	1.576574615	4.659235191	17.592566490

H	3.110639276	4.174267898	16.878565760
C	1.768165193	5.125863483	15.481691789
H	0.930954957	5.837566291	15.516553512
H	1.366703818	4.152324421	15.160067175
C	1.288779423	7.160918896	12.278029544
H	0.810862334	6.882932077	11.331737885
C	2.119043229	8.438880653	12.018176693
H	2.876784302	8.261989786	11.250229602
H	2.649662539	8.739974715	12.929349970
C	1.203944640	9.586038629	11.552451948
H	1.808252522	10.482938388	11.375427531
H	0.755329256	9.310210405	10.587638599
C	0.090530883	9.877432602	12.567275738
H	0.537760690	10.231114556	13.507405737
H	-0.555996526	10.684069990	12.204049175
C	-0.734456583	8.613157995	12.838774488
H	-1.260314908	8.317676292	11.923180048
H	-1.501370217	8.803197464	13.599527900
C	0.160340188	7.448088349	13.293261692
H	-0.457924699	6.557585376	13.428291935
H	0.598046495	7.697692209	14.268147376
O	-0.841061378	4.225124305	13.654366435
H	-0.779354493	4.803439934	14.425383337
C	-2.133950531	4.244174221	13.129178806
C	-3.082159752	5.004372123	13.810207891
C	-2.375308092	3.550516236	11.939726250
C	-4.364650730	5.108510783	13.262336709
C	-3.672350786	3.744892180	11.379765689
C	-4.649292803	4.487943346	12.041960044
H	-2.813989735	5.496660954	14.737756910
H	-5.638061644	4.624967270	11.626523902
O	-3.880456767	3.217802042	10.156211609
C	-5.166864944	3.299468559	9.546781950
H	-5.933711038	2.822077622	10.167738085
H	-5.448166272	4.340318098	9.346936653
H	-5.071332211	2.759119876	8.604546253
O	-5.379926150	5.804325488	13.817907123
C	-5.158253309	6.473984914	15.056900079
H	-4.380590989	7.242843243	14.961087930
H	-6.105505936	6.949475931	15.312033900
H	-4.881920544	5.766925472	15.849097629
H	-0.239955980	1.179159354	11.977938303
O	-0.544780003	2.019282125	12.356194647
C	-1.265177288	2.758107460	11.243553046
C	-0.101697786	3.606939402	10.672848712
C	-1.749162294	1.673816876	10.284489958
C	-0.318948298	4.870739955	9.917313519
C	-2.410106701	0.556356821	10.814590494
C	-1.525872913	1.746652772	8.905723896
C	-2.829493621	-0.477322063	9.978613948
H	-2.611282979	0.509200353	11.881331302
C	-1.955118291	0.715650130	8.070614470
H	-1.050312850	2.619069246	8.471438383
C	-2.602455466	-0.400400341	8.603245978
H	-3.338585598	-1.339130534	10.400186218
H	-1.781165673	0.785187944	7.000615866
H	-2.929532243	-1.204252197	7.950255847
C	0.477251451	5.063082822	8.769251745
C	-1.248522573	5.878795244	10.236798001
C	0.361755824	6.202583899	7.978774413
H	1.197709986	4.296489426	8.495495718
C	-1.378385826	7.012121070	9.433676313
H	-1.875041105	5.790272013	11.112124430
C	-0.573356335	7.186706462	8.306996873
H	0.992027487	6.316462196	7.101421679
H	-2.117023713	7.765432519	9.693022963
H	-0.679436035	8.072482895	7.687698032
H	0.477093583	2.940188690	10.034058547

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Ru	0.941331155	3.676764206	12.409868356
P	2.297686994	5.679442055	12.590684882
O	2.945442262	2.124913865	10.834428423
C	2.228503014	2.749432445	11.500496284
C	3.993241370	5.670659116	11.775274707
H	4.447278536	6.640835899	12.009858614
C	3.848101100	5.570801185	10.240220344
H	3.216435631	6.382915247	9.862607687
H	3.337749667	4.633909471	9.989533069
C	5.215859231	5.591508491	9.539282844
H	5.074553393	5.497766136	8.456276062
H	5.700161267	6.563266842	9.710561825
C	6.118618061	4.469694063	10.068344100
H	7.093096312	4.492940531	9.568419025
H	5.663325781	3.497594689	9.833878046
C	6.296405210	4.595476408	11.587107356
H	6.823938740	5.532632345	11.813178333
H	6.922219350	3.783097797	11.972386837
C	4.945812683	4.585121951	12.326194702
H	4.493507816	3.593772278	12.225458561
H	5.128058606	4.743280479	13.394375738
C	2.732272966	5.684474885	14.428936248
H	3.397795792	4.814274443	14.485439039
C	3.520175867	6.898638245	14.953911153
H	4.369385357	7.119742874	14.299035211
H	2.875085018	7.785181989	14.944960748
C	4.013543402	6.651619406	16.390433119
H	4.734071790	5.823484073	16.383104125
H	4.552602643	7.531787718	16.754634878
C	2.850922492	6.309682944	17.332165531
H	3.225021640	6.096939860	18.339016997
H	2.188680654	7.181172149	17.421311000
C	2.043619630	5.114152117	16.808222913
H	1.191178892	4.908044187	17.464715627
H	2.672511982	4.215286126	16.819800447
C	1.551630954	5.351276241	15.369500682
H	0.825898358	6.174785700	15.372696040
H	1.029805400	4.448073727	15.023968049
C	1.568758669	7.358573772	12.117237568
H	1.116398241	7.157935009	11.143339938
C	2.581471597	8.509266841	11.924633288
H	3.333783826	8.232396507	11.182031641
H	3.116161870	8.710299761	12.859367333
C	1.874207662	9.794069020	11.459339941
H	2.612236797	10.592621045	11.329966966
H	1.423155850	9.615659614	10.474669017
C	0.782299866	10.218804827	12.446809354
H	1.239488088	10.452798185	13.417373376
H	0.288554345	11.134677738	12.104031639
C	-0.243241975	9.093097849	12.614995244
H	-0.752881353	8.922694944	11.661401817
H	-1.011193132	9.374437953	13.344417674
C	0.426940276	7.783399604	13.064415572
H	-0.330173161	6.993184940	13.100856521
H	0.818282255	7.920617422	14.078176165
O	-0.941489925	4.610292700	13.288261180
H	-0.891629350	5.288701793	13.975048572
C	-2.247946174	4.325156838	12.953241854
C	-3.250304684	4.878875377	13.728297474
C	-2.476822632	3.445318508	11.858257130
C	-4.587395702	4.553747049	13.433694702
C	-3.864475117	3.104007783	11.631668507
C	-4.882838972	3.663242529	12.397707043
H	-2.995260795	5.526038039	14.558684626

H	-5.924196393	3.437539114	12.212006492
O	-4.121193230	2.281211204	10.610200336
C	-5.465524102	1.915255451	10.285495132
H	-5.946109173	1.400910020	11.123407424
H	-6.054204316	2.792610885	9.995164332
H	-5.373800552	1.235141382	9.439757598
O	-5.643700535	5.039217406	14.100619889
C	-5.443642154	5.998164127	15.144764753
H	-4.943551080	6.896272265	14.762841959
H	-6.441513492	6.258511322	15.497363274
H	-4.865775293	5.568933585	15.971679389
H	-0.739769753	2.109476071	13.470445429
O	-0.145478642	1.939433339	12.724598733
C	-1.411276530	2.997602138	10.981602887
C	-0.236259015	3.823844275	10.610994473
C	-1.575511286	1.798468730	10.135782155
C	-0.416070181	5.210853209	10.063853580
C	-1.704790976	0.502140850	10.654228004
C	-1.627191419	2.001891390	8.745317607
C	-1.874709596	-0.573297591	9.787510455
H	-1.598468855	0.355986418	11.722087638
C	-1.856122461	0.926087864	7.889570083
H	-1.539734222	3.006971398	8.345027780
C	-1.965827454	-0.364198389	8.407027832
H	-1.926650272	-1.583705155	10.185382180
H	-1.926654121	1.093599117	6.819343513
H	-2.109892838	-1.208716460	7.738275917
C	0.524922261	5.611982667	9.094594915
C	-1.466370711	6.096430467	10.354726254
C	0.436171266	6.846292806	8.457285322
H	1.335395143	4.936303327	8.839909681
C	-1.566732341	7.326835563	9.701703395
H	-2.237978769	5.827306245	11.063368640
C	-0.616604285	7.714798676	8.757376684
H	1.180327515	7.123217418	7.716112323
H	-2.402056844	7.983120794	9.931024875
H	-0.701893666	8.672829919	8.253145334
H	0.342704667	3.254722899	9.888701484

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Ru	0.780467612	3.224697399	12.419606616
P	1.956232658	5.300471696	12.613062480
O	2.796937825	1.791197193	10.736933141
C	2.059321674	2.419971830	11.371641236
C	3.577556474	5.376005164	11.680614722
H	3.949912610	6.394140283	11.850349220
C	3.384625911	5.207627790	10.155403518
H	2.671259772	5.945449803	9.770425809
H	2.959032976	4.222931983	9.938307531
C	4.725500142	5.338499575	9.411797348
H	4.564942072	5.186833179	8.338220252
H	5.108170956	6.362255094	9.531540820
C	5.758760554	4.339895817	9.953176969
H	6.710461447	4.452598008	9.422105206
H	5.407812949	3.315824544	9.762348472
C	5.965234238	4.534105720	11.462024535
H	6.395384126	5.529325964	11.644307071
H	6.686046038	3.805598616	11.850139267
C	4.643050405	4.406267568	12.239814270
H	4.285743098	3.373394651	12.177948658
H	4.823451617	4.610282820	13.300080992
C	2.430792495	5.622075081	14.396903074
H	3.078303202	4.755542887	14.581507673
C	3.238867422	6.919384274	14.623188480
H	4.058733605	7.016924162	13.903731675
H	2.581801530	7.788007222	14.480564643

C	3.807636440	6.951255868	16.054178265
H	4.525749407	6.126459118	16.170024640
H	4.368900145	7.881003503	16.206114515
C	2.695292489	6.812220158	17.104074266
H	3.125339239	6.796781660	18.112107029
H	2.040899465	7.695402447	17.054081589
C	1.859516620	5.547964770	16.855823014
H	1.038747643	5.481104162	17.581147871
H	2.484686608	4.656327777	17.007886728
C	1.284921759	5.509234973	15.428952201
H	0.577839162	6.338703022	15.304478054
H	0.741321008	4.577862919	15.282718222
C	0.955098678	6.722179586	11.883490837
H	0.588593973	6.289935203	10.937315116
C	1.750641570	8.009409879	11.541323415
H	2.630510458	7.791967913	10.927910790
H	2.117203401	8.470447126	12.468565050
C	0.854769733	9.011410221	10.788206472
H	1.430783202	9.919666215	10.569231347
H	0.572860448	8.577041055	9.815701456
C	-0.415316512	9.355816430	11.582082751
H	-0.133911779	9.896514434	12.499864700
H	-1.053583810	10.032021163	11.001578146
C	-1.189262427	8.082446661	11.967004534
H	-1.568841261	7.589361137	11.057386740
H	-2.064896838	8.331786063	12.581659438
C	-0.283766954	7.101863729	12.732360455
H	-0.853261438	6.214882809	13.044783436
H	0.057380514	7.584716702	13.663732390
O	-0.891337539	3.910461504	13.729342579
H	-1.573756151	4.303371755	13.150361007
C	-1.536132043	2.916601440	14.497292070
C	-2.152577844	3.356576869	15.659273744
C	-1.536573506	1.593614229	14.052123604
C	-2.840831127	2.416688416	16.437194810
C	-2.289482879	0.675515566	14.843901006
C	-2.920674201	1.081577322	16.016396436
H	-2.059583948	4.398213034	15.934699219
H	-3.487350734	0.393048959	16.628828174
O	-2.361430412	-0.581627188	14.354210299
C	-2.949101540	-1.611458001	15.149736044
H	-2.444500285	-1.697809411	16.119097388
H	-4.019735977	-1.433259109	15.304474661
H	-2.811945695	-2.532259682	14.582551430
O	-3.467459065	2.699743398	17.598750220
C	-3.411359094	4.034308734	18.101699366
H	-3.888008045	4.741030286	17.410994100
H	-3.962310274	4.020515124	19.042304378
H	-2.376059846	4.345301707	18.289140744
H	2.049565353	1.832947883	14.034215064
O	1.699931191	2.731038499	14.130583326
C	-0.737501440	1.090448100	12.898974492
C	-0.746639181	1.604692075	11.610218635
C	0.126006506	-0.092741644	13.163240952
C	-1.449242888	2.770971879	11.055402669
C	0.774371073	-0.211257387	14.406413013
C	0.350606256	-1.078298857	12.188197289
C	1.651649041	-1.266585486	14.649066239
H	0.595004135	0.535841999	15.172351282
C	1.221322137	-2.136083141	12.437500854
H	-0.184389543	-1.041237091	11.243920438
C	1.882330693	-2.229680765	13.664702530
H	2.153107381	-1.338152112	15.609911886
H	1.375192424	-2.895120895	11.676163213
H	2.561823140	-3.054886251	13.855993253
C	-0.792065587	3.481195996	10.018642081
C	-2.690052884	3.269492257	11.525981017
C	-1.333098029	4.672341826	9.511020157

H	0.095637994	3.059817348	9.555628364
C	-3.219322165	4.443607356	11.004160571
H	-3.233679484	2.709717956	12.279082605
C	-2.536831880	5.159470658	10.005026034
H	-0.815059800	5.196382122	8.713402506
H	-4.180295826	4.801959391	11.362109146
H	-2.964761586	6.072531777	9.603386026
H	-0.151907243	1.063785600	10.880093628

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Ru	2.001515228	5.283245665	10.460261725
P	3.367233064	6.267247034	12.040292541
O	2.710378435	7.349072439	8.345772751
C	2.511533038	6.599019514	9.209618343
C	4.905098261	7.276620837	11.714327692
H	5.275154798	7.533749659	12.716291729
C	4.678747972	8.603876630	10.958229846
H	3.971610314	9.243504561	11.496080133
H	4.251028631	8.408040925	9.970537416
C	6.010925963	9.357765213	10.784789563
H	5.830241509	10.287463608	10.234372317
H	6.394872554	9.647033202	11.773109187
C	7.057503649	8.498523990	10.061373046
H	8.000296202	9.047652837	9.965023610
H	6.709129258	8.286851722	9.040306363
C	7.284455447	7.173476539	10.802276640
H	7.737720388	7.373902619	11.783286910
H	7.987114079	6.538157350	10.250270171
C	5.962656046	6.415459051	10.997667647
H	5.560598720	6.132616755	10.018585636
H	6.140076118	5.484410533	11.548815686
C	3.881189030	4.993682242	13.318197587
H	4.422102361	4.262956678	12.700308064
C	4.858332122	5.490628371	14.408990156
H	5.736493682	5.970125519	13.965575928
H	4.362694719	6.243013646	15.033880954
C	5.322491404	4.313741635	15.287858018
H	5.916517922	3.624023925	14.669263776
H	5.993647861	4.685956232	16.069749365
C	4.141880933	3.551897822	15.905226708
H	4.503886350	2.699164249	16.489881973
H	3.611543134	4.211084114	16.606374460
C	3.161364375	3.086588348	14.820562717
H	2.299775927	2.577520996	15.265971235
H	3.660584282	2.344248303	14.176281432
C	2.678195141	4.260870835	13.954912188
H	2.123875992	4.960023187	14.593008626
H	1.983152954	3.909957076	13.189069574
C	2.082925243	7.453532813	12.687894972
H	2.208378996	8.318540383	12.024383019
C	2.193821105	7.954400154	14.138493610
H	3.178714757	8.404128936	14.311935882
H	2.099176111	7.110623812	14.831898623
C	1.079012148	8.976454518	14.429631874
H	1.138030096	9.298111981	15.475074838
H	1.243473344	9.872322908	13.814840884
C	-0.312318558	8.396803378	14.124864385
H	-0.513912708	7.556612902	14.803889977
H	-1.085421003	9.148261578	14.317528403
C	-0.416628767	7.905755178	12.670106666
H	-0.305361060	8.756624529	11.984479014
H	-1.400141502	7.464432877	12.478883495
C	0.683568930	6.870537567	12.382035714
H	0.589350888	6.597983920	11.295646755
H	0.497526047	5.955261119	12.950838758
H	1.061919285	3.011233100	11.203184155

O	0.800724666	3.943024434	11.190831417
O	3.118716460	2.181251351	11.245071795
H	3.713614069	1.751360840	11.875976420
C	3.803148058	2.909135997	10.344325176
C	5.186317674	2.975425538	10.348915009
C	3.005232573	3.595071467	9.358001830
C	5.827431336	3.635781141	9.280379713
H	5.753586134	2.497425810	11.137874698
C	3.728913814	4.129704944	8.214056133
H	2.062667684	3.110999316	9.103539645
C	5.108883919	4.201700974	8.206454808
O	7.151959567	3.778351494	9.194823871
O	2.938397809	4.526039788	7.218283215
H	5.674092159	4.645976843	7.398971431
C	8.008214133	3.215259098	10.199476192
C	3.516057326	5.184084070	6.077657139
H	4.016761721	6.106308286	6.387047722
H	4.214758471	4.518949709	5.560291890
H	2.677149041	5.421300699	5.425525123
H	7.899054155	2.126660149	10.241517274
H	9.021532494	3.469601021	9.891812054
H	7.799823289	3.656370481	11.180096549

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Ru	1.986903397	5.056606196	10.560456833
P	3.158596230	6.346506723	12.178240371
O	1.018458558	7.494973121	9.154805519
C	1.409410078	6.557968514	9.708845416
C	4.543314983	7.474071074	11.628703997
H	4.812178882	8.090882513	12.497545834
C	4.081956059	8.408901543	10.488411987
H	3.217620772	9.007368797	10.796016748
H	3.757793893	7.798767451	9.636974025
C	5.219624290	9.335189700	10.029295030
H	4.864505820	9.972012560	9.211106522
H	5.500345910	10.007547730	10.851571645
C	6.447315576	8.525295635	9.591235068
H	7.258521343	9.193354883	9.282120581
H	6.185914425	7.917385911	8.712027248
C	6.918993906	7.593340840	10.714839236
H	7.274905581	8.195000835	11.562552488
H	7.769660377	6.987077381	10.381247474
C	5.786493529	6.668593855	11.190297185
H	5.502399411	6.001666991	10.370225789
H	6.153921742	6.033160611	12.001880052
C	3.940883071	5.176612085	13.412633243
H	4.576333346	4.564950525	12.754840622
C	4.850653443	5.787925176	14.500759874
H	5.579741041	6.480210554	14.068709433
H	4.244979264	6.369966215	15.202941237
C	5.578833977	4.669155655	15.267729353
H	6.254384348	4.141705621	14.578131166
H	6.210307808	5.106396189	16.049015839
C	4.587280124	3.667903859	15.879909847
H	5.125544181	2.858388055	16.384971655
H	3.992732407	4.176624636	16.651484654
C	3.636124267	3.093998592	14.818660357
H	2.903013767	2.423689107	15.281156727
H	4.212027148	2.486270200	14.102886865
C	2.914741062	4.216391170	14.054462097
H	2.280417141	4.774378133	14.753872301
H	2.245015437	3.786418534	13.297741113
C	1.894271501	7.455980857	12.997474092
H	1.737957294	8.225128627	12.226428201
C	2.303215450	8.169182264	14.300117826
H	3.263371728	8.684235963	14.181975082

H	2.434654844	7.422731305	15.093357604
C	1.212362883	9.165404588	14.733414566
H	1.508329776	9.652886142	15.668960506
H	1.128662127	9.958731362	13.977491585
C	-0.146835962	8.467716823	14.898429405
H	-0.086001456	7.751712765	15.730490892
H	-0.917825933	9.196973780	15.169529024
C	-0.554700460	7.720644624	13.618289608
H	-0.726131344	8.443989648	12.809215702
H	-1.499051136	7.186070745	13.768908567
C	0.538846227	6.731166840	13.180597963
H	0.228044343	6.237294438	12.243899055
H	0.636428455	5.941590765	13.934765474
H	0.934563143	2.876873907	9.692941801
O	0.940163963	3.766220923	9.304662735
O	3.454499357	2.981951631	10.877738384
H	3.832652615	2.184023260	11.273812286
C	4.198021109	3.504654171	9.856775470
C	5.510549938	3.184893677	9.601054234
C	3.444788424	4.468975495	9.120807257
C	6.139009356	3.891817494	8.543801586
H	6.040764954	2.448837088	10.192200051
C	4.161907573	5.226908498	8.127739257
H	2.435211033	3.998091586	8.745268524
C	5.477255776	4.908997479	7.821561804
O	7.398654153	3.673240955	8.166268413
O	3.442660740	6.177035863	7.532517136
H	6.037937681	5.412887399	7.045631231
C	8.176151933	2.642791316	8.795369977
C	3.996663047	6.901902553	6.422563009
H	4.870149288	7.482177203	6.737349657
H	4.267939399	6.217934496	5.612016704
H	3.205002524	7.573527993	6.093792065
H	7.699686394	1.664557022	8.671716155
H	9.135833372	2.649697902	8.280377234
H	8.327508115	2.861085142	9.857895614

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O	-2.144560860	0.395493545	9.574987276
H	-2.309296593	-0.555346776	9.560063123
C	-1.064189664	0.678826493	8.788755648
C	-0.316867497	-0.349885193	8.195755393
C	-0.730071515	2.029952268	8.635890312
C	0.796664627	-0.012072896	7.426449985
C	0.398923533	2.333176734	7.836611286
C	1.161330189	1.328791733	7.244480901
H	-0.609595190	-1.381336288	8.355444192
H	2.028458042	1.542291298	6.634633887
O	0.676760657	3.655946484	7.697244759
C	1.910055822	4.035079853	7.108104474
H	2.759488104	3.600124502	7.649931329
H	1.965240895	3.743421677	6.050816682
H	1.952942926	5.122743169	7.183495206
O	1.604291529	-0.918063474	6.803992175
C	1.299879982	-2.296954921	6.940978970
H	0.310112006	-2.537458505	6.529938211
H	2.062535937	-2.832887603	6.373264627
H	1.339621694	-2.618904640	7.990439269
C	-1.556813126	3.092169674	9.268378401
C	-1.061647865	4.019610081	10.123637832
C	-2.983396233	3.160309133	8.852781417
C	0.288501635	4.151895624	10.686508856
C	-3.358270077	2.825015618	7.540142570
C	-3.988463106	3.568905782	9.744513973
C	-4.684525309	2.924945479	7.125686691
H	-2.595245254	2.493238354	6.842360368

C	-5.315640375	3.666856535	9.331449466
H	-3.726309042	3.780701935	10.776793085
C	-5.670807013	3.349045231	8.018568095
H	-4.948895225	2.672367405	6.102057386
H	-6.077588301	3.977423304	10.041389582
H	-6.706354078	3.421113373	7.697941669
C	0.727979483	5.436472173	11.061955419
C	1.167410811	3.072631984	10.896720144
C	2.003169976	5.644780996	11.583311975
H	0.058178639	6.282252267	10.926352278
C	2.439714897	3.279649661	11.422817565
H	0.845523719	2.068017822	10.650587912
C	2.870543703	4.565775291	11.762383044
H	2.317986321	6.649521215	11.852660118
H	3.098453575	2.428957591	11.575911766
H	3.864543506	4.722243570	12.171385743
H	-1.735272990	4.828449146	10.400479406

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Ru	0.912339376	4.070648984	11.394615085
P	2.259766679	5.619321999	12.864925552
O	3.231802975	3.234400128	9.705770896
C	2.355789814	3.601434369	10.383906651
C	4.112292302	5.570717729	12.549671172
H	4.573719426	6.232921682	13.292087872
C	4.506350789	6.117894966	11.159274511
H	4.198393454	7.164481383	11.062258686
H	3.989717232	5.563730514	10.370140690
C	6.026023492	6.013926879	10.936012947
H	6.272256988	6.371104444	9.929262899
H	6.541491530	6.682475399	11.640597473
C	6.531670843	4.578038425	11.137798764
H	7.614921331	4.530747823	10.978116073
H	6.069327943	3.922974160	10.386094045
C	6.174448634	4.066109230	12.540689376
H	6.700826690	4.669028775	13.294839757
H	6.507310695	3.029460282	12.673481230
C	4.659910206	4.146198381	12.782981069
H	4.158024825	3.445153285	12.111041416
H	4.425629636	3.811415841	13.800048755
C	2.169110631	5.328280832	14.735125685
H	2.213177397	4.235110677	14.772736858
C	3.327432207	5.846192118	15.617158052
H	4.299828419	5.553369473	15.214086367
H	3.315320536	6.942309091	15.644190551
C	3.195396492	5.293056862	17.048575238
H	3.308342754	4.197494939	17.017408686
H	4.015125137	5.669845062	17.670622246
C	1.840825443	5.643977703	17.680272897
H	1.754326119	5.199547963	18.678130843
H	1.778780710	6.732799475	17.815225415
C	0.677335448	5.192794984	16.786533215
H	-0.284478840	5.496578389	17.216034976
H	0.665097112	4.088770480	16.755441262
C	0.825468210	5.754796692	15.363760765
H	0.789719799	6.848803331	15.423209414
H	-0.021816459	5.460841839	14.738822328
C	1.821292094	7.415192216	12.513936983
H	2.046179542	7.476895850	11.438367988
C	2.669940289	8.478139762	13.243576282
H	3.740525048	8.265419537	13.158065682
H	2.426488943	8.459052023	14.314210823
C	2.375910773	9.883735210	12.687039531
H	2.970127381	10.629177772	13.228276062
H	2.701296300	9.924933548	11.637467143

C	0.880172515	10.224013732	12.770416977
H	0.585260673	10.297794991	13.827223698
H	0.688635944	11.206053874	12.322808098
C	0.028888569	9.145477932	12.083092621
H	0.248287487	9.140333664	11.007313936
H	-1.039036915	9.375371525	12.186276440
C	0.320664033	7.749719271	12.660241190
H	-0.290911630	6.989800562	12.170218240
H	0.039359282	7.747546547	13.719119544
O	-0.914095574	4.442551954	12.657769086
H	-0.619987107	3.978981732	13.471019225
C	-2.265657473	4.087695931	12.505587287
C	-3.100250698	4.597040418	13.507283989
C	-2.713706461	3.285795372	11.458463932
C	-4.447740683	4.239545894	13.515883598
C	-4.066776204	2.849360004	11.582089407
C	-4.926956472	3.334880105	12.557593483
H	-2.668542013	5.256827976	14.248691593
H	-5.960379202	3.019385976	12.619285923
O	-4.437597043	1.886388659	10.693957573
C	-5.822239137	1.683045362	10.407895304
H	-6.339726567	1.207529210	11.249114311
H	-6.309114649	2.632487925	10.159432570
H	-5.849502960	1.021466415	9.541360351
O	-5.359876364	4.682351122	14.413682959
C	-4.942924495	5.624767020	15.396189222
H	-4.554735305	6.540917190	14.932355856
H	-5.833254104	5.863336233	15.979101157
H	-4.177819212	5.200738322	16.059758908
H	-2.477081512	0.938313248	10.499275437
O	-1.618082145	1.386933539	10.466186863
C	-1.906945560	2.783252484	10.249403629
C	-0.529026009	3.405862250	9.944850984
C	-2.684038494	2.959076709	8.921382760
C	-0.394859237	4.804007366	9.506039771
C	-2.407324403	2.076911248	7.870205143
C	-3.568878015	4.019780018	8.694656263
C	-3.000788743	2.251705733	6.619661890
H	-1.729017258	1.247613073	8.043375091
C	-4.162937797	4.194800680	7.445085083
H	-3.814289787	4.704921484	9.499718222
C	-3.878247220	3.314479088	6.399598378
H	-2.776029514	1.555315036	5.815972361
H	-4.851170133	5.021478463	7.288824035
H	-4.338797265	3.453061282	5.425586645
C	0.658645488	5.145151581	8.603545217
C	-1.223468710	5.872052714	9.953820560
C	0.847144485	6.450014282	8.158167019
H	1.278114778	4.349021325	8.202993591
C	-1.045585245	7.165459454	9.483219627
H	-2.027545833	5.669350912	10.648525120
C	-0.013946570	7.462973030	8.585082746
H	1.647408133	6.668221408	7.456078133
H	-1.708835187	7.953482621	9.827327821
H	0.115258426	8.478411989	8.221162264
O	0.059145561	2.620199446	14.379378187
H	0.298761365	2.713638718	15.312650600
C	1.094560985	2.072873117	13.664294796
C	2.296335577	1.752997344	14.281661340
C	0.837575525	1.839910432	12.289051729
C	3.289230027	1.126921192	13.507592795
H	2.453867975	1.979007123	15.328714210
C	1.849165930	1.096909804	11.573631394
C	3.067856185	0.788812630	12.160695394
O	4.509753508	0.817367519	13.974872166
O	1.505238860	0.755027602	10.326740563
H	3.866583564	0.291281639	11.628282584
C	2.455824636	0.070209994	9.501871630

H	3.345050362	0.689081914	9.346388839
H	2.733892802	-0.894495281	9.940663938
H	1.949158680	-0.093118820	8.551078391
C	4.840540025	1.106696115	15.335556195
H	4.196970660	0.548856270	16.025447184
H	5.873498914	0.783264574	15.460849595
H	4.767950622	2.181548998	15.540501377
H	-0.040954353	2.705774269	9.267944617
H	-0.187528823	1.687973051	11.958524462

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11-TS

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Ru	0.785369144	4.613073623	11.044985656
P	2.265020805	5.716429936	12.695546542
O	2.786330270	5.228323202	8.906546030
C	2.042458424	4.928242480	9.749654047
C	3.999805683	5.044345089	12.965923291
H	4.508717568	5.736605321	13.650274546
C	4.816402164	4.978699104	11.657024694
H	4.878710907	5.961508848	11.178815675
H	4.305517546	4.314758814	10.949532880
C	6.234999461	4.440774214	11.913900294
H	6.786168926	4.394129767	10.967322856
H	6.778477981	5.145338598	12.559261175
C	6.198402699	3.059520492	12.584507435
H	7.215093231	2.703210373	12.786232185
H	5.738322360	2.335876335	11.895030963
C	5.375881020	3.103348827	13.880736687
H	5.882814653	3.741748327	14.618242448
H	5.307652043	2.102292423	14.325832825
C	3.962842141	3.645670845	13.613750952
H	3.459483977	2.966375011	12.922739910
H	3.378765006	3.648484527	14.541370707
C	1.534098449	5.814212541	14.429484945
H	1.229636804	4.769950435	14.603236766
C	2.462402599	6.202634225	15.601301219
H	3.380031630	5.606880416	15.600531355
H	2.767940768	7.249761396	15.497674441
C	1.729231873	6.010742537	16.943167419
H	1.515950284	4.939682830	17.080257312
H	2.385116342	6.304970121	17.770667915
C	0.411929172	6.800857248	16.999616778
H	-0.110913536	6.602313944	17.942280115
H	0.637013292	7.876418133	16.986450838
C	-0.491460883	6.471912702	15.800607878
H	-1.399613189	7.086387745	15.823132207
H	-0.818743888	5.421532732	15.867101412
C	0.255778873	6.683670273	14.474178238
H	0.544449288	7.739113563	14.401000679
H	-0.399634245	6.474419808	13.624786415
C	2.573673136	7.455944673	12.056810730
H	3.190365448	7.246626977	11.170279911
C	3.368886292	8.416690467	12.961605849
H	4.280992703	7.942336438	13.341208809
H	2.758126083	8.680055958	13.835057114
C	3.727795317	9.703337458	12.194627789
H	4.274269783	10.388465682	12.853217901
H	4.409498547	9.448325294	11.370526411
C	2.474872756	10.388968966	11.626245371
H	1.849827244	10.742850933	12.459175483
H	2.757637307	11.276162220	11.048275086
C	1.652403191	9.423995986	10.758135690
H	2.227708976	9.150424689	9.861653549
H	0.734704103	9.907761280	10.405043565
C	1.294081910	8.145140509	11.531794279
H	0.725016905	7.469453883	10.884241197
H	0.634768499	8.405743622	12.367005007

O	-0.879991870	4.437941149	12.541001636
H	-0.337899576	4.004088041	13.230304573
C	-2.044720749	3.668517127	12.487979842
C	-2.793587550	3.649969368	13.667126097
C	-2.398269686	2.955685090	11.343525996
C	-3.904987687	2.808809352	13.750281107
C	-3.432302799	1.993889951	11.533471253
C	-4.203542735	1.944803839	12.685915899
H	-2.484082567	4.291001625	14.482547219
H	-5.011042382	1.234305727	12.807018971
O	-3.547046226	1.082287468	10.528921858
C	-4.785451459	0.392668107	10.335515383
H	-4.952700172	-0.355131988	11.119146839
H	-5.619405119	1.101827868	10.310068048
H	-4.697520758	-0.102706677	9.368206915
O	-4.719096842	2.715239717	14.825695714
C	-4.491588337	3.586455361	15.931420647
H	-4.556538766	4.639150053	15.629385384
H	-5.279443220	3.365566290	16.652168156
H	-3.513644497	3.400178188	16.393762323
H	-1.306048044	1.068531320	10.149366863
O	-0.795479563	1.864066871	9.916819297
C	-1.719963156	3.034061942	9.977973370
C	-0.756101732	4.177892858	9.637610069
C	-2.712036337	2.951446752	8.815511765
C	-1.186102178	5.597167861	9.577415168
C	-2.376516373	2.266043843	7.644591012
C	-3.909362681	3.673440412	8.865677096
C	-3.238170431	2.282671266	6.548042206
H	-1.442777724	1.715888084	7.594330735
C	-4.767594405	3.690882983	7.767138854
H	-4.174235461	4.218549916	9.765556190
C	-4.437322164	2.993135278	6.604896999
H	-2.969332105	1.740008863	5.646513551
H	-5.695325914	4.253158748	7.819914822
H	-5.106333696	3.006687583	5.749789983
C	-0.553708038	6.432341995	8.618846865
C	-2.087362105	6.225725319	10.471101620
C	-0.783185391	7.803180002	8.573792531
H	0.129764346	5.978763722	7.906123896
C	-2.314564126	7.600732266	10.423732285
H	-2.627171782	5.636699006	11.200730124
C	-1.659582410	8.400826236	9.485670919
H	-0.274162229	8.407892749	7.828956457
H	-3.011244574	8.048550936	11.127349517
H	-1.835858876	9.471983198	9.457316989
O	0.540949302	2.479004271	13.537445918
H	0.536959982	1.949691397	14.345835520
C	1.320681011	1.881889469	12.575949701
C	2.016576864	0.732223425	12.927238865
C	1.337014805	2.490594380	11.281154685
C	2.873052907	0.152639770	11.977204356
H	1.931936784	0.327829200	13.929812166
C	2.260063928	1.843366058	10.367716389
C	2.994838755	0.710094883	10.696046328
O	3.614790239	-0.947010245	12.198966477
O	2.283390298	2.377552801	9.135410679
H	3.660142315	0.220601074	9.997467191
C	3.119724788	1.816704903	8.122957578
H	4.171622563	1.854285159	8.419616355
H	2.834704038	0.783215428	7.900966103
H	2.968586606	2.440198894	7.243438684
C	3.572872952	-1.577807941	13.481156375
H	2.561313309	-1.934504202	13.715362262
H	4.249939757	-2.431134534	13.412102376
H	3.921226826	-0.896759274	14.267798726
H	-0.317089810	3.880020508	8.684532751
H	0.213471978	2.192467548	10.667931994

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Ru	0.750063236	5.398205284	10.256581420
P	2.595668452	6.194178660	11.526999378
O	1.415563114	7.396194458	8.132364863
C	1.174840392	6.619192011	8.958636555
C	4.298925823	5.912190472	10.773924397
H	4.942627871	6.567338983	11.378722724
C	4.394660996	6.392267132	9.309459779
H	4.034374891	7.421283975	9.204412861
H	3.750098179	5.768255773	8.683771632
C	5.838996780	6.302499682	8.789287687
H	5.869332110	6.625898928	7.742136407
H	6.476013455	6.999820975	9.351676564
C	6.392139536	4.878409208	8.933142618
H	7.429127500	4.832472192	8.581689204
H	5.810584483	4.198253677	8.293187714
C	6.294639443	4.396606397	10.386918970
H	6.945830230	5.016168329	11.020374815
H	6.658157351	3.366248696	10.475753345
C	4.847770669	4.472641591	10.906224031
H	4.227548315	3.786951272	10.327335297
H	4.815484142	4.123807000	11.941368131
C	2.705168597	5.330768034	13.183829121
H	2.714070754	4.279571701	12.863171286
C	3.967018270	5.564312957	14.049329188
H	4.889280672	5.488607029	13.467559158
H	3.945370749	6.571962011	14.473331974
C	3.985051892	4.545360923	15.204052551
H	4.053624686	3.529141023	14.789219620
H	4.882784403	4.696581446	15.814438871
C	2.721043504	4.666825926	16.070863228
H	2.728289415	3.910469994	16.863983917
H	2.725484337	5.645760082	16.570990759
C	1.445046375	4.541475233	15.223604837
H	0.555718848	4.705081863	15.844544645
H	1.367052963	3.520635019	14.822148472
C	1.442946542	5.524088256	14.040655461
H	1.407918299	6.557351837	14.414416990
H	0.552164485	5.365311469	13.435458225
C	2.591002497	8.070792698	11.705924678
H	2.975342219	8.389756662	10.726671852
C	3.538732883	8.635736796	12.785924561
H	4.542197301	8.205854365	12.703226459
H	3.152723023	8.363293190	13.775646808
C	3.614964469	10.170246212	12.695264768
H	4.295000770	10.548581401	13.466951644
H	4.047671512	10.455849884	11.726052618
C	2.223014846	10.800563745	12.844984771
H	1.840403116	10.593884069	13.854889278
H	2.283034607	11.890240912	12.748863646
C	1.249460834	10.227462854	11.805834832
H	1.570967357	10.532113323	10.799664275
H	0.243538502	10.638754811	11.950460776
C	1.189346972	8.690551324	11.859668880
H	0.532507562	8.329517303	11.064381727
H	0.747792097	8.367267162	12.812070283
O	-3.577250433	1.257074625	12.120031596
H	-3.817027589	0.638866873	12.822831353
C	-2.488676862	0.789990829	11.442578161
C	-1.779110536	-0.326518881	11.912587947
C	-2.138503126	1.451493854	10.258436888
C	-0.731855686	-0.838885354	11.144623517
C	-1.052384951	0.907803918	9.530450683
C	-0.364793765	-0.224804571	9.938139694
H	-2.077467982	-0.790691353	12.845679945

H	0.471012221	-0.624710999	9.379683604
O	-0.734421554	1.599986319	8.392749525
C	-0.101944706	0.904000270	7.312422304
H	0.935432523	0.654809132	7.553187679
H	-0.665561091	-0.001148798	7.064760271
H	-0.125199934	1.592226261	6.465845001
O	0.024175598	-1.913183064	11.496144359
C	-0.330390883	-2.650975689	12.664011264
H	-1.351080385	-3.045267510	12.590323238
H	0.374758491	-3.481047594	12.718253934
H	-0.239734061	-2.037417170	13.569471525
H	-0.745702381	3.507681164	8.506654464
O	-0.608276612	4.471386760	8.411628004
C	-3.016609616	2.439909821	9.562622653
C	-3.199500850	3.735026289	9.890325941
C	-3.684149795	1.914078279	8.332774824
C	-2.600891620	4.569129559	10.943729201
C	-3.742150150	2.681772467	7.157324776
C	-4.259204553	0.633856193	8.323679668
C	-4.386248095	2.196825471	6.020028657
H	-3.250338055	3.650269555	7.130433989
C	-4.907750966	0.151500244	7.187333923
H	-4.212297518	0.021257809	9.218844792
C	-4.978073154	0.931567473	6.031077488
H	-4.416920896	2.804327235	5.119613592
H	-5.362453005	-0.835096479	7.206310782
H	-5.480611908	0.554116498	5.145434757
C	-2.205294056	5.877222967	10.580629155
C	-2.484056111	4.192611725	12.290632256
C	-1.726904309	6.776543044	11.535272451
H	-2.314819620	6.191575751	9.547618579
C	-2.010194990	5.098775188	13.246054765
H	-2.837544271	3.217311828	12.600040293
C	-1.639694204	6.390328747	12.880001061
H	-1.485750757	7.790910612	11.238207775
H	-1.949962225	4.794281531	14.287307231
H	-1.294439654	7.096734369	13.628113344
O	0.658447436	3.482894261	11.660373589
H	-0.198851956	3.015108047	11.657307441
C	1.538356256	2.899852011	10.702123659
C	1.795977477	3.788156651	9.676263021
C	2.067408969	1.622004639	10.806910129
C	2.469593737	3.301357259	8.551862125
H	0.143227623	4.537463667	7.799138344
C	2.836638455	1.193161107	9.713996698
C	3.019198428	2.015953866	8.583778531
O	2.481680561	4.133940303	7.463268821
O	3.400513622	-0.040090370	9.617809161
H	3.578649242	1.603025570	7.753180123
C	3.386266073	-0.887944820	10.767617692
H	3.849372403	-0.389861215	11.629219744
H	2.369691191	-1.204431101	11.028505256
H	3.977330389	-1.763577767	10.495483355
C	3.182646618	3.712678066	6.292133847
H	2.754253724	2.789593265	5.882277911
H	3.069457831	4.521145219	5.569085739
H	4.247203390	3.556445730	6.502095577
H	-3.852353309	4.298391872	9.226644803
H	1.830614363	0.984992419	11.648269458

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Ru	1.067173606	4.898456210	11.398693259
P	2.759115367	6.146886436	12.338033216
O	1.202773199	6.394677216	8.814005421
C	1.164602394	5.818129551	9.816679216
C	4.463508810	6.027505365	11.592293442

H	5.033785284	6.822702332	12.095248698
C	4.453832644	6.329473351	10.077116445
H	3.992785461	7.302293916	9.873473299
H	3.851697740	5.571740974	9.565629642
C	5.881228824	6.305624647	9.505042711
H	5.843001471	6.499455846	8.426949366
H	6.470182183	7.120031008	9.950133501
C	6.568527829	4.963420838	9.790487732
H	7.589304115	4.964250535	9.392391816
H	6.024878371	4.161132790	9.270108418
C	6.581665491	4.663427857	11.295753922
H	7.195925426	5.414717698	11.812363836
H	7.045384826	3.689903043	11.491206670
C	5.158458189	4.676969748	11.880150454
H	4.574780253	3.869320730	11.427728370
H	5.200886347	4.473672671	12.954839301
C	2.933947970	5.637153259	14.122980335
H	3.120112214	4.559123206	14.025361030
C	4.122589315	6.255117189	14.896173377
H	5.056160803	6.173949360	14.331749433
H	3.943679967	7.323423074	15.058339608
C	4.271574112	5.551519414	16.257956596
H	4.532425860	4.496981782	16.088843164
H	5.106407721	5.996293770	16.811107511
C	2.976939634	5.636241495	17.081925698
H	3.091520970	5.090997312	18.025154257
H	2.788657586	6.686020139	17.347601464
C	1.770844666	5.095755218	16.296682257
H	0.849448803	5.220812054	16.876882672
H	1.895866952	4.016616550	16.125450193
C	1.630539853	5.799834743	14.936243708
H	1.437534025	6.866802477	15.102982848
H	0.766907277	5.401649325	14.390340284
C	2.252552439	7.935027207	12.156286705
H	2.406442176	8.104033206	11.080866714
C	3.096116367	8.970659523	12.927231918
H	4.166967749	8.825516913	12.745627202
H	2.931691071	8.839791552	14.003857843
C	2.677992386	10.397658961	12.528290387
H	3.270371480	11.125738391	13.093606724
H	2.912694884	10.556965900	11.466830793
C	1.176757477	10.627678002	12.763186244
H	0.969039631	10.575476401	13.841629636
H	0.892916639	11.634683368	12.438487721
C	0.327338427	9.574343254	12.034560205
H	0.446209605	9.694260534	10.948262117
H	-0.737829073	9.711377520	12.249964332
C	0.745121920	8.148692509	12.428538286
H	0.129135383	7.427966247	11.871061863
H	0.529257592	7.988009727	13.490561688
O	1.324164169	3.140819109	13.021168465
H	0.707744286	2.552211883	13.478721178
C	2.007564286	2.468456050	11.976321759
C	2.515697469	1.180616695	12.079084652
C	2.127299061	3.296716054	10.872523094
C	3.194890127	0.706661215	10.943577188
C	2.786166205	2.785355467	9.741525275
C	3.340801672	1.504718558	9.792009609
H	2.402431344	0.598443757	12.985143226
H	3.856167996	1.064317894	8.948256761
O	2.824549421	3.598657510	8.649555653
C	3.459132679	3.120278445	7.463417212
H	4.521774344	2.910174483	7.635281561
H	2.962740241	2.216799132	7.088670284
H	3.362887405	3.923236057	6.731470036
O	3.758961777	-0.522832130	10.854596608
C	3.671815421	-1.401148677	11.971355230
H	2.627766027	-1.638095642	12.215548732

H	4.188133262	-2.314636240	11.674544502
H	4.164865910	-0.977236578	12.855551186
H	-0.339609742	3.862839619	7.873316713
O	-1.095888091	4.105192818	8.442279143
C	-1.271895181	3.144404142	9.412191708
C	-1.861765892	3.480153344	10.599427616
C	-0.778484917	1.793929612	9.072080019
H	-2.056031740	2.667737474	11.300095869
C	-2.182183669	4.825065716	11.097962169
C	-0.347570442	0.889392298	10.068768220
C	-0.694916189	1.406855076	7.713597665
C	0.149631214	-0.361563969	9.720257387
H	-0.364780840	1.185944631	11.117012655
C	-0.191685641	0.153555512	7.365740406
H	-1.065704122	2.071939717	6.927744195
C	0.233308670	-0.733905095	8.368495702
H	0.490770764	-1.043852161	10.504235954
H	-0.146383467	-0.132680241	6.313080602
H	0.627692146	-1.709524175	8.099479003
C	-2.278734310	5.986863381	10.292772219
C	-2.349919478	4.977816110	12.499477311
C	-2.555102328	7.225821666	10.869419640
H	-2.163849686	5.906974657	9.218028922
C	-2.607332510	6.222292673	13.069892935
H	-2.292904350	4.097072045	13.139940698
C	-2.725919465	7.353434758	12.253422231
H	-2.643727989	8.100105842	10.226723770
H	-2.738221060	6.304777555	14.148363873
H	-2.944398631	8.322960361	12.691997209

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Ru	0.827539027	4.776070236	11.376416440
P	2.540624431	6.149248500	12.279595018
O	1.192081240	6.075617203	8.718020576
C	1.061918002	5.569983300	9.754038324
C	4.290709337	5.915080937	11.650577493
H	4.846796591	6.763888011	12.071584339
C	4.359941581	6.019581497	10.111365297
H	3.937880770	6.971187527	9.768331260
H	3.755158399	5.222976742	9.667674750
C	5.806416160	5.888194305	9.605238949
H	5.812362688	5.933260391	8.509909579
H	6.398905121	6.744416075	9.957810062
C	6.452000386	4.586240279	10.099388094
H	7.484725474	4.510313018	9.741018638
H	5.904973133	3.727641585	9.682383871
C	6.408440602	4.509907012	11.631910051
H	7.015622412	5.323534245	12.053991208
H	6.851028461	3.571333517	11.984938686
C	4.965576004	4.618804917	12.155134289
H	4.398130037	3.751447395	11.810251875
H	4.970717975	4.581837992	13.249368924
C	2.659558069	5.873462105	14.126134090
H	2.905079393	4.803864847	14.162491263
C	3.777286631	6.643090097	14.865191728
H	4.738234805	6.553778503	14.349747340
H	3.530685753	7.710468829	14.893835757
C	3.908540308	6.116146381	16.306610185
H	4.235605038	5.066841571	16.274338136
H	4.692763588	6.672454784	16.832342081
C	2.578241727	6.215435998	17.069532275
H	2.684446157	5.793410495	18.075071065
H	2.316928587	7.275201600	17.199773514
C	1.442487694	5.511520009	16.310429351
H	0.490570057	5.641854242	16.839024290
H	1.639846941	4.429843329	16.273832029

C	1.319875984	6.043968673	14.873153321
H	1.051351591	7.106400866	14.908298660
H	0.509887590	5.533930535	14.345147470
C	2.128552006	7.926531676	11.850460502
H	2.143760992	7.894062936	10.751389184
C	3.127785942	9.016925196	12.288998162
H	4.151516408	8.761887105	11.995696602
H	3.119173092	9.105581303	13.381638212
C	2.733146572	10.371985200	11.670643786
H	3.436330064	11.144731084	12.001405300
H	2.828803305	10.307279329	10.577464361
C	1.292939155	10.764792102	12.036102142
H	1.231068177	10.936924114	13.120274509
H	1.024572835	11.710880800	11.552963537
C	0.296745050	9.661826237	11.645583306
H	0.268435153	9.560127618	10.551155952
H	-0.718307871	9.927130539	11.963281588
C	0.693128741	8.312621696	12.264971669
H	-0.021063976	7.538682627	11.966937493
H	0.634074983	8.391424299	13.356502475
O	1.218826586	3.218354910	13.245183966
H	0.695008109	2.618198790	13.793253584
C	1.980122991	2.505221025	12.289639843
C	2.587104273	1.279482999	12.542861867
C	2.037737097	3.197289128	11.093098090
C	3.298984553	0.716895509	11.471329476
C	2.725820400	2.594470239	10.030064595
C	3.367669857	1.368306727	10.226658130
H	2.514977885	0.806378738	13.514598753
H	3.911331815	0.867475181	9.435935477
O	2.693038383	3.263292800	8.842502284
C	3.316849600	2.667410563	7.707174693
H	4.393534816	2.532368548	7.866173113
H	2.856430041	1.701232420	7.467072030
H	3.159401193	3.363545905	6.882435763
O	3.954252374	-0.472008649	11.531472654
C	3.944610964	-1.193270255	12.757825390
H	2.924621196	-1.476993758	13.050091599
H	4.531138995	-2.095374809	12.580212345
H	4.406287896	-0.614755667	13.568576315
H	-0.816625806	4.203248590	7.912220077
O	-1.326645998	4.399489539	8.711429134
C	-1.112353458	3.453086716	9.651726915
C	-1.329754857	3.780335035	10.978631751
C	-0.752815265	2.102962829	9.179327619
H	-1.345772302	2.938236372	11.662441495
C	-1.806956343	5.050882435	11.553432491
C	-0.221266668	1.125570067	10.038713262
C	-0.955238627	1.769435751	7.826329508
C	0.118084807	-0.132487466	9.555236534
H	-0.031773349	1.356816527	11.078063560
C	-0.612519563	0.508842772	7.344596405
H	-1.429446730	2.473183186	7.147912840
C	-0.068762228	-0.444655120	8.206421697
H	0.548167753	-0.865176010	10.230539439
H	-0.785098425	0.268523497	6.299951087
H	0.201706813	-1.426883741	7.830840562
C	-2.247430908	6.175524182	10.812577984
C	-1.829554757	5.145647300	12.968076569
C	-2.698974032	7.317363636	11.466513282
H	-2.250120286	6.135451426	9.733168697
C	-2.272559005	6.298390147	13.612625148
H	-1.524224717	4.284636651	13.557958344
C	-2.714412316	7.388424777	12.863110288
H	-3.043918756	8.162269010	10.877910347
H	-2.279874850	6.338157133	14.697673809
H	-3.070201157	8.285734968	13.360208241

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Ru	0.358368681	4.949002104	10.302604692
P	2.136352749	5.986509800	11.542637271
O	1.042364404	6.857146360	8.132474474
C	0.799510599	6.085827545	8.967341828
C	3.886780855	5.450126577	11.143372213
H	4.547668874	5.969712982	11.850392932
C	4.308075386	5.840298651	9.711089295
H	4.219844353	6.920844062	9.556342094
H	3.627612938	5.362124614	8.994839909
C	5.756627163	5.404249320	9.427340448
H	6.026091597	5.668741675	8.397542114
H	6.433795244	5.972574412	10.080288858
C	5.962786653	3.900756156	9.667656189
H	7.014724496	3.632692997	9.517544058
H	5.381594564	3.333606082	8.927806609
C	5.504010126	3.489936352	11.075320140
H	6.171056601	3.938981814	11.824718075
H	5.584632039	2.402405415	11.197351631
C	4.056956960	3.932539460	11.347445454
H	3.389825786	3.417114130	10.655279462
H	3.759070274	3.632410704	12.358937598
C	1.887479430	5.546713126	13.348327783
H	1.634040807	4.475867502	13.280783155
C	3.095482971	5.676054197	14.298379457
H	3.983700553	5.187100899	13.887552791
H	3.349102045	6.735637937	14.424056903
C	2.748797330	5.062376462	15.668472065
H	2.580885515	3.982747752	15.542021738
H	3.602338665	5.168710663	16.347532077
C	1.494094646	5.705380439	16.282292615
H	1.243618524	5.219347381	17.231794720
H	1.708444041	6.757808021	16.515859124
C	0.297901554	5.644283649	15.318488942
H	-0.565058961	6.168004567	15.745903694
H	-0.006585825	4.597178994	15.173845446
C	0.657494534	6.258412127	13.955554370
H	0.891853513	7.320414474	14.099009625
H	-0.198968566	6.212374111	13.271220926
C	2.173773206	7.848380734	11.331647198
H	2.456655657	7.935668569	10.273295620
C	3.227088958	8.607763510	12.163055494
H	4.215281664	8.143568145	12.068997869
H	2.952338336	8.564531706	13.225215084
C	3.299830871	10.081600968	11.719701152
H	4.031429283	10.616462612	12.336228194
H	3.669498546	10.123755267	10.685189484
C	1.926629875	10.767264611	11.797557116
H	1.609499546	10.820931296	12.849133253
H	1.997348334	11.799760298	11.437407847
C	0.871803642	9.989387701	10.995642951
H	1.128229550	10.016296518	9.926951974
H	-0.113114590	10.461024370	11.093911080
C	0.789307415	8.522576119	11.449891848
H	0.046259645	7.988291350	10.850737992
H	0.439576153	8.488317038	12.487967645
O	0.207332339	2.103050136	11.230336454
H	0.323792462	1.345920915	11.820431899
C	1.112305733	2.056948140	10.206302047
C	2.081594371	1.065764755	10.166299111
C	0.971746025	3.087660433	9.232992743
C	2.971311993	1.055420512	9.081243898
C	1.966256407	3.065610087	8.197146736
C	2.922738997	2.063139684	8.101681662
H	2.153397371	0.338653662	10.966982560
H	3.652580759	2.022044157	7.304485745

O	1.874902138	4.067733373	7.297121016
C	2.808710386	4.144046726	6.217178018
H	3.832688368	4.252972097	6.592449001
H	2.745795595	3.261931475	5.568680025
H	2.528485959	5.036185828	5.657257349
O	3.935454365	0.137018902	8.905402027
C	4.064798842	-0.934988818	9.843864579
H	3.148930369	-1.535978881	9.884763579
H	4.887657407	-1.548770523	9.477930160
H	4.308048837	-0.556656487	10.843794352
H	-0.486442423	3.401023717	6.676101946
O	-0.863292731	3.905481743	7.407421613
C	-0.849854584	3.165424394	8.564720691
C	-1.427878477	3.922898022	9.676716487
C	-1.233455187	1.724121364	8.351859184
C	-2.013108070	5.249189084	9.712660290
C	-0.635000760	1.001023009	7.308006992
C	-2.186058685	1.088710483	9.154094361
C	-0.998730388	-0.317582303	7.053996741
H	0.150606614	1.452866120	6.705945400
C	-2.548815689	-0.235055175	8.901596131
H	-2.671888856	1.628547623	9.958822410
C	-1.967143457	-0.939823364	7.848064499
H	-0.527290684	-0.860230429	6.239816702
H	-3.299555183	-0.711115273	9.525738617
H	-2.258505113	-1.967006723	7.649808313
C	-2.131371472	5.808723168	11.026242622
C	-2.361321324	6.074987697	8.606425185
C	-2.565513916	7.129626222	11.212930604
H	-1.999620744	5.165101971	11.895012655
C	-2.795856637	7.370514650	8.817788092
H	-2.275184487	5.677369480	7.605234563
C	-2.890185645	7.912464598	10.114735730
H	-2.657145607	7.526073419	12.219792934
H	-3.068207390	7.982533453	7.962456380
H	-3.231007694	8.934259216	10.251243458
H	-1.652895472	3.325001618	10.555068981

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Ru	0.640340578	4.847834634	10.289992651
P	2.440351356	5.789344502	11.549657598
O	1.314734953	6.870714391	8.222202086
C	1.076553480	6.085502648	9.047297328
C	4.140623347	5.157171726	11.093634479
H	4.851222914	5.612812953	11.795853502
C	4.553690520	5.561687466	9.662455241
H	4.517881141	6.648025979	9.530567439
H	3.834549411	5.129241893	8.952984922
C	5.973125613	5.058969321	9.342662206
H	6.242812876	5.342294791	8.318065559
H	6.686201739	5.571159315	10.003630704
C	6.100292078	3.540051157	9.528658602
H	7.137742375	3.225262368	9.369019518
H	5.499493371	3.027300924	8.769726950
C	5.623036684	3.101626592	10.921119367
H	6.318785076	3.478653665	11.683803680
H	5.639334665	2.007856994	10.998702485
C	4.209716509	3.622684730	11.235776804
H	3.486479241	3.178892747	10.542367249
H	3.915981145	3.301506067	12.241280674
C	2.193097043	5.274086378	13.342786684
H	1.886090655	4.219799465	13.245154828
C	3.438449519	5.305147534	14.260398753
H	4.278562472	4.765683037	13.814242542
H	3.765970368	6.341510368	14.397847637
C	3.104132575	4.687310323	15.631462358

H	2.866920488	3.622209618	15.494204604
H	3.988900124	4.729554352	16.276654519
C	1.915663844	5.391664006	16.302949035
H	1.673554234	4.905396274	17.254300825
H	2.197479847	6.426964864	16.541583957
C	0.687124162	5.407757872	15.381494400
H	-0.136005935	5.962569246	15.846509825
H	0.327356003	4.379571776	15.228420459
C	1.027976110	6.030624965	14.018084527
H	1.320843754	7.077031911	14.168134325
H	0.147118546	6.042678378	13.371694221
C	2.618797736	7.653846647	11.417783592
H	3.012458425	7.763364945	10.397355207
C	3.635502627	8.295001898	12.385078701
H	4.594603739	7.765981415	12.362644306
H	3.253924954	8.222886662	13.411293018
C	3.848948848	9.779707524	12.037035525
H	4.559428315	10.223813043	12.743443071
H	4.309473515	9.851600352	11.041367365
C	2.524517467	10.557371950	12.043787551
H	2.118727545	10.571114832	13.065655010
H	2.696270626	11.601705489	11.760503076
C	1.500817490	9.906805648	11.102699899
H	1.853817105	9.985014229	10.064477138
H	0.542322652	10.437420941	11.147268994
C	1.282470006	8.423822187	11.445170640
H	0.573138550	7.983743650	10.743176755
H	0.827380936	8.346847775	12.439474758
O	0.138334114	1.342524716	10.574271089
H	0.299446439	0.465233636	10.946133996
C	1.112536321	1.660777588	9.678753731
C	2.303124248	0.937094935	9.672158076
C	0.824475110	2.718368671	8.763722155
C	3.267424627	1.235623565	8.704840310
C	1.895418919	3.033270234	7.852934086
C	3.069011749	2.298016333	7.808712927
H	2.455666303	0.152639994	10.403685920
H	3.857280826	2.515488662	7.102082162
O	1.689010286	4.094283548	7.028177210
C	2.672880180	4.465688949	6.055433459
H	3.617097813	4.730125629	6.542835954
H	2.833143343	3.659613000	5.332099806
H	2.264403430	5.342130681	5.553734030
O	4.445190696	0.597085234	8.577754698
C	4.724550780	-0.528375980	9.414479698
H	3.978271080	-1.318757152	9.274778393
H	5.703346117	-0.891417869	9.102044739
H	4.764160185	-0.235404732	10.470267717
H	-0.083874234	4.308637329	7.101646723
O	-0.890368394	3.805341571	7.288444192
C	-0.709931135	3.021838549	8.453776920
C	-1.149329690	3.752230024	9.714044864
C	-1.485345935	1.730953149	8.181869501
C	-1.629378936	5.088303081	9.865485124
C	-0.935915311	0.761542285	7.336030381
C	-2.778941264	1.553782668	8.673440513
C	-1.664562815	-0.376841739	6.999973341
H	0.062739103	0.901622056	6.931684959
C	-3.513459890	0.415220172	8.334820656
H	-3.223805612	2.309130970	9.315613951
C	-2.957200302	-0.553836110	7.500758002
H	-1.229016201	-1.122458014	6.340696508
H	-4.521263045	0.289393197	8.720104001
H	-3.527536077	-1.439635503	7.236773832
C	-2.107518301	5.971702622	8.837888402
C	-1.409478652	5.645176090	11.183715072
C	-2.414737788	7.274837692	9.145997979
H	-2.248436932	5.574828649	7.842464942

C	-1.764138528	6.990468167	11.464116029
H	-1.283979470	4.960043891	12.024039535
C	-2.246024296	7.795421554	10.458087197
H	-2.809825542	7.922744147	8.368682770
H	-1.655532636	7.370093489	12.474683149
H	-2.515235824	8.826907707	10.663088313
H	-1.271095179	3.099392237	10.577973492

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Ru	0.553585556	5.028069361	10.339296172
P	2.278159963	5.817808117	11.706916985
O	1.204125384	7.141935084	8.344402249
C	0.981191648	6.349296961	9.160825372
C	3.750225074	4.731877544	11.294560023
H	4.512332006	4.842784561	12.075906744
C	4.384427489	5.110059767	9.938229962
H	4.794221450	6.124711109	9.975751751
H	3.607314056	5.108873119	9.160951716
C	5.494084013	4.120268407	9.542312721
H	5.904452879	4.405389818	8.566826206
H	6.319432315	4.196014395	10.264116001
C	4.975263918	2.675683287	9.508570987
H	5.783244142	1.984594114	9.241448775
H	4.202897920	2.583367501	8.732975587
C	4.359723141	2.278680519	10.857037936
H	5.140134895	2.265203284	11.631130480
H	3.941236045	1.266737377	10.807573806
C	3.256019041	3.263910697	11.273307684
H	2.432459944	3.176735274	10.539042734
H	2.842670466	2.977784793	12.247526049
C	1.840397512	5.424480059	13.487005244
H	1.317646948	4.458173424	13.395133783
C	3.022372509	5.212888237	14.459070113
H	3.720121699	4.464478315	14.069968600
H	3.583688795	6.148933831	14.562666237
C	2.507812087	4.763759278	15.839923180
H	2.048149210	3.769775710	15.741921065
H	3.354731072	4.650044248	16.525788507
C	1.476498144	5.745317570	16.416354567
H	1.102659634	5.380011171	17.379053239
H	1.965333910	6.709678426	16.614363222
C	0.312870516	5.966085051	15.438336075
H	-0.393283455	6.702459558	15.838858606
H	-0.246685130	5.027524868	15.313050000
C	0.830329224	6.435622370	14.069619952
H	1.328162295	7.404415125	14.196256522
H	0.001149198	6.593820839	13.372490646
C	2.833528719	7.583346677	11.494817445
H	3.202986877	7.563522829	10.459575998
C	3.998901838	8.032108069	12.399039357
H	4.813489365	7.298232969	12.384810282
H	3.647441045	8.101599734	13.436620836
C	4.518190807	9.409612557	11.945097154
H	5.327518122	9.736424025	12.607669054
H	4.954255048	9.311350429	10.940770823
C	3.393121242	10.456682706	11.913859405
H	3.042159974	10.638766565	12.939808708
H	3.778165005	11.412225618	11.540843363
C	2.208282092	9.987135135	11.054644495
H	2.519984203	9.908128492	10.003527823
H	1.396961443	10.723544717	11.086604017
C	1.685838762	8.619372073	11.525456228
H	0.847319590	8.294654021	10.902459160
H	1.299574750	8.716856876	12.546119352
O	-2.364446388	1.176889828	10.185979868
H	-2.954674541	0.498024102	10.535739154
C	-1.160806045	0.620601189	9.857060898

C	-0.885926029	-0.698542816	10.222337516
C	-0.247395104	1.431291939	9.150661539
C	0.349380731	-1.263197318	9.896785837
C	0.985156696	0.815334264	8.849071903
C	1.297176102	-0.484775584	9.226223457
H	-1.638243250	-1.262927807	10.760790212
H	2.267570308	-0.912270555	9.004654144
O	1.966918110	1.544797068	8.172350365
C	2.421796841	1.001956964	6.914210894
H	2.794817907	-0.016227878	7.033590387
H	1.607891324	1.008859127	6.181261068
H	3.235212352	1.650311194	6.584498269
O	0.721463804	-2.530422529	10.194315817
C	-0.233133569	-3.400434343	10.800878211
H	-1.128142642	-3.504681714	10.176964253
H	0.259991664	-4.368517907	10.891172933
H	-0.521076183	-3.046667413	11.798836979
H	1.191197967	2.966106316	8.020779798
O	0.439488918	3.584048990	8.143221899
C	-0.686217702	2.832182274	8.662710371
C	-1.142483839	3.692660092	9.847097734
C	-1.715458782	2.661584649	7.536674575
C	-1.661903583	5.016573109	9.806064738
C	-1.251736951	2.405888707	6.240510995
C	-3.094094234	2.735265944	7.759651587
C	-2.145886116	2.226482202	5.186326691
H	-0.183880549	2.378086180	6.051181257
C	-3.991010151	2.563106843	6.703374880
H	-3.465760240	2.940458362	8.755610888
C	-3.521159392	2.305789531	5.415081157
H	-1.769159624	2.033304839	4.186428457
H	-5.058812857	2.637694949	6.888250885
H	-4.218881764	2.175757087	4.594778619
C	-2.058436707	5.758720610	8.637203367
C	-1.476737007	5.755852099	11.049329752
C	-2.353599914	7.092748927	8.742717493
H	-2.129956507	5.244495421	7.687882916
C	-1.825968961	7.142089630	11.110845373
H	-1.459672483	5.197624072	11.987708525
C	-2.246309881	7.794905318	9.981662972
H	-2.676330262	7.634599537	7.858741767
H	-1.762592676	7.660207003	12.062522710
H	-2.507577355	8.847760888	10.020854443
H	-1.252503846	3.174649871	10.800322565

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Ru	1.330966177	3.043696384	13.220602005
P	2.258970237	5.171757024	12.769570347
O	3.558675004	1.524897999	11.918566811
C	2.715699013	2.167949449	12.388138493
C	3.770766290	5.261554424	11.665355148
H	3.977376087	6.333666450	11.553363194
C	3.460399988	4.686502273	10.262678934
H	2.605941955	5.200397411	9.811018736
H	3.167573255	3.636189367	10.345465315
C	4.679169001	4.789865724	9.331895571
H	4.429845416	4.336185461	8.365973315
H	4.903895540	5.848439464	9.136311903
C	5.909982849	4.113607140	9.951090741
H	6.773615917	4.204506009	9.282924664
H	5.711825399	3.039338768	10.071710763
C	6.232796312	4.727768091	11.320522598
H	6.503233269	5.785321594	11.189913515
H	7.101804530	4.235297146	11.771325983
C	5.036420194	4.627683307	12.285610772
H	4.861562875	3.573876370	12.522862590

H	5.292772640	5.128959942	13.225705304
C	2.834154091	5.908198802	14.401294700
H	3.736229949	5.315748930	14.609619585
C	3.246013045	7.393766980	14.361789432
H	3.951489477	7.578164715	13.544381764
H	2.359533598	8.009270102	14.163448576
C	3.864671505	7.827399859	15.702681851
H	4.798219133	7.270819299	15.866083104
H	4.135330775	8.888072479	15.658394298
C	2.901733274	7.566154658	16.870365255
H	3.366053695	7.852261737	17.820238094
H	2.009779476	8.198539047	16.753123944
C	2.475691906	6.091708020	16.915375732
H	1.758400839	5.919632939	17.726362347
H	3.351777548	5.465047855	17.132865266
C	1.866619735	5.636686085	15.576835053
H	0.921701176	6.176199490	15.411397557
H	1.637430382	4.563647761	15.638747372
C	1.031472832	6.312001363	11.910240407
H	0.691444908	5.665718618	11.092023618
C	1.600647385	7.598540136	11.266002422
H	2.452745883	7.372374248	10.620226457
H	1.962373585	8.280410953	12.043624182
C	0.516879071	8.306632352	10.432113762
H	0.934265442	9.219450704	9.992455459
H	0.231149505	7.656274357	9.592866397
C	-0.725207490	8.632650553	11.272468093
H	-0.455594128	9.360610145	12.051030470
H	-1.493679055	9.106674313	10.652045833
C	-1.281768031	7.366723023	11.937278310
H	-1.648045351	6.676786762	11.163116157
H	-2.141606402	7.607805207	12.573405371
C	-0.204286745	6.651214678	12.771071065
H	-0.632875276	5.742932826	13.201288330
H	0.095945277	7.301844846	13.603258499
O	-0.487083259	3.695998900	14.363281142
H	-0.481105634	4.517313600	14.872652770
C	-1.798383662	3.231350098	14.189740601
C	-2.785590849	3.861836273	14.939109748
C	-2.015460994	2.150951013	13.316897003
C	-4.093394285	3.371643077	14.851894488
C	-3.343982431	1.621790020	13.345359983
C	-4.360637654	2.245744280	14.069466151
H	-2.525533585	4.686192882	15.592814488
H	-5.371715100	1.862628158	14.069639010
O	-3.559745261	0.487045059	12.656223491
C	-4.881325172	-0.024643823	12.491602816
H	-5.302733229	-0.357625960	13.447193308
H	-5.542737249	0.720991971	12.035344483
H	-4.773568279	-0.877186329	11.820624445
O	-5.150152020	3.894187171	15.508416892
C	-4.952998881	5.040011630	16.334476015
H	-4.569691668	5.888697694	15.753999473
H	-5.935578711	5.290515409	16.734517750
H	-4.269273152	4.820636592	17.164182480
H	-0.218665528	0.875162074	14.218862228
O	0.200853027	1.148153756	13.389264289
C	-0.863398318	1.624437050	12.445898328
C	-0.124155730	2.826738656	11.730574693
C	-1.191035412	0.502589472	11.472417938
C	-0.645253819	-0.771418322	11.616987528
C	-1.985469930	0.782685391	10.351594700
C	-0.892894621	-1.756964085	10.655649166
H	-0.008404822	-0.995818076	12.464596932
C	-2.231755464	-0.195202123	9.396445781
H	-2.405571043	1.775732216	10.224967051
C	-1.682331897	-1.473282500	9.544332168
H	-0.456427126	-2.744236835	10.777077483

H	-2.842204524	0.040033728	8.529291355
H	-1.864467978	-2.236177772	8.792975276
H	-0.719002284	3.734781154	11.854814507
C	0.308840270	2.739657183	10.310110935
C	-0.055941489	3.777876108	9.436583191
C	1.091733399	1.690242431	9.795537417
C	0.368027090	3.790716206	8.107192851
C	1.514124583	1.698710669	8.471016900
C	1.162120245	2.752841122	7.620877462
H	-0.698740370	4.577160292	9.798913950
H	1.361306848	0.858396302	10.434973592
H	0.072083258	4.606169269	7.453209713
H	2.119691835	0.878134707	8.097347768
H	1.496448611	2.756789354	6.587524798

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Ru	1.024673272	3.449648411	12.548401132
P	2.394337973	5.416471303	12.728068004
O	3.116380702	1.817548547	11.171152638
C	2.336649419	2.504793058	11.683996029
C	4.069168316	5.394188484	11.882126433
H	4.497066905	6.390439471	12.052016707
C	3.904214365	5.200585875	10.355737061
H	3.258934862	5.976919595	9.932009788
H	3.402345439	4.250534396	10.152479383
C	5.262635381	5.205032712	9.636314785
H	5.101883081	5.024196503	8.567353657
H	5.722218177	6.200340848	9.723510986
C	6.208674668	4.152894002	10.230908483
H	7.176494688	4.173816400	9.717394706
H	5.784388135	3.151673517	10.071343135
C	6.401524733	4.389161208	11.735323978
H	6.892237759	5.360750075	11.890132071
H	7.065507772	3.630475043	12.164843818
C	5.059067320	4.375197015	12.490331243
H	4.641550928	3.364218353	12.450807445
H	5.241397315	4.604164859	13.546351323
C	2.808222514	5.677350361	14.543804215
H	3.529566797	4.869208603	14.728636452
C	3.496305414	7.010058614	14.898045911
H	4.355826288	7.185911733	14.242523659
H	2.793712215	7.835645668	14.730226277
C	3.940602260	7.026288936	16.371100238
H	4.707143691	6.254394826	16.525858426
H	4.411396212	7.987298891	16.604931933
C	2.754985612	6.765735650	17.311658149
H	3.089152355	6.752192126	18.354733259
H	2.034366308	7.591382173	17.222750478
C	2.055862583	5.443564944	16.965345180
H	1.189005513	5.281367222	17.616431482
H	2.745701979	4.608191997	17.147469458
C	1.616670436	5.404881758	15.490454535
H	0.834359213	6.162111608	15.329088233
H	1.183309758	4.418001544	15.274431829
C	1.588267446	6.962265010	12.014083855
H	1.271728522	6.587681065	11.033750925
C	2.491937987	8.189399066	11.750910760
H	3.384072160	7.908036876	11.185923189
H	2.837702049	8.614430916	12.699604345
C	1.719677781	9.263562036	10.962561576
H	2.369091187	10.129268255	10.790178469
H	1.462747685	8.862247423	9.971513791
C	0.437120033	9.690560026	11.689704402
H	0.704480389	10.183709319	12.635225189
H	-0.112623890	10.428826549	11.095433920
C	-0.453809777	8.477210697	11.990137219

H	-0.814255543	8.044885883	11.045132228
H	-1.343793478	8.780901766	12.554239398
C	0.314864469	7.396639708	12.771090528
H	-0.342300577	6.539666039	12.941644332
H	0.592646169	7.795874748	13.755613394
O	-0.832854420	4.298539866	13.556968870
H	-0.762896835	4.924899841	14.290783271
C	-2.149526921	4.166762206	13.129582233
C	-3.133936586	4.758956490	13.903167707
C	-2.400378470	3.386240171	11.972057953
C	-4.477426849	4.554941506	13.545830094
C	-3.791791718	3.102961288	11.727453776
C	-4.795675958	3.714503796	12.476110452
H	-2.860749457	5.328695266	14.783591007
H	-5.842254772	3.542689217	12.266371485
O	-4.068023027	2.249151954	10.734763877
C	-5.416192492	2.026996748	10.315420379
H	-6.004235030	1.554340424	11.109962140
H	-5.892433055	2.963950061	10.004810704
H	-5.338154870	1.352714081	9.462805862
O	-5.522520869	5.096686438	14.194173012
C	-5.285957826	5.970759548	15.300250973
H	-4.685265287	6.837163135	14.998287190
H	-6.270184756	6.307315918	15.625621676
H	-4.791689128	5.441873205	16.124127192
H	-0.868040752	1.736887004	13.148466448
O	-0.235241675	1.755702673	12.414554842
C	-1.309351890	2.980733931	11.069845984
C	-0.178655812	3.967634047	10.889210015
C	-1.565660036	2.053618370	9.926147701
C	-1.329373022	0.680643823	9.980816790
C	-2.027631194	2.632915555	8.732695727
C	-1.550790500	-0.105425930	8.847956272
H	-0.945792158	0.248790794	10.895277357
C	-2.264286731	1.841732561	7.615849995
H	-2.199106257	3.703281663	8.681715223
C	-2.020715017	0.467033328	7.667994696
H	-1.346760975	-1.170968862	8.892034766
H	-2.623013502	2.300816675	6.699527185
H	-2.187695099	-0.149154474	6.789678090
H	-0.513278019	4.954995567	11.215601610
C	0.485484766	4.101738659	9.556159438
C	0.455975083	5.355126821	8.924224439
C	1.143056611	3.046469282	8.901657796
C	1.087718277	5.562714944	7.696877219
C	1.772977669	3.250201522	7.678381047
C	1.755674096	4.510525187	7.072201183
H	-0.085324796	6.175744568	9.389303181
H	1.151717053	2.059717813	9.348167544
H	1.050819378	6.542889387	7.229995760
H	2.278840828	2.420377663	7.193624723
H	2.250714011	4.665190446	6.118002004

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Ru	0.714080655	3.080298192	12.494554270
P	1.994669011	5.072012321	12.534208208
O	2.855632251	1.385858042	11.284250902
C	2.046988748	2.098569660	11.703915724
C	3.658239457	5.032915399	11.680008771
H	4.027022899	6.065118707	11.734619117
C	3.529664103	4.667529122	10.182335661
H	2.857437723	5.365682362	9.672479017
H	3.082166145	3.674711417	10.071241664
C	4.904037018	4.677636618	9.491547595
H	4.786024685	4.376922721	8.444233192
H	5.298200130	5.703855606	9.481503721

C	5.897918528	3.756538181	10.212059589
H	6.872455147	3.784502388	9.712346422
H	5.540513184	2.718858963	10.153005288
C	6.045490673	4.160115573	11.685449758
H	6.476080301	5.169725037	11.745776488
H	6.741789833	3.490644837	12.202597509
C	4.688884643	4.145460456	12.412859050
H	4.327849439	3.112995432	12.468056989
H	4.825931349	4.493112653	13.442880002
C	2.385844103	5.650450981	14.277665257
H	3.073329511	4.866867950	14.623834047
C	3.121259310	7.006643794	14.344086472
H	3.987388446	7.021923315	13.674463117
H	2.442954918	7.799890756	14.008380567
C	3.569701851	7.318815153	15.782357789
H	4.304830403	6.567245377	16.103144421
H	4.080965285	8.287735721	15.802572161
C	2.376411984	7.315205698	16.747870875
H	2.712061125	7.516988301	17.770885371
H	1.687991020	8.128297493	16.475581972
C	1.632670063	5.974870512	16.685877277
H	0.756900057	5.984923815	17.345575317
H	2.290081203	5.174693827	17.053350079
C	1.188081059	5.621317542	15.254336258
H	0.418531200	6.335008277	14.929504985
H	0.788192958	4.603758982	15.265145894
C	1.035685028	6.363772684	11.564896788
H	0.853100416	5.808896587	10.637739184
C	1.776595288	7.661931628	11.170348745
H	2.761401865	7.448881888	10.744682677
H	1.941039896	8.284793832	12.055872776
C	0.934996844	8.447985635	10.147436842
H	1.457831319	9.371328122	9.874295008
H	0.846685851	7.854864186	9.225277193
C	-0.465391276	8.765748934	10.691718106
H	-0.371777911	9.453515298	11.543930819
H	-1.059115474	9.287460525	9.933154269
C	-1.191419577	7.493717907	11.152748596
H	-1.398110613	6.853983963	10.281929178
H	-2.163172268	7.743535388	11.593380069
C	-0.346482399	6.701259530	12.166148418
H	-0.883704154	5.793499198	12.461211013
H	-0.211392596	7.306901536	13.071358764
O	-1.073941906	3.744900698	13.798952637
H	-0.794065300	4.442868639	14.410165418
C	-1.634448890	2.706413792	14.571717615
C	-2.158584726	3.053881526	15.811873499
C	-1.629904175	1.395839260	14.069124041
C	-2.712535030	2.043204591	16.606329573
C	-2.231662445	0.404010698	14.896681351
C	-2.750791002	0.720107550	16.147640064
H	-2.126121495	4.085025201	16.141789933
H	-3.212729703	-0.022497655	16.783887504
O	-2.283507959	-0.834899645	14.361167881
C	-2.720391764	-1.930875652	15.162076873
H	-2.113791367	-2.024894914	16.070463184
H	-3.778019274	-1.830706439	15.433478091
H	-2.586388101	-2.816573938	14.540219004
O	-3.250604112	2.248167610	17.829191970
C	-3.279556441	3.571943208	18.355655953
H	-3.866043071	4.243363647	17.715615120
H	-3.759041837	3.494086257	19.331673897
H	-2.266209644	3.974813723	18.480203089
H	2.262606783	2.498511213	14.408436623
O	1.305329953	2.622640297	14.369316969
C	-0.998470469	1.056840109	12.769319933
C	-1.272381208	1.927952063	11.729449067
C	-0.194705093	-0.190617822	12.655187863

C	-0.613477782	2.220844728	10.445952273
C	0.840193764	-0.449607458	13.565944094
C	-0.507079094	-1.148101836	11.680763555
C	1.581737640	-1.624447971	13.464941925
H	1.065601978	0.296532539	14.321569003
C	0.230925221	-2.327688133	11.588446018
H	-1.353284574	-0.981036239	11.020732125
C	1.283712682	-2.564097538	12.474480615
H	2.394278961	-1.810263466	14.161836218
H	-0.022079564	-3.064946345	10.831835576
H	1.861076931	-3.481215793	12.401017441
C	0.082504723	1.317966936	9.599559801
C	-0.654920583	3.590657072	10.063213673
C	0.708676385	1.772560010	8.452311649
H	0.136029725	0.271482870	9.863502422
C	-0.015247790	4.032869690	8.894885302
H	-1.273413110	4.283468637	10.627730213
C	0.668196148	3.130794287	8.092914665
H	1.232730059	1.063518119	7.818218739
H	-0.085856701	5.077913754	8.607777858
H	1.152790303	3.465887099	7.180844211
H	-2.042210096	2.662490724	11.951309801

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O	-1.874415591	0.502501015	10.051385783
H	-1.929078885	-0.448905349	10.209170478
C	-0.923009603	0.746892214	9.100184803
C	-0.159274809	-0.293917412	8.549983662
C	-0.745698374	2.078490837	8.716383386
C	0.797564220	0.015813693	7.581913264
C	0.219035749	2.352156082	7.724121474
C	0.991534837	1.338377341	7.159189587
H	-0.321369883	-1.312399138	8.885887124
H	1.737118106	1.525146599	6.397919390
O	0.307663338	3.663945364	7.352844943
C	1.274501229	4.027766444	6.379021946
H	2.292858405	3.786754050	6.711439156
H	1.085677575	3.534743256	5.415783016
H	1.182346419	5.108484284	6.255127271
O	1.602790999	-0.904915896	6.975210088
C	1.461545331	-2.268916936	7.340182243
H	0.453344517	-2.646739128	7.119499965
H	2.188380127	-2.818886561	6.739683929
H	1.679547682	-2.429870734	8.405413779
C	-1.584136930	3.161371330	9.314362651
C	-1.085739483	3.901430656	10.325175022
C	-2.953506697	3.299253099	8.747239835
C	-1.684610730	5.061315377	11.010550365
C	-3.128597443	3.462655716	7.364198312
C	-4.086318995	3.239091296	9.572398316
C	-4.406994929	3.592026791	6.823087116
H	-2.251288991	3.507695279	6.725382429
C	-5.363772973	3.361375400	9.029474373
H	-3.950406360	3.099008161	10.639921871
C	-5.528720175	3.542419602	7.653887698
H	-4.528830580	3.730836602	5.751833679
H	-6.233008037	3.312482207	9.680042338
H	-6.525162450	3.639962136	7.231666557
C	-1.380801691	5.277374901	12.366604168
C	-2.511976691	5.995391906	10.360254959
C	-1.911130605	6.363689983	13.060346196
H	-0.726625634	4.575924752	12.878940166
C	-3.036204804	7.084322435	11.051761442
H	-2.734000410	5.866849222	9.307626653
C	-2.745542899	7.271185437	12.405652618
H	-1.669112123	6.504461590	14.110371674

H	-3.671254859	7.794754576	10.529301140
H	-3.158695337	8.120825395	12.942100869
H	-0.100756514	3.615376452	10.691961154

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Ru	0.055741571	5.047545336	10.608583046
P	1.915785945	6.248938142	11.634061108
O	0.709036235	6.635877888	8.161472928
C	0.425612905	6.019463790	9.102673598
C	3.572002759	5.490282238	11.187348735
H	4.353801991	6.117007791	11.636701110
C	3.783620935	5.462621963	9.655969793
H	3.711480349	6.467946128	9.228511544
H	2.984504839	4.864211635	9.199485487
C	5.147072997	4.847953963	9.294541967
H	5.258495541	4.820485384	8.204092710
H	5.949298335	5.496838610	9.672483983
C	5.308154356	3.440758206	9.888924205
H	6.299072073	3.036420505	9.654831617
H	4.571990322	2.765294011	9.430568508
C	5.077007400	3.453844222	11.406281171
H	5.864962899	4.042904031	11.895664272
H	5.146903317	2.438307704	11.813503359
C	3.706213601	4.060241379	11.750795472
H	2.917829518	3.433895036	11.308663783
H	3.563340805	4.049512675	12.837715393
C	1.823325272	6.156775701	13.501185075
H	1.722716391	5.070708903	13.659744947
C	3.047971138	6.591961204	14.331702914
H	3.964910543	6.124925152	13.956345558
H	3.186107735	7.674532376	14.246452070
C	2.833071281	6.219325828	15.811501109
H	2.788323010	5.123893145	15.902225260
H	3.694589386	6.546279800	16.404155323
C	1.537887508	6.830554054	16.371575233
H	1.387471991	6.516041233	17.410010378
H	1.632859402	7.925447946	16.385642967
C	0.316963888	6.452357594	15.517202377
H	-0.586556277	6.943267376	15.896282713
H	0.137662142	5.367572198	15.597756171
C	0.541733937	6.828854044	14.043801221
H	0.653797809	7.917237179	13.967182708
H	-0.329776174	6.571078238	13.429279523
C	2.080540182	8.027009819	11.053878145
H	2.348547396	7.880050069	9.998430788
C	3.198651552	8.866491446	11.705472601
H	4.150805440	8.324786596	11.723438630
H	2.929639197	9.078685020	12.747538531
C	3.367113837	10.202660619	10.956935887
H	4.155448909	10.795310199	11.434949402
H	3.704630885	9.999098920	9.930751120
C	2.049275102	10.991955828	10.916098377
H	1.775348932	11.288517527	11.938927342
H	2.179876286	11.918633380	10.346076199
C	0.915362063	10.148120973	10.314865004
H	1.129359466	9.943193145	9.256261282
H	-0.031433221	10.700584952	10.340960325
C	0.751897177	8.809974243	11.055845726
H	-0.039978060	8.221166307	10.592238730
H	0.437033793	9.005153766	12.089131353
O	-2.018229930	0.786419392	9.975212916
H	-2.176251872	0.032237926	10.558654033
C	-0.717435503	0.837226507	9.580359919
C	0.156628795	-0.209955118	9.888015273
C	-0.315390953	1.984324371	8.862884026
C	1.503064356	-0.105193667	9.540409486

C	1.062257220	2.056043345	8.562704874
C	1.959886207	1.039423545	8.879594345
H	-0.223533798	-1.068751724	10.425755031
H	3.009471615	1.108113911	8.625328314
O	1.535337626	3.219253310	7.966564853
C	2.550445497	3.105949002	6.955845810
H	3.533443649	2.922537149	7.399227177
H	2.306217035	2.305451352	6.250757252
H	2.564641391	4.068780525	6.442202591
O	2.450043905	-1.038237649	9.817657375
C	2.043974825	-2.257376344	10.438588915
H	1.292027666	-2.779809410	9.834369961
H	2.943285354	-2.871174870	10.501742187
H	1.659711608	-2.075127954	11.448149219
H	0.068168659	3.946932501	7.501286556
O	-0.902586719	3.970066540	7.501041244
C	-1.368003832	3.072121270	8.507251465
C	-1.647293533	3.822470243	9.812318778
C	-2.634307146	2.458438025	7.881144773
C	-2.132123409	5.158067881	9.880509455
C	-2.474878644	1.686655868	6.724426731
C	-3.921940643	2.716758676	8.350867033
C	-3.581973718	1.178718963	6.051459521
H	-1.474460556	1.498615794	6.346422034
C	-5.036131135	2.211489797	7.675684826
H	-4.068371488	3.307457323	9.249432161
C	-4.869898609	1.443224796	6.524919960
H	-3.442617386	0.584798520	5.152225154
H	-6.033833742	2.423649331	8.050008591
H	-5.736016244	1.053666046	5.997362446
C	-2.007949103	5.824433384	11.166558502
C	-2.536141100	5.964521844	8.746533101
C	-2.335792346	7.211569024	11.287497606
H	-2.044520386	5.218259585	12.067584567
C	-2.827790216	7.288787925	8.912405876
H	-2.626388574	5.486279604	7.782020532
C	-2.715197763	7.930096386	10.185556271
H	-2.293275910	7.678319186	12.266847808
H	-3.165682571	7.869788416	8.058953835
H	-2.962733324	8.983771494	10.275063822
O	-0.269757796	3.808215019	12.579496093
H	-0.010349239	4.271311690	13.387946285
C	-0.239046442	2.414105757	12.810839951
C	1.002776678	1.788152322	12.925382382
C	-1.439786046	1.738042658	12.881834392
C	1.017137561	0.406692213	13.127123535
H	1.905807835	2.370750793	12.833876224
C	-1.397840482	0.342183026	13.059086341
C	-0.183111290	-0.318024750	13.219913000
O	2.147449304	-0.340242058	13.210244661
O	-2.606186855	-0.282276122	12.983929194
H	-0.118849427	-1.389382531	13.358216288
C	-2.677477791	-1.674236306	13.298965534
H	-2.119206623	-2.279866852	12.573185752
H	-2.296079831	-1.873463707	14.306890729
H	-3.734477025	-1.936266849	13.248049168
C	3.385558895	0.266286945	12.840240644
H	3.661158818	1.071589597	13.532811548
H	4.133545899	-0.524962521	12.897002650
H	3.338759697	0.651801077	11.815195656
H	-1.853702030	3.171245462	10.655302713
H	-2.390376104	2.242527914	12.765489383

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Ru	0.580206126	5.068192535	10.590960467
P	2.391902060	6.285524503	11.650138045

O	0.884159036	6.861822922	8.238710559
C	0.765668923	6.157187402	9.155071477
C	4.150288536	5.852154127	11.157111030
H	4.800602928	6.520999684	11.737661614
C	4.404785879	6.126463170	9.658497254
H	4.208962720	7.176914316	9.418263467
H	3.708079416	5.532009437	9.058568474
C	5.854578936	5.788470796	9.267108807
H	5.990393625	5.953103023	8.191091370
H	6.536356856	6.484538581	9.776141288
C	6.231928931	4.348829801	9.645655698
H	7.279383407	4.150182335	9.390898900
H	5.622382427	3.643781890	9.062308298
C	5.983372099	4.091891607	11.139018848
H	6.656029147	4.723511677	11.736995534
H	6.218938881	3.051478685	11.393496231
C	4.523414987	4.396603979	11.513533099
H	3.870870212	3.714883445	10.965319759
H	4.364469020	4.197242803	12.578772087
C	2.337094370	5.937680258	13.502543657
H	2.217341496	4.842773481	13.518022956
C	3.593626686	6.280689729	14.336176623
H	4.502002004	5.871327992	13.886445111
H	3.723997601	7.367556093	14.372374293
C	3.442990875	5.740621437	15.771171865
H	3.394140037	4.642094994	15.736196767
H	4.334661209	5.994690010	16.355821992
C	2.180244108	6.285632895	16.456002114
H	2.072269804	5.854292001	17.457745029
H	2.284671223	7.371532396	16.591168698
C	0.927088977	6.006677739	15.612807737
H	0.041422698	6.453626582	16.080162984
H	0.746747079	4.921831756	15.570642782
C	1.090152135	6.544390246	14.181664941
H	1.199347338	7.635630140	14.221886635
H	0.193542724	6.342326693	13.592139336
C	2.330243560	8.140035130	11.335407835
H	2.644288503	8.192689097	10.283269901
C	3.302276374	9.008627266	12.159782441
H	4.321068836	8.607161771	12.129231510
H	2.986934942	9.002232724	13.210967518
C	3.296931444	10.462142073	11.650887835
H	3.981290472	11.067614666	12.256490628
H	3.683700175	10.483513197	10.622042522
C	1.881874601	11.060006387	11.676931052
H	1.540879152	11.132700700	12.720053202
H	1.892529078	12.080986695	11.278643128
C	0.899113123	10.184420287	10.885741631
H	1.172344660	10.195700728	9.820875430
H	-0.118426243	10.588200685	10.951306673
C	0.907077570	8.731090954	11.387080174
H	0.218663078	8.131900634	10.788727970
H	0.527127798	8.702365558	12.415129389
O	-2.694696220	1.667701888	11.284367901
H	-3.117748281	1.084573327	11.927474825
C	-1.805200127	0.948111857	10.534541736
C	-1.493930389	-0.362943563	10.925562403
C	-1.234212208	1.566978208	9.409429877
C	-0.627421134	-1.122885657	10.144612541
C	-0.447791284	0.711073136	8.592435338
C	-0.124042769	-0.590052837	8.953811742
H	-1.946106584	-0.763999751	11.825962885
H	0.502251791	-1.221414740	8.339801806
O	-0.015645875	1.223864483	7.384598200
C	0.837757237	0.448404233	6.535885939
H	1.771261998	0.198787652	7.049357572
H	0.327835381	-0.460553833	6.201768351
H	1.048196457	1.085368226	5.675985031

O	-0.211158953	-2.381522189	10.438262520
C	-0.788140612	-3.047191906	11.559119227
H	-1.876521601	-3.134797022	11.453784570
H	-0.345506782	-4.043728399	11.575791992
H	-0.553212154	-2.530526955	12.498829294
H	-0.256848867	2.826366309	7.506574299
O	-0.481756303	3.546394113	8.143713281
C	-1.536141651	3.054762536	9.064646098
C	-1.357379369	3.962558948	10.289482433
C	-2.884176668	3.127346192	8.339803797
C	-1.873732466	5.307932959	10.466454118
C	-2.964423156	2.895845475	6.959751844
C	-4.066595028	3.343625343	9.057028262
C	-4.197671150	2.898768851	6.308865905
H	-2.066702593	2.709339454	6.379952273
C	-5.299881777	3.341695733	8.404942338
H	-4.019923201	3.512621710	10.126049839
C	-5.372434688	3.122262905	7.028567215
H	-4.238140176	2.725715148	5.237090558
H	-6.206719487	3.518815591	8.976214548
H	-6.332729819	3.125701214	6.521614790
C	-1.676773793	5.884420556	11.764359059
C	-2.379467850	6.163963048	9.440022268
C	-2.018048029	7.227310479	12.024505646
H	-1.438498994	5.226804821	12.597435645
C	-2.701410368	7.475904548	9.721245675
H	-2.515606774	5.767308193	8.441306716
C	-2.523801441	8.023205479	11.012844110
H	-1.885914022	7.624225340	13.026651837
H	-3.099650855	8.103073124	8.927952506
H	-2.789609148	9.057993378	11.205019416
O	0.905500076	2.808598734	11.877597519
H	0.971442501	2.173864692	12.603346868
C	1.660371273	2.421024953	10.791106697
C	1.640695987	3.353039562	9.732281785
C	2.401639568	1.249084222	10.808544574
C	2.546775908	3.073840737	8.674201071
H	0.506840919	3.572580535	8.958120448
C	3.200834622	0.975883014	9.688457016
C	3.304281840	1.901723887	8.636235554
O	2.528713532	3.988306937	7.669578050
O	3.905917611	-0.166091408	9.529789935
H	3.959306470	1.653760295	7.811087496
C	3.723481901	-1.219849529	10.477593625
H	4.072593764	-0.925528911	11.475027401
H	2.671845953	-1.529927807	10.527918885
H	4.333002401	-2.049292494	10.118107188
C	3.403060027	3.817385763	6.554695744
H	3.173440579	2.897765290	6.001849323
H	3.233136978	4.681405693	5.911927745
H	4.451710466	3.797550734	6.873444720
H	-1.359059239	3.400990310	11.214173358
H	2.347960040	0.572171384	11.652772853

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12'

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Ru	0.860260717	4.953192121	10.355764197
P	2.486170216	6.189059439	11.478531396
O	1.366164036	6.781565417	8.052554683
C	1.145545073	6.028057570	8.903470646
C	4.269472827	5.989057233	10.949021559
H	4.805494487	6.747188611	11.537263824
C	4.466863326	6.321067528	9.453516654
H	4.097292989	7.326383826	9.224905250
H	3.881574514	5.620872841	8.851126187
C	5.949018122	6.223225288	9.052801960
H	6.047631929	6.424608369	7.979554421

H	6.520982970	7.005730420	9.571483573
C	6.538210369	4.849919695	9.403920817
H	7.598381872	4.807266925	9.130045820
H	6.026622490	4.073070997	8.816918212
C	6.355319378	4.544232210	10.897243011
H	6.930550835	5.269612358	11.490488164
H	6.754381606	3.552718193	11.139998468
C	4.871807085	4.610174264	11.300180995
H	4.322745260	3.827983242	10.770305053
H	4.770729987	4.397916657	12.369557828
C	2.455008339	5.699633261	13.283920682
H	2.616203574	4.614917138	13.224529847
C	3.569761821	6.305495878	14.168294628
H	4.558016135	6.166408463	13.720627228
H	3.416470825	7.385399721	14.267198643
C	3.539057715	5.663492827	15.567624636
H	3.777125180	4.593966536	15.477014979
H	4.323267899	6.107814027	16.191191662
C	2.164511931	5.829229122	16.233667461
H	2.153391191	5.335247667	17.211636557
H	1.981267491	6.897276924	16.419229564
C	1.042498467	5.275633263	15.341222204
H	0.063798711	5.447440664	15.804700604
H	1.159414311	4.187008829	15.237902476
C	1.075450979	5.915560808	13.943332314
H	0.880460269	6.990779395	14.037798035
H	0.275133114	5.504969108	13.318090651
C	2.165695591	8.022314070	11.239652212
H	2.381761171	8.138597652	10.169120073
C	3.086709626	8.997673190	12.003161632
H	4.142222606	8.729083234	11.889880666
H	2.855930143	8.953732135	13.074335985
C	2.857732976	10.436791994	11.502758052
H	3.507498211	11.124820233	12.055654886
H	3.156903013	10.501375553	10.447023453
C	1.385822986	10.853905479	11.646690839
H	1.128348997	10.897721731	12.714855075
H	1.236884356	11.863344718	11.247207072
C	0.451164039	9.857275323	10.944063895
H	0.619636374	9.894925226	9.858442490
H	-0.597136194	10.130328633	11.107928438
C	0.687823418	8.419103515	11.434578401
H	0.025281645	7.733767200	10.899145657
H	0.418528873	8.350431135	12.494627427
O	-2.850397745	1.547276865	11.828111179
H	-3.254002788	0.923790149	12.445725357
C	-2.007918486	0.871205560	10.987197033
C	-1.639948992	-0.453620996	11.262333264
C	-1.528963507	1.562165164	9.863917628
C	-0.775348387	-1.111666199	10.385957169
C	-0.641892246	0.863908418	9.015740955
C	-0.275040524	-0.455438814	9.253906496
H	-2.037380586	-0.943360331	12.144052478
H	0.416419767	-0.986590214	8.613946754
O	-0.142238084	1.585814897	7.970786115
C	0.493753405	0.912367731	6.880984846
H	1.444687028	0.471113800	7.192698907
H	-0.162703639	0.140917603	6.463767889
H	0.672710006	1.693162558	6.140095044
O	-0.327086326	-2.383270771	10.561687382
C	-0.854945226	-3.149697467	11.641557483
H	-1.944810617	-3.247649311	11.565788659
H	-0.396859469	-4.135901130	11.560464209
H	-0.595429849	-2.708026979	12.612568371
H	-0.195683084	3.491301251	7.608814497
O	0.073416427	4.259221393	7.084172285
C	-1.973643632	2.968730944	9.608075376
C	-1.612489981	3.909699076	10.527660067

C	-2.975430526	3.227556197	8.536023107
C	-1.925506968	5.351673097	10.574014189
C	-2.859164277	2.772336798	7.213474403
C	-4.152422603	3.907969306	8.905797713
C	-3.862028705	3.037061078	6.282544376
H	-1.972864411	2.239041394	6.902518868
C	-5.159224147	4.156244496	7.979035164
H	-4.279275912	4.228405419	9.934138989
C	-5.012150976	3.731836639	6.657108734
H	-3.741186909	2.698471770	5.257647566
H	-6.059392169	4.678539464	8.290486390
H	-5.791735764	3.933344596	5.928178849
C	-2.189128307	5.949768283	11.824840702
C	-2.009722365	6.153821125	9.411015524
C	-2.592516140	7.281425499	11.907556205
H	-2.126207783	5.344122505	12.725662941
C	-2.401341561	7.485380581	9.503880422
H	-1.772421643	5.715053804	8.447515906
C	-2.713536413	8.047482958	10.746715383
H	-2.817322759	7.718446143	12.876194311
H	-2.466288708	8.087285910	8.602458761
H	-3.036371063	9.082568046	10.809404307
O	1.131603926	3.058982927	11.972218958
H	0.464090769	2.425693880	12.277744408
C	1.857323661	2.493972531	10.901281802
C	2.037039171	3.400533243	9.866955567
C	2.320436102	1.184205730	10.919383630
C	2.775484680	2.953845171	8.757519555
H	1.040622057	4.234906081	7.142398086
C	3.030457030	0.763588369	9.787932555
C	3.284474988	1.655143391	8.727922895
O	2.914596904	3.844018141	7.721956663
O	3.506257403	-0.493266832	9.604095897
H	3.848254749	1.275026207	7.885285132
C	3.231771444	-1.476328127	10.601497042
H	3.665236523	-1.193705566	11.569586770
H	2.153469922	-1.645315193	10.710197083
H	3.707719501	-2.393022501	10.251626943
C	3.743048218	3.491059590	6.612060210
H	3.336359132	2.629514781	6.069634862
H	3.746813341	4.363683088	5.958317682
H	4.765429883	3.270037209	6.938022251
H	-1.166723320	3.520483778	11.438766094
H	2.107402494	0.530607780	11.755760766

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Ketone

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O	5.666241803	2.835605522	8.825417798
C	4.786261233	2.200314417	9.406123018
C	3.346168385	2.386758328	9.007752742
C	2.291858657	1.608407737	9.517397638
C	3.059138749	3.396633012	8.073437728
C	0.981788657	1.832400290	9.095307385
C	1.751036150	3.625560135	7.659429343
C	0.708282776	2.841468871	8.167930613
H	2.480479057	0.820680779	10.241585549
H	3.883862819	3.989771109	7.687264233
H	0.174829340	1.219545156	9.491352272
H	1.541867814	4.413259707	6.939690186
H	-0.313393251	3.016374109	7.842618632
C	5.053481413	1.220390907	10.560474050
H	4.543650676	0.248558121	10.304965239
H	4.479783449	1.614303689	11.451774738
C	6.483007600	0.918865248	10.986615999
C	7.569081640	1.801113751	10.807533147
C	6.694162328	-0.299144275	11.689432788
C	8.828446185	1.460115505	11.312521673

C	7.945539101	-0.628567060	12.205334275
C	9.024311714	0.253788683	12.014544163
H	7.434891077	2.733886505	10.254644653
H	5.860115721	-0.995143320	11.838857070
H	9.661475332	2.150980219	11.152769117
H	8.079633249	-1.574638051	12.749137438
H	10.005813962	0.000216315	12.406992604

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Z-enol

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O	5.709462707	3.221809437	8.905666030
H	5.431680476	3.295633644	7.983202316
C	4.767856176	2.490925858	9.591144092
C	5.080542086	1.869789833	10.750610383
H	4.241520065	1.407464263	11.261910686
C	3.404246066	2.498006205	9.020070052
C	2.551677959	1.386516756	9.137755142
C	2.940847544	3.628143417	8.323269481
C	1.270834647	1.414402546	8.593119255
C	1.660517817	3.650597376	7.772695150
C	0.819438664	2.545057338	7.906555669
H	2.911327981	0.492339096	9.636901248
H	3.576083322	4.506380125	8.246369247
H	0.627370747	0.544459607	8.689536756
H	1.316297341	4.537223391	7.247833954
H	-0.177601808	2.561245328	7.476276740
C	6.366390177	1.736126799	11.431019805
C	7.577170018	2.304361377	10.981107768
C	6.400487912	0.977223960	12.619820054
C	8.758976270	2.109495163	11.691837467
C	7.583420915	0.785851269	13.326705646
C	8.773390202	1.352239728	12.865437363
H	7.582404865	2.897917624	10.077067548
H	5.479286121	0.530236076	12.986571623
H	9.679085619	2.557583572	11.326020013
H	7.576603692	0.195045218	14.238734451
H	9.699116889	1.207997444	13.415157771

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E-enol

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O	5.630753084	3.328370312	8.999000786
H	5.397548920	3.331359319	8.060613146
C	4.686816826	2.589326833	9.679219402
C	5.051982637	2.064872256	10.867684543
H	6.107206240	2.162821764	11.113175079
C	3.370759373	2.479034861	9.006768233
C	2.679381234	1.257609405	8.952919140
C	2.820618536	3.598454126	8.361066207
C	1.454875759	1.169035832	8.297919309
C	1.593627853	3.506799199	7.703337568
C	0.906470218	2.292974735	7.672489671
H	3.104438333	0.388485338	9.441845746
H	3.347380270	4.547832614	8.402673685
H	0.928670040	0.219200593	8.268428908
H	1.172652097	4.385000199	7.222243123
H	-0.050332367	2.220526983	7.163435553
C	4.208881752	1.410141362	11.878666636
C	2.861712146	1.754477194	12.105939504
C	4.780953499	0.417518004	12.695744750
C	2.114590719	1.105255634	13.084885760
C	4.032633671	-0.229897694	13.676821128
C	2.692079815	0.105543524	13.872609329
H	2.410183639	2.545445021	11.517059057
H	5.824203255	0.149633151	12.547848413
H	1.078112574	1.390461837	13.243887956
H	4.497380535	-0.997251877	14.290185622

H 2.107234188 -0.395480918 14.638704212

Table S5. Vibrational frequencies (in cm-1) of the optimized structures

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27.09 43.33 47.04 56.18 58.96 63.13
69.95 72.68 76.70 81.46 86.74 91.21
95.98 100.40 103.44 111.09 118.16 119.95
148.76 161.57 176.39 179.02 193.17 208.10
213.18 221.91 226.06 240.87 245.34 265.13
268.86 284.47 314.85 328.81 342.01 349.28
360.80 394.79 404.66 410.66 417.01 427.67
437.59 446.83 451.16 453.63 458.98 467.60
503.76 509.33 514.30 519.39 521.63 527.07
534.58 539.19 565.58 606.46 613.05 668.58
719.00 722.26 744.86 749.72 759.87 794.62
809.84 812.30 815.77 821.93 825.92 829.16
842.99 868.46 868.77 871.14 902.59 907.00
907.84 910.30 912.65 914.26 915.05 930.81
938.72 941.17 948.94 988.91 995.38 1001.54
1013.77 1018.97 1025.40 1028.41 1028.82 1041.82
1043.08 1048.02 1048.94 1049.69 1060.84 1064.30
1070.31 1073.91 1092.34 1093.37 1095.54 1097.56
1103.59 1108.00 1122.76 1140.37 1151.14 1158.63
1186.54 1188.23 1194.71 1206.70 1212.57 1219.02
1237.04 1237.82 1239.86 1266.48 1293.39 1301.55
1302.61 1306.75 1309.93 1312.19 1314.48 1324.62
1328.02 1334.81 1342.07 1346.54 1365.99 1367.38
1368.84 1370.51 1377.51 1379.01 1381.42 1385.14
1389.42 1393.53 1394.61 1395.50 1398.55 1399.23
1401.83 1406.75 1407.91 1492.31 1494.96 1495.76
1497.54 1499.24 1499.80 1500.59 1502.45 1503.94
1504.72 1506.62 1508.93 1511.34 1519.47 1521.42
1523.78 1539.42 1572.24 1585.69 2087.15 2153.72
2997.42 3000.55 3006.76 3015.55 3016.89 3017.77
3023.45 3024.03 3024.17 3026.73 3030.92 3037.94
3039.97 3047.63 3047.96 3051.29 3058.70 3062.15
3072.85 3073.06 3074.84 3076.08 3077.82 3080.70
3081.33 3088.01 3092.15 3097.46 3111.70 3114.21
3121.89 3136.25 3180.74 3205.38 3213.11 3217.35
3225.40 3231.29 3235.00

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79.14 90.62 192.11 202.72 217.25 240.51
252.65 288.83 295.19 306.13 374.72 425.84
500.43 541.16 561.27 621.17 625.19 654.85
686.27 770.86 815.33 832.17 958.76 1006.06
1010.18 1089.83 1107.54 1179.97 1180.49 1180.84
1201.11 1211.02 1233.07 1250.42 1312.69 1367.81
1415.33 1479.98 1496.73 1505.52 1505.86 1511.55
1518.86 1524.85 1547.58 1653.18 1680.99 3006.82
3011.01 3067.39 3072.73 3142.01 3142.81 3208.98
3238.55 3246.88 3829.34

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9.63 22.70 26.59 31.63 42.95 48.04
54.25 63.42 68.36 71.03 79.72 86.29
93.87 100.28 105.92 120.94 135.93 151.50
165.27 177.31 185.92 191.34 206.86 207.46
212.74 219.21 229.23 234.36 254.28 257.21
270.35 272.29 281.49 283.31 301.95 310.05

328.89 343.57 372.26 398.97 403.69 420.91
429.23 435.20 440.50 445.30 448.29 451.49
460.23 493.97 505.36 521.98 525.77 533.49
534.80 540.11 545.86 555.84 579.72 615.50
643.23 658.13 685.44 697.47 721.21 748.79
755.54 768.87 806.93 808.31 811.71 820.21
824.07 825.98 829.09 850.19 853.94 865.31
866.48 867.66 899.74 902.48 902.79 908.58
909.91 912.38 936.90 941.16 942.26 951.11
979.31 990.75 1022.49 1025.79 1026.83 1038.57
1043.24 1048.79 1056.62 1065.14 1069.01 1071.13
1088.93 1089.09 1093.31 1095.19 1100.17 1106.75
1113.39 1138.30 1141.26 1154.31 1159.70 1176.34
1176.87 1193.15 1204.68 1206.25 1211.49 1218.13
1218.32 1232.07 1237.67 1261.47 1267.14 1292.10
1296.66 1300.77 1302.02 1303.11 1305.24 1307.76
1310.50 1317.43 1328.84 1330.68 1337.85 1342.61
1364.65 1367.97 1369.34 1371.78 1374.42 1378.98
1380.75 1381.73 1389.19 1393.71 1394.64 1395.87
1397.45 1399.10 1400.29 1403.18 1410.49 1473.99
1481.40 1490.46 1495.02 1497.44 1499.32 1499.80
1500.67 1501.80 1503.09 1504.69 1506.48 1506.69
1508.28 1509.14 1509.99 1510.42 1511.39 1519.06
1520.33 1524.99 1525.53 1528.28 1603.58 1655.77
2066.71 2201.55 2992.69 2999.89 3019.73 3021.32
3022.33 3023.64 3024.96 3025.15 3028.08 3028.13
3029.84 3031.80 3032.17 3033.51 3035.51 3037.80
3039.00 3040.73 3043.74 3062.48 3070.82 3077.15
3081.45 3083.23 3085.70 3086.44 3087.44 3088.36
3088.83 3090.21 3090.84 3093.06 3093.98 3095.61
3101.12 3111.39 3115.16 3174.28 3178.35 3236.38
3240.00 3252.71 3781.40

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4-TS

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-583.39 17.76 22.42 25.05 32.68 42.33
47.11 54.24 60.16 66.82 70.97 79.72
89.29 92.28 99.15 110.29 115.54 131.36
148.10 154.74 166.71 179.99 191.17 202.95
206.87 212.66 218.23 221.53 231.13 255.96
257.85 266.91 274.56 280.40 283.85 310.44
326.91 343.19 372.88 388.63 397.81 402.38
413.62 431.20 432.08 436.45 444.57 447.94
449.19 461.03 498.15 506.02 518.53 523.36
525.03 534.15 539.26 546.25 562.79 571.74
622.02 655.89 669.13 704.18 721.54 744.79
749.10 755.16 782.23 808.02 808.69 811.93
820.27 824.47 828.97 846.15 856.38 864.80
866.09 867.19 899.29 901.72 903.06 908.85
909.38 912.19 936.67 940.88 942.56 957.95
980.86 992.33 1022.88 1025.62 1027.16 1038.07
1042.86 1048.26 1056.72 1069.39 1071.20 1076.19
1087.66 1088.01 1092.72 1095.07 1100.15 1107.05
1113.47 1137.87 1140.31 1142.77 1158.57 1176.86
1177.54 1189.74 1205.41 1206.80 1211.30 1217.47
1218.26 1229.76 1237.54 1257.67 1267.06 1271.64
1292.17 1296.62 1301.03 1302.64 1305.04 1306.98
1310.50 1316.92 1328.76 1330.59 1338.28 1342.68
1365.33 1367.94 1369.47 1370.79 1374.61 1379.67
1381.28 1381.89 1384.78 1389.78 1393.79 1394.95
1395.86 1397.32 1399.15 1400.02 1403.40 1453.30
1478.64 1489.13 1493.51 1496.79 1498.89 1499.79
1500.94 1501.79 1502.92 1504.36 1506.12 1507.54
1507.95 1509.13 1509.55 1510.28 1510.70 1514.64
1518.46 1520.23 1524.46 1525.49 1538.61 1613.37
1668.87 1940.77 2077.54 2993.86 3001.79 3004.65
3009.16 3019.51 3022.69 3023.78 3024.90 3025.86

3028.27 3028.87 3029.27 3032.25 3034.03 3034.34
3035.15 3035.76 3040.04 3043.03 3061.76 3070.76
3078.32 3082.29 3083.66 3085.61 3086.60 3087.57
3088.86 3090.28 3090.84 3091.12 3093.00 3093.72
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8-TS

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10-TS

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349.33 351.71 362.90 377.32 391.15 398.92
400.91 403.98 412.17 418.69 419.51 433.75
440.07 442.97 446.60 449.01 452.66 459.11
463.67 484.99 506.59 508.72 514.50 524.69
525.88 529.86 533.59 534.42 538.92 549.52
553.93 570.29 579.56 582.86 590.45 606.82
610.07 623.08 630.45 631.83 638.89 644.12
648.04 667.84 680.83 703.37 706.13 708.58
716.19 716.73 719.01 726.98 734.96 752.72
757.16 763.79 776.60 790.65 795.22 809.72
815.19 815.48 818.63 825.08 826.46 831.48
841.00 842.58 846.10 860.99 868.29 869.51
870.38 883.92 902.26 906.69 907.35 909.12
911.37 913.22 914.23 937.16 939.09 942.73

943.17 943.95 950.53 957.19 964.54 967.94
976.04 997.06 1005.02 1006.96 1009.01 1014.18
1019.60 1026.24 1028.35 1030.30 1039.34 1040.06
1044.95 1048.79 1058.01 1059.92 1060.32 1070.68
1074.92 1081.46 1083.74 1091.19 1094.72 1095.21
1103.34 1106.05 1111.59 1113.34 1114.16 1118.71
1123.36 1141.80 1147.87 1160.16 1160.98 1178.49
1179.22 1179.89 1184.51 1186.94 1195.47 1198.24
1198.47 1200.28 1208.27 1209.43 1213.72 1214.46
1220.86 1222.47 1222.64 1222.81 1228.84 1239.82
1241.88 1247.38 1248.93 1249.51 1267.38 1268.99
1289.22 1293.39 1297.36 1302.19 1304.86 1308.01
1311.06 1314.13 1323.37 1331.00 1331.31 1334.33
1340.75 1342.33 1344.47 1346.69 1350.38 1365.90
1366.08 1367.73 1369.74 1371.28 1372.72 1375.47
1379.73 1381.75 1384.61 1392.97 1394.64 1396.02
1397.13 1398.40 1400.11 1402.09 1404.61 1410.80
1415.19 1452.68 1465.72 1480.15 1481.11 1487.18
1492.03 1492.77 1496.55 1496.66 1498.41 1500.10
1500.55 1500.84 1501.53 1502.22 1503.18 1503.88
1505.79 1507.00 1507.67 1508.71 1509.75 1512.51
1515.22 1516.08 1517.61 1519.45 1520.78 1523.91
1525.41 1528.31 1531.89 1533.53 1537.73 1545.66
1620.76 1622.60 1629.69 1635.09 1649.25 1654.40
1655.24 1668.43 1678.14 1699.65 2058.01 3014.20
3016.57 3018.25 3019.56 3020.28 3021.48 3022.14
3022.95 3023.97 3024.14 3025.10 3026.46 3026.84
3027.02 3029.72 3035.95 3039.17 3045.57 3047.87
3062.10 3070.77 3074.70 3075.76 3078.34 3078.55
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3096.43 3096.76 3098.26 3099.21 3108.38 3124.08
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3194.10 3200.52 3202.01 3207.49 3209.86 3211.34
3224.96 3227.66 3241.12 3243.35 3244.68 3617.72
3658.75 3770.69 3823.28

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5'-TS

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129.65 143.13 153.47 163.85 173.09 174.39
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222.29 233.47 235.43 241.27 263.61 271.71
274.54 278.22 287.96 288.83 291.04 300.68
309.66 327.32 331.99 347.68 351.10 355.75
381.79 398.76 402.52 417.04 426.39 432.26
435.73 440.38 443.30 445.98 451.28 453.11
463.50 495.15 505.40 511.75 523.49 525.72
529.17 534.61 537.44 541.72 551.10 575.59
582.38 583.34 596.66 610.88 631.03 631.53
637.37 659.51 680.21 680.84 708.18 713.51
722.12 723.61 745.59 758.18 775.93 789.51
794.06 809.44 811.39 812.40 821.77 826.62
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866.69 867.96 879.35 885.79 899.55 903.99
905.60 909.50 910.48 912.19 935.91 936.89
940.95 943.84 953.66 958.79 975.03 987.99
996.86 1006.00 1007.43 1015.18 1019.16 1024.44
1027.28 1028.40 1037.76 1039.71 1040.67 1044.52
1047.84 1053.34 1056.67 1066.90 1069.49 1070.17
1088.48 1089.78 1092.58 1094.32 1101.02 1107.38
1114.52 1116.21 1118.58 1123.31 1139.83 1145.48
1159.22 1177.49 1178.11 1180.87 1198.27 1199.06
1200.31 1206.13 1211.12 1216.48 1218.36 1218.93

1227.32 1230.26 1231.17 1237.56 1239.59 1255.17
1255.63 1267.98 1292.44 1297.95 1299.86 1303.59
1307.06 1307.97 1308.26 1310.80 1320.59 1321.30
1329.86 1331.49 1337.77 1341.76 1343.06 1349.37
1363.88 1366.42 1366.56 1369.40 1371.47 1373.36
1377.40 1379.76 1382.18 1383.62 1391.92 1395.01
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1404.75 1456.25 1478.86 1484.09 1486.74 1489.44
1493.37 1497.16 1499.43 1499.75 1501.10 1501.84
1502.66 1502.96 1504.58 1507.20 1507.41 1508.26
1510.96 1512.86 1513.76 1515.76 1518.58 1521.81
1526.51 1527.12 1528.24 1532.48 1603.95 1608.68
1613.43 1643.94 1650.30 1656.85 1661.54 2071.04
3008.12 3014.66 3016.09 3017.80 3018.19 3021.39
3022.46 3023.95 3025.11 3025.37 3027.51 3029.01
3030.82 3033.16 3034.70 3040.67 3042.10 3057.17
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3116.38 3119.53 3120.99 3139.16 3148.18 3150.59
3157.38 3160.33 3164.10 3164.99 3169.97 3199.25
3201.82 3227.10 3234.41 3238.75 3670.55 3810.78

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12.96 20.90 27.16 28.91 29.84 42.98
46.51 53.25 57.18 65.40 67.81 68.86
76.57 80.85 83.44 86.21 89.51 94.56
96.44 105.19 109.06 116.32 123.31 133.92
144.19 149.52 157.50 174.97 179.71 180.38
186.88 195.08 197.37 208.94 217.13 220.66
221.70 228.98 235.11 238.68 261.98 268.67
275.75 281.65 288.50 290.41 298.32 310.63
312.41 324.85 327.27 342.22 348.33 353.10
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715.51 721.82 742.03 752.27 770.43 785.64
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829.56 830.56 843.87 845.94 855.64 856.38
865.62 867.87 868.87 870.99 902.31 904.76
906.87 910.08 910.58 915.94 935.74 937.50
942.05 942.67 943.65 959.45 978.39 980.47
985.54 1010.77 1013.08 1013.87 1015.21 1024.79
1027.87 1028.21 1040.45 1043.25 1045.21 1049.16
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1089.50 1092.98 1094.07 1095.63 1100.05 1108.63
1115.18 1118.13 1123.14 1132.20 1139.49 1143.89
1160.60 1177.07 1179.61 1180.89 1198.81 1202.22
1204.91 1206.89 1212.89 1216.79 1217.73 1220.16
1228.74 1231.76 1232.96 1236.76 1239.36 1240.43
1255.89 1268.92 1291.68 1299.31 1302.15 1304.80
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1334.84 1341.07 1341.45 1345.76 1351.66 1364.44
1365.00 1367.66 1370.00 1372.74 1373.23 1375.49
1379.99 1382.00 1382.66 1384.58 1393.68 1394.50
1395.49 1397.17 1398.07 1398.70 1402.27 1405.91
1416.68 1455.89 1481.11 1484.84 1486.68 1492.78
1494.20 1496.67 1499.42 1500.11 1501.24 1501.59
1502.02 1503.53 1504.35 1507.07 1507.75 1507.83
1511.43 1512.43 1514.15 1517.64 1518.38 1522.10
1527.32 1528.30 1529.25 1541.14 1613.59 1619.33
1623.24 1642.97 1651.04 1657.60 1659.19 2052.32
3013.10 3013.52 3015.09 3019.19 3020.83 3021.76

3022.66 3023.25 3025.25 3026.77 3028.61 3029.14
3031.37 3041.32 3047.48 3051.73 3056.40 3059.66
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3081.41 3083.65 3084.13 3084.81 3086.70 3087.48
3095.34 3098.62 3105.28 3109.52 3118.94 3121.38
3137.93 3156.84 3158.70 3172.99 3182.34 3192.41
3195.76 3199.96 3202.11 3206.23 3214.36 3216.20
3223.59 3237.86 3245.95 3270.06 3791.21 3813.96

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137.46 155.88 164.42 169.55 178.47 184.30
186.22 192.88 202.62 206.47 210.00 213.85
218.44 223.42 230.81 233.36 240.16 261.71
270.84 272.50 278.34 285.22 286.21 290.33
300.65 312.56 323.45 340.69 344.43 380.78
387.26 398.13 400.36 404.82 411.62 420.19
425.72 438.56 441.63 447.31 450.79 454.88
455.36 462.55 500.67 505.25 506.10 517.13
521.21 524.22 534.42 537.67 538.48 556.28
561.93 582.00 589.64 619.45 626.84 632.25
645.19 657.76 673.10 682.84 704.59 709.56
724.15 737.98 745.30 751.67 757.73 786.85
800.88 806.50 811.68 813.66 814.98 823.22
824.81 831.16 836.41 837.80 843.71 851.93
867.83 868.93 869.60 894.14 901.93 903.24
905.38 907.82 910.08 914.91 922.67 928.59
938.66 941.34 942.78 950.48 961.07 973.87
976.99 1000.56 1004.48 1009.57 1012.64 1015.37
1022.52 1026.52 1028.39 1033.75 1040.67 1045.83
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1089.46 1090.26 1094.44 1098.19 1101.42 1107.99
1113.72 1114.84 1117.31 1123.46 1140.00 1144.68
1158.91 1176.42 1177.74 1189.91 1201.66 1202.53
1202.95 1206.17 1208.36 1212.80 1215.17 1219.00
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1266.63 1267.56 1285.48 1293.40 1299.15 1302.04
1305.15 1308.31 1309.78 1311.17 1318.59 1327.73
1328.07 1334.39 1341.39 1345.18 1350.26 1359.67
1366.38 1367.09 1368.80 1370.80 1372.66 1375.98
1377.23 1380.81 1382.29 1384.97 1391.51 1394.53
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1502.13 1503.72 1504.17 1507.35 1508.09 1508.58
1509.60 1510.10 1510.38 1511.83 1514.89 1520.04
1520.75 1522.46 1527.07 1528.36 1544.76 1593.92
1597.19 1638.23 1645.38 1648.12 1658.73 2037.44
2979.33 3014.91 3017.43 3018.73 3022.30 3022.78
3025.08 3026.87 3027.56 3029.25 3029.78 3030.62
3031.28 3033.05 3035.74 3037.25 3046.54 3056.35
3059.14 3061.91 3067.35 3074.11 3076.90 3078.44
3081.27 3083.57 3083.61 3084.21 3085.75 3087.59
3089.13 3095.33 3102.83 3103.65 3107.44 3113.77
3151.50 3155.37 3161.93 3169.71 3170.81 3183.81
3189.18 3189.47 3197.72 3198.55 3210.71 3211.29
3212.73 3219.76 3246.67 3264.33 3813.09 3838.94

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24.44 28.22 32.33 37.27 42.64 49.52
53.65 60.92 61.47 69.78 72.37 75.65

81.78 84.82 88.51 91.33 95.46 99.95
107.52 112.40 118.42 121.05 131.04 142.89
157.71 161.15 175.97 182.69 185.68 193.94
198.82 207.08 211.40 214.36 220.21 223.05
233.98 235.91 256.28 260.38 268.58 273.47
275.59 284.42 287.73 288.80 294.22 313.81
327.02 335.26 340.19 343.00 352.95 377.55
387.72 398.45 401.93 404.45 413.62 422.70
424.01 441.83 447.73 450.20 456.88 459.43
463.70 474.47 489.53 504.20 508.23 520.98
524.22 534.70 535.43 537.05 558.39 565.85
583.48 594.54 602.27 620.97 627.86 632.89
655.27 662.80 694.31 708.57 716.42 719.21
726.74 744.15 752.61 758.93 770.11 798.19
802.27 805.51 810.37 812.97 823.36 823.67
825.01 831.94 838.53 840.48 858.43 865.61
866.74 867.94 869.83 892.14 900.10 901.25
905.26 907.69 910.23 913.58 926.85 937.79
940.18 941.09 942.59 960.47 973.92 984.99
992.74 1005.76 1007.75 1015.88 1018.41 1022.12
1022.41 1025.43 1027.95 1037.95 1041.21 1046.68
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1092.12 1094.54 1095.40 1098.28 1102.48 1106.56
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1365.38 1367.52 1368.11 1370.07 1376.31 1378.83
1382.23 1384.47 1385.21 1391.24 1394.89 1395.54
1396.31 1397.97 1399.04 1400.22 1401.68 1404.00
1408.52 1451.19 1471.54 1473.06 1483.59 1491.54
1491.81 1497.08 1497.90 1499.73 1500.46 1501.31
1501.66 1503.01 1503.87 1504.07 1507.61 1507.97
1508.86 1509.08 1510.23 1511.99 1516.32 1517.88
1520.90 1521.60 1525.37 1528.79 1540.90 1574.46
1604.34 1644.62 1653.91 1658.04 1661.66 2028.38
2981.37 3016.26 3019.00 3019.75 3023.33 3025.30
3025.73 3027.45 3028.64 3029.72 3031.76 3032.96
3038.89 3043.73 3044.54 3051.13 3056.55 3059.36
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3083.34 3085.65 3086.27 3089.07 3090.47 3093.46
3102.73 3104.56 3111.08 3115.13 3121.93 3122.30
3128.11 3143.35 3154.41 3172.03 3177.73 3178.19
3180.98 3191.18 3192.98 3198.97 3203.49 3210.09
3217.59 3218.79 3255.56 3263.86 3744.46 3823.21

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-27.97 14.57 16.09 26.72 32.37 37.91
42.18 51.11 53.94 57.93 67.76 69.39
73.95 75.38 80.66 85.77 87.41 90.78
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142.75 145.65 150.53 159.51 174.48 180.55
185.99 198.18 209.89 212.02 212.91 219.58
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279.21 282.56 291.73 302.37 308.86 312.25
315.64 333.41 335.55 342.16 396.02 397.61
399.55 406.22 408.36 420.02 420.87 425.83
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485.06 495.37 505.34 505.82 519.95 525.76
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741.77 746.94 749.78 755.98 759.72 776.49

805.60 807.52 807.80 810.58 812.60 819.03
823.53 831.14 831.58 844.35 847.02 858.27
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904.49 908.68 909.27 911.78 913.69 936.81
938.00 940.43 941.34 954.65 974.62 979.69
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1020.29 1025.10 1027.31 1029.31 1040.33 1044.04
1049.11 1055.22 1056.74 1065.60 1068.19 1071.08
1082.55 1090.52 1093.69 1093.92 1096.74 1100.73
1105.63 1110.90 1111.04 1131.15 1135.11 1138.93
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1220.46 1221.37 1225.58 1225.80 1232.87 1236.15
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2927.10 2978.72 3017.65 3020.28 3021.35 3022.59
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3057.24 3063.80 3069.22 3079.45 3079.84 3081.33
3081.52 3082.55 3084.86 3085.63 3088.13 3089.19
3089.26 3092.30 3095.54 3102.07 3104.59 3112.95
3117.49 3140.25 3142.46 3164.72 3168.42 3187.94
3193.65 3193.67 3202.47 3209.78 3214.41 3215.60
3218.69 3229.22 3232.01 3248.08 3473.82 3836.53

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16.59 22.81 27.21 28.27 35.11 47.33
48.28 54.17 56.83 61.06 69.90 73.37
78.02 85.38 89.71 89.99 97.44 102.47
113.12 121.75 127.81 135.77 147.15 149.35
152.24 173.93 179.66 185.16 186.25 192.01
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241.45 250.84 254.68 262.57 265.33 273.17
274.80 277.42 287.17 300.21 311.89 315.78
323.01 329.89 346.92 378.84 398.45 399.22
411.68 415.01 423.31 426.30 432.13 437.59
441.72 446.63 449.58 452.42 458.10 474.39
495.49 499.66 511.91 521.67 522.78 529.31
530.70 542.09 547.45 560.60 576.32 586.69
606.13 607.74 615.95 625.31 633.01 639.00
641.30 665.73 702.33 713.10 716.40 721.07
727.84 731.67 743.69 746.64 771.04 775.15
789.70 802.97 811.67 813.52 823.90 827.03
833.54 837.27 844.42 861.20 863.57 865.53
866.54 868.68 898.68 900.64 903.13 907.08
911.71 913.37 914.67 927.12 938.20 938.75
941.06 942.82 950.66 961.77 976.35 982.85
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1357.36 1367.00 1367.65 1368.12 1369.65 1371.22
1374.48 1379.98 1381.35 1385.04 1387.03 1390.42
1395.19 1396.04 1397.29 1397.90 1400.48 1403.03
1404.65 1418.56 1466.81 1487.30 1489.54 1492.50
1497.01 1498.41 1499.16 1500.09 1500.97 1501.99
1503.03 1504.71 1507.08 1507.72 1508.70 1509.37
1510.75 1510.92 1511.16 1513.54 1518.58 1520.62
1523.70 1525.09 1536.43 1539.69 1548.03 1615.28
1631.01 1642.97 1655.07 1662.98 1676.42 2050.75
2995.53 3018.03 3019.43 3020.39 3020.68 3020.76
3021.45 3023.07 3026.82 3028.43 3030.79 3030.88
3031.82 3035.53 3039.77 3042.34 3048.75 3057.63
3059.62 3069.22 3073.33 3076.83 3080.49 3081.98
3084.26 3086.18 3087.29 3087.55 3088.76 3088.89
3089.83 3089.85 3094.37 3103.70 3115.83 3119.42
3124.38 3125.51 3164.12 3165.81 3166.32 3181.16
3186.17 3188.68 3195.24 3198.15 3208.07 3208.30
3212.51 3222.19 3227.08 3253.18 3784.89 3813.15

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8'-TS

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-234.71 17.62 21.03 25.27 31.86 35.14
43.96 47.99 55.26 57.56 61.92 70.46
74.57 77.30 85.34 88.19 89.32 97.38
101.68 114.76 120.68 127.13 137.11 143.25
149.84 151.28 177.01 180.29 184.08 190.37
191.80 203.45 207.73 213.01 215.86 219.42
227.32 242.21 250.54 255.14 258.10 261.45
266.67 271.18 276.62 281.24 286.88 312.97
313.22 328.36 338.74 346.82 367.94 399.20
399.72 406.45 416.70 420.76 427.46 435.56
438.84 446.87 449.62 450.62 455.20 458.20
480.16 499.70 510.79 514.32 521.13 523.59
528.45 531.40 534.37 556.09 569.97 575.28
597.67 601.57 613.58 627.16 632.80 644.91
647.10 660.52 696.20 707.03 711.91 717.45
723.30 735.02 742.82 746.19 747.21 775.23
787.52 791.59 796.96 803.34 811.48 812.82
824.08 828.12 833.49 843.74 846.41 862.82
864.13 866.36 868.44 869.45 901.06 903.28
906.87 911.30 913.32 913.88 930.11 938.18
940.28 940.95 942.82 953.67 962.71 980.61
984.51 999.38 1001.61 1008.64 1009.99 1016.15
1017.97 1023.59 1027.29 1029.73 1041.68 1045.50
1049.17 1053.45 1060.52 1061.42 1070.31 1074.32
1077.24 1092.65 1092.84 1095.53 1096.65 1102.74
1106.83 1116.38 1117.17 1119.40 1125.50 1139.32
1141.84 1158.98 1174.77 1177.38 1199.10 1199.75
1202.83 1205.53 1209.28 1214.40 1218.18 1219.28
1219.80 1221.50 1223.35 1234.74 1237.43 1243.64
1262.34 1263.33 1269.42 1294.21 1296.17 1300.12
1302.29 1304.45 1307.00 1307.52 1312.04 1320.95
1324.12 1329.96 1331.09 1340.74 1347.28 1349.19
1363.02 1365.39 1367.60 1368.41 1369.92 1371.41
1374.52 1380.06 1382.01 1385.49 1387.37 1390.37
1394.90 1395.47 1396.81 1397.55 1400.41 1402.84
1404.66 1431.97 1470.09 1481.79 1486.61 1492.91
1496.97 1498.83 1499.97 1500.87 1500.93 1501.95
1503.10 1504.78 1507.10 1507.63 1508.66 1510.03
1510.36 1511.21 1511.23 1512.64 1520.78 1522.44
1524.75 1526.02 1532.93 1537.00 1541.85 1599.17
1633.19 1634.46 1655.92 1657.61 1671.25 2053.76
2993.70 3016.25 3018.75 3019.71 3021.19 3021.54
3022.45 3027.09 3027.76 3028.65 3031.20 3032.31
3034.87 3035.93 3040.49 3042.73 3048.31 3056.61

3061.88 3069.96 3072.27 3074.84 3080.69 3081.04
3082.95 3085.17 3086.11 3087.67 3088.61 3089.72
3093.73 3095.93 3098.90 3110.31 3112.78 3116.16
3119.83 3124.53 3166.79 3170.53 3172.35 3185.61
3187.15 3194.00 3196.26 3203.28 3208.88 3212.92
3215.12 3229.56 3250.77 3255.29 3792.98 3802.79

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9'

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17.03 25.21 29.67 32.33 39.34 44.43
50.77 52.11 56.96 65.14 69.27 73.67
77.30 88.15 90.71 93.06 99.81 104.73
108.71 110.15 121.94 130.72 135.87 138.02
155.83 158.42 167.80 177.54 184.23 190.55
193.94 200.85 209.20 211.39 216.17 218.61
220.15 222.05 240.09 248.09 250.42 260.65
268.19 273.74 282.20 284.45 288.37 308.96
312.80 322.61 327.56 346.48 349.13 392.99
398.28 403.41 417.52 423.20 424.19 425.71
433.25 439.82 446.30 449.28 452.31 459.16
478.18 488.61 505.76 512.52 518.58 521.52
528.48 531.44 538.85 544.11 552.54 559.03
561.08 588.40 598.93 608.89 622.08 629.98
637.66 644.84 654.51 706.18 708.41 717.06
723.62 741.69 744.13 744.31 747.72 773.98
785.68 791.91 803.89 811.27 814.10 825.93
828.11 832.47 837.04 845.71 860.17 864.71
867.17 868.18 878.92 901.39 903.36 910.43
912.58 913.65 921.17 927.44 934.60 938.70
942.32 946.49 961.39 965.07 967.68 983.26
989.19 992.98 995.81 1008.63 1015.09 1018.35
1020.52 1023.46 1028.02 1030.64 1041.99 1047.05
1048.50 1055.93 1059.07 1060.90 1070.15 1075.34
1089.01 1090.39 1095.65 1096.50 1103.10 1108.83
1110.43 1113.84 1116.66 1117.58 1141.06 1142.66
1161.57 1162.94 1177.16 1179.15 1199.23 1203.30
1204.48 1207.71 1212.70 1216.31 1219.09 1220.73
1222.79 1228.76 1234.79 1236.76 1246.93 1257.74
1265.42 1267.20 1291.51 1297.98 1300.16 1303.25
1305.40 1308.16 1309.66 1311.91 1321.14 1326.82
1332.09 1337.36 1341.66 1347.24 1347.95 1356.66
1362.99 1368.40 1369.12 1371.17 1373.00 1374.39
1376.80 1381.07 1383.47 1384.82 1388.84 1393.30
1396.85 1398.15 1400.02 1401.48 1402.15 1403.59
1434.74 1470.28 1480.23 1487.97 1488.81 1489.36
1496.41 1499.11 1500.03 1500.37 1501.70 1503.05
1505.29 1506.71 1507.06 1508.79 1509.57 1510.50
1511.47 1513.60 1514.79 1519.68 1520.87 1524.71
1525.66 1538.08 1539.40 1548.94 1583.47 1610.97
1617.84 1633.15 1648.51 1657.67 1676.34 2066.41
3014.78 3016.92 3018.23 3019.93 3021.06 3023.03
3024.43 3027.21 3029.07 3030.41 3031.07 3032.46
3035.16 3041.41 3042.21 3048.80 3057.06 3062.47
3065.77 3074.23 3077.27 3081.43 3082.46 3085.31
3085.50 3086.14 3086.81 3088.81 3089.12 3089.27
3096.14 3098.60 3100.59 3106.09 3108.18 3111.87
3115.80 3161.43 3163.38 3171.11 3180.70 3182.66
3186.77 3192.92 3196.60 3199.97 3205.71 3210.45
3212.61 3220.23 3249.75 3257.77 3768.46 3828.15

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2b'

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16.32 31.15 31.83 43.90 45.72 70.45
81.63 89.57 127.26 139.54 160.18 184.81
198.47 212.07 223.68 229.13 261.56 273.66
290.53 299.29 312.85 347.07 384.32 394.53

414.19 419.69 432.82 476.62 502.79 538.47
544.92 555.64 580.76 615.97 626.06 632.51
638.24 645.03 647.41 707.12 711.02 715.51
736.39 748.75 774.64 775.22 793.60 816.71
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955.18 970.95 976.03 976.42 995.53 997.89
1014.43 1015.01 1016.78 1057.27 1059.47 1093.64
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1194.09 1195.25 1199.25 1209.95 1216.73 1219.59
1230.57 1240.77 1245.99 1268.25 1297.62 1332.78
1343.00 1353.62 1364.13 1366.97 1399.84 1407.71
1467.44 1484.88 1488.79 1492.89 1504.54 1505.81
1506.28 1516.98 1521.62 1536.02 1539.35 1555.88
1629.52 1631.08 1642.89 1658.08 1660.00 1668.60
1695.93 3002.70 3009.81 3063.13 3073.11 3142.32
3142.79 3148.14 3168.14 3169.56 3176.84 3179.33
3187.28 3193.34 3200.43 3201.60 3201.70 3208.91
3225.06 3241.16 3822.52

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11'

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4.57 17.64 23.28 25.41 34.20 35.33
40.03 43.70 47.45 51.05 57.58 62.40
65.35 70.78 74.78 75.60 78.94 81.89
87.33 89.29 94.93 97.84 99.36 102.51
111.65 116.52 119.89 124.30 127.93 132.43
142.62 151.32 156.96 164.70 169.81 171.13
179.55 184.56 186.45 191.83 199.08 200.59
207.61 210.29 217.83 218.99 223.72 229.54
234.70 238.32 264.70 267.11 269.00 271.69
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297.17 302.76 311.16 323.25 327.88 343.51
346.45 367.13 375.52 392.69 399.61 403.87
406.60 415.36 416.42 418.37 427.98 434.04
438.90 447.09 451.91 460.07 460.32 462.09
477.61 504.47 507.19 511.20 513.82 525.23
529.75 536.14 541.21 543.81 549.14 553.17
556.44 565.67 568.62 578.62 596.10 607.37
617.75 620.13 625.80 628.64 633.37 646.12
657.48 661.19 684.70 691.32 704.31 712.68
721.78 732.75 747.04 752.99 760.40 771.14
792.30 803.52 808.65 810.51 814.30 818.60
819.65 820.81 823.72 827.13 830.10 849.85
852.70 855.27 858.26 866.98 869.12 870.35
881.08 901.16 902.45 903.42 904.66 908.59
910.91 913.92 931.30 938.39 941.17 942.38
946.25 951.42 954.57 971.18 981.32 983.48
995.81 1000.51 1005.65 1007.57 1012.39 1012.72
1015.39 1022.94 1026.64 1027.63 1031.72 1038.82
1043.95 1048.00 1056.56 1057.99 1071.29 1073.78
1076.16 1080.68 1083.98 1089.55 1093.69 1094.85
1097.89 1101.48 1104.74 1107.21 1115.15 1116.05
1137.31 1141.79 1146.43 1155.20 1159.40 1167.15
1176.12 1179.22 1184.65 1187.03 1190.25 1196.56
1197.04 1200.26 1203.39 1205.68 1206.98 1212.70
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1234.88 1235.86 1241.10 1256.39 1262.75 1264.51
1281.64 1285.66 1292.87 1299.44 1301.84 1305.43
1305.96 1306.91 1309.08 1319.76 1327.37 1333.35
1341.46 1342.96 1344.33 1346.55 1349.62 1351.37
1366.44 1366.70 1369.33 1370.76 1375.21 1382.20
1383.13 1384.59 1390.63 1391.75 1393.02 1394.48
1395.42 1396.36 1397.71 1397.97 1401.33 1404.01
1407.46 1419.95 1445.37 1468.19 1473.94 1478.19
1487.22 1489.93 1491.31 1492.70 1494.02 1497.45
1498.05 1499.12 1500.42 1500.99 1501.74 1502.04
1504.30 1505.21 1506.74 1507.42 1508.34 1508.91

1510.35 1510.77 1512.45 1513.11 1513.71 1517.90
1519.70 1520.88 1521.84 1524.89 1528.23 1530.39
1537.12 1541.83 1574.18 1630.76 1642.37 1644.05
1659.31 1664.29 1665.92 1674.45 2046.39 2978.81
2989.05 3012.31 3016.33 3019.74 3022.60 3023.62
3024.12 3025.71 3028.30 3028.63 3029.10 3030.23
3030.97 3032.27 3036.42 3039.19 3041.73 3046.53
3048.61 3050.44 3061.34 3073.92 3077.43 3077.57
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3229.59 3239.17 3239.99 3240.72 3268.61 3284.96
3672.10 3803.54 3817.11

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11'-TS

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-1380.60 11.09 15.92 19.09 28.89 32.30
35.75 45.33 51.74 55.15 58.34 59.86
66.84 68.52 72.99 74.19 77.53 83.17
83.54 88.59 93.30 95.05 98.11 99.54
103.14 109.23 116.08 121.31 123.89 132.27
135.41 144.35 161.61 163.63 169.17 175.51
185.19 188.55 197.59 201.80 207.71 208.75
211.49 214.32 215.43 220.39 223.58 230.56
231.90 235.66 238.79 240.31 258.69 267.37
275.35 275.81 280.12 283.82 288.33 291.60
293.53 305.40 312.27 318.85 325.22 340.29
344.30 344.89 378.39 387.73 394.87 398.53
400.85 413.26 419.62 423.53 425.01 436.12
442.32 448.25 450.01 453.20 459.76 474.56
486.76 491.65 505.01 519.13 522.40 524.26
527.05 531.97 536.52 541.05 545.28 552.54
555.99 567.15 577.81 580.27 590.42 609.30
622.08 627.77 632.41 633.71 638.15 649.74
653.68 677.14 689.76 705.24 712.00 714.64
719.08 732.92 738.88 742.94 750.93 761.08
770.40 775.33 785.52 789.42 806.24 810.11
813.00 820.07 823.41 825.37 827.58 830.67
832.52 834.41 853.01 867.40 868.12 869.52
875.88 900.72 901.86 903.66 904.98 908.00
909.63 913.26 915.09 937.58 938.15 940.62
942.93 954.90 960.53 969.16 974.44 977.27
1000.80 1002.90 1004.32 1005.56 1007.22 1010.53
1018.11 1023.69 1026.64 1027.45 1040.76 1045.20
1046.24 1048.96 1055.73 1057.96 1067.63 1067.81
1072.33 1088.31 1091.01 1091.41 1094.51 1096.19
1100.80 1105.81 1113.09 1113.85 1118.39 1123.40
1136.56 1138.03 1144.17 1157.80 1163.72 1177.11
1178.36 1178.54 1181.58 1189.77 1191.51 1199.76
1200.99 1201.24 1205.37 1209.55 1209.90 1212.51
1215.42 1217.92 1218.70 1222.54 1229.41 1234.13
1235.29 1237.05 1240.68 1246.90 1257.46 1264.38
1274.99 1290.71 1293.15 1298.30 1300.18 1305.14
1307.31 1308.06 1309.48 1319.28 1324.88 1332.45
1333.73 1337.32 1337.72 1341.88 1345.45 1346.34
1366.24 1367.65 1370.47 1372.76 1375.74 1376.29
1379.35 1381.81 1383.05 1385.15 1388.23 1393.33
1394.22 1394.94 1395.79 1397.02 1398.58 1400.78
1403.84 1404.83 1449.05 1456.53 1466.72 1479.36
1487.07 1490.45 1492.19 1493.41 1494.02 1496.15
1498.86 1500.10 1500.56 1501.32 1501.96 1502.45
1503.07 1504.68 1507.07 1507.52 1507.77 1508.28
1509.56 1510.66 1510.96 1512.31 1514.09 1516.06
1518.22 1518.80 1520.61 1522.84 1525.64 1526.13
1528.60 1541.71 1547.16 1589.20 1604.74 1635.63

1640.69 1649.34 1654.85 1659.96 1672.07 2041.05
2994.22 3009.11 3014.60 3017.00 3019.26 3019.33
3020.91 3021.18 3022.14 3023.82 3024.80 3025.75
3026.36 3027.02 3028.33 3038.12 3046.06 3047.09
3059.34 3061.31 3065.51 3068.22 3070.74 3073.55
3074.82 3076.30 3079.31 3080.63 3081.43 3082.30
3084.41 3087.27 3089.84 3091.73 3095.77 3117.46
3117.62 3129.58 3133.89 3134.70 3150.85 3160.04
3161.58 3162.53 3162.55 3164.44 3183.14 3184.84
3190.93 3194.20 3204.47 3205.69 3210.88 3211.80
3215.81 3225.38 3229.94 3230.54 3235.93 3255.25
3407.53 3819.11 3827.29

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12'

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4.96 13.56 17.50 20.29 25.52 32.52
38.91 40.30 44.66 47.56 49.95 55.06
63.74 65.58 68.12 72.91 75.53 79.96
84.85 87.71 92.61 94.02 95.43 96.81
105.05 108.26 111.91 122.49 127.01 133.12
143.32 145.94 154.31 158.38 160.76 166.18
173.06 179.25 180.49 189.90 191.93 201.38
201.96 209.02 209.07 214.37 221.71 223.67
229.45 230.73 234.53 238.79 239.64 259.82
271.69 273.97 276.47 278.08 282.12 283.48
286.04 293.54 304.93 310.07 326.60 338.44
349.37 351.48 367.82 368.95 381.21 386.51
395.41 398.14 401.44 416.32 425.01 429.99
432.94 434.66 436.53 444.06 445.11 451.11
451.69 461.73 476.46 501.09 503.48 514.15
519.78 524.20 530.43 534.57 539.14 542.73
546.88 549.22 553.69 572.21 583.32 590.42
599.34 607.80 609.82 627.70 631.03 635.66
637.10 646.14 655.71 660.09 679.51 709.34
711.24 713.12 714.94 719.99 735.56 739.68
741.18 753.38 779.48 783.87 795.18 797.76
807.70 808.55 813.63 822.25 824.92 825.77
830.03 835.91 848.17 860.27 864.82 867.12
868.77 872.33 897.94 900.92 904.41 905.86
909.57 910.14 914.90 934.13 936.49 942.16
942.66 948.88 952.60 958.24 964.35 979.54
981.47 996.15 1007.04 1008.41 1012.86 1018.11
1021.03 1024.10 1027.47 1027.85 1040.51 1041.45
1045.13 1048.80 1056.69 1059.71 1062.49 1070.37
1073.61 1087.87 1088.79 1089.37 1093.78 1095.61
1100.83 1109.07 1114.21 1115.03 1118.18 1123.10
1125.25 1139.47 1144.47 1159.90 1164.56 1178.81
1179.56 1180.60 1185.68 1187.62 1199.21 1200.15
1200.70 1201.68 1206.94 1210.85 1213.45 1219.38
1219.88 1221.97 1228.41 1229.51 1232.69 1239.06
1241.40 1242.07 1248.34 1252.92 1268.92 1269.45
1287.79 1292.42 1298.60 1301.86 1305.02 1308.31
1309.78 1313.18 1323.74 1331.80 1334.38 1334.67
1339.55 1341.11 1344.12 1345.78 1351.45 1365.53
1367.95 1369.50 1369.97 1373.33 1373.51 1377.86
1381.95 1383.03 1383.97 1393.56 1394.41 1395.61
1396.39 1397.32 1398.33 1398.60 1402.58 1406.41
1407.06 1456.38 1464.50 1481.45 1482.24 1486.90
1488.63 1491.95 1494.71 1495.61 1498.05 1499.32
1500.49 1500.82 1501.48 1501.65 1502.99 1503.80
1504.21 1505.36 1507.92 1507.93 1509.96 1511.67
1512.56 1512.93 1518.02 1518.61 1521.20 1521.65
1522.94 1526.31 1527.47 1530.07 1536.61 1552.73
1611.06 1619.51 1625.16 1632.24 1646.47 1649.93
1653.81 1656.70 1667.89 1685.30 2065.06 3017.05
3017.62 3019.31 3019.72 3021.17 3021.67 3022.02
3025.24 3025.99 3027.63 3028.19 3029.90 3032.79

3035.67 3039.47 3042.72 3044.37 3047.27 3061.16
3064.49 3066.55 3069.39 3076.18 3076.93 3081.65
3082.48 3083.75 3083.94 3084.41 3086.17 3087.54
3087.95 3092.10 3094.78 3096.47 3105.03 3113.53
3115.29 3124.81 3127.66 3132.31 3158.02 3159.03
3160.75 3163.62 3172.93 3176.58 3183.96 3188.92
3193.23 3198.80 3206.01 3208.52 3210.46 3214.50
3217.32 3229.51 3231.65 3246.06 3271.85 3751.12
3773.84 3825.89 3827.66

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Ketone

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49.29 87.99 99.65 131.78 162.72 205.34
253.89 296.92 349.44 415.67 429.31 441.63
465.99 510.58 582.26 627.07 629.91 630.61
681.71 708.54 721.77 770.43 788.45 805.78
821.20 871.17 896.62 935.60 952.94 995.40
996.02 999.43 1008.05 1009.19 1013.62 1019.78
1026.12 1041.07 1056.80 1116.18 1121.37 1194.35
1197.07 1203.08 1218.91 1229.94 1230.78 1278.51
1310.65 1345.85 1364.66 1367.74 1423.12 1477.98
1488.30 1498.11 1529.14 1534.43 1596.95 1628.68
1648.96 1654.42 1723.28 2753.42 2798.26 3065.77
3093.47 3117.31 3152.59 3169.28 3178.38 3186.35
3193.35 3199.19 3204.53

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Z-enol

==========

43.18 51.16 82.85 95.12 168.91 207.80
267.85 306.24 328.04 384.75 413.96 419.25
425.16 496.65 534.31 582.18 627.94 630.45
650.72 678.49 707.64 715.44 771.68 780.78
828.26 849.80 852.34 865.77 876.76 930.12
938.52 977.28 982.69 999.57 1003.33 1004.10
1012.43 1048.64 1059.30 1078.46 1117.77 1120.27
1195.80 1197.60 1219.42 1222.58 1237.63 1247.73
1318.58 1336.24 1357.39 1367.26 1373.33 1415.25
1487.18 1492.94 1534.47 1541.21 1625.93 1630.84
1656.88 1661.55 1719.65 3165.45 3175.93 3176.86
3183.44 3185.90 3188.08 3193.47 3201.61 3202.86
3210.13 3253.11 3808.98

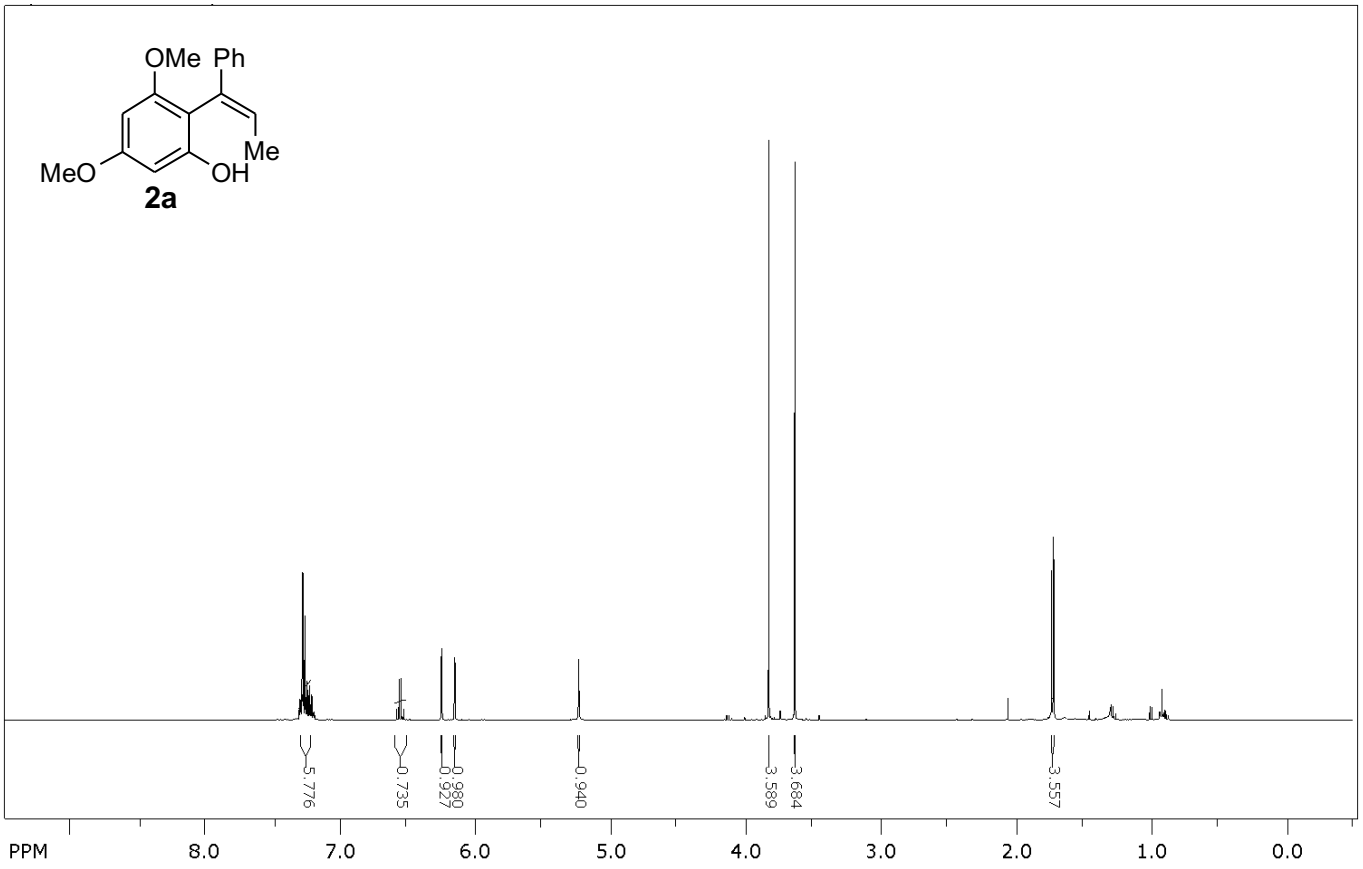
==========

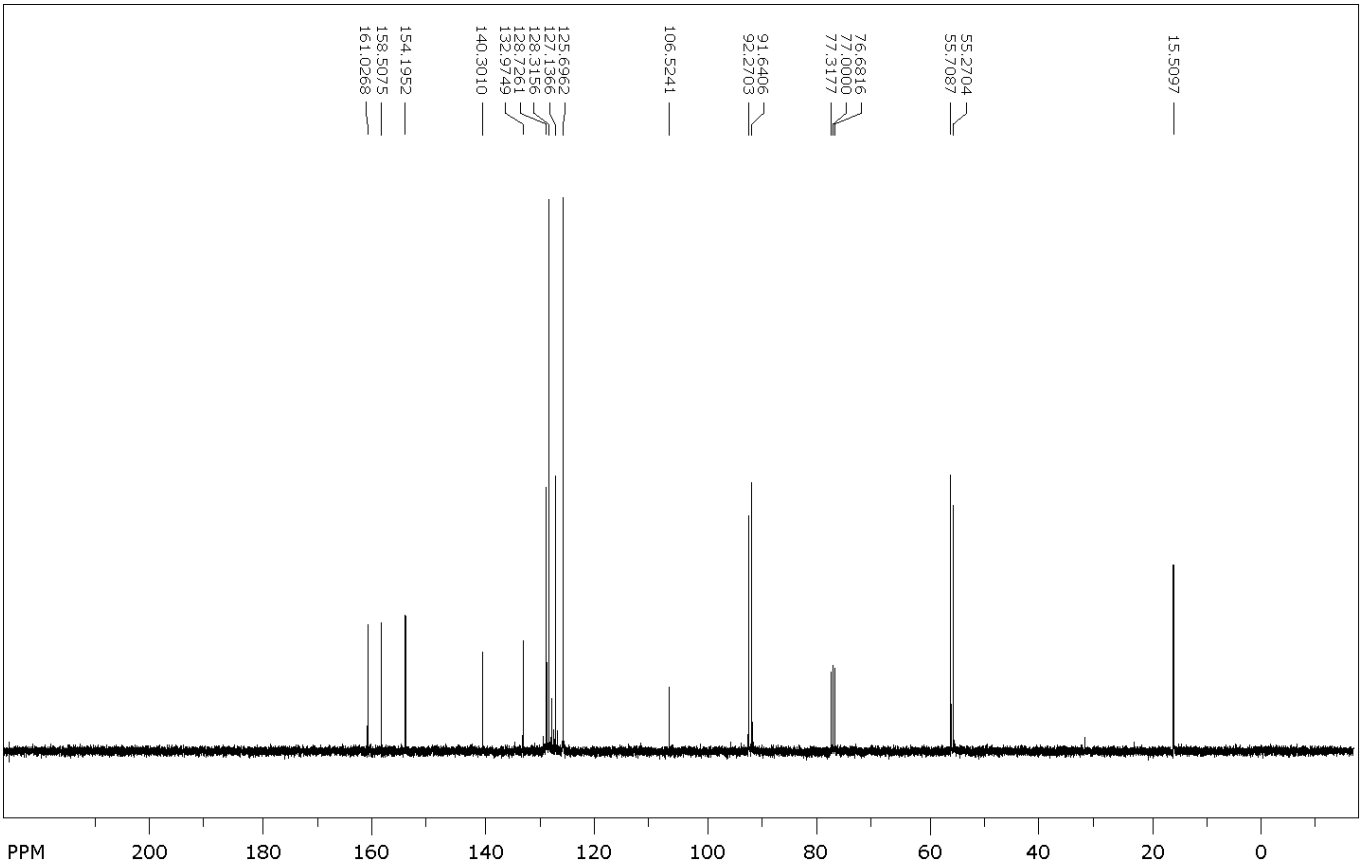
E-enol

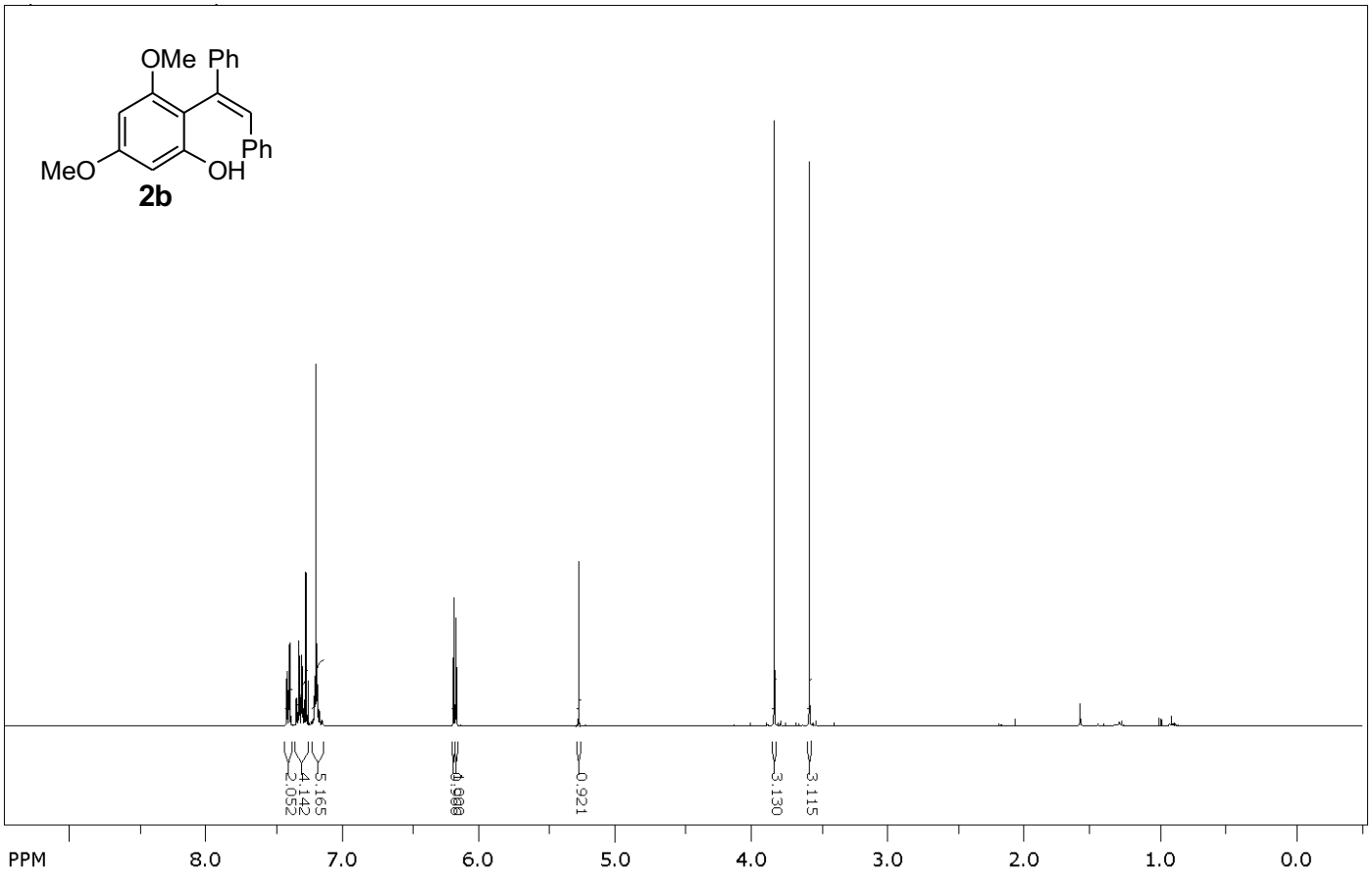
==========

37.13 50.06 77.99 124.81 162.35 202.16
259.31 329.86 340.93 401.10 407.10 419.92
431.24 496.00 520.61 590.43 619.36 634.58
637.67 652.47 712.62 716.46 748.03 774.13
788.74 859.02 867.22 871.54 881.15 931.61
942.86 975.83 984.45 996.07 1003.66 1013.36
1015.02 1053.54 1059.27 1104.04 1114.27 1131.18
1195.01 1197.12 1215.29 1219.57 1224.13 1237.11
1292.48 1339.09 1343.43 1365.05 1367.88 1421.59
1485.96 1489.89 1536.19 1540.93 1627.76 1631.76
1658.60 1660.59 1718.35 3168.19 3171.10 3177.74
3177.87 3186.10 3187.76 3195.43 3200.82 3205.97
3212.96 3221.95 3800.37

9. ^{1}H and ^{13}C NMR Spectra of Products.



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Ph
MeO
OH
2b
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4.142
5.165
0.921
3.130
3.115
PPM
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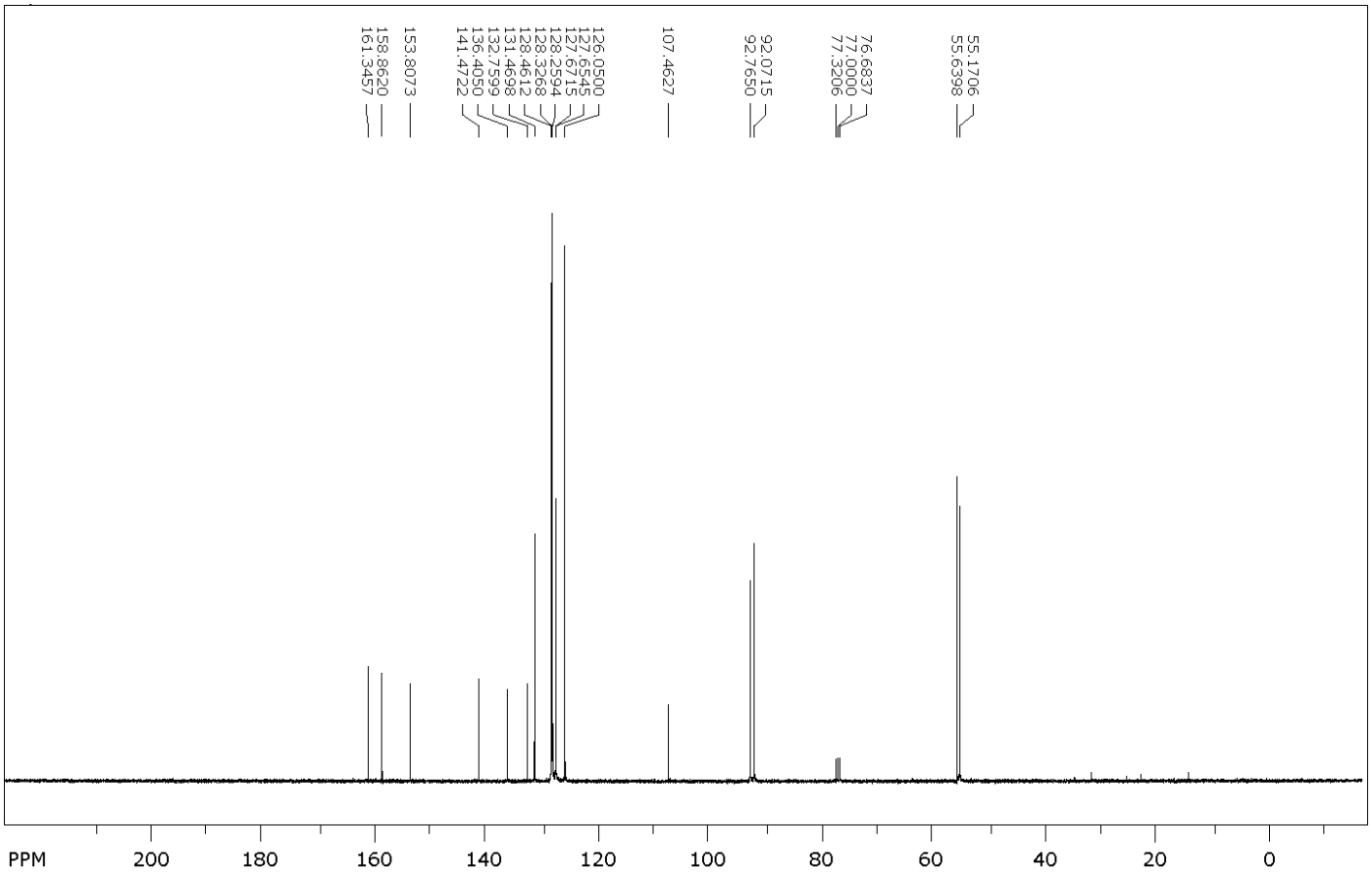
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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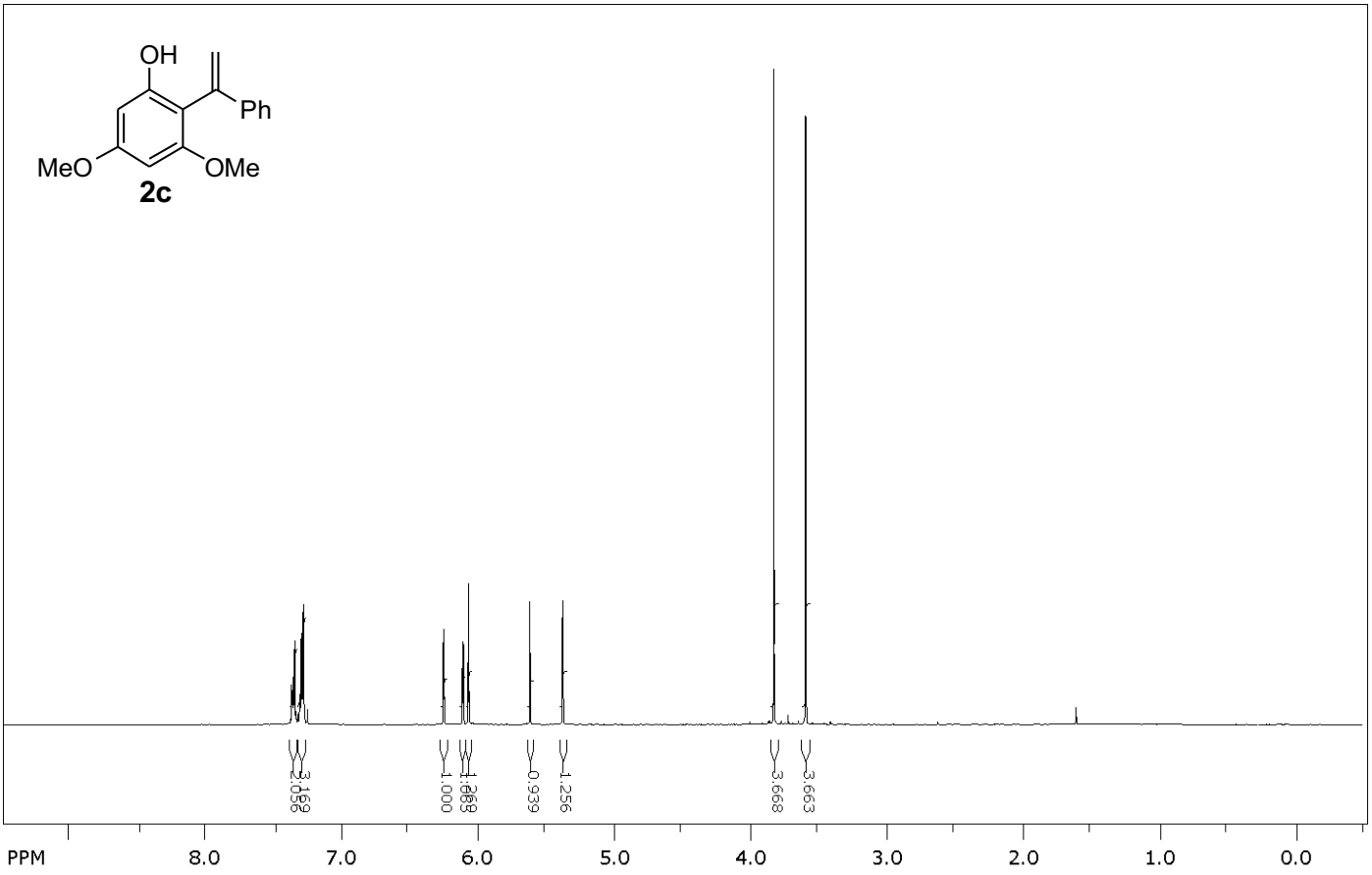
153.8073
141.4722
136.4050
132.7599
131.4698
128.4612
128.3268
128.3594
127.6715
127.6545
126.0500
107.4627
92.7650
92.0715
77.3206
77.0000
76.6837
55.6398
55.1706
PPM
200
180
160
140
120
100
80
60
40
20
0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Ph
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OMe
2c
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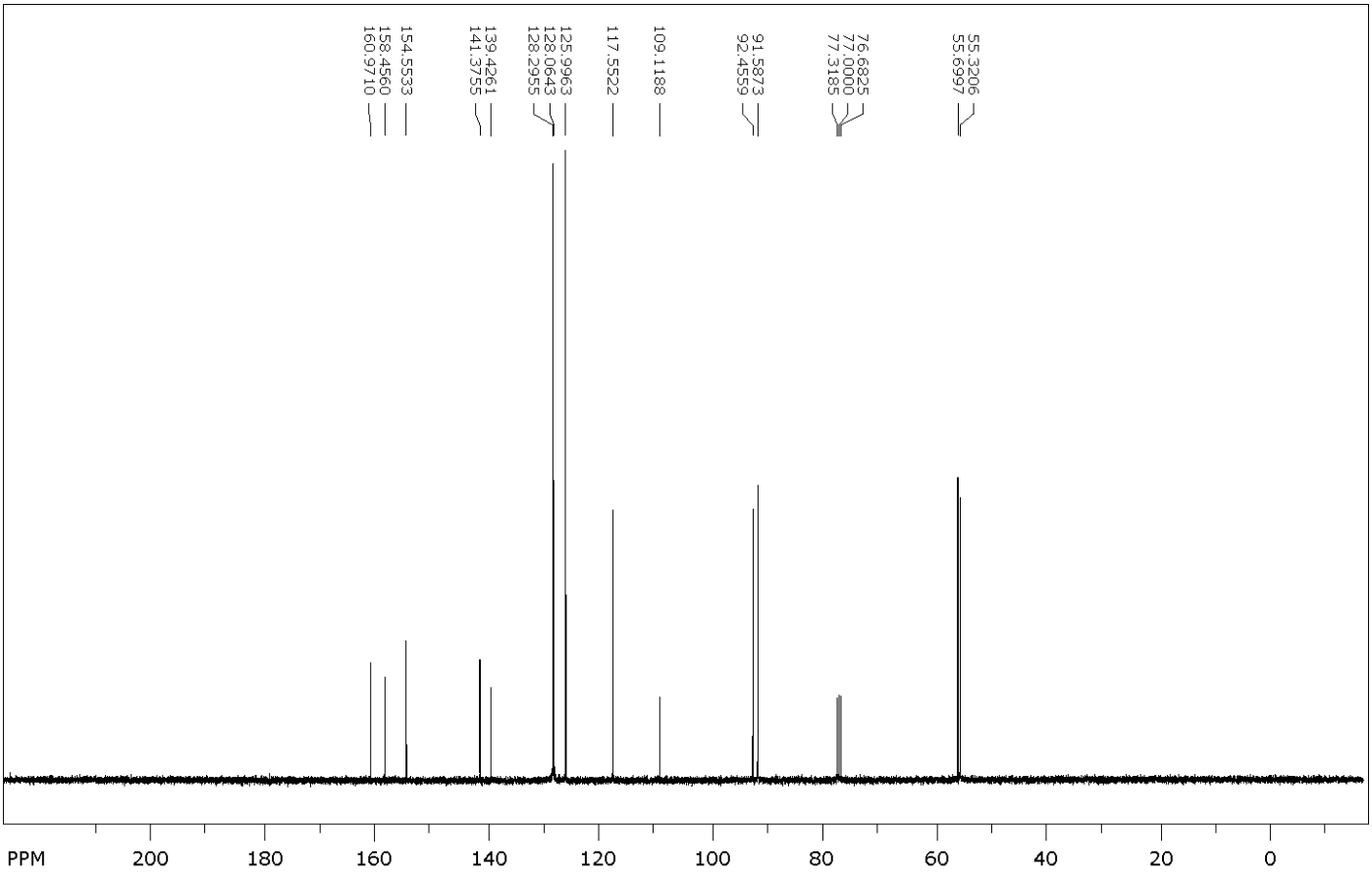
1.000
1.256
0.939
3.668
3.663
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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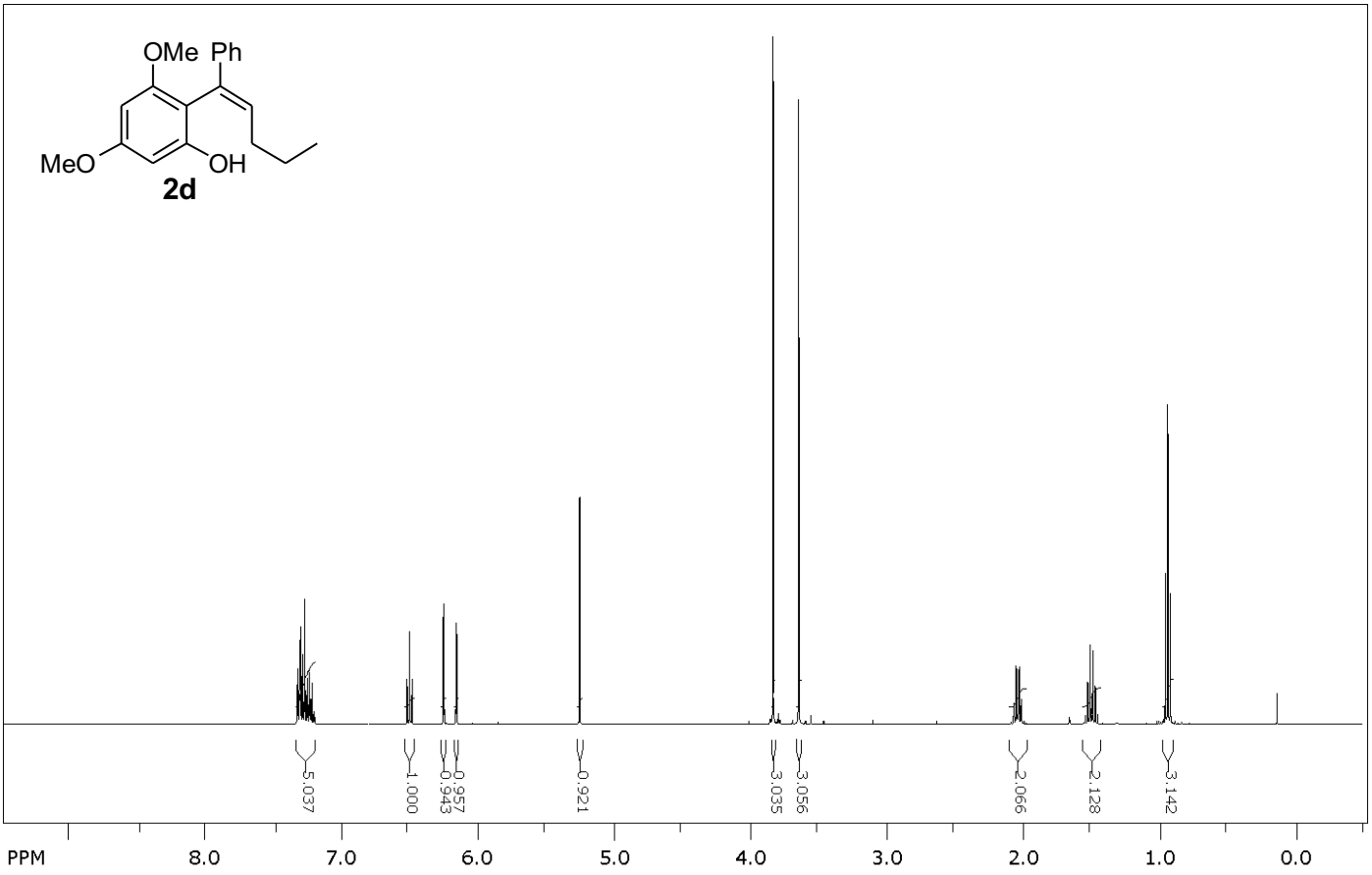
154.5533
141.3755
139.4261
128.2955
128.0643
125.9963
117.5522
109.1188
92.4559
91.5873
77.3185
77.0000
76.6825
55.6997
55.3206
PPM
200
180
160
140
120
100
80
60
40
20
0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MeO
OH
2d
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1.000
0.957
0.943
0.921
3.035
3.056
2.066
2.128
3.142
PPM
8.0
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6.0
5.0
4.0
3.0
2.0
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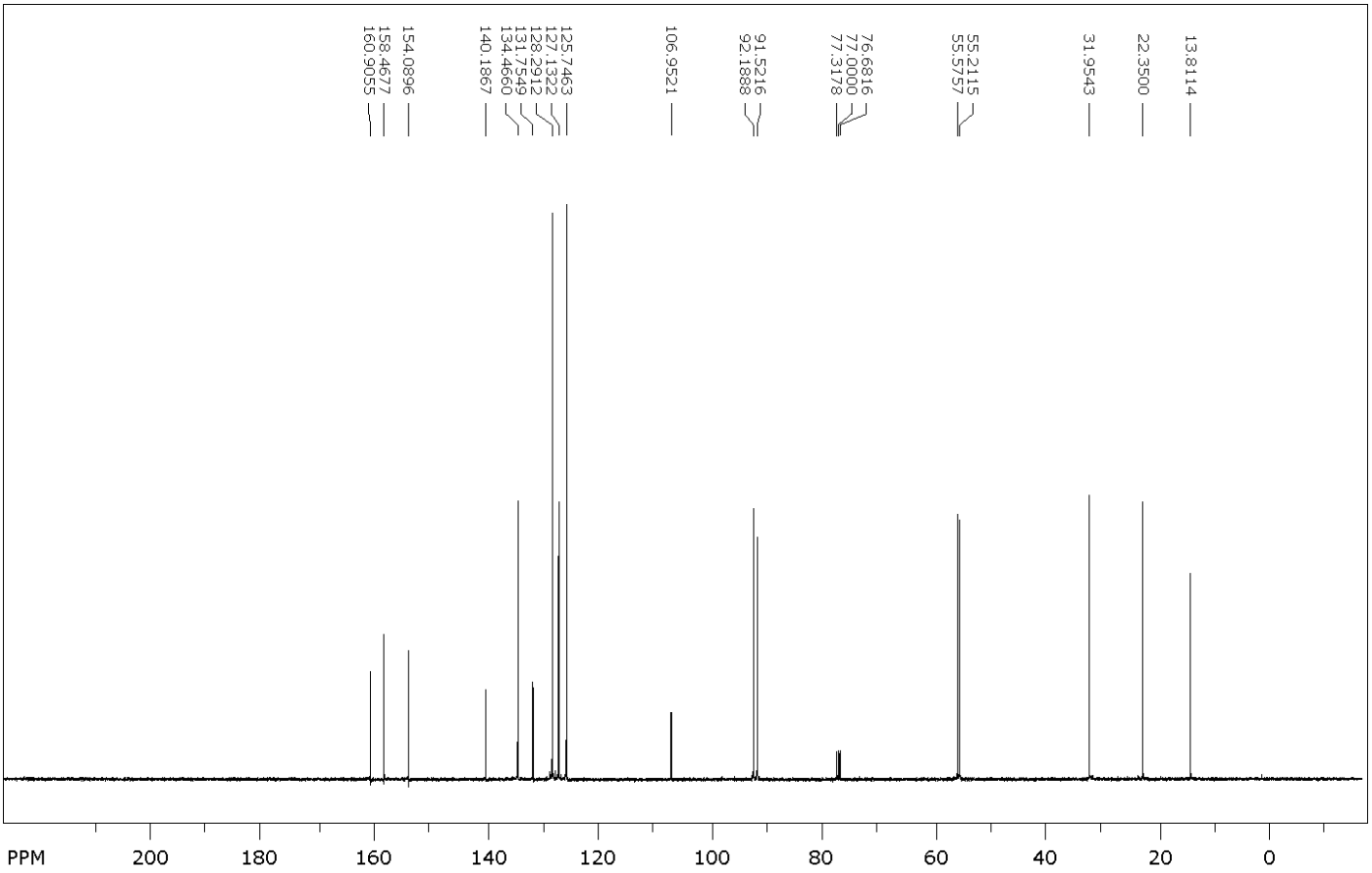
0.0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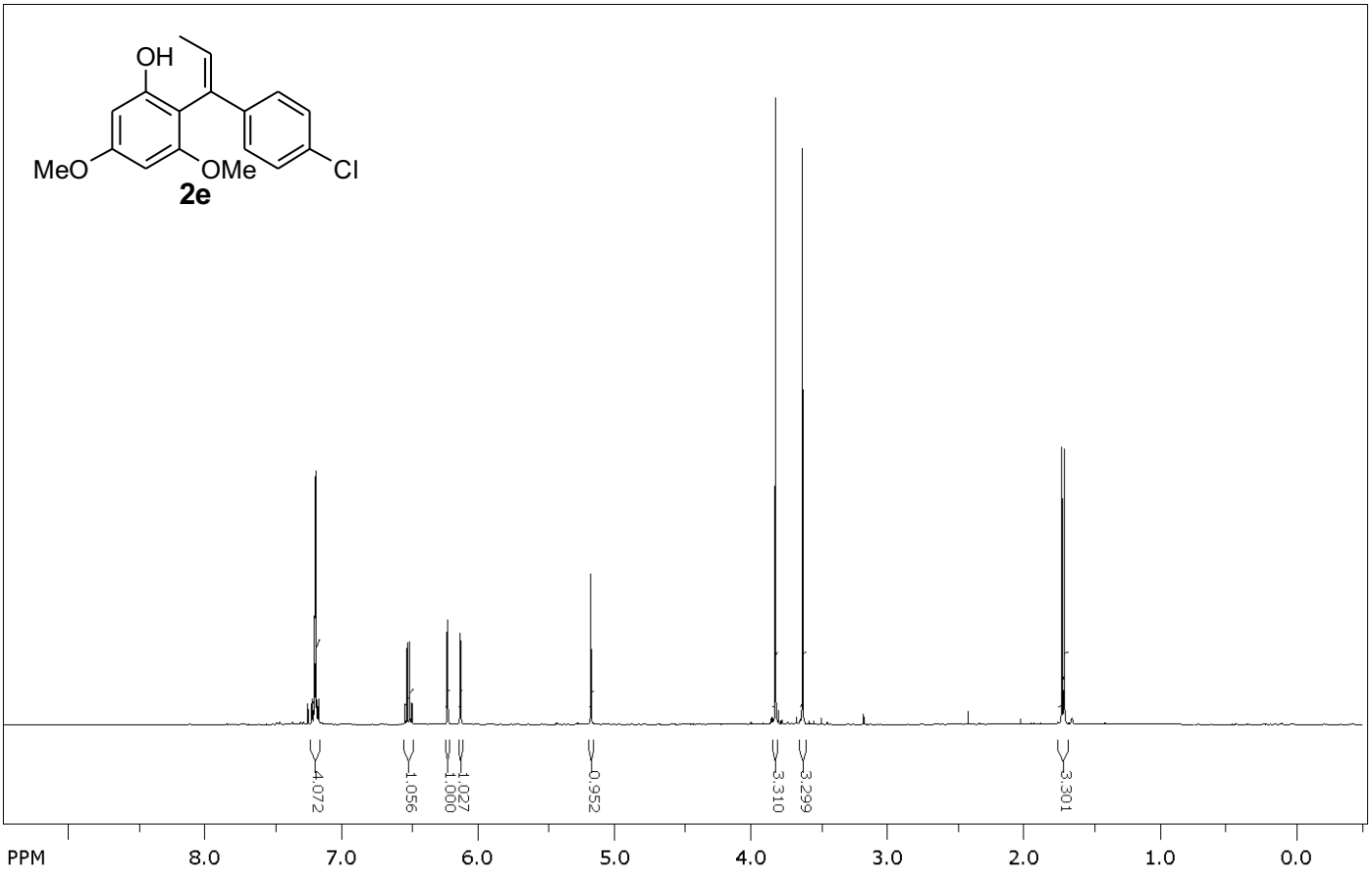
154.0896
140.1867
134.4660
131.7549
128.2912
127.1322
125.7463
106.9521
92.1888
91.5216
77.3178
77.0000
76.6816
55.5757
55.2115
31.9543
22.3500
13.8114
PPM
200
180
160
140
120
100
80
60
40
20
0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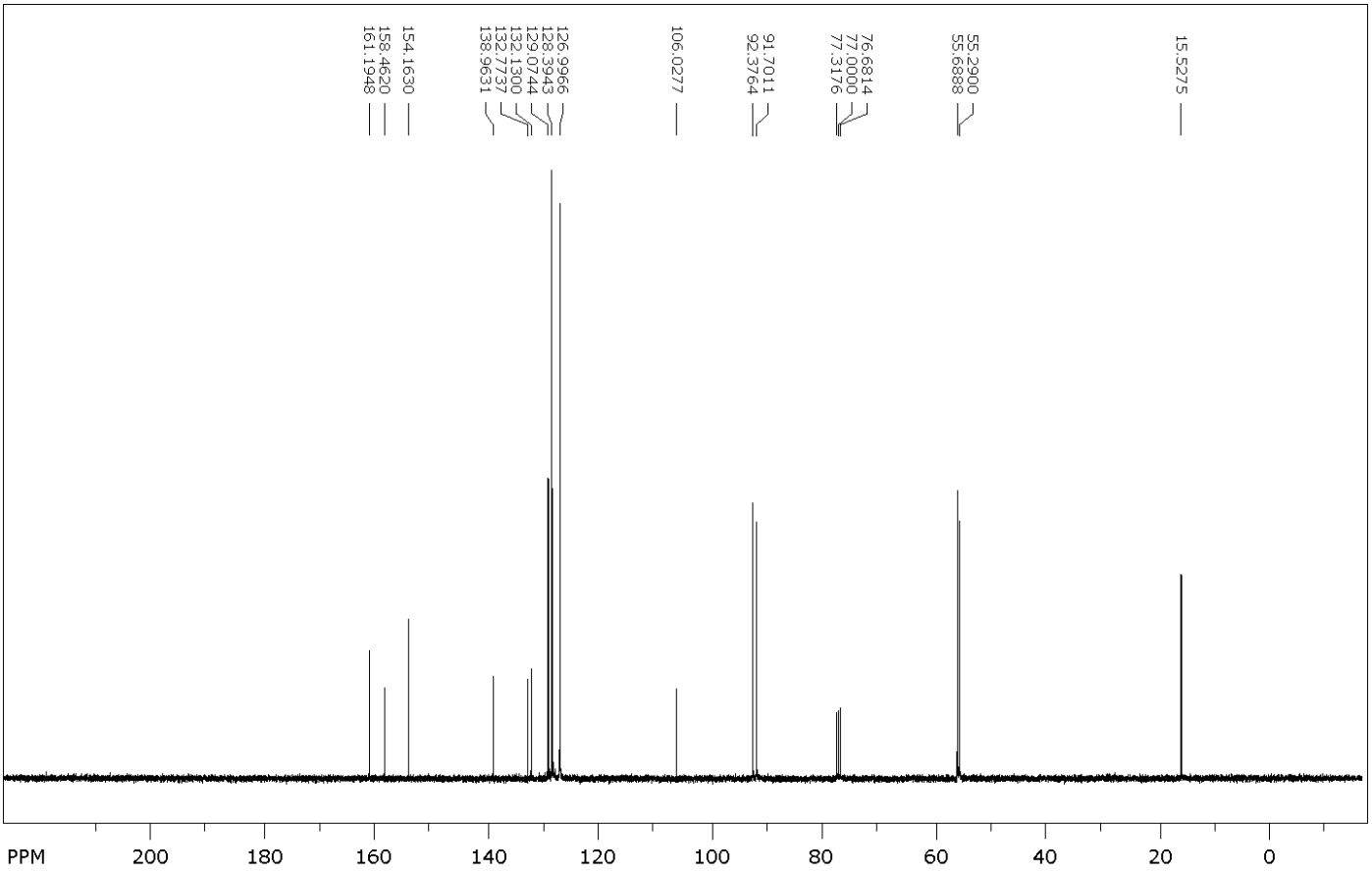
MeO
OMe
Cl
2e
4.072
1.056
1.000
1.027
0.952
3.310
3.299
3.301
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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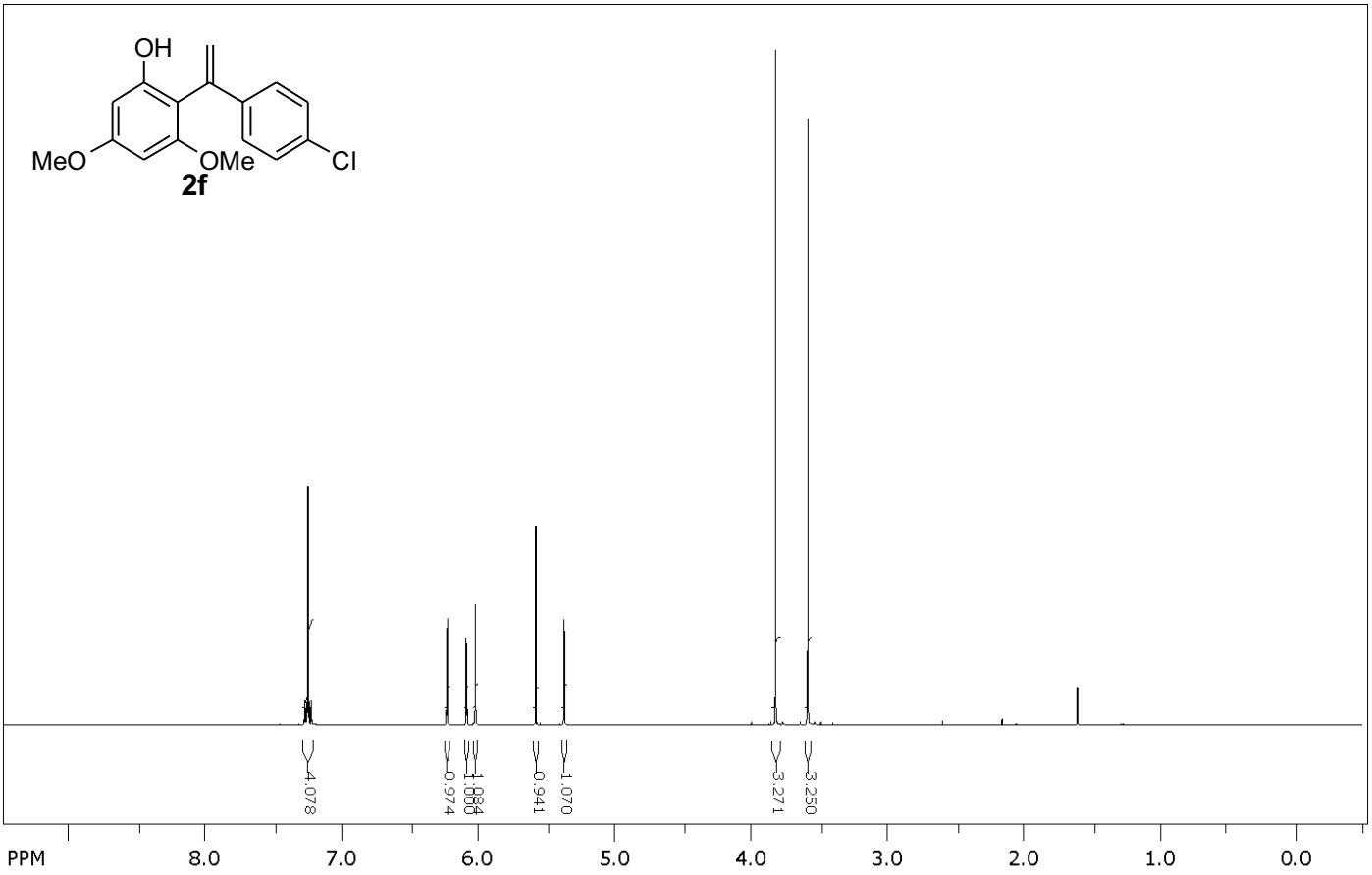
138.9631
132.7737
132.1300
129.0744
128.3943
126.9966
106.0277
92.3764
91.7011
77.3176
77.0000
76.6814
55.6888
55.2900
15.5275
PPM
200
180
160
140
120
100
80
60
40
20
0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MeO
OMe
Cl
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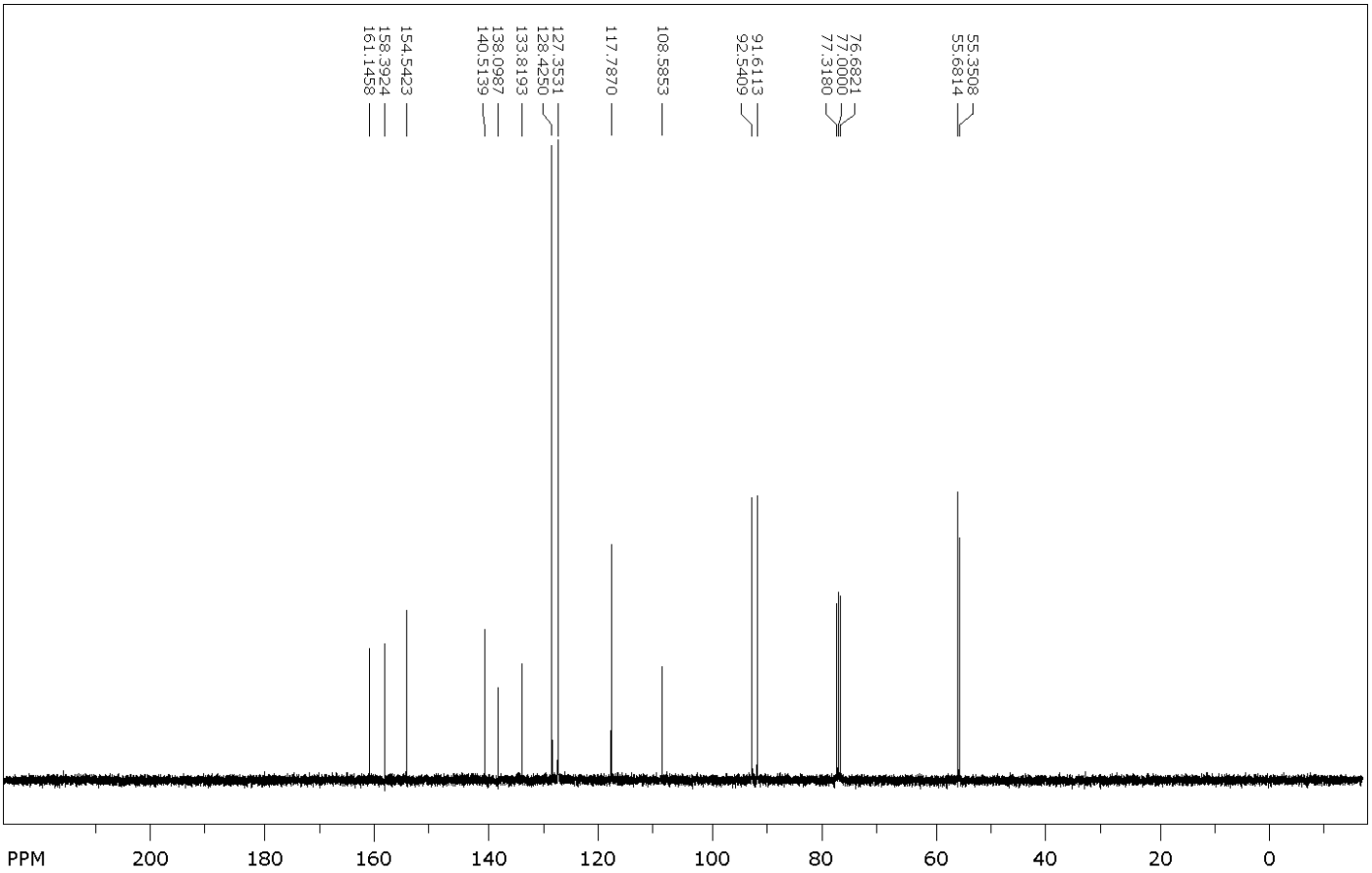
1.000
1.084
0.941
1.070
3.271
3.250
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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154.5423
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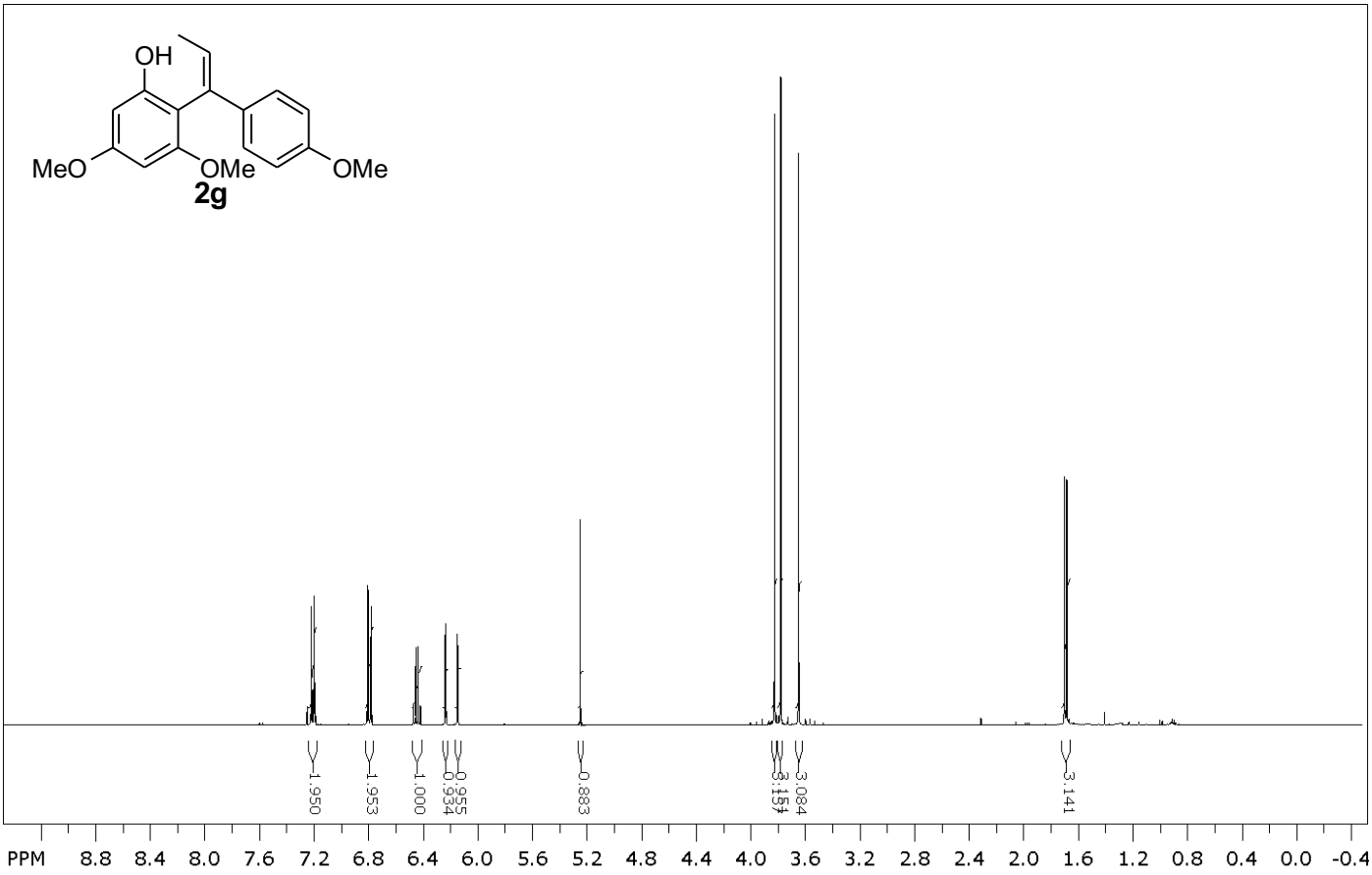
138.0987
133.8193
128.4250
127.3531
117.7870
108.5853
92.5409
91.6113
77.3180
77.0000
76.6821
55.6814
55.3508
PPM
200
180
160
140
120
100
80
60
40
20
0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MeO
OMe
OMe
2g
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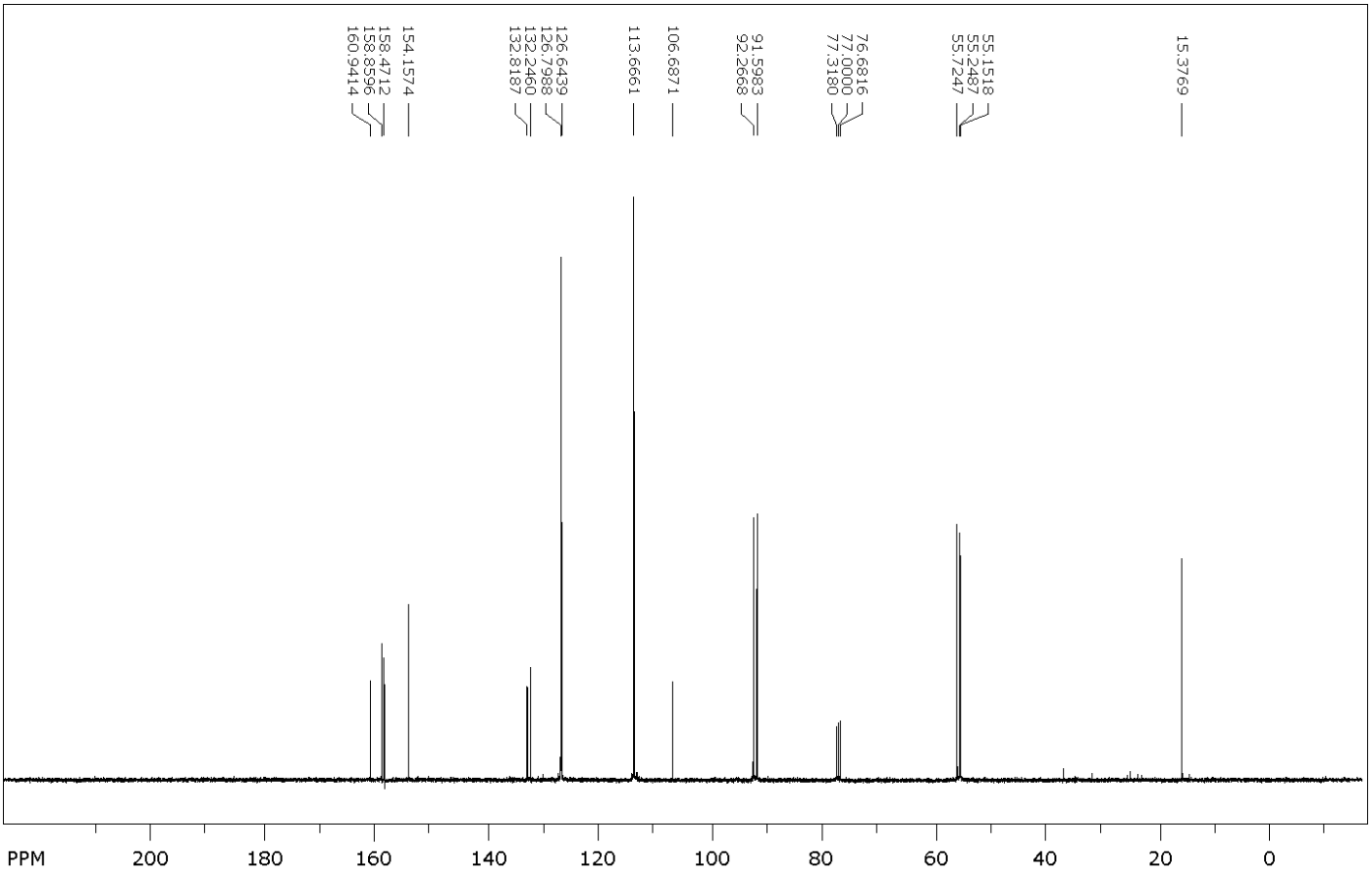
1.953
1.000
0.955
0.934
0.883
3.157
3.084
3.141
PPM
8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0 -0.4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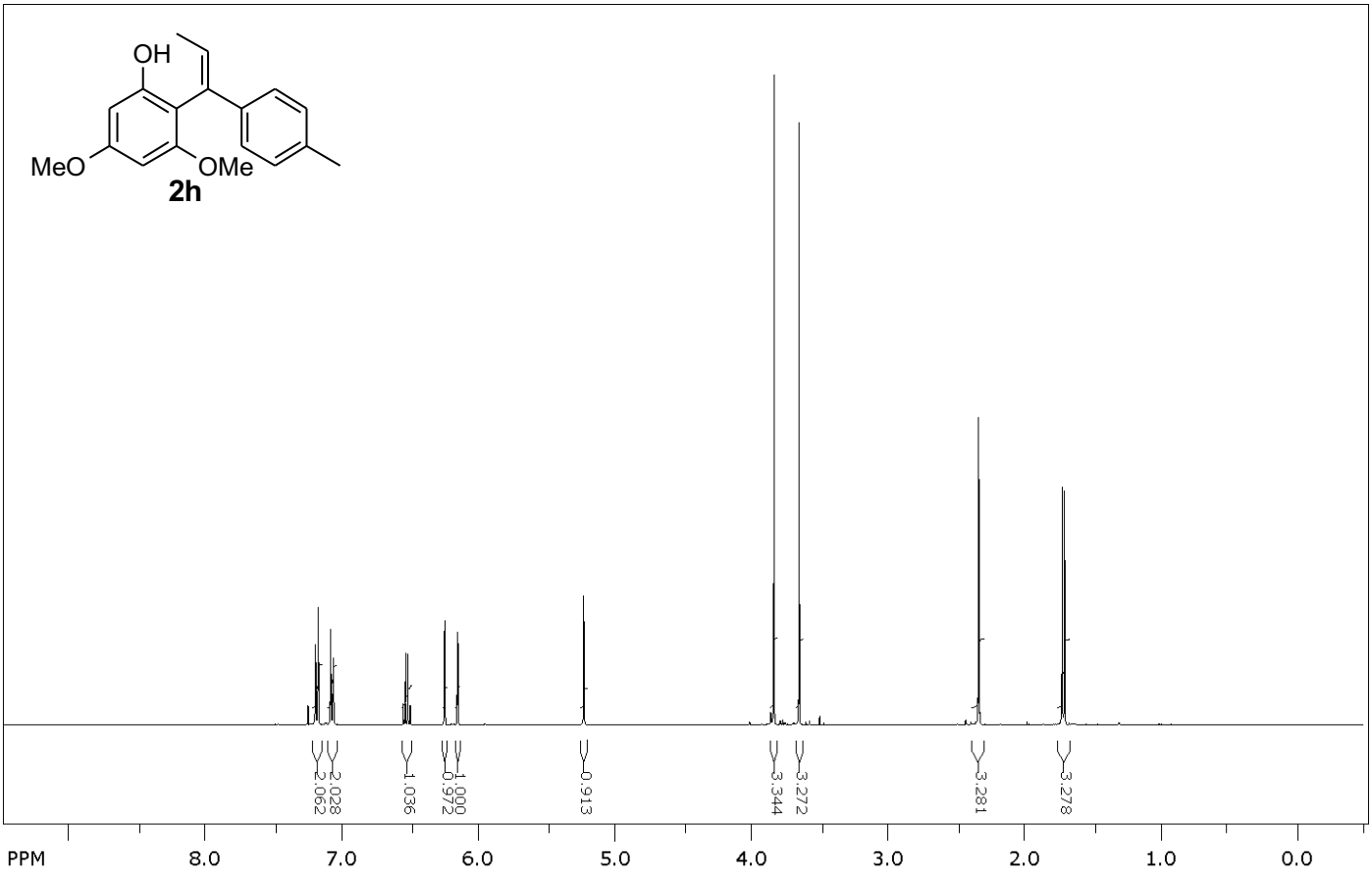
158.4712
154.1574
132.8187
132.2460
126.7988
126.6439
113.6661
106.6871
92.2668
91.5983
77.3180
77.0000
76.6816
55.7247
55.2487
55.1518
15.3769
PPM
200 180 160 140 120 100 80 60 40 20 0


OH
MeO
OMe
2h
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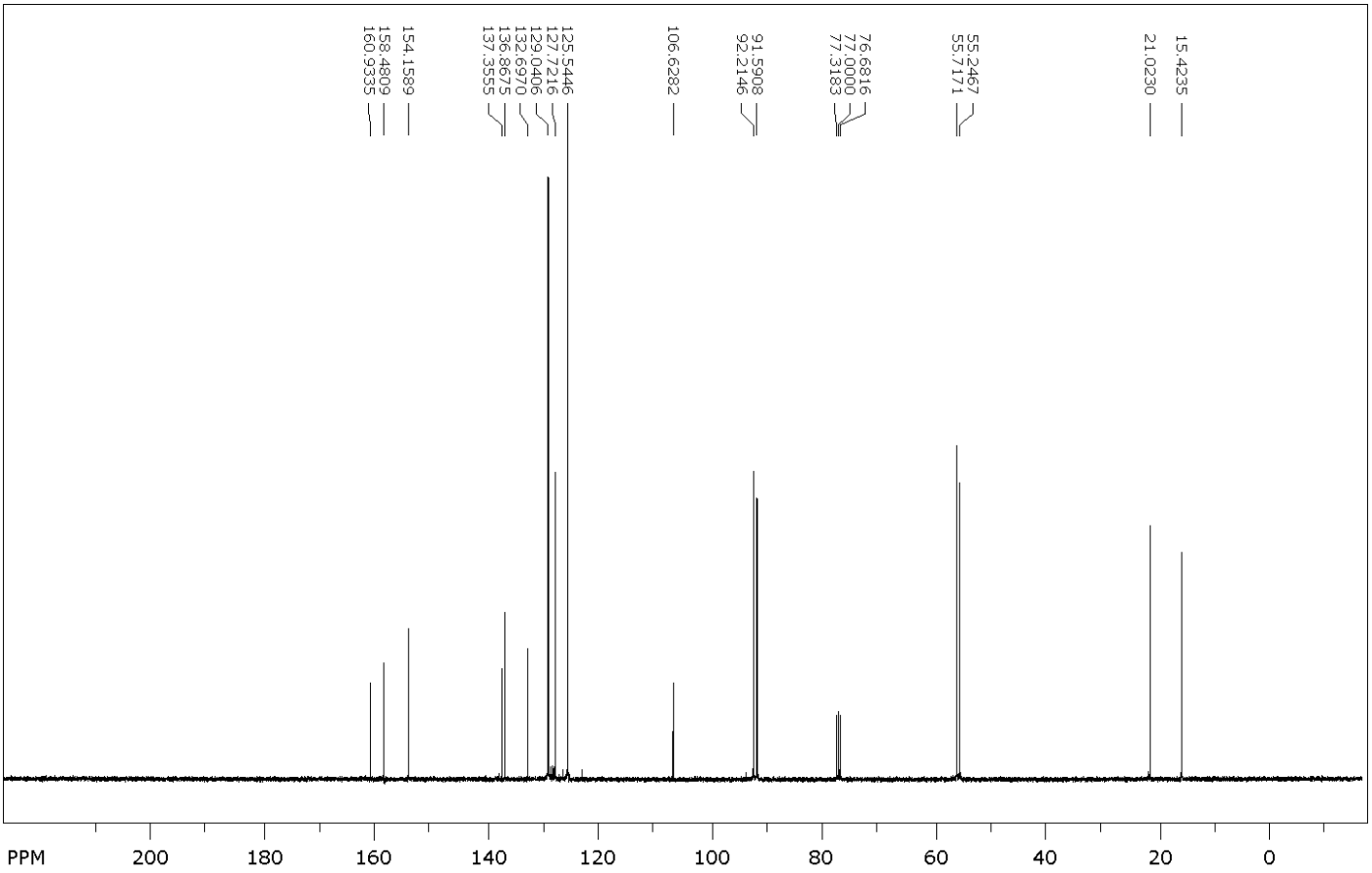
2.028
1.036
1.000
0.972
0.913
3.344
3.272
3.281
3.278
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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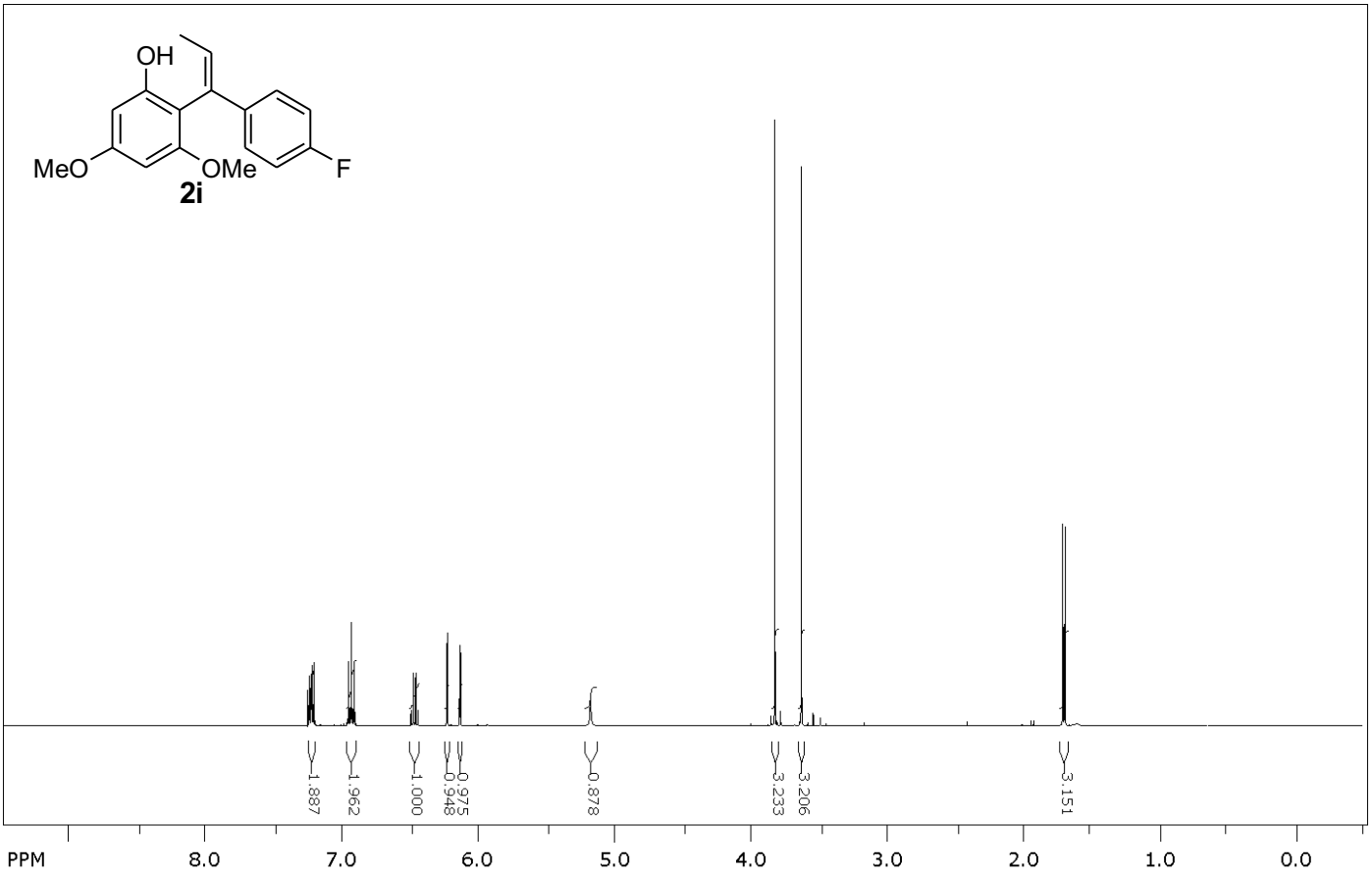
136.8675
132.6970
129.0406
127.7216
125.5446
106.6282
92.2146
91.5908
77.3183
77.0000
76.6816
55.7171
55.2467
21.0230
15.4235
PPM
200
180
160
140
120
100
80
60
40
20
0


OH
MeO
OMe
F
2i
1.887
1.962
1.000
0.948
0.975
0.878
3.233
3.206
3.151
PPM
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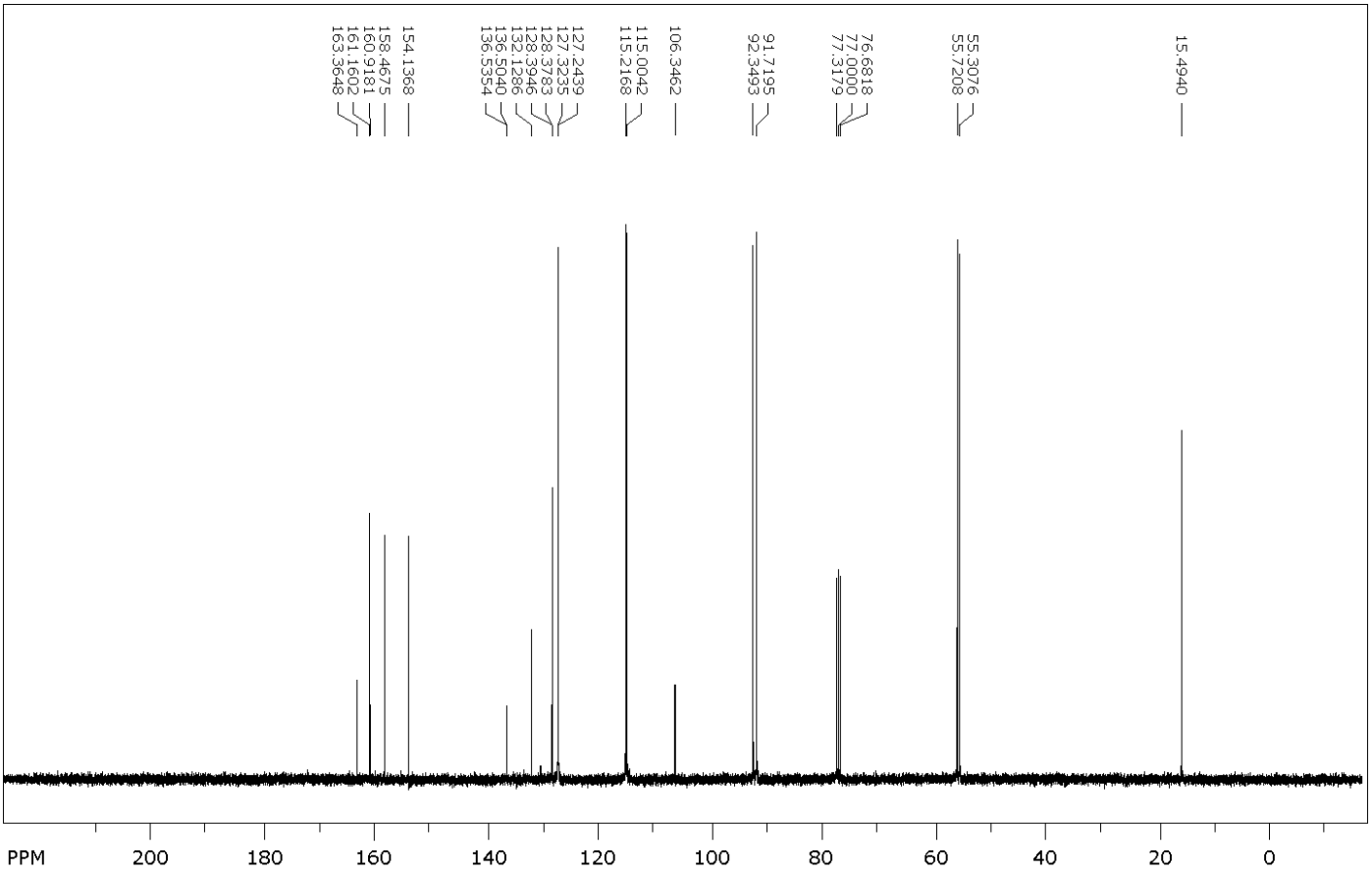
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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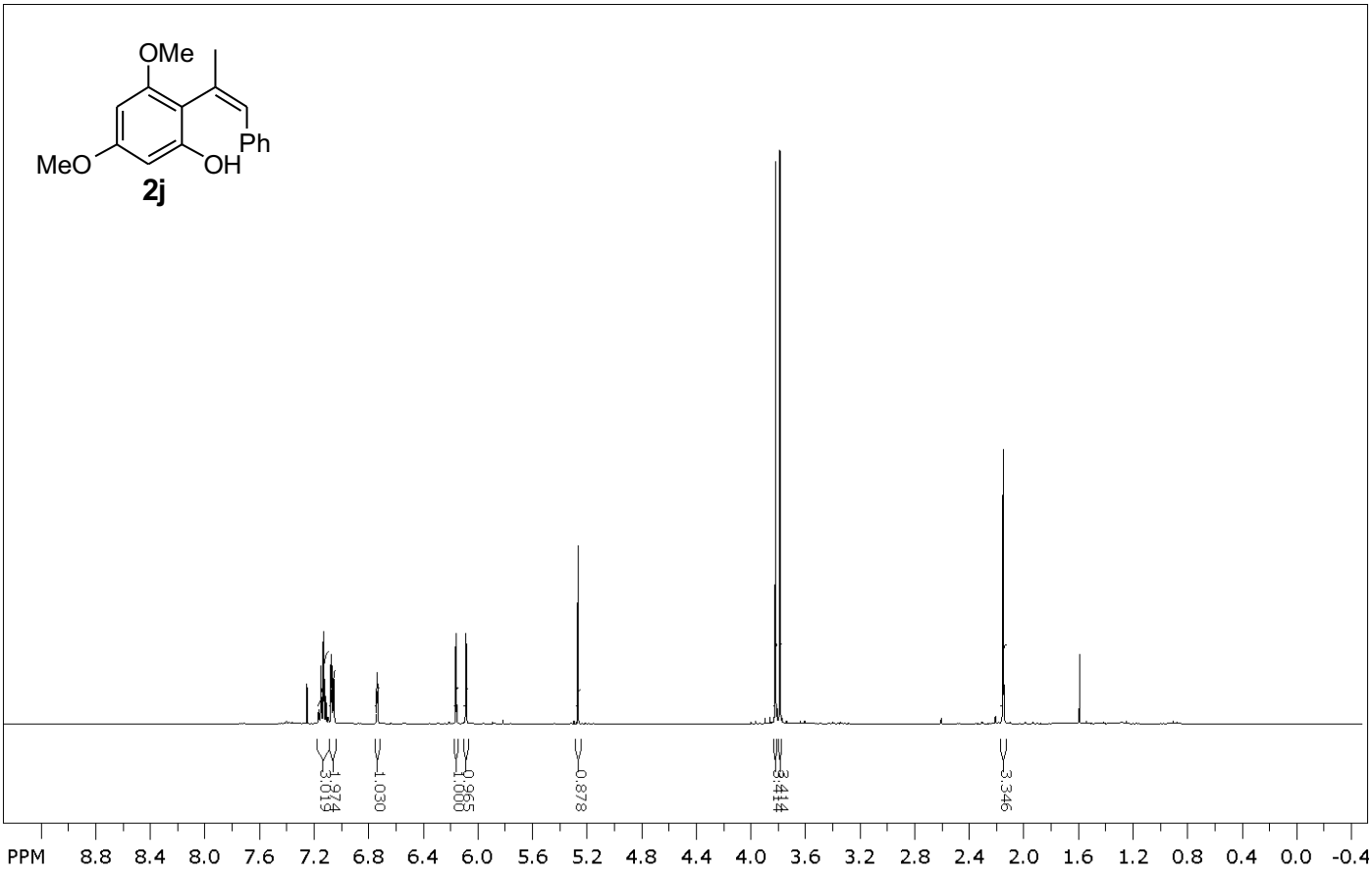
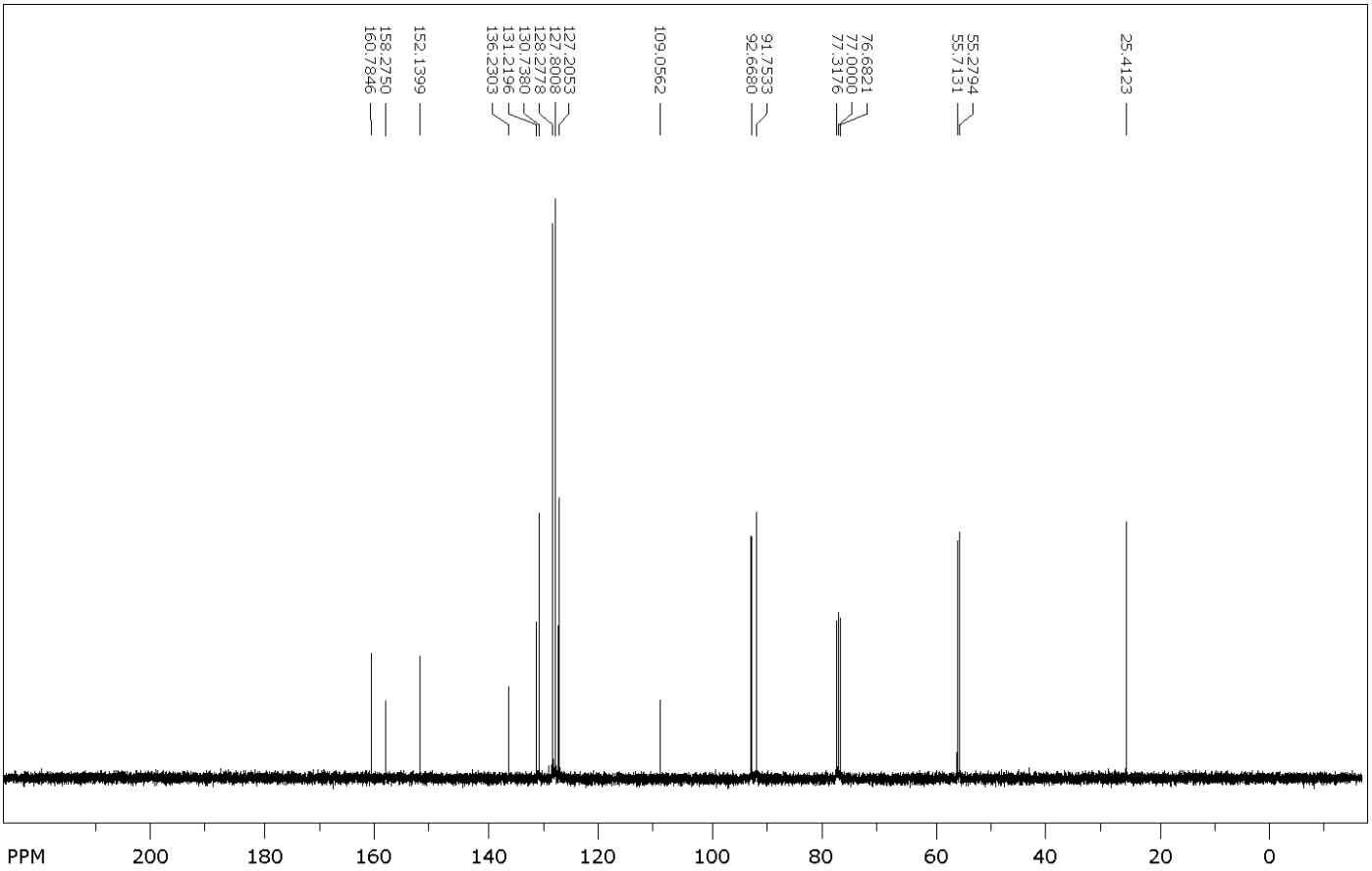
160.9181
158.4675
154.1368
136.5354
136.5040
132.1286
128.3946
128.3783
127.3235
127.2439
115.2168
115.0042
106.3462
92.3493
91.7195
77.3179
77.0000
76.6818
55.7208
55.3076
15.4940
PPM
200
180
160
140
120
100
80
60
40
20
0


OMe
Ph
MeO
OH
2j
3.019
1.974
1.030
1.000
0.965
0.878
3.414
3.346
PPM
8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0 -0.4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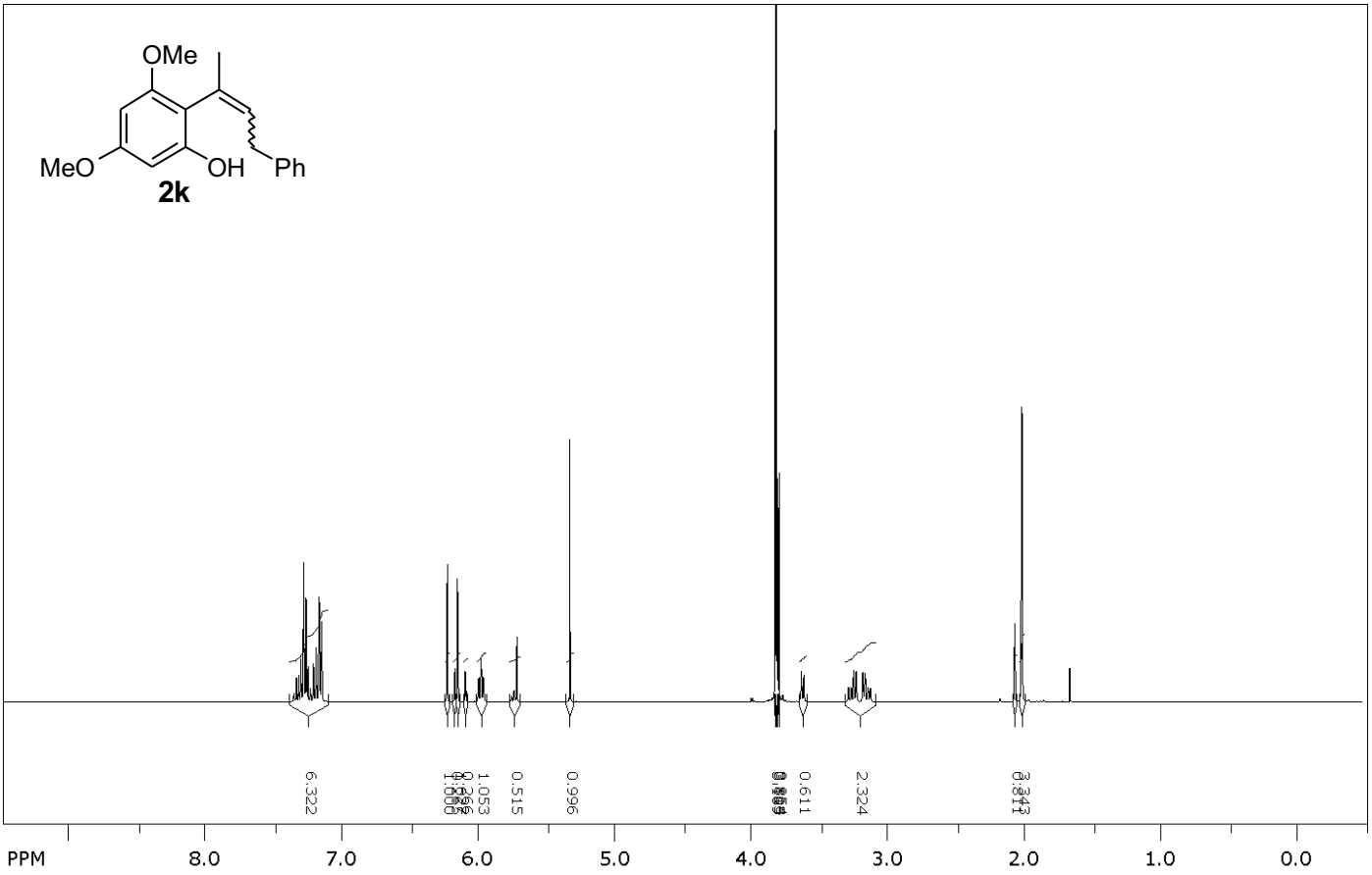
152.1399
136.2303
131.2196
130.7380
128.2778
127.8008
127.2053
109.0562
92.6680
91.7533
77.3176
77.0000
76.6821
55.7131
55.2794
25.4123
PPM
200 180 160 140 120 100 80 60 40 20 0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MeO
OH
Ph
2k
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1.000
1.053
0.515
0.996
0.611
2.324
3.811
PPM
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3.0
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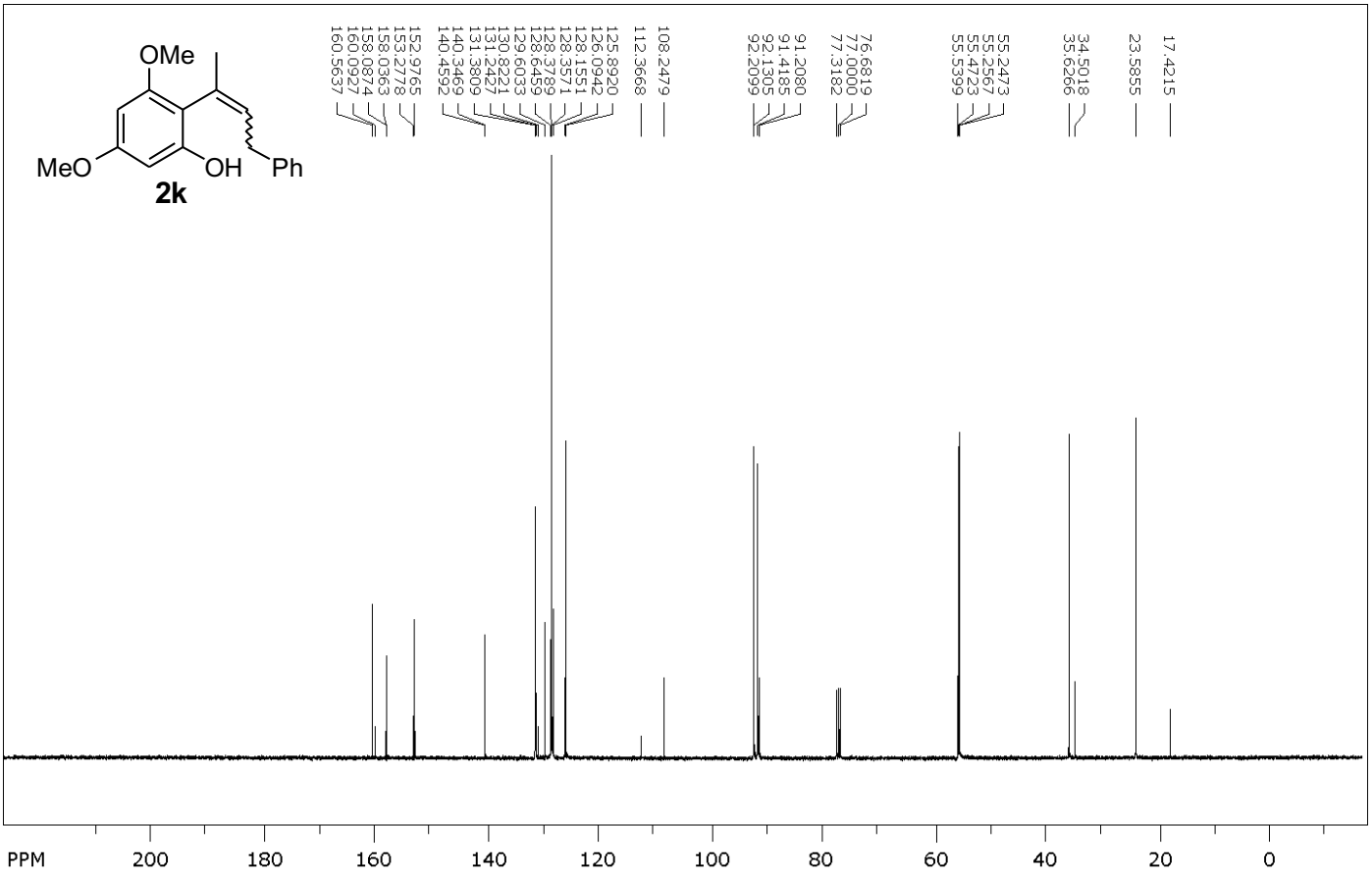
1.0
0.0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OH
Ph
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158.0363
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152.9765
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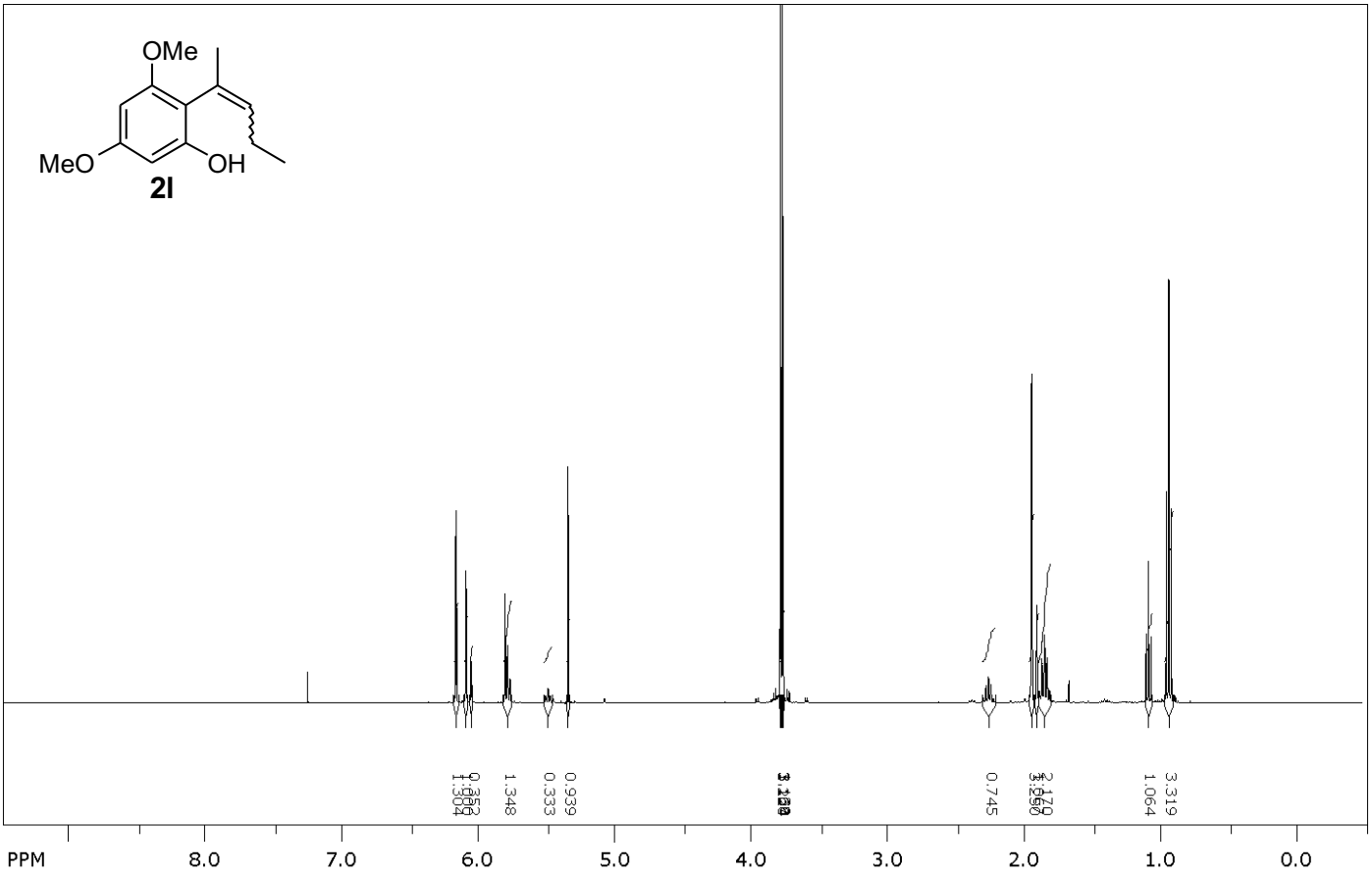
140.3469
131.3809
131.2427
130.8221
129.6033
128.6459
128.3789
128.3571
128.1551
126.0942
125.8920
112.3668
108.2479
92.2099
92.1305
91.4185
91.2080
77.3182
77.0000
76.6819
55.5399
55.4723
55.2567
55.2473
35.6266
34.5018
23.5855
17.4215
PPM
200
180
160
140
120
100
80
60
40
20
0


OMe
MeO
OH
2l
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0.333
0.939
0.745
1.064
3.319
PPM
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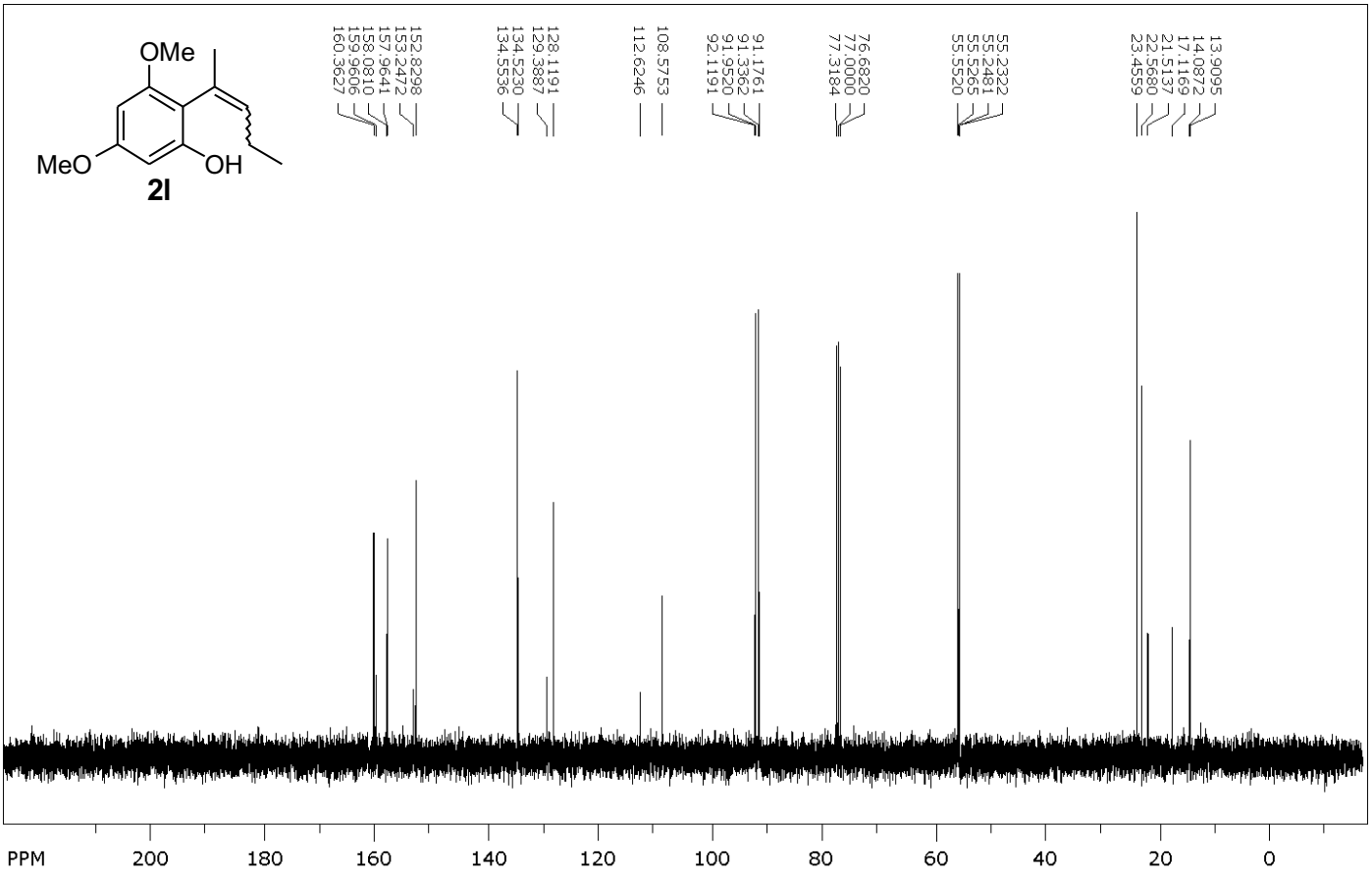
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


OMe
MeO
OH
2l
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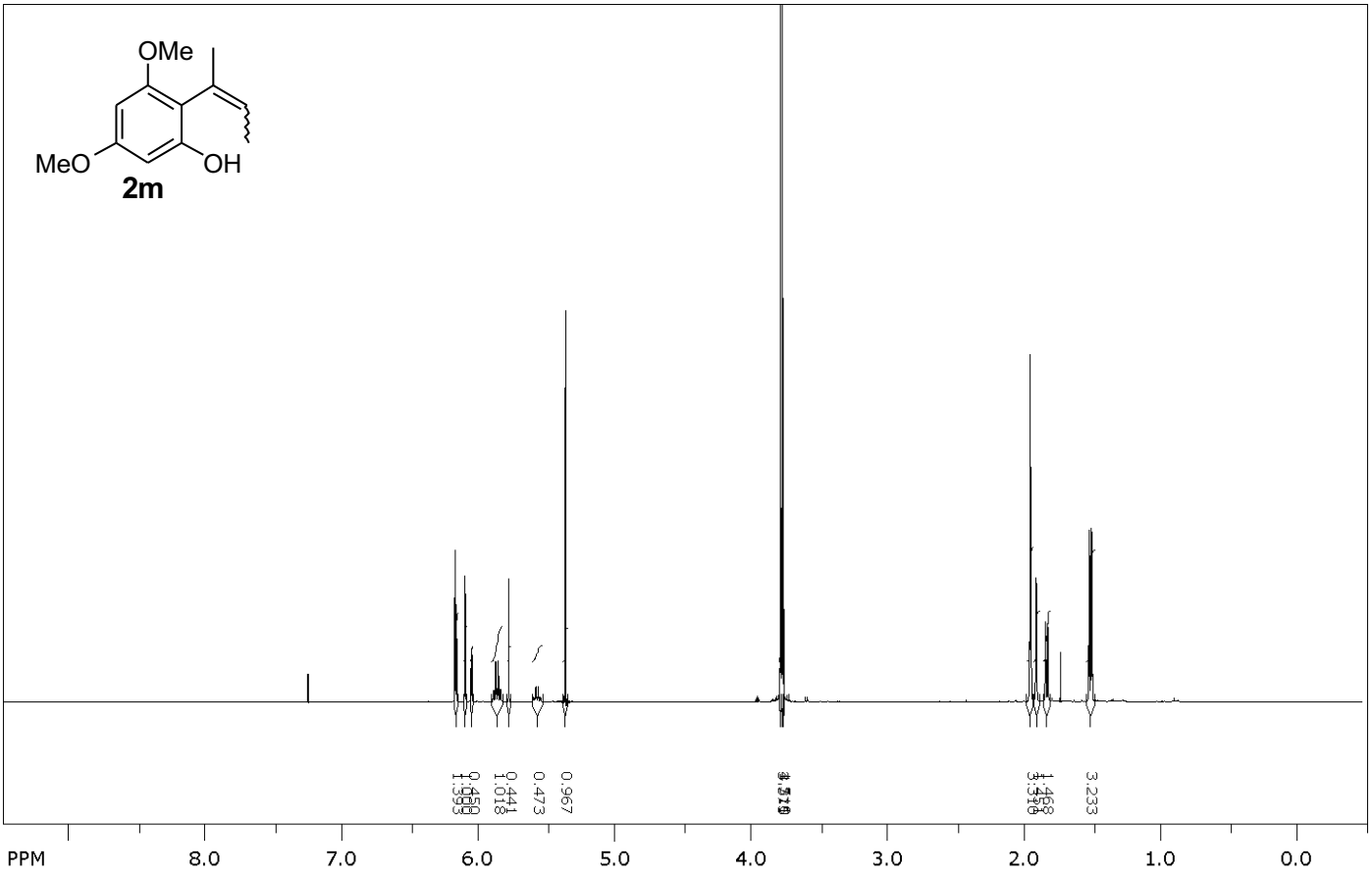
158.0810
157.9641
153.2472
152.8298
134.5536
134.5230
129.3887
128.1191
112.6246
108.5753
92.1191
91.9520
91.3362
91.1761
77.3184
77.0000
76.6820
55.5520
55.5265
55.2481
55.2322
23.4559
22.5680
21.5137
17.1169
14.0872
13.9095
PPM
200
180
160
140
120
100
80
60
40
20
0


OMe
MeO
OH
2m
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0.967
1.018
0.441
0.473
3.310
3.233
PPM
8.0
7.0
6.0
5.0
4.0
3.0
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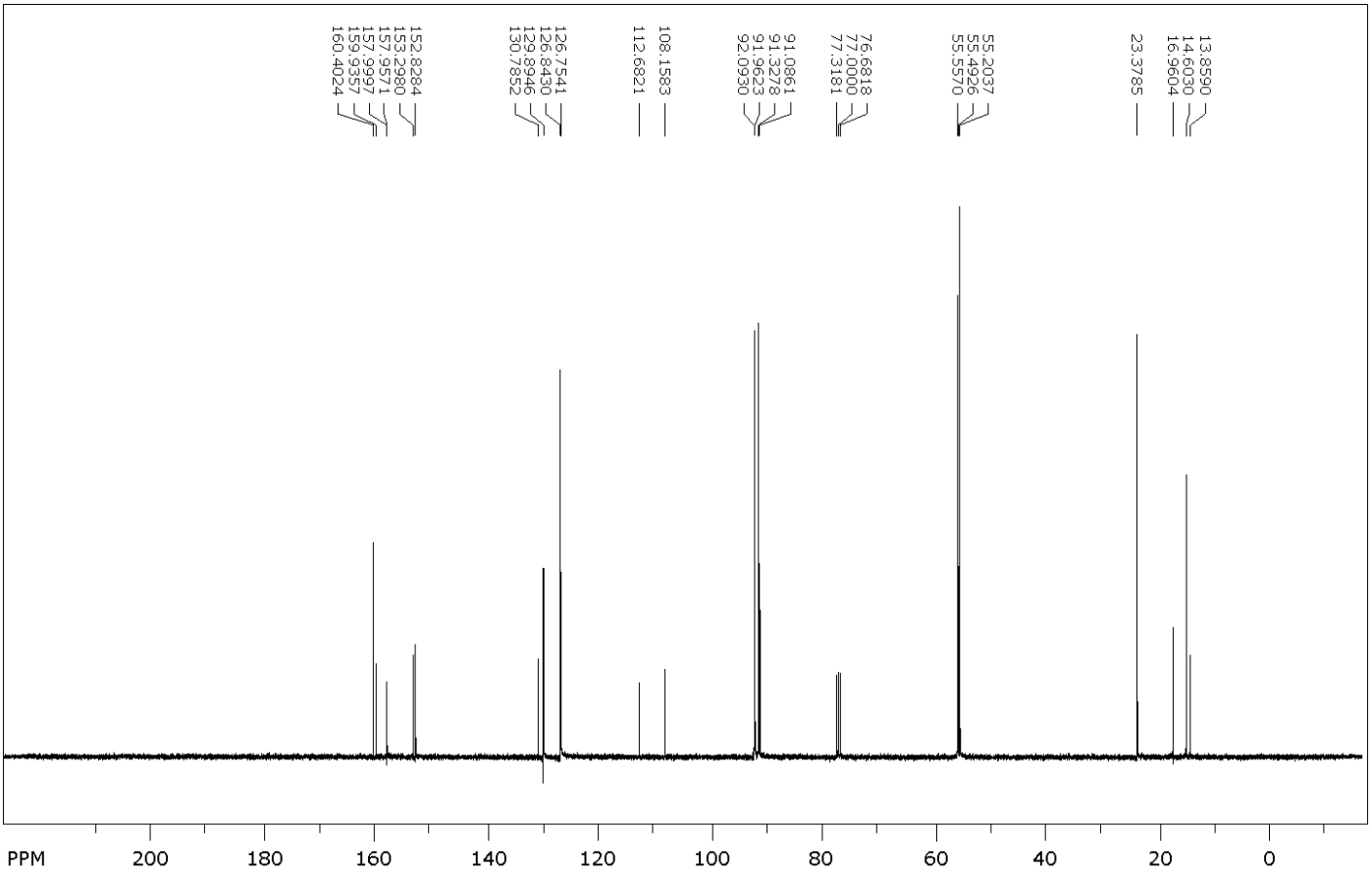
1.0
0.0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153.2980
152.8284
130.7852
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112.6821
108.1583
92.0930
91.9623
91.3278
91.0861
77.3181
77.0000
76.6818
55.5570
55.4926
55.2037
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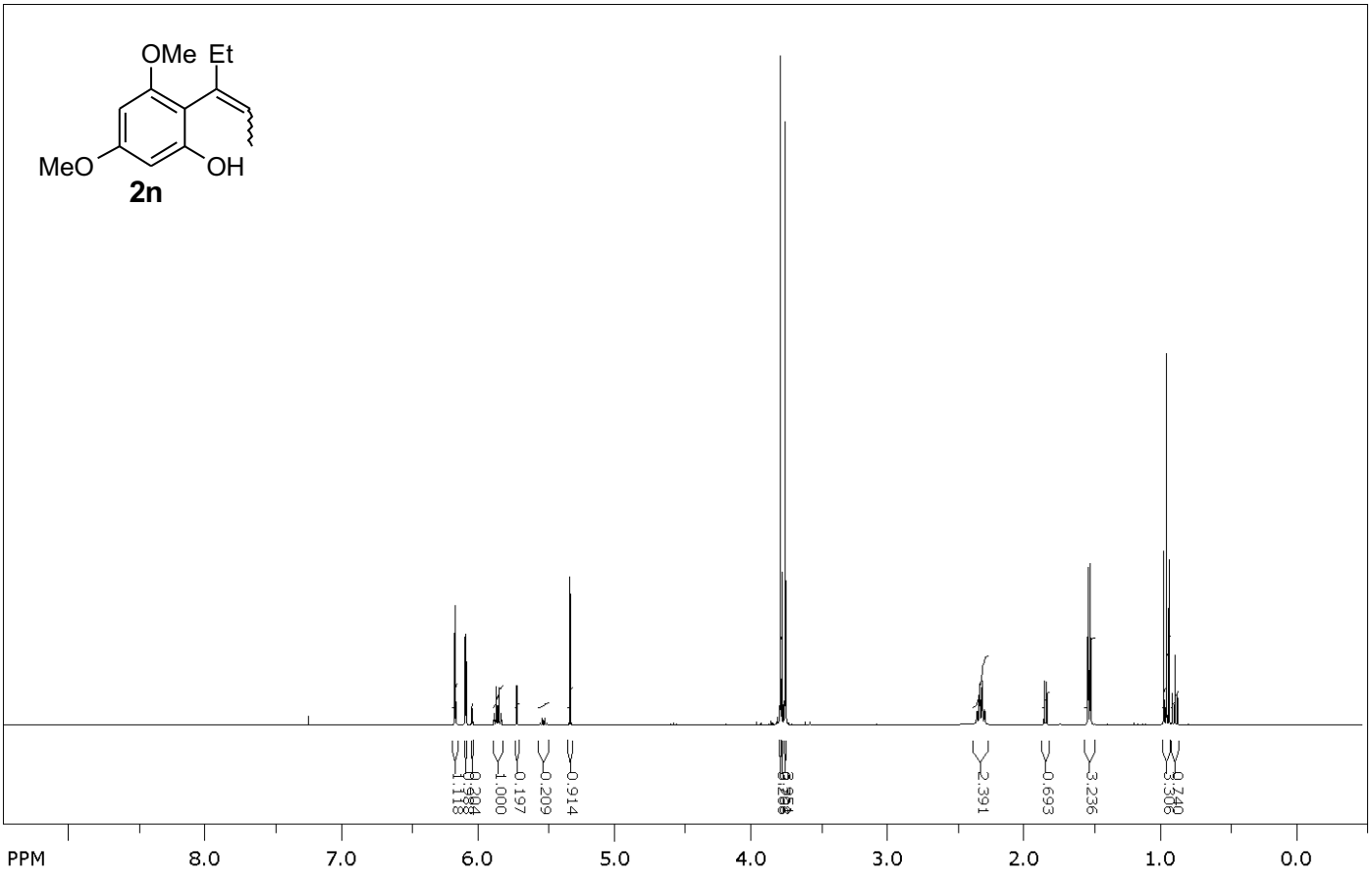
14.6030
13.8590
PPM
200
180
160
140
120
100
80
60
40
20
0


OMe Et
MeO
OH
2n
1.118
1.000
0.197
0.209
0.914
2.391
0.693
3.236
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PPM
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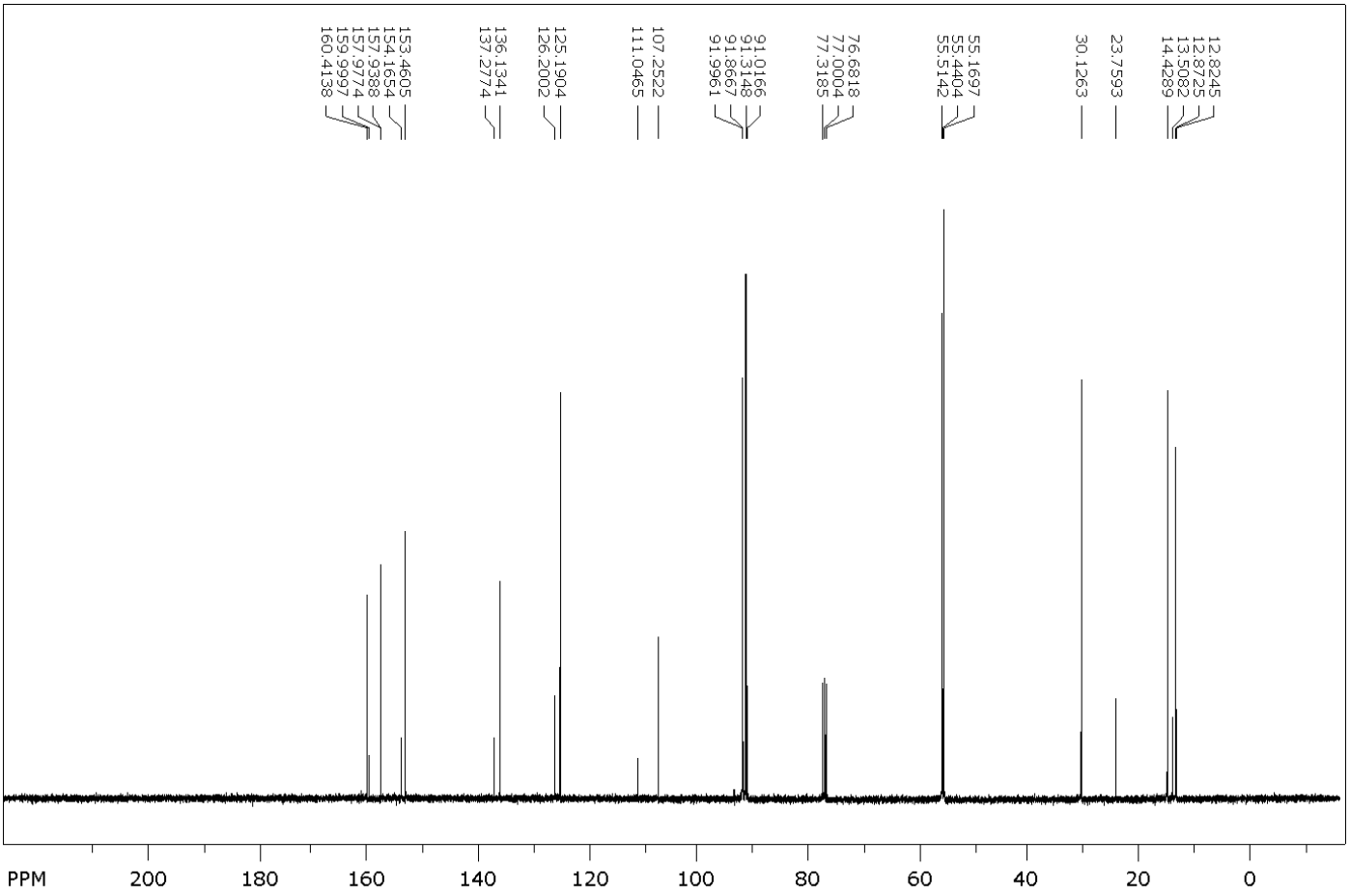
4.0
3.0
2.0
1.0
0.0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157.9388
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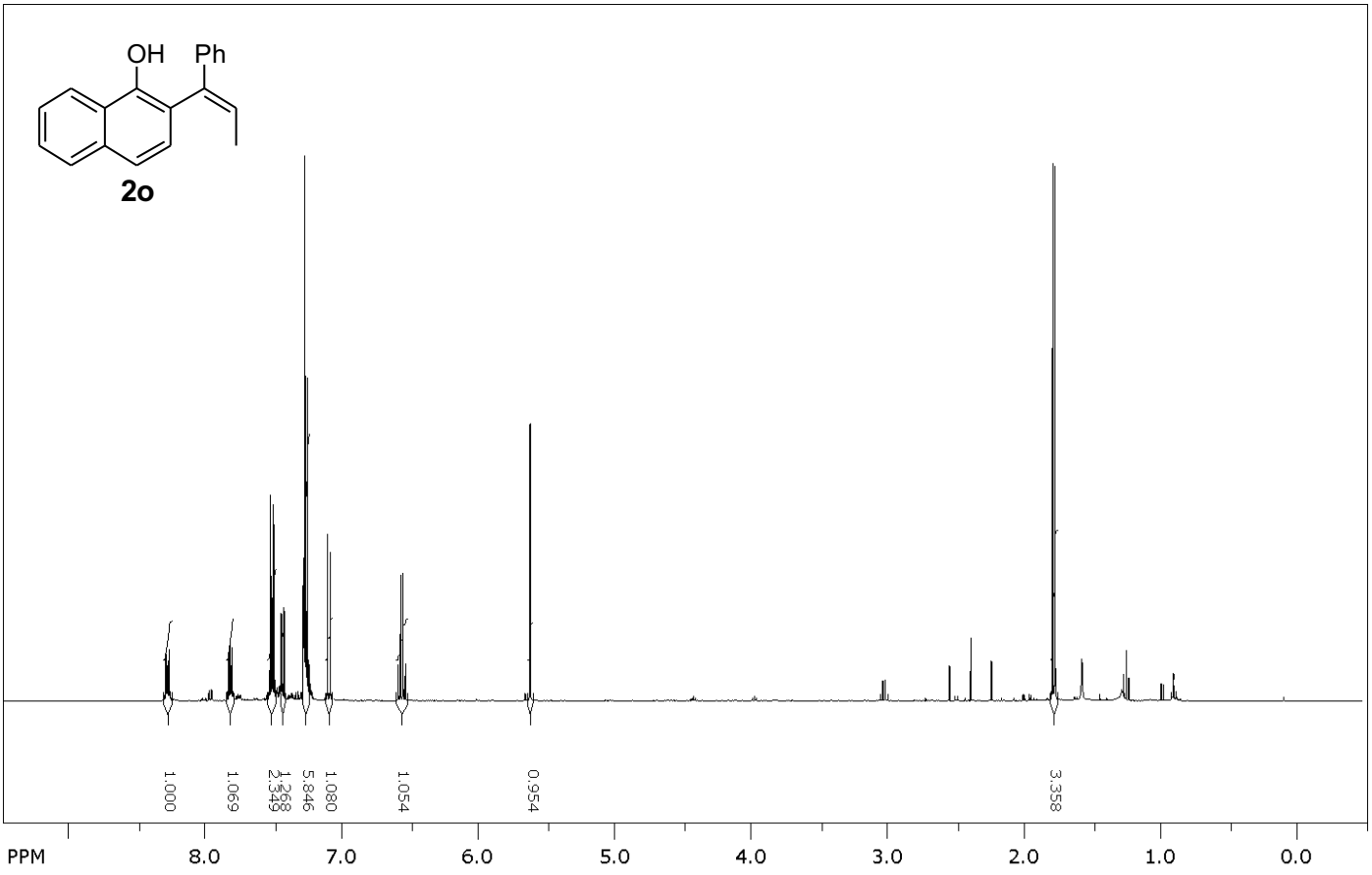
153.4605
137.2774
136.1341
126.2002
125.1904
111.0465
107.2522
91.9961
91.8667
91.3148
91.0166
77.3185
77.0004
76.6818
55.5142
55.4404
55.1697
30.1263
23.7593
14.4289
13.5082
12.8725
12.8245
PPM
200
180
160
140
120
100
80
60
40
20
0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Ph
2o
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1.069
1.268
2.349
5.846
1.080
1.054
0.954
3.358
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
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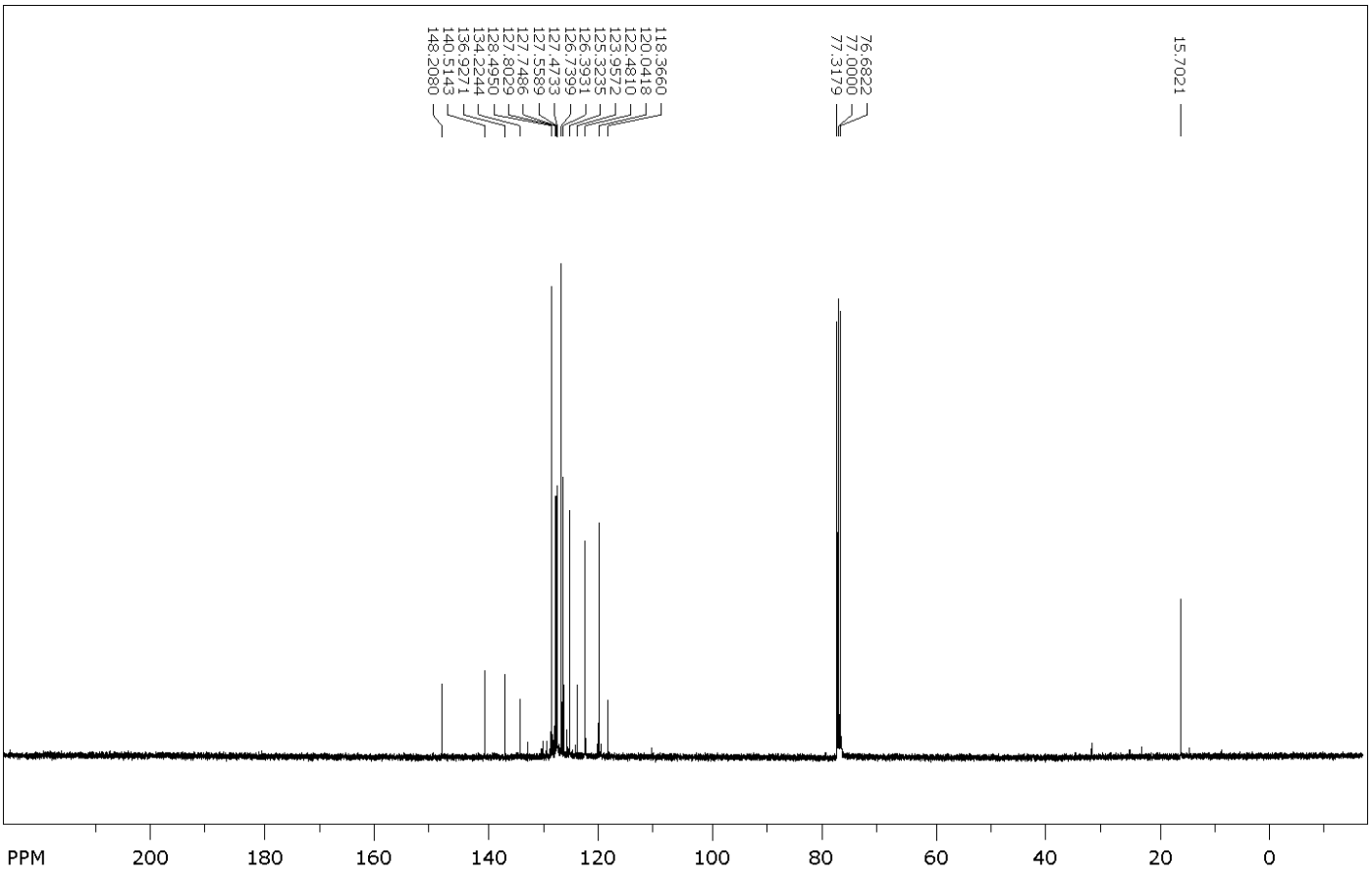
0.0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123.9572
122.4810
120.0418
118.3660
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140
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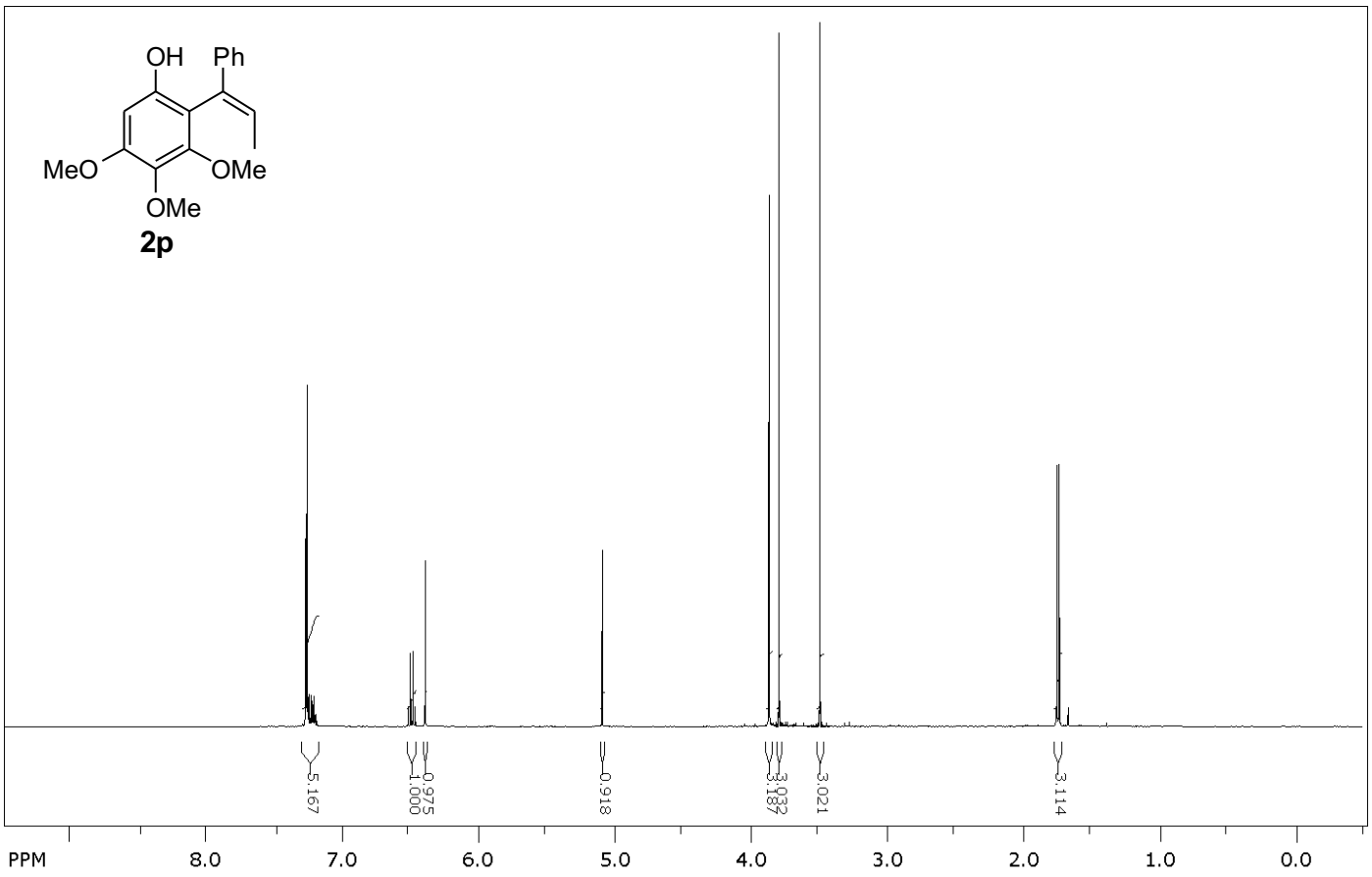
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Ph
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OMe
OMe
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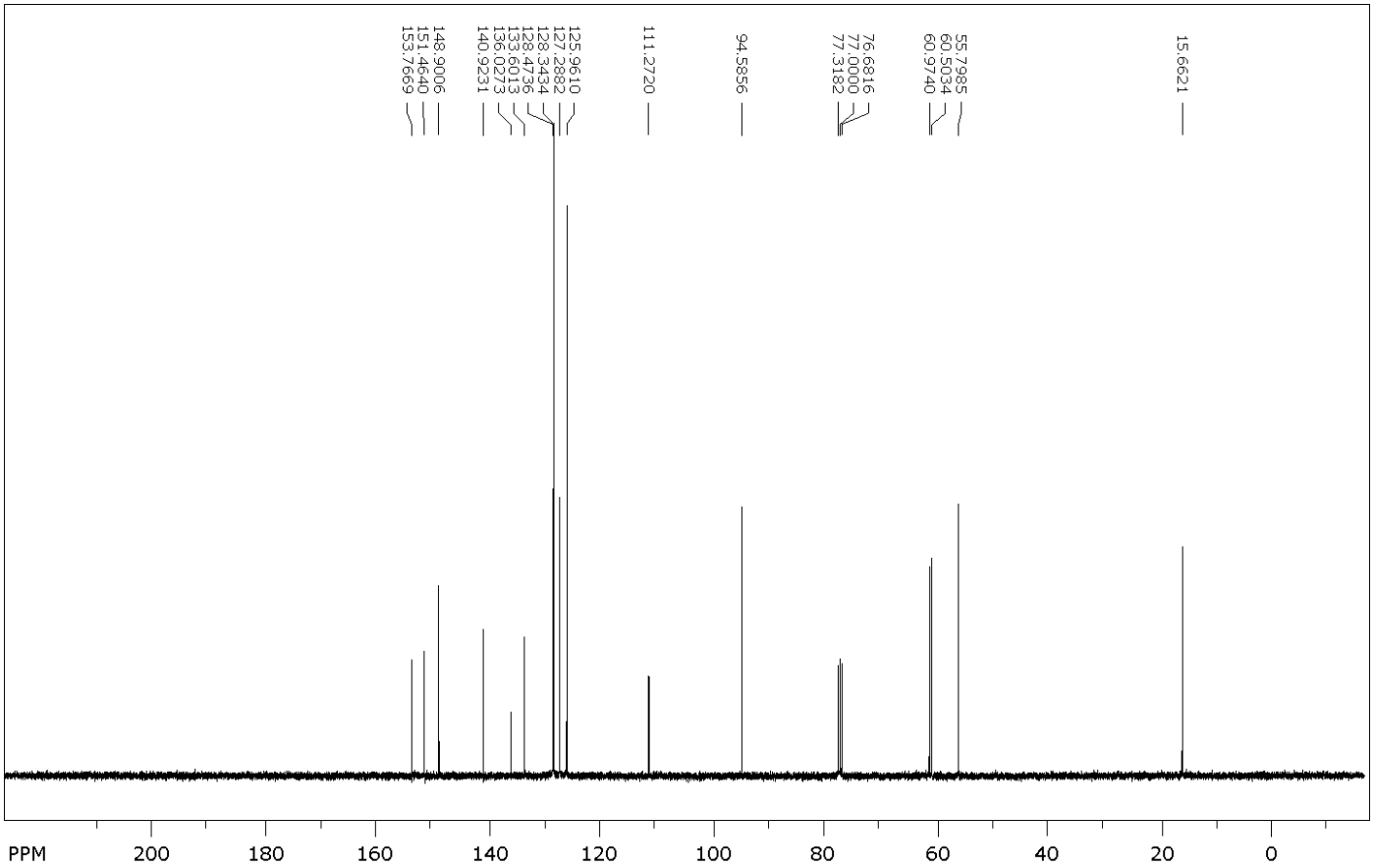
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111.2720
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77.3182
77.0000
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140
120
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20
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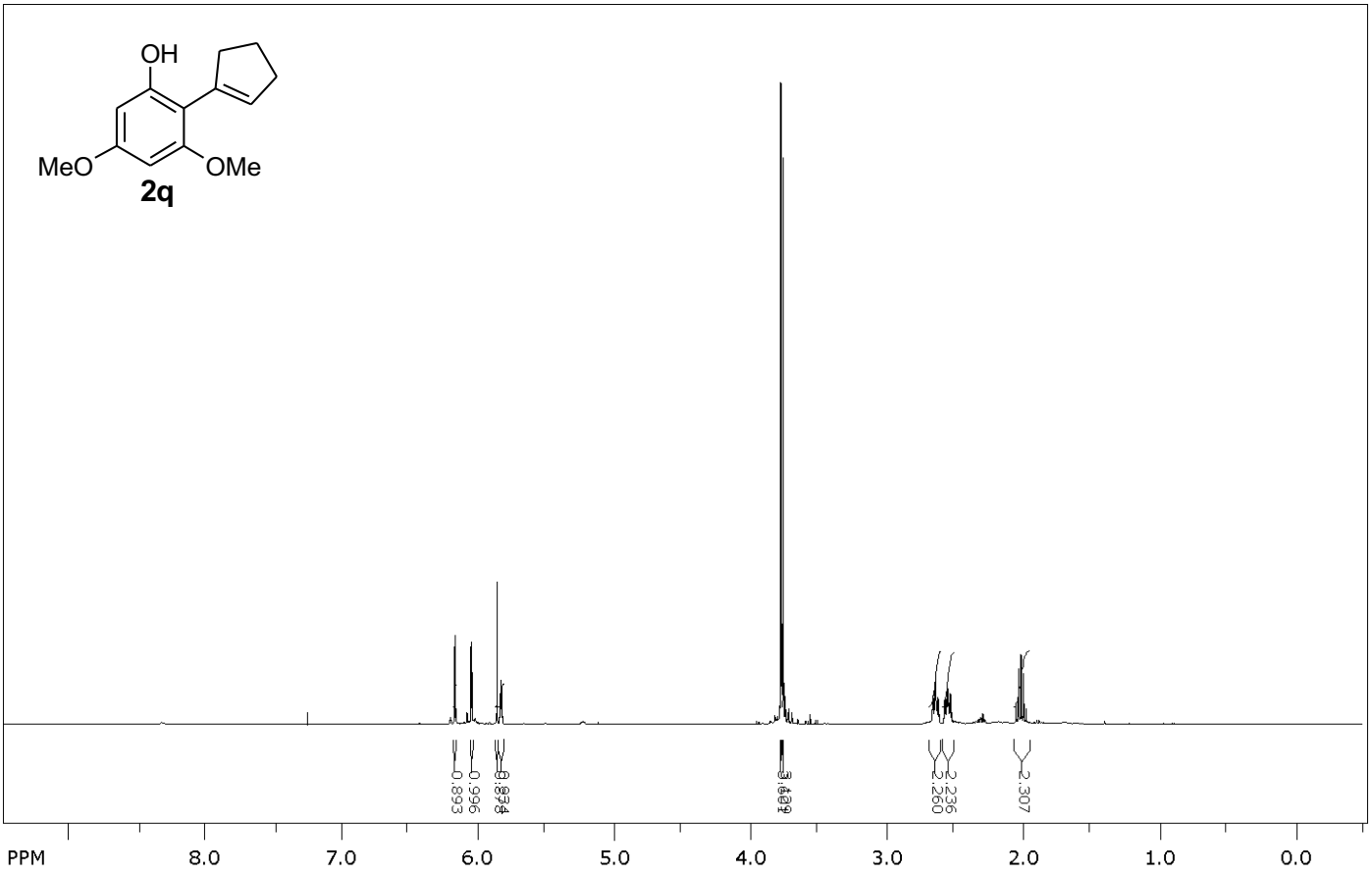
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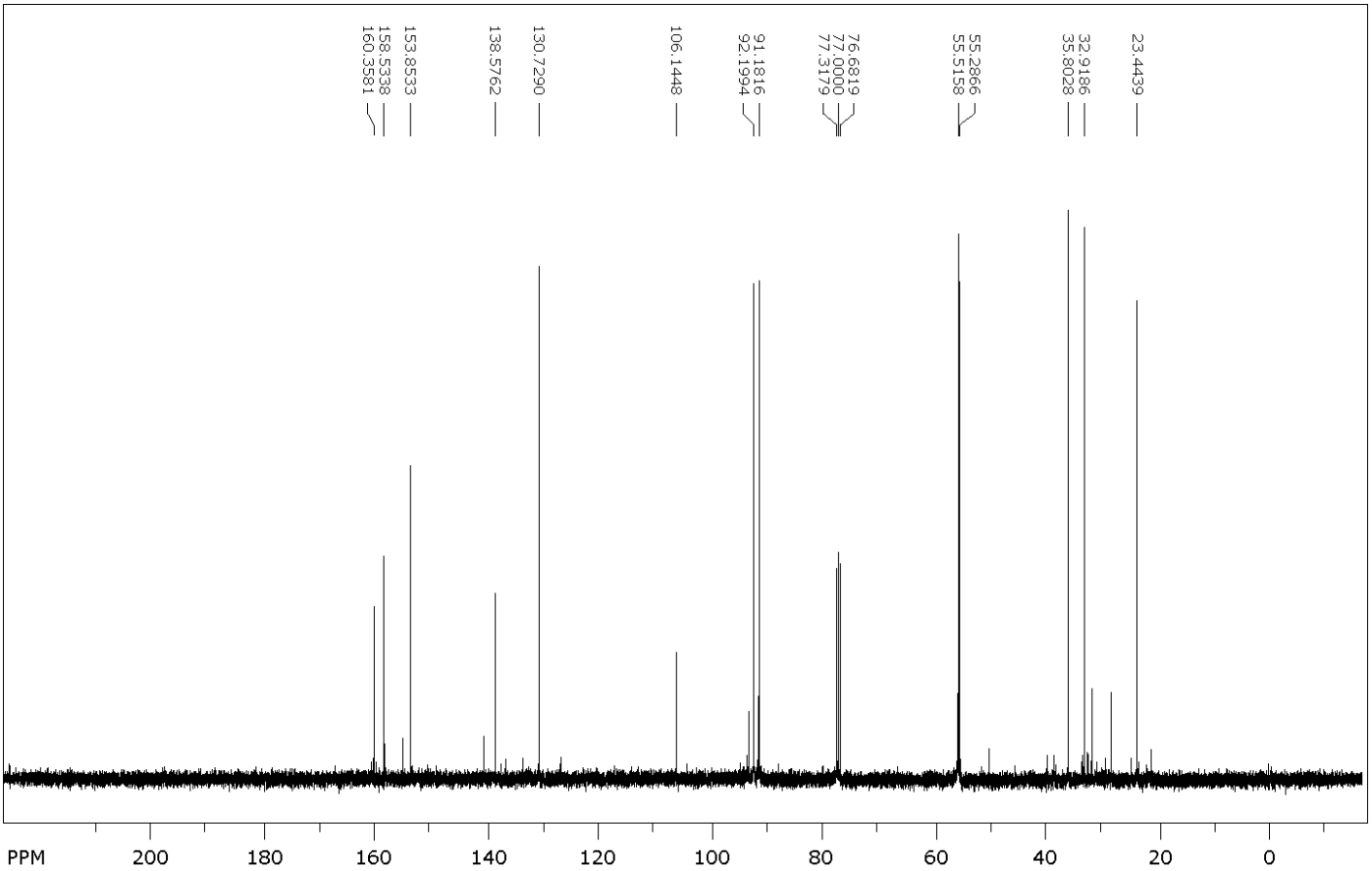
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PPM
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20
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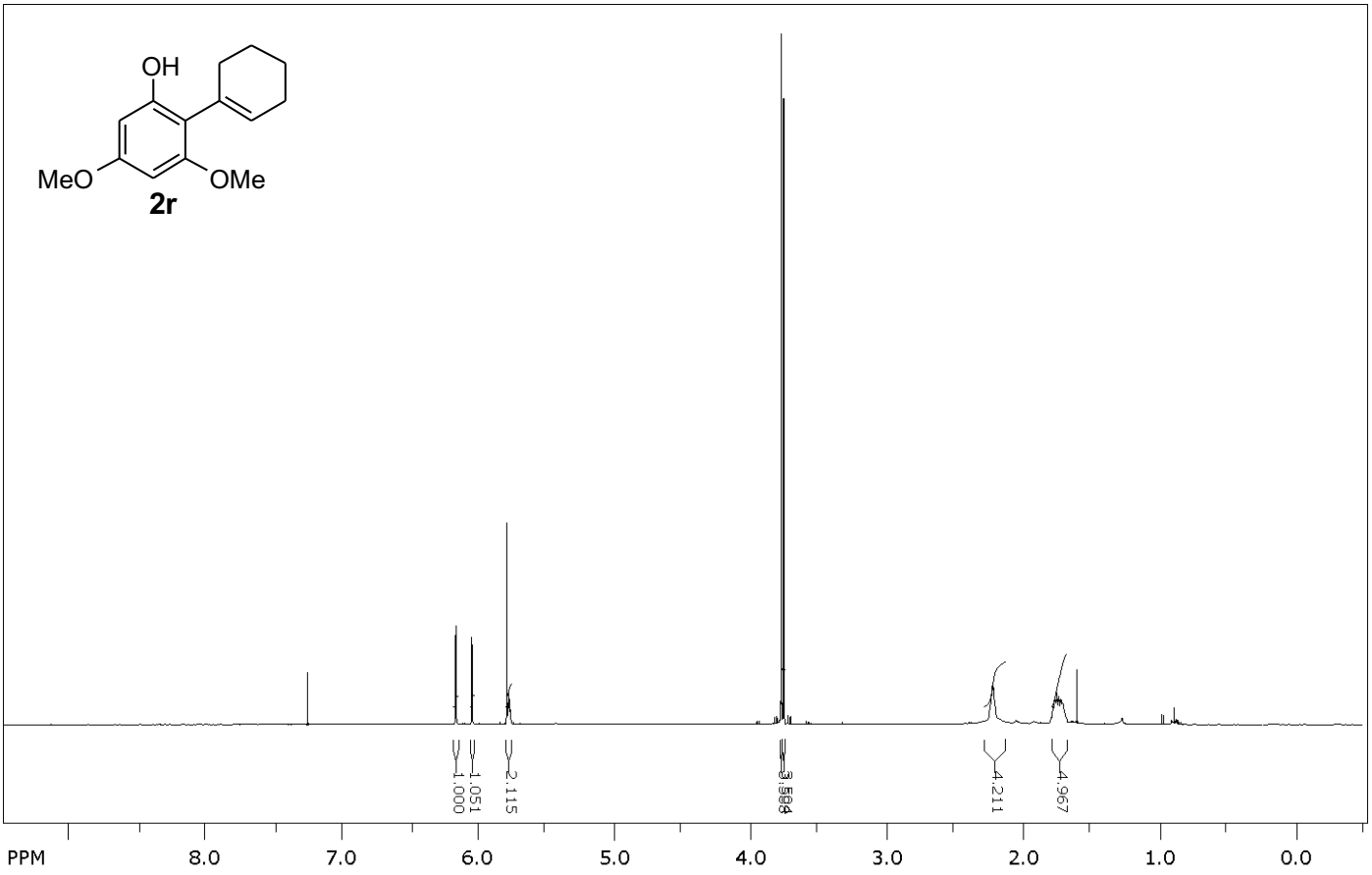
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OMe
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4.211
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PPM
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6.0
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4.0
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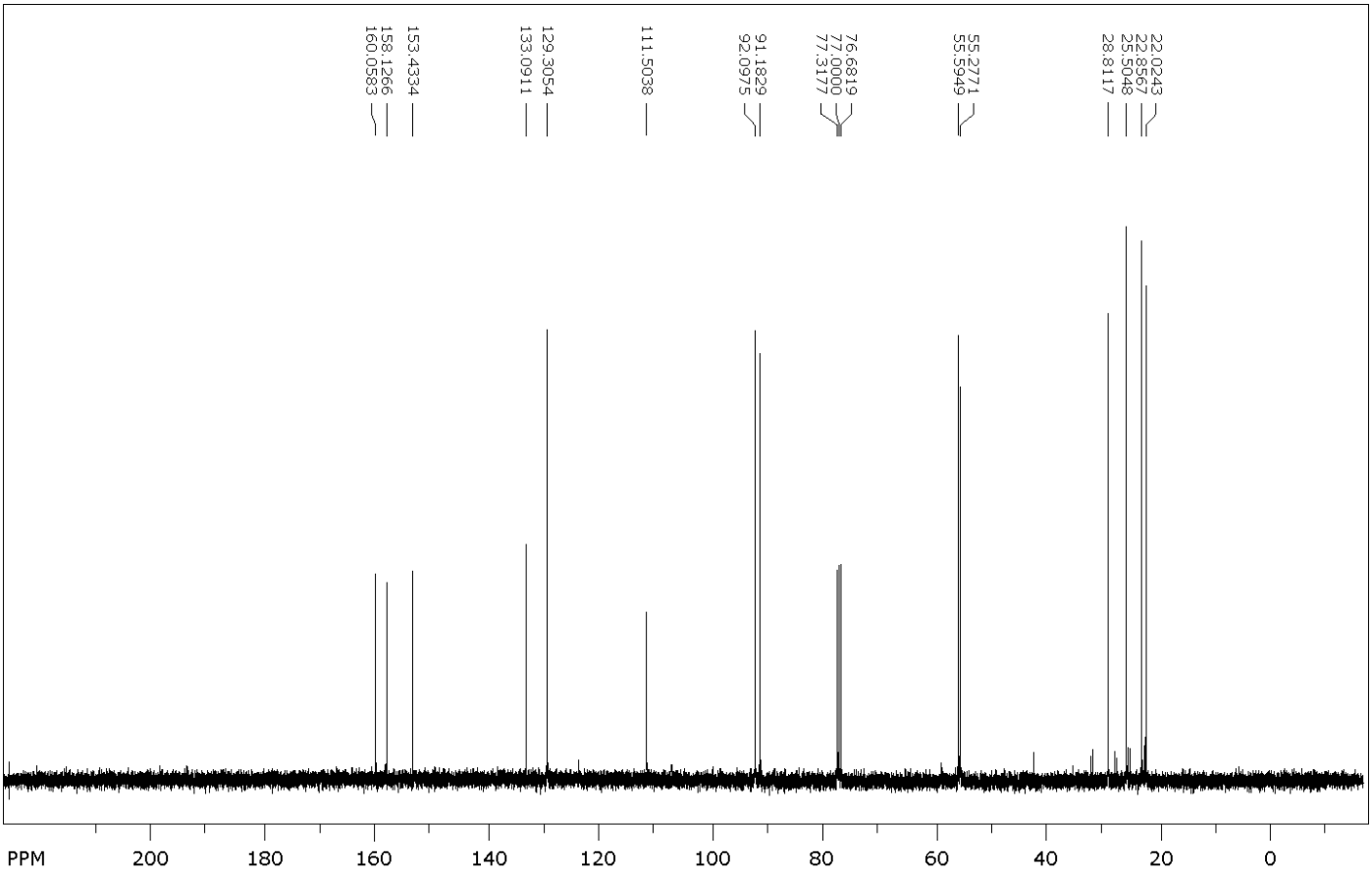
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77.0000
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55.2771
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PPM
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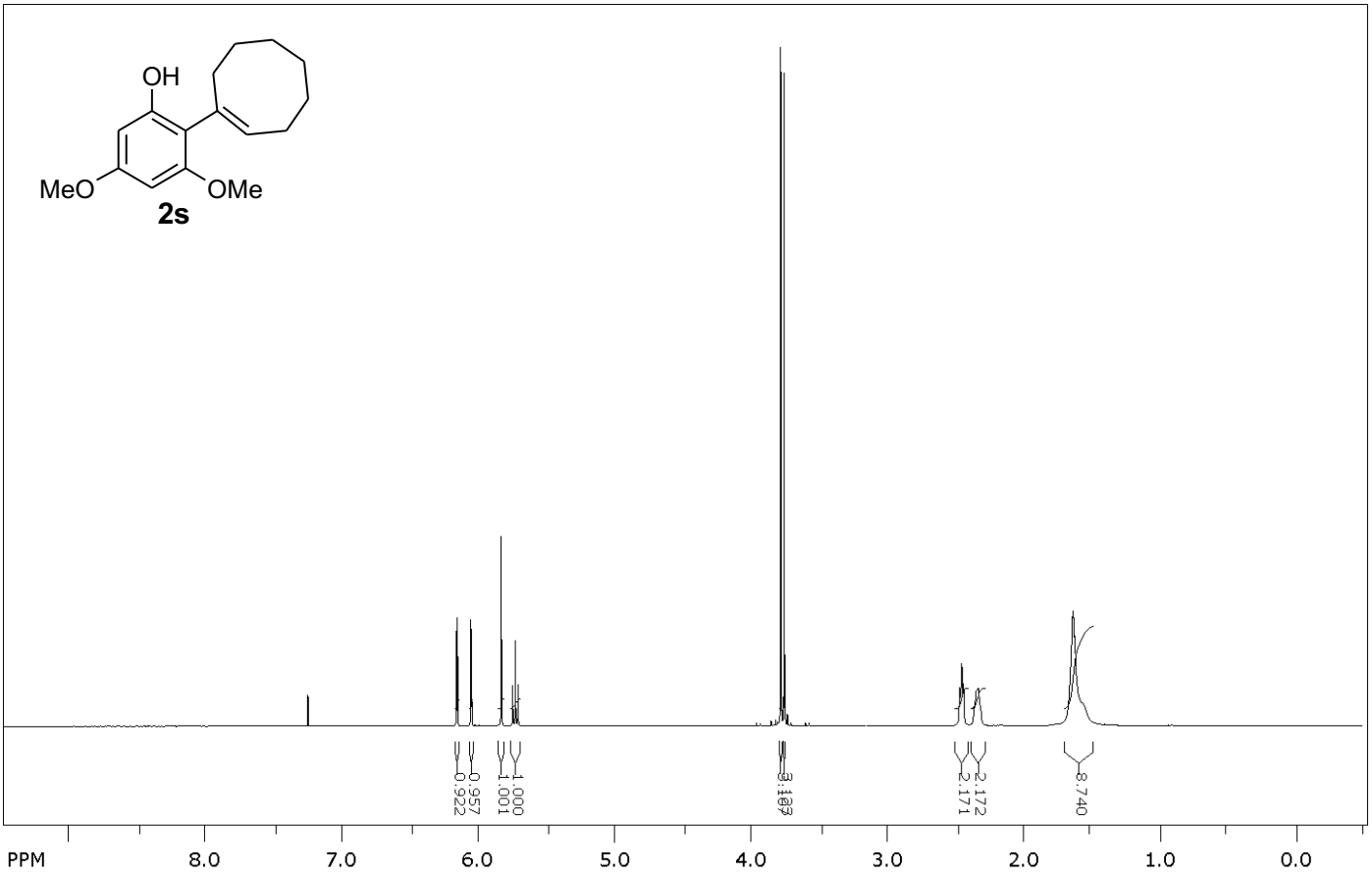
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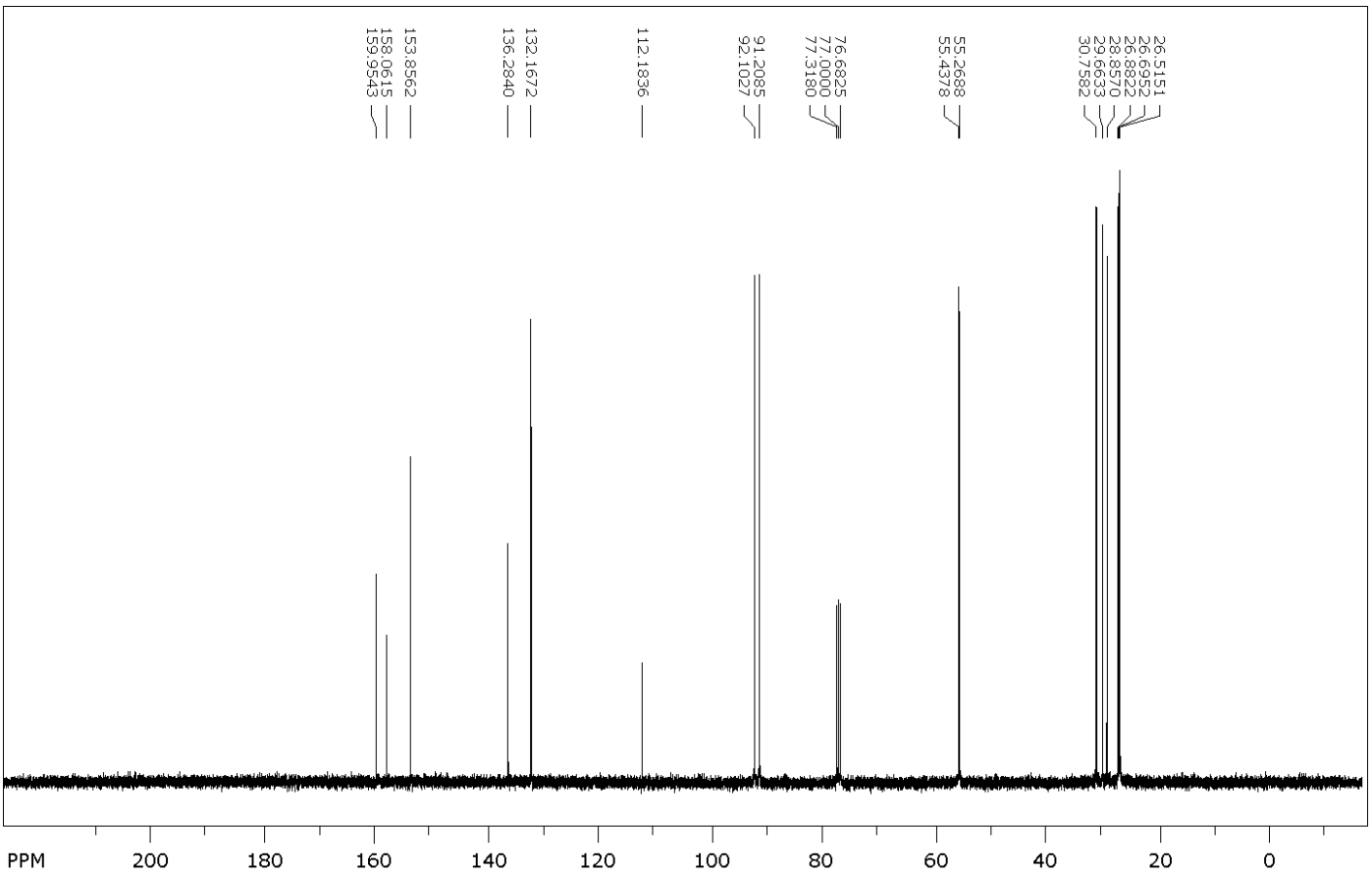
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91.2085
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77.0000
76.6825
55.4378
55.2688
30.7582
29.6633
28.8570
26.8822
26.6952
26.5151
PPM
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160
140
120
100
80
60
40
20
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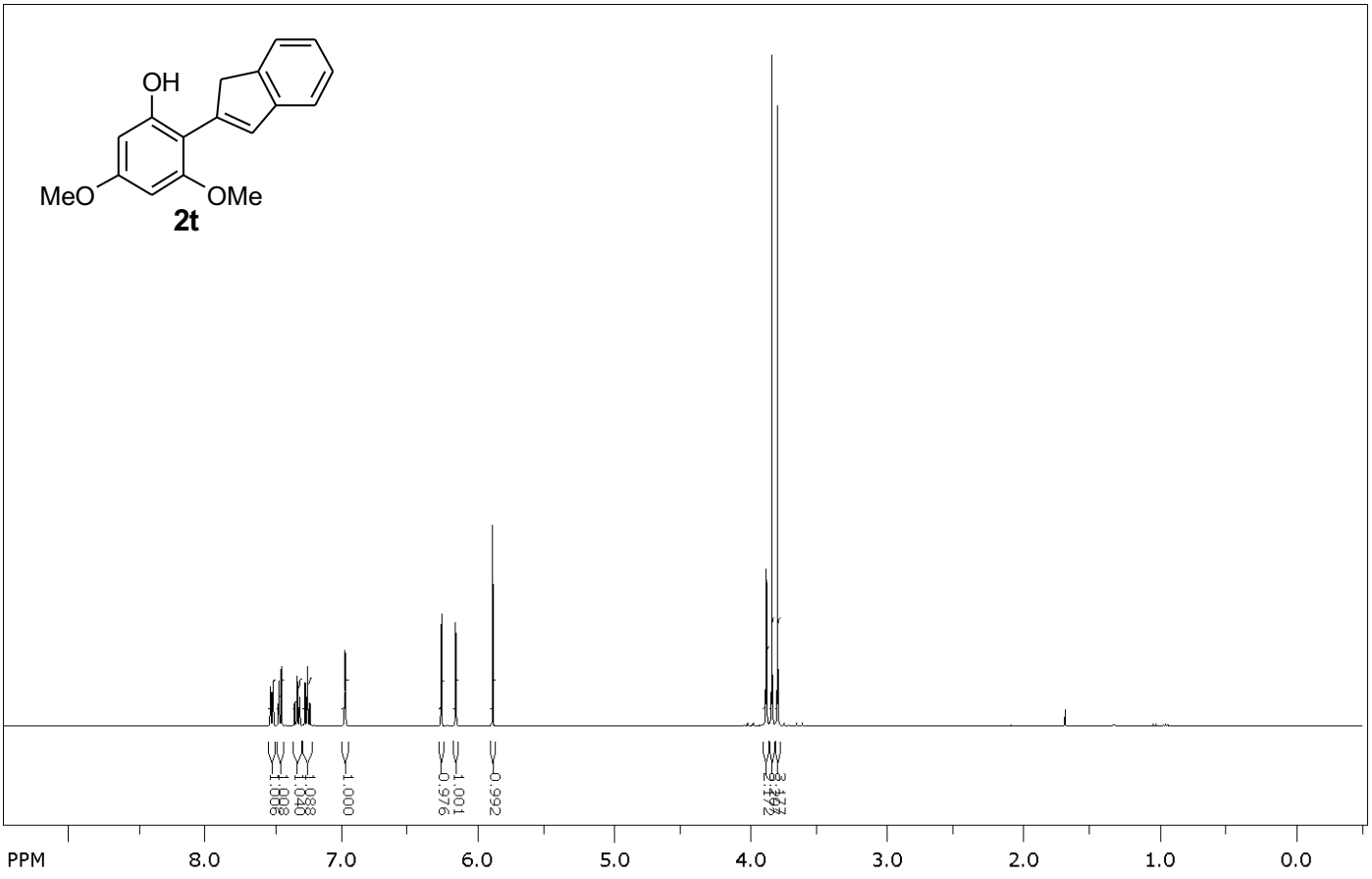
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MeO
OMe
2t
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1.000
0.976
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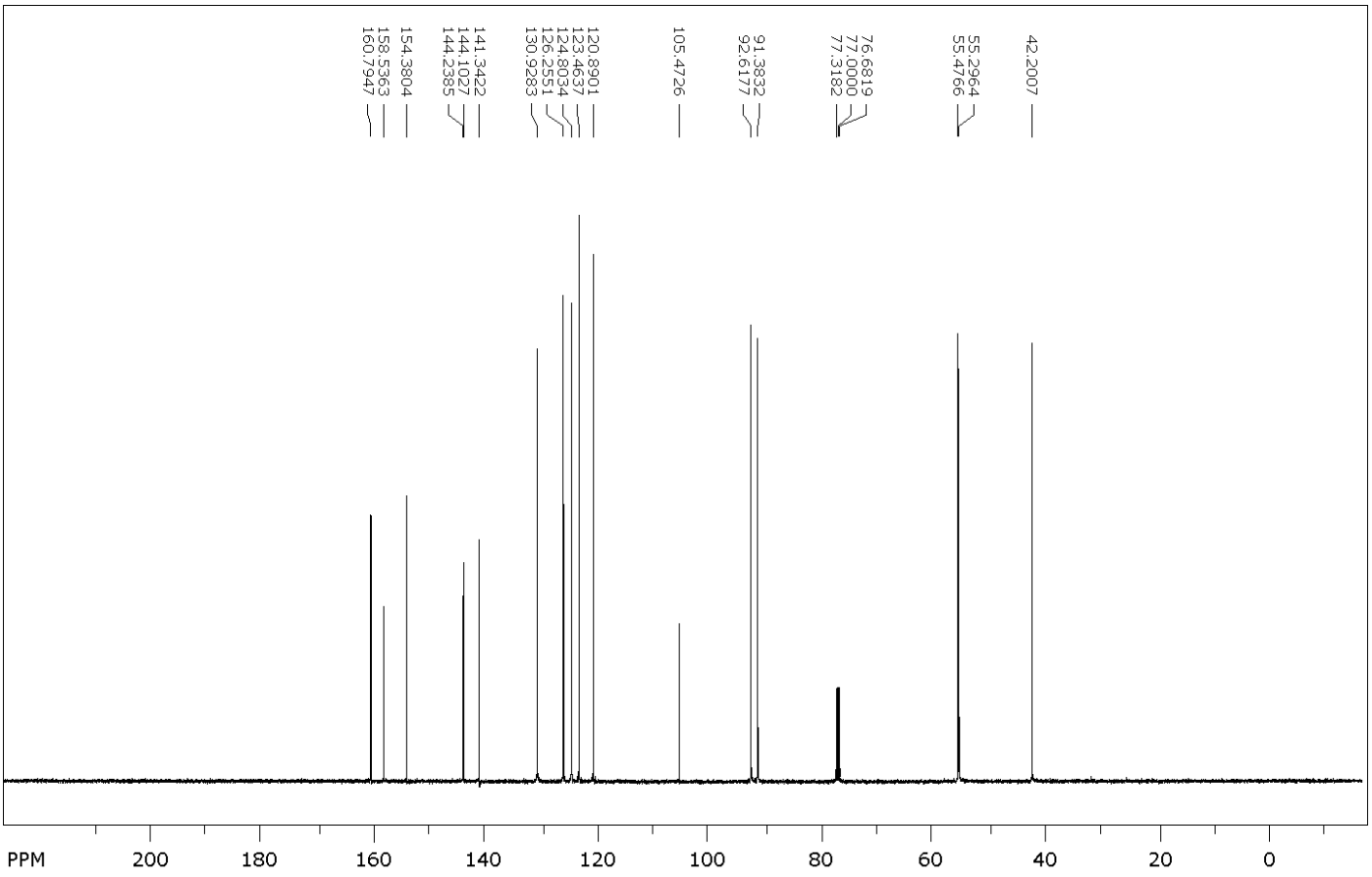
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92.6177
91.3832
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77.0000
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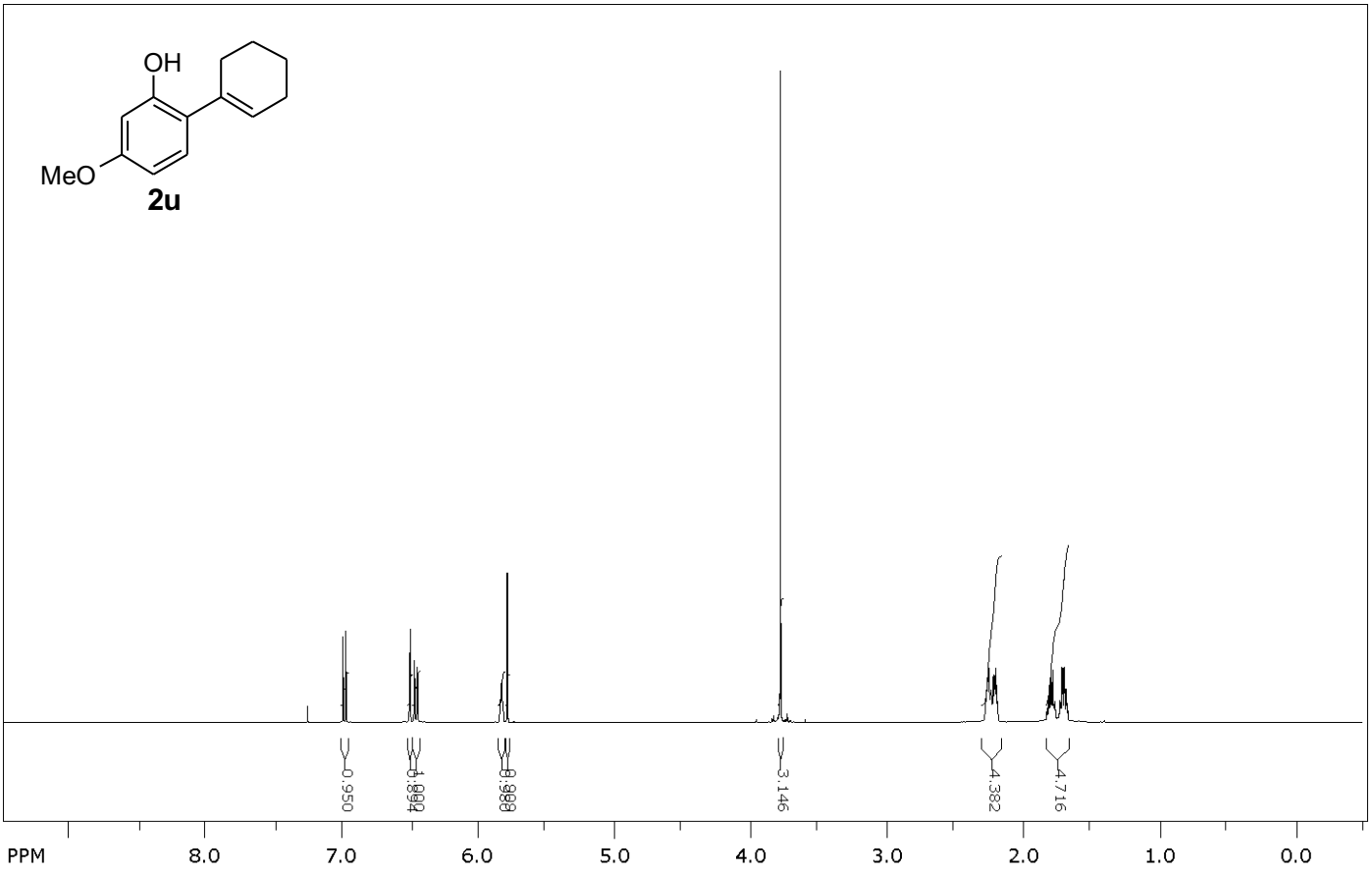
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0.988
3.146
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4.0
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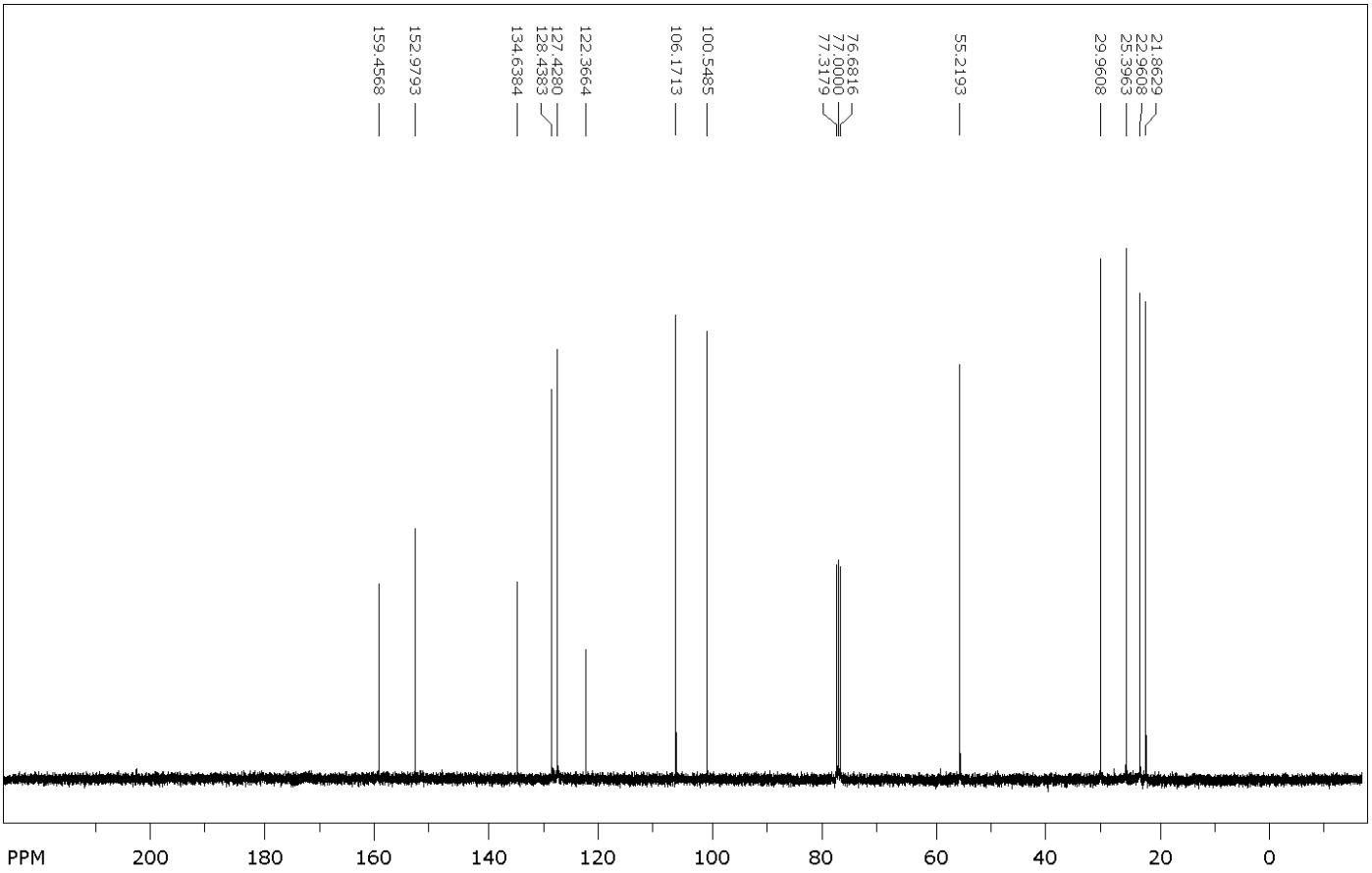
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55.2193
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22.9608
21.8629
PPM
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140
120
100
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60
40
20
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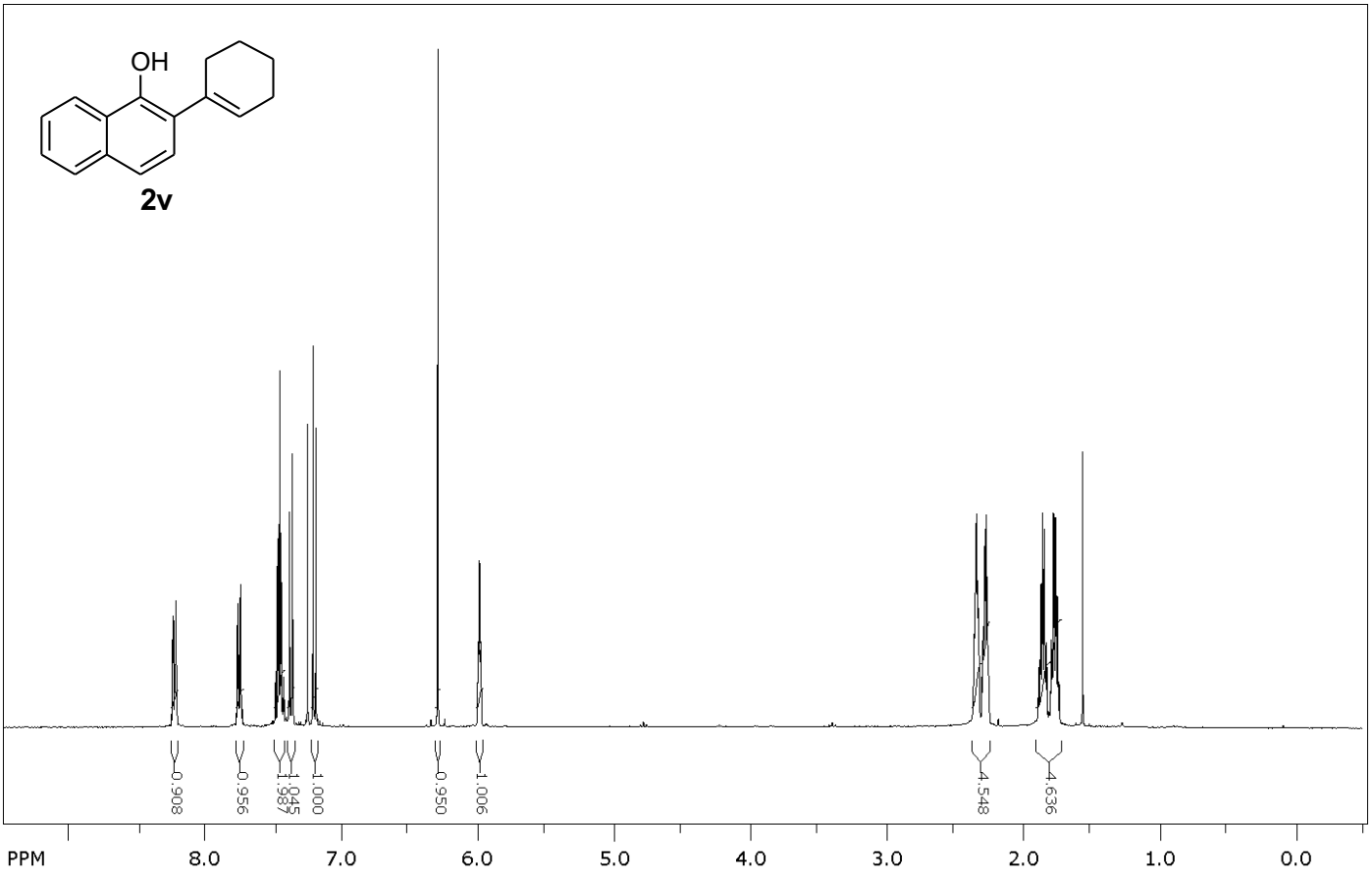
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0.950
1.006
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4.0
3.0
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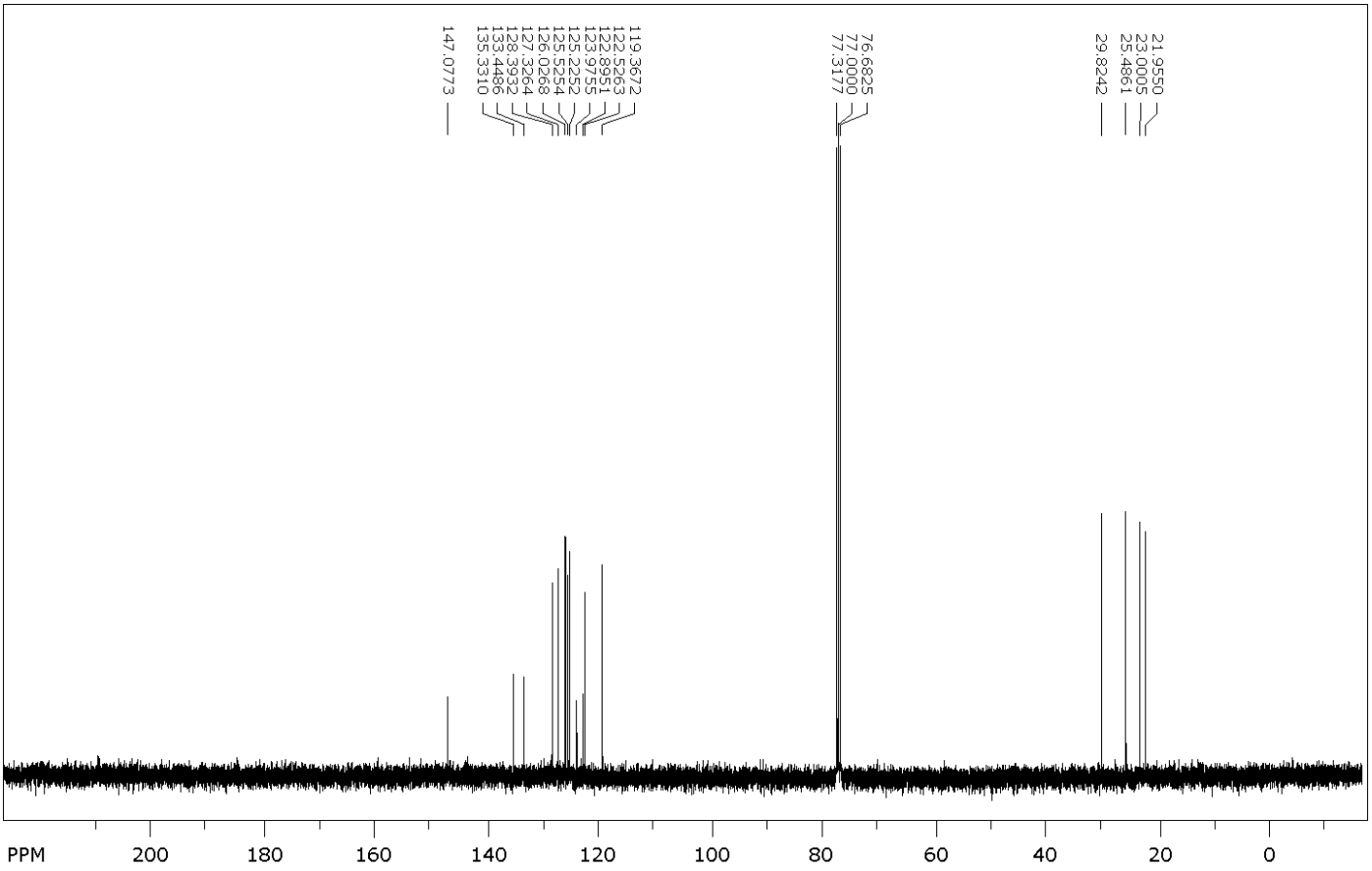
1.0
0.0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119.3672
77.3177
77.0000
76.6825
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23.0005
21.9550
PPM
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140
120
100
80
60
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20
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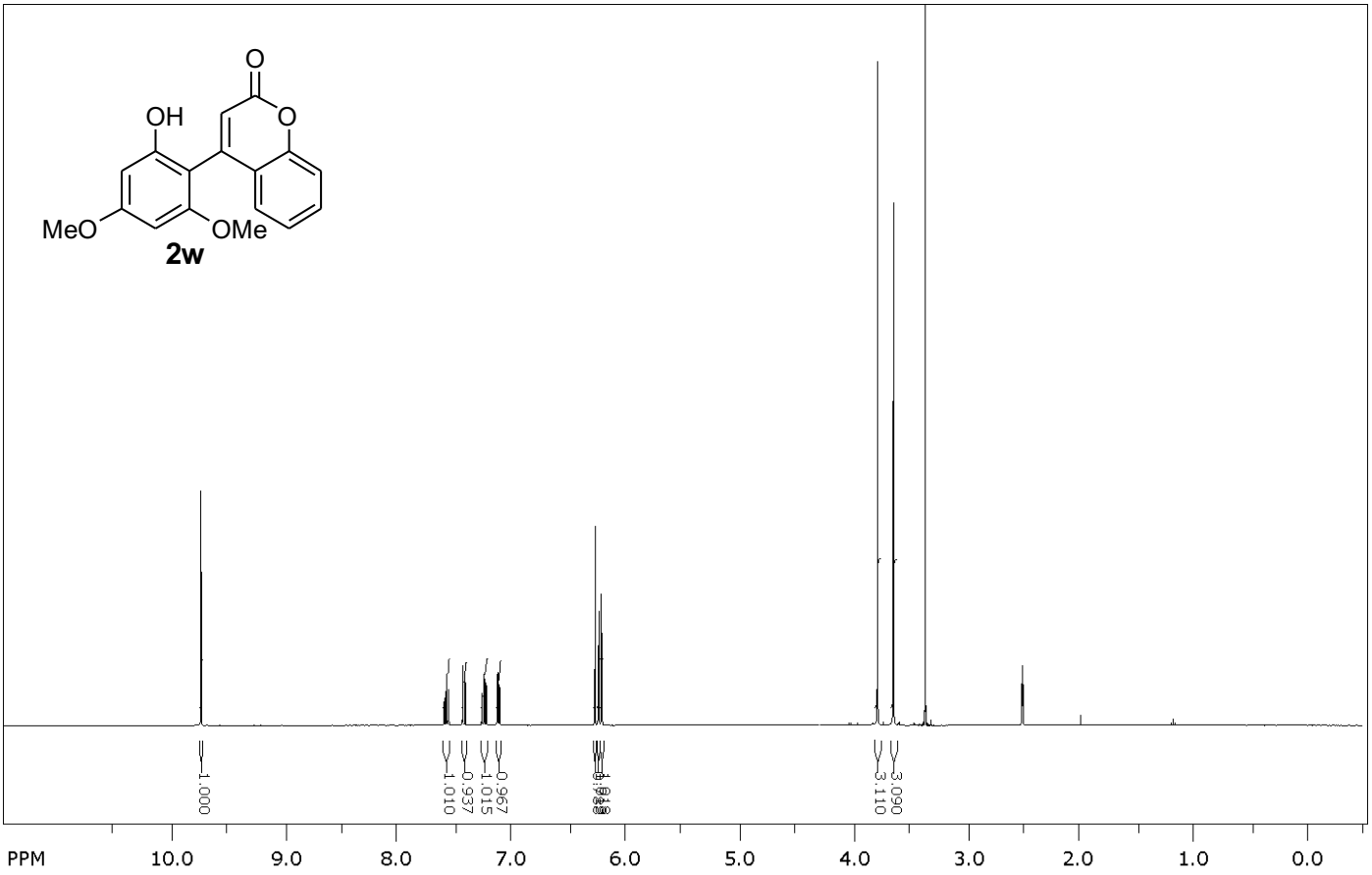
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OH
O
MeO
OMe
2w
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1.015
0.967
3.110
3.090
PPM
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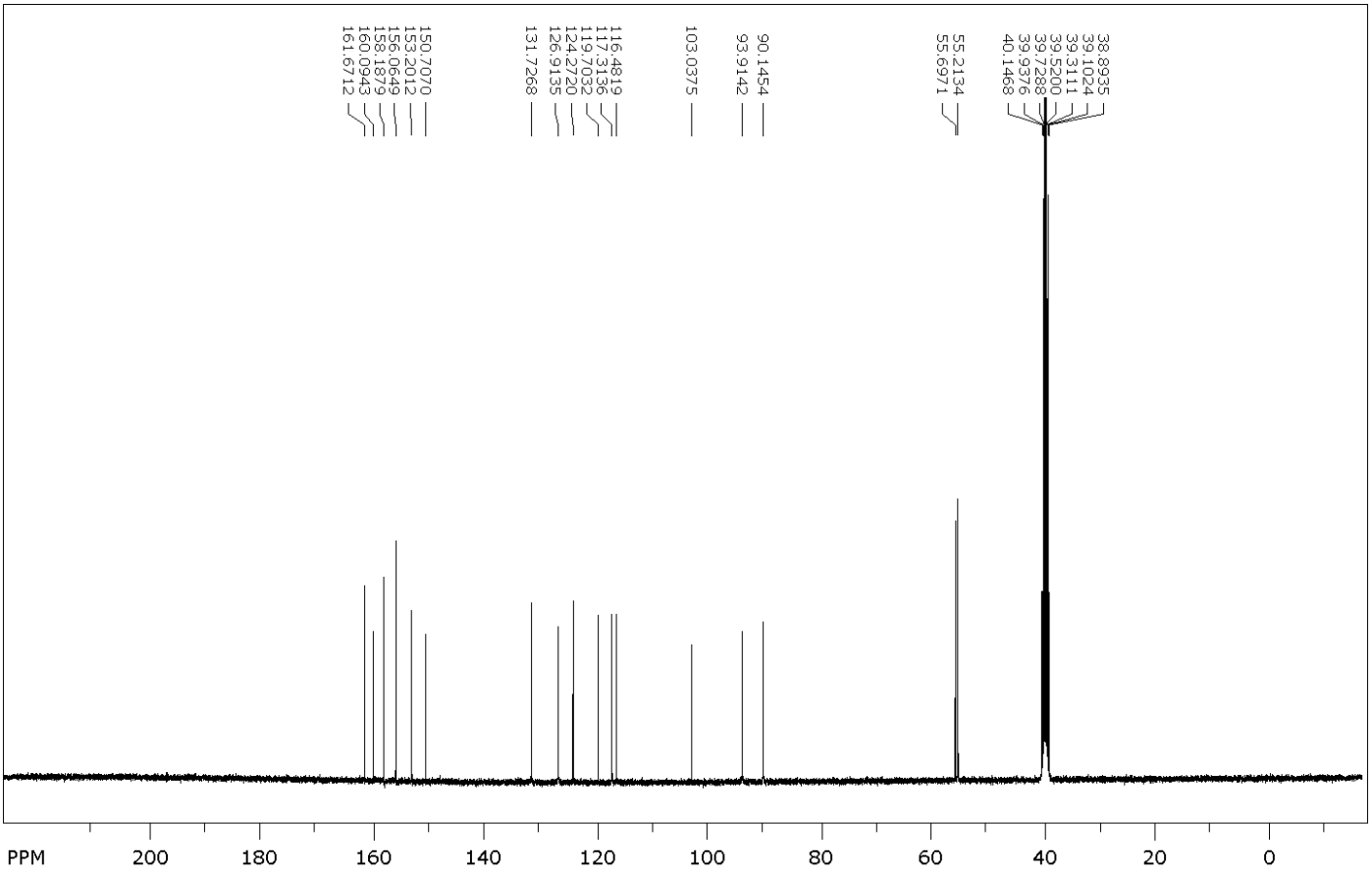
4.0
3.0
2.0
1.0
0.0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116.4819
103.0375
93.9142
90.1454
55.6971
55.2134
40.1468
39.9376
39.7288
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39.1024
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PPM
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120
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20
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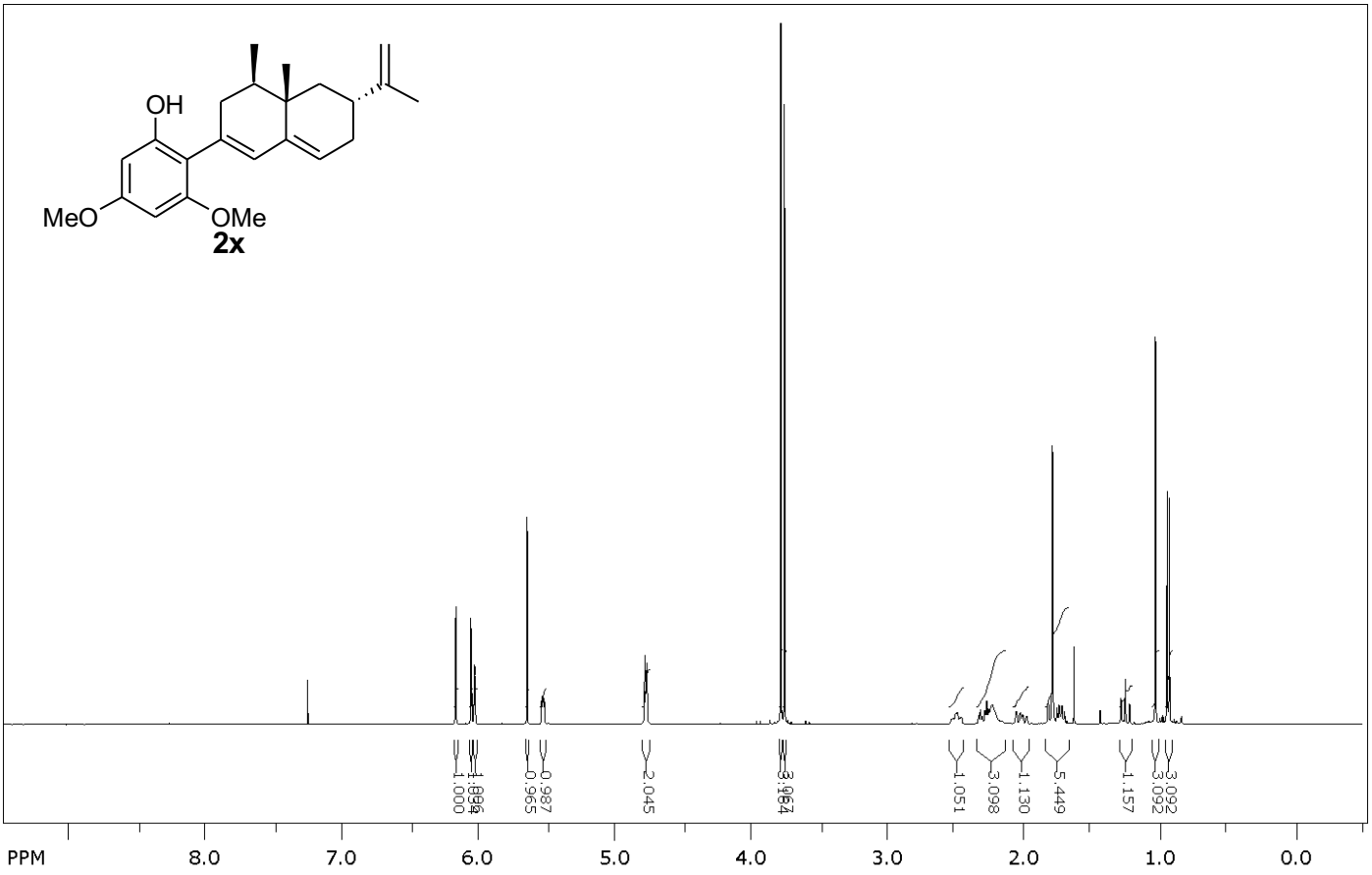
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0.987
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3.964
1.051
3.098
1.130
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1.157
3.092
3.092
PPM
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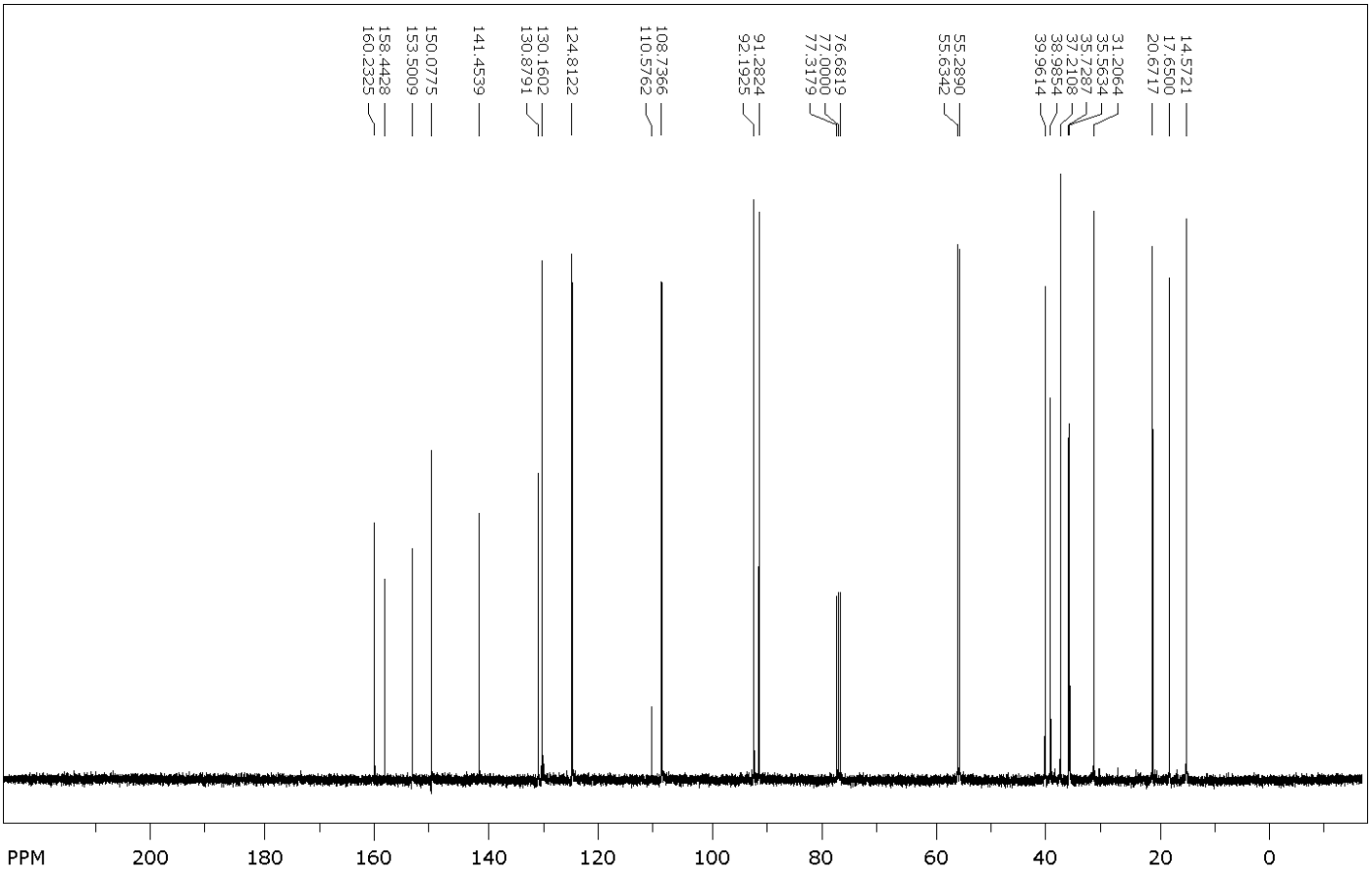
4.0
3.0
2.0
1.0
0.0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91.2824
77.3179
77.0000
76.6819
55.6342
55.2890
39.9614
38.9854
37.2108
35.7287
35.5634
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17.6500
14.5721
PPM
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140
120
100
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60
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20
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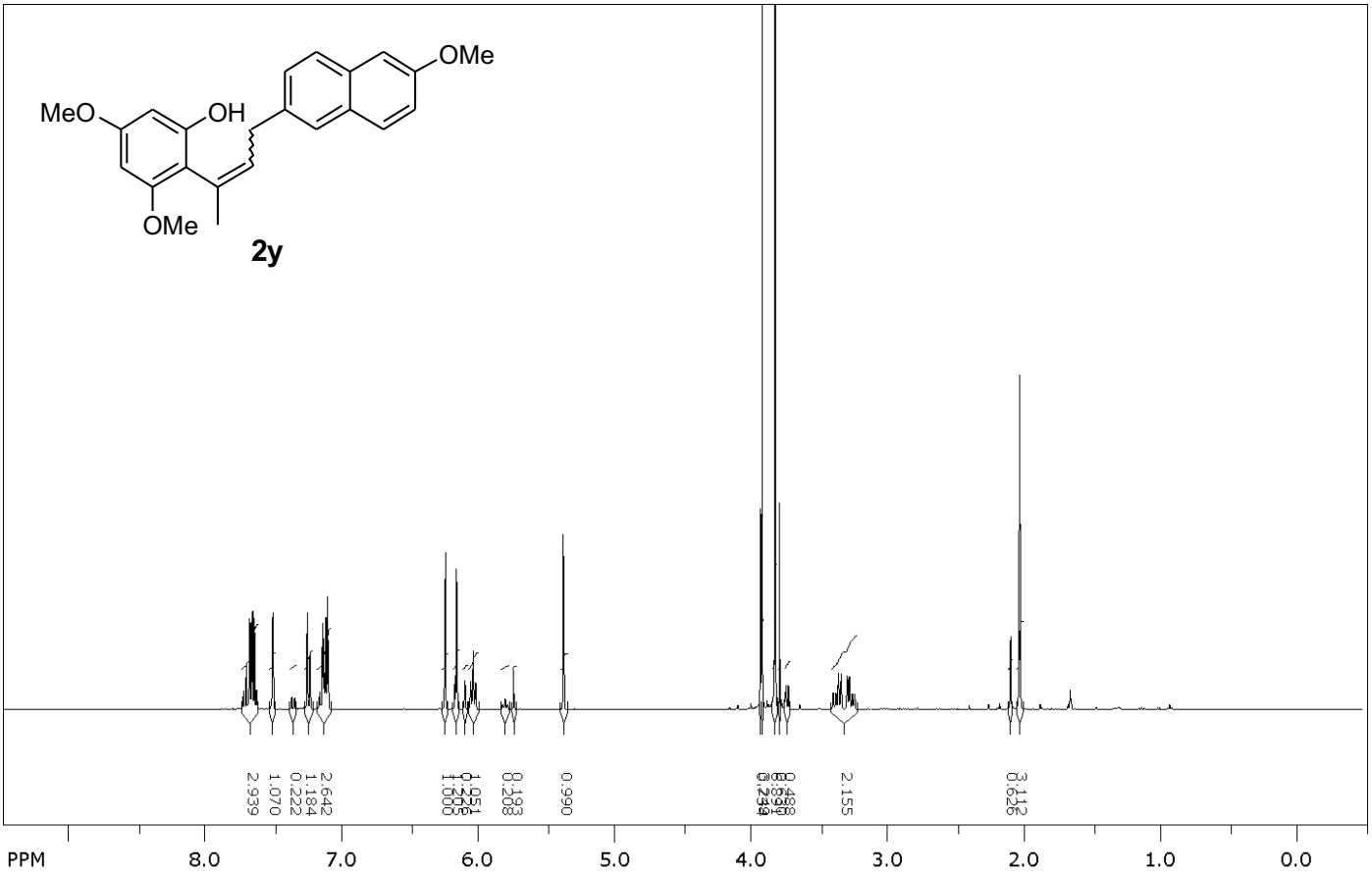
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MeO
OH
OMe
2y
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1.184
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0.990
2.155
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PPM
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4.0
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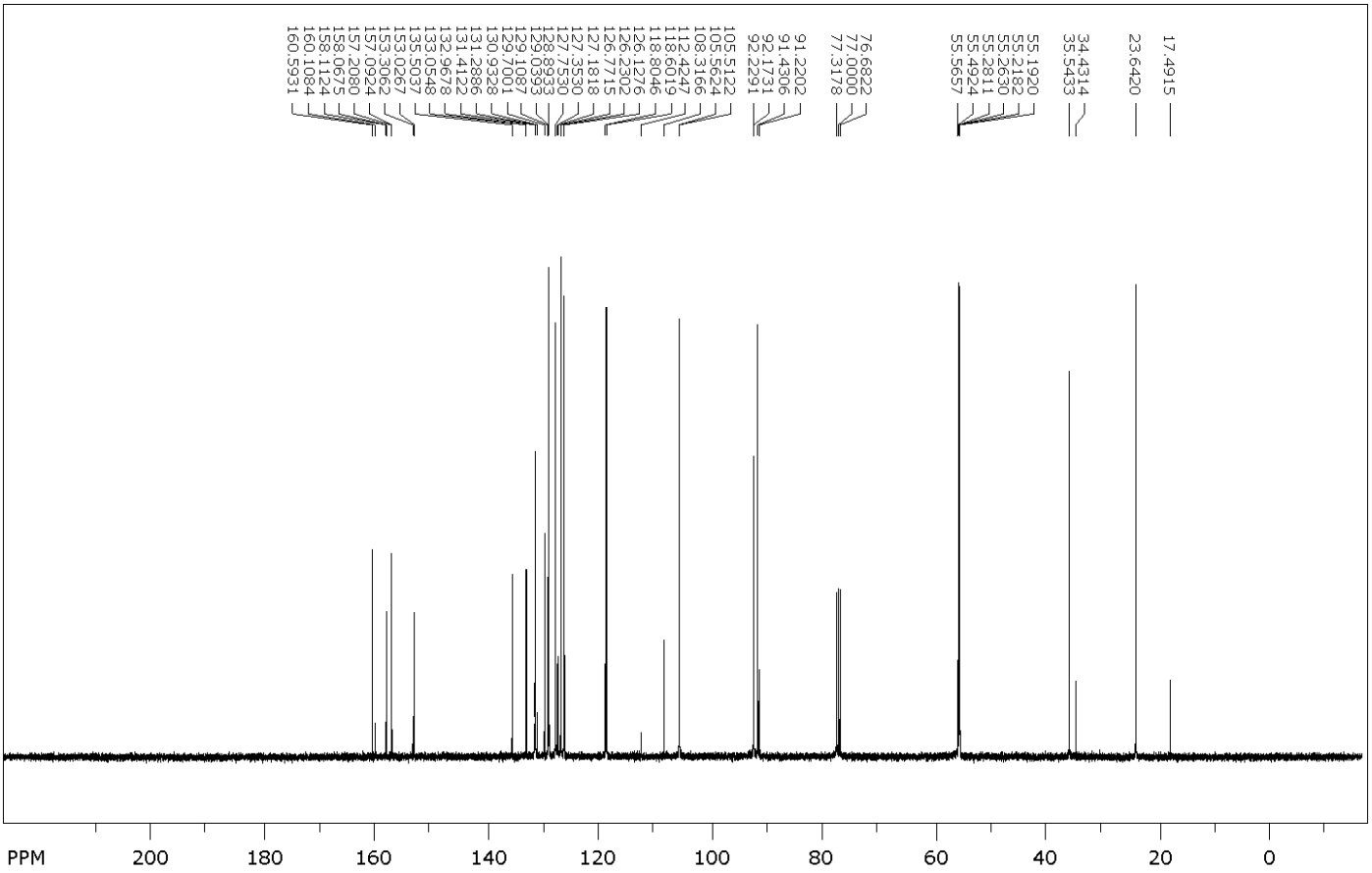
0.0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105.5122
92.2291
92.1731
91.4306
91.2202
77.3178
77.0000
76.6822
55.5657
55.4924
55.2811
55.2630
55.2182
55.1920
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23.6420
17.4915
PPM
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140
120
100
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60
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20
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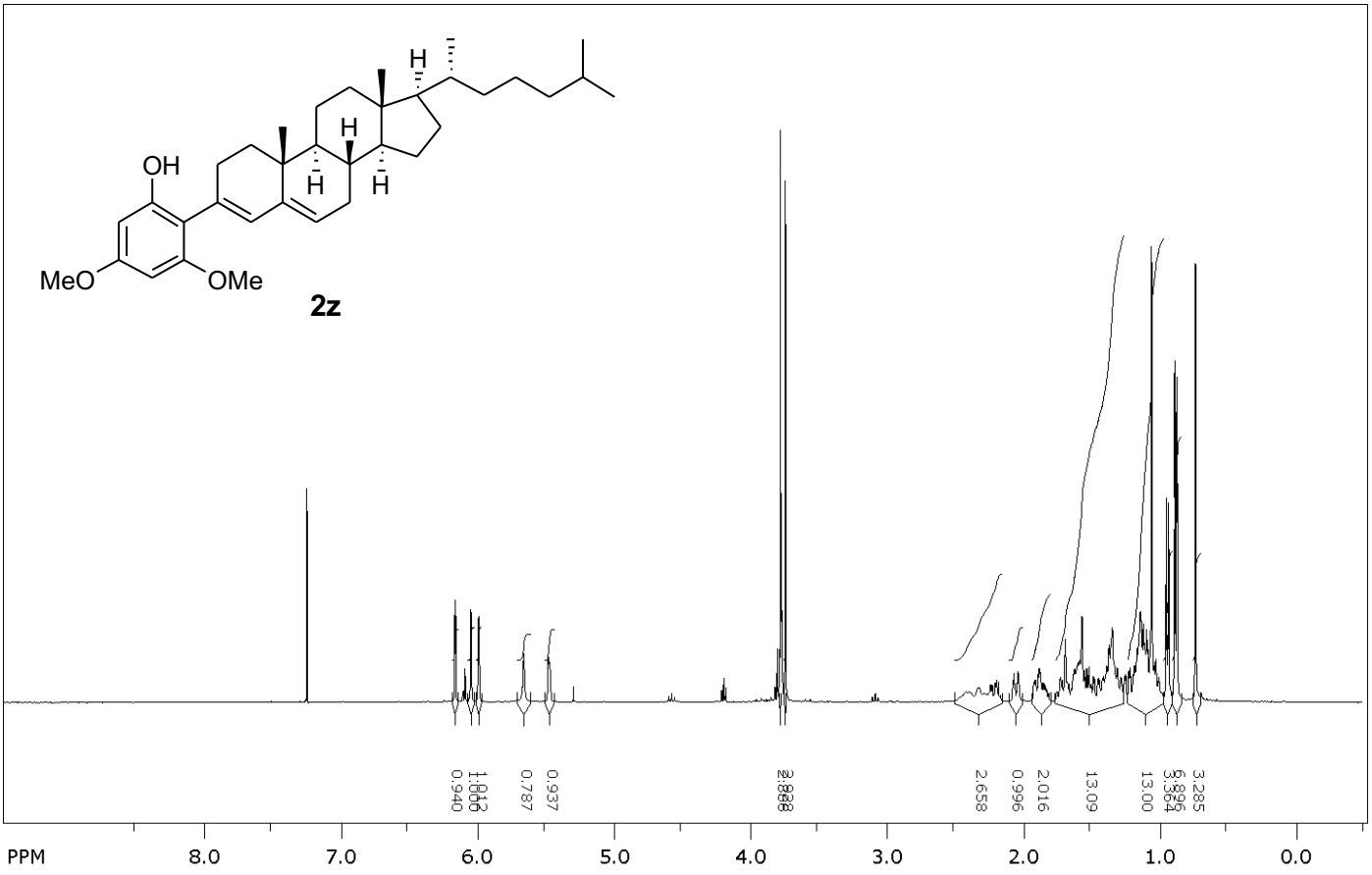
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MeO
OMe
H
H
H
H
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1.006
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0.937
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2.658
0.996
2.016
13.09
13.00
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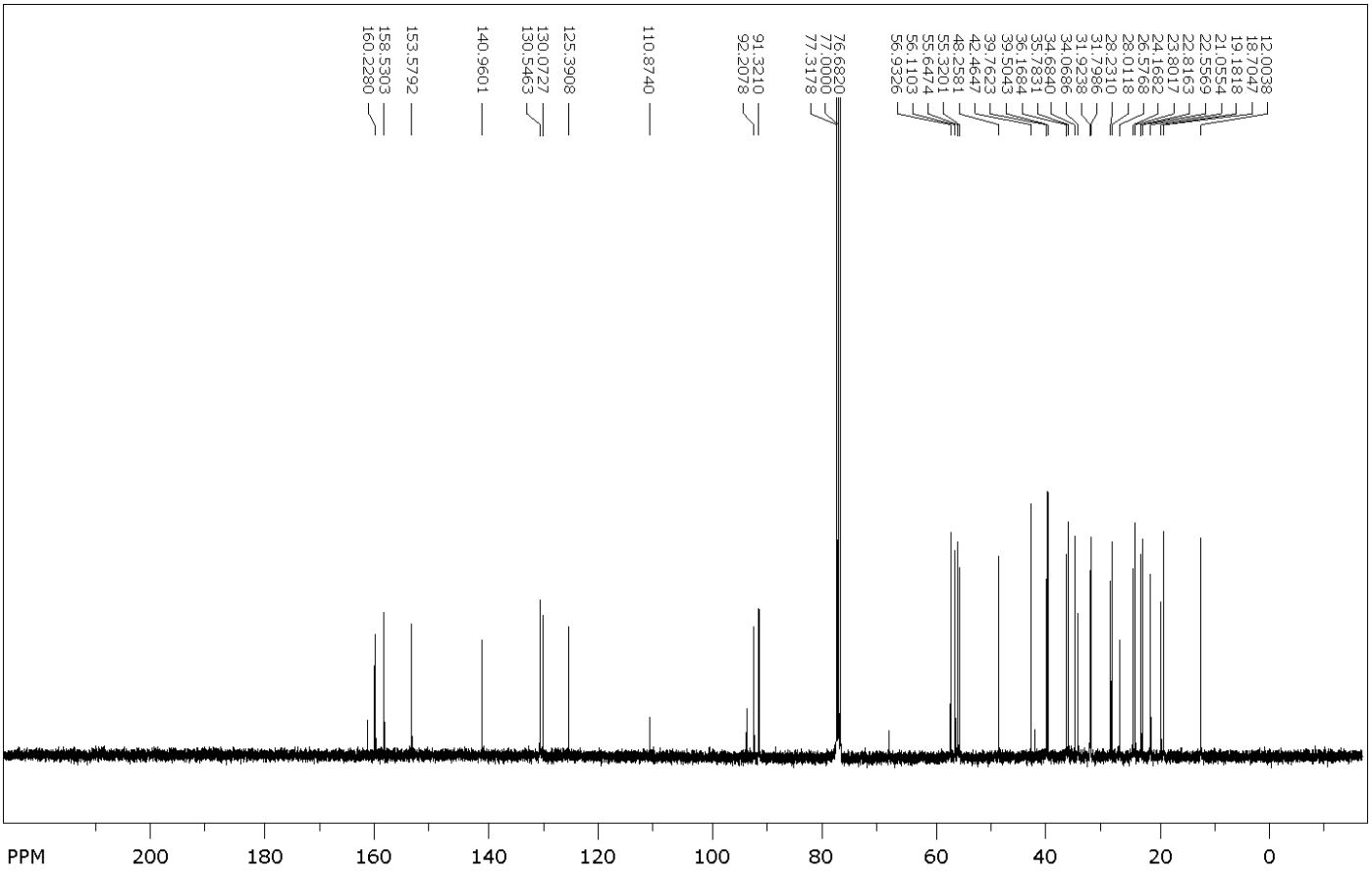
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125.3908
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77.3178
77.0000
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56.9326
56.1103
55.6474
55.3201
48.2581
42.4647
39.7623
39.5043
36.1684
35.7831
34.6840
34.0686
31.9238
31.7986
28.2310
28.0118
26.5768
24.1682
23.8017
22.8163
22.5569
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18.7047
12.0038
PPM
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140
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100
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20
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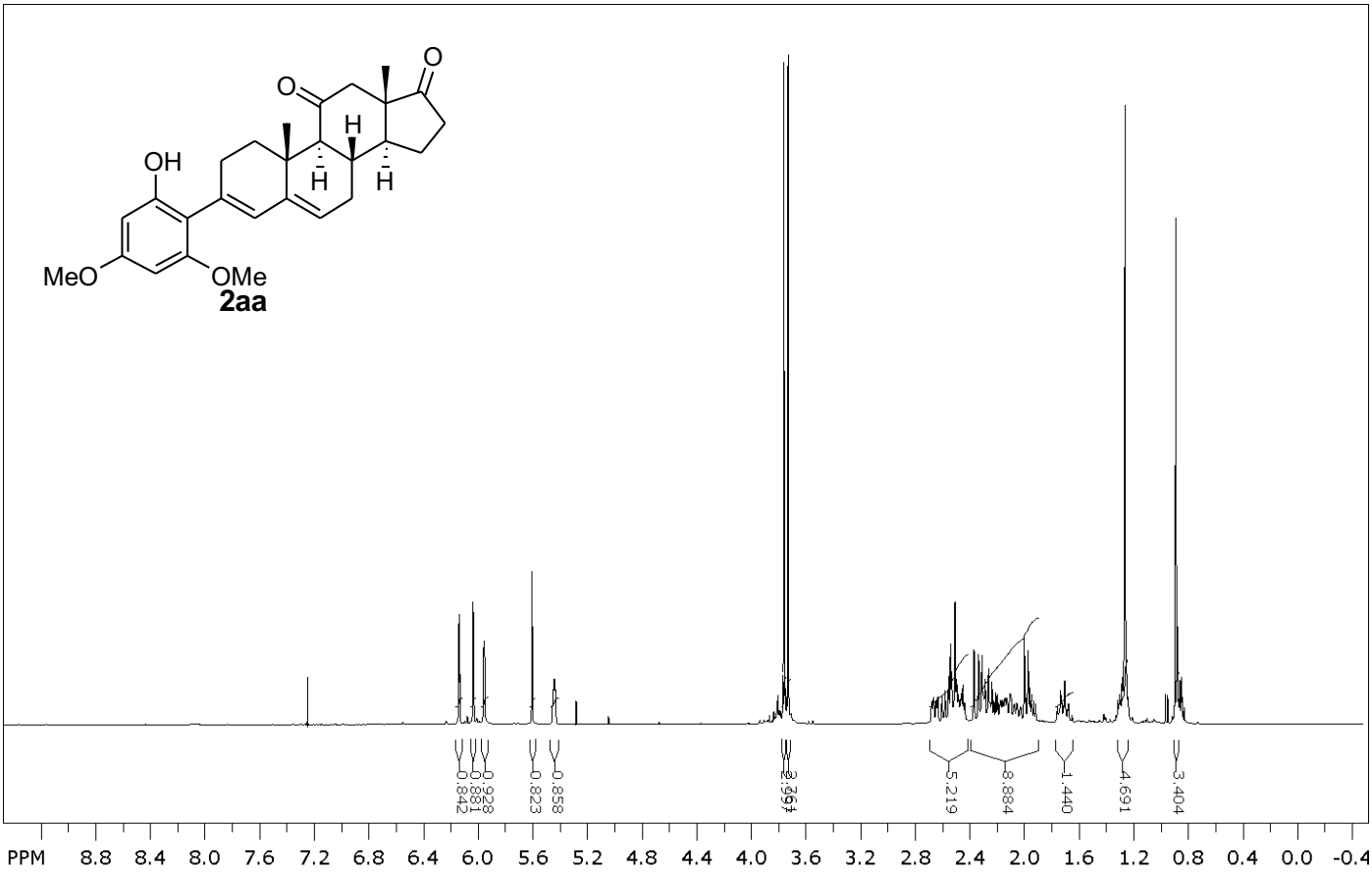
O
O
H
H
H
OH
MeO
OMe
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0.823
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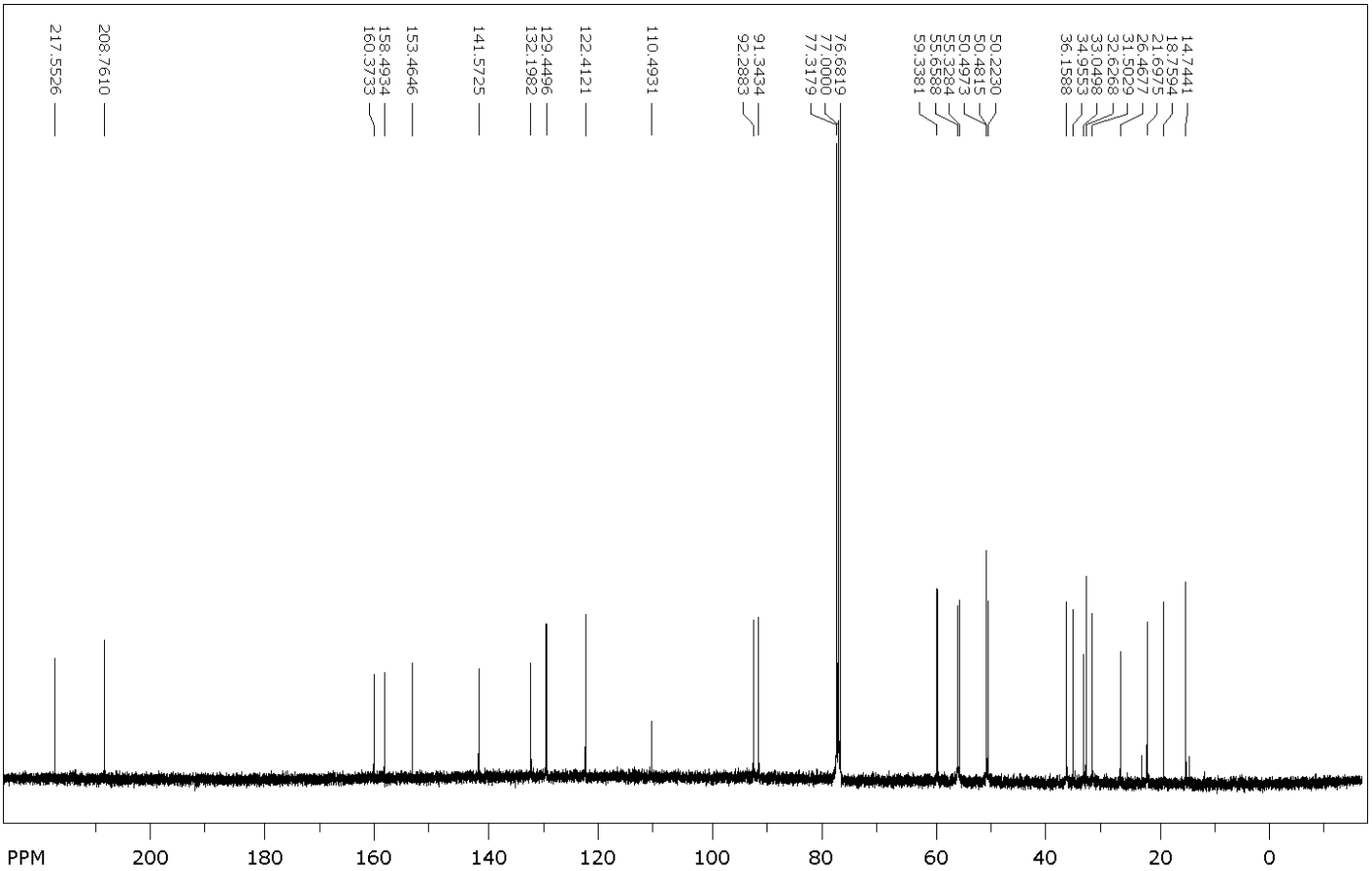
5.219
8.884
1.440
4.691
3.404
PPM
8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0 -0.4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91.3434
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77.0000
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50.2230
36.1588
34.9553
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21.6975
18.7594
14.7441
PPM
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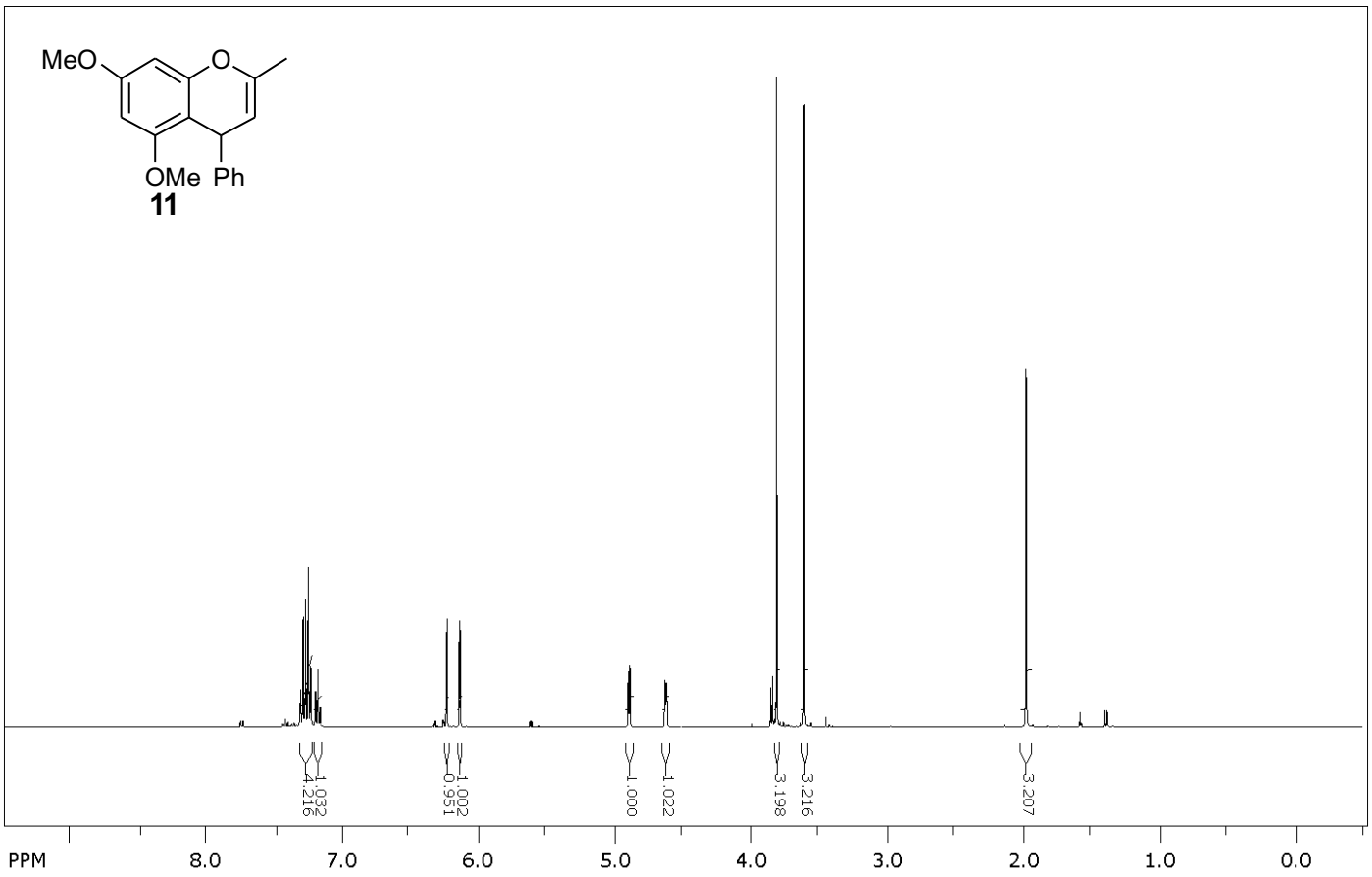
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O
OMe Ph
11
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1.002
0.951
1.000
1.022
3.198
3.216
3.207
PPM
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6.0
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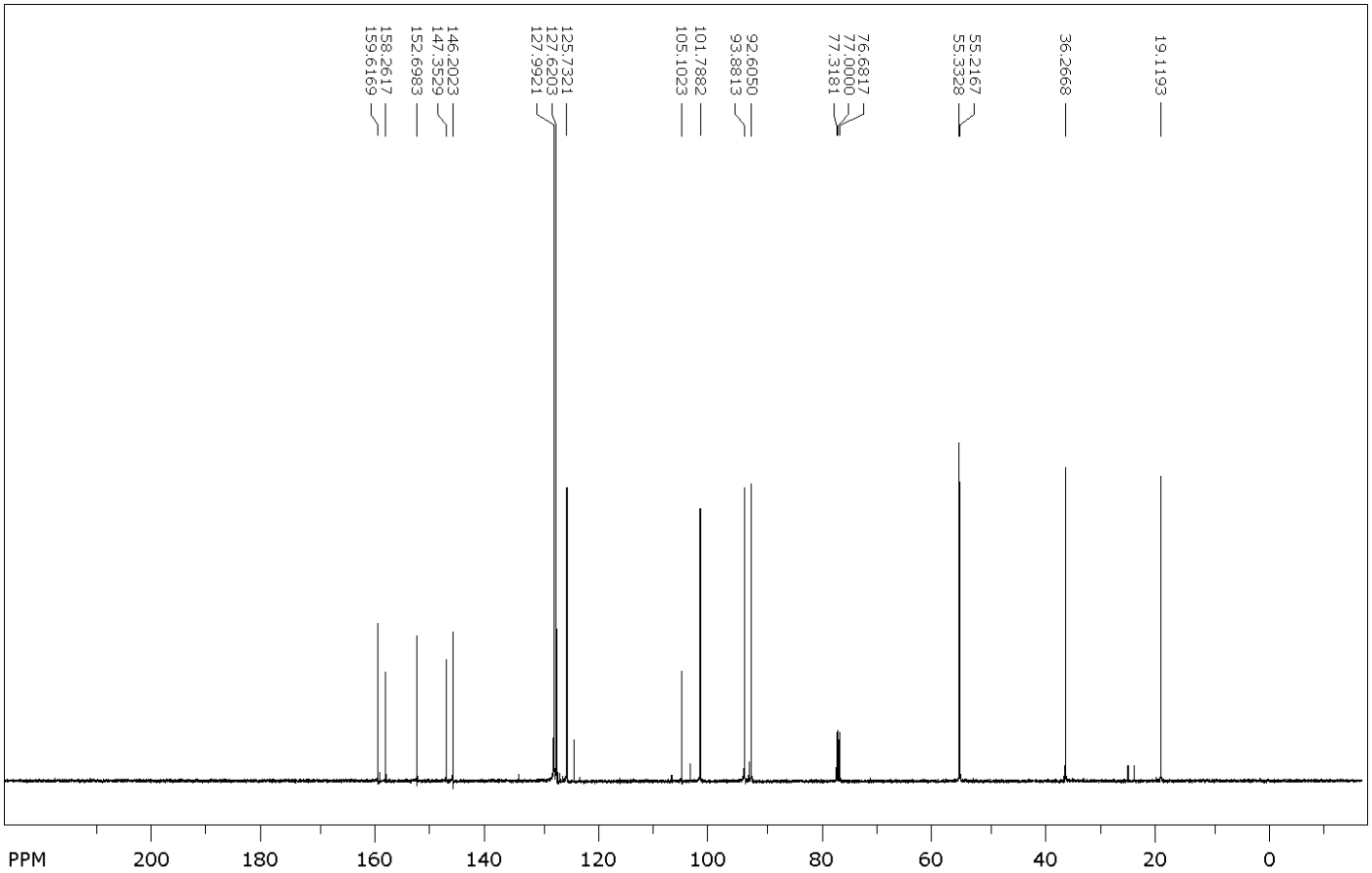
4.0
3.0
2.0
1.0
0.0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93.8813
92.6050
77.3181
77.0000
76.6817
55.3328
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36.2668
19.1193
PPM
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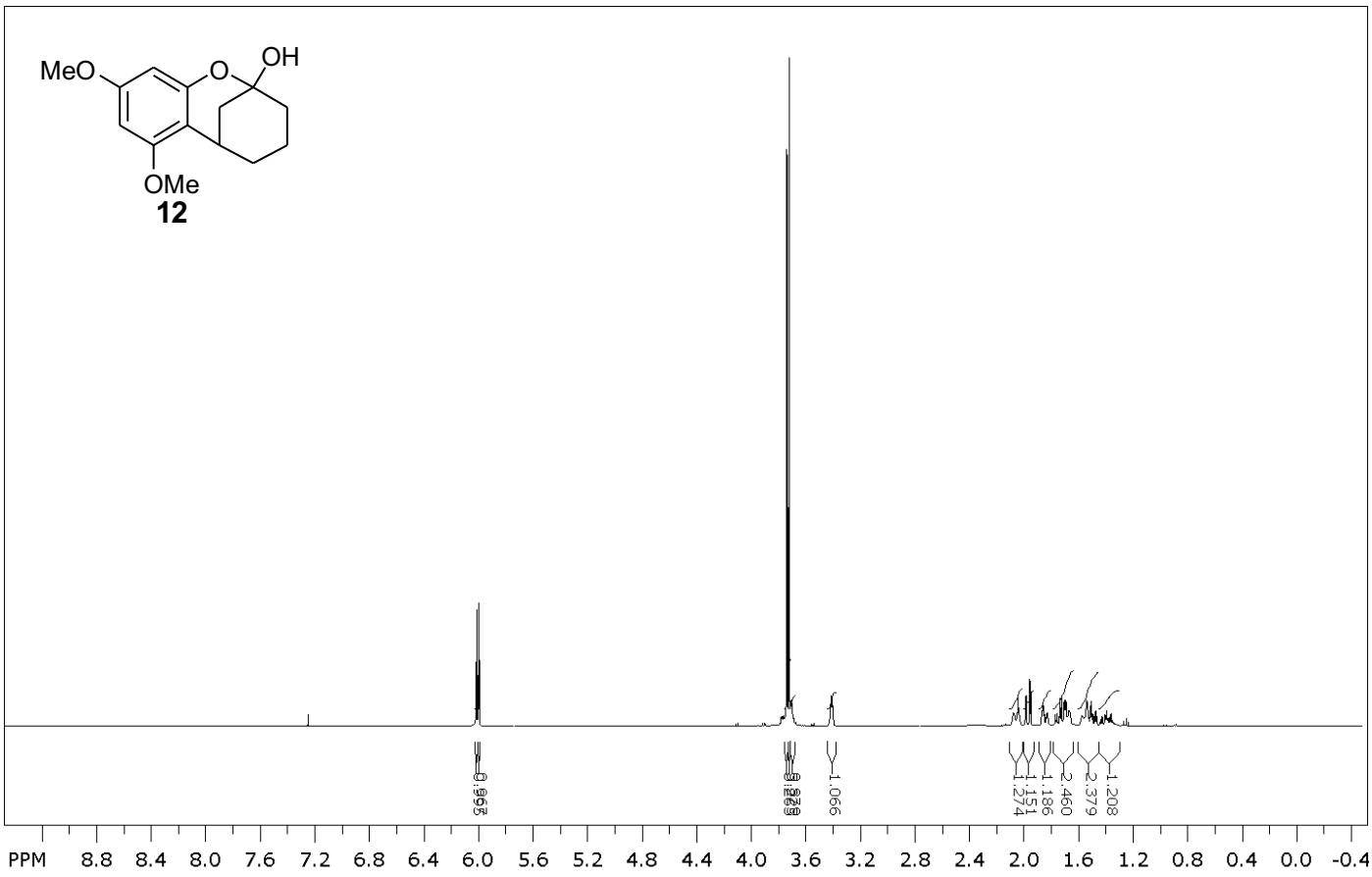
140
120
100
80
60
40
20
0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O
OH
OMe
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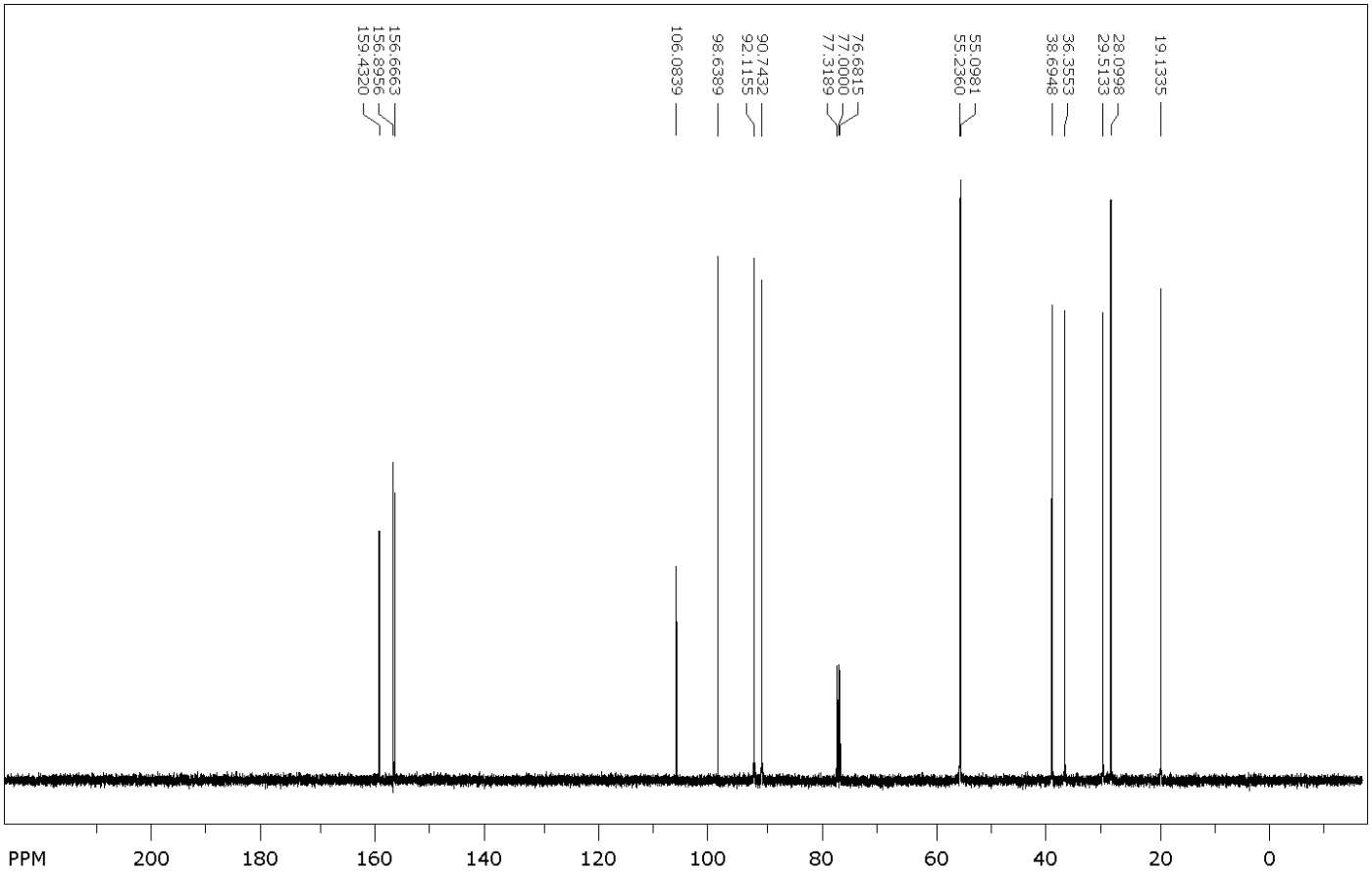
1.151
1.186
2.460
2.379
1.208
PPM
8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0 -0.4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77.0000
76.6815
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29.5133
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19.1335
PPM
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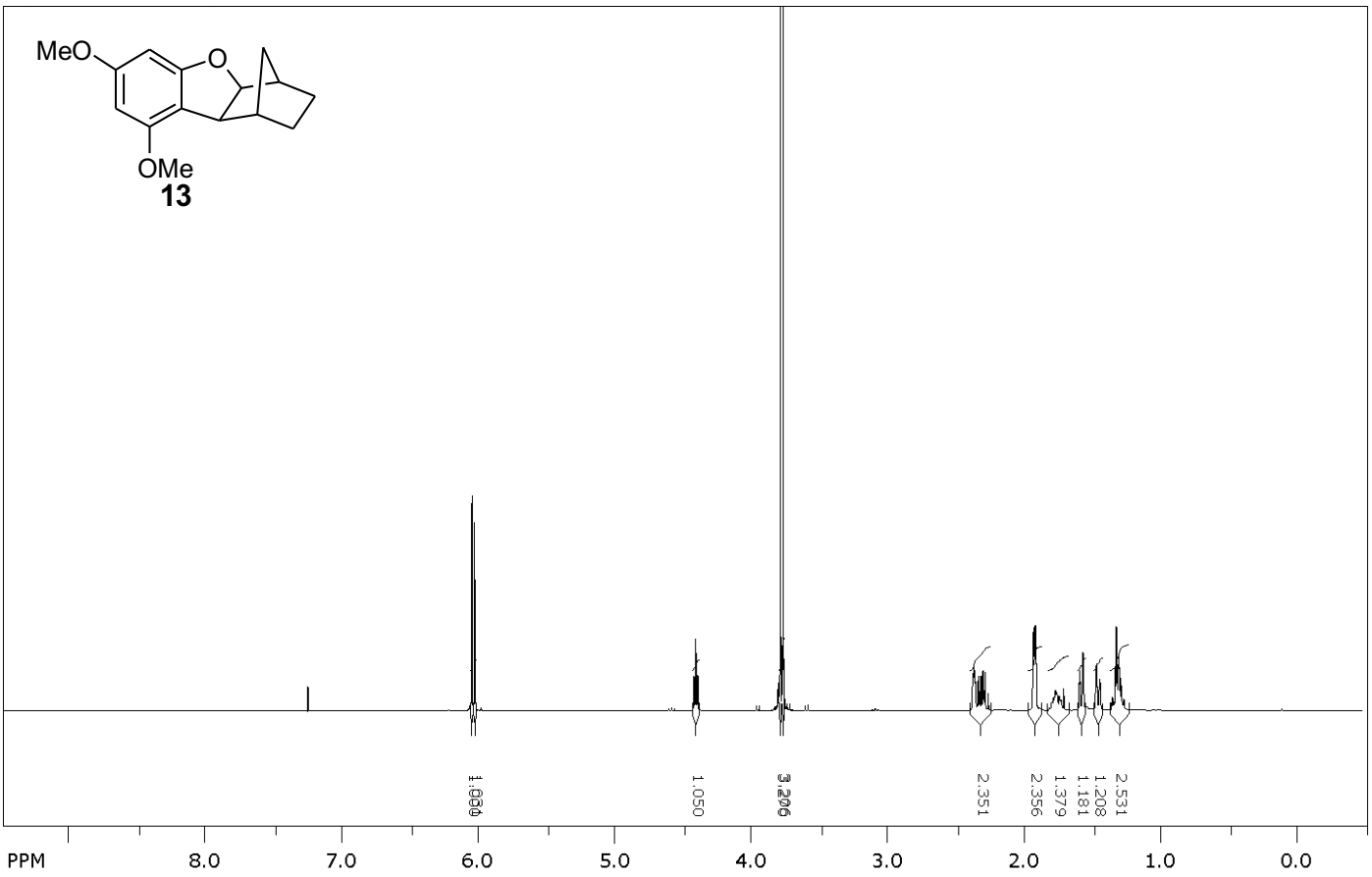
MeO
O
OMe
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2.351
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1.379
1.181
1.208
2.531
PPM
8.0
7.0
6.0
5.0
4.0
3.0
2.0
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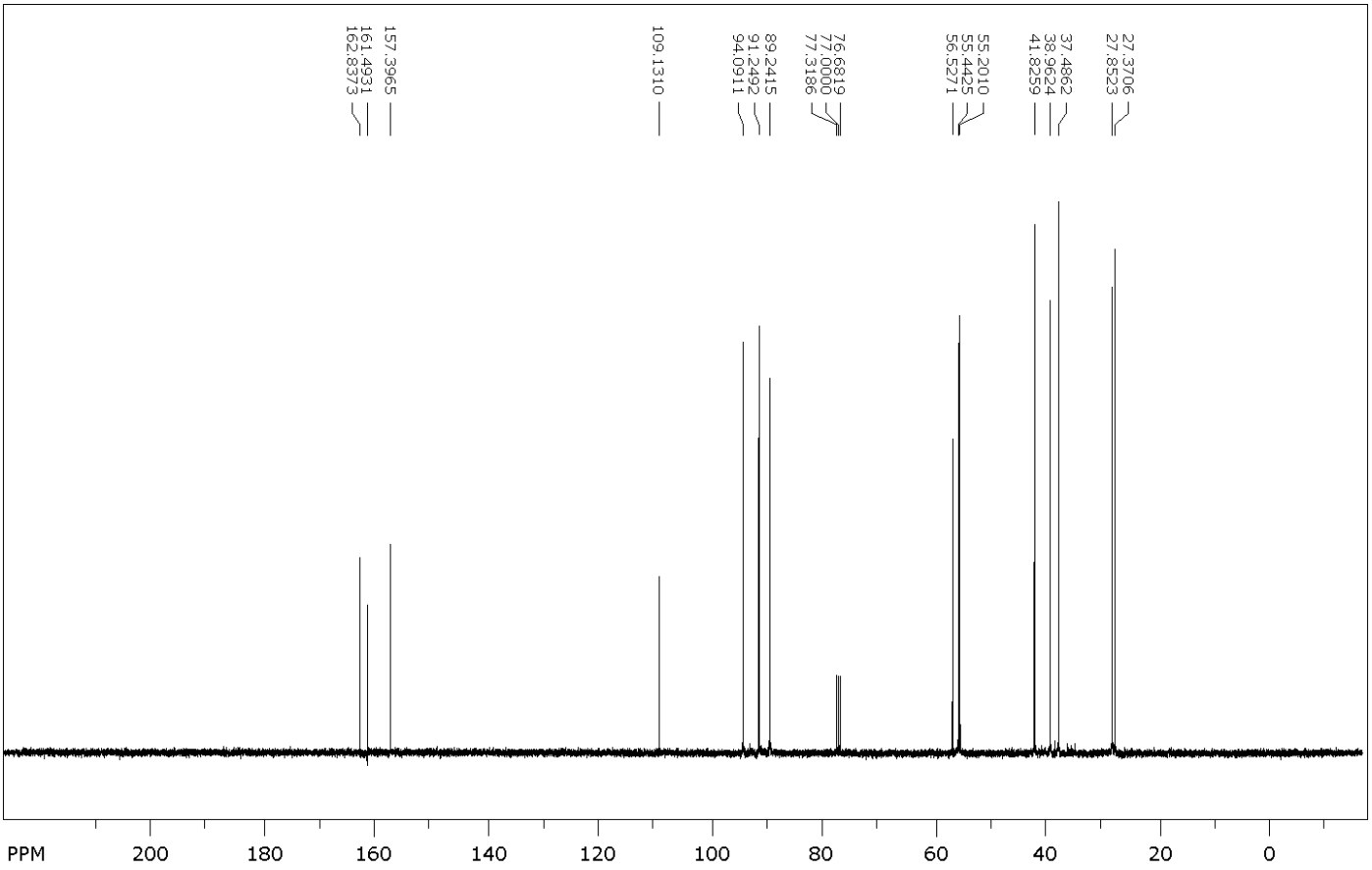
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140
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100
80
60
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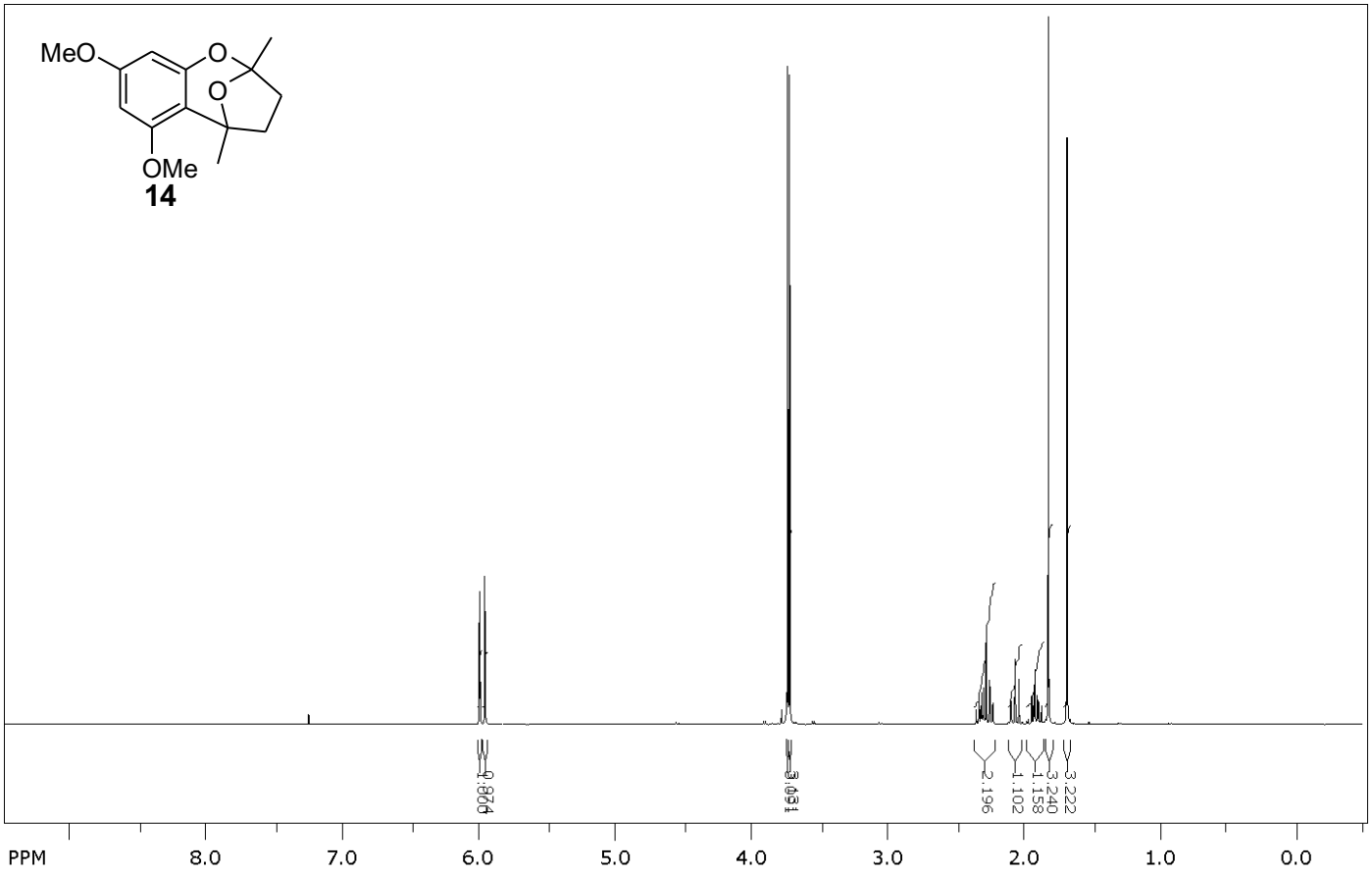
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OMe
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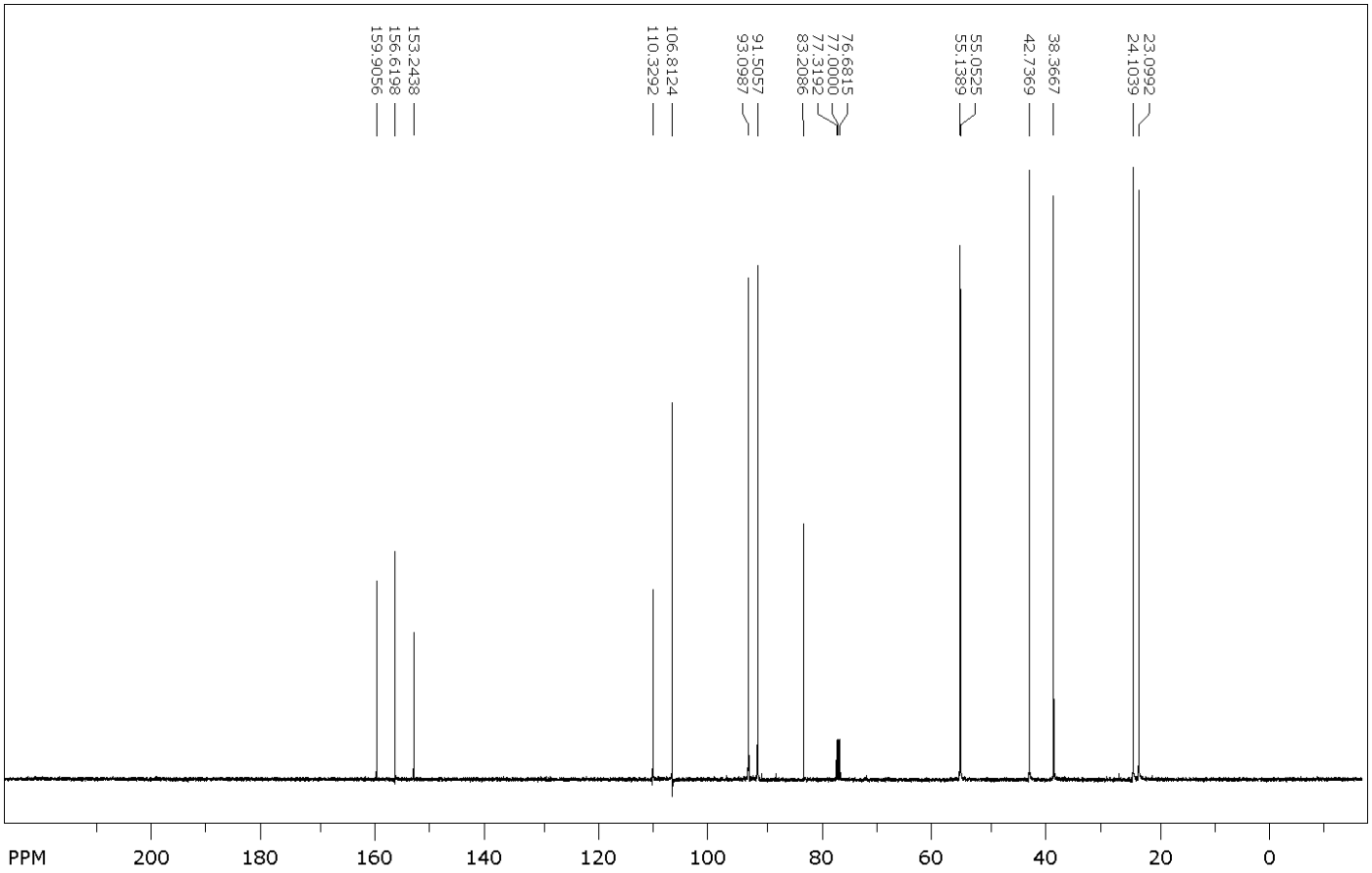
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PPM
200
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