Supporting Information

Nickel-Catalyzed Asymmetric Hydrogenation of ß-Acylamino Nitroolefins: An Efficient Approach to Chiral Amines

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1. General Information

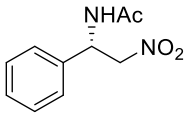
All the reactions dealing with air- or moisture-sensitive compounds were carried out in a dry reaction vessel under a positive pressure of nitrogen or in the nitrogen-filled glovebox. Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers and used without further purification. NMR spectra were recorded on Bruker ADVANCE III (400 MHz) spectrometers for ^{1}H NMR and ^{13}C NMR. $CDCl_3$ was the solvent used for the NMR analysis, with tetramethylsilane as the internal standard. Chemical shifts were reported upfield to TMS (0.00 ppm) for ^{1}H NMR and relative to $CDCl_3$ (77.0 ppm) for ^{13}C NMR. Optical rotation was determined using a Perkin Elmer 343 polarimeter. HPLC analysis was conducted on an Agilent 1260 Series instrument. Column Chromatography was performed with silica gel Merck 60 (300-400 mesh). All new products were further characterized by HRMS. A positive ion mass spectrum of sample was acquired on a Thermo LTQ-FT mass spectrometer with an electrospray ionization source.

All the (*Z*)-β-Acylamino Nitroolefins were pepared according the literature.[1] The absolute configuration of products were determined by comparison of analytical data with the literature.

2. General Procedure for Asymmetric Hydrogenation of (Z)-β-Acylamino Nitroolefins 1

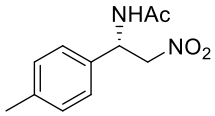
In a nitrogen-filled glovebox, the $Ni(OAc)_2$ (0.01 mmol) and (*S*)-Bianpine (0.011 mmol) were dissolved in 1.0 mL anhydrous MeOH and THF (1:1), and the solution was stirred for 30 min at rt. Then the solution was equally divided into 10 vials charged with substrates (0.1 mmol) in anhydrous TFE solution (1.0 mL). The resulting vials were transferred to an autoclave, which was charged with 5-10 atm H_2, and the reaction was stirred at rt for 24h. When the reaction was completed, the H_2 was released slowly and the solution was passed through a short column of silica gel

with EA. The solution was concentrated under reduced pressure to got the target compound. The chiral compounds were the analyzed by using HPLC on a chiral stationary phase to determine the ee.



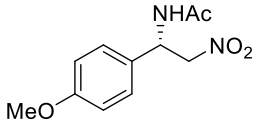
(*S*)-N-(2-nitro-1-phenylethyl)acetamide 2a

White solid; 20.7 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +34.20 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 11.5 min (major), 20.1 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.33 (m, 3H), 7.33 – 7.28 (m, 2H), 6.37 (brs, 1H), 5.70-5.65 (m, 1H), 4.91 (dd, *J* = 13.0, 6.5 Hz, 1H), 4.73 (dd, *J* = 13.0, 5.6 Hz, 1H), 2.05 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 136.3, 129.3, 128.9, 126.4, 78.2, 51.2, 23.3.



(*S*)-N-(2-nitro-1-(p-tolyl)ethyl)acetamide 2b

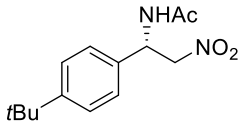
White solid; 22.0 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +72.30 (c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 11.9 min (major), 16.7 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (s, 4H), 6.32 (brs, 1H), 5.67-5.58 (m, 1H), 4.89 (dd, *J* = 12.8, 6.4, 1H), 4.70 (dd, *J* = 12.8, 5.7, 1H), 2.34 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 138.8, 133.3, 129.9, 126.4, 78.2, 51.1, 23.3, 21.1.



(*S*)-N-(1-(4-methoxyphenyl)-2-nitroethyl)acetamide 2c

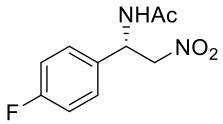
White solid; 23.7 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +59.00 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85:15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 9.9 min

(major), 15.3 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.19 (m, 2H), 7.03 – 6.62 (m, 2H), 6.31 (brs, 1H), 5.63-5.58 (m, 1H), 4.89 (dd, *J* = 12.8, 6.5 Hz, 1H), 4.68 (dd, *J* = 12.8, 5.9 Hz, 1H), 3.79 (s, 3H), 2.03 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 159.8, 128.3, 127.8, 114.6, 78.2, 55.4, 50.9, 23.3.



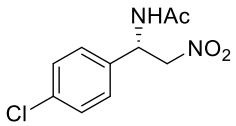
(*S*)-N-(1-(4-(tert-butyl)phenyl)-2-nitroethyl)acetamide 2d

White solid; 26.3 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +58.20 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 9.0 min (major), 13.4 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.35 (m, 2H), 7.26 – 7.20 (m, 2H), 6.34 (brs, 1H), 5.70-5.60 (m, 1H), 4.90 (dd, *J* = 12.9, 6.6 Hz, 1H), 4.71 (dd, *J* = 12.9, 5.8 Hz, 1H), 2.03 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 151.9, 133.3, 126.2, 78.1, 51.0, 34.6, 31.2, 23.3.



(*S*)-N-(1-(4-fluorophenyl)-2-nitroethyl)acetamide 2e

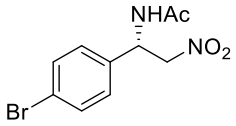
White solid; 22.5 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +43.20 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 12.2 min (major), 24.0 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.28 (m, 2H), 7.18 – 6.99 (m, 2H), 6.44 (brs, 1H), 5.68-5.66 (m, 1H), 4.90 (dd, *J* = 13.0, 6.5 Hz, 1H), 4.71 (dd, *J* = 13.0, 5.5 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 164.0, 161.5, 132.2, 132.2, 128.4, 128.3, 116.4, 116.2, 78.2, 50.7, 23.3.



(*S*)-N-(1-(4-chlorophenyl)-2-nitroethyl)acetamide 2f

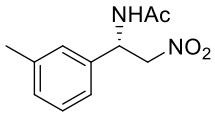
White solid; 24.1 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +52.00 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane:

isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 13.3 min (major), 25.0 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 2H), 7.27-7.23 (m, 2H), 6.51 (brs, 1H), 5.71 – 5.47 (m, 1H), 4.89 (dd, *J* = 13.1, 6.5 Hz, 1H), 4.71 (dd, *J* = 13.1, 5.3 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 134.9, 134.8, 129.5, 127.9, 78.0, 50.7, 23.3.



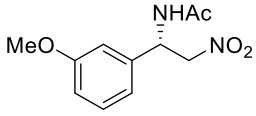
(*S*)-N-(1-(4-bromophenyl)-2-nitroethyl)acetamide 2g

White solid; 28.0 mg, 97% yield; 99% ee; $[\alpha]_D^{20}$ = +48.80 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85:15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 8.3 min (major), 15.2 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.49 (m, 2H), 7.24 – 7.10 (m, 2H), 6.50 (brs, 1H), 5.66-5.61 (m, 1H), 4.88 (dd, *J* = 13.1, 6.5 Hz, 1H), 4.71 (dd, *J* = 13.1, 5.3 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 135.4, 132.4, 128.2, 122.9, 78.0, 50.7, 23.3.



(*S*)-N-(2-nitro-1-(m-tolyl)ethyl)acetamide 2h

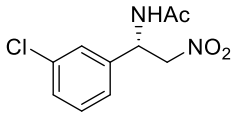
White solid; 22.1 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +47.00 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85:15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 6.3 min (major), 9.9 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.22 (m, 1H),7.19-7.05 (m, 3H), 6.41 (brs, 1H), 5.70-5.60 (m, 1H), 4.88 (dd, *J* = 12.9, 6.7, 1H), 4.70 (dd, *J* = 12.9, 5.7 Hz, 1H), 2.35 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 139.1, 136.3, 129.6, 129.2, 127.3, 123.4, 78.2, 51.3, 23.3, 21.5.



(*S*)-N-(1-(3-methoxyphenyl)-2-nitroethyl)acetamide 2i

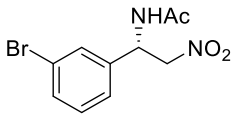
White solid; 23.6 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +44.00 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane:

isopropanol = 85: 15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 8.8 min (major), 12.9 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.22 (m,, 1H), 7.05 – 6.70 (m, 3H), 6.38 (brs, 1H), 5.70-5.60 (m, 1H), 4.89 (dd, *J* = 12.9, 6.6 Hz, 1H), 4.71 (dd, *J* = 12.9, 5.6 Hz, 1H), 3.80 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 160.1, 137.9, 130.4, 118.4, 113.8, 112.7, 78.1, 55.4, 51.2, 23.3.



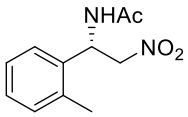
(*S*)-N-(1-(3-chlorophenyl)-2-nitroethyl)acetamide 2j

White solid; 23.7 mg, 98% yield; 99% ee; $[\alpha]_D^{20}$ = +46.80 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85: 15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 6.5 min (major), 9.3 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 3H), 7.24-7.16 (m, 1H), 6.61 (brs, 1H), 5.72-5.62 (m, 1H), 4.88 (dd, *J* = 13.2, 6.7 Hz, 1H), 4.71 (dd, *J* = 13.2, 5.2 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 138.4, 135.2, 130.5, 129.0, 126.7, 124.7, 78.0, 50.7, 23.2.



(*S*)-N-(1-(3-bromophenyl)-2-nitroethyl)acetamide 2k

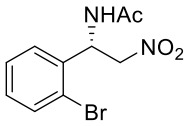
White solid; 28.0 mg, 97% yield; 99% ee; $[\alpha]_D^{20}$ = +99.40 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85: 15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 6.8 min (major), 9.6 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.33 (m, 2H), 7.32 – 7.09 (m, 2H), 6.63 (brs, 1H), 5.86 – 5.33 (m, 1H), 4.87 (dd, *J* = 13.2, 6.8 Hz, 1H), 4.71 (dd, *J* = 13.2, 5.2 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 138.7, 132.0, 130.8, 129.6, 125.2, 123.3, 78.0, 50.7, 23.2.



(*S*)-N-(2-nitro-1-(o-tolyl)ethyl)acetamide 2l

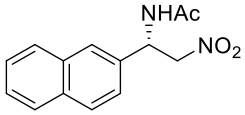
White solid; 22.1 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +62.60 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85:15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 5.8 min

(major), 6.8 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.18 (m, 4H), 6.19 (brs, 1H), 5.95-5.90 (m, 1H), 4.84 (dd, *J* = 12.7, 7.1 Hz, 1H), 4.69 (dd, *J* = 12.7, 6.4 Hz, 1H), 2.45 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 136.4, 134.7, 131.4, 128.9, 126.8, 125.0, 77.3, 47.9, 23.1, 19.3.



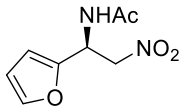
(*S*)-N-(1-(2-bromophenyl)-2-nitroethyl)acetamide 2m

White solid; 28.6 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +13.20 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 11.1 min (major), 13.9 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.56 (m, 1H), 7.40 – 7.29 (m, 2H), 7.23-7.18 (m, 1H), 6.66 (brs, 1H), 6.02-5.93 (m, 1H), 4.97 (dd, *J* = 13.0, 6.7 Hz, 1H), 4.81 (dd, *J* = 13.0, 4.8 Hz, 1H), 2.07 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 136.3, 133.2, 129.8, 128.1, 128.0, 122.9, 76.8, 51.1, 22.8.



(*S*)-N-(1-(naphthalen-2-yl)-2-nitroethyl)acetamide 2n

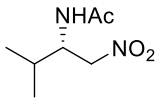
White solid; 25.7 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = +82.80 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 85: 15; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 9.3 min (major), 16.9 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.67 (m, 4H), 7.59 – 7.44 (m, 2H), 7.41-7.35 (m, 1H), 6.51 (brs, 1H), 5.88-5.80 (m, 1H), 4.99 (dd, *J* = 13.0, 6.6 Hz, 1H), 4.81 (dd, *J* = 13.0, 5.6 Hz, 1H), 2.08 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 132.6, 132.1, 128.3, 127.0, 126.7, 125.8, 125.7, 124.7, 122.8, 77.1, 50.4, 22.3.



(*S*)-N-(1-(furan-2-yl)-2-nitroethyl)acetamide 2o

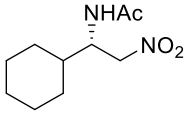
White solid; 14.0 mg, 87% yield; 96% ee; $[\alpha]_D^{20}$ = +45.40 (c = 0.5, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane:

isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 12.1 min (major), 13.3 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (m, 1H), 6.43 – 6.27 (m, 3H), 5.77 (dd, *J* = 13.2, 5.5 Hz, 1H), 4.90 (dd, *J* = 13.2, 5.5 Hz, 1H), 4.73 (dd, *J* = 13.2, 5.7 Hz, 1H), 2.07 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 148.9, 143.0, 110.8, 108.1, 76.1, 45.5, 23.2.



(*S*)-N-(3-methyl-1-nitrobutan-2-yl)acetamide 2p

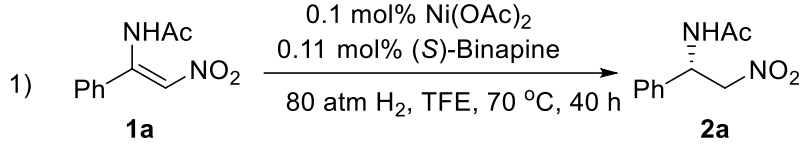
White solid; 17.4 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = -50.40 (c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 97: 3; flow rate = 0.9 mL/min; UV detection at 210 nm; t_R = 38.0 min (major), 40.6 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.92 (brs, 1H), 4.63 (dd, *J* = 12.8, 5.8 Hz, 1H), 4.54 (dd, *J* = 12.8, 3.9 Hz, 1H), 4.30 – 4.16 (m, 1H), 2.04 (s, 3H), 1.97 – 1.81 (m, 1H), 1.02 (d, *J* =6.7 Hz, 3H), 0.99 (d, *J*=6.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 76.6, 53.2, 29.7, 23.3, 19.5, 19.1.



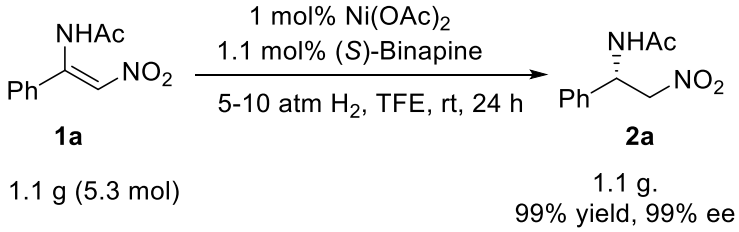
(*S*)-N-(1-cyclohexyl-2-nitroethyl)acetamide 2q

White solid; 21.3 mg, 99% yield; 99% ee; $[\alpha]_D^{20}$ = -31.70 (c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 7.6 min (major), 10.4 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.96 (brs, 1H), 4.65 (dd, *J* = 13.0, 5.7 Hz, 1H), 4.54 (dd, *J* = 13.0, 3.8 Hz, 1H), 4.23 (m, 1H), 2.03 (s, 3H), 1.84 – 1.61 (m, 5H), 1.62 – 1.46 (m, 1H), 1.31 – 1.11 (m, 3H), 1.10 – 0.77 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 76.3, 52.3, 38.9, 29.8, 29.5, 25.9, 25.7, 23.3.

3. Gram-scale Reaction and S/C Evaluation



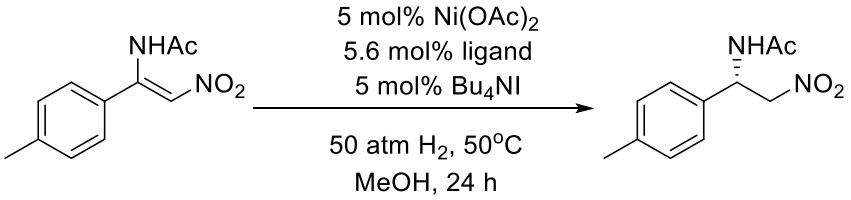
In a nitrogen-filled glovebox, the $Ni(OAc)_2$ (0.01 mmol) and (*S*)-Bianpine (0.011 mmol) were dissolved in 1.0 mL anhydrous MeOH and THF (1:1), and the solution was stirred for 30 min at rt. Then the catalyst solution (0.2 mL) was transferred by syringe into the vials charged with substrates **1a** (0.414g, 2 mmol) in anhydrous TFE solution (5.0 mL). The resulting vials were transferred to an autoclave, which was charged with 80 atm H_2, and the reaction was stirred at 70°C for 40h. When the reaction was completed, the H_2 was released slowly and the solution was passed through a short column of silica gel with EA. The solution was concentrated under reduced pressure to got the target compound. The conversion of **1a** was confirmed by ^1H NMR. The chiral compounds were the analyzed by using HPLC on a chiral stationary phase to determine the ee.



In a nitrogen-filled glovebox, the $Ni(OAc)_2$ (0.05 mmol) and (*S*)-Bianpine (0.055 mmol) were dissolved in 1.0 mL anhydrous MeOH and THF (1:1), and the solution was stirred for 30 min at rt. Then the catalyst solution was transferred by syringe into the vials charged with substrates **1a** (1.1g, 5.3 mmol) in anhydrous TFE solution (30.0 mL). The resulting vials were transferred to an autoclave, which was charged with 10 atm H_2, and the reaction was stirred at rt for 24h. When the reaction was completed, the H_2 was released slowly and the solution was passed through a short column of silica gel with EA. The solution was concentrated under reduced pressure to got the

target compound. The chiral compounds were the analyzed by using HPLC on a chiral stationary phase to determine the ee. The yield of **2a** is 99%, ee is 99%.

4. The Influence of additive Bu_4NI



Entry	Ligand	Additive	Conv. (%)	Ee (%)
1	(*Rc,Sp*)-DuanPhos	Bu_4NI	71	68
2	(*Rc,Sp*)-DuanPhos	-	85	65
3	(*R,R*)-QuinoxP*	Bu_4NI	80	95
4	(*R,R*)-QuinoxP*	-	>99	97
5	(*S*)-DuPhos	Bu_4NI	>99	30
6	(*S*)-DuPhos	-	>99	37

5. Deuterium Labeling Studies

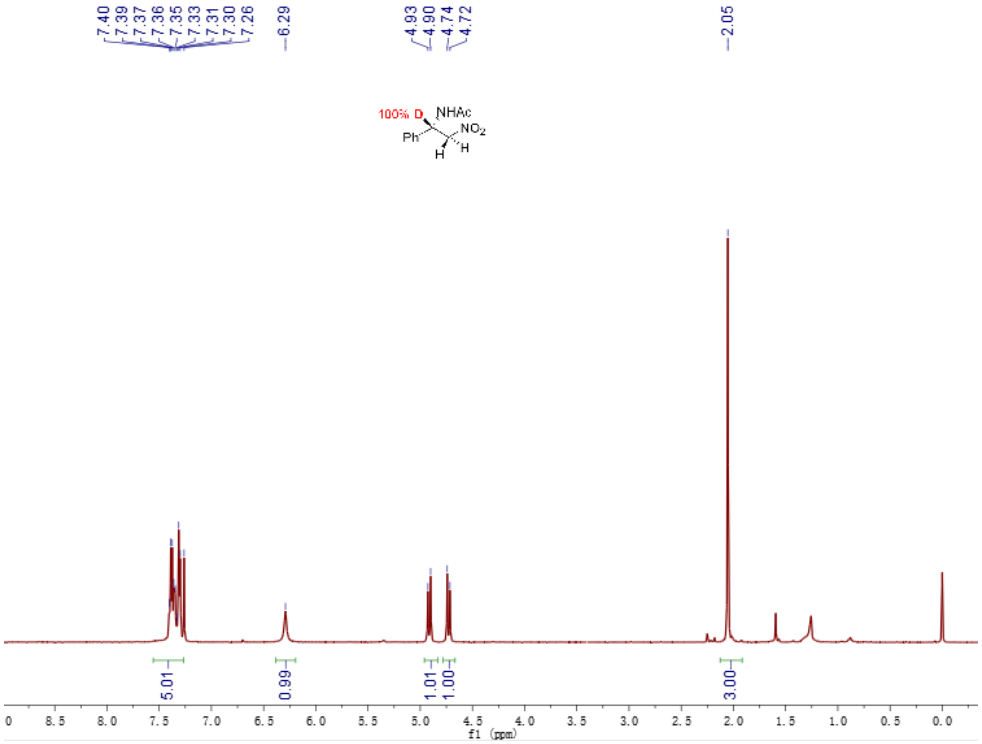
(1) Asymmetric hydrogenation of **1a** in TFE solution under D_2: In a nitrogen-filled glovebox, the $Ni(OAc)_2$ (0.01 mmol) and (*S*)-Bianpine (0.011 mmol) were dissolved in 1.0 mL anhydrous MeOH and THF (1:1), and the solution was stirred for 30 min at rt. Then the solution was equally divided into 10 vials charged with **1a** (0.1 mmol) in anhydrous TFE solution (1.0 mL). The resulting vials were transferred to an autoclave, which was charged with 5-10 atm D_2, and the reaction was stirred at rt for 24h. When the reaction was completed, the D_2 was released slowly and the solution was passed through a short column of silica gel with EA. The solution was concentrated under reduced pressure to got the target compound. The chiral compounds were the analyzed by using HPLC on a chiral stationary phase to determine the ee.

(2) Asymmetric hydrogenation of **1a** in CD_3OD solution under H_2 (D_2): In a nitrogen-filled glovebox, the $Ni(OAc)_2$ (0.01 mmol) and (*S*)-Bianpine (0.011 mmol) were dissolved in 1.0 mL anhydrous CD_3OD and THF (1:1), and the solution was stirred for 30 min at rt. Then the solution was equally divided into 10 vials charged with **1a** (0.1 mmol) in anhydrous CD_3OD solution (1.0 mL). The resulting vials were transferred to an autoclave, which was charged with 30-50 atm H_2 (D_2), and the reaction was stirred at 50 ºC for 24h. When the reaction was completed, the D_2 was released slowly and the solution was passed through a short column of silica gel with EA. The solution was concentrated under reduced pressure to got the target compound. The chiral compounds were the analyzed by using HPLC on a chiral stationary phase to determine the ee.

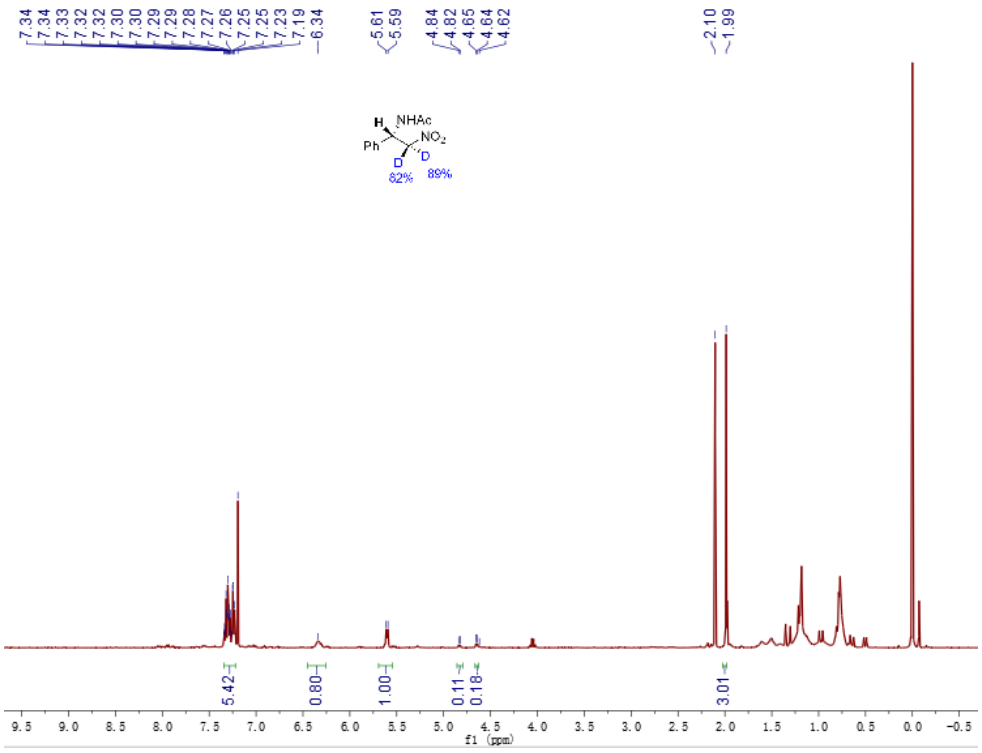
(3) Asymmetric hydrogenation of **2a** in CD_3OD solution under H_2: A vials charged with **2a** (0.1 mmol) in anhydrous CD_3OD solution (1.0 mL). The resulting vials were transferred to an autoclave, which was charged with 30 H_2, and the reaction was stirred at 50 ºC for 24h. When the reaction was completed, the H_2 was released slowly and the solution was passed through a short column of silica gel with EA. The

solution was concentrated under reduced pressure to got the target compound. The chiral compounds were the analyzed by using HPLC on a chiral stationary phase to determine the ee.

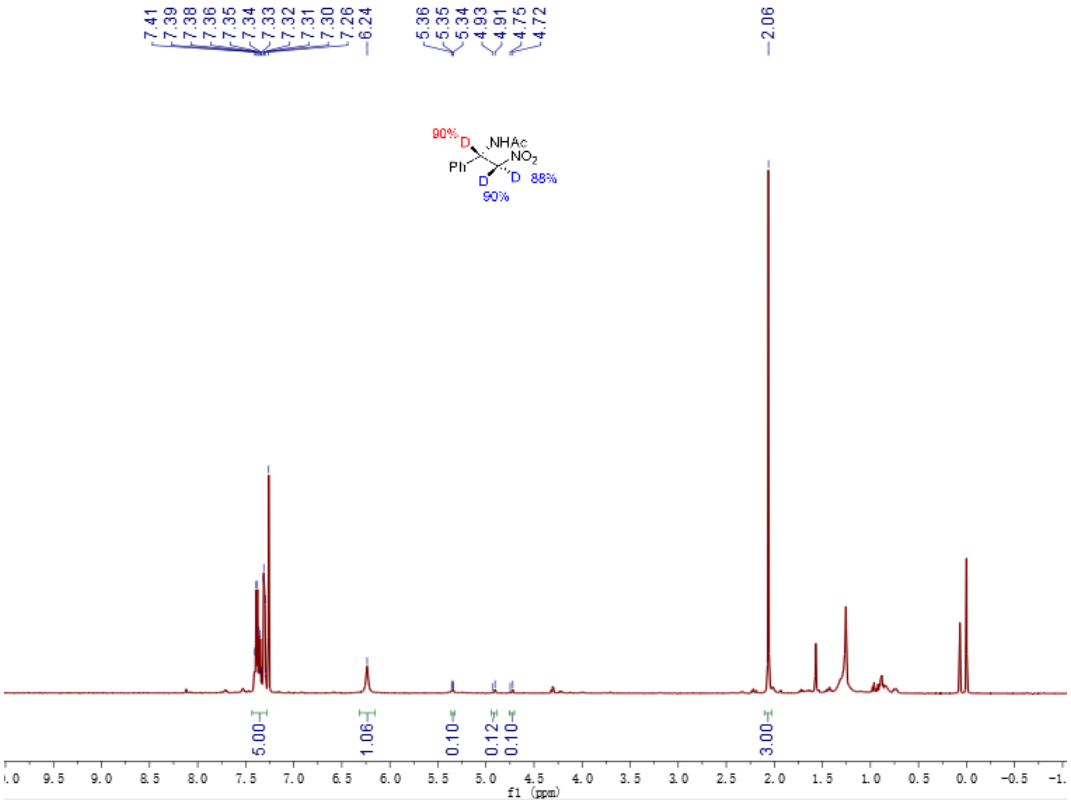
^{1}H NMR spectrum of **2a**: asymmetric hydrogenation of **1a** under TFE and 10atm D_2



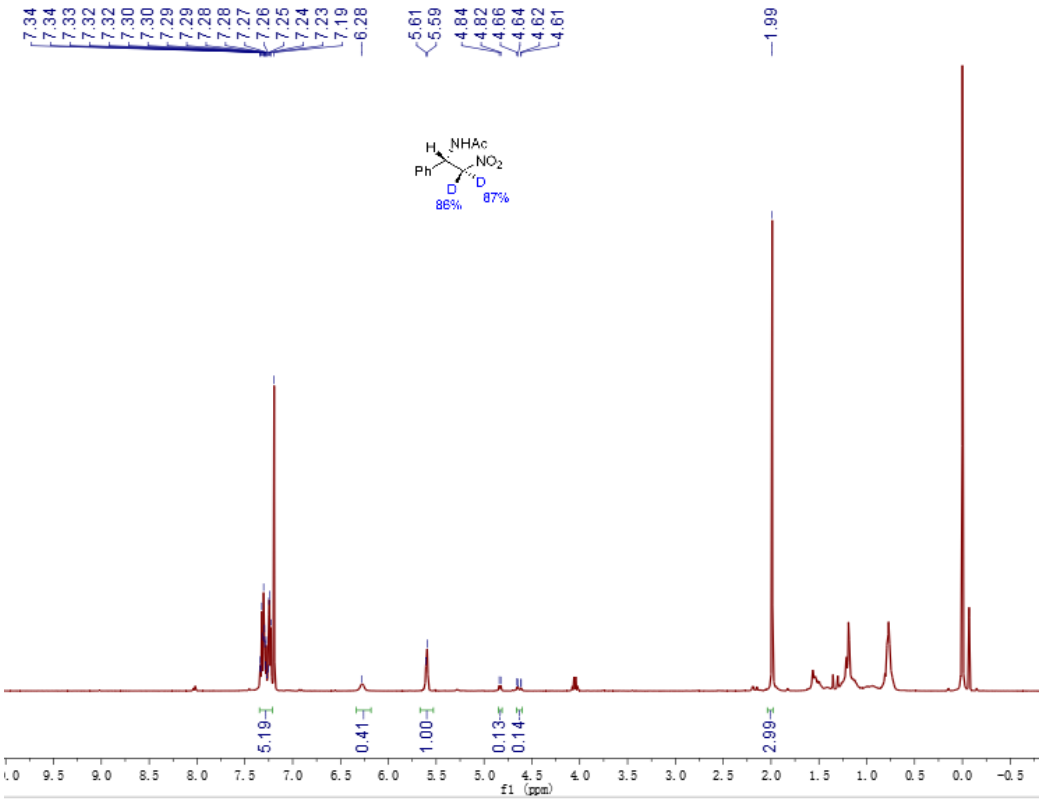
^{1}H NMR spectrum of **2a:** asymmetric hydrogenation of **1a** CD_3OD and 50 atm H_2



^{1}H NMR spectrum of **2a:** asymmetric hydrogenation of **1a** CD_3OD and 30 atm D_2



^{1}H NMR spectrum of **2a**: **2a** was stirred in CD_3OD and 30 atm H_2



6. Computational Details

We carried out density functional theory (DFT) calculations to understand the mechanism of the Ni-catalyzed asymmetric hydrogenation of (*Z*)-*N*-(2-nitro-1-(p-tolyl)vinyl)acetamide **1b** using a (S)-Binapine ligand. M06-L[3] method combined with 6-31G* basis set[4] and Grimme's dispersion correction[5] was used to optimize all the structures in gas phase. The vibrational frequency calculations were computed on the optimized structures at the same level of theory to check whether every optimized structure is either an energy minimum or a transition state. The effect of the solvent (2,2,2-TriFluoroEthanol, TFE) was then included by single-point calculations with an implicit solvent model SMD[6] (by the M06L-D3 and B3LYP-D3[7] methods). All the computations were carried out by Gaussian 09 package.[8] All 3D images of the optimized structures were illustrated by CYLview.[9]

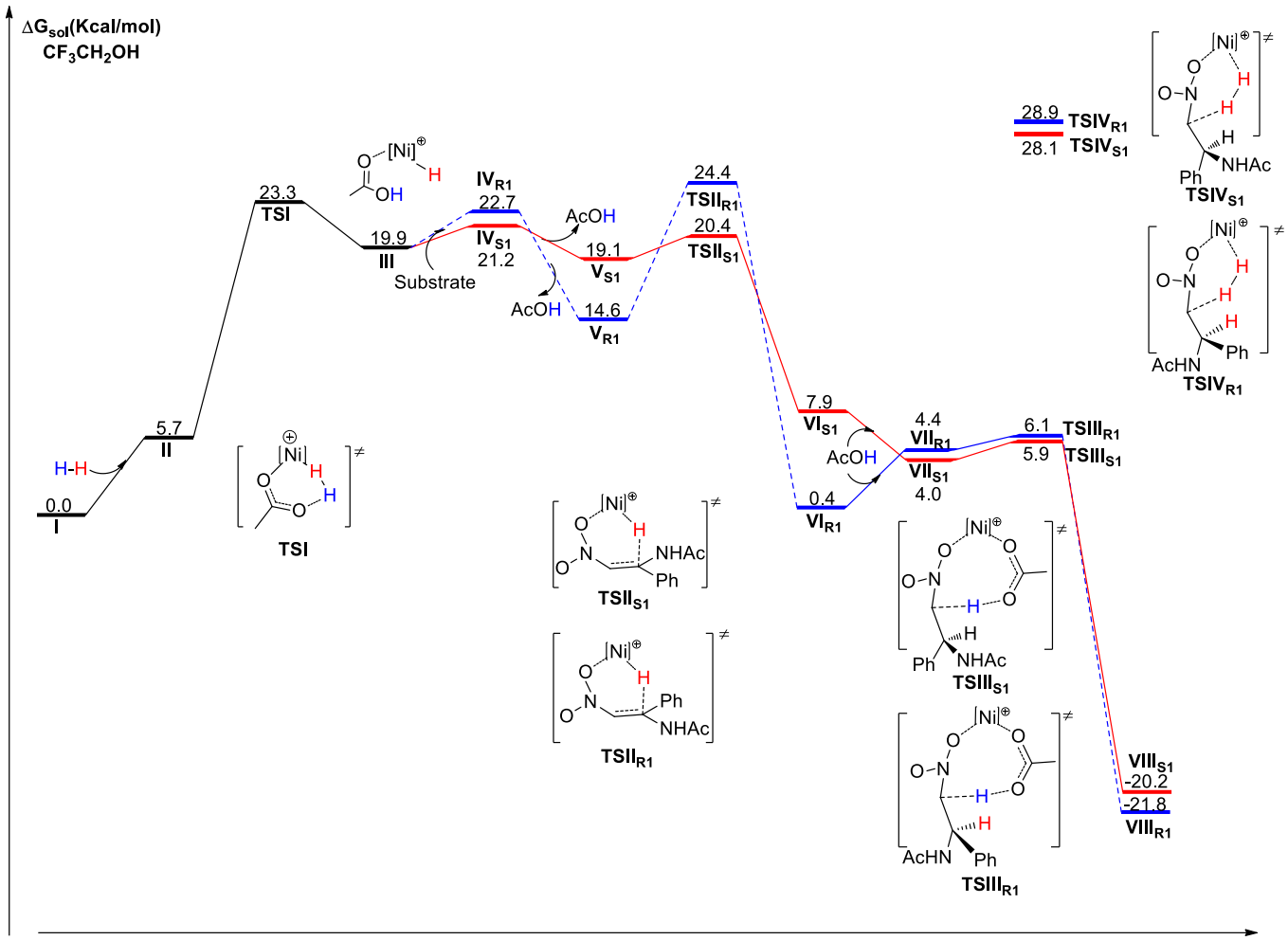


Figure S1. Free energy profiles of the of the Ni-catalyzed asymmetric hydrogenation reaction pathways for the S1, & R1 (most favorable 1,4-addition) isomers in solution by the M06L/6-31G* method.

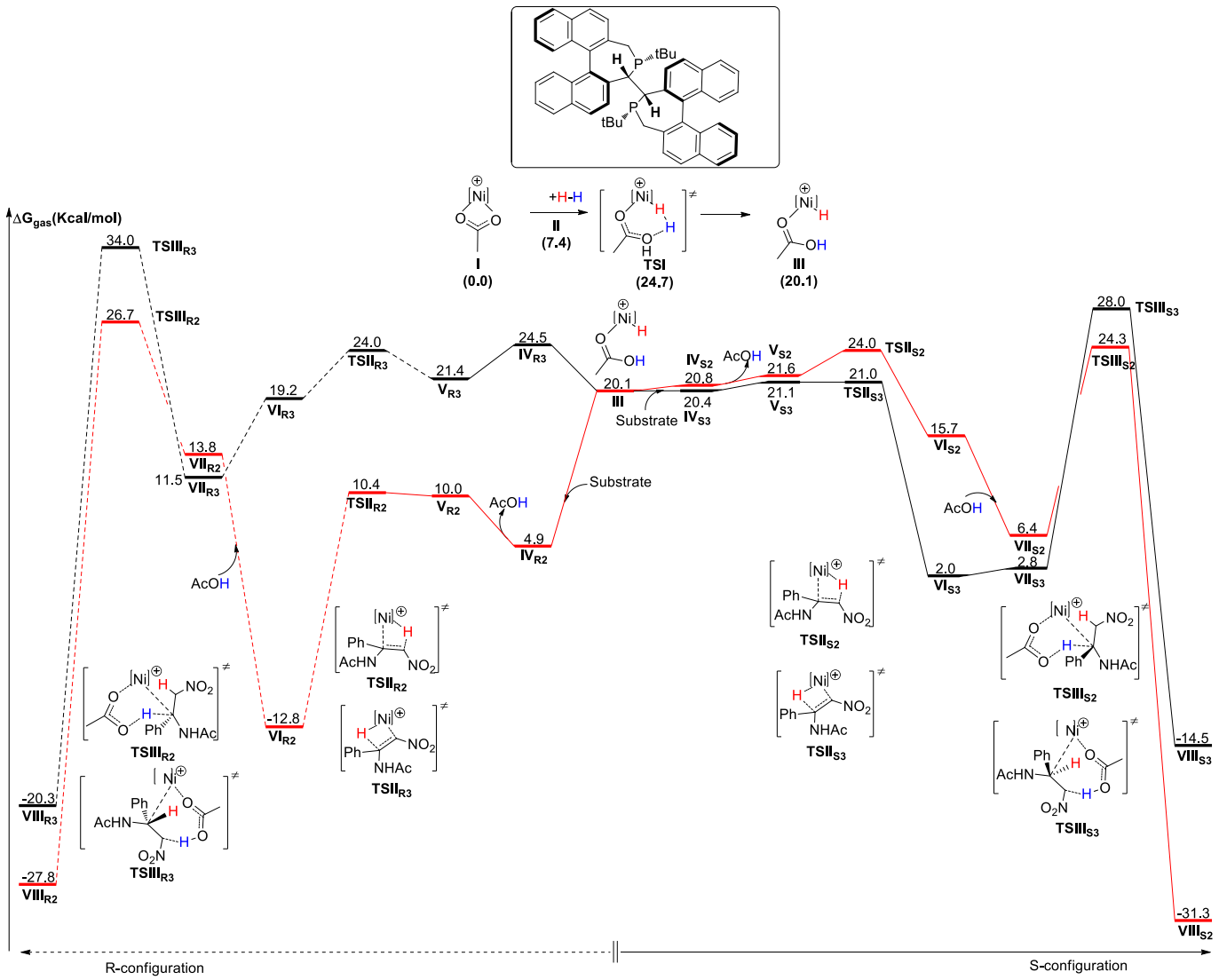


Figure S2. Free energy profiles of the of the Ni-catalyzed asymmetric hydrogenation reaction pathways for the S2, S3 & R2, R3 (less favorable) isomers in gas phase by the M06L/6-31G* method.

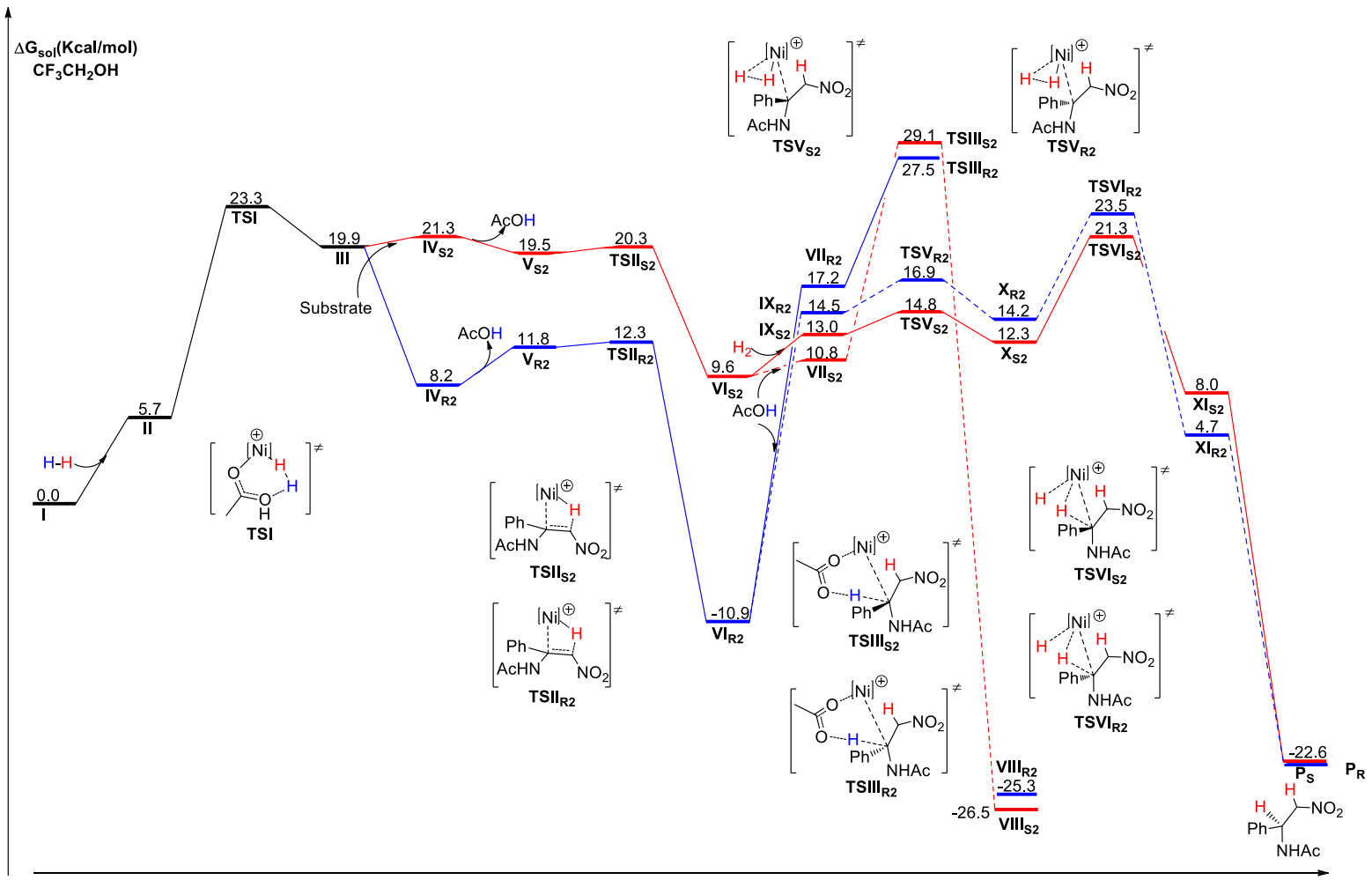


Figure S3. Free energy profiles of the of the Ni-catalyzed asymmetric hydrogenation reaction pathways for the S2, S3 & R2, R3 (less favorable) isomers in solution by the M06L/6-31G* method.

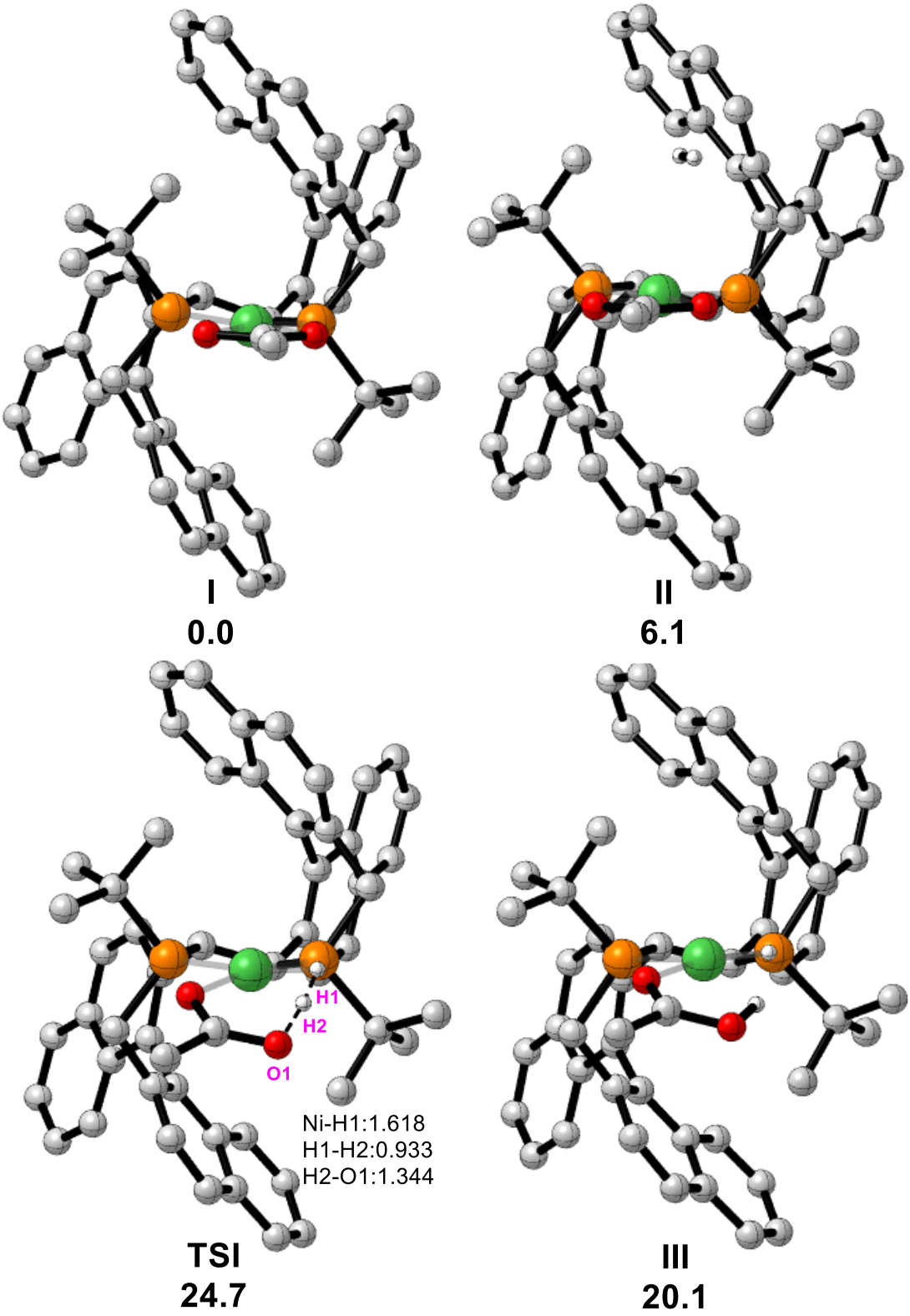


Figure S4. Optimized structures of the key intermediates and transition states in the cationic form. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

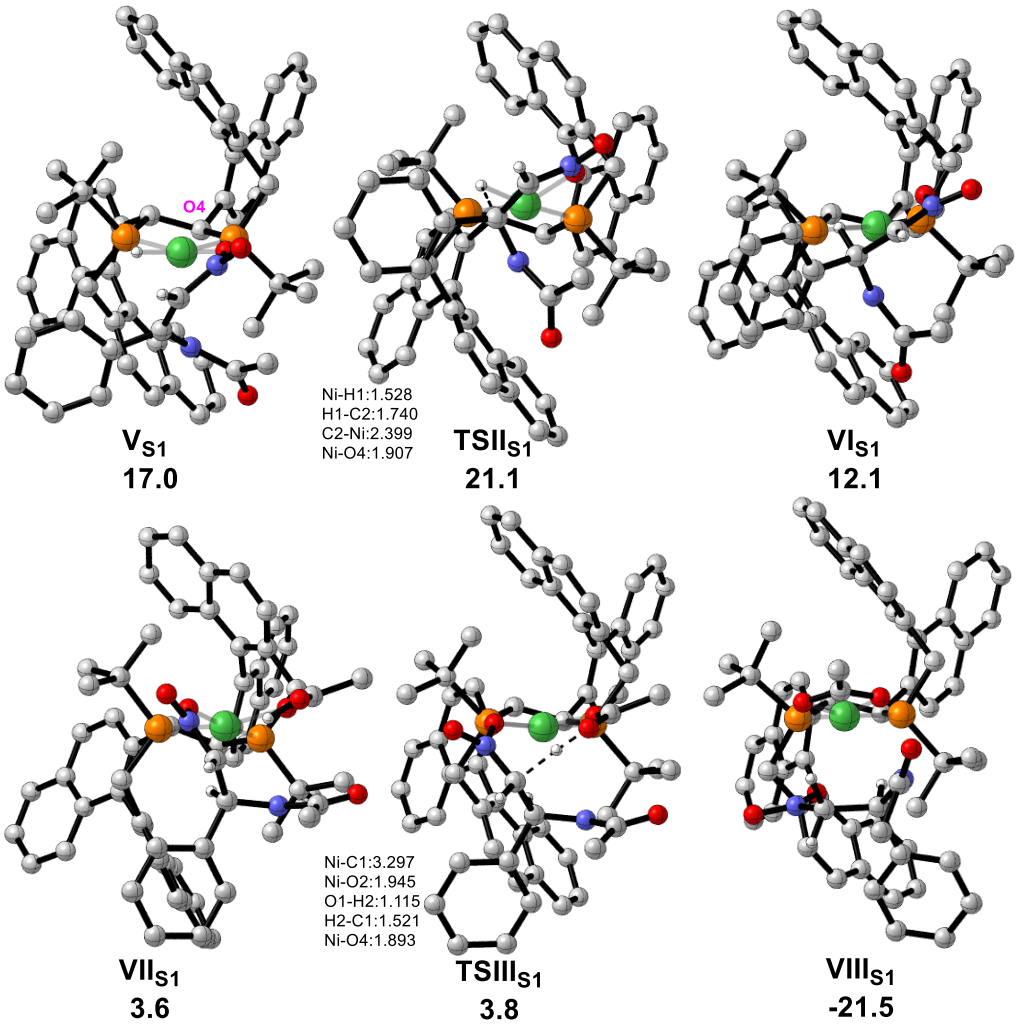


Figure S5. Optimized structures of the key intermediates and transition states for the S1 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

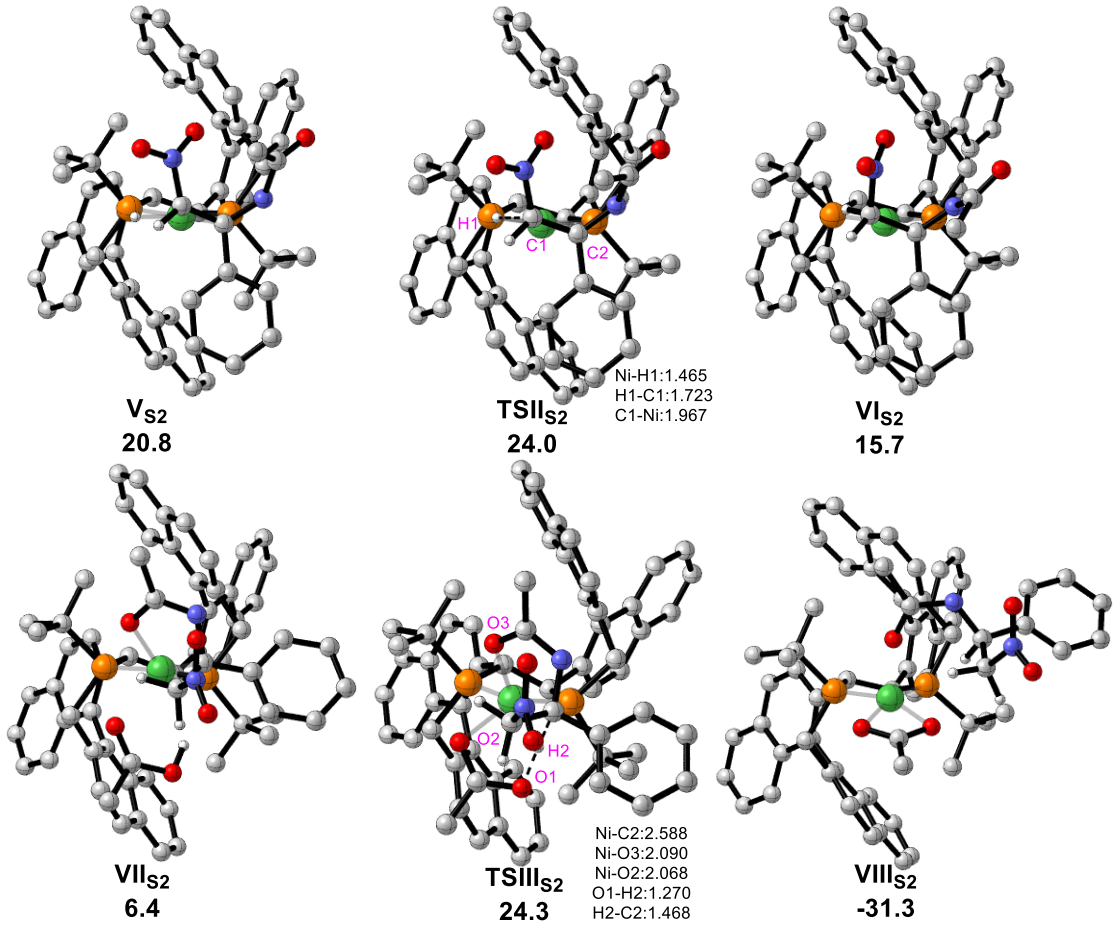


Figure S6. Optimized structures of the key intermediates and transition states for the S2 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

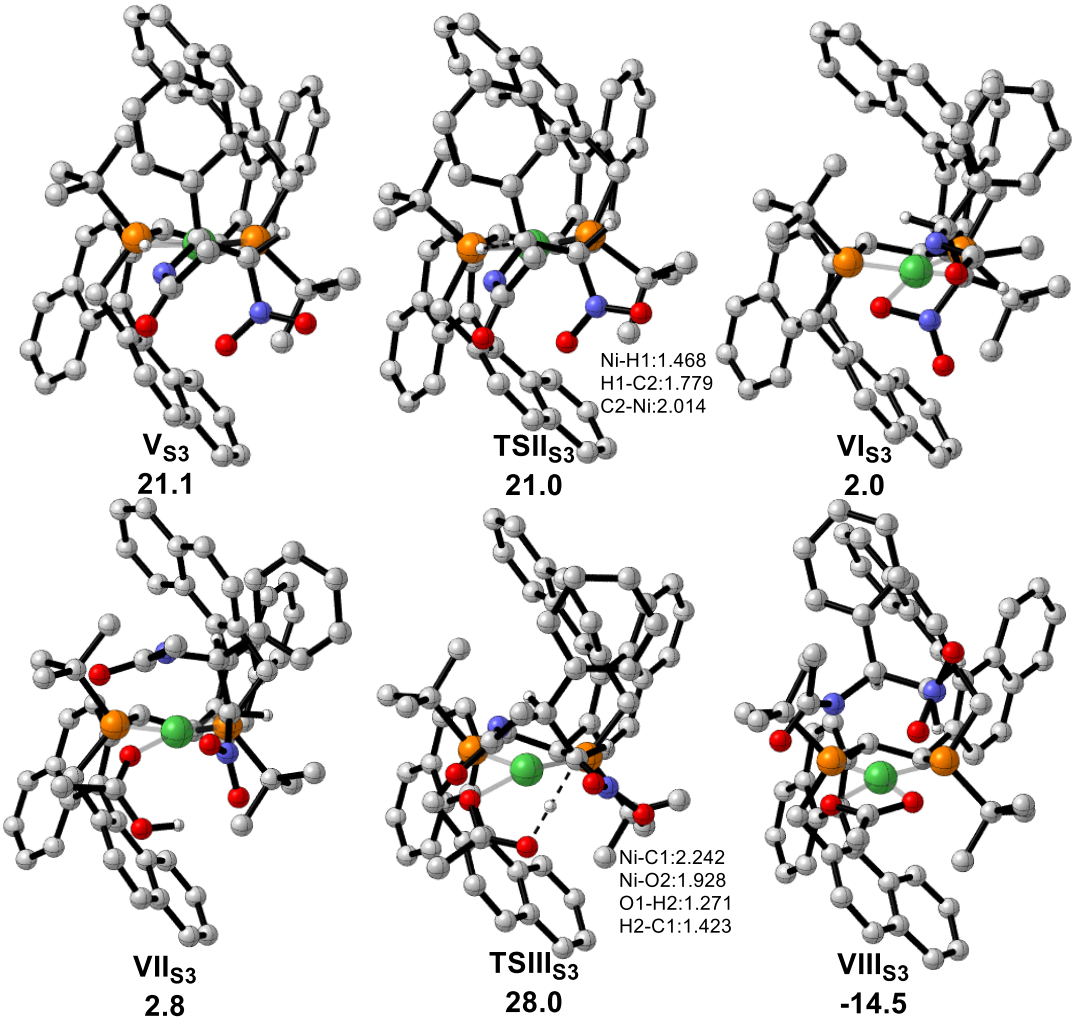


Figure S7. Optimized structures of the key intermediates and transition states for the S3 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

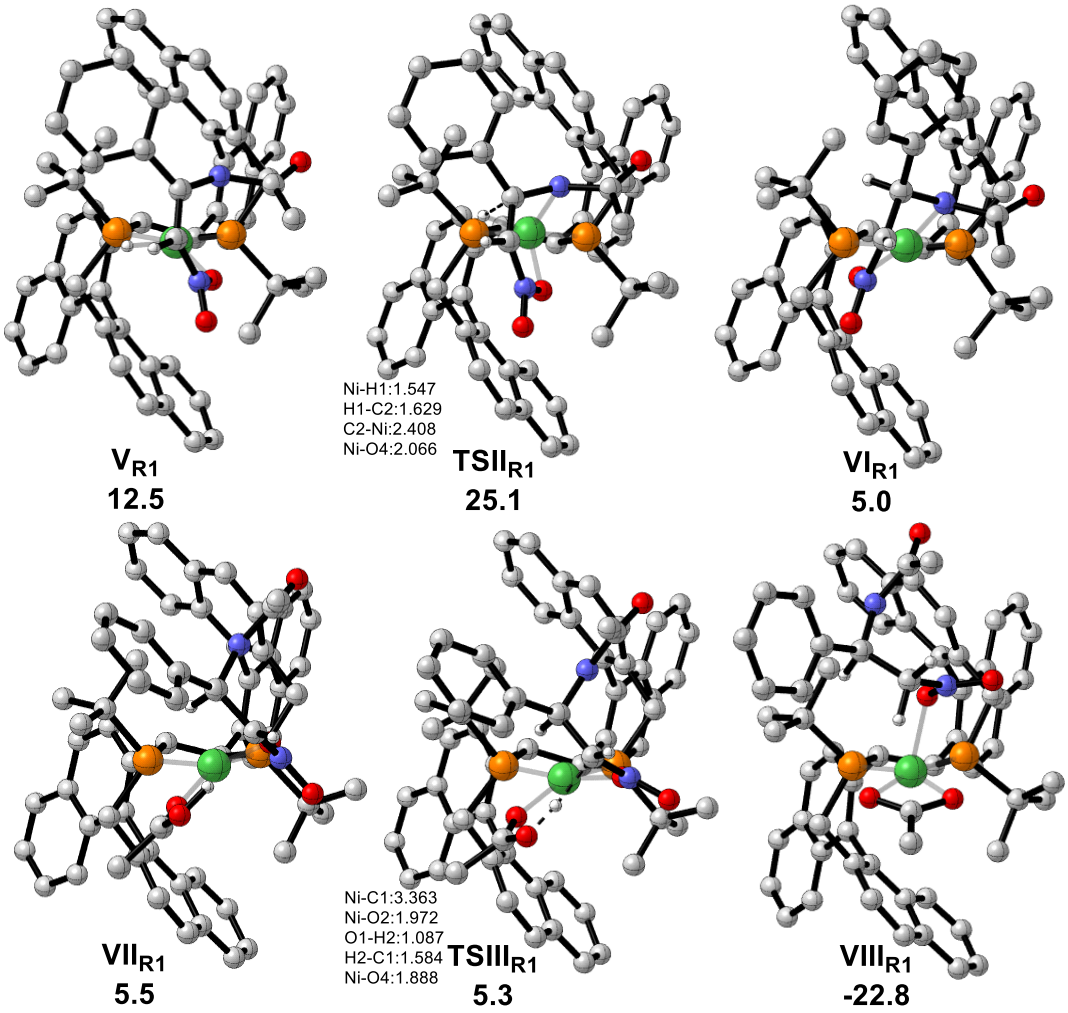


Figure S8. Optimized structures of the key intermediates and transition states for the R1 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

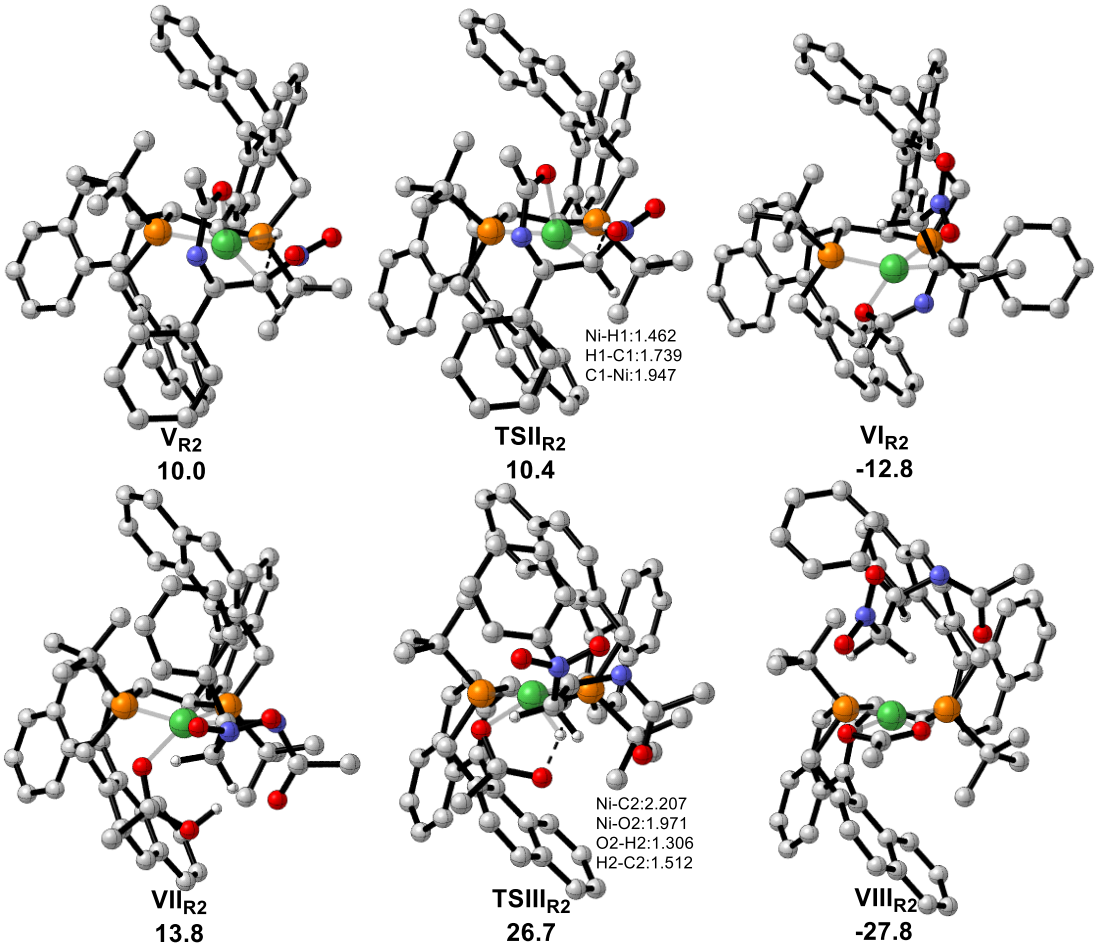


Figure S9. Optimized structures of the key intermediates and transition states for the R2 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

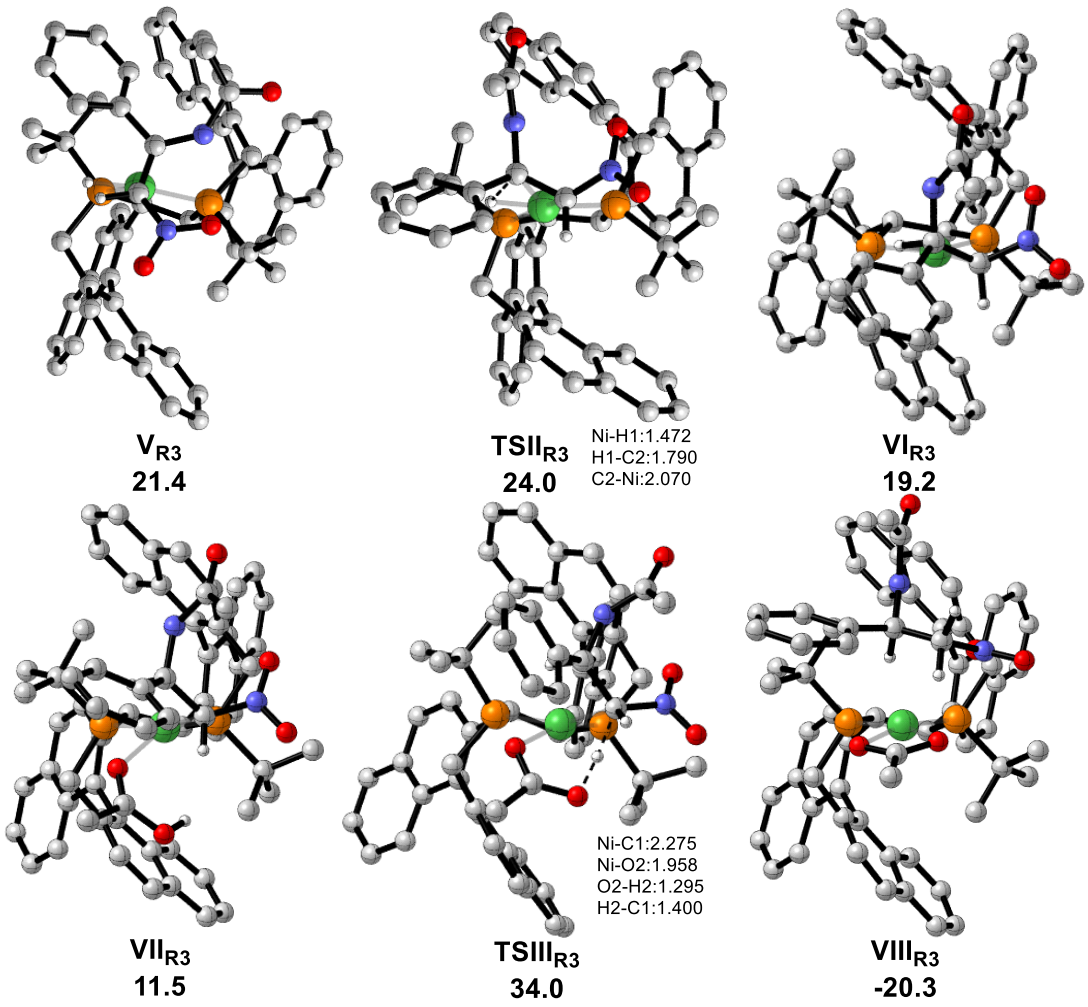


Figure S10. Optimized structures of the key intermediates and transition states for the R3 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

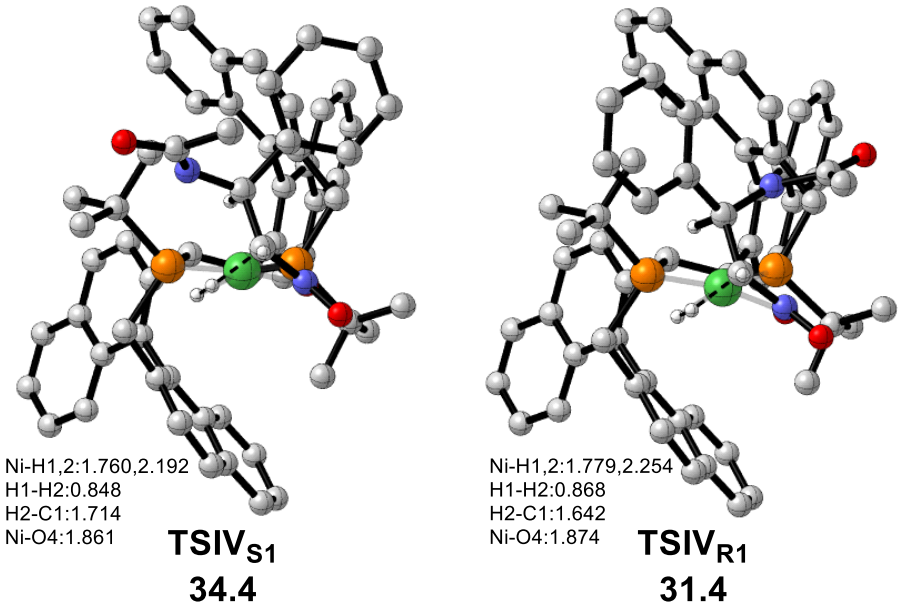


Figure S11. Optimized structures of the transition states involving H_2 splitting for the S1 & R1 isomers. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

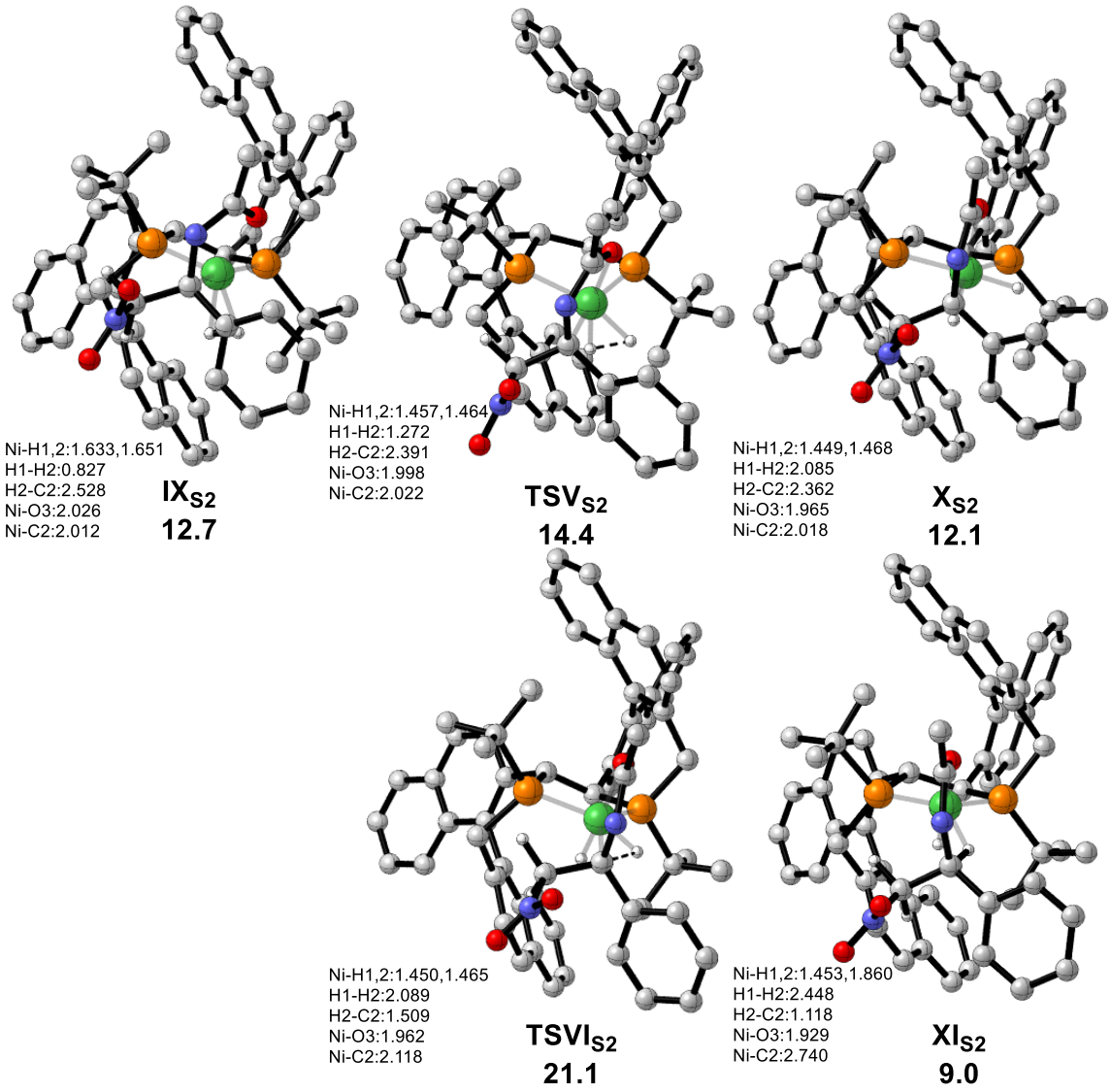


Figure S12. Optimized structures of the transition states involving H_2 splitting for the S2 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

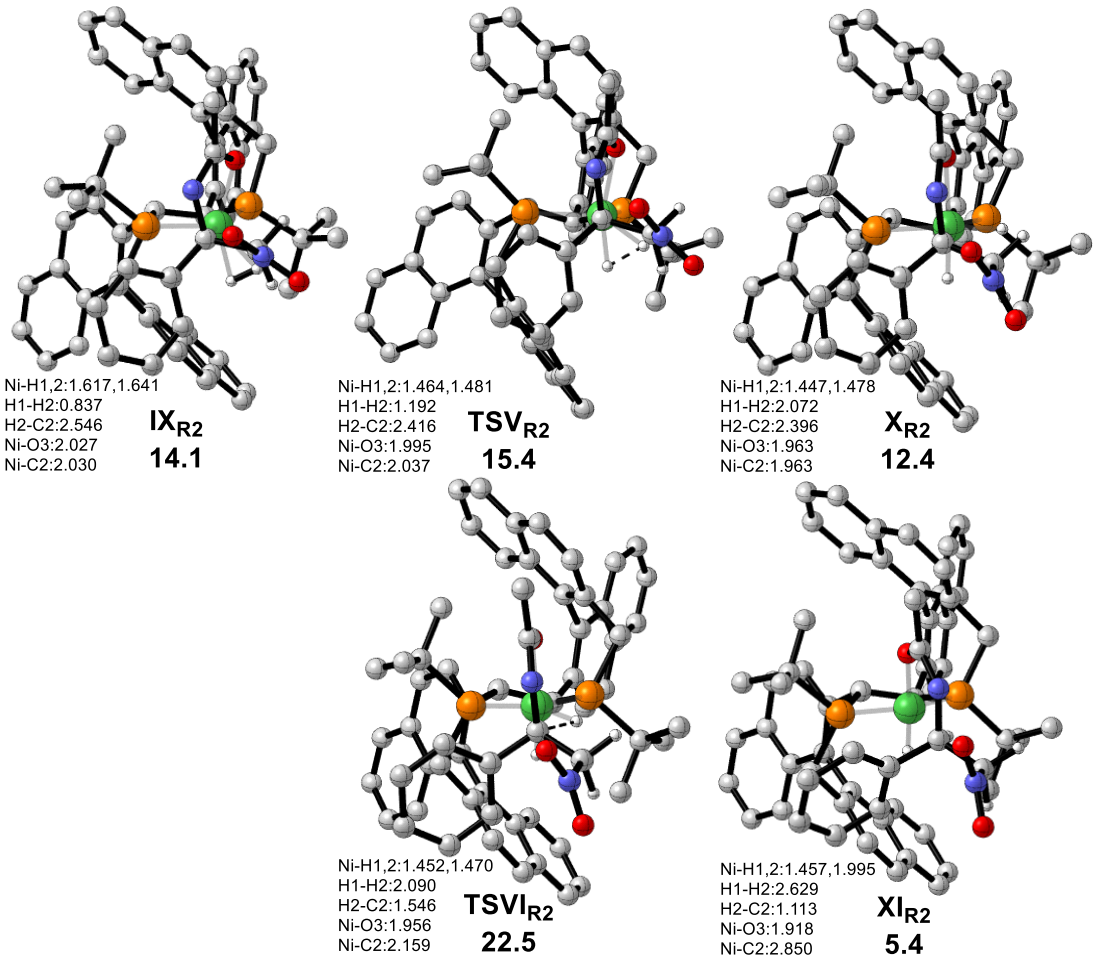


Figure S13. Optimized structures of the transition states involving H_2 splitting for the R2 isomer. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

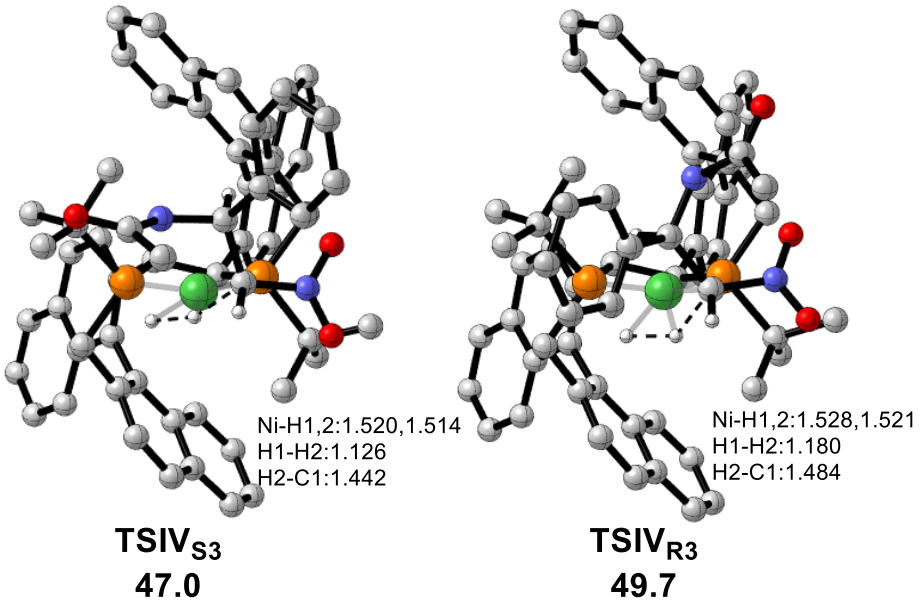


Figure S14. Optimized structures of the transition states involving H_2 splitting for the S3 & R3 isomers. The key bond lengths (in angstrom) and relative free energies (in kcal/mol) in gas phase are given. Unimportant hydrogen atoms are not shown for clarity.

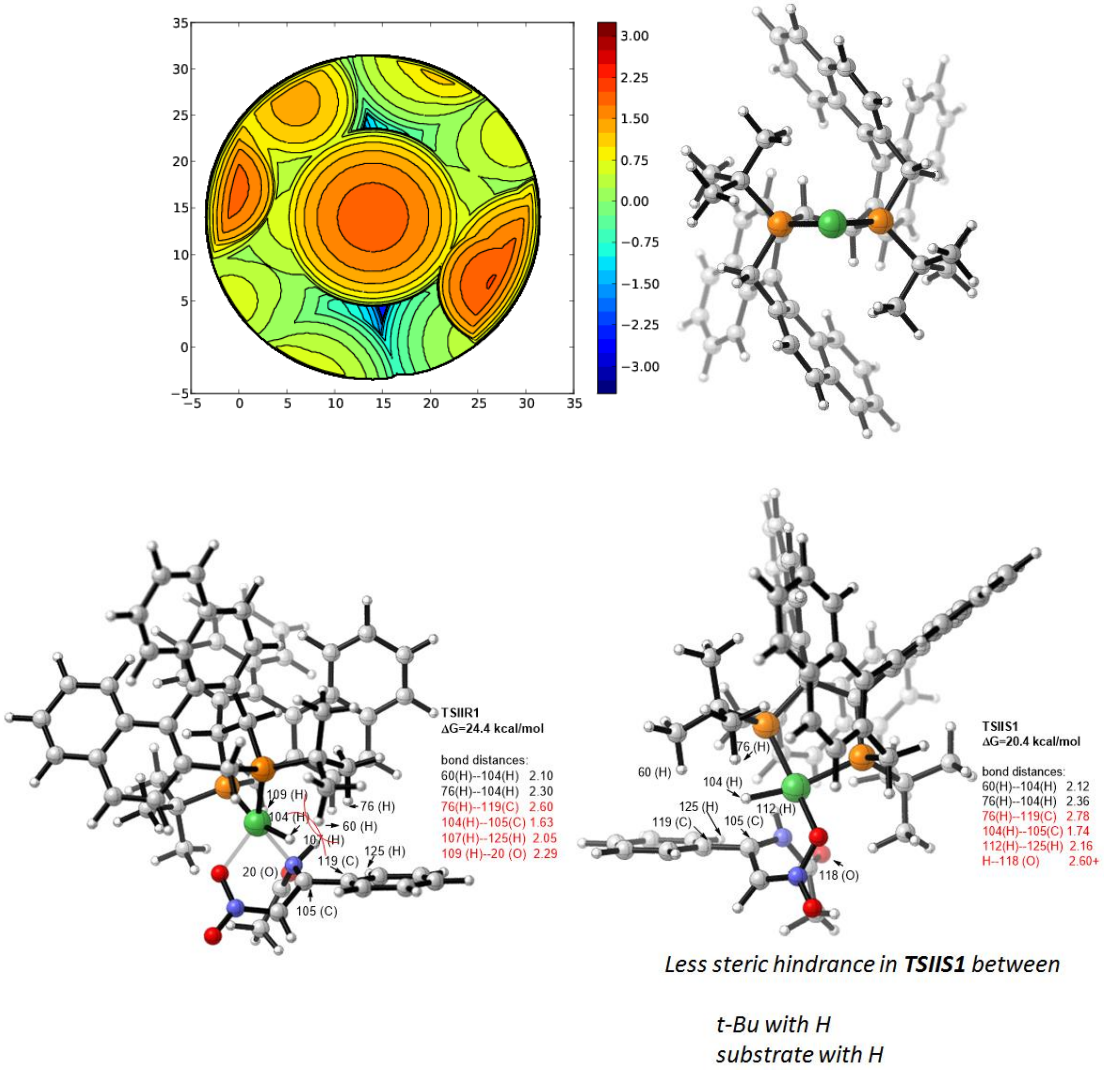


Figure S15. (top) The steric map[10] for **TSIIS1** and (bottom) The regio-determining transition states **TSIIR1** (left) and **TSIIS1** (right) to illustrate the larger steric effect on the stereoselectivity in **TSIIR1**.

Table S1. The absolute (in Hartree) and relative (in kcal/mol) energies for S isomer in gas phase by M06L/6-31G* method.

	E	E+ZPE	G	ΔE_{gas}	$\Delta E_{gas+ZPE}$	ΔG_{gas}
H_2	-1.167913	-1.158003	-1.169494			
Sub	-722.083326	-721.890567	-721.931901			
AcOH	-229.056125	-228.993765	-229.020702			
I	-4429.445753	-4428.534385	-4428.61447	0.0	0.0	0.0
II	-4430.616853	-4429.691448	-4429.774171	-2.0	0.6	6.1
TSI	-4430.589486	-4429.664058	-4429.744656	15.2	17.8	24.7
III	-4430.599646	-4429.669984	-4429.751874	8.8	14.1	20.1
S1 isomer						
IV_{S1}	-5152.712677	-5151.587988	-5151.685241	-9.8	-3.2	19.2
V_{S1}	-4923.638698	-4922.577172	-4922.668052	1.4	7.5	17.0
$TSII_{S1}$	-4923.629306	-4922.571295	-4922.66147	7.3	11.2	21.1
VI_{S1}	-4923.645825	-4922.583676	-4922.675879	-3.1	3.5	12.1
VII_{S1}	-5152.741101	-5151.61341	-5151.710159	-27.7	-19.1	3.6
$TSIII_{S1}$	-5152.740304	-5151.615022	-5151.709737	-27.2	-20.1	3.8
$VIII_{S1}$	-5152.784518	-5151.65355	-5151.750064	-54.9	-44.3	-21.5
the second step as the H_2 splitting						
$TSIV_{S1}$	-4924.795065	-4923.717246	-4923.809842	8.6	18.8	34.4
S2 isomer						
IV_{S2}	-5152.715133	-5151.587572	-5151.682768	-11.4	-2.9	20.8
V_{S2}	-4923.629605	-4922.569423	-4922.660809	7.1	12.4	21.6
$TSII_{S2}$	-4923.628109	-4922.567982	-4922.656934	8.0	13.3	24.0
VI_{S2}	-4923.642711	-4922.579463	-4922.670268	-1.2	6.1	15.6
VII_{S2}	-5152.74026	-5151.609546	-5151.705656	-27.2	-16.7	6.4
$TSIII_{S2}$	-5152.706214	-5151.581461	-5151.677208	-5.8	0.9	24.3
$VIII_{S2}$	-5152.797434	-5151.667395	-5151.765762	-63.0	-53.0	-31.3
the second step as the H_2 splitting						
IX_{S2}	-4924.836817	-4923.754403	-4923.844465	-17.6	-4.5	12.7
TSV_{S2}	-4924.828402	-4923.749646	-4923.841781	-12.3	-1.5	14.4
X_{S2}	-4924.834676	-4923.753899	-4923.845382	-16.2	-4.2	12.1
$TSVI_{S2}$	-4924.817377	-4923.738884	-4923.831062	-5.4	5.2	21.1
XI_{S2}	-4924.840318	-4923.756624	-4923.850435	-19.8	-5.9	8.9
S3 isomer						
IV_{S3}	-5152.713277	-5151.586546	-5151.683473	-10.2	-2.1	21.6
V_{S3}	-4923.63086	-4922.57056	-4922.661549	6.3	11.7	21.1
$TSII_{S3}$	-4923.630155	-4922.570663	-4922.661768	6.7	11.6	21.0
VI_{S3}	-4923.665269	-4922.601476	-4922.69209	-15.3	-7.7	1.9
VII_{S3}	-5152.747765	-5151.616745	-5151.711467	-31.9	-21.2	2.8
$TSIII_{S3}$	-5152.700612	-5151.575417	-5151.671329	-2.3	4.7	27.9
$VIII_{S3}$	-5152.771223	-5151.641609	-5151.738986	-46.6	-36.8	-14.5
the second step as the H_2 splitting						

$TSIV_{S3}$	-4924.779819	-4923.699488	-4923.789807	18.2	29.9	47.0

Table S2. The absolute (in Hartree) and relative (in kcal/mol) energies for R isomer in gas phase by M06L/6-31G* method.

	E	**E+ZPE**	**G**	**ΔE_{gas}**	**$\Delta E_{gas+ZPE}$**	**ΔG_{gas}**
R1 isomer						
IV_{R1}	-5152.712189	-5151.586983	-5151.684316	-9.5	-2.5	19.8
V_{R1}	-4923.643563	-4922.583527	-4922.67531	-1.7	3.6	12.5
$TSII_{R1}$	-4923.626688	-4922.566498	-4922.655212	8.9	14.2	25.1
VI_{R1}	-4923.661337	-4922.596433	-4922.687133	-12.8	-4.5	5.0
VII_{R1}	-5152.737764	-5151.609726	-5151.707086	-25.6	-16.8	5.5
$TSIII_{R1}$	-5152.736818	-5151.611313	-5151.707482	-25.0	-17.8	5.3
$VIII_{R1}$	-5152.7828	-5151.653866	-5151.752251	-53.8	-44.5	-22.8
the second step as the H_2 splitting						
$TSIV_{R1}$	-4924.804037	-4923.72435	-4923.814598	3.0	14.3	31.4
R2 isomer						
IV_{R2}	-5152.736332	-5151.611563	-5151.708054	-24.7	-18.0	4.9
V_{R2}	-4923.649559	-4922.588797	-4922.679268	-5.5	0.2	10.0
$TSII_{R2}$	-4923.649149	-4922.58939	-4922.678632	-5.2	-0.1	10.4
VI_{R2}	-4923.689092	-4922.624351	-4922.715696	-30.3	-22.1	-12.9
VII_{R2}	-5152.731704	-5151.599999	-5151.693859	-21.8	-10.7	13.8
$TSIII_{R2}$	-5152.70137	-5151.575156	-5151.6677	-2.1	3.3	26.6
$VIII_{R2}$	-5152.789277	-5151.659551	-5151.760284	-57.9	-48.1	-27.9
the second step as the H_2 splitting						
IX_{R2}	-4924.834189	-4923.751484	-4923.842223	-15.9	-2.7	14.1
TSV_{R2}	-4924.828498	-4923.749549	-4923.840072	-12.4	-1.5	15.4
X_{R2}	-4924.834929	-4923.754273	-4923.844887	-16.4	-4.4	12.4
$TSVI_{R2}$	-4924.816815	-4923.737779	-4923.828779	-5.0	5.9	22.5
XI_{R2}	-4924.844795	-4923.761682	-4923.856024	-22.6	-9.1	5.4
R3 isomer						
IV_{R3}	-5152.709277	-5151.58168	-5151.676831	-7.7	0.8	24.5
V_{R3}	-4923.633023	-4922.571734	-4922.66116	4.9	11.0	21.3
$TSII_{R3}$	-4923.627854	-4922.567266	-4922.657002	8.2	13.8	23.9
VI_{R3}	-4923.637926	-4922.574043	-4922.6646	1.8	9.5	19.2
VII_{R3}	-5152.734004	-5151.603138	-5151.697629	-23.2	-12.7	11.4
$TSIII_{R3}$	-5152.693515	-5151.567422	-5151.661795	2.2	9.7	33.9
$VIII_{R3}$	-5152.780877	-5151.650022	-5151.748343	-52.6	-42.1	-20.4
the second step as the H_2 splitting						
$TSIV_{R3}$	-4924.774419	-4923.695431	-4923.785588	21.6	32.5	49.6

Table S3. The absolute (in Hartree) and relative (in kcal/mol) single-point energies for the S- and R isomers in gas phase and in CF_3CH_2OH as solution with SMD model by B3LYP/6-31G* method.

	E_{gas}	E_{SMD}	ΔE_{gas}	ΔE_{SMD}	ΔG_{gas}	ΔG_{SMD}
H_2	-1.175481	-1.174926				
Sub2	-722.17706	-722.193087				
AcOH	-229.08468	-229.090818				
I	-4429.963459	-4430.045596	0.0	0.0	0.0	0.0
TSI	-4431.113795	-4431.197205	15.8	14.6	25.3	24.1
III	-4431.124908	-4431.20592	8.8	9.2	20.1	20.5
S isomer						
$TSII_{S2}$	-4924.209696	-4924.307447	13.6	9.6	29.6	25.6
VI_{S2}	-4924.225869	-4924.327816	3.4	-3.2	20.2	13.6
VII_{S2}	-5153.355856		-25.0		8.6	
$TSIII_{S2}$	-5153.32496	-5153.415593	-5.6	-1.2	24.5	28.8
$TSII_{S3}$	-4924.212606		11.7		26.0	
$TSIII_{S3}$	-5153.323868		-4.9		25.3	
V_{S1}	-4924.224794	-4924.312552	4.1	6.4	19.7	22.1
$TSII_{S1}$	-4924.212285	-4924.305562	11.9	10.8	25.8	24.7
VI_{S1}	-4924.232134	-4924.332039	-0.5	-5.8	14.7	9.4
VII_{S1}	-5153.366738	-5153.46545	-31.8	-32.5	-0.5	-1.3
$TSIII_{S1}$	-5153.365022	-5153.460532	-30.8	-29.4	0.3	1.6
$VIII_{S1}$	-5153.401124	-5153.497112	-53.4	-52.4	-20.0	-18.9
the second step as the H_2 splitting						
TSV_{S2}	-4925.416275	-4925.506765	-5.9	-5.7	20.8	21.0
X_{S2}	-4925.422182	-4925.513019	-9.7	-9.6	18.7	18.7
$TSVI_{S2}$	-4925.407793	-4925.498404	-0.6	-0.4	25.9	26.0
$TSIV_{S3}$	-4925.372863		21.3		50.1	
$TSIV_{S1}$	-4925.388136	-4925.490619	11.7	4.5	37.5	30.2
R isomer						
$TSII_{R2}$	-4924.227475		2.4		18.0	
VI_{R2}	-4924.278604		-29.7		-11.2	
VII_{R2}	-5153.344705		-18.0		17.6	
$TSIII_{R2}$	-5153.314029	-5153.410567	1.2	1.9	30.0	30.6
$TSII_{R3}$	-4924.213814		11.0		26.8	
$TSIII_{R3}$	-5153.31257		2.1		33.9	
V_{R1}	-4924.228664	-4924.316291	1.7	4.1	15.8	18.2
$TSII_{R1}$	-4924.209907	-4924.302834	13.4	12.5	29.6	28.7
VI_{R1}	-4924.254676	-4924.302578	-14.7	12.7	3.2	27.3
VII_{R1}	-5153.364893	-4924.355739	-30.7	-20.7	0.4	-2.8
$TSIII_{R1}$	-5153.362527	-5153.466083	-29.2	-32.9	1.1	-1.8
$VIII_{R1}$	-5153.398934	-5153.460171	-52.0	-29.2	-21.0	1.0
the second step as the H_2 splitting						

TSV_{R2}	-4925.417482	-4925.505922	-6.7	-5.1	21.1	22.7
$TSVI_{R2}$	-4925.408586	-4925.497282	-1.1	0.3	26.4	27.8
$TSIV_{R3}$	-4925.360961		28.8		56.9	
$TSIV_{R1}$	-4925.395769	-4925.492032	6.9	3.6	35.4	32.0

Table S4. The absolute (in Hartree) and relative (in kcal/mol) single-point energies for the S- and R isomers in CF_3CH_2OH as solution with SMD model by M06L/6-31G* method.

	E_{SMD}	**ΔE_{SMD}**	**ΔG_{SMD}**
H_2	-1.167359		
Sub	-722.099159		
AcOH	-229.06254		
I	-4429.526063	0.0	0.0
II	-4430.697295	-2.4	5.8
TSII	-4430.671398	13.8	23.4
III	-4430.679782	8.6	19.9
S1 isomer			
IV_{S1}	-5152.805026	-7.8	21.3
V_{S1}	-4923.724541	3.5	19.1
$TSII_{S1}$	-4923.719647	6.5	20.4
VI_{S1}	-4923.741717	-7.3	7.9
VII_{S1}	-5152.836036	-27.3	4.0
$TSIII_{S1}$	-5152.832691	-25.2	5.9
$VIII_{S1}$	-5152.87809	-53.7	-20.2
the second step as the H_2 splitting			
$TSIV_{S1}$	-4924.89379	2.3	28.1
S2 isomer			
IV_{S2}	-5152.810001	-10.9	21.3
V_{S2}	-4923.722199	4.9	19.5
$TSII_{S2}$	-4923.723261	4.3	20.3
VI_{S2}	-4923.741585	-7.2	9.6
VII_{S2}	-5152.828906	-22.8	10.8
$TSIII_{S2}$	-5152.794223	-1.0	29.1
$VIII_{S2}$	-5152.88546	-58.3	-24.1
the second step as the H_2 splitting			
IX_{S2}	-4924.924895	-17.3	13.0
TSV_{S2}	-4924.916361	-11.9	14.8
X_{S2}	-4924.922993	-16.1	12.3
$TSVI_{S2}$	-4924.905759	-5.2	21.3
XI_{S2}	-4924.930417	-20.7	8.0
R1 isomer			

IV_{R1}	-5152.803219	-6.7	22.7
V_{R1}	-4923.729393	0.4	14.6
$TSII_{R1}$	-4923.716948	8.2	24.4
VI_{R1}	-4923.757888	-17.5	0.4
VII_{R1}	-5152.835193	-26.7	4.4
$TSIII_{R1}$	-5152.831081	-24.2	6.1
$VIII_{R1}$	-5152.876807	-52.9	-21.8
the second step as the H_2 splitting			
$TSIV_{R1}$	-4924.896708	0.4	28.9
R2 isomer			
IV_{R2}	-5152.826749	-21.4	8.2
V_{R2}	-4923.735822	-3.6	11.8
$TSII_{R2}$	-4923.735302	-3.3	12.3
VI_{R2}	-4923.775239	-28.4	-10.9
VII_{R2}	-5152.821959	-18.4	17.2
$TSIII_{R2}$	-5152.794575	-1.3	27.5
$VIII_{R2}$	-5152.880789	-55.4	-25.3
the second step as the H_2 splitting			
IX_{R2}	-4924.922067	-15.5	14.5
TSV_{R2}	-4924.914832	-10.9	16.9
X_{R2}	-4924.920749	-14.7	14.2
$TSVI_{R2}$	-4924.903839	-4.0	23.5
XI_{R2}	-4924.934486	-23.3	4.7

Cartesian coordinates of all optimized structures

H_2

H	0.000000	0.000000	0.372098
H	0.000000	0.000000	-0.372098

Sub

C	3.497754	0.872800	0.867963
C	2.110785	0.922997	0.796686
C	1.410801	0.067204	-0.063633
C	2.138176	-0.836178	-0.851360
C	3.525939	-0.878773	-0.783265
C	4.210477	-0.027044	0.079298
H	4.023722	1.535601	1.552203
H	1.555471	1.607241	1.435836
H	1.621831	-1.480927	-1.563597
H	4.074446	-1.575787	-1.413818
H	5.296187	-0.064757	0.137162
C	-0.063688	0.116692	-0.147536
C	-0.680508	1.321662	-0.131640
H	-0.119253	2.233772	0.027500
N	-2.063029	1.584229	-0.402765
N	-0.712051	-1.106913	-0.230038
H	-0.117685	-1.890148	-0.472030
O	-2.725149	0.752886	-1.027528
O	-2.475690	2.691653	-0.044910
C	-1.870524	-1.443346	0.496685
O	-2.428012	-0.664574	1.235972
C	-2.347082	-2.844204	0.230404
H	-1.536309	-3.556840	0.041491
H	-2.946927	-3.189515	1.074314
H	-2.987893	-2.830433	-0.659322

AcOH

C	-1.387709	-0.098415	-0.000010
H	-1.910216	0.858955	-0.000688
H	-1.683160	-0.681705	-0.878229
H	-1.683258	-0.680407	0.879044
C	0.092058	0.126793	-0.000020
O	0.655543	1.197154	0.000003
O	0.762429	-1.053419	-0.000002
H	1.706765	-0.816997	0.000040

I

P	-0.413424	1.517202	-1.462356
P	0.419508	1.513195	1.466394
C	0.805150	-1.304261	1.340776
C	2.990568	-0.364420	0.477888
C	4.300319	-2.590410	1.830292
H	4.896315	-1.800451	1.380179
C	3.049029	0.950446	0.928356
C	-2.992692	-0.349473	-0.477525
C	-2.197762	-1.376225	-1.211980
C	-0.595767	1.746934	3.010627
C	3.755064	-0.736872	-0.676478
C	-0.811684	-1.298314	-1.341628
C	-2.896965	-2.474363	-1.820135
C	-0.100865	-2.338355	-1.987851
H	0.986088	-2.265088	-2.044692
C	-0.000306	-0.157772	0.775726
H	-1.046489	-0.295168	1.089078
C	-3.045310	0.966579	-0.925130
C	-2.151094	1.424526	-2.034769
H	-2.436710	2.420087	-2.394471
H	-2.177335	0.739483	-2.895779
C	2.137336	-3.529608	2.461268
C	2.190782	-1.389047	1.210053
C	4.654535	0.211351	-1.264430
C	-4.653451	0.229900	1.266589
C	-0.000903	-0.156581	-0.774521
H	1.044608	-0.298276	-1.088195
C	2.819622	-4.623121	3.046517
H	2.231063	-5.404671	3.525746
C	-2.842295	-4.602802	-3.056061
H	-2.257595	-5.386337	-3.536753
C	2.156753	1.410297	2.038705
H	2.447669	2.403176	2.401485
H	2.178768	0.722475	2.897620
C	-2.154646	-3.514264	-2.467861
C	5.391144	-0.153827	-2.416691
H	6.075282	0.576217	-2.848173
C	-3.642816	-1.997628	1.284479
H	-2.974523	-2.734996	0.843158
C	-4.358608	-2.312661	2.417039
H	-4.244769	-3.295012	2.871090
C	4.757194	1.505323	-0.701494
H	5.459414	2.215932	-1.135718
C	2.884705	-2.492155	1.815410

C	-0.745715	-3.423336	-2.518948
H	-0.182206	-4.221920	-2.999753
C	0.728948	-3.431402	2.513621
H	0.161622	-4.228080	2.993110
C	-3.758484	-0.721071	0.676198
C	4.348603	-2.327119	-2.420844
H	4.230505	-3.307915	-2.877156
C	0.089388	-2.341973	1.985276
H	-0.997130	-2.263302	2.043016
C	-5.391306	-0.134627	2.418273
H	-6.071999	0.597495	2.851689
C	-4.750223	1.525659	0.706664
H	-5.448839	2.238616	1.142841
C	0.053073	2.847236	3.852615
H	-0.610256	3.091775	4.691940
H	0.217424	3.767127	3.280018
H	1.009563	2.527347	4.282422
C	-4.951865	-3.629679	-2.427710
H	-6.039191	-3.669175	-2.430590
C	3.633808	-2.011449	-1.287813
H	2.962052	-2.746846	-0.848504
C	-4.313050	-2.565149	-1.836024
H	-4.905049	-1.773134	-1.384276
C	-3.935957	1.893774	-0.333739
H	-3.978135	2.907077	-0.734043
C	5.240071	-1.394059	-2.989703
H	5.806137	-1.658715	-3.880092
C	4.933870	-3.659677	2.419057
H	6.020972	-3.704883	2.421188
C	-1.990758	2.167735	2.561531
H	-2.410588	1.442621	1.855803
H	-1.983902	3.151234	2.070869
H	-2.671128	2.221599	3.422110
C	-0.040013	2.854166	-3.846057
H	0.625122	3.097534	-4.684294
H	-0.201194	3.773558	-3.271762
H	-0.997463	2.539202	-4.277362
C	-5.245616	-1.376847	2.988373
H	-5.812531	-1.640976	3.878377
C	-4.213868	-4.665869	-3.034668
H	-4.732252	-5.504407	-3.494584
C	2.000163	2.162210	-2.555571
H	2.680999	2.215019	-3.415844
H	2.416377	1.433514	-1.851434
H	1.997837	3.144488	-2.062333
C	4.190829	-4.693406	3.024046
H	4.705107	-5.535753	3.481639
C	0.603247	1.749222	-3.005844
C	3.944286	1.874750	0.339487
H	3.991417	2.886716	0.742605
C	-0.692526	0.450624	3.816609
H	0.284439	0.005697	4.044230
H	-1.301006	-0.307374	3.307425
H	-1.184235	0.667221	4.773920
C	0.693948	0.454060	-3.814413
H	-0.285165	0.014500	-4.043202
H	1.298500	-0.308010	-3.306667
H	1.186962	0.670208	-4.771156
Ni	0.003772	3.013232	0.003711
O	-0.361143	4.604452	-1.021116
C	0.007399	5.279604	0.002980
O	0.364545	4.604695	1.031083
C	0.045469	6.761046	-0.011989
H	1.030832	7.091538	-0.361579
H	-0.701769	7.160304	-0.701580
H	-0.102288	7.163384	0.992750

II

P	-0.639489	-1.392863	1.494044
P	0.245775	-1.595668	-1.407709
C	1.042175	1.135205	-1.348296
C	3.051030	-0.082108	-0.405444
C	4.697967	1.823708	-1.859323
H	5.157553	0.975763	-1.356790
C	2.938416	-1.414446	-0.789890
C	-2.874038	0.834387	0.425629
C	-1.948766	1.730624	1.175539
C	-0.699695	-1.671473	-3.016265
C	3.838344	0.245146	0.747086
C	-0.593120	1.442487	1.326805
C	-2.488146	2.915164	1.781704
C	0.252805	2.361112	1.995254
H	1.315812	2.128009	2.070818
C	0.069545	0.139415	-0.763527
H	-0.941050	0.413825	-1.103262
C	-3.130849	-0.454898	0.877770
C	-2.352208	-1.022856	2.024413
H	-2.796524	-1.958650	2.383184

H	-2.300158	-0.326156	2.874432
C	2.713708	3.059323	-2.567519
C	2.422009	1.008100	-1.205939
C	4.594211	-0.780454	1.402671
C	-4.543206	0.486818	-1.370730
C	0.041819	0.181099	0.786399
H	1.090204	0.165264	1.119778
C	3.564030	3.993196	-3.206478
H	3.109423	4.831107	-3.733920
C	-2.144595	4.993492	3.054634
H	-1.460720	5.675462	3.558850
C	2.004579	-1.808108	-1.891196
H	2.140070	-2.858984	-2.174902
H	2.161043	-1.198260	-2.794532
C	-1.613042	3.824109	2.460125
C	5.345152	-0.456804	2.558333
H	5.916640	-1.247176	3.044030
C	-3.234615	2.554869	-1.350223
H	-2.482850	3.191193	-0.885738
C	-3.865402	2.963942	-2.502727
H	-3.604522	3.921271	-2.949756
C	4.547604	-2.099618	0.893325
H	5.153169	-2.871394	1.367216
C	3.284985	1.953432	-1.858197
C	-0.234424	3.523443	2.531820
H	0.433773	4.222986	3.032702
C	1.307437	3.188802	-2.620303
H	0.874201	4.042543	-3.140041
C	-3.544747	1.307155	-0.749779
C	4.599568	1.831713	2.427618
H	4.604464	2.842274	2.831594
C	0.501194	2.245662	-2.041110
H	-0.584017	2.341843	-2.100290
C	-5.185248	0.947520	-2.545472
H	-5.943659	0.313944	-3.004471
C	-4.830034	-0.785184	-0.820658
H	-5.599252	-1.400150	-1.286518
C	-0.224324	-2.896067	-3.801591
H	-0.865969	-3.021471	-4.682832
H	-0.284602	-3.818671	-3.214309
H	0.802512	-2.777942	-4.167765
C	-4.361805	4.353450	2.367545
H	-5.430871	4.555149	2.349497
C	3.875128	1.555138	1.290764
H	3.317856	2.348636	0.795909
C	-3.875088	3.215161	1.769298
H	-4.567049	2.526272	1.290428
C	-4.113681	-1.256424	0.249496
H	-4.308350	-2.252657	0.647958
C	5.344425	0.819516	3.067778
H	5.918915	1.053221	3.961456
C	5.495941	2.741774	-2.500563
H	6.576410	2.613836	-2.491677
C	-2.175046	-1.802215	-2.656318
H	-2.492402	-0.979127	-2.006650
H	-2.386094	-2.746439	-2.137426
H	-2.795761	-1.762696	-3.561558
C	-0.489299	-2.774409	3.874877
H	0.116570	-3.097380	4.730777
H	-0.752315	-3.666936	3.295525
H	-1.411766	-2.341092	4.279067
C	-4.853098	2.157584	-3.105248
H	-5.348954	2.495764	-4.012538
C	-3.491311	5.258950	3.008143
H	-3.889733	6.159314	3.471027
C	1.647666	-2.352142	2.625113
H	2.290039	-2.522913	3.499224
H	2.182881	-1.671834	1.953650
H	1.520559	-3.311334	2.103813
C	4.928768	3.843205	-3.173239
H	5.572666	4.565250	-3.670863
C	0.309945	-1.761635	3.053101
C	3.712945	-2.411235	-0.149366
H	3.655143	-3.434679	-0.517523
C	-0.491771	-0.404027	-3.845172
H	0.565108	-0.154155	-4.003800
H	-0.981086	0.467185	-3.393321
H	-0.945393	-0.551960	-4.833930
C	0.551683	-0.487401	3.864074
H	-0.367348	0.073886	4.075284
H	1.255368	0.190286	3.364251
H	0.997974	-0.761552	4.828891
Ni	-0.580241	-2.943870	0.032114
O	-1.442383	-4.336974	1.044765
C	-1.321410	-5.089083	0.014099
O	-0.775151	-4.561741	-1.014866
C	-1.756554	-6.505799	0.028304
H	-0.903090	-7.137551	0.303292

H	-2.543771	-6.664520	0.768526
H	-2.090566	-6.818435	-0.963976
H	1.836495	-5.444770	0.099843
H	1.920433	-4.779235	0.431087

TSI

P	-0.847207	1.355167	-1.343879
P	-0.026291	1.452110	1.608617
C	1.376634	-1.005477	1.261696
C	3.033749	0.750167	0.507726
C	5.110264	-0.928528	1.669557
H	5.358185	0.059396	1.288931
C	2.620280	1.950499	1.075911
C	-2.558554	-1.360706	-0.510831
C	-1.449170	-2.005037	-1.273525
C	-1.021050	1.137697	3.161601
C	3.843987	0.783347	-0.673947
C	-0.192963	-1.412116	-1.409811
C	-1.707251	-3.256352	-1.930153
C	0.830323	-2.075830	-2.128189
H	1.807437	-1.596124	-2.200209
C	0.193320	-0.199777	0.779735
H	-0.721015	-0.736197	1.075265
C	-3.077013	-0.138434	-0.928216
C	-2.398386	0.648780	-2.004506
H	-3.021013	1.485712	-2.340612
H	-2.148665	0.034319	-2.881950
C	3.467547	-2.651728	2.211897
C	2.689967	-0.555383	1.141144
C	4.319658	2.040373	-1.169814
C	-4.316006	-1.448583	1.232621
C	0.161264	-0.091026	-0.765397
H	1.181142	0.177256	-1.081067
C	4.522292	-3.454527	2.708597
H	4.279394	-4.434703	3.117548
C	-0.899714	-5.156535	-3.271328
H	-0.079651	-5.643515	-3.797757
C	1.636345	1.948943	2.203623
H	1.546485	2.940959	2.660581
H	1.924032	1.239916	2.994772
C	-0.650986	-3.913800	-2.640275
C	5.087986	2.069110	-2.358890
H	5.445323	3.031821	-2.723210
C	-2.586237	-3.177787	1.205747
H	-1.704640	-3.625091	0.748467
C	-3.141876	-3.749150	2.328340
H	-2.689039	-4.639302	2.760833
C	3.973773	3.226996	-0.480520
H	4.360378	4.179264	-0.841467
C	3.759556	-1.363376	1.657902
C	0.617606	-3.297153	-2.711712
H	1.420859	-3.801562	-3.247189
C	2.125566	-3.092118	2.256643
H	1.907249	-4.079690	2.661202
C	-3.145271	-2.009589	0.625600
C	4.897832	-0.325439	-2.566150
H	5.123035	-1.237917	-3.114750
C	1.114198	-2.284586	1.809244
H	0.078716	-2.624022	1.858609
C	-4.874515	-2.074442	2.372428
H	-5.766558	-1.636691	2.819801
C	-4.860749	-0.251762	0.710566
H	-5.761148	0.161266	1.163996
C	-0.780218	2.281515	4.147556
H	-1.468181	2.173712	4.995079
H	-0.963818	3.268480	3.705134
H	0.238036	2.270803	4.553626
C	-3.199655	-5.071116	-2.567667
H	-4.193252	-5.514704	-2.558793
C	4.166402	-0.390975	-1.402166
H	3.822198	-1.354389	-1.028827
C	-2.987576	-3.868736	-1.934811
H	-3.819242	-3.374812	-1.438942
C	-4.230599	0.405263	-0.314850
H	-4.627423	1.348820	-0.691024
C	5.366368	0.913861	-3.049538
H	5.949784	0.951390	-3.966878
C	6.111097	-1.728418	2.168938
H	7.137558	-1.367479	2.169441
C	-2.490102	1.080862	2.751762
H	-2.644587	0.355799	1.945069
H	-2.868522	2.053417	2.407468
H	-3.111427	0.763120	3.599990
C	-0.980833	2.900018	-3.632867
H	-0.445643	3.463147	-4.407759
H	-1.539288	3.616504	-3.020099
H	-1.698202	2.248149	-4.145674
C	-4.298297	-3.196790	2.917178

H	-4.731756	-3.662081	3.799876
C	-2.146274	-5.730811	-3.232839
H	-2.326650	-6.684910	-3.723435
C	1.108016	3.019456	-2.241442
H	1.740195	3.422636	-3.044045
H	1.759681	2.470247	-1.553914
H	0.673355	3.866375	-1.690741
C	5.820769	-3.007597	2.684994
H	6.623480	-3.632394	3.070824
C	0.032061	2.102625	-2.809872
C	3.112262	3.183649	0.586043
H	2.803895	4.104604	1.081245
C	-0.627165	-0.190833	3.810466
H	0.451422	-0.283660	3.989761
H	-0.948884	-1.052809	3.213276
H	-1.129796	-0.270648	4.783097
C	0.679874	1.021464	-3.676893
H	-0.018510	0.224952	-3.963349
H	1.544499	0.555483	-3.186206
H	1.049928	1.483267	-4.601600
Ni	-1.102436	2.733539	0.290781
O	-2.339277	3.738239	-0.747505
C	-3.180436	4.465607	-0.102597
O	-3.145441	4.621921	1.149336
C	-4.225155	5.175506	-0.899650
H	-5.096203	5.405626	-0.283758
H	-3.809493	6.122703	-1.262290
H	-4.513744	4.587572	-1.774574
H	-1.964495	4.051121	1.441025
H	-1.084675	3.758050	1.543250

III

P	-0.871082	-1.337341	1.371877
P	-0.061720	-1.453635	-1.596132
C	1.358194	1.003217	-1.259963
C	3.012847	-0.757141	-0.517772
C	5.087643	0.909372	-1.704621
H	5.334122	-0.079264	-1.324912
C	2.580242	-1.955157	-1.076191
C	-2.560531	1.400487	0.522528
C	-1.441029	2.041822	1.272214
C	-1.055374	-1.122962	-3.146514
C	3.834575	-0.792856	0.655878
C	-0.190061	1.437474	1.405103
C	-1.683884	3.301979	1.917478
C	0.845564	2.104536	2.102652
H	1.820891	1.620173	2.167949
C	0.174512	0.202695	-0.769978
H	-0.738100	0.743440	-1.062811
C	-3.083681	0.185904	0.954966
C	-2.403774	-0.586410	2.040455
H	-3.042476	-1.395529	2.413734
H	-2.133325	0.052491	2.893832
C	3.448496	2.640311	-2.231696
C	2.671213	0.548646	-1.150983
C	4.299439	-2.052677	1.154948
C	-4.322775	1.481618	-1.216262
C	0.145887	0.103459	0.776838
H	1.165082	-0.168521	1.092361
C	4.502074	3.436779	-2.740929
H	4.259859	4.417665	-3.148714
C	-0.851143	5.209323	3.232410
H	-0.022864	5.695700	3.746511
C	1.595119	-1.947752	-2.202378
H	1.500134	-2.937807	-2.661498
H	1.884551	-1.235359	-2.989541
C	-0.616574	3.959057	2.610722
C	5.081893	-2.083480	2.334520
H	5.430984	-3.048522	2.700871
C	-2.585621	3.203253	-1.208470
H	-1.700691	3.650145	-0.757478
C	-3.142257	3.768636	-2.333485
H	-2.686955	4.653543	-2.774046
C	3.923511	-3.240010	0.482627
H	4.296896	-4.195244	0.849845
C	3.739309	1.351208	-1.679214
C	0.648417	3.334289	2.674057
H	1.461510	3.839183	3.194073
C	2.108223	3.087005	-2.262725
H	1.890320	4.075564	-2.665232
C	-3.147656	2.041945	-0.617549
C	4.922368	0.314058	2.530148
H	5.163263	1.226856	3.071552
C	1.097925	2.283912	-1.805419
H	0.063683	2.628087	-1.845345
C	-4.881474	2.100448	-2.359826
H	-5.776910	1.663257	-2.801136
C	-4.872018	0.292760	-0.680590

H	-5.776761	-0.118924	-1.126847
C	-0.814498	-2.254925	-4.145267
H	-1.508332	-2.144171	-4.987847
H	-0.984672	-3.245193	-3.704415
H	0.201267	-2.234092	-4.557188
C	-3.158245	5.132758	2.551944
H	-4.149075	5.582698	2.548617
C	4.178158	0.381427	1.374498
H	3.838909	1.346597	1.001224
C	-2.959946	3.923162	1.928250
H	-3.799720	3.429617	1.445607
C	-4.242619	-0.356328	0.350612
H	-4.645104	-1.292678	0.739774
C	5.382608	-0.927743	3.014825
H	5.976134	-0.966943	3.925591
C	6.087387	1.703045	-2.216010
H	7.111861	1.336496	-2.227113
C	-2.523292	-1.072444	-2.737327
H	-2.682737	-0.346184	-1.933133
H	-2.883709	-2.047696	-2.380647
H	-3.151538	-0.769339	-3.585891
C	-0.995249	-2.846874	3.678890
H	-0.461789	-3.395088	4.465807
H	-1.527506	-3.582303	3.063752
H	-1.736085	-2.208991	4.175776
C	-4.302359	3.216251	-2.914945
H	-4.736460	3.676317	-3.800083
C	-2.094248	5.791477	3.200961
H	-2.263561	6.751175	3.684527
C	1.113856	-2.932454	2.319960
H	1.737214	-3.323263	3.135799
H	1.769800	-2.372216	1.645570
H	0.708442	-3.787850	1.759542
C	5.798362	2.982986	-2.730932
H	6.600075	3.602866	-3.126772
C	0.010166	-2.032681	2.863141
C	3.051992	-3.191932	-0.575433
H	2.720918	-4.111817	-1.057856
C	-0.667240	0.212065	-3.785833
H	0.411150	0.309954	-3.963294
H	-0.992620	1.069329	-3.183741
H	-1.168702	0.297257	-4.758658
C	0.624982	-0.935912	3.732313
H	-0.092183	-0.151977	4.007425
H	1.482828	-0.454553	3.245035
H	0.998183	-1.382242	4.663598
Ni	-1.061160	-2.746337	-0.281363
O	-2.235032	-3.937956	0.694213
C	-3.067161	-4.675425	0.126804
O	-3.142458	-4.787069	-1.176517
C	-4.038690	-5.498158	0.887206
H	-5.043286	-5.381152	0.470504
H	-3.777136	-6.557049	0.781961
H	-4.030317	-5.229338	1.943731
H	-2.362490	-4.260736	-1.536069
H	-0.969935	-3.626344	-1.533721

IV$_{S2}$

P	-0.607459	0.596351	1.410536
P	-0.408871	0.036506	-1.826017
C	2.217450	-0.944314	-1.339914
C	0.809535	-2.977923	-0.884983
C	2.979454	-4.550277	-2.071384
H	2.054366	-5.038903	-1.775234
C	-0.391771	-2.689673	-1.526944
C	2.146834	2.576095	0.841850
C	2.737942	1.413202	1.564576
C	-0.081035	1.219970	-3.255102
C	0.818430	-3.914797	0.198791
C	2.189913	0.133246	1.493561
C	3.887610	1.638681	2.398085
C	2.826007	-0.943262	2.158089
H	2.387217	-1.937359	2.069080
C	1.158284	0.001552	-0.813726
H	1.549397	1.018233	-0.934196
C	0.855036	3.004583	1.135601
C	-0.005094	2.221056	2.077279
H	-0.870994	2.807872	2.407943
H	0.571165	1.972528	2.977584
C	4.321971	-2.532259	-2.364356
C	2.064585	-2.330200	-1.358345
C	-0.395700	-4.585095	0.563061
C	2.394159	4.510305	-0.690883
C	0.936288	-0.193237	0.712495
H	0.728573	-1.261806	0.858958
C	5.357089	-3.337454	-2.897253
H	6.274892	-2.850776	-3.225884
C	5.656569	0.749253	3.862293

H	6.122564	-0.109862	4.343777
C	-0.444978	-1.636391	-2.588728
H	-1.348261	-1.725075	-3.202750
H	0.425880	-1.711115	-3.251549
C	4.514875	0.530658	3.054461
C	-0.390862	-5.488476	1.653816
H	-1.321821	-5.992758	1.913746
C	4.198212	2.868233	-0.558936
H	4.622551	1.961314	-0.132418
C	4.898631	3.563524	-1.518120
H	5.869924	3.197733	-1.845613
C	-1.574745	-4.315152	-0.168606
H	-2.489493	-4.853961	0.079210
C	3.107975	-3.145770	-1.913601
C	3.964423	-0.760409	2.897026
H	4.447017	-1.604946	3.387989
C	4.447619	-1.127098	-2.292111
H	5.369679	-0.660166	-2.637699
C	2.921889	3.306254	-0.119672
C	1.953086	-5.066419	2.019234
H	2.861294	-5.258310	2.587452
C	3.417125	-0.361394	-1.813558
H	3.512444	0.724599	-1.784539
C	3.149499	5.213001	-1.660235
H	2.734113	6.130169	-2.076969
C	1.122919	4.966638	-0.275573
H	0.741987	5.910494	-0.665474
C	-1.433782	1.537109	-3.896826
H	-1.281411	2.185900	-4.769711
H	-2.101630	2.052593	-3.195928
H	-1.953571	0.635138	-4.234994
C	5.524714	3.113424	3.434491
H	5.908910	4.117934	3.600004
C	1.985150	-4.191596	0.957533
H	2.917860	-3.698273	0.689902
C	4.422817	2.932089	2.631913
H	3.945908	3.797443	2.178451
C	0.375426	4.222017	0.599970
H	-0.587712	4.596750	0.941026
C	0.756161	-5.723832	2.372669
H	0.745613	-6.416138	3.211784
C	3.999215	-5.303194	-2.604125
H	3.870752	-6.377681	-2.717367
C	0.559925	2.496972	-2.711237
H	1.630867	2.367118	-2.509327
H	0.089268	2.850636	-1.784892
H	0.482919	3.296613	-3.462014
C	-0.998603	-1.864833	2.635314
H	-1.531138	-2.425201	3.414962
H	0.021056	-2.270095	2.585524
H	-1.492599	-2.091162	1.681893
C	4.374592	4.748876	-2.074025
H	4.942246	5.292711	-2.825924
C	6.158477	2.013940	4.047694
H	7.033521	2.171794	4.674438
C	-0.015671	-0.130699	4.127005
H	-0.233298	-0.852980	4.924570
H	-0.126434	0.865779	4.569172
H	1.031964	-0.269799	3.839348
C	5.205583	-4.697587	-3.011287
H	6.005972	-5.306852	-3.425799
C	-0.999070	-0.373463	2.978191
C	-1.575071	-3.380960	-1.174002
H	-2.489642	-3.184296	-1.734276
C	0.840589	0.607966	-4.312964
H	0.363812	-0.217409	-4.852708
H	1.787954	0.246677	-3.892862
H	1.085296	1.378329	-5.056552
C	-2.386396	0.088738	3.430608
H	-3.156468	-0.126673	2.686326
H	-2.401693	1.165990	3.650525
H	-2.668437	-0.432069	4.355097
Ni	-2.103318	0.501501	-0.320343
H	-1.854274	-0.895520	-0.105910
C	-4.506545	-2.979011	1.996072
C	-4.068333	-2.045119	1.071864
C	-4.682734	-0.789635	0.955044
C	-5.774640	-0.522653	1.798002
C	-6.222182	-1.463889	2.720635
C	-5.584618	-2.693128	2.834709
H	-3.992236	-3.937057	2.069901
H	-3.230674	-2.295056	0.427552
H	-6.298110	0.427733	1.726633
H	-7.076075	-1.227010	3.351569
H	-5.925044	-3.425322	3.563613
C	-4.199111	0.282737	0.048397
C	-3.752312	0.152980	-1.305176
N	-4.748316	1.565828	0.320323

H	-4.583625	1.935081	1.249918
N	-3.945910	-1.037201	-2.128820
O	-4.573179	-1.996168	-1.691256
O	-3.462564	-0.985178	-3.266109
H	-3.836818	1.023909	-1.951458
C	-5.797678	2.212682	-0.322852
O	-6.150796	3.312276	0.082391
C	-6.457232	1.514292	-1.479678
H	-6.452830	0.423214	-1.381797
H	-7.486637	1.873113	-1.541155
H	-5.972588	1.771570	-2.429171
C	-2.517005	3.622625	-0.460525
O	-2.182404	2.481201	-0.786884
C	-3.116096	4.054648	0.826360
H	-4.211669	4.094327	0.714834
H	-2.869313	3.341906	1.618444
H	-2.780106	5.059196	1.095583
O	-2.362279	4.626316	-1.317510
H	-1.973960	4.267481	-2.138159

V_{S2}

P	-1.058829	0.118270	1.144772
P	-0.378340	-0.443379	-1.880052
C	2.383849	-0.451048	-1.190176
C	1.669272	-2.816398	-0.665949
C	4.252129	-3.664001	-1.723201
H	3.491637	-4.404397	-1.485796
C	0.458995	-3.010768	-1.320524
C	0.622739	3.011346	0.663720
C	1.598486	2.274463	1.513087
C	-0.334696	0.653300	-3.395990
C	1.976415	-3.613118	0.485171
C	1.692493	0.885377	1.501497
C	2.463843	3.028763	2.377531
C	2.731657	0.245772	2.221438
H	2.822170	-0.838602	2.147566
C	1.041152	0.133744	-0.811133
H	1.073132	1.211518	-1.031925
C	-0.746666	2.853082	0.845862
C	-1.275930	1.826886	1.801338
H	-2.341221	2.010375	1.994674
H	-0.754533	1.867780	2.769538
C	4.954926	-1.337820	-1.963541
C	2.659185	-1.816936	-1.158095
C	1.088203	-4.668270	0.874696
C	0.146482	4.751394	-1.031608
C	0.759757	0.000630	0.700128
H	0.991290	-1.041663	0.966519
C	6.223789	-1.798919	-2.387778
H	6.982141	-1.061820	-2.649529
C	4.327088	3.097174	3.983517
H	5.098534	2.565391	4.539511
C	0.079964	-2.121982	-2.466461
H	-0.770482	-2.529983	-3.025348
H	0.914887	-2.008419	-3.172419
C	3.480504	2.354218	3.126863
C	1.389200	-5.438452	2.024404
H	0.707616	-6.241095	2.305104
C	2.463275	4.050784	-0.674612
H	3.196509	3.444243	-0.145296
C	2.876266	4.913690	-1.663882
H	3.932711	4.976743	-1.917580
C	-0.092526	-4.882063	0.124852
H	-0.760895	-5.693683	0.412174
C	3.943032	-2.284699	-1.601573
C	3.609726	0.953023	2.997437
H	4.405313	0.442147	3.538380
C	4.658252	0.042090	-1.895200
H	5.435947	0.763458	-2.143049
C	1.091760	3.935336	-0.327544
C	3.373371	-4.125462	2.410462
H	4.253409	-3.914535	3.014533
C	3.405787	0.465950	-1.540948
H	3.177557	1.532347	-1.508327
C	0.609213	5.645487	-2.027383
H	-0.121763	6.263065	-2.548610
C	-1.231045	4.618901	-0.740131
H	-1.946479	5.256912	-1.257828
C	-1.274792	0.069474	-4.450931
H	-1.274088	0.723824	-5.331198
H	-2.315528	0.011213	-4.106132
H	-0.961471	-0.926113	-4.788569
C	3.159210	5.121895	3.404883
H	3.027241	6.194600	3.529844
C	3.122877	-3.374227	1.285834
H	3.811249	-2.580397	1.002789
C	2.330101	4.430214	2.552899
H	1.546575	4.962157	2.018334

C	-1.665609	3.676912	0.156282
H	-2.726498	3.565785	0.370014
C	2.504140	-5.171515	2.782460
H	2.718425	-5.764478	3.668855
C	5.490600	-4.080202	-2.153010
H	5.697914	-5.144450	-2.244653
C	-0.787510	2.051713	-2.988227
H	-0.138239	2.480543	-2.216145
H	-1.814285	2.081953	-2.609251
H	-0.735020	2.722152	-3.856185
C	-1.216469	-2.429880	2.179006
H	-1.184912	-3.117143	3.035519
H	-0.339877	-2.647306	1.559020
H	-2.109659	-2.665966	1.589226
C	1.944015	5.724539	-2.343769
H	2.285216	6.410142	-3.116523
C	4.173576	4.455198	4.121637
H	4.825398	5.016503	4.787694
C	-0.019644	-0.797479	3.615702
H	-0.244797	-1.314723	4.557464
H	0.194768	0.250177	3.859717
H	0.897636	-1.245309	3.219519
C	6.491895	-3.142889	-2.478942
H	7.469190	-3.486637	-2.810822
C	-1.202133	-0.984708	2.662798
C	-0.412551	-4.051662	-0.919770
H	-1.332664	-4.207867	-1.483998
C	1.085273	0.742922	-3.961555
H	1.557058	-0.232209	-4.134514
H	1.746443	1.327175	-3.312906
H	1.045025	1.261299	-4.927780
C	-2.495646	-0.668819	3.412216
H	-3.381963	-0.924522	2.822635
H	-2.559553	0.377054	3.740210
H	-2.547086	-1.288086	4.316585
Ni	-2.200436	-0.371853	-0.732596
H	-2.212560	-0.727709	-2.163118
C	-4.128106	-4.145884	0.038352
C	-3.873246	-2.828241	-0.315190
C	-4.411959	-1.765431	0.431776
C	-5.212007	-2.064492	1.541822
C	-5.460854	-3.385892	1.896808
C	-4.920504	-4.429827	1.149840
H	-3.708250	-4.956125	-0.554944
H	-3.234795	-2.614264	-1.175402
H	-5.655312	-1.250553	2.112422
H	-6.091270	-3.600748	2.756749
H	-5.123468	-5.461976	1.426040
C	-4.141821	-0.358060	0.042927
C	-4.076186	-0.140274	-1.359752
N	-4.461744	0.641905	0.972687
H	-3.921479	0.644145	1.829801
C	-5.216705	1.813578	0.861023
O	-5.007122	2.707713	1.661060
C	-6.328596	1.842749	-0.145687
H	-6.453751	0.910155	-0.704678
H	-7.257892	2.048667	0.394268
H	-6.178375	2.667992	-0.847940
N	-4.131276	1.169223	-1.992814
O	-3.692446	2.147663	-1.374934
O	-4.569926	1.204348	-3.137727
H	-4.473772	-0.893025	-2.032886

TSII$_{S2}$

P	-0.997297	0.101804	1.194361
P	-0.345378	-0.402096	-1.842981
C	2.416599	-0.432498	-1.190295
C	1.689617	-2.798934	-0.673989
C	4.241091	-3.657151	-1.793078
H	3.478104	-4.393153	-1.550204
C	0.466738	-2.994769	-1.305421
C	0.641381	3.017498	0.688846
C	1.646064	2.297166	1.519511
C	-0.299064	0.666283	-3.378462
C	2.020465	-3.600219	0.467384
C	1.745284	0.906524	1.518840
C	2.522383	3.062369	2.362316
C	2.789596	0.276488	2.239338
H	2.880990	-0.808604	2.178390
C	1.081778	0.155958	-0.791679
H	1.115515	1.235554	-1.003103
C	-0.718475	2.822548	0.898680
C	-1.185701	1.796953	1.883206
H	-2.230969	1.981103	2.158681
H	-0.597955	1.830156	2.812339
C	4.962425	-1.335384	-2.019524
C	2.675905	-1.801253	-1.180205
C	1.149529	-4.667414	0.861985

C	0.077340	4.726378	-1.010032
C	0.817123	0.010319	0.724159
H	1.065652	-1.030004	0.984304
C	6.218757	-1.803790	-2.472016
H	6.979504	-1.070981	-2.738871
C	4.410728	3.151906	3.938459
H	5.190765	2.627285	4.489115
C	0.054259	-2.096434	-2.431724
H	-0.830056	-2.486407	-2.950858
H	0.855484	-1.999405	-3.179230
C	3.550878	2.397821	3.104891
C	1.475027	-5.441928	2.001857
H	0.806854	-6.254399	2.286307
C	2.422191	4.098470	-0.694299
H	3.183727	3.517532	-0.176303
C	2.789255	4.967205	-1.696201
H	3.837824	5.059385	-1.972635
C	-0.038489	-4.889877	0.126222
H	-0.692929	-5.712363	0.414461
C	3.947381	-2.276543	-1.651045
C	3.676445	0.994865	2.995403
H	4.477461	0.491193	3.535030
C	4.683102	0.046788	-1.926584
H	5.464607	0.762642	-2.178342
C	1.062280	3.946595	-0.317844
C	3.449273	-4.108601	2.370178
H	4.334626	-3.891255	2.964176
C	3.442007	0.479107	-1.543515
H	3.224496	1.547239	-1.492316
C	0.494177	5.629469	-2.017896
H	-0.265168	6.219583	-2.530213
C	-1.292186	4.537105	-0.709240
H	-2.038088	5.133610	-1.233520
C	-1.248709	0.069693	-4.418046
H	-1.268605	0.720719	-5.300467
H	-2.285768	0.000139	-4.060610
H	-0.932528	-0.924545	-4.756328
C	3.232111	5.168389	3.353299
H	3.101200	6.242444	3.467172
C	3.175108	-3.353067	1.253765
H	3.850136	-2.548889	0.967129
C	2.389491	4.465737	2.523968
H	1.597331	4.991069	1.995864
C	-1.680563	3.586905	0.199753
H	-2.736466	3.422595	0.411616
C	2.597392	-5.167398	2.746384
H	2.830544	-5.763867	3.625592
C	5.467692	-4.080277	-2.249588
H	5.662899	-5.145371	-2.356610
C	-0.751618	2.066272	-2.981285
H	-0.091625	2.503348	-2.223699
H	-1.770857	2.084833	-2.579241
H	-0.721830	2.731414	-3.854339
C	-1.200555	-2.455127	2.170264
H	-1.173197	-3.161252	3.011424
H	-0.334918	-2.675234	1.535517
H	-2.105025	-2.659315	1.586947
C	1.819679	5.746726	-2.360446
H	2.124366	6.437122	-3.144120
C	4.258882	4.511457	4.061570
H	4.920736	5.081582	4.709935
C	0.043543	-0.883915	3.633308
H	-0.181707	-1.431737	4.557616
H	0.270612	0.152038	3.913302
H	0.953143	-1.327442	3.213238
C	6.471999	-3.149112	-2.583386
H	7.439732	-3.498497	-2.936531
C	-1.148189	-1.021985	2.684908
C	-0.385409	-4.050956	-0.902729
H	-1.314418	-4.210511	-1.450789
C	1.115158	0.745676	-3.957748
H	1.584248	-0.233213	-4.117037
H	1.780915	1.337655	-3.320797
H	1.070479	1.249114	-4.931703
C	-2.431341	-0.669847	3.435896
H	-3.318241	-0.738548	2.796899
H	-2.393236	0.328700	3.889096
H	-2.579840	-1.388051	4.252336
Ni	-2.170442	-0.292328	-0.670757
H	-2.443088	-0.393208	-2.107111
C	-4.157769	-4.127436	0.102662
C	-3.876413	-2.824427	-0.283413
C	-4.366131	-1.730569	0.452924
C	-5.149796	-1.986068	1.584413
C	-5.430679	-3.292938	1.969655
C	-4.935996	-4.367203	1.234491
H	-3.769920	-4.960594	-0.481122
H	-3.251061	-2.650739	-1.163025

H	-5.548841	-1.149023	2.154727
H	-6.048640	-3.471696	2.846912
H	-5.161449	-5.387523	1.536043
C	-4.048878	-0.338752	0.034880
C	-3.994756	-0.160087	-1.395234
N	-4.427638	0.721962	0.890629
H	-3.806829	0.948615	1.656596
C	-5.482746	1.630152	0.810208
O	-5.487153	2.584152	1.565493
C	-6.583367	1.340282	-0.170902
H	-6.546392	0.339348	-0.613132
H	-7.536962	1.459129	0.350661
H	-6.571815	2.084409	-0.974471
N	-4.274257	1.144600	-2.014153
O	-3.777238	2.150569	-1.505203
O	-4.984259	1.126005	-3.012930
H	-4.418368	-0.946794	-2.015198

VI$_{S2}$

P	-0.959123	0.201791	1.176175
P	-0.337865	-0.371957	-1.849719
C	2.430915	-0.524570	-1.198054
C	1.593504	-2.848226	-0.664121
C	4.119707	-3.834542	-1.734028
H	3.322176	-4.532573	-1.490347
C	0.372697	-2.981073	-1.314960
C	0.820140	3.015806	0.663109
C	1.789080	2.246366	1.493070
C	-0.263751	0.699380	-3.382180
C	1.860110	-3.658992	0.488401
C	1.814225	0.852423	1.502538
C	2.699896	2.971214	2.334513
C	2.814170	0.172575	2.240970
H	2.845996	-0.916624	2.190929
C	1.120208	0.125485	-0.813510
H	1.205005	1.201130	-1.030887
C	-0.547028	2.903396	0.890539
C	-1.062152	1.898873	1.872872
H	-2.100302	2.108846	2.158380
H	-0.471489	1.899833	2.800942
C	4.945071	-1.550480	-1.986879
C	2.632808	-1.903187	-1.164182
C	0.914986	-4.662611	0.883221
C	0.341738	4.749037	-1.038663
C	0.845378	0.005394	0.705476
H	1.030779	-1.046446	0.971677
C	6.184960	-2.080797	-2.416744
H	6.980162	-1.386649	-2.686742
C	4.575276	2.972883	3.928219
H	5.319860	2.412162	4.492330
C	0.026037	-2.071555	-2.452724
H	-0.853817	-2.436539	-2.997153
H	0.852164	-2.000595	-3.175684
C	3.683180	2.258154	3.093797
C	1.172531	-5.440252	2.038550
H	0.445553	-6.199800	2.325207
C	2.647335	3.985396	-0.741796
H	3.377914	3.362277	-0.228283
C	3.054692	4.825813	-1.752596
H	4.103993	4.855048	-2.039206
C	-0.275412	-4.817762	0.134296
H	-0.989771	-5.586794	0.428801
C	3.886281	-2.440210	-1.614772
C	3.730891	0.849112	3.000230
H	4.497361	0.307992	3.553710
C	4.722735	-0.156508	-1.923311
H	5.535609	0.520782	-2.182568
C	1.284608	3.914757	-0.352407
C	3.230593	-4.243319	2.412682
H	4.123657	-4.081888	3.013044
C	3.497152	0.334715	-1.560064
H	3.324814	1.411855	-1.531717
C	0.799600	5.620363	-2.056503
H	0.071390	6.252947	-2.563338
C	-1.032264	4.648452	-0.718466
H	-1.746358	5.290053	-1.233632
C	-1.237263	0.118914	-4.408928
H	-1.307153	0.793905	-5.270723
H	-2.256935	0.007153	-4.012907
H	-0.913327	-0.858155	-4.786790
C	3.516939	5.045620	3.309681
H	3.445167	6.126507	3.410474
C	3.020028	-3.482439	1.286344
H	3.750904	-2.729669	0.997464
C	2.644096	4.381462	2.480323
H	1.887195	4.944069	1.938991
C	-1.464509	3.727671	0.200727
H	-2.526926	3.645315	0.427349

C	2.302231	-5.234426	2.792935
H	2.483560	-5.833274	3.682778
C	5.331312	-4.318300	-2.169316
H	5.479944	-5.392437	-2.259013
C	-0.687794	2.105512	-2.974206
H	-0.015854	2.522674	-2.215327
H	-1.703187	2.139562	-2.560480
H	-0.651471	2.779802	-3.840374
C	-1.351162	-2.336801	2.119084
H	-1.425666	-3.049204	2.952409
H	-0.473484	-2.620062	1.528224
H	-2.235157	-2.462546	1.485170
C	2.126337	5.657240	-2.412758
H	2.463515	6.324477	-3.203126
C	4.498453	4.340130	4.035401
H	5.184986	4.879305	4.684649
C	-0.012836	-0.880424	3.612047
H	-0.288715	-1.422015	4.526453
H	0.284715	0.132862	3.908986
H	0.866966	-1.384408	3.195057
C	6.379904	-3.437595	-2.503952
H	7.335209	-3.834205	-2.840684
C	-1.201516	-0.916731	2.651109
C	-0.549712	-3.975262	-0.912311
H	-1.480818	-4.075906	-1.469676
C	1.143704	0.753066	-3.977597
H	1.586295	-0.235900	-4.149375
H	1.830502	1.322209	-3.340993
H	1.103140	1.267033	-4.946802
C	-2.461593	-0.447666	3.379958
H	-3.298997	-0.265919	2.697193
H	-2.283385	0.473674	3.947794
H	-2.779246	-1.216831	4.095880
Ni	-2.153638	-0.132885	-0.609427
H	-2.965779	0.098195	-2.066661
C	-4.157661	-3.886756	-0.272428
C	-3.957368	-2.552077	-0.604488
C	-4.327740	-1.518888	0.280304
C	-4.925167	-1.880519	1.498531
C	-5.132472	-3.214646	1.822496
C	-4.742730	-4.225278	0.944873
H	-3.868473	-4.666474	-0.975020
H	-3.509318	-2.319833	-1.574799
H	-5.226382	-1.102700	2.196520
H	-5.607489	-3.467150	2.768317
H	-4.911305	-5.269040	1.199799
C	-3.984500	-0.114048	-0.037739
C	-3.997306	0.162496	-1.548091
N	-4.512080	0.902570	0.803344
H	-3.874419	1.642199	1.074214
C	-5.845538	1.321284	0.949751
O	-6.070666	2.342312	1.567386
C	-6.923879	0.460898	0.351772
H	-6.576068	-0.252396	-0.400389
H	-7.422239	-0.103604	1.147762
H	-7.673067	1.118011	-0.096458
N	-4.457512	1.544381	-1.843925
O	-3.704297	2.453912	-1.502944
O	-5.567573	1.661802	-2.339395
H	-4.610771	-0.537510	-2.120804

VII$_{S2}$

P	-0.668032	-0.255976	0.807921
P	0.618275	-1.071055	-1.801702
C	3.112000	-0.020524	-0.940533
C	3.100219	-2.324392	0.095650
C	5.963251	-2.421597	-0.484439
H	5.454155	-3.303540	-0.103483
C	2.127373	-3.029470	-0.606571
C	0.099357	2.920286	-0.072779
C	1.042711	2.702205	1.059937
C	0.449279	-0.402664	-3.538628
C	3.446688	-2.749149	1.420612
C	1.557423	1.446204	1.372943
C	1.424477	3.835715	1.856325
C	2.543079	1.321124	2.382555
H	2.964169	0.332984	2.574010
C	1.615917	0.137296	-0.809519
H	1.349755	1.106656	-1.250870
C	-1.165883	2.342817	-0.075071
C	-1.553621	1.351644	0.975394
H	-2.630303	1.143837	0.944793
H	-1.332031	1.734694	1.982858
C	5.911358	-0.125034	-1.310839
C	3.797077	-1.165177	-0.533869
C	2.878463	-3.955338	1.946588
C	-0.489953	4.126185	-2.156122
C	1.138310	0.180470	0.662117

H	1.621867	-0.663492	1.176283
C	7.309889	-0.202390	-1.516748
H	7.821277	0.666386	-1.930259
C	2.781343	4.794034	3.672199
H	3.534603	4.653201	4.446546
C	1.680995	-2.556201	-1.954855
H	1.105333	-3.326081	-2.481727
H	2.541880	-2.283875	-2.579898
C	2.404663	3.677605	2.888415
C	3.225949	-4.373829	3.253652
H	2.792659	-5.298267	3.634563
C	1.797834	4.275837	-1.307598
H	2.547414	4.019444	-0.561064
C	2.142469	5.063798	-2.382507
H	3.164703	5.424173	-2.480181
C	1.946671	-4.676954	1.163625
H	1.522029	-5.596740	1.564796
C	5.213860	-1.248134	-0.757944
C	2.969672	2.401184	3.107654
H	3.735167	2.285459	3.873908
C	5.181881	1.033326	-1.659351
H	5.714422	1.888462	-2.074255
C	0.477259	3.779076	-1.157652
C	4.618256	-2.426802	3.529773
H	5.284156	-1.832649	4.152477
C	3.822280	1.072121	-1.496206
H	3.260133	1.961886	-1.786863
C	-0.107831	4.956555	-3.236796
H	-0.858063	5.214752	-3.983788
C	-1.799849	3.604993	-2.052027
H	-2.547128	3.904162	-2.787620
C	-0.500388	-1.334728	-4.295713
H	-0.575447	-0.996847	-5.337847
H	-1.502927	-1.324305	-3.855084
H	-0.148340	-2.373213	-4.311378
C	1.218405	6.180526	2.476360
H	0.748305	7.151024	2.331417
C	4.318342	-2.003465	2.255335
H	4.754553	-1.081390	1.875103
C	0.841006	5.118030	1.688440
H	0.071049	5.260230	0.933714
C	-2.112643	2.712699	-1.059057
H	-3.115147	2.289649	-0.997032
C	4.076809	-3.627505	4.033211
H	4.330165	-3.956849	5.038656
C	7.319235	-2.469467	-0.708649
H	7.866891	-3.385061	-0.494475
C	-0.164706	0.989697	-3.443911
H	0.540216	1.735504	-3.054816
H	-1.057449	0.991360	-2.807855
H	-0.463280	1.330382	-4.445233
C	-2.383546	-1.109073	2.789124
H	-2.543455	-1.629456	3.742640
H	-2.931141	-1.664673	2.019240
H	-2.831777	-0.112056	2.890706
C	1.182361	5.414579	-3.353781
H	1.466601	6.043896	-4.194276
C	2.203993	6.024296	3.471836
H	2.497206	6.874729	4.083500
C	-0.285765	-2.453316	2.430789
H	0.772845	-2.420608	2.146180
H	-0.808213	-3.097121	1.715114
H	-0.339374	-2.925544	3.421267
C	8.005445	-1.348056	-1.217543
H	9.079463	-1.398029	-1.383561
C	-0.883604	-1.051512	2.491970
C	1.551654	-4.201041	-0.060186
H	0.806941	-4.737189	-0.649302
C	1.800506	-0.330357	-4.251400
H	2.215029	-1.321386	-4.467000
H	2.548209	0.240664	-3.686862
H	1.662523	0.175565	-5.216193
C	-0.165909	-0.263472	3.589119
H	-0.422946	0.802553	3.614693
H	0.923005	-0.345359	3.503868
H	-0.446472	-0.687608	4.562304
Ni	-1.183916	-1.589830	-0.792971
H	-5.228343	-2.565586	0.662904
C	-6.230824	0.364904	3.455416
C	-5.834909	-0.361340	2.336563
C	-5.298653	0.285606	1.217980
C	-5.181281	1.678539	1.247683
C	-5.573239	2.405450	2.368139
C	-6.097526	1.750236	3.477901
H	-6.652475	-0.158219	4.311105
H	-5.951426	-1.444336	2.349765
H	-4.780154	2.204939	0.382097
H	-5.473659	3.488970	2.367339

H	-6.408680	2.316781	4.352661
C	-4.781710	-0.507210	0.035032
C	-5.442919	-1.865226	-0.146182
N	-4.814768	0.263871	-1.200030
H	-5.702234	0.695932	-1.431081
N	-6.945252	-1.761426	-0.243968
O	-7.405940	-0.725106	-0.720620
O	-7.592423	-2.724927	0.133967
H	-5.116103	-2.326091	-1.084088
C	-3.112740	-4.838810	-1.169432
H	-3.591498	-4.858525	-2.154135
H	-2.420860	-5.687894	-1.142112
H	-3.864602	-4.967489	-0.387608
C	-2.357071	-3.569993	-0.992576
O	-1.479658	-3.207674	-1.845608
O	-2.550239	-2.804246	0.010935
H	-3.715759	-0.738137	0.191472
C	-3.886904	0.086345	-2.170853
C	-4.095504	0.847035	-3.447031
H	-4.082615	0.152869	-4.293351
H	-5.025796	1.422299	-3.471879
H	-3.252626	1.534393	-3.587820
O	-2.897358	-0.643769	-2.012536

TSIII$_{S2}$

P	0.807401	-0.074469	1.071626
P	-0.082557	0.737611	-1.723117
C	-2.779672	0.274964	-1.076172
C	-2.462094	2.640078	-0.231495
C	-5.044416	3.245553	-1.438631
H	-4.419230	4.050722	-1.059783
C	-1.255994	3.108171	-0.745255
C	-0.662310	-3.052938	0.491057
C	-1.647239	-2.474890	1.446653
C	-0.136164	-0.003061	-3.451482
C	-2.989641	3.229156	0.964385
C	-1.840302	-1.101359	1.559592
C	-2.419466	-3.364713	2.267737
C	-2.871128	-0.602799	2.394420
H	-3.027975	0.476177	2.435739
C	-1.371023	-0.139210	-0.728582
H	-1.243400	-1.185543	-1.039037
C	0.697683	-2.795831	0.628257
C	1.190475	-1.795298	1.628140
H	2.278282	-1.864652	1.757115
H	0.727976	-1.947006	2.613011
C	-5.385634	0.889217	-1.978474
C	-3.248877	1.577653	-0.921802
C	-2.335141	4.364217	1.544149
C	-0.153997	-4.550471	-1.416600
C	-1.039954	-0.086107	0.776276
H	-1.339131	0.908374	1.132463
C	-6.671127	1.221065	-2.468312
H	-7.293283	0.423726	-2.873562
C	-4.225477	-3.713824	3.902884
H	-5.010144	-3.290624	4.529291
C	-0.657553	2.470550	-1.959589
H	0.202878	3.037829	-2.331025
H	-1.403048	2.432297	-2.765071
C	-3.452062	-2.835402	3.107744
C	-2.864360	4.942596	2.724055
H	-2.357941	5.808104	3.150411
C	-2.489352	-4.112972	-0.847297
H	-3.234936	-3.631580	-0.217545
C	-2.892402	-4.904521	-1.898487
H	-3.954544	-5.041984	-2.092312
C	-1.166339	4.868554	0.927108
H	-0.682761	5.748030	1.351414
C	-4.550692	1.915100	-1.428554
C	-3.667432	-1.438999	3.130043
H	-4.463855	-1.035557	3.754738
C	-4.899298	-0.436768	-2.031147
H	-5.542746	-1.220536	-2.429491
C	-1.113264	-3.904686	-0.570785
C	-4.623989	3.296657	2.766604
H	-5.507316	2.882533	3.249068
C	-3.627151	-0.724918	-1.614686
H	-3.242067	-1.742331	-1.696912
C	-0.601786	-5.372989	-2.477905
H	0.142892	-5.861741	-3.105710
C	1.222510	-4.342302	-1.171956
H	1.952086	-4.879788	-1.778003
C	1.012279	0.591757	-4.274088
H	0.919672	0.236642	-5.308750
H	1.996085	0.304251	-3.902909
H	0.960005	1.687439	-4.303102
C	-2.949492	-5.590098	3.098511
H	-2.745596	-6.658861	3.112458

C	-4.144286	2.720168	1.614010
H	-4.651826	1.853934	1.194682
C	-2.188758	-4.763660	2.304353
H	-1.388060	-5.188947	1.703753
C	1.629941	-3.472296	-0.192965
H	2.690728	-3.314956	-0.001523
C	-3.984724	4.422199	3.325823
H	-4.377733	4.873271	4.234464
C	-6.292318	3.538132	-1.936871
H	-6.640647	4.568909	-1.940476
C	-0.031285	-1.527063	-3.318476
H	-0.994373	-1.972195	-3.033170
H	0.720922	-1.846102	-2.589626
H	0.242744	-1.959412	-4.289875
C	2.426830	0.907770	3.118205
H	2.520039	1.497113	4.039910
H	3.119598	1.339915	2.391687
H	2.759471	-0.110520	3.352836
C	-1.943143	-5.546265	-2.720418
H	-2.274863	-6.175916	-3.543115
C	-3.985852	-5.066317	3.897797
H	-4.584235	-5.731766	4.516243
C	0.604813	2.402051	2.305611
H	-0.446636	2.494092	2.010715
H	1.228520	2.817195	1.506817
H	0.741437	3.030697	3.195987
C	-7.121637	2.518473	-2.446063
H	-8.110082	2.763207	-2.828972
C	0.981330	0.964293	2.638648
C	-0.628709	4.236252	-0.165320
H	0.286050	4.614171	-0.622678
C	-1.443503	0.331314	-4.185784
H	-1.500770	1.383311	-4.485273
H	-2.345763	0.075799	-3.622272
H	-1.459909	-0.258646	-5.111651
C	0.058186	0.466545	3.753066
H	0.213740	-0.584617	4.021598
H	-1.000957	0.603131	3.514093
H	0.263330	1.059154	4.654607
Ni	1.839976	0.550900	-0.722756
H	5.259897	2.030283	-1.000845
C	6.411449	1.435577	2.851593
C	5.745979	1.408124	1.633570
C	5.065967	0.256777	1.206068
C	5.083831	-0.864201	2.050783
C	5.752182	-0.836256	3.270323
C	6.419193	0.314259	3.677879
H	6.936911	2.339509	3.151844
H	5.754532	2.299550	1.012071
H	4.554704	-1.772667	1.764290
H	5.751988	-1.722578	3.901583
H	6.947551	0.335590	4.628469
C	4.334142	0.237866	-0.107181
C	5.101497	0.977339	-1.225765
N	4.186268	-1.164239	-0.518917
H	5.010707	-1.726601	-0.315414
N	6.480492	0.400173	-1.404259
O	6.548909	-0.726937	-1.902948
O	7.429460	1.060163	-1.006669
H	4.586992	0.867193	-2.184227
C	3.083871	4.504636	-1.150773
H	2.518272	4.804911	-2.035384
H	2.799820	5.113293	-0.287143
H	4.146508	4.702454	-1.336669
C	2.901126	3.052938	-0.850648
O	2.414447	2.273057	-1.712506
O	3.306322	2.636638	0.297856
H	3.422880	1.378603	0.170043
C	3.584168	-1.465073	-1.690775
C	4.020073	-2.690369	-2.419020
H	4.873577	-2.426000	-3.055461
H	4.355593	-3.484544	-1.743434
H	3.210477	-3.058003	-3.053341
O	2.710458	-0.705132	-2.148204

VIII$_{S2}$

P	-0.836581	0.068190	1.139996
P	-0.012090	-0.563207	-1.832150
C	2.727659	-0.305029	-1.065380
C	2.219799	-2.691985	-0.370878
C	4.905916	-3.357238	-1.274415
H	4.210134	-4.148626	-1.006454
C	1.059172	-3.044735	-1.055702
C	0.641401	3.065572	0.463246
C	1.669689	2.477860	1.366838
C	0.118603	0.293888	-3.508002
C	2.575462	-3.422405	0.811438
C	1.831781	1.098651	1.489386

C	2.500168	3.354455	2.144220	H	-2.111835	4.826258	-1.697428
C	2.874761	0.581104	2.297592	C	-0.905192	-0.344843	-4.453729
H	2.993168	-0.502376	2.357331	H	-0.850689	0.162104	-5.426425
C	1.323007	0.179865	-0.786633	H	-1.930916	-0.272702	-4.090473
H	1.274123	1.242028	-1.063699	H	-0.674812	-1.401938	-4.637337
C	-0.706301	2.782332	0.658186	C	3.127418	5.573777	2.923301
C	-1.123737	1.799707	1.706222	H	2.951179	6.647532	2.935872
H	-2.181040	1.903999	1.970186	C	3.657954	-3.039100	1.645292
H	-0.536008	1.940976	2.621397	H	4.264499	-2.179619	1.366163
C	5.398413	-1.002828	-1.679039	C	2.306145	4.759347	2.179022
C	3.126926	-1.629987	-0.896933	H	1.486201	5.198854	1.616225
C	1.800750	-4.562524	1.202522	C	-1.689890	3.422303	-0.132668
C	0.015096	4.577282	-1.397726	H	-2.738550	3.212605	0.074446
C	0.998226	0.095916	0.721233	C	3.190474	-4.860703	3.170619
H	1.320924	-0.903426	1.037751	H	3.438267	-5.406164	4.078660
C	6.719990	-1.372579	-2.025887	C	6.192196	-3.686567	-1.633418
H	7.414407	-0.588456	-2.326363	H	6.496926	-4.730987	-1.638213
C	4.393331	3.673180	3.684588	C	-0.121593	1.792684	-3.310332
H	5.196970	3.235800	4.276193	H	0.766284	2.282287	-2.888936
C	0.594443	-2.258634	-2.238405	H	-0.970494	2.015829	-2.659015
H	-0.215993	-2.777010	-2.761681	H	-0.305753	2.266194	-4.284648
H	1.421422	-2.127936	-2.948282	C	-2.295841	-1.188119	3.166554
C	3.556453	2.806579	2.941731	H	-2.309420	-1.733021	4.119961
C	2.141000	-5.266542	2.382254	H	-2.843260	-1.801205	2.444953
H	1.543803	-6.135115	2.658215	H	-2.857984	-0.258014	3.311240
C	2.382455	4.169323	-0.955761	C	1.719464	5.626635	-2.771829
H	3.167790	3.692104	-0.373209	H	1.998964	6.274216	-3.600038
C	2.718836	4.983144	-2.013707	C	4.190578	5.031471	3.673725
H	3.767126	5.137035	-2.262244	H	4.836840	5.687713	4.252630
C	0.703351	-4.955981	0.403980	C	-0.155100	-2.274182	2.492536
H	0.148345	-5.855170	0.671337	H	0.934717	-2.192708	2.576236
C	4.465457	-2.008266	-1.266264	H	-0.380573	-2.691387	1.501169
C	3.727204	1.404709	2.983771	H	-0.475059	-3.014528	3.237434
H	4.535622	0.988491	3.583968	C	7.115988	-2.687327	-2.000430
C	4.972091	0.342060	-1.747469	H	8.132787	-2.960413	-2.274229
H	5.686641	1.109287	-2.043798	C	-0.853191	-0.938675	2.752297
C	1.026124	3.938050	-0.608525	C	0.338172	-4.201529	-0.680790
C	3.950095	-3.732522	2.798167	H	-0.486771	-4.518384	-1.316500
H	4.780806	-3.411275	3.423501	C	1.500203	0.138232	-4.154944
C	3.671589	0.670770	-1.471703	H	1.729195	-0.891135	-4.450626
H	3.336832	1.705788	-1.562486	H	2.315337	0.505233	-3.524430
C	0.395300	5.426723	-2.464012	H	1.507229	0.735840	-5.076384
H	-0.388816	5.910516	-3.046111	C	-0.156948	-0.219414	3.909886
C	-1.344998	4.315799	-1.113930	H	-0.725121	0.648612	4.262277

H	0.861744	0.103689	3.674135
H	-0.088743	-0.917591	4.755069
Ni	-2.006073	-0.340206	-0.672668
H	-4.650603	-2.063237	-0.432629
C	-5.711811	-0.746147	3.246482
C	-5.175555	-0.909463	1.975122
C	-4.571012	0.161352	1.294273
C	-4.573581	1.410369	1.936540
C	-5.098520	1.574625	3.214132
C	-5.667646	0.493042	3.880126
H	-6.175443	-1.596783	3.741770
H	-5.229643	-1.896034	1.518419
H	-4.164435	2.277411	1.419351
H	-5.077645	2.557617	3.680884
H	-6.090178	0.618747	4.874390
C	-4.017546	0.014035	-0.086754
C	-4.762987	-1.073554	-0.867283
N	-4.235693	1.288105	-0.798767
H	-5.137323	1.741562	-0.662966
N	-6.274367	-0.863605	-0.887345
O	-6.691795	0.201517	-1.342879
O	-6.971009	-1.769855	-0.454260
H	-4.469757	-1.098077	-1.919865
C	-3.148679	-4.760718	-1.370858
H	-2.855265	-4.930526	-2.408108
H	-2.746316	-5.541144	-0.718985
H	-4.242408	-4.822153	-1.308656
C	-2.714770	-3.409694	-0.921078
O	-2.435051	-2.476648	-1.667023
O	-2.706497	-3.281517	0.408739
H	-2.411810	-2.353393	0.591117
C	-3.668645	1.386004	-1.999920
C	-4.180155	2.363699	-2.996962
H	-5.001334	1.906245	-3.563343
H	-4.576181	3.264564	-2.517323
H	-3.388547	2.636132	-3.699565
O	-2.715106	0.609661	-2.267764

IV$_{S3}$

P	0.612332	0.133299	-1.574665
P	0.603182	-0.349894	1.509656
C	-2.207224	-0.285686	1.519067
C	-1.800013	-2.709740	0.942545
C	-3.909257	-3.356235	2.844722
H	-3.314551	-4.148631	2.395898
C	-0.451536	-2.955274	1.183993
C	-1.345901	2.864218	-0.942211
C	-2.311838	1.945799	-1.605523
C	0.776844	0.687247	3.078907
C	-2.505330	-3.526386	-0.001101
C	-2.190949	0.562606	-1.493873
C	-3.365072	2.496900	-2.409593
C	-3.155200	-0.281381	-2.096165
H	-3.057510	-1.359461	-1.967996
C	-1.007485	0.196368	0.740710
H	-0.962369	1.286368	0.842598
C	-0.000283	2.839793	-1.299487
C	0.494297	1.829621	-2.293353
H	1.475001	2.112274	-2.691433
H	-0.202262	1.760819	-3.138277
C	-4.382589	-0.983781	3.184745
C	-2.530953	-1.632395	1.666800
C	-1.841098	-4.644656	-0.601521
C	-0.864298	4.721237	0.621335
C	-1.052612	-0.113727	-0.765217
H	-1.210850	-1.192913	-0.853436
C	-5.439588	-1.352115	4.050824
H	-6.025129	-0.561960	4.519482
C	-5.365677	2.167120	-3.804528
H	-6.090955	1.485768	-4.247951
C	0.327222	-2.072634	2.113961
H	1.310476	-2.506495	2.332924
H	-0.206960	-1.974777	3.067737
C	-4.326275	1.622086	-3.012928
C	-2.528016	-5.432014	-1.557251
H	-2.006936	-6.278071	-2.004337
C	-3.127440	3.799109	0.543661
H	-3.847084	3.092139	0.135166
C	-3.516276	4.673637	1.531992
H	-4.543357	4.656562	1.891874
C	-0.505558	-4.924270	-0.233524
H	-0.019434	-5.806779	-0.648981
C	-3.602881	-2.003100	2.546992
C	-4.202724	0.228209	-2.817642
H	-4.941398	-0.438302	-3.262440
C	-4.069316	0.372292	2.938937
H	-4.675101	1.150203	3.403238
C	-1.793329	3.787182	0.058654

C	-4.476353	-4.031392	-1.335873
H	-5.496942	-3.793523	-1.629754
C	-3.001073	0.705121	2.148555
H	-2.749085	1.753448	1.987365
C	-1.301185	5.617218	1.627087
H	-0.582799	6.325353	2.039024
C	0.470811	4.722672	0.157098
H	1.161190	5.473492	0.541486
C	2.200318	0.539882	3.621012
H	2.269087	1.056171	4.587039
H	2.951909	0.984580	2.963041
H	2.466237	-0.511004	3.801847
C	-4.490898	4.383449	-3.455154
H	-4.548704	5.453092	-3.646084
C	-3.842255	-3.255843	-0.393497
H	-4.362645	-2.404873	0.041596
C	-3.477700	3.887429	-2.669016
H	-2.741770	4.569940	-2.250322
C	0.893664	3.798510	-0.765737
H	1.919345	3.814072	-1.127044
C	-3.817301	-5.130978	-1.924304
H	-4.331752	-5.737484	-2.666609
C	-4.934368	-3.680915	3.701708
H	-5.143309	-4.726409	3.918534
C	0.486175	2.147589	2.715204
H	-0.591724	2.342254	2.643419
H	0.944570	2.459950	1.768439
H	0.879846	2.806179	3.500326
C	2.051499	-1.299134	-3.495645
H	2.041707	-1.902224	-4.413212
H	2.602201	-1.862648	-2.733994
H	2.602313	-0.379086	-3.723076
C	-2.598532	5.594583	2.078768
H	-2.921652	6.285715	2.854371
C	-5.451395	3.520428	-4.021521
H	-6.250362	3.927690	-4.637546
C	0.002804	-2.376686	-2.604870
H	0.242677	-3.150111	-3.347068
H	-1.091128	-2.341333	-2.531887
H	0.407287	-2.707433	-1.638879
C	-5.715200	-2.673691	4.304806
H	-6.528367	-2.945721	4.974359
C	0.610569	-1.047235	-3.053287
C	0.176903	-4.085685	0.611168
H	1.215579	-4.288289	0.865391
C	-0.185656	0.246046	4.189802
H	0.117365	-0.701790	4.648446
H	-1.228296	0.164004	3.868012
H	-0.150877	1.002731	4.984008
C	-0.186432	-0.483250	-4.230759
H	0.315287	0.369209	-4.702543
H	-1.204008	-0.181144	-3.954174
H	-0.276089	-1.265039	-4.996379
Ni	2.161151	-0.138727	0.012414
H	2.544112	-0.445999	1.404383
C	4.150685	0.217669	0.280074
C	3.755429	0.147941	-1.099950
H	4.007305	-0.784926	-1.595131
N	3.959706	1.247036	-2.037244
O	4.518290	0.947403	-3.093415
O	3.594529	2.384688	-1.740902
N	4.896220	-0.943858	0.683470
H	4.446728	-1.609893	1.298355
C	5.986954	-1.453105	0.027345
C	6.729657	-0.545418	-0.909681
H	6.346003	-0.648759	-1.932426
H	6.655210	0.513180	-0.637214
H	7.778549	-0.848354	-0.923429
O	6.347680	-2.610388	0.247341
C	4.452292	1.453301	1.045203
C	5.599869	1.504507	1.850666
C	3.578910	2.549327	1.063735
C	5.878650	2.629946	2.618169
H	6.274762	0.652782	1.879487
C	3.850303	3.665819	1.840854
H	2.670522	2.514355	0.467956
C	5.006708	3.714795	2.617941
H	6.779862	2.652337	3.226655
H	3.147733	4.497982	1.846254
H	5.222437	4.590822	3.225753
C	3.435286	-3.939166	-0.863088
O	3.037040	-2.852839	-0.443298
C	2.677516	-4.807508	-1.818223
H	1.625539	-4.522668	-1.851545
H	3.107092	-4.690717	-2.820716
H	2.782254	-5.863584	-1.552896
O	4.601620	-4.477629	-0.545872
H	5.165738	-3.829417	-0.039701

V_{S3}

P	0.569373	0.123405	-1.639239
P	0.719566	-0.388508	1.449263
C	-2.122147	-0.610756	1.474070
C	-1.363241	-2.919439	0.792050
C	-3.588797	-3.946729	2.381009
H	-2.864765	-4.632575	1.948010
C	-0.029063	-2.977964	1.177826
C	-1.043229	2.958111	-0.725166
C	-2.170307	2.173913	-1.306058
C	1.057680	0.799708	2.844033
C	-1.817008	-3.776044	-0.264225
C	-2.202781	0.781397	-1.291781
C	-3.266230	2.893878	-1.895391
C	-3.365369	0.098371	-1.726421
H	-3.384392	-0.990058	-1.649242
C	-0.964246	0.066100	0.772944
H	-1.016744	1.141901	1.001226
C	0.243850	2.864978	-1.244350
C	0.570990	1.846666	-2.290185
H	1.559017	2.036721	-2.728460
H	-0.158109	1.873129	-3.113344
C	-4.357072	-1.673558	2.839854
C	-2.305067	-1.994676	1.485509
C	-0.911810	-4.732228	-0.831597
C	-0.249518	4.751489	0.792866
C	-1.067489	-0.066492	-0.761041
H	-1.317073	-1.118730	-0.968530
C	-5.447754	-2.221796	3.556302
H	-6.162054	-1.539231	4.015321
C	-5.503812	2.887331	-2.920984
H	-6.375294	2.323310	-3.251399
C	0.491389	-2.031146	2.214617
H	1.452076	-2.364992	2.623411
H	-0.211048	-1.913709	3.051816
C	-4.420193	2.177895	-2.350479
C	-1.356629	-5.567791	-1.884611
H	-0.658069	-6.292673	-2.300980
C	-2.528628	3.902038	1.051501
H	-3.332236	3.240692	0.731787
C	-2.724065	4.753930	2.114115
H	-3.679371	4.755353	2.635406
C	0.427545	-4.774490	-0.378833
H	1.117867	-5.488670	-0.825768
C	-3.409484	-2.548748	2.216070
C	-4.449098	0.771064	-2.222830
H	-5.339167	0.228733	-2.539180
C	-4.172489	-0.276661	2.736898
H	-4.905443	0.388782	3.191300
C	-1.290511	3.866595	0.358054
C	-3.514814	-4.495532	-1.852148
H	-4.519367	-4.401487	-2.259877
C	-3.078113	0.233393	2.090709
H	-2.935893	1.313210	2.026314
C	-0.491601	5.629085	1.876925
H	0.309570	6.297434	2.191362
C	1.011035	4.696386	0.153447
H	1.796423	5.383201	0.469207
C	2.183959	0.231335	3.706542
H	2.496720	0.988012	4.437300
H	3.073845	-0.029852	3.117992
H	1.869795	-0.656650	4.267697
C	-4.310020	4.959742	-2.648829
H	-4.263370	6.038325	-2.784346
C	-3.123509	-3.685983	-0.809965
H	-3.824364	-2.965984	-0.390566
C	-3.246475	4.300891	-2.077391
H	-2.368609	4.866598	-1.774424
C	1.254990	3.753116	-0.810868
H	2.236334	3.687723	-1.277402
C	-2.629063	-5.451837	-2.390190
H	-2.954038	-6.091475	-3.207916
C	-4.651656	-4.447474	3.095220
H	-4.760614	-5.523492	3.213138
C	1.466938	2.119876	2.203499
H	0.673613	2.493157	1.547698
H	2.380986	2.025392	1.603500
H	1.643385	2.883723	2.973130
C	0.526253	-2.375580	-2.795923
H	0.437173	-3.013155	-3.685300
H	-0.286730	-2.660228	-2.118623
H	1.469327	-2.622027	-2.298822
C	-1.700414	5.630250	2.529915
H	-1.870867	6.304409	3.366448
C	-5.455725	4.252290	-3.065743
H	-6.291960	4.786984	-3.510952
C	-0.950168	-0.712636	-3.874826

H	-0.926342	-1.228539	-4.843502
H	-1.204433	0.335956	-4.073609
H	-1.768415	-1.155134	-3.297213
C	-5.597660	-3.581337	3.680915
H	-6.437078	-3.992082	4.237868
C	0.407038	-0.909536	-3.194060
C	0.863794	-3.894472	0.577544
H	1.903683	-3.912526	0.903212
C	-0.192101	1.011345	3.699217
H	-0.638740	0.074523	4.054939
H	-0.965170	1.574483	3.164064
H	0.079199	1.601880	4.583376
C	1.507888	-0.496335	-4.173401
H	2.518114	-0.569596	-3.760305
H	1.358330	0.522307	-4.551448
H	1.480467	-1.166828	-5.041423
Ni	2.165486	-0.358844	-0.150487
H	2.579331	-0.667667	1.232903
C	4.175961	-0.366768	-0.048603
C	3.690157	-0.561468	-1.384531
N	4.811241	-1.426483	0.670354
H	4.246647	-2.242560	0.869731
C	6.157398	-1.800281	0.481958
C	7.049650	-0.821248	-0.228675
H	6.606419	-0.449062	-1.160757
H	7.256465	0.052060	0.400840
H	7.993952	-1.318446	-0.454509
O	6.531202	-2.868022	0.919663
C	4.549805	1.002324	0.390239
C	5.038545	1.190216	1.695086
C	4.391590	2.133670	-0.425269
C	5.339211	2.459126	2.169866
H	5.187830	0.319905	2.330196
C	4.699533	3.403038	0.051174
H	4.039573	2.032509	-1.451372
C	5.166406	3.574367	1.351810
H	5.718442	2.576865	3.182968
H	4.582960	4.264179	-0.604845
H	5.409080	4.568898	1.719734
N	3.832570	-1.893421	-1.941952
O	4.289391	-1.984781	-3.077276
O	3.480163	-2.851469	-1.239645
H	3.837228	0.195291	-2.149718

$TSII_{S3}$

P	0.538989	0.089953	-1.658023
P	0.689559	-0.415410	1.424414
C	-2.152594	-0.548186	1.478119
C	-1.475602	-2.879416	0.773011
C	-3.715139	-3.842823	2.375468
H	-3.015317	-4.548043	1.934173
C	-0.139612	-2.990452	1.141765
C	-0.926281	2.988167	-0.716147
C	-2.097028	2.263378	-1.288430
C	1.090134	0.725201	2.844143
C	-1.974743	-3.719665	-0.277271
C	-2.195401	0.873405	-1.283939
C	-3.162921	3.039029	-1.861551
C	-3.391778	0.248932	-1.714397
H	-3.461438	-0.837893	-1.645087
C	-0.978407	0.095975	0.772821
H	-0.995503	1.172342	1.004667
C	0.347923	2.836303	-1.253179
C	0.609017	1.809953	-2.309581
H	1.595795	1.954943	-2.767224
H	-0.135183	1.871153	-3.117396
C	-4.408721	-1.550562	2.854918
C	-2.377233	-1.925988	1.482110
C	-1.116846	-4.716644	-0.848046
C	-0.029031	4.739359	0.792381
C	-1.097682	-0.027783	-0.763959
H	-1.396344	-1.067029	-0.972754
C	-5.511944	-2.069464	3.574032
H	-6.201671	-1.368067	4.042202
C	-5.408545	3.145784	-2.863886
H	-6.308838	2.625844	-3.189560
C	0.439065	-2.066097	2.167324
H	1.404847	-2.431171	2.536862
H	-0.225260	-1.940519	3.034795
C	-4.354083	2.381725	-2.309429
C	-1.605012	-5.536650	-1.893910
H	-0.940779	-6.292245	-2.312045
C	-2.339470	3.993204	1.086017
H	-3.176358	3.367503	0.780186
C	-2.480068	4.852693	2.151446
H	-3.425649	4.895554	2.688409
C	0.222772	-4.816416	-0.406098
H	0.876915	-5.563361	-0.853938

C	-3.492956	-2.450106	2.218396
C	-4.447608	0.976543	-2.193617
H	-5.365102	0.479720	-2.506628
C	-4.180915	-0.159415	2.760867
H	-4.889199	0.525275	3.225640
C	-1.115760	3.904205	0.372541
C	-3.713694	-4.371805	-1.850353
H	-4.716172	-4.235764	-2.251280
C	-3.076594	0.320790	2.108734
H	-2.899729	1.396069	2.051238
C	-0.214941	5.628058	1.878453
H	0.620315	6.259399	2.180163
C	1.220023	4.623728	0.139037
H	2.040793	5.272213	0.445206
C	2.198826	0.086559	3.679496
H	2.560908	0.813887	4.417248
H	3.067728	-0.209983	3.074845
H	1.849895	-0.794167	4.231389
C	-4.114518	5.157061	-2.592083
H	-4.017623	6.232944	-2.721928
C	-3.280033	-3.575592	-0.814497
H	-3.946136	-2.824221	-0.393247
C	-3.077950	4.444607	-2.035913
H	-2.171165	4.966913	-1.740323
C	1.407482	3.670835	-0.828769
H	2.378861	3.561943	-1.308329
C	-2.874911	-5.368162	-2.390619
H	-3.233864	-5.996970	-3.202550
C	-4.789178	-4.315314	3.092124
H	-4.930691	-5.388332	3.203110
C	1.553996	2.040740	2.232071
H	0.773997	2.465780	1.591725
H	2.458645	1.917671	1.622810
H	1.771270	2.777517	3.017488
C	0.398539	-2.409754	-2.804383
H	0.260221	-3.043890	-3.689951
H	-0.410636	-2.657058	-2.108200
H	1.341481	-2.697664	-2.329215
C	-1.412506	5.683739	2.549557
H	-1.540086	6.365639	3.387533
C	-5.297133	4.507909	-3.000732
H	-6.111762	5.084713	-3.433293
C	-1.012951	-0.691277	-3.885988
H	-1.011923	-1.211704	-4.852447
H	-1.223692	0.366298	-4.087963
H	-1.848006	-1.096748	-3.304555
C	-5.704579	-3.424403	3.689180
H	-6.553621	-3.812295	4.247907
C	0.335596	-0.940921	-3.205322
C	0.705705	-3.949525	0.539212
H	1.746821	-4.009331	0.854872
C	-0.142623	0.971513	3.714658
H	-0.624161	0.046526	4.056037
H	-0.895949	1.573190	3.192638
H	0.156470	1.535421	4.607188
C	1.456964	-0.572310	-4.179442
H	2.460155	-0.669898	-3.752481
H	1.341829	0.446571	-4.568431
H	1.418593	-1.250945	-5.040618
Ni	2.125245	-0.408861	-0.189651
H	2.757593	-0.593103	1.122431
C	4.129532	-0.473190	-0.004092
C	3.665881	-0.643931	-1.364495
N	4.745550	-1.564373	0.696338
H	4.148936	-2.348423	0.929021
C	6.058678	-2.011072	0.449783
C	6.973361	-1.081599	-0.297904
H	6.520499	-0.698637	-1.221054
H	7.238242	-0.211758	0.314543
H	7.885879	-1.624956	-0.546724
O	6.390124	-3.098604	0.873235
C	4.610446	0.879448	0.409710
C	5.144678	1.044220	1.697699
C	4.502960	2.008511	-0.413163
C	5.552711	2.293248	2.146512
H	5.247014	0.172217	2.340120
C	4.917046	3.257960	0.036294
H	4.100835	1.923805	-1.421814
C	5.439265	3.408014	1.318135
H	5.969090	2.394799	3.146522
H	4.839039	4.118408	-0.626172
H	5.766536	4.385569	1.665104
N	3.739702	-1.987252	-1.905474
O	4.210059	-2.126374	-3.029768
O	3.309912	-2.910253	-1.196471
H	3.898378	0.093879	-2.127452

VI$_{S3}$

P	0.787904	-0.124208	-1.267359
P	0.092962	-0.964164	1.624863
C	-2.584361	-0.132278	1.237097
C	-2.540931	-2.493777	0.339373
C	-5.214163	-2.803390	1.455190
H	-4.705340	-3.653740	1.007566
C	-1.418279	-3.091873	0.902292
C	-0.034508	2.986484	-0.292681
C	-1.210781	2.664504	-1.150773
C	0.636862	-0.125706	3.195224
C	-3.065041	-3.011972	-0.888535
C	-1.662403	1.359366	-1.340752
C	-1.888744	3.744012	-1.813102
C	-2.843481	1.122253	-2.086195
H	-3.199454	0.095605	-2.181056
C	-1.157261	0.134579	0.815318
H	-0.884359	1.136408	1.181782
C	1.233634	2.517750	-0.617464
C	1.412572	1.536633	-1.733145
H	2.469288	1.439970	-2.005990
H	0.857569	1.840541	-2.634140
C	-5.233776	-0.466140	2.163141
C	-3.216980	-1.357931	1.031011
C	-2.481301	-4.187154	-1.463717
C	0.972014	4.265192	1.575708
C	-0.983566	0.157103	-0.724224
H	-1.487393	-0.745243	-1.104768
C	-6.546066	-0.660409	2.656498
H	-7.051620	0.180012	3.130803
C	-3.752126	4.542148	-3.209688
H	-4.657870	4.317155	-3.771787
C	-0.781071	-2.492136	2.118851
H	-0.041466	-3.171859	2.556982
H	-1.520462	-2.242585	2.893768
C	-3.076949	3.477069	-2.567654
C	-2.990880	-4.684053	-2.687689
H	-2.539789	-5.580712	-3.112026
C	-1.463481	4.225268	1.340560
H	-2.354750	3.909581	0.800928
C	-1.585223	4.998175	2.472293
H	-2.573674	5.283278	2.827303
C	-1.384856	-4.802383	-0.813790
H	-0.949998	-5.702137	-1.247740
C	-4.548223	-1.552879	1.530385
C	-3.543365	2.146931	-2.664783
H	-4.458286	1.946315	-3.220993
C	-4.575158	0.776552	2.295409
H	-5.102284	1.606871	2.763641
C	-0.189752	3.828108	0.857758
C	-4.599901	-2.890511	-2.773151
H	-5.420323	-2.392540	-3.285986
C	-3.286033	0.929788	1.858154
H	-2.778297	1.888342	1.977094
C	0.810728	5.076330	2.724996
H	1.702967	5.403520	3.258234
C	2.250013	3.839938	1.141303
H	3.134855	4.187724	1.675032
C	1.423237	-1.134172	4.032943
H	1.821754	-0.630488	4.922617
H	2.274027	-1.558269	3.484448
H	0.798339	-1.963388	4.384351
C	-2.085053	6.091712	-2.425733
H	-1.693507	7.106228	-2.388341
C	-4.136839	-2.388443	-1.578254
H	-4.599456	-1.501487	-1.148016
C	-1.413406	5.080558	-1.778901
H	-0.495095	5.307924	-1.242525
C	2.371740	2.959271	0.097191
H	3.352933	2.600757	-0.211309
C	-4.025895	-4.050476	-3.333578
H	-4.404865	-4.441836	-4.275090
C	-6.486514	-2.962372	1.952302
H	-6.971462	-3.934148	1.886365
C	1.523132	1.049409	2.799580
H	0.999779	1.735195	2.124945
H	2.444035	0.728382	2.289563
H	1.814988	1.625240	3.688054
C	0.474061	-2.534736	-2.544662
H	0.267062	-3.116410	-3.453027
H	-0.380396	-2.668940	-1.871688
H	1.356709	-2.978023	-2.062690
C	-0.439487	5.433113	3.170370
H	-0.548365	6.050270	4.059554
C	-3.271557	5.826789	-3.139357
H	-3.795818	6.637257	-3.640819
C	-0.499534	-0.575589	-3.735054
H	-0.425357	-1.026867	-4.732902
H	-0.521627	0.513525	-3.865384

H	-1.463685	-0.887032	-3.315618
C	-7.165579	-1.881894	2.551938
H	-8.172771	-2.021299	2.938791
C	0.676169	-1.062746	-2.886518
C	-0.844471	-4.247418	0.319189
H	0.024908	-4.702228	0.794561
C	-0.572457	0.392492	3.975577
H	-1.318050	-0.385295	4.181287
H	-1.077062	1.214215	3.452073
H	-0.233128	0.785473	4.942736
C	1.980148	-0.870237	-3.657598
H	2.849928	-1.198312	-3.076902
H	2.141175	0.170130	-3.964264
H	1.955610	-1.479263	-4.569820
Ni	1.726417	-1.331327	0.247123
H	3.892920	-0.770379	1.413959
C	4.475397	-1.032428	0.518077
C	3.533572	-1.800988	-0.422380
N	5.554427	-1.856558	1.051073
H	5.379521	-2.298249	1.946807
C	6.679014	-2.382458	0.429003
C	7.006329	-1.895544	-0.957379
H	6.141922	-1.912869	-1.631577
H	7.371907	-0.861916	-0.931674
H	7.791186	-2.533672	-1.366483
O	7.371161	-3.179958	1.034471
C	4.959979	0.275117	-0.074582
C	5.577663	1.190961	0.784766
C	4.852242	0.596976	-1.427701
C	6.075817	2.395545	0.301667
H	5.679577	0.941245	1.841188
C	5.352453	1.803196	-1.917382
H	4.395255	-0.104473	-2.124659
C	5.965781	2.705725	-1.054277
H	6.555073	3.094066	0.984640
H	5.268833	2.029838	-2.978898
H	6.360328	3.645041	-1.435029
N	3.041852	-3.021292	0.121326
O	3.016761	-4.107646	-0.419361
O	2.419199	-2.781472	1.271740
H	3.881383	-1.997897	-1.436277

VII$_{S3}$

P	-0.478373	0.158949	1.376223
P	0.040347	-0.925282	-1.450160
C	2.793602	-0.202344	-1.208971
C	2.671920	-2.510949	-0.187042
C	5.326387	-2.974263	-1.310743
H	4.784685	-3.790729	-0.839604
C	1.508394	-3.077475	-0.699068
C	0.398598	3.167742	0.192326
C	1.613558	2.845446	0.994029
C	-0.499414	-0.121981	-3.054056
C	3.202279	-3.009022	1.048190
C	2.034264	1.539863	1.233284
C	2.379923	3.938113	1.529604
C	3.267577	1.304238	1.889219
H	3.596499	0.271729	2.015254
C	1.388197	0.162084	-0.782950
H	1.162274	1.144203	-1.222925
C	-0.872032	2.798665	0.622515
C	-1.042256	1.865634	1.782795
H	-2.094730	1.814645	2.093247
H	-0.463698	2.195361	2.659195
C	5.434807	-0.667587	-2.101885
C	3.382621	-1.437571	-0.940255
C	2.587772	-4.141223	1.675570
C	-0.645178	4.405273	-1.686349
C	1.272534	0.328285	0.750276
H	1.752997	-0.560338	1.187618
C	6.741761	-0.926229	-2.578705
H	7.278801	-0.121982	-3.080064
C	4.381199	4.748453	2.711483
H	5.323758	4.524346	3.209942
C	0.861571	-2.495104	-1.917635
H	0.102741	-3.170461	-2.329998
H	1.595011	-2.287572	-2.709220
C	3.617154	3.672195	2.200432
C	3.101792	-4.617607	2.905268
H	2.625128	-5.481853	3.367088
C	1.790357	4.204243	-1.606277
H	2.694258	3.861203	-1.106111
C	1.884834	4.890450	-2.795268
H	2.863114	5.074929	-3.234678
C	1.450110	-4.730025	1.075457
H	0.993365	-5.599441	1.547091
C	4.706968	-1.703132	-1.431187
C	4.047515	2.333611	2.341743

H	5.001389	2.133271	2.828109
C	4.821584	0.591034	-2.290615
H	5.380534	1.382688	-2.787884
C	0.529525	3.931287	-1.015485
C	4.765696	-2.874631	2.909180
H	5.606694	-2.384137	3.395264
C	3.535669	0.804646	-1.873133
H	3.061531	1.773487	-2.037293
C	-0.511065	5.130550	-2.894557
H	-1.414320	5.488375	-3.387954
C	-1.914493	4.113059	-1.135037
H	-2.807067	4.514809	-1.614085
C	-1.418024	-1.075687	-3.820277
H	-1.745268	-0.586654	-4.746493
H	-2.325048	-1.357261	-3.270134
H	-0.897437	-1.996223	-4.114153
C	2.709314	6.310464	1.964194
H	2.351224	7.335328	1.891229
C	4.303183	-2.399126	1.703011
H	4.791588	-1.545653	1.235616
C	1.950602	5.287750	1.445002
H	0.998263	5.517162	0.972742
C	-2.021150	3.309525	-0.028802
H	-3.003040	3.092791	0.392825
C	4.165262	-3.997021	3.515882
H	4.544998	-4.368170	4.465197
C	6.593495	-3.197981	-1.796546
H	7.040403	-4.184911	-1.696145
C	-1.231256	1.172171	-2.708551
H	-0.610885	1.840134	-2.101685
H	-2.164660	1.005403	-2.156217
H	-1.489948	1.713573	-3.628190
C	-0.003990	-2.167122	2.768159
H	0.231836	-2.693921	3.702855
H	0.853704	-2.297738	2.099041
H	-0.874766	-2.655544	2.313638
C	0.726370	5.364428	-3.444900
H	0.815417	5.913536	-4.379771
C	3.942064	6.044414	2.593583
H	4.535796	6.863960	2.992826
C	0.925468	-0.097941	3.799085
H	0.933448	-0.512008	4.815503
H	0.891001	0.994521	3.892438
H	1.882354	-0.368880	3.339977
C	7.315890	-2.165024	-2.427676
H	8.319337	-2.354698	-2.802603
C	-0.270450	-0.691833	3.047976
C	0.905885	-4.187164	-0.060492
H	0.016767	-4.633084	-0.507894
C	0.720967	0.219217	-3.912830
H	1.343268	-0.653331	-4.143590
H	1.360048	0.979200	-3.447163
H	0.373684	0.632249	-4.868870
C	-1.526308	-0.535958	3.906965
H	-2.371299	-1.106558	3.510166
H	-1.821735	0.511358	4.049362
H	-1.318638	-0.943356	4.904450
Ni	-1.597235	-1.050640	0.017723
H	-3.392767	1.117008	-0.076896
C	-4.106250	0.284132	0.067396
C	-3.309749	-0.660389	0.957616
N	-4.299881	-0.220713	-1.297037
H	-3.410583	-0.442961	-1.737326
C	-5.257407	-1.069344	-1.834827
C	-6.680119	-0.968494	-1.370814
H	-7.256201	-1.750576	-1.868439
H	-6.776443	-1.076006	-0.288449
H	-7.099229	0.007726	-1.640971
O	-4.920500	-1.795743	-2.765096
C	-5.338975	0.906944	0.683457
C	-5.874514	0.471125	1.895732
C	-5.943823	1.985640	0.026970
C	-7.004301	1.083816	2.432297
H	-5.423685	-0.360666	2.434904
C	-7.071893	2.597258	0.560405
H	-5.528740	2.325977	-0.923559
C	-7.608124	2.144145	1.765243
H	-7.414767	0.724507	3.373572
H	-7.535952	3.429927	0.035394
H	-8.492944	2.620204	2.182572
C	-2.739020	-3.702663	-1.105806
O	-2.357774	-2.523116	-1.002825
O	-2.952353	-4.505822	-0.089670
C	-2.983963	-4.315004	-2.435185
H	-3.832755	-3.788362	-2.889509
H	-2.125350	-4.151301	-3.094237
H	-3.203328	-5.379958	-2.353268
H	-2.952244	-4.013662	0.775745

N	-3.886253	-1.963475	1.203238
O	-3.254147	-2.735321	1.974315
O	-4.870065	-2.337934	0.571431
H	-3.121254	-0.215915	1.936176

TSIII$_{S3}$

P	-0.371191	-0.067525	1.397213
P	0.050524	-0.871435	-1.539778
C	2.771804	-0.115817	-1.343697
C	2.741397	-2.448726	-0.377504
C	5.376445	-2.809338	-1.589743
H	4.885869	-3.642381	-1.092484
C	1.573635	-3.019461	-0.876216
C	0.397729	3.047663	0.358233
C	1.642629	2.716676	1.107956
C	-0.545685	-0.060456	-3.123075
C	3.295190	-2.957280	0.842428
C	2.076160	1.403539	1.290869
C	2.397178	3.791010	1.693481
C	3.289395	1.146469	1.974133
H	3.609364	0.110191	2.087078
C	1.387757	0.193329	-0.822309
H	1.117735	1.205404	-1.154736
C	-0.836771	2.585628	0.802460
C	-0.913781	1.607892	1.929531
H	-1.930387	1.547399	2.337500
H	-0.249686	1.893823	2.759060
C	5.366888	-0.500551	-2.386724
C	3.406082	-1.339836	-1.124241
C	2.679083	-4.081735	1.482730
C	-0.779092	4.346024	-1.392800
C	1.342562	0.207951	0.724963
H	1.872431	-0.695161	1.053053
C	6.657914	-0.715661	-2.925620
H	7.143370	0.104963	-3.452408
C	4.384735	4.564229	2.925003
H	5.323297	4.324589	3.423736
C	0.887211	-2.414414	-2.059605
H	0.129704	-3.084215	-2.482183
H	1.602227	-2.153667	-2.850502
C	3.629820	3.505131	2.366180
C	3.202679	-4.556146	2.709569
H	2.722537	-5.412629	3.181994
C	1.666135	4.265603	-1.414415
H	2.603824	3.926314	-0.977092
C	1.679717	5.036940	-2.554782
H	2.629390	5.299128	-3.017227
C	1.546901	-4.683372	0.885493
H	1.098784	-5.554991	1.361352
C	4.709821	-1.560270	-1.680714
C	4.056579	2.163082	2.477092
H	4.996729	1.947728	2.983609
C	4.701231	0.734611	-2.550151
H	5.204906	1.539428	-3.083844
C	0.444221	3.893453	-0.797419
C	4.896107	-2.842141	2.673223
H	5.755510	-2.364948	3.140213
C	3.435301	0.912584	-2.055913
H	2.918096	1.863889	-2.197184
C	-0.727033	5.163585	-2.547305
H	-1.665261	5.507912	-2.981404
C	-2.011755	3.926976	-0.839897
H	-2.942149	4.290770	-1.275385
C	-1.804837	-0.774701	-3.614272
H	-2.072243	-0.381424	-4.603118
H	-2.657585	-0.587293	-2.949877
H	-1.681275	-1.859017	-3.705510
C	2.708384	6.145195	2.230752
H	2.343484	7.169747	2.198987
C	4.418245	-2.362438	1.474249
H	4.907055	-1.514136	0.997812
C	1.958927	5.140436	1.665613
H	1.007217	5.384901	1.200803
C	-2.036927	3.040427	0.206610
H	-2.990449	2.704039	0.615569
C	4.285880	-3.949078	3.298682
H	4.675470	-4.320399	4.243863
C	6.627322	-2.989043	-2.132659
H	7.113748	-3.958890	-2.051466
C	-0.879351	1.399388	-2.836930
H	0.014212	2.013493	-2.676734
H	-1.537338	1.517200	-1.964271
H	-1.405467	1.827217	-3.700404
C	-0.570293	-2.511239	2.717162
H	-0.308022	-3.132726	3.584391
H	-0.019237	-2.911679	1.857116
H	-1.645274	-2.642742	2.546008
C	0.474604	5.499842	-3.122818

H	0.499530	6.118647	-4.016993
C	3.939696	5.861496	2.855615
H	4.525113	6.667326	3.293024
C	1.202843	-0.966732	3.575466
H	1.213558	-1.476802	4.547598
H	1.534700	0.065547	3.742555
H	1.947062	-1.472229	2.946935
C	7.282125	-1.932545	-2.798241
H	8.273235	-2.087455	-3.218883
C	-0.215269	-1.052953	3.008708
C	0.993671	-4.146339	-0.248686
H	0.105007	-4.594237	-0.694088
C	0.547999	-0.143021	-4.192505
H	0.690822	-1.163491	-4.564402
H	1.516034	0.237515	-3.842078
H	0.245143	0.472819	-5.049230
C	-1.198031	-0.495896	4.040478
H	-2.231473	-0.485185	3.677087
H	-0.923998	0.506633	4.386563
H	-1.190578	-1.156108	4.916814
Ni	-1.500400	-1.204619	-0.072304
H	-3.198603	0.275949	-0.711376
C	-4.083765	-0.192602	-0.219422
C	-3.454061	-0.902063	0.986020
N	-4.618962	-1.078215	-1.245873
H	-3.899617	-1.635746	-1.695078
C	-5.822355	-1.781052	-1.322488
C	-7.095939	-1.118525	-0.888839
H	-7.867304	-1.884295	-0.789470
H	-7.010677	-0.562087	0.045461
H	-7.407553	-0.411814	-1.668598
O	-5.805589	-2.866206	-1.887991
C	-4.976624	0.989113	0.100511
C	-5.309952	1.375898	1.399634
C	-5.403269	1.783443	-0.970940
C	-6.072773	2.522275	1.621319
H	-4.989988	0.790291	2.260553
C	-6.161508	2.925392	-0.750470
H	-5.137681	1.483944	-1.985960
C	-6.500427	3.298619	0.550220
H	-6.335159	2.801711	2.639388
H	-6.490041	3.528035	-1.595198
H	-7.097048	4.191042	0.726136
C	-2.720209	-3.578224	-0.662025
O	-2.082490	-2.623955	-1.240724
O	-3.106771	-3.473291	0.538819
C	-3.070830	-4.783562	-1.452904
H	-4.065125	-4.595835	-1.881565
H	-2.366118	-4.946942	-2.271659
H	-3.141612	-5.664875	-0.812410
H	-2.986631	-2.227136	0.759554
N	-4.448645	-1.557141	1.916437
O	-4.053639	-1.806856	3.052432
O	-5.557783	-1.823935	1.477721
H	-2.985784	-0.174013	1.651691

VIII$_{S3}$

P	0.018468	-0.490387	1.645209
P	0.193887	-1.030602	-1.357585
C	2.700218	0.279885	-1.456818
C	3.312969	-2.054266	-0.704543
C	5.719420	-1.775297	-2.334448
H	5.492126	-2.725964	-1.858796
C	2.223649	-2.849127	-1.050069
C	-0.054194	2.749025	0.792684
C	1.314464	2.659169	1.380100
C	-0.723015	-0.294357	-2.808844
C	4.186981	-2.491967	0.343707
C	2.061831	1.482004	1.374697
C	1.870965	3.837718	1.986309
C	3.390728	1.484053	1.864249
H	3.963228	0.556889	1.811731
C	1.377926	0.248001	-0.729559
H	0.858100	1.192888	-0.941121
C	-1.108239	2.011246	1.320046
C	-0.861055	0.957131	2.350392
H	-1.801151	0.599789	2.788563
H	-0.234961	1.331177	3.175361
C	5.118592	0.523661	-2.895302
C	3.593836	-0.790873	-1.446668
C	3.994426	-3.784260	0.931488
C	-1.666358	3.854686	-0.733253
C	1.539408	0.180445	0.810987
H	2.285437	-0.601333	1.019812
C	6.326854	0.626127	-3.626520
H	6.546783	1.564443	-4.134664
C	3.773568	4.978340	3.055119
H	4.802978	4.940118	3.409638

C	1.233663	-2.364609	-2.063849
H	0.571585	-3.171772	-2.400022
H	1.741734	-1.952766	-2.946101
C	3.218092	3.813272	2.474677
C	4.851666	-4.203790	1.977557
H	4.695530	-5.190484	2.412511
C	0.721674	4.314764	-0.991937
H	1.751913	4.174027	-0.668326
C	0.445637	5.124436	-2.070787
H	1.261000	5.615815	-2.597825
C	2.922715	-4.592709	0.483987
H	2.787141	-5.580052	0.923925
C	4.808752	-0.694649	-2.207034
C	3.962782	2.616922	2.377520
H	4.992725	2.605139	2.731811
C	4.200712	1.596140	-2.843102
H	4.440161	2.521972	-3.364878
C	-0.317086	3.648787	-0.292494
C	6.035958	-2.106506	1.877681
H	6.825953	-1.458775	2.252793
C	3.020101	1.467575	-2.159210
H	2.306045	2.293414	-2.135080
C	-1.916630	4.710466	-1.832629
H	-2.949543	4.852770	-2.151280
C	-2.717932	3.170773	-0.081932
H	-3.749009	3.353015	-0.385526
C	-1.859032	-1.250752	-3.172616
H	-2.356951	-0.893708	-4.083358
H	-2.613601	-1.293599	-2.378619
H	-1.517610	-2.275233	-3.361456
C	1.693454	6.146480	2.737393
H	1.098167	7.048973	2.860096
C	5.231949	-1.675532	0.847517
H	5.395765	-0.694025	0.406198
C	1.129670	5.035990	2.153832
H	0.092840	5.073883	1.829387
C	-2.434648	2.252900	0.895888
H	-3.248253	1.721746	1.389613
C	5.849563	-3.383545	2.446667
H	6.495696	-3.715173	3.256588
C	6.880202	-1.646507	-3.060111
H	7.558299	-2.493319	-3.142570
C	-1.301323	1.052909	-2.388971
H	-0.534158	1.831660	-2.303633
H	-1.842219	1.001220	-1.432798
H	-2.017682	1.399674	-3.146331
C	1.103871	-2.796194	2.644090
H	1.533621	-3.371063	3.475385
H	1.893263	-2.669196	1.895495
H	0.301069	-3.394293	2.194977
C	-0.883809	5.330327	-2.494624
H	-1.087502	5.977574	-3.344845
C	3.031008	6.126418	3.181951
H	3.466127	7.015265	3.633816
C	1.741403	-0.716672	3.849702
H	1.965772	-1.243693	4.786248
H	1.502326	0.322522	4.108001
H	2.661816	-0.713622	3.252808
C	7.196963	-0.433170	-3.703974
H	8.121606	-0.344282	-4.270175
C	0.600509	-1.445865	3.138715
C	2.037860	-4.118021	-0.451188
H	1.187757	-4.724426	-0.765588
C	0.205182	-0.105355	-4.011713
H	0.511911	-1.057856	-4.457620
H	1.107716	0.468775	-3.766779
H	-0.336768	0.451618	-4.787068
C	-0.585703	-1.624243	4.088968
H	-1.455317	-2.069461	3.592693
H	-0.888454	-0.678283	4.553260
H	-0.291919	-2.299727	4.902224
Ni	-0.976962	-1.796769	0.259896
H	-3.331034	-0.254683	-0.066015
C	-4.415202	-0.487091	0.016001
C	-4.575232	-0.747287	1.531316
N	-4.581693	-1.679304	-0.795111
H	-3.754545	-2.242238	-0.957846
C	-5.727161	-2.355540	-1.191712
C	-7.048433	-1.646050	-1.106280
H	-7.842371	-2.392730	-1.160334
H	-7.182454	-1.041444	-0.205341
H	-7.151707	-0.964828	-1.960272
O	-5.603576	-3.478235	-1.658905
C	-5.131456	0.727513	-0.544480
C	-5.909351	1.592093	0.227332
C	-4.924770	1.028975	-1.895998
C	-6.463872	2.738570	-0.343203
H	-6.123091	1.363762	1.269484

C	-5.468593	2.174878	-2.461992
H	-4.333824	0.343392	-2.504415
C	-6.241031	3.037664	-1.683534
H	-7.080724	3.393717	0.268180
H	-5.295168	2.393381	-3.514512
H	-6.677040	3.931828	-2.124666
C	-2.382026	-3.592147	0.438819
O	-1.829715	-3.248904	-0.673072
O	-2.097994	-2.847278	1.444157
C	-3.321585	-4.726200	0.511947
H	-4.171422	-4.526275	-0.160037
H	-2.839324	-5.636270	0.139782
H	-3.684160	-4.876003	1.529940
H	-3.789460	-1.429407	1.864348
N	-5.862077	-1.429225	1.881672
O	-5.884170	-2.648445	1.745693
O	-6.804696	-0.730215	2.243505
H	-4.546470	0.183654	2.103183

IV_{S1}

P	0.151170	-1.074219	-1.496531
P	-0.571745	-0.267304	1.403049
C	1.583380	1.643303	1.344824
C	-0.359350	2.907244	0.340945
C	0.702781	5.285025	1.642061
H	-0.259007	5.324059	1.136515
C	-1.494486	2.242182	0.786347
C	3.179875	-1.961192	-0.222408
C	3.539700	-0.751908	-1.018013
C	-0.235207	-1.137540	3.030919
C	-0.439734	3.702623	-0.848608
C	2.640610	0.291052	-1.226560
C	4.847937	-0.679474	-1.608345
C	3.054733	1.449273	-1.930137
H	2.333593	2.258011	-2.061133
C	1.109802	0.312837	0.804880
H	1.785372	-0.460291	1.199440
C	2.162379	-2.813499	-0.643608
C	1.320084	-2.460215	-1.831977
H	0.719258	-3.318949	-2.155072
H	1.959353	-2.161516	-2.673673
C	2.642524	4.033947	2.433782
C	0.904028	2.841133	1.127734
C	-1.700425	3.869035	-1.509723
C	3.676807	-3.526558	1.632198
C	1.212391	0.261012	-0.738000
H	0.727580	1.178552	-1.097220
C	3.141916	5.230800	3.000942
H	4.089947	5.193619	3.536808
C	6.529079	0.573375	-2.899394
H	6.806627	1.482828	-3.431613
C	-1.419957	1.280039	1.925512
H	-2.421314	1.008036	2.280058
H	-0.860265	1.704165	2.770423
C	5.239395	0.499807	-2.321029
C	-1.765467	4.624214	-2.704392
H	-2.732245	4.738944	-3.193614
C	4.875947	-1.398864	1.526815
H	5.074133	-0.448887	1.033702
C	5.550645	-1.721638	2.681700
H	6.275286	-1.023178	3.095636
C	-2.851767	3.265581	-0.951264
H	-3.820663	3.446246	-1.420451
C	1.404382	4.053204	1.714606
C	4.317712	1.562867	-2.447685
H	4.619782	2.464107	-2.980351
C	3.333238	2.809105	2.572122
H	4.282836	2.794480	3.106267
C	3.917445	-2.281899	0.964737
C	0.609344	5.020407	-2.605051
H	1.503484	5.465405	-3.037562
C	2.807463	1.653556	2.058622
H	3.340143	0.709775	2.184150
C	4.399931	-3.834653	2.809539
H	4.208306	-4.788270	3.301398
C	2.705236	-4.409091	1.105990
H	2.546220	-5.369727	1.595904
C	-1.565350	-1.382279	3.744724
H	-1.374518	-1.918470	4.683730
H	-2.240801	-1.997960	3.139351
H	-2.079274	-0.447662	4.006947
C	7.016466	-1.655076	-2.132866
H	7.703191	-2.497520	-2.077914
C	0.703004	4.306724	-1.431964
H	1.667575	4.194995	-0.940022
C	5.774644	-1.752559	-1.549142
H	5.493333	-2.673696	-1.044127
C	1.950584	-4.045365	0.020560

H	1.178701	-4.710032	-0.361893
C	-0.634656	5.185537	-3.247807
H	-0.695329	5.755784	-4.172171
C	1.209312	6.428840	2.213202
H	0.646159	7.357651	2.145930
C	0.445442	-2.464729	2.718462
H	1.399558	-2.312306	2.201829
H	-0.175172	-3.105891	2.086077
H	0.668182	-3.001700	3.650905
C	-0.934225	0.959023	-3.007142
H	-1.490651	1.241807	-3.908840
H	-0.182749	1.739578	-2.832450
H	-1.650191	0.985127	-2.171483
C	5.316916	-2.952427	3.328955
H	5.863213	-3.200355	4.236666
C	7.405847	-0.479496	-2.806501
H	8.393347	-0.413704	-3.258496
C	0.904457	-0.291719	-4.143175
H	0.571892	0.210258	-5.061820
H	1.302865	-1.267691	-4.443921
H	1.726201	0.300814	-3.726596
C	2.445394	6.409419	2.890012
H	2.837792	7.323423	3.330849
C	-0.291694	-0.416260	-3.197880
C	-2.739439	2.459425	0.153472
H	-3.621543	2.009107	0.610705
C	0.693961	-0.316649	3.927113
H	0.326769	0.694503	4.140107
H	1.700495	-0.229243	3.502158
H	0.798449	-0.831685	4.891332
C	-1.298745	-1.387375	-3.815886
H	-2.222335	-1.436631	-3.235835
H	-0.895966	-2.405605	-3.896694
H	-1.556155	-1.049774	-4.828573
Ni	-1.488806	-1.416695	-0.073746
H	-2.451492	-1.263243	1.075174
C	-4.977532	-0.599727	-0.230490
C	-4.889767	-1.967647	-0.117374
H	-5.510116	-2.533224	0.566267
N	-3.962777	-2.747233	-0.800544
O	-4.148826	-3.966936	-0.899976
O	-2.903912	-2.205414	-1.276489
N	-4.545204	0.107710	-1.321021
H	-4.228753	1.060937	-1.152393
C	-4.531606	-0.189699	-2.704578
C	-5.161575	-1.459566	-3.186350
H	-4.402114	-2.243876	-3.287886
H	-5.950328	-1.837880	-2.529591
H	-5.568640	-1.268955	-4.181592
O	-4.067280	0.653954	-3.444095
C	-5.526703	0.185859	0.871560
C	-5.243873	-0.194203	2.194104
C	-6.251135	1.365107	0.631882
C	-5.675110	0.593709	3.253363
H	-4.639006	-1.084443	2.369963
C	-6.689784	2.141724	1.695229
H	-6.483764	1.652762	-0.393029
C	-6.397975	1.760171	3.005393
H	-5.435972	0.305934	4.275048
H	-7.261909	3.046850	1.505208
H	-6.732657	2.377300	3.836397
C	-1.871431	-4.549185	0.542403
O	-2.632848	-4.171934	1.592712
H	-3.184516	-4.916858	1.882788
O	-1.143894	-3.726624	0.018118
C	-1.954556	-5.985200	0.131432
H	-1.638184	-6.641196	0.951346
H	-2.983474	-6.247573	-0.136372
H	-1.314836	-6.163277	-0.733533

V_{S1}

P	-0.025381	-1.178580	-1.474235
P	-0.741618	-0.275107	1.394644
C	1.414566	1.606387	1.279740
C	-0.507189	2.828055	0.185854
C	0.500554	5.245101	1.466066
H	-0.451195	5.262875	0.940017
C	-1.662089	2.179953	0.603022
C	2.883514	-2.176612	-0.096028
C	3.340045	-1.025426	-0.927554
C	-0.452332	-1.062045	3.066614
C	-0.532244	3.572866	-1.038334
C	2.516803	0.063645	-1.203778
C	4.673986	-1.048548	-1.461051
C	3.025797	1.171780	-1.924699
H	2.362686	2.020654	-2.103755
C	0.944773	0.258851	0.781955
H	1.603912	-0.506901	1.217180

C	1.836580	-2.993275	-0.513453
C	1.056777	-2.640776	-1.741340
H	0.412773	-3.471598	-2.054744
H	1.733108	-2.407963	-2.575241
C	2.437496	4.029667	2.321151
C	0.728711	2.791830	1.019697
C	-1.761097	3.707408	-1.765046
C	3.210524	-3.663497	1.856972
C	1.076398	0.135760	-0.756943
H	0.647992	1.058106	-1.175140
C	2.916586	5.243720	2.868481
H	3.855625	5.228071	3.420870
C	6.482544	0.064657	-2.706530
H	6.836695	0.938645	-3.252332
C	-1.638825	1.278060	1.793875
H	-2.654419	1.003078	2.108673
H	-1.132312	1.743801	2.652598
C	5.164427	0.082670	-2.190826
C	-1.770884	4.420410	-2.987556
H	-2.714204	4.516926	-3.524268
C	4.524506	-1.605719	1.698531
H	4.801316	-0.701537	1.158953
C	5.118357	-1.891107	2.906032
H	5.856499	-1.206585	3.319398
C	-2.932038	3.099416	-1.255493
H	-3.871103	3.219587	-1.796060
C	1.210142	4.021825	1.582785
C	4.313455	1.192924	-2.390861
H	4.692388	2.058034	-2.934016
C	3.139597	2.815874	2.495643
H	4.082834	2.824054	3.040885
C	3.549982	-2.471636	1.137569
C	0.598607	4.816315	-2.797746
H	1.512931	5.240183	-3.208366
C	2.631095	1.642723	2.004941
H	3.168865	0.706293	2.160388
C	3.852514	-3.934453	3.089666
H	3.584519	-4.845023	3.625120
C	2.212311	-4.520098	1.334937
H	1.969559	-5.436395	1.872325
C	-1.756019	-1.037398	3.863073
H	-1.622924	-1.618218	4.784595
H	-2.585966	-1.488140	3.304540
H	-2.049820	-0.022365	4.157252
C	6.806577	-2.158581	-1.843312
H	7.442191	-3.033986	-1.726021
C	0.638518	4.147353	-1.595569
H	1.582117	4.049000	-1.061385
C	5.534773	-2.168082	-1.320296
H	5.177985	-3.053014	-0.798357
C	1.517877	-4.170912	0.204074
H	0.714723	-4.807735	-0.167938
C	-0.616137	4.963064	-3.498534
H	-0.635167	5.502614	-4.442939
C	0.987009	6.406054	2.020088
H	0.418326	7.328549	1.921000
C	-0.010137	-2.497305	2.818776
H	0.896902	-2.524104	2.207324
H	-0.784170	-3.077082	2.297899
H	0.220591	-2.998990	3.768522
C	-1.157164	0.737339	-3.074645
H	-1.670429	0.989847	-4.011173
H	-0.443783	1.544862	-2.869040
H	-1.917990	0.746612	-2.282750
C	4.783127	-3.066606	3.609669
H	5.263266	-3.284112	4.561478
C	7.293039	-1.030351	-2.534464
H	8.303596	-1.034702	-2.937548
C	0.754558	-0.456807	-4.128842
H	0.405931	-0.088751	-5.103134
H	1.272535	-1.404544	-4.314921
H	1.487238	0.264553	-3.750863
C	2.210856	6.412468	2.719457
H	2.587228	7.339525	3.146461
C	-0.451808	-0.610023	-3.203302
C	-2.871849	2.342624	-0.112186
H	-3.778183	1.902241	0.309245
C	0.638946	-0.326766	3.847307
H	0.468417	0.755176	3.920458
H	1.632834	-0.485110	3.410483
H	0.673932	-0.723748	4.870023
C	-1.394072	-1.672487	-3.771575
H	-2.213902	-1.890811	-3.080951
H	-0.872558	-2.617328	-3.969637
H	-1.829777	-1.323792	-4.716656
Ni	-1.636367	-1.515321	-0.028811
H	-2.439548	-1.668084	1.232144
C	-4.624213	-1.455924	-0.046428

C	-4.547147	-2.827339	-0.001605
H	-5.227049	-3.438297	0.578886
N	-3.559525	-3.574977	-0.649212
O	-3.759123	-4.754379	-0.915196
O	-2.413596	-3.037444	-0.908871
N	-4.131827	-0.724979	-1.116848
H	-3.926111	0.255172	-0.920970
C	-4.438402	-0.873942	-2.501841
C	-4.966164	-2.187112	-2.985995
H	-4.174918	-2.945376	-3.021651
H	-5.765291	-2.583357	-2.350988
H	-5.342372	-2.041243	-3.999718
O	-4.260453	0.095932	-3.207960
C	-5.307664	-0.712534	1.007587
C	-5.285534	-1.197056	2.326177
C	-5.950427	0.507871	0.737784
C	-5.883175	-0.475728	3.349238
H	-4.758187	-2.126409	2.539019
C	-6.547922	1.226337	1.764972
H	-6.004874	0.877120	-0.286903
C	-6.511301	0.738775	3.070890
H	-5.848257	-0.852150	4.369191
H	-7.051789	2.165052	1.546583
H	-6.975711	1.306118	3.874404

$TSII_{S1}$

P	0.116157	0.928158	-1.634591
P	0.911406	0.130835	1.229505
C	-1.494053	-1.407153	1.412915
C	0.143210	-2.994785	0.320248
C	-1.117862	-5.116944	1.863459
H	-0.210854	-5.319762	1.298655
C	1.416537	-2.510084	0.600158
C	-2.495184	2.448139	-0.183333
C	-3.179146	1.316949	-0.876798
C	0.838854	1.043477	2.863035
C	-0.046509	-3.831870	-0.826349
C	-2.543035	0.100961	-1.123892
C	-4.526510	1.506442	-1.336278
C	-3.250181	-0.956821	-1.746996
H	-2.730987	-1.904179	-1.907005
C	-0.869634	-0.188206	0.772638
H	-1.374769	0.698892	1.185315
C	-1.380720	3.058168	-0.752196
C	-0.765609	2.492778	-1.994216
H	-0.037998	3.185126	-2.432723
H	-1.530672	2.274883	-2.751733
C	-2.801625	-3.559082	2.699536
C	-1.006696	-2.698275	1.221690
C	1.086858	-4.232319	-1.607532
C	-2.441471	4.140074	1.622525
C	-1.101852	-0.161742	-0.757595
H	-0.843098	-1.163274	-1.128510
C	-3.425631	-4.641083	3.364621
H	-4.320585	-4.440371	3.952604
C	-6.547705	0.610869	-2.419041
H	-7.057806	-0.227824	-2.891632
C	1.619086	-1.507624	1.691635
H	2.686370	-1.361261	1.911361
H	1.133861	-1.818061	2.629310
C	-5.219770	0.423112	-1.967205
C	0.889298	-5.029474	-2.761193
H	1.762122	-5.326974	-3.341205
C	-4.053305	2.305118	1.764374
H	-4.501367	1.406563	1.342841
C	-4.507771	2.796426	2.967062
H	-5.306485	2.278581	3.494304
C	2.374460	-3.790635	-1.230115
H	3.238876	-4.097094	-1.816411
C	-1.629570	-3.794225	1.910402
C	-4.553120	-0.810053	-2.143392
H	-5.085169	-1.635913	-2.614036
C	-3.307211	-2.243612	2.801008
H	-4.211329	-2.067774	3.382680
C	-3.008283	2.952510	1.055842
C	-1.493242	-4.994846	-2.399498
H	-2.492403	-5.286785	-2.717141
C	-2.659886	-1.202177	2.191776
H	-3.046605	-0.186680	2.288375
C	-2.944142	4.627356	2.853005
H	-2.506606	5.534376	3.269611
C	-1.364834	4.774976	0.958993
H	-0.945464	5.685491	1.385986
C	2.191476	0.910158	3.557609
H	2.199999	1.538797	4.457171
H	3.019102	1.244940	2.921345
H	2.401155	-0.117651	3.878078
C	-6.489711	2.902670	-1.684574

H	-6.980723	3.869274	-1.592136
C	-1.334318	-4.240018	-1.260071
H	-2.206761	-3.941856	-0.681448
C	-5.202423	2.749037	-1.225773
H	-4.689153	3.598624	-0.782103
C	-0.823234	4.223664	-0.174527
H	0.036756	4.685696	-0.659382
C	-0.373427	-5.400790	-3.155334
H	-0.513411	-6.003721	-4.049894
C	-1.741398	-6.145478	2.530852
H	-1.323850	-7.149063	2.480921
C	0.535850	2.504453	2.558486
H	-0.387272	2.600458	1.976835
H	1.339933	2.980549	1.981651
H	0.396719	3.068830	3.490603
C	0.929453	-1.274560	-3.067602
H	1.395635	-1.670381	-3.979433
H	0.097597	-1.943785	-2.816429
H	1.682323	-1.345796	-2.270970
C	-3.953506	3.971000	3.516377
H	-4.326173	4.354527	4.463689
C	-7.176209	1.824206	-2.279041
H	-8.195544	1.959021	-2.634678
C	-0.787050	0.147862	-4.198197
H	-0.554944	-0.409942	-5.114845
H	-1.092258	1.154547	-4.505006
H	-1.645901	-0.343080	-3.725348
C	-2.912027	-5.912130	3.280821
H	-3.399063	-6.736118	3.797717
C	0.453753	0.156344	-3.303377
C	2.525033	-2.936238	-0.167417
H	3.524604	-2.607445	0.124938
C	-0.259520	0.485129	3.770343
H	-0.206413	-0.602808	3.903520
H	-1.262254	0.731797	3.402060
H	-0.162620	0.942118	4.763564
C	1.559017	0.978533	-3.968518
H	2.481399	0.961539	-3.379549
H	1.279286	2.029958	-4.106659
H	1.781900	0.556355	-4.956600
Ni	1.850078	1.219684	-0.341540
H	2.784342	1.506023	0.832655
C	4.234669	1.215811	-0.083564
C	4.505323	2.499150	-0.612881
H	5.400324	3.061831	-0.383321
N	3.606376	3.146287	-1.405847
O	3.895189	4.131533	-2.081220
O	2.359124	2.718541	-1.405632
N	3.820821	0.184322	-0.983949
H	3.504579	-0.673791	-0.531075
C	4.441673	-0.186031	-2.213653
C	5.257004	0.824021	-2.958205
H	4.668773	1.692304	-3.275670
H	6.079332	1.208056	-2.344092
H	5.666186	0.332499	-3.842447
O	4.258260	-1.325298	-2.594244
C	5.049609	0.785886	1.073728
C	5.341084	1.716629	2.081833
C	5.541526	-0.520986	1.190564
C	6.104737	1.350960	3.180851
H	4.933575	2.725261	2.004335
C	6.300827	-0.887068	2.297965
H	5.372839	-1.246582	0.394749
C	6.580205	0.044328	3.294601
H	6.321211	2.081708	3.956749
H	6.686840	-1.901038	2.374131
H	7.173303	-0.245477	4.158933

VI_{S1}

P	-0.165581	-0.911999	-1.622690
P	-0.933736	0.034183	1.176098
C	1.641821	1.218458	1.479545
C	0.293853	3.033689	0.351671
C	1.778347	4.937840	1.986278
H	0.950765	5.278600	1.368897
C	-1.040175	2.714524	0.586940
C	2.313042	-2.625881	-0.192174
C	3.075372	-1.558480	-0.902057
C	-1.113563	-0.953572	2.763085
C	0.623141	3.852379	-0.776699
C	2.536836	-0.293932	-1.132828
C	4.396011	-1.853722	-1.381580
C	3.310877	0.705144	-1.772253
H	2.866214	1.690458	-1.923322
C	0.885309	0.107793	0.786030
H	1.253512	-0.848837	1.184992
C	1.149788	-3.155948	-0.743110
C	0.564003	-2.551359	-1.982370

H	-0.235330	-3.174388	-2.399214
H	1.330104	-2.405585	-2.756028
C	3.154167	3.139360	2.899633
C	1.357464	2.569807	1.287411
C	-0.427738	4.388498	-1.591965
C	2.117335	-4.244089	1.670061
C	1.128454	0.082301	-0.742683
H	0.944553	1.103177	-1.101754
C	3.878958	4.109718	3.632100
H	4.690919	3.773271	4.275995
C	6.465456	-1.116139	-2.491371
H	7.033161	-0.319404	-2.970525
C	-1.408054	1.743769	1.663296
H	-2.488893	1.754611	1.861315
H	-0.901291	1.969109	2.614164
C	5.162351	-0.826010	-2.022322
C	-0.097212	5.165579	-2.728911
H	-0.908570	5.566866	-3.335316
C	3.897034	-2.567135	1.738033
H	4.424849	-1.730076	1.284668
C	4.307770	-3.052021	2.958275
H	5.155436	-2.592750	3.463284
C	-1.771556	4.102109	-1.263659
H	-2.573512	4.507516	-1.878542
C	2.088559	3.553939	2.036501
C	4.590947	0.455787	-2.189968
H	5.178434	1.237558	-2.669992
C	3.450365	1.762601	3.010876
H	4.272045	1.448348	3.653500
C	2.789633	-3.137473	1.057688
C	2.250610	4.864396	-2.277033
H	3.287729	5.049206	-2.550406
C	2.704410	0.835214	2.333831
H	2.928251	-0.226584	2.440540
C	2.575172	-4.727025	2.920443
H	2.055816	-5.571661	3.372330
C	0.995659	-4.812104	1.020484
H	0.499505	-5.668120	1.476949
C	-2.447092	-0.584380	3.416073
H	-2.631326	-1.257252	4.262946
H	-3.302236	-0.692165	2.734633
H	-2.453680	0.439145	3.808398
C	6.239783	-3.397778	-1.754782
H	6.656995	-4.398872	-1.667654
C	1.964511	4.119879	-1.155348
H	2.776023	3.721490	-0.548669
C	4.974819	-3.145385	-1.278184
H	4.402751	-3.952218	-0.826074
C	0.504920	-4.260090	-0.136481
H	-0.391181	-4.663461	-0.607607
C	1.213228	5.397138	-3.070511
H	1.454638	5.989027	-3.950616
C	2.494331	5.854698	2.719768
H	2.229796	6.908744	2.667437
C	-1.098167	-2.434600	2.400402
H	-0.199704	-2.697475	1.832068
H	-1.967154	-2.726337	1.791595
H	-1.105805	-3.048139	3.311418
C	-0.803111	1.372257	-3.036362
H	-1.208914	1.817605	-3.954293
H	0.096687	1.944419	-2.777069
H	-1.552996	1.528898	-2.248943
C	3.644710	-4.143206	3.556594
H	3.982996	-4.521722	4.518719
C	6.999007	-2.375086	-2.359101
H	8.000334	-2.588160	-2.727108
C	0.690996	-0.256814	-4.217370
H	0.502971	0.340112	-5.119109
H	0.838996	-1.292451	-4.542823
H	1.627504	0.105372	-3.775116
C	3.561959	5.442891	3.543081
H	4.123547	6.180124	4.112819
C	-0.507172	-0.106064	-3.276292
C	-2.062903	3.272986	-0.211274
H	-3.104748	3.053685	0.022886
C	0.034176	-0.662211	3.731237
H	0.181710	0.408426	3.920547
H	0.986106	-1.078563	3.378088
H	-0.185769	-1.139405	4.695226
C	-1.738644	-0.782313	-3.884941
H	-2.632359	-0.588675	-3.280172
H	-1.634352	-1.869853	-3.975571
H	-1.913190	-0.371664	-4.887256
Ni	-1.916931	-1.005917	-0.433976
H	-3.388209	-1.220925	0.610238
C	-4.306838	-0.938484	-0.029584
C	-4.672387	-2.103059	-0.848799
H	-5.697019	-2.425858	-0.974572

N	-3.775613	-2.751168	-1.594127
O	-4.035682	-3.615493	-2.430692
O	-2.454293	-2.489192	-1.395781
N	-3.841429	0.230509	-0.819130
H	-3.468175	0.985544	-0.243113
C	-4.490275	0.828144	-1.923718
C	-5.431606	0.013822	-2.759912
H	-4.962520	-0.882237	-3.180673
H	-6.290815	-0.324383	-2.168706
H	-5.788894	0.649359	-3.572107
O	-4.230306	1.994150	-2.165063
C	-5.365631	-0.600895	0.997780
C	-5.808100	-1.619097	1.849405
C	-5.878831	0.688925	1.145487
C	-6.757536	-1.354147	2.828026
H	-5.398327	-2.624131	1.737025
C	-6.835754	0.950505	2.124602
H	-5.556025	1.493765	0.484896
C	-7.274017	-0.066386	2.966575
H	-7.097625	-2.153643	3.482595
H	-7.241428	1.954995	2.223644
H	-8.019855	0.141783	3.730419

VII$_{S1}$

P	-0.281749	-0.022620	1.590820
P	-0.026737	-1.057052	-1.289731
C	2.634802	-0.045885	-1.390161
C	2.895365	-2.302685	-0.283279
C	5.388212	-2.570565	-1.760975
H	4.987474	-3.417159	-1.208455
C	1.743122	-3.020371	-0.583643
C	0.049238	3.030374	0.223911
C	1.358441	2.895972	0.924655
C	-0.733456	-0.423660	-2.904058
C	3.647632	-2.646841	0.886412
C	1.976399	1.663896	1.131444
C	2.008780	4.091779	1.386830
C	3.284323	1.611942	1.672582
H	3.761694	0.637080	1.777044
C	1.264456	0.177514	-0.788331
H	0.872773	1.124017	-1.191922
C	-1.115542	2.481751	0.750651
C	-1.059527	1.596454	1.956393
H	-2.060837	1.396477	2.361080
H	-0.465750	2.048780	2.765593
C	5.175744	-0.289410	-2.607316
C	3.371601	-1.209037	-1.176377
C	3.265883	-3.789156	1.660808
C	-1.309276	4.065958	-1.572803
C	1.335497	0.349253	0.748459
H	1.981558	-0.459780	1.121419
C	6.436408	-0.439917	-3.233953
H	6.831406	0.395256	-3.811454
C	3.970418	5.188265	2.392091
H	4.974055	5.103419	2.807371
C	0.874390	-2.592774	-1.725588
H	0.121050	-3.350937	-1.963120
H	1.461607	-2.397714	-2.634535
C	3.324900	4.010217	1.946634
C	3.997260	-4.108340	2.830478
H	3.696791	-4.981268	3.409099
C	1.128836	4.236239	-1.681637
H	2.110012	4.030805	-1.257083
C	1.027100	4.922707	-2.869756
H	1.929570	5.249301	-3.382744
C	2.135664	-4.542770	1.263911
H	1.852673	-5.417338	1.848337
C	4.639856	-1.367343	-1.830986
C	3.949645	2.746970	2.049504
H	4.961238	2.687965	2.449197
C	4.426823	0.902237	-2.732981
H	4.843577	1.730652	-3.304545
C	-0.027667	3.784326	-0.994371
C	5.427586	-2.199070	2.484027
H	6.264688	-1.584998	2.810163
C	3.188181	1.008629	-2.157349
H	2.609093	1.926937	-2.269944
C	-1.377895	4.795369	-2.784265
H	-2.359800	5.006240	-3.207083
C	-2.473068	3.569217	-0.940740
H	-3.450604	3.797468	-1.365341
C	-1.531504	-1.536465	-3.586541
H	-1.967602	-1.144136	-4.513683
H	-2.364707	-1.927101	-2.991799
H	-0.894429	-2.385031	-3.865318
C	2.036088	6.491008	1.795778
H	1.532054	7.454551	1.756517
C	4.750075	-1.872672	1.331952

H	5.061723	-1.008247	0.748519
C	1.387739	5.366800	1.340764
H	0.375618	5.454827	0.952896
C	-2.372399	2.769066	0.168509
H	-3.273336	2.374754	0.638035
C	5.052573	-3.328603	3.240248
H	5.600206	-3.580992	4.145651
C	6.603731	-2.689774	-2.392737
H	7.153581	-3.626453	-2.328258
C	-1.607478	0.786635	-2.592579
H	-1.031512	1.572768	-2.093273
H	-2.466444	0.560210	-1.948796
H	-2.000441	1.216062	-3.523730
C	0.446470	-2.223495	3.081455
H	0.863415	-2.647457	4.004981
H	1.189102	-2.379034	2.290612
H	-0.458309	-2.782834	2.823327
C	-0.236437	5.213568	-3.424612
H	-0.303109	5.766176	-4.359315
C	3.343442	6.407757	2.316629
H	3.846755	7.306810	2.665955
C	1.442129	-0.064105	3.800734
H	1.601865	-0.409986	4.830029
H	1.381658	1.031164	3.830714
H	2.335436	-0.345563	3.230845
C	7.142141	-1.613125	-3.126452
H	8.109098	-1.718641	-3.613537
C	0.168658	-0.736518	3.273321
C	1.372320	-4.142053	0.195974
H	0.474036	-4.696421	-0.077704
C	0.394531	0.029627	-3.836831
H	1.160535	-0.736724	-4.005359
H	0.893513	0.933353	-3.469462
H	-0.039553	0.276170	-4.814464
C	-0.951530	-0.503831	4.289771
H	-1.891440	-0.980417	4.005452
H	-1.125347	0.563181	4.475681
H	-0.637509	-0.942730	5.245320
Ni	-1.406505	-1.395897	0.354911
H	-3.306849	-0.156945	0.333507
C	-4.352038	-0.502079	0.187342
C	-4.618053	-1.529138	1.251258
H	-5.621452	-1.638968	1.654473
N	-3.689577	-1.862464	2.176043
O	-3.960703	-2.382892	3.259804
O	-2.380948	-1.720324	1.928610
N	-4.333396	-1.036457	-1.182363
H	-3.407576	-1.135629	-1.580120
C	-5.216928	-1.910626	-1.773484
C	-6.598436	-2.000759	-1.191394
H	-6.652175	-2.875910	-0.531507
H	-6.891428	-1.116001	-0.617029
H	-7.314327	-2.166176	-1.999887
O	-4.848681	-2.580383	-2.733819
C	-5.236052	0.724501	0.336568
C	-5.562470	1.190340	1.615094
C	-5.637782	1.467203	-0.776863
C	-6.277257	2.373287	1.776508
H	-5.251894	0.622976	2.493345
C	-6.357979	2.647640	-0.614020
H	-5.380336	1.112416	-1.773722
C	-6.677250	3.106169	0.661631
H	-6.526233	2.720109	2.777419
H	-6.672517	3.210897	-1.490895
H	-7.240133	4.028727	0.786948
C	-2.898893	-3.878423	-0.766327
O	-2.074890	-2.950111	-0.647815
O	-3.994426	-4.000160	-0.066221
C	-2.715003	-4.944607	-1.784644
H	-3.320715	-4.662479	-2.655760
H	-1.670662	-5.025034	-2.092461
H	-3.087694	-5.905320	-1.422346
H	-4.190941	-3.163986	0.467417

TSIII$_{S1}$

P	-0.264028	-0.009168	1.596017
P	-0.018000	-1.065379	-1.274345
C	2.645675	-0.063798	-1.385738
C	2.895373	-2.314054	-0.261211
C	5.387914	-2.603418	-1.733971
H	4.983095	-3.444025	-1.175411
C	1.742279	-3.032055	-0.558165
C	0.051103	3.029293	0.201908
C	1.365092	2.906265	0.896459
C	-0.723062	-0.437399	-2.891197
C	3.646246	-2.652993	0.910880
C	1.986983	1.678363	1.117537
C	2.014401	4.109517	1.340528

C	3.295196	1.635908	1.658651
H	3.774387	0.663288	1.775869
C	1.276817	0.170357	-0.785496
H	0.888223	1.113765	-1.198909
C	-1.108472	2.483079	0.742613
C	-1.041245	1.610531	1.956775
H	-2.039569	1.412603	2.369735
H	-0.442875	2.071952	2.757334
C	5.186164	-0.328159	-2.598534
C	3.376804	-1.228651	-1.161953
C	3.264452	-3.792903	1.688781
C	-1.325039	4.047448	-1.591302
C	1.350023	0.357828	0.748681
H	1.999108	-0.445828	1.127682
C	6.446712	-0.489132	-3.222800
H	6.845852	0.339687	-3.806571
C	3.977595	5.223691	2.323199
H	4.982784	5.146505	2.736210
C	0.872342	-2.608507	-1.700485
H	0.111353	-3.361979	-1.928265
H	1.456272	-2.422825	-2.613589
C	3.332257	4.038152	1.897649
C	3.995624	-4.107767	2.859749
H	3.695904	-4.979360	3.440759
C	1.111859	4.219258	-1.723966
H	2.096967	4.018722	-1.306167
C	0.998410	4.895952	-2.916625
H	1.895679	5.218811	-3.440889
C	2.134765	-4.548471	1.293802
H	1.852758	-5.422033	1.880208
C	4.644943	-1.397575	-1.814146
C	3.959059	2.777529	2.018228
H	4.971411	2.726076	2.417028
C	4.442895	0.865897	-2.734276
H	4.863985	1.687900	-3.311845
C	-0.037755	3.772170	-1.022286
C	5.424452	-2.198081	2.508404
H	6.260772	-1.582259	2.833257
C	3.204228	0.982403	-2.160546
H	2.629279	1.902391	-2.280513
C	-1.405616	4.767568	-2.807493
H	-2.391549	4.974002	-3.223059
C	-2.482565	3.552734	-0.946078
H	-3.463905	3.775802	-1.364707
C	-1.512496	-1.552669	-3.579023
H	-1.962441	-1.157105	-4.498048
H	-2.332109	-1.961957	-2.979695
H	-0.866116	-2.389599	-3.870899
C	2.039304	6.514606	1.714344
H	1.533605	7.476668	1.662698
C	4.747426	-1.876007	1.354750
H	5.058808	-1.013452	0.768195
C	1.391001	5.382771	1.278648
H	0.377241	5.463583	0.893754
C	-2.370972	2.761348	0.168324
H	-3.266520	2.367156	0.648569
C	5.050089	-3.325849	3.267637
H	5.597675	-3.575220	4.173912
C	6.603564	-2.732901	-2.363558
H	7.149110	-3.671513	-2.291227
C	-1.599072	0.771547	-2.581397
H	-1.022541	1.558355	-2.084118
H	-2.455096	0.546656	-1.933586
H	-1.994854	1.198936	-3.512195
C	0.452100	-2.208121	3.090288
H	0.859898	-2.637330	4.015438
H	1.196328	-2.371655	2.302683
H	-0.456178	-2.760010	2.827034
C	-0.270533	5.181574	-3.461780
H	-0.346593	5.726363	-4.400342
C	3.348712	6.441117	2.231345
H	3.852141	7.345952	2.565164
C	1.471149	-0.056234	3.800078
H	1.632940	-0.401168	4.829386
H	1.419237	1.039467	3.827651
H	2.359803	-0.345753	3.226777
C	7.147306	-1.664433	-3.105227
H	8.114210	-1.777889	-3.590620
C	0.189453	-0.718066	3.279594
C	1.370940	-4.151257	0.224824
H	0.472486	-4.705828	-0.047678
C	0.407671	0.018799	-3.820064
H	1.182611	-0.741326	-3.975916
H	0.895038	0.930867	-3.457954
H	-0.022615	0.251991	-4.802570
C	-0.924273	-0.469730	4.299588
H	-1.874877	-0.926023	4.016578
H	-1.077890	0.599579	4.489543

H	-0.617184	-0.918235	5.252900
Ni	-1.401248	-1.388224	0.370099
H	-3.300659	-0.221660	0.261731
C	-4.350856	-0.554767	0.121034
C	-4.595099	-1.648815	1.144826
H	-5.602757	-1.721805	1.552387
N	-3.691655	-1.813103	2.173643
O	-4.016994	-2.199759	3.291608
O	-2.399592	-1.677073	1.952642
N	-4.371265	-1.021232	-1.266486
H	-3.455847	-1.120778	-1.687167
C	-5.272629	-1.876171	-1.866996
C	-6.639978	-1.981432	-1.254169
H	-6.678334	-2.873081	-0.616194
H	-6.919614	-1.110631	-0.652161
H	-7.374778	-2.126617	-2.049365
O	-4.929566	-2.508344	-2.859037
C	-5.221051	0.666134	0.362698
C	-5.513597	1.062614	1.672916
C	-5.645858	1.470821	-0.698080
C	-6.216147	2.238970	1.916755
H	-5.193097	0.446820	2.514420
C	-6.353464	2.644402	-0.452348
H	-5.416529	1.168945	-1.718822
C	-6.637966	3.034226	0.854074
H	-6.439754	2.530132	2.940963
H	-6.686850	3.255992	-1.289030
H	-7.192017	3.951026	1.043921
C	-2.940844	-3.815486	-0.769066
O	-2.070514	-2.914573	-0.633415
O	-4.042482	-3.897148	-0.111101
C	-2.743507	-4.873620	-1.800707
H	-3.339965	-4.585051	-2.675990
H	-1.695856	-4.957881	-2.097868
H	-3.123596	-5.836242	-1.450874
H	-4.275100	-2.965987	0.455642

VIII$_{S1}$

P	-0.076094	-0.139009	-1.829672
P	0.321269	-0.804927	1.104522
C	-2.402026	-0.188355	1.628366
C	-2.486653	-2.587640	0.845819
C	-4.605221	-2.989210	2.815349
H	-4.198356	-3.839164	2.272705
C	-1.191265	-3.073500	0.985401
C	-0.732287	2.985892	-0.779305
C	-2.092695	2.545748	-1.205706
C	1.243207	0.139983	2.420909
C	-3.364618	-3.207718	-0.103199
C	-2.499908	1.213602	-1.175275
C	-3.013997	3.545691	-1.672512
C	-3.838326	0.872409	-1.488575
H	-4.136489	-0.174463	-1.413500
C	-1.226335	0.143169	0.737568
H	-0.929982	1.181423	0.951829
C	0.407790	2.578420	-1.466839
C	0.323169	1.516782	-2.518192
H	1.266575	1.421309	-3.065446
H	-0.470560	1.739007	-3.247602
C	-4.582142	-0.612813	3.376432
C	-2.971633	-1.459602	1.691727
C	-2.931534	-4.379557	-0.805840
C	0.687344	4.477741	0.600042
C	-1.585183	0.083589	-0.767474
H	-2.127854	-0.861006	-0.927071
C	-5.653113	-0.847084	4.271715
H	-6.047324	-0.004998	4.839587
C	-5.272253	4.160317	-2.437044
H	-6.293610	3.856760	-2.664385
C	-0.214321	-2.373897	1.880247
H	0.679593	-2.984645	2.049565
H	-0.653728	-2.133577	2.859359
C	-4.361051	3.174282	-1.989805
C	-3.795897	-4.979132	-1.753278
H	-3.453740	-5.871866	-2.276124
C	-1.678483	4.237075	1.169130
H	-2.660604	3.812238	0.967863
C	-1.505780	5.082509	2.241093
H	-2.351755	5.317084	2.884227
C	-1.629470	-4.881382	-0.571289
H	-1.307544	-5.777893	-1.100256
C	-4.050181	-1.699681	2.609095
C	-4.749974	1.821985	-1.863063
H	-5.779540	1.544819	-2.085925
C	-4.015149	0.672789	3.230287
H	-4.431562	1.502215	3.800692
C	-0.593922	3.901369	0.317426
C	-5.455593	-3.279995	-1.346269

H	-6.432917	-2.854410	-1.565243
C	-2.947956	0.869849	2.395223
H	-2.505847	1.862504	2.297684
C	0.825548	5.359239	1.698451
H	1.806314	5.791416	1.895217
C	1.790815	4.132032	-0.214635
H	2.756379	4.600440	-0.024475
C	2.328926	-0.774365	2.989839
H	2.973539	-0.195176	3.663150
H	2.969517	-1.200897	2.207124
H	1.909619	-1.605568	3.569538
C	-3.545027	5.831923	-2.320073
H	-3.226547	6.861598	-2.469639
C	-4.648148	-2.683617	-0.405268
H	-4.993223	-1.794169	0.118774
C	-2.639477	4.900321	-1.868341
H	-1.613984	5.205206	-1.673928
C	1.657799	3.187343	-1.198473
H	2.512604	2.904294	-1.809532
C	-5.031604	-4.441917	-2.023342
H	-5.682828	-4.907797	-2.759667
C	-5.638362	-3.185911	3.701347
H	-6.041223	-4.186669	3.843124
C	1.853195	1.369166	1.757122
H	1.081836	1.987130	1.282808
H	2.589243	1.112366	0.986143
H	2.352810	1.995371	2.509286
C	-0.753570	-2.583777	-2.890819
H	-1.175078	-3.180296	-3.711248
H	-1.437690	-2.674581	-2.039031
H	0.205753	-3.029014	-2.603117
C	-0.245194	5.655569	2.507496
H	-0.124285	6.329741	3.352752
C	-4.877987	5.465865	-2.596454
H	-5.585301	6.214177	-2.947395
C	-1.948543	-0.638668	-3.868547
H	-2.143287	-1.143140	-4.824207
H	-1.979973	0.441433	-4.058205
H	-2.778878	-0.888576	-3.196854
C	-6.177662	-2.106438	4.430392
H	-6.998390	-2.275974	5.124026
C	-0.605921	-1.129078	-3.323817
C	-0.770993	-4.220375	0.269256
H	0.244221	-4.587813	0.423196
C	0.292881	0.587234	3.534084
H	-0.297311	-0.233936	3.959923
H	-0.404114	1.361590	3.190388
H	0.884570	1.024253	4.349153
C	0.484173	-0.980900	-4.388246
H	1.481757	-1.222367	-4.003638
H	0.510497	0.029515	-4.812832
H	0.274422	-1.672065	-5.214377
Ni	1.396057	-1.242380	-0.684194
H	3.827131	-0.577078	0.339619
C	4.913500	-0.525504	0.179886
C	5.081780	-0.402193	-1.336183
H	5.974039	0.144271	-1.657154
N	3.926779	0.307640	-1.995928
O	4.057090	0.635601	-3.165296
O	2.895268	0.485269	-1.328580
N	5.386329	-1.810079	0.671175
H	4.654639	-2.466373	0.923874
C	6.591859	-2.427129	0.404818
C	7.730739	-1.550597	-0.047144
H	7.924055	-1.718363	-1.113480
H	7.567889	-0.481120	0.121673
H	8.635504	-1.858956	0.482998
O	6.701701	-3.636378	0.545708
C	5.401930	0.682390	0.957099
C	5.386796	1.959230	0.386838
C	5.766562	0.550708	2.299913
C	5.725658	3.078436	1.142657
H	5.108210	2.101442	-0.658287
C	6.104788	1.669026	3.055031
H	5.791221	-0.442237	2.746505
C	6.081995	2.937678	2.480525
H	5.718147	4.063157	0.678533
H	6.394519	1.546738	4.097021
H	6.350758	3.811324	3.070230
C	2.881065	-2.966752	-1.108111
O	2.515529	-2.647011	0.083632
O	2.453797	-2.224401	-2.052131
C	3.750433	-4.144325	-1.353508
H	4.625989	-4.146666	-0.689559
H	3.189057	-5.059233	-1.128824
H	4.070519	-4.179819	-2.397145
H	5.091562	-1.384304	-1.822902

IV_{R2}

P	-0.322946	0.591718	1.367967
P	-0.201356	-0.342741	-1.555793
C	2.601611	-0.853518	-1.218522
C	1.507243	-2.964970	-0.363722
C	3.710323	-4.421472	-1.588511
H	2.858773	-4.960683	-1.180528
C	0.210964	-2.984877	-0.866416
C	1.765742	3.048090	0.347828
C	2.680372	2.242578	1.209375
C	-0.145558	0.554358	-3.198805
C	1.805781	-3.696782	0.831824
C	2.506450	0.871553	1.394392
C	3.749031	2.912445	1.897537
C	3.425435	0.142460	2.188579
H	3.276603	-0.933979	2.294722
C	1.456778	0.023345	-0.764910
H	1.663617	1.043123	-1.122790
C	0.416033	3.165738	0.666950
C	-0.158723	2.374571	1.798636
H	-1.153821	2.742801	2.079911
H	0.489017	2.446686	2.682384
C	4.818214	-2.327475	-2.176022
C	2.601703	-2.237686	-1.066960
C	0.803960	-4.537217	1.414785
C	1.415954	4.632622	-1.524972
C	1.368034	0.093657	0.779187
H	1.450514	-0.942933	1.132970
C	5.900596	-3.081798	-2.688399
H	6.745431	-2.547330	-3.121870
C	5.719611	2.810933	3.371365
H	6.405793	2.210773	3.968170
C	-0.162517	-2.120265	-2.030486
H	-1.156854	-2.374937	-2.420401
H	0.556171	-2.225631	-2.857287
C	4.663399	2.152429	2.697361
C	1.098351	-5.243997	2.605548
H	0.329075	-5.889693	3.029549
C	3.597593	3.555367	-1.274372
H	4.262351	2.884322	-0.732916
C	4.045709	4.201510	-2.403453
H	5.062338	4.033193	-2.753440
C	-0.467954	-4.610767	0.801197
H	-1.214840	-5.284414	1.222506
C	3.697736	-3.002823	-1.593839
C	4.480818	0.755957	2.810426
H	5.183319	0.177434	3.409455
C	4.813762	-0.915450	-2.230133
H	5.677185	-0.399673	-2.649182
C	2.273160	3.741344	-0.799878
C	3.299896	-4.266020	2.667472
H	4.262844	-4.156550	3.162734
C	3.731828	-0.208221	-1.779517
H	3.726015	0.880810	-1.842311
C	1.915670	5.296034	-2.671409
H	1.251167	5.970438	-3.211120
C	0.074841	4.792468	-1.103842
H	-0.570166	5.482808	-1.646669
C	1.227491	0.415233	-3.863266
H	1.165176	0.811803	-4.884815
H	1.578237	-0.621804	-3.936402
H	1.997285	0.995475	-3.341495
C	4.958322	4.930872	2.525558
H	5.066379	6.012440	2.474486
C	3.055503	-3.588605	1.494380
H	3.827138	-2.950172	1.067020
C	3.927418	4.319593	1.850590
H	3.230238	4.927857	1.279641
C	-0.415935	4.046822	-0.063172
H	-1.456419	4.154175	0.246395
C	2.317617	-5.109897	3.225899
H	2.527686	-5.651393	4.146019
C	4.771927	-5.126428	-2.105388
H	4.750242	-6.214334	-2.095440
C	-1.213785	-0.013912	-4.129186
H	-2.216867	0.015021	-3.690936
H	-1.011434	-1.052765	-4.415031
H	-1.233199	0.580348	-5.051784
C	-0.343219	-1.728920	2.849918
H	-0.745270	-2.281141	3.711628
H	0.726055	-1.970434	2.800574
H	-0.821438	-2.114129	1.940600
C	3.200975	5.083696	-3.108329
H	3.568620	5.591970	-3.997213
C	5.871434	4.173133	3.286445
H	6.684960	4.669629	3.810951
C	0.348146	0.294715	4.133204
H	0.215149	-0.320871	5.033296

H	0.119337	1.327691	4.418581
H	1.407940	0.241509	3.857005
C	5.883855	-4.454674	-2.652662
H	6.719605	-5.024703	-3.053204
C	-0.578021	-0.230893	3.035837
C	-0.767398	-3.827212	-0.284407
H	-1.760320	-3.853841	-0.732780
C	-0.401319	2.031731	-2.932860
H	0.304191	2.431059	-2.196691
H	-1.413017	2.218502	-2.551656
H	-0.275587	2.611970	-3.857360
C	-2.030655	0.044864	3.436248
H	-2.739960	-0.338383	2.696157
H	-2.225706	1.118968	3.552599
H	-2.242283	-0.433463	4.402483
Ni	-1.743702	0.187481	-0.244257
H	-2.418795	0.093389	-1.604311
C	-5.439466	-0.911448	-0.216141
C	-4.924407	-0.969565	-1.472846
N	-4.123811	-2.021919	-2.021420
O	-3.976873	-3.083373	-1.404804
O	-3.648348	-1.803894	-3.142140
H	-5.120463	-0.197369	-2.205717
N	-5.049554	-1.770817	0.807862
H	-5.784096	-2.107898	1.418575
C	-3.756421	-2.162852	1.089940
O	-2.779721	-1.614873	0.591176
C	-3.648594	-3.314536	2.038060
H	-3.723955	-4.241039	1.453583
H	-2.675580	-3.302651	2.533930
H	-4.446500	-3.332498	2.788186
C	-6.435041	0.102441	0.151232
C	-6.552059	0.513056	1.490271
C	-7.286876	0.675153	-0.808186
C	-7.496571	1.461752	1.860206
H	-5.869352	0.108219	2.236276
C	-8.219040	1.634465	-0.436795
H	-7.238176	0.339812	-1.842501
C	-8.331303	2.026624	0.898132
H	-7.573516	1.770165	2.900678
H	-8.878683	2.062958	-1.187896
H	-9.073554	2.767657	1.187012
C	-3.851391	2.133214	-0.083069
O	-3.158121	1.361778	0.601901
C	-4.731678	3.173725	0.508212
H	-4.410155	4.162666	0.163176
H	-5.762839	3.038225	0.161471
H	-4.699098	3.132270	1.597584
O	-3.841905	2.111541	-1.399073
H	-3.203122	1.366537	-1.638266

V_{R2}

P	-0.968999	-0.086033	1.311166
P	-0.365833	-0.900791	-1.663925
C	2.348219	-0.115498	-1.256146
C	2.300816	-2.490524	-0.423177
C	4.968616	-2.787032	-1.567527
H	4.451959	-3.649558	-1.153197
C	1.149143	-3.033630	-0.979423
C	0.002245	3.025559	0.345803
C	1.147371	2.628508	1.213126
C	-0.795764	0.006661	-3.243502
C	2.825757	-3.047064	0.785802
C	1.534908	1.299469	1.366298
C	1.856986	3.651954	1.929907
C	2.694791	0.985541	2.116193
H	3.000112	-0.060071	2.180776
C	0.928567	0.153903	-0.803396
H	0.656026	1.164907	-1.144304
C	-1.288507	2.597416	0.635055
C	-1.535329	1.616228	1.736474
H	-2.605401	1.562541	1.968807
H	-1.010145	1.919560	2.651892
C	5.003834	-0.424506	-2.187036
C	2.982402	-1.346940	-1.089419
C	2.197070	-4.198609	1.361019
C	-0.914997	4.382832	-1.514170
C	0.793748	0.142368	0.732975
H	1.274390	-0.784454	1.079514
C	6.316860	-0.607713	-2.682790
H	6.829413	0.247039	-3.123046
C	3.710989	4.313513	3.408158
H	4.591091	4.028134	3.983430
C	0.552832	-2.398524	-2.198038
H	-0.154146	-3.070197	-2.699973
H	1.327533	-2.111300	-2.921473
C	3.013061	3.305537	2.701270
C	2.713487	-4.739966	2.563517

H	2.229692	-5.620450	2.986101
C	1.510105	4.268590	-1.214107
H	2.377472	3.913871	-0.660095
C	1.684797	5.067137	-2.320733
H	2.690549	5.336006	-2.637893
C	1.041404	-4.732307	0.743277
H	0.558692	-5.601101	1.189999
C	4.310980	-1.530138	-1.597343
C	3.424513	1.954824	2.750596
H	4.317279	1.693613	3.317640
C	4.350061	0.825045	-2.270767
H	4.882108	1.672689	-2.701340
C	0.213203	3.891121	-0.778334
C	4.396034	-3.015620	2.644518
H	5.242949	-2.556835	3.151074
C	3.059018	0.965520	-1.834749
H	2.559451	1.931353	-1.917750
C	-0.699219	5.214294	-2.639789
H	-1.567220	5.580690	-3.187541
C	-2.216868	4.002969	-1.110937
H	-3.076846	4.401815	-1.649663
C	-1.503203	-0.962426	-4.190546
H	-1.880824	-0.406338	-5.057845
H	-2.352149	-1.481417	-3.730378
H	-0.821470	-1.731445	-4.572835
C	2.130264	5.961719	2.648227
H	1.781084	6.992261	2.644400
C	3.932532	-2.477069	1.466362
H	4.420849	-1.600400	1.044386
C	1.438527	5.007522	1.938882
H	0.546321	5.295058	1.387725
C	-2.391552	3.110449	-0.084976
H	-3.390693	2.798252	0.211078
C	3.788321	-4.162285	3.196252
H	4.169658	-4.584551	4.123491
C	6.241591	-2.934841	-2.066003
H	6.721027	-3.911202	-2.035642
C	-1.687541	1.189704	-2.885715
H	-1.203666	1.838151	-2.147825
H	-2.654873	0.891775	-2.461543
H	-1.882672	1.799112	-3.778436
C	-0.296662	-2.326795	2.826905
H	-0.280215	-2.830278	3.803716
H	0.739197	-2.316609	2.466774
H	-0.890361	-2.933738	2.137454
C	0.571920	5.547549	-3.041580
H	0.723300	6.182765	-3.911718
C	3.282745	5.618278	3.383407
H	3.823157	6.384480	3.935117
C	0.108928	-0.170838	3.958051
H	0.019467	-0.632756	4.950473
H	-0.117201	0.894818	4.080314
H	1.156626	-0.259970	3.655399
C	6.928776	-1.835953	-2.621791
H	7.936868	-1.966493	-3.009617
C	-0.831320	-0.907294	3.000889
C	0.513442	-4.146271	-0.379764
H	-0.396630	-4.540105	-0.833145
C	0.467890	0.547931	-3.918151
H	1.249738	-0.208443	-4.055954
H	0.900726	1.388433	-3.363014
H	0.199344	0.925827	-4.913154
C	-2.238251	-0.914577	3.603339
H	-2.985907	-1.343208	2.927424
H	-2.569938	0.096496	3.873576
H	-2.239844	-1.510615	4.525471
Ni	-2.036795	-1.197259	-0.334842
H	-1.774963	-1.991924	-1.541021
C	-4.130905	-0.975702	-0.030541
C	-3.728056	-1.482519	-1.284481
N	-4.016800	-2.890083	-1.698641
O	-5.022903	-3.431066	-1.256055
O	-3.245799	-3.398088	-2.510584
H	-3.757599	-0.852729	-2.170532
N	-4.480888	-1.918974	0.987468
H	-5.449625	-1.934266	1.287719
C	-3.700383	-2.997899	1.233949
O	-2.558900	-3.061785	0.745245
C	-4.254069	-4.074332	2.103451
H	-4.551713	-4.920000	1.472166
H	-3.475327	-4.432594	2.782973
H	-5.126042	-3.755502	2.681848
C	-4.751094	0.351046	0.135945
C	-4.986414	0.857004	1.424930
C	-5.198786	1.103512	-0.961706
C	-5.641474	2.069258	1.610480
H	-4.648825	0.284584	2.289883
C	-5.849402	2.317193	-0.774687

H	-5.075811	0.720984	-1.973656
C	-6.075488	2.807179	0.510536
H	-5.815151	2.438813	2.619192
H	-6.199354	2.875310	-1.640865
H	-6.592912	3.752959	0.654358

$TSII_{R2}$

P	-0.987015	-0.068203	1.300922
P	-0.325995	-0.873518	-1.659071
C	2.376209	-0.088806	-1.214835
C	2.320224	-2.466065	-0.373951
C	4.982335	-2.774388	-1.516408
H	4.456129	-3.636408	-1.113128
C	1.174320	-3.026903	-0.925782
C	-0.072264	3.048200	0.330445
C	1.084733	2.684004	1.196779
C	-0.698940	0.015832	-3.265408
C	2.856800	-3.014991	0.834488
C	1.496770	1.364298	1.367790
C	1.784407	3.731170	1.888245
C	2.668912	1.082355	2.111790
H	2.993782	0.043248	2.189260
C	0.948208	0.184054	-0.791615
H	0.686283	1.193763	-1.143418
C	-1.352526	2.595741	0.628012
C	-1.573077	1.620776	1.740252
H	-2.638897	1.552650	1.988199
H	-1.037450	1.933501	2.646262
C	5.039543	-0.408381	-2.118656
C	3.000914	-1.323938	-1.044806
C	2.256382	-4.184404	1.403586
C	-1.025273	4.365108	-1.540369
C	0.781643	0.186017	0.742991
H	1.273761	-0.727358	1.108619
C	6.355270	-0.597324	-2.604726
H	6.877382	0.257092	-3.034312
C	3.649965	4.451058	3.323959
H	4.543359	4.190900	3.890711
C	0.555270	-2.408483	-2.141923
H	-0.174023	-3.083275	-2.606007
H	1.312562	-2.156016	-2.897763
C	2.957545	3.418291	2.648318
C	2.783842	-4.718614	2.604186
H	2.322041	-5.613536	3.020982
C	1.403190	4.297838	-1.254570
H	2.279866	3.968125	-0.700033
C	1.557090	5.083810	-2.373233
H	2.555965	5.364560	-2.701622
C	1.118501	-4.746653	0.779005
H	0.662503	-5.635003	1.215375
C	4.333554	-1.512856	-1.542681
C	3.390922	2.075231	2.718078
H	4.295443	1.839048	3.277446
C	4.396365	0.847124	-2.197716
H	4.939430	1.694656	-2.614459
C	0.116055	3.904624	-0.804588
C	4.422901	-2.953707	2.696557
H	5.256928	-2.476121	3.206958
C	3.101748	0.992259	-1.775266
H	2.607604	1.961085	-1.857680
C	-0.831279	5.187504	-2.676513
H	-1.709019	5.530501	-3.223904
C	-2.317310	3.956171	-1.132857
H	-3.186868	4.326849	-1.676358
C	-1.398973	-0.948704	-4.222438
H	-1.690441	-0.403994	-5.129351
H	-2.308179	-1.394662	-3.801675
H	-0.745392	-1.771416	-4.535190
C	2.029553	6.058231	2.559387
H	1.662684	7.082524	2.542318
C	3.948232	-2.421337	1.519785
H	4.415689	-1.530565	1.103428
C	1.342463	5.079274	1.879906
H	0.436620	5.341454	1.338276
C	-2.469140	3.069687	-0.097943
H	-3.459568	2.734163	0.204147
C	3.843065	-4.117804	3.241694
H	4.233249	-4.535087	4.167525
C	6.258051	-2.928080	-2.006273
H	6.729765	-3.908324	-1.979636
C	-1.594849	1.207425	-2.943833
H	-1.136093	1.859052	-2.192626
H	-2.578578	0.912792	-2.554717
H	-1.756716	1.812717	-3.845968
C	-0.281142	-2.323227	2.779943
H	-0.257543	-2.842700	3.748123
H	0.754203	-2.294251	2.420164
H	-0.866663	-2.926348	2.080198

C	0.431324	5.536880	-3.091653
H	0.565566	6.163180	-3.971015
C	3.200144	5.748059	3.280768
H	3.736775	6.533520	3.808439
C	0.090517	-0.173363	3.938353
H	0.026843	-0.658213	4.921707
H	-0.166344	0.881950	4.085394
H	1.137097	-0.225001	3.622926
C	6.957884	-1.830376	-2.548167
H	7.968099	-1.965420	-2.928901
C	-0.839264	-0.916692	2.976292
C	0.573640	-4.164130	-0.337247
H	-0.325367	-4.578281	-0.792658
C	0.584845	0.535785	-3.916629
H	1.360116	-0.231865	-4.029746
H	1.016720	1.373730	-3.357639
H	0.345023	0.910006	-4.920257
C	-2.240746	-0.969238	3.586024
H	-2.967259	-1.461514	2.930168
H	-2.622127	0.032038	3.825266
H	-2.207606	-1.533855	4.527090
Ni	-2.040848	-1.125331	-0.368491
H	-2.027452	-1.750931	-1.689787
C	-4.073647	-1.057392	-0.009120
C	-3.703953	-1.474429	-1.318092
N	-3.990571	-2.879759	-1.786860
O	-5.036215	-3.393235	-1.414968
O	-3.185627	-3.385053	-2.563978
H	-3.874503	-0.807165	-2.162033
N	-4.379786	-2.082885	0.945511
H	-5.339052	-2.142222	1.270317
C	-3.561357	-3.151449	1.100638
O	-2.439978	-3.154694	0.565895
C	-4.057781	-4.291881	1.924665
H	-4.360796	-5.107674	1.257679
H	-3.244800	-4.669111	2.551872
H	-4.912931	-4.029617	2.554422
C	-4.765049	0.225651	0.231903
C	-4.984727	0.662940	1.547693
C	-5.273858	1.008396	-0.816085
C	-5.674100	1.842094	1.807256
H	-4.603044	0.063540	2.374612
C	-5.963422	2.186934	-0.556040
H	-5.162123	0.685122	-1.849675
C	-6.165001	2.612828	0.755351
H	-5.831834	2.158088	2.836638
H	-6.359092	2.768958	-1.386126
H	-6.709710	3.532377	0.956693

VI_{R2}

P	-0.979279	-0.072863	1.078381
P	-0.105615	-0.769518	-1.819248
C	2.596419	-0.193504	-1.136496
C	2.283179	-2.588234	-0.389995
C	5.069642	-3.022710	-1.159601
H	4.457017	-3.858109	-0.829323
C	1.192867	-3.041392	-1.126257
C	0.132215	3.025321	0.409653
C	1.257049	2.562348	1.269405
C	-0.396989	0.176995	-3.411793
C	2.595594	-3.231839	0.853240
C	1.575914	1.212872	1.409821
C	1.999682	3.542379	2.013808
C	2.680183	0.829058	2.209614
H	2.922287	-0.231717	2.282012
C	1.157219	0.175113	-0.849139
H	1.009176	1.216758	-1.166198
C	-1.174030	2.644413	0.700763
C	-1.441162	1.588593	1.726282
H	-2.497123	1.559936	2.021680
H	-0.847011	1.749746	2.637640
C	5.318993	-0.663424	-1.735814
C	3.120684	-1.467875	-0.912728
C	1.824596	-4.364757	1.274459
C	-0.741069	4.478432	-1.398144
C	0.845461	0.117418	0.666419
H	1.251640	-0.842581	1.009195
C	6.672667	-0.919507	-2.060565
H	7.284409	-0.092009	-2.418523
C	3.856051	4.092515	3.534217
H	4.705468	3.755876	4.127638
C	0.744954	-2.304484	-2.348334
H	0.034005	-2.899234	-2.933112
H	1.590648	-2.035723	-2.994371
C	3.114656	3.127327	2.811525
C	2.105979	-4.972867	2.521460
H	1.509327	-5.832949	2.824303
C	1.678171	4.227309	-1.138185

H	2.532170	3.814837	-0.602848
C	1.878257	5.030684	-2.237554
H	2.891634	5.243864	-2.572324
C	0.778400	-4.836621	0.447849
H	0.210229	-5.710840	0.764175
C	4.491868	-1.729387	-1.251314
C	3.439980	1.753973	2.874673
H	4.295077	1.440983	3.472586
C	4.756303	0.621631	-1.900840
H	5.387310	1.432557	-2.262894
C	0.369483	3.918030	-0.685777
C	3.866344	-3.379195	2.925697
H	4.657540	-3.001086	3.570288
C	3.432664	0.839692	-1.624695
H	2.998104	1.830112	-1.771899
C	-0.498779	5.322333	-2.508782
H	-1.353851	5.745976	-3.034911
C	-2.054903	4.152130	-0.990517
H	-2.902311	4.611411	-1.498584
C	-1.479145	-0.551302	-4.210816
H	-1.622343	-0.046376	-5.174671
H	-2.443554	-0.546994	-3.687798
H	-1.223305	-1.597419	-4.418823
C	2.391337	5.831450	2.745398
H	2.101439	6.880051	2.737701
C	3.625025	-2.770424	1.714558
H	4.231577	-1.920942	1.405888
C	1.658198	4.919663	2.022485
H	0.793000	5.260084	1.459399
C	-2.258587	3.247131	0.019981
H	-3.275785	3.011891	0.335016
C	3.101840	-4.490915	3.336109
H	3.304093	-4.964196	4.294569
C	6.385296	-3.240971	-1.494571
H	6.799387	-4.244351	-1.418332
C	-0.869916	1.586563	-3.066762
H	-0.065921	2.197589	-2.641265
H	-1.706755	1.593225	-2.353690
H	-1.208026	2.099472	-3.977109
C	-1.365581	-2.607665	2.132027
H	-1.353855	-3.305513	2.981402
H	-0.637658	-2.975014	1.399631
H	-2.364453	-2.649405	1.678201
C	0.782416	5.589440	-2.927625
H	0.955246	6.230674	-3.789251
C	3.508394	5.420778	3.500402
H	4.082975	6.153732	4.062731
C	0.320805	-1.238966	3.349082
H	0.185773	-1.821166	4.270733
H	0.672367	-0.242145	3.641200
H	1.115982	-1.736149	2.780593
C	7.201323	-2.181165	-1.939903
H	8.241899	-2.368062	-2.196306
C	-1.017325	-1.200510	2.610451
C	0.454190	-4.171895	-0.706011
H	-0.381108	-4.505249	-1.321649
C	0.884785	0.264903	-4.242965
H	1.207727	-0.710095	-4.625383
H	1.718123	0.704112	-3.680287
H	0.703658	0.909055	-5.113490
C	-2.078467	-0.694953	3.588997
H	-3.053608	-0.539761	3.124044
H	-1.775946	0.240995	4.072920
H	-2.210150	-1.442221	4.382364
Ni	-1.939645	-1.019290	-0.626754
H	-3.706348	0.202465	-2.149280
C	-3.910418	-0.846615	-0.249913
C	-4.025224	0.387979	-1.116098
N	-5.469321	0.906567	-1.284160
O	-5.613880	2.120038	-1.315528
O	-6.359405	0.069328	-1.393049
H	-3.474512	1.252529	-0.741772
N	-4.484540	-1.995562	-0.967219
H	-5.495658	-2.099272	-0.983684
C	-3.713917	-2.676485	-1.798452
O	-2.470283	-2.414340	-1.816637
C	-4.273130	-3.713369	-2.705053
H	-4.221308	-3.357695	-3.740776
H	-3.663930	-4.620157	-2.649036
H	-5.312154	-3.961174	-2.475813
C	-4.565278	-0.723230	1.080438
C	-4.909536	-1.876266	1.804191
C	-4.888172	0.520645	1.646975
C	-5.521242	-1.792142	3.049140
H	-4.682752	-2.855165	1.382518
C	-5.497628	0.606032	2.895207
H	-4.684693	1.443951	1.104832
C	-5.813216	-0.548899	3.605793

H	-5.772906	-2.704104	3.587152
H	-5.740848	1.584204	3.305363
H	-6.294588	-0.480132	4.578606

VII_{R2}

P	-0.687708	0.258037	1.358815
P	-0.379064	-0.453327	-1.654226
C	2.463235	-0.538832	-1.335159
C	1.754712	-2.867680	-0.685276
C	4.233008	-3.802092	-1.915292
H	3.491108	-4.520379	-1.574881
C	0.496297	-3.024031	-1.257479
C	1.255588	2.991029	0.695117
C	2.249983	2.135695	1.392631
C	-0.532404	0.693700	-3.121702
C	2.111944	-3.663029	0.454103
C	2.178586	0.747051	1.377697
C	3.326227	2.780176	2.096342
C	3.251194	-0.008748	1.912071
H	3.203587	-1.093447	1.833075
C	1.181870	0.087986	-0.823474
H	1.229924	1.160876	-1.058294
C	-0.082711	2.990219	1.075381
C	-0.605201	1.978394	2.050116
H	-1.610241	2.245194	2.402005
H	0.042064	1.912652	2.938013
C	4.934424	-1.501371	-2.328794
C	2.727024	-1.905875	-1.274350
C	1.193240	-4.643744	0.951017
C	0.767662	4.812841	-0.912852
C	1.058539	-0.023478	0.708333
H	1.203567	-1.087358	0.950838
C	6.151255	-2.000118	-2.851734
H	6.886506	-1.286983	-3.222846
C	5.447298	2.624681	3.333469
H	6.244302	2.003787	3.741625
C	0.032639	-2.108209	-2.351707
H	-0.863620	-2.498192	-2.846932
H	0.809786	-1.969777	-3.116160
C	4.382208	1.990278	2.651777
C	1.525763	-5.389325	2.107535
H	0.811586	-6.127112	2.472083
C	3.003356	3.829827	-0.888652
H	3.727151	3.136174	-0.466073
C	3.371170	4.643007	-1.936118
H	4.380550	4.579122	-2.338095
C	-0.032427	-4.838996	0.274305
H	-0.713920	-5.615524	0.621319
C	3.953285	-2.413893	-1.823526
C	4.329169	0.585391	2.508857
H	5.147636	-0.019054	2.898849
C	4.655208	-0.117059	-2.306009
H	5.405031	0.580609	-2.677415
C	1.690584	3.873379	-0.350294
C	3.631505	-4.232172	2.270740
H	4.579005	-4.078817	2.783744
C	3.450322	0.340599	-1.843450
H	3.237221	1.409582	-1.848688
C	1.183492	5.649161	-1.976615
H	0.466746	6.358417	-2.389390
C	-0.543715	4.874545	-0.390905
H	-1.229266	5.631951	-0.770946
C	-1.635492	0.140786	-4.025560
H	-1.870560	0.870340	-4.811380
H	-2.560685	-0.069774	-3.479184
H	-1.317017	-0.783873	-4.523376
C	4.419711	4.771110	2.971675
H	4.428484	5.849788	3.114631
C	3.342044	-3.498943	1.142884
H	4.066264	-2.777981	0.770408
C	3.378424	4.184475	2.290101
H	2.573126	4.806818	1.906501
C	-0.951892	3.979644	0.563360
H	-1.956939	4.041660	0.969746
C	2.715955	-5.184930	2.762757
H	2.957634	-5.759839	3.654017
C	5.420397	-4.256191	-2.440205
H	5.605669	-5.326700	-2.502148
C	-0.875165	2.078909	-2.570195
H	-0.025919	2.511847	-2.026921
H	-1.732101	2.073588	-1.887410
H	-1.108298	2.766685	-3.394787
C	-1.631379	-0.215368	3.949831
H	-1.955710	-0.993951	4.651936
H	-2.519003	0.222822	3.492922
H	-1.151034	0.577286	4.536203
C	2.456202	5.563589	-2.486864
H	2.761153	6.204405	-3.311436

C	5.471255	3.989235	3.490478
H	6.292119	4.467088	4.020861
C	-0.993799	-2.225981	2.508157
H	-0.338416	-2.559706	1.692419
H	-2.028099	-2.310696	2.174346
H	-0.852376	-2.921196	3.346829
C	6.396393	-3.350429	-2.903275
H	7.334001	-3.723766	-3.309323
C	-0.647963	-0.803185	2.931553
C	-0.367158	-4.041745	-0.789625
H	-1.295250	-4.218892	-1.327430
C	0.764807	0.799782	-3.925159
H	1.152859	-0.168711	-4.263070
H	1.557598	1.308000	-3.365272
H	0.571787	1.401799	-4.823169
C	0.720916	-0.844690	3.613053
H	1.159360	0.146177	3.780915
H	1.446176	-1.458482	3.067997
H	0.588396	-1.314425	4.597274
Ni	-2.164646	-0.420371	-0.254854
H	-5.466730	-1.661949	0.652549
C	-4.053999	0.002903	0.392392
C	-5.228614	-0.876679	-0.068811
N	-6.505614	-0.052157	-0.183603
O	-7.092397	-0.087580	-1.255576
O	-6.854292	0.596476	0.801865
H	-5.124155	-1.308682	-1.059457
C	-3.749806	-4.022098	-1.939148
H	-3.232638	-3.893587	-2.891966
H	-3.580449	-5.023029	-1.534293
H	-4.828283	-3.930940	-2.122622
C	-3.347074	-2.972011	-0.963429
O	-2.877766	-1.886345	-1.354992
O	-3.587305	-3.293357	0.280112
H	-3.519770	-2.531362	0.931509
N	-4.278189	0.348205	1.783421
C	-4.475506	-0.652726	2.688522
O	-4.138457	-1.821483	2.457951
C	-5.139849	-0.256968	3.971121
H	-4.909267	0.772124	4.266019
H	-6.227838	-0.328835	3.846161
H	-4.847666	-0.943374	4.768409
H	-4.855564	1.171269	1.940571
C	-3.958007	1.193182	-0.494583
C	-4.214370	1.059867	-1.879387
C	-3.781319	2.496635	0.001122
C	-4.301559	2.169355	-2.709070
H	-4.391346	0.075838	-2.306933
C	-3.883436	3.604425	-0.829428
H	-3.586830	2.639630	1.063258
C	-4.150113	3.451205	-2.187988
H	-4.509536	2.027103	-3.767933
H	-3.770568	4.601532	-0.407028
H	-4.244908	4.323164	-2.831034

TSIII$_{R2}$

P	-0.677005	0.215929	1.322629
P	-0.298917	-0.458933	-1.680715
C	2.525224	-0.526843	-1.307044
C	1.815858	-2.852664	-0.649906
C	4.316889	-3.786194	-1.833260
H	3.575509	-4.504587	-1.491905
C	0.567795	-3.023019	-1.240034
C	1.224064	2.982780	0.677457
C	2.221439	2.153366	1.403135
C	-0.464337	0.674386	-3.154396
C	2.154563	-3.624371	0.510351
C	2.166664	0.762987	1.418092
C	3.275155	2.825087	2.115922
C	3.222841	0.029078	2.011046
H	3.180973	-1.057669	1.968718
C	1.234595	0.094359	-0.810759
H	1.278562	1.168832	-1.040242
C	-0.120662	2.958884	1.036966
C	-0.638930	1.939144	2.004153
H	-1.648747	2.188445	2.352639
H	0.004752	1.875996	2.895143
C	5.009833	-1.485464	-2.265540
C	2.792815	-1.892595	-1.233439
C	1.227023	-4.594827	1.010435
C	0.724549	4.789930	-0.944192
C	1.083563	-0.031497	0.718045
H	1.246848	-1.092223	0.956362
C	6.234497	-1.982979	-2.770794
H	6.969765	-1.270158	-3.142326
C	5.373014	2.718039	3.398370
H	6.165487	2.113859	3.838828
C	0.115886	-2.119802	-2.348692

H	-0.773959	-2.509356	-2.853224
H	0.902733	-1.976104	-3.102740
C	4.324773	2.058069	2.714563
C	1.538522	-5.315066	2.188992
H	0.818239	-6.045475	2.556017
C	2.975106	3.841918	-0.890445
H	3.704582	3.162454	-0.454887
C	3.341393	4.654297	-1.939049
H	4.355961	4.604315	-2.329692
C	0.015783	-4.808472	0.313617
H	-0.670925	-5.577469	0.666131
C	4.028409	-2.398663	-1.761566
C	4.281270	0.649209	2.617294
H	5.090642	0.062766	3.051040
C	4.723634	-0.102258	-2.258717
H	5.473970	0.595422	-2.628860
C	1.655955	3.867582	-0.367217
C	3.639355	-4.150537	2.367595
H	4.576242	-3.983953	2.895873
C	3.512419	0.354251	-1.811572
H	3.294359	1.421974	-1.827385
C	1.138890	5.626693	-2.008200
H	0.416305	6.323296	-2.432090
C	-0.593093	4.835032	-0.435754
H	-1.284769	5.582813	-0.823360
C	-1.520252	0.089931	-4.093045
H	-1.718470	0.804688	-4.902157
H	-2.468848	-0.112758	-3.585870
H	-1.177191	-0.842483	-4.558281
C	4.336958	4.845933	2.962455
H	4.334005	5.927771	3.078818
C	3.370456	-3.441415	1.219334
H	4.099288	-2.724921	0.846948
C	3.312213	4.234075	2.278116
H	2.508731	4.841419	1.868318
C	-0.999756	3.934185	0.513586
H	-2.009664	3.984548	0.910885
C	2.716187	-5.094898	2.861715
H	2.941939	-5.650447	3.769334
C	5.512537	-4.238972	-2.340205
H	5.705430	-5.308824	-2.387218
C	-0.881705	2.041489	-2.618217
H	-0.107916	2.473430	-1.971789
H	-1.810849	1.998640	-2.041447
H	-1.033536	2.742837	-3.449958
C	-1.643906	-0.189772	3.927332
H	-1.967042	-0.936720	4.663524
H	-2.539201	0.256422	3.491738
H	-1.110936	0.599461	4.471166
C	2.417976	5.557196	-2.504910
H	2.721629	6.197778	-3.330082
C	5.385528	4.086274	3.518736
H	6.193562	4.583854	4.050492
C	-1.275313	-2.231703	2.481081
H	-0.751162	-2.624254	1.598395
H	-2.346129	-2.217403	2.268531
H	-1.112092	-2.947063	3.298947
C	6.487443	-3.332472	-2.804326
H	7.431028	-3.704882	-3.197040
C	-0.741081	-0.861846	2.887001
C	-0.304286	-4.032313	-0.770595
H	-1.228241	-4.214207	-1.313478
C	0.861826	0.820191	-3.903962
H	1.304301	-0.136220	-4.207663
H	1.607711	1.371940	-3.320847
H	0.679495	1.398466	-4.819348
C	0.632660	-1.050214	3.531584
H	1.150347	-0.108006	3.747275
H	1.297225	-1.690968	2.939759
H	0.477119	-1.562816	4.490470
Ni	-2.058431	-0.459875	-0.355826
H	-5.621251	-1.741645	0.772649
C	-4.110684	-0.207570	0.414507
C	-5.368761	-1.009180	0.001156
N	-6.569818	-0.106682	-0.156955
O	-7.171309	-0.164336	-1.220405
O	-6.861296	0.621763	0.791027
H	-5.273171	-1.503240	-0.963398
C	-3.678594	-3.961520	-1.854932
H	-3.170921	-4.000393	-2.821665
H	-3.532430	-4.892315	-1.301253
H	-4.755328	-3.867707	-2.045381
C	-3.234572	-2.787476	-1.046293
O	-2.779818	-1.759672	-1.651092
O	-3.395530	-2.807872	0.211741
H	-3.389502	-1.533732	0.498068
N	-4.278647	0.307281	1.763553
C	-4.644296	-0.546689	2.789576

O	-4.464440	-1.754509	2.720663
C	-5.266419	0.136477	3.974599
H	-4.841300	1.128949	4.161637
H	-6.339988	0.267486	3.789966
H	-5.147525	-0.487751	4.862300
H	-4.790897	1.185197	1.789161
C	-3.940484	0.942137	-0.563466
C	-4.285149	0.788970	-1.926252
C	-3.714195	2.254639	-0.111285
C	-4.415167	1.885272	-2.767911
H	-4.475735	-0.200759	-2.331283
C	-3.861487	3.351026	-0.952771
H	-3.435794	2.413883	0.927974
C	-4.228092	3.176919	-2.283144
H	-4.692370	1.723163	-3.807794
H	-3.706769	4.352919	-0.556739
H	-4.366819	4.036783	-2.934453

VIII$_{R2}$

P	-0.076704	-0.396561	1.631249
P	0.038236	-1.053715	-1.329777
C	2.600680	0.153958	-1.529387
C	3.121113	-2.187144	-0.740482
C	5.499648	-2.059375	-2.425677
H	5.236687	-2.987513	-1.924366
C	1.988347	-2.935092	-1.044168
C	0.074991	2.837748	0.700825
C	1.422947	2.651615	1.310475
C	-0.953103	-0.305080	-2.713225
C	3.988048	-2.632231	0.310825
C	2.087367	1.427427	1.301155
C	2.051859	3.784422	1.932619
C	3.413308	1.339542	1.791816
H	3.924481	0.377746	1.731377
C	1.288630	0.198047	-0.780223
H	0.805780	1.158125	-1.015963
C	-1.039878	2.172396	1.201305
C	-0.888973	1.121630	2.254753
H	-1.857429	0.820729	2.668367
H	-0.257567	1.480461	3.082247
C	5.003467	0.257278	-3.015714
C	3.444120	-0.956883	-1.518564
C	3.728856	-3.882890	0.959597
C	-1.408031	4.076211	-0.847151
C	1.471931	0.159261	0.758759
H	2.166636	-0.667383	0.970935
C	6.197152	0.284470	-3.776384
H	6.453393	1.201251	-4.306451
C	4.007258	4.779579	3.049897
H	5.024927	4.666511	3.422388
C	0.998870	-2.434068	-2.053561
H	0.290493	-3.219892	-2.340141
H	1.494565	-2.068633	-2.964426
C	3.386751	3.664106	2.439196
C	4.574649	-4.306314	2.013226
H	4.365477	-5.261218	2.494783
C	1.012996	4.347494	-1.058460
H	2.022584	4.117079	-0.721345
C	0.822953	5.196105	-2.124952
H	1.684443	5.629212	-2.629662
C	2.604001	-4.644222	0.563594
H	2.416061	-5.600202	1.051496
C	4.646871	-0.932313	-2.301805
C	4.053973	2.424040	2.326941
H	5.077746	2.339295	2.689624
C	4.145713	1.377588	-2.953834
H	4.423412	2.285917	-3.487303
C	-0.089142	3.757524	-0.387294
C	5.879797	-2.291298	1.803492
H	6.712823	-1.676155	2.138072
C	2.973823	1.317435	-2.246154
H	2.311237	2.184079	-2.210246
C	-1.568537	4.968523	-1.934355
H	-2.579747	5.198944	-2.270201
C	-2.519127	3.460236	-0.226814
H	-3.520019	3.725103	-0.564204
C	-1.867612	-1.390763	-3.282282
H	-2.510134	-0.949856	-4.055334
H	-2.519806	-1.823850	-2.513774
H	-1.307815	-2.210717	-3.747654
C	2.017347	6.090411	2.712058
H	1.483114	7.030337	2.835975
C	5.087675	-1.859212	0.764508
H	5.303249	-0.908042	0.281159
C	1.391283	5.028575	2.101449
H	0.366089	5.140161	1.756084
C	-2.336547	2.504242	0.739963
H	-3.192124	1.998342	1.190862

C	5.626475	-3.527609	2.432793
H	6.262946	-3.860413	3.249896
C	6.648532	-2.003554	-3.179422
H	7.282114	-2.884527	-3.258492
C	-1.778923	0.826151	-2.114061
H	-1.141752	1.620275	-1.709046
H	-2.432249	0.475705	-1.304918
H	-2.423163	1.281269	-2.879057
C	-0.760233	-1.397573	4.092658
H	-0.510111	-2.039654	4.947079
H	-1.627900	-1.831056	3.585925
H	-1.057851	-0.422195	4.494652
C	-0.477971	5.516770	-2.565384
H	-0.613619	6.195281	-3.404932
C	3.340529	5.972623	3.183658
H	3.825005	6.822103	3.660322
C	0.964899	-2.669399	2.767207
H	1.783793	-2.592189	2.041723
H	0.170407	-3.280138	2.322207
H	1.356876	-3.205917	3.641990
C	7.009740	-0.819885	-3.854852
H	7.923338	-0.788789	-4.444560
C	0.463196	-1.289628	3.179160
C	1.737857	-4.163199	-0.385372
H	0.851759	-4.733579	-0.665314
C	-0.041266	0.252734	-3.805868
H	0.619569	-0.504989	-4.243260
H	0.582092	1.078822	-3.442453
H	-0.663671	0.649568	-4.618663
C	1.594116	-0.550598	3.895317
H	1.379457	0.508623	4.084562
H	2.539204	-0.611049	3.342843
H	1.759284	-1.028394	4.870087
Ni	-1.081181	-1.781941	0.326346
H	-4.579326	-2.227762	1.080998
C	-4.792363	-0.313633	0.139334
C	-4.872359	-1.826170	0.104323
N	-6.252090	-2.368272	-0.161828
O	-6.318335	-3.560147	-0.439626
O	-7.202556	-1.600439	-0.064433
H	-4.227129	-2.276353	-0.657197
C	-3.160234	-4.901279	0.671546
H	-2.751940	-5.700239	0.046681
H	-3.232998	-5.225761	1.711669
H	-4.173986	-4.690287	0.299904
C	-2.342055	-3.672075	0.552100
O	-1.847049	-3.309116	-0.576720
O	-2.140025	-2.887242	1.538390
H	-3.720812	-0.114869	0.338299
N	-5.481153	0.223613	1.300084
C	-4.897001	0.184941	2.533143
O	-3.731312	-0.186466	2.679891
C	-5.751619	0.641450	3.681484
H	-6.746338	0.985521	3.383255
H	-5.862378	-0.178631	4.398011
H	-5.241050	1.452868	4.209036
H	-6.482892	0.343272	1.216067
C	-5.186128	0.399916	-1.133681
C	-5.256086	-0.258345	-2.364178
C	-5.408532	1.779352	-1.101237
C	-5.531017	0.447541	-3.532838
H	-5.107137	-1.336455	-2.428688
C	-5.682690	2.486286	-2.267316
H	-5.370599	2.300452	-0.144833
C	-5.741470	1.822703	-3.490066
H	-5.592913	-0.086557	-4.479236
H	-5.859172	3.559893	-2.218312
H	-5.963647	2.371707	-4.402584

IV_{R3}

P	0.643542	-0.249235	-1.574875
P	0.367244	-0.744041	1.562617
C	-2.344741	0.104507	1.395763
C	-2.545016	-2.325490	0.764183
C	-5.098319	-2.320244	2.200813
H	-4.698559	-3.252141	1.808559
C	-1.374349	-2.903864	1.247630
C	-0.226071	2.986064	-0.747784
C	-1.495625	2.521975	-1.368448
C	0.883573	0.245299	3.083932
C	-3.238614	-2.955340	-0.322313
C	-1.880336	1.182553	-1.369922
C	-2.348529	3.501972	-1.986456
C	-3.170351	0.832286	-1.838967
H	-3.470557	-0.212717	-1.786907
C	-0.981968	0.247217	0.756914
H	-0.649849	1.278057	0.928892
C	0.999836	2.519720	-1.210211

C	1.070021	1.431180	-2.233489
H	2.059208	1.404855	-2.706521
H	0.339011	1.616151	-3.034915
C	-4.888080	0.073567	2.629131
C	-3.075180	-1.082459	1.391770
C	-2.743432	-4.188631	-0.856406
C	0.974565	4.512187	0.795169
C	-1.036674	0.067675	-0.777538
H	-1.562177	-0.879957	-0.968825
C	-6.149883	0.037743	3.268574
H	-6.543872	0.962737	3.688162
C	-4.498338	4.087330	-3.032320
H	-5.485318	3.773281	-3.370570
C	-0.530348	-2.199853	2.267019
H	0.201358	-2.881549	2.719917
H	-1.154537	-1.803656	3.078525
C	-3.645166	3.117150	-2.455104
C	-3.381139	-4.770625	-1.977664
H	-2.985062	-5.706116	-2.371560
C	-1.460054	4.384247	0.923977
H	-2.407134	3.985475	0.567332
C	-1.450610	5.282213	1.966810
H	-2.390387	5.581999	2.426717
C	-1.629324	-4.804743	-0.241936
H	-1.299729	-5.779541	-0.601176
C	-4.348479	-1.123845	2.056232
C	-4.037668	1.765251	-2.338590
H	-5.032379	1.471200	-2.672449
C	-4.132833	1.266054	2.564967
H	-4.544518	2.177876	2.996728
C	-0.254108	3.959690	0.307098
C	-4.981201	-2.971717	-2.024697
H	-5.853702	-2.505356	-2.478391
C	-2.892674	1.269800	1.985573
H	-2.303244	2.187351	1.963972
C	0.948363	5.448300	1.856803
H	1.894304	5.860092	2.208279
C	2.189095	4.102923	0.200993
H	3.120450	4.573476	0.520274
C	2.139544	-0.383093	3.688970
H	2.387785	0.138257	4.623302
H	3.007279	-0.303692	3.025932
H	1.993959	-1.443201	3.939457
C	-2.795753	5.766299	-2.760945
H	-2.459506	6.791199	-2.904621
C	-4.386760	-2.384236	-0.931068
H	-4.796833	-1.460602	-0.527912
C	-1.951085	4.850445	-2.178118
H	-0.954813	5.162023	-1.872992
C	2.195939	3.124313	-0.759939
H	3.126031	2.835802	-1.242262
C	-4.472717	-4.173050	-2.559828
H	-4.950693	-4.626980	-3.425289
C	-6.316157	-2.324707	2.839897
H	-6.866051	-3.258383	2.940215
C	1.174314	1.678988	2.635927
H	0.255475	2.266611	2.514258
H	1.729165	1.723877	1.688646
H	1.779127	2.190875	3.396563
C	0.261461	-2.683871	-2.928170
H	-0.161128	-3.204997	-3.798031
H	-0.325704	-2.976395	-2.047679
H	1.282257	-3.047307	-2.778825
C	-0.237620	5.824043	2.439166
H	-0.245129	6.538029	3.259997
C	-4.088132	5.389617	-3.179221
H	-4.750038	6.126655	-3.628863
C	-1.173435	-0.817783	-3.702288
H	-1.296831	-1.274202	-4.693455
H	-1.330130	0.261132	-3.819661
H	-1.974675	-1.217076	-3.068729
C	-6.856268	-1.135626	3.370549
H	-7.823512	-1.153517	3.868352
C	0.217731	-1.179741	-3.183682
C	-0.970158	-4.174600	0.779859
H	-0.122676	-4.655093	1.267179
C	-0.207035	0.267925	4.160612
H	-0.313702	-0.698725	4.665244
H	-1.188086	0.568202	3.775178
H	0.077650	0.998207	4.929233
C	1.233786	-0.806338	-4.266520
H	2.269742	-0.947496	-3.948958
H	1.108327	0.223886	-4.618269
H	1.075287	-1.461257	-5.132724
Ni	1.877518	-1.232775	0.106658
H	2.324547	-1.591094	1.491039
C	4.233012	-0.370970	-0.326245
N	4.243785	0.453440	-1.416098

H	3.758078	0.066251	-2.225384
C	5.096170	1.512529	-1.820684
O	4.806406	2.062983	-2.864431
C	6.300409	1.872638	-1.006717
H	6.727591	1.031813	-0.454042
H	7.042269	2.284647	-1.694284
H	6.054832	2.654775	-0.279414
C	3.834162	-1.719988	-0.444102
H	4.134724	-2.380707	0.361331
N	3.944160	-2.440254	-1.692231
O	3.808822	-1.836049	-2.766948
O	4.142624	-3.651078	-1.609297
C	4.725896	0.114530	0.969371
C	5.509078	-0.704417	1.798276
C	4.414224	1.412653	1.397084
C	5.972399	-0.225728	3.018717
H	5.793343	-1.702795	1.469000
C	4.867893	1.881927	2.621293
H	3.778934	2.037409	0.772419
C	5.653853	1.065837	3.434949
H	6.594456	-0.862499	3.643281
H	4.599658	2.887137	2.943854
H	6.017862	1.435021	4.391159
C	2.109527	-4.286878	0.185598
H	1.762213	-5.710997	-1.347796
H	3.211988	-6.019103	-0.351407
H	1.616429	-6.353461	0.319522
O	2.634148	-4.142801	1.405655
H	2.533824	-3.179789	1.615079
O	1.599472	-3.346707	-0.417383
C	2.173332	-5.675846	-0.337699

V_{R3}

P	0.705688	-0.394329	-1.489305
P	0.344262	-0.790241	1.679060
C	-2.319226	0.186864	1.390749
C	-2.551089	-2.241566	0.743940
C	-5.174180	-2.162612	2.054471
H	-4.779452	-3.104992	1.682636
C	-1.405621	-2.837456	1.261745
C	0.397489	2.878682	-0.714446
C	-0.935840	2.637275	-1.335597
C	0.967626	0.153404	3.170005
C	-3.209681	-2.858517	-0.370110
C	-1.556117	1.390381	-1.318867
C	-1.594690	3.741523	-1.978302
C	-2.881509	1.259784	-1.802633
H	-3.367096	0.286327	-1.721251
C	-0.917876	0.291674	0.830840
H	-0.551584	1.303702	1.053037
C	1.534861	2.238966	-1.193927
C	1.417288	1.148159	-2.207673
H	2.393292	0.906722	-2.649653
H	0.750024	1.446736	-3.030199
C	-4.922473	0.226905	2.487587
C	-3.079734	-0.983935	1.349810
C	-2.731002	-4.115688	-0.864800
C	1.834574	4.187411	0.823388
C	-0.916498	0.158455	-0.713236
H	-1.567095	-0.698689	-0.942812
C	-6.214267	0.225719	3.065569
H	-6.604379	1.161798	3.463436
C	-3.574397	4.663055	-3.113803
H	-4.587221	4.515177	-3.487230
C	-0.650590	-2.166039	2.366470
H	0.018929	-2.863758	2.881966
H	-1.337513	-1.737388	3.106958
C	-2.923177	3.574973	-2.485765
C	-3.365833	-4.708452	-1.982337
H	-2.988657	-5.663684	-2.346226
C	-0.594790	4.402976	0.998135
H	-1.593747	4.146091	0.648730
C	-0.440392	5.270550	2.055533
H	-1.319210	5.688876	2.542504
C	-1.589959	-4.705562	-0.270871
H	-1.222374	-5.654971	-0.658391
C	-4.386637	-0.986789	1.945957
C	-3.554189	2.317667	-2.351869
H	-4.576798	2.198233	-2.708046
C	-4.138167	1.401334	2.452636
H	-4.551713	2.326022	2.853280
C	0.529700	3.829195	0.350285
C	-4.886212	-2.844591	-2.134577
H	-5.718072	-2.353423	-2.635464
C	-2.869978	1.371842	1.937421
H	-2.260036	2.277189	1.928357
C	1.957825	5.104333	1.894631
H	2.957808	5.375484	2.233220

C	2.969130	3.597466	0.220176
H	3.963018	3.913592	0.538924
C	2.068491	-0.672818	3.834141
H	2.413059	-0.153917	4.738544
H	2.934112	-0.808570	3.177622
H	1.714023	-1.664671	4.143281
C	-1.624536	6.036314	-2.790767
H	-1.116598	6.988795	-2.928275
C	-4.303998	-2.250818	-1.037830
H	-4.688367	-1.300884	-0.670588
C	-0.969632	5.001580	-2.163914
H	0.052101	5.147461	-1.821232
C	2.817423	2.634145	-0.746042
H	3.689223	2.193216	-1.231467
C	-4.417498	-4.086102	-2.611636
H	-4.889257	-4.547409	-3.476609
C	-6.421267	-2.133417	2.633612
H	-7.000614	-3.051498	2.707338
C	1.514805	1.498408	2.695813
H	0.711480	2.208928	2.467592
H	2.146731	1.408331	1.802406
H	2.124726	1.952116	3.488668
C	-0.154703	-2.745824	-2.643207
H	-0.650851	-3.274364	-3.468164
H	-0.843458	-2.760873	-1.791649
H	0.733599	-3.322644	-2.373893
C	0.846196	5.632947	2.505344
H	0.954691	6.330672	3.332938
C	-2.942294	5.873442	-3.262960
H	-3.449986	6.701338	-3.752999
C	-1.101370	-0.703398	-3.664642
H	-1.273948	-1.186158	-4.635693
H	-1.024933	0.375777	-3.846422
H	-1.994741	-0.886792	-3.056869
C	-6.954753	-0.928863	3.135712
H	-7.945186	-0.919738	3.585809
C	0.159297	-1.311608	-3.046683
C	-0.923433	-4.061691	0.740455
H	-0.022455	-4.500915	1.171463
C	-0.158349	0.396567	4.178856
H	-0.493333	-0.527011	4.664180
H	-1.031635	0.887079	3.732129
H	0.217432	1.057793	4.970217
C	1.270559	-1.237421	-4.095608
H	2.251693	-1.544930	-3.724610
H	1.362757	-0.232462	-4.522574
H	1.027551	-1.920354	-4.919490
Ni	1.765379	-1.458270	0.218597
H	1.966115	-1.978228	1.595725
C	3.889642	-1.656862	-0.313873
N	4.124677	-0.983043	-1.484461
H	3.550323	-1.292323	-2.267155
C	5.117889	-0.066003	-1.901736
O	4.885341	0.556319	-2.920765
C	6.413813	0.041341	-1.156890
H	6.646680	-0.828686	-0.538522
H	7.197816	0.185645	-1.904815
H	6.417011	0.926631	-0.512044
C	3.136169	-2.856561	-0.274546
H	3.206486	-3.479332	0.609821
N	2.933629	-3.703802	-1.430337
O	3.118665	-3.243167	-2.566634
O	2.549582	-4.846581	-1.202675
C	4.504526	-1.159621	0.927461
C	5.108052	-2.036250	1.841826
C	4.491876	0.215444	1.204402
C	5.707831	-1.536412	2.991221
H	5.143192	-3.103407	1.628753
C	5.080899	0.708349	2.360577
H	3.992916	0.893936	0.512813
C	5.700156	-0.165777	3.252579
H	6.193812	-2.220145	3.683335
H	5.049002	1.777170	2.566650
H	6.173049	0.217957	4.153989

$TSII_{R3}$

P	0.449637	0.028554	-1.678958
P	0.539037	-0.736077	1.379838
C	-2.292348	-0.497839	1.447119
C	-1.939000	-2.794599	0.466703
C	-4.285205	-3.635890	1.983952
H	-3.695370	-4.368324	1.437383
C	-0.634766	-3.144130	0.797853
C	-0.583586	2.977460	-0.403476
C	-1.874275	2.506257	-0.981335
C	1.025463	0.126692	2.963192
C	-2.546124	-3.385662	-0.689080
C	-2.144799	1.151677	-1.171313

C	-2.840135	3.481547	-1.403368
C	-3.394562	0.746939	-1.699857
H	-3.587067	-0.320983	-1.813900
C	-1.040731	0.046082	0.792409
H	-0.916688	1.090642	1.117075
C	0.612245	2.700072	-1.056521
C	0.628560	1.775373	-2.231904
H	1.553945	1.873568	-2.806332
H	-0.217824	1.971004	-2.905991
C	-4.650395	-1.346953	2.755692
C	-2.699278	-1.823855	1.304733
C	-1.831971	-4.384809	-1.427259
C	0.683351	4.329103	1.241523
C	-1.182039	0.063135	-0.750233
H	-1.632180	-0.898382	-1.024565
C	-5.807248	-1.795976	3.436254
H	-6.388974	-1.070806	4.004282
C	-5.059830	4.007056	-2.329719
H	-6.014335	3.654208	-2.718620
C	0.075144	-2.432484	1.905725
H	0.986719	-2.960975	2.207271
H	-0.561170	-2.327173	2.797161
C	-4.100504	3.046532	-1.928224
C	-2.412587	-4.932421	-2.596801
H	-1.857700	-5.693882	-3.144288
C	-1.706550	3.944373	1.605141
H	-2.656557	3.530208	1.271002
C	-1.638771	4.641551	2.790042
H	-2.533900	4.763133	3.397050
C	-0.546166	-4.778919	-0.989524
H	-0.019037	-5.559752	-1.536649
C	-3.871585	-2.278872	1.995918
C	-4.351813	1.661696	-2.051423
H	-5.314201	1.331908	-2.440978
C	-4.238903	0.003695	2.813689
H	-4.844514	0.716854	3.371635
C	-0.554282	3.756412	0.799334
C	-4.345963	-3.519496	-2.322067
H	-5.317907	-3.183442	-2.677877
C	-3.089034	0.407728	2.189180
H	-2.770626	1.449170	2.247949
C	0.711881	5.060070	2.454238
H	1.659456	5.490381	2.777152
C	1.858183	4.104881	0.483916
H	2.798573	4.553061	0.802482
C	1.910112	-0.823751	3.770615
H	2.385159	-0.269379	4.590096
H	2.716815	-1.261742	3.164918
H	1.339169	-1.644696	4.219672
C	-3.539887	5.785062	-1.760980
H	-3.318698	6.849508	-1.717239
C	-3.817975	-2.980227	-1.170854
H	-4.377675	-2.225266	-0.621496
C	-2.591238	4.877678	-1.351927
H	-1.629307	5.236418	-0.994654
C	1.826425	3.285234	-0.617856
H	2.732284	3.119919	-1.202256
C	-3.641350	-4.506556	-3.042044
H	-4.071994	-4.927630	-3.947967
C	-5.409827	-4.042085	2.663285
H	-5.701143	-5.090074	2.643124
C	1.805014	1.376628	2.571406
H	1.263072	1.959417	1.817850
H	2.791440	1.133151	2.156699
H	1.954378	2.028172	3.442227
C	0.868891	-2.324404	-3.105476
H	0.573629	-2.987835	-3.929797
H	0.578818	-2.816909	-2.169266
H	1.961153	-2.236171	-3.135892
C	-0.420252	5.207538	3.219486
H	-0.381364	5.763518	4.153817
C	-4.791129	5.350941	-2.244283
H	-5.533556	6.080505	-2.560641
C	-1.294526	-1.167254	-3.576173
H	-1.385241	-1.675335	-4.545270
H	-1.843091	-0.220343	-3.649428
H	-1.798372	-1.804896	-2.839037
C	-6.184909	-3.115856	3.390861
H	-7.074125	-3.450125	3.920953
C	0.190937	-0.964515	-3.273522
C	0.048188	-4.150543	0.075407
H	1.054095	-4.432830	0.388732
C	-0.195793	0.530007	3.788743
H	-0.894984	-0.297250	3.963503
H	-0.750353	1.352263	3.319601
H	0.142315	0.891508	4.768407
C	0.831700	-0.223099	-4.452069
H	1.886770	0.023378	-4.293170

H	0.297403	0.699292	-4.704309
H	0.788492	-0.873818	-5.334560
Ni	1.989794	-0.644491	-0.227261
H	2.833897	-0.874314	0.974736
C	4.055723	-0.444726	-0.107252
N	4.216703	0.933802	0.160660
H	3.405534	1.514399	-0.048460
C	5.377763	1.734651	0.069969
O	5.228993	2.938319	0.126279
C	6.703779	1.061447	-0.119158
H	6.673513	0.330256	-0.935998
H	7.442788	1.830562	-0.348764
H	7.019932	0.523053	0.781112
C	3.508688	-0.868132	-1.382019
H	3.608549	-1.929031	-1.608335
N	3.767098	-0.096072	-2.582566
O	4.058052	-0.746150	-3.587722
O	3.678741	1.136094	-2.544930
C	5.006192	-1.346239	0.611491
C	5.723057	-2.340379	-0.058572
C	5.242531	-1.135665	1.976425
C	6.651734	-3.117625	0.629287
H	5.592744	-2.482158	-1.130885
C	6.167536	-1.910357	2.660941
H	4.702225	-0.338693	2.489858
C	6.873866	-2.907591	1.986518
H	7.213558	-3.880638	0.095437
H	6.344408	-1.735258	3.720003
H	7.604137	-3.512641	2.519310

VI_{R3}

P	0.494457	0.064759	-1.638799
P	0.442680	-0.837203	1.367260
C	-2.381236	-0.450823	1.365069
C	-2.136418	-2.773182	0.383438
C	-4.555931	-3.475570	1.849000
H	-3.991255	-4.245440	1.328926
C	-0.862996	-3.205850	0.740153
C	-0.465109	3.001786	-0.357446
C	-1.745022	2.589796	-1.001172
C	0.899203	-0.066644	3.008503
C	-2.776199	-3.367811	-0.754369
C	-2.072403	1.249368	-1.205179
C	-2.647612	3.609468	-1.455477
C	-3.327842	0.905705	-1.763530
H	-3.577243	-0.151219	-1.870067
C	-1.080425	0.036967	0.766777
H	-0.912637	1.065111	1.124368
C	0.751674	2.692330	-0.953983
C	0.795208	1.796078	-2.155213
H	1.766868	1.850513	-2.655527
H	0.012521	2.051872	-2.884527
C	-4.822825	-1.167092	2.594373
C	-2.854751	-1.752139	1.200816
C	-2.157300	-4.481693	-1.409583
C	0.764554	4.268449	1.381636
C	-1.167973	0.113791	-0.778155
H	-1.633776	-0.826466	-1.110170
C	-6.022519	-1.548163	3.241339
H	-6.580213	-0.787644	3.786687
C	-4.806261	4.241627	-2.455329
H	-5.764496	3.935976	-2.874029
C	-0.113865	-2.525369	1.841379
H	0.768923	-3.104191	2.136919
H	-0.741603	-2.405062	2.737441
C	-3.910125	3.235960	-2.020814
C	-2.780544	-5.052595	-2.544880
H	-2.299599	-5.901916	-3.029286
C	-1.655709	3.989439	1.604403
H	-2.603169	3.619443	1.215622
C	-1.624066	4.673225	2.798685
H	-2.546238	4.829914	3.355139
C	-0.910152	-4.955094	-0.938431
H	-0.452726	-5.815395	-1.425774
C	-4.071114	-2.141775	1.860926
C	-4.228550	1.864974	-2.143485
H	-5.196613	1.581846	-2.555081
C	-4.343367	0.159921	2.664244
H	-4.927951	0.906419	3.200569
C	-0.469949	3.759182	0.860687
C	-4.558919	-3.431109	-2.409405
H	-5.486167	-3.023648	-2.807229
C	-3.152583	0.497575	2.079935
H	-2.778727	1.519888	2.150374
C	0.757176	4.989150	2.600348
H	1.703183	5.374683	2.979063
C	1.970189	3.994375	0.692852
H	2.912001	4.388281	1.073714

C	1.819786	-1.044886	3.741383
H	2.280339	-0.539690	4.599933
H	2.639543	-1.408364	3.102816
H	1.282094	-1.918178	4.127858
C	-3.218831	5.943804	-1.838923
H	-2.946386	6.995931	-1.789937
C	-3.993421	-2.870046	-1.286879
H	-4.482057	-2.029472	-0.796435
C	-2.330946	4.991450	-1.396638
H	-1.364005	5.303733	-1.010027
C	1.965811	3.199252	-0.426835
H	2.898246	2.992819	-0.950249
C	-3.952811	-4.535768	-3.042692
H	-4.414859	-4.975795	-3.923841
C	-5.719868	-3.816524	2.497478
H	-6.062297	-4.849054	2.477353
C	1.643144	1.231760	2.716630
H	1.112478	1.846207	1.979821
H	2.656858	1.042873	2.340675
H	1.741804	1.834098	3.629180
C	0.211911	-2.390044	-2.780366
H	-0.044133	-3.028779	-3.635977
H	-0.539882	-2.565748	-2.003809
H	1.182318	-2.724222	-2.387651
C	-0.409181	5.183696	3.300932
H	-0.399385	5.732760	4.240116
C	-4.473497	5.570784	-2.362938
H	-5.168124	6.335215	-2.704422
C	-1.083824	-0.557781	-3.869390
H	-1.141961	-1.074825	-4.835682
H	-1.187831	0.516489	-4.066340
H	-1.949728	-0.881103	-3.280439
C	-6.468701	-2.845920	3.193325
H	-7.389726	-3.129303	3.698311
C	0.241046	-0.924133	-3.196275
C	-0.262533	-4.303401	0.080034
H	0.718570	-4.642305	0.413897
C	-0.333243	0.236853	3.859716
H	-1.014706	-0.616828	3.962889
H	-0.907187	1.078638	3.454533
H	-0.008390	0.523882	4.868231
C	1.400165	-0.665477	-4.156367
H	2.362329	-0.992261	-3.750177
H	1.485259	0.387530	-4.449735
H	1.235577	-1.243124	-5.074534
Ni	1.946777	-0.643852	-0.225840
H	3.161476	-0.779479	0.878700
C	4.050533	-0.531610	0.126711
N	4.342498	0.841437	0.485095
H	3.525447	1.449523	0.518091
C	5.464738	1.616810	0.151801
O	5.369282	2.823776	0.268438
C	6.715694	0.916159	-0.290026
H	6.536943	0.245157	-1.138717
H	7.442863	1.674050	-0.584947
H	7.140214	0.306386	0.516131
C	3.511712	-0.775343	-1.264617
H	3.607437	-1.813366	-1.595352
N	4.069051	0.067865	-2.313835
O	4.686367	-0.507853	-3.212557
O	3.912977	1.289362	-2.247735
C	5.087480	-1.521390	0.618452
C	5.782002	-2.362403	-0.251725
C	5.397525	-1.536760	1.982697
C	6.765366	-3.217547	0.239985
H	5.592122	-2.323429	-1.323787
C	6.377442	-2.391546	2.471735
H	4.884011	-0.848645	2.655991
C	7.061380	-3.237479	1.599268
H	7.310438	-3.859939	-0.447940
H	6.614192	-2.393237	3.533449
H	7.831656	-3.904574	1.979988

VII$_{R3}$

P	-0.320692	0.198553	1.561615
P	-0.283824	-0.682864	-1.427220
C	2.556349	-0.559647	-1.412903
C	2.053402	-2.826823	-0.433513
C	4.415273	-3.795503	-1.838935
H	3.766565	-4.492319	-1.312459
C	0.755672	-3.125157	-0.829647
C	1.055376	3.043081	0.363341
C	2.280304	2.450188	0.969577
C	-0.720612	0.224671	-3.000897
C	2.573612	-3.420434	0.762949
C	2.402094	1.077128	1.188663
C	3.333469	3.324485	1.408098
C	3.581070	0.554395	1.773102

H	3.651778	-0.523752	1.919802
C	1.302191	0.048030	-0.820658
H	1.239789	1.093409	-1.161339
C	-0.175522	2.873708	0.990406
C	-0.320301	1.940966	2.147457
H	-1.238352	2.133370	2.707967
H	0.529307	2.017964	2.841489
C	4.925765	-1.534805	-2.612617
C	2.893736	-1.901492	-1.245098
C	1.769336	-4.350282	1.500349
C	-0.052381	4.520726	-1.290376
C	1.365238	0.076745	0.726514
H	1.708545	-0.918794	1.032555
C	6.088791	-2.046964	-3.236276
H	6.730399	-1.357552	-3.784035
C	5.575786	3.624942	2.381964
H	6.477122	3.178137	2.800441
C	0.129061	-2.388382	-1.971707
H	-0.798950	-2.869789	-2.299360
H	0.804130	-2.321392	-2.836677
C	4.526122	2.767124	1.974440
C	2.261437	-4.883963	2.716345
H	1.637542	-5.589793	3.264364
C	2.298994	3.926435	-1.615599
H	3.201763	3.424427	-1.270188
C	2.317779	4.643558	-2.790484
H	3.231787	4.690968	-3.379393
C	0.492426	-4.699454	1.001736
H	-0.101006	-5.441209	1.536687
C	4.070369	-2.420021	-1.880901
C	4.621519	1.367532	2.136582
H	5.529802	0.946042	2.565890
C	4.581107	-0.167124	-2.700204
H	5.242646	0.510673	-3.238336
C	1.120252	3.833591	-0.831457
C	4.290775	-3.606312	2.477728
H	5.267294	-3.319565	2.862985
C	3.426311	0.298206	-2.128447
H	3.162079	1.353414	-2.208155
C	0.009955	5.271547	-2.488426
H	-0.886889	5.795940	-2.817075
C	-1.256187	4.400900	-0.554987
H	-2.146223	4.944656	-0.871203
C	-1.790554	-0.583547	-3.737710
H	-2.165088	-0.000413	-4.588671
H	-2.649908	-0.821948	-3.094879
H	-1.396110	-1.525278	-4.137971
C	4.271039	5.545528	1.749824
H	4.166483	6.626553	1.685255
C	3.847255	-3.078824	1.286122
H	4.476164	-2.380761	0.736992
C	3.238164	4.738685	1.333749
H	2.327972	5.194203	0.952813
C	-1.318587	3.576830	0.540650
H	-2.248214	3.493017	1.102265
C	3.493580	-4.516544	3.201919
H	3.857290	-4.926973	4.141270
C	5.547042	-4.263356	-2.464020
H	5.785977	-5.324032	-2.422090
C	-1.264218	1.599513	-2.619840
H	-0.642800	2.090160	-1.860849
H	-2.290915	1.545139	-2.235322
H	-1.284195	2.259960	-3.496686
C	-1.021113	-2.118144	2.988424
H	-0.877866	-2.771343	3.860084
H	-0.669135	-2.676805	2.108753
H	-2.099224	-1.912337	2.913748
C	1.165895	5.328273	-3.230528
H	1.196346	5.902236	-4.154222
C	5.458410	4.988198	2.266345
H	6.270199	5.638439	2.585358
C	1.211810	-1.157381	3.544519
H	1.215774	-1.657139	4.522502
H	1.839102	-0.262231	3.633067
H	1.688367	-1.846539	2.836515
C	6.398584	-3.383208	-3.162934
H	7.293945	-3.766248	-3.647966
C	-0.234442	-0.821680	3.175609
C	-0.003672	-4.086231	-0.120859
H	-0.986126	-4.360406	-0.504250
C	0.512856	0.405267	-3.887378
H	1.054360	-0.529374	-4.078854
H	1.220950	1.123705	-3.457575
H	0.196874	0.807018	-4.858977
C	-0.853414	-0.023494	4.328307
H	-1.878536	0.307801	4.138376
H	-0.252728	0.852632	4.593593
H	-0.887613	-0.669791	5.214657

Ni	-1.784350	-0.556692	0.172496
H	-3.246360	0.102172	-0.963402
C	-3.992070	0.367432	-0.163893
N	-4.012024	1.812207	-0.260102
H	-3.107959	2.239427	-0.444189
C	-4.860592	2.722497	0.357364
O	-4.548271	3.902292	0.361929
C	-6.152256	2.212283	0.931025
H	-6.012686	1.340874	1.580513
H	-6.611155	3.016196	1.508607
H	-6.842744	1.911223	0.133863
C	-3.445285	-0.279168	1.124433
H	-3.894085	-1.255768	1.298551
N	-3.627448	0.420800	2.381623
O	-4.023601	-0.258766	3.338008
O	-3.356312	1.623512	2.463774
C	-5.271381	-0.283994	-0.668395
C	-6.127734	-1.027553	0.146941
C	-5.591826	-0.129723	-2.021275
C	-7.283985	-1.601313	-0.381264
H	-5.921409	-1.133855	1.212567
C	-6.738667	-0.707777	-2.551501
H	-4.935843	0.468172	-2.656163
C	-7.588226	-1.450035	-1.731075
H	-7.951852	-2.160169	0.271330
H	-6.974053	-0.576362	-3.605738
H	-8.490815	-1.897762	-2.141687
C	-3.366127	-3.143371	-0.392628
C	-4.314013	-3.911658	-1.235792
H	-4.268354	-4.981400	-1.018672
H	-5.332482	-3.568229	-1.009737
H	-4.120582	-3.714431	-2.291961
O	-3.214825	-3.621776	0.834637
H	-2.570289	-3.053889	1.312478
O	-2.773766	-2.136996	-0.795505

$TSIII_{R3}$

P	0.296989	0.161399	-1.639027
P	0.342294	-0.738514	1.334434
C	-2.473908	-0.453479	1.464342
C	-2.162534	-2.750273	0.477653
C	-4.537036	-3.549323	1.981016
H	-3.967403	-4.290801	1.425544
C	-0.865575	-3.111102	0.825965
C	-0.936998	3.067107	-0.400437
C	-2.208942	2.505527	-0.936491
C	0.971552	0.201476	2.823906
C	-2.761933	-3.336719	-0.685276
C	-2.382535	1.136629	-1.148463
C	-3.260087	3.410362	-1.315440
C	-3.608963	0.649114	-1.660093
H	-3.718512	-0.425853	-1.803334
C	-1.222208	0.080988	0.799743
H	-1.090349	1.123221	1.127410
C	0.254931	2.858034	-1.087805
C	0.305400	1.905749	-2.235275
H	1.172935	2.073366	-2.873317
H	-0.596687	1.982690	-2.859853
C	-4.843245	-1.260707	2.778725
C	-2.912417	-1.768502	1.310694
C	-2.034497	-4.317590	-1.435764
C	0.290471	4.535397	1.175778
C	-1.355057	0.102142	-0.739488
H	-1.745357	-0.883206	-1.021409
C	-6.008125	-1.688402	3.459203
H	-6.569137	-0.955450	4.037869
C	-5.548847	3.775521	-2.149630
H	-6.486603	3.354474	-2.510397
C	-0.153202	-2.397762	1.933792
H	0.750563	-2.928249	2.248079
H	-0.797256	-2.256777	2.812337
C	-4.501208	2.888112	-1.805013
C	-2.600941	-4.851125	-2.618524
H	-2.033575	-5.596397	-3.175282
C	-2.050428	3.991610	1.634986
H	-2.982451	3.510768	1.342234
C	-1.986220	4.705794	2.810026
H	-2.863892	4.771562	3.450063
C	-0.753924	-4.717270	-0.989151
H	-0.217967	-5.488551	-1.541221
C	-4.091170	-2.202431	2.003944
C	-4.646308	1.491841	-1.958833
H	-5.590088	1.096491	-2.332499
C	-4.394769	0.076752	2.856418
H	-4.976312	0.796848	3.430690
C	-0.919999	3.871231	0.787207
C	-4.554985	-3.471735	-2.326265
H	-5.531873	-3.145584	-2.677789

C	-3.238592	0.459414	2.230029
H	-2.894529	1.491825	2.300926
C	0.311872	5.288709	2.374257
H	1.235862	5.795897	2.650793
C	1.447237	4.386285	0.372828
H	2.358762	4.924306	0.633682
C	2.129965	-0.571261	3.455226
H	2.518855	0.003735	4.305318
H	2.960835	-0.731143	2.757547
H	1.820014	-1.551110	3.837474
C	-4.151006	5.657746	-1.609268
H	-4.010184	6.735392	-1.557261
C	-4.038431	-2.944020	-1.164424
H	-4.612168	-2.208480	-0.603930
C	-3.118680	4.821480	-1.254459
H	-2.173739	5.251849	-0.934085
C	1.434628	3.548229	-0.714641
H	2.327105	3.447986	-1.333234
C	-3.833007	-4.433818	-3.062437
H	-4.253867	-4.843943	-3.977831
C	-5.668621	-3.934952	2.660697
H	-5.984806	-4.975512	2.631495
C	1.436831	1.582658	2.373166
H	0.681174	2.101833	1.773934
H	2.361544	1.542247	1.787086
H	1.637678	2.211112	3.250513
C	0.827109	-2.188810	-3.064123
H	0.573042	-2.860195	-3.895944
H	0.547750	-2.705888	-2.136079
H	1.915315	-2.059135	-3.083533
C	-0.797143	5.365727	3.183047
H	-0.762723	5.938645	4.107224
C	-5.384466	5.134918	-2.047790
H	-6.194928	5.808169	-2.318838
C	-1.382531	-1.122601	-3.537487
H	-1.450249	-1.619840	-4.514233
H	-1.973280	-0.200294	-3.597551
H	-1.857036	-1.793383	-2.810491
C	-6.418530	-2.997811	3.400733
H	-7.313443	-3.316074	3.931023
C	0.094290	-0.860522	-3.237611
C	-0.180474	-4.112847	0.099678
H	0.810650	-4.414915	0.435463
C	-0.164989	0.376012	3.837094
H	-0.628484	-0.569191	4.142738
H	-0.953167	1.038502	3.461506
H	0.246390	0.843884	4.740941
C	0.704013	-0.098906	-4.419061
H	1.746602	0.194857	-4.260429
H	0.128633	0.796438	-4.678080
H	0.686106	-0.758542	-5.295902
Ni	1.778380	-0.824428	-0.272448
H	3.216028	0.122062	0.713977
C	4.087535	0.238594	0.036418
N	4.180390	1.676597	-0.083665
H	3.295052	2.170722	-0.029882
C	5.118741	2.419633	-0.784373
O	4.896552	3.598974	-1.004575
C	6.389512	1.720955	-1.184528
H	6.212389	0.738339	-1.639636
H	6.928291	2.352094	-1.892808
H	7.026466	1.549987	-0.308253
C	3.808434	-0.570715	-1.266865
H	4.693280	-1.167696	-1.504717
N	3.614484	0.149994	-2.537829
O	3.944314	-0.465677	-3.551365
O	3.101124	1.270864	-2.547388
C	5.230810	-0.341103	0.866418
C	5.858171	-1.563880	0.618926
C	5.617980	0.385022	2.000972
C	6.860424	-2.035102	1.467692
H	5.589747	-2.177906	-0.239498
C	6.613020	-0.084821	2.847677
H	5.138099	1.342194	2.201613
C	7.243490	-1.298910	2.582237
H	7.347896	-2.982402	1.243368
H	6.902021	0.503203	3.716325
H	8.028815	-1.666293	3.239179
C	3.083525	-3.208206	0.122158
C	3.513037	-4.443384	0.839883
H	3.401791	-5.322463	0.200671
H	4.577647	-4.347000	1.086984
H	2.966945	-4.572413	1.777464
O	3.268100	-3.120482	-1.130557
H	3.214701	-1.838053	-1.304657
O	2.587460	-2.247610	0.801049

VIII$_{R3}$

P	0.022444	-0.021154	-1.754849	C	-4.542010	2.201941	-1.889491
P	0.152620	-0.982794	1.143209	H	-5.560276	2.005332	-2.223112
C	-2.554289	-0.236985	1.534993	C	-4.220224	0.578439	3.105838
C	-2.714975	-2.558025	0.552438	H	-4.630406	1.380758	3.718058
C	-4.955282	-3.004600	2.358905	C	-0.381003	3.788931	0.758091
H	-4.559375	-3.826025	1.766079	C	-5.556259	-2.811978	-1.882205
C	-1.470961	-3.151512	0.733354	H	-6.476823	-2.286657	-2.129195
C	-0.553205	3.012098	-0.435402	C	-3.096118	0.785474	2.351487
C	-1.916897	2.703419	-0.955701	H	-2.601618	1.757815	2.361627
C	1.010480	-0.220228	2.609023	C	1.102829	4.952657	2.337062
C	-3.565956	-3.025878	-0.500565	H	2.108507	5.270787	2.609799
C	-2.380760	1.398193	-1.118486	C	2.040086	3.870864	0.326051
C	-2.760062	3.798477	-1.350786	H	3.042872	4.207807	0.590783
C	-3.703153	1.168075	-1.570006	C	1.944748	-1.265739	3.220168
H	-4.051357	0.137425	-1.651491	H	2.546927	-0.791046	4.006251
C	-1.302686	0.087878	0.753221	H	2.637418	-1.695801	2.486342
H	-0.960162	1.083931	1.072445	H	1.391496	-2.087262	3.690680
C	0.573857	2.605557	-1.142873	C	-3.145127	6.171928	-1.732701
C	0.437688	1.678917	-2.307751	H	-2.775005	7.195078	-1.722266
H	1.352975	1.630029	-2.901294	C	-4.779119	-2.371546	-0.836106
H	-0.387191	1.984512	-2.968032	H	-5.089815	-1.502883	-0.258220
C	-4.853239	-0.685000	3.117705	C	-2.316561	5.146702	-1.340855
C	-3.187604	-1.475652	1.461465	H	-1.298674	5.372125	-1.032691
C	-3.174647	-4.166862	-1.272699	C	1.859206	3.068569	-0.772057
C	0.934284	4.215234	1.140572	H	2.707128	2.808660	-1.405064
C	-1.552573	0.181247	-0.772028	C	-5.173252	-3.942289	-2.633539
H	-2.132500	-0.710018	-1.056283	H	-5.799693	-4.284615	-3.454427
C	-5.982154	-0.936703	3.933621	C	-6.042324	-3.220319	3.172864
H	-6.369079	-0.124301	4.547940	H	-6.497279	-4.208017	3.211673
C	-4.923333	4.617615	-2.195169	C	1.799056	0.968776	2.076805
H	-5.934741	4.396400	-2.534644	H	1.153245	1.668327	1.534109
C	-0.507075	-2.587578	1.732027	H	2.591494	0.644946	1.389894
H	0.346706	-3.256690	1.888765	H	2.271056	1.527662	2.896636
H	-0.982269	-2.410938	2.708999	C	-0.624942	-2.395091	-2.968261
C	-4.091547	3.538550	-1.811387	H	-0.996811	-2.953679	-3.838014
C	-4.009100	-4.606758	-2.328679	H	-1.359509	-2.518099	-2.164153
H	-3.701572	-5.478111	-2.906044	H	0.315298	-2.858085	-2.644700
C	-1.467129	4.131421	1.604604	C	0.028848	5.255215	3.140063
H	-2.474255	3.831696	1.319012	H	0.173264	5.818899	4.059339
C	-1.265752	4.837903	2.768421	C	-4.464653	5.911352	-2.154177
H	-2.115005	5.084096	3.402916	H	-5.110269	6.733312	-2.456014
C	-1.940503	-4.798252	-0.986267	C	-1.749401	-0.388029	-3.905944
H	-1.652761	-5.678156	-1.560655	H	-1.918748	-0.861145	-4.882194
C	-4.329823	-1.732582	2.292388	H	-1.746931	0.696886	-4.066904

H	-2.611713	-0.635284	-3.274342
C	-6.570102	-2.177439	3.961253
H	-7.434511	-2.361686	4.595479
C	-0.440787	-0.924083	-3.324071
C	-1.096142	-4.278676	-0.037242
H	-0.128495	-4.744456	0.153400
C	-0.002268	0.258885	3.650109
H	-0.717470	-0.518594	3.947045
H	-0.571806	1.128106	3.299359
H	0.539532	0.571075	4.552411
C	0.703499	-0.745307	-4.324011
H	1.672081	-1.044088	-3.908866
H	0.785948	0.289291	-4.676741
H	0.510948	-1.373135	-5.203175
Ni	1.364843	-1.274428	-0.585465
H	3.754598	-0.530154	-0.108763
C	4.798919	-0.175041	-0.186333
N	4.699283	1.249709	0.098636
H	3.786267	1.661332	-0.061890
C	5.681442	2.198134	0.296633
O	5.368166	3.377637	0.382053
C	7.104162	1.726379	0.440625
H	7.379044	0.937157	-0.268676
H	7.767118	2.582526	0.304585
H	7.269200	1.314652	1.443614
C	5.224622	-0.456064	-1.619785
H	6.181150	0.001486	-1.893208
N	4.235690	0.065983	-2.630499
O	4.523838	-0.089448	-3.803578
O	3.202081	0.594781	-2.215474
C	5.605506	-0.938062	0.847324
C	6.567047	-1.895777	0.519082
C	5.350263	-0.681314	2.199143
C	7.252403	-2.585156	1.519233
H	6.814556	-2.106217	-0.520766
C	6.027457	-1.371107	3.196406
H	4.624543	0.089622	2.459455
C	6.983334	-2.328263	2.858768
H	8.008081	-3.318099	1.244070
H	5.815000	-1.155208	4.242036
H	7.521439	-2.863368	3.637939
C	2.899473	-2.934750	-0.970433
C	3.808268	-4.086514	-1.197821
H	4.284425	-4.026007	-2.179176
H	4.562099	-4.132843	-0.405089
H	3.235375	-5.019563	-1.145014
O	2.587541	-2.115213	-1.896626
H	5.288659	-1.524296	-1.848154
O	2.390176	-2.716740	0.185840

IV_{R1}

P	0.236440	-0.350572	-1.739800
P	0.347245	-0.804913	1.317377
C	-2.275398	0.324076	1.560240
C	-2.738527	-2.100590	1.055337
C	-4.969368	-1.916542	2.913999
H	-4.678821	-2.880754	2.503090
C	-1.570024	-2.790642	1.355570
C	-0.180396	2.935493	-0.928641
C	-1.539939	2.599778	-1.440437
C	1.250040	0.150455	2.650758
C	-3.660648	-2.654223	0.109564
C	-2.055403	1.306730	-1.377888
C	-2.305173	3.633104	-2.081383
C	-3.351418	1.039315	-1.882887
H	-3.736760	0.021104	-1.807439
C	-1.012338	0.338964	0.728262
H	-0.549611	1.329142	0.847430
C	0.942712	2.347944	-1.503462
C	0.801867	1.236606	-2.497969
H	1.750897	1.050592	-3.013811
H	0.052849	1.507030	-3.253737
C	-4.588660	0.479520	3.189359
C	-3.056672	-0.815227	1.732857
C	-3.413883	-3.951061	-0.443946
C	1.313799	4.326529	0.479990
C	-1.292491	0.148738	-0.783233
H	-1.930839	-0.740153	-0.864912
C	-5.725185	0.530160	4.031199
H	-6.006733	1.489325	4.465037
C	-4.375220	4.356988	-3.201137
H	-5.373228	4.110935	-3.562978
C	-0.516017	-2.160850	2.216479
H	0.247768	-2.891350	2.507597
H	-0.945247	-1.731920	3.134835
C	-3.616544	3.337814	-2.577065
C	-4.313758	-4.480707	-1.399971
H	-4.114816	-5.471566	-1.807884

C	-1.102762	4.465834	0.818252
H	-2.113055	4.179574	0.531837
C	-0.907414	5.351108	1.853365
H	-1.765971	5.756476	2.385572
C	-2.264004	-4.662455	-0.029166
H	-2.097396	-5.666847	-0.419357
C	-4.204097	-0.765163	2.594728
C	-4.117617	2.023047	-2.450563
H	-5.116852	1.800297	-2.823715
C	-3.811512	1.629662	2.925584
H	-4.114118	2.583247	3.357546
C	-0.006360	3.908143	0.110878
C	-5.649047	-2.478055	-1.282350
H	-6.514630	-1.908438	-1.615212
C	-2.683838	1.544124	2.153573
H	-2.080517	2.433464	1.973997
C	1.479238	5.246056	1.543247
H	2.490529	5.551749	1.811288
C	2.418042	3.815669	-0.242492
H	3.415617	4.198651	-0.022180
C	2.035312	-0.831774	3.518725
H	2.675034	-0.271139	4.213576
H	2.682505	-1.484643	2.918035
H	1.374933	-1.467277	4.121433
C	-2.561617	5.910394	-2.905039
H	-2.147103	6.905723	-3.052095
C	-4.803231	-1.942419	-0.338243
H	-5.003202	-0.952472	0.067584
C	-1.803531	4.945016	-2.284963
H	-0.796080	5.188694	-1.957217
C	2.232650	2.845223	-1.195074
H	3.062239	2.477776	-1.797469
C	-5.408083	-3.760690	-1.816240
H	-6.088463	-4.176291	-2.556437
C	-6.059491	-1.837358	3.748576
H	-6.623763	-2.737698	3.983371
C	2.194833	1.102757	1.926266
H	1.643271	1.781792	1.265872
H	2.909758	0.544387	1.307419
H	2.763122	1.716506	2.641064
C	-1.325089	-2.424489	-2.708073
H	-1.479106	-3.176354	-3.494597
H	-2.315404	-2.012599	-2.470924
H	-0.949146	-2.948838	-1.821103
C	0.394844	5.743846	2.224877
H	0.536388	6.447314	3.042713
C	-3.864572	5.622191	-3.358995
H	-4.454863	6.396707	-3.844120
C	-1.055691	-0.511594	-4.287227
H	-1.485320	-1.185967	-5.040186
H	-0.360358	0.151654	-4.813996
H	-1.877167	0.096039	-3.887104
C	-6.451571	-0.603025	4.305364
H	-7.321448	-0.553902	4.956894
C	-0.361390	-1.349677	-3.213350
C	-1.362198	-4.086941	0.829015
H	-0.471963	-4.630832	1.139920
C	0.299830	0.959359	3.533524
H	-0.497403	0.352220	3.981347
H	-0.170024	1.783349	2.983895
H	0.870254	1.408624	4.357038
C	0.894082	-2.000206	-3.806817
H	1.347244	-2.711432	-3.108866
H	1.657582	-1.254866	-4.071931
H	0.628949	-2.538137	-4.727073
Ni	1.510779	-1.408765	-0.296654
H	2.162428	-1.822938	0.992109
C	5.080803	-0.327763	0.107880
N	4.664864	0.434462	-0.959769
H	4.242802	1.333622	-0.738575
C	4.673211	0.145775	-2.337445
O	4.051653	0.876255	-3.086637
C	5.542181	-0.967196	-2.840377
H	4.914307	-1.807822	-3.155628
H	6.056025	-0.600533	-3.732707
H	6.278355	-1.329958	-2.118771
C	4.957041	-1.697193	0.124270
H	5.533659	-2.325418	0.790971
N	4.132058	-2.431356	-0.730793
O	4.352483	-3.641456	-0.874539
O	3.155445	-1.863258	-1.339094
C	5.641762	0.397400	1.244796
C	5.605888	-0.155833	2.536484
C	6.160339	1.692975	1.076499
C	6.078094	0.564099	3.623304
H	5.164282	-1.139573	2.687129
C	6.623861	2.413423	2.168574
H	6.226034	2.121863	0.077751

C	6.583609	1.852392	3.443845
H	6.036390	0.127637	4.618991
H	7.029978	3.411976	2.023828
H	6.944779	2.418870	4.299463
C	1.693738	-4.545653	-0.468430
C	1.943420	-5.746154	-1.323121
H	2.994301	-5.743918	-1.635493
H	1.744173	-6.684839	-0.794473
H	1.321586	-5.695183	-2.218639
O	2.086852	-4.607075	0.819496
H	2.567277	-5.435871	0.980027
O	1.145121	-3.537492	-0.874095

V_{R1}

P	0.425070	-0.347192	-1.697903
P	0.444413	-0.792728	1.372945
C	-2.273056	0.101545	1.472363
C	-2.493389	-2.342801	0.883240
C	-4.934880	-2.347361	2.493991
H	-4.551561	-3.279306	2.086480
C	-1.278044	-2.894431	1.272806
C	0.077683	2.875069	-0.814085
C	-1.301223	2.618503	-1.322840
C	1.278620	0.182874	2.734148
C	-3.265355	-3.007558	-0.125892
C	-1.867780	1.344222	-1.335855
C	-2.044146	3.724363	-1.862193
C	-3.198823	1.170836	-1.787019
H	-3.634023	0.170961	-1.743354
C	-0.963010	0.248944	0.729476
H	-0.593384	1.269601	0.907668
C	1.173284	2.289891	-1.439921
C	0.969252	1.229758	-2.475103
H	1.890053	1.041419	-3.032937
H	0.189343	1.527518	-3.189979
C	-4.725229	0.052504	2.882883
C	-2.989300	-1.095875	1.532696
C	-2.824797	-4.276562	-0.627555
C	1.638667	4.148648	0.630453
C	-1.150313	0.123928	-0.803671
H	-1.801747	-0.746050	-0.975141
C	-5.937731	0.008258	3.611228
H	-6.312712	0.932994	4.048684
C	-4.121819	4.610073	-2.842307
H	-5.142819	4.431593	-3.178227
C	-0.391364	-2.172003	2.236341
H	0.376868	-2.835027	2.648158
H	-0.960764	-1.743407	3.074082
C	-3.385331	3.519249	-2.320440
C	-3.573803	-4.919839	-1.641250
H	-3.226569	-5.885406	-2.008019
C	-0.764380	4.293962	1.061467
H	-1.787742	4.040786	0.790275
C	-0.521026	5.105482	2.146325
H	-1.354282	5.479257	2.738229
C	-1.609739	-4.824041	-0.154552
H	-1.276397	-5.785216	-0.544125
C	-4.212328	-1.143882	2.284362
C	-3.942807	2.222873	-2.251480
H	-4.969554	2.070708	-2.582375
C	-3.995152	1.253952	2.747673
H	-4.390513	2.166409	3.192710
C	0.299978	3.776137	0.279205
C	-5.118403	-3.071580	-1.702502
H	-6.001681	-2.603470	-2.132954
C	-2.799756	1.267399	2.080472
H	-2.232159	2.194710	1.997557
C	1.852242	5.000506	1.740758
H	2.876135	5.274549	1.994591
C	2.717170	3.628581	-0.124581
H	3.731135	3.953348	0.111172
C	1.970951	-0.793085	3.684367
H	2.593828	-0.228495	4.390740
H	2.628921	-1.490378	3.148863
H	1.254987	-1.377863	4.273755
C	-2.232240	6.063115	-2.514037
H	-1.780961	7.048757	-2.608582
C	-4.429584	-2.432284	-0.696478
H	-4.776010	-1.467086	-0.330189
C	-1.494040	5.026316	-1.993474
H	-0.465643	5.206894	-1.690455
C	2.489819	2.699497	-1.109460
H	3.312259	2.303100	-1.706817
C	-4.694234	-4.330659	-2.175491
H	-5.251616	-4.828630	-2.965871
C	-6.104596	-2.359871	3.217309
H	-6.633162	-3.299395	3.366123
C	2.302894	1.079357	2.052923

H	1.825931	1.707754	1.294421
H	3.078856	0.478004	1.560716
H	2.796527	1.742676	2.777737
C	-0.523878	-2.755268	-2.581759
H	-0.834101	-3.426207	-3.394734
H	-1.380022	-2.655237	-1.905827
H	0.288514	-3.242259	-2.029356
C	0.798587	5.462713	2.492581
H	0.978542	6.107967	3.349785
C	-3.562256	5.861006	-2.933982
H	-4.136193	6.691542	-3.339552
C	-1.277791	-0.796135	-3.916184
H	-1.501668	-1.429242	-4.785165
H	-1.076945	0.213235	-4.295558
H	-2.188097	-0.754239	-3.306370
C	-6.621034	-1.171772	3.773456
H	-7.550060	-1.195357	4.339145
C	-0.107322	-1.401958	-3.145833
C	-0.837335	-4.127888	0.738039
H	0.120364	-4.530019	1.070077
C	0.280165	1.041684	3.510698
H	-0.562518	0.464713	3.912433
H	-0.126356	1.857651	2.899889
H	0.795235	1.508517	4.360680
C	1.109148	-1.562207	-4.058271
H	1.956825	-2.003256	-3.519116
H	1.434887	-0.613556	-4.501380
H	0.859484	-2.241746	-4.883371
Ni	1.671335	-1.380877	-0.209790
H	2.203339	-1.947386	1.078011
C	4.705940	-1.270435	-0.031443
N	4.176051	-0.451629	-1.018082
H	3.922869	0.494288	-0.731132
C	4.337469	-0.537436	-2.424050
O	3.969661	0.413466	-3.087254
C	4.988579	-1.742424	-3.025712
H	4.246417	-2.523127	-3.229654
H	5.410793	-1.437101	-3.984814
H	5.770514	-2.181520	-2.400005
C	4.620144	-2.638302	-0.104687
H	5.279013	-3.301059	0.442094
N	3.678056	-3.323938	-0.880859
O	3.879342	-4.495686	-1.183422
O	2.590083	-2.732939	-1.236894
C	5.406961	-0.608931	1.063959
C	5.482816	-1.219719	2.327310
C	5.958315	0.672957	0.891365
C	6.095812	-0.566523	3.386088
H	5.020027	-2.194119	2.478201
C	6.566544	1.323896	1.955048
H	5.937101	1.147356	-0.089312
C	6.635362	0.707313	3.203561
H	6.142472	-1.044667	4.361933
H	7.000294	2.310283	1.808418
H	7.112015	1.219339	4.036485

$TSII_{R1}$

P	0.488415	-0.163651	-1.731399
P	0.555070	-0.853297	1.244440
C	-2.173283	-0.039551	1.487925
C	-2.374942	-2.432952	0.712352
C	-4.625066	-2.673759	2.554845
H	-4.224120	-3.558720	2.066180
C	-1.132726	-3.020999	0.923642
C	-0.006016	2.981744	-0.660231
C	-1.359044	2.685554	-1.216899
C	1.265419	-0.023980	2.769400
C	-3.246384	-2.978355	-0.285906
C	-1.867096	1.388459	-1.285312
C	-2.134904	3.770625	-1.751537
C	-3.170540	1.164242	-1.791889
H	-3.553938	0.141781	-1.802012
C	-0.891414	0.196714	0.720730
H	-0.540118	1.206833	0.980966
C	1.129955	2.465019	-1.274227
C	0.996363	1.475713	-2.387017
H	1.939516	1.362702	-2.932577
H	0.226008	1.793349	-3.102576
C	-4.516849	-0.285940	3.052200
C	-2.827285	-1.269413	1.525159
C	-2.874495	-4.184971	-0.963594
C	1.463276	4.232394	0.894863
C	-1.098355	0.177083	-0.812707
H	-1.709187	-0.709768	-1.035820
C	-5.664722	-0.436115	3.866180
H	-6.057168	0.443001	4.376525
C	-4.209131	4.583720	-2.799661
H	-5.205752	4.367616	-3.183213

C	-0.173493	-2.411685	1.897657	H	3.037279	0.746413	1.750933
H	0.652668	-3.094932	2.127229	H	2.505027	1.720964	3.135792
H	-0.670559	-2.158977	2.846769	C	-0.518008	-2.496044	-2.794258
C	-3.446018	3.515635	-2.269428	H	-0.731500	-3.126465	-3.667871
C	-3.736330	-4.717060	-1.953258	H	-1.464424	-2.376833	-2.253807
H	-3.443138	-5.638539	-2.455639	H	0.181797	-3.043283	-2.152535
C	-0.958006	4.299652	1.236757	C	0.516055	5.478051	2.751912
H	-1.963092	4.019349	0.925719	H	0.643736	6.108749	3.629017
C	-0.778297	5.088467	2.349875	C	-3.703158	5.859645	-2.843173
H	-1.643150	5.420176	2.920934	H	-4.296165	6.671805	-3.258298
C	-1.629674	-4.786122	-0.662741	C	-0.967028	-0.435302	-4.134443
H	-1.347378	-5.703155	-1.178771	H	-1.223002	-1.081345	-4.984585
C	-3.986463	-1.421931	2.359980	H	-0.582949	0.503175	-4.550045
C	-3.945301	2.193967	-2.256202	H	-1.898896	-0.216999	-3.600210
H	-4.948700	2.004164	-2.635484	C	-6.265802	-1.661932	4.018767
C	-3.874442	0.964470	2.908670	H	-7.145805	-1.766680	4.649793
H	-4.293840	1.835637	3.410808	C	0.050678	-1.159503	-3.254798
C	0.148787	3.840345	0.477357	C	-0.767509	-4.196879	0.226729
C	-5.262513	-2.877280	-1.644287	H	0.209232	-4.641325	0.417869
H	-6.183671	-2.368403	-1.921740	C	0.165806	0.548179	3.665674
C	-2.729716	1.073384	2.166346	H	-0.621642	-0.176784	3.907973
H	-2.224269	2.036296	2.081435	H	-0.311727	1.426638	3.215491
C	1.610616	5.061240	2.032849	H	0.614498	0.875927	4.612541
H	2.616046	5.355199	2.333511	C	1.349283	-1.395661	-4.027433
C	2.586108	3.753919	0.178658	H	2.047159	-1.998457	-3.433886
H	3.582041	4.080269	0.479317	H	1.845327	-0.464187	-4.329833
C	2.075012	-1.055925	3.552057	H	1.129887	-1.960340	-4.942551
H	2.661570	-0.547565	4.328399	Ni	1.903548	-1.087247	-0.356835
H	2.784693	-1.597934	2.913587	H	2.855701	-1.350311	0.833687
H	1.434890	-1.791943	4.052308	C	4.271200	-1.297231	0.029893
C	-2.403197	6.112536	-2.360824	N	3.787727	-0.439838	-1.025931
H	-1.994430	7.119508	-2.415826	H	3.667668	0.526480	-0.710110
C	-4.458640	-2.344483	-0.663261	C	4.263503	-0.388280	-2.383143
H	-4.749782	-1.419161	-0.169356	O	4.126823	0.675540	-2.953095
C	-1.640742	5.098794	-1.829817	C	4.876450	-1.597784	-3.000514
H	-0.635031	5.317251	-1.479169	H	4.166360	-2.429004	-3.068347
C	2.422484	2.867830	-0.856148	H	5.204742	-1.327703	-4.005472
H	3.282532	2.512883	-1.427456	H	5.731107	-1.957072	-2.417337
C	-4.906174	-4.079110	-2.289734	C	4.511898	-2.662917	-0.214654
H	-5.555553	-4.495089	-3.057095	H	5.323023	-3.204839	0.252165
C	-5.731045	-2.790053	3.363964	N	3.585113	-3.446787	-0.859205
H	-6.195573	-3.764203	3.501818	O	3.810341	-4.631185	-1.106092
C	2.154733	1.115704	2.288167	O	2.450032	-2.905015	-1.172287
H	1.606178	1.777665	1.609269	C	5.124037	-0.621822	1.035915

C	5.371971	-1.268359	2.254743
C	5.665496	0.653628	0.821389
C	6.125957	-0.650966	3.242297
H	4.947772	-2.256929	2.428858
C	6.421439	1.269415	1.813034
H	5.528555	1.165393	-0.131662
C	6.645942	0.624665	3.026772
H	6.302855	-1.161977	4.186138
H	6.844449	2.254769	1.631204
H	7.231207	1.113141	3.802550

VI$_{R1}$

P	0.524861	-0.099692	-1.582059
P	0.231528	-1.051984	1.300790
C	-2.407397	-0.017754	1.402693
C	-2.692804	-2.353492	0.469409
C	-5.118081	-2.527824	2.066916
H	-4.737376	-3.407800	1.553411
C	-1.542222	-3.072376	0.777182
C	0.129856	2.992094	-0.467852
C	-1.214798	2.803461	-1.087049
C	0.992944	-0.318522	2.851921
C	-3.494122	-2.763583	-0.645219
C	-1.793703	1.543252	-1.236596
C	-1.913940	3.958043	-1.579292
C	-3.095180	1.422113	-1.781464
H	-3.537117	0.427094	-1.851727
C	-1.053699	0.169850	0.758317
H	-0.646574	1.128688	1.116080
C	1.260630	2.450203	-1.069035
C	1.127478	1.506484	-2.220823
H	2.090359	1.340064	-2.715985
H	0.411558	1.870220	-2.971101
C	-4.889749	-0.191850	2.741317
C	-3.136612	-1.200056	1.303973
C	-3.166744	-3.970127	-1.344593
C	1.602701	4.067515	1.211388
C	-1.122723	0.267548	-0.784081
H	-1.747934	-0.574756	-1.117414
C	-6.116650	-0.306356	3.436947
H	-6.492061	0.564910	3.972746
C	-3.924590	4.945236	-2.602951
H	-4.926460	4.807705	-3.008257
C	-0.612138	-2.580527	1.844250
H	0.179652	-3.309110	2.051475
H	-1.142712	-2.363741	2.782919
C	-3.229843	3.807693	-2.126729
C	-3.945368	-4.353312	-2.463667
H	-3.686563	-5.274570	-2.985117
C	-0.823697	4.249626	1.468380
H	-1.830024	4.041872	1.108340
C	-0.645342	4.961142	2.632660
H	-1.512819	5.303194	3.193546
C	-2.042486	-4.722316	-0.927228
H	-1.803698	-5.648170	-1.449769
C	-4.376947	-1.318460	2.019691
C	-3.802602	2.518615	-2.196452
H	-4.808385	2.407842	-2.599910
C	-4.150666	1.012927	2.747882
H	-4.551739	1.876410	3.277329
C	0.286001	3.777670	0.720944
C	-5.314862	-2.385151	-2.214972
H	-6.145885	-1.772953	-2.560006
C	-2.940353	1.086145	2.113153
H	-2.363807	2.012323	2.136669
C	1.749446	4.824071	2.398682
H	2.756370	5.042973	2.753157
C	2.726326	3.555776	0.519701
H	3.726209	3.797769	0.879715
C	1.846666	-1.379812	3.545125
H	2.351298	-0.925923	4.407416
H	2.613721	-1.801847	2.885806
H	1.243216	-2.213263	3.923760
C	-2.039488	6.340447	-2.063586
H	-1.573294	7.323690	-2.058742
C	-4.590693	-1.993836	-1.112409
H	-4.857297	-1.076465	-0.590347
C	-1.343215	5.257316	-1.580685
H	-0.331804	5.398766	-1.207273
C	2.554105	2.744053	-0.572811
H	3.417458	2.365036	-1.124407
C	-4.994400	-3.577506	-2.896286
H	-5.577904	-3.879840	-3.763130
C	-6.300531	-2.610634	2.763984
H	-6.844413	-3.552743	2.789145
C	1.840631	0.887571	2.457882
H	1.270386	1.614085	1.867958
H	2.725550	0.613465	1.867726

H	2.195264	1.407088	3.358068
C	-0.280436	-2.512787	-2.626963
H	-0.573487	-3.138296	-3.480877
H	-1.135551	-2.472900	-1.945542
H	0.540300	-3.023685	-2.101494
C	0.651112	5.259539	3.100524
H	0.777811	5.831984	4.016843
C	-3.346618	6.190112	-2.570166
H	-3.887653	7.057327	-2.942670
C	-1.051113	-0.495894	-3.871430
H	-1.199533	-1.057095	-4.803500
H	-0.879266	0.551598	-4.146683
H	-1.993441	-0.551763	-3.313410
C	-6.813409	-1.489984	3.448249
H	-7.753965	-1.568199	3.989330
C	0.113984	-1.120477	-3.102655
C	-1.228250	-4.262377	0.077549
H	-0.327050	-4.809126	0.354563
C	-0.113430	0.158363	3.799212
H	-0.859341	-0.612704	4.026168
H	-0.641090	1.034069	3.404826
H	0.345256	0.457864	4.750583
C	1.348786	-1.210138	-3.995938
H	2.169407	-1.735649	-3.494121
H	1.723298	-0.235897	-4.329144
H	1.099964	-1.792331	-4.892107
Ni	1.728205	-1.274283	-0.217720
H	3.829190	-0.931435	1.287216
C	4.449812	-1.250412	0.431169
N	3.624246	-0.720460	-0.739263
H	3.486300	0.287770	-0.600202
C	4.129542	-0.834986	-2.087184
O	4.029480	0.133093	-2.814283
C	4.696874	-2.147485	-2.513971
H	4.070608	-2.993953	-2.211382
H	4.825480	-2.135168	-3.598211
H	5.678664	-2.299073	-2.048021
C	4.526834	-2.724346	0.427770
H	5.449784	-3.276081	0.304093
N	3.434084	-3.462886	0.526094
O	3.378674	-4.694379	0.515578
O	2.219276	-2.831284	0.664305
C	5.801792	-0.582403	0.558405
C	6.708791	-1.093211	1.494423
C	6.151167	0.566576	-0.156906
C	7.936981	-0.477035	1.702829
H	6.442212	-1.978172	2.071416
C	7.386004	1.179234	0.048803
H	5.479898	0.999613	-0.896849
C	8.281625	0.661150	0.977181
H	8.628576	-0.890640	2.433598
H	7.644836	2.065664	-0.526382
H	9.245146	1.140520	1.135336

VII$_{R1}$

P	-0.011576	0.113499	-1.727715
P	0.189226	-0.987431	1.077759
C	-2.530108	-0.310680	1.572381
C	-2.654821	-2.581708	0.478993
C	-4.896440	-3.148983	2.248341
H	-4.501327	-3.928726	1.601608
C	-1.399355	-3.154966	0.646591
C	-0.701463	3.070817	-0.346109
C	-2.045696	2.715165	-0.883967
C	1.116503	-0.228101	2.511809
C	-3.483510	-3.016796	-0.604895
C	-2.456926	1.396350	-1.067875
C	-2.927912	3.783526	-1.268064
C	-3.758419	1.119672	-1.552745
H	-4.060156	0.078234	-1.667361
C	-1.301241	0.079311	0.783040
H	-0.979367	1.072043	1.132294
C	0.452930	2.749806	-1.053715
C	0.403672	1.824691	-2.229570
H	1.370560	1.780187	-2.744061
H	-0.356493	2.124598	-2.967489
C	-4.802325	-0.883014	3.155635
C	-3.149362	-1.551579	1.435604
C	-3.050085	-4.099414	-1.436514
C	0.699963	4.327098	1.268366
C	-1.579694	0.212717	-0.735622
H	-2.116073	-0.698516	-1.037530
C	-5.921551	-1.195691	3.963880
H	-6.308033	-0.428528	4.633953
C	-5.111118	4.527382	-2.130190
H	-6.106584	4.270679	-2.491130
C	-0.453568	-2.599860	1.667913
H	0.404016	-3.263321	1.823004

H	-0.944969	-2.445264	2.639010
C	-4.239672	3.476964	-1.755802
C	-3.855941	-4.498713	-2.530089
H	-3.514283	-5.324333	-3.153669
C	-1.691741	4.064051	1.720088
H	-2.674400	3.702255	1.421135
C	-1.540591	4.737305	2.910610
H	-2.404604	4.899446	3.552260
C	-1.809162	-4.721020	-1.161649
H	-1.490154	-5.559194	-1.780094
C	-4.280302	-1.870763	2.258901
C	-4.631719	2.124591	-1.870990
H	-5.633533	1.893482	-2.231367
C	-4.176687	0.382037	3.221014
H	-4.582400	1.137592	3.892693
C	-0.582965	3.825586	0.867514
C	-5.468159	-2.787895	-1.992886
H	-6.405468	-2.281807	-2.216086
C	-3.066833	0.650528	2.463333
H	-2.582688	1.626104	2.529260
C	0.814517	5.033028	2.490801
H	1.794384	5.411961	2.780022
C	1.821262	4.085094	0.439679
H	2.790466	4.509456	0.701857
C	2.242371	-1.176562	2.930562
H	2.807746	-0.725297	3.755742
H	2.954944	-1.355019	2.113791
H	1.869945	-2.146593	3.283948
C	-3.409951	6.146123	-1.603026
H	-3.084944	7.183645	-1.563818
C	-4.716108	-2.385787	-0.912902
H	-5.061874	-1.566230	-0.285024
C	-2.543286	5.148880	-1.221211
H	-1.541204	5.411871	-0.891652
C	1.700805	3.299819	-0.678560
H	2.573636	3.146287	-1.314489
C	-5.037766	-3.854659	-2.809248
H	-5.643037	-4.165130	-3.658013
C	-5.976307	-3.424188	3.053839
H	-6.426439	-4.414561	3.029241
C	1.705923	1.096684	2.035609
H	0.935985	1.773425	1.649580
H	2.452069	0.959820	1.240374
H	2.201980	1.611792	2.869310
C	-0.249146	-2.290277	-3.058440
H	-0.579145	-2.862014	-3.936398
H	-0.867260	-2.606711	-2.211051
H	0.794918	-2.567888	-2.855173
C	-0.277807	5.229166	3.300959
H	-0.173279	5.766865	4.241003
C	-4.710016	5.838498	-2.052123
H	-5.386074	6.638562	-2.346268
C	-1.819075	-0.486911	-3.782881
H	-1.967793	-0.924058	-4.778688
H	-2.025167	0.587895	-3.862049
H	-2.574721	-0.931259	-3.122347
C	-6.502739	-2.438999	3.914126
H	-7.361039	-2.669562	4.541319
C	-0.390780	-0.795328	-3.328021
C	-0.993130	-4.235385	-0.171699
H	-0.011881	-4.679834	-0.006000
C	0.174117	0.032437	3.687721
H	-0.355067	-0.866135	4.027394
H	-0.574426	0.797986	3.450715
H	0.759656	0.406211	4.537903
C	0.606715	-0.361307	-4.402878
H	1.645016	-0.528405	-4.097348
H	0.480045	0.689590	-4.687553
H	0.426166	-0.962440	-5.303024
Ni	1.435973	-1.027768	-0.658850
H	3.853777	-0.433613	0.276777
C	4.783113	-0.121921	-0.239041
N	4.533081	1.303444	-0.481018
H	3.554291	1.522249	-0.630436
C	5.367581	2.232450	-1.068285
O	4.907325	3.302404	-1.447775
C	6.830933	1.896302	-1.161993
H	7.005684	0.888138	-1.555623
H	7.314335	2.628221	-1.811214
H	7.303302	1.934734	-0.173077
C	4.865181	-0.968917	-1.476883
H	5.792105	-1.271678	-1.956729
N	3.793224	-1.096831	-2.275294
O	3.737993	-1.778864	-3.302371
O	2.685515	-0.409061	-1.903442
C	5.911847	-0.344736	0.750815
C	6.889060	-1.329938	0.598669
C	5.942555	0.457322	1.898560

C	7.882316	-1.499400	1.562734
H	6.899475	-1.978609	-0.275564
C	6.930620	0.288787	2.859772
H	5.190458	1.237878	2.014297
C	7.908681	-0.691076	2.692928
H	8.641677	-2.265285	1.419913
H	6.942532	0.928148	3.740412
H	8.688225	-0.820267	3.440641
C	3.193982	-3.547045	0.171087
C	2.883867	-4.790807	0.932029
H	3.134718	-5.671769	0.333124
H	3.511748	-4.833665	1.828548
H	1.832905	-4.830247	1.222051
O	4.442498	-3.486050	-0.215047
H	4.612545	-2.617346	-0.702202
O	2.350198	-2.667727	-0.050806

TSIII$_{R1}$

P	0.040316	0.168751	-1.756523
P	0.312488	-0.932135	1.064717
C	-2.430559	-0.382399	1.569373
C	-2.467988	-2.653619	0.470590
C	-4.663626	-3.320888	2.266352
H	-4.239915	-4.082293	1.615865
C	-1.184418	-3.167428	0.616418
C	-0.780570	3.084842	-0.348491
C	-2.108286	2.666419	-0.881366
C	1.185412	-0.146347	2.517393
C	-3.290766	-3.120763	-0.604407
C	-2.461390	1.330082	-1.054413
C	-3.041757	3.693145	-1.256551
C	-3.762416	0.993897	-1.501631
H	-4.023078	-0.060326	-1.597450
C	-1.224101	0.064731	0.773419
H	-0.948033	1.070650	1.123974
C	0.388160	2.824240	-1.056922
C	0.376609	1.906005	-2.240431
H	1.336875	1.915125	-2.770406
H	-0.404326	2.177319	-2.967965
C	-4.662026	-1.052500	3.171700
C	-2.995795	-1.649183	1.436994
C	-2.816813	-4.174819	-1.451467
C	0.555858	4.394821	1.278395
C	-1.519447	0.191284	-0.741516
H	-2.010434	-0.744997	-1.044650
C	-5.759729	-1.413038	3.989247
H	-6.173947	-0.662841	4.661909
C	-5.268775	4.336583	-2.084554
H	-6.259012	4.035772	-2.425154
C	-0.254514	-2.579881	1.633199
H	0.635154	-3.202330	1.771138
H	-0.745402	-2.454532	2.608618
C	-4.347947	3.326804	-1.716596
C	-3.617022	-4.602141	-2.538683
H	-3.243648	-5.403841	-3.175244
C	-1.821625	4.017010	1.720853
H	-2.785420	3.612089	1.416764
C	-1.705256	4.687458	2.916919
H	-2.577533	4.803334	3.557354
C	-1.543999	-4.738650	-1.197736
H	-1.194454	-5.556958	-1.826347
C	-4.104140	-2.016912	2.271426
C	-4.685179	1.957752	-1.807451
H	-5.684828	1.680289	-2.139960
C	-4.094000	0.239735	3.229610
H	-4.527698	0.978094	3.902882
C	-0.700636	3.836540	0.870245
C	-5.304041	-2.978457	-1.962732
H	-6.269024	-2.518624	-2.166914
C	-3.004024	0.555732	2.461877
H	-2.564438	1.552263	2.522190
C	0.634424	5.096876	2.506064
H	1.594709	5.519356	2.800489
C	1.688328	4.211952	0.450715
H	2.635869	4.679633	0.718177
C	2.339048	-1.053211	2.950286
H	2.875218	-0.580836	3.783277
H	3.071288	-1.210844	2.148433
H	1.992894	-2.034275	3.299520
C	-3.627006	6.030023	-1.602242
H	-3.344969	7.080405	-1.578107
C	-4.557520	-2.549392	-0.889635
H	-4.935182	-1.754408	-0.248784
C	-2.713535	5.073287	-1.226183
H	-1.718117	5.380227	-0.914660
C	1.607039	3.432033	-0.675532
H	2.489325	3.327012	-1.307657
C	-4.832394	-4.013978	-2.796257

H	-5.433004	-4.345460	-3.640403
C	-5.724130	-3.642598	3.080414
H	-6.130648	-4.651725	3.059995
C	1.717550	1.208153	2.060366
H	0.920898	1.854563	1.674410
H	2.478514	1.114559	1.274886
H	2.179462	1.736162	2.905754
C	-0.185188	-2.216224	-3.122914
H	-0.537022	-2.786214	-3.993488
H	-0.768860	-2.550802	-2.257433
H	0.868017	-2.474239	-2.954140
C	-0.467850	5.235189	3.314627
H	-0.391300	5.770867	4.258478
C	-4.920514	5.663836	-2.026027
H	-5.634406	6.431901	-2.316045
C	-1.823984	-0.451197	-3.763665
H	-1.990739	-0.877127	-4.761402
H	-2.068001	0.616987	-3.818568
H	-2.542166	-0.932482	-3.088471
C	-6.286354	-2.680670	3.944425
H	-7.129391	-2.947446	4.578019
C	-0.369076	-0.722146	-3.368430
C	-0.738517	-4.223213	-0.214182
H	0.262060	-4.626456	-0.058160
C	0.216903	0.067876	3.681914
H	-0.290985	-0.849223	4.002807
H	-0.548502	0.816986	3.447767
H	0.782410	0.444497	4.544288
C	0.550525	-0.241097	-4.492463
H	1.608642	-0.394931	-4.266916
H	0.384737	0.814390	-4.737952
H	0.314535	-0.818339	-5.395535
Ni	1.544672	-0.974743	-0.699092
H	3.561839	-0.397194	0.136900
C	4.541647	-0.071522	-0.260863
N	4.316500	1.350481	-0.528545
H	3.349589	1.613670	-0.688967
C	5.206075	2.315766	-0.956291
O	4.785391	3.408161	-1.316207
C	6.674360	1.991415	-0.907359
H	6.905877	0.980860	-1.260504
H	7.208451	2.721927	-1.517542
H	7.046306	2.059596	0.122072
C	4.810459	-0.898454	-1.496807
H	5.811356	-0.893209	-1.925466
N	3.882445	-0.898855	-2.503902
O	4.150150	-1.161702	-3.670993
O	2.606831	-0.660688	-2.227486
C	5.558176	-0.300559	0.841991
C	6.520673	-1.310721	0.781103
C	5.511783	0.511337	1.982650
C	7.415673	-1.504222	1.831652
H	6.593153	-1.956947	-0.090219
C	6.401962	0.317069	3.031750
H	4.779013	1.317471	2.028316
C	7.360261	-0.693340	2.959240
H	8.165626	-2.289000	1.757416
H	6.355203	0.963290	3.906297
H	8.064693	-0.840121	3.775266
C	3.329987	-3.439207	0.071187
C	3.186129	-4.656909	0.924807
H	3.485348	-5.552502	0.373531
H	3.869787	-4.567928	1.777549
H	2.167337	-4.768957	1.301575
O	4.446843	-3.373890	-0.572078
H	4.592301	-2.390780	-1.013117
O	2.427249	-2.572650	0.048027

$VIII_{R1}$

P	-0.224077	-0.096121	-1.800649
P	0.086716	-1.054599	1.063771
C	-2.553247	-0.160404	1.643426
C	-2.917950	-2.451545	0.643195
C	-5.131772	-2.743041	2.534480
H	-4.830317	-3.585958	1.917407
C	-1.691884	-3.098046	0.759435
C	-0.372178	2.975958	-0.441539
C	-1.781706	2.797749	-0.899527
C	1.118502	-0.379267	2.462331
C	-3.836296	-2.884527	-0.370301
C	-2.400578	1.552438	-0.991449
C	-2.527670	3.973891	-1.257202
C	-3.774796	1.464092	-1.323455
H	-4.238923	0.476561	-1.348858
C	-1.330339	0.109375	0.797941
H	-0.918646	1.077440	1.119446
C	0.701282	2.459766	-1.162454
C	0.469664	1.526189	-2.309805

H	1.401846	1.319294	-2.847072
H	-0.248534	1.949324	-3.028940
C	-4.809925	-0.453034	3.316114
C	-3.283464	-1.347176	1.577012
C	-3.523729	-4.039899	-1.158592
C	1.242677	4.130688	1.044351
C	-1.679592	0.256660	-0.704866
H	-2.361763	-0.571432	-0.952368
C	-5.920604	-0.624445	4.176413
H	-6.212446	0.207406	4.816504
C	-4.653932	5.018832	-1.927367
H	-5.710061	4.907994	-2.171251
C	-0.656726	-2.596414	1.716536
H	0.149822	-3.326350	1.850468
H	-1.086863	-2.374930	2.703477
C	-3.915121	3.858459	-1.595486
C	-4.419148	-4.450190	-2.174720
H	-4.168620	-5.333748	-2.761074
C	-1.134515	4.170123	1.617497
H	-2.165920	3.905993	1.388947
C	-0.847166	4.885809	2.757796
H	-1.652869	5.174776	3.430082
C	-2.295059	-4.708946	-0.948921
H	-2.065896	-5.590386	-1.546847
C	-4.407423	-1.525046	2.454735
C	-4.518145	2.580435	-1.597221
H	-5.577859	2.496034	-1.835027
C	-4.076977	0.754410	3.301147
H	-4.394426	1.574193	3.944360
C	-0.106469	3.765255	0.727694
C	-5.866906	-2.589097	-1.678742
H	-6.771468	-2.023584	-1.893704
C	-2.973624	0.884663	2.501508
H	-2.402787	1.814891	2.502692
C	1.499681	4.891244	2.210129
H	2.530198	5.168564	2.429613
C	2.292093	3.693423	0.201443
H	3.319958	4.000336	0.397572
C	2.152858	-1.443147	2.838390
H	2.859006	-1.022229	3.566128
H	2.730952	-1.792503	1.974209
H	1.693166	-2.322413	3.304899
C	-2.681823	6.370892	-1.656858
H	-2.201329	7.346140	-1.702078
C	-5.032055	-2.179777	-0.663696
H	-5.285191	-1.299935	-0.074084
C	-1.939296	5.263973	-1.317463
H	-0.879454	5.380089	-1.104994
C	2.026193	2.850295	-0.847222
H	2.842195	2.497143	-1.476952
C	-5.564709	-3.738357	-2.437760
H	-6.237446	-4.055990	-3.231529
C	-6.198627	-2.882260	3.391162
H	-6.730717	-3.830421	3.436180
C	1.803264	0.884898	1.959871
H	1.075480	1.670726	1.730292
H	2.387714	0.706776	1.049714
H	2.470070	1.284785	2.737335
C	-1.282209	-2.267648	-3.113278
H	-1.783593	-2.694110	-3.992698
H	-1.984620	-2.339432	-2.274201
H	-0.408880	-2.887287	-2.882061
C	0.479897	5.257672	3.055849
H	0.693146	5.833475	3.953942
C	-4.054870	6.254286	-1.952769
H	-4.631897	7.139141	-2.212271
C	-2.135523	-0.055259	-3.859336
H	-2.397674	-0.405557	-4.866474
H	-1.988834	1.030324	-3.919036
H	-3.003059	-0.244125	-3.215915
C	-6.606966	-1.813123	4.214112
H	-7.455986	-1.936291	4.883115
C	-0.896871	-0.817630	-3.385659
C	-1.387134	-4.222889	-0.043763
H	-0.423525	-4.715223	0.094629
C	0.251875	-0.027644	3.672702
H	-0.314997	-0.880808	4.063687
H	-0.456793	0.779252	3.449493
H	0.902516	0.328200	4.482522
C	0.209428	-0.732461	-4.440932
H	1.152633	-1.175080	-4.101143
H	0.403817	0.301638	-4.748558
H	-0.109313	-1.280943	-5.336296
Ni	1.081869	-1.478137	-0.780567
H	4.177100	-0.564652	0.854202
C	5.107181	-0.296977	0.332904
N	5.102674	1.157332	0.316042
H	4.329521	1.602397	0.798269

C	5.801778	2.055849	-0.465311
O	5.488951	3.237885	-0.454506
C	6.929650	1.535043	-1.318280
H	7.401570	0.627528	-0.927690
H	6.559525	1.330061	-2.331252
H	7.682732	2.320926	-1.409045
C	4.967737	-0.894189	-1.073874
H	5.843223	-0.766704	-1.711564
N	3.819979	-0.258673	-1.786630
O	3.929327	0.035461	-2.969481
O	2.792220	-0.070229	-1.106365
C	6.253314	-0.956518	1.076917
C	6.217071	-2.342188	1.271251
C	7.318122	-0.227695	1.604506
C	7.237908	-2.988633	1.958313
H	5.366602	-2.920108	0.900955
C	8.342067	-0.875356	2.292497
H	7.337542	0.854684	1.492698
C	8.309093	-2.255224	2.464944
H	7.194269	-4.066078	2.104402
H	9.167549	-0.293847	2.697813
H	9.110541	-2.759290	3.000378
C	2.333160	-3.318849	-1.373096
C	3.031988	-4.578326	-1.739450
H	3.621276	-4.443452	-2.650522
H	3.661422	-4.933851	-0.920113
H	2.284671	-5.352860	-1.950887
O	1.881281	-2.525292	-2.261173
H	4.729376	-1.963186	-1.015786
O	2.142472	-2.995092	-0.147131

IX$_{S2}$

P	0.388689	-0.687885	1.560503
P	0.813839	0.017351	-1.475101
C	-1.817138	1.229114	-1.398228
C	-0.304663	3.062851	-0.573383
C	-2.082514	4.938239	-1.941132
H	-1.151064	5.293423	-1.506316
C	0.960719	2.709302	-1.027582
C	-2.209142	-2.573458	0.448225
C	-2.900364	-1.477925	1.190411
C	0.601843	-1.050102	-3.016353
C	-0.427800	3.899532	0.584271
C	-2.370586	-0.192249	1.299237
C	-4.147103	-1.775223	1.842183
C	-3.096179	0.821283	1.972094
H	-2.660579	1.820715	2.025028
C	-0.947560	0.142109	-0.803168
H	-1.381157	-0.820454	-1.109231
C	-0.963609	-3.042842	0.858056
C	-0.229725	-2.368369	1.975228
H	0.631696	-2.963896	2.297563
H	-0.896844	-2.250026	2.838611
C	-3.598963	3.116915	-2.529116
C	-1.518059	2.586351	-1.293048
C	0.750945	4.427002	1.205161
C	-2.279931	-4.376499	-1.250910
C	-1.019431	0.193726	0.745256
H	-0.834424	1.241288	1.021775
C	-4.464050	4.070067	-3.117562
H	-5.386209	3.717711	-3.578557
C	-6.100139	-1.019642	3.138976
H	-6.631512	-0.207206	3.633327
C	1.105464	1.719991	-2.142251
H	2.106219	1.765735	-2.588625
H	0.378001	1.915109	-2.941326
C	-4.864619	-0.731097	2.511225
C	0.627063	5.236372	2.359776
H	1.533870	5.637354	2.812008
C	-4.046952	-2.686556	-1.241461
H	-4.501319	-1.796287	-0.809367
C	-4.628298	-3.288275	-2.334057
H	-5.535554	-2.866905	-2.762632
C	2.016864	4.097398	0.666850
H	2.912737	4.519153	1.121932
C	-2.385889	3.552589	-1.904655
C	-4.314342	0.569516	2.545655
H	-4.865320	1.363844	3.047833
C	-3.900591	1.736903	-2.549152
H	-4.832883	1.405647	-3.005241
C	-2.856174	-3.201736	-0.667079
C	-1.766453	4.965054	2.316306
H	-2.740334	5.169036	2.757116
C	-3.026980	0.826480	-2.015990
H	-3.262794	-0.238233	-2.048271
C	-2.916221	-4.983925	-2.359768
H	-2.468233	-5.879997	-2.788782
C	-1.065376	-4.878662	-0.726611

H	-0.643069	-5.788772	-1.153211
C	1.903135	-1.054842	-3.815628
H	1.766905	-1.653906	-4.725293
H	2.721707	-1.514250	-3.248086
H	2.207138	-0.051021	-4.140998
C	-5.894585	-3.333474	2.512733
H	-6.288343	-4.347713	2.532559
C	-1.681847	4.193575	1.179066
H	-2.588841	3.796997	0.726425
C	-4.697385	-3.082959	1.883776
H	-4.159309	-3.905127	1.418844
C	-0.409563	-4.205608	0.272262
H	0.547521	-4.565197	0.648238
C	-0.604672	5.500551	2.909282
H	-0.685469	6.117990	3.801195
C	-2.938736	5.838281	-2.531350
H	-2.678066	6.894436	-2.550022
C	0.302336	-2.468066	-2.545623
H	-0.667054	-2.533038	-2.041226
H	1.058949	-2.843855	-1.847249
H	0.258196	-3.150348	-3.405782
C	1.988475	-0.410953	3.812134
H	2.076372	-0.109355	4.863911
H	2.865839	-0.011319	3.288614
H	2.056384	-1.506773	3.780590
C	-4.063939	-4.451392	-2.896807
H	-4.537937	-4.923639	-3.754633
C	-6.612637	-2.293450	3.136951
H	-7.561938	-2.504690	3.624642
C	0.706739	1.628704	3.091988
H	-0.286195	2.057252	2.900263
H	1.374005	1.963034	2.287781
H	1.072942	2.080502	4.023123
C	-4.146592	5.406427	-3.116430
H	-4.817810	6.130681	-3.572885
C	0.657481	0.109702	3.250954
C	2.113926	3.244329	-0.403576
H	3.094557	3.006017	-0.818375
C	-0.540881	-0.575552	-3.913941
H	-0.430697	0.461589	-4.252569
H	-1.517182	-0.672143	-3.427232
H	-0.569007	-1.205470	-4.813155
C	-0.455831	-0.245323	4.244996
H	-0.391434	-1.282999	4.589677
H	-1.461516	-0.073199	3.844192
H	-0.344243	0.389823	5.133205
Ni	2.178718	-0.571876	0.228116
H	4.112054	1.340069	-1.393165
C	6.178173	0.970546	2.110882
C	5.384116	0.778126	0.990177
C	4.952801	-0.505492	0.607378
C	5.366215	-1.585241	1.399982
C	6.159751	-1.393432	2.527421
C	6.567486	-0.116207	2.893278
H	6.499825	1.976659	2.372116
H	5.085189	1.652628	0.411982
H	5.080689	-2.601126	1.136622
H	6.464408	-2.255057	3.117812
H	7.189637	0.033713	3.772608
C	4.022846	-0.676949	-0.569593
C	4.308329	0.303999	-1.671484
N	4.059595	-2.050180	-1.084718
H	4.876356	-2.320076	-1.631252
N	5.772710	0.289093	-2.110542
O	6.285450	-0.821660	-2.260526
O	6.322909	1.360798	-2.293815
H	3.752057	0.074442	-2.582916
H	2.831209	0.432533	1.364413
C	3.305379	-2.961567	-0.467260
C	3.482307	-4.410677	-0.770148
H	2.538322	-4.819900	-1.149033
H	4.270337	-4.602176	-1.502599
H	3.715101	-4.953950	0.151855
O	2.429741	-2.578057	0.353200
H	2.523909	0.926472	0.776904

TSV_{S2}

P	0.391117	-0.674421	1.583083
P	0.783425	0.002043	-1.489267
C	-1.832505	1.223672	-1.383876
C	-0.327568	3.064203	-0.555717
C	-2.103342	4.927994	-1.946713
H	-1.174501	5.287645	-1.510108
C	0.942264	2.703506	-0.991792
C	-2.183029	-2.598353	0.501328
C	-2.884380	-1.500444	1.226657
C	0.559418	-1.025259	-3.051273
C	-0.459286	3.915282	0.591300

C	-2.384289	-0.201504	1.294592
C	-4.136454	-1.801313	1.867013
C	-3.166504	0.826522	1.875903
H	-2.765888	1.841197	1.876570
C	-0.959718	0.139074	-0.789529
H	-1.399925	-0.824695	-1.082529
C	-0.933660	-3.056253	0.905835
C	-0.185586	-2.368806	2.007338
H	0.703417	-2.943609	2.291050
H	-0.815702	-2.272708	2.903747
C	-3.613556	3.100063	-2.529567
C	-1.536104	2.581528	-1.280914
C	0.715172	4.453162	1.212776
C	-2.253485	-4.406184	-1.192876
C	-1.024805	0.193095	0.760290
H	-0.847996	1.241811	1.046061
C	-4.477922	4.047612	-3.128187
H	-5.397265	3.690289	-3.591013
C	-6.136002	-1.041360	3.086211
H	-6.701526	-0.221960	3.528643
C	1.098682	1.716903	-2.108256
H	2.104023	1.765887	-2.543031
H	0.381555	1.924208	-2.913343
C	-4.898470	-0.746839	2.465838
C	0.583506	5.271528	2.360370
H	1.487334	5.678436	2.813141
C	-4.024394	-2.721404	-1.184565
H	-4.479776	-1.829915	-0.756409
C	-4.603773	-3.325343	-2.277091
H	-5.510776	-2.905222	-2.707398
C	1.984659	4.118187	0.687965
H	2.876922	4.546588	1.143833
C	-2.404071	3.542080	-1.902210
C	-4.392606	0.571645	2.428229
H	-4.983720	1.377906	2.861017
C	-3.912915	1.719515	-2.543906
H	-4.842577	1.384217	-3.002358
C	-2.833258	-3.234005	-0.608793
C	-1.808209	4.989375	2.310563
H	-2.784551	5.192607	2.746127
C	-3.038842	0.813841	-2.003484
H	-3.269666	-0.252418	-2.033054
C	-2.889157	-5.018156	-2.299394
H	-2.438549	-5.913388	-2.727432
C	-1.033334	-4.898341	-0.672967
H	-0.607823	-5.808295	-1.096642
C	1.893284	-1.072440	-3.795939
H	1.779277	-1.667935	-4.710945
H	2.678615	-1.548792	-3.195281
H	2.238369	-0.077600	-4.107844
C	-5.850242	-3.376795	2.580693
H	-6.214795	-4.400099	2.643365
C	-1.716582	4.213209	1.177567
H	-2.620891	3.815892	0.720581
C	-4.649780	-3.120924	1.959887
H	-4.078958	-3.948191	1.545149
C	-0.378402	-4.220202	0.322313
H	0.581181	-4.575335	0.693709
C	-0.650754	5.532530	2.904968
H	-0.737316	6.154095	3.793464
C	-2.958270	5.822313	-2.547428
H	-2.699225	6.878732	-2.572455
C	0.171844	-2.438483	-2.626003
H	-0.826232	-2.472403	-2.174870
H	0.871653	-2.865384	-1.899865
H	0.140911	-3.097004	-3.505026
C	1.621697	-0.748779	4.046845
H	1.861713	-0.255915	4.997263
H	2.570213	-0.906539	3.514482
H	1.195801	-1.729611	4.289599
C	-4.038193	-4.489009	-2.837054
H	-4.511593	-4.963900	-3.693761
C	-6.609329	-2.329444	3.140709
H	-7.560469	-2.545156	3.622838
C	1.227355	1.534299	3.088703
H	0.631933	2.146419	2.399656
H	2.263813	1.528498	2.732740
H	1.218938	2.047646	4.059070
C	-4.162748	5.384443	-3.134992
H	-4.833029	6.104342	-3.599675
C	0.646763	0.131173	3.259501
C	2.090065	3.249741	-0.367883
H	3.073507	3.008180	-0.771825
C	-0.520371	-0.475535	-3.982849
H	-0.330336	0.552778	-4.312027
H	-1.516104	-0.507776	-3.528197
H	-0.558633	-1.099107	-4.886005
C	-0.672749	0.260864	4.028522

H	-1.261830	-0.663662	4.068224
H	-1.311212	1.042790	3.604186
H	-0.448280	0.548326	5.063507
Ni	2.182234	-0.613284	0.256090
H	4.078109	1.379121	-1.283273
C	6.235438	0.951108	2.181808
C	5.377116	0.780057	1.105408
C	5.041825	-0.501875	0.638636
C	5.600520	-1.601905	1.297655
C	6.459305	-1.431264	2.381020
C	6.783295	-0.156331	2.828359
H	6.480944	1.957044	2.516669
H	4.938249	1.663605	0.638620
H	5.374397	-2.613199	0.963683
H	6.882275	-2.306390	2.870567
H	7.458320	-0.022683	3.670620
C	4.058684	-0.658730	-0.497066
C	4.292051	0.354686	-1.586372
N	4.120364	-2.013304	-1.063860
H	4.964256	-2.263754	-1.576851
N	5.745089	0.386166	-2.061499
O	6.295656	-0.705216	-2.219006
O	6.249597	1.476256	-2.266048
H	3.719716	0.123692	-2.488740
H	2.830710	-0.198207	1.501800
C	3.267995	-2.938846	-0.633915
C	3.450834	-4.364048	-1.030919
H	2.527313	-4.737322	-1.487299
H	4.279198	-4.511288	-1.728239
H	3.631249	-4.971561	-0.137322
O	2.295098	-2.601214	0.094957
H	2.460817	0.737850	0.723723

X_{S2}

P	0.417622	-0.724836	1.560795
P	0.711386	-0.084832	-1.562460
C	-1.821457	1.241955	-1.375143
C	-0.202881	3.029508	-0.633168
C	-1.953248	4.948855	-1.975788
H	-1.002271	5.278140	-1.564318
C	1.031508	2.617751	-1.126357
C	-2.249695	-2.541484	0.632547
C	-2.907095	-1.390344	1.313960
C	0.421057	-1.138873	-3.090196
C	-0.244570	3.913878	0.494800
C	-2.349954	-0.113222	1.343158
C	-4.168499	-1.621404	1.962937
C	-3.084257	0.960760	1.905138
H	-2.643161	1.957707	1.876256
C	-0.982807	0.131826	-0.782721
H	-1.473104	-0.818669	-1.034174
C	-1.030718	-3.040880	1.077181
C	-0.265300	-2.324605	2.148078
H	0.581469	-2.925935	2.499354
H	-0.900481	-2.108594	3.020473
C	-3.543629	3.174990	-2.510110
C	-1.462026	2.586665	-1.298492
C	0.977534	4.436886	1.031015
C	-2.360498	-4.386980	-1.014640
C	-0.986790	0.209409	0.767513
H	-0.752077	1.251590	1.034184
C	-4.385187	4.150475	-3.096469
H	-5.326563	3.824117	-3.537172
C	-6.130284	-0.747907	3.166053
H	-6.660206	0.104853	3.589280
C	1.098297	1.594744	-2.217936
H	2.088311	1.574093	-2.690591
H	0.364590	1.818586	-3.003205
C	-4.882598	-0.521077	2.537672
C	0.933955	5.281180	2.166190
H	1.872422	5.672734	2.557330
C	-4.071215	-2.641725	-1.072422
H	-4.502385	-1.727019	-0.668639
C	-4.653409	-3.248762	-2.161978
H	-5.538547	-2.807541	-2.616258
C	2.204913	4.061396	0.437180
H	3.132587	4.481171	0.825352
C	-2.304972	3.575582	-1.910719
C	-4.317954	0.772038	2.468289
H	-4.870846	1.613874	2.883550
C	-3.892408	1.806169	-2.517011
H	-4.838418	1.504030	-2.964965
C	-2.907989	-3.183006	-0.466787
C	-1.464044	5.067632	2.257895
H	-2.408099	5.311458	2.741445
C	-3.046329	0.870539	-1.982405
H	-3.312587	-0.187811	-2.007625
C	-2.999423	-5.000907	-2.118357

H	-2.574807	-5.921486	-2.518209
C	-1.168979	-4.911786	-0.462043
H	-0.769055	-5.844480	-0.859575
C	1.784975	-1.447421	-3.711317
H	1.646165	-2.068927	-4.605340
H	2.441857	-2.000567	-3.027281
H	2.307094	-0.537976	-4.037880
C	-5.945405	-3.105290	2.716093
H	-6.353385	-4.110126	2.804127
C	-1.458737	4.265174	1.139608
H	-2.398454	3.889563	0.739124
C	-4.736703	-2.915513	2.087992
H	-4.201088	-3.775561	1.693547
C	-0.509461	-4.239122	0.534073
H	0.430331	-4.622726	0.926977
C	-0.259019	5.585228	2.776104
H	-0.277495	6.224455	3.655932
C	-2.787854	5.870366	-2.563670
H	-2.489830	6.916002	-2.602861
C	-0.251708	-2.439723	-2.656626
H	-1.314560	-2.293962	-2.431367
H	0.225799	-2.894063	-1.779903
H	-0.207759	-3.166482	-3.479412
C	1.713283	-0.686746	4.007985
H	2.038155	-0.114483	4.885817
H	2.622453	-1.024394	3.490506
H	1.171865	-1.566479	4.376427
C	-4.119456	-4.443357	-2.687591
H	-4.595387	-4.920090	-3.541871
C	-6.657805	-2.013144	3.251613
H	-7.616641	-2.176387	3.738933
C	1.622805	1.469479	2.745725
H	1.108628	2.041708	1.963869
H	2.634066	1.238746	2.387337
H	1.713919	2.124664	3.622117
C	-4.021272	5.474493	-3.120004
H	-4.674625	6.215633	-3.575242
C	0.846170	0.210388	3.123756
C	2.227625	3.157169	-0.593471
H	3.178699	2.885397	-1.052955
C	-0.448693	-0.438314	-4.134991
H	0.049143	0.427488	-4.586303
H	-1.412970	-0.108625	-3.731292
H	-0.660595	-1.145496	-4.947881
C	-0.422882	0.620654	3.876428
H	-1.131417	-0.203335	4.028942
H	-0.955494	1.427774	3.360137
H	-0.142242	1.001593	4.866465
Ni	2.060063	-0.845723	0.111122
H	3.996428	1.100566	-1.381988
C	5.772522	1.147438	2.277875
C	5.005332	0.810998	1.169707
C	4.879192	-0.521763	0.751769
C	5.553092	-1.503346	1.484326
C	6.322379	-1.167649	2.596045
C	6.438612	0.158065	2.999045
H	5.846547	2.190388	2.581182
H	4.461565	1.598453	0.643155
H	5.474103	-2.548732	1.190064
H	6.838697	-1.952804	3.144930
H	7.040233	0.420306	3.866196
C	4.004199	-0.856785	-0.430363
C	4.270896	0.067038	-1.591391
N	4.184316	-2.250652	-0.863701
H	5.095268	-2.519429	-1.230089
N	5.746943	0.133933	-1.988118
O	6.391622	-0.912899	-1.914740
O	6.173726	1.210440	-2.369218
H	3.764059	-0.257986	-2.505486
H	2.598775	-1.102322	1.452151
C	3.200087	-3.131430	-0.738314
C	3.402275	-4.551262	-1.144300
H	2.580896	-4.856723	-1.801578
H	4.354667	-4.720705	-1.652280
H	3.357725	-5.194644	-0.258985
O	2.076868	-2.770384	-0.284619
H	2.193643	0.585087	0.296626

TSVI$_{S2}$

P	-0.425632	0.784071	1.560094
P	-0.615544	0.128016	-1.652778
C	1.856157	-1.263619	-1.324177
C	0.143859	-3.000969	-0.670705
C	1.895334	-4.972916	-1.925992
H	0.916306	-5.271410	-1.559301
C	-1.051419	-2.562354	-1.233572
C	2.327222	2.501584	0.695636
C	2.943233	1.322128	1.366802

C	-0.238835	1.162312	-3.177341
C	0.102724	-3.886151	0.455966
C	2.328535	0.071037	1.389656
C	4.202413	1.501149	2.035340
C	3.003922	-1.029306	1.973270
H	2.519460	-2.005893	1.942878
C	1.023877	-0.127336	-0.774939
H	1.551913	0.807805	-1.009201
C	1.121126	3.021645	1.151920
C	0.354500	2.310882	2.224004
H	-0.445942	2.945181	2.622579
H	1.008596	2.029954	3.062591
C	3.564048	-3.251351	-2.384793
C	1.448870	-2.595943	-1.269419
C	-1.159006	-4.375325	0.927720
C	2.460043	4.354441	-0.940354
C	0.964653	-0.193664	0.785585
H	0.689482	-1.228223	1.041979
C	4.400529	-4.253900	-2.931397
H	5.371213	-3.958112	-3.328117
C	6.101284	0.550255	3.279734
H	6.585870	-0.322557	3.716441
C	-1.026162	-1.540457	-2.326828
H	-1.994033	-1.479978	-2.841912
H	-0.270351	-1.799343	-3.079224
C	4.857147	0.373848	2.628093
C	-1.196846	-5.220325	2.062714
H	-2.164349	-5.586098	2.405437
C	4.159375	2.597986	-0.999034
H	4.583735	1.679418	-0.597051
C	4.753839	3.209366	-2.079621
H	5.640446	2.766524	-2.529469
C	-2.342329	-3.973183	0.265973
H	-3.298583	-4.375066	0.600298
C	2.287119	-3.611491	-1.843537
C	4.234803	-0.892525	2.557926
H	4.740579	-1.755121	2.990524
C	3.955851	-1.894152	-2.375568
H	4.930134	-1.622813	-2.780700
C	2.995971	3.142757	-0.396565
C	1.199265	-5.077609	2.273298
H	2.110306	-5.351059	2.802051
C	3.117471	-0.932129	-1.877241
H	3.417013	0.117343	-1.888962
C	3.109799	4.970538	-2.036468
H	2.693392	5.896318	-2.433092
C	1.269979	4.886591	-0.391948
H	0.875194	5.820182	-0.792603
C	-1.585269	1.506277	-3.819681
H	-1.420236	2.094562	-4.731760
H	-2.213125	2.111187	-3.150722
H	-2.150737	0.612301	-4.116516
C	6.024607	2.911740	2.820044
H	6.472171	3.899018	2.914359
C	1.272712	-4.273774	1.158932
H	2.241040	-3.926656	0.803201
C	4.822034	2.770866	2.168141
H	4.329561	3.650616	1.760496
C	0.608628	4.222549	0.608723
H	-0.323274	4.618638	1.009288
C	-0.044785	-5.559122	2.730572
H	-0.087785	-6.199540	3.608715
C	2.726811	-5.921644	-2.473655
H	2.398008	-6.957497	-2.526552
C	0.455185	2.447637	-2.734006
H	1.499516	2.271392	-2.451493
H	-0.051962	2.933716	-1.890701
H	0.476112	3.160574	-3.569646
C	-1.844598	0.743659	3.913846
H	-2.271821	0.173775	4.748479
H	-2.686846	1.140101	3.328461
H	-1.293681	1.587756	4.345829
C	4.230639	4.410424	-2.601502
H	4.715760	4.890172	-3.448903
C	6.679481	1.792583	3.372925
H	7.634164	1.917533	3.879462
C	-1.744039	-1.400527	2.639267
H	-1.194508	-1.998877	1.902375
H	-2.712410	-1.128708	2.199194
H	-1.938215	-2.048520	3.504516
C	3.996670	-5.565891	-2.971814
H	4.647024	-6.327647	-3.396381
C	-0.948946	-0.174861	3.078860
C	-2.288063	-3.075764	-0.769856
H	-3.205311	-2.797662	-1.291794
C	0.635897	0.428751	-4.192983
H	0.123530	-0.423595	-4.653475
H	1.573639	0.068147	-3.753867

H	0.899608	1.120672	-5.004057
C	0.249540	-0.640226	3.907921
H	0.961225	0.160879	4.142220
H	0.801914	-1.443045	3.405283
H	-0.109538	-1.046349	4.862515
Ni	-1.930661	0.945865	-0.030559
H	-3.718074	-0.902841	-1.272748
C	-6.053231	-1.172851	2.098818
C	-5.177092	-0.760888	1.101262
C	-5.039528	0.597196	0.787233
C	-5.788615	1.529992	1.507270
C	-6.668775	1.115113	2.503141
C	-6.807261	-0.236332	2.801438
H	-6.146189	-2.233102	2.325749
H	-4.578436	-1.507778	0.576278
H	-5.684226	2.593086	1.295890
H	-7.249888	1.857268	3.046620
H	-7.496146	-0.559379	3.578552
C	-4.034187	1.016943	-0.269705
C	-4.100856	0.095921	-1.472486
N	-4.209186	2.408043	-0.675400
H	-5.129923	2.681727	-1.009276
N	-5.538942	-0.112905	-1.961834
O	-6.276868	0.870817	-1.930896
O	-5.834909	-1.226052	-2.364184
H	-3.577094	0.514867	-2.336740
H	-3.064921	1.102879	0.883469
C	-3.171469	3.246185	-0.746416
C	-3.387291	4.650988	-1.194295
H	-2.721815	4.866187	-2.037182
H	-4.418946	4.857190	-1.489164
H	-3.106808	5.335863	-0.387097
O	-2.012895	2.863528	-0.435015
H	-1.890617	-0.484349	0.202520

XI$_{S2}$

P	0.543242	-0.781013	1.550920
P	0.513251	0.040653	-1.759380
C	-2.077380	1.090433	-1.234740
C	-0.574311	3.011027	-0.586559
C	-2.595874	4.777007	-1.743944
H	-1.653105	5.186221	-1.388932
C	0.641394	2.737004	-1.205820
C	-2.092055	-2.689201	0.725971
C	-2.796608	-1.580397	1.428333
C	0.187045	-0.955072	-3.316738
C	-0.594055	3.857672	0.569544
C	-2.275479	-0.287037	1.451243
C	-4.029375	-1.858636	2.109290
C	-3.016642	0.752015	2.065387
H	-2.605825	1.761134	2.039931
C	-1.085771	0.053183	-0.758107
H	-1.506682	-0.933007	-0.995850
C	-0.829732	-3.091330	1.145507
C	-0.137388	-2.345811	2.244733
H	0.695863	-2.926157	2.657051
H	-0.829198	-2.109177	3.066253
C	-4.050580	2.871512	-2.201698
C	-1.840415	2.462482	-1.154151
C	0.623558	4.457893	1.029166
C	-2.043847	-4.460303	-1.002594
C	-0.956017	0.085840	0.808308
H	-0.750635	1.136373	1.068861
C	-5.015517	3.772247	-2.712537
H	-5.950933	3.366324	-3.096209
C	-5.981667	-1.060865	3.377240
H	-6.522599	-0.231137	3.831238
C	0.691343	1.777503	-2.352048
H	1.639503	1.860123	-2.899863
H	-0.119489	1.984349	-3.062739
C	-4.756493	-0.788565	2.722762
C	0.605566	5.257135	2.197319
H	1.540911	5.702651	2.535325
C	-3.948467	-2.929072	-0.927002
H	-4.469432	-2.091373	-0.467703
C	-4.498730	-3.558123	-2.020056
H	-5.447791	-3.208869	-2.422072
C	1.822222	4.213751	0.318119
H	2.739566	4.701554	0.646653
C	-2.815228	3.376380	-1.681440
C	-4.224656	0.518811	2.667073
H	-4.783225	1.336757	3.121019
C	-4.269213	1.475905	-2.216790
H	-5.211470	1.092581	-2.606703
C	-2.708368	-3.352749	-0.383004
C	-1.761694	4.881807	2.444237
H	-2.684817	5.053319	2.994587
C	-3.302282	0.617043	-1.765195

H	-3.466538	-0.460925	-1.800845
C	-2.648326	-5.099213	-2.112134
H	-2.133265	-5.944388	-2.568715
C	-0.776428	-4.858613	-0.516637
H	-0.272442	-5.702334	-0.988176
C	1.557995	-1.147098	-3.973464
H	1.448329	-1.704281	-4.913176
H	2.236966	-1.717448	-3.325552
H	2.041205	-0.192017	-4.222179
C	-5.747350	-3.403764	2.874549
H	-6.128173	-4.420284	2.950719
C	-1.780527	4.110307	1.304858
H	-2.718695	3.685719	0.953457
C	-4.558859	-3.170032	2.223316
H	-4.010580	-4.006196	1.795661
C	-0.178437	-4.176530	0.512432
H	0.810260	-4.469902	0.865101
C	-0.558411	5.459589	2.899095
H	-0.556415	6.069451	3.799786
C	-3.548711	5.625229	-2.258414
H	-3.349992	6.694350	-2.298900
C	-0.382886	-2.312644	-2.913349
H	-1.435162	-2.244407	-2.611333
H	0.177145	-2.777964	-2.090225
H	-0.346593	-2.998489	-3.770963
C	1.973158	-0.624407	3.877911
H	2.419270	-0.019540	4.677417
H	2.798917	-1.041998	3.284096
H	1.440274	-1.454427	4.356543
C	-3.848252	-4.657500	-2.617164
H	-4.297651	-5.153082	-3.475177
C	-6.474104	-2.340960	3.449177
H	-7.416120	-2.539163	3.956284
C	1.802994	1.471202	2.525653
H	1.211463	2.045354	1.802024
H	2.750152	1.199001	2.036864
H	2.038321	2.141404	3.363750
C	-4.775658	5.124196	-2.738465
H	-5.521969	5.807437	-3.137968
C	1.043512	0.247719	3.030595
C	1.831050	3.360038	-0.755424
H	2.753658	3.190245	-1.312824
C	-0.760299	-0.259923	-4.293457
H	-0.319313	0.641823	-4.733721
H	-1.713082	0.018177	-3.826471
H	-0.988521	-0.943002	-5.122647
C	-0.150187	0.711772	3.864303
H	-0.829119	-0.105469	4.139104
H	-0.738274	1.475094	3.339931
H	0.209207	1.167164	4.796729
Ni	1.732484	-0.782150	-0.218021
H	4.004802	1.481417	-0.678877
C	7.106256	0.923672	2.071482
C	6.167719	0.793565	1.051837
C	5.539513	-0.432980	0.821358
C	5.855743	-1.519887	1.643490
C	6.791840	-1.388678	2.662292
C	7.422980	-0.165486	2.876865
H	7.594694	1.882569	2.229395
H	5.942864	1.664460	0.437572
H	5.360470	-2.477713	1.481377
H	7.030318	-2.244939	3.289451
H	8.159893	-0.061841	3.670015
C	4.465962	-0.597760	-0.230082
C	4.317801	0.566816	-1.190283
N	4.578894	-1.876116	-0.923140
H	5.498689	-2.093453	-1.289276
N	5.581864	0.890311	-1.943409
O	6.386009	-0.025194	-2.107898
O	5.679802	2.027610	-2.379065
H	3.576471	0.344510	-1.968203
H	3.503012	-0.647792	0.335248
C	3.574463	-2.755530	-1.087642
C	3.895968	-4.079171	-1.698018
H	3.166854	-4.301722	-2.483317
H	4.905500	-4.132345	-2.113349
H	3.791533	-4.860632	-0.937020
O	2.394946	-2.518625	-0.735886
H	1.411842	0.601331	0.088721

$TSIV_{S3}$

P	0.416588	-0.014514	-1.505792
P	0.075066	-0.803305	1.487424
C	-2.664241	-0.138480	1.350454
C	-2.620497	-2.470344	0.388489
C	-5.204521	-2.882344	1.698696
H	-4.712182	-3.708682	1.192099
C	-1.410695	-2.993897	0.837254

C	-0.486914	3.072125	-0.409441
C	-1.761709	2.692914	-1.080931
C	0.623084	0.035561	3.076733
C	-3.207974	-3.005580	-0.804476
C	-2.117753	1.356730	-1.280685
C	-2.616934	3.729021	-1.589798
C	-3.350263	1.039959	-1.901117
H	-3.611287	-0.011231	-2.026335
C	-1.303401	0.200705	0.783528
H	-1.056292	1.225319	1.090138
C	0.726449	2.636921	-0.933240
C	0.741509	1.695096	-2.090436
H	1.678905	1.728459	-2.643060
H	-0.074262	1.918470	-2.792255
C	-5.217731	-0.567511	2.477828
C	-3.283035	-1.375248	1.155437
C	-2.571970	-4.102180	-1.473429
C	0.768602	4.370053	1.283226
C	-1.296867	0.193533	-0.760486
H	-1.803269	-0.729485	-1.061861
C	-6.487217	-0.804432	3.057427
H	-6.973127	0.010377	3.592741
C	-4.728429	4.402520	-2.664293
H	-5.680643	4.114304	-3.108409
C	-0.711822	-2.373795	2.004826
H	0.062411	-3.025371	2.422076
H	-1.422191	-2.125610	2.803269
C	-3.869164	3.380816	-2.193542
C	-3.126202	-4.600389	-2.677040
H	-2.629094	-5.435046	-3.170277
C	-1.668816	4.251673	1.449496
H	-2.625404	3.900608	1.065909
C	-1.627506	5.015560	2.594375
H	-2.552043	5.259096	3.114428
C	-1.385476	-4.648889	-0.933346
H	-0.918656	-5.497304	-1.432460
C	-4.562253	-1.618528	1.757651
C	-4.211931	2.017319	-2.324542
H	-5.165873	1.753434	-2.779931
C	-4.571277	0.681117	2.613722
H	-5.073619	1.479756	3.157895
C	-0.480653	3.905754	0.756054
C	-4.885692	-2.958287	-2.568054
H	-5.782019	-2.516504	-2.999099
C	-3.324435	0.879823	2.079996
H	-2.821247	1.841333	2.200905
C	0.771843	5.179411	2.444718
H	1.728821	5.534268	2.826544
C	1.974951	3.959327	0.666747
H	2.922489	4.323960	1.063518
C	1.958063	-0.547451	3.538466
H	2.175089	-0.182510	4.550019
H	2.778596	-0.204182	2.897041
H	1.972300	-1.642913	3.566092
C	-3.116880	6.071795	-2.025809
H	-2.817847	7.117039	-1.984782
C	-4.380145	-2.459011	-1.388728
H	-4.882006	-1.628810	-0.894998
C	-2.265623	5.103590	-1.547745
H	-1.301702	5.398306	-1.141254
C	1.956293	3.080040	-0.386559
H	2.887124	2.734369	-0.837654
C	-4.257203	-4.039533	-3.219741
H	-4.669328	-4.425962	-4.149220
C	-6.433625	-3.083548	2.282111
H	-6.901758	-4.064052	2.224300
C	0.802984	1.524814	2.801103
H	-0.151341	2.059191	2.725153
H	1.373751	1.711424	1.880445
H	1.358247	1.985542	3.628469
C	0.766001	-2.447359	-2.837760
H	0.503940	-3.105819	-3.677391
H	0.351846	-2.908330	-1.930391
H	1.859849	-2.446771	-2.769190
C	-0.398639	5.494323	3.092963
H	-0.380283	6.107497	3.991218
C	-4.367566	5.724312	-2.576306
H	-5.034489	6.501385	-2.943531
C	-1.273565	-1.162996	-3.487565
H	-1.325810	-1.688675	-4.450259
H	-1.752075	-0.185421	-3.622755
H	-1.869147	-1.749446	-2.778341
C	-7.089803	-2.034762	2.958450
H	-8.064602	-2.206007	3.409771
C	0.200040	-1.050040	-3.091187
C	-0.810565	-4.091840	0.179775
H	0.109346	-4.510066	0.587901
C	-0.431099	-0.171422	4.168718

H	-0.458421	-1.205088	4.530402
H	-1.441092	0.112884	3.847820
H	-0.169176	0.463792	5.024761
C	0.951418	-0.384008	-4.248172
H	2.005918	-0.188050	-4.036305
H	0.479579	0.556851	-4.552891
H	0.916764	-1.058886	-5.112774
Ni	1.634540	-1.115890	0.013319
H	3.324276	0.298413	0.607114
C	4.213743	-0.263376	0.248746
C	3.814734	-1.173497	-0.928576
H	4.620386	-1.906251	-1.072249
N	3.723084	-0.528195	-2.239052
O	3.939740	-1.225817	-3.229576
O	3.420656	0.669517	-2.282477
N	4.589663	-1.124337	1.376563
H	3.797555	-1.513665	1.876305
C	5.627430	-2.044812	1.449158
C	6.909560	-1.761634	0.721541
H	7.626602	-2.545092	0.972007
H	6.772854	-1.748946	-0.366681
H	7.317910	-0.782855	0.995309
O	5.476407	-3.032621	2.157630
C	5.267795	0.794840	-0.020709
C	6.134411	0.775919	-1.113562
C	5.386778	1.827007	0.914679
C	7.104947	1.761710	-1.264659
H	6.076752	-0.017144	-1.859421
C	6.354992	2.813622	0.767331
H	4.714522	1.841174	1.775578
C	7.218428	2.782612	-0.326123
H	7.772614	1.729810	-2.122808
H	6.438185	3.606701	1.508069
H	7.976387	3.553444	-0.446434
C	2.587475	-3.598791	0.634405
O	2.133613	-2.544227	1.208914
O	2.908708	-3.595884	-0.591746
C	2.797041	-4.816160	1.460537
H	3.765966	-4.699067	1.964653
H	2.031621	-4.909770	2.235796
H	2.831398	-5.711943	0.838060
H	3.053236	-2.352344	-0.844253

TSIV$_{S1}$

P	0.382783	-0.293229	-1.595787
P	0.119199	-1.161534	1.329846
C	-2.465998	0.019841	1.431806
C	-2.904569	-2.273397	0.468468
C	-5.370097	-2.282289	2.033367
H	-5.061968	-3.175716	1.495211
C	-1.791338	-3.043812	0.789842
C	0.256524	2.826797	-0.408133
C	-1.076414	2.737974	-1.071052
C	0.913745	-0.504686	2.888312
C	-3.698005	-2.638039	-0.666896
C	-1.762981	1.533458	-1.218467
C	-1.664294	3.945720	-1.580626
C	-3.068284	1.524707	-1.768431
H	-3.597640	0.572816	-1.831091
C	-1.104434	0.118953	0.782800
H	-0.640321	1.055643	1.126756
C	1.371149	2.196829	-0.952561
C	1.224734	1.253083	-2.103549
H	2.200026	0.972502	-2.520436
H	0.623630	1.683426	-2.919489
C	-4.953834	0.009285	2.768531
C	-3.286588	-1.100006	1.306948
C	-3.395011	-3.841609	-1.382846
C	1.728609	3.834157	1.311112
C	-1.197805	0.208879	-0.759396
H	-1.892889	-0.583224	-1.077868
C	-6.183760	-0.025178	3.466889
H	-6.486087	0.857988	4.028380
C	-3.567429	5.101690	-2.630489
H	-4.574235	5.052815	-3.043876
C	-0.868000	-2.604517	1.882635
H	-0.173874	-3.403384	2.169021
H	-1.420183	-2.302745	2.784903
C	-2.982931	3.909840	-2.139722
C	-4.158851	-4.178028	-2.526281
H	-3.916079	-5.095797	-3.061182
C	-0.690201	4.161866	1.481202
H	-1.693732	4.012142	1.086466
C	-0.511023	4.874330	2.644587
H	-1.375345	5.276744	3.169394
C	-2.308436	-4.642246	-0.957737
H	-2.089929	-5.564618	-1.494625
C	-4.534481	-1.135814	2.016503

C	-3.670329	2.676550	-2.198772
H	-4.681251	2.653614	-2.603841
C	-4.121619	1.150583	2.804525
H	-4.451670	2.028593	3.358290
C	0.415481	3.614395	0.779528
C	-5.474139	-2.174990	-2.264686
H	-6.279721	-1.531915	-2.613747
C	-2.909655	1.145015	2.168296
H	-2.264587	2.023792	2.210754
C	1.877882	4.589457	2.499232
H	2.882800	4.750195	2.888779
C	2.841404	3.254798	0.657172
H	3.842420	3.438183	1.047714
C	1.599383	-1.674537	3.596487
H	2.254065	-1.296957	4.392159
H	2.216358	-2.276245	2.914465
H	0.878946	-2.354219	4.065479
C	-1.569490	6.326296	-2.079377
H	-1.016785	7.263524	-2.075568
C	-4.760758	-1.825968	-1.140697
H	-5.009940	-0.911091	-0.605795
C	-0.978435	5.188181	-1.583123
H	0.037510	5.239677	-1.199363
C	2.661696	2.429257	-0.423036
H	3.519424	1.961752	-0.906756
C	-5.174059	-3.361991	-2.964743
H	-5.747664	-3.629064	-3.849473
C	-6.554908	-2.288293	2.731819
H	-7.172834	-3.183668	2.733930
C	1.921524	0.569065	2.493133
H	1.462414	1.329299	1.851498
H	2.788140	0.164873	1.955793
H	2.298536	1.082012	3.388049
C	-0.429689	-2.588726	-2.866508
H	-0.832939	-3.094032	-3.754581
H	-1.200176	-2.636387	-2.088829
H	0.446273	-3.149176	-2.520722
C	0.783699	5.096125	3.158127
H	0.912077	5.667498	4.074918
C	-2.879675	6.290057	-2.598339
H	-3.336571	7.199938	-2.981589
C	-1.319716	-0.466114	-3.813210
H	-1.482425	-0.894927	-4.810348
H	-1.209709	0.618432	-3.937431
H	-2.231111	-0.654489	-3.232636
C	-6.973435	-1.149217	3.449703
H	-7.914648	-1.167000	3.994965
C	-0.088587	-1.140714	-3.199097
C	-1.504912	-4.231297	0.075682
H	-0.642046	-4.828279	0.372132
C	-0.132456	0.123519	3.811696
H	-0.979911	-0.538383	4.028461
H	-0.529627	1.058685	3.399600
H	0.345808	0.368664	4.768914
C	1.077538	-1.057993	-4.186431
H	2.001624	-1.478760	-3.780458
H	1.265591	-0.029118	-4.516077
H	0.814809	-1.637186	-5.080461
Ni	1.468313	-1.607660	-0.271763
H	3.346388	-1.084360	0.529049
C	4.401198	-1.421588	0.412185
N	4.861419	-1.621254	1.775296
H	4.155565	-1.769320	2.486934
C	6.119180	-2.001966	2.226627
O	6.258516	-2.313998	3.396078
C	7.266754	-1.948747	1.253361
H	7.742221	-0.962173	1.307846
H	8.009335	-2.690152	1.556334
H	6.988159	-2.108871	0.207166
C	4.339835	-2.742225	-0.321242
H	5.195241	-3.410048	-0.271144
N	3.675753	-2.867507	-1.504546
O	3.979729	-3.650439	-2.399083
O	2.545685	-2.171011	-1.680229
C	5.121232	-0.274779	-0.287507
C	5.285490	-0.232006	-1.674935
C	5.568261	0.809957	0.476651
C	5.875049	0.875550	-2.283125
H	4.979949	-1.068317	-2.300056
C	6.170525	1.906940	-0.130681
H	5.449259	0.782370	1.559171
C	6.319959	1.947810	-1.515387
H	6.002023	0.887234	-3.363779
H	6.526860	2.733468	0.482208
H	6.792548	2.804116	-1.991730
H	2.866580	-3.125911	0.467080
H	2.061849	-2.964792	0.679365

IX_{R2}

P	-0.161101	-0.832036	-1.742720
P	-1.034638	0.065113	1.137699
C	1.563552	1.300036	1.392801
C	0.216942	3.077371	0.236509
C	1.669489	5.022196	1.870963
H	0.830137	5.345786	1.259488
C	-1.110503	2.723083	0.447300
C	2.304351	-2.557492	-0.151886
C	3.056869	-1.495042	-0.881782
C	-1.026783	-0.840846	2.788828
C	0.562496	3.861218	-0.914879
C	2.521910	-0.231410	-1.127231
C	4.378788	-1.797332	-1.359973
C	3.315260	0.768568	-1.741391
H	2.878141	1.756807	-1.893470
C	0.801012	0.177180	0.722156
H	1.185357	-0.763136	1.140368
C	1.124605	-3.086657	-0.668274
C	0.535743	-2.525042	-1.925468
H	-0.261076	-3.171479	-2.309442
H	1.314804	-2.457577	-2.696033
C	3.082618	3.247507	2.775118
C	1.272458	2.647012	1.192757
C	-0.472113	4.330863	-1.787359
C	2.206802	-4.228887	1.674689
C	1.096318	0.142466	-0.795972
H	0.930061	1.163982	-1.161971
C	3.800080	4.231052	3.496772
H	4.625154	3.910009	4.131877
C	6.462128	-1.066310	-2.451407
H	7.038990	-0.267669	-2.916491
C	-1.488232	1.803921	1.570309
H	-2.570071	1.835844	1.760103
H	-0.975108	2.082551	2.501064
C	5.158843	-0.770707	-1.985530
C	-0.128141	5.082420	-2.936478
H	-0.930064	5.437097	-3.583671
C	3.949613	-2.515338	1.729217
H	4.436731	-1.647117	1.289218
C	4.427642	-3.038910	2.908532
H	5.284397	-2.576963	3.395178
C	-1.816544	4.008149	-1.492127
H	-2.605999	4.392587	-2.137950
C	2.000018	3.643785	1.926014
C	4.600851	0.518134	-2.140446
H	5.201094	1.302474	-2.600327
C	3.404863	1.875298	2.876947
H	4.246668	1.574178	3.499484
C	2.829199	-3.087614	1.072787
C	2.209155	4.879464	-2.392401
H	3.248979	5.091258	-2.633696
C	2.657062	0.936812	2.217462
H	2.899820	-0.122289	2.317939
C	2.733616	-4.752088	2.880064
H	2.252385	-5.624531	3.321602
C	1.064518	-4.791988	1.058130
H	0.608674	-5.677364	1.502218
C	-2.443374	-0.803560	3.349086
H	-2.470433	-1.334362	4.310134
H	-3.139240	-1.305442	2.670675
H	-2.810873	0.214884	3.526472
C	6.209863	-3.354605	-1.750487
H	6.614960	-4.361930	-1.677694
C	1.906612	4.161204	-1.257143
H	2.709444	3.812521	-0.610440
C	4.945943	-3.095767	-1.274240
H	4.365160	-3.904960	-0.838106
C	0.522029	-4.213639	-0.060890
H	-0.374500	-4.626823	-0.521284
C	1.185397	5.350835	-3.239087
H	1.437933	5.925129	-4.127753
C	2.378615	5.952648	2.594379
H	2.098292	7.002634	2.541603
C	-0.630500	-2.289356	2.523079
H	0.397588	-2.375038	2.154640
H	-1.284861	-2.770464	1.786229
H	-0.683625	-2.868947	3.454932
C	-1.364011	-0.777616	-4.238104
H	-1.298783	-0.534198	-5.306206
H	-2.327767	-0.396047	-3.879963
H	-1.384669	-1.872461	-4.153544
C	3.821075	-4.171932	3.488148
H	4.212966	-4.581749	4.416504
C	6.983514	-2.331541	-2.335133
H	7.984707	-2.549158	-2.700931
C	-0.308124	1.362804	-3.444999
H	0.626688	1.849677	-3.137947

H	-1.096700	1.701108	-2.760223
H	-0.554322	1.749218	-4.442679
C	3.460106	5.559000	3.408457
H	4.015667	6.306420	3.970876
C	-0.168903	-0.158096	-3.502296
C	-2.119031	3.210045	-0.417839
H	-3.153820	2.969170	-0.184803
C	-0.052616	-0.240626	3.800391
H	-0.202569	0.832122	3.970984
H	0.991369	-0.392410	3.509175
H	-0.194241	-0.743389	4.766673
C	1.105429	-0.512398	-4.278659
H	1.153479	-1.575188	-4.539744
H	2.024045	-0.242814	-3.745720
H	1.100535	0.044922	-5.224369
Ni	-2.146230	-0.726563	-0.681536
H	-4.308196	-1.929953	-2.080229
C	-5.965843	0.923985	2.631959
C	-5.299716	-0.090297	1.950384
C	-4.789820	0.113124	0.661574
C	-5.021567	1.366266	0.069311
C	-5.686764	2.380827	0.744827
C	-6.155309	2.168332	2.039023
H	-6.351586	0.730605	3.630805
H	-5.191539	-1.057395	2.435887
H	-4.665033	1.558850	-0.943308
H	-5.842218	3.340644	0.255264
H	-6.676759	2.959400	2.572379
C	-4.089213	-0.937528	-0.130983
C	-4.749059	-1.112551	-1.496317
N	-4.078715	-2.251639	0.526215
H	-4.960709	-2.586287	0.907700
N	-6.243702	-1.471256	-1.420804
O	-6.661700	-2.021251	-0.404168
O	-6.906959	-1.191537	-2.404947
H	-4.738787	-0.215942	-2.116916
H	-2.690295	0.129554	-1.971629
C	-3.210351	-3.147072	0.042619
C	-3.332739	-4.584754	0.414302
H	-2.466091	-4.873903	1.021373
H	-4.242467	-4.805054	0.977969
H	-3.311654	-5.204842	-0.487050
O	-2.273189	-2.749055	-0.700187
H	-2.504712	0.688430	-1.377043

TSV_{R2}

P	-0.183084	-0.828040	-1.771935
P	-1.025152	0.045697	1.159009
C	1.565212	1.258211	1.390934
C	0.255719	3.062005	0.230463
C	1.700264	4.972275	1.917119
H	0.882045	5.313309	1.286778
C	-1.076787	2.704874	0.408362
C	2.281559	-2.585145	-0.246297
C	3.033713	-1.506393	-0.948686
C	-1.002913	-0.816182	2.838434
C	0.622663	3.868914	-0.898199
C	2.511313	-0.230581	-1.147186
C	4.361567	-1.799350	-1.415346
C	3.335810	0.793610	-1.674693
H	2.914960	1.794799	-1.778090
C	0.797244	0.155030	0.697260
H	1.185469	-0.797763	1.078357
C	1.109106	-3.116911	-0.772000
C	0.492402	-2.526685	-2.004400
H	-0.336515	-3.148875	-2.361496
H	1.232101	-2.463953	-2.816361
C	3.065580	3.169088	2.839088
C	1.292134	2.610517	1.199934
C	-0.397075	4.359610	-1.777700
C	2.184041	-4.261958	1.574746
C	1.079865	0.141488	-0.824767
H	0.915175	1.164404	-1.193519
C	3.776763	4.135708	3.589595
H	4.579457	3.796676	4.243799
C	6.473359	-1.041202	-2.427869
H	7.069701	-0.227848	-2.840121
C	-1.477931	1.795727	1.532352
H	-2.561637	1.836248	1.709528
H	-0.971750	2.088327	2.461506
C	5.165565	-0.752328	-1.971341
C	-0.032631	5.135654	-2.904261
H	-0.823156	5.502676	-3.558482
C	3.913043	-2.537043	1.646854
H	4.398502	-1.664384	1.214281
C	4.376869	-3.051942	2.836024
H	5.222161	-2.580675	3.333663
C	-1.746208	4.027832	-1.516552

H	-2.522570	4.420588	-2.173074
C	2.012016	3.589181	1.964389
C	4.627145	0.551501	-2.057463
H	5.247708	1.355677	-2.451451
C	3.362185	1.791182	2.941849
H	4.176594	1.472382	3.591621
C	2.805695	-3.119104	0.977220
C	2.294243	4.924683	-2.321002
H	3.337907	5.143662	-2.538078
C	2.621814	0.868469	2.250968
H	2.837494	-0.196237	2.358463
C	2.698208	-4.779138	2.787955
H	2.217828	-5.654554	3.224604
C	1.054222	-4.833609	0.944637
H	0.603525	-5.726301	1.379104
C	-2.451458	-1.041427	3.262472
H	-2.469926	-1.518110	4.251737
H	-2.987813	-1.694119	2.565883
H	-3.012010	-0.102002	3.341064
C	6.181798	-3.358195	-1.843592
H	6.574641	-4.372464	-1.811138
C	1.972299	4.180332	-1.208605
H	2.763377	3.819123	-0.554328
C	4.912451	-3.106732	-1.378001
H	4.314435	-3.927631	-0.988814
C	0.518630	-4.258750	-0.178940
H	-0.370028	-4.681058	-0.644062
C	1.285403	5.412409	-3.176542
H	1.553251	6.005198	-4.048353
C	2.402066	5.885332	2.668874
H	2.136530	6.939360	2.620474
C	-0.304657	-2.166354	2.673853
H	0.786628	-2.068648	2.618251
H	-0.636067	-2.705933	1.776952
H	-0.516048	-2.800295	3.545975
C	-1.032502	-1.087485	-4.379150
H	-1.162554	-0.653083	-5.378113
H	-2.035390	-1.268853	-3.968199
H	-0.535732	-2.056398	-4.508647
C	3.771365	-4.187757	3.410795
H	4.153046	-4.591410	4.346074
C	6.976924	-2.317571	-2.365081
H	7.982118	-2.529626	-2.723122
C	-0.859086	1.258119	-3.502769
H	-0.396644	1.925489	-2.764731
H	-1.935432	1.228236	-3.301112
H	-0.725402	1.727493	-4.486196
C	3.456971	5.468871	3.506373
H	4.007370	6.202785	4.091222
C	-0.214643	-0.127022	-3.512166
C	-2.068564	3.205453	-0.467789
H	-3.106564	2.952181	-0.264476
C	-0.307898	-0.009101	3.935345
H	-0.847290	0.911871	4.184010
H	0.726015	0.252591	3.692186
H	-0.284027	-0.616596	4.850205
C	1.197037	0.015622	-4.091933
H	1.818474	-0.881365	-3.982308
H	1.737419	0.850610	-3.634872
H	1.115727	0.228132	-5.165684
Ni	-2.164470	-0.786140	-0.703372
H	-4.488375	-2.023661	-2.106498
C	-5.859586	1.006546	2.561830
C	-5.230763	-0.033308	1.881757
C	-4.771184	0.131919	0.569806
C	-4.996608	1.374859	-0.043670
C	-5.626338	2.413299	0.630119
C	-6.056682	2.236970	1.943433
H	-6.210697	0.843367	3.578894
H	-5.110340	-0.991057	2.382676
H	-4.660174	1.537387	-1.069100
H	-5.783034	3.364977	0.125143
H	-6.552428	3.046888	2.473102
C	-4.135550	-0.963985	-0.221636
C	-4.850068	-1.146692	-1.556844
N	-4.167224	-2.255739	0.479715
H	-5.073489	-2.583158	0.808032
N	-6.358210	-1.386848	-1.412669
O	-6.757391	-1.951499	-0.393777
O	-7.057694	-1.014742	-2.338651
H	-4.784826	-0.282889	-2.218920
H	-2.654633	-0.421023	-2.051997
C	-3.181914	-3.124030	0.262615
C	-3.283529	-4.516533	0.783127
H	-2.462767	-4.695367	1.487953
H	-4.232475	-4.716646	1.286423
H	-3.159532	-5.230598	-0.037226
O	-2.146417	-2.749825	-0.353510

H	-2.459671	0.505183	-1.327535

X_{R2}

P	-0.229904	-0.876461	-1.772779
P	-1.008573	0.042288	1.178391
C	1.574824	1.209526	1.382230
C	0.279034	3.043495	0.250983
C	1.738779	4.914286	1.961956
H	0.936187	5.274068	1.322210
C	-1.059597	2.715264	0.443913
C	2.299793	-2.580893	-0.328552
C	3.030964	-1.477752	-1.014102
C	-0.986125	-0.845279	2.840717
C	0.648546	3.861340	-0.867498
C	2.475452	-0.213969	-1.205025
C	4.364864	-1.736084	-1.482054
C	3.273497	0.829481	-1.735721
H	2.831627	1.821041	-1.834283
C	0.795116	0.127603	0.670039
H	1.178235	-0.836518	1.026313
C	1.144323	-3.127437	-0.875061
C	0.531618	-2.517736	-2.100273
H	-0.253798	-3.161992	-2.512806
H	1.286109	-2.371929	-2.888402
C	3.067415	3.083264	2.883314
C	1.314453	2.566063	1.209418
C	-0.371462	4.388881	-1.724984
C	2.197746	-4.267242	1.481503
C	1.041438	0.129560	-0.857223
H	0.847164	1.148535	-1.223655
C	3.776611	4.031743	3.658491
H	4.563111	3.674547	4.322576
C	6.456775	-0.924092	-2.493596
H	7.032302	-0.095828	-2.905685
C	-1.462409	1.786976	1.552196
H	-2.545924	1.821770	1.730645
H	-0.958305	2.067890	2.486151
C	5.142212	-0.668729	-2.036888
C	-0.003327	5.166629	-2.849324
H	-0.793121	5.559476	-3.489180
C	3.916275	-2.531986	1.576468
H	4.401049	-1.655737	1.150371
C	4.370915	-3.047371	2.768820
H	5.209304	-2.573555	3.275687
C	-1.725630	4.105650	-1.434050
H	-2.502745	4.538365	-2.063771
C	2.033676	3.527048	1.996123
C	4.569267	0.620153	-2.122427
H	5.167049	1.440940	-2.517595
C	3.343908	1.700503	2.976196
H	4.139598	1.363361	3.639820
C	2.818346	-3.117958	0.894967
C	2.325425	4.905815	-2.291330
H	3.370605	5.110862	-2.514825
C	2.607268	0.794792	2.258857
H	2.807051	-0.273372	2.358722
C	2.702646	-4.784357	2.698859
H	2.223991	-5.664550	3.127790
C	1.079098	-4.845674	0.837304
H	0.627138	-5.739911	1.266704
C	-2.434276	-1.169661	3.198592
H	-2.465351	-1.683046	4.168915
H	-2.905829	-1.824039	2.457371
H	-3.051368	-0.267457	3.283901
C	6.223970	-3.248223	-1.909502
H	6.642996	-4.251949	-1.876577
C	2.000632	4.154848	-1.184640
H	2.790516	3.772418	-0.541032
C	4.948066	-3.029402	-1.445361
H	4.370328	-3.864942	-1.056646
C	0.555212	-4.275526	-0.294303
H	-0.324488	-4.705235	-0.770224
C	1.317223	5.418048	-3.133677
H	1.587633	6.013408	-4.002925
C	2.438375	5.809087	2.737073
H	2.186096	6.866725	2.697631
C	-0.184106	-2.140374	2.697683
H	0.898314	-1.959596	2.705039
H	-0.433311	-2.699950	1.787032
H	-0.394658	-2.791755	3.556905
C	-1.077899	-1.093678	-4.400106
H	-1.275264	-0.609303	-5.364511
H	-2.043042	-1.440731	-4.006909
H	-0.450873	-1.970519	-4.599904
C	3.765239	-4.187659	3.334742
H	4.139545	-4.591638	4.272856
C	6.992535	-2.187350	-2.430705
H	8.002819	-2.373806	-2.788706

C	-1.235471	1.177344	-3.351789
H	-0.857404	1.848638	-2.570342
H	-2.287228	0.961700	-3.126161
H	-1.200428	1.729279	-4.300321
C	3.473777	5.369528	3.587192
H	4.022313	6.089131	4.191263
C	-0.396059	-0.092627	-3.466898
C	-2.053564	3.276137	-0.392699
H	-3.094684	3.057566	-0.169657
C	-0.392852	0.004834	3.965713
H	-1.027684	0.860373	4.222286
H	0.613626	0.374204	3.742804
H	-0.319711	-0.617608	4.867502
C	0.975450	0.283480	-4.036442
H	1.714726	-0.525113	-3.979689
H	1.398035	1.159667	-3.531252
H	0.858911	0.548221	-5.095024
Ni	-2.104825	-0.910507	-0.590711
H	-4.527749	-1.860831	-2.272486
C	-5.854388	0.760544	2.613883
C	-5.247826	-0.235679	1.852017
C	-4.736937	0.037714	0.578743
C	-4.890570	1.342323	0.084511
C	-5.499346	2.337177	0.838398
C	-5.980330	2.052738	2.115141
H	-6.243663	0.515449	3.600244
H	-5.176990	-1.242472	2.258916
H	-4.512890	1.584611	-0.909977
H	-5.604555	3.338328	0.423235
H	-6.461133	2.827944	2.707214
C	-4.121235	-1.005732	-0.306483
C	-4.780840	-0.975002	-1.680527
N	-4.278415	-2.359306	0.250456
H	-5.228276	-2.700037	0.389602
N	-6.306396	-0.996403	-1.595917
O	-6.805339	-1.744380	-0.751277
O	-6.924835	-0.290581	-2.373468
H	-4.545788	-0.086008	-2.267281
H	-2.429254	-1.313358	-1.975368
C	-3.238432	-3.179027	0.334184
C	-3.418108	-4.577114	0.818984
H	-2.709189	-4.764804	1.633099
H	-4.432202	-4.782552	1.169956
H	-3.175060	-5.281309	0.016048
O	-2.081724	-2.772602	0.028778
H	-2.273139	0.480637	-0.949732

$TSVI_{R2}$

P	-0.404795	-0.883786	-1.737373
P	-0.966124	0.114486	1.323183
C	1.703620	1.071574	1.353163
C	0.509945	3.024527	0.322695
C	2.245104	4.738166	1.953271
H	1.433337	5.177288	1.377955
C	-0.836385	2.782499	0.580749
C	2.145548	-2.671103	-0.414238
C	2.882557	-1.590008	-1.128071
C	-0.905839	-0.774902	2.984979
C	0.876961	3.832744	-0.803949
C	2.347069	-0.313476	-1.296389
C	4.184634	-1.882236	-1.660876
C	3.138980	0.704662	-1.881446
H	2.713816	1.704368	-1.967426
C	0.793437	0.069061	0.679137
H	1.126412	-0.926471	0.997025
C	0.944564	-3.162140	-0.914249
C	0.321709	-2.531967	-2.123266
H	-0.483112	-3.160461	-2.523381
H	1.064712	-2.397192	-2.923463
C	3.463642	2.781579	2.760231
C	1.555960	2.449739	1.212674
C	-0.147485	4.426842	-1.611686
C	2.024158	-4.339111	1.412597
C	0.943718	0.070703	-0.872077
H	0.765432	1.100578	-1.217630
C	4.318270	3.651290	3.479083
H	5.117119	3.214666	4.077793
C	6.242635	-1.123908	-2.778726
H	6.814518	-0.311353	-3.225675
C	-1.248026	1.891885	1.716970
H	-2.314527	2.017278	1.951118
H	-0.671334	2.136025	2.618245
C	4.957130	-0.836637	-2.261522
C	0.214647	5.205411	-2.737654
H	-0.579451	5.650261	-3.336796
C	3.849723	-2.714531	1.413793
H	4.367740	-1.872412	0.959640
C	4.325614	-3.250097	2.588703

H	5.215335	-2.827060	3.051639
C	-1.502069	4.209726	-1.269837
H	-2.279811	4.685618	-1.867026
C	2.411619	3.329348	1.956584
C	4.407794	0.462923	-2.333847
H	5.000655	1.265913	-2.771188
C	3.610946	1.378276	2.831326
H	4.413790	0.960105	3.438314
C	2.686062	-3.233135	0.788586
C	2.546589	4.814826	-2.281315
H	3.591384	4.967994	-2.545266
C	2.742895	0.554302	2.164529
H	2.846541	-0.528000	2.247104
C	2.549828	-4.877736	2.612038
H	2.035535	-5.721683	3.071373
C	0.842947	-4.850738	0.826620
H	0.352565	-5.706857	1.290057
C	-2.354122	-1.056675	3.385154
H	-2.376504	-1.533618	4.374217
H	-2.844688	-1.733753	2.674909
H	-2.955117	-0.140997	3.444596
C	5.988167	-3.437901	-2.166547
H	6.385701	-4.450733	-2.146807
C	2.228642	4.059090	-1.176212
H	3.024870	3.620567	-0.578345
C	4.740204	-3.188209	-1.644947
H	4.164102	-4.009563	-1.225105
C	0.310792	-4.263534	-0.292418
H	-0.611257	-4.645070	-0.728364
C	1.533392	5.396599	-3.071004
H	1.799117	5.995260	-3.939489
C	3.084571	5.555598	2.673309
H	2.930796	6.632721	2.657032
C	-0.162096	-2.098967	2.806607
H	0.925878	-1.962518	2.758231
H	-0.482356	-2.641904	1.907771
H	-0.357283	-2.745325	3.673186
C	-1.476084	-1.031728	-4.260090
H	-1.749200	-0.542898	-5.203697
H	-2.410379	-1.314516	-3.753552
H	-0.934014	-1.950090	-4.514907
C	3.674985	-4.344660	3.193947
H	4.064639	-4.763563	4.119276
C	6.754243	-2.397629	-2.730842
H	7.742362	-2.608094	-3.134498
C	-1.377299	1.245989	-3.234772
H	-0.862232	1.918749	-2.537303
H	-2.398662	1.101177	-2.858607
H	-1.443298	1.764604	-4.200485
C	4.139021	5.012191	3.435594
H	4.798978	5.670795	3.996194
C	-0.635297	-0.076013	-3.411221
C	-1.831146	3.397023	-0.215796
H	-2.872872	3.229193	0.046744
C	-0.244135	0.053573	4.087189
H	-0.846375	0.923959	4.372002
H	0.759393	0.402059	3.818022
H	-0.143760	-0.571411	4.984695
C	0.696789	0.206736	-4.109000
H	1.367726	-0.660355	-4.146907
H	1.238573	1.025958	-3.623247
H	0.503654	0.515121	-5.144754
Ni	-2.134798	-0.779830	-0.370829
H	-4.947909	-1.551536	-2.456987
C	-5.560201	0.877451	2.664283
C	-5.115900	-0.112470	1.792862
C	-4.702060	0.205246	0.494541
C	-4.772717	1.546464	0.089373
C	-5.220631	2.533892	0.959045
C	-5.613817	2.206372	2.255225
H	-5.881160	0.600062	3.666710
H	-5.098556	-1.147601	2.127067
H	-4.456914	1.825901	-0.916889
H	-5.268977	3.566548	0.617237
H	-5.972105	2.977796	2.932670
C	-4.289059	-0.857912	-0.490599
C	-5.073718	-0.688334	-1.793462
N	-4.500835	-2.214531	0.009200
H	-5.469017	-2.520376	0.088304
N	-6.568286	-0.591965	-1.551307
O	-7.045364	-1.395788	-0.745679
O	-7.189641	0.250782	-2.171574
H	-4.806446	0.219314	-2.337710
H	-3.095385	-0.992725	-1.462988
C	-3.490181	-3.014464	0.352079
C	-3.780757	-4.379841	0.874639
H	-3.294928	-4.499550	1.849308
H	-4.849290	-4.582586	0.979820

H	-3.342561	-5.129634	0.207856
O	-2.297085	-2.629568	0.244507
H	-1.987036	0.619363	-0.727930

XI_{R2}

P	-0.441303	-0.660108	-1.846755
P	-0.825160	0.329742	1.402370
C	1.947191	0.906276	1.326086
C	0.968932	3.013172	0.354880
C	2.999282	4.471920	1.878687
H	2.241305	5.016393	1.320578
C	-0.376764	2.964138	0.707706
C	1.720883	-2.879787	-0.539790
C	2.692317	-1.908921	-1.116019
C	-0.898792	-0.596151	3.036347
C	1.366095	3.782660	-0.787448
C	2.368753	-0.562032	-1.278342
C	3.974458	-2.386869	-1.551786
C	3.343515	0.330140	-1.787891
H	3.079333	1.383132	-1.877882
C	0.891755	0.035732	0.682079
H	1.089730	-0.998094	0.993217
C	0.518407	-3.125076	-1.192869
C	0.139585	-2.321739	-2.398524
H	-0.675759	-2.800089	-2.953645
H	0.990402	-2.197675	-3.084357
C	3.958835	2.372159	2.672138
C	1.979067	2.293245	1.182080
C	0.384314	4.538395	-1.508320
C	1.103749	-4.573525	1.156743
C	1.029344	0.025600	-0.882670
H	1.029057	1.079715	-1.199393
C	4.942360	3.120271	3.362411
H	5.690053	2.580980	3.943265
C	6.210750	-1.928991	-2.472751
H	6.932930	-1.205056	-2.848786
C	-0.823413	2.113274	1.856238
H	-1.841027	2.376656	2.174565
H	-0.157601	2.254349	2.717321
C	4.941059	-1.460259	-2.058749
C	0.773434	5.269597	-2.656227
H	0.012155	5.836032	-3.192199
C	3.179388	-3.316415	1.441307
H	3.889654	-2.571714	1.088074
C	3.421690	-3.982796	2.620996
H	4.317683	-3.753964	3.194820
C	-0.960317	4.514478	-1.069917
H	-1.700939	5.107893	-1.605665
C	2.970516	3.053158	1.889792
C	4.594153	-0.094036	-2.149525
H	5.330745	0.615304	-2.525708
C	3.916054	0.962594	2.754508
H	4.671392	0.444504	3.344737
C	2.017653	-3.583606	0.671748
C	3.048896	4.528667	-2.382441
H	4.082325	4.530859	-2.723406
C	2.929915	0.258782	2.114405
H	2.889079	-0.827830	2.202036
C	1.392531	-5.255448	2.363313
H	0.689322	-6.010803	2.713895
C	-0.082876	-4.827383	0.430207
H	-0.767058	-5.595080	0.792728
C	-2.387769	-0.653142	3.394925
H	-2.515802	-1.089221	4.394882
H	-2.944757	-1.272676	2.680727
H	-2.857619	0.340381	3.404217
C	5.565164	-4.187334	-1.947366
H	5.805462	-5.248317	-1.922793
C	2.705140	3.815635	-1.256808
H	3.470228	3.266157	-0.712396
C	4.326395	-3.761471	-1.528134
H	3.599886	-4.492937	-1.182817
C	-0.372868	-4.106298	-0.699511
H	-1.296484	-4.287574	-1.249880
C	2.076380	5.262579	-3.092456
H	2.360976	5.825024	-3.979046
C	3.961456	5.170476	2.569891
H	3.956191	6.258396	2.546605
C	-0.364582	-2.013291	2.828815
H	0.731859	-2.039204	2.780546
H	-0.756737	-2.484854	1.917085
H	-0.657455	-2.643082	3.680066
C	-1.415451	-0.423501	-4.390341
H	-1.654305	0.201079	-5.260559
H	-2.368050	-0.724930	-3.928783
H	-0.919125	-1.326692	-4.764284
C	2.524851	-4.966049	3.086889
H	2.731997	-5.493111	4.015930

C	6.523435	-3.265070	-2.414612
H	7.501139	-3.615220	-2.738994
C	-1.200150	1.689102	-3.071857
H	-0.665687	2.212549	-2.270798
H	-2.238703	1.554996	-2.734338
H	-1.208338	2.347908	-3.951172
C	4.950739	4.492626	3.311349
H	5.710089	5.057445	3.847939
C	-0.535694	0.359810	-3.413406
C	-1.328488	3.727892	-0.009161
H	-2.365963	3.697897	0.319584
C	-0.121036	0.094743	4.155574
H	-0.582372	1.041641	4.458664
H	0.922749	0.292104	3.881524
H	-0.110992	-0.554794	5.041188
C	0.831522	0.635437	-4.037368
H	1.439440	-0.268859	-4.164905
H	1.411831	1.350168	-3.440073
H	0.698183	1.083416	-5.031130
Ni	-1.869780	-0.437356	-0.280004
H	-5.509500	-0.791244	-2.714886
C	-5.772022	0.924220	2.670743
C	-5.566098	0.046000	1.609097
C	-4.879822	0.466736	0.470351
C	-4.407909	1.781856	0.402496
C	-4.623620	2.660239	1.458599
C	-5.304703	2.232230	2.597841
H	-6.307619	0.583446	3.554156
H	-5.942198	-0.973741	1.673503
H	-3.858973	2.115099	-0.482857
H	-4.266392	3.687105	1.394282
H	-5.474404	2.921494	3.421982
C	-4.684417	-0.443221	-0.728643
C	-5.602775	-0.078095	-1.888405
N	-4.797074	-1.858329	-0.410390
H	-5.742333	-2.228728	-0.394347
N	-7.055802	-0.106658	-1.480739
O	-7.431939	-1.112648	-0.870621
O	-7.749368	0.845788	-1.781187
H	-5.409250	0.934368	-2.247607
H	-3.662480	-0.295787	-1.143922
C	-3.786552	-2.575772	0.113136
C	-4.076497	-3.967355	0.569754
H	-3.700927	-4.090302	1.591261
H	-5.139100	-4.221017	0.542789
H	-3.528259	-4.681213	-0.054548
O	-2.623154	-2.131507	0.212762
H	-1.396469	0.909359	-0.573595

TSIV$_{R3}$

P	0.459512	-0.023672	-1.659366
P	0.417644	-0.938508	1.373055
C	-2.346936	-0.300597	1.456645
C	-2.284526	-2.642532	0.502033
C	-4.797916	-3.110691	1.912817
H	-4.295362	-3.932041	1.408233
C	-1.057995	-3.158136	0.909831
C	-0.270901	2.999658	-0.430762
C	-1.635726	2.645262	-0.915555
C	1.143467	-0.080574	2.871612
C	-2.916986	-3.198835	-0.659021
C	-2.030601	1.320433	-1.104805
C	-2.543715	3.703268	-1.265772
C	-3.334177	1.028661	-1.573283
H	-3.616897	-0.017402	-1.697734
C	-1.027629	0.077679	0.818618
H	-0.759802	1.089684	1.163473
C	0.844576	2.620223	-1.172435
C	0.707716	1.674518	-2.319167
H	1.592136	1.681298	-2.960659
H	-0.168064	1.902332	-2.943952
C	-4.860182	-0.784478	2.652142
C	-2.936433	-1.555708	1.291077
C	-2.311424	-4.314593	-1.324128
C	1.234357	4.241916	1.098517
C	-1.160451	0.143131	-0.721469
H	-1.695347	-0.769826	-1.009905
C	-6.108025	-1.047465	3.266692
H	-6.604414	-0.237101	3.799158
C	-4.768907	4.420364	-2.040045
H	-5.771212	4.150748	-2.371430
C	-0.293934	-2.498116	2.013803
H	0.527627	-3.130134	2.368609
H	-0.938975	-2.258320	2.870228
C	-3.864745	3.379997	-1.716998
C	-2.911936	-4.836960	-2.494576
H	-2.435907	-5.684278	-2.987295
C	-1.144399	4.076871	1.647976

H	-2.151273	3.749231	1.392392
C	-0.923903	4.778716	2.811201
H	-1.755559	4.987532	3.481418
C	-1.109317	-4.858158	-0.814401
H	-0.669055	-5.722843	-1.309801
C	-4.191116	-1.827982	1.934150
C	-4.233224	2.023309	-1.852670
H	-5.238841	1.780663	-2.194277
C	-4.251178	0.486605	2.744765
H	-4.766891	1.282449	3.280345
C	-0.080184	3.779183	0.757723
C	-4.664194	-3.189462	-2.354905
H	-5.577290	-2.757289	-2.759496
C	-3.023823	0.710763	2.179087
H	-2.552613	1.691234	2.260627
C	1.420447	4.983870	2.289322
H	2.423615	5.336072	2.528322
C	2.322623	3.912020	0.254564
H	3.318552	4.291971	0.484338
C	2.098736	-1.051437	3.567718
H	2.643692	-0.521439	4.358895
H	2.851185	-1.468423	2.882458
H	1.570980	-1.887031	4.041753
C	-3.079907	6.061566	-1.545661
H	-2.772011	7.104139	-1.501819
C	-4.112501	-2.665090	-1.207560
H	-4.598749	-1.829536	-0.707125
C	-2.181714	5.074571	-1.213767
H	-1.172677	5.350923	-0.919066
C	2.134092	3.099678	-0.835603
H	2.978585	2.852136	-1.479771
C	-4.061158	-4.284852	-3.007075
H	-4.508647	-4.690751	-3.911724
C	-6.005823	-3.337052	2.530156
H	-6.445786	-4.331849	2.501208
C	1.889201	1.181095	2.428330
H	1.374512	1.705883	1.614098
H	2.916156	0.969498	2.105645
H	1.963896	1.887090	3.265059
C	0.447956	-2.508588	-2.928820
H	0.105401	-3.151742	-3.751146
H	-0.007092	-2.888615	-2.005327
H	1.536707	-2.628515	-2.853998
C	0.368036	5.242109	3.135314
H	0.527381	5.805643	4.052186
C	-4.390705	5.737226	-1.950315
H	-5.092468	6.529215	-2.203245
C	-1.433569	-0.992460	-3.549520
H	-1.586779	-1.479933	-4.521602
H	-1.803312	0.036783	-3.638723
H	-2.065407	-1.526000	-2.828672
C	-6.676343	-2.296061	3.204167
H	-7.634764	-2.487377	3.681970
C	0.055304	-1.059595	-3.205152
C	-0.484922	-4.273714	0.256833
H	0.458368	-4.672894	0.629806
C	0.013481	0.330373	3.821838
H	-0.662632	-0.491920	4.083947
H	-0.590356	1.146105	3.406916
H	0.457165	0.699836	4.755194
C	0.847315	-0.524781	-4.402353
H	1.925753	-0.468001	-4.229801
H	0.499934	0.465623	-4.717003
H	0.692220	-1.204479	-5.249851
Ni	1.817538	-1.123367	-0.250928
H	3.195290	-0.404685	0.750809
C	4.095985	-0.521293	0.088624
N	4.465723	0.850288	-0.139978
H	3.739492	1.537783	0.038248
C	5.448576	1.350544	-0.980386
O	5.475556	2.546517	-1.215516
C	6.454972	0.382503	-1.541425
H	6.303289	-0.663139	-1.253394
H	6.442015	0.461490	-2.633464
H	7.456003	0.680777	-1.214244
C	3.651598	-1.363538	-1.136668
H	4.268367	-2.259398	-1.246367
N	3.679260	-0.781331	-2.503228
O	3.903873	-1.583081	-3.406349
O	3.460095	0.418155	-2.667450
C	5.067991	-1.284686	0.983503
C	5.019468	-2.678551	1.105030
C	5.958671	-0.574606	1.794708
C	5.852126	-3.344906	1.999343
H	4.326169	-3.273412	0.511964
C	6.793211	-1.242594	2.684644
H	5.997842	0.509702	1.720338
C	6.744851	-2.629597	2.790674

H	5.801974	-4.429172	2.071190
H	7.486870	-0.671297	3.298060
H	7.399506	-3.150511	3.485746
H	2.631327	-2.336768	-0.672880
H	2.124904	-2.478690	0.383791

TSIV$_{R1}$

P	0.393416	-0.206550	-1.666973
P	0.389317	-1.061263	1.271371
C	-2.279453	-0.122066	1.551498
C	-2.573887	-2.458932	0.658937
C	-4.894313	-2.670082	2.427291
H	-4.548666	-3.541948	1.876523
C	-1.367106	-3.108626	0.891179
C	-0.054057	2.919417	-0.513431
C	-1.390071	2.638974	-1.113934
C	1.263586	-0.268625	2.721426
C	-3.413556	-2.906977	-0.411586
C	-1.935432	1.359291	-1.185468
C	-2.131996	3.746521	-1.653140
C	-3.255416	1.178238	-1.666479
H	-3.673481	0.170649	-1.665860
C	-0.987146	0.086800	0.794550
H	-0.592916	1.072038	1.083159
C	1.113981	2.431512	-1.092354
C	1.060676	1.424151	-2.198756
H	2.057246	1.263098	-2.635062
H	0.399048	1.758403	-3.013889
C	-4.637810	-0.334127	3.093695
C	-2.998767	-1.314904	1.514096
C	-3.042478	-4.069305	-1.161744
C	1.331846	4.214819	1.082517
C	-1.187742	0.125433	-0.739725
H	-1.797685	-0.752717	-1.004989
C	-5.798823	-0.467454	3.891733
H	-6.136975	0.396108	4.463295
C	-4.181072	4.620613	-2.700718
H	-5.186046	4.435547	-3.078488
C	-0.417746	-2.574268	1.922128
H	0.366833	-3.300669	2.164638
H	-0.936824	-2.312204	2.854741
C	-3.453140	3.532590	-2.162751
C	-3.861975	-4.490222	-2.237141
H	-3.568064	-5.376577	-2.798429
C	-1.097980	4.198181	1.363660
H	-2.085405	3.884224	1.028661
C	-0.972505	4.987291	2.483940
H	-1.862023	5.287624	3.034181
C	-1.839088	-4.741103	-0.838887
H	-1.561647	-5.628894	-1.405866
C	-4.174553	-1.451381	2.325992
C	-4.000436	2.230062	-2.126499
H	-5.016123	2.072608	-2.487533
C	-3.914384	0.878663	3.045984
H	-4.277045	1.733632	3.615372
C	0.042859	3.779044	0.630991
C	-5.357679	-2.639603	-1.849259
H	-6.252930	-2.085853	-2.125071
C	-2.762933	0.971148	2.310991
H	-2.199018	1.904921	2.294261
C	1.423166	5.041778	2.227907
H	2.409890	5.370262	2.553137
C	2.483073	3.801180	0.372883
H	3.457234	4.185378	0.674776
C	2.230973	-1.287626	3.326551
H	2.834230	-0.798972	4.102301
H	2.935316	-1.700359	2.593690
H	1.705250	-2.125355	3.800146
C	-2.322181	6.090666	-2.281757
H	-1.879006	7.082153	-2.347867
C	-4.592810	-2.213945	-0.787812
H	-4.890088	-1.328284	-0.229415
C	-1.593662	5.056618	-1.741910
H	-0.580566	5.245000	-1.395140
C	2.377246	2.916888	-0.670568
H	3.259228	2.626720	-1.243203
C	-4.994308	-3.789710	-2.579626
H	-5.609589	-4.118383	-3.414313
C	-6.012321	-2.770702	3.221904
H	-6.541259	-3.719327	3.287572
C	2.011286	0.962435	2.217587
H	1.335977	1.676118	1.732604
H	2.808638	0.719149	1.505136
H	2.483344	1.485477	3.060068
C	-0.373530	-2.513177	-2.948597
H	-0.801543	-3.009949	-3.829837
H	-1.109590	-2.598947	-2.139675
H	0.526233	-3.062187	-2.652155

C	0.297420	5.418201	2.920297
H	0.381034	6.049518	3.802171
C	-3.631071	5.877853	-2.758534
H	-4.196755	6.705865	-3.180293
C	-1.348871	-0.415043	-3.852517
H	-1.498087	-0.816523	-4.863114
H	-1.296312	0.677755	-3.937486
H	-2.242118	-0.668811	-3.269426
C	-6.477113	-1.659987	3.955619
H	-7.365981	-1.752819	4.575843
C	-0.083927	-1.049020	-3.266917
C	-1.006484	-4.249718	0.135045
H	-0.061185	-4.748052	0.353125
C	0.250508	0.175194	3.780697
H	-0.418273	-0.629507	4.109157
H	-0.368761	1.009957	3.432562
H	0.797749	0.525666	4.665291
C	1.069516	-0.904674	-4.262983
H	2.024846	-1.248889	-3.856131
H	1.187475	0.129367	-4.607498
H	0.847416	-1.516118	-5.146367
Ni	1.601943	-1.510048	-0.424938
H	3.354304	-0.992254	0.620419
C	4.330155	-1.015418	0.085192
N	4.167731	0.060896	-0.881878
H	3.347860	0.647721	-0.765867
C	4.874013	0.332823	-2.031327
O	4.462712	1.195197	-2.800406
C	6.131128	-0.456578	-2.267589
H	5.901858	-1.406078	-2.767200
H	6.780834	0.116814	-2.931221
H	6.665459	-0.684846	-1.337960
C	4.465912	-2.396222	-0.517094
H	5.438582	-2.879536	-0.492403
N	3.811559	-2.675466	-1.698012
O	4.268181	-3.403779	-2.572906
O	2.585419	-2.216355	-1.855223
C	5.380363	-0.761390	1.147875
C	5.807184	-1.802962	1.978862
C	5.849525	0.532242	1.388163
C	6.692147	-1.556491	3.023500
H	5.441127	-2.816973	1.815203
C	6.739229	0.776505	2.430342
H	5.514902	1.349640	0.749981
C	7.162530	-0.265654	3.250599
H	7.018154	-2.377784	3.658265
H	7.105695	1.787228	2.598692
H	7.860300	-0.073738	4.062877
H	3.164696	-2.958110	0.311168
H	2.339294	-2.812797	0.535387

(NOAc-H)

TSII$_{S1}$

P	-0.288748	-1.034807	-1.693314
P	-1.251179	-0.197177	1.115750
C	1.059423	1.471696	1.349078
C	-0.588495	2.953342	0.130225
C	0.455933	5.159844	1.714744
H	-0.431391	5.303315	1.102890
C	-1.852790	2.407966	0.326054
C	2.380060	-2.311623	-0.103659
C	3.012981	-1.148025	-0.791077
C	-1.213676	-0.999414	2.806790
C	-0.361200	3.796187	-1.007482
C	2.291130	0.001515	-1.114824
C	4.392925	-1.238866	-1.179682
C	2.936859	1.088520	-1.752972
H	2.350252	1.981333	-1.978378
C	0.525480	0.210957	0.710076
H	1.056873	-0.641856	1.159431
C	1.334745	-2.997922	-0.714151
C	0.760803	-2.500592	-2.005656
H	0.140267	-3.263518	-2.487525
H	1.554821	-2.201508	-2.702655
C	2.180304	3.712894	2.658809
C	0.514580	2.729976	1.106853
C	-1.460946	4.164500	-1.848973
C	2.324386	-3.966186	1.736317
C	0.818850	0.167743	-0.812511
H	0.509874	1.143387	-1.211463
C	2.706505	4.837758	3.337845
H	3.580364	4.697412	3.973140
C	6.388084	-0.209708	-2.191511
H	6.851259	0.654278	-2.667070
C	-2.096219	1.411867	1.418339
H	-3.167960	1.202091	1.533901
H	-1.729724	1.783157	2.387604
C	5.025772	-0.121981	-1.816414

C	-1.226427	4.976431	-2.984715
H	-2.075447	5.254196	-3.608574
C	3.833991	-2.049898	1.914603
H	4.254340	-1.136567	1.496454
C	4.254895	-2.496307	3.146691
H	5.000207	-1.928506	3.700333
C	-2.753416	3.686535	-1.534079
H	-3.598636	4.004161	-2.143822
C	1.038804	3.869645	1.808249
C	4.266988	1.040035	-2.078711
H	4.750908	1.889837	-2.558810
C	2.755322	2.430227	2.804367
H	3.639716	2.315499	3.429911
C	2.859061	-2.763246	1.170196
C	1.132009	5.016246	-2.492156
H	2.137447	5.340677	-2.753225
C	2.197731	1.345101	2.183281
H	2.633681	0.354132	2.317121
C	2.794689	-4.407344	2.996682
H	2.383570	-5.328013	3.409998
C	1.304931	-4.662443	1.045076
H	0.906287	-5.579436	1.478002
C	-2.632893	-0.986882	3.376149
H	-2.650112	-1.558865	4.312233
H	-3.358888	-1.451983	2.695835
H	-2.983140	0.026583	3.607060
C	6.480634	-2.474340	-1.381936
H	7.044058	-3.393219	-1.232569
C	0.934305	4.250117	-1.366405
H	1.783465	3.975559	-0.743306
C	5.162648	-2.416438	-0.993766
H	4.698767	-3.292570	-0.547687
C	0.796672	-4.168961	-0.129282
H	-0.015265	-4.682767	-0.642191
C	0.043283	5.391456	-3.306280
H	0.212595	6.005917	-4.187836
C	0.983535	6.230989	2.397055
H	0.512195	7.207851	2.310575
C	-0.717164	-2.431599	2.634734
H	0.258251	-2.457442	2.134647
H	-1.408225	-3.045537	2.042965
H	-0.592061	-2.907294	3.616582
C	-1.333225	1.033710	-3.201140
H	-1.717063	1.391709	-4.165465
H	-0.608813	1.779712	-2.852340
H	-2.175314	1.025714	-2.494802
C	3.737367	-3.689134	3.692251
H	4.085718	-4.037172	4.662328
C	7.106635	-1.359708	-1.976268
H	8.151548	-1.417727	-2.273219
C	0.533520	-0.245961	-4.263721
H	0.263449	0.248573	-5.205898
H	0.942261	-1.228990	-4.522774
H	1.332786	0.345804	-3.799841
C	2.125371	6.075806	3.208864
H	2.536919	6.933204	3.737194
C	-0.709590	-0.346428	-3.377852
C	-2.932643	2.811288	-0.493675
H	-3.927551	2.442361	-0.251459
C	-0.268006	-0.266251	3.760775
H	-0.455603	0.812669	3.827716
H	0.782056	-0.408439	3.481377
H	-0.392138	-0.682393	4.768706
C	-1.731674	-1.295517	-4.009710
H	-2.670755	-1.320639	-3.440489
H	-1.365902	-2.326228	-4.086198
H	-1.969550	-0.951383	-5.024140
Ni	-1.980900	-1.526231	-0.387567
H	-2.866274	-1.875784	0.766822
C	-4.206074	-1.712002	-0.530792
C	-4.400183	-3.033570	-0.926960
H	-5.314019	-3.600329	-0.800746
N	-3.357044	-3.709578	-1.491584
O	-3.456637	-4.787573	-2.067184
O	-2.166025	-3.145511	-1.369705
C	-5.219497	-1.003225	0.242625
C	-5.897823	-1.630637	1.297800
C	-5.536345	0.322496	-0.080169
C	-6.867406	-0.941488	2.013900
H	-5.638172	-2.655004	1.566140
C	-6.511975	1.009546	0.631638
H	-5.026740	0.793475	-0.921159
C	-7.175568	0.378586	1.683050
H	-7.384142	-1.431978	2.835623
H	-6.761410	2.034252	0.363615
H	-7.936234	0.915555	2.245446
H	-3.636558	-1.055039	-1.227975

$TSIII_{S1}$

P	-0.759020	-0.245243	1.433265
P	-0.155333	-1.166463	-1.398070
C	2.333780	0.216227	-1.337110
C	2.888118	-2.001701	-0.274757
C	5.486555	-1.806844	-1.608784
H	5.222482	-2.707891	-1.060145
C	1.858833	-2.850048	-0.669981
C	-0.570137	2.901420	0.238111
C	0.672970	2.832538	1.056056
C	-0.948794	-0.606331	-2.994196
C	3.601471	-2.288466	0.935232
C	1.370475	1.644201	1.263744
C	1.158247	4.045063	1.654921
C	2.606715	1.665730	1.955289
H	3.153666	0.729247	2.068856
C	0.923094	0.215583	-0.793472
H	0.424382	1.118608	-1.172587
C	-1.724922	2.229474	0.625887
C	-1.704669	1.285900	1.788923
H	-2.717787	0.980847	2.080703
H	-1.227188	1.743170	2.670089
C	4.914029	0.403977	-2.473250
C	3.243787	-0.814822	-1.105348
C	3.293168	-3.479285	1.670296
C	-1.845348	3.931438	-1.619496
C	0.884308	0.306504	0.751127
H	1.568673	-0.468179	1.129232
C	6.198246	0.470003	-3.064758
H	6.460565	1.359586	-3.636214
C	2.885102	5.235795	2.942448
H	3.838242	5.209536	3.469622
C	1.009691	-2.504438	-1.854762
H	0.417752	-3.364604	-2.184500
H	1.616323	-2.157392	-2.701703
C	2.403190	4.038157	2.362137
C	3.970050	-3.739347	2.886299
H	3.722072	-4.648017	3.434146
C	0.563692	4.327145	-1.476412
H	1.518175	4.180248	-0.973486
C	0.505582	5.088290	-2.621419
H	1.415636	5.534077	-3.018296
C	2.294793	-4.353679	1.181000
H	2.073274	-5.264692	1.735907
C	4.544715	-0.750248	-1.709287
C	3.120435	2.825280	2.471626
H	4.078683	2.821783	2.990067
C	3.979050	1.450514	-2.632956
H	4.265611	2.333510	-3.202825
C	-0.602241	3.723236	-0.937166
C	5.220579	-1.692672	2.652087
H	5.968205	-1.002875	3.038645
C	2.724284	1.348634	-2.092737
H	2.001536	2.155062	-2.230722
C	-1.871976	4.734882	-2.784866
H	-2.827349	4.887715	-3.286278
C	-3.012380	3.304992	-1.124791
H	-3.965132	3.479975	-1.624818
C	-1.794889	-1.757729	-3.543955
H	-2.242178	-1.452009	-4.498187
H	-2.618695	-2.022491	-2.867977
H	-1.204065	-2.662077	-3.739057
C	0.921942	6.408062	2.189324
H	0.339999	7.326235	2.142564
C	4.587313	-1.414603	1.462541
H	4.840882	-0.509373	0.913866
C	0.432974	5.263954	1.603947
H	-0.533519	5.291501	1.106701
C	-2.945136	2.453701	-0.052121
H	-3.844490	1.956832	0.307263
C	4.911619	-2.864560	3.373097
H	5.420615	-3.073682	4.311563
C	6.723333	-1.716027	-2.203710
H	7.424761	-2.543074	-2.114197
C	-1.845534	0.587286	-2.683519
H	-1.275995	1.451351	-2.321592
H	-2.608315	0.351637	-1.930190
H	-2.366989	0.909419	-3.595129
C	-0.081253	-2.500732	2.873503
H	0.285639	-2.953139	3.805010
H	0.713015	-2.607871	2.125202
H	-0.955239	-3.070752	2.537437
C	-0.722667	5.301577	-3.280679
H	-0.755629	5.912774	-4.179918
C	2.164097	6.401785	2.855351
H	2.542337	7.316263	3.307299
C	0.762096	-0.339838	3.789119
H	0.846529	-0.731030	4.811207

H	0.645459	0.748601	3.863277
H	1.715489	-0.550572	3.289465
C	7.090071	-0.565718	-2.931881
H	8.073736	-0.505641	-3.392642
C	-0.423674	-1.032439	3.111948
C	1.575816	-4.028553	0.059393
H	0.771154	-4.678054	-0.284783
C	0.109629	-0.199638	-4.020453
H	0.760916	-1.030654	-4.314256
H	0.744121	0.619916	-3.663045
H	-0.394417	0.152272	-4.930154
C	-1.653172	-0.903860	4.014188
H	-2.539189	-1.371835	3.578770
H	-1.878031	0.140627	4.260560
H	-1.436480	-1.415609	4.960553
Ni	-1.594306	-1.721120	0.102901
H	-3.589412	-1.171522	-0.781292
C	-4.667495	-1.397669	-0.666232
C	-4.804641	-2.566257	0.254495
H	-5.782355	-3.012018	0.424962
N	-4.017054	-2.690593	1.350304
O	-4.256955	-3.441281	2.295025
O	-2.884496	-1.975859	1.438705
C	-5.391954	-0.137511	-0.257115
C	-5.649948	0.161538	1.083963
C	-5.782243	0.778831	-1.238491
C	-6.271475	1.358502	1.434680
H	-5.373607	-0.549753	1.862877
C	-6.407661	1.971890	-0.890464
H	-5.593612	0.548855	-2.288756
C	-6.648840	2.268315	0.449833
H	-6.470059	1.575837	2.482486
H	-6.717920	2.668428	-1.667983
H	-7.142012	3.198592	0.724214
C	-2.419077	-4.415535	-1.290309
O	-1.789756	-3.476361	-0.768211
O	-3.713732	-4.528706	-1.301970
C	-1.710882	-5.546229	-1.958965
H	-2.250514	-5.857851	-2.856898
H	-0.680358	-5.283286	-2.207140
H	-1.694953	-6.408552	-1.282338
H	-4.145344	-3.789155	-0.705499
H	-5.001386	-1.693943	-1.672350

$TSII_{R1}$

P	0.473415	-0.157854	-1.929493
P	0.958535	-0.895530	1.034457
C	-1.742943	-0.156871	1.597983
C	-1.967157	-2.531678	0.761973
C	-4.041170	-2.876767	2.787213
H	-3.682766	-3.734853	2.223485
C	-0.698982	-3.096269	0.845344
C	0.147120	2.973231	-0.751012
C	-1.266931	2.679064	-1.124500
C	1.815648	-0.082559	2.481083
C	-2.907942	-3.070158	-0.176189
C	-1.789377	1.386075	-1.113422
C	-2.115026	3.774610	-1.506187
C	-3.169513	1.181782	-1.358539
H	-3.561157	0.165566	-1.292281
C	-0.557394	0.135711	0.706248
H	-0.204518	1.148504	0.953675
C	1.205666	2.459586	-1.491841
C	0.945280	1.486553	-2.597203
H	1.829107	1.350929	-3.232060
H	0.122210	1.822147	-3.245789
C	-3.911489	-0.510687	3.374596
C	-2.368156	-1.401587	1.648656
C	-2.572405	-4.252305	-0.913130
C	1.780493	4.226117	0.629079
C	-0.960260	0.162643	-0.787832
H	-1.593179	-0.722473	-0.957368
C	-4.966940	-0.714250	4.295067
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C	-4.342358	4.619040	-2.128622
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C	0.340478	-2.480228	1.727514
H	1.202309	-3.145104	1.855608
H	-0.062131	-2.262991	2.727762
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H	-1.065167	5.337018	3.043326
C	-1.301171	-4.844177	-0.724106
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C	-4.007819	2.222780	-1.654741
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H	3.874148	-0.190939	-0.884803

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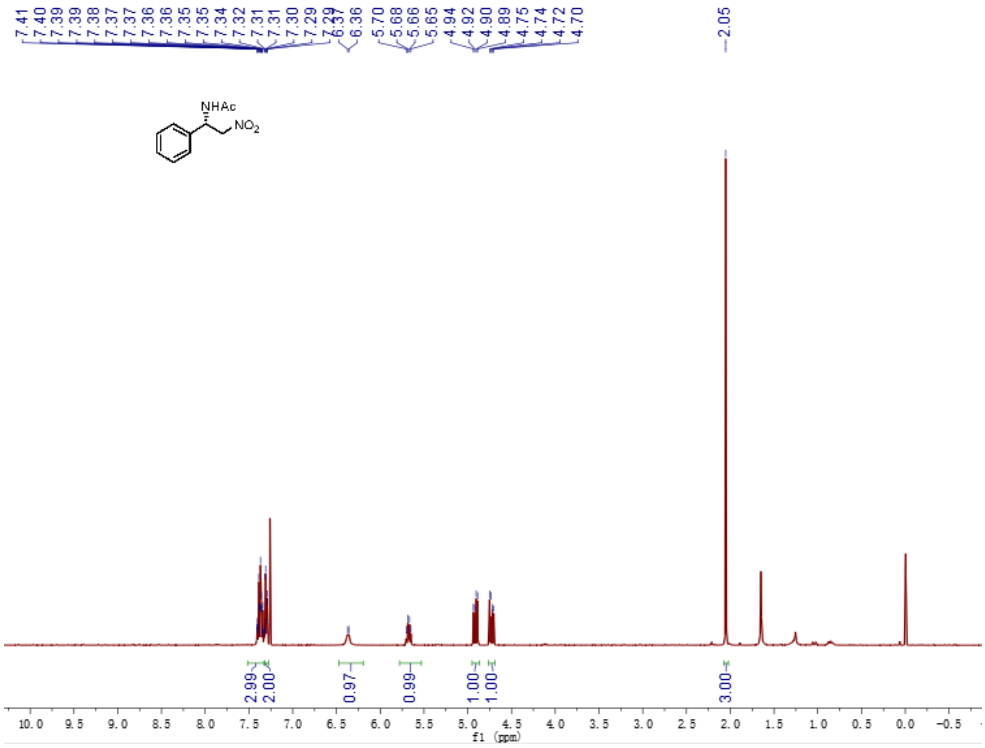
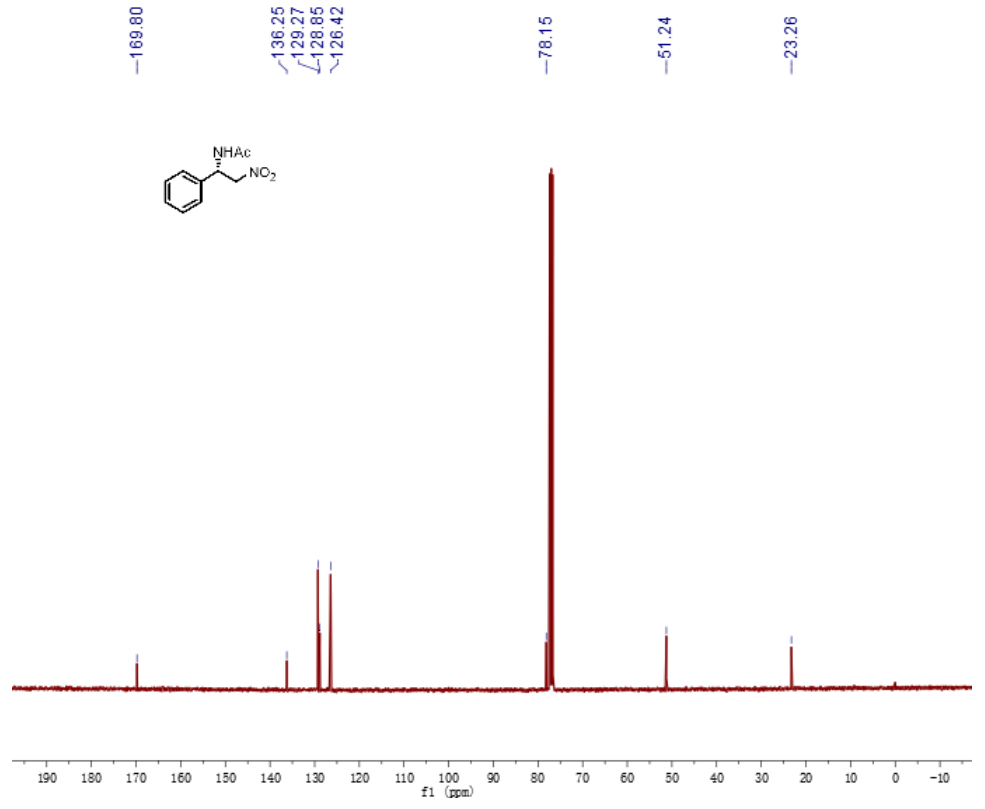
8. NMR and HPLC

^{1}H NMR and ^{13}C NMR of **2a**





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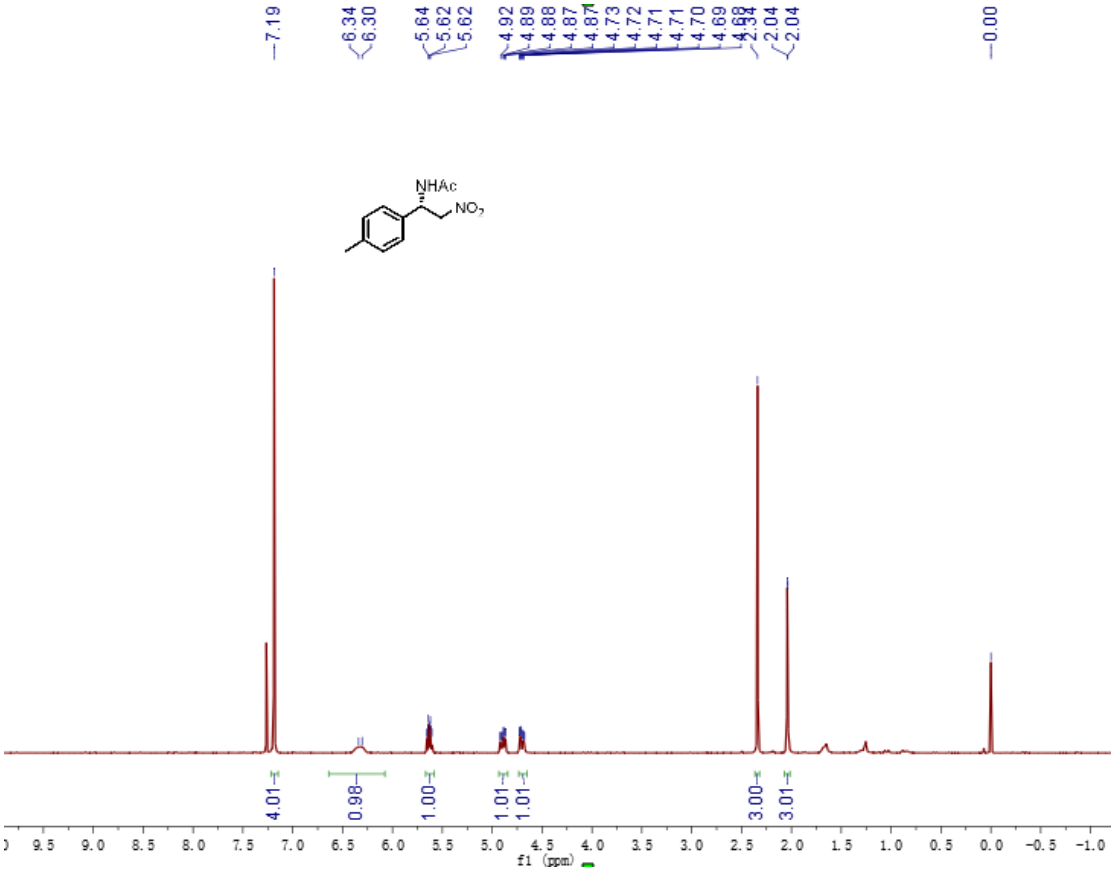

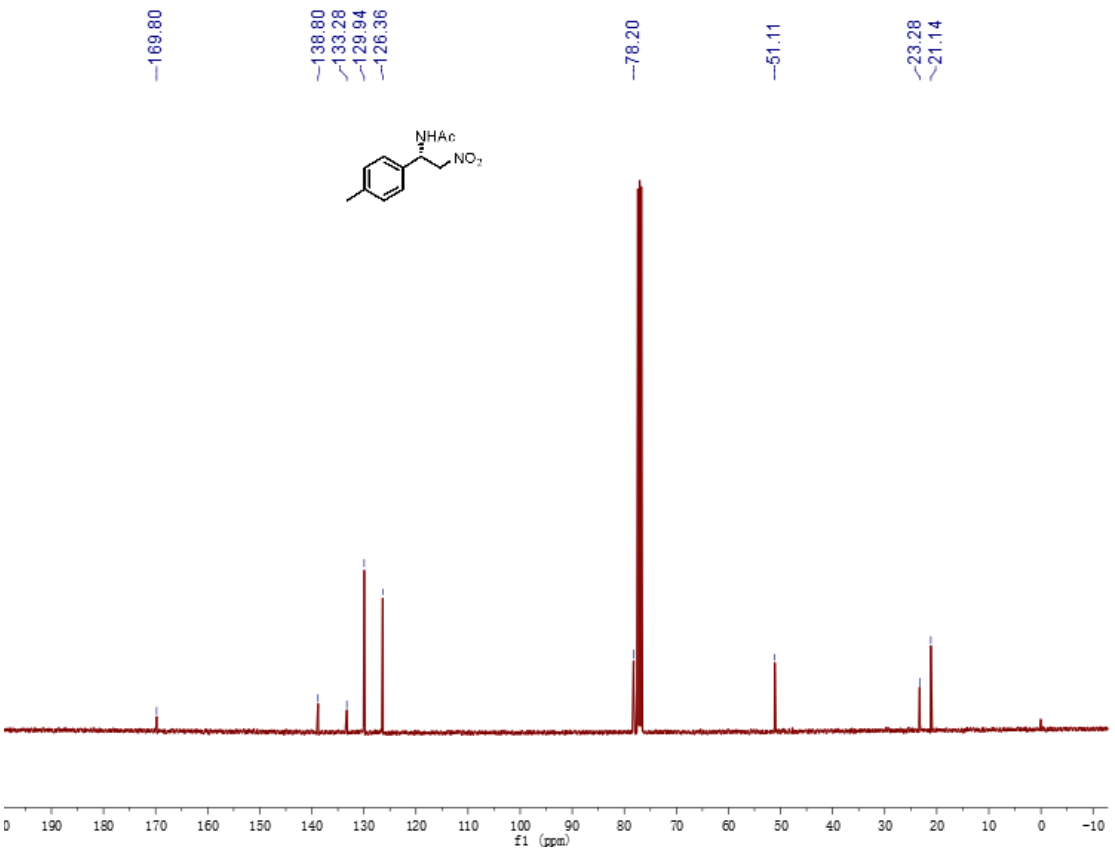

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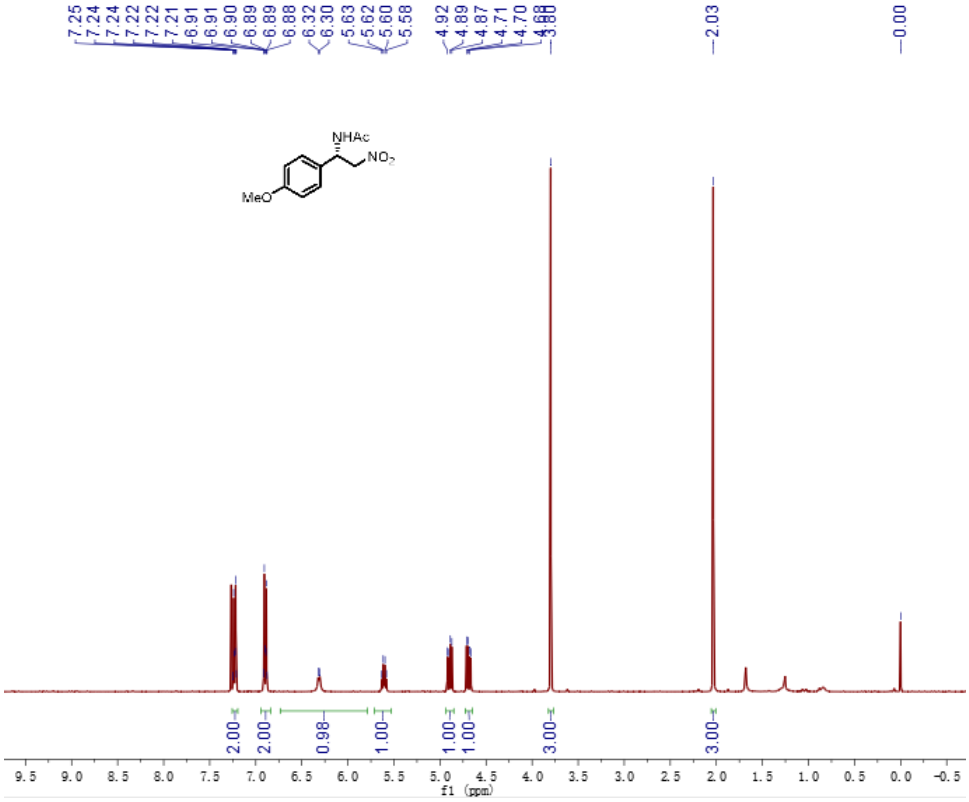

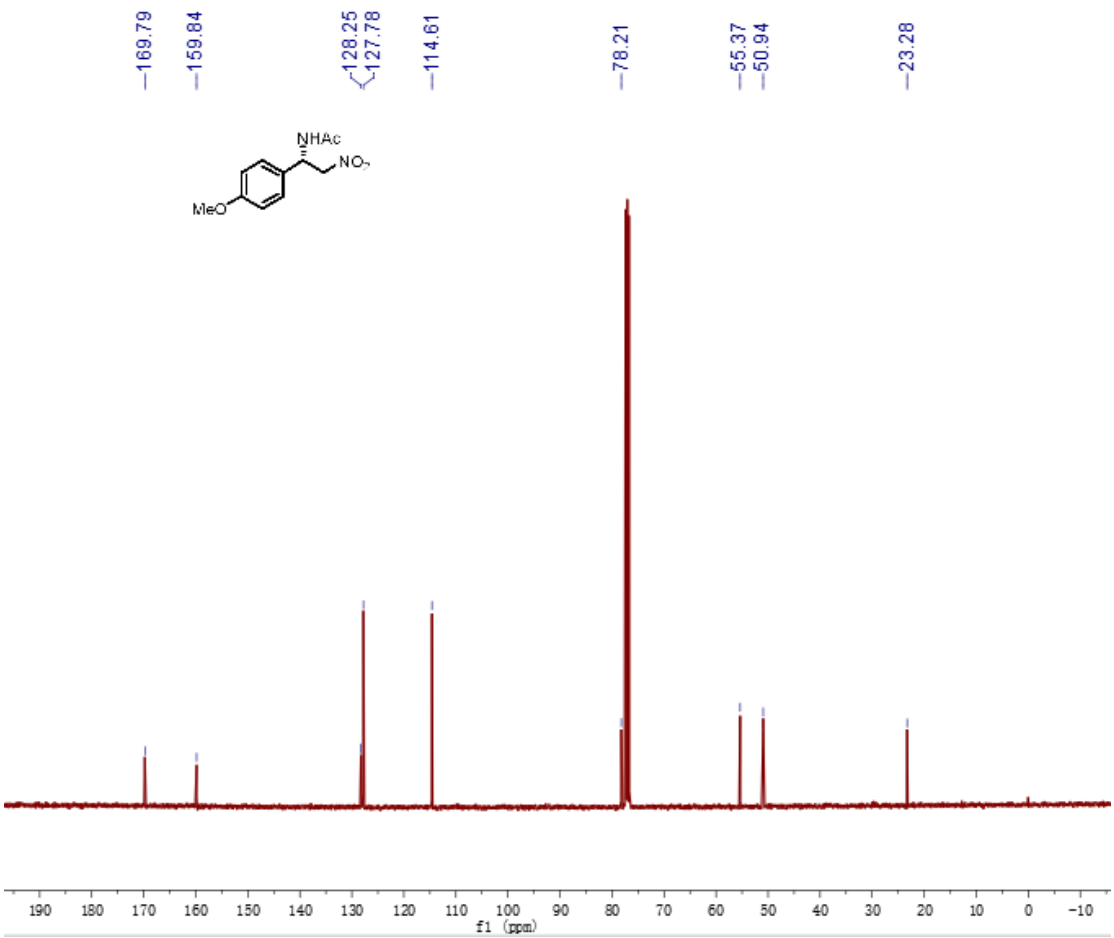

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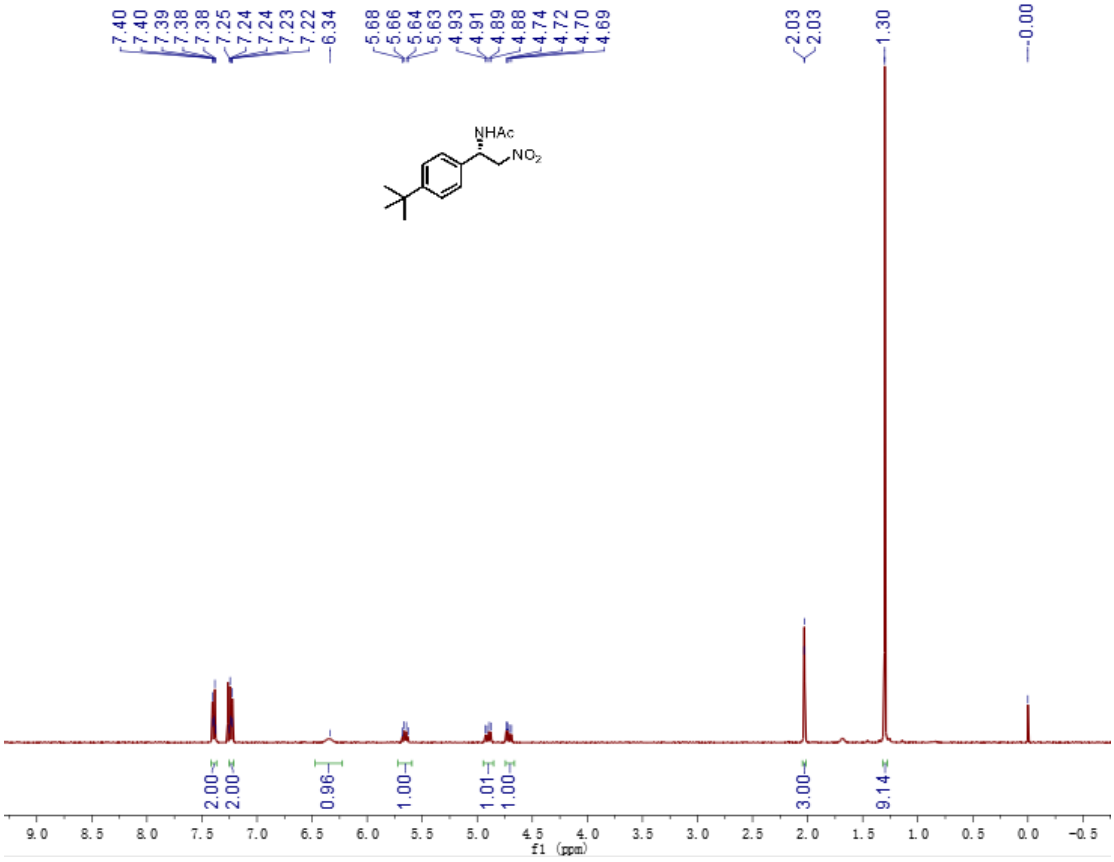

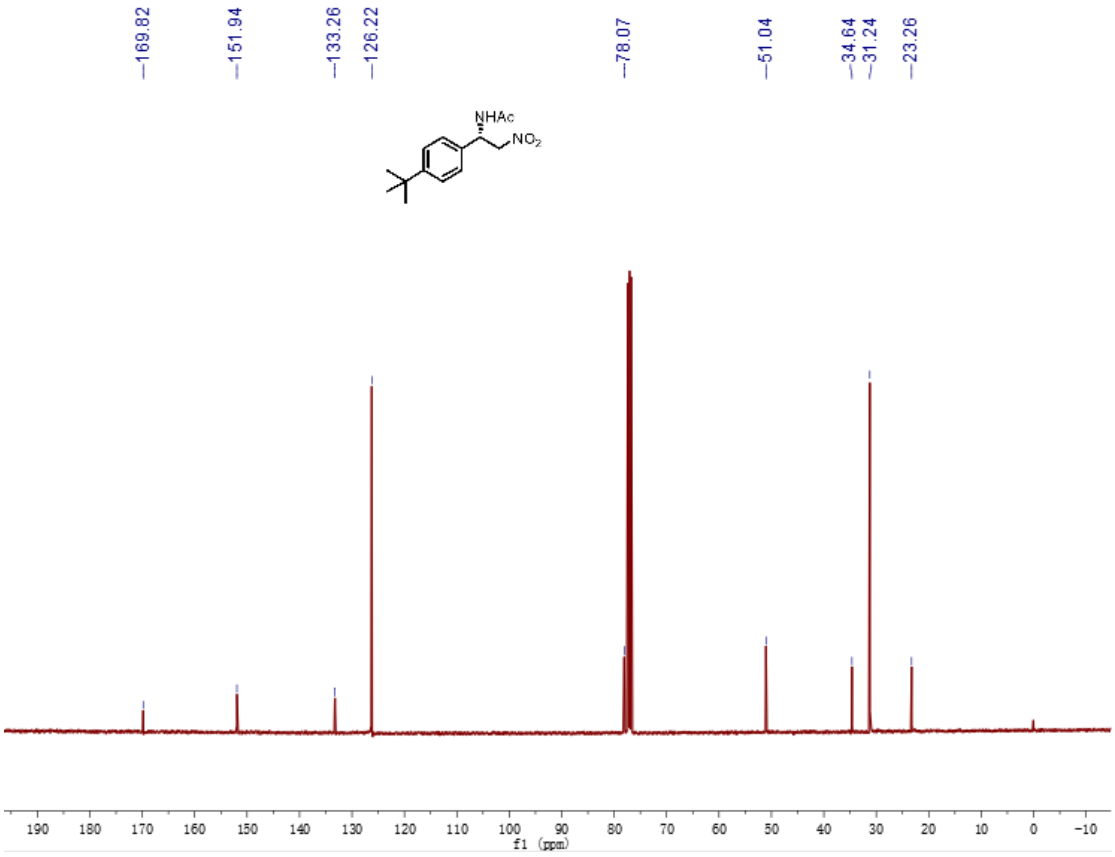

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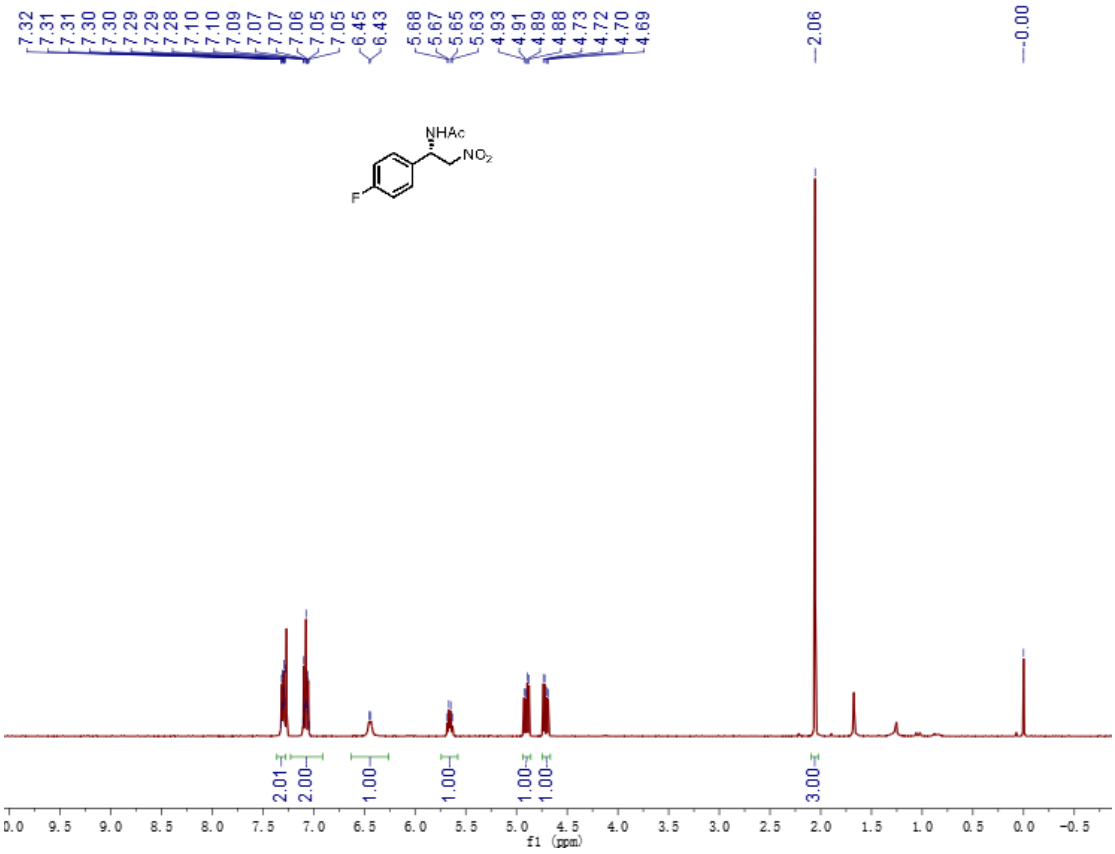

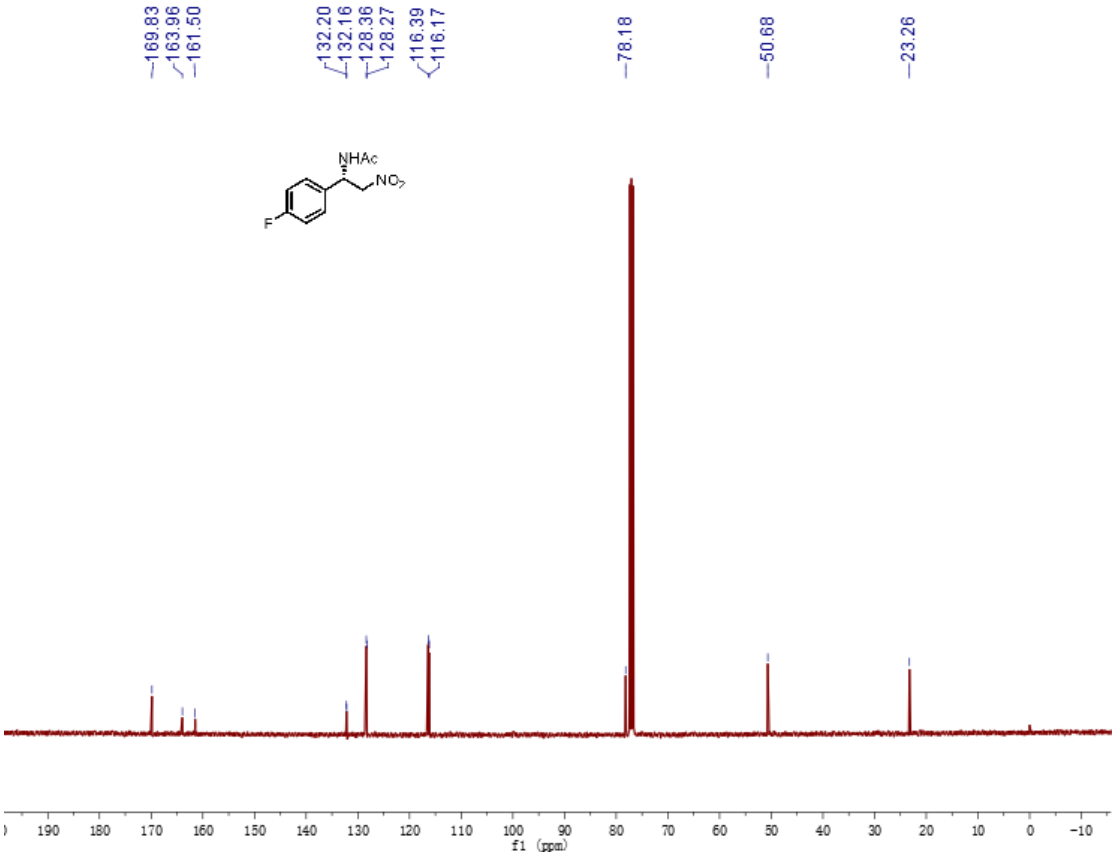

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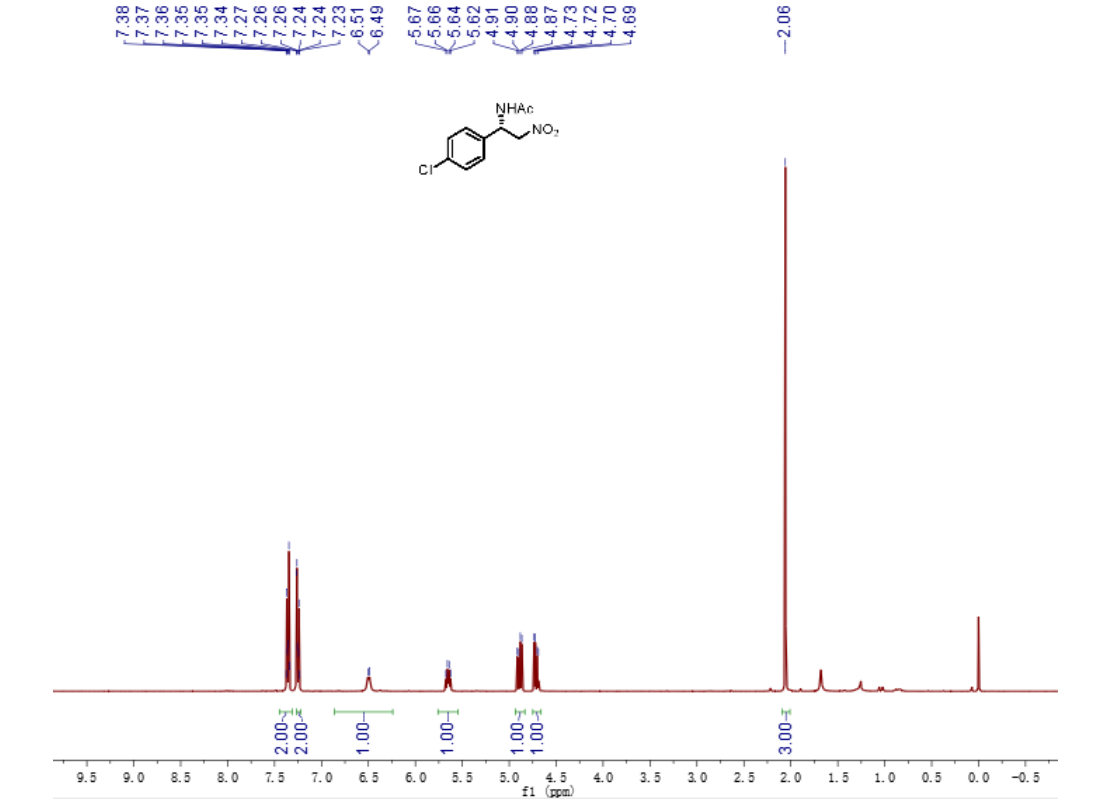

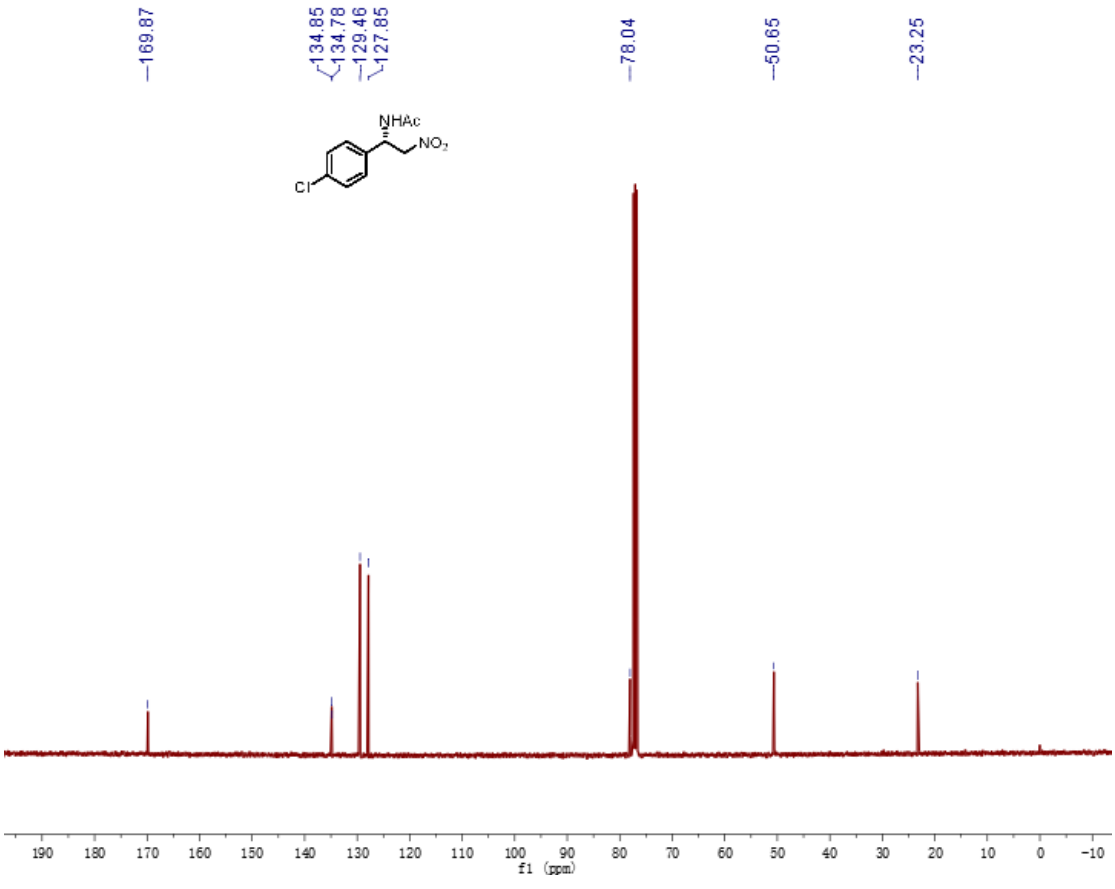

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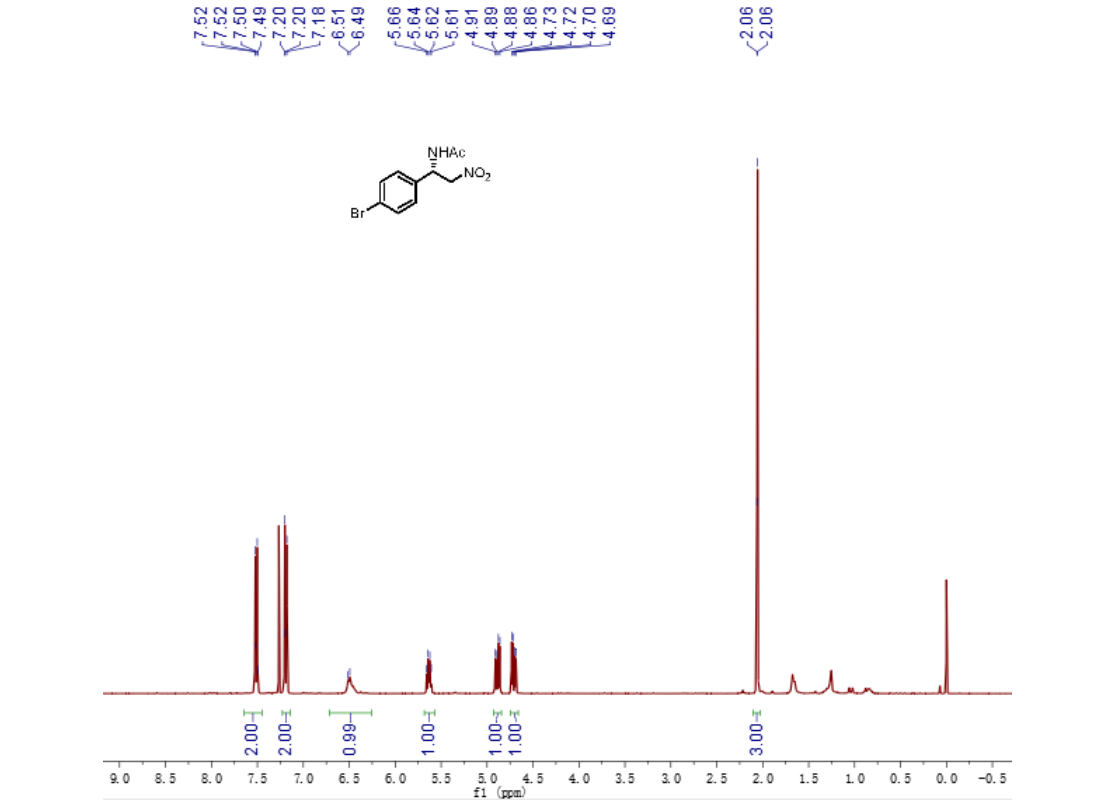
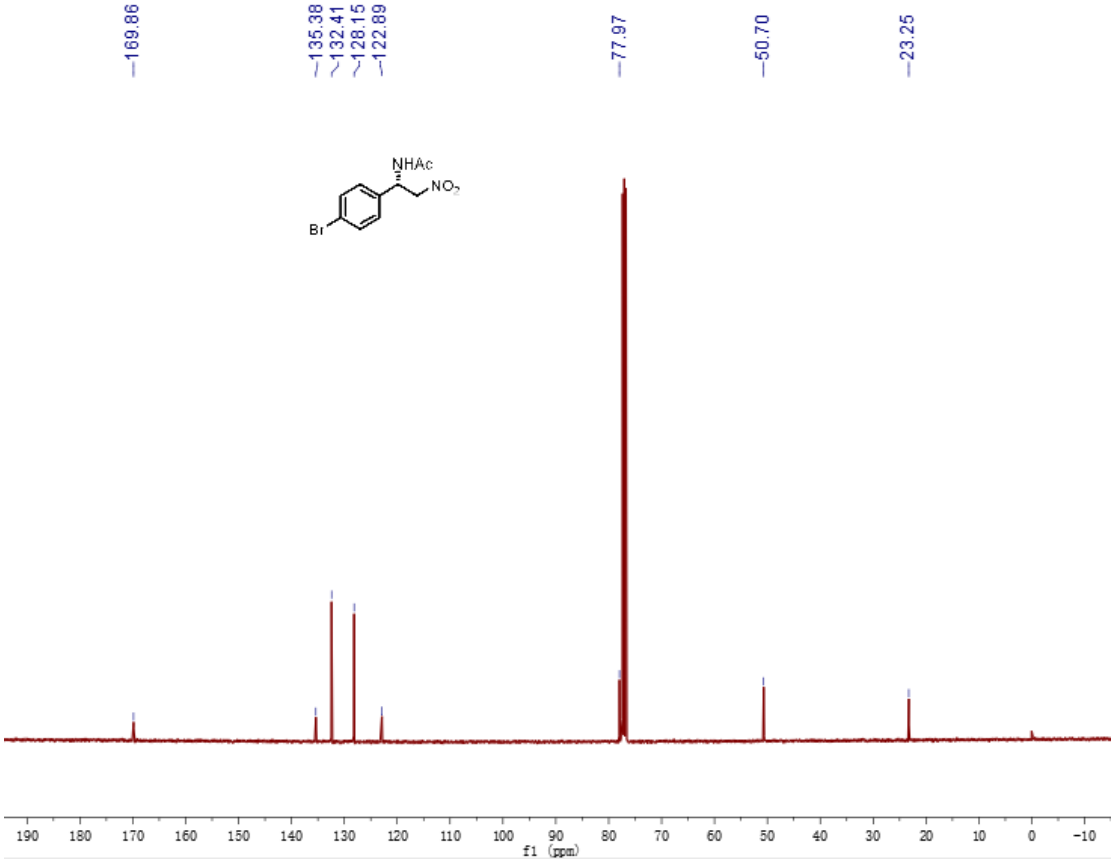
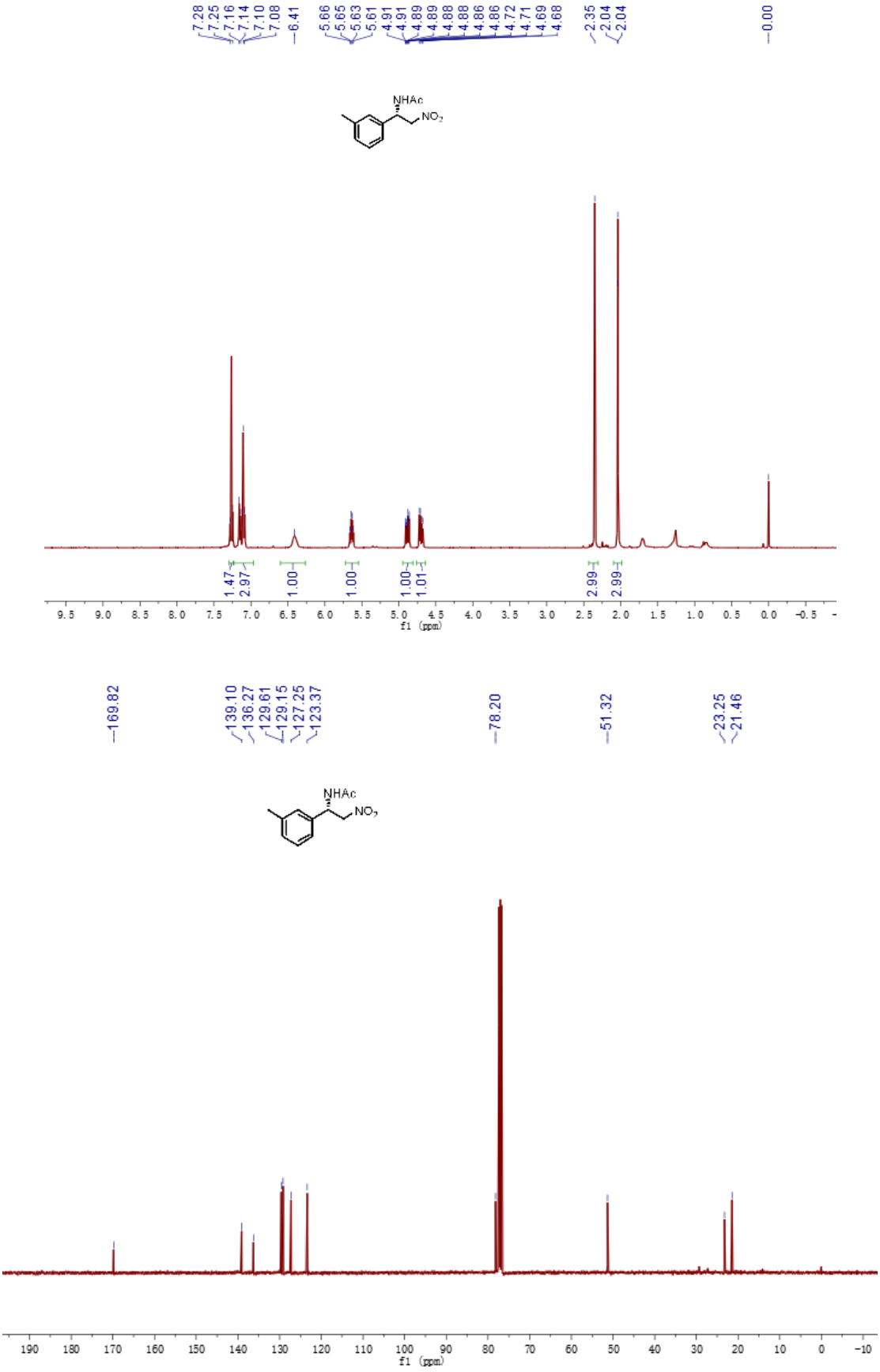




^{1}H NMR and ^{13}C NMR of **2h**



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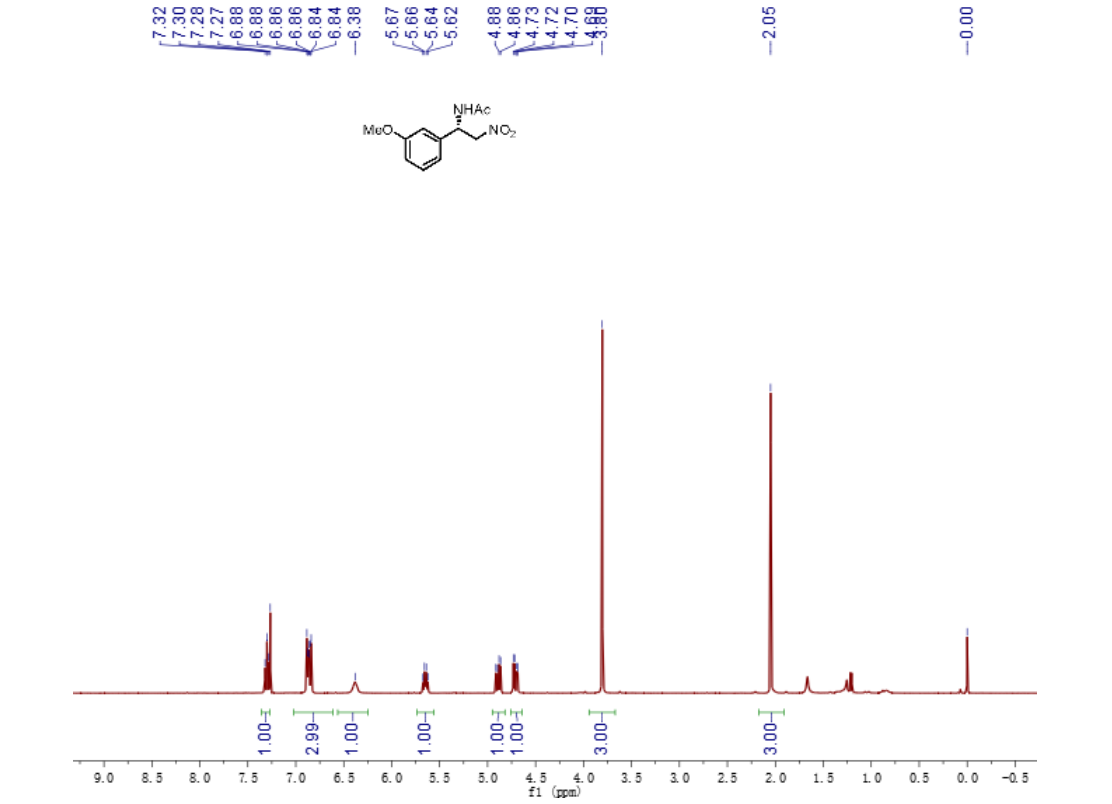

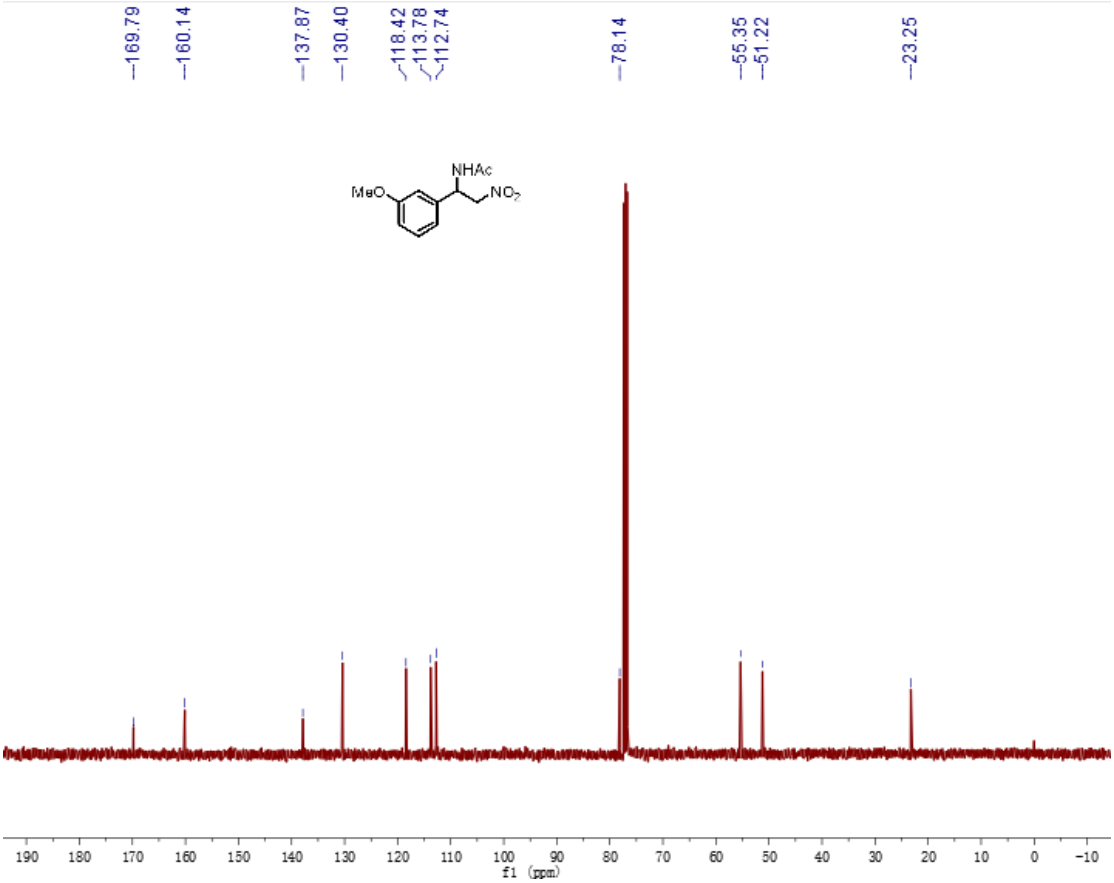

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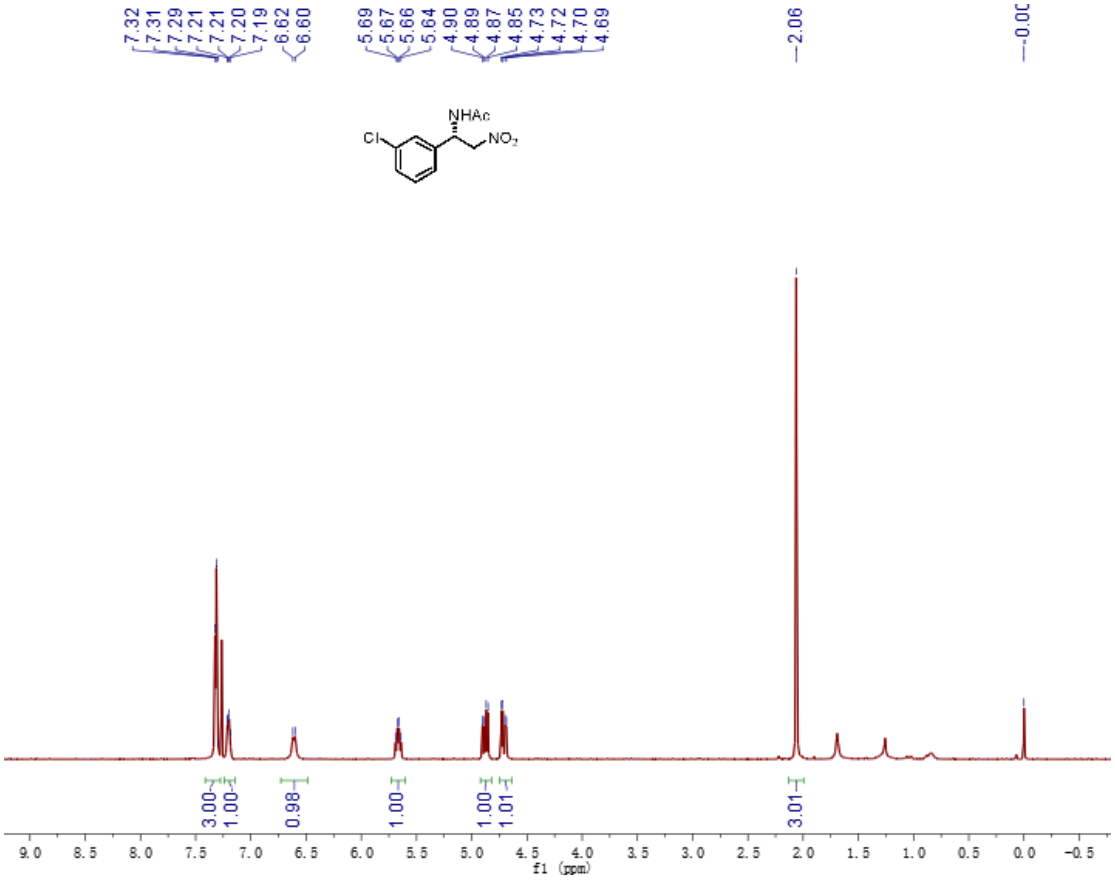

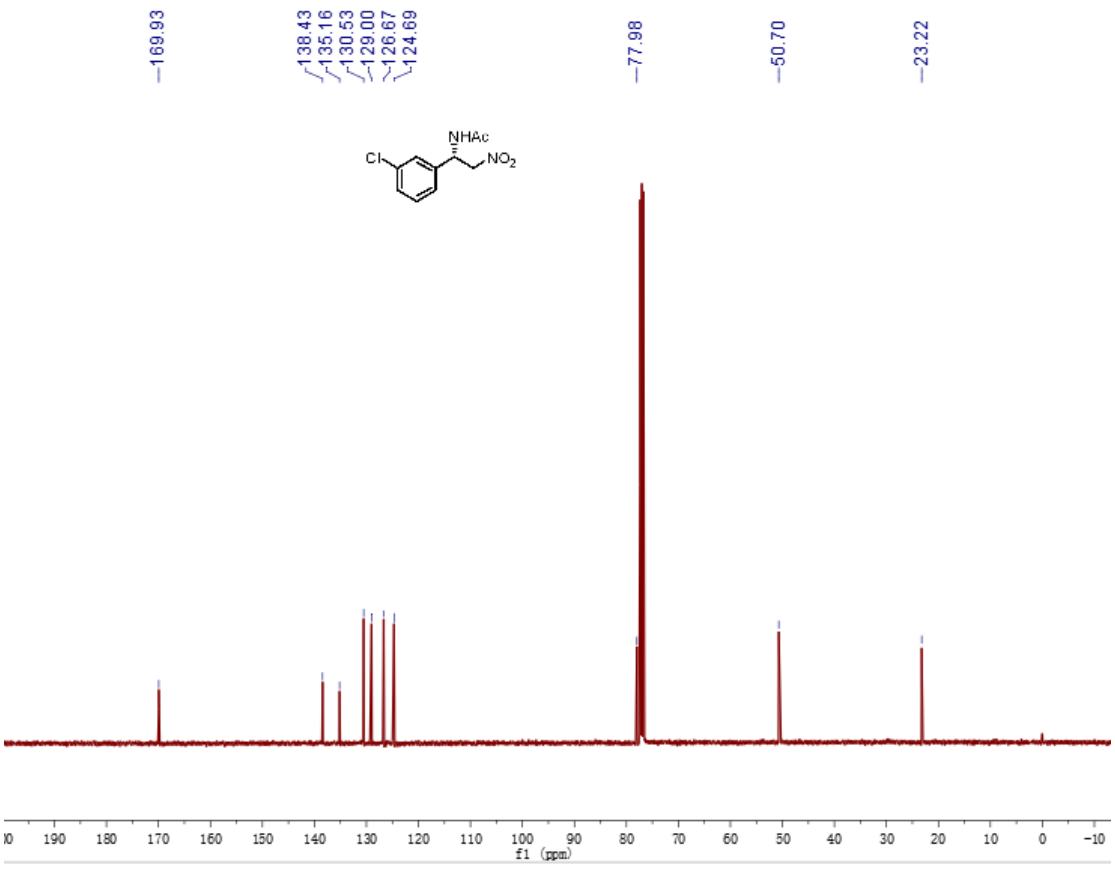

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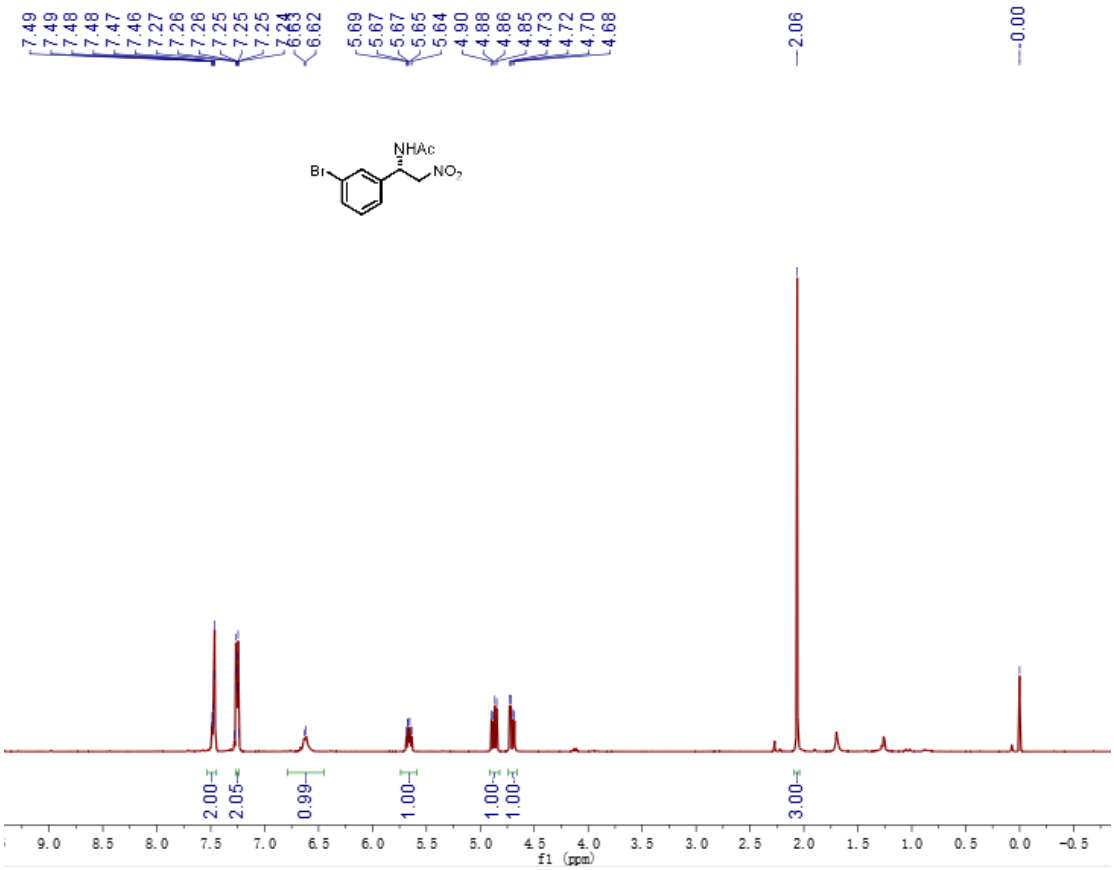

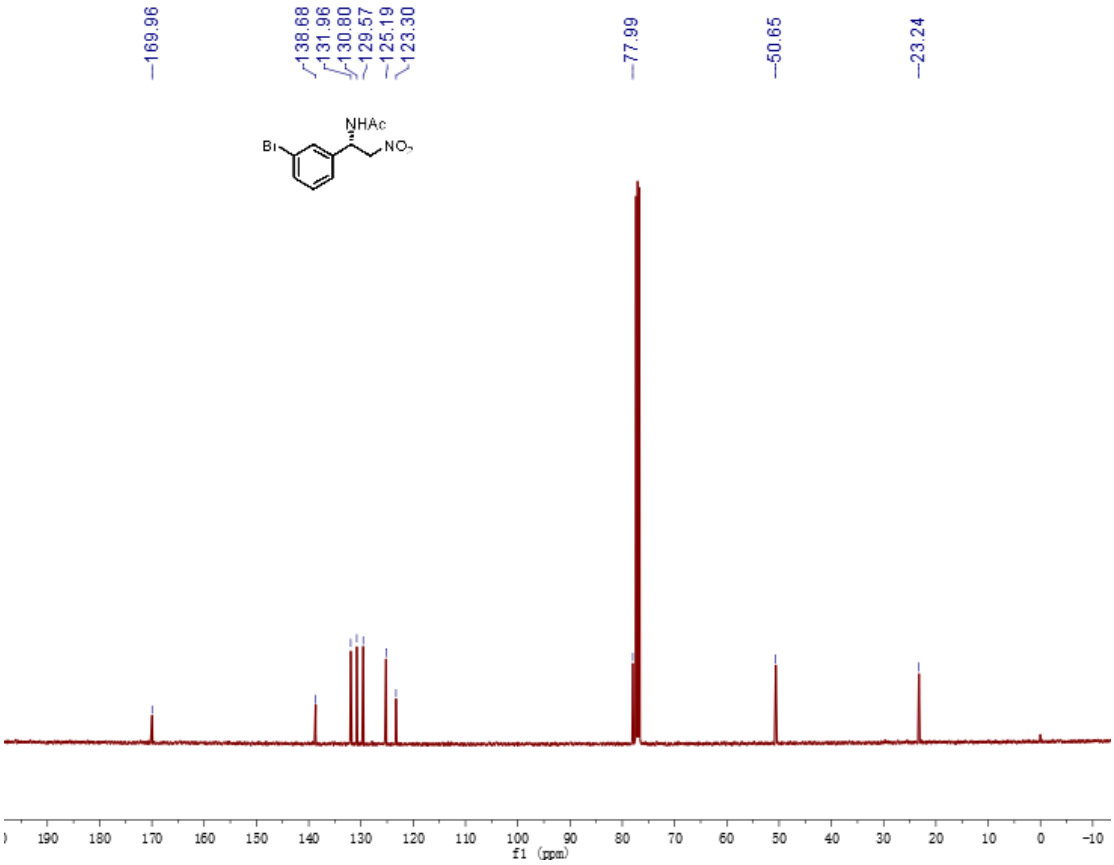

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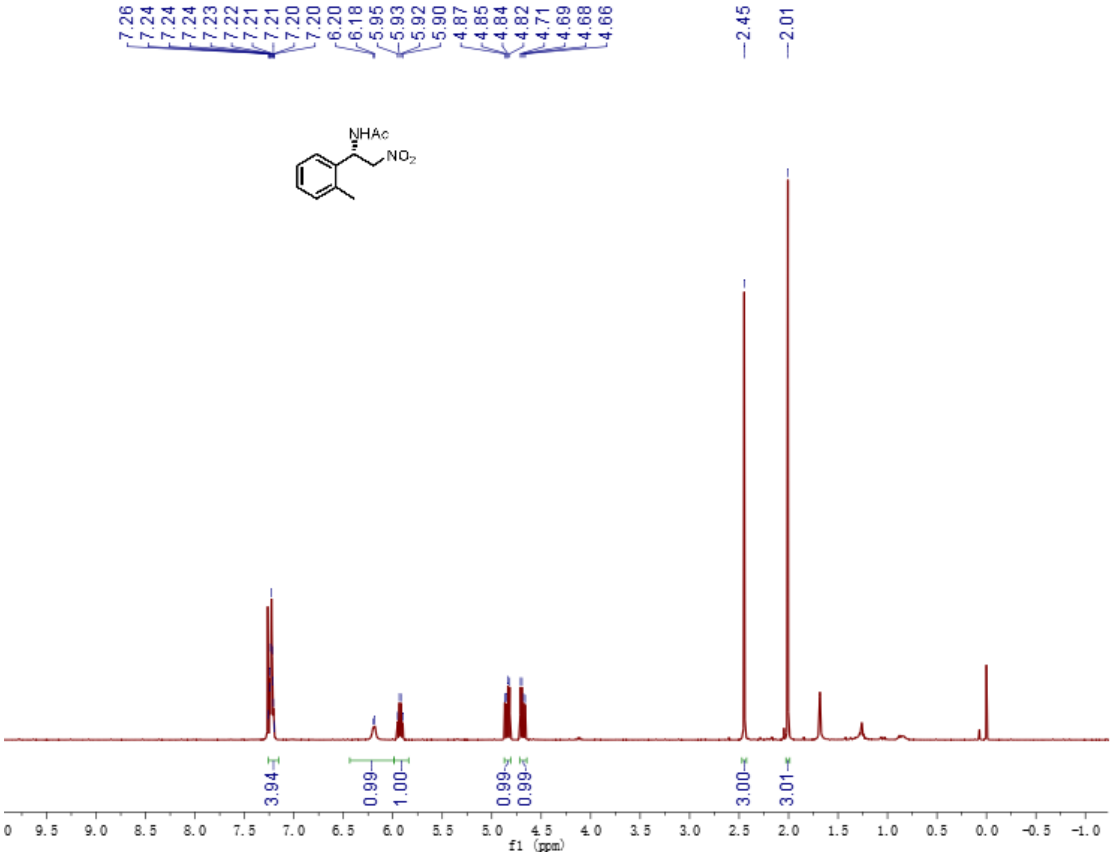

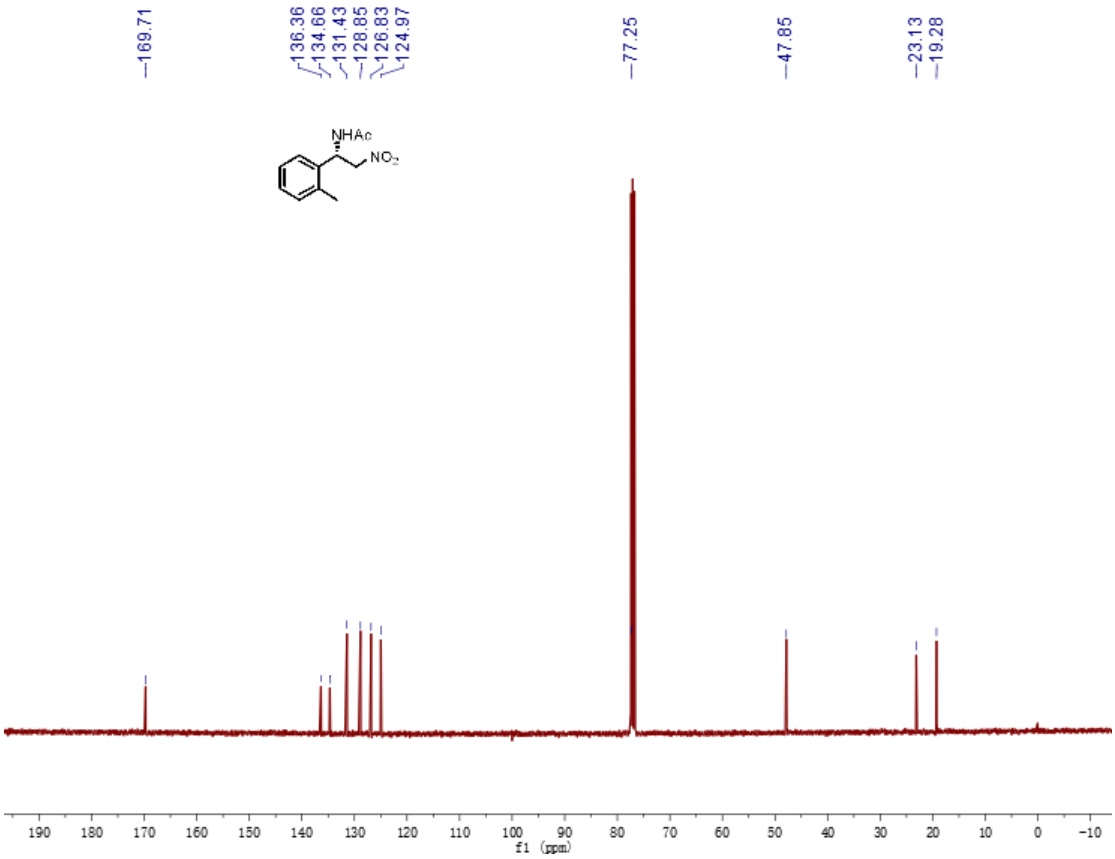

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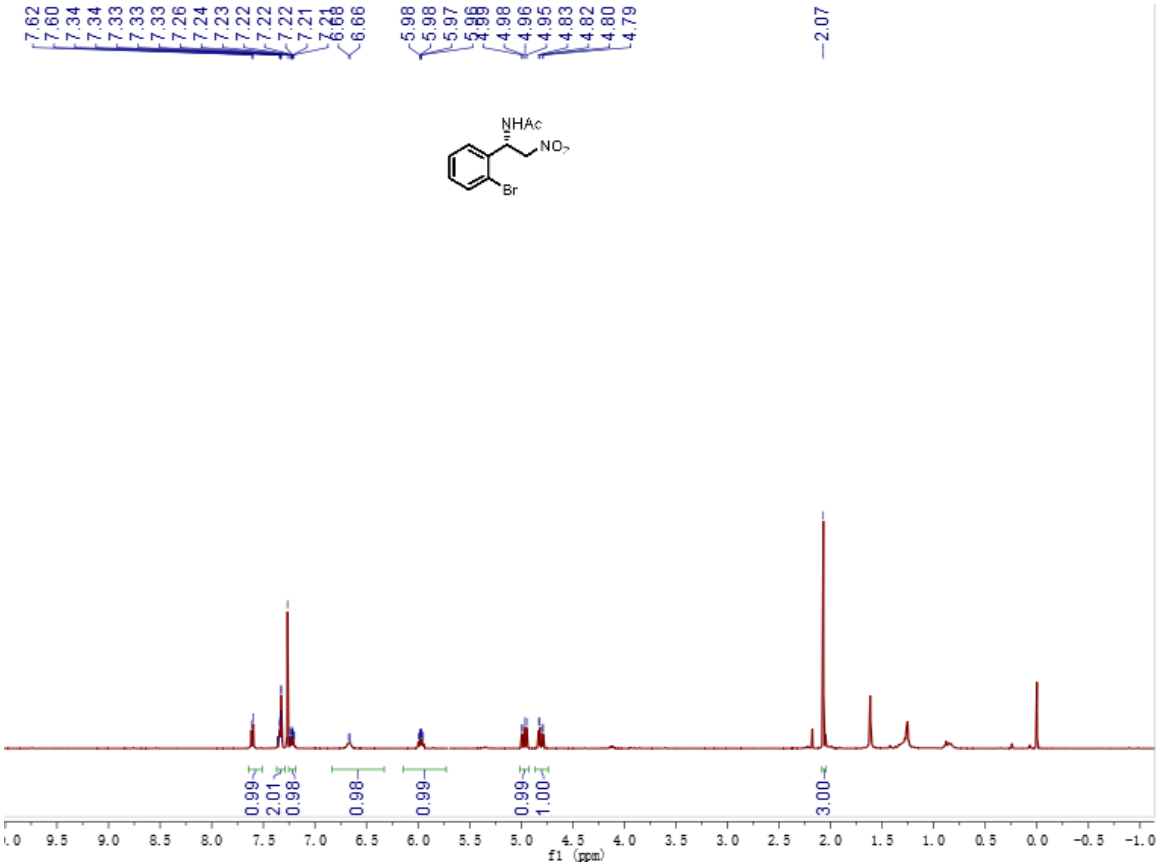

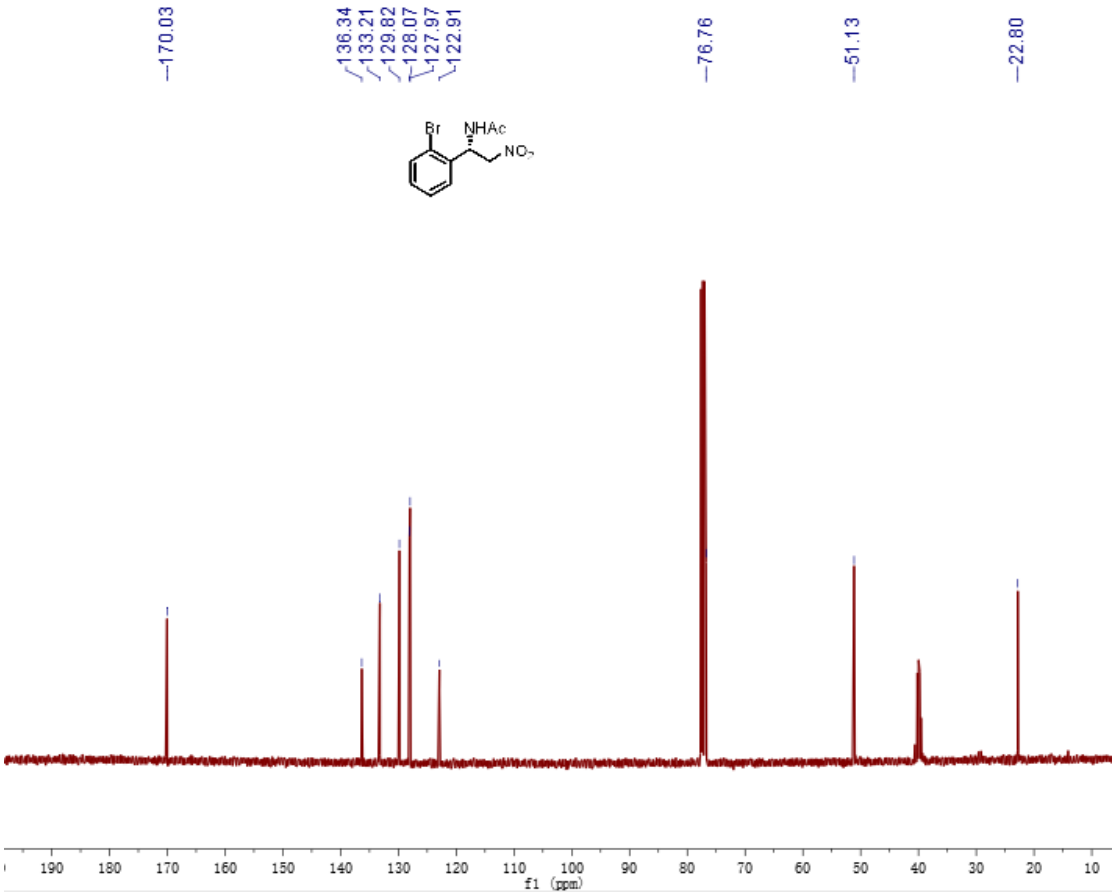

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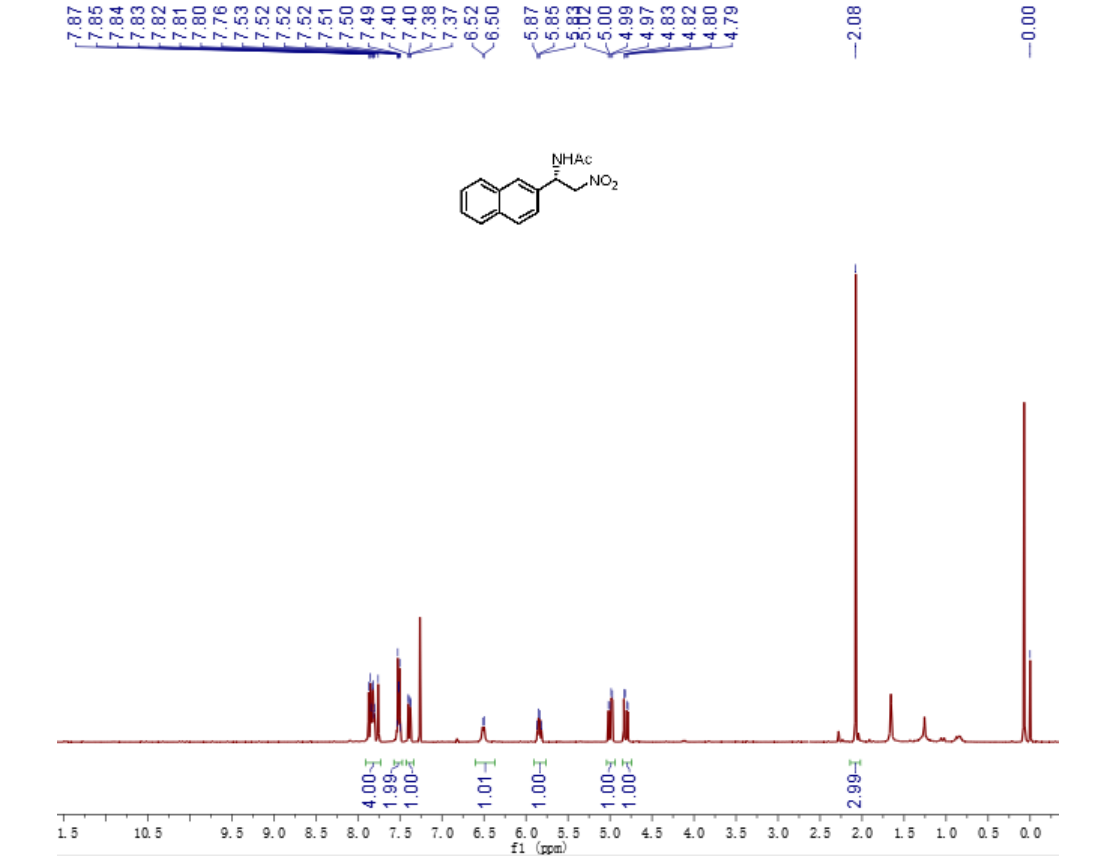

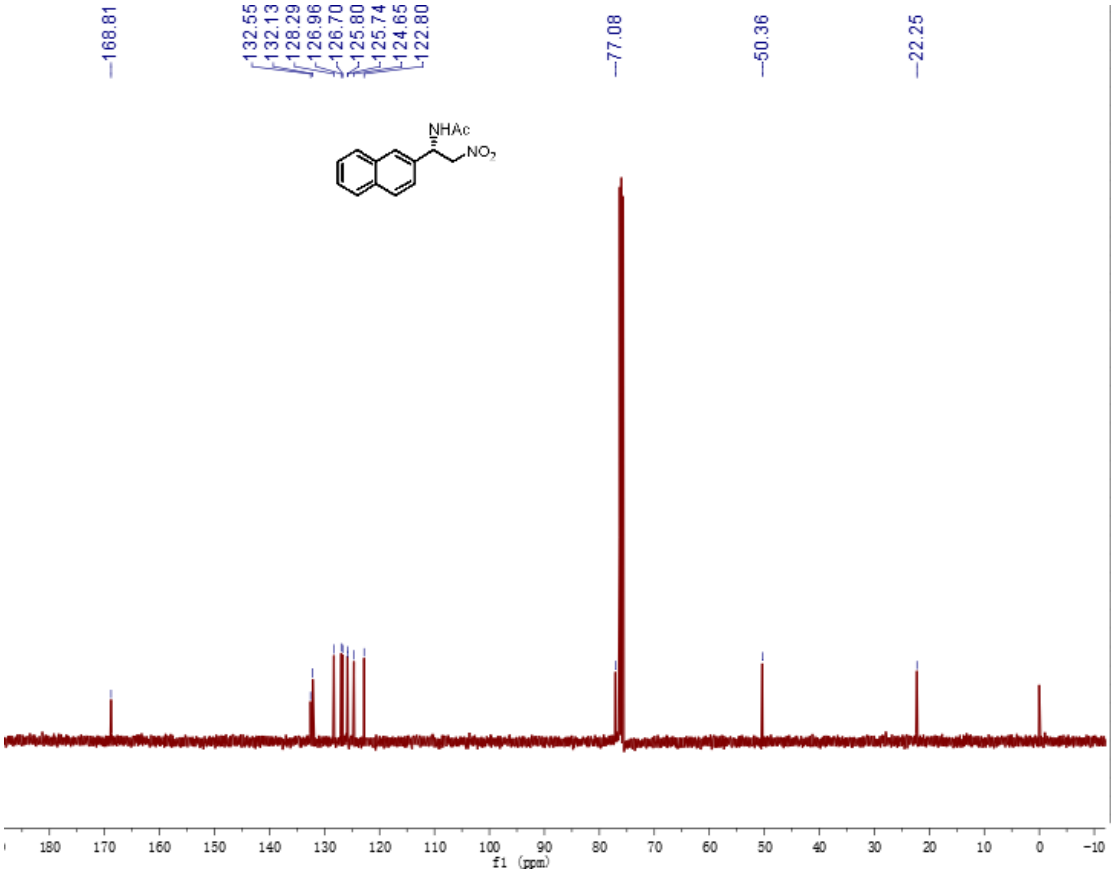

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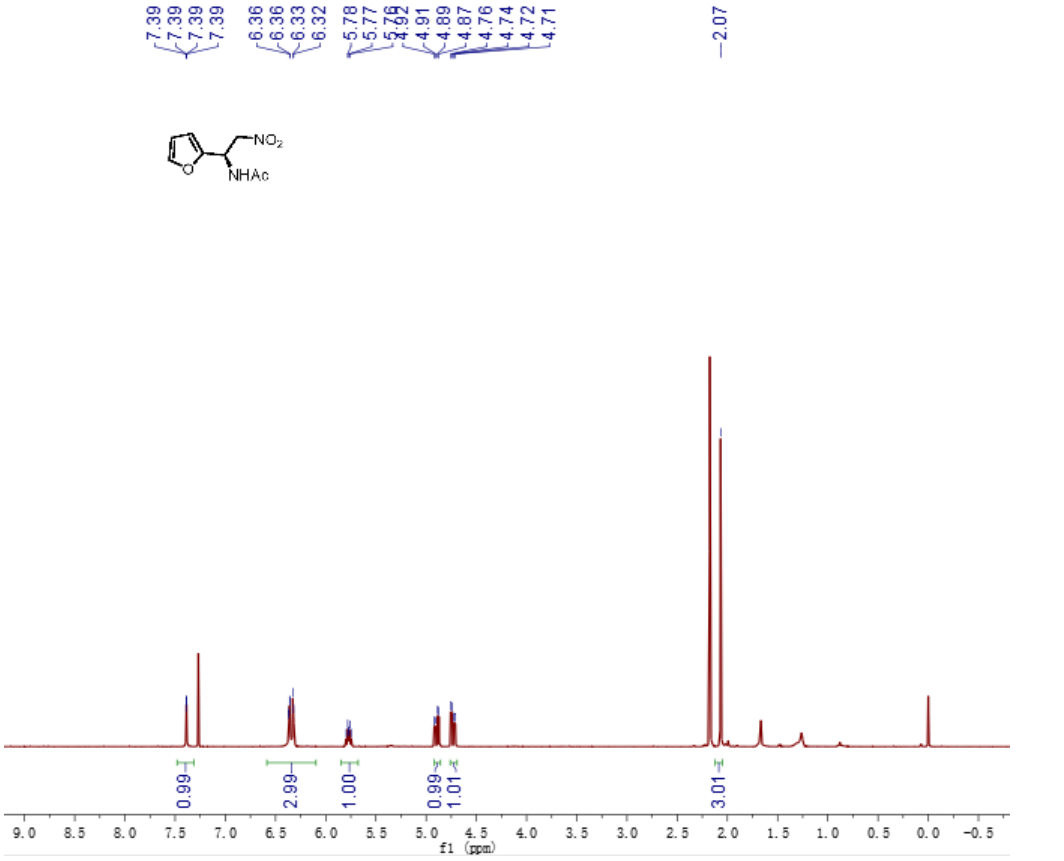

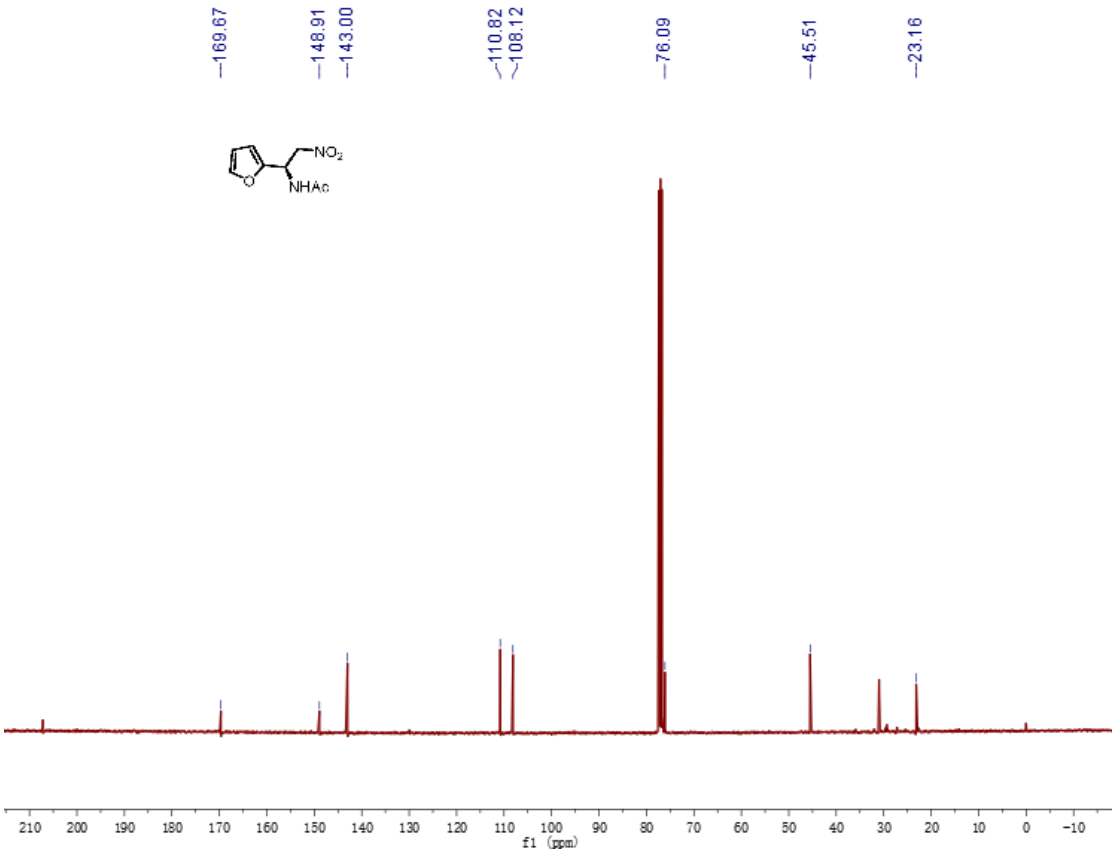

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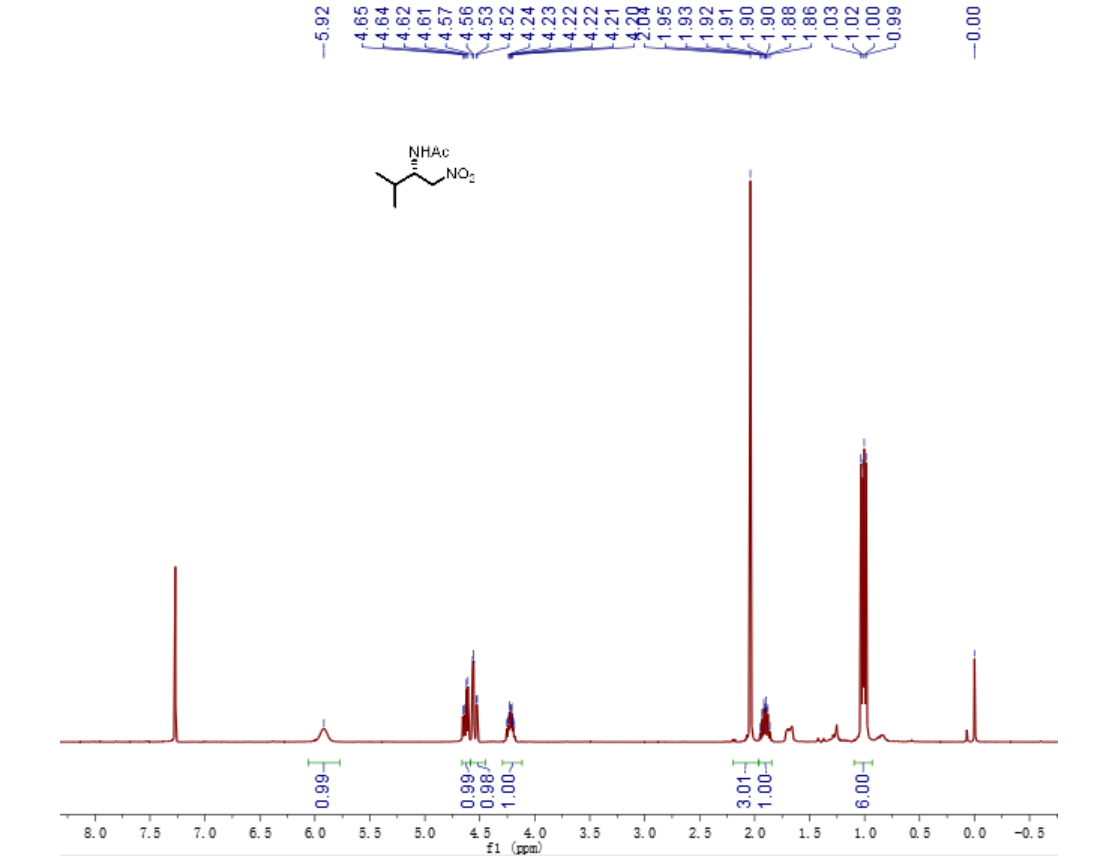
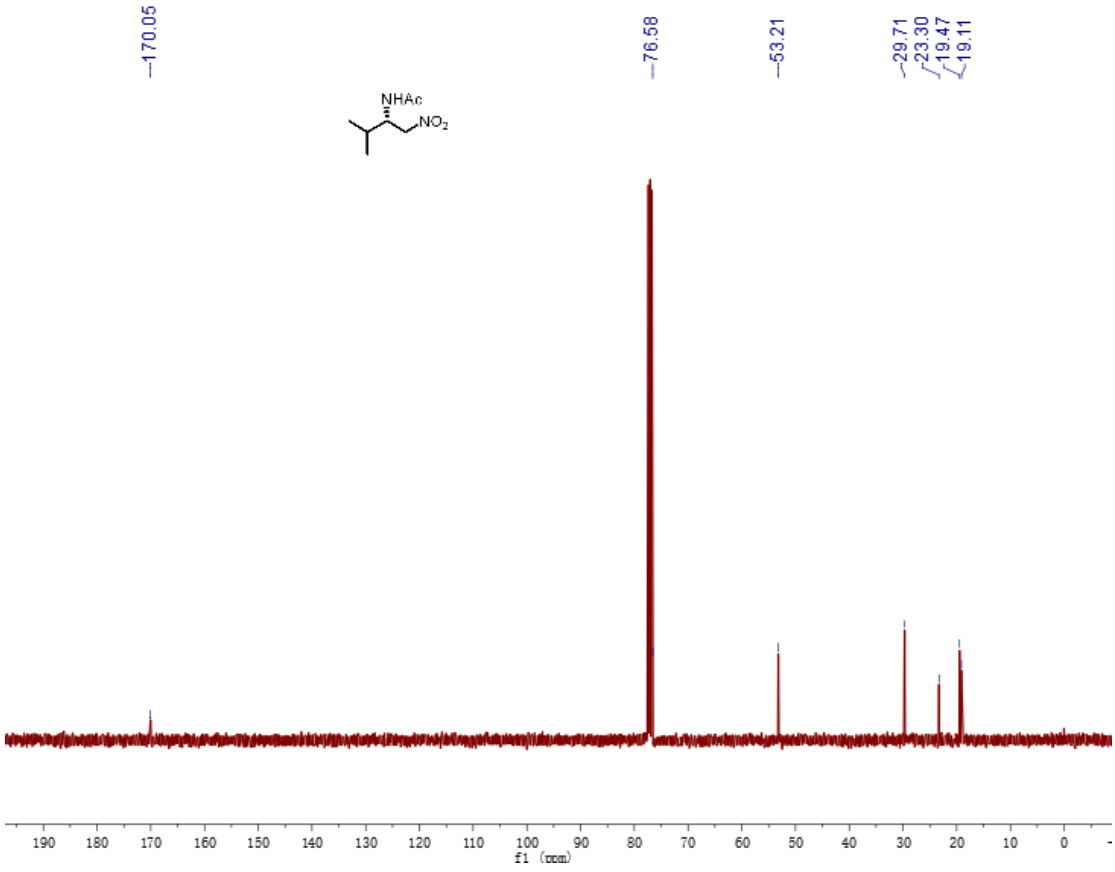
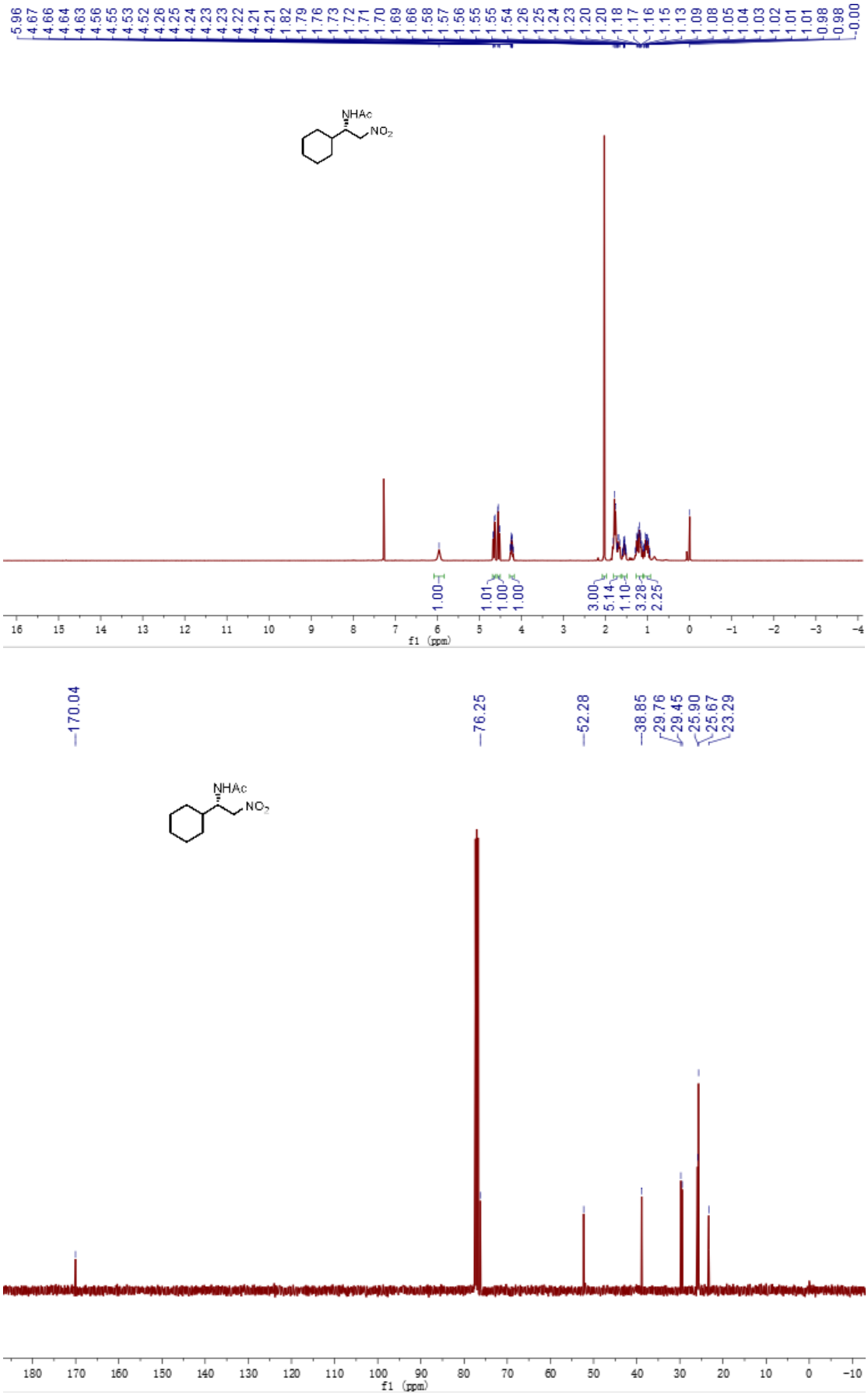




^{1}H NMR and ^{13}C NMR of **2q**



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                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
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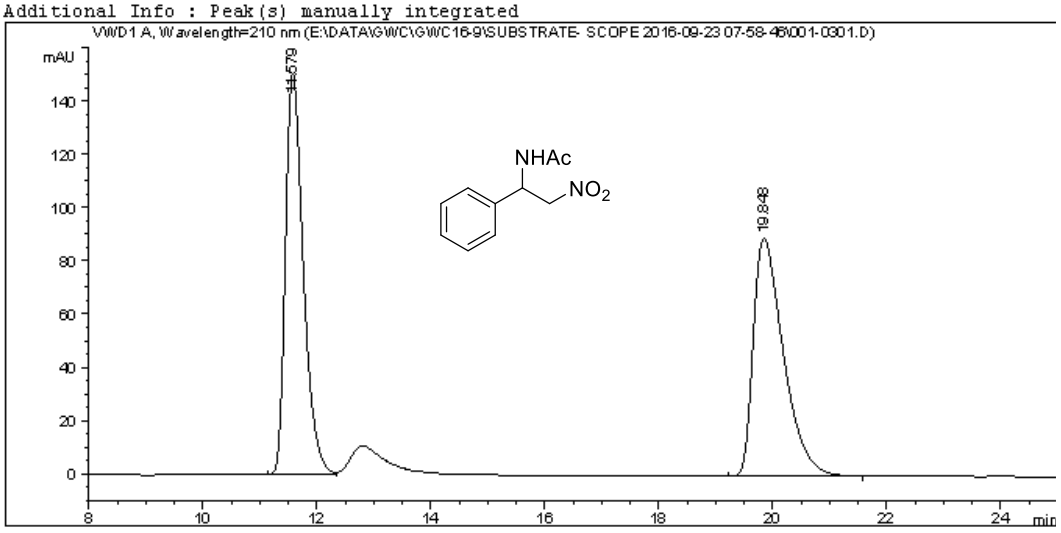


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                            Area Percent Report
    ======================================================================

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    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.579 BV    0.3331 3282.81226  150.73700  50.0626
       2  19.848 BB    0.5575 3274.59888   89.36766  49.9374

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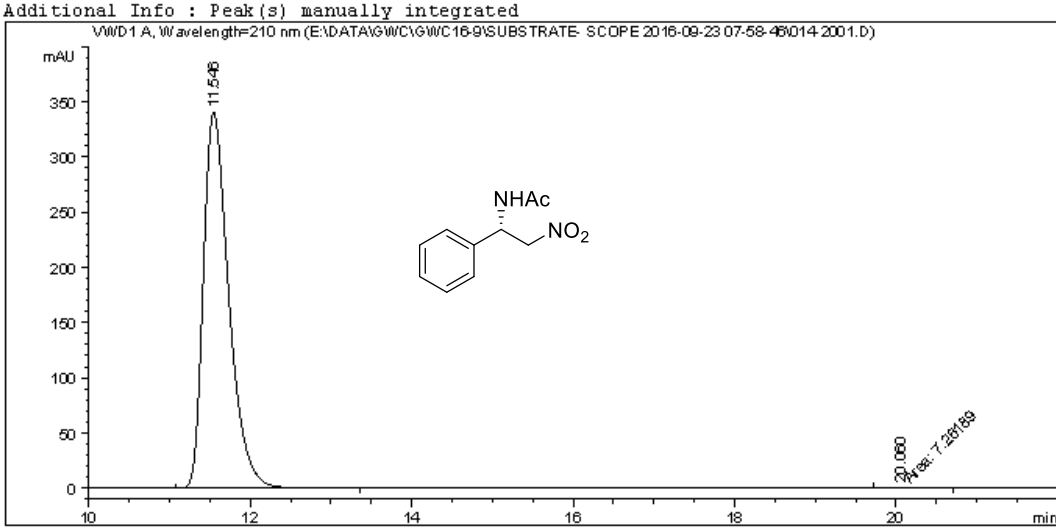
HPLC-2a-**cat**

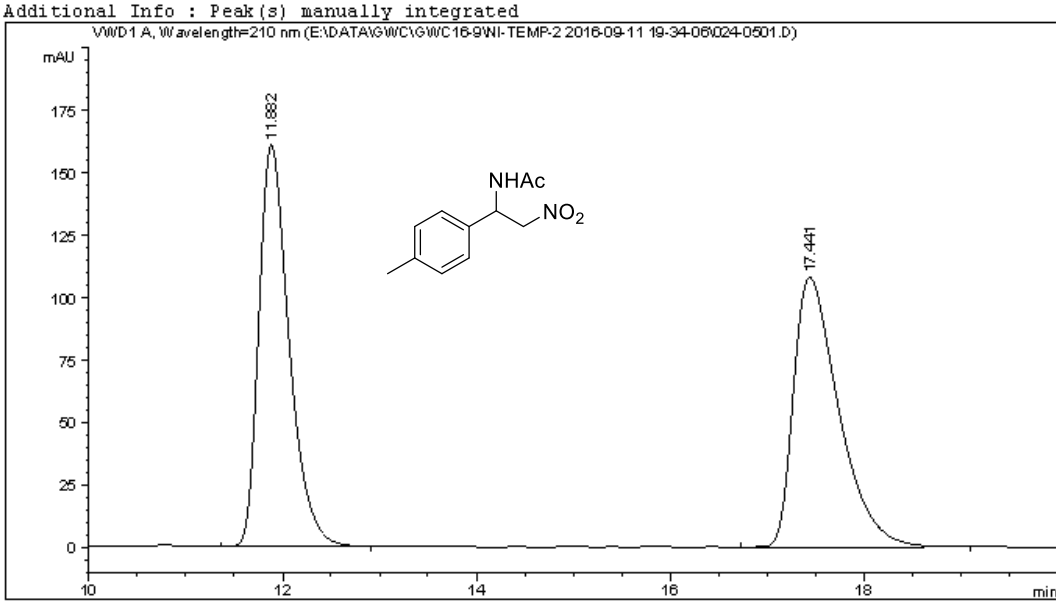
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\014-2001.D
Sample Name: biao-cat

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  20
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 14
    Injection Date  : 9/23/2016 2:15:31 PM               Inj :  1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 2:18:34 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:28:02 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.546 BB    0.3353 7448.50586  340.40121  99.9026
       2  20.060 MM    0.4875    7.26189 2.48253e-1   0.0974

    Totals :                  7455.76775  340.64947

    ======================================================================
                               *** End of Report ***


1260HPLC-DAD 10/25/2016 8:28:08 PM SYSTEM                       Page 1 of 1
```

HPLC-2b-rac

```
Data File E:\DATA\GWC\GWC16-9\NI-TEMP-2 2016-09-11 19-34-06\024-0501.D
Sample Name: rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 24
    Injection Date  : 9/11/2016 8:48:00 PM               Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\NI-TEMP-2 2016-09-11 19-34-06\VWD-ADH(1-6)-90-10-
                      210NM-20MIN.M
    Last changed    : 9/11/2016 7:34:06 PM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-9\NI-TEMP-2 2016-09-11 19-34-06\VWD-ADH(1-6)-90-10-
                      210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 9:05:10 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

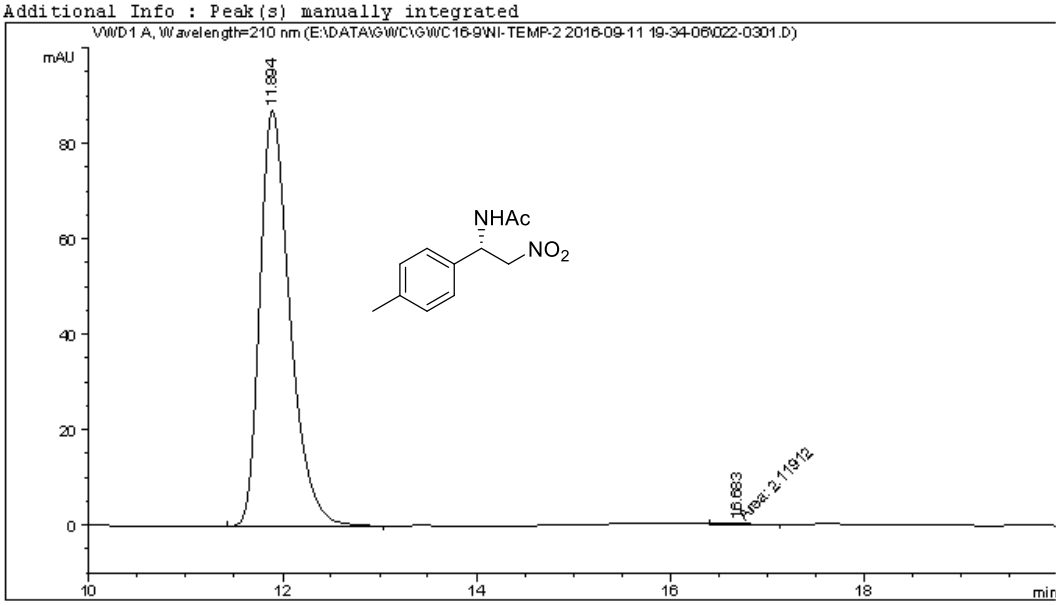



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.882 BB    0.3322 3490.79248  160.83640  49.9750
       2  17.441 BB    0.4915 3494.28735  107.97732  50.0250

    Totals :                  6985.07983  268.81371


    ======================================================================
                            *** End of Report ***

1260HPLC-DAD 10/25/2016 9:05:17 PM SYSTEM                    Page 1 of 1
```

HPLC-2b-cat

Data File E:\DATA\GWC\GWC16-9\NI-TEMP-2 2016-09-11 19-34-06\022-0301.D
Sample Name: 4

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 22
    Injection Date  : 9/11/2016 8:06:26 PM               Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\NI-TEMP-2 2016-09-11 19-34-06\VWD-ADH(1-6)-90-10-
                      210NM-20MIN.M
    Last changed    : 9/11/2016 7:34:06 PM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-9\NI-TEMP-2 2016-09-11 19-34-06\VWD-ADH(1-6)-90-10-
                      210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 9:05:37 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

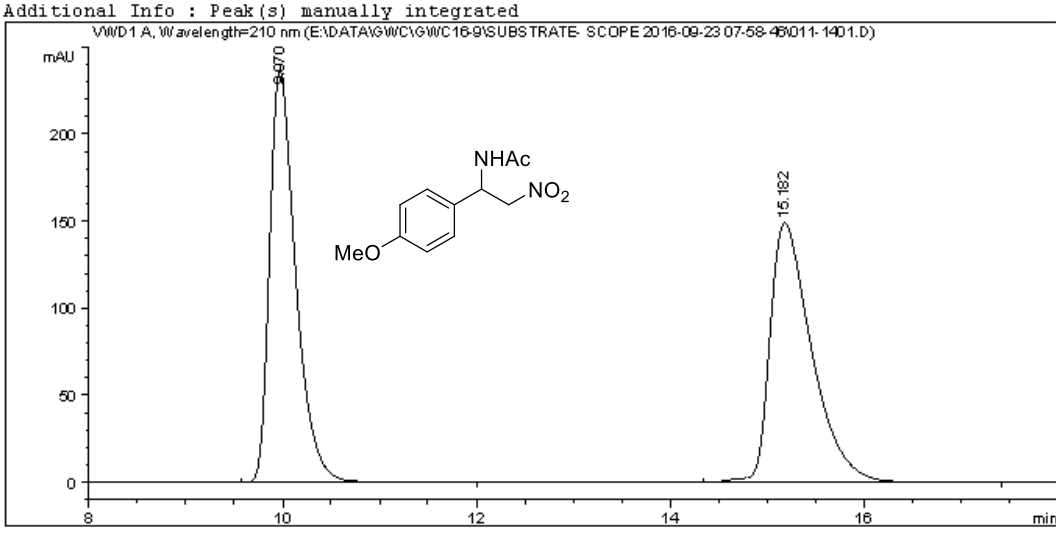



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.894 BB    0.3290 1878.40344   86.97512  99.8873
       2  16.683 MM    0.2885    2.11912 1.22423e-1   0.1127

    Totals :                  1880.52256   87.09754


    ======================================================================
                               *** End of Report ***

1260HPLC-DAD 10/25/2016 9:05:41 PM SYSTEM                    Page 1 of 1
```

HPLC-2c-rac

Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\011-1401.D
Sample Name: OMe-rac

```
    ==================================================================
    Acq. Operator   : SYSTEM                       Seq. Line :  14
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 11
    Injection Date  : 9/23/2016 12:26:45 PM              Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 12:30:57 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:14:43 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

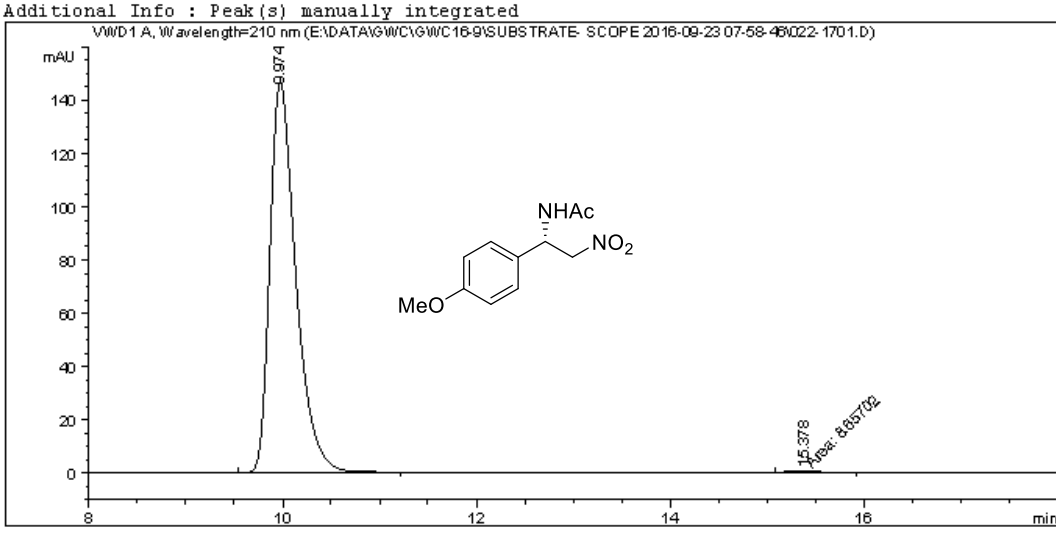



```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]       [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.970 BB    0.2851 4435.74561  236.17282  49.8124
       2  15.182 BB    0.4532 4469.14990  148.88206  50.1876

    Totals :                  8904.89551  385.05489


    ==================================================================
                          *** End of Report ***
```

HPLC-2c-cat

Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\022-1701.D
Sample Name: 4-ome-cat

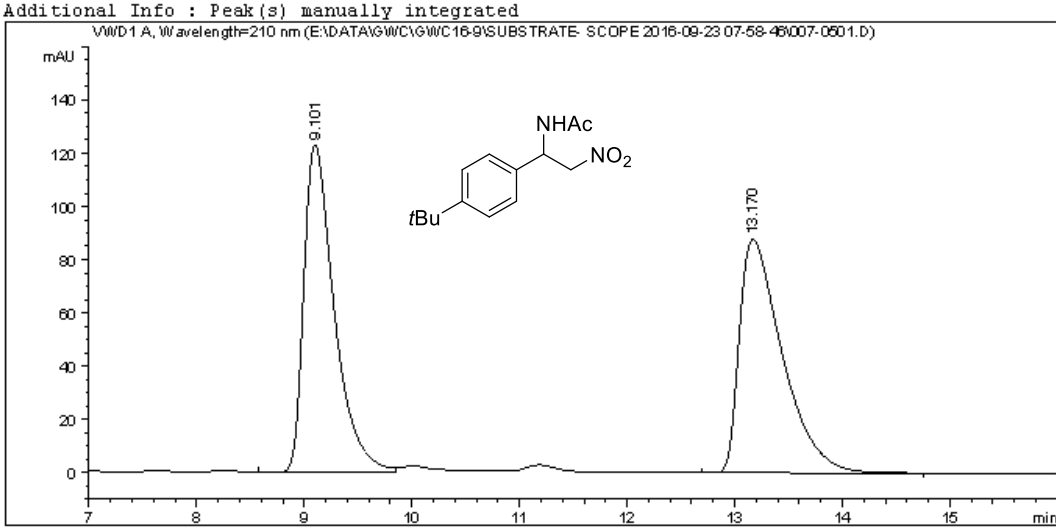
```
    ======================================================================
    Acq. Operator   : SYSTEM                       Seq. Line :  17
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 22
    Injection Date  : 9/23/2016 1:23:05 PM               Inj :  1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 1:23:17 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:25:15 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]       [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.974 BB    0.2836 2728.93823  146.27979  99.6838
       2  15.378 MM    0.4133    8.65702 3.49128e-1   0.3162

    Totals :                  2737.59526  146.62891


    ======================================================================
                            *** End of Report ***
```

HPLC-2d-rac

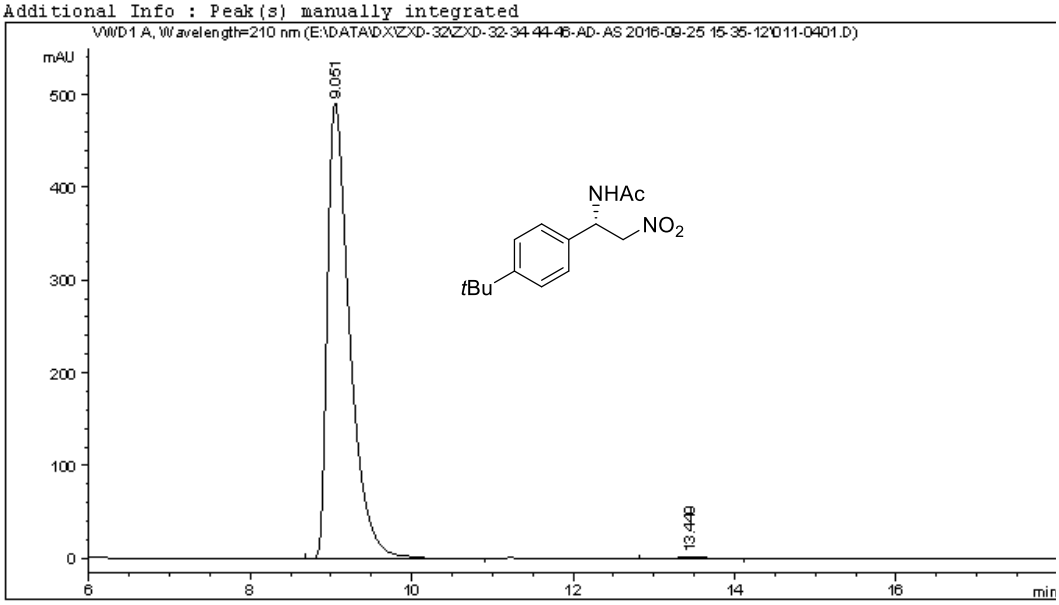
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\007-0501.D
Sample Name: tBu-rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 7
    Injection Date  : 9/23/2016 9:32:37 AM               Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 9:47:19 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:05:00 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.101 BV    0.2952 2405.08936  122.98277  49.7564
       2  13.170 BB    0.4168 2428.64331   87.78138  50.2436

    Totals :                  4833.73267  210.76415

    ======================================================================
                            *** End of Report ***


1260HPLC-DAD 10/25/2016 8:05:05 PM SYSTEM                    Page 1 of 1
```

HPLC-2d-cat

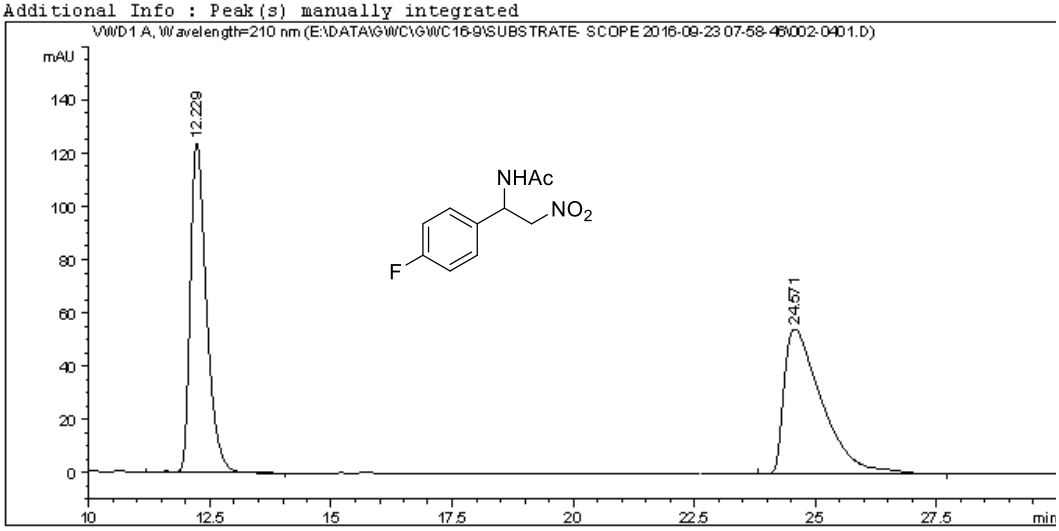
```
Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-25 15-35-12\011-0401.D
Sample Name: tBu-cat

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 11
    Injection Date  : 9/25/2016 4:28:15 PM                 Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-25 15-35-12\VWD-ADH(1-6)
                      -90-10-210NM-20MIN.M
    Last changed    : 9/25/2016 3:35:13 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-25 15-35-12\VWD-ADH(1-6)
                      -90-10-210NM-20MIN.M (Sequence Method)
    Last changed    : 12/16/2016 10:16:21 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.051 BB    0.2895 9401.23535  490.67557  99.5203
       2  13.449 BB    0.3760   45.31156    1.77419   0.4797

    Totals :                  9446.54691  492.44976


    ======================================================================
                            *** End of Report ***

1260HPLC-VWD 12/16/2016 10:16:27 AM SYSTEM                    Page 1 of 1
```

HPLC-2e-rac

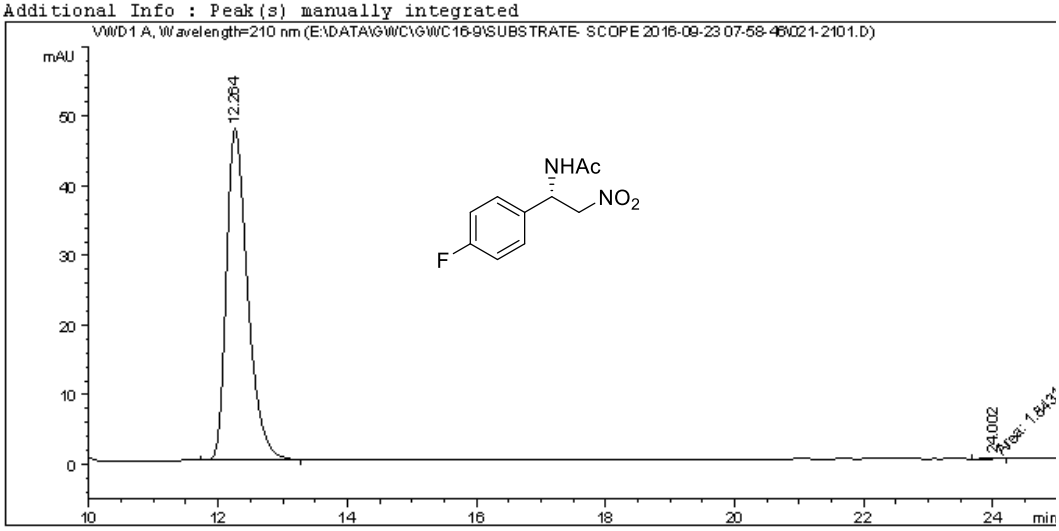
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\002-0401.D
Sample Name: F-rac

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 2
    Injection Date  : 9/23/2016 9:01:49 AM                 Inj :   1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 9:17:36 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:02:58 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.229 BB    0.3536 2873.46655  123.86520  49.2803
       2  24.571 BB    0.7853 2957.39014   54.47705  50.7197

    Totals :                  5830.85669  178.34226

    ======================================================================
                              *** End of Report ***


1260HPLC-DAD 10/25/2016 8:03:06 PM SYSTEM                       Page 1 of 1
```

HPLC-2e-cat

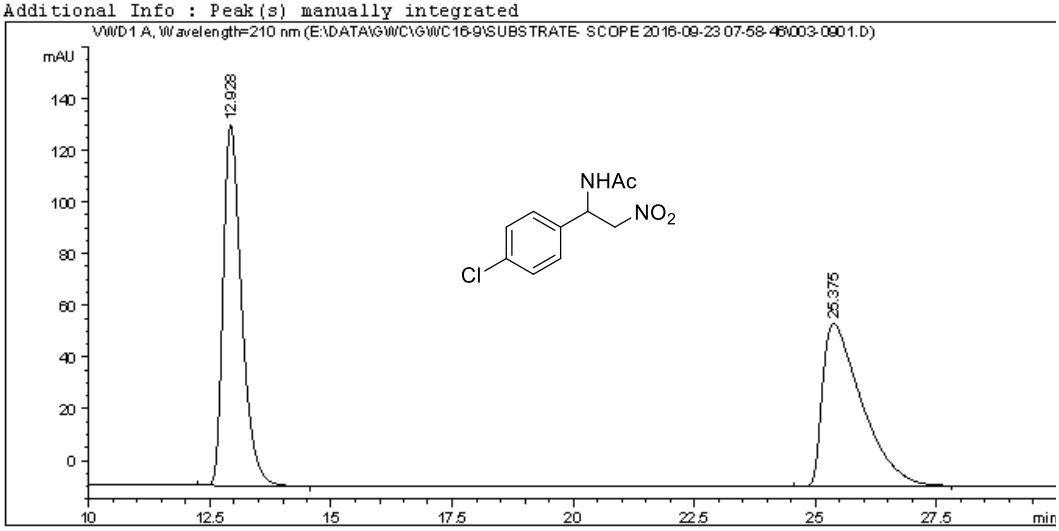
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\021-2101.D
Sample Name: 4-f-cat

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  21
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 21
    Injection Date  : 9/23/2016 2:41:47 PM               Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 2:42:30 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:30:14 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.264 BB    0.3478 1087.23499   47.55069  99.8308
       2  24.002 MM    0.3073    1.84314 9.99646e-2   0.1692

    Totals :                  1089.07812   47.65066

    ======================================================================
                            *** End of Report ***
```

HPLC-2f-rac

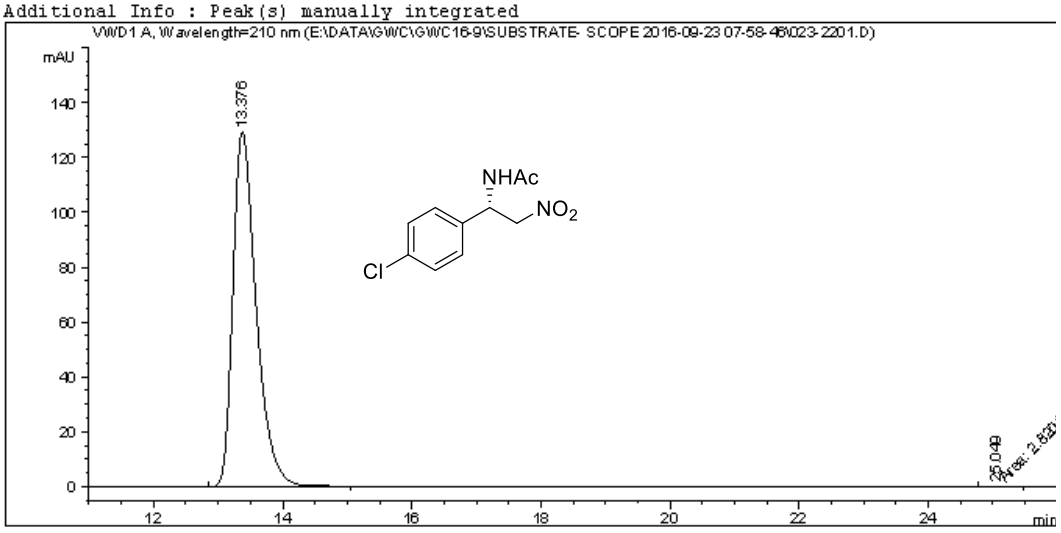
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\003-0901.D
Sample Name: Cl-rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   9
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 3
    Injection Date  : 9/23/2016 10:45:44 AM              Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 11:16:28 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:09:49 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.928 BB    0.4035 3685.12231  139.38007  50.9043
       2  25.375 BB    0.8318 3554.19092   62.84177  49.0957

    Totals :                  7239.31323  202.22183


    ======================================================================
                            *** End of Report ***


1260HPLC-DAD 10/25/2016 8:09:53 PM SYSTEM                    Page 1 of 1
```

HPLC-2f-cat

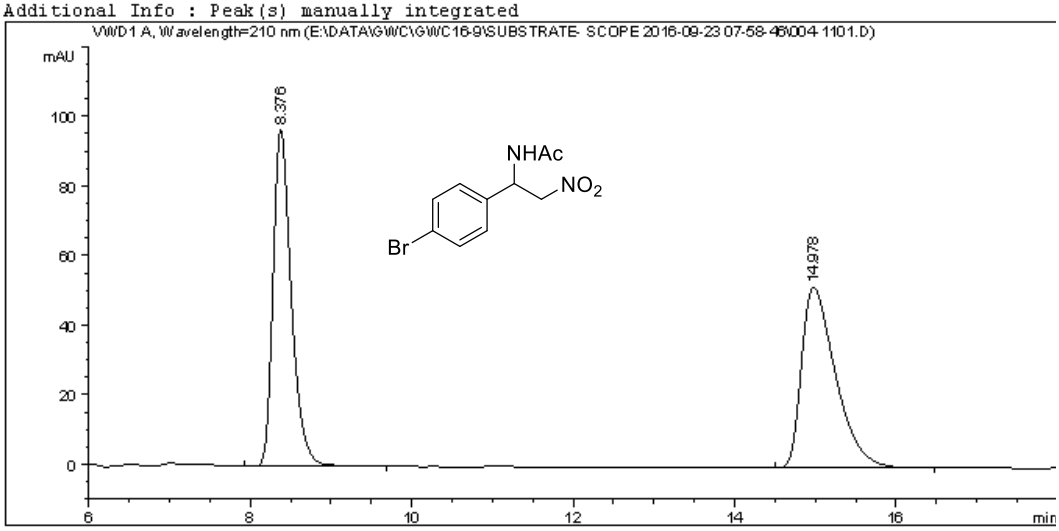
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\023-2201.D
Sample Name: 4-cl-cat

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  22
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 23
    Injection Date  : 9/23/2016 3:12:34 PM                 Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 2:42:30 PM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:34:19 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.376 BB    0.3811 3233.29492  129.12560  99.9128
       2  25.049 MM    0.4247    2.82047 1.10689e-1   0.0872

    Totals :                  3236.11540  129.23628


    ======================================================================
                            *** End of Report ***
```

HPLC-2g-rac

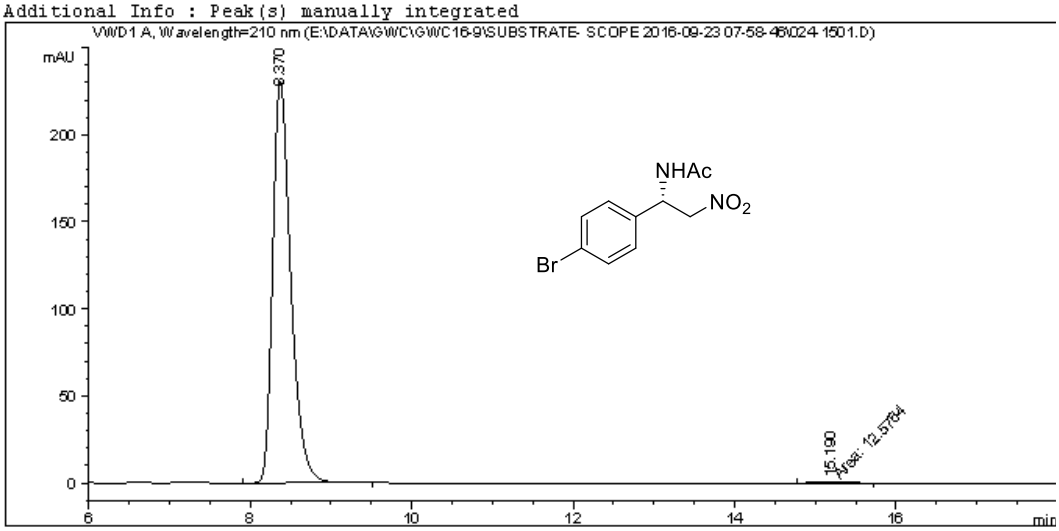
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\004-1101.D
Sample Name: Br-rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  11
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 4
    Injection Date  : 9/23/2016 11:29:23 AM              Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 11:47:07 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:10:49 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.376 BB    0.2391 1517.92566   96.70007  50.0947
       2  14.978 BB    0.4456 1512.18921   51.79261  49.9053

    Totals :                  3030.11487  148.49268

    ======================================================================
                            *** End of Report ***


1260HPLC-DAD 10/25/2016 8:10:55 PM SYSTEM                       Page 1 of 1
```

HPLC-2g-cat

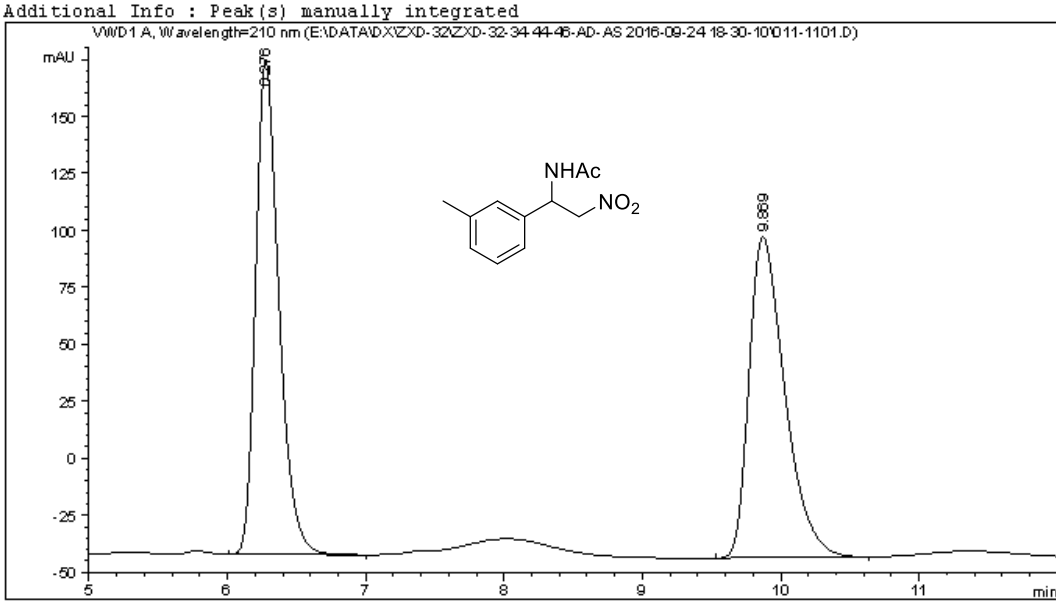
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\024-1501.D
Sample Name: 4-br-cat

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  15
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 24
    Injection Date  : 9/23/2016 12:47:32 PM              Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 12:30:57 PM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:20:39 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.370 BB    0.2369 3599.86133  230.84367  99.6519
       2  15.190 MM    0.4652   12.57644 4.50604e-1   0.3481

    Totals :                  3612.43776  231.29428


    ======================================================================
                            *** End of Report ***
```

HPLC-2h-rac

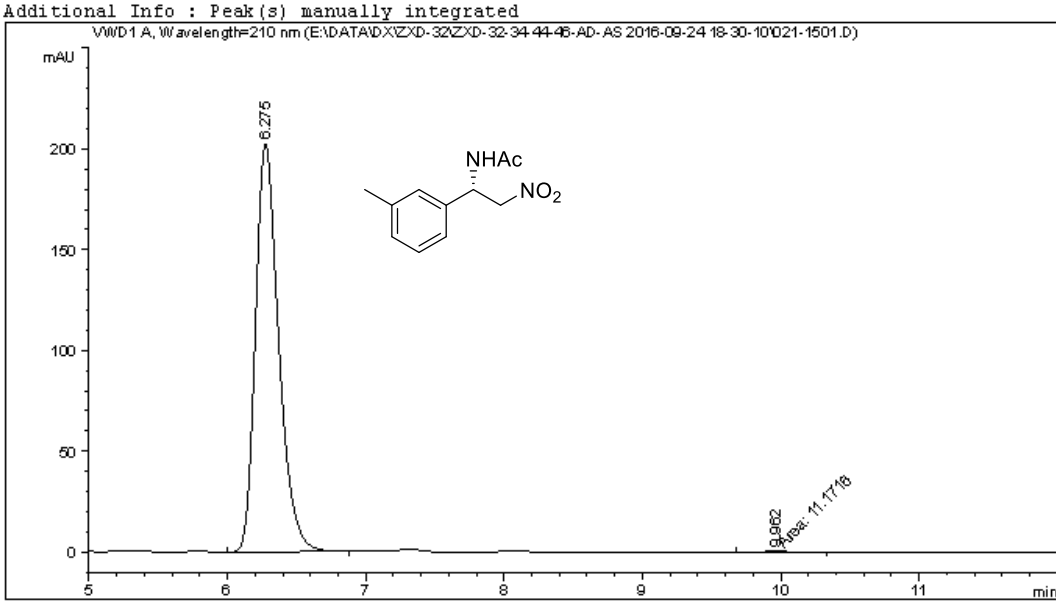
```
Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\011-1101.D
Sample Name: 3-ME-rac

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  11
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 11
    Injection Date  : 9/25/2016 12:38:59 AM                Inj :  1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:38:23 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.276 VB    0.1799 2538.25171  216.25807  50.0981
       2   9.869 BB    0.2755 2528.31250  140.77724  49.9019

    Totals :                   5066.56421  357.03531


    ======================================================================
                               *** End of Report ***

1260HPLC-DAD 10/25/2016 8:38:34 PM SYSTEM                    Page 1 of 1
```

HPLC-2h-cat

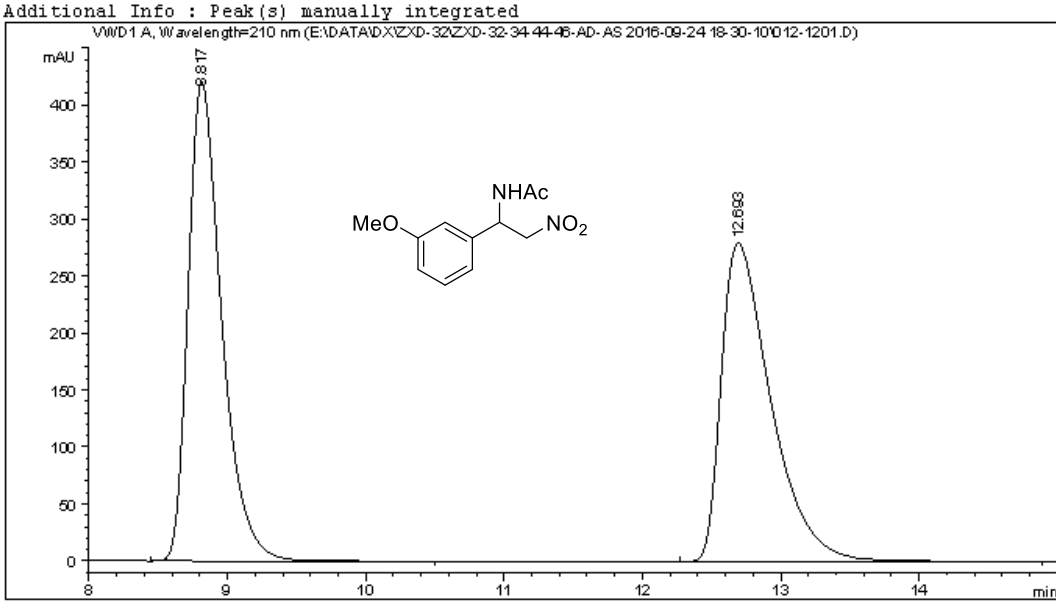
```
Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\021-1501.D
Sample Name: 3-me-cat

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  15
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 21
    Injection Date  : 9/25/2016 2:02:01 AM                 Inj :  1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:44:33 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.275 BB    0.1784 2362.60815  202.04823  99.5294
       2   9.962 MM    0.3113   11.17162 5.98206e-1   0.4706

    Totals :                  2373.77978  202.64644


    ======================================================================
                              *** End of Report ***

1260HPLC-DAD 10/25/2016 8:44:36 PM SYSTEM                       Page 1 of 1
```

HPLC-2i-rac

```
Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\012-1201.D
Sample Name: 3-ome-rac

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  12
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 12
    Injection Date  : 9/25/2016 12:59:43 AM                Inj :  1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:40:38 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

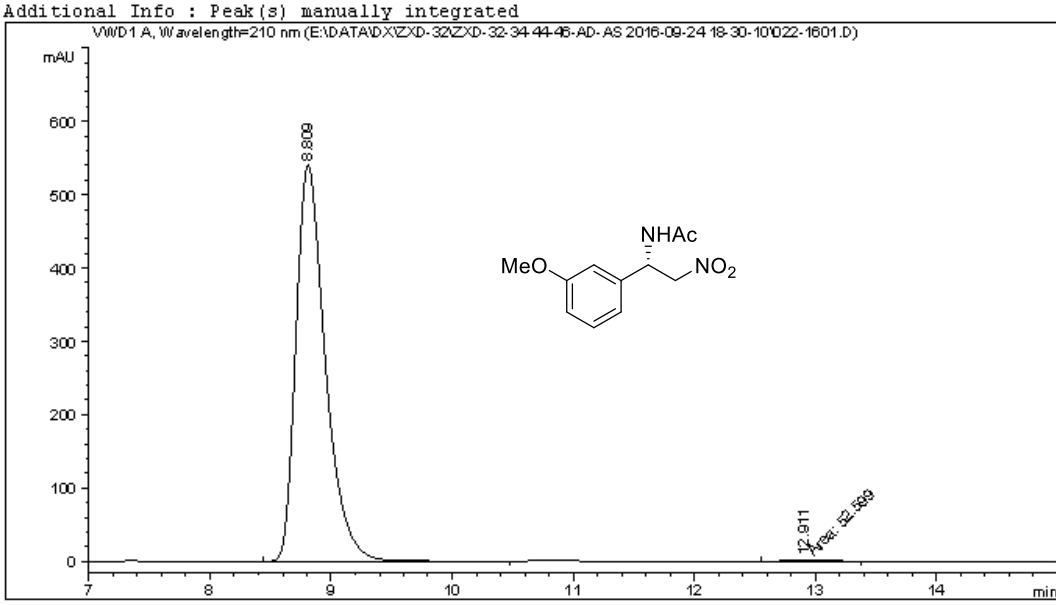



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.817 BB    0.2570 7102.33496  420.51407  50.4378
       2  12.693 BB    0.3772 6979.04395  279.57132  49.5622

    Totals :                  1.40814e4   700.08539


    ======================================================================
                            *** End of Report ***

1260HPLC-DAD 10/25/2016 8:40:42 PM SYSTEM                    Page 1 of 1
```

HPLC-2i-cat

Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\022-1601.D
Sample Name: 3-ome-cat

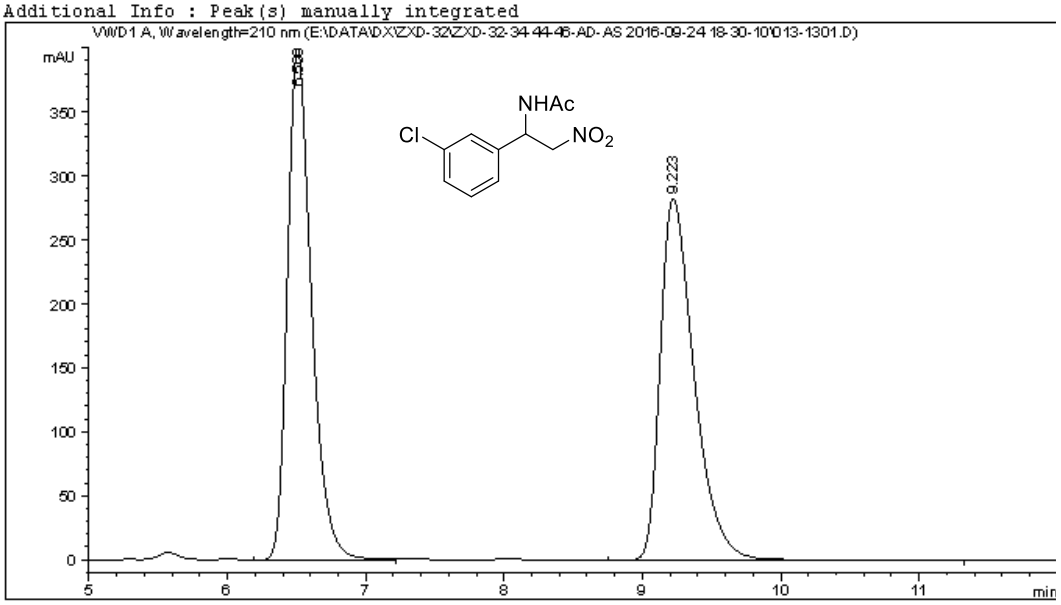
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  16
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 22
    Injection Date  : 9/25/2016 2:22:47 AM                 Inj :  1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:47:10 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.809 BB    0.2569 9113.59473  540.10608  99.4262
       2  12.911 MM    0.3741   52.59902    2.34333   0.5738

    Totals :                  9166.19375  542.44941


    ======================================================================
                              *** End of Report ***
```

HPLC-2j-rac

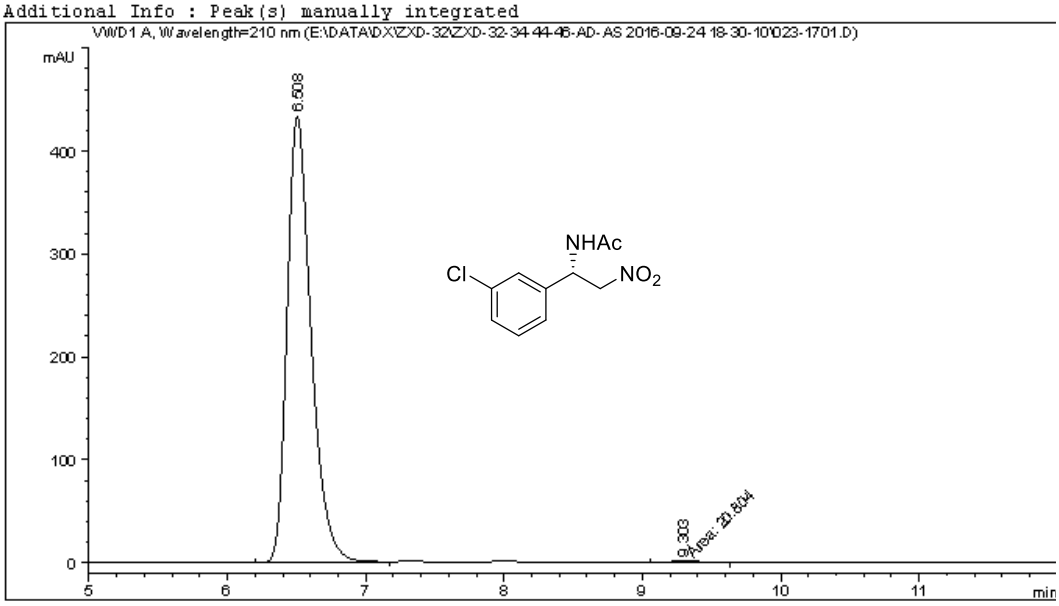
```
Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\013-1301.D
Sample Name: 3-cl-rac

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  13
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 13
    Injection Date  : 9/25/2016 1:20:28 AM                 Inj :  1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:41:42 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.509 BV    0.1842 4849.09326  400.60236  50.1704
       2   9.223 BB    0.2598 4816.15283  282.63071  49.8296

    Totals :                   9665.24609  683.23306


    ======================================================================
                              *** End of Report ***

1260HPLC-DAD 10/25/2016 8:41:46 PM SYSTEM                    Page 1 of 1
```

HPLC-2j-cat

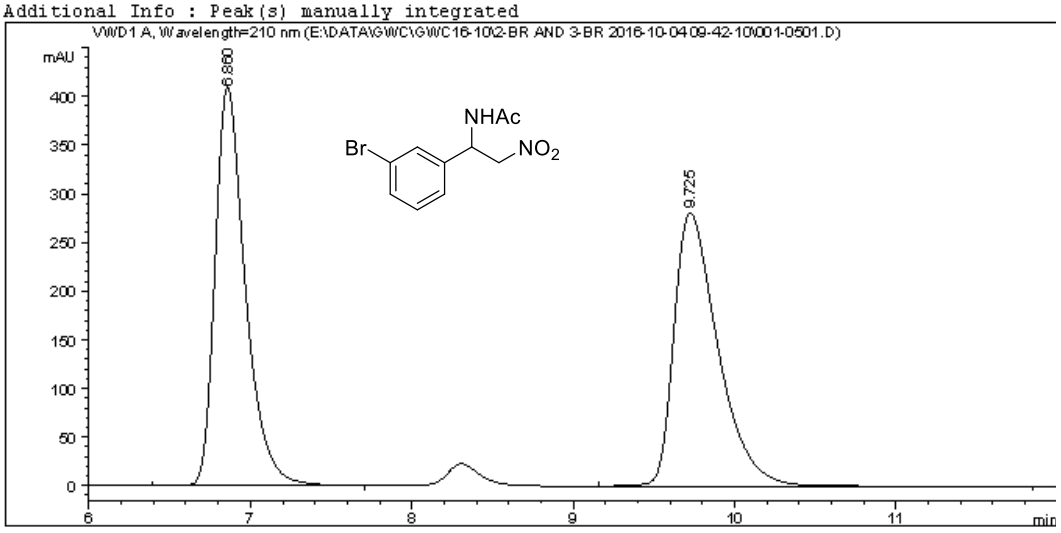
```
Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\023-1701.D
Sample Name: 3-cl-cat

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  17
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 23
    Injection Date  : 9/25/2016 2:43:33 AM                 Inj :  1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:48:31 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.508 BB    0.1846 5222.48682  433.45673  99.6032
       2   9.303 MM    0.2542   20.80397    1.36397   0.3968

    Totals :                   5243.29078  434.82070


    ======================================================================
                               *** End of Report ***

1260HPLC-DAD 10/25/2016 8:48:36 PM SYSTEM                       Page 1 of 1
```

HPLC-2k-rac

```
Data File E:\DATA\GWC\GWC16-10\2-BR AND 3-BR 2016-10-04 09-42-10\001-0501.D
Sample Name: 3-Br-rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 1
    Injection Date  : 10/4/2016 10:56:01 AM              Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-10\2-BR AND 3-BR 2016-10-04 09-42-10\VWD-ADH(1-6)-85-
                      15-210NM-30MIN.M
    Last changed    : 10/4/2016 10:35:17 AM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-10\2-BR AND 3-BR 2016-10-04 09-42-10\VWD-ADH(1-6)-85-
                      15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:50:53 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

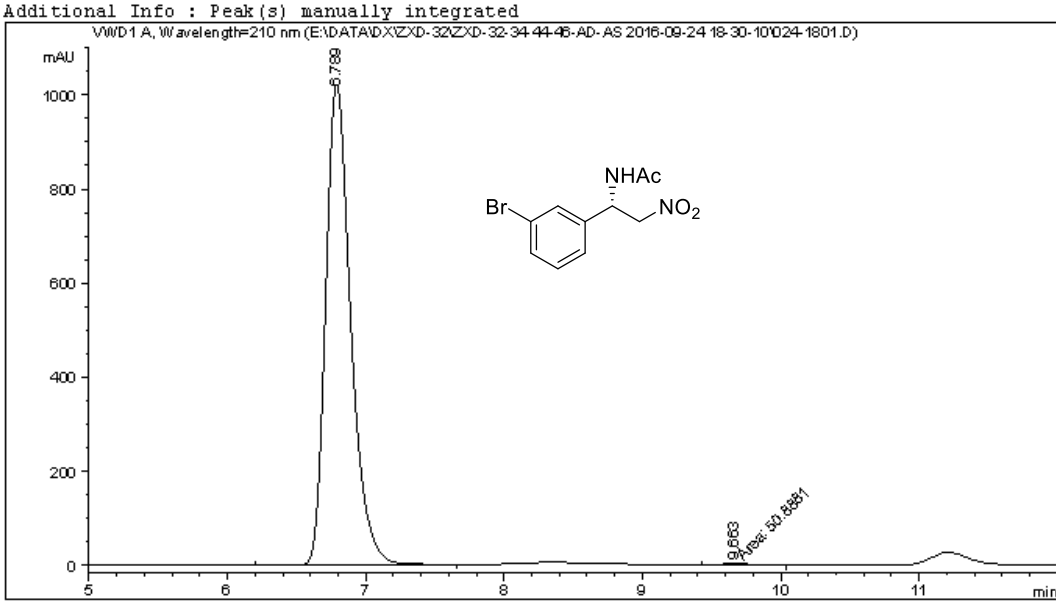



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.860 BB    0.1975 5363.68115  410.22986  50.1193
       2   9.725 BB    0.2886 5338.14404  281.02087  49.8807

    Totals :                  1.07018e4   691.25073


    ======================================================================
                            *** End of Report ***
```

HPLC-2k-cat

Data File E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\024-1801.D
Sample Name: 3-br-cat

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  18
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 24
    Injection Date  : 9/25/2016 3:04:20 AM                 Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M
    Last changed    : 9/24/2016 10:04:57 PM by SYSTEM
    Analysis Method : E:\DATA\DX\ZXD-32\ZXD-32-34-44-46-AD-AS 2016-09-24 18-30-10\VWD-ADH(1-6)
                      -85-15-210NM-20MIN.M (Sequence Method)
    Last changed    : 10/25/2016 9:02:20 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



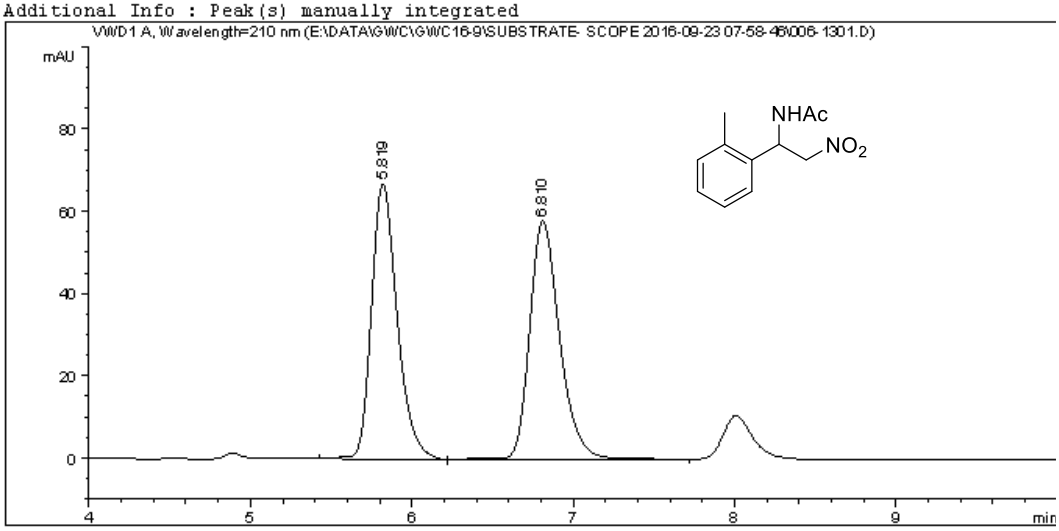

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.789 BB    0.1915 1.28355e4  1022.09790  99.6051
       2   9.663 MM    0.2817   50.88806    3.01076   0.3949

    Totals :                  1.28863e4  1025.10866


    ======================================================================
                            *** End of Report ***
```

1260HPLC-DAD 10/25/2016 9:02:24 PM SYSTEM Page 1 of 1

HPLC-2l-rac

Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\006-1301.D
Sample Name: 2-me-rac

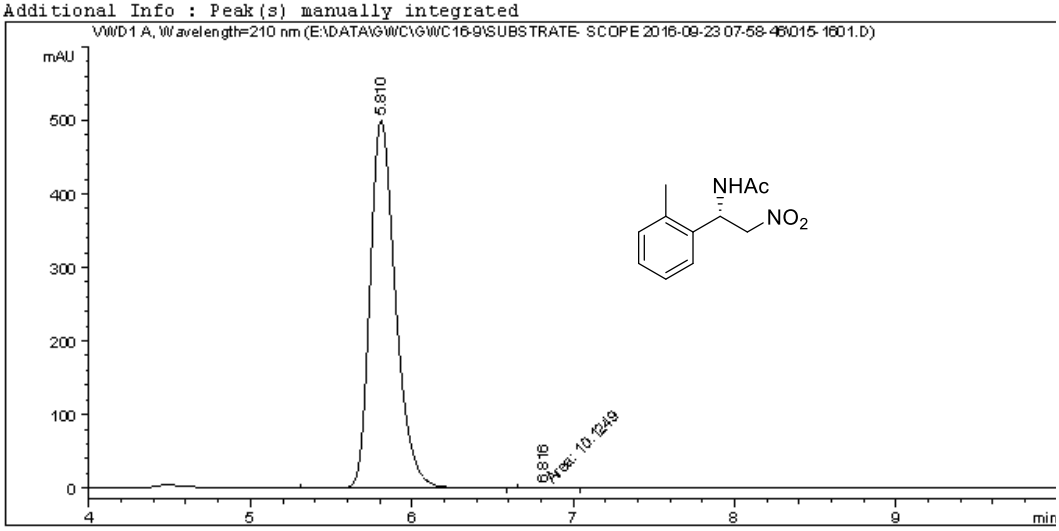
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  13
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 6
    Injection Date  : 9/23/2016 12:11:00 PM               Inj :  1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 12:20:36 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:13:50 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   5.819 BB    0.1692  741.97858   67.01857  49.7411
       2   6.810 BB    0.1968  749.70227   57.99751  50.2589

    Totals :                   1491.68085  125.01608

    ======================================================================
                            *** End of Report ***
```

HPLC-2l-cat

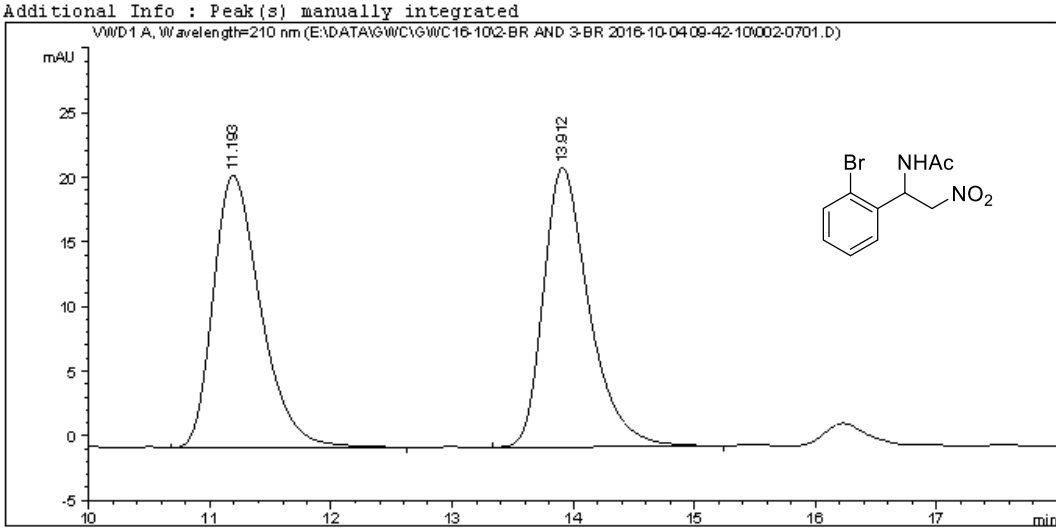
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\015-1601.D
Sample Name: 2-me-cat

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  16
    Acq. Instrument : 1260HPLC-VWD                    Location : Vial 15
    Injection Date  : 9/23/2016 1:08:19 PM                 Inj :   1
                                                     Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 1:21:47 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:23:45 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   5.810 BB    0.1679 5471.99609  499.22159  99.8153
       2   6.816 MM    0.1899   10.12492 8.88631e-1   0.1847

    Totals :                   5482.12102  500.11022

    ======================================================================
                            *** End of Report ***


1260HPLC-DAD 10/25/2016 8:23:48 PM SYSTEM                    Page 1 of 1
```

HPLC-2m-rac

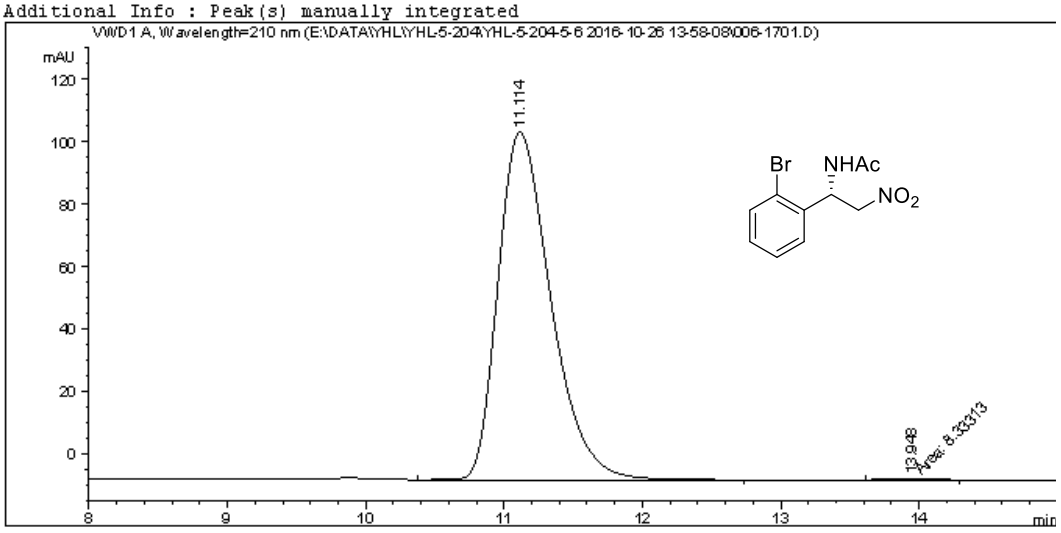
```
Data File E:\DATA\GWC\GWC16-10\2-BR AND 3-BR 2016-10-04 09-42-10\002-0701.D
Sample Name: 2-Br-RAC

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 2
    Injection Date  : 10/4/2016 11:22:39 AM               Inj :   1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-10\2-BR AND 3-BR 2016-10-04 09-42-10\VWD-ADH(1-6)-90-
                      10-210NM-40MIN.M
    Last changed    : 10/4/2016 11:09:48 AM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-10\2-BR AND 3-BR 2016-10-04 09-42-10\VWD-ADH(1-6)-90-
                      10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/26/2016 10:28:22 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.193 BB    0.4187  575.57806   21.06749  50.3137
       2  13.912 BB    0.3979  568.40088   21.60568  49.6863

    Totals :                  1143.97894   42.67317


    ======================================================================
                              *** End of Report ***
```

HPLC-2m-cat

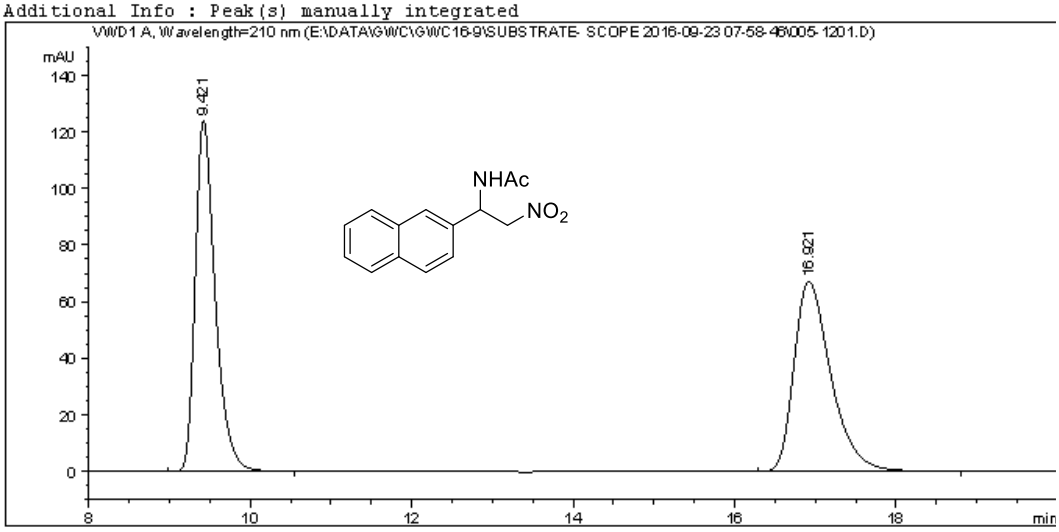
```
Data File E:\DATA\YHL\YHL-5-204\YHL-5-204-5-6 2016-10-26 13-58-08\006-1701.D
Sample Name: 2

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  17
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 6
    Injection Date  : 10/26/2016 7:41:47 PM              Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\YHL\YHL-5-204\YHL-5-204-5-6 2016-10-26 13-58-08\VWD-ADH(1-6)-90-
                      10-210NM-40MIN.M
    Last changed    : 10/26/2016 2:15:48 PM by SYSTEM
    Analysis Method : E:\DATA\YHL\YHL-5-204\YHL-5-204-5-6 2016-10-26 13-58-08\VWD-ADH(1-6)-90-
                      10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/27/2016 11:46:18 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.114 BB    0.4091 2962.12622  111.44106  99.7195
       2  13.948 MM    0.3647    8.33313 3.80846e-1   0.2805

    Totals :                  2970.45935  111.82191


    ======================================================================
                              *** End of Report ***
```

HPLC-2n-rac

```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\005-1201.D
Sample Name: Nai-rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  12
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 5
    Injection Date  : 9/23/2016 11:50:12 AM               Inj :  1
                                                  Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-10MIN.M
    Last changed    : 9/23/2016 11:58:04 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-10MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:12:23 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

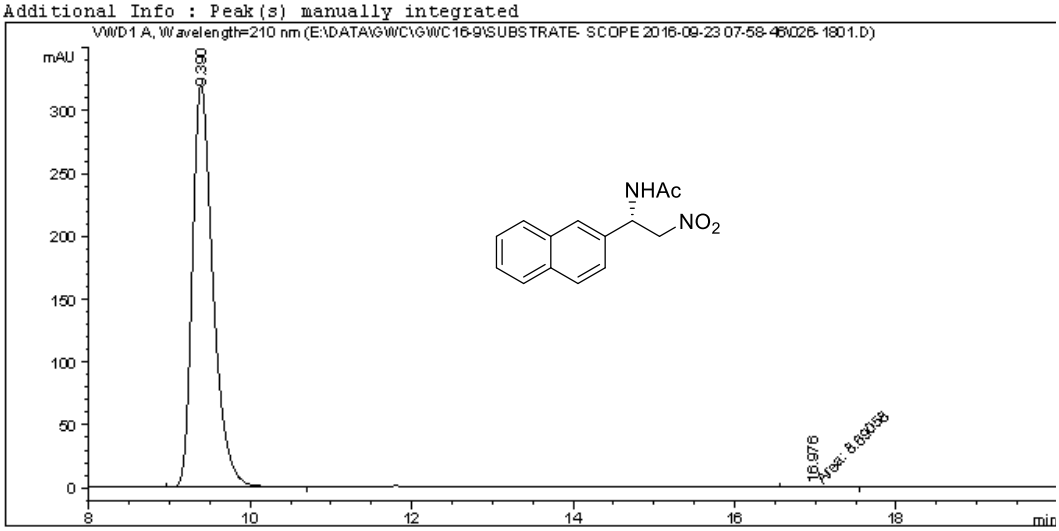



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.421 BB    0.2616 2143.52905  124.06277  50.0649
       2  16.921 BB    0.4825 2137.96875   67.32954  49.9351

    Totals :                  4281.49780  191.39231

    ======================================================================
                              *** End of Report ***


1260HPLC-DAD 10/25/2016 8:12:29 PM SYSTEM                    Page 1 of 1
```

HPLC-2n-cat

Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\026-1801.D
Sample Name: nai-cat

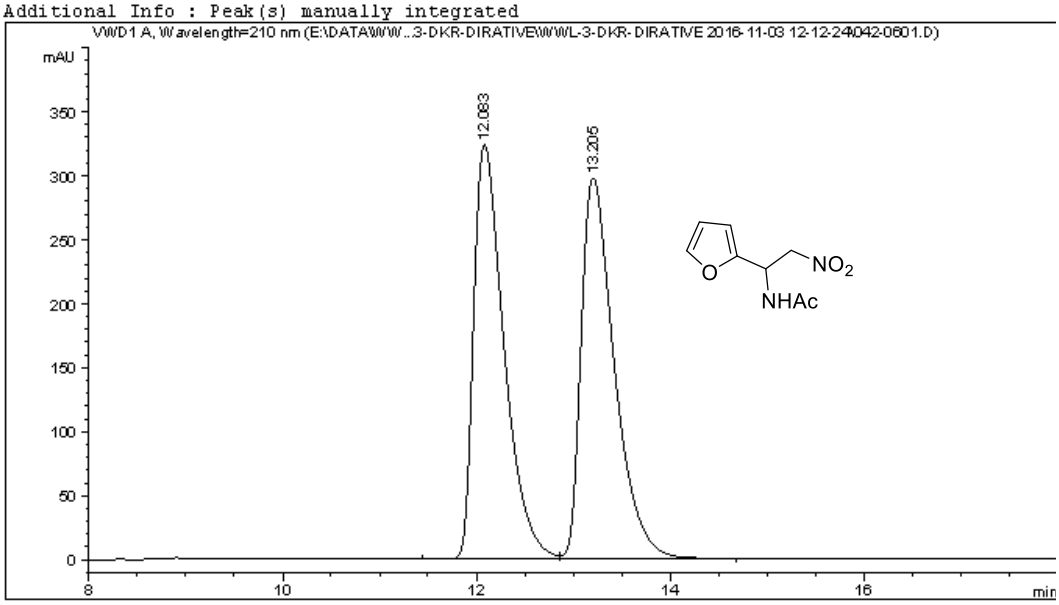
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  18
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 26
    Injection Date  : 9/23/2016 1:43:50 PM                Inj :  1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M
    Last changed    : 9/23/2016 1:23:17 PM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-85
                      -15-210NM-30MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:26:28 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.390 BB    0.2708 5709.43457  320.51248  99.8480
       2  16.976 MM    0.4998    8.69058 2.89791e-1   0.1520

    Totals :                  5718.12515  320.80227


    ======================================================================
                            *** End of Report ***
```

HPLC-2o-rac

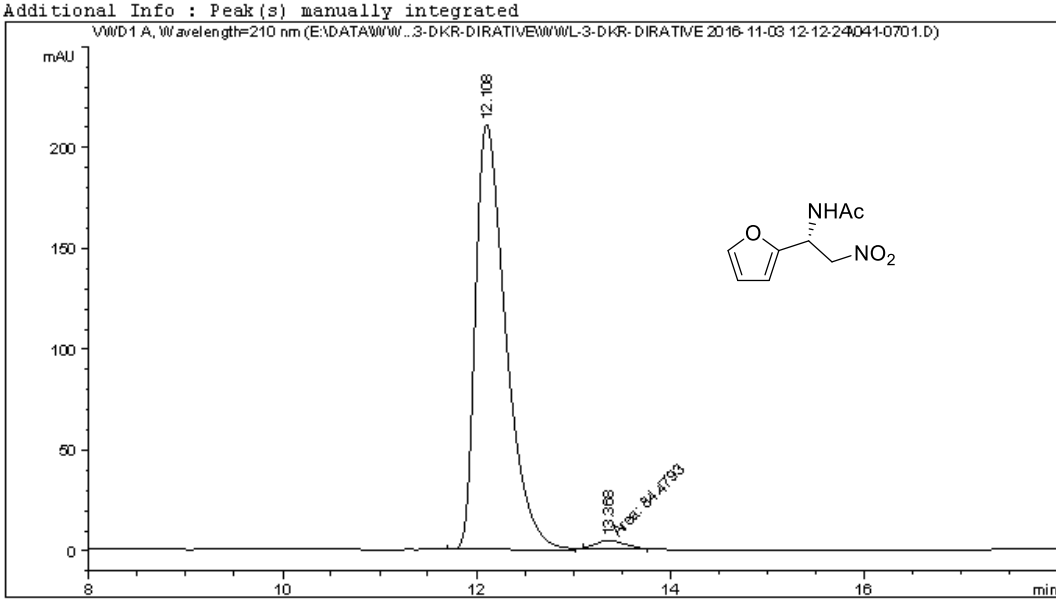
```
Data File E:\DATA\WWL\WWL-3-DKR-DIRATIVE\WWL-3-DKR-DIRATIVE 2016-11-03 12-12-24\042-0601.D
Sample Name: rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   6
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 42
    Injection Date  : 11/3/2016 2:02:08 PM               Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\WWL\WWL-3-DKR-DIRATIVE\WWL-3-DKR-DIRATIVE 2016-11-03 12-12-24
                      \VWD-ADH(1-6)-90-10-210NM-20MIN.M
    Last changed    : 11/3/2016 12:14:22 PM by SYSTEM
    Analysis Method : E:\DATA\WWL\WWL-3-DKR-DIRATIVE\WWL-3-DKR-DIRATIVE 2016-11-03 12-12-24
                      \VWD-ADH(1-6)-90-10-210NM-20MIN.M (Sequence Method)
    Last changed    : 11/3/2016 2:36:58 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                           Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.083 BV    0.3320 7048.88770  323.80307  49.8933
       2  13.205 VB    0.3614 7079.03027  297.73203  50.1067

    Totals :                  1.41279e4   621.53510


    ======================================================================
                           *** End of Report ***

1260HPLC-VWD 11/3/2016 2:37:08 PM SYSTEM                       Page 1 of 1
```

HPLC-2o-cat

```
Data File E:\DATA\WWL\WWL-3-DKR-DIRATIVE\WWL-3-DKR-DIRATIVE 2016-11-03 12-12-24\041-0701.D
Sample Name: cat

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 41
    Injection Date  : 11/3/2016 2:22:54 PM               Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\WWL\WWL-3-DKR-DIRATIVE\WWL-3-DKR-DIRATIVE 2016-11-03 12-12-24
                      \VWD-ADH(1-6)-90-10-210NM-20MIN.M
    Last changed    : 11/3/2016 2:39:26 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\WWL\WWL-3-DKR-DIRATIVE\WWL-3-DKR-DIRATIVE 2016-11-03 12-12-24
                      \VWD-ADH(1-6)-90-10-210NM-20MIN.M (Sequence Method)
    Last changed    : 11/3/2016 2:43:02 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

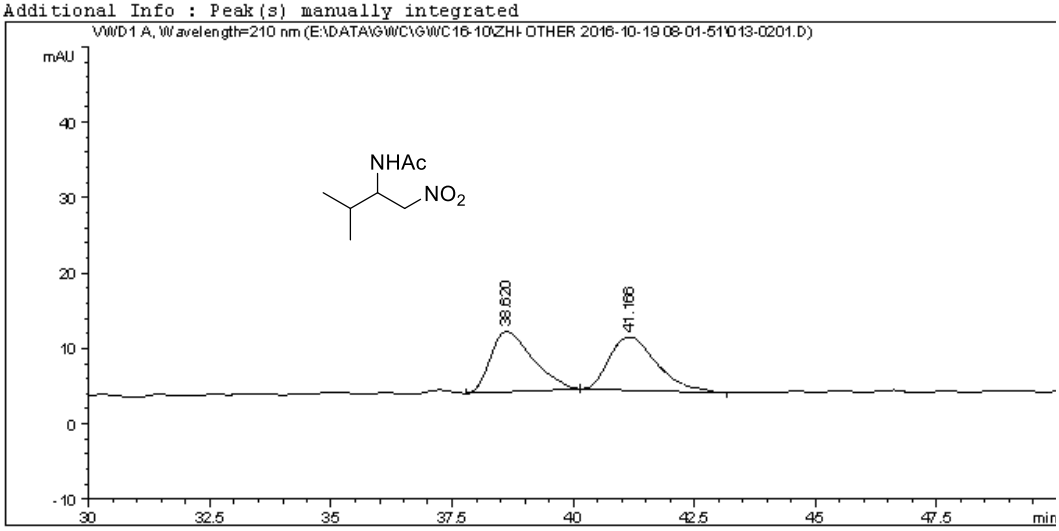



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]       [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.108 BV    0.3320 4585.45508  210.59842  98.1910
       2  13.368 MM    0.3501   84.47933    4.02145   1.8090

    Totals :                  4669.93441  214.61987


    ======================================================================

1260HPLC-VWD 11/3/2016 2:43:05 PM SYSTEM                       Page 1 of 1
```

HPLC-2p-rac

Data File E:\DATA\GWC\GWC16-10\ZHI-OTHER 2016-10-19 08-01-51\013-0201.D
Sample Name: zhi-rac

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 13
    Injection Date  : 10/19/2016 8:13:24 AM               Inj :   1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-10\ZHI-OTHER 2016-10-19 08-01-51\VWD-ADH(1-6)-97-3-0.9
                      -210NM-40MIN.M
    Last changed    : 10/19/2016 8:43:09 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-10\ZHI-OTHER 2016-10-19 08-01-51\VWD-ADH(1-6)-97-3-0.9
                      -210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 10:51:16 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

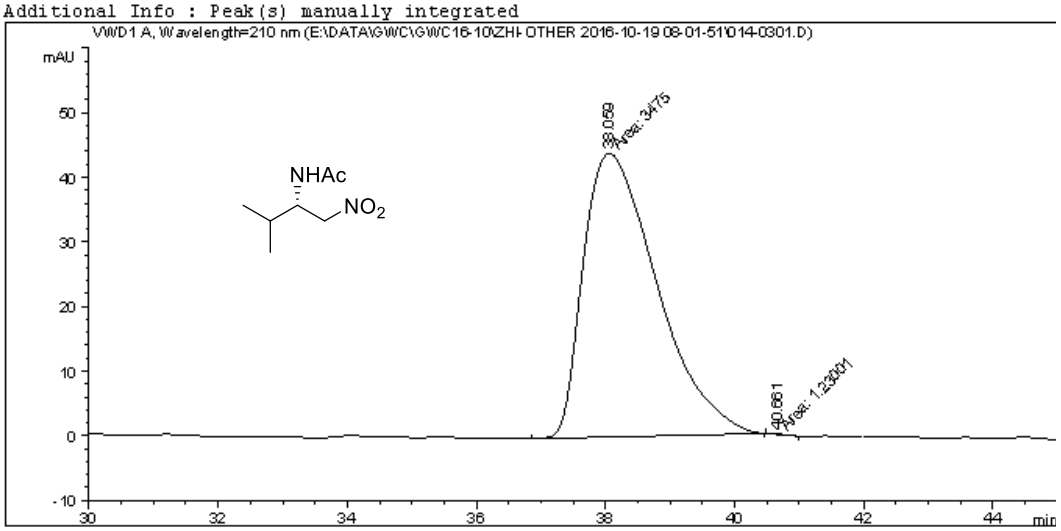



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  38.620 BB    0.8918  481.31561    7.97812  50.0437
       2  41.166 BB    0.9897  480.47427    7.03635  49.9563

    Totals :                   961.78989   15.01447

    ======================================================================
                              *** End of Report ***
```

HPLC-2p-cat

Data File E:\DATA\GWC\GWC16-10\ZHI-OTHER 2016-10-19 08-01-51\014-0301.D
Sample Name: ZHI-CAT

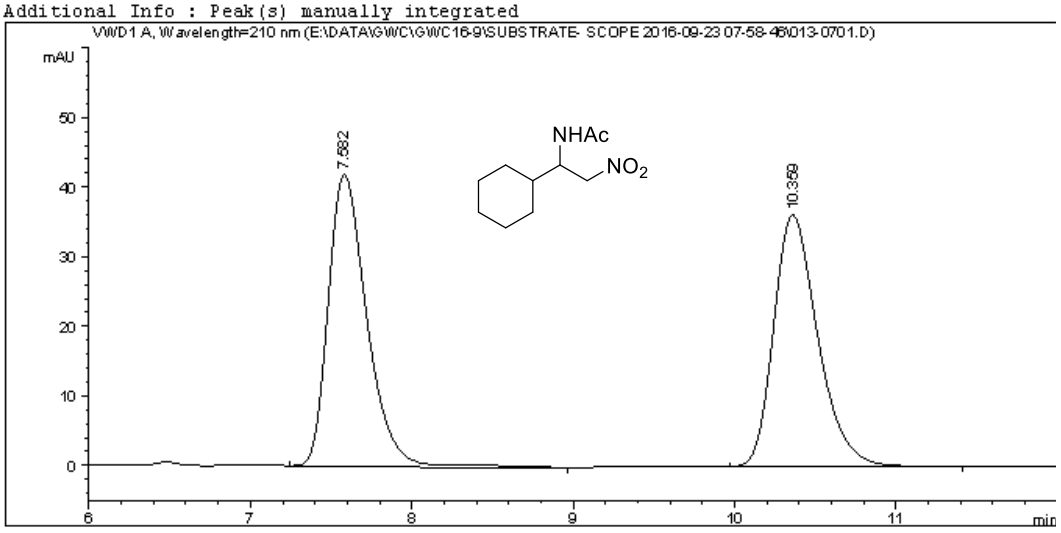
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 14
    Injection Date  : 10/19/2016 9:04:09 AM               Inj :   1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-10\ZHI-OTHER 2016-10-19 08-01-51\VWD-ADH(1-6)-97-3-0.9
                      -210NM-40MIN.M
    Last changed    : 10/19/2016 8:43:09 AM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-10\ZHI-OTHER 2016-10-19 08-01-51\VWD-ADH(1-6)-97-3-0.9
                      -210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 7:57:42 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  38.059 MM    1.3206 3474.99585   43.85545  99.9646
       2  40.661 MM    0.2434    1.23001 8.42135e-2   0.0354

    Totals :                  3476.22586   43.93966


    ======================================================================
                              *** End of Report ***
```

HPLC-2q-rac

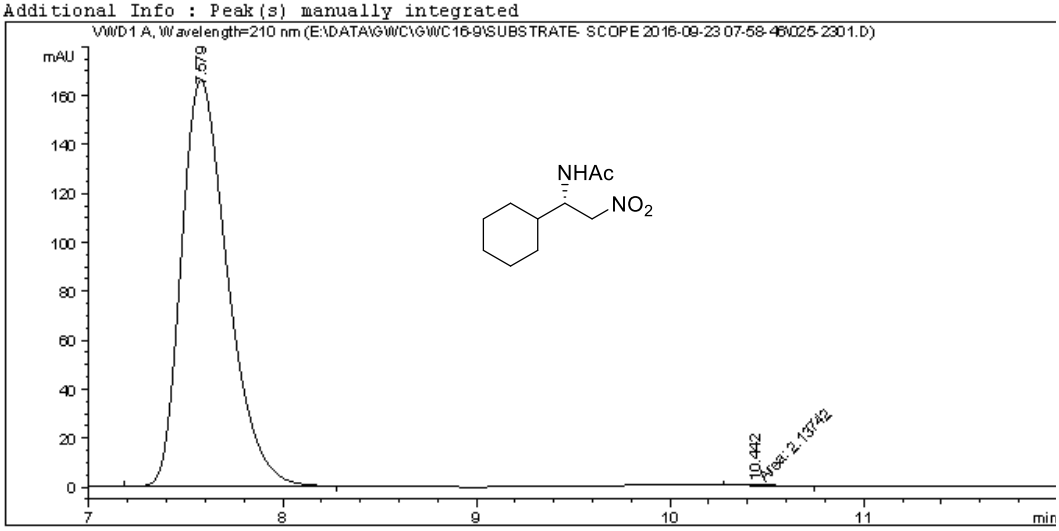
```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\013-0701.D
Sample Name: six-huan-rac

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 13
    Injection Date  : 9/23/2016 10:14:07 AM               Inj :   1
                                                  Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 9:47:19 AM by SYSTEM
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:07:41 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.582 BB    0.2558  704.48138   41.96710  50.7415
       2  10.359 BB    0.2910  683.89142   36.11015  49.2585

    Totals :                  1388.37280   78.07725


    ======================================================================
                            *** End of Report ***
```

HPLC-2q-cat

```
Data File E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\025-2301.D
Sample Name: sixhuan-cat

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  23
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 25
    Injection Date  : 9/23/2016 3:43:20 PM               Inj :  1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M
    Last changed    : 9/23/2016 3:45:05 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\GWC\GWC16-9\SUBSTRATE- SCOPE 2016-09-23 07-58-46\VWD-ADH(1-6)-90
                      -10-210NM-40MIN.M (Sequence Method)
    Last changed    : 10/25/2016 8:36:03 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.579 BB    0.2563 2750.34399  165.97928  99.9223
       2  10.442 MM    0.2352    2.13742 1.51444e-1   0.0777

    Totals :                  2752.48141  166.13072

    ======================================================================
                            *** End of Report ***


1260HPLC-DAD 10/25/2016 8:36:13 PM SYSTEM                    Page 1 of 1
```