Supporting Information

Aminoquinoline–rhodium(II) conjugates as Src-family SH3 ligands

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General methods

Synthesis procedures: Large scale reactions were performed in oven-dried round-bottom flasks. Small scale reactions were performed in 4-mL vials or scintillation vials. Air- or moisture-sensitive reactions were performed in vials sealed with septum caps. Insensitive reactions used bulk solvent without further purification, while air- or moisture-sensitive ones used solvent stored under argon or nitrogen. Reaction vessels were stirred magnetically; flasks were heated in an oil bath and vials in an aluminum heating block. Flash chromatography was performed with 40-63 μM particle size silica gel (Silicycle).

Chemicals: Chemical reagents were purchased and used without further purification. All solvents used were ACS reagent grade. Solvents used under inert atmosphere were bought and maintained in inert packaging or purified and degassed by a solvent dispensing system (Pure Process Technology).

NMR spectroscopy: NMR data was acquired with Bruker Avance 400 MHz, Bruker Avance 500 MHz, or Bruker Avance III 600 MHz instrument. ^{1}H and ^{13}C NMR spectra were referenced relative to residual solvent or TMS.

Mass spectroscopy: Compatible samples were analyzed using an Agilent 6890 gas chromatograph. All other samples were analyzed by electrospray ionization (ESI–MS) by direct injection into a Bruker Daltonics microTOF instrument.

Synthesis of known compounds: N-Boc-piperazine,[1] *tert*-butyl 4-bromobutanoate,[2] methyl 6-bromohexanoate,[3] and $Rh_2(OAc)_3(tfa)$[4] were prepared according to previously reported protocols.

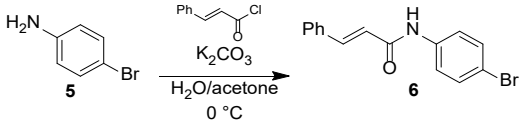
HPLC: HPLC analyses were performed on reverse phase columns using a Shimadzu CBM-20A instrument monitoring at 254 and 350 nm. Mobile phase consisted of acetonitrile/water mixtures with 0.1% trifluoroacetic acid in both constituents. Analytical and preparative separations employed a Phenomenex Jupiter 4μ Proteo 90A (250 × 4.6 mm) column at 1 mL/min and a Phenomenex Jupiter 4μ Proteo 90A (250 × 15 mm) at 8 mL/min, respectively.

ITC analysis: ITC experiments were performed using a MicroCal ITC200 instrument at 25 ˚C. Solutions of 275 μM ligand were titrated into 18-20 μM solutions of SH3 domain. Heats of dilution were measured independently for each experiment by titrating the ligand solution into buffer (20 mM phosphate buffer, pH 7.0, 150 mM NaCl, 1 mM EDTA). The linear regression for the heat of dilution and the observed baseline were subtracted from the raw data. The experimental data were fit in Origin (MicroCal) using a one set of sites binding model minimizing the residual sum of squared deviations.

Computational docking and model building: Docking was performed using the GOLD program (v. 5.7.2, CSD-Discovery suite). Docking was conducting assuming protonation at both basic nitrogens of the ligand **4.2**, and the GOLD program found 10 low-energy docked structures. A promising candidate was used as a starting point to build a two-point binding model: the ligand was locked in place except for the 3-carbon alkyl linker. Manual manipulation of the linker torsional angles (Swiss PDB Viewer) was then used to build a reasonable binding model based on the docked structure.

Chemical synthesis

N-(4-bromophenyl)cinnamamide (6)



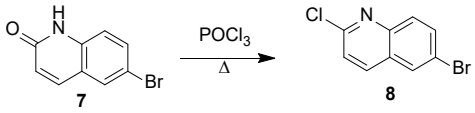
The procedure was adapted from the literature.[5] A 500-mL round-bottom flask was charged with 4-bromoaniline, **5**, (5.3 g, 31 mmol), water (70 mL), and potassium carbonate (60.0 g, 434 mmol). The mixture was gently heated to dissolve the solid then held at 0 °C. With stirring, a solution of cinnamoyl chloride in acetone (7.1 g, 43 mmol in 25 mL) was added dropwise by addition funnel over 30 min. The flask was placed in the freezer for 30 min to precipitate the product. The mixture was filtered on a glass frit, washed with cold water (20 mL) and cold diethyl ether (15 mL), and dried under vacuum to afford the product as a white powder (9.2 g, 99%). Spectral data was consistent with that previously reported.[6] ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.37 (s, 1H), 7.70–7.66 (m, 2H), 7.65–7.63 (m, 2H), 7.61 (d, 1H, J = 15.7 Hz), 7.48–7.40 (m, 3H), 6.81 (d, 1H, J = 15.7 Hz). ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.7, 140.6, 138.6, 134.6, 131.6, 129.9, 129.1, 127.8, 121.9, 121.1, 115.0. GC–MS, m/z: calculated for $C_{15}H_{12}BrNO^{\bullet}$ $[M^{\bullet}]^{+}$ 303.0, found 302.9.

6-bromoquinolin-2(1H)-one (7)

The procedure was adapted from the literature.[5] A 500-mL round-bottom flask was charged with amide **6** (9.2 g, 30 mmol), chlorobenzene (150 mL), and aluminum chloride (24.3 g, 182 mmol). The flask was fitted with a reflux condenser, and the solution was heated at reflux, quickly turning yellow to black. After 2 h, the mixture was concentrated by rotary evaporation to ~65 mL, then poured onto ice (900 mL). The reaction flask was rinsed with water, and the resulting aqueous suspension was filtered on a glass frit. The solid was

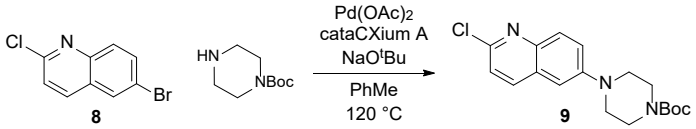
dried under vacuum to afford the product as a light orange solid (3.75 g, 55%). Spectral data were consistent with that previously reported.[7] ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.87 (br s, 1H), 7.91 (d, 1H, *J* = 2.3 Hz), 7.87 (d, 1H, *J* = 9.6 Hz), 7.63 (dd, 1H, *J* = 8.7, 2.3 Hz), 7.24 (d, 1H, *J* = 8.8 Hz), 6.55 (d, 1H, *J* = 9.6 Hz). ^{13}C NMR (125 MHz, DMSO-d_6) δ 161.7, 139.2, 138.0, 132.9, 129.9, 123.2, 120.9, 117.3, 113.4, 39.5. GC–MS, m/z: calculated for $C_9H_6BrNO^{\bullet}$ $[M^{\bullet}]^+$ 223.0, found 222.9.

6-bromo-2-chloroquinoline (8)



The procedure was adapted from the literature.[5] To a 500-mL round-bottom flask charged with phosphoryl chloride (20.5 g), lactam **7** (1.50 g, 6.69 mmol) was slowly added. The mixture was refluxed for 75 min, then cooled to rt and quenched by slowly pouring the solution onto ice. The flask was rinsed with cold water, and the precipitate was collected on a glass frit and washed with cold water. The solid was dried under vacuum to afford the product as an orange solid (1.62 g, 100%). Spectral data were consistent with that previously reported.[8] ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (ddd, 1H, J = 8.6, 0.7, 0.4 Hz), 7.98 (d, 1H, J = 2.2 Hz), 7.89 (dt, 1H, J = 9, 0.6 Hz), 7.80 (dd, 1H, J = 9, 2.2 Hz), 7.41 (d, 1H, J = 8.6 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 146.4, 137.7, 134.0, 130.3, 129.63, 127.9, 123.3, 120.9. GC–MS, m/z: calculated for $C_9H_5BrClN^{\bullet}$ $[M^{\bullet}]^+$ 242.9, found 243.0.

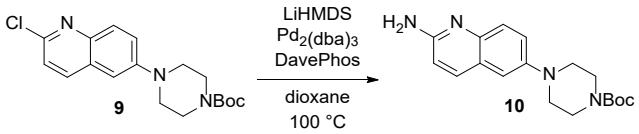
tert-butyl 4-(2-chloroquinolin-6-yl)piperazine-1-carboxylate (9)



The procedure was adapted from the literature.[5] To a 4-mL vial, charged with bromide **8** (200 mg, 825 μmol), *N*-Boc-piperazine (154 mg, 825 μmol), $Pd(OAc)_2$ (3.6 mg, 16 μmol), and cataCXium® A (11.8 mg, 33 μmol) and equipped with a magnetic stir bar under nitrogen, was added sodium *tert*-butoxide (95 mg, 990 μmol) and toluene (1 mL). The vial was sealed and stirred at 120 °C in an aluminum heating block for 24 h. Upon cooling, the mixture was extracted with ethyl acetate, the combined organic phases were washed with brine, dried over sodium sulfate, filtered, and concentrated by rotary evaporation. Purification on silica gel column (Et_2O/hexanes, 20→50% v/v)afforded the product as a yellow-orange solid (126 mg, 44% yield). Spectral data were consistent with that previously reported.[5] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, 1H, *J* = 8.6 Hz), 7.89 (d, 1H, *J* = 9.3 Hz), 7.48 (dd, 1H, *J* = 9.3, 2.7 Hz), 7.29 (d, 1H, *J* = 8.6 Hz), 7.01 (d, 1H, *J* = 2.7 Hz), 3.66–3.61 (m, 4H), 3.28–3.24 (m, 4H), 1.50 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.6,

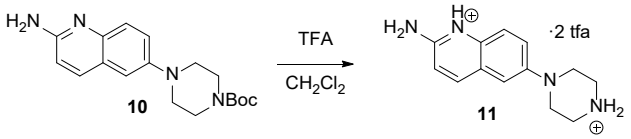
149.5, 147.8, 143.3, 137.5, 129.3, 127.9, 123.4, 122.5, 109.4, 80.1, 49.1, 28.4. GC–MS, m/z: calculated for $C_{18}H_{22}ClN_3O_2^{\bullet}$ $[M^{\bullet}]^+$ 347.1, found 347.2.

tert-butyl 4-(2-aminoquinolin-6-yl)piperazine-1-carboxylate (10)



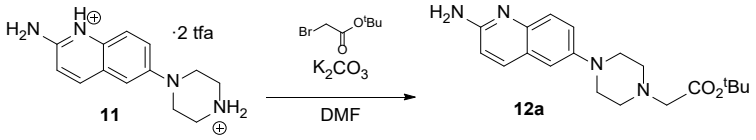
The procedure was adapted from the literature.[5] To a 4-mL vial, charged with chloride **9** (45 mg, 129 μmol), $Pd_2(dba)_3$ (1.8 mg, 1.9 μmol), and DavePhos (1.5 mg, 3.9 μmol) and equipped with a magnetic stir bar under nitrogen, was added anhydrous dioxane (1.5 mL). The vial was sealed, and lithium bis(trimethylsilyl)amide (1.0 M in tetrahydrofuran, 170 μL) was added via syringe. The vial was stirred at 100 °C in an aluminum heating block for 20 h. Upon cooling, the mixture was quenched with 5 drops of 2.0 M hydrochloric acid, stirred for 10 minutes, then adjusted to pH 12 with 1.0 M potassium hydroxide. The mixture was then extracted with methylene chloride, washed with brine, dried over sodium sulfate, filtered, and concentrated by rotary evaporation. Purification on silica gel column (methanol/methylene chloride/triethylamine, 5:94:1→15:84:1 v/v) afforded the product as a yellow-orange solid (32 mg, 73% yield). Spectral data were consistent with that previously reported.[5] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, 1H, J = 8.7 Hz), 7.60 (d, 1H, J = 9.1 Hz), 7.35 (dd, 1H, J = 9.2, 2.8 Hz), 6.98 (d, 1H, J = 2.7 Hz), 6.70 (d, 1H, J = 8.8 Hz), 4.78 (br s, 2H), 3.65–3.60 (m, 4H), 3.18–3.13 (m, 4H), 1.49 (s, 9H). GC–MS, m/z: calculated for $C_{18}H_{24}N_4O_2^{\bullet}$ $[M^{\bullet}]^+$ 328.2, found 328.2.

6-(piperazin-1-yl)quinolin-2-amine (11)



A scintillation vial was charged with Boc-amine 1**0** (260 mg, 792 μmol), trifluoroacetic acid (4.0 mL), and methylene chloride (4.0 mL) and equipped with a magnetic stir bar. After 4 h, starting material was consumed, and the mixture was concentrated by rotary evaporation, resuspended in toluene, and concentrated once more to obtain the pure bis(trifluoroacetate) salt as a dark yellow solid (350 mg, 97%). ^{1}H NMR (500 MHz, CD_3OD) δ 8.26 (d, 1H, *J* = 9.4 Hz), 7.62–7.61 (m, 2H), 7.39 (t, 1H, *J* = 1.3 Hz), 7.03 (d, 1H, *J* = 9.4 Hz), 3.53–3.50 (m, 4H), 3.44–3.41 (m, 4H). ^{13}C NMR (150 MHz, CD_3OD) δ 149.3, 144.5, 132.1, 125.6, 123.7, 119.3, 114.7, 114.4, 47.7, 44.7. GC–MS, m/z: calculated for $C_{13}H_{16}N_4^{\bullet}$ $[M^{\bullet}]^+$ 228.1, found 228.1.

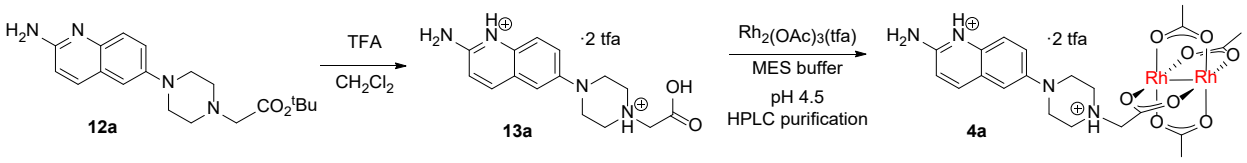
tert-butyl 2-(4-(2-aminoquinolin-6-yl)piperazin-1-yl)acetate (12a)



To a 4-mL vial was added the bis-TFA salt **11** (105 mg, 230 µmol), *tert*-butyl bromoacetate (37 µL, 253 µmol), potassium carbonate (163 mg, 1.15 mmol), and dry *N*,*N*-dimethylformamide (1.0 mL). The vial was equipped with a magnetic stir bar and stirred at 40 °C for 16 h. The mixture was extracted with ethyl acetate, dried over sodium sulfate, filtered, and concentrated by rotary evaporation. Purification on silica gel column (ethyl acetate/hexanes/triethylamine, 80:19:1→99:0:1 v/v) afforded the product as a light orange solid (71 mg, 90% yield). ^{1}H NMR (600 MHz, CD_3OD) δ 7.83 (d, 1H, J = 8.9 Hz), 7.45 (d, 1H, J = 9.2 Hz), 7.36 (dd, 1H, J = 9.2, 2.7 Hz), 7.07 (d, 1H, J = 2.6 Hz), 6.77 (d, 1H, J = 8.9 Hz), 3.25–3.22 (m, 4H), 3.20 (s, 2H), 2.78–2.76 (m, 4H), 1.49 (s, 9H). ^{13}C NMR (150 MHz, CD_3OD) δ 171.0, 158.3, 148.0, 143.5, 138.8, 126.2, 125.1, 124.0, 113.6, 112.8, 82.5, 60.7, 54.0, 50.9, 28.4. GC–MS, m/z: calculated for $C_{19}H_{26}N_4O_2^{\bullet}$ $[M^{\bullet}]^+$ 342.2, found 342.2.

dirhodium ligation of 2-(4-(2-aminoquinolin-6-yl)piperazin-1-yl)acetic acid (4a)

Two steps:



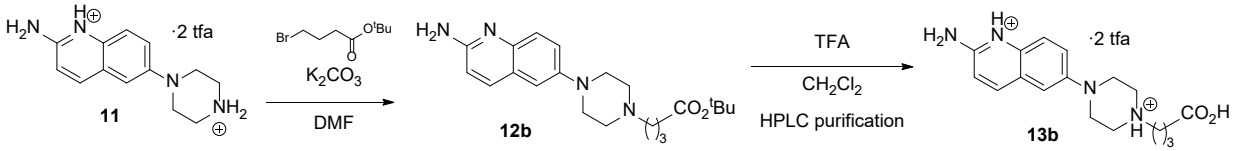
A 4-mL vial was charged with ester **12a** (8 mg, 23 µmol), trifluoroacetic acid (1 mL), and dry methylene chloride (1 mL) and equipped with a magnetic stir bar. After 3 h stirring at rt, the starting material was consumed, and the mixture was concentrated by rotary evaporation, resuspended in toluene, and concentrated once more to obtain the bis(trifluoroacetate) intermediate **13a** as a yellow solid (12 mg, 99% yield). ^{1}H NMR (400 MHz, CD_3OD) δ 8.25 (d, 1H, J = 9.4 Hz), 7.62 (s, 1H), 7.61 (s, 1H), 7.39 (s, 1H), 7.03 (d, 1H, J = 9.3 Hz), 4.17 (s, 2H), 3.61 (br s, 8H). ESI–MS, m/z: calculated for $C_{15}H_{19}N_4O_2$ $[M+H]^+$ 287.2, found 287.0.

A 4-mL vial was charged with acid **13a** as the bis(trifluoroacetate) salt (2.0 mg, 3.9 µmol), $Rh_2(OAc)_3(tfa)$ (4.2 mg, 8.7 µmol), and MES buffer (1.4 mL, 25 mg/mL, pH = 4.5) and equipped with a magnetic stir bar. The vial was stirred at rt, and the reaction was monitored by analytical HPLC. After 24 h, the mixture was purified by preparative HPLC. Fractions were combined, concentrated by rotary evaporation, and dried by

lyophilization to afford the product as the bis(trifluoroacetate) salt as a light green solid (3.0 mg, 86%). ESI–MS, m/z: calculated for $C_{21}H_{27}N_4O_8Rh_2$ $[M+H]^+$ 669.0, found 668.8.

4-(4-(2-aminoquinolin-6-yl)piperazin-1-yl)butanoic acid (13b)

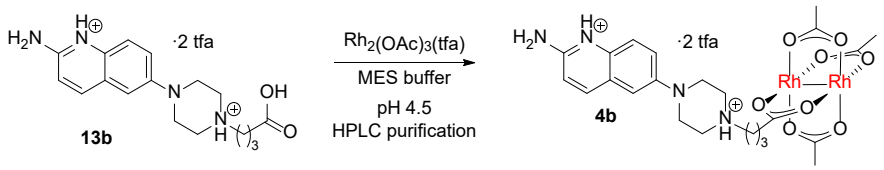
Two steps:



To a 4-mL vial was added the bis-TFA salt **11** (81 mg, 178 µmol), *tert*-butyl 4-bromobutyrate (50 mg, 213 µmol), potassium carbonate (120 mg, 888 mmol), and dry *N*,*N*-dimethylformamide (1.0 mL) and equipped with a magnetic stir bar. The vial was stirred at 40 °C for 16 h. The mixture was extracted with ethyl acetate, dried over sodium sulfate, filtered, and concentrated by rotary evaporation. Purification on silica gel column (methanol/methylene chloride/triethylamine, 0:99:1→10:89:1 v/v) afforded the ester intermediate **12b** as a light orange solid (52 mg, 78%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.85 (d, 1H, J = 8.9 Hz), 7.45 (d, 1H, J = 9.2 Hz), 7.37 (dd, 1H, J = 9.2, 2.7 Hz), 7.08 (d, 1H, J = 2.7 Hz), 6.77 (d, 1H, J = 8.9 Hz), 3.24–3.21 (m, 4H), 2.70–2.66 (m, 4H), 2.47–2.42 (m, 2H), 2.30 (t, 2H, J = 7.3 Hz), 1.86–1.79 (m, 2H), 1.46 (s, 9H). ^{13}C NMR (125 MHz, CD_3OD) δ 174.5, 158.3, 148.0, 143.3, 138.9, 126.1, 125.1, 123.9, 113.6, 112.8, 81.5, 58.8, 54.3, 51.0, 34.2, 28.4, 23.0.

A 4-mL vial was charged with ester **12b** (24 mg, 60 µmol), trifluoroacetic acid (0.5 mL), and dry methylene chloride (0.5 mL) and equipped with a magnetic stir bar. After stirring at rt for 4.5 h, the starting material was consumed, and the mixture was concentrated by rotary evaporation. Purification was performed by preparative HPLC. Fractions were combined, concentrated by rotary evaporation, and dried by lyophilization to obtain the pure bis(trifluoroacetate) salt as a yellow solid (12 mg, 38%). ^{1}H NMR (600 MHz, CD_3OD) δ 8.25 (d, 1H, J = 9.4 Hz), 7.63–7.61 (m, 2H), 7.38 (d, 1H, J = 2.0 Hz), 7.03 (d, 1H, J = 9.4 Hz), 3.53 (br s, 1H), 3.30–3.27 (m, 2H), 2.50 (t, 2H, J = 6.9 Hz), 2.11–2.05 (m, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 175.8, 155.2, 148.8, 144.5, 132.1, 125.5, 123.7, 119.4, 114.8, 114.4, 57.4, 53.0, 47.9, 31.4, 20.4. ESI–MS, m/z: calculated for $C_{17}H_{23}N_4O_2$ $[M+H]^+$ 315.2, found 315.1.

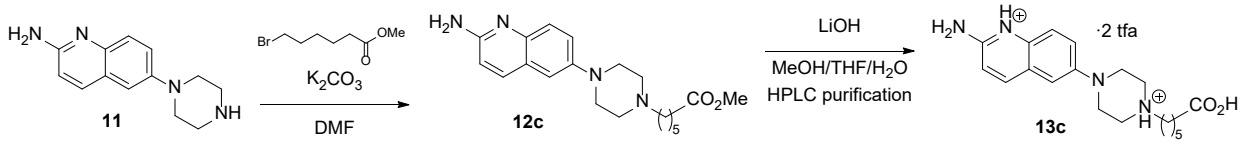
dirhodium ligation of 4-(4-(2-aminoquinolin-6-yl)piperazin-1-yl)butanoic acid (4b)



A 4-mL vial was charged with acid **13b** as the bis(trifluoroacetate) salt (3.3 mg, 6.1 μmol), $Rh_2(OAc)_3(tfa)$ (6.3 mg, 9.1 μmol), and MES buffer (1.2 mL, 25 mg/mL, pH = 4.5) and equipped with a magnetic stir bar. The vial was stirred at 40 °C and monitored by analytical HPLC. After 24 h, the mixture was purified by preparative HPLC. Fractions were combined, concentrated by rotary evaporation, and dried by lyophilization to afford the product as the bis(trifluoroacetate) salt as a light green solid (5.5 mg, 98%). ESI–MS, m/z: calculated for $C_{23}H_{31}N_4O_8Rh_2$ $[M+H]^+$ 697.0, found 696.8; calculated for $[M+2H]^{2+}$ 349.0, found 348.9; calculated for $[M+2H+MeOH]^{2+}$ 365.0, found 364.9.

6-(4-(2-aminoquinolin-6-yl)piperazin-1-yl)hexanoic acid (13c)

Two steps:

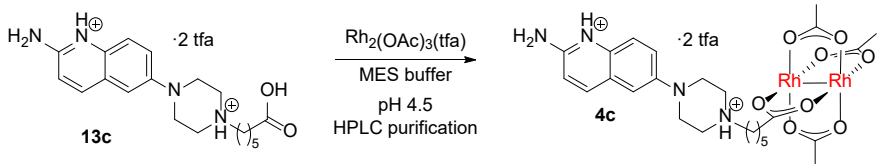


A 4-mL vial was charged with **11** as the free amine (55 mg, 240 μmol), methyl 6-bromohexanoate (64 mg, 290 μmol), potassium carbonate (167 mg, 1.21 mmol), and dry *N*,*N*-dimethylformamide (1.0 mL) and equipped with a magnetic stir bar. After 25 h stirring at rt, *N*,*N*-diisopropylethylamine (42 μL, 240 μmol) was added to speed the reaction. After an additional 19 h, 6-bromohexanoate (30 mg, 140 μmol) was added. After 3 h, the mixture was extracted with ethyl acetate, dried over sodium sulfate, filtered, and concentrated by rotary evaporation. Purification on silica gel column (methanol/ethyl acetate/hexanes/triethylamine, 0:80:19:1→0:99:0:1→2:97:0:1 v/v) afforded the ester intermediate **12c** as a light orange solid (42 mg, 30%). ^{1}H NMR (600 MHz, CD_3OD) δ 7.85 (d, 1H, *J* = 8.9 Hz), 7.46 (d, 1H, *J* = 9.2 Hz), 7.38 (dd, 1H, *J* = 9.2, 2.7 Hz), 7.08 (d, 1H, *J* = 2.7 Hz), 6.78 (d, 1H, *J* = 8.9 Hz), 3.66 (s, 3H), 3.25–3.22 (m, 4H), 2.71–2.67 (m, 4H), 2.47–2.43 (m, 2H), 2.36 (t, 2H, *J* = 7.4 Hz), 1.70–1.63 (m, 2H), 1.63–1.56 (m, 2H), 1.41–1.35 (m, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 175.9, 158.3, 148.0, 143.3, 138.9, 126.1, 125.1, 123.9, 113.6, 112.8, 59.5, 54.3, 52.0, 50.9, 34.7, 28.1, 27.2, 25.9.

A 4-mL vial was charged with ester **12c** (20 mg, 56 μmol), lithium hydroxide (5.2 mg, 224 μmol), methanol (1.7 mL), water (0.5 mL), and tetrahydrofuran (0.2 mL) and equipped with a magnetic stir bar. After stirring

at 40 °C for 20 h, the starting material was consumed, and the mixture was dried under a gentle stream of nitrogen, resuspended in methanol, and filtered. Purification was performed by preparative HPLC. Fractions were combined, concentrated by rotary evaporation, and dried by lyophilization to obtain the pure bis(trifluoroacetate) salt as a yellow solid (9.0 mg, 28%). ^{1}H NMR (600 MHz, CD_3OD) δ 8.26 (d, 1H, J = 9.4 Hz), 7.62 (d, 2H, J = 1.3 Hz), 7.39 (s, 1H), 7.04 (d, 1H, J = 9.4 Hz), 3.51 (br s, 8H), 3.26–3.21 (m, 2H), 2.36 (t, 2H, J = 7.3 Hz), 1.86–1.79 (m, 2H), 1.73–1.67 (m, 2H), 1.51–1.44 (m, 2H). ^{13}C NMR (150 MHz, CD_3OD) δ 177.2, 155.1, 148.8, 144.5, 132.1, 125.5, 123.7, 119.4, 114.8, 114.4, 57.8, 52.9, 47.8, 34.4, 27.0, 25.3, 24.8. ESI–MS, m/z: calculated for $C_{19}H_{27}N_4O_2$ $[M+H]^+$ 343.2, found 343.1.

dirhodium ligation of 6-(4-(2-aminoquinolin-6-yl)piperazin-1-yl)hexanoic acid (4c)



A 4-mL vial was charged with acid **13c** as the bis(trifluoroacetate) salt (3.2 mg, 5.6 μmol), $Rh_2(OAc)_3(tfa)$ (4.2 mg, 8.4 μmol), and MES buffer (1.2 mL, 25 mg/mL, pH = 4.5) and equipped with a magnetic stir bar. The vial was stirred at 40 °C, and the reaction was monitored by analytical HPLC. After 36 h, the mixture was purified by preparative HPLC. Fractions were combined, concentrated by rotary evaporation, and dried by lyophilization, to afford the product as the bis(trifluoroacetate) salt as a light green solid (5.1 mg, 95%). ESI–MS, m/z: calculated for $C_{25}H_{35}N_4O_8Rh_2$ $[M+H]^+$ 725.1, found 724.9; calculated for $[M+2H]^{2+}$ 363.0, found 362.9; calculated for $[M+2H+MeOH]^{2+}$ 379.0, found 378.9.

Compound characterization

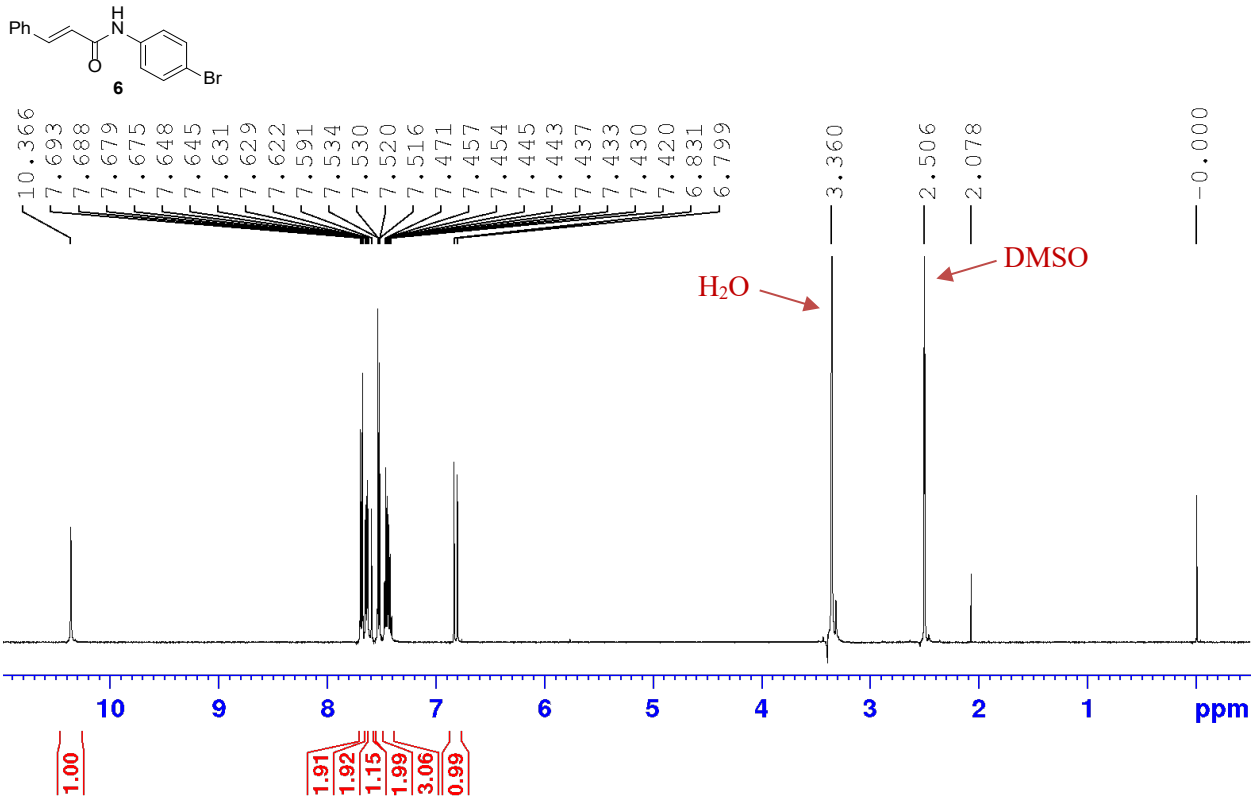


Figure 1. ^{1}H NMR spectrum of compound **6** in DMSO-d_6.

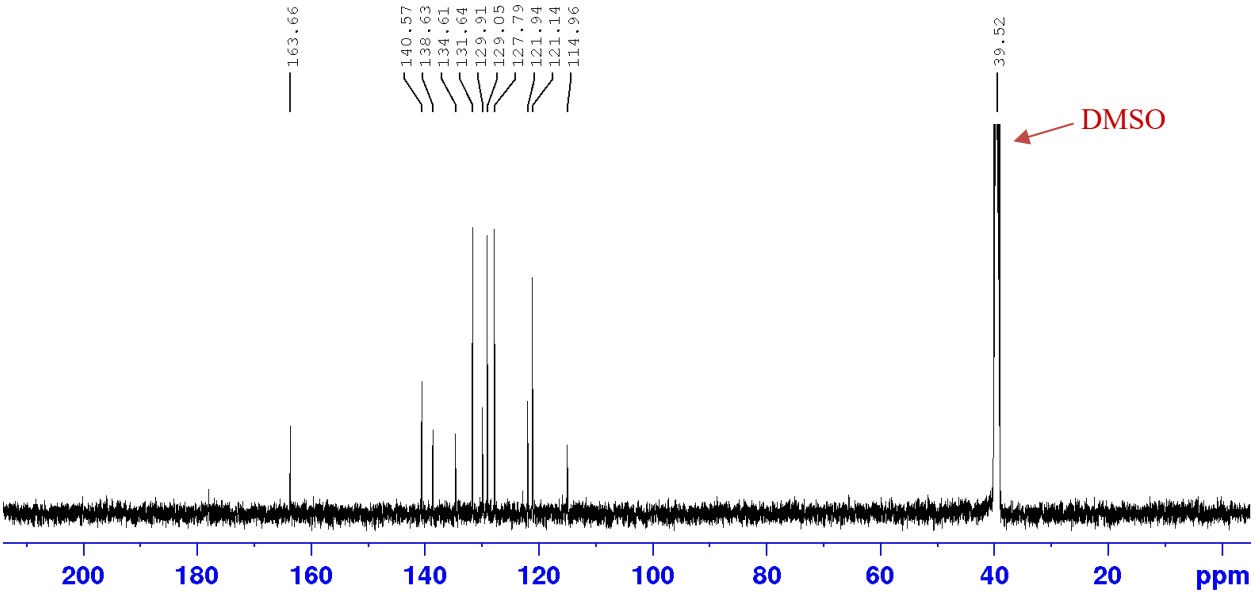


Figure 2. ^{13}C NMR spectrum of compound **6** in DMSO-d_6.

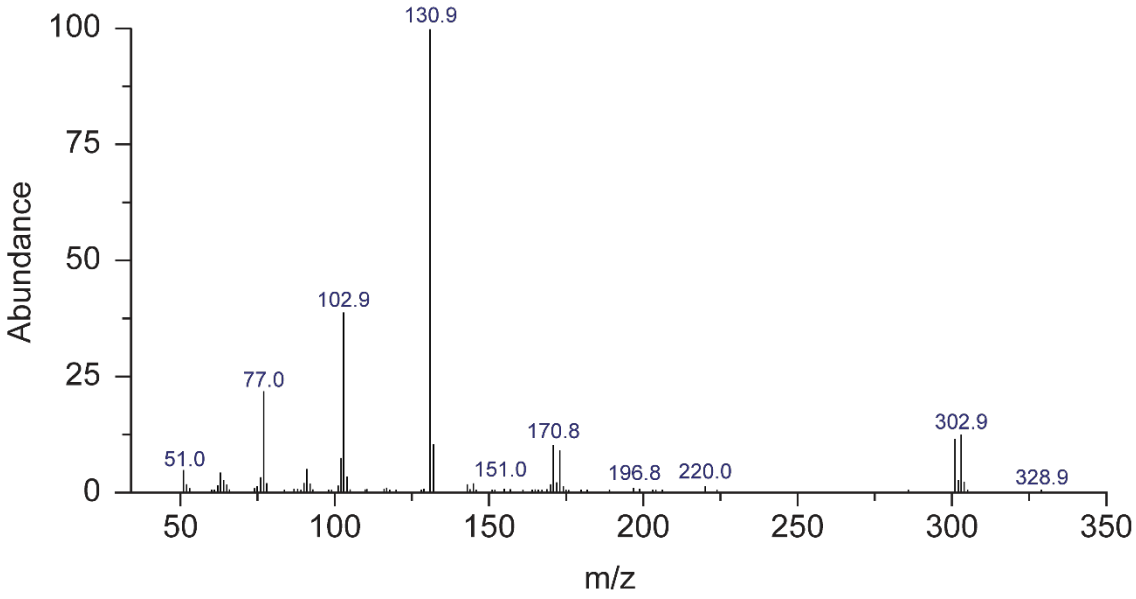


Figure 3. GC–MS spectrum of compound **6**.

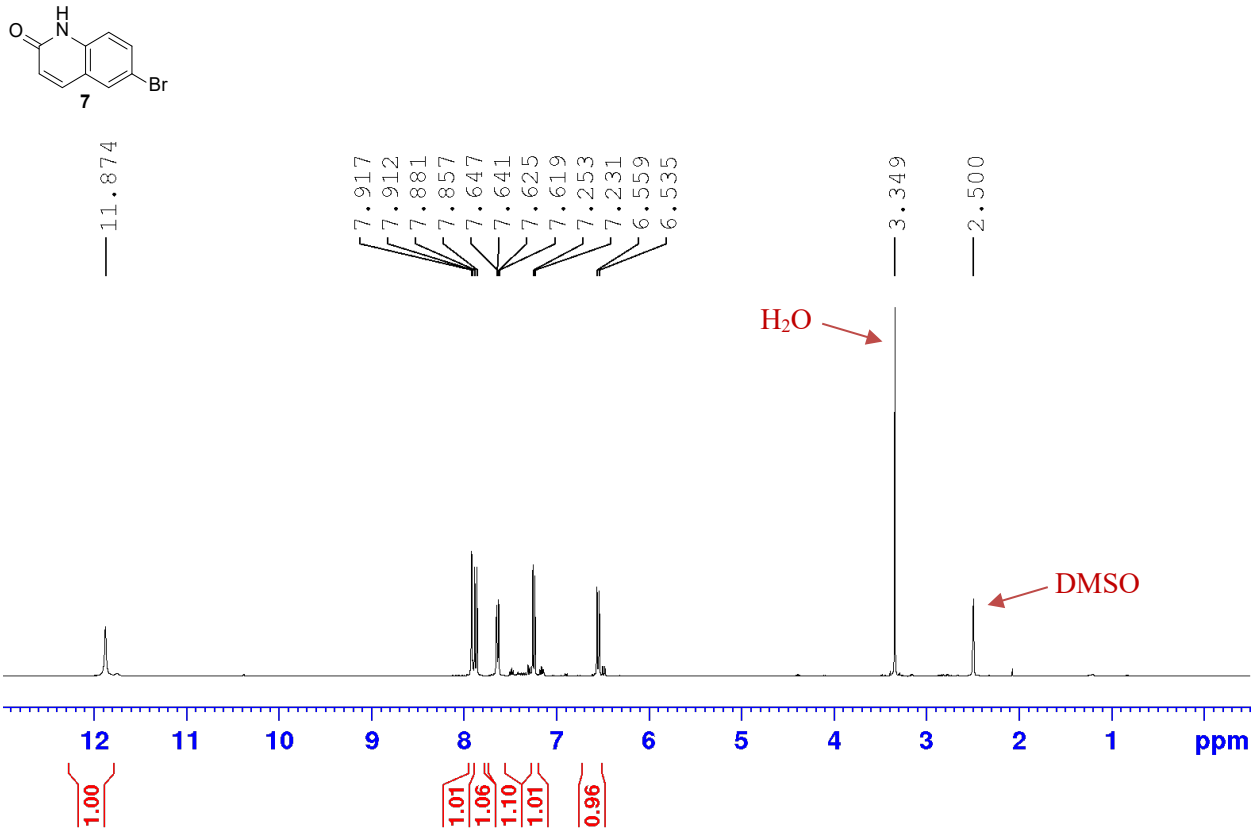


Figure 4. ^{1}H NMR spectrum of compound **7** in DMSO-d_6.

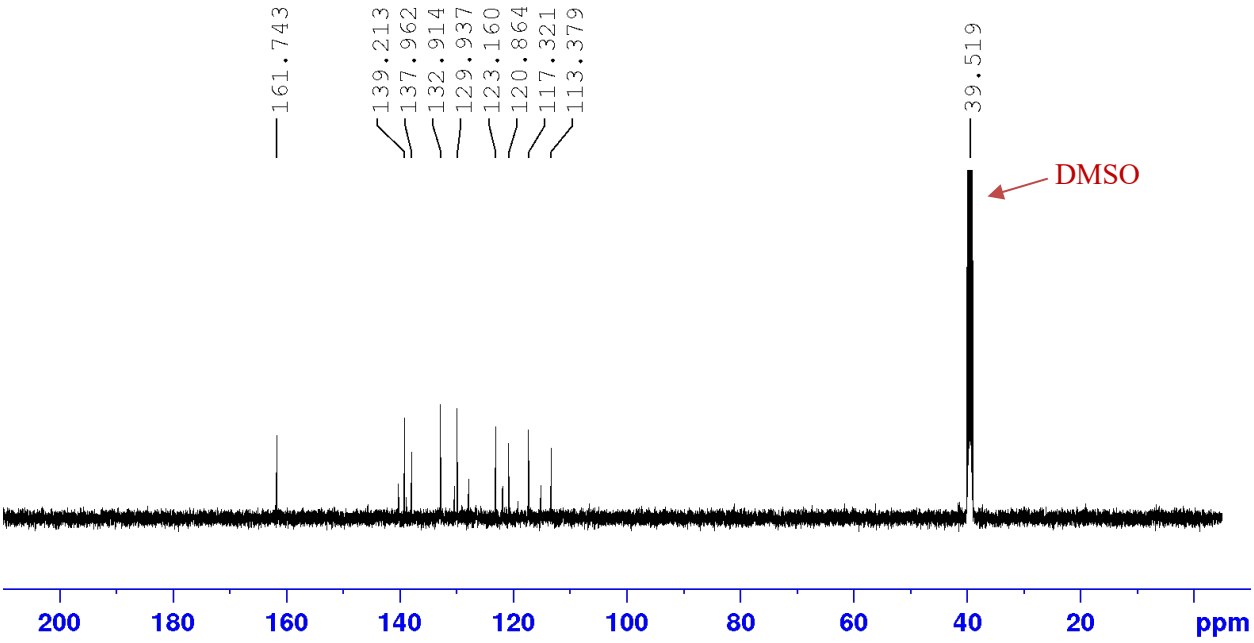


Figure 5. ^{13}C NMR spectrum of compound **7** in DMSO-d_6.

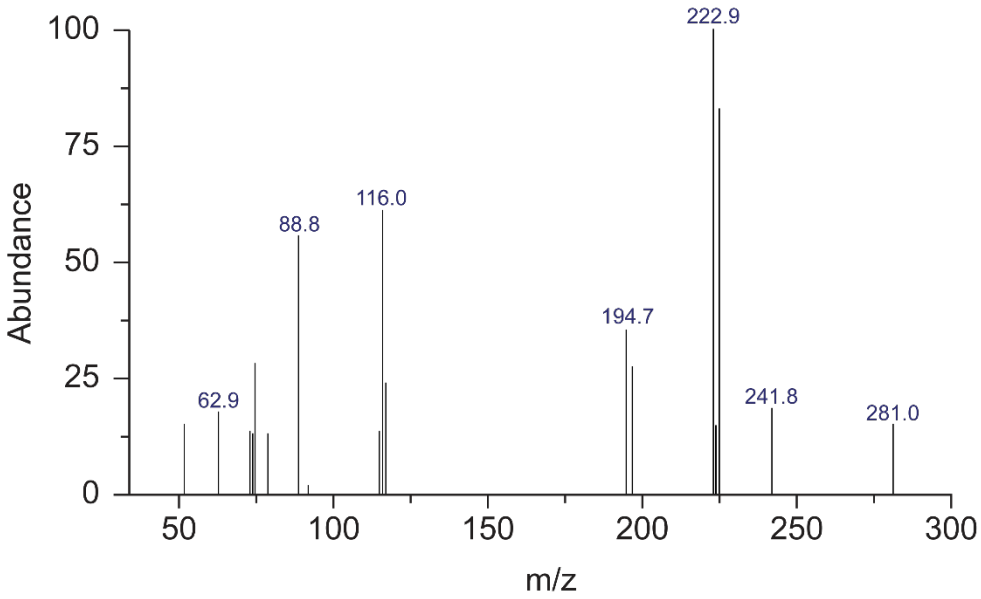


Figure 6. GC–MS spectrum of compound **7**.

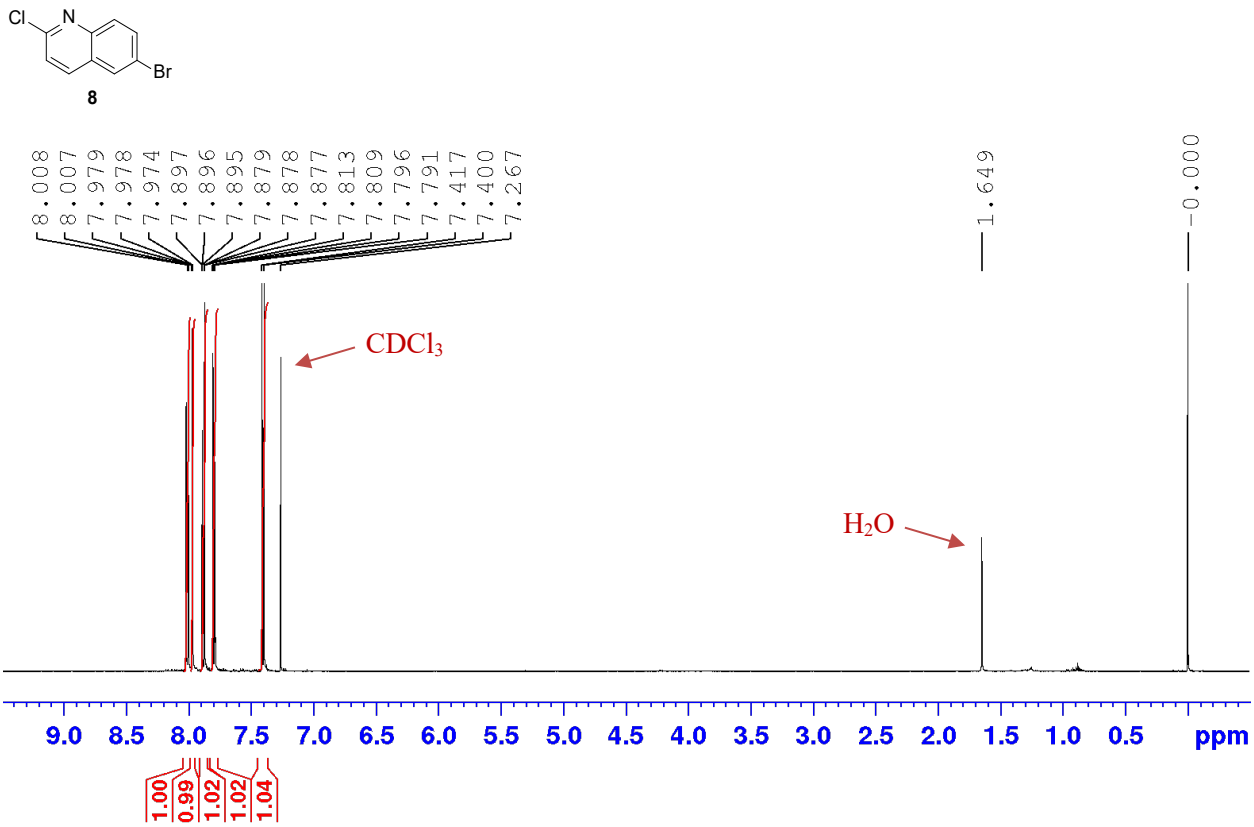


Figure 7. ^{1}H NMR spectrum of compound **8** in $CDCl_3$.

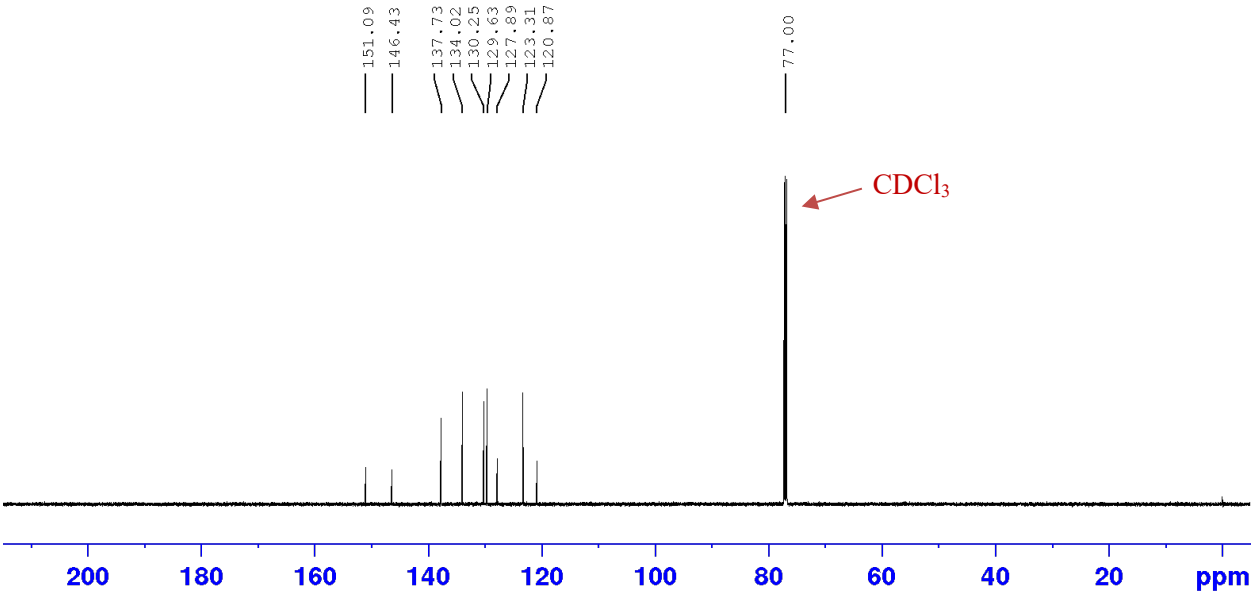


Figure 8. ^{13}C NMR spectrum of compound **8** in $CDCl_3$.

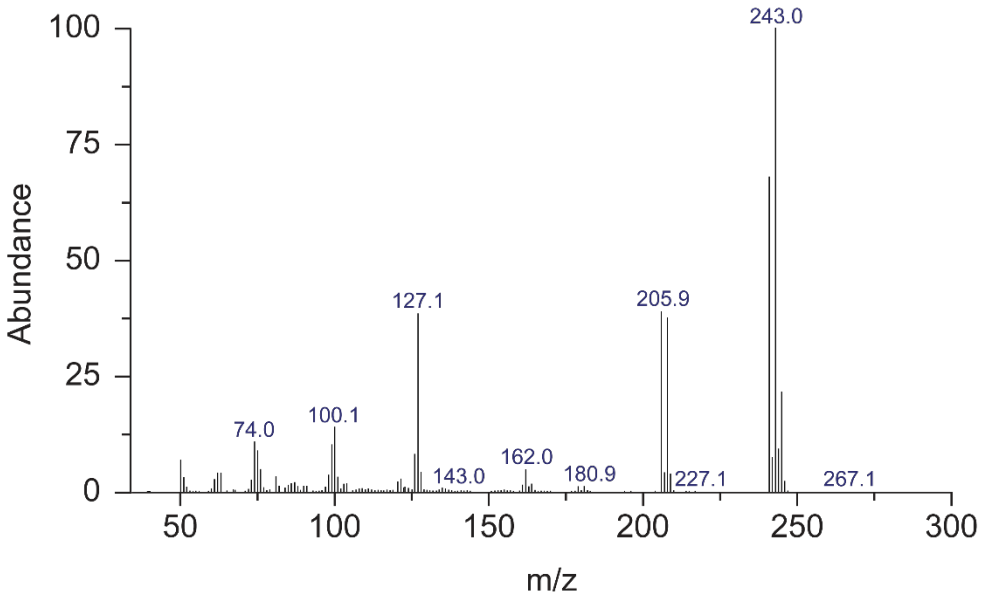


Figure 9. GC–MS spectrum of compound **8**.

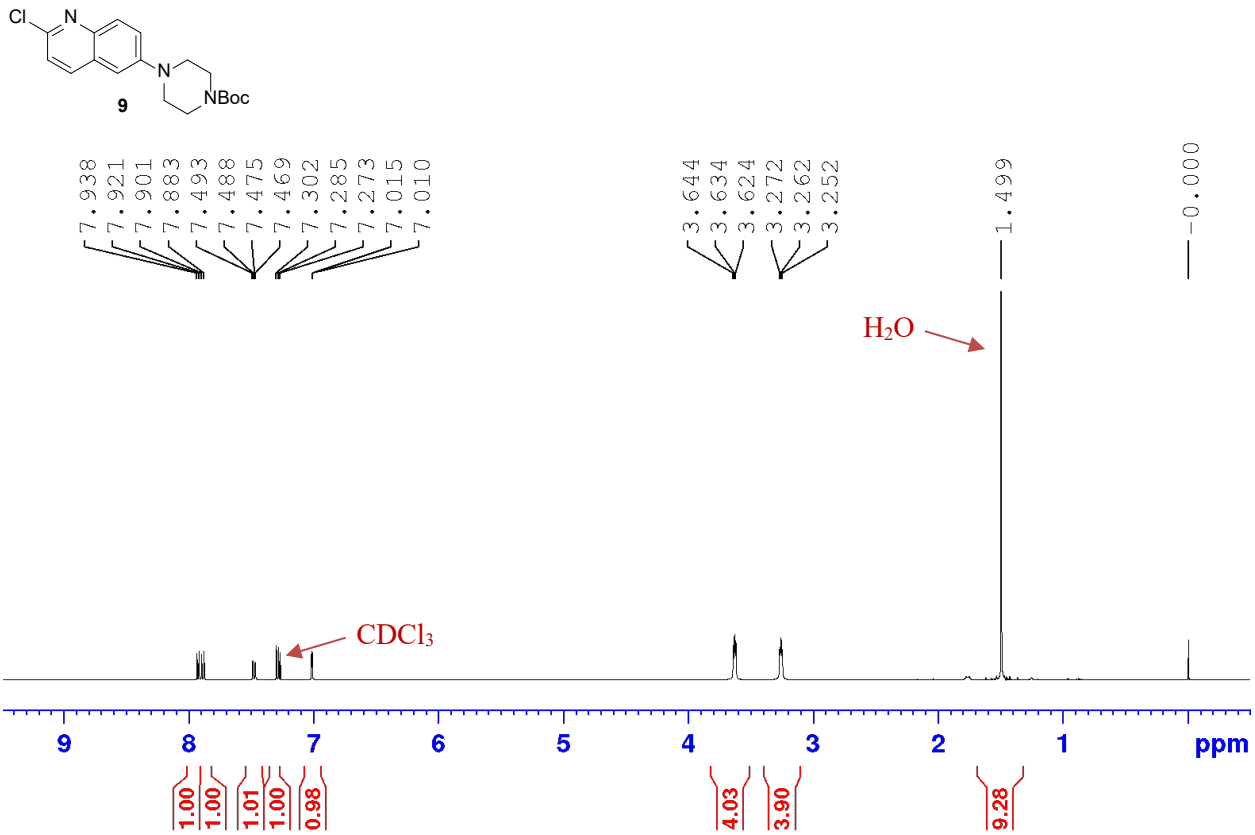


Figure 10. ^{1}H NMR spectrum of compound **9** in $CDCl_3$.

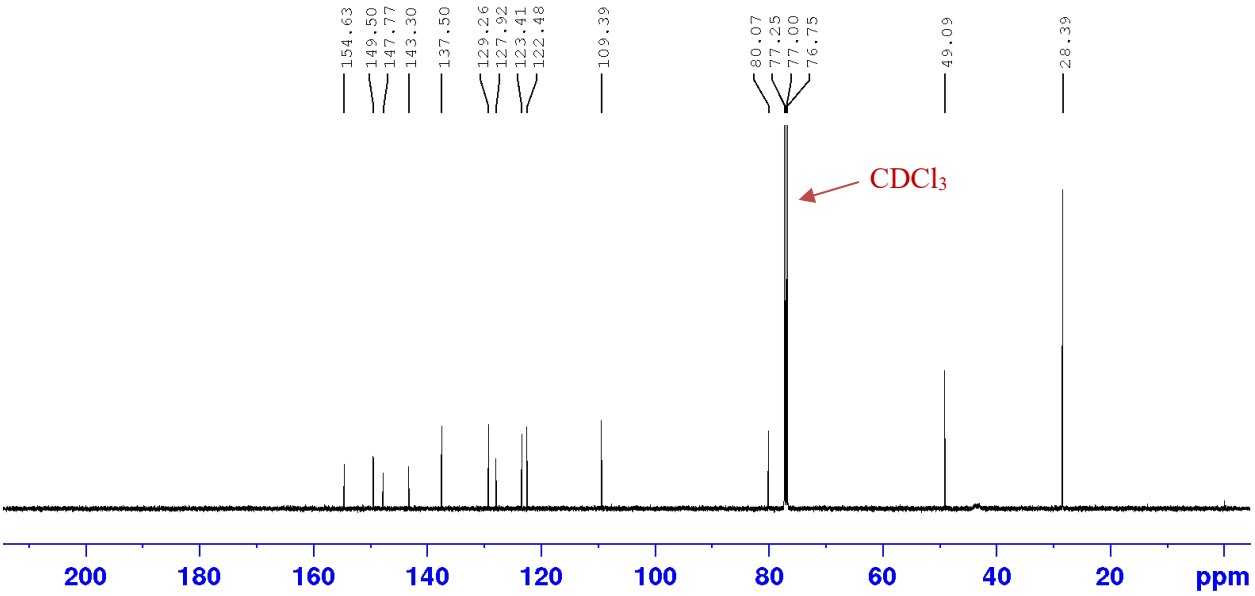


Figure 11. ^{13}C NMR spectrum of compound **9** in $CDCl_3$.

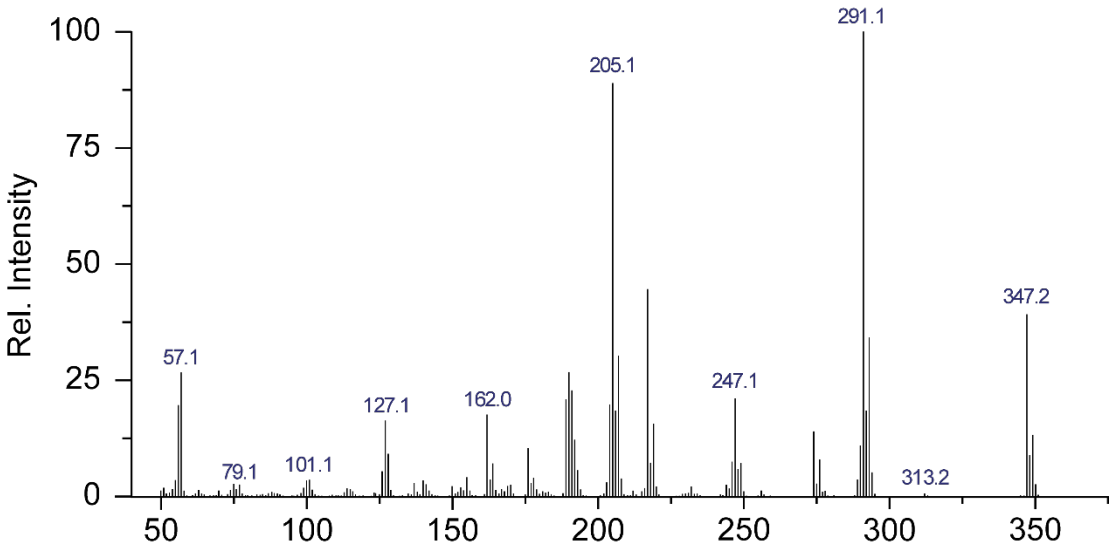


Figure 12. GC–MS spectrum of compound **9**.

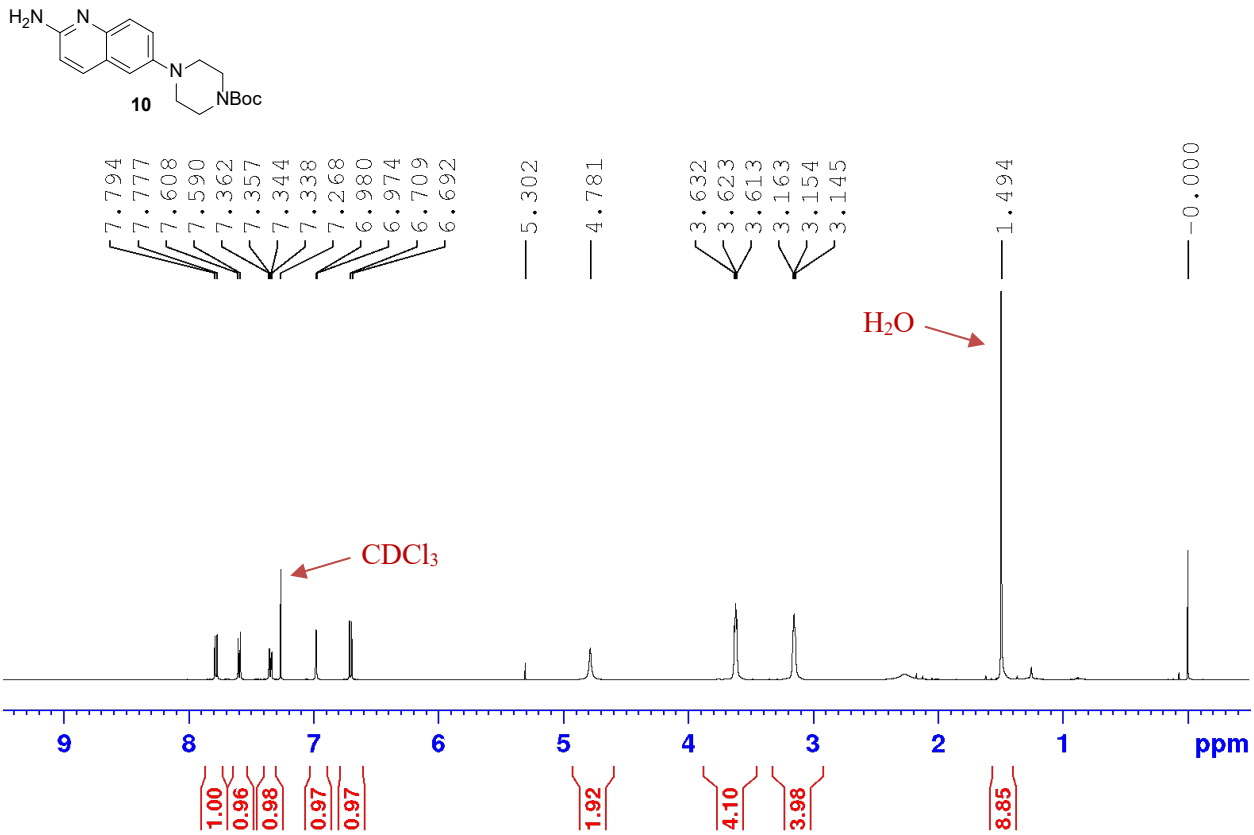


Figure 13. ^{1}H NMR spectrum of compound **10** in $CDCl_3$.

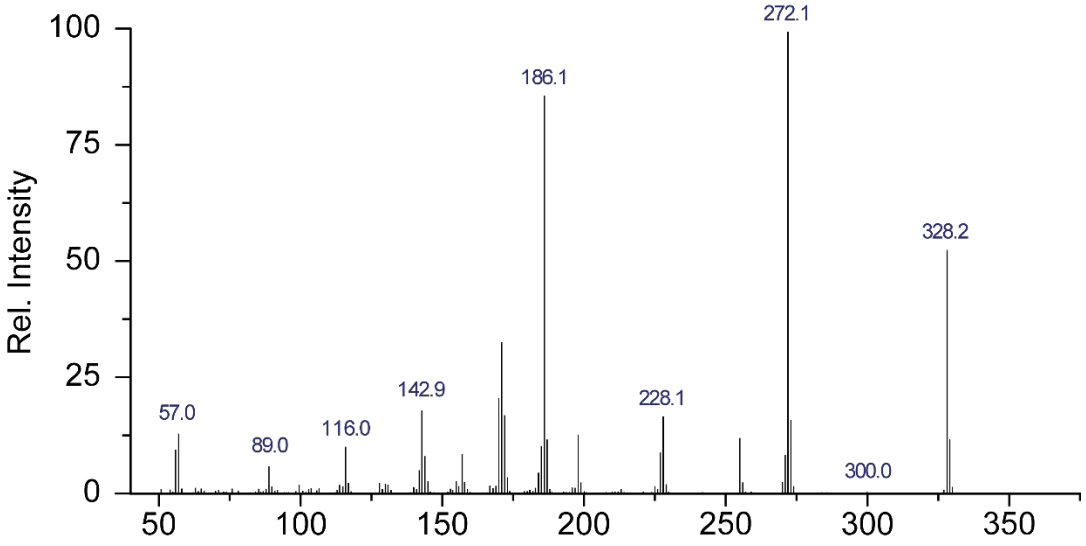


Figure 14. GC–MS spectrum of compound **10**.

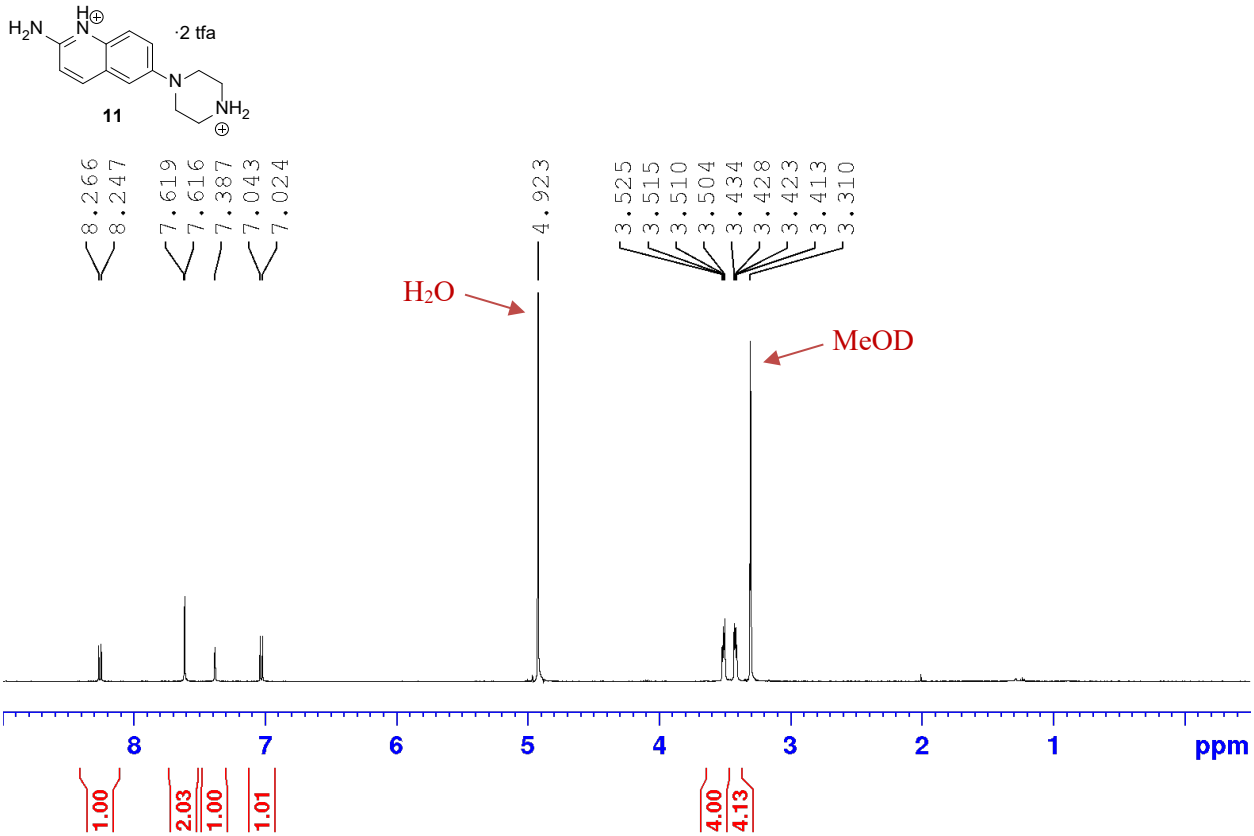


Figure 15. ^{1}H NMR spectrum of compound **11** in CD_3OD.

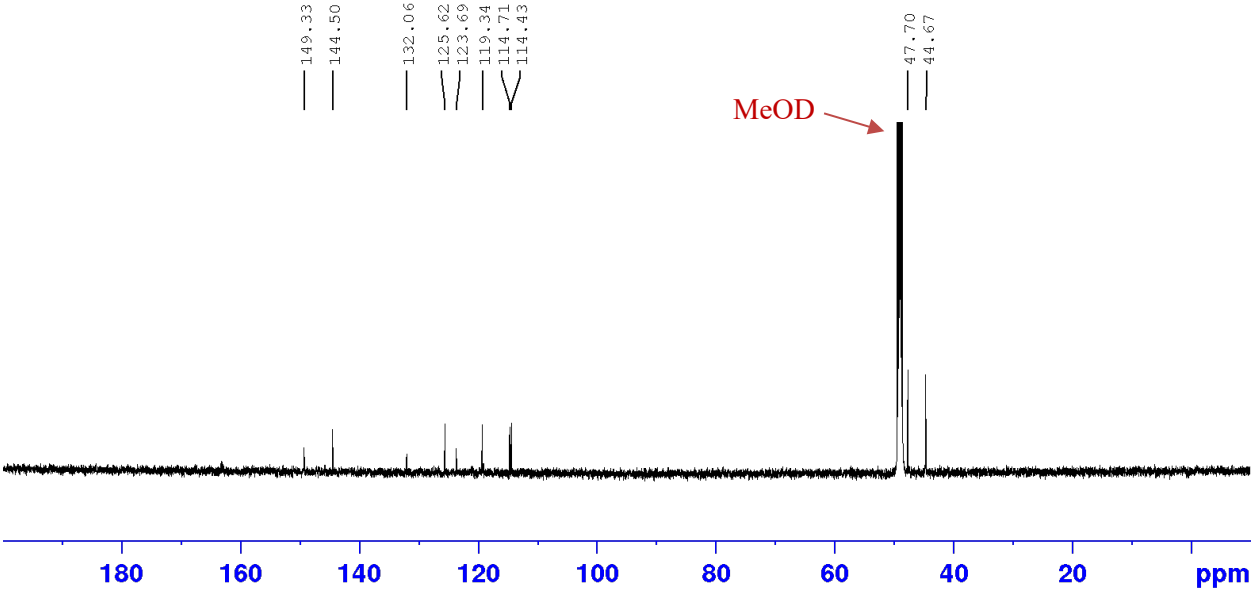


Figure 16. ^{13}C NMR spectrum of compound **11** in CD_3OD.

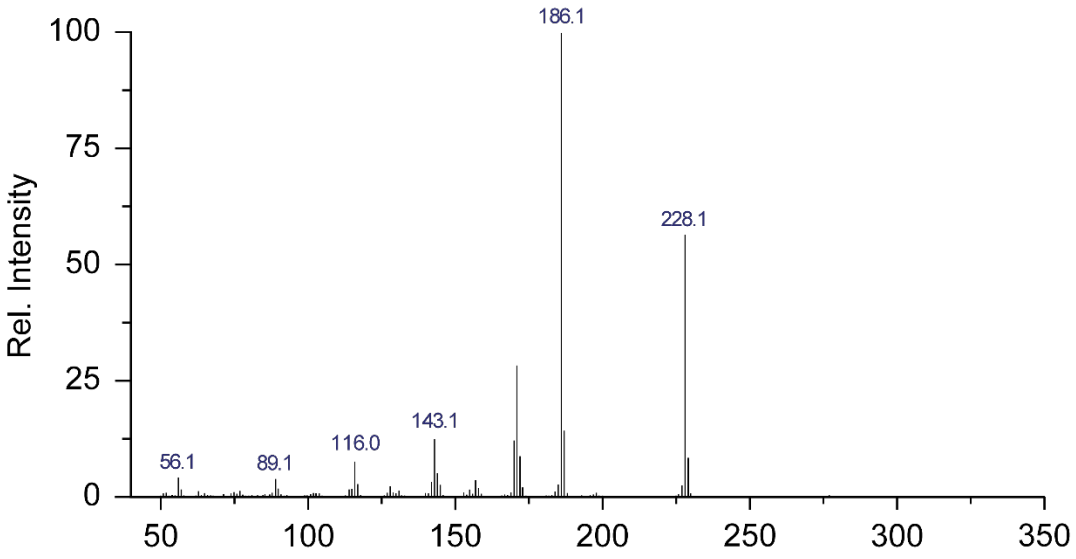


Figure 17. GC–MS spectrum of compound **11**.

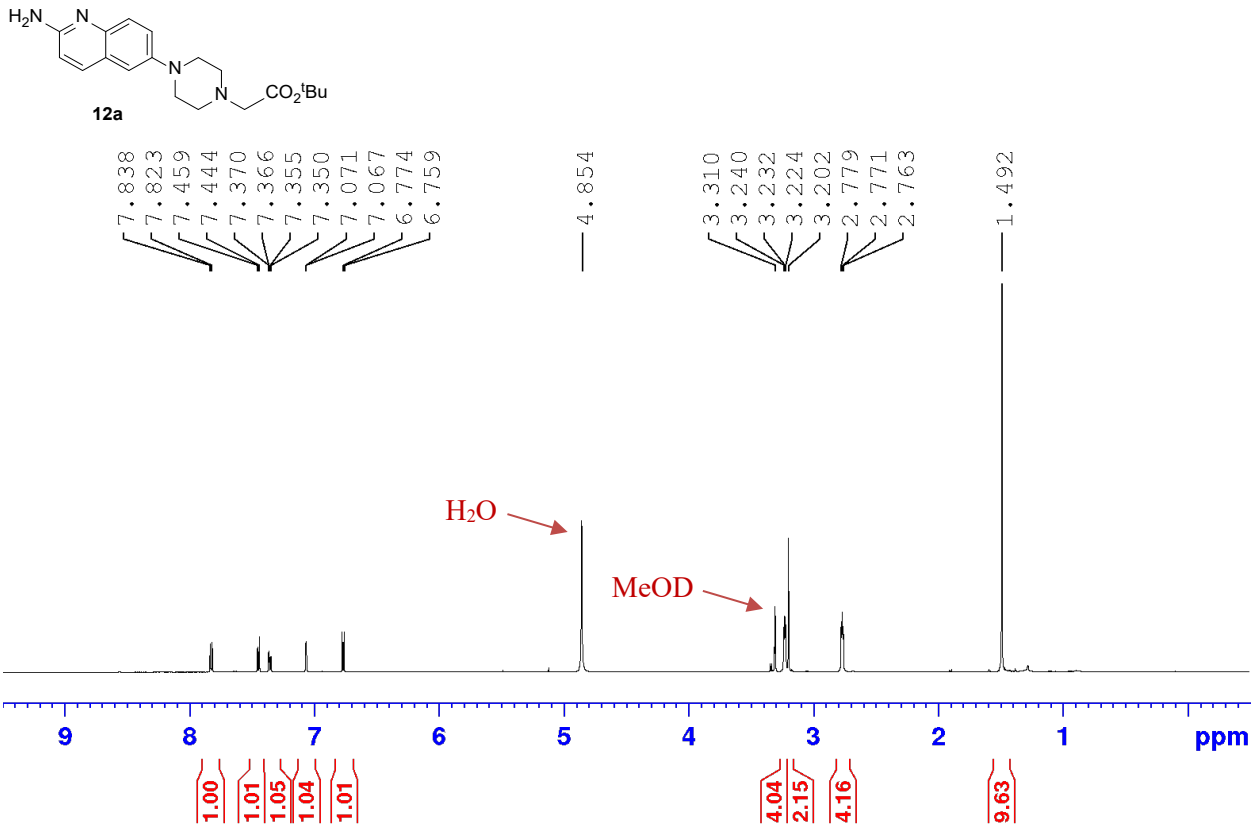


Figure 18. ^{1}H NMR spectrum of compound **12a** in CD_3OD.

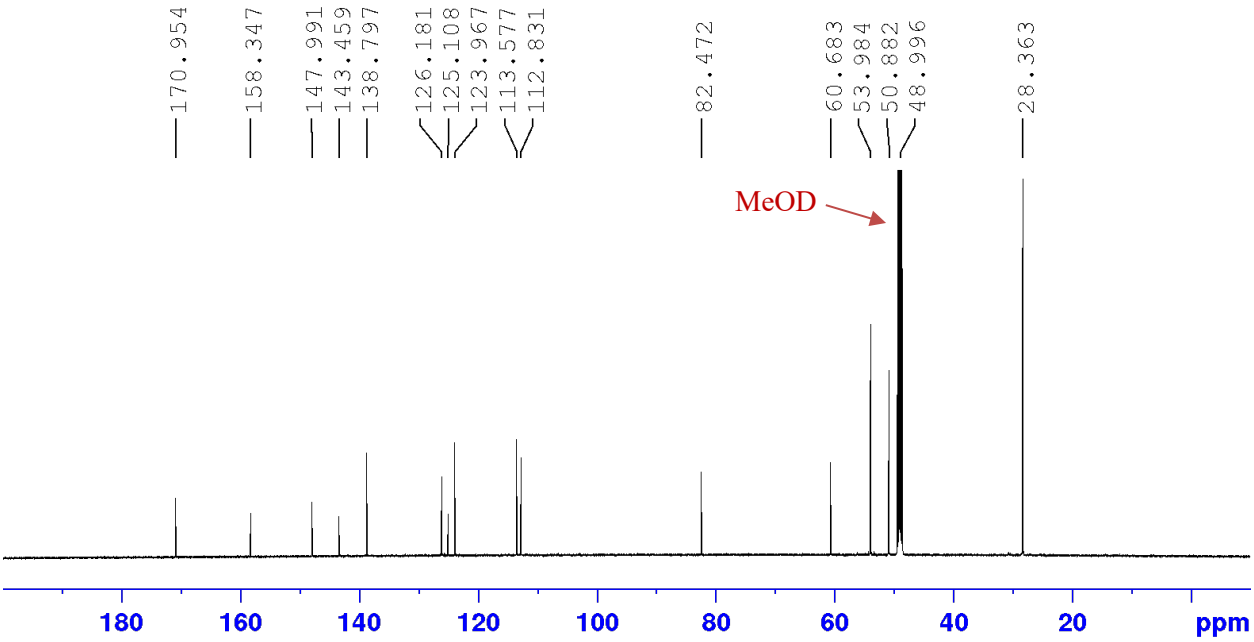


Figure 19. ^{13}C NMR spectrum of compound **12a** in CD_3OD.

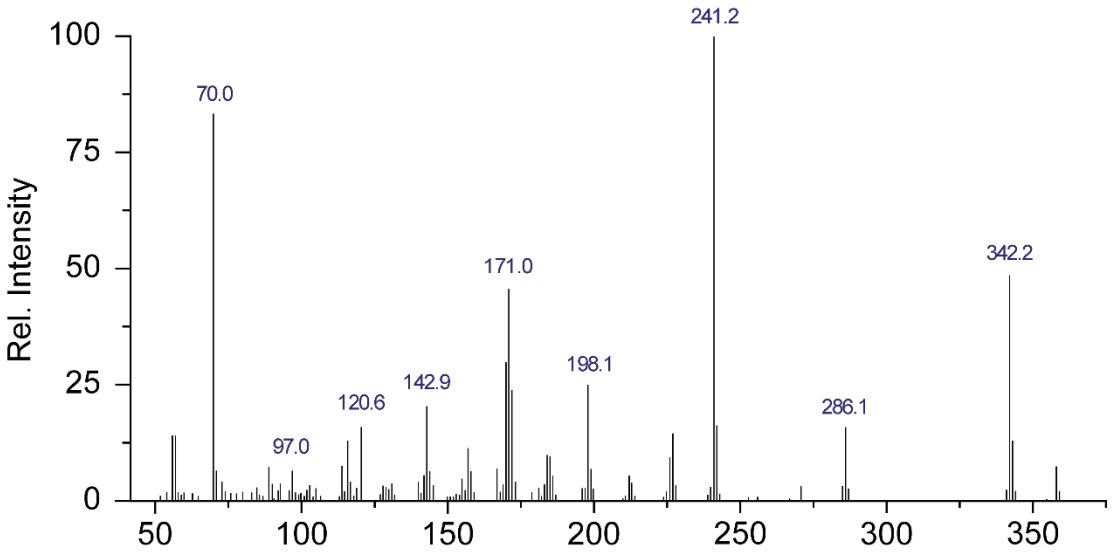


Figure 20. GC–MS spectrum of compound **12a**.

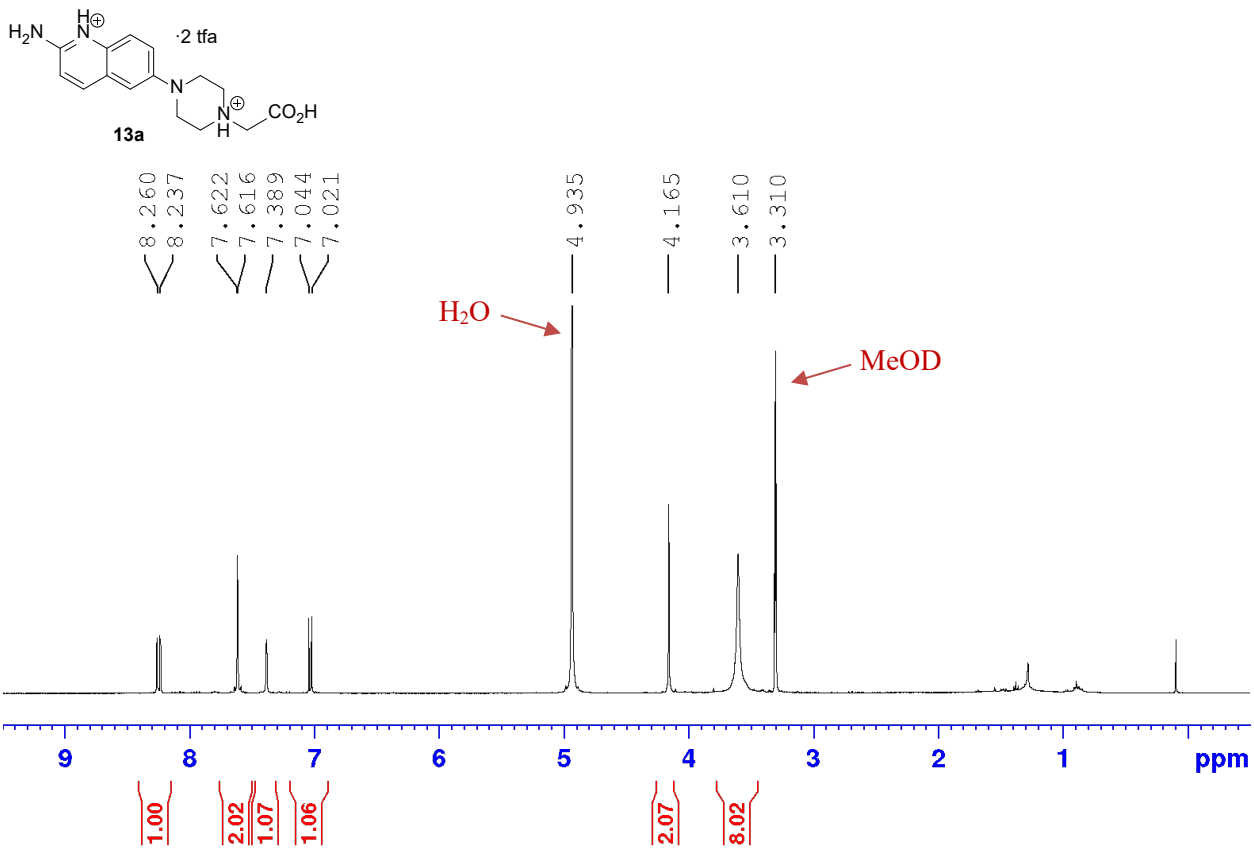


Figure 21. ^{1}H NMR spectrum of compound **13a** in CD_3OD.

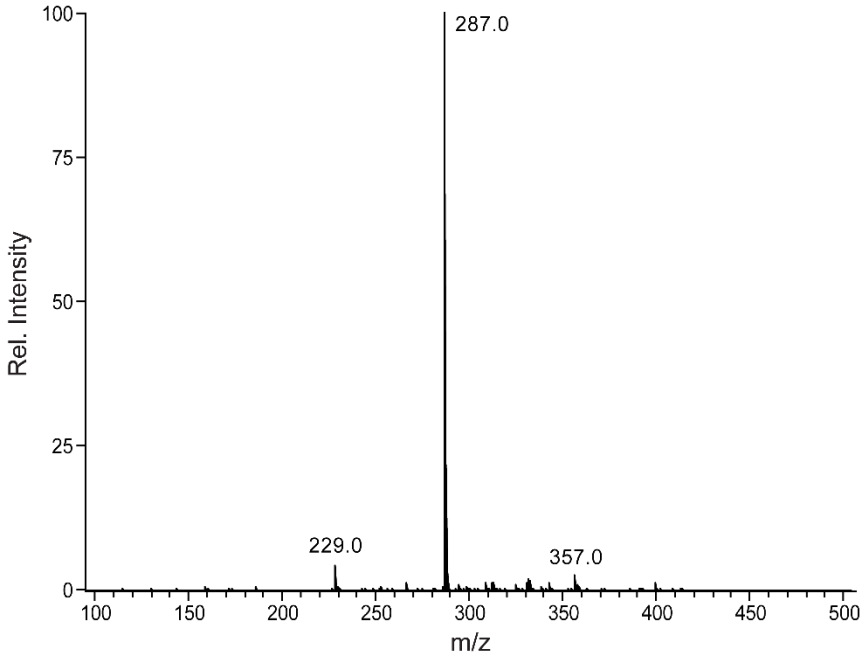


Figure 22. ESI–MS spectrum of compound **13a**.

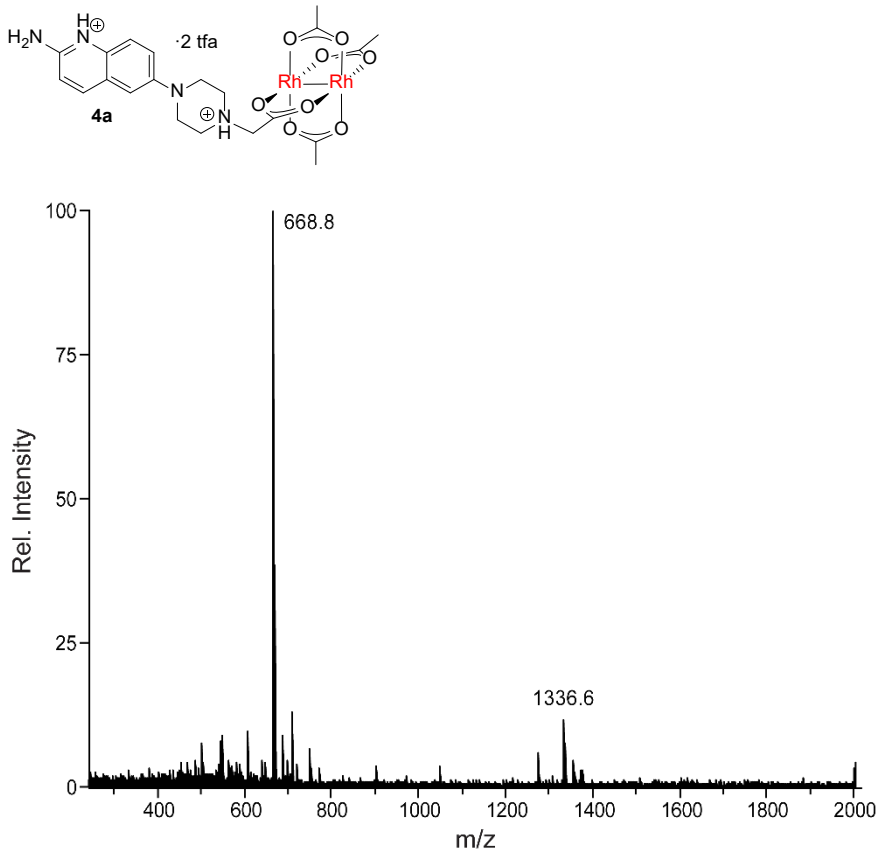


Figure 23. ESI–MS spectrum of compound **4a**.

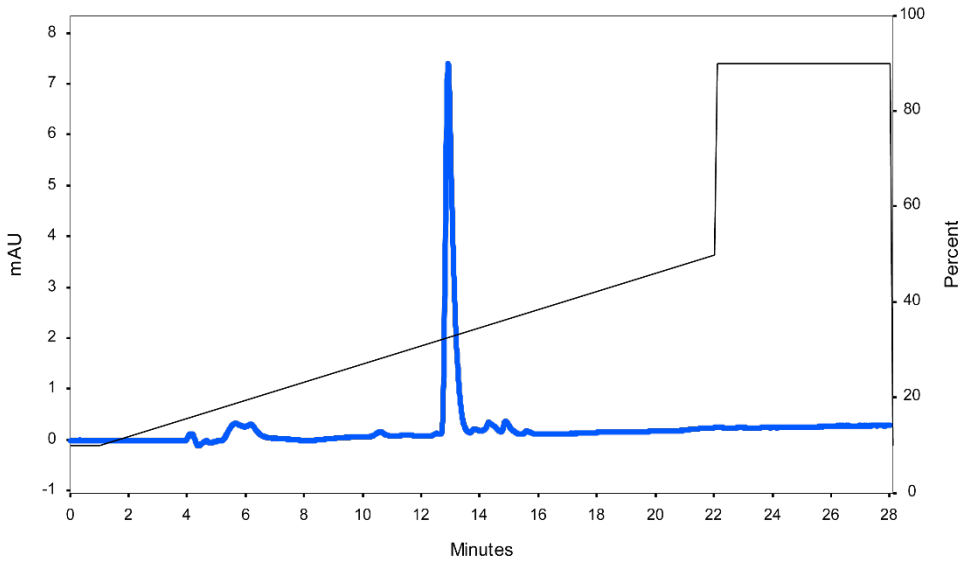


Figure 24.HPLC chromatogram of compound **4a**.

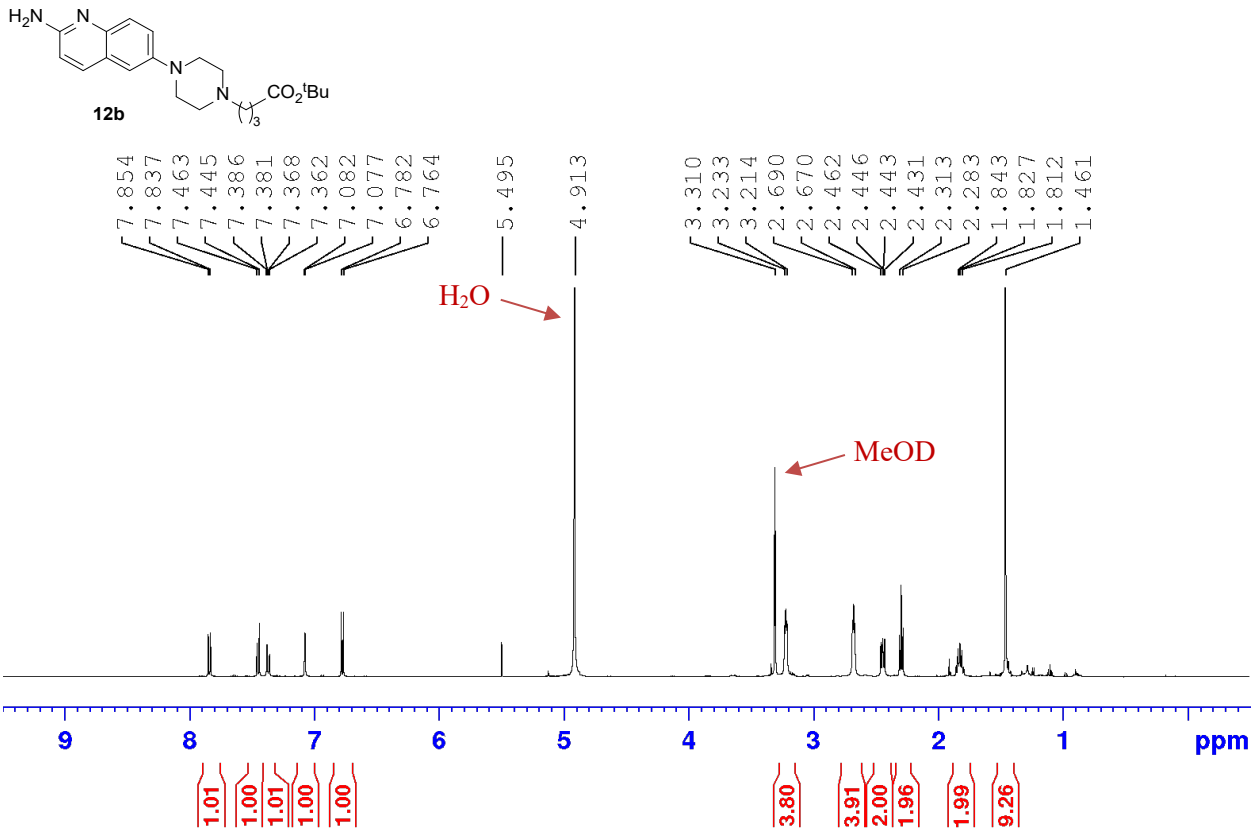


Figure 25. ^{1}H NMR spectrum of compound **12b** in CD_3OD.

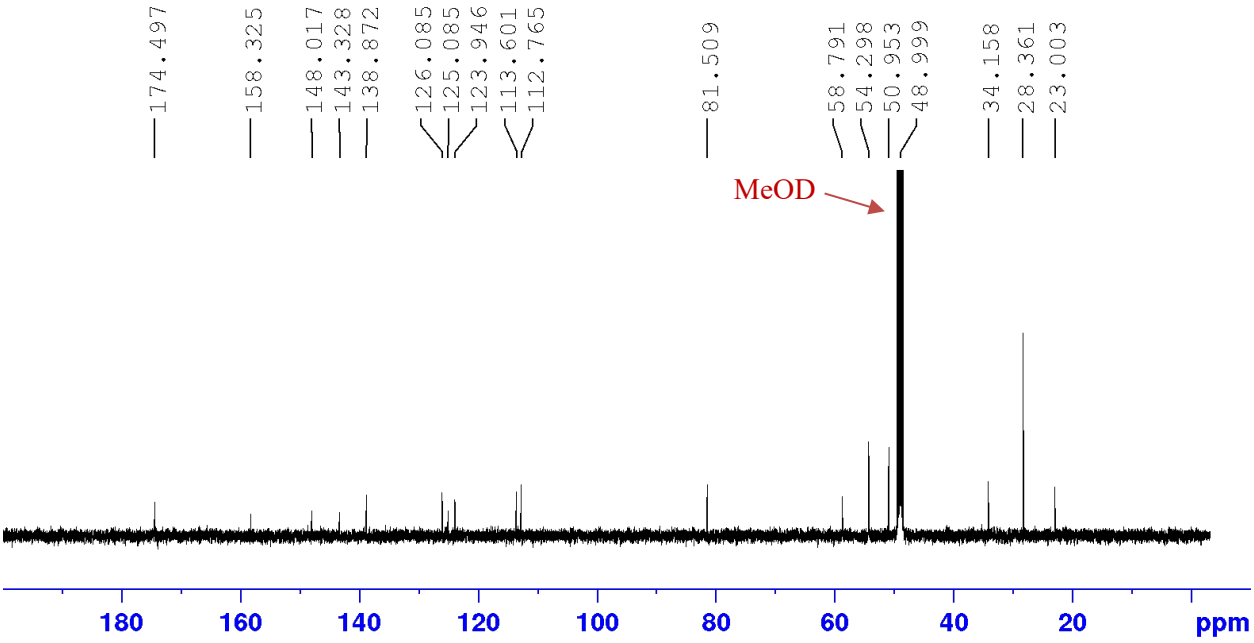


Figure 26. ^{13}C NMR spectrum of compound **12b** in CD_3OD.

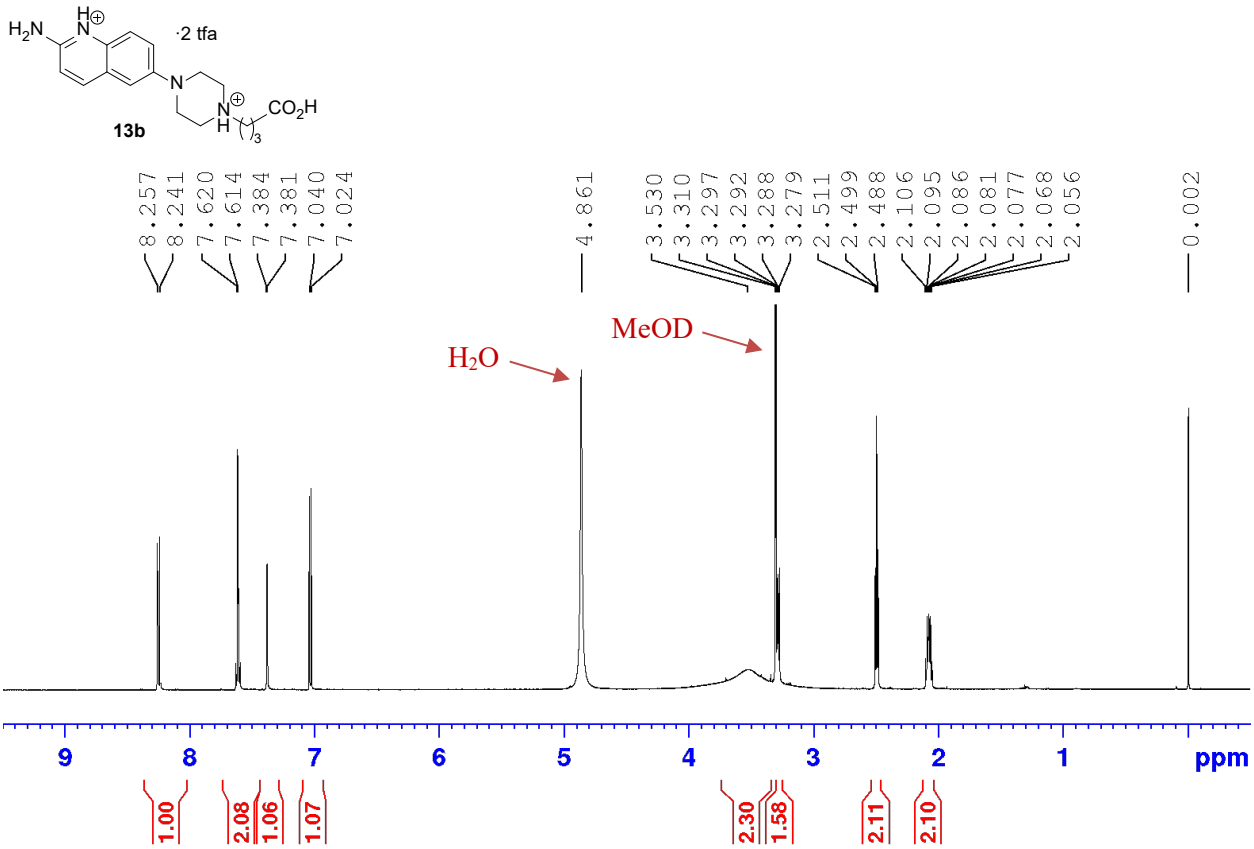


Figure 27. ^{1}H NMR spectrum of compound **13b** in CD_3OD.

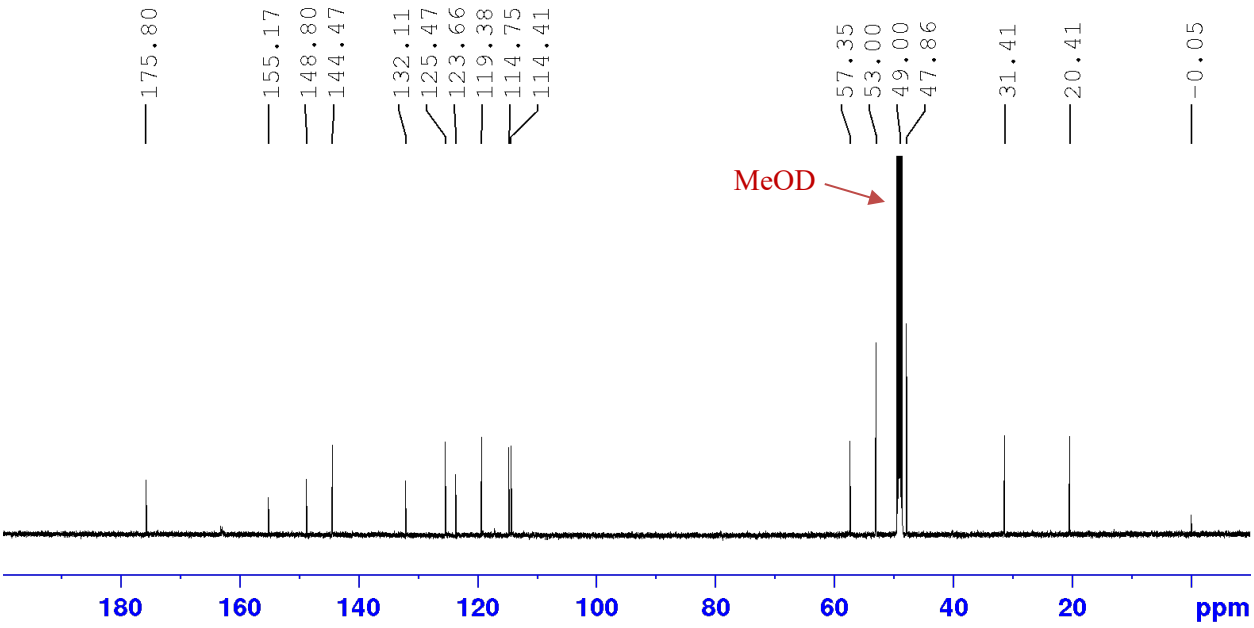


Figure 28. ^{13}C NMR spectrum of compound **13b** in CD_3OD.

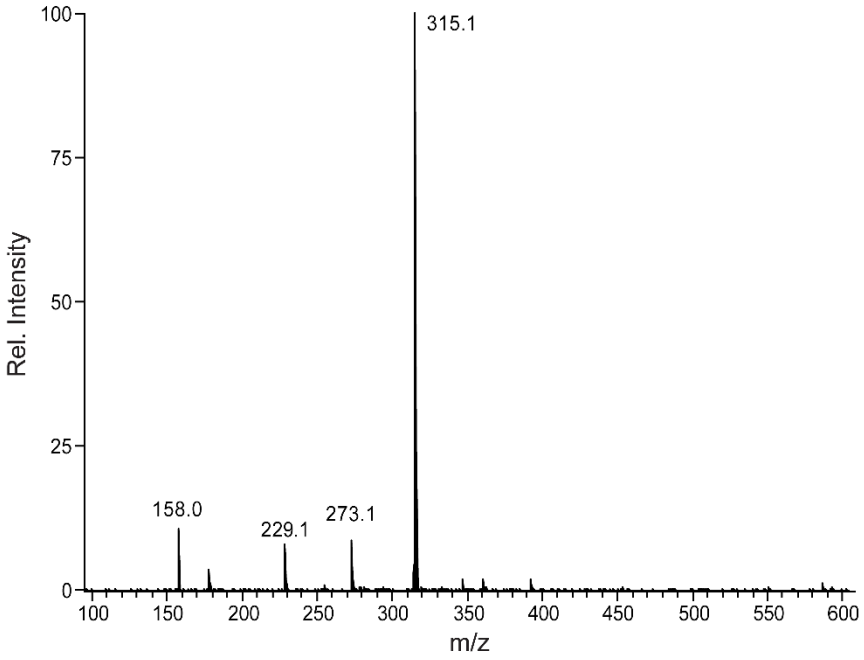


Figure 29.ESI–MS spectrum of compound **13b**.

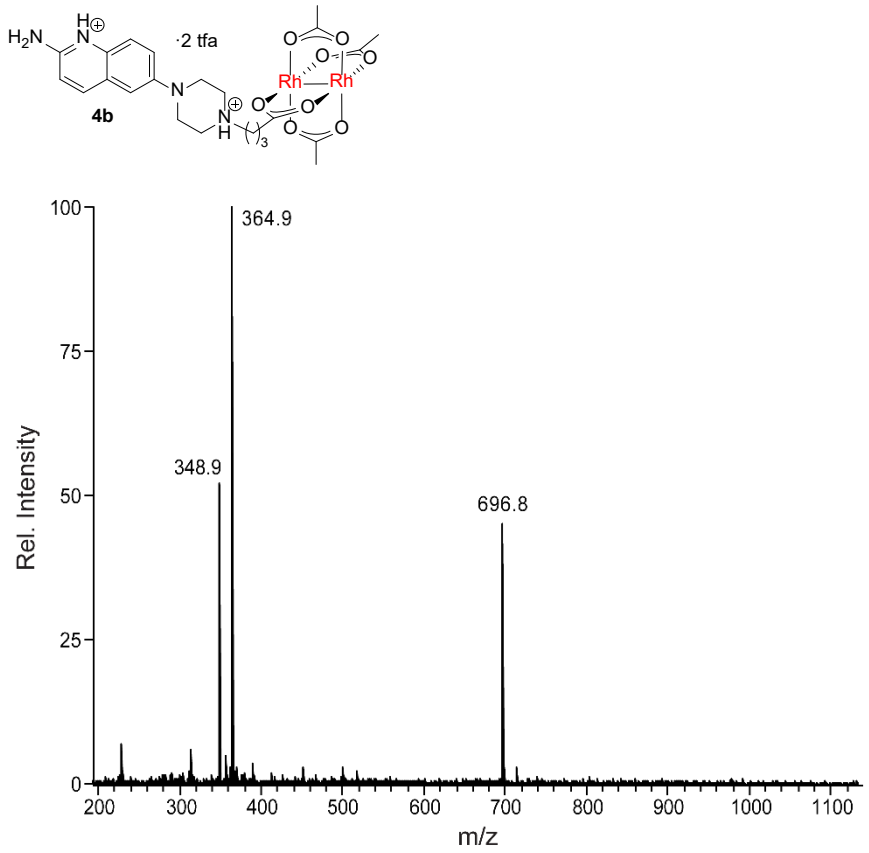


Figure 30.ESI–MS spectrum of compound **4b**.

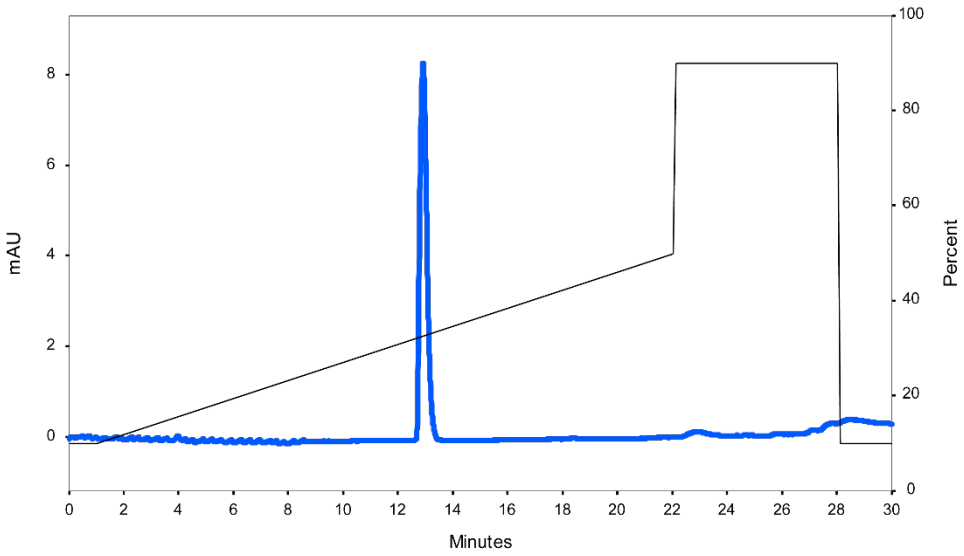


Figure 31. HPLC chromatogram of compound **4b**.

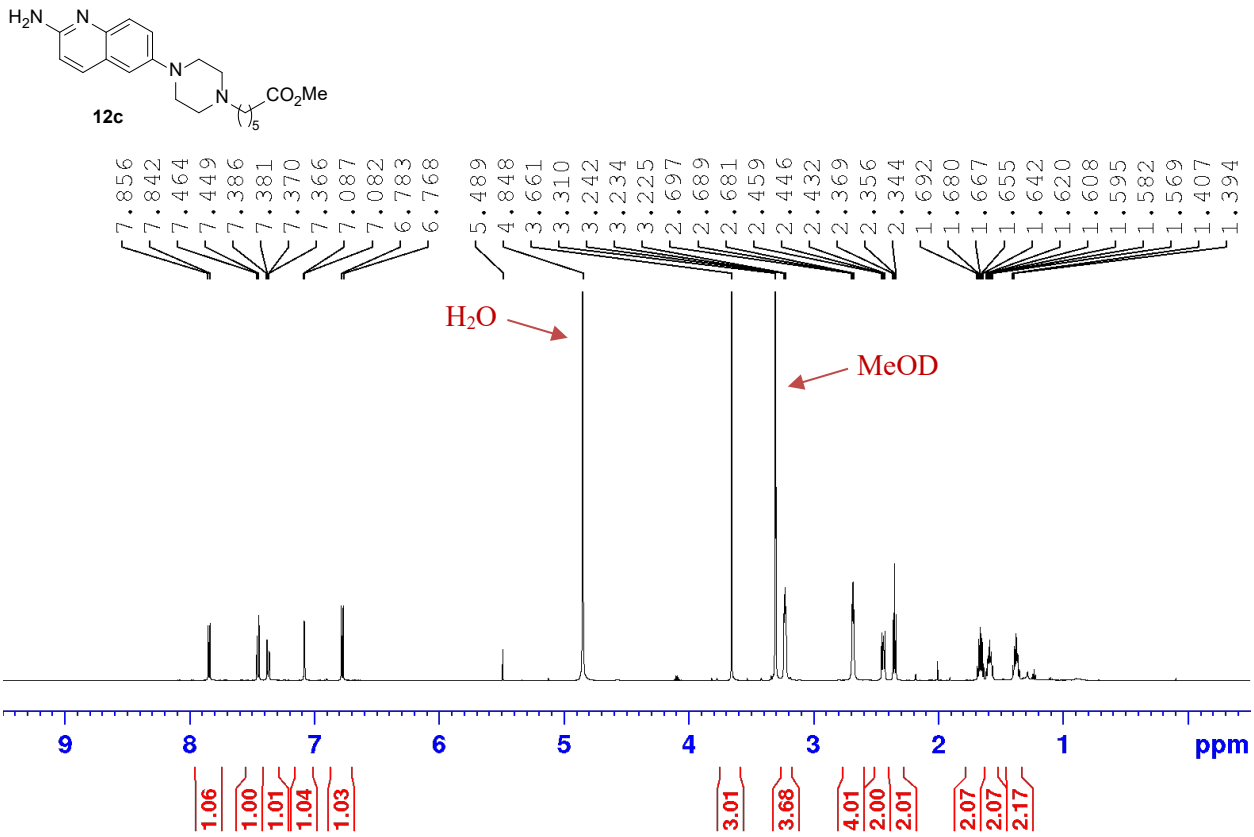


Figure 32. ^{1}H NMR spectrum of compound **12c** in CD_3OD.

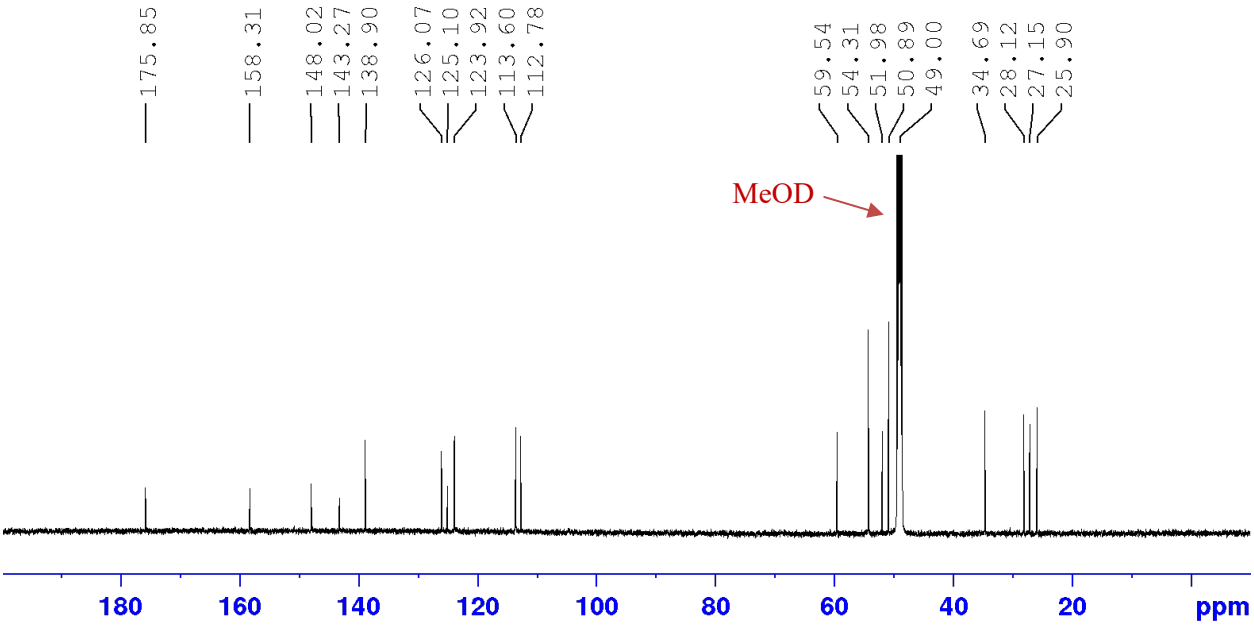


Figure 33. ^{13}C NMR spectrum of compound **12c** in CD_3OD.

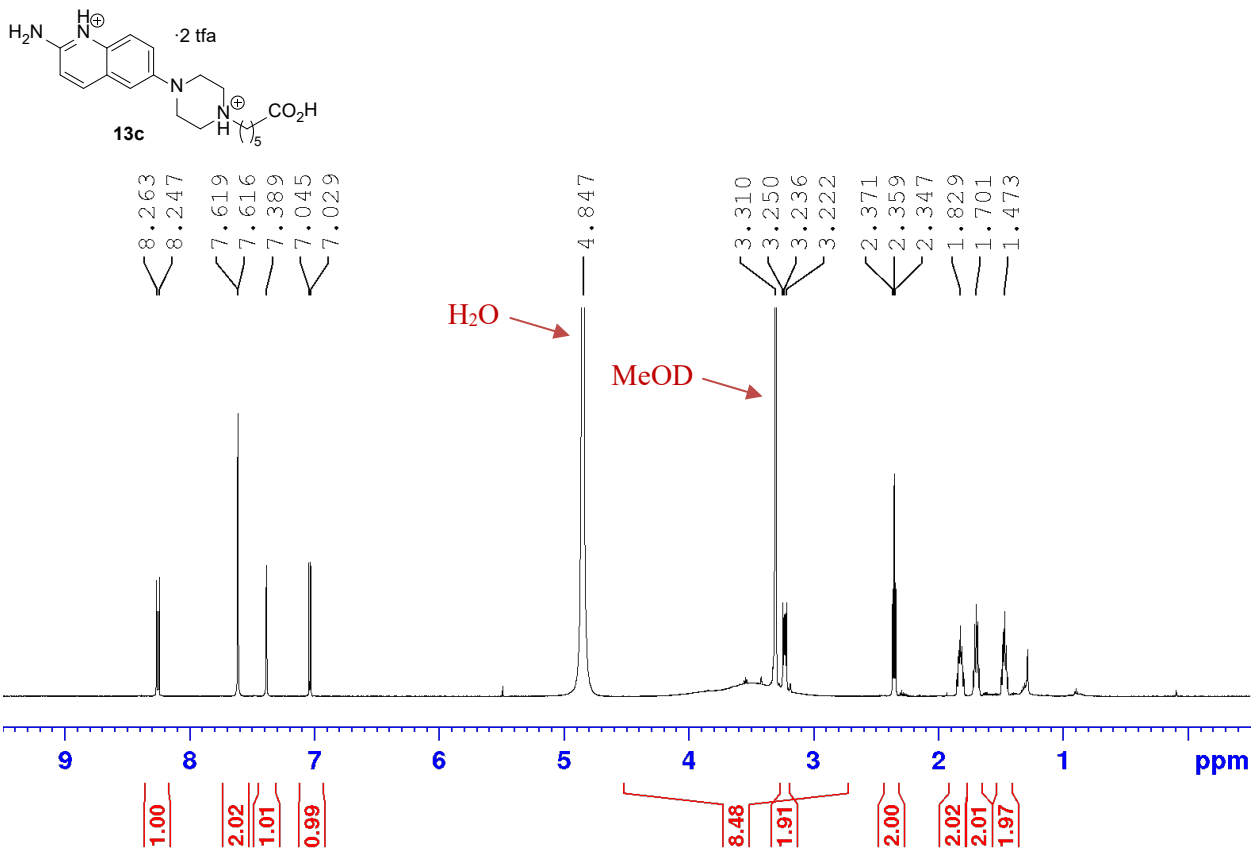


Figure 34. ^{1}H NMR spectrum of compound **13c** in CD_3OD.

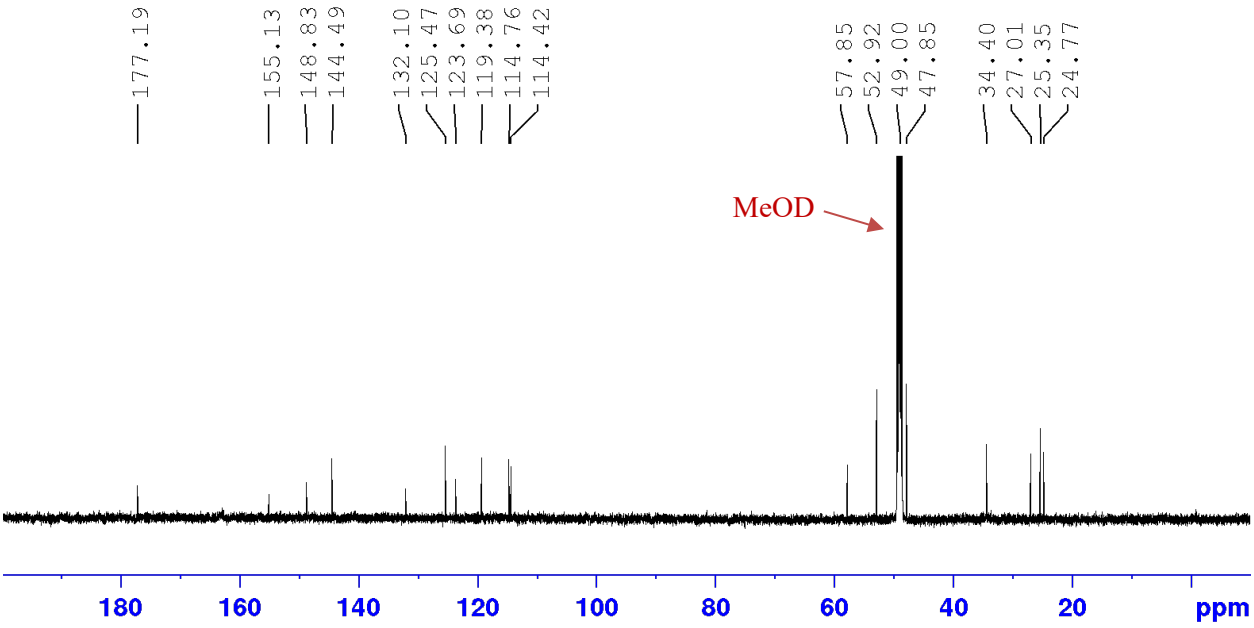


Figure 35. ^{13}C NMR spectrum of compound **13c** in CD_3OD.

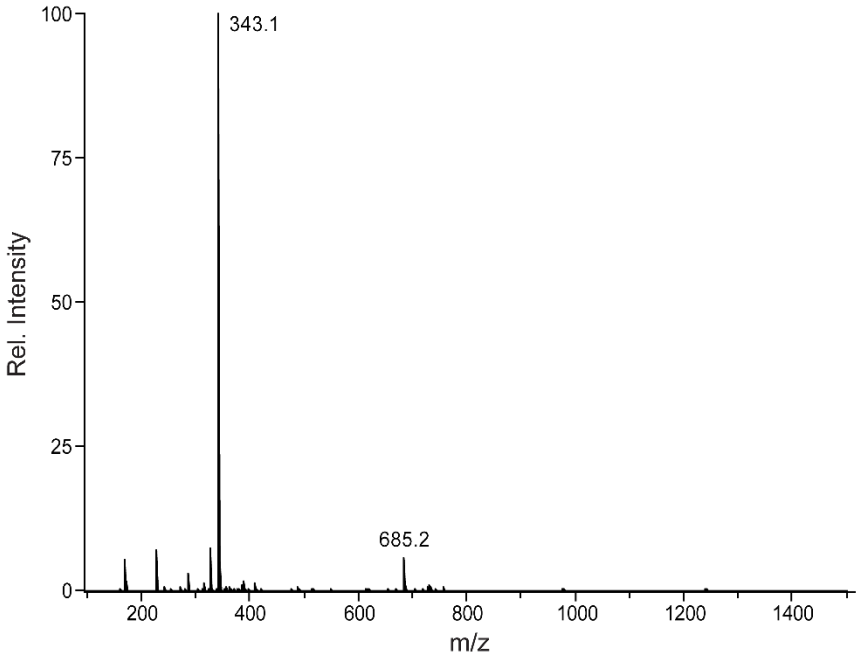


Figure 36. ESI–MS spectrum of compound **13c**.

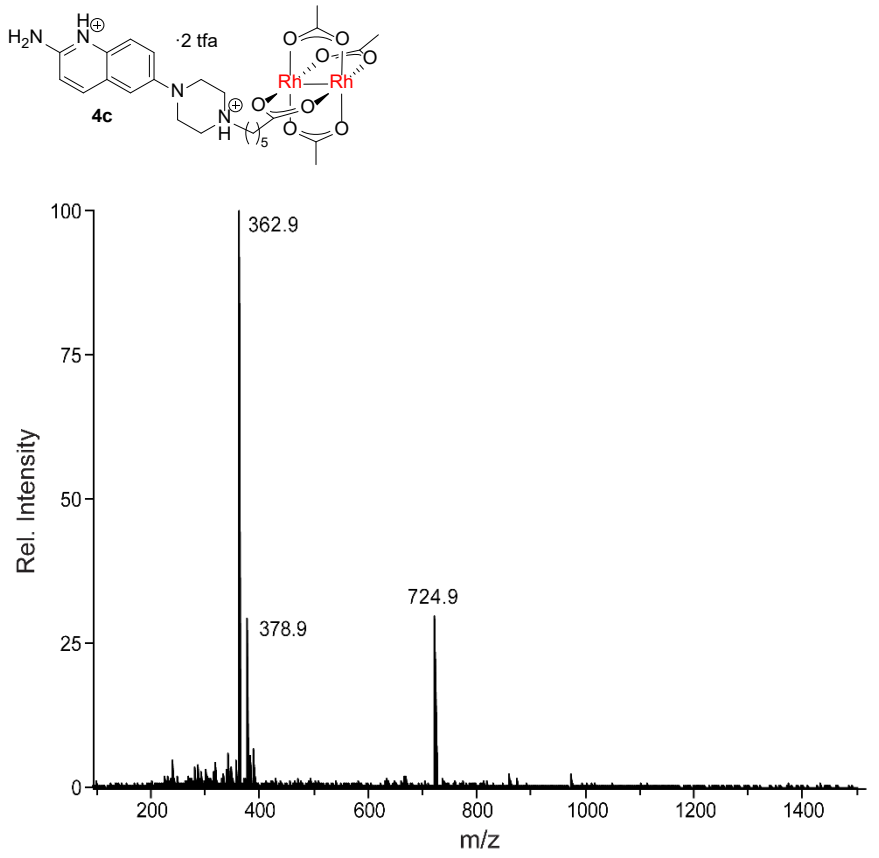


Figure 37.ESI–MS spectrum of compound **4c**.

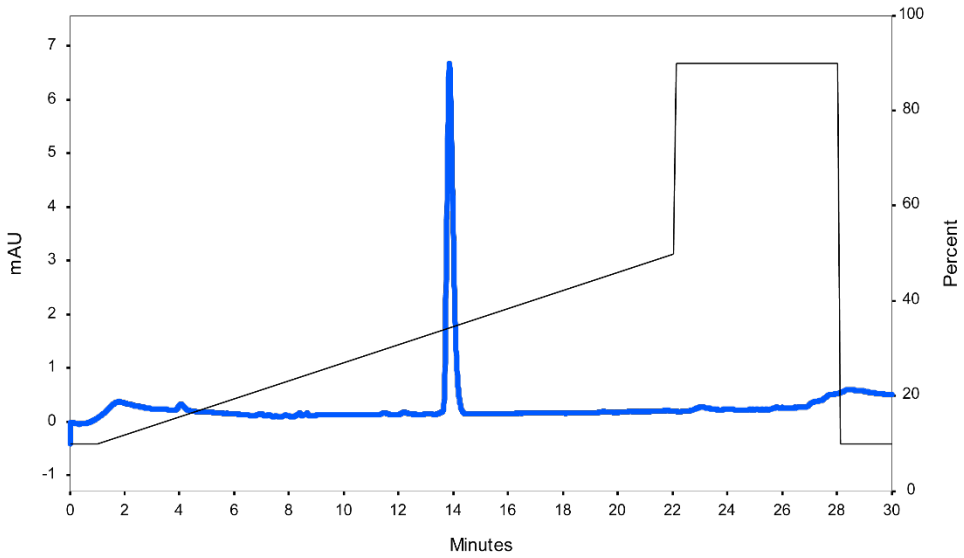
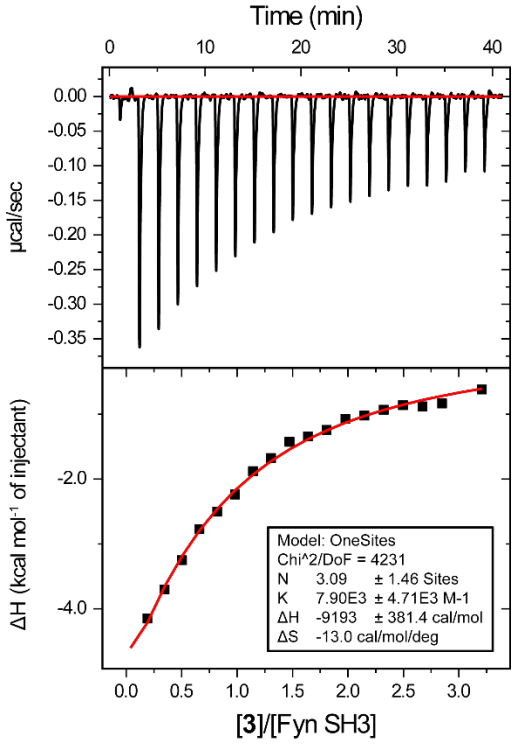
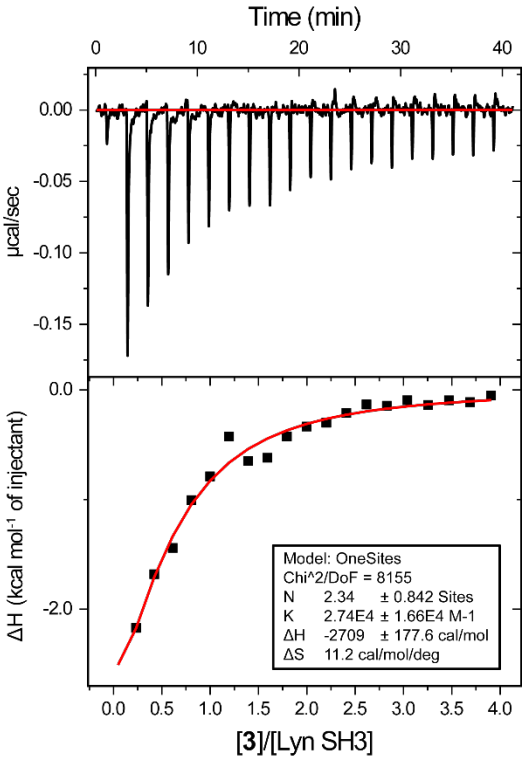
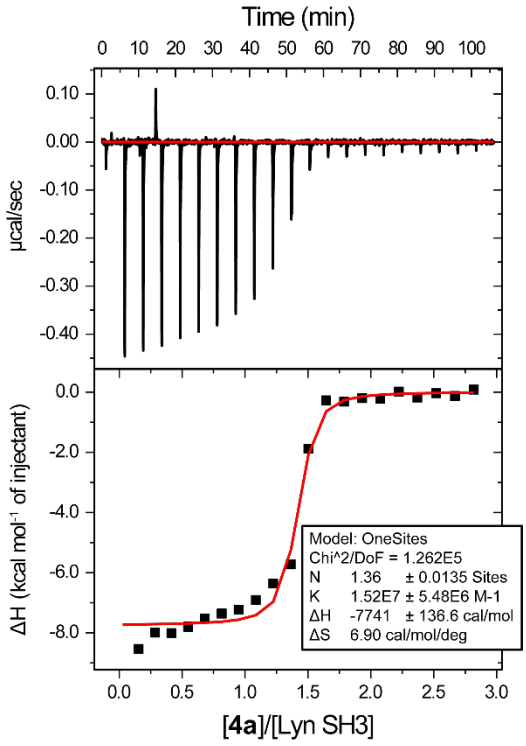


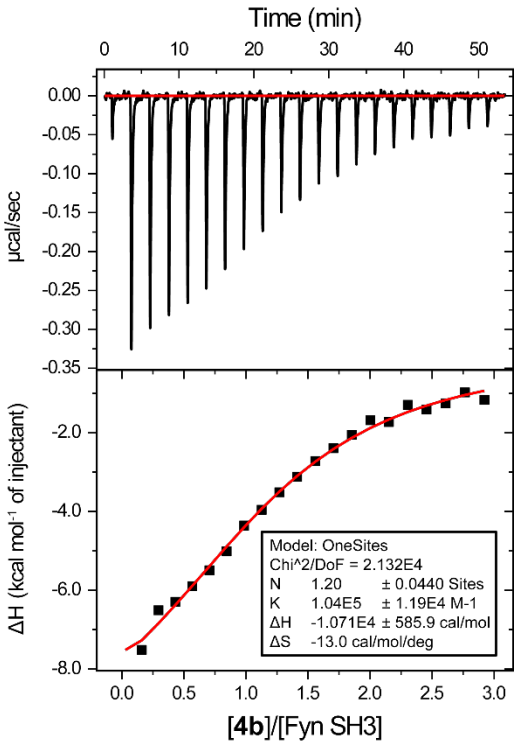
Figure 38. HPLC chromatogram of compound **4c**.

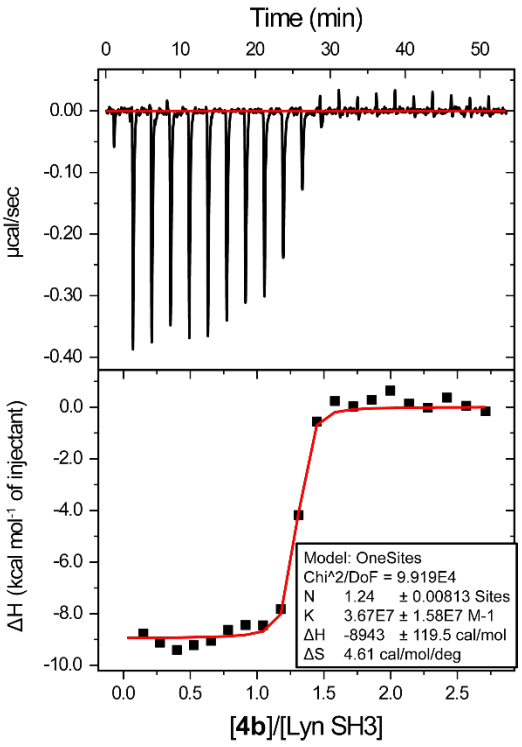
ITC binding data








Time (min)
µcal/sec
ΔH (kcal mol-1 of injectant)
Model: OneSites
Chi^2/DoF = 2.132E4
N 1.20 ± 0.0440 Sites
K 1.04E5 ± 1.19E4 M-1
ΔH -1.071E4 ± 585.9 cal/mol
ΔS -13.0 cal/mol/deg
[4b]/[Fyn SH3]


Time (min)
µcal/sec
ΔH (kcal mol-1 of injectant)
Model: OneSites
Chi^2/DoF = 9.919E4
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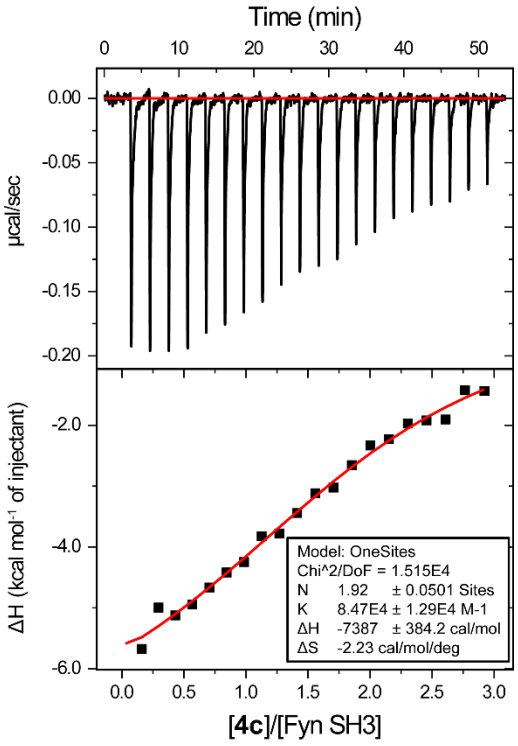
K 3.67E7 ± 1.58E7 M-1
ΔH -8943 ± 119.5 cal/mol
ΔS 4.61 cal/mol/deg
[4b]/[Lyn SH3]


Time (min)
µcal/sec
ΔH (kcal mol-1 of injectant)
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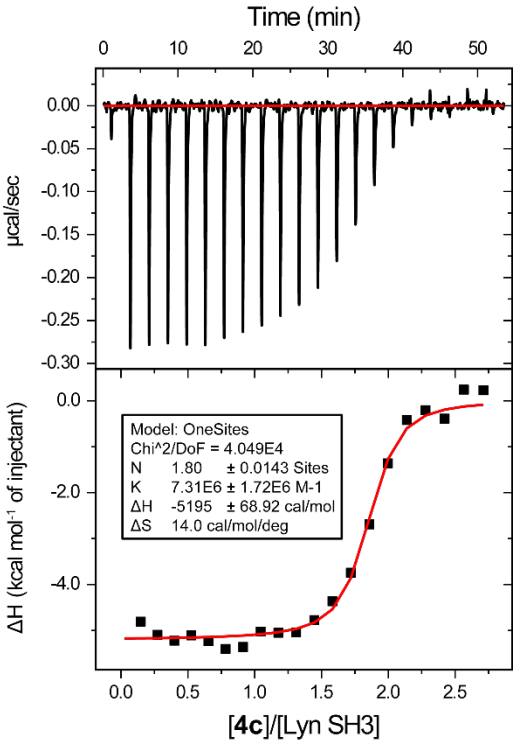
K 8.47E4 ± 1.29E4 M-1
ΔH -7387 ± 384.2 cal/mol
ΔS -2.23 cal/mol/deg
[4c]/[Fyn SH3]


Time (min)
µcal/sec
ΔH (kcal mol-1 of injectant)
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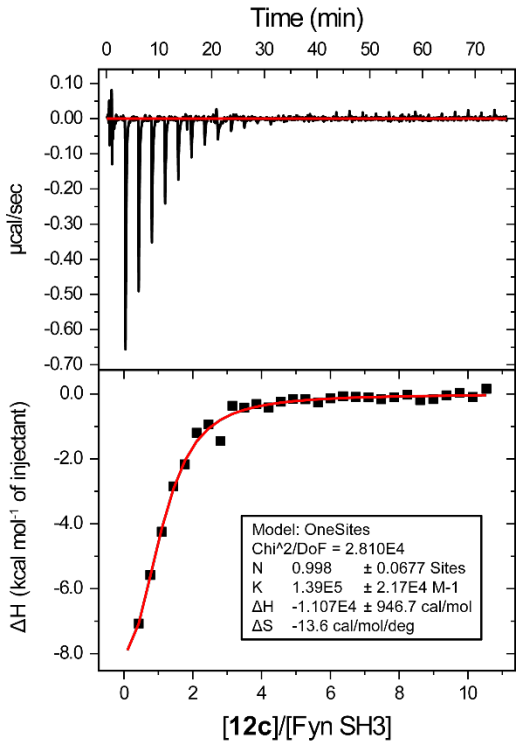
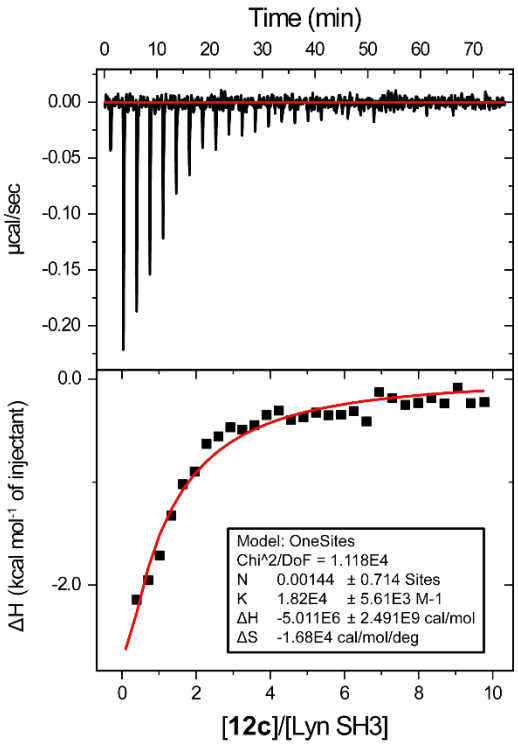
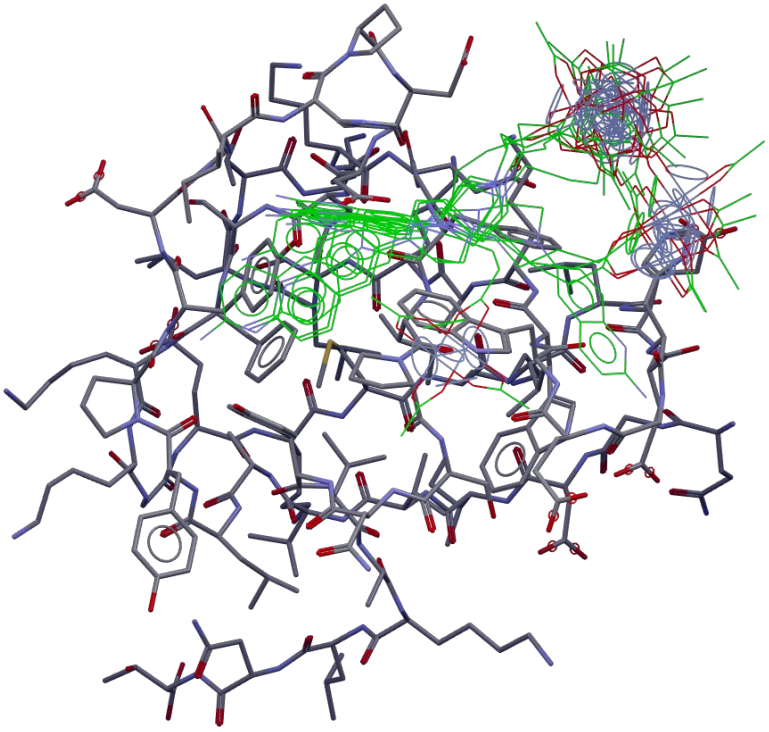
K 7.31E6 ± 1.72E6 M-1
ΔH -5195 ± 68.92 cal/mol
ΔS 14.0 cal/mol/deg
[4c]/[Lyn SH3]


Time (min)
µcal/sec
ΔH (kcal mol-1 of injectant)
Model: OneSites
Chi^2/DoF = 2.810E4
N 0.998 ± 0.0677 Sites
K 1.39E5 ± 2.17E4 M-1
ΔH -1.107E4 ± 946.7 cal/mol
ΔS -13.6 cal/mol/deg
[12c]/[Fyn SH3]

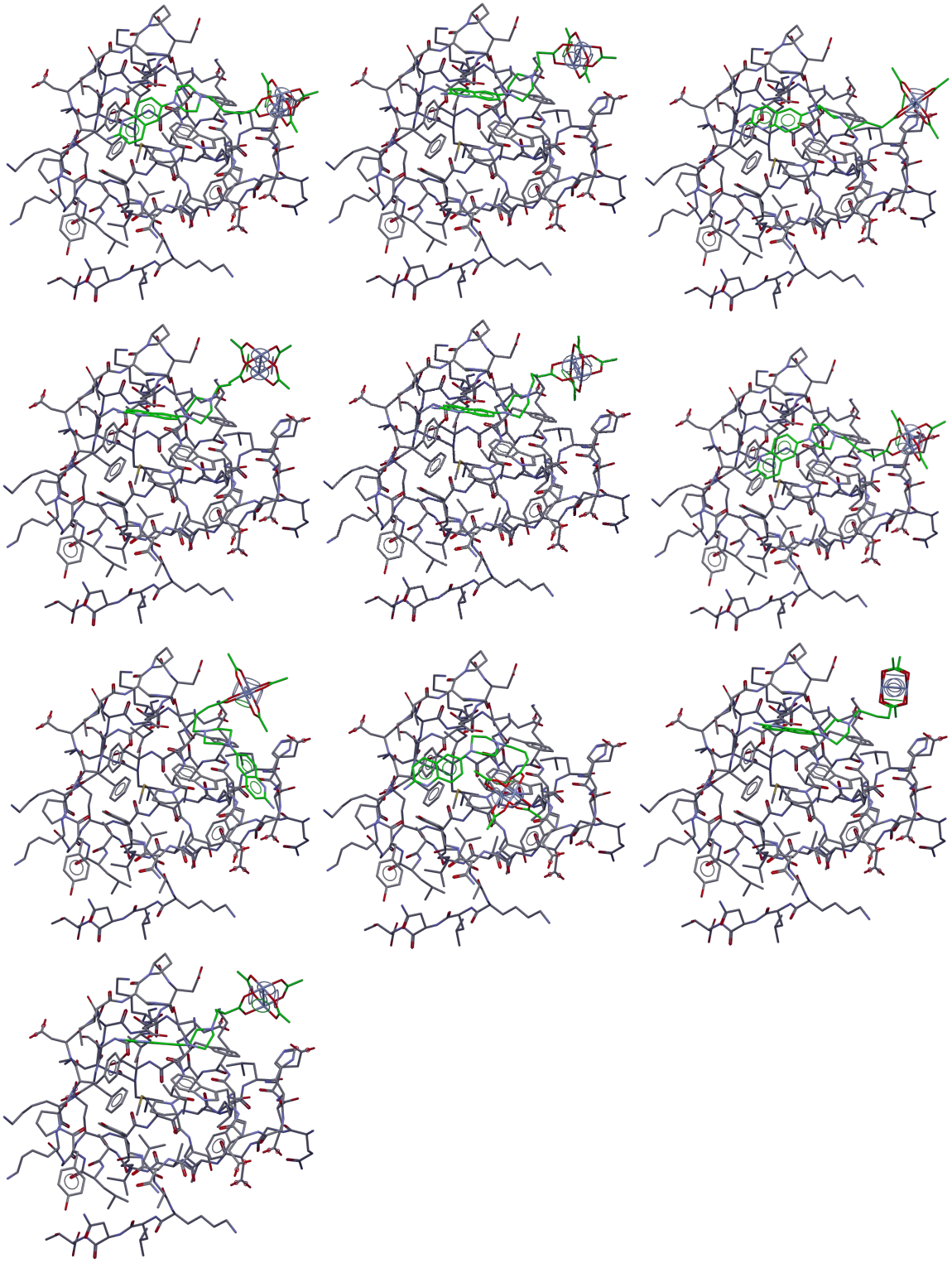

Time (min)
µcal/sec
ΔH (kcal mol-1 of injectant)
Model: OneSites
Chi^2/DoF = 1.118E4
N 0.00144 ± 0.714 Sites
K 1.82E4 ± 5.61E3 M-1
ΔH -5.011E6 ± 2.491E9 cal/mol
ΔS -1.68E4 cal/mol/deg
[12c]/[Lyn SH3]

Computational docking

Overlay of the top 10 docked conformations identified by GOLD:



Individual images of the top 10 docked conformations identified by Gold:



Coordinates of final binding model:

HETATM 1 N d 1 10.619 -4.445 -30.483 1.00 99.99 N

HETATM 2 N d 1 11.993 -2.499 -31.882 1.00 99.99 N

HETATM 3 N d 1 19.244 -1.024 -32.077 1.00 99.99 N

HETATM 4 N d 1 17.194 -1.268 -31.204 1.00 99.99 N

HETATM 5 C d 1 4.279 -5.456 -28.891 1.00 99.99 C

HETATM 6 C d 1 3.825 -4.061 -29.134 1.00 99.99 C

HETATM 7 C d 1 7.123 -7.792 -29.808 1.00 99.99 C

HETATM 8 C d 1 8.348 -7.770 -30.659 1.00 99.99 C

HETATM 9 C d 1 5.714 -10.394 -27.737 1.00 99.99 C

HETATM 10 C d 1 2.871 -8.058 -26.820 1.00 99.99 C

HETATM 11 C d 1 6.169 -11.789 -27.495 1.00 99.99 C

HETATM 12 C d 1 1.646 -8.080 -25.969 1.00 99.99 C

HETATM 13 C d 1 10.874 -1.988 -31.048 1.00 99.99 C

HETATM 14 C d 1 10.755 -3.031 -29.928 1.00 99.99 C

HETATM 15 C d 1 11.503 -4.792 -31.681 1.00 99.99 C

HETATM 16 C d 1 11.556 -3.651 -32.708 1.00 99.99 C

HETATM 17 C d 1 15.922 -1.535 -31.384 1.00 99.99 C

HETATM 18 C d 1 15.044 -1.496 -30.366 1.00 99.99 C

HETATM 19 C d 1 13.745 -1.790 -30.541 1.00 99.99 C

HETATM 20 C d 1 13.222 -2.155 -31.732 1.00 99.99 C

HETATM 21 C d 1 14.124 -2.159 -32.741 1.00 99.99 C

HETATM 22 C d 1 15.430 -1.856 -32.593 1.00 99.99 C

HETATM 23 C d 1 16.275 -1.880 -33.641 1.00 99.99 C

HETATM 24 C d 1 17.570 -1.591 -33.457 1.00 99.99 C

HETATM 25 C d 1 18.011 -1.290 -32.224 1.00 99.99 C

HETATM 26 C d 1 10.755 -5.558 -29.462 1.00 99.99 C

HETATM 27 C d 1 9.962 -7.065 -30.233 1.00 99.99 C

HETATM 28 O d 1 3.846 -6.388 -29.627 1.00 99.99 O

HETATM 29 O d 1 4.910 -10.191 -28.697 1.00 99.99 O

HETATM 30 O d 1 6.032 -8.159 -30.335 1.00 99.99 O

HETATM 31 O d 1 2.763 -8.402 -28.029 1.00 99.99 O

HETATM 32 O d 1 5.084 -5.658 -27.933 1.00 99.99 O

HETATM 33 O d 1 7.231 -7.449 -28.600 1.00 99.99 O

HETATM 34 O d 1 6.148 -9.462 -27.001 1.00 99.99 O

HETATM 35 O d 1 3.962 -7.692 -26.293 1.00 99.99 O

HETATM 36 Cr d 1 4.361 -8.311 -29.231 1.00 99.99 Cr

HETATM 37 Cr d 1 5.633 -7.539 -27.398 1.00 99.99 Cr

HETATM 38 H d 1 3.545 -3.705 -28.361 1.00 99.99 H

HETATM 39 H d 1 3.325 -3.981 -29.754 1.00 99.99 H

HETATM 40 H d 1 4.552 -3.434 -29.263 1.00 99.99 H

HETATM 41 H d 1 8.054 -7.814 -31.741 1.00 99.99 H

HETATM 42 H d 1 8.428 -8.734 -31.226 1.00 99.99 H

HETATM 43 H d 1 6.449 -12.146 -28.267 1.00 99.99 H

HETATM 44 H d 1 6.669 -11.869 -26.876 1.00 99.99 H

HETATM 45 H d 1 5.442 -12.416 -27.365 1.00 99.99 H

HETATM 46 H d 1 1.631 -7.359 -25.444 1.00 99.99 H

HETATM 47 H d 1 0.921 -8.238 -26.422 1.00 99.99 H

HETATM 48 H d 1 1.817 -8.648 -25.379 1.00 99.99 H

HETATM 49 H d 1 10.987 -0.951 -30.672 1.00 99.99 H

HETATM 50 H d 1 9.927 -1.952 -31.636 1.00 99.99 H

HETATM 51 H d 1 9.870 -2.795 -29.292 1.00 99.99 H

HETATM 52 H d 1 11.685 -2.920 -29.330 1.00 99.99 H

HETATM 53 H d 1 9.636 -4.501 -30.845 1.00 99.99 H

HETATM 54 H d 1 11.102 -5.710 -32.172 1.00 99.99 H

HETATM 55 H d 1 12.545 -4.998 -31.341 1.00 99.99 H

HETATM 56 H d 1 12.182 -3.890 -33.590 1.00 99.99 H

HETATM 57 H d 1 10.542 -3.472 -33.136 1.00 99.99 H

HETATM 58 H d 1 19.906 -1.036 -32.893 1.00 99.99 H

HETATM 59 H d 1 19.621 -0.791 -31.124 1.00 99.99 H

HETATM 60 H d 1 15.395 -1.237 -29.353 1.00 99.99 H

HETATM 61 H d 1 13.141 -1.752 -29.621 1.00 99.99 H

HETATM 62 H d 1 13.826 -2.437 -33.762 1.00 99.99 H

HETATM 63 H d 1 15.926 -2.128 -34.657 1.00 99.99 H

HETATM 64 H d 1 18.256 -1.600 -34.322 1.00 99.99 H

HETATM 65 H d 1 17.554 -1.033 -30.269 1.00 99.99 H

HETATM 66 H d 1 10.136 -5.364 -28.552 1.00 99.99 H

HETATM 67 H d 1 11.741 -5.936 -29.093 1.00 99.99 H

HETATM 68 H d 1 10.632 -7.406 -31.056 1.00 99.99 H

HETATM 69 H d 1 10.184 -7.788 -29.402 1.00 99.99 H

ATOM 70 N GLN A 1 10.473 -14.506 -14.094 1.00 0.00 N

ATOM 71 CA GLN A 1 11.422 -14.806 -12.985 1.00 0.00 C

ATOM 72 C GLN A 1 12.711 -14.008 -13.187 1.00 0.00 C

ATOM 73 O GLN A 1 13.327 -13.554 -12.243 1.00 0.00 O

ATOM 74 CB GLN A 1 11.745 -16.301 -12.981 1.00 0.00 C

ATOM 75 CG GLN A 1 11.817 -16.803 -11.537 1.00 0.00 C

ATOM 76 CD GLN A 1 13.260 -17.185 -11.202 1.00 0.00 C

ATOM 77 NE2 GLN A 1 13.490 -18.051 -10.254 1.00 0.00 N

ATOM 78 OE1 GLN A 1 14.188 -16.689 -11.810 1.00 0.00 O

ATOM 79 H GLN A 1 10.139 -13.593 -14.219 1.00 99.99 H

ATOM 80 HA GLN A 1 10.974 -14.531 -12.043 1.00 99.99 H

ATOM 81 HB2 GLN A 1 10.973 -16.838 -13.511 1.00 99.99 H

ATOM 82 HB3 GLN A 1 12.696 -16.465 -13.466 1.00 99.99 H

ATOM 83 HG2 GLN A 1 11.486 -16.023 -10.868 1.00 99.99 H

ATOM 84 HG3 GLN A 1 11.180 -17.668 -11.425 1.00 99.99 H

ATOM 85 HE21 GLN A 1 12.742 -18.451 -9.764 1.00 99.99 H

ATOM 86 HE22 GLN A 1 14.411 -18.302 -10.033 1.00 99.99 H

ATOM 87 N GLY A 2 13.122 -13.835 -14.412 1.00 0.00 N

ATOM 88 CA GLY A 2 14.370 -13.068 -14.678 1.00 0.00 C

ATOM 89 C GLY A 2 15.465 -14.025 -15.155 1.00 0.00 C

ATOM 90 O GLY A 2 15.910 -14.887 -14.424 1.00 0.00 O

ATOM 91 H GLY A 2 12.608 -14.211 -15.156 1.00 99.99 H

ATOM 92 HA2 GLY A 2 14.692 -12.577 -13.772 1.00 99.99 H

ATOM 93 HA3 GLY A 2 14.182 -12.327 -15.441 1.00 99.99 H

ATOM 94 N ASP A 3 15.902 -13.880 -16.376 1.00 0.00 N

ATOM 95 CA ASP A 3 16.968 -14.781 -16.897 1.00 0.00 C

ATOM 96 C ASP A 3 18.304 -14.037 -16.900 1.00 0.00 C

ATOM 97 O ASP A 3 18.353 -12.831 -17.034 1.00 0.00 O

ATOM 98 CB ASP A 3 16.619 -15.209 -18.324 1.00 0.00 C

ATOM 99 CG ASP A 3 17.202 -16.597 -18.597 1.00 0.00 C

ATOM 100 OD1 ASP A 3 16.785 -17.534 -17.936 1.00 0.00 O

ATOM 101 OD2 ASP A 3 18.056 -16.699 -19.463 1.00 0.00 O1-

ATOM 102 H ASP A 3 15.531 -13.177 -16.950 1.00 99.99 H

ATOM 103 HA ASP A 3 17.042 -15.654 -16.267 1.00 99.99 H

ATOM 104 HB2 ASP A 3 15.546 -15.241 -18.439 1.00 99.99 H

ATOM 105 HB3 ASP A 3 17.035 -14.500 -19.025 1.00 99.99 H

ATOM 106 N ILE A 4 19.391 -14.745 -16.755 1.00 0.00 N

ATOM 107 CA ILE A 4 20.720 -14.071 -16.753 1.00 0.00 C

ATOM 108 C ILE A 4 21.432 -14.350 -18.079 1.00 0.00 C

ATOM 109 O ILE A 4 21.537 -15.480 -18.514 1.00 0.00 O

ATOM 110 CB ILE A 4 21.564 -14.595 -15.586 1.00 0.00 C

ATOM 111 CG1 ILE A 4 22.523 -13.498 -15.119 1.00 0.00 C

ATOM 112 CG2 ILE A 4 22.372 -15.816 -16.035 1.00 0.00 C

ATOM 113 CD1 ILE A 4 21.952 -12.816 -13.874 1.00 0.00 C

ATOM 114 H ILE A 4 19.333 -15.718 -16.651 1.00 99.99 H

ATOM 115 HA ILE A 4 20.578 -13.006 -16.643 1.00 99.99 H

ATOM 116 HB ILE A 4 20.915 -14.875 -14.770 1.00 99.99 H

ATOM 117 HG12 ILE A 4 23.482 -13.935 -14.882 1.00 99.99 H

ATOM 118 HG13 ILE A 4 22.644 -12.768 -15.905 1.00 99.99 H

ATOM 119 HG21 ILE A 4 21.725 -16.502 -16.561 1.00 99.99 H

ATOM 120 HG22 ILE A 4 23.169 -15.497 -16.692 1.00 99.99 H

ATOM 121 HG23 ILE A 4 22.793 -16.307 -15.171 1.00 99.99 H

ATOM 122 HD11 ILE A 4 21.819 -13.549 -13.091 1.00 99.99 H

ATOM 123 HD12 ILE A 4 22.635 -12.050 -13.538 1.00 99.99 H

ATOM 124 HD13 ILE A 4 20.999 -12.368 -14.114 1.00 99.99 H

ATOM 125 N VAL A 5 21.919 -13.328 -18.723 1.00 0.00 N

ATOM 126 CA VAL A 5 22.622 -13.524 -20.019 1.00 0.00 C

ATOM 127 C VAL A 5 23.968 -12.808 -19.964 1.00 0.00 C

ATOM 128 O VAL A 5 24.138 -11.854 -19.231 1.00 0.00 O

ATOM 129 CB VAL A 5 21.779 -12.925 -21.148 1.00 0.00 C

ATOM 130 CG1 VAL A 5 20.763 -13.961 -21.631 1.00 0.00 C

ATOM 131 CG2 VAL A 5 21.041 -11.688 -20.632 1.00 0.00 C

ATOM 132 H VAL A 5 21.822 -12.424 -18.355 1.00 99.99 H

ATOM 133 HA VAL A 5 22.771 -14.577 -20.205 1.00 99.99 H

ATOM 134 HB VAL A 5 22.424 -12.643 -21.967 1.00 99.99 H

ATOM 135 HG11 VAL A 5 20.498 -14.614 -20.813 1.00 99.99 H

ATOM 136 HG12 VAL A 5 19.878 -13.457 -21.991 1.00 99.99 H

ATOM 137 HG13 VAL A 5 21.196 -14.544 -22.431 1.00 99.99 H

ATOM 138 HG21 VAL A 5 21.638 -11.202 -19.875 1.00 99.99 H

ATOM 139 HG22 VAL A 5 20.870 -11.003 -21.450 1.00 99.99 H

ATOM 140 HG23 VAL A 5 20.093 -11.985 -20.208 1.00 99.99 H

ATOM 141 N VAL A 6 24.924 -13.240 -20.733 1.00 0.00 N

ATOM 142 CA VAL A 6 26.239 -12.550 -20.706 1.00 0.00 C

ATOM 143 C VAL A 6 26.468 -11.873 -22.055 1.00 0.00 C

ATOM 144 O VAL A 6 26.242 -12.452 -23.100 1.00 0.00 O

ATOM 145 CB VAL A 6 27.358 -13.555 -20.421 1.00 0.00 C

ATOM 146 CG1 VAL A 6 27.233 -14.743 -21.376 1.00 0.00 C

ATOM 147 CG2 VAL A 6 28.715 -12.879 -20.623 1.00 0.00 C

ATOM 148 H VAL A 6 24.775 -14.003 -21.330 1.00 99.99 H

ATOM 149 HA VAL A 6 26.212 -11.797 -19.934 1.00 99.99 H

ATOM 150 HB VAL A 6 27.277 -13.903 -19.402 1.00 99.99 H

ATOM 151 HG11 VAL A 6 26.778 -14.417 -22.299 1.00 99.99 H

ATOM 152 HG12 VAL A 6 28.214 -15.146 -21.580 1.00 99.99 H

ATOM 153 HG13 VAL A 6 26.618 -15.507 -20.922 1.00 99.99 H

ATOM 154 HG21 VAL A 6 28.724 -11.929 -20.110 1.00 99.99 H

ATOM 155 HG22 VAL A 6 29.495 -13.511 -20.223 1.00 99.99 H

ATOM 156 HG23 VAL A 6 28.885 -12.721 -21.678 1.00 99.99 H

ATOM 157 N ALA A 7 26.899 -10.644 -22.037 1.00 0.00 N

ATOM 158 CA ALA A 7 27.129 -9.916 -23.312 1.00 0.00 C

ATOM 159 C ALA A 7 28.104 -10.701 -24.187 1.00 0.00 C

ATOM 160 O ALA A 7 29.260 -10.871 -23.852 1.00 0.00 O

ATOM 161 CB ALA A 7 27.714 -8.535 -23.012 1.00 0.00 C

ATOM 162 H ALA A 7 27.065 -10.195 -21.182 1.00 99.99 H

ATOM 163 HA ALA A 7 26.191 -9.802 -23.834 1.00 99.99 H

ATOM 164 HB1 ALA A 7 28.484 -8.625 -22.260 1.00 99.99 H

ATOM 165 HB2 ALA A 7 26.932 -7.883 -22.651 1.00 99.99 H

ATOM 166 HB3 ALA A 7 28.139 -8.120 -23.915 1.00 99.99 H

ATOM 167 N LEU A 8 27.652 -11.159 -25.319 1.00 0.00 N

ATOM 168 CA LEU A 8 28.558 -11.906 -26.231 1.00 0.00 C

ATOM 169 C LEU A 8 29.243 -10.891 -27.141 1.00 0.00 C

ATOM 170 O LEU A 8 30.346 -11.093 -27.608 1.00 0.00 O

ATOM 171 CB LEU A 8 27.748 -12.896 -27.071 1.00 0.00 C

ATOM 172 CG LEU A 8 27.162 -13.977 -26.160 1.00 0.00 C

ATOM 173 CD1 LEU A 8 26.037 -14.708 -26.895 1.00 0.00 C

ATOM 174 CD2 LEU A 8 28.258 -14.975 -25.783 1.00 0.00 C

ATOM 175 H LEU A 8 26.723 -10.986 -25.578 1.00 99.99 H

ATOM 176 HA LEU A 8 29.303 -12.434 -25.653 1.00 99.99 H

ATOM 177 HB2 LEU A 8 26.947 -12.373 -27.571 1.00 99.99 H

ATOM 178 HB3 LEU A 8 28.392 -13.355 -27.807 1.00 99.99 H

ATOM 179 HG LEU A 8 26.769 -13.518 -25.265 1.00 99.99 H

ATOM 180 HD11 LEU A 8 26.177 -14.606 -27.961 1.00 99.99 H

ATOM 181 HD12 LEU A 8 26.054 -15.755 -26.628 1.00 99.99 H

ATOM 182 HD13 LEU A 8 25.086 -14.281 -26.614 1.00 99.99 H

ATOM 183 HD21 LEU A 8 29.125 -14.810 -26.405 1.00 99.99 H

ATOM 184 HD22 LEU A 8 28.528 -14.838 -24.746 1.00 99.99 H

ATOM 185 HD23 LEU A 8 27.895 -15.981 -25.930 1.00 99.99 H

ATOM 186 N TYR A 9 28.587 -9.790 -27.380 1.00 0.00 N

ATOM 187 CA TYR A 9 29.173 -8.732 -28.243 1.00 0.00 C

ATOM 188 C TYR A 9 28.919 -7.370 -27.592 1.00 0.00 C

ATOM 189 O TYR A 9 27.859 -7.122 -27.054 1.00 0.00 O

ATOM 190 CB TYR A 9 28.504 -8.769 -29.619 1.00 0.00 C

ATOM 191 CG TYR A 9 29.024 -9.952 -30.400 1.00 0.00 C

ATOM 192 CD1 TYR A 9 28.485 -11.226 -30.184 1.00 0.00 C

ATOM 193 CD2 TYR A 9 30.045 -9.774 -31.341 1.00 0.00 C

ATOM 194 CE1 TYR A 9 28.967 -12.322 -30.908 1.00 0.00 C

ATOM 195 CE2 TYR A 9 30.528 -10.871 -32.065 1.00 0.00 C

ATOM 196 CZ TYR A 9 29.989 -12.145 -31.849 1.00 0.00 C

ATOM 197 OH TYR A 9 30.464 -13.225 -32.563 1.00 0.00 O

ATOM 198 H TYR A 9 27.701 -9.656 -26.984 1.00 99.99 H

ATOM 199 HA TYR A 9 30.234 -8.897 -28.353 1.00 99.99 H

ATOM 200 HB2 TYR A 9 27.434 -8.861 -29.497 1.00 99.99 H

ATOM 201 HB3 TYR A 9 28.728 -7.858 -30.153 1.00 99.99 H

ATOM 202 HD1 TYR A 9 27.697 -11.362 -29.458 1.00 99.99 H

ATOM 203 HD2 TYR A 9 30.461 -8.792 -31.508 1.00 99.99 H

ATOM 204 HE1 TYR A 9 28.551 -13.305 -30.741 1.00 99.99 H

ATOM 205 HE2 TYR A 9 31.315 -10.734 -32.791 1.00 99.99 H

ATOM 206 HH TYR A 9 30.630 -12.936 -33.463 1.00 99.99 H

ATOM 207 N PRO A 10 29.908 -6.470 -27.649 1.00 0.00 N

ATOM 208 CA PRO A 10 29.792 -5.123 -27.072 1.00 0.00 C

ATOM 209 C PRO A 10 28.658 -4.321 -27.718 1.00 0.00 C

ATOM 210 O PRO A 10 28.421 -4.402 -28.907 1.00 0.00 O

ATOM 211 CB PRO A 10 31.154 -4.491 -27.383 1.00 0.00 C

ATOM 212 CG PRO A 10 31.651 -5.268 -28.554 1.00 0.00 C

ATOM 213 CD PRO A 10 31.216 -6.678 -28.284 1.00 0.00 C

ATOM 214 HA PRO A 10 29.653 -5.150 -26.004 1.00 99.99 H

ATOM 215 HB2 PRO A 10 31.025 -3.446 -27.621 1.00 99.99 H

ATOM 216 HB3 PRO A 10 31.807 -4.593 -26.529 1.00 99.99 H

ATOM 217 HG2 PRO A 10 31.204 -4.892 -29.463 1.00 99.99 H

ATOM 218 HG3 PRO A 10 32.727 -5.198 -28.613 1.00 99.99 H

ATOM 219 HD2 PRO A 10 31.131 -7.241 -29.198 1.00 99.99 H

ATOM 220 HD3 PRO A 10 31.909 -7.170 -27.617 1.00 99.99 H

ATOM 221 N TYR A 11 27.948 -3.555 -26.934 1.00 0.00 N

ATOM 222 CA TYR A 11 26.818 -2.753 -27.482 1.00 0.00 C

ATOM 223 C TYR A 11 26.905 -1.321 -26.955 1.00 0.00 C

ATOM 224 O TYR A 11 26.929 -1.094 -25.761 1.00 0.00 O

ATOM 225 CB TYR A 11 25.497 -3.373 -27.023 1.00 0.00 C

ATOM 226 CG TYR A 11 24.350 -2.774 -27.806 1.00 0.00 C

ATOM 227 CD1 TYR A 11 23.752 -1.581 -27.377 1.00 0.00 C

ATOM 228 CD2 TYR A 11 23.881 -3.416 -28.958 1.00 0.00 C

ATOM 229 CE1 TYR A 11 22.686 -1.031 -28.101 1.00 0.00 C

ATOM 230 CE2 TYR A 11 22.815 -2.866 -29.682 1.00 0.00 C

ATOM 231 CZ TYR A 11 22.218 -1.674 -29.254 1.00 0.00 C

ATOM 232 OH TYR A 11 21.169 -1.133 -29.967 1.00 0.00 O

ATOM 233 H TYR A 11 28.156 -3.512 -25.977 1.00 99.99 H

ATOM 234 HA TYR A 11 26.855 -2.755 -28.562 1.00 99.99 H

ATOM 235 HB2 TYR A 11 25.526 -4.440 -27.189 1.00 99.99 H

ATOM 236 HB3 TYR A 11 25.354 -3.178 -25.971 1.00 99.99 H

ATOM 237 HD1 TYR A 11 24.112 -1.085 -26.489 1.00 99.99 H

ATOM 238 HD2 TYR A 11 24.341 -4.335 -29.290 1.00 99.99 H

ATOM 239 HE1 TYR A 11 22.225 -0.112 -27.770 1.00 99.99 H

ATOM 240 HE2 TYR A 11 22.454 -3.362 -30.570 1.00 99.99 H

ATOM 241 HH TYR A 11 21.012 -1.691 -30.733 1.00 99.99 H

ATOM 242 N ASP A 12 26.943 -0.350 -27.823 1.00 0.00 N

ATOM 243 CA ASP A 12 27.017 1.058 -27.345 1.00 0.00 C

ATOM 244 C ASP A 12 25.633 1.695 -27.461 1.00 0.00 C

ATOM 245 O ASP A 12 25.130 1.914 -28.544 1.00 0.00 O

ATOM 246 CB ASP A 12 28.026 1.842 -28.187 1.00 0.00 C

ATOM 247 CG ASP A 12 28.959 2.627 -27.264 1.00 0.00 C

ATOM 248 OD1 ASP A 12 28.466 3.474 -26.537 1.00 0.00 O

ATOM 249 OD2 ASP A 12 30.151 2.368 -27.299 1.00 0.00 O1-

ATOM 250 H ASP A 12 26.916 -0.545 -28.783 1.00 99.99 H

ATOM 251 HA ASP A 12 27.321 1.060 -26.309 1.00 99.99 H

ATOM 252 HB2 ASP A 12 28.605 1.156 -28.786 1.00 99.99 H

ATOM 253 HB3 ASP A 12 27.498 2.528 -28.833 1.00 99.99 H

ATOM 254 N GLY A 13 25.014 1.976 -26.343 1.00 0.00 N

ATOM 255 CA GLY A 13 23.652 2.587 -26.351 1.00 0.00 C

ATOM 256 C GLY A 13 23.439 3.419 -27.618 1.00 0.00 C

ATOM 257 O GLY A 13 23.705 4.604 -27.647 1.00 0.00 O

ATOM 258 H GLY A 13 25.447 1.774 -25.488 1.00 99.99 H

ATOM 259 HA2 GLY A 13 23.543 3.224 -25.485 1.00 99.99 H

ATOM 260 HA3 GLY A 13 22.910 1.803 -26.311 1.00 99.99 H

ATOM 261 N ILE A 14 22.944 2.809 -28.661 1.00 0.00 N

ATOM 262 CA ILE A 14 22.696 3.567 -29.917 1.00 0.00 C

ATOM 263 C ILE A 14 21.239 4.028 -29.925 1.00 0.00 C

ATOM 264 O ILE A 14 20.843 4.877 -30.700 1.00 0.00 O

ATOM 265 CB ILE A 14 22.957 2.664 -31.125 1.00 0.00 C

ATOM 266 CG1 ILE A 14 24.458 2.400 -31.250 1.00 0.00 C

ATOM 267 CG2 ILE A 14 22.453 3.353 -32.394 1.00 0.00 C

ATOM 268 CD1 ILE A 14 24.718 0.893 -31.182 1.00 0.00 C

ATOM 269 H ILE A 14 22.725 1.855 -28.612 1.00 99.99 H

ATOM 270 HA ILE A 14 23.351 4.426 -29.955 1.00 99.99 H

ATOM 271 HB ILE A 14 22.436 1.728 -30.992 1.00 99.99 H

ATOM 272 HG12 ILE A 14 24.814 2.784 -32.195 1.00 99.99 H

ATOM 273 HG13 ILE A 14 24.979 2.891 -30.442 1.00 99.99 H

ATOM 274 HG21 ILE A 14 22.961 4.298 -32.517 1.00 99.99 H

ATOM 275 HG22 ILE A 14 22.652 2.723 -33.249 1.00 99.99 H

ATOM 276 HG23 ILE A 14 21.390 3.524 -32.313 1.00 99.99 H

ATOM 277 HD11 ILE A 14 23.966 0.426 -30.563 1.00 99.99 H

ATOM 278 HD12 ILE A 14 24.676 0.476 -32.177 1.00 99.99 H

ATOM 279 HD13 ILE A 14 25.695 0.715 -30.758 1.00 99.99 H

ATOM 280 N HIS A 15 20.441 3.471 -29.055 1.00 0.00 N

ATOM 281 CA HIS A 15 19.008 3.864 -28.984 1.00 0.00 C

ATOM 282 C HIS A 15 18.751 4.563 -27.649 1.00 0.00 C

ATOM 283 O HIS A 15 19.622 4.646 -26.806 1.00 0.00 O

ATOM 284 CB HIS A 15 18.133 2.613 -29.080 1.00 0.00 C

ATOM 285 CG HIS A 15 17.330 2.660 -30.351 1.00 0.00 C

ATOM 286 CD2 HIS A 15 17.638 3.096 -31.616 1.00 0.00 C

ATOM 287 ND1 HIS A 15 16.018 2.216 -30.413 1.00 0.00 N

ATOM 288 CE1 HIS A 15 15.590 2.393 -31.676 1.00 0.00 C

ATOM 289 NE2 HIS A 15 16.538 2.927 -32.451 1.00 0.00 N

ATOM 290 H HIS A 15 20.791 2.794 -28.439 1.00 99.99 H

ATOM 291 HA HIS A 15 18.771 4.533 -29.798 1.00 99.99 H

ATOM 292 HB2 HIS A 15 18.760 1.734 -29.084 1.00 99.99 H

ATOM 293 HB3 HIS A 15 17.464 2.575 -28.233 1.00 99.99 H

ATOM 294 HD1 HIS A 15 15.498 1.841 -29.672 1.00 99.99 H

ATOM 295 HD2 HIS A 15 18.590 3.508 -31.917 1.00 99.99 H

ATOM 296 HE1 HIS A 15 14.599 2.136 -32.022 1.00 99.99 H

ATOM 297 N PRO A 16 17.530 5.077 -27.455 1.00 0.00 N

ATOM 298 CA PRO A 16 17.155 5.773 -26.220 1.00 0.00 C

ATOM 299 C PRO A 16 17.009 4.809 -25.038 1.00 0.00 C

ATOM 300 O PRO A 16 17.300 5.150 -23.909 1.00 0.00 O

ATOM 301 CB PRO A 16 15.801 6.395 -26.556 1.00 0.00 C

ATOM 302 CG PRO A 16 15.246 5.532 -27.640 1.00 0.00 C

ATOM 303 CD PRO A 16 16.422 5.022 -28.425 1.00 0.00 C

ATOM 304 HA PRO A 16 17.849 6.553 -25.964 1.00 99.99 H

ATOM 305 HB2 PRO A 16 15.170 6.386 -25.679 1.00 99.99 H

ATOM 306 HB3 PRO A 16 15.942 7.412 -26.890 1.00 99.99 H

ATOM 307 HG2 PRO A 16 14.693 4.712 -27.205 1.00 99.99 H

ATOM 308 HG3 PRO A 16 14.592 6.117 -28.270 1.00 99.99 H

ATOM 309 HD2 PRO A 16 16.242 4.012 -28.763 1.00 99.99 H

ATOM 310 HD3 PRO A 16 16.612 5.658 -29.277 1.00 99.99 H

ATOM 311 N ASP A 17 16.548 3.615 -25.284 1.00 0.00 N

ATOM 312 CA ASP A 17 16.369 2.641 -24.168 1.00 0.00 C

ATOM 313 C ASP A 17 17.362 1.481 -24.301 1.00 0.00 C

ATOM 314 O ASP A 17 17.509 0.678 -23.401 1.00 0.00 O

ATOM 315 CB ASP A 17 14.944 2.086 -24.211 1.00 0.00 C

ATOM 316 CG ASP A 17 13.968 3.212 -24.558 1.00 0.00 C

ATOM 317 OD1 ASP A 17 13.595 3.944 -23.656 1.00 0.00 O

ATOM 318 OD2 ASP A 17 13.610 3.322 -25.719 1.00 0.00 O1-

ATOM 319 H ASP A 17 16.303 3.362 -26.198 1.00 99.99 H

ATOM 320 HA ASP A 17 16.523 3.143 -23.224 1.00 99.99 H

ATOM 321 HB2 ASP A 17 14.882 1.312 -24.962 1.00 99.99 H

ATOM 322 HB3 ASP A 17 14.689 1.673 -23.246 1.00 99.99 H

ATOM 323 N ASP A 18 18.038 1.374 -25.412 1.00 0.00 N

ATOM 324 CA ASP A 18 19.003 0.252 -25.584 1.00 0.00 C

ATOM 325 C ASP A 18 20.086 0.332 -24.507 1.00 0.00 C

ATOM 326 O ASP A 18 20.857 1.271 -24.465 1.00 0.00 O

ATOM 327 CB ASP A 18 19.658 0.351 -26.962 1.00 0.00 C

ATOM 328 CG ASP A 18 18.764 -0.330 -28.001 1.00 0.00 C

ATOM 329 OD1 ASP A 18 17.722 -0.835 -27.616 1.00 0.00 O

ATOM 330 OD2 ASP A 18 19.135 -0.334 -29.163 1.00 0.00 O1-

ATOM 331 H ASP A 18 17.906 2.022 -26.135 1.00 99.99 H

ATOM 332 HA ASP A 18 18.473 -0.686 -25.509 1.00 99.99 H

ATOM 333 HB2 ASP A 18 19.790 1.390 -27.225 1.00 99.99 H

ATOM 334 HB3 ASP A 18 20.621 -0.140 -26.938 1.00 99.99 H

ATOM 335 N LEU A 19 20.168 -0.642 -23.642 1.00 0.00 N

ATOM 336 CA LEU A 19 21.219 -0.607 -22.588 1.00 0.00 C

ATOM 337 C LEU A 19 22.548 -1.041 -23.214 1.00 0.00 C

ATOM 338 O LEU A 19 22.610 -1.999 -23.959 1.00 0.00 O

ATOM 339 CB LEU A 19 20.815 -1.552 -21.445 1.00 0.00 C

ATOM 340 CG LEU A 19 22.044 -1.998 -20.646 1.00 0.00 C

ATOM 341 CD1 LEU A 19 22.792 -3.090 -21.415 1.00 0.00 C

ATOM 342 CD2 LEU A 19 22.969 -0.803 -20.411 1.00 0.00 C

ATOM 343 H LEU A 19 19.553 -1.404 -23.684 1.00 99.99 H

ATOM 344 HA LEU A 19 21.313 0.400 -22.209 1.00 99.99 H

ATOM 345 HB2 LEU A 19 20.138 -1.034 -20.785 1.00 99.99 H

ATOM 346 HB3 LEU A 19 20.318 -2.420 -21.854 1.00 99.99 H

ATOM 347 HG LEU A 19 21.724 -2.392 -19.693 1.00 99.99 H

ATOM 348 HD11 LEU A 19 22.126 -3.545 -22.134 1.00 99.99 H

ATOM 349 HD12 LEU A 19 23.634 -2.656 -21.930 1.00 99.99 H

ATOM 350 HD13 LEU A 19 23.142 -3.842 -20.723 1.00 99.99 H

ATOM 351 HD21 LEU A 19 22.504 0.094 -20.790 1.00 99.99 H

ATOM 352 HD22 LEU A 19 23.153 -0.695 -19.353 1.00 99.99 H

ATOM 353 HD23 LEU A 19 23.904 -0.966 -20.921 1.00 99.99 H

ATOM 354 N SER A 20 23.609 -0.336 -22.930 1.00 0.00 N

ATOM 355 CA SER A 20 24.930 -0.695 -23.521 1.00 0.00 C

ATOM 356 C SER A 20 25.600 -1.797 -22.697 1.00 0.00 C

ATOM 357 O SER A 20 25.625 -1.755 -21.484 1.00 0.00 O

ATOM 358 CB SER A 20 25.830 0.542 -23.525 1.00 0.00 C

ATOM 359 OG SER A 20 26.616 0.560 -22.342 1.00 0.00 O

ATOM 360 H SER A 20 23.540 0.438 -22.333 1.00 99.99 H

ATOM 361 HA SER A 20 24.797 -1.036 -24.536 1.00 99.99 H

ATOM 362 HB2 SER A 20 26.478 0.513 -24.388 1.00 99.99 H

ATOM 363 HB3 SER A 20 25.219 1.432 -23.564 1.00 99.99 H

ATOM 364 HG SER A 20 27.513 0.312 -22.579 1.00 99.99 H

ATOM 365 N PHE A 21 26.168 -2.771 -23.353 1.00 0.00 N

ATOM 366 CA PHE A 21 26.862 -3.861 -22.615 1.00 0.00 C

ATOM 367 C PHE A 21 28.151 -4.213 -23.357 1.00 0.00 C

ATOM 368 O PHE A 21 28.227 -4.109 -24.565 1.00 0.00 O

ATOM 369 CB PHE A 21 25.960 -5.097 -22.513 1.00 0.00 C

ATOM 370 CG PHE A 21 25.277 -5.367 -23.834 1.00 0.00 C

ATOM 371 CD1 PHE A 21 24.029 -4.794 -24.108 1.00 0.00 C

ATOM 372 CD2 PHE A 21 25.883 -6.207 -24.775 1.00 0.00 C

ATOM 373 CE1 PHE A 21 23.389 -5.058 -25.325 1.00 0.00 C

ATOM 374 CE2 PHE A 21 25.242 -6.474 -25.991 1.00 0.00 C

ATOM 375 CZ PHE A 21 23.995 -5.899 -26.267 1.00 0.00 C

ATOM 376 H PHE A 21 26.158 -2.772 -24.333 1.00 99.99 H

ATOM 377 HA PHE A 21 27.104 -3.516 -21.619 1.00 99.99 H

ATOM 378 HB2 PHE A 21 26.558 -5.953 -22.240 1.00 99.99 H

ATOM 379 HB3 PHE A 21 25.211 -4.928 -21.753 1.00 99.99 H

ATOM 380 HD1 PHE A 21 23.562 -4.145 -23.382 1.00 99.99 H

ATOM 381 HD2 PHE A 21 26.846 -6.649 -24.564 1.00 99.99 H

ATOM 382 HE1 PHE A 21 22.428 -4.615 -25.537 1.00 99.99 H

ATOM 383 HE2 PHE A 21 25.710 -7.122 -26.717 1.00 99.99 H

ATOM 384 HZ PHE A 21 23.499 -6.107 -27.204 1.00 99.99 H

ATOM 385 N LYS A 22 29.170 -4.616 -22.651 1.00 0.00 N

ATOM 386 CA LYS A 22 30.450 -4.956 -23.331 1.00 0.00 C

ATOM 387 C LYS A 22 30.659 -6.467 -23.297 1.00 0.00 C

ATOM 388 O LYS A 22 30.390 -7.112 -22.304 1.00 0.00 O

ATOM 389 CB LYS A 22 31.606 -4.271 -22.600 1.00 0.00 C

ATOM 390 CG LYS A 22 32.827 -4.210 -23.520 1.00 0.00 C

ATOM 391 CD LYS A 22 34.063 -4.696 -22.760 1.00 0.00 C

ATOM 392 CE LYS A 22 35.059 -5.312 -23.745 1.00 0.00 C

ATOM 393 NZ LYS A 22 35.333 -4.345 -24.846 1.00 0.00 N1+

ATOM 394 H LYS A 22 29.096 -4.691 -21.674 1.00 99.99 H

ATOM 395 HA LYS A 22 30.423 -4.613 -24.354 1.00 99.99 H

ATOM 396 HB2 LYS A 22 31.314 -3.270 -22.322 1.00 99.99 H

ATOM 397 HB3 LYS A 22 31.854 -4.833 -21.711 1.00 99.99 H

ATOM 398 HG2 LYS A 22 32.662 -4.842 -24.380 1.00 99.99 H

ATOM 399 HG3 LYS A 22 32.982 -3.192 -23.845 1.00 99.99 H

ATOM 400 HD2 LYS A 22 34.527 -3.861 -22.255 1.00 99.99 H

ATOM 401 HD3 LYS A 22 33.770 -5.438 -22.033 1.00 99.99 H

ATOM 402 HE2 LYS A 22 35.980 -5.542 -23.230 1.00 99.99 H

ATOM 403 HE3 LYS A 22 34.641 -6.218 -24.159 1.00 99.99 H

ATOM 404 HZ1 LYS A 22 34.896 -3.429 -24.619 1.00 99.99 H

ATOM 405 HZ2 LYS A 22 36.359 -4.220 -24.951 1.00 99.99 H

ATOM 406 HZ3 LYS A 22 34.934 -4.710 -25.735 1.00 99.99 H

ATOM 407 N LYS A 23 31.147 -7.041 -24.365 1.00 0.00 N

ATOM 408 CA LYS A 23 31.377 -8.511 -24.359 1.00 0.00 C

ATOM 409 C LYS A 23 31.988 -8.897 -23.013 1.00 0.00 C

ATOM 410 O LYS A 23 32.648 -8.104 -22.371 1.00 0.00 O

ATOM 411 CB LYS A 23 32.332 -8.903 -25.485 1.00 0.00 C

ATOM 412 CG LYS A 23 33.545 -7.971 -25.473 1.00 0.00 C

ATOM 413 CD LYS A 23 34.333 -8.142 -26.773 1.00 0.00 C

ATOM 414 CE LYS A 23 35.209 -9.394 -26.678 1.00 0.00 C

ATOM 415 NZ LYS A 23 35.966 -9.568 -27.949 1.00 0.00 N1+

ATOM 416 H LYS A 23 31.368 -6.509 -25.157 1.00 99.99 H

ATOM 417 HA LYS A 23 30.438 -9.031 -24.477 1.00 99.99 H

ATOM 418 HB2 LYS A 23 32.657 -9.923 -25.334 1.00 99.99 H

ATOM 419 HB3 LYS A 23 31.823 -8.823 -26.434 1.00 99.99 H

ATOM 420 HG2 LYS A 23 33.211 -6.947 -25.387 1.00 99.99 H

ATOM 421 HG3 LYS A 23 34.178 -8.215 -24.633 1.00 99.99 H

ATOM 422 HD2 LYS A 23 33.646 -8.246 -27.600 1.00 99.99 H

ATOM 423 HD3 LYS A 23 34.959 -7.277 -26.932 1.00 99.99 H

ATOM 424 HE2 LYS A 23 35.902 -9.286 -25.857 1.00 99.99 H

ATOM 425 HE3 LYS A 23 34.583 -10.258 -26.510 1.00 99.99 H

ATOM 426 HZ1 LYS A 23 36.297 -8.642 -28.286 1.00 99.99 H

ATOM 427 HZ2 LYS A 23 36.784 -10.190 -27.783 1.00 99.99 H

ATOM 428 HZ3 LYS A 23 35.346 -9.994 -28.667 1.00 99.99 H

ATOM 429 N GLY A 24 31.765 -10.102 -22.572 1.00 0.00 N

ATOM 430 CA GLY A 24 32.325 -10.528 -21.258 1.00 0.00 C

ATOM 431 C GLY A 24 31.463 -9.962 -20.119 1.00 0.00 C

ATOM 432 O GLY A 24 31.540 -10.410 -18.992 1.00 0.00 O

ATOM 433 H GLY A 24 31.229 -10.727 -23.103 1.00 99.99 H

ATOM 434 HA2 GLY A 24 33.335 -10.158 -21.161 1.00 99.99 H

ATOM 435 HA3 GLY A 24 32.330 -11.606 -21.202 1.00 99.99 H

ATOM 436 N GLU A 25 30.644 -8.982 -20.402 1.00 0.00 N

ATOM 437 CA GLU A 25 29.783 -8.391 -19.334 1.00 0.00 C

ATOM 438 C GLU A 25 28.529 -9.250 -19.146 1.00 0.00 C

ATOM 439 O GLU A 25 28.074 -9.916 -20.054 1.00 0.00 O

ATOM 440 CB GLU A 25 29.378 -6.969 -19.726 1.00 0.00 C

ATOM 441 CG GLU A 25 29.128 -6.143 -18.463 1.00 0.00 C

ATOM 442 CD GLU A 25 29.999 -4.885 -18.495 1.00 0.00 C

ATOM 443 OE1 GLU A 25 31.202 -5.025 -18.637 1.00 0.00 O

ATOM 444 OE2 GLU A 25 29.447 -3.803 -18.379 1.00 0.00 O1-

ATOM 445 H GLU A 25 30.595 -8.632 -21.314 1.00 99.99 H

ATOM 446 HA GLU A 25 30.321 -8.370 -18.401 1.00 99.99 H

ATOM 447 HB2 GLU A 25 30.171 -6.515 -20.302 1.00 99.99 H

ATOM 448 HB3 GLU A 25 28.476 -7.002 -20.319 1.00 99.99 H

ATOM 449 HG2 GLU A 25 28.087 -5.859 -18.418 1.00 99.99 H

ATOM 450 HG3 GLU A 25 29.379 -6.732 -17.592 1.00 99.99 H

ATOM 451 N LYS A 26 27.975 -9.243 -17.961 1.00 0.00 N

ATOM 452 CA LYS A 26 26.756 -10.060 -17.690 1.00 0.00 C

ATOM 453 C LYS A 26 25.528 -9.153 -17.605 1.00 0.00 C

ATOM 454 O LYS A 26 25.598 -8.028 -17.152 1.00 0.00 O

ATOM 455 CB LYS A 26 26.930 -10.803 -16.364 1.00 0.00 C

ATOM 456 CG LYS A 26 27.319 -12.257 -16.640 1.00 0.00 C

ATOM 457 CD LYS A 26 28.365 -12.708 -15.618 1.00 0.00 C

ATOM 458 CE LYS A 26 27.671 -13.059 -14.300 1.00 0.00 C

ATOM 459 NZ LYS A 26 28.662 -13.659 -13.362 1.00 0.00 N1+

ATOM 460 H LYS A 26 28.367 -8.701 -17.244 1.00 99.99 H

ATOM 461 HA LYS A 26 26.614 -10.777 -18.485 1.00 99.99 H

ATOM 462 HB2 LYS A 26 27.707 -10.327 -15.784 1.00 99.99 H

ATOM 463 HB3 LYS A 26 26.002 -10.777 -15.812 1.00 99.99 H

ATOM 464 HG2 LYS A 26 26.444 -12.885 -16.561 1.00 99.99 H

ATOM 465 HG3 LYS A 26 27.731 -12.337 -17.635 1.00 99.99 H

ATOM 466 HD2 LYS A 26 28.885 -13.576 -15.994 1.00 99.99 H

ATOM 467 HD3 LYS A 26 29.072 -11.909 -15.450 1.00 99.99 H

ATOM 468 HE2 LYS A 26 27.256 -12.164 -13.861 1.00 99.99 H

ATOM 469 HE3 LYS A 26 26.878 -13.768 -14.488 1.00 99.99 H

ATOM 470 HZ1 LYS A 26 29.250 -14.348 -13.873 1.00 99.99 H

ATOM 471 HZ2 LYS A 26 29.267 -12.909 -12.970 1.00 99.99 H

ATOM 472 HZ3 LYS A 26 28.161 -14.137 -12.586 1.00 99.99 H

ATOM 473 N MET A 27 24.403 -9.642 -18.045 1.00 0.00 N

ATOM 474 CA MET A 27 23.154 -8.833 -18.009 1.00 0.00 C

ATOM 475 C MET A 27 21.985 -9.705 -17.559 1.00 0.00 C

ATOM 476 O MET A 27 21.980 -10.907 -17.735 1.00 0.00 O

ATOM 477 CB MET A 27 22.843 -8.306 -19.407 1.00 0.00 C

ATOM 478 CG MET A 27 23.342 -6.864 -19.535 1.00 0.00 C

ATOM 479 SD MET A 27 23.192 -6.322 -21.257 1.00 0.00 S

ATOM 480 CE MET A 27 23.963 -7.769 -22.025 1.00 0.00 C

ATOM 481 H MET A 27 24.376 -10.551 -18.411 1.00 99.99 H

ATOM 482 HA MET A 27 23.244 -7.993 -17.334 1.00 99.99 H

ATOM 483 HB2 MET A 27 23.330 -8.926 -20.144 1.00 99.99 H

ATOM 484 HB3 MET A 27 21.774 -8.329 -19.561 1.00 99.99 H

ATOM 485 HG2 MET A 27 22.746 -6.221 -18.904 1.00 99.99 H

ATOM 486 HG3 MET A 27 24.375 -6.809 -19.228 1.00 99.99 H

ATOM 487 HE1 MET A 27 24.617 -8.250 -21.311 1.00 99.99 H

ATOM 488 HE2 MET A 27 23.199 -8.464 -22.335 1.00 99.99 H

ATOM 489 HE3 MET A 27 24.533 -7.455 -22.890 1.00 99.99 H

ATOM 490 N LYS A 28 20.988 -9.093 -16.990 1.00 0.00 N

ATOM 491 CA LYS A 28 19.795 -9.855 -16.530 1.00 0.00 C

ATOM 492 C LYS A 28 18.565 -9.288 -17.236 1.00 0.00 C

ATOM 493 O LYS A 28 18.416 -8.091 -17.359 1.00 0.00 O

ATOM 494 CB LYS A 28 19.636 -9.699 -15.016 1.00 0.00 C

ATOM 495 CG LYS A 28 18.406 -10.481 -14.549 1.00 0.00 C

ATOM 496 CD LYS A 28 17.833 -9.827 -13.290 1.00 0.00 C

ATOM 497 CE LYS A 28 17.750 -10.864 -12.169 1.00 0.00 C

ATOM 498 NZ LYS A 28 19.071 -10.966 -11.488 1.00 0.00 N1+

ATOM 499 H LYS A 28 21.024 -8.121 -16.871 1.00 99.99 H

ATOM 500 HA LYS A 28 19.910 -10.899 -16.781 1.00 99.99 H

ATOM 501 HB2 LYS A 28 20.516 -10.083 -14.521 1.00 99.99 H

ATOM 502 HB3 LYS A 28 19.513 -8.654 -14.772 1.00 99.99 H

ATOM 503 HG2 LYS A 28 17.660 -10.476 -15.329 1.00 99.99 H

ATOM 504 HG3 LYS A 28 18.690 -11.499 -14.328 1.00 99.99 H

ATOM 505 HD2 LYS A 28 18.475 -9.014 -12.982 1.00 99.99 H

ATOM 506 HD3 LYS A 28 16.845 -9.445 -13.501 1.00 99.99 H

ATOM 507 HE2 LYS A 28 16.999 -10.563 -11.455 1.00 99.99 H

ATOM 508 HE3 LYS A 28 17.485 -11.825 -12.587 1.00 99.99 H

ATOM 509 HZ1 LYS A 28 19.547 -10.041 -11.516 1.00 99.99 H

ATOM 510 HZ2 LYS A 28 18.931 -11.255 -10.499 1.00 99.99 H

ATOM 511 HZ3 LYS A 28 19.659 -11.674 -11.973 1.00 99.99 H

ATOM 512 N VAL A 29 17.690 -10.128 -17.714 1.00 0.00 N

ATOM 513 CA VAL A 29 16.489 -9.604 -18.424 1.00 0.00 C

ATOM 514 C VAL A 29 15.292 -9.566 -17.473 1.00 0.00 C

ATOM 515 O VAL A 29 14.874 -10.575 -16.940 1.00 0.00 O

ATOM 516 CB VAL A 29 16.168 -10.500 -19.619 1.00 0.00 C

ATOM 517 CG1 VAL A 29 15.467 -9.675 -20.696 1.00 0.00 C

ATOM 518 CG2 VAL A 29 17.465 -11.083 -20.183 1.00 0.00 C

ATOM 519 H VAL A 29 17.826 -11.092 -17.615 1.00 99.99 H

ATOM 520 HA VAL A 29 16.705 -8.603 -18.764 1.00 99.99 H

ATOM 521 HB VAL A 29 15.520 -11.303 -19.302 1.00 99.99 H

ATOM 522 HG11 VAL A 29 14.755 -9.008 -20.234 1.00 99.99 H

ATOM 523 HG12 VAL A 29 16.200 -9.098 -21.240 1.00 99.99 H

ATOM 524 HG13 VAL A 29 14.952 -10.337 -21.376 1.00 99.99 H

ATOM 525 HG21 VAL A 29 18.257 -10.356 -20.091 1.00 99.99 H

ATOM 526 HG22 VAL A 29 17.728 -11.974 -19.632 1.00 99.99 H

ATOM 527 HG23 VAL A 29 17.325 -11.333 -21.225 1.00 99.99 H

ATOM 528 N LEU A 30 14.741 -8.404 -17.256 1.00 0.00 N

ATOM 529 CA LEU A 30 13.574 -8.289 -16.339 1.00 0.00 C

ATOM 530 C LEU A 30 12.277 -8.555 -17.109 1.00 0.00 C

ATOM 531 O LEU A 30 11.250 -8.836 -16.525 1.00 0.00 O

ATOM 532 CB LEU A 30 13.530 -6.879 -15.745 1.00 0.00 C

ATOM 533 CG LEU A 30 14.815 -6.612 -14.958 1.00 0.00 C

ATOM 534 CD1 LEU A 30 15.142 -7.825 -14.084 1.00 0.00 C

ATOM 535 CD2 LEU A 30 15.968 -6.360 -15.932 1.00 0.00 C

ATOM 536 H LEU A 30 15.101 -7.604 -17.693 1.00 99.99 H

ATOM 537 HA LEU A 30 13.672 -9.010 -15.542 1.00 99.99 H

ATOM 538 HB2 LEU A 30 13.440 -6.156 -16.542 1.00 99.99 H

ATOM 539 HB3 LEU A 30 12.680 -6.794 -15.085 1.00 99.99 H

ATOM 540 HG LEU A 30 14.679 -5.744 -14.330 1.00 99.99 H

ATOM 541 HD11 LEU A 30 14.224 -8.273 -13.732 1.00 99.99 H

ATOM 542 HD12 LEU A 30 15.696 -8.548 -14.664 1.00 99.99 H

ATOM 543 HD13 LEU A 30 15.736 -7.510 -13.239 1.00 99.99 H

ATOM 544 HD21 LEU A 30 15.577 -5.966 -16.858 1.00 99.99 H

ATOM 545 HD22 LEU A 30 16.656 -5.649 -15.500 1.00 99.99 H

ATOM 546 HD23 LEU A 30 16.485 -7.289 -16.126 1.00 99.99 H

ATOM 547 N GLU A 31 12.307 -8.470 -18.413 1.00 0.00 N

ATOM 548 CA GLU A 31 11.063 -8.719 -19.194 1.00 0.00 C

ATOM 549 C GLU A 31 11.423 -9.193 -20.602 1.00 0.00 C

ATOM 550 O GLU A 31 12.357 -8.711 -21.211 1.00 0.00 O

ATOM 551 CB GLU A 31 10.250 -7.427 -19.282 1.00 0.00 C

ATOM 552 CG GLU A 31 8.757 -7.763 -19.280 1.00 0.00 C

ATOM 553 CD GLU A 31 7.953 -6.521 -19.668 1.00 0.00 C

ATOM 554 OE1 GLU A 31 8.555 -5.577 -20.154 1.00 0.00 O

ATOM 555 OE2 GLU A 31 6.749 -6.534 -19.473 1.00 0.00 O1-

ATOM 556 H GLU A 31 13.141 -8.240 -18.877 1.00 99.99 H

ATOM 557 HA GLU A 31 10.476 -9.479 -18.699 1.00 99.99 H

ATOM 558 HB2 GLU A 31 10.479 -6.799 -18.434 1.00 99.99 H

ATOM 559 HB3 GLU A 31 10.500 -6.905 -20.194 1.00 99.99 H

ATOM 560 HG2 GLU A 31 8.566 -8.553 -19.992 1.00 99.99 H

ATOM 561 HG3 GLU A 31 8.463 -8.088 -18.293 1.00 99.99 H

ATOM 562 N GLU A 32 10.682 -10.129 -21.126 1.00 0.00 N

ATOM 563 CA GLU A 32 10.972 -10.631 -22.497 1.00 0.00 C

ATOM 564 C GLU A 32 9.883 -10.141 -23.451 1.00 0.00 C

ATOM 565 O GLU A 32 8.707 -10.196 -23.148 1.00 0.00 O

ATOM 566 CB GLU A 32 10.996 -12.161 -22.489 1.00 0.00 C

ATOM 567 CG GLU A 32 11.111 -12.679 -23.924 1.00 0.00 C

ATOM 568 CD GLU A 32 12.017 -13.912 -23.950 1.00 0.00 C

ATOM 569 OE1 GLU A 32 11.803 -14.798 -23.140 1.00 0.00 O

ATOM 570 OE2 GLU A 32 12.911 -13.948 -24.780 1.00 0.00 O1-

ATOM 571 H GLU A 32 9.929 -10.500 -20.620 1.00 99.99 H

ATOM 572 HA GLU A 32 11.932 -10.256 -22.824 1.00 99.99 H

ATOM 573 HB2 GLU A 32 11.844 -12.505 -21.914 1.00 99.99 H

ATOM 574 HB3 GLU A 32 10.085 -12.533 -22.044 1.00 99.99 H

ATOM 575 HG2 GLU A 32 10.130 -12.946 -24.290 1.00 99.99 H

ATOM 576 HG3 GLU A 32 11.533 -11.909 -24.552 1.00 99.99 H

ATOM 577 N HIS A 33 10.262 -9.661 -24.602 1.00 0.00 N

ATOM 578 CA HIS A 33 9.253 -9.167 -25.576 1.00 0.00 C

ATOM 579 C HIS A 33 9.381 -9.958 -26.878 1.00 0.00 C

ATOM 580 O HIS A 33 9.184 -9.410 -27.960 1.00 0.00 O

ATOM 581 CB HIS A 33 9.507 -7.686 -25.855 1.00 99.99 C

ATOM 582 CG HIS A 33 8.519 -6.853 -25.087 1.00 99.99 C

ATOM 583 CD2 HIS A 33 8.673 -5.990 -24.029 1.00 99.99 C

ATOM 584 ND1 HIS A 33 7.165 -6.849 -25.383 1.00 99.99 N

ATOM 585 CE1 HIS A 33 6.563 -6.009 -24.521 1.00 99.99 C

ATOM 586 NE2 HIS A 33 7.437 -5.458 -23.674 1.00 99.99 N

ATOM 587 N GLY A 34 9.703 -11.219 -26.786 1.00 0.00 N

ATOM 588 CA GLY A 34 9.847 -12.042 -28.018 1.00 0.00 C

ATOM 589 C GLY A 34 11.318 -12.069 -28.441 1.00 0.00 C

ATOM 590 O GLY A 34 12.149 -12.674 -27.794 1.00 0.00 O

ATOM 591 H GLY A 34 9.851 -11.624 -25.906 1.00 99.99 H

ATOM 592 HA2 GLY A 34 9.252 -11.613 -28.810 1.00 99.99 H

ATOM 593 HA3 GLY A 34 9.511 -13.049 -27.820 1.00 99.99 H

ATOM 594 N GLU A 35 11.644 -11.423 -29.527 1.00 0.00 N

ATOM 595 CA GLU A 35 13.060 -11.417 -29.994 1.00 0.00 C

ATOM 596 C GLU A 35 13.833 -10.295 -29.296 1.00 0.00 C

ATOM 597 O GLU A 35 15.035 -10.183 -29.433 1.00 0.00 O

ATOM 598 CB GLU A 35 13.095 -11.193 -31.507 1.00 0.00 C

ATOM 599 CG GLU A 35 14.164 -12.092 -32.130 1.00 0.00 C

ATOM 600 CD GLU A 35 13.537 -13.429 -32.529 1.00 0.00 C

ATOM 601 OE1 GLU A 35 12.357 -13.439 -32.837 1.00 0.00 O

ATOM 602 OE2 GLU A 35 14.248 -14.420 -32.520 1.00 0.00 O1-

ATOM 603 H GLU A 35 10.957 -10.946 -30.037 1.00 99.99 H

ATOM 604 HA GLU A 35 13.518 -12.367 -29.762 1.00 99.99 H

ATOM 605 HB2 GLU A 35 12.131 -11.434 -31.929 1.00 99.99 H

ATOM 606 HB3 GLU A 35 13.330 -10.159 -31.712 1.00 99.99 H

ATOM 607 HG2 GLU A 35 14.573 -11.610 -33.007 1.00 99.99 H

ATOM 608 HG3 GLU A 35 14.953 -12.264 -31.413 1.00 99.99 H

ATOM 609 N TRP A 36 13.159 -9.460 -28.553 1.00 0.00 N

ATOM 610 CA TRP A 36 13.871 -8.349 -27.859 1.00 0.00 C

ATOM 611 C TRP A 36 13.477 -8.325 -26.380 1.00 0.00 C

ATOM 612 O TRP A 36 12.337 -8.550 -26.028 1.00 0.00 O

ATOM 613 CB TRP A 36 13.489 -7.017 -28.507 1.00 0.00 C

ATOM 614 CG TRP A 36 14.308 -6.809 -29.740 1.00 0.00 C

ATOM 615 CD1 TRP A 36 14.096 -7.423 -30.927 1.00 0.00 C

ATOM 616 CD2 TRP A 36 15.461 -5.938 -29.931 1.00 0.00 C

ATOM 617 CE2 TRP A 36 15.909 -6.070 -31.266 1.00 0.00 C

ATOM 618 CE3 TRP A 36 16.154 -5.056 -29.082 1.00 0.00 C

ATOM 619 NE1 TRP A 36 15.046 -6.986 -31.833 1.00 0.00 N

ATOM 620 CZ2 TRP A 36 17.006 -5.352 -31.743 1.00 0.00 C

ATOM 621 CZ3 TRP A 36 17.259 -4.332 -29.560 1.00 0.00 C

ATOM 622 CH2 TRP A 36 17.684 -4.479 -30.887 1.00 0.00 C

ATOM 623 H TRP A 36 12.190 -9.561 -28.455 1.00 99.99 H

ATOM 624 HA TRP A 36 14.937 -8.499 -27.947 1.00 99.99 H

ATOM 625 HB2 TRP A 36 12.441 -7.031 -28.769 1.00 99.99 H

ATOM 626 HB3 TRP A 36 13.675 -6.212 -27.812 1.00 99.99 H

ATOM 627 HD1 TRP A 36 13.313 -8.139 -31.133 1.00 99.99 H

ATOM 628 HE1 TRP A 36 15.114 -7.278 -32.766 1.00 99.99 H

ATOM 629 HE3 TRP A 36 15.835 -4.935 -28.058 1.00 99.99 H

ATOM 630 HZ2 TRP A 36 17.330 -5.469 -32.767 1.00 99.99 H

ATOM 631 HZ3 TRP A 36 17.784 -3.657 -28.900 1.00 99.99 H

ATOM 632 HH2 TRP A 36 18.534 -3.920 -31.248 1.00 99.99 H

ATOM 633 N TRP A 37 14.411 -8.041 -25.512 1.00 0.00 N

ATOM 634 CA TRP A 37 14.083 -7.992 -24.058 1.00 0.00 C

ATOM 635 C TRP A 37 14.816 -6.819 -23.407 1.00 0.00 C

ATOM 636 O TRP A 37 15.715 -6.238 -23.981 1.00 0.00 O

ATOM 637 CB TRP A 37 14.527 -9.284 -23.368 1.00 0.00 C

ATOM 638 CG TRP A 37 14.637 -10.400 -24.355 1.00 0.00 C

ATOM 639 CD1 TRP A 37 13.646 -10.828 -25.169 1.00 0.00 C

ATOM 640 CD2 TRP A 37 15.789 -11.247 -24.630 1.00 0.00 C

ATOM 641 CE2 TRP A 37 15.434 -12.180 -25.631 1.00 0.00 C

ATOM 642 CE3 TRP A 37 17.096 -11.294 -24.112 1.00 0.00 C

ATOM 643 NE1 TRP A 37 14.117 -11.885 -25.928 1.00 0.00 N

ATOM 644 CZ2 TRP A 37 16.343 -13.127 -26.101 1.00 0.00 C

ATOM 645 CZ3 TRP A 37 18.014 -12.245 -24.583 1.00 0.00 C

ATOM 646 CH2 TRP A 37 17.638 -13.161 -25.575 1.00 0.00 C

ATOM 647 H TRP A 37 15.321 -7.854 -25.822 1.00 99.99 H

ATOM 648 HA TRP A 37 13.015 -7.873 -23.940 1.00 99.99 H

ATOM 649 HB2 TRP A 37 15.489 -9.124 -22.907 1.00 99.99 H

ATOM 650 HB3 TRP A 37 13.806 -9.548 -22.609 1.00 99.99 H

ATOM 651 HD1 TRP A 37 12.650 -10.413 -25.220 1.00 99.99 H

ATOM 652 HE1 TRP A 37 13.598 -12.376 -26.597 1.00 99.99 H

ATOM 653 HE3 TRP A 37 17.395 -10.593 -23.347 1.00 99.99 H

ATOM 654 HZ2 TRP A 37 16.046 -13.831 -26.864 1.00 99.99 H

ATOM 655 HZ3 TRP A 37 19.015 -12.272 -24.178 1.00 99.99 H

ATOM 656 HH2 TRP A 37 18.350 -13.889 -25.934 1.00 99.99 H

ATOM 657 N LYS A 38 14.453 -6.483 -22.202 1.00 0.00 N

ATOM 658 CA LYS A 38 15.141 -5.367 -21.498 1.00 0.00 C

ATOM 659 C LYS A 38 15.956 -5.953 -20.346 1.00 0.00 C

ATOM 660 O LYS A 38 15.425 -6.578 -19.450 1.00 0.00 O

ATOM 661 CB LYS A 38 14.105 -4.382 -20.959 1.00 0.00 C

ATOM 662 CG LYS A 38 14.701 -2.974 -20.932 1.00 0.00 C

ATOM 663 CD LYS A 38 13.656 -1.989 -20.403 1.00 0.00 C

ATOM 664 CE LYS A 38 13.993 -0.579 -20.892 1.00 0.00 C

ATOM 665 NZ LYS A 38 13.465 -0.392 -22.272 1.00 0.00 N1+

ATOM 666 H LYS A 38 13.735 -6.977 -21.752 1.00 99.99 H

ATOM 667 HA LYS A 38 15.804 -4.860 -22.184 1.00 99.99 H

ATOM 668 HB2 LYS A 38 13.238 -4.393 -21.601 1.00 99.99 H

ATOM 669 HB3 LYS A 38 13.820 -4.671 -19.959 1.00 99.99 H

ATOM 670 HG2 LYS A 38 15.567 -2.962 -20.286 1.00 99.99 H

ATOM 671 HG3 LYS A 38 14.992 -2.687 -21.931 1.00 99.99 H

ATOM 672 HD2 LYS A 38 12.679 -2.272 -20.765 1.00 99.99 H

ATOM 673 HD3 LYS A 38 13.659 -2.006 -19.323 1.00 99.99 H

ATOM 674 HE2 LYS A 38 13.542 0.148 -20.232 1.00 99.99 H

ATOM 675 HE3 LYS A 38 15.065 -0.445 -20.895 1.00 99.99 H

ATOM 676 HZ1 LYS A 38 12.956 -1.249 -22.568 1.00 99.99 H

ATOM 677 HZ2 LYS A 38 12.815 0.420 -22.288 1.00 99.99 H

ATOM 678 HZ3 LYS A 38 14.254 -0.218 -22.926 1.00 99.99 H

ATOM 679 N ALA A 39 17.246 -5.773 -20.373 1.00 0.00 N

ATOM 680 CA ALA A 39 18.099 -6.338 -19.291 1.00 0.00 C

ATOM 681 C ALA A 39 18.766 -5.216 -18.495 1.00 0.00 C

ATOM 682 O ALA A 39 18.484 -4.050 -18.680 1.00 0.00 O

ATOM 683 CB ALA A 39 19.177 -7.231 -19.909 1.00 0.00 C

ATOM 684 H ALA A 39 17.652 -5.275 -21.114 1.00 99.99 H

ATOM 685 HA ALA A 39 17.495 -6.930 -18.620 1.00 99.99 H

ATOM 686 HB1 ALA A 39 19.061 -7.244 -20.983 1.00 99.99 H

ATOM 687 HB2 ALA A 39 19.075 -8.236 -19.524 1.00 99.99 H

ATOM 688 HB3 ALA A 39 20.153 -6.845 -19.656 1.00 99.99 H

ATOM 689 N LYS A 40 19.656 -5.572 -17.608 1.00 0.00 N

ATOM 690 CA LYS A 40 20.357 -4.545 -16.787 1.00 0.00 C

ATOM 691 C LYS A 40 21.824 -4.950 -16.625 1.00 0.00 C

ATOM 692 O LYS A 40 22.156 -6.120 -16.637 1.00 0.00 O

ATOM 693 CB LYS A 40 19.696 -4.453 -15.411 1.00 0.00 C

ATOM 694 CG LYS A 40 20.052 -3.114 -14.761 1.00 0.00 C

ATOM 695 CD LYS A 40 19.836 -3.208 -13.249 1.00 0.00 C

ATOM 696 CE LYS A 40 18.521 -2.518 -12.879 1.00 0.00 C

ATOM 697 NZ LYS A 40 18.679 -1.816 -11.574 1.00 0.00 N1+

ATOM 698 H LYS A 40 19.867 -6.521 -17.486 1.00 99.99 H

ATOM 699 HA LYS A 40 20.298 -3.588 -17.283 1.00 99.99 H

ATOM 700 HB2 LYS A 40 18.624 -4.525 -15.521 1.00 99.99 H

ATOM 701 HB3 LYS A 40 20.049 -5.261 -14.787 1.00 99.99 H

ATOM 702 HG2 LYS A 40 21.087 -2.880 -14.963 1.00 99.99 H

ATOM 703 HG3 LYS A 40 19.421 -2.338 -15.168 1.00 99.99 H

ATOM 704 HD2 LYS A 40 19.793 -4.246 -12.955 1.00 99.99 H

ATOM 705 HD3 LYS A 40 20.654 -2.722 -12.738 1.00 99.99 H

ATOM 706 HE2 LYS A 40 18.262 -1.802 -13.644 1.00 99.99 H

ATOM 707 HE3 LYS A 40 17.738 -3.257 -12.797 1.00 99.99 H

ATOM 708 HZ1 LYS A 40 19.479 -1.154 -11.630 1.00 99.99 H

ATOM 709 HZ2 LYS A 40 17.810 -1.288 -11.356 1.00 99.99 H

ATOM 710 HZ3 LYS A 40 18.859 -2.515 -10.824 1.00 99.99 H

ATOM 711 N SER A 41 22.708 -3.999 -16.489 1.00 0.00 N

ATOM 712 CA SER A 41 24.150 -4.348 -16.344 1.00 0.00 C

ATOM 713 C SER A 41 24.499 -4.506 -14.863 1.00 0.00 C

ATOM 714 O SER A 41 24.257 -3.623 -14.065 1.00 0.00 O

ATOM 715 CB SER A 41 25.007 -3.236 -16.953 1.00 0.00 C

ATOM 716 OG SER A 41 26.324 -3.312 -16.427 1.00 0.00 O

ATOM 717 H SER A 41 22.427 -3.060 -16.495 1.00 99.99 H

ATOM 718 HA SER A 41 24.336 -5.273 -16.871 1.00 99.99 H

ATOM 719 HB2 SER A 41 25.040 -3.353 -18.026 1.00 99.99 H

ATOM 720 HB3 SER A 41 24.577 -2.276 -16.708 1.00 99.99 H

ATOM 721 HG SER A 41 26.888 -3.705 -17.097 1.00 99.99 H

ATOM 722 N LEU A 42 25.063 -5.619 -14.486 1.00 0.00 N

ATOM 723 CA LEU A 42 25.418 -5.816 -13.052 1.00 0.00 C

ATOM 724 C LEU A 42 26.568 -4.876 -12.680 1.00 0.00 C

ATOM 725 O LEU A 42 26.888 -4.697 -11.522 1.00 0.00 O

ATOM 726 CB LEU A 42 25.847 -7.266 -12.824 1.00 0.00 C

ATOM 727 CG LEU A 42 25.071 -7.847 -11.641 1.00 0.00 C

ATOM 728 CD1 LEU A 42 23.725 -8.387 -12.129 1.00 0.00 C

ATOM 729 CD2 LEU A 42 25.878 -8.982 -11.009 1.00 0.00 C

ATOM 730 H LEU A 42 25.247 -6.323 -15.142 1.00 99.99 H

ATOM 731 HA LEU A 42 24.555 -5.595 -12.442 1.00 99.99 H

ATOM 732 HB2 LEU A 42 25.640 -7.847 -13.711 1.00 99.99 H

ATOM 733 HB3 LEU A 42 26.906 -7.299 -12.612 1.00 99.99 H

ATOM 734 HG LEU A 42 24.903 -7.073 -10.906 1.00 99.99 H

ATOM 735 HD11 LEU A 42 23.885 -9.044 -12.971 1.00 99.99 H

ATOM 736 HD12 LEU A 42 23.247 -8.936 -11.331 1.00 99.99 H

ATOM 737 HD13 LEU A 42 23.094 -7.564 -12.429 1.00 99.99 H

ATOM 738 HD21 LEU A 42 26.844 -9.047 -11.488 1.00 99.99 H

ATOM 739 HD22 LEU A 42 26.011 -8.786 -9.955 1.00 99.99 H

ATOM 740 HD23 LEU A 42 25.350 -9.915 -11.138 1.00 99.99 H

ATOM 741 N LEU A 43 27.194 -4.276 -13.657 1.00 0.00 N

ATOM 742 CA LEU A 43 28.325 -3.350 -13.367 1.00 0.00 C

ATOM 743 C LEU A 43 27.780 -1.966 -13.013 1.00 0.00 C

ATOM 744 O LEU A 43 28.075 -1.418 -11.970 1.00 0.00 O

ATOM 745 CB LEU A 43 29.223 -3.242 -14.602 1.00 0.00 C

ATOM 746 CG LEU A 43 30.233 -2.111 -14.401 1.00 0.00 C

ATOM 747 CD1 LEU A 43 31.199 -2.484 -13.275 1.00 0.00 C

ATOM 748 CD2 LEU A 43 31.020 -1.894 -15.696 1.00 0.00 C

ATOM 749 H LEU A 43 26.920 -4.437 -14.584 1.00 99.99 H

ATOM 750 HA LEU A 43 28.900 -3.728 -12.539 1.00 99.99 H

ATOM 751 HB2 LEU A 43 29.749 -4.174 -14.747 1.00 99.99 H

ATOM 752 HB3 LEU A 43 28.616 -3.032 -15.470 1.00 99.99 H

ATOM 753 HG LEU A 43 29.710 -1.202 -14.141 1.00 99.99 H

ATOM 754 HD11 LEU A 43 31.665 -3.432 -13.499 1.00 99.99 H

ATOM 755 HD12 LEU A 43 31.959 -1.722 -13.185 1.00 99.99 H

ATOM 756 HD13 LEU A 43 30.655 -2.560 -12.345 1.00 99.99 H

ATOM 757 HD21 LEU A 43 31.037 -2.811 -16.265 1.00 99.99 H

ATOM 758 HD22 LEU A 43 30.546 -1.117 -16.279 1.00 99.99 H

ATOM 759 HD23 LEU A 43 32.031 -1.599 -15.457 1.00 99.99 H

ATOM 760 N THR A 44 26.985 -1.400 -13.874 1.00 0.00 N

ATOM 761 CA THR A 44 26.415 -0.052 -13.592 1.00 0.00 C

ATOM 762 C THR A 44 24.922 -0.188 -13.291 1.00 0.00 C

ATOM 763 O THR A 44 24.211 0.790 -13.167 1.00 0.00 O

ATOM 764 CB THR A 44 26.614 0.855 -14.809 1.00 0.00 C

ATOM 765 CG2 THR A 44 26.316 0.069 -16.086 1.00 0.00 C

ATOM 766 OG1 THR A 44 25.734 1.967 -14.717 1.00 0.00 O

ATOM 767 H THR A 44 26.759 -1.863 -14.705 1.00 99.99 H

ATOM 768 HA THR A 44 26.910 0.379 -12.734 1.00 99.99 H

ATOM 769 HB THR A 44 27.634 1.204 -14.835 1.00 99.99 H

ATOM 770 HG1 THR A 44 25.536 2.262 -15.609 1.00 99.99 H

ATOM 771 HG21 THR A 44 25.655 -0.754 -15.857 1.00 99.99 H

ATOM 772 HG22 THR A 44 25.845 0.720 -16.808 1.00 99.99 H

ATOM 773 HG23 THR A 44 27.239 -0.314 -16.496 1.00 99.99 H

ATOM 774 N LYS A 45 24.443 -1.394 -13.166 1.00 0.00 N

ATOM 775 CA LYS A 45 22.999 -1.602 -12.865 1.00 0.00 C

ATOM 776 C LYS A 45 22.142 -0.803 -13.845 1.00 0.00 C

ATOM 777 O LYS A 45 21.014 -0.457 -13.555 1.00 0.00 O

ATOM 778 CB LYS A 45 22.707 -1.136 -11.438 1.00 0.00 C

ATOM 779 CG LYS A 45 23.846 -1.575 -10.516 1.00 0.00 C

ATOM 780 CD LYS A 45 23.317 -1.733 -9.089 1.00 0.00 C

ATOM 781 CE LYS A 45 23.350 -0.378 -8.380 1.00 0.00 C

ATOM 782 NZ LYS A 45 23.000 -0.560 -6.943 1.00 0.00 N1+

ATOM 783 H LYS A 45 25.033 -2.170 -13.265 1.00 99.99 H

ATOM 784 HA LYS A 45 22.769 -2.654 -12.952 1.00 99.99 H

ATOM 785 HB2 LYS A 45 22.624 -0.060 -11.419 1.00 99.99 H

ATOM 786 HB3 LYS A 45 21.780 -1.575 -11.099 1.00 99.99 H

ATOM 787 HG2 LYS A 45 24.243 -2.520 -10.859 1.00 99.99 H

ATOM 788 HG3 LYS A 45 24.628 -0.830 -10.529 1.00 99.99 H

ATOM 789 HD2 LYS A 45 22.300 -2.098 -9.121 1.00 99.99 H

ATOM 790 HD3 LYS A 45 23.935 -2.436 -8.551 1.00 99.99 H

ATOM 791 HE2 LYS A 45 24.341 0.045 -8.458 1.00 99.99 H

ATOM 792 HE3 LYS A 45 22.637 0.289 -8.843 1.00 99.99 H

ATOM 793 HZ1 LYS A 45 23.527 -1.369 -6.558 1.00 99.99 H

ATOM 794 HZ2 LYS A 45 23.249 0.301 -6.414 1.00 99.99 H

ATOM 795 HZ3 LYS A 45 21.980 -0.740 -6.855 1.00 99.99 H

ATOM 796 N LYS A 46 22.656 -0.518 -15.008 1.00 0.00 N

ATOM 797 CA LYS A 46 21.851 0.244 -16.000 1.00 0.00 C

ATOM 798 C LYS A 46 20.925 -0.732 -16.720 1.00 0.00 C

ATOM 799 O LYS A 46 21.281 -1.867 -16.963 1.00 0.00 O

ATOM 800 CB LYS A 46 22.781 0.915 -17.013 1.00 0.00 C

ATOM 801 CG LYS A 46 22.330 2.359 -17.238 1.00 0.00 C

ATOM 802 CD LYS A 46 23.360 3.087 -18.104 1.00 0.00 C

ATOM 803 CE LYS A 46 22.786 4.430 -18.559 1.00 0.00 C

ATOM 804 NZ LYS A 46 21.566 4.195 -19.382 1.00 0.00 N1+

ATOM 805 H LYS A 46 23.561 -0.817 -15.235 1.00 99.99 H

ATOM 806 HA LYS A 46 21.264 0.994 -15.491 1.00 99.99 H

ATOM 807 HB2 LYS A 46 23.792 0.909 -16.633 1.00 99.99 H

ATOM 808 HB3 LYS A 46 22.744 0.376 -17.947 1.00 99.99 H

ATOM 809 HG2 LYS A 46 21.373 2.363 -17.739 1.00 99.99 H

ATOM 810 HG3 LYS A 46 22.241 2.862 -16.287 1.00 99.99 H

ATOM 811 HD2 LYS A 46 24.259 3.255 -17.529 1.00 99.99 H

ATOM 812 HD3 LYS A 46 23.594 2.484 -18.969 1.00 99.99 H

ATOM 813 HE2 LYS A 46 22.528 5.022 -17.693 1.00 99.99 H

ATOM 814 HE3 LYS A 46 23.523 4.956 -19.148 1.00 99.99 H

ATOM 815 HZ1 LYS A 46 21.541 3.202 -19.689 1.00 99.99 H

ATOM 816 HZ2 LYS A 46 20.720 4.405 -18.814 1.00 99.99 H

ATOM 817 HZ3 LYS A 46 21.587 4.814 -20.217 1.00 99.99 H

ATOM 818 N GLU A 47 19.740 -0.312 -17.063 1.00 0.00 N

ATOM 819 CA GLU A 47 18.807 -1.237 -17.762 1.00 0.00 C

ATOM 820 C GLU A 47 18.426 -0.646 -19.120 1.00 0.00 C

ATOM 821 O GLU A 47 18.312 0.554 -19.277 1.00 0.00 O

ATOM 822 CB GLU A 47 17.549 -1.433 -16.913 1.00 0.00 C

ATOM 823 CG GLU A 47 16.752 -2.626 -17.445 1.00 0.00 C

ATOM 824 CD GLU A 47 15.313 -2.546 -16.933 1.00 0.00 C

ATOM 825 OE1 GLU A 47 15.120 -2.033 -15.844 1.00 0.00 O

ATOM 826 OE2 GLU A 47 14.428 -3.000 -17.640 1.00 0.00 O1-

ATOM 827 H GLU A 47 19.464 0.607 -16.864 1.00 99.99 H

ATOM 828 HA GLU A 47 19.296 -2.188 -17.912 1.00 99.99 H

ATOM 829 HB2 GLU A 47 17.832 -1.618 -15.888 1.00 99.99 H

ATOM 830 HB3 GLU A 47 16.939 -0.543 -16.963 1.00 99.99 H

ATOM 831 HG2 GLU A 47 16.752 -2.606 -18.525 1.00 99.99 H

ATOM 832 HG3 GLU A 47 17.206 -3.544 -17.102 1.00 99.99 H

ATOM 833 N GLY A 48 18.234 -1.480 -20.104 1.00 0.00 N

ATOM 834 CA GLY A 48 17.869 -0.967 -21.453 1.00 0.00 C

ATOM 835 C GLY A 48 17.339 -2.116 -22.306 1.00 0.00 C

ATOM 836 O GLY A 48 17.051 -3.189 -21.815 1.00 0.00 O

ATOM 837 H GLY A 48 18.336 -2.444 -19.956 1.00 99.99 H

ATOM 838 HA2 GLY A 48 18.742 -0.542 -21.925 1.00 99.99 H

ATOM 839 HA3 GLY A 48 17.106 -0.209 -21.359 1.00 99.99 H

ATOM 840 N PHE A 49 17.213 -1.901 -23.583 1.00 0.00 N

ATOM 841 CA PHE A 49 16.704 -2.983 -24.468 1.00 0.00 C

ATOM 842 C PHE A 49 17.884 -3.707 -25.118 1.00 0.00 C

ATOM 843 O PHE A 49 18.813 -3.095 -25.606 1.00 0.00 O

ATOM 844 CB PHE A 49 15.804 -2.384 -25.551 1.00 0.00 C

ATOM 845 CG PHE A 49 14.526 -3.185 -25.647 1.00 0.00 C

ATOM 846 CD1 PHE A 49 13.904 -3.653 -24.483 1.00 0.00 C

ATOM 847 CD2 PHE A 49 13.964 -3.458 -26.899 1.00 0.00 C

ATOM 848 CE1 PHE A 49 12.719 -4.394 -24.573 1.00 0.00 C

ATOM 849 CE2 PHE A 49 12.780 -4.199 -26.989 1.00 0.00 C

ATOM 850 CZ PHE A 49 12.157 -4.667 -25.826 1.00 0.00 C

ATOM 851 H PHE A 49 17.461 -1.028 -23.955 1.00 99.99 H

ATOM 852 HA PHE A 49 16.141 -3.688 -23.874 1.00 99.99 H

ATOM 853 HB2 PHE A 49 15.569 -1.361 -25.298 1.00 99.99 H

ATOM 854 HB3 PHE A 49 16.317 -2.411 -26.501 1.00 99.99 H

ATOM 855 HD1 PHE A 49 14.337 -3.443 -23.517 1.00 99.99 H

ATOM 856 HD2 PHE A 49 14.445 -3.097 -27.797 1.00 99.99 H

ATOM 857 HE1 PHE A 49 12.239 -4.755 -23.675 1.00 99.99 H

ATOM 858 HE2 PHE A 49 12.347 -4.410 -27.955 1.00 99.99 H

ATOM 859 HZ PHE A 49 11.244 -5.239 -25.895 1.00 99.99 H

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ATOM 862 C ILE A 50 18.393 -6.762 -26.769 1.00 0.00 C

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ATOM 869 HA ILE A 50 19.663 -5.116 -26.213 1.00 99.99 H

ATOM 870 HB ILE A 50 20.456 -7.194 -25.094 1.00 99.99 H

ATOM 871 HG12 ILE A 50 18.201 -6.906 -23.132 1.00 99.99 H

ATOM 872 HG13 ILE A 50 17.945 -7.833 -24.610 1.00 99.99 H

ATOM 873 HG21 ILE A 50 19.960 -4.611 -23.835 1.00 99.99 H

ATOM 874 HG22 ILE A 50 20.078 -5.906 -22.644 1.00 99.99 H

ATOM 875 HG23 ILE A 50 21.403 -5.624 -23.774 1.00 99.99 H

ATOM 876 HD11 ILE A 50 20.443 -8.386 -23.081 1.00 99.99 H

ATOM 877 HD12 ILE A 50 18.930 -8.954 -22.375 1.00 99.99 H

ATOM 878 HD13 ILE A 50 19.410 -9.494 -23.984 1.00 99.99 H

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ATOM 880 CA PRO A 51 18.644 -7.874 -28.942 1.00 0.00 C

ATOM 881 C PRO A 51 18.858 -9.333 -28.528 1.00 0.00 C

ATOM 882 O PRO A 51 19.677 -9.622 -27.678 1.00 0.00 O

ATOM 883 CB PRO A 51 19.532 -7.526 -30.133 1.00 0.00 C

ATOM 884 CG PRO A 51 20.775 -6.951 -29.534 1.00 0.00 C

ATOM 885 CD PRO A 51 20.387 -6.324 -28.220 1.00 0.00 C

ATOM 886 HA PRO A 51 17.613 -7.686 -29.193 1.00 99.99 H

ATOM 887 HB2 PRO A 51 19.742 -8.420 -30.701 1.00 99.99 H

ATOM 888 HB3 PRO A 51 19.027 -6.808 -30.763 1.00 99.99 H

ATOM 889 HG2 PRO A 51 21.497 -7.738 -29.380 1.00 99.99 H

ATOM 890 HG3 PRO A 51 21.187 -6.209 -30.201 1.00 99.99 H

ATOM 891 HD2 PRO A 51 21.134 -6.534 -27.468 1.00 99.99 H

ATOM 892 HD3 PRO A 51 20.280 -5.255 -28.330 1.00 99.99 H

ATOM 893 N SER A 52 18.138 -10.259 -29.098 1.00 0.00 N

ATOM 894 CA SER A 52 18.331 -11.678 -28.693 1.00 0.00 C

ATOM 895 C SER A 52 19.410 -12.333 -29.560 1.00 0.00 C

ATOM 896 O SER A 52 19.394 -13.528 -29.782 1.00 0.00 O

ATOM 897 CB SER A 52 17.016 -12.436 -28.845 1.00 0.00 C

ATOM 898 OG SER A 52 17.204 -13.790 -28.462 1.00 0.00 O

ATOM 899 H SER A 52 17.469 -10.026 -29.775 1.00 99.99 H

ATOM 900 HA SER A 52 18.654 -11.699 -27.664 1.00 99.99 H

ATOM 901 HB2 SER A 52 16.266 -11.980 -28.217 1.00 99.99 H

ATOM 902 HB3 SER A 52 16.694 -12.395 -29.875 1.00 99.99 H

ATOM 903 HG SER A 52 17.924 -13.822 -27.828 1.00 99.99 H

ATOM 904 N ASN A 53 20.353 -11.571 -30.042 1.00 0.00 N

ATOM 905 CA ASN A 53 21.430 -12.171 -30.880 1.00 0.00 C

ATOM 906 C ASN A 53 22.785 -11.582 -30.477 1.00 0.00 C

ATOM 907 O ASN A 53 23.812 -11.939 -31.020 1.00 0.00 O

ATOM 908 CB ASN A 53 21.162 -11.879 -32.355 1.00 0.00 C

ATOM 909 CG ASN A 53 21.944 -12.867 -33.222 1.00 0.00 C

ATOM 910 ND2 ASN A 53 21.306 -13.829 -33.832 1.00 0.00 N

ATOM 911 OD1 ASN A 53 23.148 -12.764 -33.346 1.00 0.00 O

ATOM 912 H ASN A 53 20.355 -10.610 -29.850 1.00 99.99 H

ATOM 913 HA ASN A 53 21.452 -13.238 -30.713 1.00 99.99 H

ATOM 914 HB2 ASN A 53 20.106 -11.979 -32.556 1.00 99.99 H

ATOM 915 HB3 ASN A 53 21.478 -10.871 -32.580 1.00 99.99 H

ATOM 916 HD21 ASN A 53 20.334 -13.912 -33.731 1.00 99.99 H

ATOM 917 HD22 ASN A 53 21.797 -14.467 -34.389 1.00 99.99 H

ATOM 918 N TYR A 54 22.800 -10.691 -29.524 1.00 0.00 N

ATOM 919 CA TYR A 54 24.092 -10.092 -29.084 1.00 0.00 C

ATOM 920 C TYR A 54 24.475 -10.667 -27.717 1.00 0.00 C

ATOM 921 O TYR A 54 25.634 -10.718 -27.356 1.00 0.00 O

ATOM 922 CB TYR A 54 23.945 -8.574 -28.975 1.00 0.00 C

ATOM 923 CG TYR A 54 24.064 -7.955 -30.347 1.00 0.00 C

ATOM 924 CD1 TYR A 54 23.154 -8.302 -31.353 1.00 0.00 C

ATOM 925 CD2 TYR A 54 25.085 -7.035 -30.614 1.00 0.00 C

ATOM 926 CE1 TYR A 54 23.265 -7.728 -32.626 1.00 0.00 C

ATOM 927 CE2 TYR A 54 25.196 -6.461 -31.887 1.00 0.00 C

ATOM 928 CZ TYR A 54 24.286 -6.808 -32.893 1.00 0.00 C

ATOM 929 OH TYR A 54 24.395 -6.243 -34.147 1.00 0.00 O

ATOM 930 H TYR A 54 21.964 -10.421 -29.094 1.00 99.99 H

ATOM 931 HA TYR A 54 24.863 -10.330 -29.803 1.00 99.99 H

ATOM 932 HB2 TYR A 54 22.980 -8.335 -28.554 1.00 99.99 H

ATOM 933 HB3 TYR A 54 24.722 -8.182 -28.335 1.00 99.99 H

ATOM 934 HD1 TYR A 54 22.367 -9.012 -31.148 1.00 99.99 H

ATOM 935 HD2 TYR A 54 25.787 -6.767 -29.838 1.00 99.99 H

ATOM 936 HE1 TYR A 54 22.563 -7.996 -33.402 1.00 99.99 H

ATOM 937 HE2 TYR A 54 25.984 -5.752 -32.092 1.00 99.99 H

ATOM 938 HH TYR A 54 25.078 -5.569 -34.110 1.00 99.99 H

ATOM 939 N VAL A 55 23.507 -11.101 -26.955 1.00 0.00 N

ATOM 940 CA VAL A 55 23.809 -11.676 -25.612 1.00 0.00 C

ATOM 941 C VAL A 55 23.239 -13.092 -25.523 1.00 0.00 C

ATOM 942 O VAL A 55 22.415 -13.491 -26.322 1.00 0.00 O

ATOM 943 CB VAL A 55 23.167 -10.806 -24.530 1.00 0.00 C

ATOM 944 CG1 VAL A 55 23.657 -9.365 -24.676 1.00 0.00 C

ATOM 945 CG2 VAL A 55 21.644 -10.847 -24.681 1.00 0.00 C

ATOM 946 H VAL A 55 22.580 -11.052 -27.269 1.00 99.99 H

ATOM 947 HA VAL A 55 24.879 -11.706 -25.464 1.00 99.99 H

ATOM 948 HB VAL A 55 23.442 -11.183 -23.556 1.00 99.99 H

ATOM 949 HG11 VAL A 55 24.065 -9.222 -25.666 1.00 99.99 H

ATOM 950 HG12 VAL A 55 22.831 -8.687 -24.525 1.00 99.99 H

ATOM 951 HG13 VAL A 55 24.423 -9.170 -23.939 1.00 99.99 H

ATOM 952 HG21 VAL A 55 21.349 -11.788 -25.123 1.00 99.99 H

ATOM 953 HG22 VAL A 55 21.183 -10.747 -23.710 1.00 99.99 H

ATOM 954 HG23 VAL A 55 21.323 -10.035 -25.317 1.00 99.99 H

ATOM 955 N ALA A 56 23.663 -13.857 -24.552 1.00 0.00 N

ATOM 956 CA ALA A 56 23.132 -15.243 -24.416 1.00 0.00 C

ATOM 957 C ALA A 56 23.382 -15.755 -22.998 1.00 0.00 C

ATOM 958 O ALA A 56 23.691 -15.000 -22.097 1.00 0.00 O

ATOM 959 CB ALA A 56 23.824 -16.162 -25.424 1.00 0.00 C

ATOM 960 H ALA A 56 24.326 -13.517 -23.912 1.00 99.99 H

ATOM 961 HA ALA A 56 22.070 -15.237 -24.601 1.00 99.99 H

ATOM 962 HB1 ALA A 56 23.706 -15.759 -26.419 1.00 99.99 H

ATOM 963 HB2 ALA A 56 23.379 -17.146 -25.380 1.00 99.99 H

ATOM 964 HB3 ALA A 56 24.875 -16.231 -25.187 1.00 99.99 H

ATOM 965 N LYS A 57 23.246 -17.034 -22.795 1.00 0.00 N

ATOM 966 CA LYS A 57 23.469 -17.605 -21.436 1.00 0.00 C

ATOM 967 C LYS A 57 24.940 -17.993 -21.277 1.00 0.00 C

ATOM 968 O LYS A 57 25.504 -18.681 -22.104 1.00 0.00 O

ATOM 969 CB LYS A 57 22.593 -18.847 -21.254 1.00 0.00 C

ATOM 970 CG LYS A 57 21.128 -18.478 -21.493 1.00 0.00 C

ATOM 971 CD LYS A 57 20.272 -19.747 -21.465 1.00 0.00 C

ATOM 972 CE LYS A 57 18.861 -19.421 -21.959 1.00 0.00 C

ATOM 973 NZ LYS A 57 18.225 -20.657 -22.494 1.00 0.00 N1+

ATOM 974 H LYS A 57 22.997 -17.621 -23.539 1.00 99.99 H

ATOM 975 HA LYS A 57 23.209 -16.869 -20.689 1.00 99.99 H

ATOM 976 HB2 LYS A 57 22.893 -19.606 -21.962 1.00 99.99 H

ATOM 977 HB3 LYS A 57 22.710 -19.226 -20.250 1.00 99.99 H

ATOM 978 HG2 LYS A 57 20.796 -17.803 -20.718 1.00 99.99 H

ATOM 979 HG3 LYS A 57 21.029 -17.998 -22.455 1.00 99.99 H

ATOM 980 HD2 LYS A 57 20.715 -20.494 -22.107 1.00 99.99 H

ATOM 981 HD3 LYS A 57 20.221 -20.125 -20.455 1.00 99.99 H

ATOM 982 HE2 LYS A 57 18.272 -19.039 -21.139 1.00 99.99 H

ATOM 983 HE3 LYS A 57 18.916 -18.677 -22.740 1.00 99.99 H

ATOM 984 HZ1 LYS A 57 18.849 -21.087 -23.207 1.00 99.99 H

ATOM 985 HZ2 LYS A 57 18.068 -21.331 -21.718 1.00 99.99 H

ATOM 986 HZ3 LYS A 57 17.313 -20.417 -22.931 1.00 99.99 H

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ATOM 988 CA LEU A 58 26.999 -17.904 -20.001 1.00 0.00 C

ATOM 989 C LEU A 58 27.775 -17.700 -21.303 1.00 0.00 C

ATOM 990 O LEU A 58 27.259 -17.172 -22.268 1.00 0.00 O

ATOM 991 CB LEU A 58 27.111 -19.366 -19.562 1.00 0.00 C

ATOM 992 CG LEU A 58 28.079 -19.471 -18.382 1.00 0.00 C

ATOM 993 CD1 LEU A 58 27.478 -18.764 -17.165 1.00 0.00 C

ATOM 994 CD2 LEU A 58 28.319 -20.944 -18.048 1.00 0.00 C

ATOM 995 H LEU A 58 25.091 -17.008 -19.560 1.00 99.99 H

ATOM 996 HA LEU A 58 27.410 -17.266 -19.233 1.00 99.99 H

ATOM 997 HB2 LEU A 58 26.138 -19.728 -19.264 1.00 99.99 H

ATOM 998 HB3 LEU A 58 27.480 -19.961 -20.385 1.00 99.99 H

ATOM 999 HG LEU A 58 29.017 -19.003 -18.643 1.00 99.99 H

ATOM 1000 HD11 LEU A 58 26.401 -18.816 -17.215 1.00 99.99 H

ATOM 1001 HD12 LEU A 58 27.821 -19.247 -16.263 1.00 99.99 H

ATOM 1002 HD13 LEU A 58 27.789 -17.729 -17.160 1.00 99.99 H

ATOM 1003 HD21 LEU A 58 27.617 -21.556 -18.594 1.00 99.99 H

ATOM 1004 HD22 LEU A 58 29.327 -21.217 -18.325 1.00 99.99 H

ATOM 1005 HD23 LEU A 58 28.183 -21.099 -16.988 1.00 99.99 H

ATOM 1006 N ASN A 59 29.013 -18.112 -21.337 1.00 0.00 N

ATOM 1007 CA ASN A 59 29.822 -17.940 -22.577 1.00 0.00 C

ATOM 1008 C ASN A 59 31.276 -18.320 -22.294 1.00 0.00 C

ATOM 1009 O ASN A 59 31.682 -19.450 -22.482 1.00 0.00 O

ATOM 1010 CB ASN A 59 29.757 -16.480 -23.031 1.00 0.00 C

ATOM 1011 CG ASN A 59 30.750 -16.256 -24.173 1.00 0.00 C

ATOM 1012 ND2 ASN A 59 30.866 -15.066 -24.697 1.00 0.00 N

ATOM 1013 OD1 ASN A 59 31.428 -17.173 -24.593 1.00 0.00 O

ATOM 1014 H ASN A 59 29.411 -18.534 -20.548 1.00 99.99 H

ATOM 1015 HA ASN A 59 29.429 -18.576 -23.355 1.00 99.99 H

ATOM 1016 HB2 ASN A 59 28.758 -16.254 -23.374 1.00 99.99 H

ATOM 1017 HB3 ASN A 59 30.008 -15.834 -22.203 1.00 99.99 H

ATOM 1018 HD21 ASN A 59 30.319 -14.327 -24.358 1.00 99.99 H

ATOM 1019 HD22 ASN A 59 31.499 -14.913 -25.428 1.00 99.99 H

ATOM 1020 N THR A 60 32.065 -17.383 -21.844 1.00 0.00 N

ATOM 1021 CA THR A 60 33.493 -17.688 -21.550 1.00 0.00 C

ATOM 1022 C THR A 60 33.654 -17.988 -20.058 1.00 0.00 C

ATOM 1023 O THR A 60 33.181 -17.196 -19.260 1.00 0.00 O

ATOM 1024 CB THR A 60 34.358 -16.482 -21.924 1.00 0.00 C

ATOM 1025 CG2 THR A 60 35.798 -16.722 -21.469 1.00 0.00 C

ATOM 1026 OG1 THR A 60 34.327 -16.299 -23.332 1.00 0.00 O

ATOM 1027 OXT THR A 60 34.247 -19.006 -19.739 1.00 0.00 O1-

ATOM 1028 H THR A 60 31.717 -16.479 -21.701 1.00 99.99 H

ATOM 1029 HA THR A 60 33.804 -18.547 -22.126 1.00 99.99 H

ATOM 1030 HB THR A 60 33.975 -15.598 -21.437 1.00 99.99 H

ATOM 1031 HG1 THR A 60 34.830 -17.010 -23.735 1.00 99.99 H

ATOM 1032 HG21 THR A 60 35.844 -17.626 -20.879 1.00 99.99 H

ATOM 1033 HG22 THR A 60 36.436 -16.826 -22.335 1.00 99.99 H

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CONECT 3 25 58 59

CONECT 4 65 17 25

CONECT 5 6 28 32

CONECT 6 5 38 39 40

CONECT 7 8 30 33

CONECT 8 7 27 41 42

CONECT 9 11 34 29

CONECT 10 12 35 31

CONECT 11 9 43 44 45

CONECT 12 10 46 47 48

CONECT 13 2 14 49 50

CONECT 14 13 1 51 52

CONECT 15 1 16 54 55

CONECT 16 15 2 56 57

CONECT 17 4 18 22

CONECT 18 17 19 60

CONECT 19 18 20 61

CONECT 20 2 19 21

CONECT 21 20 22 62

CONECT 22 17 21 23

CONECT 23 22 24 63

CONECT 24 23 25 64

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CONECT 40 6

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CONECT 50 13

CONECT 51 14

CONECT 52 14

CONECT 53 1

CONECT 54 15

CONECT 55 15

CONECT 56 16

CONECT 57 16

CONECT 58 3

CONECT 59 3

CONECT 60 18

CONECT 61 19

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CONECT 66 26

CONECT 67 26

CONECT 68 27

CONECT 69 27

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Data for computed docked structures:

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:08 2019

File generated by GOLD software.

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85 91 1

SMALL

USER_CHARGES

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4	C	9.2046	-1.9687	-25.5349	C.2	1 <1> 0.0000
5	C	8.8230	-3.0595	-26.4782	C.3	1 <1> 0.0000
6	H	10.0273	3.5294	-26.3730	H	1 <1> 0.0000
7	H	8.6162	3.2940	-26.4916	H	1 <1> 0.0000
8	H	9.5657	2.7491	-27.4110	H	1 <1> 0.0000
9	H	8.0970	-3.7521	-25.9759	H	1 <1> 0.0000
10	H	9.1722	-4.0453	-26.0718	H	1 <1> 0.0000
11	O	8.5167	1.4653	-24.8403	O.co2	1 <1> 0.0000
12	O	9.1192	-1.4862	-22.1212	O.co2	1 <1> 0.0000
13	O	8.2949	-1.4278	-24.8412	O.co2	1 <1> 0.0000
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15	Cr	10.9949	-0.2351	-24.1621	Cr.oh	1 <1> 0.0000
16	O	10.6199	1.2293	-25.5183	O.co2	1 <1> 0.0000
17	C	10.2443	-2.0700	-22.0786	C.2	1 <1> 0.0000
18	O	10.4197	-1.6367	-25.4696	O.co2	1 <1> 0.0000
19	C	10.5345	1.7118	-22.1046	C.2	1 <1> 0.0000

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21 O	11.4443	1.1709	-22.7983	O.co2	1 <1>	0.0000
22 C	10.3949	-3.2201	-21.1470	C.3	1 <1>	0.0000
23 C	10.9161	2.8026	-21.1613	C.3	1 <1>	0.0000
24 H	9.7119	-3.7864	-21.2665	H	1 <1>	0.0000
25 H	11.1230	-3.5509	-21.1479	H	1 <1>	0.0000
26 H	10.1735	-3.0060	-20.2285	H	1 <1>	0.0000
27 H	11.5174	3.3381	-21.5477	H	1 <1>	0.0000
28 H	10.2309	3.1951	-20.8012	H	1 <1>	0.0000
29 H	11.4305	2.4308	-20.6146	H	1 <1>	0.0000
30 C	11.3670	-3.0003	-32.8549	C.3	1 <1>	0.0000
31 C	10.4567	-2.0963	-32.0127	C.3	1 <1>	0.0000
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33 C	11.0547	-3.6143	-29.9945	C.3	1 <1>	0.0000
34 C	11.9126	-4.4464	-30.9585	C.3	1 <1>	0.0000
35 N	12.4244	-3.4182	-31.8974	N.pl3	1 <1>	0.0000
36 N	19.1014	-0.2332	-32.1335	N.pl3	1 <1>	0.0000
37 C	16.0389	-1.6000	-31.4063	C.ar	1 <1>	0.0000
38 C	15.2381	-1.8863	-30.3649	C.ar	1 <1>	0.0000
39 C	14.0361	-2.4619	-30.5348	C.ar	1 <1>	0.0000
40 C	13.5443	-2.8071	-31.7448	C.ar	1 <1>	0.0000
41 C	14.3617	-2.4829	-32.7732	C.ar	1 <1>	0.0000

42	C	15.5661	-1.8937	-32.6305	C.ar	1 <1> 0.0000
43	C	16.3302	-1.5977	-33.6982	C.ar	1 <1> 0.0000
44	C	17.5292	-1.0281	-33.5206	C.ar	1 <1> 0.0000
45	C	17.9593	-0.7697	-32.2740	C.ar	1 <1> 0.0000
46	N	17.2208	-1.0572	-31.2344	N.pl3	1 <1> 0.0000
47	C	9.3153	-1.8900	-29.7192	C.3	1 <1> 0.0000
48	C	8.8410	-2.9945	-28.2886	C.3	1 <1> 0.0000
49	H	11.7243	-2.5170	-33.7868	H	1 <1> 0.0000
50	H	10.7929	-3.8827	-33.2204	H	1 <1> 0.0000
51	H	9.5647	-1.8018	-32.6133	H	1 <1> 0.0000
52	H	11.0701	-1.1966	-31.7883	H	1 <1> 0.0000
53	H	9.2780	-3.4812	-31.0406	H	1 <1> 0.0000
54	H	10.5415	-4.2968	-29.2761	H	1 <1> 0.0000
55	H	11.7346	-2.9424	-29.4200	H	1 <1> 0.0000
56	H	12.6738	-5.0619	-30.4407	H	1 <1> 0.0000
57	H	11.2783	-5.1915	-31.4922	H	1 <1> 0.0000
58	H	19.6988	0.0046	-32.9648	H	1 <1> 0.0000
59	H	19.4690	-0.0232	-31.1713	H	1 <1> 0.0000
60	H	15.5775	-1.6649	-29.3390	H	1 <1> 0.0000
61	H	13.4958	-2.6730	-29.5988	H	1 <1> 0.0000
62	H	14.0774	-2.7096	-33.8112	H	1 <1> 0.0000
63	H	15.9898	-1.8080	-34.7262	H	1 <1> 0.0000

64	H	18.1468	-0.7766	-34.4004	H	1 <1> 0.0000
65	H	17.5706	-0.8476	-30.2895	H	1 <1> 0.0000
66	H	8.3372	-1.5075	-30.0998	H	1 <1> 0.0000
67	H	9.8196	-1.0203	-29.2284	H	1 <1> 0.0000
68	H	7.9160	-3.5430	-28.5867	H	1 <1> 0.0000
69	H	9.6504	-3.7619	-28.4202	H	1 <1> 0.0000
70	****	8.6120	0.7004	-24.2032	LP	1 <1> 0.0000
71	****	7.6473	1.9549	-24.9073	LP	1 <1> 0.0000
72	****	8.9786	-0.7164	-22.7437	LP	1 <1> 0.0000
73	****	8.3727	-1.7958	-21.5322	LP	1 <1> 0.0000
74	****	8.5239	-0.6960	-24.1993	LP	1 <1> 0.0000
75	****	7.3469	-1.7322	-24.9348	LP	1 <1> 0.0000
76	****	9.0325	0.6535	-22.7946	LP	1 <1> 0.0000
77	****	8.6431	1.8426	-21.5970	LP	1 <1> 0.0000
78	****	10.7605	0.4594	-24.8958	LP	1 <1> 0.0000
79	****	11.3665	1.5389	-26.1073	LP	1 <1> 0.0000
80	****	10.7067	-0.9105	-24.8449	LP	1 <1> 0.0000
81	****	11.0961	-2.0996	-26.0425	LP	1 <1> 0.0000
82	****	11.1272	-0.9574	-23.4363	LP	1 <1> 0.0000
83	****	12.0919	-2.2118	-22.7322	LP	1 <1> 0.0000
84	****	11.2153	0.4390	-23.4402	LP	1 <1> 0.0000
85	****	12.3922	1.4753	-22.7047	LP	1 <1> 0.0000

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2 1 12 ar

3 1 13 ar

4 1 14 ar

5 1 15 1

6 2 3 1

7 2 11 ar

8 2 16 ar

9 3 6 1

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11 3 8 1

12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

21 15 18 ar

22 15 20 ar

23 15 21 ar

24 17 20 ar

25 17 22 1

26 19 21 ar

27 19 23 1

28 22 24 1

29 22 25 1

30 22 26 1

31 23 27 1

32 23 28 1

33 23 29 1

34 30 31 1

35 30 35 1

36 30 49 1

37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

41 32 33 1

42 32 47 1

43 32 53 1

44 33 34 1

45 33 54 1

46 33 55 1

47 34 35 1

48 34 56 1

49 34 57 1

50 35 40 1

51 36 45 1

52 36 58 1

53 36 59 1

54 37 38 ar

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65 43 44 ar

66 43 63 1

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76 11 70 1

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81 13 75 1

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@<TRIPOS>SUBSTRUCTURE

1 **** 1

@<TRIPOS>SET

LONE_PAIRS STATIC ATOMS <user> **** ""

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DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

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> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final -113.50 input 2.31 | X-H torsion

[841 836 835 832] final 78.73 input 27.02 | X-H torsion

[172 163 162 160] final -21.43 input 178.05 | X-H torsion

[876 867 866 864] final -86.52 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

> <Gold.Protein.RotatedAtoms>

20.6822 -0.5482 -29.3807 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 172 bound_to 163

14.2583 -0.2864 -22.9358 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

12.8958 -1.2201 -22.5412 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.8731 0.4618 -22.3055 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

17.1972 -13.8310 -27.5030 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

24.9208 -6.8326 -34.6930 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

18.0808 -14.1223 -28.8096 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

16.4643 -14.3528 -28.8309 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

20.5685 -1.8628 -30.2937 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

21.5201 -0.6158 -30.7475 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

24.8438 -5.3519 -34.0800 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

23.4861 -6.1291 -34.5482 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score	S(PLP)	S(hbond)	S(cho)	S(metal)	DE(clash)	DE(tors)	intcor
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78.9906

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-60.0518

> <Gold.PLP.part.hbond>

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7.2320

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0.0000

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0.0000

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donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

L1 H 36 59 P1 261 1.76

L1 H 46 65 P1 261 1.89

P1 H 603 615 L1 20 1.66

P1 H 603 616 L1 21 1.92

> <Gold.PLP.Chemscore.Internal.Correction>

0.2167

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:09 2019

File generated by GOLD software.

#

@<TRIPOS>MOLECULE

*****|pRh-6|mol2|1|dock2

85 91 1

SMALL

USER_CHARGES

@<TRIPOS>ATOM

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3	C	16.8883	-7.4479	-35.8341	C.3	1 <1> 0.0000
4	C	12.8458	-5.0195	-34.0961	C.2	1 <1> 0.0000
5	C	12.7980	-3.6420	-33.5256	C.3	1 <1> 0.0000
6	H	16.9994	-7.8317	-36.6352	H	1 <1> 0.0000
7	H	17.3461	-7.7366	-35.2454	H	1 <1> 0.0000
8	H	17.2556	-6.5901	-36.0946	H	1 <1> 0.0000
9	H	12.1606	-2.9884	-34.1779	H	1 <1> 0.0000
10	H	13.2754	-2.9229	-34.2425	H	1 <1> 0.0000
11	O	15.0341	-7.8251	-34.3926	O.co2	1 <1> 0.0000
12	O	11.0317	-7.9297	-33.7307	O.co2	1 <1> 0.0000
13	O	13.0653	-5.9880	-33.3117	O.co2	1 <1> 0.0000
14	O	13.0197	-9.7139	-34.7893	O.co2	1 <1> 0.0000
15	Cr	12.6359	-6.9902	-36.1375	Cr.oh	1 <1> 0.0000
16	O	14.6498	-6.9408	-36.3949	O.co2	1 <1> 0.0000
17	C	10.2450	-7.4702	-34.6129	C.2	1 <1> 0.0000
18	O	12.6618	-5.1565	-35.3364	O.co2	1 <1> 0.0000
19	C	12.8357	-9.8510	-36.0296	C.2	1 <1> 0.0000
20	O	10.6474	-7.0454	-35.7331	O.co2	1 <1> 0.0000
21	O	12.6162	-8.8824	-36.8140	O.co2	1 <1> 0.0000

22	C	8.7932	-7.4226	-34.2916	C.3	1 <1> 0.0000
23	C	12.8835	-11.2285	-36.6000	C.3	1 <1> 0.0000
24	H	8.6821	-7.0387	-33.4905	H	1 <1> 0.0000
25	H	8.3354	-7.1338	-34.8802	H	1 <1> 0.0000
26	H	8.4259	-8.2803	-34.0311	H	1 <1> 0.0000
27	H	13.3214	-11.2171	-37.3783	H	1 <1> 0.0000
28	H	13.1422	-11.8252	-36.0252	H	1 <1> 0.0000
29	H	12.1132	-11.3512	-36.9053	H	1 <1> 0.0000
30	C	11.8232	0.2478	-29.3426	C.3	1 <1> 0.0000
31	C	12.2598	-1.0344	-30.0642	C.3	1 <1> 0.0000
32	N	13.7785	-1.1511	-30.1422	N.4	1 <1> 0.0000
33	C	14.5558	-0.7443	-28.8898	C.3	1 <1> 0.0000
34	C	13.9950	0.5357	-28.2536	C.3	1 <1> 0.0000
35	N	12.5653	0.1928	-28.0558	N.pl3	1 <1> 0.0000
36	N	8.8775	-2.9128	-22.4401	N.pl3	1 <1> 0.0000
37	C	11.0001	-1.3015	-24.6021	C.ar	1 <1> 0.0000
38	C	12.1285	-0.5708	-24.6152	C.ar	1 <1> 0.0000
39	C	12.6545	-0.1029	-25.7595	C.ar	1 <1> 0.0000
40	C	12.0964	-0.3129	-26.9718	C.ar	1 <1> 0.0000
41	C	10.9774	-1.0724	-26.9276	C.ar	1 <1> 0.0000
42	C	10.4368	-1.5645	-25.7946	C.ar	1 <1> 0.0000
43	C	9.3198	-2.3147	-25.8218	C.ar	1 <1> 0.0000

44	C	8.7988	-2.7738	-24.6766	C.ar	1 <1> 0.0000
45	C	9.3941	-2.4684	-23.5112	C.ar	1 <1> 0.0000
46	N	10.4784	-1.7388	-23.4806	N.pl3	1 <1> 0.0000
47	C	14.3028	-2.4976	-30.6032	C.3	1 <1> 0.0000
48	C	13.0268	-3.1688	-31.7919	C.3	1 <1> 0.0000
49	H	10.7223	0.3515	-29.2601	H	1 <1> 0.0000
50	H	12.1270	1.1403	-29.9368	H	1 <1> 0.0000
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53	H	14.0663	-0.4608	-30.8769	H	1 <1> 0.0000
54	H	15.6248	-0.5805	-29.1648	H	1 <1> 0.0000
55	H	14.5070	-1.5577	-28.1284	H	1 <1> 0.0000
56	H	14.5539	0.8528	-27.3517	H	1 <1> 0.0000
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58	H	8.0084	-3.5036	-22.4573	H	1 <1> 0.0000
59	H	9.3160	-2.6873	-21.5116	H	1 <1> 0.0000
60	H	12.6315	-0.3271	-23.6641	H	1 <1> 0.0000
61	H	13.5608	0.5086	-25.6276	H	1 <1> 0.0000
62	H	10.4272	-1.3178	-27.8477	H	1 <1> 0.0000
63	H	8.8198	-2.5693	-26.7717	H	1 <1> 0.0000
64	H	7.8891	-3.3985	-24.7056	H	1 <1> 0.0000
65	H	10.9177	-1.5201	-22.5760	H	1 <1> 0.0000

66 H 14.3153 -3.2439 -29.7720 H 1 <1> 0.0000

67 H 15.2701 -2.6257 -31.1506 H 1 <1> 0.0000

68 H 12.4034 -3.9029 -31.2281 H 1 <1> 0.0000

69 H 12.3736 -2.2563 -31.8376 H 1 <1> 0.0000

70 **** 14.0589 -7.8073 -34.1721 LP 1 <1> 0.0000

71 **** 15.6909 -8.1790 -33.7267 LP 1 <1> 0.0000

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74 **** 13.1000 -6.9218 -33.6678 LP 1 <1> 0.0000

75 **** 13.2041 -5.8195 -32.3358 LP 1 <1> 0.0000

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81 **** 12.4923 -4.3540 -35.9084 LP 1 <1> 0.0000

82 **** 11.6226 -7.0632 -35.9536 LP 1 <1> 0.0000

83 **** 9.9906 -6.6914 -36.3989 LP 1 <1> 0.0000

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5 1 15 1

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7 2 11 ar

8 2 16 ar

9 3 6 1

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11 3 8 1

12 4 5 1

13 4 13 ar

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16 5 10 1

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19 14 19 ar

20 15 16 ar

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22 15 20 ar

23 15 21 ar

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25 17 22 l

26 19 21 ar

27 19 23 l

28 22 24 l

29 22 25 l

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31 23 27 l

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35 30 35 l

36 30 49 l

37 30 50 l

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39 31 51 l

40 31 52 l

41 32 33 l

42 32 47 l

43 32 53 l

44 33 34 l

45 33 54 l

46 33 55 l

47 34 35 l

48 34 56 l

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50 35 40 l

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53 36 59 l

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56 37 46 ar

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60 39 61 l

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62 41 42 ar

63 41 62 l

64 42 43 ar

65 43 44 ar

66 43 63 l

67 44 45 ar

68 44 64 1

69 45 46 ar

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71 47 48 1

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73 47 67 1

74 48 68 1

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76 11 70 1

77 11 71 1

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79 12 73 1

80 13 74 1

81 13 75 1

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88 20 82 1

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@<TRIPOS>SET

LONE_PAIRS STATIC ATOMS <user> **** ""

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DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

unknown|gold_protein|mol2

> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final 133.44 input 2.31 | X-H torsion

[841 836 835 832] final -73.76 input 27.02 | X-H torsion

[172 163 162 160] final 87.56 input 178.05 | X-H torsion

[876 867 866 864] final 131.20 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

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12.9697 0.5201 -22.3335 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

14.2537 -0.4044 -22.9502 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.8010 -1.1593 -22.4976 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

17.7016 -14.2285 -29.1559 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

24.4856 -5.2933 -34.0373 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

16.3166 -14.2364 -28.3469 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

17.7122 -13.8318 -27.6018 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

20.5441 -0.6604 -29.3455 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

20.6758 -1.8579 -30.4479 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

23.5758 -6.4462 -34.6833 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

25.1992 -6.6088 -34.6154 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score	S(PLP)	S(hbond)	S(cho)	S(metal)	DE(clash)	DE(tors)	intcor
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-53.8877

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-3.0000

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donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

P1 H 557 566 L1 11 1.00

> <Gold.PLP.Chemscore.Internal.Correction>

0.1743

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:10 2019

File generated by GOLD software.

#

@<TRIPOS>MOLECULE

*****|pRh-6|mol2|1|dock3

85 91 1

SMALL

USER_CHARGES

@<TRIPOS>ATOM

1 Cr 11.2132 3.8450 -30.0532 Cr.oh 1 <1> 0.0000

2 C 8.3729 3.7788 -30.5000 C.2 1 <1> 0.0000

3 C 6.9565 3.3963 -30.2536 C.3 1 <1> 0.0000

4 C 11.2869 2.8601 -32.7477 C.2 1 <1> 0.0000

5	C	11.5924	1.8698	-33.8206	C.3	1 <1> 0.0000
6	H	6.4650	4.1379	-30.1544	H	1 <1> 0.0000
7	H	6.8600	2.8389	-29.6884	H	1 <1> 0.0000
8	H	6.4946	3.0888	-31.0477	H	1 <1> 0.0000
9	H	11.8562	2.4120	-34.7668	H	1 <1> 0.0000
10	H	10.8376	1.9661	-34.6452	H	1 <1> 0.0000
11	O	9.2892	3.2439	-29.8134	O.co2	1 <1> 0.0000
12	O	13.0854	4.5720	-30.3544	O.co2	1 <1> 0.0000
13	O	11.5053	2.5310	-31.5454	O.co2	1 <1> 0.0000
14	O	10.8630	5.2370	-28.6588	O.co2	1 <1> 0.0000
15	Cr	10.4765	5.3758	-31.6944	Cr.oh	1 <1> 0.0000
16	O	8.6042	4.6489	-31.3933	O.co2	1 <1> 0.0000
17	C	13.3167	5.4421	-31.2476	C.2	1 <1> 0.0000
18	O	10.8266	3.9838	-33.0888	O.co2	1 <1> 0.0000
19	C	10.4028	6.3608	-28.9999	C.2	1 <1> 0.0000
20	O	12.4004	5.9770	-31.9342	O.co2	1 <1> 0.0000
21	O	10.1843	6.6899	-30.2022	O.co2	1 <1> 0.0000
22	C	14.7331	5.8246	-31.4940	C.3	1 <1> 0.0000
23	C	10.0973	7.3511	-27.9271	C.3	1 <1> 0.0000
24	H	15.2247	5.0830	-31.5932	H	1 <1> 0.0000
25	H	14.8296	6.3820	-32.0593	H	1 <1> 0.0000
26	H	15.1950	6.1320	-30.6999	H	1 <1> 0.0000

27 H	9.3282	7.7664	-28.1106	H	1 <1>	0.0000
28 H	10.1710	7.0198	-27.1282	H	1 <1>	0.0000
29 H	10.6127	7.9919	-28.0863	H	1 <1>	0.0000
30 C	15.4264	-2.1695	-31.7880	C.3	1 <1>	0.0000
31 C	14.8110	-1.3730	-32.9465	C.3	1 <1>	0.0000
32 N	13.6440	-2.1165	-33.5878	N.4	1 <1>	0.0000
33 C	12.6866	-2.8302	-32.6326	C.3	1 <1>	0.0000
34 C	13.4333	-3.5601	-31.5068	C.3	1 <1>	0.0000
35 N	14.2602	-2.4776	-30.9194	N.pl3	1 <1>	0.0000
36 N	10.9964	1.4093	-25.5322	N.pl3	1 <1>	0.0000
37 C	13.0278	-0.0789	-27.8635	C.ar	1 <1>	0.0000
38 C	14.2863	-0.0420	-28.3350	C.ar	1 <1>	0.0000
39 C	14.6944	-0.8535	-29.3248	C.ar	1 <1>	0.0000
40 C	13.8849	-1.7512	-29.9283	C.ar	1 <1>	0.0000
41 C	12.6335	-1.7818	-29.4144	C.ar	1 <1>	0.0000
42 C	12.2030	-0.9877	-28.4134	C.ar	1 <1>	0.0000
43 C	10.9427	-1.0701	-27.9487	C.ar	1 <1>	0.0000
44 C	10.5418	-0.2547	-26.9648	C.ar	1 <1>	0.0000
45 C	11.4031	0.6456	-26.4613	C.ar	1 <1>	0.0000
46 N	12.6276	0.7298	-26.9112	N.pl3	1 <1>	0.0000
47 C	12.8143	-1.3035	-34.5632	C.3	1 <1>	0.0000
48 C	12.1901	0.1734	-33.6036	C.3	1 <1>	0.0000

49	H	16.2699	-1.6454	-31.2946	H	1 <1> 0.0000
50	H	15.8900	-3.1061	-32.1750	H	1 <1> 0.0000
51	H	15.5914	-1.1721	-33.7170	H	1 <1> 0.0000
52	H	14.4774	-0.4143	-32.4933	H	1 <1> 0.0000
53	H	14.0866	-2.8818	-34.1512	H	1 <1> 0.0000
54	H	12.0814	-3.5679	-33.2112	H	1 <1> 0.0000
55	H	11.9929	-2.0929	-32.1648	H	1 <1> 0.0000
56	H	12.7560	-4.0937	-30.8119	H	1 <1> 0.0000
57	H	14.0763	-4.3656	-31.9312	H	1 <1> 0.0000
58	H	10.0147	1.3444	-25.1627	H	1 <1> 0.0000
59	H	11.6440	2.1279	-25.1207	H	1 <1> 0.0000
60	H	15.0039	0.6845	-27.9178	H	1 <1> 0.0000
61	H	15.7382	-0.6986	-29.6398	H	1 <1> 0.0000
62	H	11.8764	-2.4705	-29.8172	H	1 <1> 0.0000
63	H	10.2252	-1.8025	-28.3560	H	1 <1> 0.0000
64	H	9.5105	-0.3346	-26.5793	H	1 <1> 0.0000
65	H	13.2698	1.4257	-26.5080	H	1 <1> 0.0000
66	H	11.8830	-1.8422	-34.8641	H	1 <1> 0.0000
67	H	13.2310	-0.8558	-35.4999	H	1 <1> 0.0000
68	H	11.5861	-0.2177	-32.7505	H	1 <1> 0.0000
69	H	13.1637	0.4583	-33.1219	H	1 <1> 0.0000
70	****	10.2432	3.5029	-29.9644	LP	1 <1> 0.0000

71 **** 9.0602 2.5616 -29.1191 LP 1 <1> 0.0000

72 **** 12.1462 4.2828 -30.1694 LP 1 <1> 0.0000

73 **** 13.8423 4.1752 -29.8350 LP 1 <1> 0.0000

74 **** 11.3116 3.1770 -30.8071 LP 1 <1> 0.0000

75 **** 11.8716 1.6249 -31.3337 LP 1 <1> 0.0000

76 **** 11.0753 4.5514 -29.3551 LP 1 <1> 0.0000

77 **** 11.0157 5.0318 -27.6921 LP 1 <1> 0.0000

78 **** 9.5434 4.9381 -31.5783 LP 1 <1> 0.0000

79 **** 7.8473 5.0457 -31.9126 LP 1 <1> 0.0000

80 **** 10.6144 4.6695 -32.3926 LP 1 <1> 0.0000

81 **** 10.6739 4.1891 -34.0556 LP 1 <1> 0.0000

82 **** 11.4465 5.7180 -31.7832 LP 1 <1> 0.0000

83 **** 12.6294 6.6593 -32.6285 LP 1 <1> 0.0000

84 **** 10.3781 6.0439 -30.9406 LP 1 <1> 0.0000

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9 3 6 1

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12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

21 15 18 ar

22 15 20 ar

23 15 21 ar

24 17 20 ar

25 17 22 1

26 19 21 ar

27 19 23 1

28 22 24 1

29 22 25 1

30 22 26 1

31 23 27 1

32 23 28 1

33 23 29 1

34 30 31 1

35 30 35 1

36 30 49 1

37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

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44 33 34 1

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46 33 55 1

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49 34 57 1

50 35 40 1

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76 11 70 1

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81 13 75 1

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@<TRIPOS>SUBSTRUCTURE

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DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

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5.7.2

> <Gold.Id.Protein>

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> <Gold.Protein.RotatedTorsions>

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[841 836 835 832] final 87.01 input 27.02 | X-H torsion

[172 163 162 160] final -75.59 input 178.05 | X-H torsion

[876 867 866 864] final -58.42 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

> <Gold.Protein.RotatedAtoms>

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13.1825 0.5999 -22.4041 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

14.2035 -0.6368 -22.9625 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.6388 -1.0064 -22.4148 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

17.0677 -13.8520 -27.5139 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

24.5039 -6.9535 -34.7837 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

18.1327 -14.0816 -28.6910 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

16.5449 -14.3720 -28.9384 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

21.1201 -1.5554 -30.8721 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

21.2990 -0.1465 -30.0662 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

25.1885 -5.6352 -34.1777 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

23.5678 -5.7221 -34.3577 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

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donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

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L1 H 46 65 P1 249 2.00

> <Gold.PLP.Chemscore.Internal.Correction>

0.1743

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:11 2019

File generated by GOLD software.

#

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*****|pRh-6|mol2|1|dock4

85 91 1

SMALL

USER_CHARGES

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6 H 21.9838 -4.7076 -31.8871 H 1 <1> 0.0000

7 H 21.3655 -5.5128 -32.9021 H 1 <1> 0.0000

8 H 20.7165 -5.2022 -31.6667 H 1 <1> 0.0000

9	H	15.7564	-2.9572	-34.1981	H	1 <1> 0.0000
10	H	15.5496	-1.9274	-34.5827	H	1 <1> 0.0000
11	O	20.5800	-3.6298	-34.2869	O.co2	1 <1> 0.0000
12	O	19.5344	-0.0947	-35.9836	O.co2	1 <1> 0.0000
13	O	18.0848	-2.2548	-34.8372	O.co2	1 <1> 0.0000
14	O	21.9777	-1.4984	-35.4210	O.co2	1 <1> 0.0000
15	Cr	20.1071	-0.8308	-33.0889	Cr.oh	1 <1> 0.0000
16	O	20.6029	-2.6352	-32.2996	O.co2	1 <1> 0.0000
17	C	19.3528	0.9188	-35.2432	C.2	1 <1> 0.0000
18	O	18.1596	-1.2316	-32.8622	O.co2	1 <1> 0.0000
19	C	22.6017	-0.8946	-34.5062	C.2	1 <1> 0.0000
20	O	19.5574	0.8999	-33.9963	O.co2	1 <1> 0.0000
21	O	22.0525	-0.4751	-33.4460	O.co2	1 <1> 0.0000
22	C	18.8632	2.1685	-35.8849	C.3	1 <1> 0.0000
23	C	24.0652	-0.6674	-34.6842	C.3	1 <1> 0.0000
24	H	18.1535	1.9777	-36.3961	H	1 <1> 0.0000
25	H	18.7718	2.7829	-35.3812	H	1 <1> 0.0000
26	H	19.4208	2.4723	-36.6165	H	1 <1> 0.0000
27	H	24.4888	-0.8131	-33.9115	H	1 <1> 0.0000
28	H	24.3896	-1.0728	-35.3797	H	1 <1> 0.0000
29	H	24.1431	0.1665	-34.7004	H	1 <1> 0.0000
30	C	12.3929	0.9091	-29.1585	C.3	1 <1> 0.0000

31	C	12.8522	-0.2540	-30.0481	C.3	1 <1> 0.0000
32	N	14.2883	-0.6671	-29.7433	N.4	1 <1> 0.0000
33	C	14.6845	-0.7063	-28.2668	C.3	1 <1> 0.0000
34	C	14.1348	0.4988	-27.4903	C.3	1 <1> 0.0000
35	N	12.6818	0.4293	-27.7816	N.pl3	1 <1> 0.0000
36	N	8.5108	-2.8071	-22.5940	N.pl3	1 <1> 0.0000
37	C	10.0800	-1.6183	-25.4048	C.ar	1 <1> 0.0000
38	C	10.0685	-1.7399	-26.7437	C.ar	1 <1> 0.0000
39	C	10.9110	-1.0426	-27.5241	C.ar	1 <1> 0.0000
40	C	11.8335	-0.1844	-27.0368	C.ar	1 <1> 0.0000
41	C	11.8025	-0.0650	-25.6893	C.ar	1 <1> 0.0000
42	C	10.9590	-0.7433	-24.8852	C.ar	1 <1> 0.0000
43	C	10.9812	-0.5769	-23.5499	C.ar	1 <1> 0.0000
44	C	10.1414	-1.2790	-22.7781	C.ar	1 <1> 0.0000
45	C	9.2933	-2.1513	-23.3487	C.ar	1 <1> 0.0000
46	N	9.2699	-2.3168	-24.6452	N.pl3	1 <1> 0.0000
47	C	14.7399	-1.9651	-30.3850	C.3	1 <1> 0.0000
48	C	15.0540	-1.5695	-32.1840	C.3	1 <1> 0.0000
49	H	11.3463	1.2214	-29.3504	H	1 <1> 0.0000
50	H	12.9863	1.8231	-29.3917	H	1 <1> 0.0000
51	H	12.7706	0.0417	-31.1200	H	1 <1> 0.0000
52	H	12.1410	-1.0809	-29.8331	H	1 <1> 0.0000

53	H	14.8827	0.0868	-30.1643	H	1 <1> 0.0000
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55	H	14.2895	-1.6335	-27.7894	H	1 <1> 0.0000
56	H	14.4226	0.4938	-26.4210	H	1 <1> 0.0000
57	H	14.5745	1.4438	-27.8854	H	1 <1> 0.0000
58	H	8.5211	-2.6761	-21.5513	H	1 <1> 0.0000
59	H	7.8391	-3.5012	-23.0088	H	1 <1> 0.0000
60	H	9.3660	-2.4436	-27.2215	H	1 <1> 0.0000
61	H	10.8205	-1.2596	-28.6000	H	1 <1> 0.0000
62	H	12.5026	0.6035	-25.1673	H	1 <1> 0.0000
63	H	11.6750	0.1335	-23.0693	H	1 <1> 0.0000
64	H	10.1557	-1.1299	-21.6844	H	1 <1> 0.0000
65	H	8.6098	-2.9890	-25.0593	H	1 <1> 0.0000
66	H	13.9174	-2.7205	-30.4150	H	1 <1> 0.0000
67	H	15.6594	-2.5191	-30.0696	H	1 <1> 0.0000
68	H	14.0714	-1.3010	-32.6400	H	1 <1> 0.0000
69	H	15.5491	-0.5730	-32.0314	H	1 <1> 0.0000
70	****	20.2615	-2.7911	-34.7287	LP	1 <1> 0.0000
71	****	20.7366	-4.4535	-34.8319	LP	1 <1> 0.0000
72	****	19.8524	-0.9548	-35.5846	LP	1 <1> 0.0000
73	****	19.3597	-0.0339	-36.9663	LP	1 <1> 0.0000
74	****	19.0640	-2.1133	-34.9828	LP	1 <1> 0.0000

75	****	17.5396	-2.7277	-35.5294	LP	1 <1> 0.0000
76	****	20.9965	-1.6677	-35.3293	LP	1 <1> 0.0000
77	****	22.4643	-1.8077	-36.2381	LP	1 <1> 0.0000
78	****	20.2849	-1.7751	-32.6986	LP	1 <1> 0.0000
79	****	20.7777	-2.6960	-31.3169	LP	1 <1> 0.0000
80	****	19.1409	-1.0622	-32.9539	LP	1 <1> 0.0000
81	****	17.6730	-0.9222	-32.0451	LP	1 <1> 0.0000
82	****	19.8759	0.0612	-33.5545	LP	1 <1> 0.0000
83	****	19.4007	1.7236	-33.4513	LP	1 <1> 0.0000
84	****	21.0733	-0.6166	-33.3004	LP	1 <1> 0.0000
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8	2	16	ar
9	3	6	1
10	3	7	1

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14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

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DONOR_HYDROGENS STATIC ATOMS <user> **** ""

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ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

unknown|gold_protein|mol2

> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final 160.93 input 2.31 | X-H torsion

[841 836 835 832] final -90.20 input 27.02 | X-H torsion

[172 163 162 160] final -177.98 input 178.05 | X-H torsion

[876 867 866 864] final -48.41 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

> <Gold.Protein.RotatedAtoms>

20.9711 -1.7241 -30.6979 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 172 bound_to 163

13.3982 0.6239 -22.4834 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

14.1062 -0.8463 -22.9536 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.5208 -0.8207 -22.3446 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

17.4621 -14.2861 -29.2421 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

24.3450 -6.9493 -34.7956 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

16.3517 -14.1593 -28.0916 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

17.9222 -13.8499 -27.7688 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

21.4260 -0.2328 -30.3185 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

20.3672 -1.0437 -29.3761 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

25.2707 -5.7673 -34.2300 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

23.6481 -5.5944 -34.2932 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score	S(PLP)	S(hbond)	S(cho)	S(metal)	DE(clash)	DE(tors)	intcor
61.18	-60.16	1.00	0.00	0.00	0.00	1.08	0.17

> <Gold.PLP.Fitness>

61.1772

> <Gold.PLP.PLP>

-60.1569

> <Gold.PLP.part.hbond>

-2.0000

> <Gold.PLP.part.metal>

0.0000

> <Gold.PLP.part.buried>

-1.9107

> <Gold.PLP.part.nonpolar>

-57.2527

> <Gold.PLP.part.repulsive>

0.3575

> <Gold.PLP.ligand.clash>

0.0000

> <Gold.PLP.ligand.torsion>

1.0759

> <Gold.PLP.Chemscore.Hbond>

1.0000

> <Gold.PLP.Chemscore.CHOScore>

0.0000

> <Gold.PLP.Chemscore.Metal>

0.0000

> <Gold.Chemscore.Hbonds>

donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

P1 H 163 172 L1 16 1.00

> <Gold.PLP.Chemscore.Internal.Correction>

0.1721

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:13 2019

File generated by GOLD software.

#

@<TRIPOS>MOLECULE

*****|pRh-6|mol2|1|dock5

85 91 1

SMALL

USER_CHARGES

@<TRIPOS>ATOM

1 Cr 8.5420 -0.0156 -25.9235 Cr.oh 1 <1> 0.0000

2 C 11.3959 -0.3707 -25.9378 C.2 1 <1> 0.0000

3 C 12.8065 -0.1080 -26.3306 C.3 1 <1> 0.0000

4 C 8.5655 -2.7807 -26.6913 C.2 1 <1> 0.0000

5 C 8.3038 -3.9384 -27.5948 C.3 1 <1> 0.0000

6 H 13.2883 0.0662 -25.5964 H 1 <1> 0.0000

7 H 12.8890 0.4141 -26.9306 H 1 <1> 0.0000

8 H 13.2969 -0.9080 -26.5712 H 1 <1> 0.0000

9 H 7.4377 -3.7004 -28.2672 H 1 <1> 0.0000

10 H 7.2876 -4.3612 -27.3773 H 1 <1> 0.0000

11 O 10.4620 0.2402 -26.5309 O.co2 1 <1> 0.0000

12 O 6.6746 -0.3207 -25.1856 O.co2 1 <1> 0.0000

13 O 8.3102 -1.6163 -27.1163 O.co2 1 <1> 0.0000

14	O	8.8343	1.4959	-24.6450	O.co2	1 <1> 0.0000
15	Cr	9.3196	-1.5044	-24.2628	Cr.oh	1 <1> 0.0000
16	O	11.1869	-1.1993	-25.0007	O.co2	1 <1> 0.0000
17	C	6.4657	-1.1493	-24.2485	C.2	1 <1> 0.0000
18	O	9.0273	-3.0159	-25.5414	O.co2	1 <1> 0.0000
19	C	9.2961	1.2607	-23.4951	C.2	1 <1> 0.0000
20	O	7.3996	-1.7602	-23.6555	O.co2	1 <1> 0.0000
21	O	9.5513	0.0963	-23.0700	O.co2	1 <1> 0.0000
22	C	5.0550	-1.4120	-23.8558	C.3	1 <1> 0.0000
23	C	9.5577	2.4184	-22.5915	C.3	1 <1> 0.0000
24	H	4.5732	-1.5861	-24.5899	H	1 <1> 0.0000
25	H	4.9725	-1.9341	-23.2557	H	1 <1> 0.0000
26	H	4.5646	-0.6119	-23.6151	H	1 <1> 0.0000
27	H	10.3290	2.2942	-22.1586	H	1 <1> 0.0000
28	H	9.4605	3.1855	-22.9858	H	1 <1> 0.0000
29	H	9.0426	2.2934	-21.9430	H	1 <1> 0.0000
30	C	10.8736	-1.9884	-31.0483	C.3	1 <1> 0.0000
31	C	10.7546	-3.0307	-29.9283	C.3	1 <1> 0.0000
32	N	10.6187	-4.4449	-30.4829	N.4	1 <1> 0.0000
33	C	11.5029	-4.7919	-31.6813	C.3	1 <1> 0.0000
34	C	11.5558	-3.6514	-32.7080	C.3	1 <1> 0.0000
35	N	11.9933	-2.4995	-31.8818	N.pl3	1 <1> 0.0000

36	N	19.2436	-1.0241	-32.0767	N.pl3	1 <1> 0.0000
37	C	15.9217	-1.5347	-31.3838	C.ar	1 <1> 0.0000
38	C	15.0441	-1.4961	-30.3660	C.ar	1 <1> 0.0000
39	C	13.7448	-1.7897	-30.5413	C.ar	1 <1> 0.0000
40	C	13.2219	-2.1545	-31.7324	C.ar	1 <1> 0.0000
41	C	14.1243	-2.1588	-32.7406	C.ar	1 <1> 0.0000
42	C	15.4300	-1.8560	-32.5935	C.ar	1 <1> 0.0000
43	C	16.2752	-1.8799	-33.6406	C.ar	1 <1> 0.0000
44	C	17.5699	-1.5905	-33.4572	C.ar	1 <1> 0.0000
45	C	18.0110	-1.2904	-32.2238	C.ar	1 <1> 0.0000
46	N	17.1935	-1.2677	-31.2040	N.pl3	1 <1> 0.0000
47	C	10.7546	-5.5581	-29.4616	C.3	1 <1> 0.0000
48	C	9.4925	-5.1955	-28.1322	C.3	1 <1> 0.0000
49	H	10.9869	-0.9514	-30.6723	H	1 <1> 0.0000
50	H	9.9273	-1.9524	-31.6359	H	1 <1> 0.0000
51	H	9.8698	-2.7950	-29.2920	H	1 <1> 0.0000
52	H	11.6852	-2.9203	-29.3304	H	1 <1> 0.0000
53	H	9.6363	-4.5014	-30.8445	H	1 <1> 0.0000
54	H	11.1025	-5.7105	-32.1723	H	1 <1> 0.0000
55	H	12.5447	-4.9981	-31.3409	H	1 <1> 0.0000
56	H	12.1820	-3.8900	-33.5896	H	1 <1> 0.0000
57	H	10.5423	-3.4716	-33.1355	H	1 <1> 0.0000

58	H	19.9058	-1.0362	-32.8927	H	1 <1> 0.0000
59	H	19.6212	-0.7907	-31.1238	H	1 <1> 0.0000
60	H	15.3950	-1.2372	-29.3527	H	1 <1> 0.0000
61	H	13.1412	-1.7524	-29.6210	H	1 <1> 0.0000
62	H	13.8259	-2.4372	-33.7619	H	1 <1> 0.0000
63	H	15.9259	-2.1280	-34.6572	H	1 <1> 0.0000
64	H	18.2564	-1.6001	-34.3216	H	1 <1> 0.0000
65	H	17.5543	-1.0327	-30.2692	H	1 <1> 0.0000
66	H	11.7329	-5.5102	-28.9244	H	1 <1> 0.0000
67	H	10.5848	-6.6373	-29.7028	H	1 <1> 0.0000
68	H	8.9976	-6.1617	-27.8736	H	1 <1> 0.0000
69	H	10.2123	-5.0388	-27.2845	H	1 <1> 0.0000
70	****	9.5113	0.0783	-26.2661	LP	1 <1> 0.0000
71	****	10.6736	0.8855	-27.2649	LP	1 <1> 0.0000
72	****	7.6096	-0.1278	-25.4833	LP	1 <1> 0.0000
73	****	5.9044	0.1399	-25.6268	LP	1 <1> 0.0000
74	****	8.4741	-0.8229	-26.5300	LP	1 <1> 0.0000
75	****	7.9447	-1.4895	-28.0384	LP	1 <1> 0.0000
76	****	8.6509	0.7407	-25.2742	LP	1 <1> 0.0000
77	****	8.6515	2.4376	-24.9274	LP	1 <1> 0.0000
78	****	10.2519	-1.3922	-24.7030	LP	1 <1> 0.0000
79	****	11.9571	-1.6598	-24.5595	LP	1 <1> 0.0000

80 **** 9.2107 -2.2607 -24.9121 LP 1 <1> 0.0000

81 **** 9.2101 -3.9576 -25.2590 LP 1 <1> 0.0000

82 **** 8.3502 -1.5983 -23.9202 LP 1 <1> 0.0000

83 **** 7.1880 -2.4054 -22.9214 LP 1 <1> 0.0000

84 **** 9.3875 -0.6971 -23.6563 LP 1 <1> 0.0000

85 **** 9.9168 -0.0304 -22.1479 LP 1 <1> 0.0000

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2 1 12 ar

3 1 13 ar

4 1 14 ar

5 1 15 1

6 2 3 1

7 2 11 ar

8 2 16 ar

9 3 6 1

10 3 7 1

11 3 8 1

12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

21 15 18 ar

22 15 20 ar

23 15 21 ar

24 17 20 ar

25 17 22 1

26 19 21 ar

27 19 23 1

28 22 24 1

29 22 25 1

30 22 26 1

31 23 27 1

32 23 28 1

33 23 29 1

34 30 31 1

35 30 35 1

36 30 49 1

37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

41 32 33 1

42 32 47 1

43 32 53 1

44 33 34 1

45 33 54 1

46 33 55 1

47 34 35 1

48 34 56 1

49 34 57 1

50 35 40 1

51 36 45 1

52 36 58 1

53 36 59 1

54 37 38 ar

55 37 42 ar

56 37 46 ar

57 38 39 ar

58 38 60 1

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60 39 61 1

61 40 41 ar

62 41 42 ar

63 41 62 1

64 42 43 ar

65 43 44 ar

66 43 63 1

67 44 45 ar

68 44 64 1

69 45 46 ar

70 46 65 1

71 47 48 1

72 47 66 1

73 47 67 1

74 48 68 1

75 48 69 1

76 11 70 1

77 11 71 1

78 12 72 1

79 12 73 1

80 13 74 1

81 13 75 1

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87 18 81 1

88 20 82 1

89 20 83 1

90 21 84 1

91 21 85 1

@<TRIPOS>SUBSTRUCTURE

1 **** 1

@<TRIPOS>SET

LONE_PAIRS STATIC ATOMS <user> **** ""

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

unknown|gold_protein|mol2

> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final -85.27 input 2.31 | X-H torsion

[841 836 835 832] final -72.43 input 27.02 | X-H torsion

[172 163 162 160] final -56.35 input 178.05 | X-H torsion

[876 867 866 864] final -1.15 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

> <Gold.Protein.RotatedAtoms>

20.4245 -1.0318 -29.3685 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 172 bound_to 163

14.1562 -0.7528 -22.9600 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

12.5700 -0.9121 -22.3748 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

13.3010 0.6193 -22.4479 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

17.7196 -14.2232 -29.1460 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

23.7020 -6.6123 -34.6997 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

16.3171 -14.2423 -28.3679 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

17.6933 -13.8314 -27.5909 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

20.9194 -1.7430 -30.7191 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

21.4326 -0.2412 -30.3346 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

25.2905 -6.4552 -34.5383 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

24.2857 -5.2510 -34.0831 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score	S(PLP)	S(hbond)	S(cho)	S(metal)	DE(clash)	DE(tors)	intcor
65.79	-56.65	3.71	0.00	0.00	0.00	1.07	0.14

> <Gold.PLP.Fitness>

65.7925

> <Gold.PLP.PLP>

-56.6550

> <Gold.PLP.part.hbond>

-3.0000

> <Gold.PLP.part.metal>

0.0000

> <Gold.PLP.part.buried>

-7.3347

> <Gold.PLP.part.nonpolar>

-47.5246

> <Gold.PLP.part.repulsive>

0.2140

> <Gold.PLP.ligand.clash>

0.0000

> <Gold.PLP.ligand.torsion>

1.0690

> <Gold.PLP.Chemscore.Hbond>

3.7120

> <Gold.PLP.Chemscore.CHOScore>

0.0000

> <Gold.PLP.Chemscore.Metal>

0.0000

> <Gold.Chemscore.Hbonds>

donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

L1 H 36 59 P1 261 1.82

L1 H 46 65 P1 261 1.89

> <Gold.PLP.Chemscore.Internal.Correction>

0.1396

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:14 2019

File generated by GOLD software.

#

@<TRIPOS>MOLECULE

*****|pRh-6|mol2|1|dock6

85 91 1

SMALL

USER_CHARGES

@<TRIPOS>ATOM

1	Cr	6.9110	-10.5355	-32.8301	Cr.oh	1 <1> 0.0000
2	C	6.1772	-9.8186	-30.1434	C.2	1 <1> 0.0000
3	C	5.4160	-9.1228	-29.0711	C.3	1 <1> 0.0000
4	C	9.4835	-9.5827	-31.9873	C.2	1 <1> 0.0000
5	C	10.6738	-8.6843	-32.0221	C.3	1 <1> 0.0000
6	H	5.0596	-9.7325	-28.5209	H	1 <1> 0.0000
7	H	4.9133	-8.5604	-29.3367	H	1 <1> 0.0000
8	H	5.9805	-8.7145	-28.3980	H	1 <1> 0.0000
9	H	11.5842	-9.2562	-31.7012	H	1 <1> 0.0000
10	H	11.0807	-8.5613	-30.9838	H	1 <1> 0.0000
11	O	5.9708	-9.5106	-31.3515	O.co2	1 <1> 0.0000
12	O	7.8746	-11.6708	-34.2111	O.co2	1 <1> 0.0000
13	O	8.5071	-9.3173	-32.7475	O.co2	1 <1> 0.0000
14	O	5.3733	-11.8160	-32.8045	O.co2	1 <1> 0.0000
15	Cr	7.9680	-11.8502	-31.1767	Cr.oh	1 <1> 0.0000
16	O	7.0044	-10.7149	-29.7957	O.co2	1 <1> 0.0000
17	C	8.7018	-12.5671	-33.8634	C.2	1 <1> 0.0000

18	O	9.5057	-10.5697	-31.2023	O.co2	1 <1> 0.0000
19	C	5.3955	-12.8030	-32.0195	C.2	1 <1> 0.0000
20	O	8.9082	-12.8751	-32.6553	O.co2	1 <1> 0.0000
21	O	6.3719	-13.0684	-31.2593	O.co2	1 <1> 0.0000
22	C	9.4630	-13.2628	-34.9357	C.3	1 <1> 0.0000
23	C	4.2052	-13.7014	-31.9847	C.3	1 <1> 0.0000
24	H	9.8194	-12.6532	-35.4859	H	1 <1> 0.0000
25	H	9.9657	-13.8252	-34.6701	H	1 <1> 0.0000
26	H	8.8985	-13.6711	-35.6088	H	1 <1> 0.0000
27	H	4.0240	-13.9287	-31.1402	H	1 <1> 0.0000
28	H	3.5380	-13.3990	-32.4502	H	1 <1> 0.0000
29	H	4.4998	-14.4426	-32.2407	H	1 <1> 0.0000
30	C	12.1269	-3.1700	-30.7788	C.3	1 <1> 0.0000
31	C	12.3079	-4.5782	-31.3613	C.3	1 <1> 0.0000
32	N	11.8061	-4.6651	-32.7989	N.4	1 <1> 0.0000
33	C	12.1327	-3.4772	-33.7049	C.3	1 <1> 0.0000
34	C	11.9374	-2.1340	-32.9870	C.3	1 <1> 0.0000
35	N	12.7861	-2.2916	-31.7806	N.pl3	1 <1> 0.0000
36	N	19.9334	-0.5267	-32.5441	N.pl3	1 <1> 0.0000
37	C	16.7186	-1.2399	-31.5786	C.ar	1 <1> 0.0000
38	C	15.9535	-1.3512	-30.4786	C.ar	1 <1> 0.0000
39	C	14.6511	-1.6725	-30.5529	C.ar	1 <1> 0.0000

40	C	14.0142	-1.9190	-31.7186	C.ar	1 <1> 0.0000
41	C	14.8041	-1.7739	-32.8076	C.ar	1 <1> 0.0000
42	C	16.1096	-1.4399	-32.7608	C.ar	1 <1> 0.0000
43	C	16.8389	-1.3120	-33.8846	C.ar	1 <1> 0.0000
44	C	18.1378	-0.9959	-33.8023	C.ar	1 <1> 0.0000
45	C	18.6996	-0.8216	-32.5941	C.ar	1 <1> 0.0000
46	N	17.9949	-0.9466	-31.5002	N.pl3	1 <1> 0.0000
47	C	12.1764	-5.9359	-33.5395	C.3	1 <1> 0.0000
48	C	10.8998	-7.2094	-33.0495	C.3	1 <1> 0.0000
49	H	12.4961	-3.0752	-29.7375	H	1 <1> 0.0000
50	H	11.0418	-2.9300	-30.6953	H	1 <1> 0.0000
51	H	11.7584	-5.3159	-30.7312	H	1 <1> 0.0000
52	H	13.4001	-4.7770	-31.3033	H	1 <1> 0.0000
53	H	10.7606	-4.6687	-32.7216	H	1 <1> 0.0000
54	H	11.4708	-3.5143	-34.6025	H	1 <1> 0.0000
55	H	13.1933	-3.5357	-34.0446	H	1 <1> 0.0000
56	H	12.1574	-1.2613	-33.6323	H	1 <1> 0.0000
57	H	10.8673	-2.0006	-32.7054	H	1 <1> 0.0000
58	H	20.5052	-0.4204	-33.4194	H	1 <1> 0.0000
59	H	20.4040	-0.3891	-31.6142	H	1 <1> 0.0000
60	H	16.4034	-1.1962	-29.4834	H	1 <1> 0.0000
61	H	14.1480	-1.7635	-29.5776	H	1 <1> 0.0000

62	H	14.4061	-1.9453	-33.8184	H	1 <1> 0.0000
63	H	16.3902	-1.4559	-34.8821	H	1 <1> 0.0000
64	H	18.7285	-0.8806	-34.7277	H	1 <1> 0.0000
65	H	18.4468	-0.8059	-30.5863	H	1 <1> 0.0000
66	H	13.1398	-6.3646	-33.1706	H	1 <1> 0.0000
67	H	12.2108	-6.0089	-34.6554	H	1 <1> 0.0000
68	H	9.9165	-6.6853	-32.9879	H	1 <1> 0.0000
69	H	10.8443	-7.7484	-34.0332	H	1 <1> 0.0000
70	****	6.4697	-9.9807	-32.0796	LP	1 <1> 0.0000
71	****	5.3085	-8.7968	-31.5794	LP	1 <1> 0.0000
72	****	7.3534	-11.1749	-33.5165	LP	1 <1> 0.0000
73	****	7.7435	-11.4600	-35.1798	LP	1 <1> 0.0000
74	****	7.6979	-9.9047	-32.7457	LP	1 <1> 0.0000
75	****	8.5449	-8.5201	-33.3501	LP	1 <1> 0.0000
76	****	6.1553	-11.1943	-32.8485	LP	1 <1> 0.0000
77	****	4.5736	-11.6551	-33.3829	LP	1 <1> 0.0000
78	****	7.5256	-11.2108	-30.4903	LP	1 <1> 0.0000
79	****	7.1355	-10.9256	-28.8270	LP	1 <1> 0.0000
80	****	8.7237	-11.1914	-31.1584	LP	1 <1> 0.0000
81	****	10.3054	-10.7306	-30.6239	LP	1 <1> 0.0000
82	****	8.4092	-12.4050	-31.9272	LP	1 <1> 0.0000
83	****	9.5705	-13.5888	-32.4274	LP	1 <1> 0.0000

84 **** 7.1811 -12.4809 -31.2611 LP 1 <1> 0.0000

85 **** 6.3341 -13.8656 -30.6568 LP 1 <1> 0.0000

@<TRIPOS>BOND

1 1 11 ar

2 1 12 ar

3 1 13 ar

4 1 14 ar

5 1 15 1

6 2 3 1

7 2 11 ar

8 2 16 ar

9 3 6 1

10 3 7 1

11 3 8 1

12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

21 15 18 ar

22 15 20 ar

23 15 21 ar

24 17 20 ar

25 17 22 1

26 19 21 ar

27 19 23 1

28 22 24 1

29 22 25 1

30 22 26 1

31 23 27 1

32 23 28 1

33 23 29 1

34 30 31 1

35 30 35 1

36 30 49 1

37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

41 32 33 1

42 32 47 l

43 32 53 l

44 33 34 l

45 33 54 l

46 33 55 l

47 34 35 l

48 34 56 l

49 34 57 l

50 35 40 l

51 36 45 l

52 36 58 l

53 36 59 l

54 37 38 ar

55 37 42 ar

56 37 46 ar

57 38 39 ar

58 38 60 l

59 39 40 ar

60 39 61 l

61 40 41 ar

62 41 42 ar

63 41 62 l

64 42 43 ar

65 43 44 ar

66 43 63 1

67 44 45 ar

68 44 64 1

69 45 46 ar

70 46 65 1

71 47 48 1

72 47 66 1

73 47 67 1

74 48 68 1

75 48 69 1

76 11 70 1

77 11 71 1

78 12 72 1

79 12 73 1

80 13 74 1

81 13 75 1

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85 16 79 1

86 18 80 1

87 18 81 1

88 20 82 1

89 20 83 1

90 21 84 1

91 21 85 1

@<TRIPOS>SUBSTRUCTURE

1 **** 1

@<TRIPOS>SET

LONE_PAIRS STATIC ATOMS <user> **** ""

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

unknown|gold_protein|mol2

> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final 123.45 input 2.31 | X-H torsion

[841 836 835 832] final 76.35 input 27.02 | X-H torsion

[172 163 162 160] final -81.97 input 178.05 | X-H torsion

[876 867 866 864] final -124.18 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

> <Gold.Protein.RotatedAtoms>

20.3513 -1.3938 -29.5355 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 172 bound_to 163

12.8300 0.4311 -22.2921 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

14.2566 -0.2351 -22.9284 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.9375 -1.2399 -22.5608 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

17.2348 -13.8258 -27.5033 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

25.2801 -6.4188 -34.4753 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

18.0626 -14.1340 -28.8421 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

16.4440 -14.3463 -28.7981 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

21.1826 -1.4782 -30.9054 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

21.2442 -0.1359 -29.9775 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

24.2442 -5.2561 -34.0890 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

23.7182 -6.6480 -34.7618 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score	S(PLP)	S(hbond)	S(cho)	S(metal)	DE(clash)	DE(tors)	intcor
59.03	-49.16	3.95	0.00	0.00	0.00	1.06	0.14

> <Gold.PLP.Fitness>

59.0256

> <Gold.PLP.PLP>

-49.1628

> <Gold.PLP.part.hbond>

-3.0000

> <Gold.PLP.part.metal>

0.0000

> <Gold.PLP.part.buried>

-7.5353

> <Gold.PLP.part.nonpolar>

-41.4689

> <Gold.PLP.part.repulsive>

0.8701

> <Gold.PLP.ligand.clash>

0.0000

> <Gold.PLP.ligand.torsion>

1.0634

> <Gold.PLP.Chemscore.Hbond>

3.9500

> <Gold.PLP.Chemscore.CHOScore>

0.0000

> <Gold.PLP.Chemscore.Metal>

0.0000

> <Gold.Chemscore.Hbonds>

donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

L1 H 36 59 P1 163 0.95

L1 H 46 65 P1 261 2.00

P1 H 532 541 L1 18 1.00

> <Gold.PLP.Chemscore.Internal.Correction>

0.1396

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:15 2019

File generated by GOLD software.

#

@<TRIPOS>MOLECULE

*****|pRh-6|mol2|1|dock7

85 91 1

SMALL

USER_CHARGES

@<TRIPOS>ATOM

1	Cr	17.9568	-8.5540	-35.1891	Cr.oh	1 <1> 0.0000
2	C	19.5194	-6.2523	-34.4602	C.2	1 <1> 0.0000
3	C	20.4598	-5.4382	-33.6440	C.3	1 <1> 0.0000
4	C	15.7976	-6.6679	-35.0623	C.2	1 <1> 0.0000
5	C	14.5186	-6.1054	-34.5397	C.3	1 <1> 0.0000
6	H	21.1412	-5.1715	-34.1597	H	1 <1> 0.0000
7	H	20.6635	-5.7720	-32.9464	H	1 <1> 0.0000
8	H	20.1357	-4.5449	-33.4557	H	1 <1> 0.0000
9	H	14.6007	-5.9559	-33.4307	H	1 <1> 0.0000
10	H	14.0468	-6.8397	-33.8347	H	1 <1> 0.0000
11	O	19.1413	-7.3796	-34.0322	O.co2	1 <1> 0.0000
12	O	16.8172	-9.6493	-36.4643	O.co2	1 <1> 0.0000
13	O	16.2907	-7.6795	-34.4834	O.co2	1 <1> 0.0000
14	O	19.6296	-9.3186	-35.9776	O.co2	1 <1> 0.0000
15	Cr	18.0015	-6.8748	-36.8498	Cr.oh	1 <1> 0.0000
16	O	19.1411	-5.7796	-35.5746	O.co2	1 <1> 0.0000
17	C	16.4389	-9.1766	-37.5787	C.2	1 <1> 0.0000
18	O	16.3286	-6.1103	-36.0612	O.co2	1 <1> 0.0000
19	C	20.1607	-8.7609	-36.9766	C.2	1 <1> 0.0000
20	O	16.8170	-8.0492	-38.0067	O.co2	1 <1> 0.0000

21	O	19.6675	-7.7494	-37.5555	O.co2	1 <1> 0.0000
22	C	15.4985	-9.9907	-38.3949	C.3	1 <1> 0.0000
23	C	21.4396	-9.3234	-37.4992	C.3	1 <1> 0.0000
24	H	14.8170	-10.2574	-37.8792	H	1 <1> 0.0000
25	H	15.2947	-9.6569	-39.0924	H	1 <1> 0.0000
26	H	15.8226	-10.8840	-38.5832	H	1 <1> 0.0000
27	H	21.9944	-8.6583	-37.7171	H	1 <1> 0.0000
28	H	21.7698	-9.9450	-36.9911	H	1 <1> 0.0000
29	H	21.2518	-9.5733	-38.2763	H	1 <1> 0.0000
30	C	11.9055	-4.2658	-31.5352	C.3	1 <1> 0.0000
31	C	12.0473	-4.9124	-32.9198	C.3	1 <1> 0.0000
32	N	11.2370	-4.1699	-33.9771	N.4	1 <1> 0.0000
33	C	11.2626	-2.6427	-33.9034	C.3	1 <1> 0.0000
34	C	11.1426	-2.1332	-32.4600	C.3	1 <1> 0.0000
35	N	12.2541	-2.8415	-31.7790	N.pl3	1 <1> 0.0000
36	N	19.2090	-0.3332	-32.1247	N.pl3	1 <1> 0.0000
37	C	16.0474	-1.4156	-31.3445	C.ar	1 <1> 0.0000
38	C	15.2539	-1.6630	-30.2877	C.ar	1 <1> 0.0000
39	C	13.9952	-2.1080	-30.4377	C.ar	1 <1> 0.0000
40	C	13.4342	-2.3523	-31.6422	C.ar	1 <1> 0.0000
41	C	14.2485	-2.0693	-32.6852	C.ar	1 <1> 0.0000
42	C	15.5101	-1.6099	-32.5619	C.ar	1 <1> 0.0000

43	C	16.2673	-1.3481	-33.6434	C.ar	1 <1> 0.0000
44	C	17.5228	-0.9091	-33.4859	C.ar	1 <1> 0.0000
45	C	18.0147	-0.7465	-32.2459	C.ar	1 <1> 0.0000
46	N	17.2829	-1.0012	-31.1931	N.pl3	1 <1> 0.0000
47	C	11.5166	-4.5753	-35.4117	C.3	1 <1> 0.0000
48	C	13.3028	-5.1223	-35.4546	C.3	1 <1> 0.0000
49	H	12.4958	-4.7788	-30.7490	H	1 <1> 0.0000
50	H	10.8543	-4.3604	-31.1776	H	1 <1> 0.0000
51	H	11.7103	-5.9742	-32.8718	H	1 <1> 0.0000
52	H	13.1350	-4.8752	-33.1464	H	1 <1> 0.0000
53	H	10.2399	-4.4344	-33.7901	H	1 <1> 0.0000
54	H	10.4170	-2.2371	-34.5082	H	1 <1> 0.0000
55	H	12.2186	-2.2554	-34.3275	H	1 <1> 0.0000
56	H	11.1467	-1.0281	-32.3882	H	1 <1> 0.0000
57	H	10.1587	-2.4296	-32.0281	H	1 <1> 0.0000
58	H	19.8017	-0.1223	-32.9665	H	1 <1> 0.0000
59	H	19.6252	-0.2008	-31.1685	H	1 <1> 0.0000
60	H	15.6451	-1.5190	-29.2664	H	1 <1> 0.0000
61	H	13.4651	-2.3024	-29.4922	H	1 <1> 0.0000
62	H	13.9111	-2.2236	-33.7206	H	1 <1> 0.0000
63	H	15.8761	-1.4809	-34.6663	H	1 <1> 0.0000
64	H	18.1354	-0.6847	-34.3763	H	1 <1> 0.0000

65 H 17.6809 -0.8667 -30.2536 H 1 <1> 0.0000

66 H 11.4868 -3.6984 -36.1032 H 1 <1> 0.0000

67 H 10.9723 -5.4016 -35.9339 H 1 <1> 0.0000

68 H 13.5718 -5.2895 -36.5247 H 1 <1> 0.0000

69 H 13.7675 -4.1262 -35.2239 H 1 <1> 0.0000

70 **** 18.5180 -7.9387 -34.5790 LP 1 <1> 0.0000

71 **** 19.4654 -7.7127 -33.1467 LP 1 <1> 0.0000

72 **** 17.4404 -9.1247 -35.8843 LP 1 <1> 0.0000

73 **** 16.4922 -10.5466 -36.1655 LP 1 <1> 0.0000

74 **** 17.1459 -8.0779 -34.8150 LP 1 <1> 0.0000

75 **** 15.8253 -8.0804 -33.6943 LP 1 <1> 0.0000

76 **** 18.7734 -8.9630 -35.6030 LP 1 <1> 0.0000

77 **** 20.0649 -10.1164 -35.5603 LP 1 <1> 0.0000

78 **** 18.5178 -6.3042 -36.1545 LP 1 <1> 0.0000

79 **** 19.4661 -4.8823 -35.8733 LP 1 <1> 0.0000

80 **** 17.1849 -6.4659 -36.4359 LP 1 <1> 0.0000

81 **** 15.8934 -5.3125 -36.4786 LP 1 <1> 0.0000

82 **** 17.4402 -7.4902 -37.4599 LP 1 <1> 0.0000

83 **** 16.4929 -7.7162 -38.8922 LP 1 <1> 0.0000

84 **** 18.8123 -7.3510 -37.2239 LP 1 <1> 0.0000

85 **** 20.1330 -7.3485 -38.3445 LP 1 <1> 0.0000

@<TRIPOS>BOND

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2 1 12 ar

3 1 13 ar

4 1 14 ar

5 1 15 1

6 2 3 1

7 2 11 ar

8 2 16 ar

9 3 6 1

10 3 7 1

11 3 8 1

12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

21 15 18 ar

22 15 20 ar

23 15 21 ar

24 17 20 ar

25 17 22 1

26 19 21 ar

27 19 23 1

28 22 24 1

29 22 25 1

30 22 26 1

31 23 27 1

32 23 28 1

33 23 29 1

34 30 31 1

35 30 35 1

36 30 49 1

37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

41 32 33 1

42 32 47 1

43 32 53 1

44 33 34 1

45 33 54 l

46 33 55 l

47 34 35 l

48 34 56 l

49 34 57 l

50 35 40 l

51 36 45 l

52 36 58 l

53 36 59 l

54 37 38 ar

55 37 42 ar

56 37 46 ar

57 38 39 ar

58 38 60 l

59 39 40 ar

60 39 61 l

61 40 41 ar

62 41 42 ar

63 41 62 l

64 42 43 ar

65 43 44 ar

66 43 63 l

67 44 45 ar

68 44 64 1

69 45 46 ar

70 46 65 1

71 47 48 1

72 47 66 1

73 47 67 1

74 48 68 1

75 48 69 1

76 11 70 1

77 11 71 1

78 12 72 1

79 12 73 1

80 13 74 1

81 13 75 1

82 14 76 1

83 14 77 1

84 16 78 1

85 16 79 1

86 18 80 1

87 18 81 1

88 20 82 1

89 20 83 1

90 21 84 1

91 21 85 1

@<TRIPOS>SUBSTRUCTURE

1 **** 1

@<TRIPOS>SET

LONE_PAIRS STATIC ATOMS <user> **** ""

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

unknown|gold_protein|mol2

> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final 14.03 input 2.31 | X-H torsion

[841 836 835 832] final 176.02 input 27.02 | X-H torsion

[172 163 162 160] final -114.09 input 178.05 | X-H torsion

[876 867 866 864] final -21.97 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

> <Gold.Protein.RotatedAtoms>

20.4236 -1.7353 -29.9010 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 172 bound_to 163

12.7953 -1.1558 -22.4939 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

12.9783 0.5251 -22.3362 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

14.2511 -0.4162 -22.9517 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

16.3529 -14.2317 -28.5052 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

23.9486 -6.8197 -34.7717 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

17.5612 -13.8322 -27.5289 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

17.8481 -14.2328 -29.0858 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

21.4316 -1.0218 -30.9255 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

20.9213 -0.2431 -29.5838 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

25.3593 -6.1538 -34.3965 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

23.9648 -5.3403 -34.1512 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score	S(PLP)	S(hbond)	S(cho)	S(metal)	DE(clash)	DE(tors)	intcor
55.70	-47.76	4.12	0.00	0.00	0.00	2.28	0.14

> <Gold.PLP.Fitness>

55.7000

> <Gold.PLP.PLP>

-47.7624

> <Gold.PLP.part.hbond>

-4.0000

> <Gold.PLP.part.metal>

0.0000

> <Gold.PLP.part.buried>

-2.3435

> <Gold.PLP.part.nonpolar>

-42.1360

> <Gold.PLP.part.repulsive>

0.1127

> <Gold.PLP.ligand.clash>

0.0000

> <Gold.PLP.ligand.torsion>

2.2799

> <Gold.PLP.Chemscore.Hbond>

4.1193

> <Gold.PLP.Chemscore.CHOScore>

0.0000

> <Gold.PLP.Chemscore.Metal>

0.0000

> <Gold.Chemscore.Hbonds>

donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

L1 H 36 59 P1 261 1.66

L1 H 46 65 P1 261 1.98

P1 H 557 566 L1 13 0.47

> <Gold.PLP.Chemscore.Internal.Correction>

0.1396

Name: *****

Creating user name zb1

Creation time: Thu Jun 13 10:31:17 2019

File generated by GOLD software.

#

@<TRIPOS>MOLECULE

*****|pRh-6|mol2|1|dock8

85 91 1

SMALL

USER_CHARGES

@<TRIPOS>ATOM

1 Cr 20.9625 -0.7128 -33.5525 Cr.oh 1 <1> 0.0000

2	C	19.7011	0.9419	-35.5379	C.2	1 <1> 0.0000
3	C	19.4130	2.1854	-36.3021	C.3	1 <1> 0.0000
4	C	18.2493	-1.1478	-32.7250	C.2	1 <1> 0.0000
5	C	17.0946	-1.0919	-31.7822	C.3	1 <1> 0.0000
6	H	19.5526	2.0338	-37.1733	H	1 <1> 0.0000
7	H	19.7600	2.8418	-36.0050	H	1 <1> 0.0000
8	H	18.4671	2.3726	-36.3948	H	1 <1> 0.0000
9	H	17.1016	-0.1100	-31.2393	H	1 <1> 0.0000
10	H	17.4742	-1.0325	-30.7281	H	1 <1> 0.0000
11	O	20.4627	0.9942	-34.5308	O.co2	1 <1> 0.0000
12	O	21.4235	-2.4959	-32.6965	O.co2	1 <1> 0.0000
13	O	19.3341	-0.5943	-32.3809	O.co2	1 <1> 0.0000
14	O	22.5043	-0.8854	-34.8165	O.co2	1 <1> 0.0000
15	Cr	19.6340	-1.9207	-35.0872	Cr.oh	1 <1> 0.0000
16	O	19.1730	-0.1376	-35.9432	O.co2	1 <1> 0.0000
17	C	20.8954	-3.5754	-33.1018	C.2	1 <1> 0.0000
18	O	18.0922	-1.7481	-33.8231	O.co2	1 <1> 0.0000
19	C	22.3473	-1.4857	-35.9147	C.2	1 <1> 0.0000
20	O	20.1339	-3.6277	-34.1089	O.co2	1 <1> 0.0000
21	O	21.2625	-2.0392	-36.2588	O.co2	1 <1> 0.0000
22	C	21.1835	-4.8188	-32.3376	C.3	1 <1> 0.0000
23	C	23.5019	-1.5416	-36.8575	C.3	1 <1> 0.0000

24	H	21.0439	-4.6673	-31.4664	H	1 <1> 0.0000
25	H	20.8366	-5.4752	-32.6347	H	1 <1> 0.0000
26	H	22.1295	-5.0060	-32.2449	H	1 <1> 0.0000
27	H	23.2152	-1.4095	-37.6929	H	1 <1> 0.0000
28	H	24.1725	-1.0531	-36.6023	H	1 <1> 0.0000
29	H	23.6731	-2.3588	-36.9244	H	1 <1> 0.0000
30	C	11.2051	-0.1303	-29.6900	C.3	1 <1> 0.0000
31	C	11.8120	-1.3844	-30.3334	C.3	1 <1> 0.0000
32	N	13.3176	-1.2460	-30.5335	N.4	1 <1> 0.0000
33	C	14.0962	-0.5881	-29.3936	C.3	1 <1> 0.0000
34	C	13.3617	0.6340	-28.8239	C.3	1 <1> 0.0000
35	N	12.0342	0.0724	-28.4730	N.pl3	1 <1> 0.0000
36	N	9.2825	-2.8512	-22.2551	N.pl3	1 <1> 0.0000
37	C	11.0284	-1.3004	-24.7697	C.ar	1 <1> 0.0000
38	C	12.1275	-0.5549	-24.9788	C.ar	1 <1> 0.0000
39	C	12.4686	-0.1271	-26.2058	C.ar	1 <1> 0.0000
40	C	11.7414	-0.3948	-27.3125	C.ar	1 <1> 0.0000
41	C	10.6569	-1.1677	-27.0730	C.ar	1 <1> 0.0000
42	C	10.3001	-1.6203	-25.8540	C.ar	1 <1> 0.0000
43	C	9.2067	-2.3868	-25.6856	C.ar	1 <1> 0.0000
44	C	8.8705	-2.8057	-24.4587	C.ar	1 <1> 0.0000
45	C	9.6257	-2.4441	-23.4076	C.ar	1 <1> 0.0000

46	N	10.6875	-1.6984	-23.5670	N.pl3	1 <1> 0.0000
47	C	14.0407	-2.5220	-30.9205	C.3	1 <1> 0.0000
48	C	15.5272	-1.9900	-31.9198	C.3	1 <1> 0.0000
49	H	10.1120	-0.2094	-29.5209	H	1 <1> 0.0000
50	H	11.3012	0.7368	-30.3833	H	1 <1> 0.0000
51	H	11.3227	-1.5728	-31.3174	H	1 <1> 0.0000
52	H	11.5735	-2.2135	-29.6324	H	1 <1> 0.0000
53	H	13.4244	-0.5939	-31.3474	H	1 <1> 0.0000
54	H	15.0964	-0.2718	-29.7741	H	1 <1> 0.0000
55	H	14.2479	-1.3172	-28.5634	H	1 <1> 0.0000
56	H	13.9172	1.1312	-28.0050	H	1 <1> 0.0000
57	H	13.2654	1.4233	-29.6050	H	1 <1> 0.0000
58	H	8.4326	-3.4545	-22.1200	H	1 <1> 0.0000
59	H	9.8491	-2.5814	-21.4117	H	1 <1> 0.0000
60	H	12.7608	-0.2650	-24.1233	H	1 <1> 0.0000
61	H	13.3719	0.5021	-26.2341	H	1 <1> 0.0000
62	H	9.9814	-1.4586	-27.8907	H	1 <1> 0.0000
63	H	8.5768	-2.6874	-26.5399	H	1 <1> 0.0000
64	H	7.9794	-3.4439	-24.3278	H	1 <1> 0.0000
65	H	11.2516	-1.4364	-22.7470	H	1 <1> 0.0000
66	H	13.4417	-3.1369	-31.6354	H	1 <1> 0.0000
67	H	14.4646	-3.2387	-30.1733	H	1 <1> 0.0000

68 H 15.7493 -2.8094 -32.6441 H 1 <1> 0.0000

69 H 15.0112 -1.2187 -32.5523 H 1 <1> 0.0000

70 **** 20.6709 0.1616 -34.0175 LP 1 <1> 0.0000

71 **** 20.8571 1.8682 -34.2470 LP 1 <1> 0.0000

72 **** 21.2431 -1.6389 -33.1793 LP 1 <1> 0.0000

73 **** 22.0203 -2.5016 -31.8941 LP 1 <1> 0.0000

74 **** 20.1243 -0.6192 -32.9931 LP 1 <1> 0.0000

75 **** 19.4010 -0.1320 -31.4967 LP 1 <1> 0.0000

76 **** 21.7479 -0.8291 -34.1649 LP 1 <1> 0.0000

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79 **** 18.5762 -0.1319 -36.7456 LP 1 <1> 0.0000

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81 **** 17.2113 -2.1676 -34.0422 LP 1 <1> 0.0000

82 **** 19.9257 -2.7951 -34.6222 LP 1 <1> 0.0000

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3 1 13 ar

4 1 14 ar

5 1 15 1

6 2 3 1

7 2 11 ar

8 2 16 ar

9 3 6 1

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12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

20 15 16 ar

21 15 18 ar

22 15 20 ar

23 15 21 ar

24 17 20 ar

25 17 22 1

26 19 21 ar

27 19 23 1

28 22 24 1

29 22 25 1

30 22 26 1

31 23 27 1

32 23 28 1

33 23 29 1

34 30 31 1

35 30 35 1

36 30 49 1

37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

41 32 33 1

42 32 47 1

43 32 53 1

44 33 34 1

45 33 54 1

46 33 55 1

47 34 35 1

48 34 56 l

49 34 57 l

50 35 40 l

51 36 45 l

52 36 58 l

53 36 59 l

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62 41 42 ar

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67 44 45 ar

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72 47 66 1

73 47 67 1

74 48 68 1

75 48 69 1

76 11 70 1

77 11 71 1

78 12 72 1

79 12 73 1

80 13 74 1

81 13 75 1

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DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

> <Gold.Version>

5.7.2

> <Gold.Id.Protein>

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> <Gold.Protein.RotatedTorsions>

[614 603 602 601] final -161.52 input 2.31 | X-H torsion

[841 836 835 832] final 119.87 input 27.02 | X-H torsion

[172 163 162 160] final 161.69 input 178.05 | X-H torsion

[876 867 866 864] final -98.25 input 173.38 | X-H torsion

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TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

PHE57 PRO59 SER60 ASN61 TYR62

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13.9441 0.4144 -22.7206 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

13.6390 -1.2526 -22.8299 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.4432 -0.2053 -22.2315 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

16.6141 -13.9756 -27.7279 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

25.0647 -6.7294 -34.6340 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

18.1525 -13.9343 -28.1799 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

16.9894 -14.3929 -29.2304 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

21.2801 -0.1415 -30.0346 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

20.3045 -1.3411 -29.5094 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

24.6648 -5.2836 -34.0648 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

23.5180 -6.3030 -34.6237 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1001 bound_to 867

> <Gold.Score>

Score S(PLP) S(hbond) S(cho) S(metal) DE(clash) DE(tors) intcor

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donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

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0.1263

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#       Creating user name   zb1
#       Creation time:       Thu Jun 13 10:31:21 2019


#       File generated by GOLD software.
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   85    91     1
SMALL
USER_CHARGES


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      2 C           20.5016  -3.6612 -32.8922 C.2          1 <1>             0.0000
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      4 C           17.0685  -2.8186 -34.2673 C.2          1 <1>             0.0000
      5 C           15.7256  -3.4599 -34.3704 C.3          1 <1>             0.0000
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9	H	15.8225	-4.4505	-34.8884	H	1 <1> 0.0000
10	H	15.4413	-3.5621	-35.4510	H	1 <1> 0.0000
11	O	20.5389	-3.6501	-34.1554	O.co2	1 <1> 0.0000
12	O	18.8618	-0.4923	-36.0746	O.co2	1 <1> 0.0000
13	O	17.9044	-3.0206	-35.1957	O.co2	1 <1> 0.0000
14	O	21.4535	-1.1645	-35.0318	O.co2	1 <1> 0.0000
15	Cr	19.0656	-1.1530	-33.1130	Cr.oh	1 <1> 0.0000
16	O	19.9006	-2.7725	-32.2160	O.co2	1 <1> 0.0000
17	C	18.2607	0.3965	-35.3983	C.2	1 <1> 0.0000
18	O	17.3089	-2.1002	-33.2588	O.co2	1 <1> 0.0000
19	C	21.6939	-0.4462	-34.0233	C.2	1 <1> 0.0000
20	O	18.2234	0.3854	-34.1351	O.co2	1 <1> 0.0000
21	O	20.8579	-0.2442	-33.0949	O.co2	1 <1> 0.0000
22	C	17.5630	1.4804	-36.1409	C.3	1 <1> 0.0000
23	C	23.0367	0.1952	-33.9201	C.3	1 <1> 0.0000
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25	H	17.2060	2.0222	-35.6735	H	1 <1> 0.0000
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31	C	12.3753	-1.1744	-30.9092	C.3	1 <1>	0.0000
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34	C	14.5750	-0.3160	-29.1265	C.3	1 <1>	0.0000
35	N	13.1182	-0.1476	-28.9027	N.pl3	1 <1>	0.0000
36	N	8.7580	-2.2748	-23.3129	N.pl3	1 <1>	0.0000
37	C	11.1523	-1.0629	-25.4518	C.ar	1 <1>	0.0000
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55	H	14.3365	-2.4588	-29.0186	H	1 <1> 0.0000
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57	H	14.9615	0.4592	-29.8280	H	1 <1> 0.0000
58	H	7.8717	-2.8392	-23.3347	H	1 <1> 0.0000
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62	H	10.9099	-1.5548	-28.7016	H	1 <1> 0.0000
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64	H	7.9845	-3.0719	-25.5738	H	1 <1> 0.0000
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66	H	12.7538	-3.6871	-31.5231	H	1 <1> 0.0000
67	H	14.4422	-4.0307	-31.0480	H	1 <1> 0.0000
68	H	13.4302	-3.5374	-33.8937	H	1 <1> 0.0000
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71	****	21.0252	-4.3722	-34.6476	LP	1 <1> 0.0000
72	****	19.3322	-1.2419	-35.6090	LP	1 <1> 0.0000

73	****	18.8652	-0.4434	-37.0734	LP	1 <1> 0.0000
74	****	18.8109	-2.6005	-35.1525	LP	1 <1> 0.0000
75	****	17.6585	-3.6003	-35.9725	LP	1 <1> 0.0000
76	****	20.5632	-1.6097	-35.1278	LP	1 <1> 0.0000
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78	****	19.4301	-2.0228	-32.6816	LP	1 <1> 0.0000
79	****	19.8971	-2.8213	-31.2172	LP	1 <1> 0.0000
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81	****	16.6092	-1.9759	-32.5552	LP	1 <1> 0.0000
82	****	18.6801	-0.3454	-33.6278	LP	1 <1> 0.0000
83	****	17.7372	1.1074	-33.6429	LP	1 <1> 0.0000
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6	2	3	1
7	2	11	ar
8	2	16	ar

9 3 6 1

10 3 7 1

11 3 8 1

12 4 5 1

13 4 13 ar

14 4 18 ar

15 5 9 1

16 5 10 1

17 5 48 1

18 12 17 ar

19 14 19 ar

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22 15 20 ar

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25 17 22 1

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28 22 24 1

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31 23 27 1

32 23 28 1

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37 30 50 1

38 31 32 1

39 31 51 1

40 31 52 1

41 32 33 1

42 32 47 1

43 32 53 1

44 33 34 1

45 33 54 1

46 33 55 1

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DONOR_HYDROGENS STATIC ATOMS <user> **** ""

4 53 58 59 65

ATOM$BLUE STATIC ATOMS COLORGROUP SYSTEM

16 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

ATOM$RED STATIC ATOMS COLORGROUP SYSTEM

4 53 58 59 65

@<TRIPOS>COMMENT

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5.7.2

> <Gold.Id.Protein>

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[841 836 835 832] final 125.78 input 27.02 | X-H torsion

[172 163 162 160] final -173.99 input 178.05 | X-H torsion

[876 867 866 864] final 104.19 input 173.38 | X-H torsion

> <Gold.Protein.ActiveResidues>

TYR19 ILE22 HIS23 ASP25 ASP26 HIS41 GLY42 GLU43 TRP44 LYS46

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14.2449 -0.4688 -22.9554 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

12.7540 -1.1240 -22.4739 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

13.0284 0.5478 -22.3533 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

16.5506 -14.0024 -27.7917 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

24.0659 -5.3423 -34.0958 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

18.1240 -13.9127 -28.0899 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

17.0829 -14.3869 -29.2551 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 988 bound_to 836

21.4476 -0.2625 -30.3728 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 998 bound_to 163

20.3879 -0.9833 -29.3607 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 999 bound_to 163

23.8516 -6.7662 -34.8035 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

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> <Gold.Score>

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donor molecule, donor type, donor heavy atom, donor atom, acceptor molecule, acceptor atom, score

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0.1263

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Creating user name zb1

Creation time: Thu Jun 13 10:31:23 2019

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      5 C           9.6071  -4.2493 -29.0839 C.3         1 <1>             0.0000
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      7 H          13.5059   0.3078 -26.9764 H           1 <1>             0.0000
      8 H          13.5968  -0.9121 -26.2366 H           1 <1>             0.0000
      9 H           8.5956  -4.6448 -29.3659 H           1 <1>             0.0000
     10 H           9.1259  -5.0568 -28.4713 H           1 <1>             0.0000
     11 O          11.1985   0.1253 -27.8269 O.co2        1 <1>             0.0000
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15 Cr	8.9701	-1.2169	-26.1759	Cr.oh	1 <1>	0.0000
16 O	10.9710	-0.9863	-25.9159	O.co2	1 <1>	0.0000
17 C	6.5193	-0.9643	-27.6595	C.2	1 <1>	0.0000
18 O	9.2630	-2.9446	-27.1422	O.co2	1 <1>	0.0000
19 C	8.7372	1.6392	-26.0194	C.2	1 <1>	0.0000
20 O	6.9919	-1.4245	-26.5816	O.co2	1 <1>	0.0000
21 O	8.6732	0.5809	-25.3283	O.co2	1 <1>	0.0000
22 C	5.0880	-1.2000	-27.9898	C.3	1 <1>	0.0000
23 C	8.5833	2.9502	-25.3245	C.3	1 <1>	0.0000
24 H	5.0279	-1.5212	-28.8232	H	1 <1>	0.0000
25 H	4.6845	-1.6070	-27.4320	H	1 <1>	0.0000
26 H	4.5936	-0.3871	-28.1718	H	1 <1>	0.0000
27 H	9.0256	2.9335	-24.5488	H	1 <1>	0.0000
28 H	8.7438	3.6290	-25.8410	H	1 <1>	0.0000
29 H	7.8064	2.9272	-25.0123	H	1 <1>	0.0000
30 C	14.3906	-1.4632	-30.3132	C.3	1 <1>	0.0000
31 C	13.7772	-2.8696	-30.2824	C.3	1 <1>	0.0000
32 N	12.6159	-3.0025	-31.2621	N.4	1 <1>	0.0000
33 C	12.8013	-2.3411	-32.6283	C.3	1 <1>	0.0000

34	C	13.4512	-0.9547	-32.5142	C.3	1 <1> 0.0000
35	N	14.6906	-1.2459	-31.7528	N.pl3	1 <1> 0.0000
36	N	20.6325	-3.6746	-35.4375	N.pl3	1 <1> 0.0000
37	C	18.2890	-2.1903	-33.4173	C.ar	1 <1> 0.0000
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13.9324 0.4244 -22.7148 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 614 bound_to 603

13.6535 -1.2464 -22.8346 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 615 bound_to 603

12.4404 -0.2214 -22.2326 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 616 bound_to 603

16.3393 -14.1992 -28.3836 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 841 bound_to 836

24.2471 -5.2982 -34.0602 H 0 0 0 0 0 0 0 0 0 0 0 0 # atno 876 bound_to 867

17.6798 -13.8311 -27.5834 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 987 bound_to 836

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23.7100 -6.6390 -34.7585 LP 0 0 0 0 0 0 0 0 0 0 0 0 # atno 1000 bound_to 867

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