

**NHC-Catalysed [3+2]-Asymmetric Annulation between Pyrazolin-4,5-diones and Enals:
Synthesis of Novel Spirocyclic Pyrazolone γ -Butyrolactones and Computational Study of
Mechanism and Stereoselectivity**

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General Information

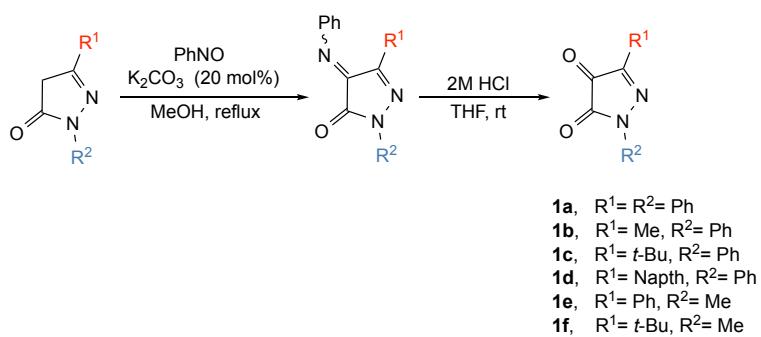
¹H NMR (500 MHz), ¹³C NMR (126 MHz) and ¹⁹F NMR (376 MHz) spectra were recorded in CDCl₃ as solvent. Chemical shifts for protons are reported in ppm from TMS with the residual CHCl₃ resonance as internal reference. Chemical shifts for carbons are reported in ppm from TMS and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s= singlet, d= doublet, t= triplet, q= quartet, m= multiplet, br= broad), coupling constants in Hertz, and integration.

Specific rotations were measured on a Perkin-Elmer 341 digital polarimeter using a 1 mL cell with a 1-dm path length, and a sodium lamp, and concentration is given in g per 100 mL. Infrared spectra were recorded on a Perkin-Elmer Spectrum One FT-IR spectrometer and are reported in frequency of absorption (only the structurally most important peaks are given).

Flash chromatography was carried out using silica gel (230–240 mesh). TLC analysis was performed on glass-backed plates coated with silica gel 60 and F254 indicator, and visualized by either UV irradiation or by staining with phosphomolybdic acid solution. Chiral HPLC analysis was performed on a JASCO HPLC system (JASCO PU-2089 and UV-2075 UV/Vis detector) with a quaternary pump, and on Hewett-Packard 1090 Series II instrument equipped with a quaternary pump, using Phenomenex Lux-amylose-1 and Lux-i-cellulose-5 analytical columns (250 × 4.6 mm). Detection was monitored at 210 and 254 nm. ESI mass spectra were obtained on an Agilent 5973 inert GC/MS system.

Commercially available organic and inorganic compounds were used without further purification. Solvents were dried and stored over microwave-activated 4Å molecular sieves. Enals and 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one were available commercially. The other 2,5-disubstituted pyrazol-3-ones were synthetized by the reaction of proper β-keto esters with hydrazines in refluxing acetic acid.¹ Pyrazolin-4,5-diones **1a–c**,² **1e**³ and triazolium salts used as pre-catalysts **A–E**⁴ were prepared according to literature procedures. The racemic samples of spiropyrazolones were prepared by using an equimolar mixture of both enantiomers of pre-catalyst **B**.

Synthesis of Pyrazolin-4,5-diones **1d** and **1f**.

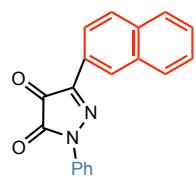


Step one

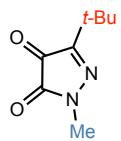
To a solution of the corresponding 2,5-disubstituted 3*H*-pyrazol-3-one (15.59 mmol, 1.0 equiv) in methanol (25 mL) at room temperature was added nitrosobenzene (15.59 mmol, 1.0 equiv) and potassium carbonate (3.12 mmol, 0.2 equiv). The mixture was brought to reflux till TLC indicated the completion of the reaction (*ca* 6 h). The solvent was removed from the reaction mixture and the residue was dissolved in EtOAc. The organic layer was washed with 30 mL of water and dried over anhydrous MgSO₄. Then the organic solvent was removed using a rotary evaporator. The phenylimine was sufficiently pure to proceed to next step.

Step two

In a 50 mL round bottomed flask a solution of 4-(phenylimino)-3*H*-pyrazol-3-one (9.43 mmol, 1 equiv) in THF (0.3M) and HCl 2M solution (47.15 mmol, 5 equiv) was added at room temperature. The reaction was controlled via TLC. After completion of the reaction (16 h), the mixture was diluted with water and the organic layer was extracted three times with dichloromethane. The combined organic layers were dried over anhydrous MgSO₄. The solvent was evaporated in vacuum. Chromatographic purification (hexane/ethyl acetate, 8/1) gave the desired product.



3-(Naphthalen-2-yl)-1-phenyl-1*H*-pyrazole-4,5-dione (1d**).** Black solid (1.8 g, 65% yield). Mp 150–152°C (from hexane/ethyl acetate). **¹H NMR** (500 MHz, CDCl₃) δ 7.34 (tt, *J*= 7.4, 1.1 Hz, 1H), 7.51–7.55 (m, 2H), 7.56–7.62 (m, 2H), 7.88 (dd, *J*= 7.5, 1.6 Hz, 1H), 7.96 (d, *J*= 8.7 Hz, 1H), 7.99 (dd, *J*= 7.2, 1.7 Hz, 1H), 8.02–8.05 (m, 2H), 8.23 (dd, *J*= 8.6, 1.7 Hz, 1H), 8.76 (s, 1H). **¹³C NMR** (126 MHz, CDCl₃) δ 118.1, 122.5, 124.0, 126.6, 127.1, 128.0, 128.3, 129.0, 129.2, 129.3, 129.4, 133.0, 134.7, 136.7, 141.0, 148.9, 184.2. **IR** $\nu_{\text{max}}/\text{cm}^{-1}$ 814, 904, 1051, 1157, 1271, 1297, 1354, 1411, 1491, 1594, 1721, 1758, 3039, 3062. **HRMS** (ESI-TOF) *m/z* calcd for C₁₉H₁₂N₂NaO₂ [M+Na]⁺ 323.0791. Found 323.0786.



3-(*tert*-Butyl)-1-methyl-1*H*-pyrazole-4,5-dione (1f**).** Dark red solid (1.5 g, 94% yield). Mp 60–63°C (from hexane/ethyl acetate). **¹H NMR** (500 MHz, CDCl₃) δ 1.28 (s, 9H), 3.38 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃) δ 27.0, 32.4, 33.3, 150.7, 151.5, 185.3. **IR** ν_{max}/cm⁻¹ 897, 1051, 1084, 1217, 1368, 1461, 1471, 1598, 1685, 1709, 1761, 2929, 2976. **HRMS** (ESI-TOF) m/z calcd for C₈H₁₃N₂O₂ [M+H]⁺ 169.0972. Found 169.0977.

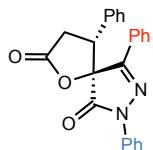
Table S2 Optimization of Reaction Conditions for **1c.^a**

Entry	Base	Solvent	Additive	Yield (%) ^b	dr ^c	er ^d
1	DABCO	Toluene	—	73	>99:<1	73:23
2	DMAP	Toluene	—	46	>99:<1	72:28
3	KOt-Bu	Toluene	—	69	>99:<1	85:15
4 ^e	KOt-Bu	Toluene	—	51	>99:<1	81:19
5	NaOAc	Toluene	—	55	>99:<1	75:25
6	Cs ₂ CO ₃	Toluene	—	38	>99:<1	86:14
7	TBD	Toluene	—	63	>99:<1	87:13
8	TBD	Toluene	LiCl	15	>99:<1	70:30
9	TBD	Toluene	ZnCl ₂	55	>99:<1	84:16
10	TBD	Toluene	MgCl ₂	n.r.	—	—
11	TBD	Toluene	FeCl ₃	n.r.	—	—
12	DIPEA	Toluene	—	69	>99:<1	84:16
13	TBD	Benzene	—	36	>99:<1	89:11
14	TBD	Et ₂ O	—	49	>99:<1	79:21
15	TBD	THF	—	12	>99:<1	79:21
16	TBD	DCM	—	71	>99:<1	84:16
17	TBD	Hexane	—	64	>99:<1	84:16

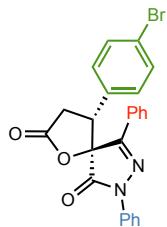
^a Reaction conditions: **1c** (0.06 mmol), **2a** (0.06 mmol), **B** (10 mol%), base (0.5 equiv), Lewis acid (2 equiv), solvent (1 mL), at rt for 16 h. ^b Yield of **3c** after column chromatography. ^c Dr values determined by ¹H NMR. ^d Er values determined via chiral HPLC analysis. ^e 0°C.

General Procedure for Spirocyclic Pyrazolone γ -Butyrolactones.

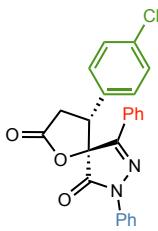
In a dried 5 mL heat gun-dried flask equipped with a magnetic stirring bar the pre-catalyst **A–E** (0.006 mmol, 0.1 equiv) was weighed. Then pyrazolin-4,5-dione **1a–f** (0.06 mmol) and enal **2a–g** (0.06 mmol, 1.0 equiv) were added under a N₂ atmosphere. Dry toluene (1 mL) was added and the mixture was stirred several minutes. Finally, the base (0.03 mmol, 0.5 equiv.) was introduced to the flask. After 16 h, the solvent was straight removed under reduced pressure and the residue was purified by column chromatography (hexane/ethyl acetate, 10/1) to give the desired compound.



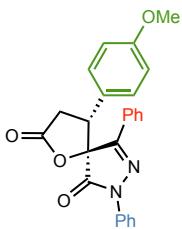
(4R,5S)-4,7,9-Triphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3a). Yellow oil (16.5 mg, 72% yield). $[\alpha]^{25}_D = -101.6$ (c 0.1, CHCl₃, er 86:14). ¹H NMR (500 MHz, CDCl₃) δ 2.93 (dd, *J*= 17.1, 8.2 Hz, 1H), 3.82 (dd, *J*= 14.0, 13.8 Hz, 1H), 4.15 (dd, *J*= 13.8, 8.2 Hz, 1H), 7.11-7.13 (m, 2H), 7.14-7.18 (m, 1H), 7.22-7.31 (m, 5H), 7.43-7.45 (m, 2H), 7.54-7.59 (m, 3H), 7.98-8.00 (m, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 30.3, 49.0, 87.8, 119.5, 126.1, 126.8, 127.6, 128.6, 128.7, 128.8, 129.1, 129.4, 130.5, 131.5, 136.5, 153.2, 168.7, 173.5. IR ν_{max}/cm^{-1} 751, 919, 1076, 1160, 1291, 1308, 1324, 1398, 1452, 1492, 1596, 1720, 1804, 2859, 2927. HRMS (ESI-TOF) m/z: calcd for C₂₄H₁₈N₂NaO₃ [M+Na]⁺ 405.1210. Found 405.1220. HPLC (Lux Amylose-1, n-hexane/2-propanol 70:30, λ = 254 nm, 0.8 mL/min): t_R (minor)= 8.2 min, t_R (major)= 9.8 min, (er 86:14).



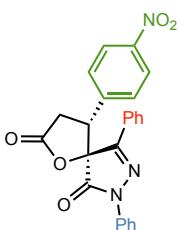
(4R,5S)-4-(4-Bromophenyl)-7,9-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3ab). Yellow oil (12.7 mg, 46% yield). $[\alpha]^{25}_D = -29.2$ (c 0.2, CHCl₃, er 81:19). ¹H NMR (500 MHz, CDCl₃) δ 2.93 (dd, *J*= 17.0, 8.2 Hz, 1H), 3.75 (dd, *J*= 17.0, 13.8 Hz, 1H), 4.11 (dd, *J*= 13.7, 8.1 Hz, 1H), 6.97-7.00 (m, 2H), 7.18-7.22 (m, 1H), 7.32-7.39 (m, 4H), 7.47-7.49 (m, 2H), 7.53-7.59 (m, 3H), 7.95-7.97 (m, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 30.4, 48.4, 87.4, 119.4, 123.3, 126.3, 126.8, 128.6, 128.9, 129.3, 129.5, 129.6, 131.6, 132.0, 136.4, 153.1, 168.4, 173.0. IR ν_{max}/cm^{-1} 1023, 1010, 1047, 1077, 1157, 1328, 1395, 1445, 1492, 1596, 1724, 1807, 2853, 29323, 2957, 3065. HRMS (ESI-TOF) m/z: calcd for C₂₄H₁₇BrN₂NaO₃ [M+Na]⁺ 483.0315. Found 483.0324. HPLC (Lux Amylose-1, n-hexane/2-propanol 90:10, λ = 210 nm, 1 mL/min): t_R (minor)= 15.0 min, t_R (major)= 26.6 min, (er 81:19).



(4R,5S)-4-(4-Chlorophenyl)-7,9-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3ac). White solid (16.9 mg, 64% yield). Mp 188-190°C (from chloroform). $[\alpha]^{25}_{D} = -43.0$ (c 0.4, CHCl_3 , er 81:19). $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 2.94 (dd, $J = 16.9, 8.1$ Hz, 1H), 3.76 (dd, $J = 16.9, 13.7$ Hz, 1H), 4.12 (dd, $J = 13.8, 8.2$ Hz, 1H), 7.05 (d, $J = 8.5$, 2H), 7.18-7.24 (m, 3H), 7.34 (t, $J = 7.6$ Hz, 2H), 7.49 (d, $J = 7.7$ Hz, 2H), 7.53-7.59 (m, 3H), 7.97 (dd, $J = 3.3, 1.6$ Hz, 2H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 30.5, 48.3, 87.5, 119.4, 126.3, 126.8, 128.6, 128.9, 129.0, 129.1, 129.2, 129.5, 131.6, 135.1, 136.4, 153.1, 168.5, 173.0. $\text{IR } \nu_{\text{max}}/\text{cm}^{-1}$ 1157, 1298, 1399, 1445, 1486, 1596, 1720, 1807, 2856, 2923, 2954, 3064. HRMS (ESI-TOF) m/z: calcd for $\text{C}_{24}\text{H}_{17}\text{ClN}_2\text{NaO}_3$ [M+Na]⁺ 439.0820. Found 439.0834. HPLC (Lux i-Cellulose-5, n-hexane/2-propanol 85:15, $\lambda = 210$ nm, 1 mL/min): t_R (minor)= 10.8 min, t_R (major)= 16.7 min, (er 81:19).

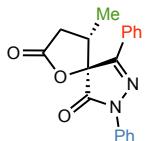


(4R,5S)-4-(4-Methoxyphenyl)-7,9-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3ad). Pale yellow oil (17.6 mg, 71% yield). $[\alpha]^{25}_{D} = -5.9$ (c 0.1, CHCl_3 , er 74:26). $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 2.89 (dd, $J = 17.0, 8.1$ Hz, 1H), 3.68 (s, 3H), 3.74 (dd, $J = 16.8, 13.9$ Hz, 1H), 4.09 (dd, $J = 13.7, 8.0$ Hz, 1H), 6.74 (d, $J = 8.7$ Hz, 2H), 7.02 (d, $J = 8.6$ Hz, 2H), 7.15 (t, $J = 7.3$ Hz, 1H), 7.30 (t, $J = 7.7$ Hz, 2H), 7.48 (d, $J = 8.2$ Hz, 2H), 7.55-7.53 (m, 3H), 7.96 (d, $J = 7.8$ Hz, 2H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 29.7, 48.4, 55.2, 87.9, 114.2, 119.4, 122.2, 126.1, 126.8, 128.7, 128.8, 128.9, 129.4, 129.5, 131.4, 136.6, 153.3, 159.9, 173.5. $\text{IR } \nu_{\text{max}}/\text{cm}^{-1}$ 802, 953, 1063, 1399, 1462, 1496, 1516, 1593, 1613, 1727, 1811, 2859, 2924, 2954. HRMS (ESI-TOF) m/z: calcd for $\text{C}_{25}\text{H}_{20}\text{KN}_2\text{O}_4$ [M+K]⁺ 451.1055. Found 451.1058. HPLC (Lux Amylose-1, n-hexane/2-propanol 90:10, $\lambda = 254$ nm, 1 mL/min): t_R (minor)= 18.1 min, t_R (major)= 29.9 min, (er 74:26).

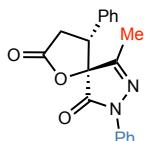


(4R,5S)-4-(4-Nitrophenyl)-7,9-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3ae). Yellow oil (23.9 mg, 93% yield). $[\alpha]^{25}_{D} = -45.8$ (c 0.2, CHCl_3 , er 77:23). $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 3.01 (dd, $J = 16.9, 8.4$ Hz, 1H), 3.83 (dd, $J = 16.9, 13.5$ Hz, 1H), 4.24 (dd, $J = 13.6, 8.1$ Hz, 1H), 7.17 (t, $J = 7.9$ Hz, 1H), 7.28-7.33 (m, 4H), 7.48 (d, $J = 8.1$ Hz, 2H), 7.56-7.61 (m, 3H), 7.98 (dd, $J = 7.1, 1.0$ Hz, 2H), 8.11 (d, $J = 8.6$ Hz, 2H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 30.4, 48.4, 87.1, 119.0, 124.0,

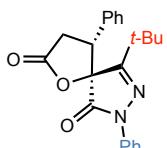
126.4, 126.7, 128.4, 128.8, 129.0, 129.6, 131.9, 136.2, 137.9, 148.2, 152.9, 168.0, 172.3. IR $\nu_{\text{max}}/\text{cm}^{-1}$ 760, 840, 1071, 1164, 1307, 1324, 1344, 1398, 1491, 1524, 1598, 1644, 1725, 1814, 2872, 2946, 3009, 3059. HRMS (ESI-TOF) m/z: calcd for $C_{24}H_{17}N_3NaO_5$ [M+Na]⁺ 450.1060. Found 450.1068. HPLC (Lux Amylose-1, n-hexane/2-propanol 90:10, λ = 210 nm, 1 mL/min): t_R (minor)= 32.5 min, t_R (major)= 51.1 min, (er 77:23).



(*4S,5S*)-4-Methyl-7,9-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (**3ag**). Pale yellow oil (11.9 mg, 62% yield). $[\alpha]^{25}_D = -70.5$ (c 0.1, CHCl₃, er 80:20). ¹H NMR (500 MHz, CDCl₃) δ 1.12 (d, J = 5.8 Hz, 3H), 2.75 (dd, J = 22.7, 14.1 Hz, 1H), 3.02-2.96 (m, 2H), 7.27 (t, J = 7.6 Hz, 1H), 7.44-7.52 (m, 5H), 7.91 (d, J = 6.9 Hz, 2H), 7.95 (d, J = 8.6 Hz, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 12.6, 33.1, 38.7, 87.6, 118.9, 126.0, 126.7, 128.5, 129.1, 129.2, 131.4, 137.2, 153.9, 169.0, 174.0. IR $\nu_{\text{max}}/\text{cm}^{-1}$ 1338, 1409, 1452, 1492, 1596, 1714, 1811, 2850, 2927, 2967. HRMS (ESI-TOF) m/z: calcd for $C_{19}H_{16}N_2NaO_3$ [M+Na]⁺ 343.1053. Found 343.1059. HPLC (Lux i-Cellulose-5, n-hexane/2-propanol 95:5, λ = 210 nm, 0.8 mL/min): t_R (minor)= 48.0 min, t_R (major)= 54.1 min, (er 80:20).

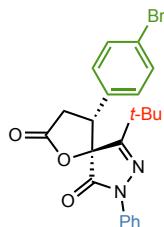


(*4R,5S*)-9-Methyl-4,7-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (**3b**). Yellow oil (9.4 mg, 49% yield). **Major diastereomer:** $[\alpha]^{25}_D = +48.0$ (c 2.0, EtOAc, er 1.5:98.5) for (*4S,5R*) enantiomer,⁵ $[\alpha]^{25}_D = -161.5$ (c 0.2, EtOAc, er 81:19) for (*4R,5S*) enantiomer. ¹H NMR (500 MHz, CDCl₃) δ 2.37 (s, 3H), 2.90 (dd, J = 16.8, 7.9 Hz, 1H), 3.76 (dd, J = 16.8, 13.7 Hz, 1H), 3.98 (dd, J = 13.6, 7.8 Hz, 1H), 7.12 (tt, J = 7.3, 1.2 Hz, 1H), 7.22-7.32 (m, 7H), 7.37 (dd, J = 8.8, 1.3 Hz, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 12.9, 30.6, 47.3, 87.3, 119.1, 125.8, 127.4, 128.7, 129.0, 129.1, 130.6, 136.5, 155.7, 168.3, 173.4. IR $\nu_{\text{max}}/\text{cm}^{-1}$ 1120, 1157, 1371, 1408, 1455, 1499, 1596, 1726, 1804, 2853, 2920, 2957, 2997, 3031, 3054. HRMS (ESI-TOF) m/z: calcd for $C_{19}H_{16}N_2NaO_3$ [M+Na]⁺ 343.1053. Found 343.1061. HPLC (Lux Amylose-1, n-hexane/2-propanol 80:20, λ = 254 nm, 0.6 mL/min): t_R (minor)= 15.9 min, t_R (major)= 19.2 min, (er 81:19).

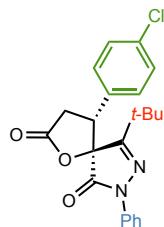


(*4R,5S*)-9-(tert-Butyl)-4,7-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (**3c**). Yellow oil (13.7 mg, 63% yield). $[\alpha]^{25}_D = -150.5$ (c 0.2, CHCl₃, er 87:13). ¹H NMR (500 MHz, CDCl₃) δ 1.52 (s, 9H), 2.86 (dd, J = 17.0, 8.4 Hz, 1H), 3.73 (dd, J = 17.0, 13.4 Hz, 1H), 4.40 (dd, J = 13.4, 8.4 Hz, 1H), 7.10 (m, 1H), 7.21-7.23 (m, 2H), 7.24-7.26 (m, 5H), 7.32-7.36 (m, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 29.3, 30.1, 36.6, 47.2, 89.1, 119.0, 125.6, 127.3, 128.6, 128.8, 128.9, 131.2, 136.5, 163.7, 168.8, 173.4. IR $\nu_{\text{max}}/\text{cm}^{-1}$ 684, 757, 890, 1087, 1107, 1381, 1494, 1598, 1718, 1761, 1805, 2925, 2969, 3029. HRMS (ESI-TOF) m/z: calcd for $C_{22}H_{23}N_2O_3$ [M+H]⁺ 363.1703. Found 363.1709. HPLC (Lux i-

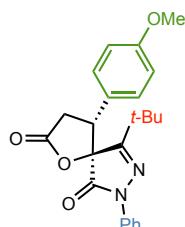
Cellulose-5, n-hexane/2-propanol 80:20, $\lambda = 254$ nm, 0.8 mL/min): t_R (minor)= 16.6 min, t_R (major)= 21.5 min, (er 87:13).



(4R,5S)-4-(4-Bromophenyl)-9-(tert-butyl)-7-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3cb). White solid (15.4 mg, 58% yield). Mp > 300°C (from hexane). $[\alpha]^{25}_D = -93.6$ (c 0.1, CHCl₃, er 93:7). **¹H NMR** (500 MHz, CDCl₃) δ 1.49 (s, 9H), 2.86 (dd, $J = 16.9, 8.3$ Hz, 1H), 3.66 (dd, $J = 16.8, 13.2$ Hz, 1H), 4.34 (dd, $J = 13.6, 8.6$ Hz, 1H), 7.16-7.10 (m, 3H), 7.31-7.27 (m, 2H), 7.41-7.36 (m, 4H). **¹³C NMR** (126 MHz, CDCl₃) δ 29.3, 30.2, 36.7, 46.7, 88.7, 119.0, 123.1, 125.9, 128.8, 129.0, 130.3, 132.0, 136.4, 163.7, 168.6, 172.9. **IR** ν_{max}/cm^{-1} 896, 1010, 1083, 1114, 1187, 1382, 1496, 1596, 1724, 1811, 2860, 2874, 2931, 2968. **HRMS** (ESI-TOF) m/z: calcd for C₂₂H₂₁BrN₂NaO₃ [M+Na]⁺ 463.0628. Found 463.0638. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 80:20, $\lambda = 254$ nm, 0.8 mL/min): t_R (minor)= 16.5 min, t_R (major)= 23.7 min, (er 93:7).

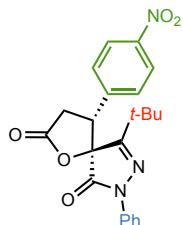


(4R,5S)-9-(tert-Butyl)-4-(4-chlorophenyl)-7-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3cc). Yellow oil (15.7 mg, 66% yield). $[\alpha]^{25}_D = -99.4$ (c 0.3, CHCl₃, er 92:8). **¹H NMR** (500 MHz, CDCl₃) δ 1.49 (s, 9H), 2.87 (dd, $J = 17.1, 8.5$ Hz, 1H), 3.67 (dd, $J = 16.9, 13.4$ Hz, 1H), 4.36 (dd, $J = 13.4, 8.4$ Hz, 1H), 7.12-7.18 (m, 3H), 7.24-7.30 (m, 4H), 7.36-7.39 (m, 2H). **¹³C NMR** (126 MHz, CDCl₃) δ 29.3, 30.3, 36.7, 46.7, 88.8, 118.9, 125.8, 128.8, 129.0, 129.8, 135.0, 136.4, 163.7, 168.7, 173.0. **IR** ν_{max}/cm^{-1} 691, 899, 1020, 1114, 1187, 1385, 1499, 1596, 1720, 1808, 2870, 2931, 2967. **HRMS** (ESI-TOF) m/z: calcd for C₂₂H₂₁ClN₂NaO₃ [M+Na]⁺ 419.1133. Found 419.1139. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 90:10, $\lambda = 254$ nm, 0.8 mL/min): t_R (minor)= 24.5 min, t_R (major)= 36.4 min, (er 92:8).

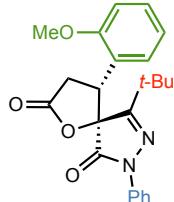


(4R,5S)-9-(tert-Butyl)-4-(4-methoxyphenyl)-7-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3cd). Pale yellow oil (16.5 mg, 70% yield). $[\alpha]^{25}_D = -56.2$ (c 0.4, CHCl₃, er 85:15). **¹H NMR** (500 MHz, CDCl₃) δ 1.49 (s, 9H), 2.83 (dd, $J = 16.9, 8.3$ Hz, 1H), 3.67 (dd, $J = 17.0, 13.5$ Hz, 1H), 3.68 (s, 3H), 4.35 (dd, $J = 13.3, 8.5$ Hz, 1H), 6.75-6.79 (m, 2H), 7.11 (tt, $J = 7.4, 1.1$ Hz, 1H), 7.15-7.18

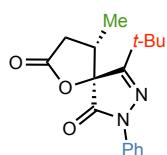
(m, 2H), 7.23-7.28 (m, 2H), 7.37-7.39 (m, 2H). **¹³C NMR** (126 MHz, CDCl₃) δ 29.3, 30.4, 36.6, 46.8, 55.2, 89.2, 114.2, 119.0, 123.0, 125.6, 128.6, 128.7, 136.6, 159.9, 163.8, 169.0, 173.5. **IR v_{max}/cm⁻¹** 1757, 894, 1111, 1187, 1237, 1271, 1384, 1494, 1594, 1611, 1721, 1805, 2872, 2932, 2966, 3083. **HRMS** (ESI-TOF) m/z: calcd for C₂₃H₂₄N₂NaO₄ [M+Na]⁺ 415.1628. Found 415.1630. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 95:5, λ= 254 nm, 1 mL/min): t_R (minor)= 53.7 min, t_R (major)= 79.2 min, (er 85:15).



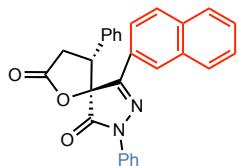
(4R,5S)-9-(tert-Butyl)-4-(4-nitrophenyl)-7-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3ce). Yellow oil (12.5 mg, 51% yield). [α]²⁵_D= -194.3 (c 0.3, CHCl₃, er 94:6). **¹H NMR** (500 MHz, CDCl₃) δ 1.52 (s, 9H), 2.95 (dd, J= 16.8, 8.5 Hz, 1H), 3.74 (dd, J= 17.1, 13.6 Hz, 1H), 4.47 (dd, J= 13.3, 8.5 Hz, 1H), 7.10-7.14 (m, 1H), 7.24-7.27 (m, 2H), 7.37-7.43 (m, 5H), 8.12-8.14 (m, 2H). **¹³C NMR** (126 MHz, CDCl₃) δ 29.2, 30.1, 36.8, 46.8, 88.4, 118.5, 123.9, 126.0, 128.5, 128.8, 138.2, 138.7, 148.0, 163.6, 168.2, 172.2. **IR v_{max}/cm⁻¹** 754, 894, 1111, 1184, 1348, 1494, 1517, 1494, 1517, 1594, 1721, 1811, 2869, 2929, 2962, 3079. **HRMS** (ESI-TOF) m/z: calcd for C₂₂H₂₀N₃O₅ [M+H]⁺ 406.1408. Found 406.1411. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 80:20, λ= 254 nm, 0.8 mL/min): t_R (minor)= 30.9 min, t_R (major)= 42.2 min, (er 94:6).



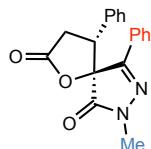
(4R,5S)-9-(tert-Butyl)-4-(2-methoxyphenyl)-7-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3cf). Pale yellow oil (5.4 mg, 23% yield). [α]²⁵_D= -204.9 (c 0.1, CHCl₃, er 77:23). **¹H NMR** (500 MHz, CDCl₃) δ 1.46 (s, 9H), 2.79 (dd, J= 17.2, 8.6 Hz, 1H), 3.64 (dd, J= 17.2, 13.5 Hz, 1H), 3.79 (s, 3H), 4.91 (dd, J= 13.6, 8.6 Hz, 1H), 6.78 (dd, J= 9.2, 0.8 Hz, 1H), 6.90 (dt, J= 7.7, 1 Hz, 1H), 7.08 (tt, J= 7.1, 1.1 Hz, 1H), 7.18 (td, J= 7.6, 1.6 Hz, 1H), 7.21-7.25 (m, 2H), 7.32-7.34 (m, 2H), 7.42 (d, J= 7.8, 1.6 Hz, 1H). **¹³C NMR** (126 MHz, CDCl₃) δ 28.4, 30.5, 36.7, 40.4, 55.1, 89.1, 110.4, 119.0, 119.6, 120.7, 125.4, 127.8, 128.6, 129.8, 137.0, 157.6, 165.5, 169.5, 174.0. **IR v_{max}/cm⁻¹** 745, 899, 1020, 1083, 1114, 1187, 1244, 1288, 1358, 1382, 1462, 1496, 1600, 1720, 1808, 2850, 2964. **HRMS** (ESI-TOF) m/z: calcd for C₂₃H₂₄N₂NaO₄ [M+Na]⁺ 415.1628. Found 415.1628. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 80:20, λ= 254 nm, 0.8 mL/min): t_R (minor)= 19.5 min, t_R (major)= 23.7 min, (er 77:23).



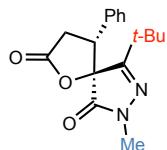
(4S,5S)-9-(tert-Butyl)-4-methyl-7-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (**3cg**).
 Pale yellow oil (10.5 mg, 58% yield). $[\alpha]^{25}_{D} = -123.8$ (c 0.3, CHCl_3 , er 92:8). **$^1\text{H NMR}$** (500 MHz, CDCl_3) δ 1.14 (d, $J = 7.3$ Hz, 9H), 2.66 (dd, $J = 16.9, 8.0$ Hz, 1H), 2.99 (dd, $J = 17.0, 12.0$ Hz, 1H), 3.14-3.25 (m, 1H), 7.22 (t, $J = 8.5$ Hz, 1H), 7.41 (t, $J = 8.3$ Hz, 2H), 7.85 (d, $J = 9.8$ Hz, 2H). **$^{13}\text{C NMR}$** (126 MHz, CDCl_3) δ 12.5, 29.0, 32.7, 36.3, 37.3, 88.7, 118.6, 125.6, 129.0, 137.2, 164.0, 169.0, 174.0. **IR** $\nu_{\text{max}}/\text{cm}^{-1}$ 1305, 1382, 1499, 1596, 1720, 1804, 2877, 2907, 2934, 2974. **HRMS** (ESI-TOF) m/z: calcd for $\text{C}_{17}\text{H}_{20}\text{N}_2\text{NaO}_3$ [M+Na]⁺ 323.1366. Found 323.1371. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 98:2, $\lambda = 210$ nm, 1 mL/min): t_R (major)= 45.4 min, t_R (minor)= 51.2 min, (er 92:8).



(4R,5S)-9-(Naphthalen-2-yl)-4,7-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (**3d**).
 Yellow oil (11.7 mg, 45% yield). $[\alpha]^{25}_{D} = -33.9$ (c 0.2, CHCl_3 , er 81:19). **$^1\text{H NMR}$** (500 MHz, CDCl_3) δ 2.99 (dd, $J = 17.1, 8.1$ Hz, 1H), 3.86 (dd, $J = 17.0, 13.8$ Hz, 1H), 4.26 (dd, $J = 11.9, 6.6$ Hz, 1H), 7.11-7.13 (m, 2H), 7.18 (t, $J = 7.4$ Hz, 1H), 7.23-7.26 (m, 2H), 7.32 (t, $J = 1.3$ Hz, 3H), 7.47 (dd, $J = 8.8, 1.2$ Hz, 2H), 7.59-7.65 (m, 2H), 7.92-7.94 (m, 1H), 7.98-8.02 (m, 2H), 8.12 (dd, $J = 8.6, 1.7$ Hz, 1H), 8.38 (br, 1H). **$^{13}\text{C NMR}$** (126 MHz, CDCl_3) δ 30.3, 49.4, 88.0, 119.6, 123.1, 126.1, 126.2, 127.2, 127.3, 127.6, 128.0, 128.1, 128.8, 128.9, 129.0, 129.1, 129.5, 130.4, 133.0, 134.5, 136.5, 153.1, 168.7, 173.6. **IR** $\nu_{\text{max}}/\text{cm}^{-1}$ 755, 775, 1164, 1362, 1459, 1502, 1600, 1723, 1804, 2927, 2947. **HRMS** (ESI-TOF) m/z: calcd for $\text{C}_{28}\text{H}_{20}\text{N}_2\text{NaO}_3$ [M+Na]⁺ 455.1366. Found 455.1360. **HPLC** (Lux i-Cellulose-5, n-hexane/2-propanol 80:20, $\lambda = 254$ nm, 0.6 mL/min): t_R (major)= 35.0 min, t_R (minor)= 47.1 min, (er 81:19).

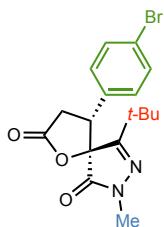


(4R,5S)-7-Methyl-4,9-diphenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (**3e**). Pale yellow oil (12.5 mg, 65% yield). $[\alpha]^{25}_{D} = -81.1$ (c 0.3, CHCl_3 , er 80:20). **$^1\text{H NMR}$** (500 MHz, CDCl_3) δ 7.86-7.88 (m, 2H), 7.50-7.53 (m, 3H), 7.27-7.31 (m, 3H), 7.04-7.06 (m, 2H), 4.05 (dd, $J = 13.8, 8.0$ Hz, 1H), 3.75 (dd, $J = 16.9, 13.9$ Hz, 1H), 2.96 (s, 1H), 2.86 (dd, $J = 16.9, 8.0$ Hz, 1H). **$^{13}\text{C NMR}$** (126 MHz, CDCl_3) δ 30.3, 31.2, 48.6, 87.1, 126.5, 127.6, 128.7, 128.9, 129.0, 129.3, 130.8, 131.1, 152.6, 170.1, 173.6. **IR** $\nu_{\text{max}}/\text{cm}^{-1}$ 758, 859, 973, 1036, 1164, 1395, 1452, 1496, 1717, 1801, 2931, 2994, 3031, 3068. **HRMS** (ESI-TOF) m/z: calcd for $\text{C}_{19}\text{H}_{16}\text{N}_2\text{NaO}_3$ [M+Na]⁺ 343.1053. Found 343.1059. **HPLC** (Lux Amylose-1, n-hexane/2-propanol 90:10, $\lambda = 254$ nm, 0.8 mL/min): t_R (minor)= 14.6 min, t_R (major)= 18.1 min, (er 80:20).



(4R,5S)-9-(tert-Butyl)-7-methyl-4-phenyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3f).

Pale yellow oil (10.5 mg, 58% yield). $[\alpha]^{25}_{D} = -122.8$ (c 0.2, CHCl_3 , er 84:16). $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 1.42 (s, 9H), 2.80 (s, 3H), 2.81 (dd, $J = 16.8, 8.3$ Hz, 1H), 3.67 (dd, $J = 16.8, 13.6$ Hz, 1H), 4.30 (dd, $J = 13.6, 8.2$ Hz, 1H), 7.18-7.20 (m, 2H), 7.31-7.33 (m, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 29.2, 30.1, 30.7, 36.3, 46.9, 88.4, 127.4, 128.7, 128.8, 131.6, 163.0, 170.3, 173.6. $\text{IR } \nu_{\text{max}}/\text{cm}^{-1}$ 1047, 1117, 1184, 1221, 1281, 1365, 1409, 1459, 1707, 1808, 2860, 2961. HRMS (ESI-TOF) m/z: calcd for $\text{C}_{17}\text{H}_{20}\text{N}_2\text{NaO}_3$ [M+Na] $^+$ 323.1366. Found 323.1371. HPLC (Lux i-Cellulose-5, n-hexane/2-propanol 80:20, $\lambda = 210$ nm, 0.8 mL/min): t_R (minor)= 24.8 min, t_R (major)= 74.8 min, (er 84:16).

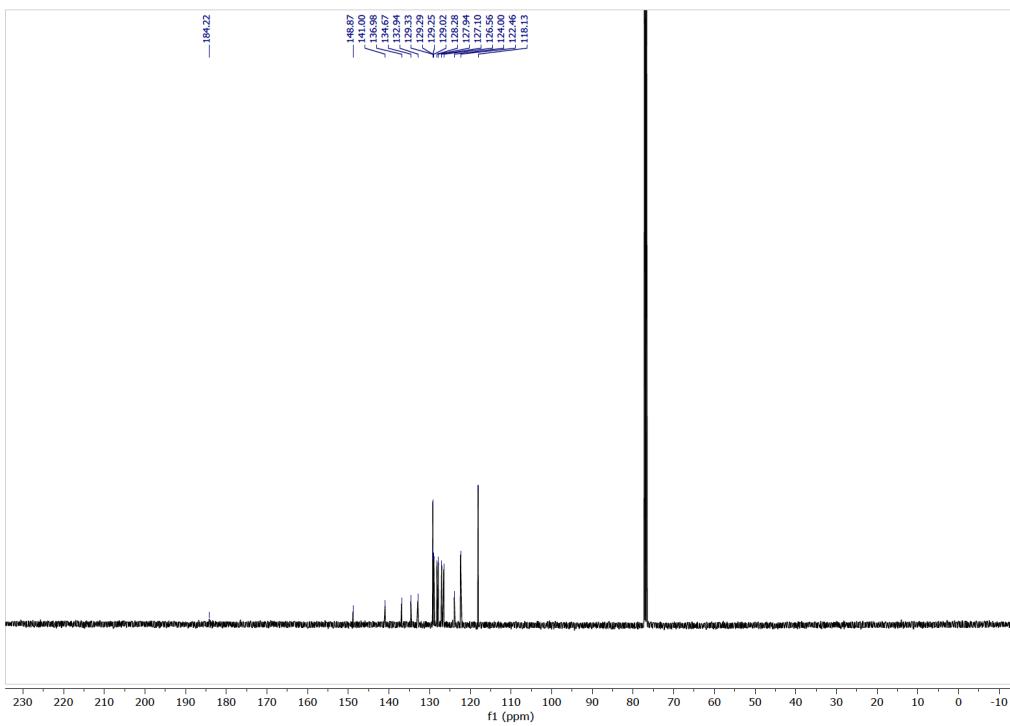
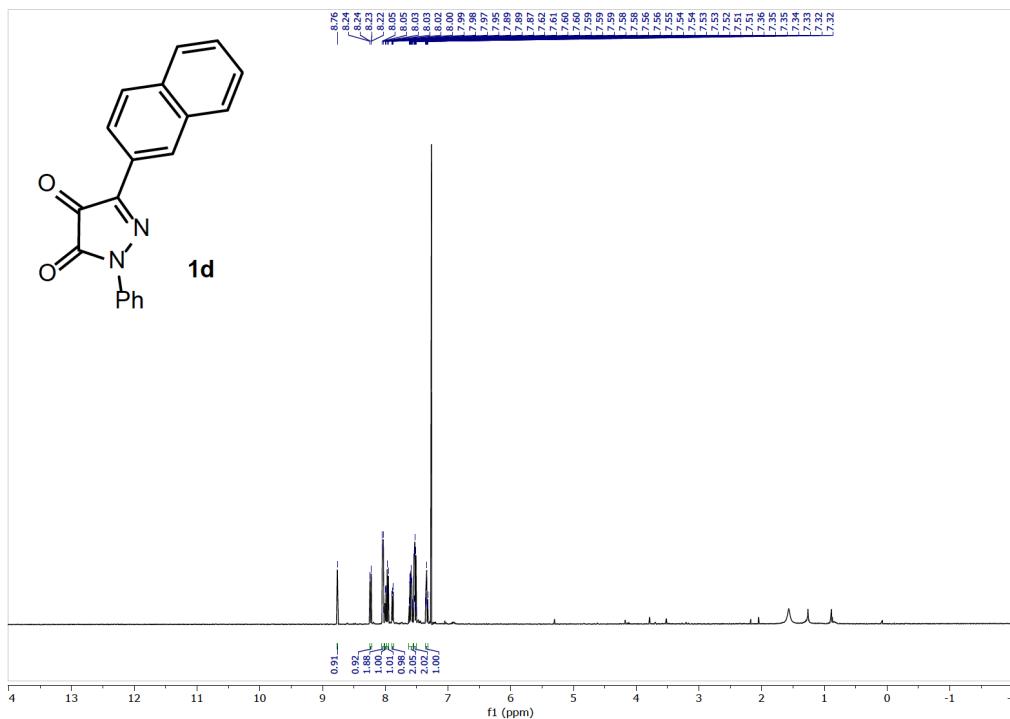


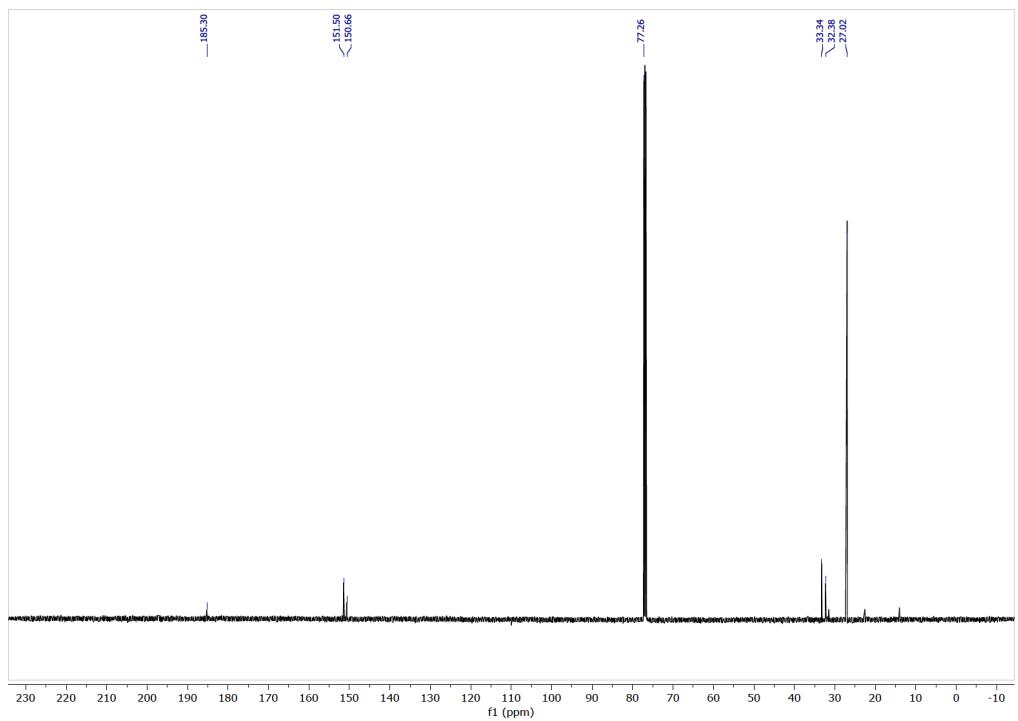
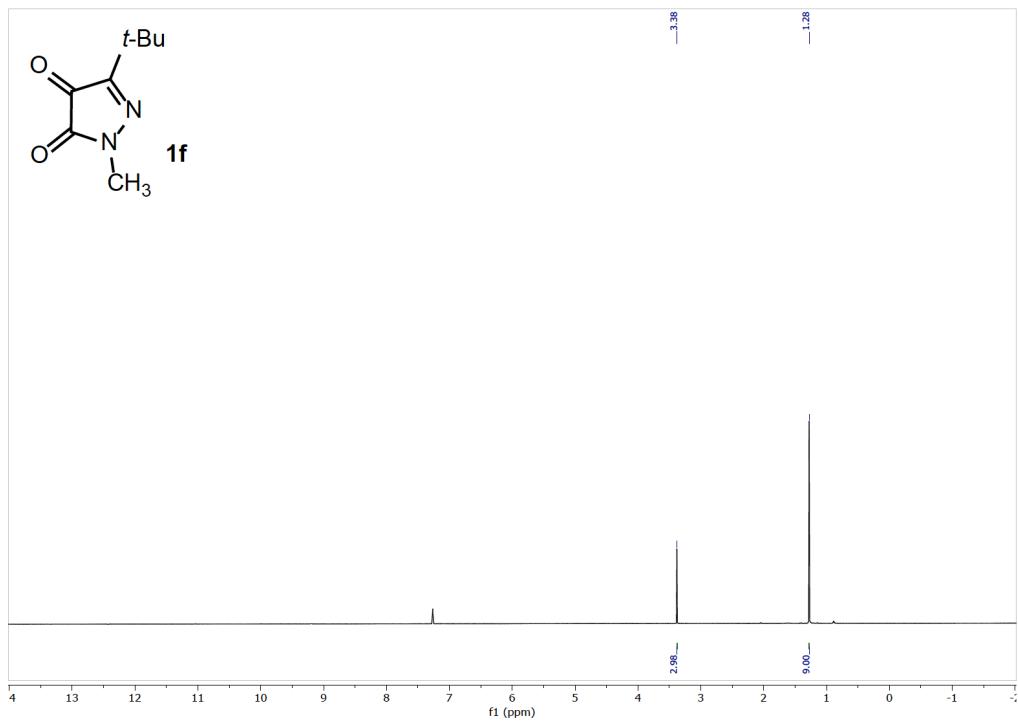
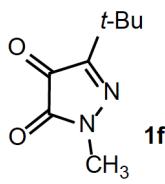
(4R,5S)-4-(4-Bromophenyl)-9-(tert-butyl)-7-methyl-1-oxa-7,8-diazaspiro[4.4]non-8-ene-2,6-dione (3fb). Yellow oil (16.2 mg, 71% yield). $[\alpha]^{25}_{D} = -108.6$ (c 0.4, CHCl_3 , er 90:10). $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 1.40 (s, 9H), 2.79 (dd, $J = 15.7, 8.1$ Hz, 1H), 2.85 (s, 3H), 3.60 (dd, $J = 15.8, 11.2$ Hz, 1H), 4.24 (dd, $J = 16.3, 8.6$ Hz, 1H), 7.07 (d, $J = 8.2$ Hz, 2H), 7.46 (d, $J = 8.5$ Hz, 2H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 29.2, 30.2, 30.9, 36.3, 46.3, 88.0, 122.9, 129., 130.7, 131.9, 162.9, 170.2, 173.0. $\text{IR } \nu_{\text{max}}/\text{cm}^{-1}$ 1047, 1114, 1181, 1211, 1419, 1462, 1492, 1720, 1801, 2870, 2921, 2967. HRMS (ESI-TOF) m/z: calcd for $\text{C}_{17}\text{H}_{19}\text{BrN}_2\text{NaO}_3$ [M+Na] $^+$ 401.0471. Found 401.0480. HPLC (Lux i-Cellulose-5, n-hexane/2-propanol 80:20, $\lambda = 210$ nm, 0.8 mL/min): t_R (minor)= 23.1 min, t_R (major)= 66.1 min, (er 90:10).

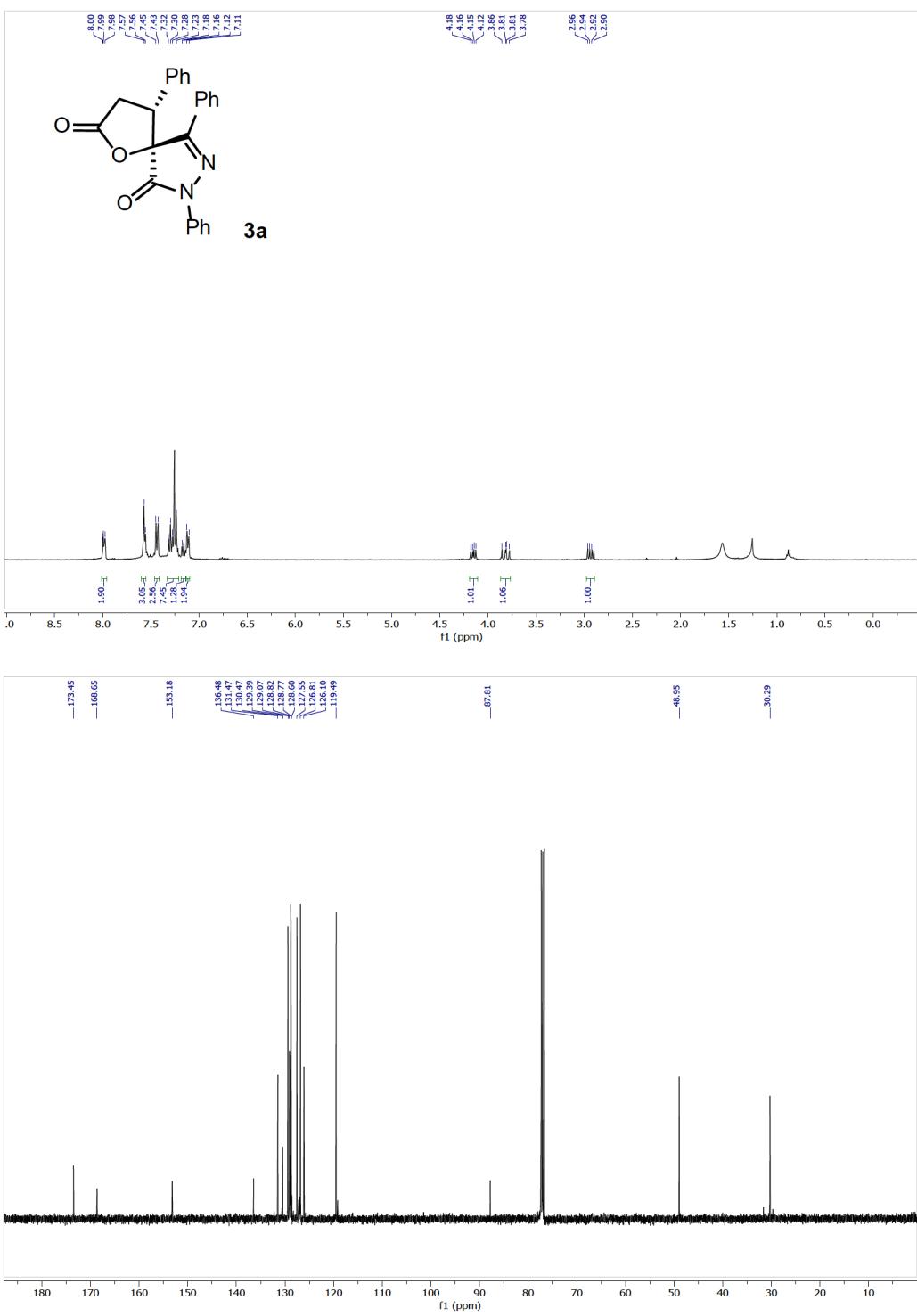
References and Notes

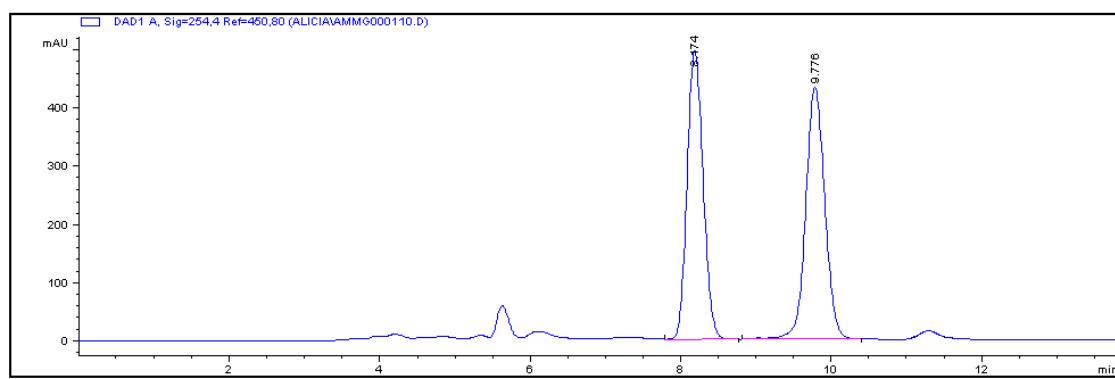
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Copies of ^1H NMR, ^{13}C NMR Spectra and HPLC Profiles

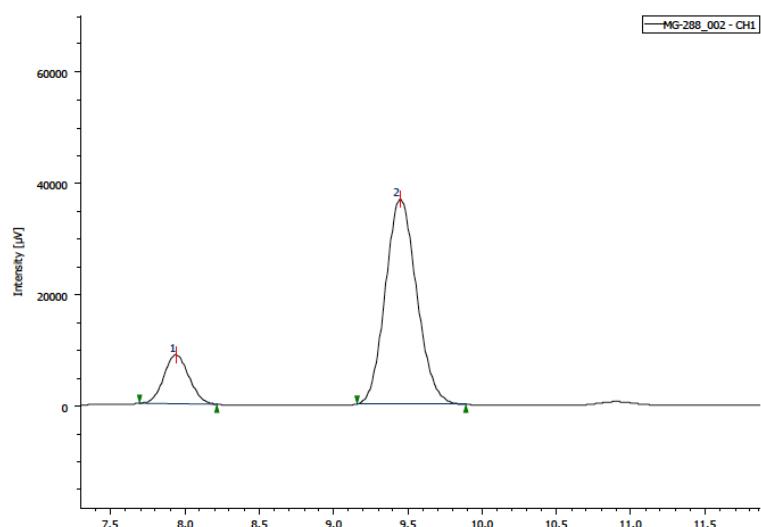




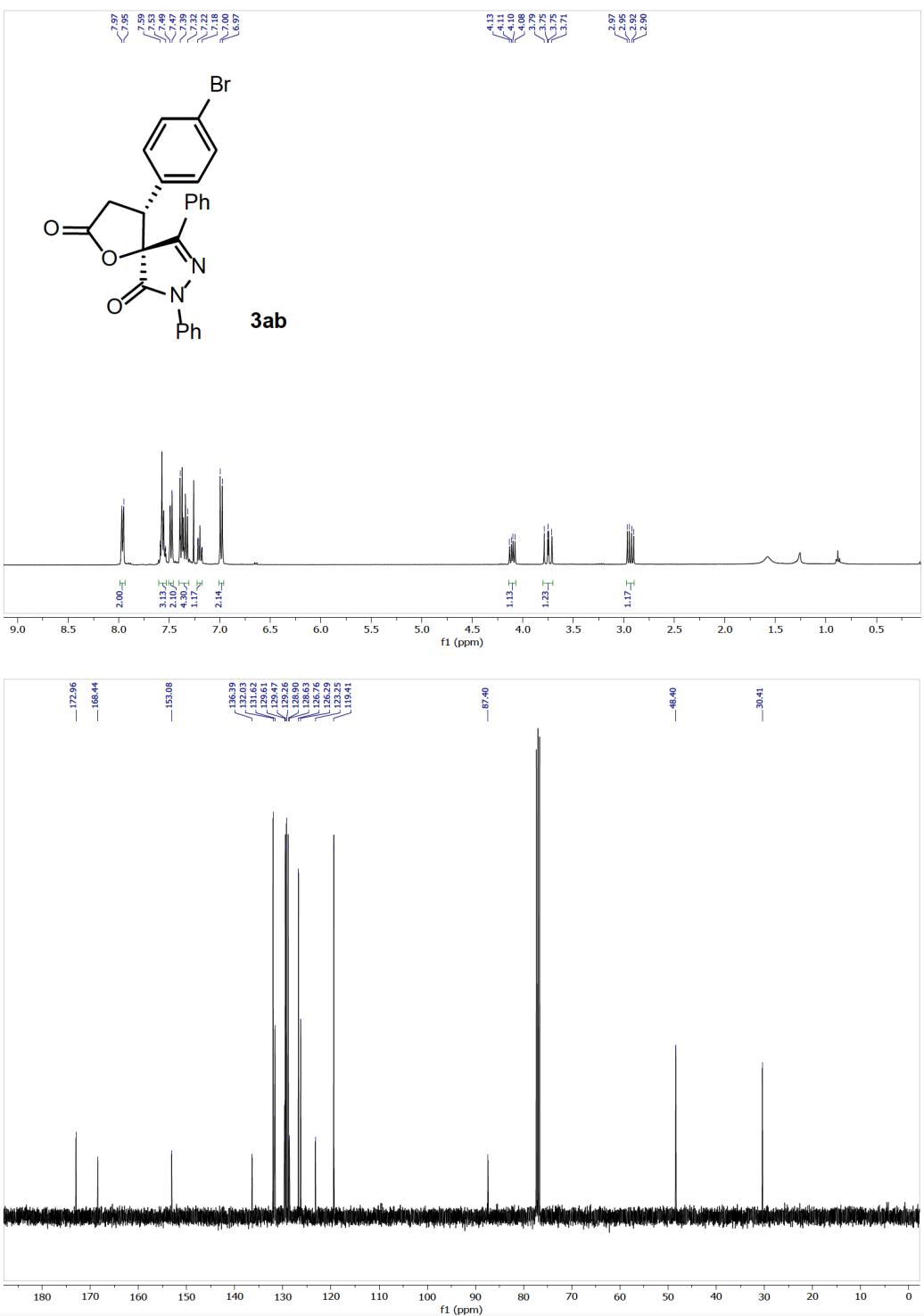


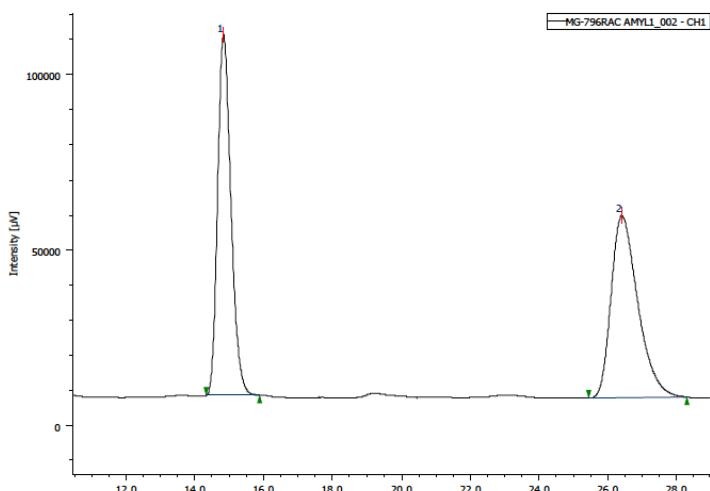


	Time	Area	Area%
1	8.174	7428.8	49.132
2	9.776	7691.5	50.868

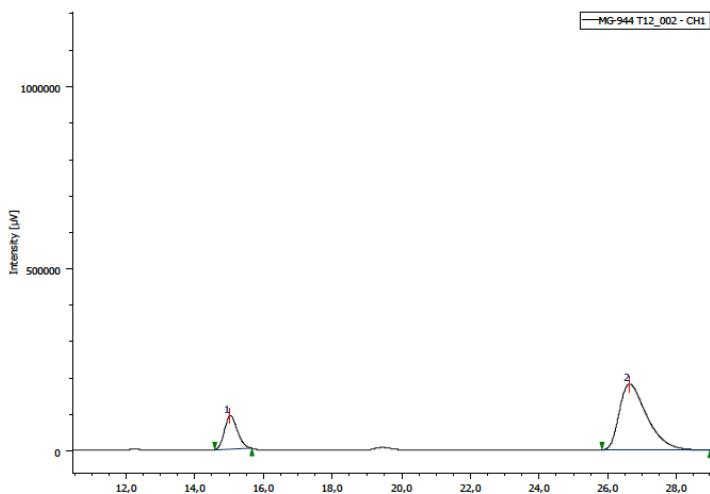


	Time	Area	Area%
1	7,942	103451	16,117
2	9,442	538427	83,883

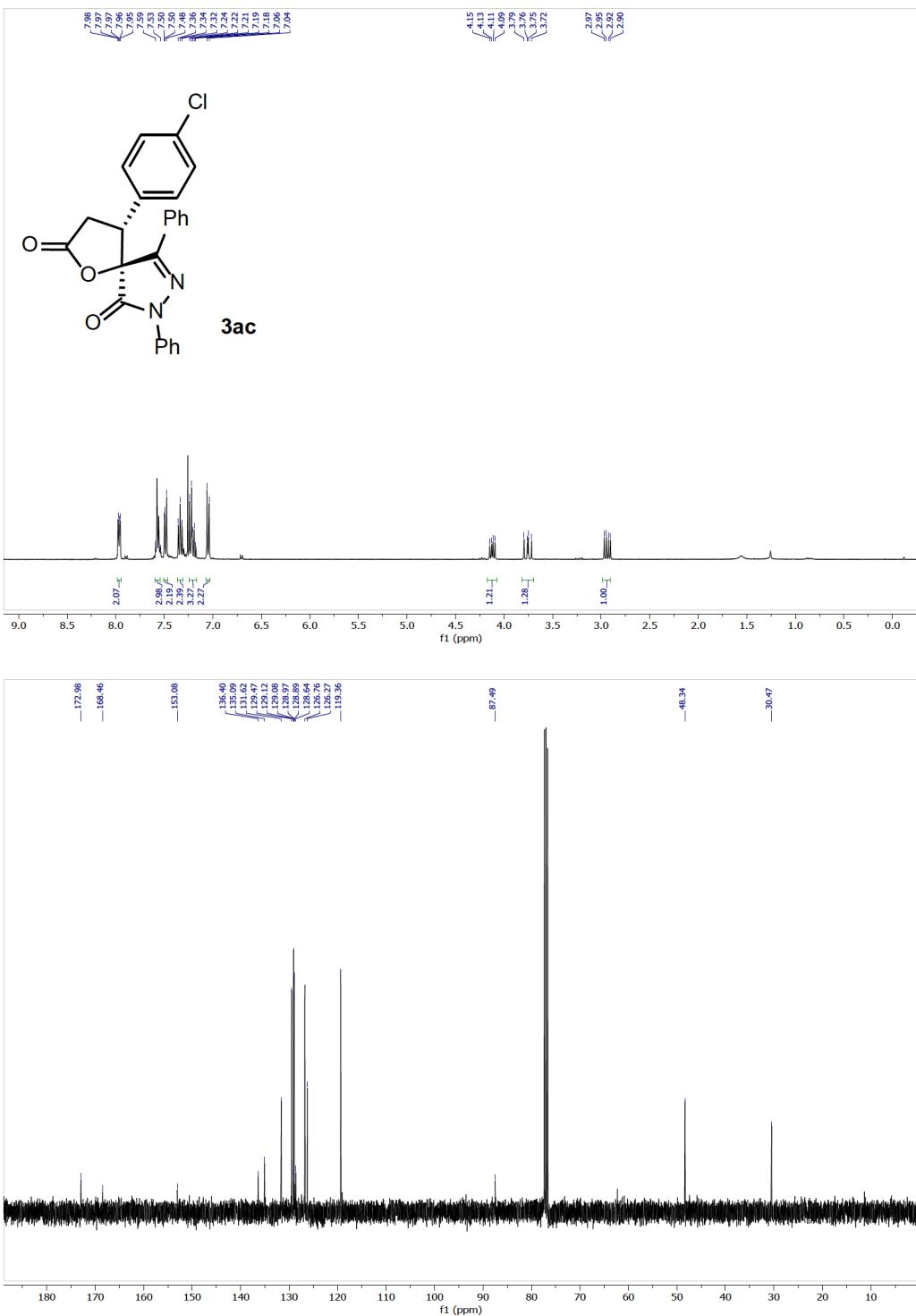


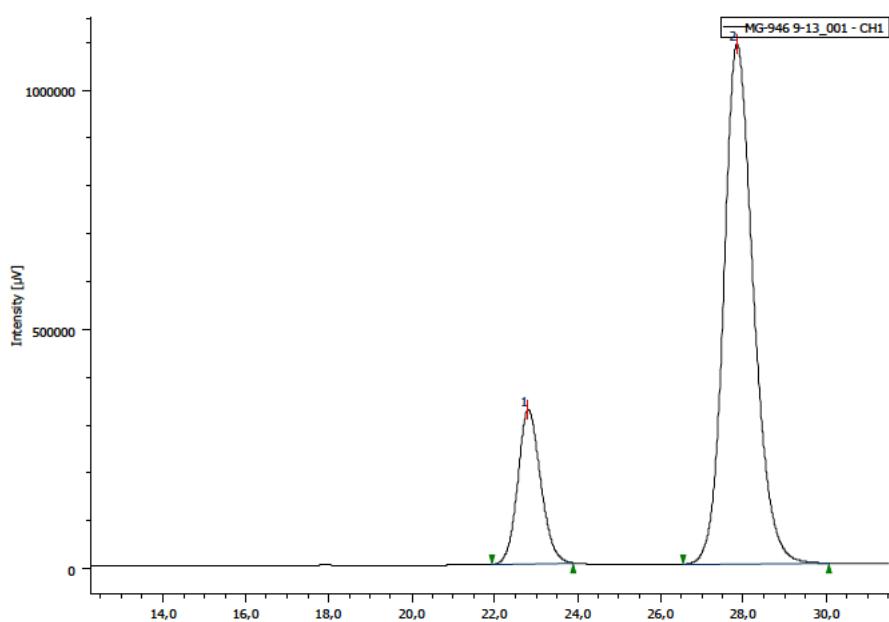
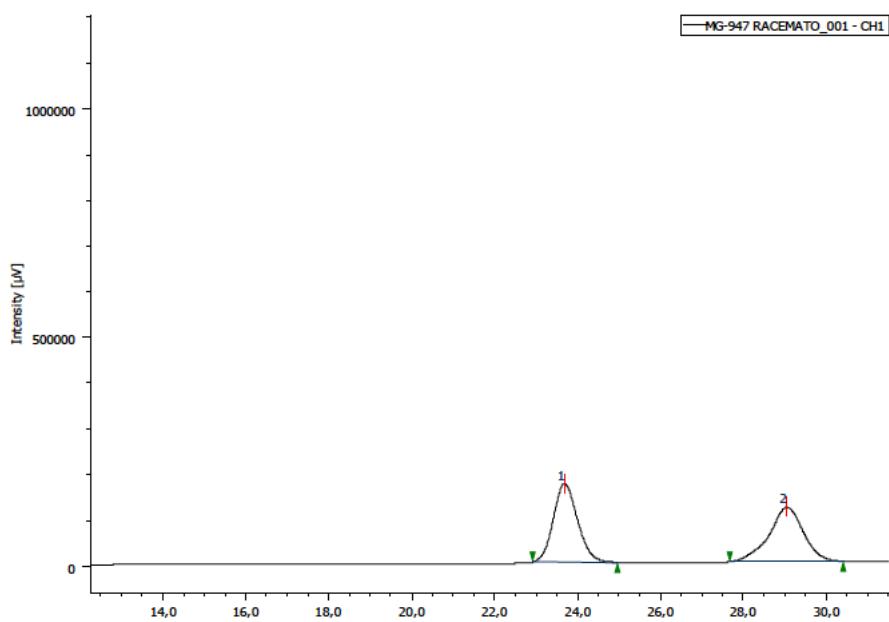


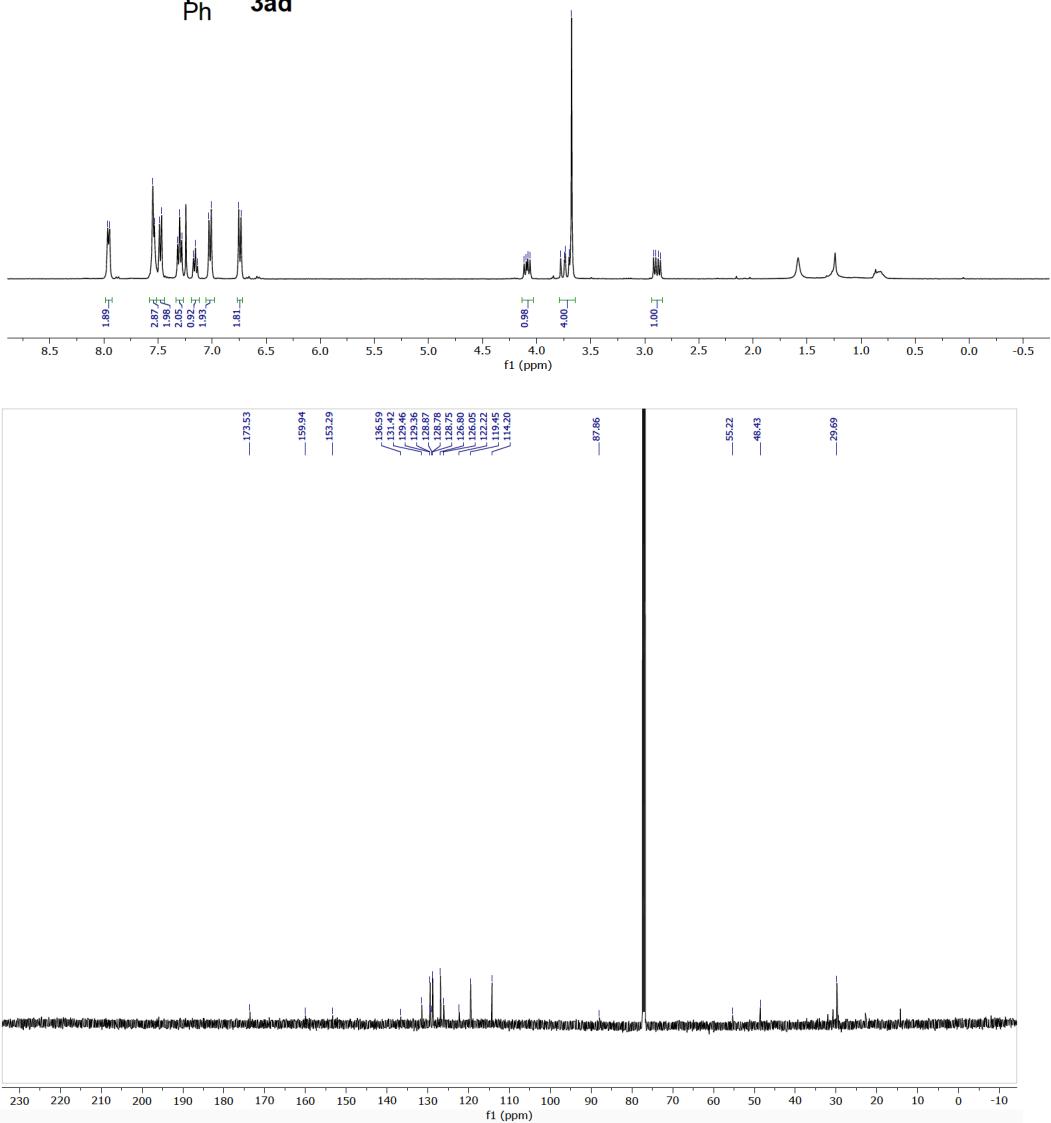
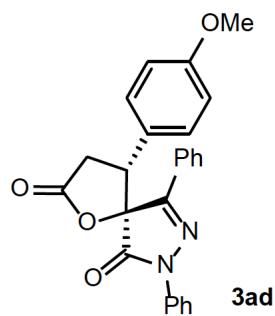
	Time	Area	Area%
1	14,825	2750882	49,471
2	26,383	2809734	50,529

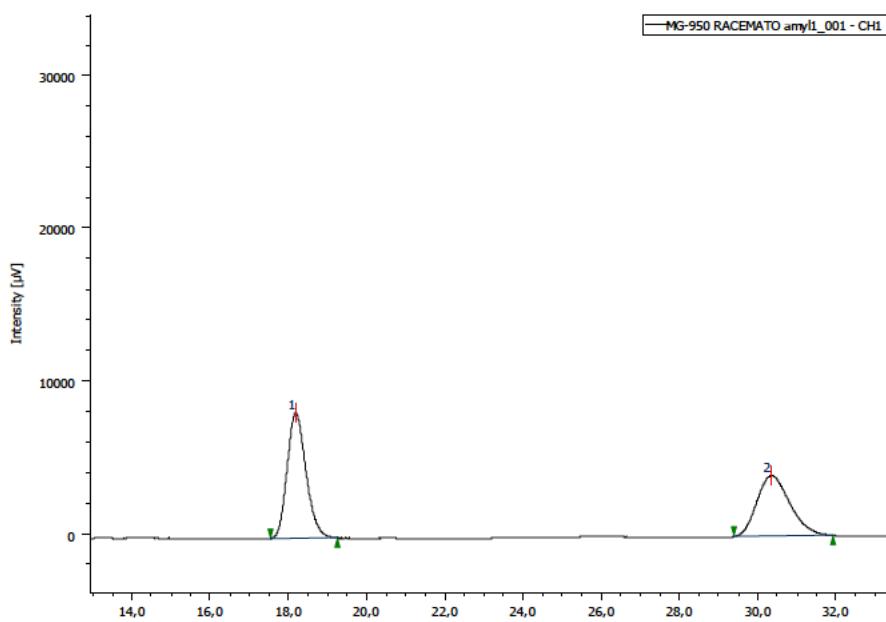


	Time	Area	Area%
1	15,025	2397865	19,287
2	26,608	10034772	80,713

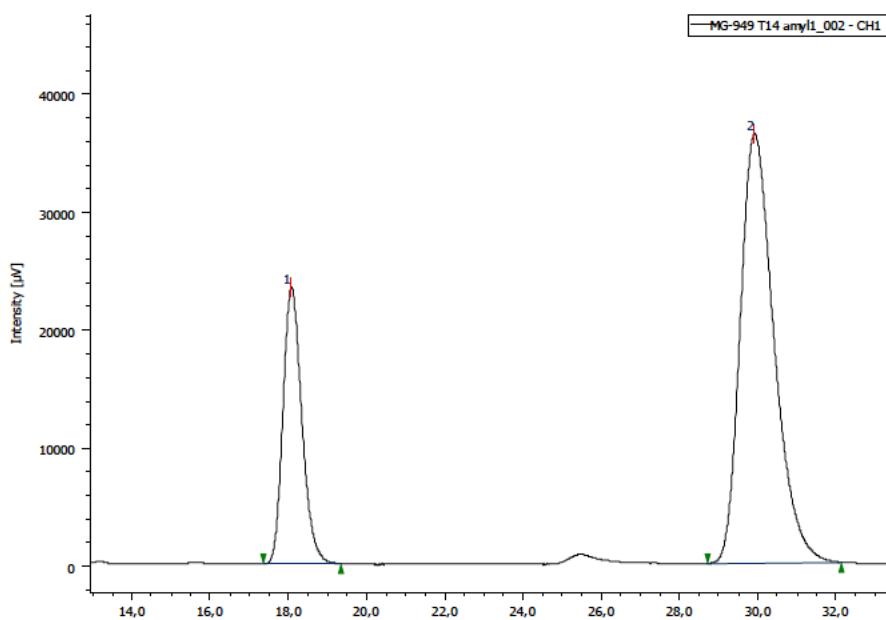




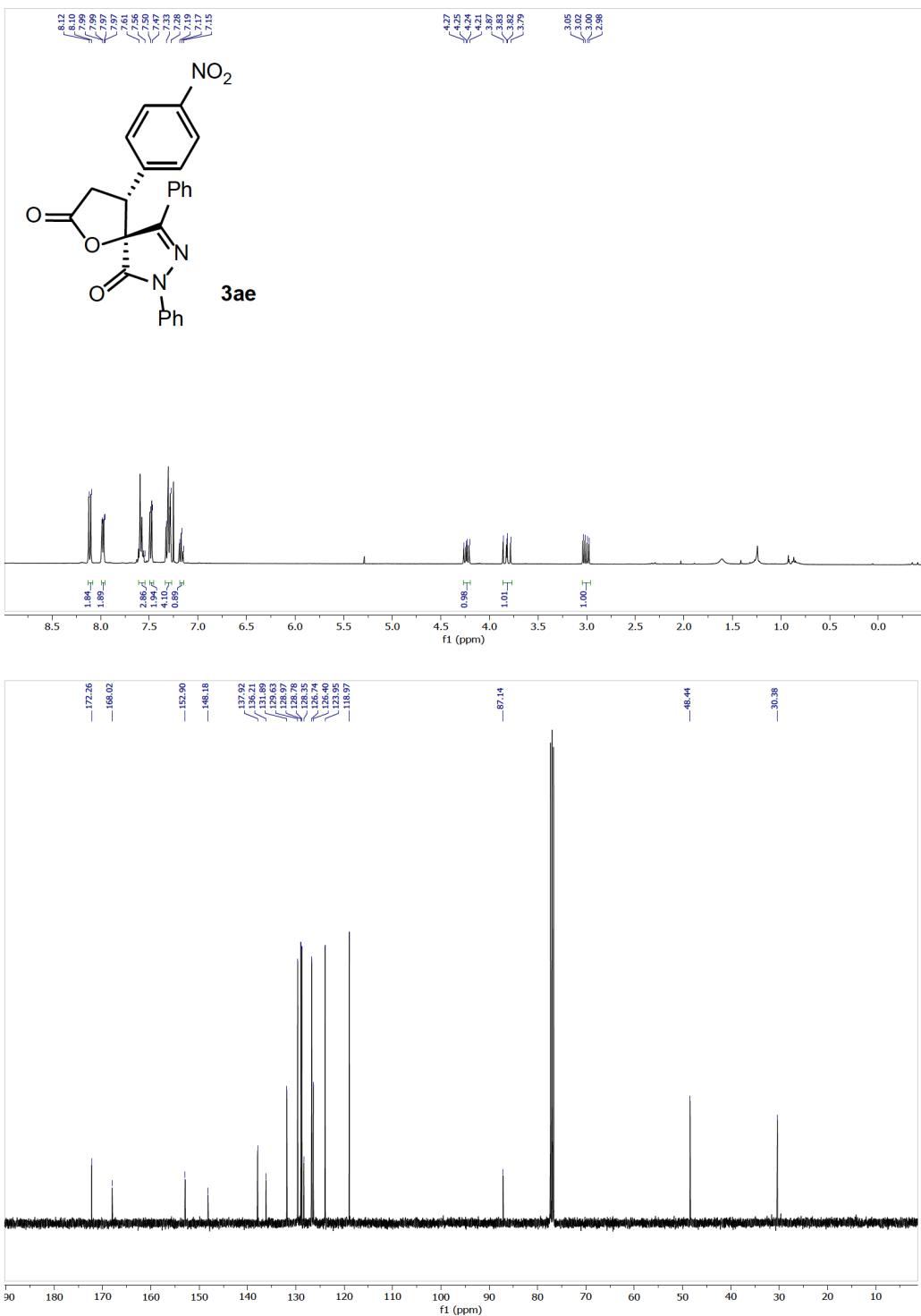


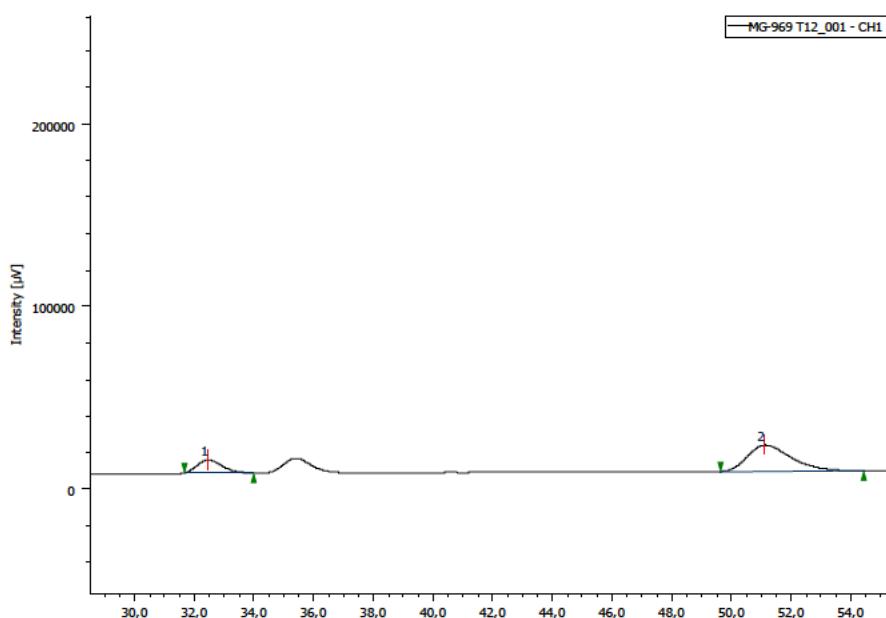
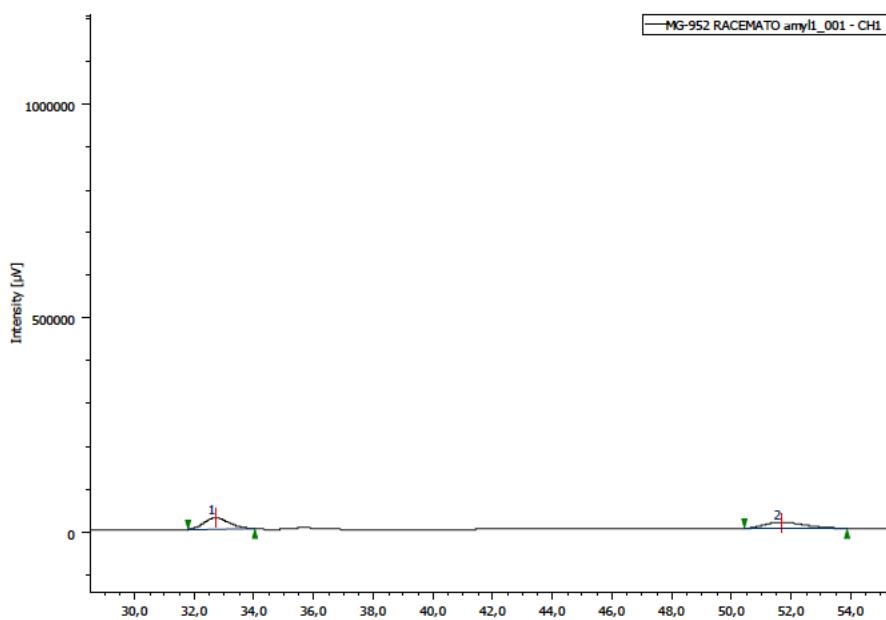


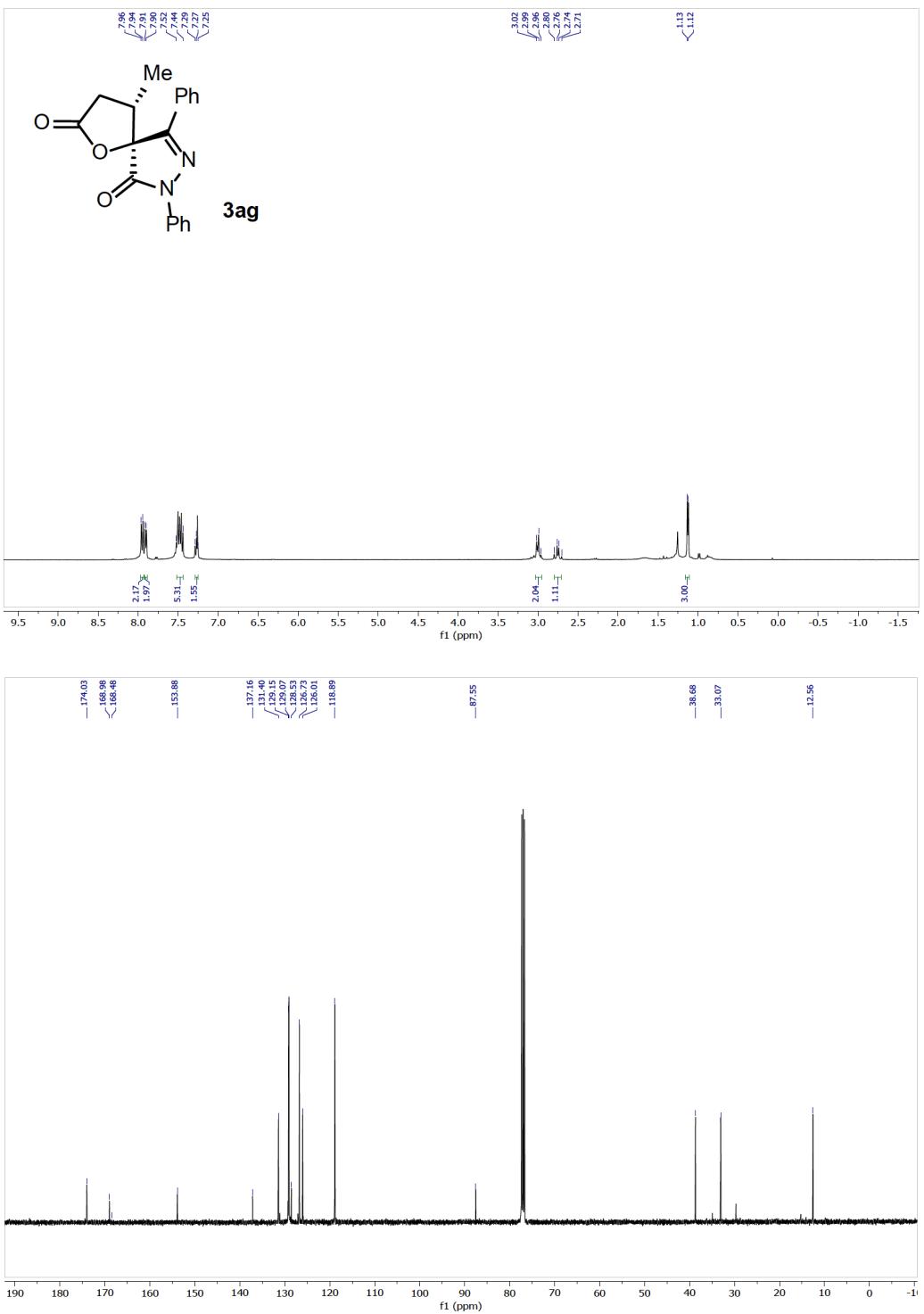
	Time	Area	Area%
1	18,175	273872	53,965
2	30,325	233629	46,035

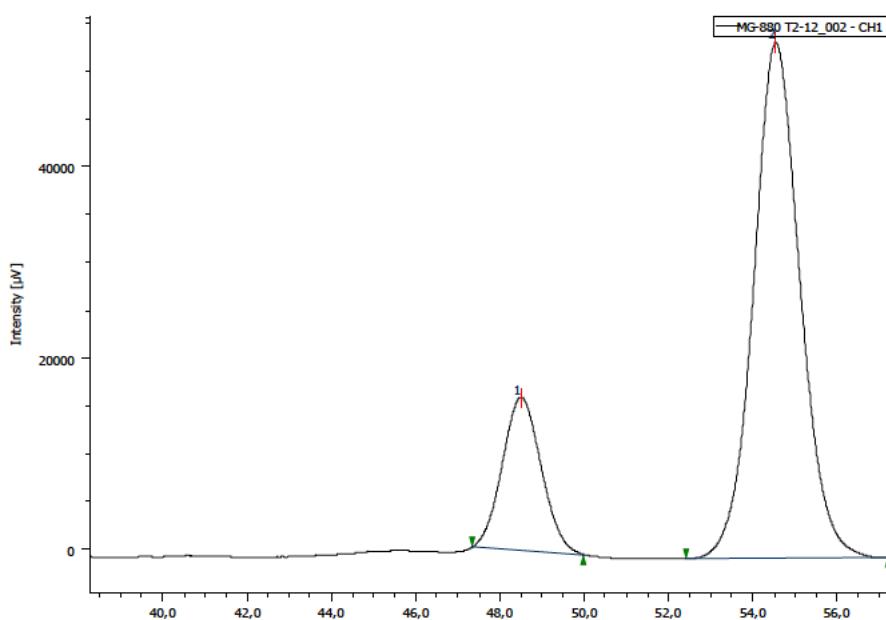
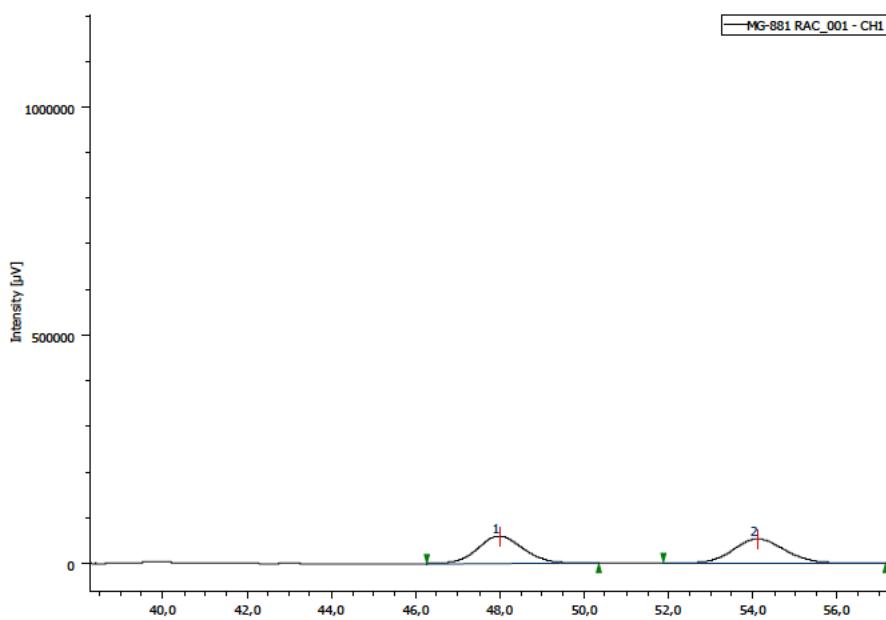


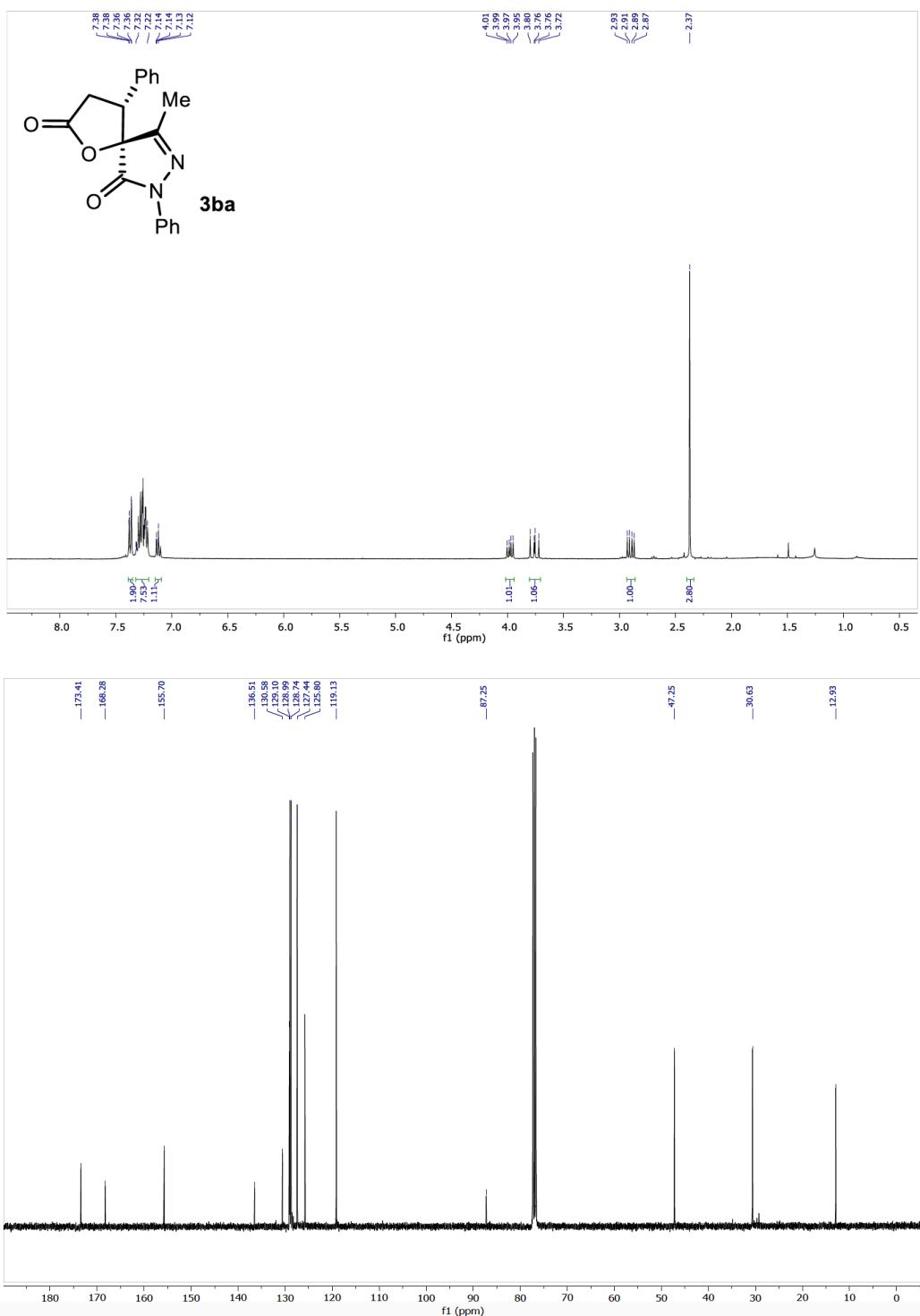
	Time	Area	Area%
1	18,067	782188	26,449
2	29,892	2175204	73,551



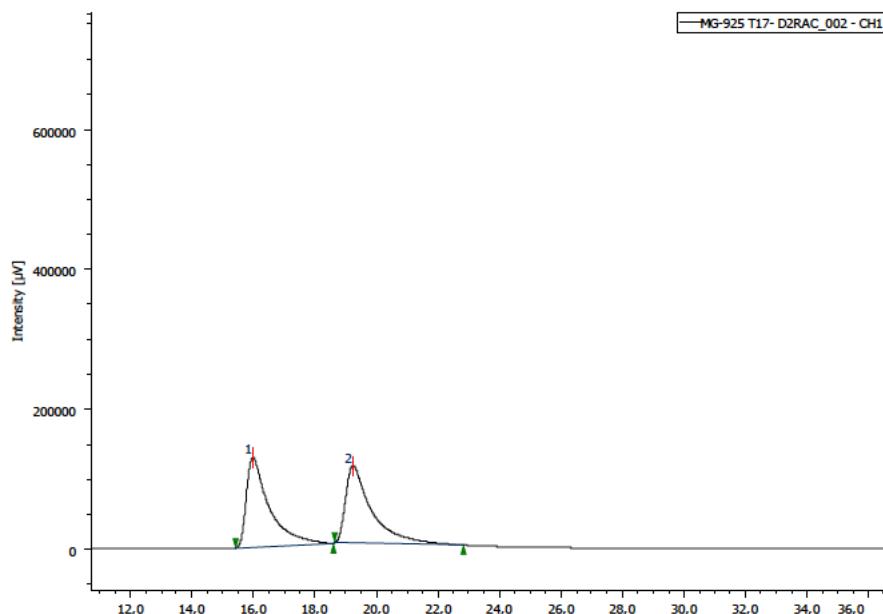






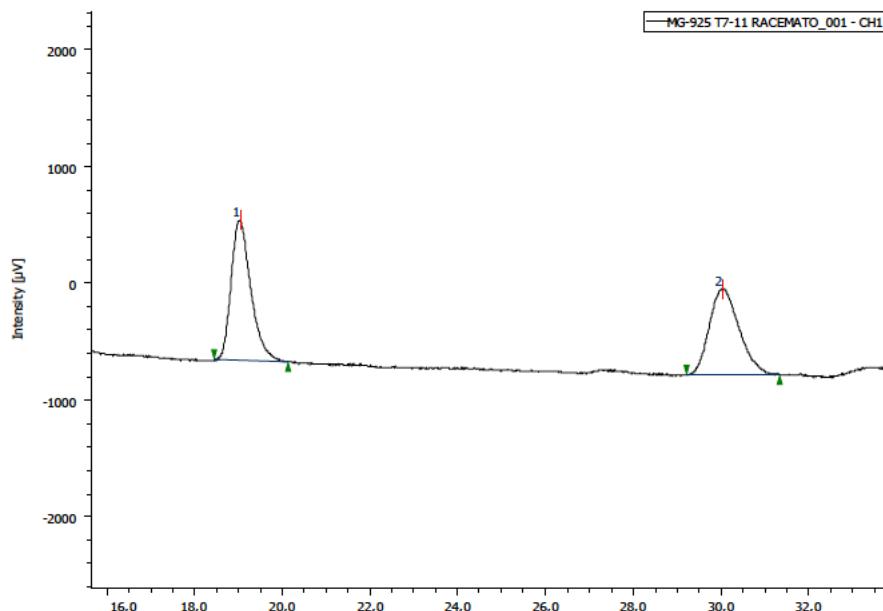


Major diastereomer

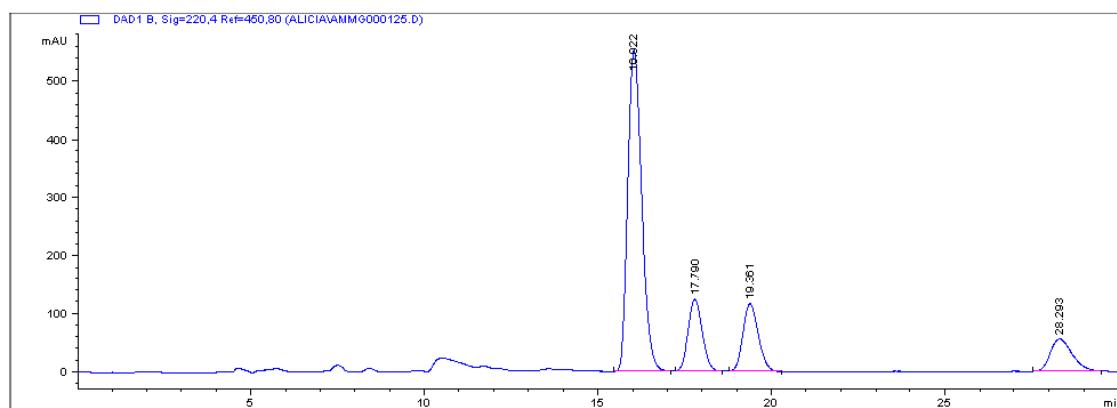


	Time	Area	Area%
1	15,975	6602845	50,442
2	19,225	6487047	49,558

Minor diastereomer

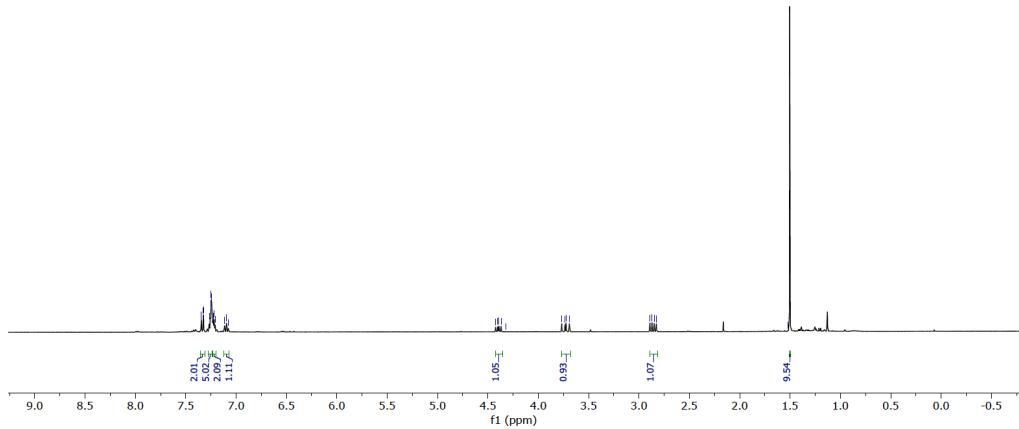
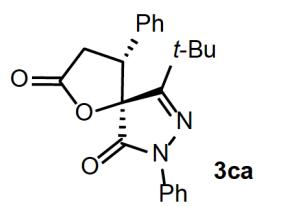


	Time	Area	Area%
1	19,033	37314	51,954
2	30,017	34507	48,046

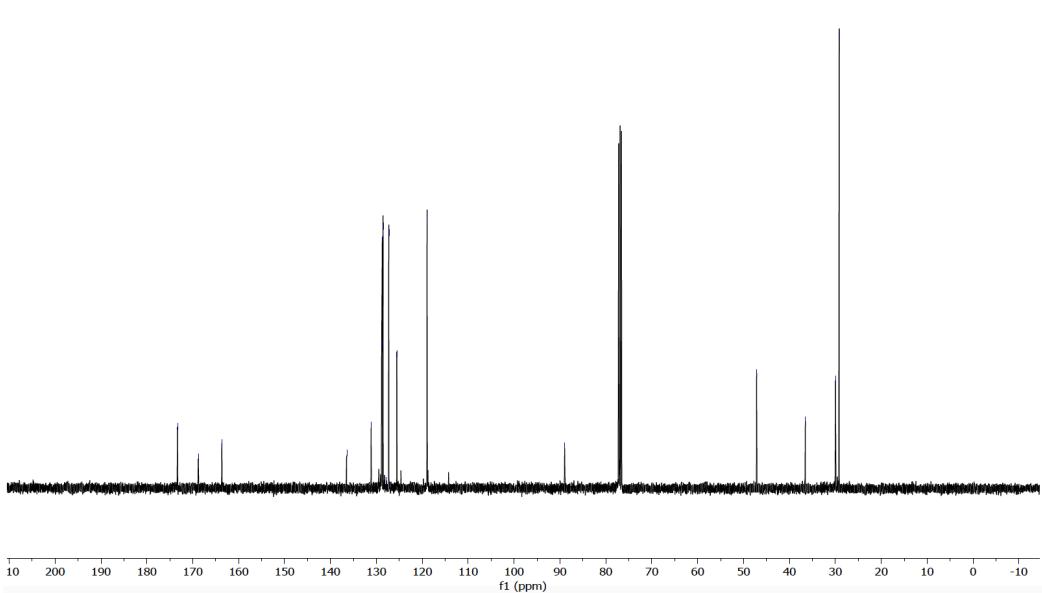


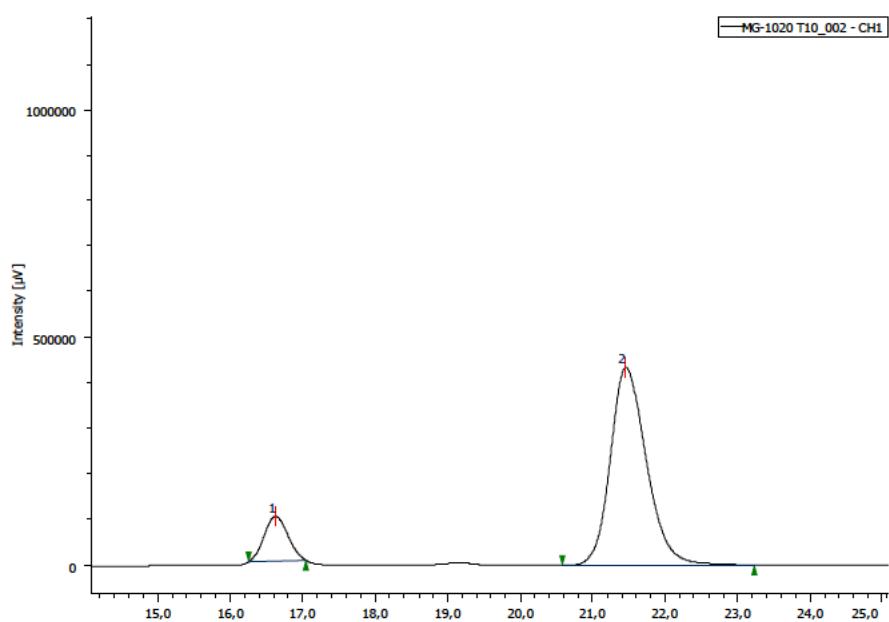
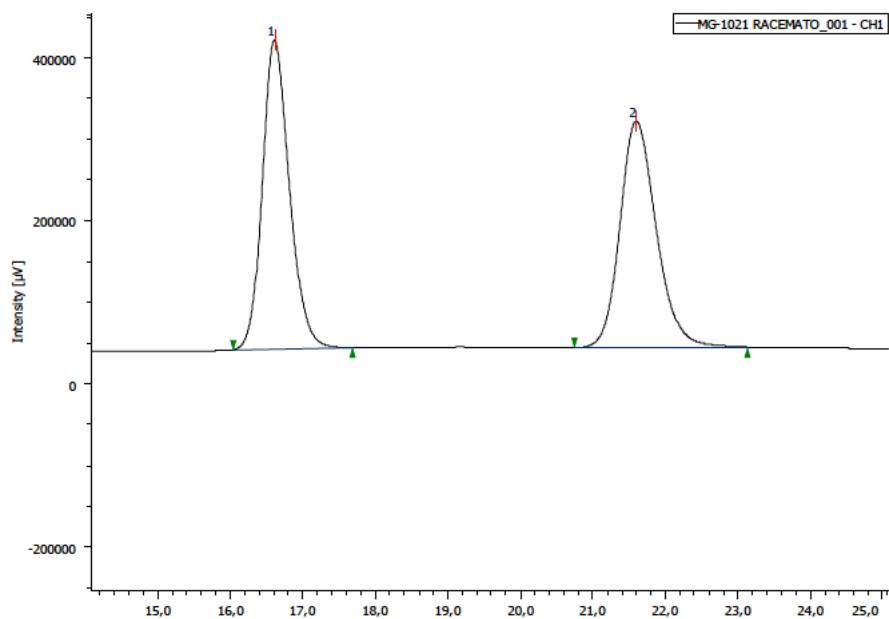
#	Time	Area	Area%
1	16.022	15241.5	61.954
2	17.79	3430.3	13.943
3	19.361	3525	14.328
4	28.293	2404.6	9.774

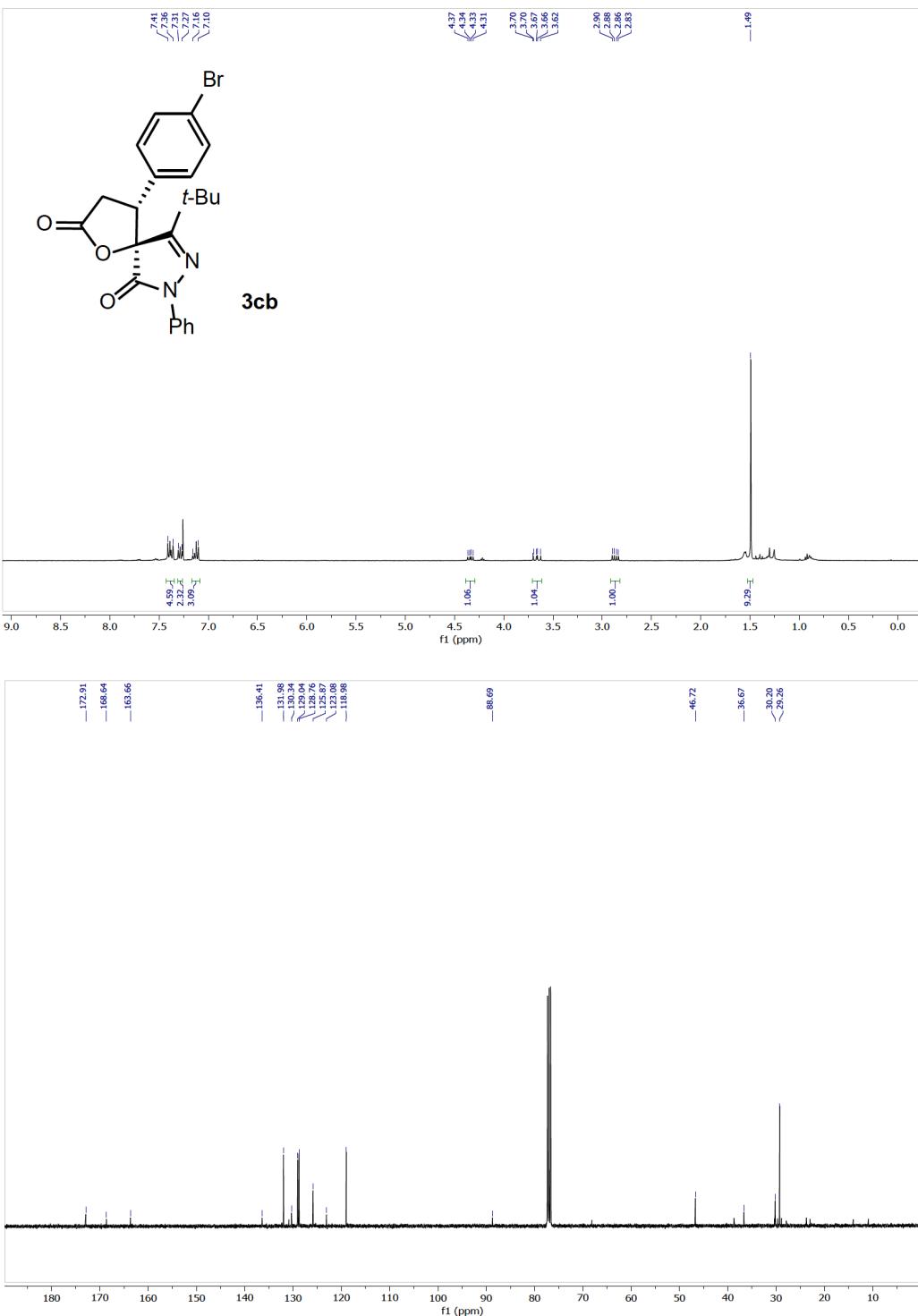
MG-468_PROTON_01
MG-468

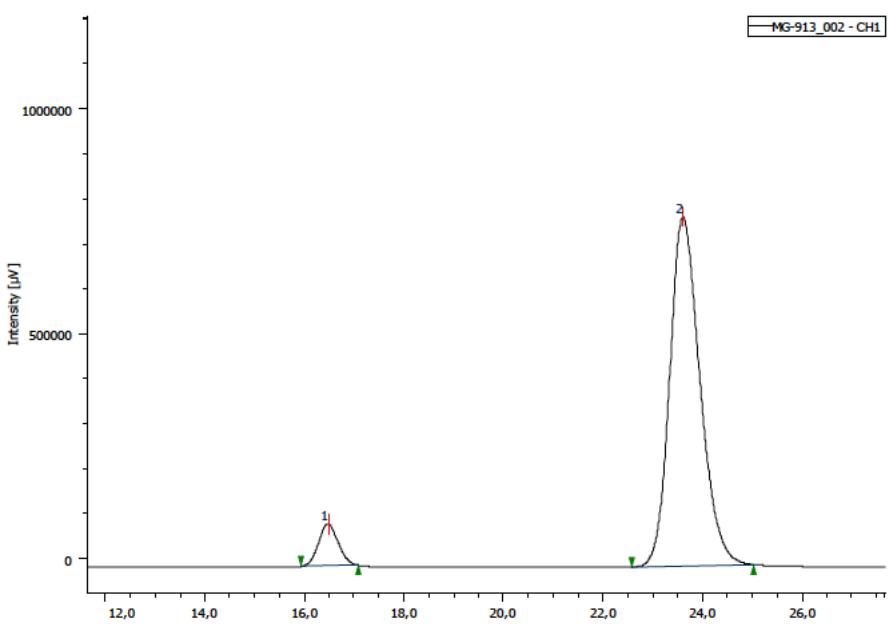
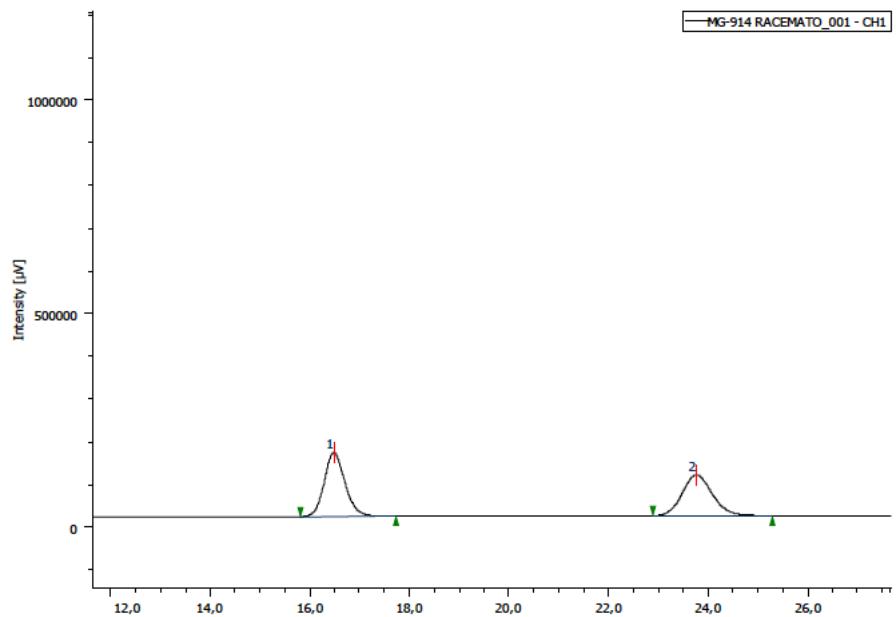


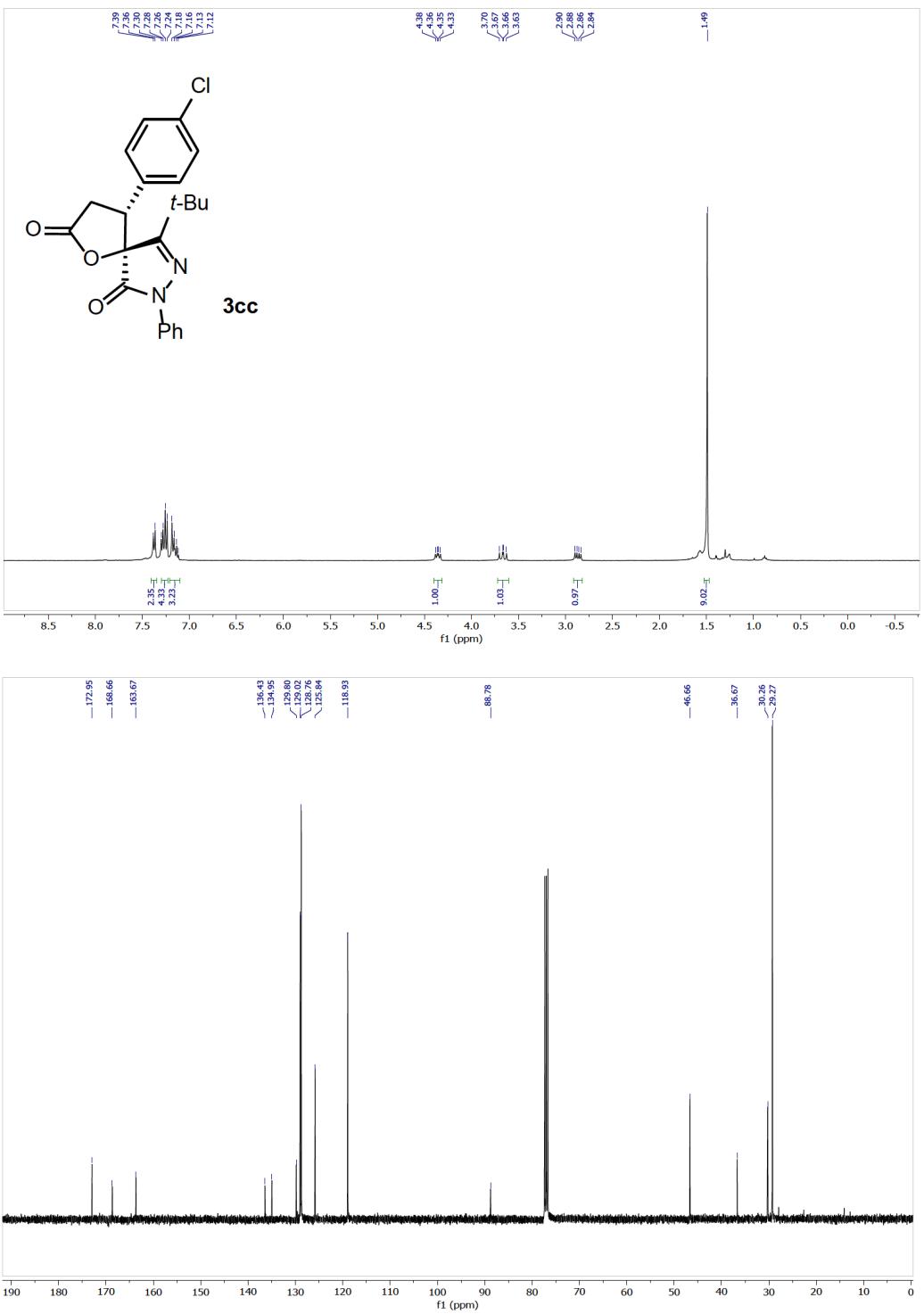
MG-468_CARBON_01
MG-468

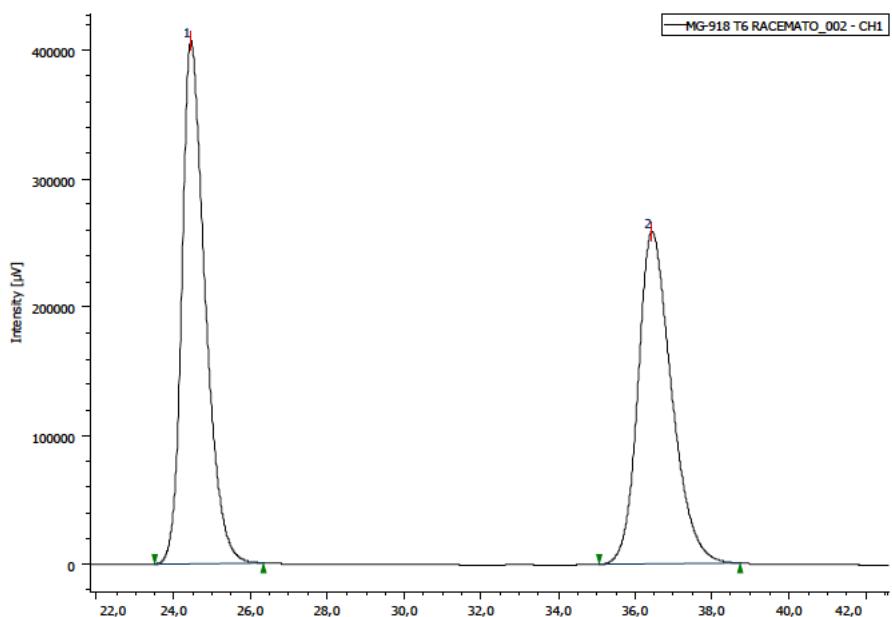




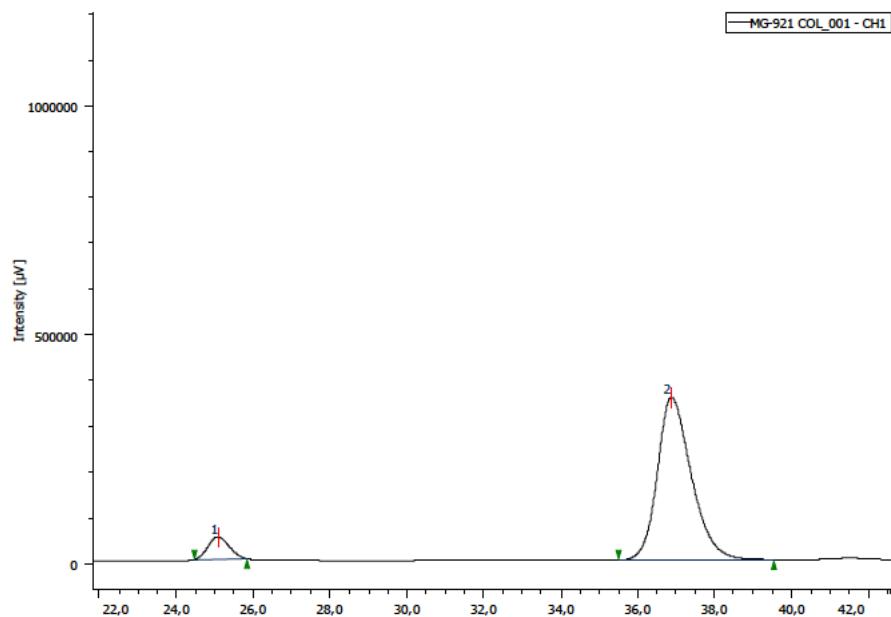




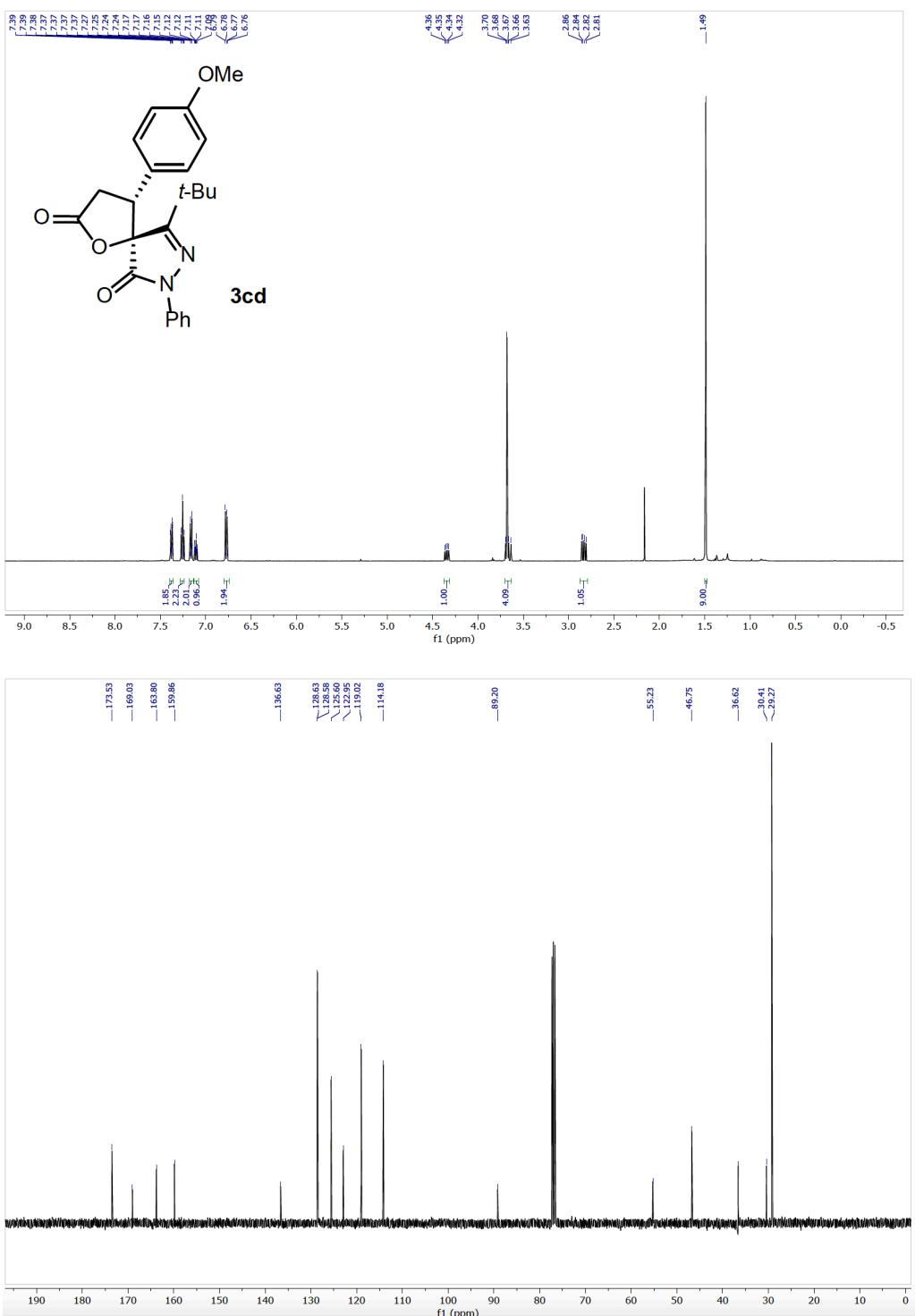


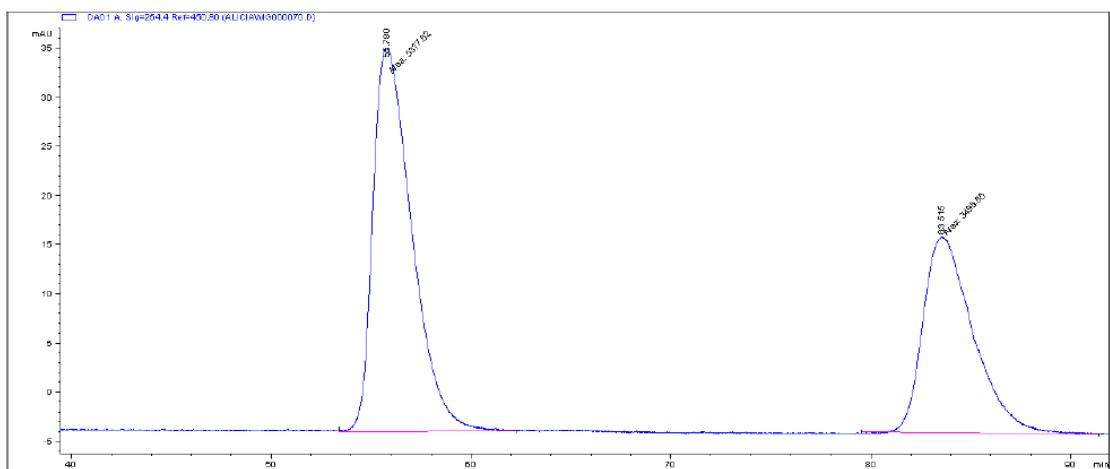


	Time	Area	Area%
1	24,450	17069497	52,139
2	36,425	15668974	47,861

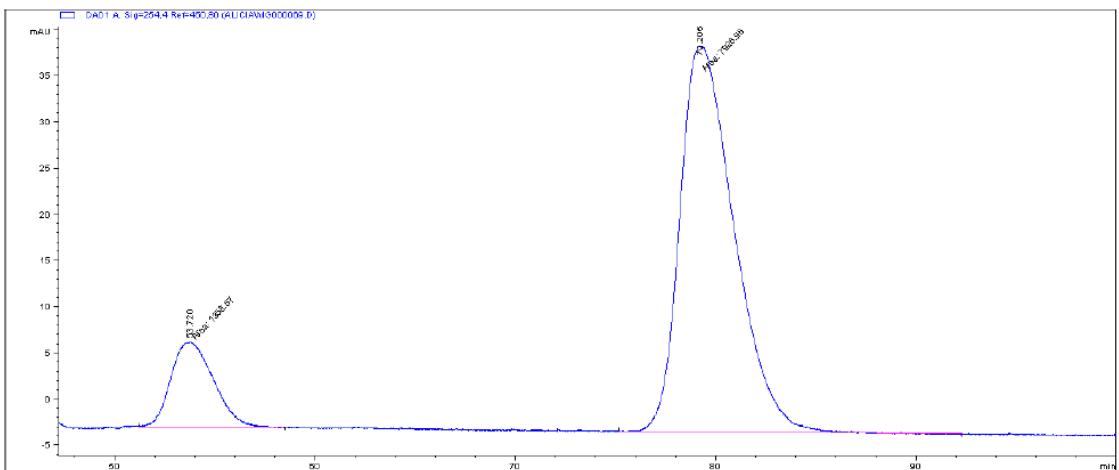


	Time	Area	Area%
1	25,075	1852294	7,844
2	36,858	21761664	92,156

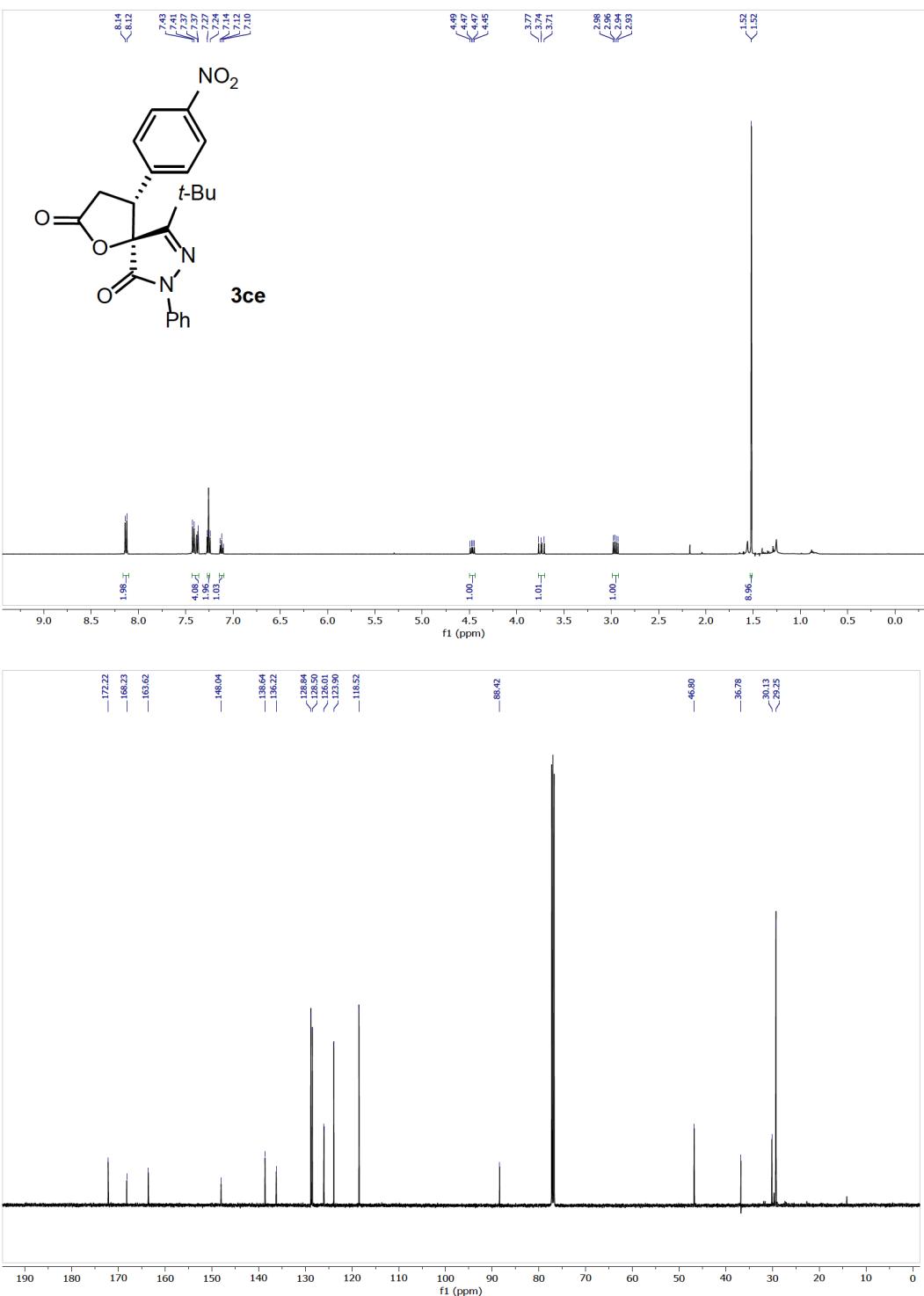


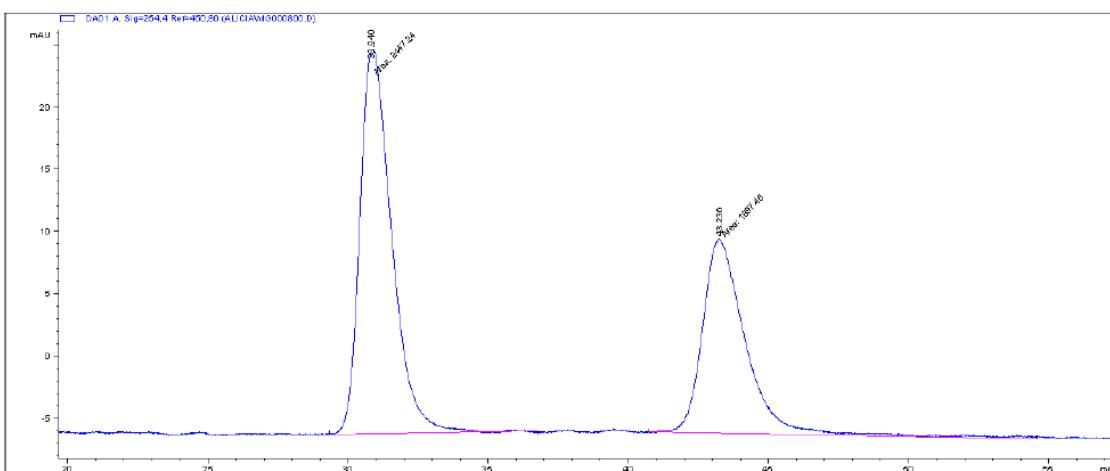


	Time	Area	Area%
1	55.78	5317.6	60.336
2	83.515	3495.7	39.664

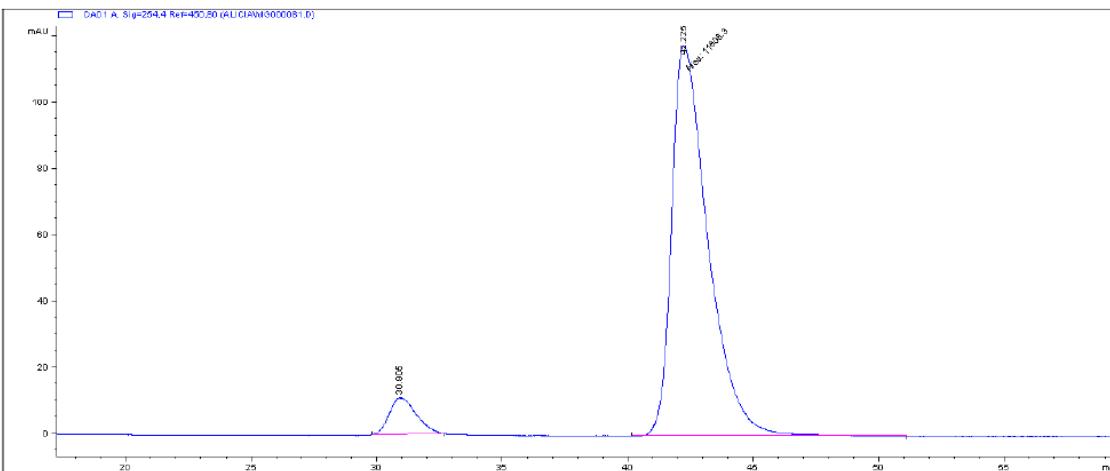


	Time	Area	Area%
1	53.72	1358.6	14.631
2	79.205	7927	85.369

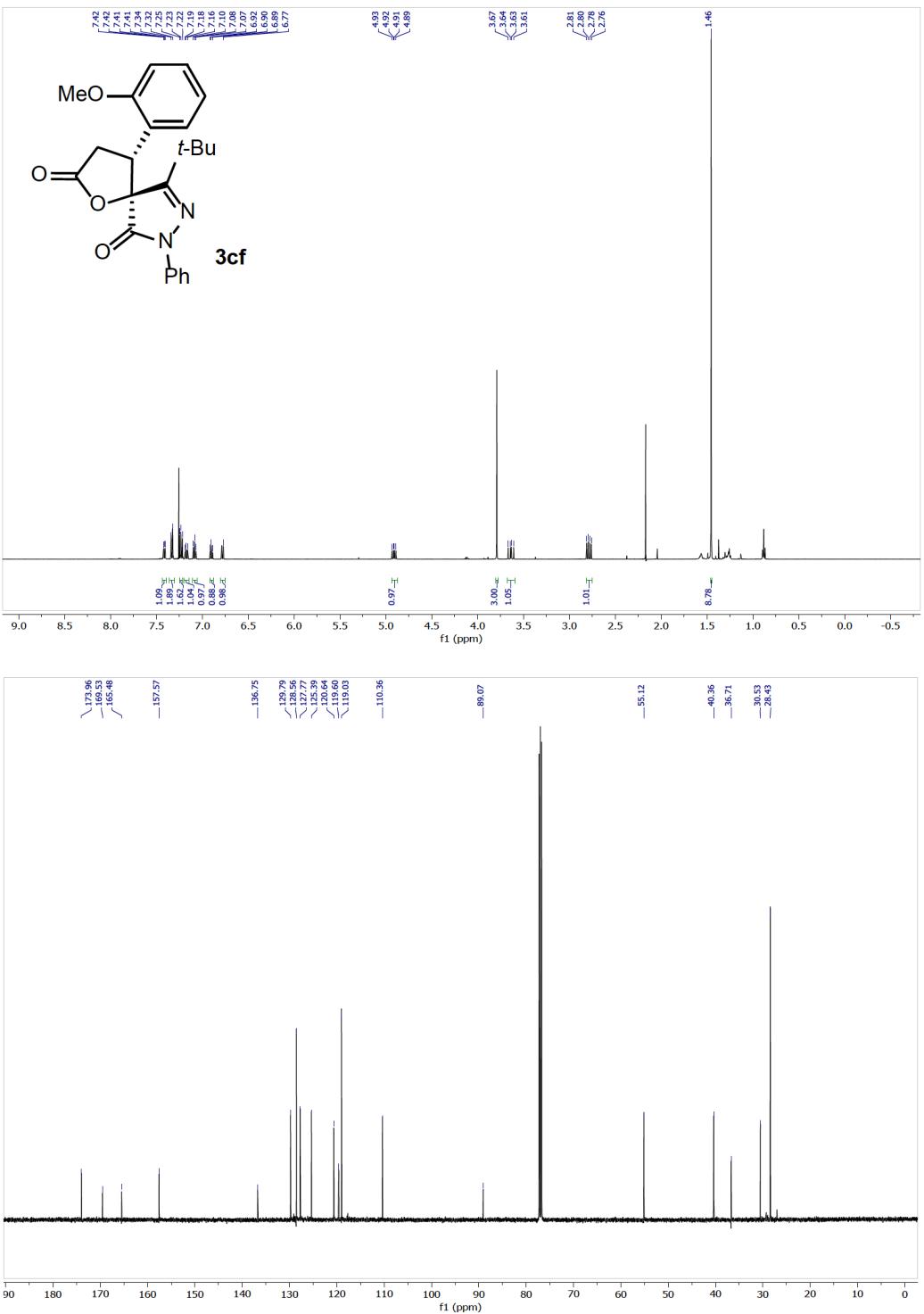


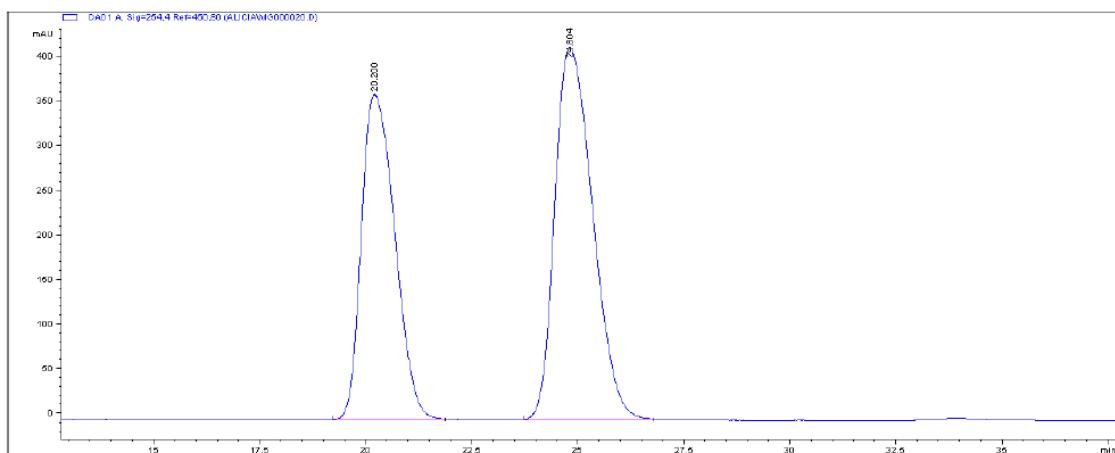


	Time	Area	Area%
1	30.84	2447.2	59.045
2	43.236	1697.5	40.955

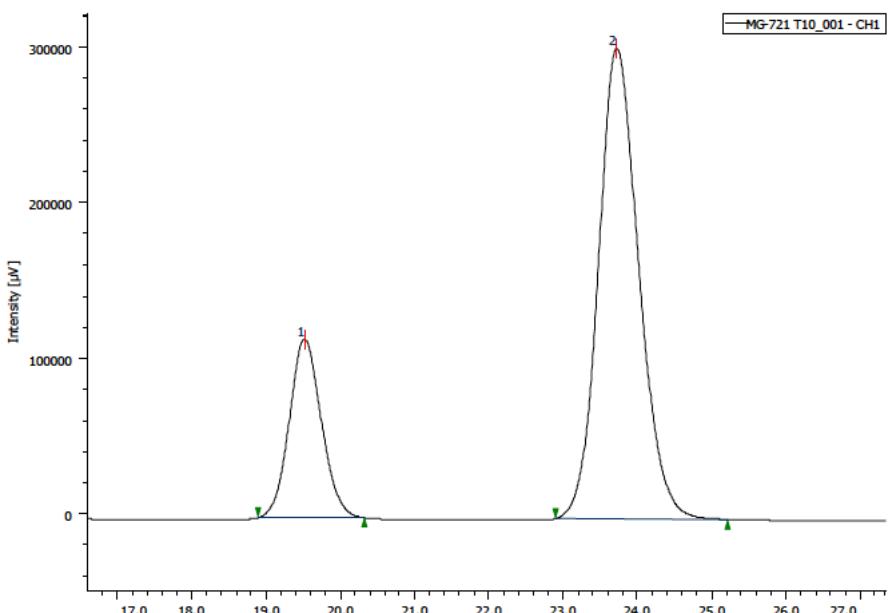


	Time	Area	Area%
1	30.905	818.2	6.480
2	42.225	11808.3	93.520

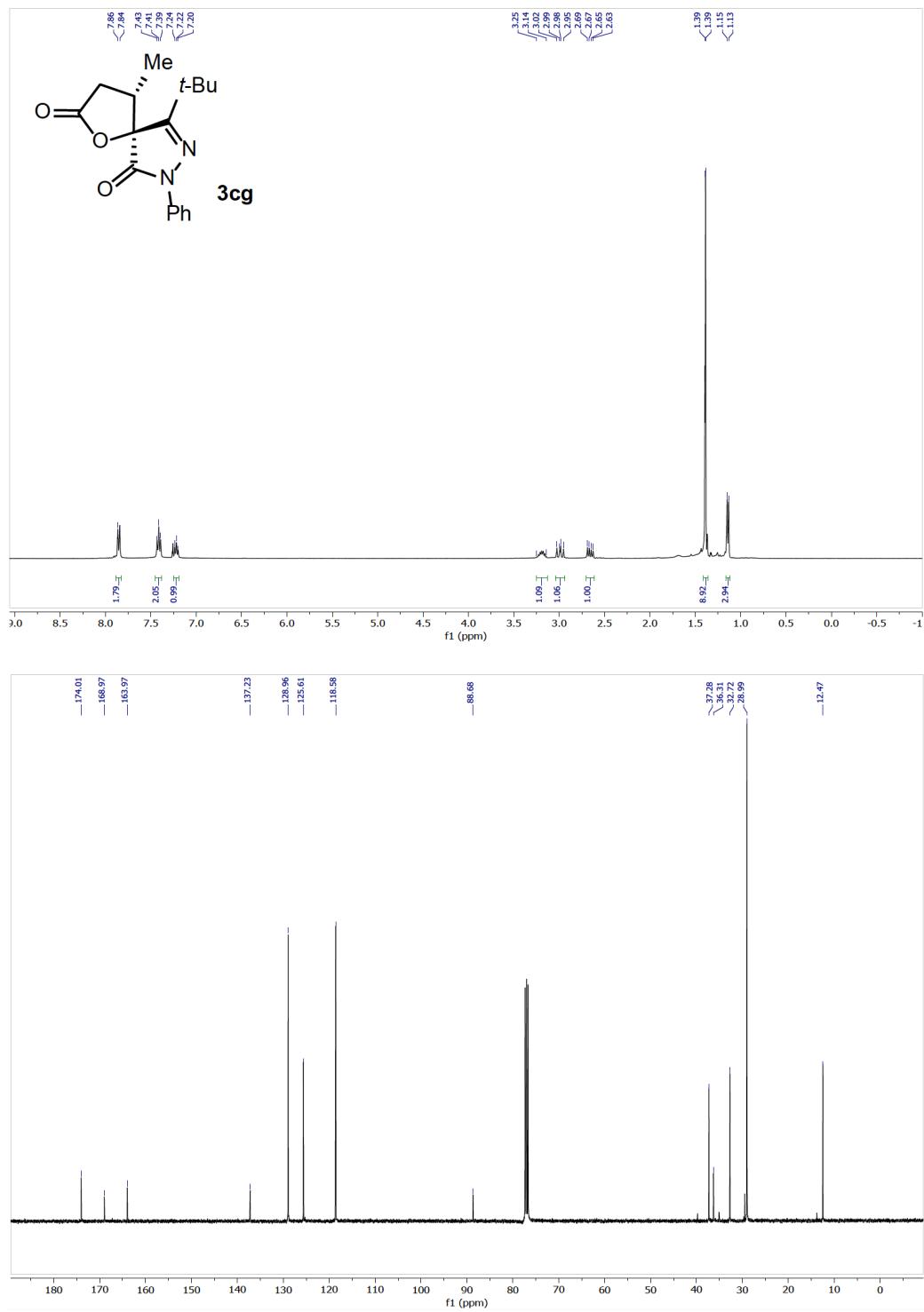


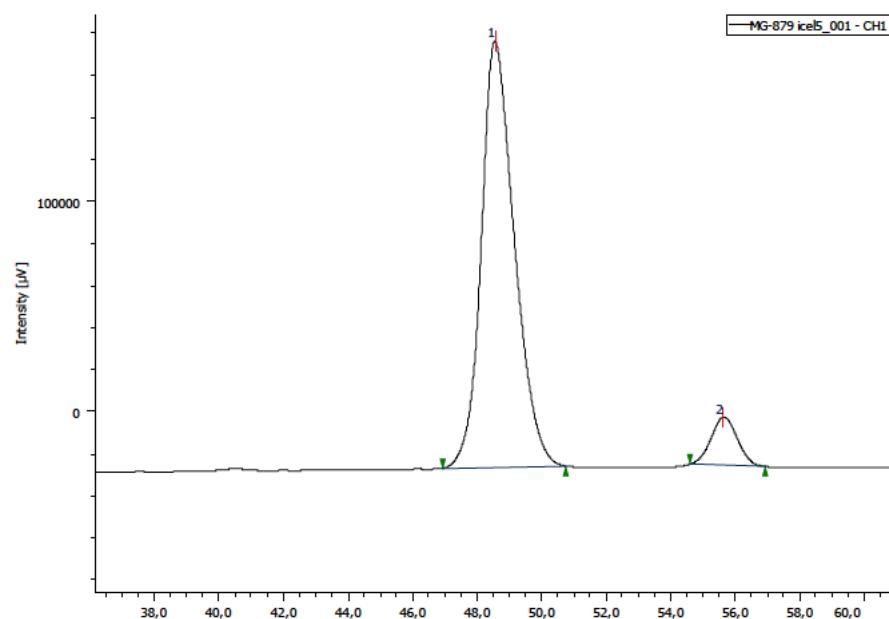
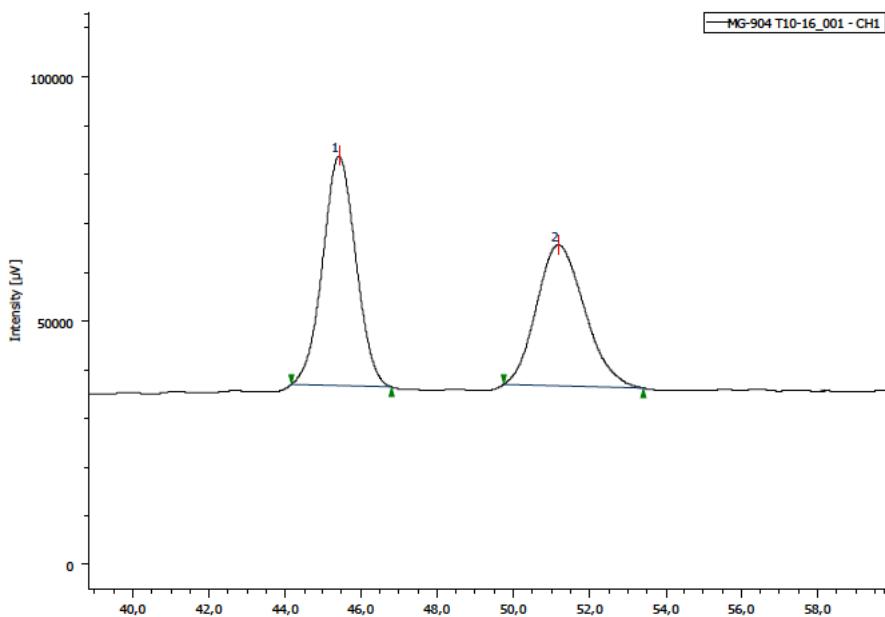


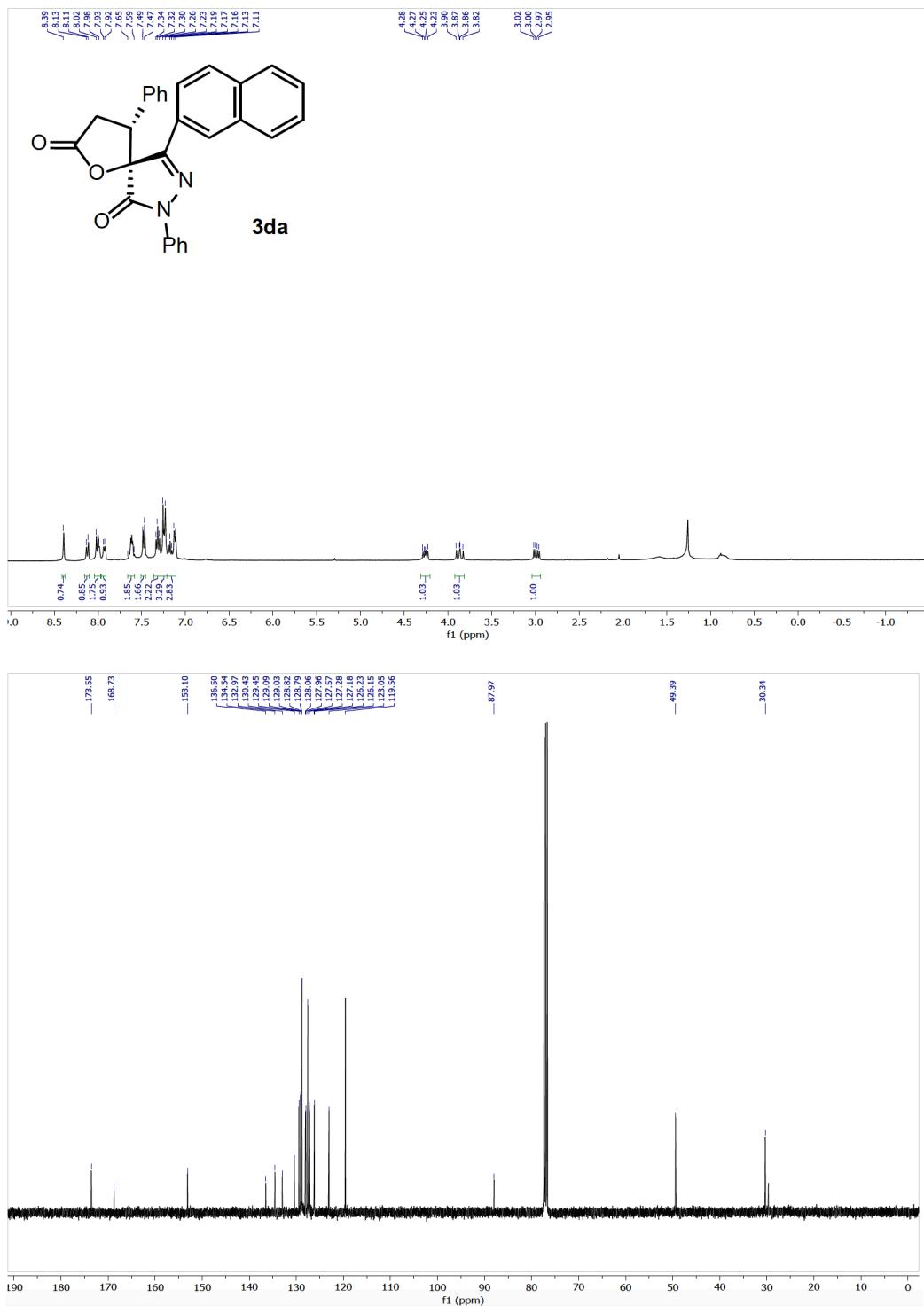
	Time	Area	Area%
1	20.2	19947.7	43.514
2	24.804	25893.8	56.486

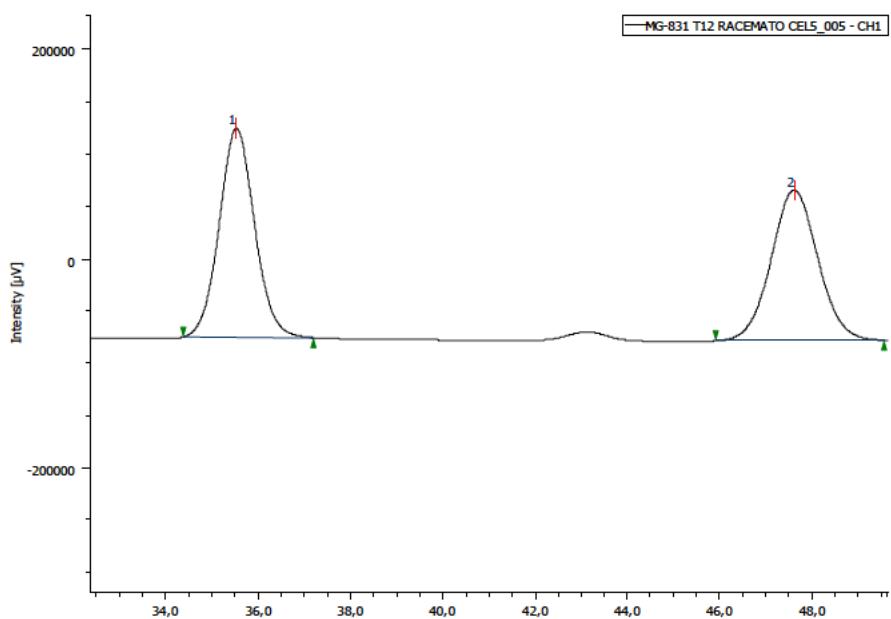


	Time	Area	Area%
1	19,517	3444418	23,234
2	23,708	11380736	76,766

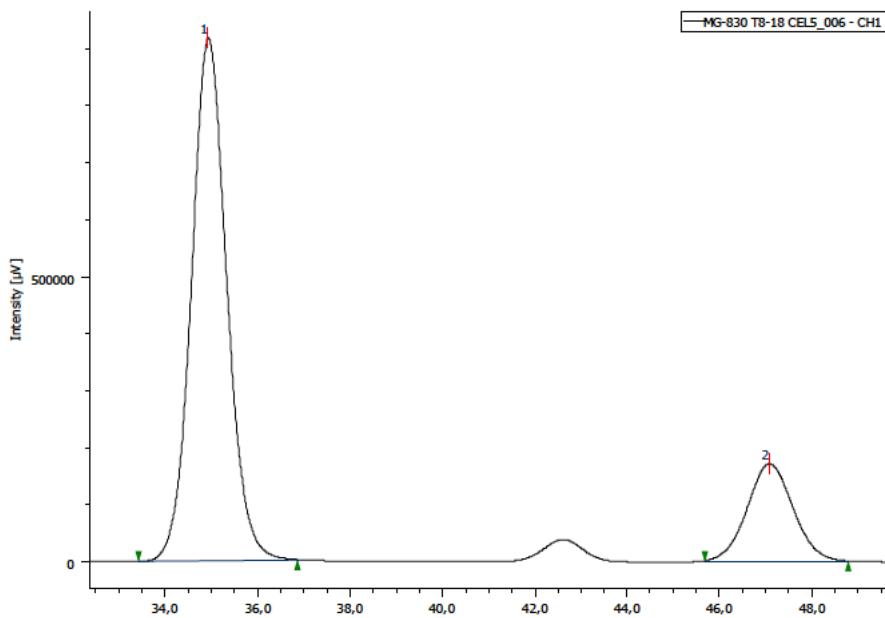




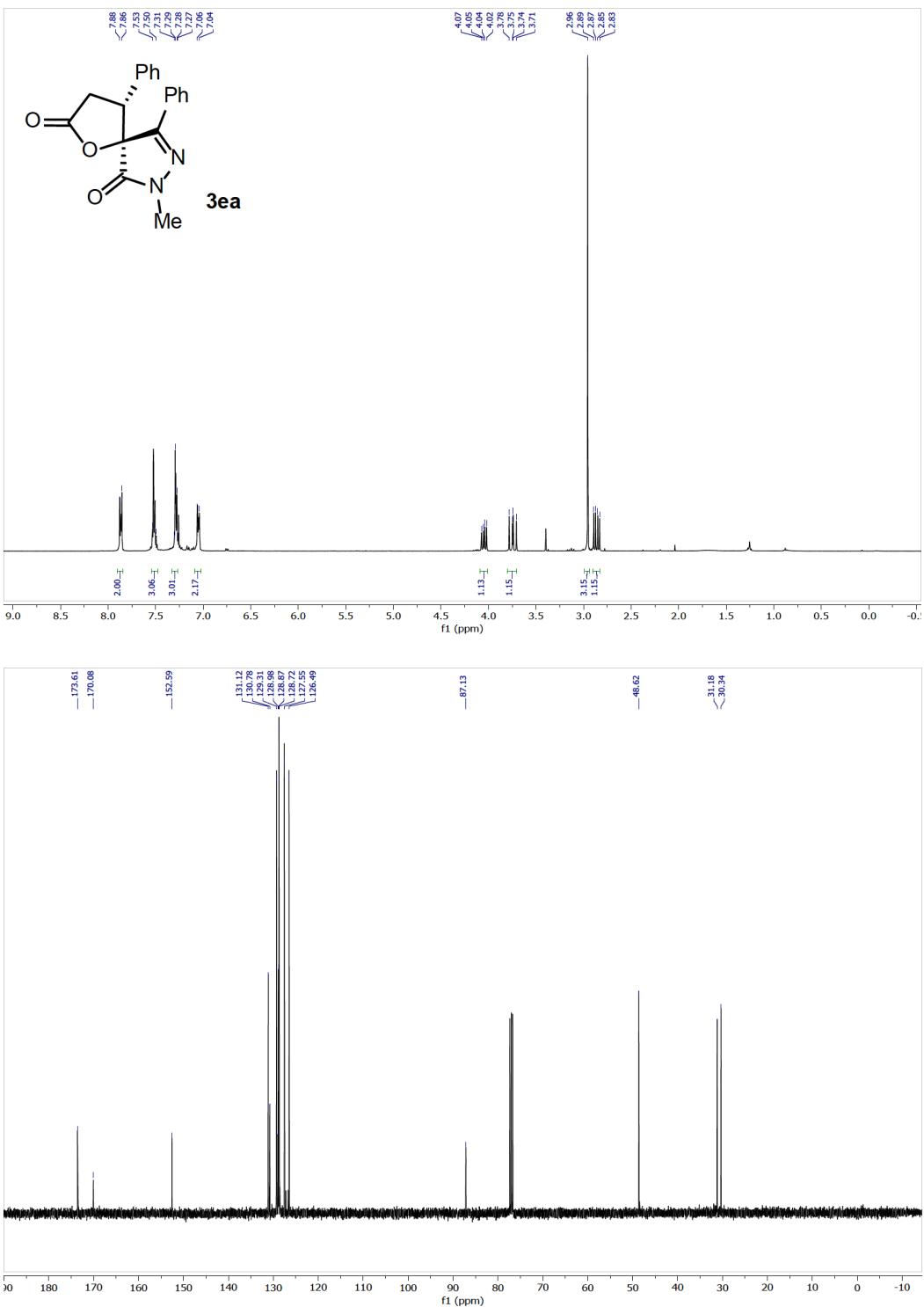


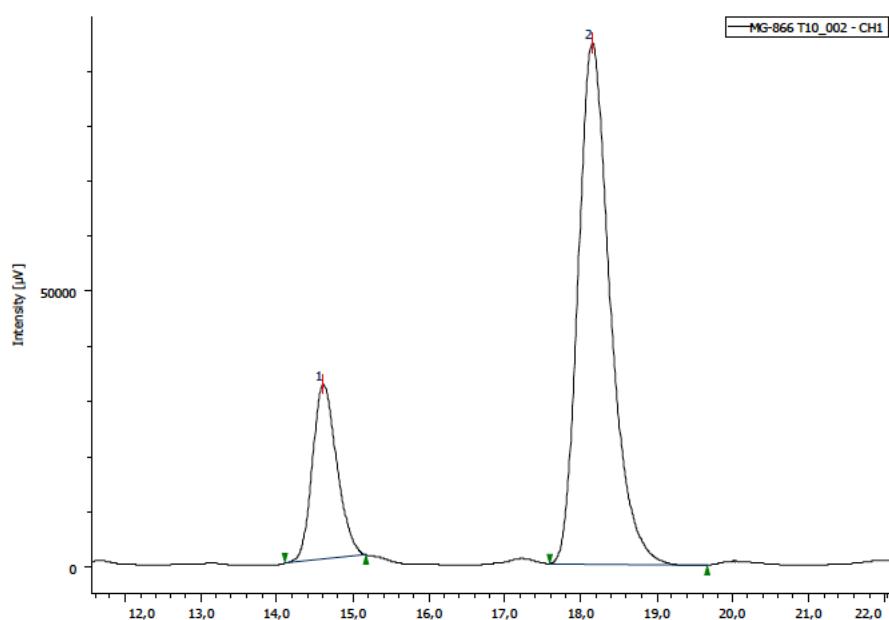
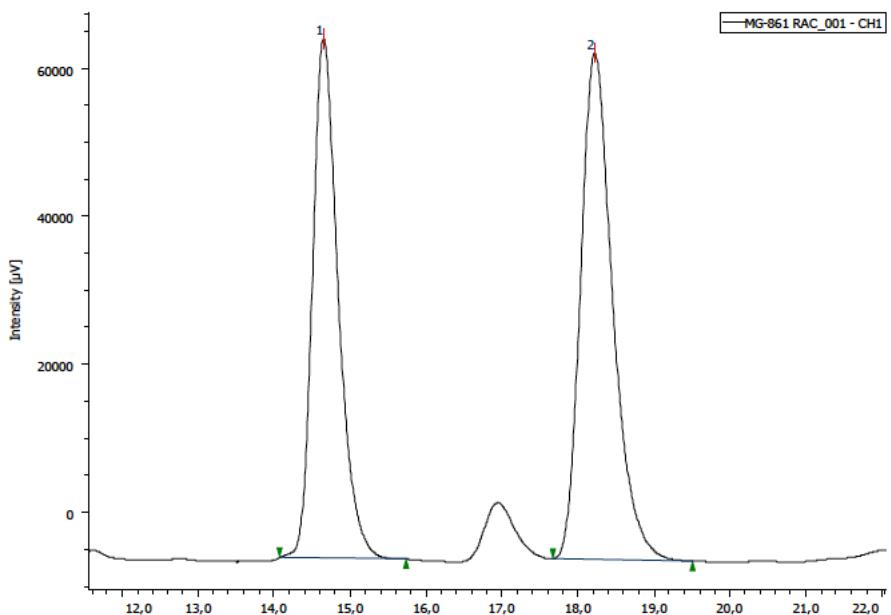


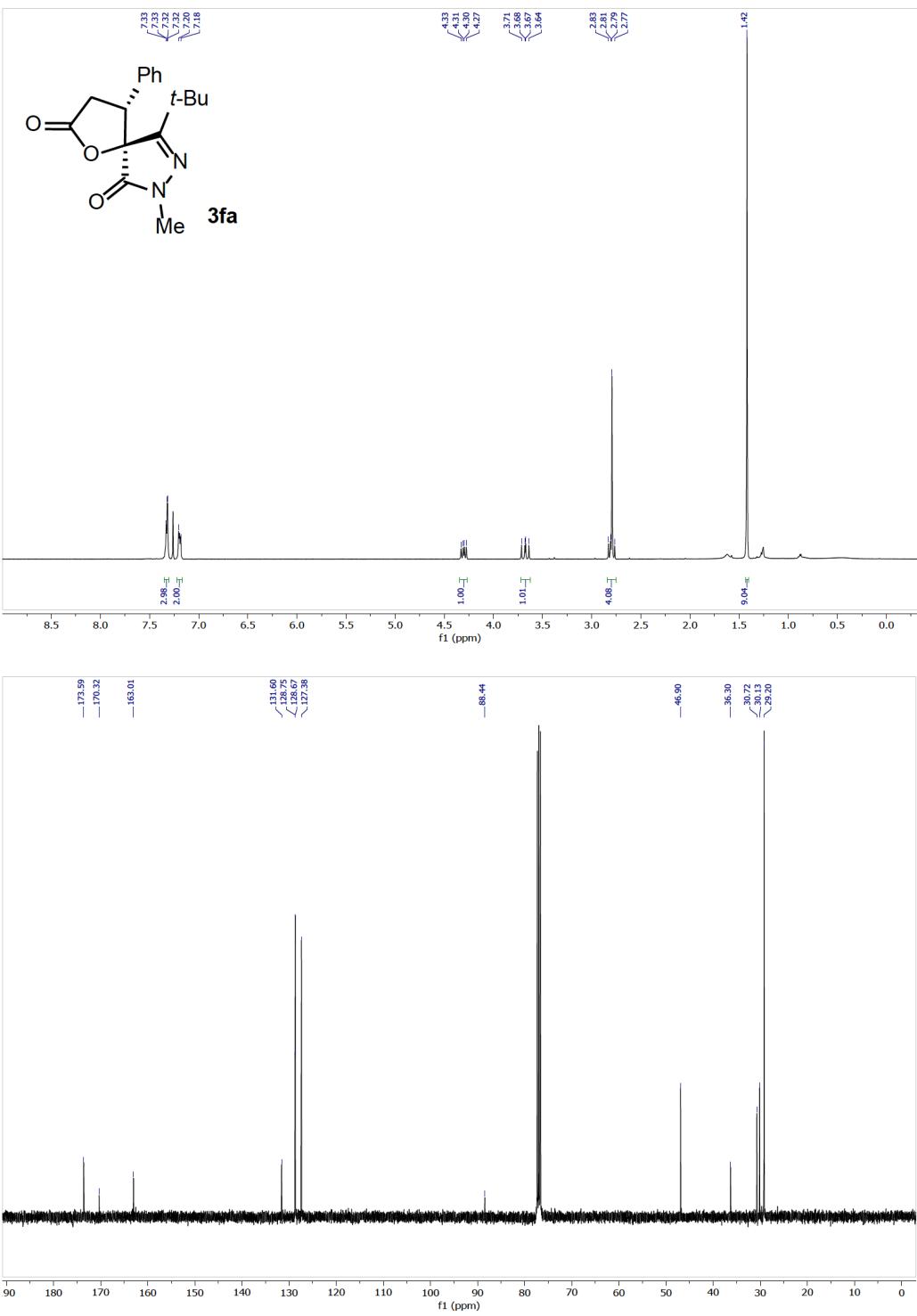
	Time	Area	Area%
1	35,525	10635812	51,205
2	47,583	10135420	48,795

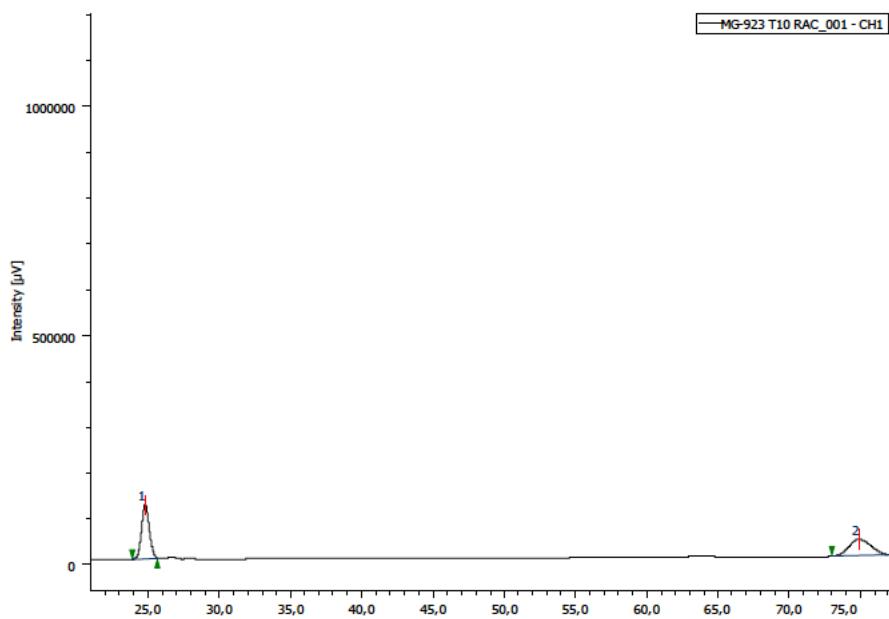


	Time	Area	Area%
1	34,933	48603938	80,635
2	47,058	11672173	19,365

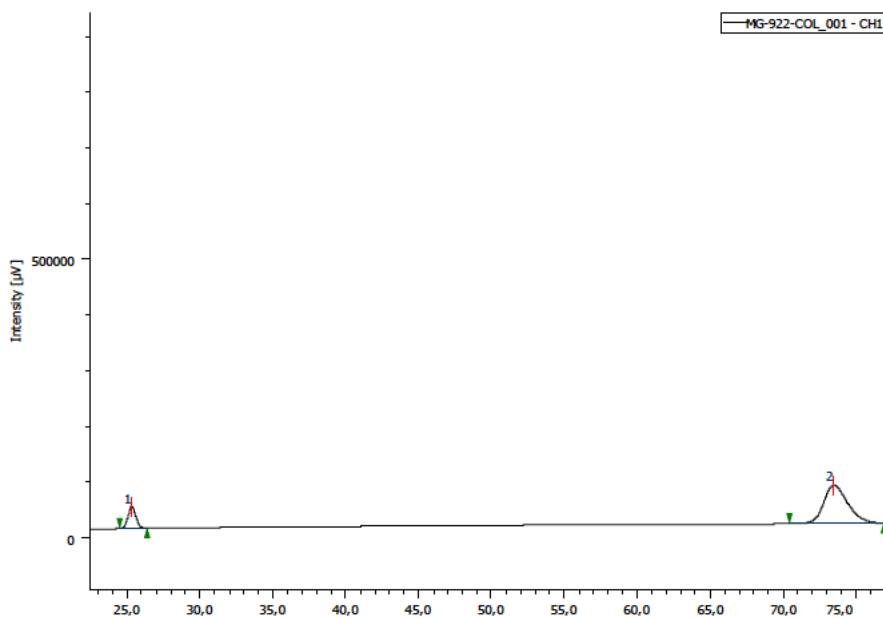




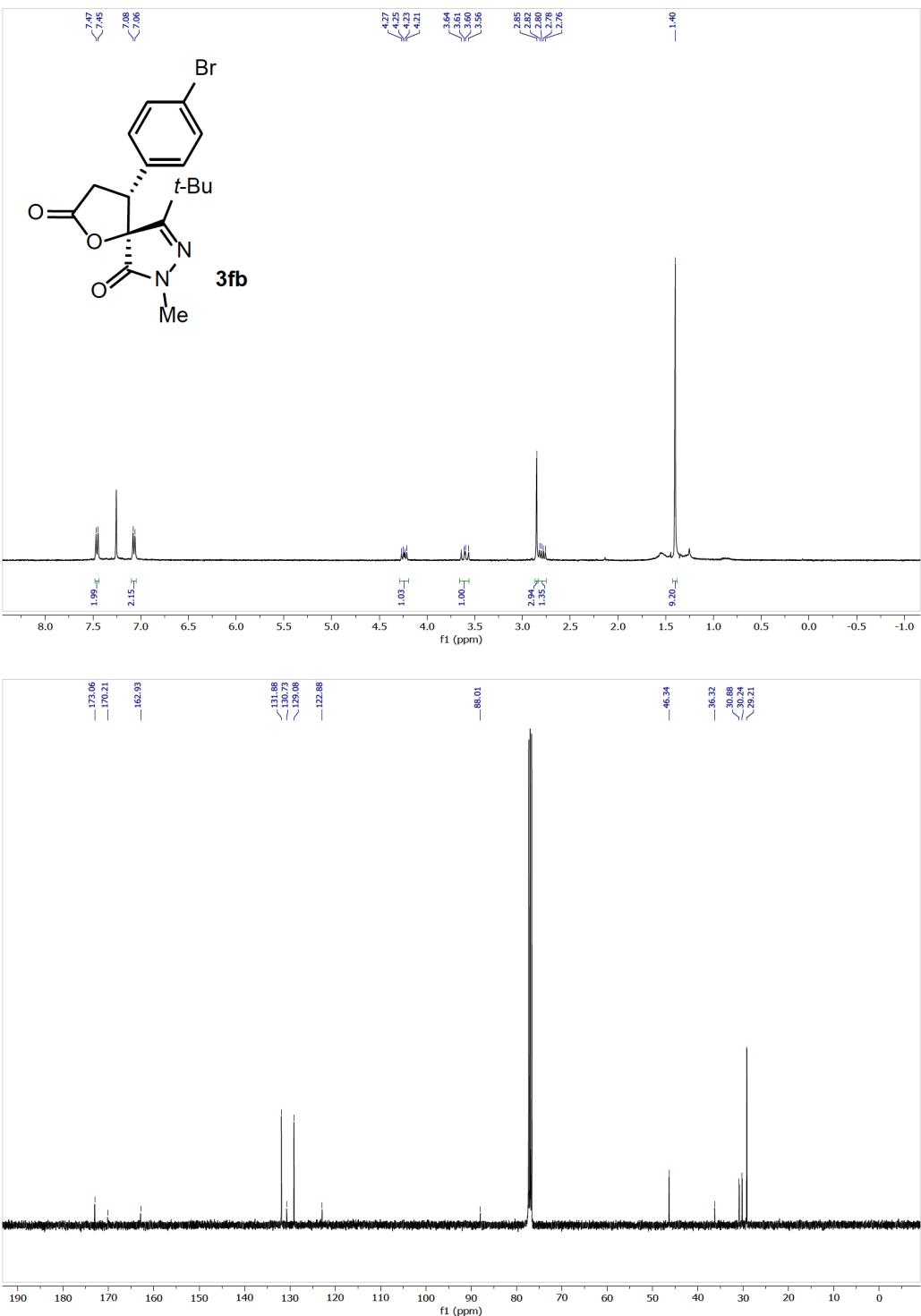


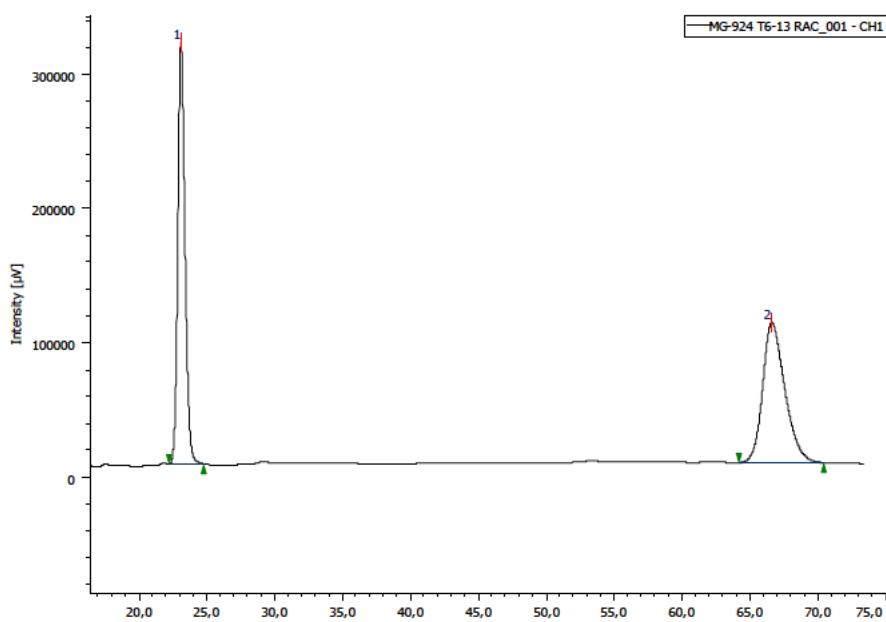


	Time	Area	Area%
1	24,783	4418833	52,363
2	74,833	4020023	47,637

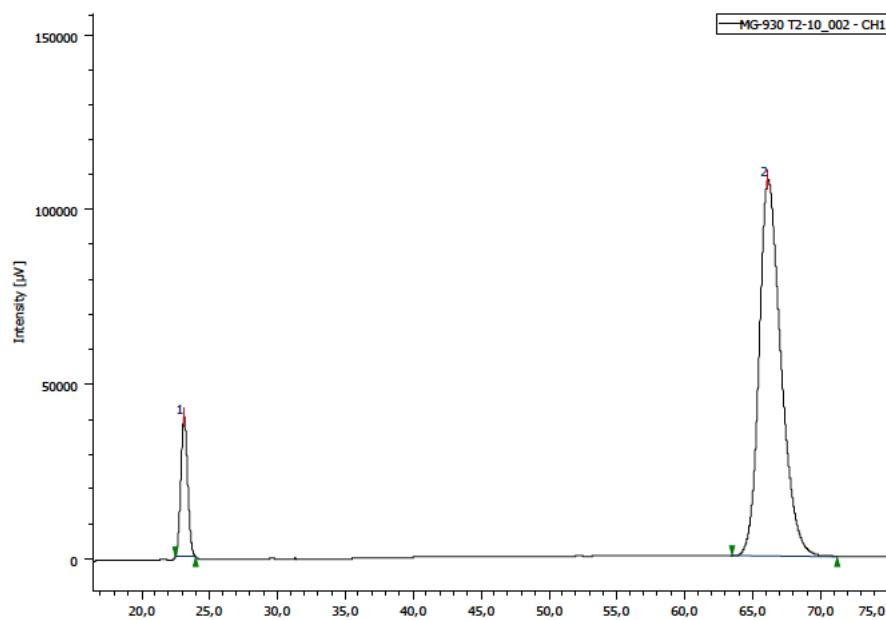


	Time	Area	Area%
1	25,317	1466177	15,686
2	73,408	7880791	84,314





	Time	Area	Area%
1	23,108	11541306	49,371
2	66,542	11835318	50,629



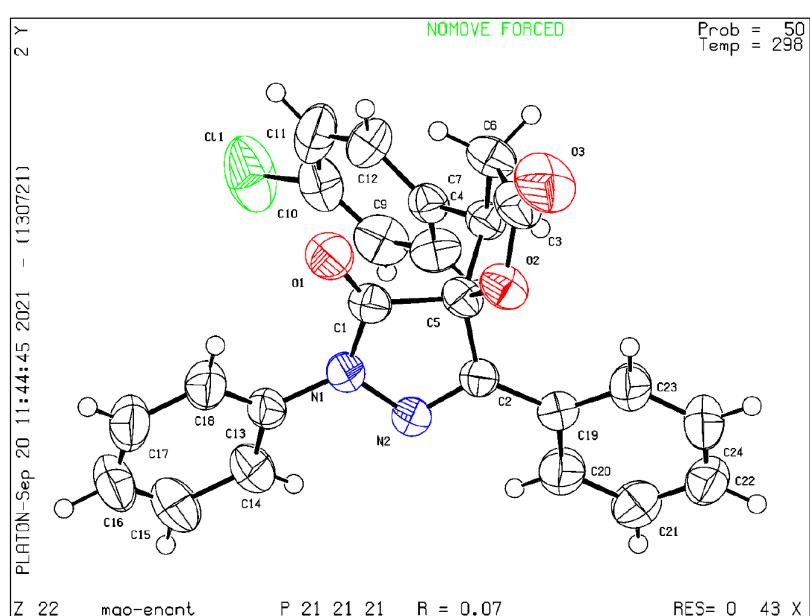
	Time	Area	Area%
1	23,142	1398250	10,403
2	66,075	12042653	89,597

Crystallographic data of spirocycle **3ac**.

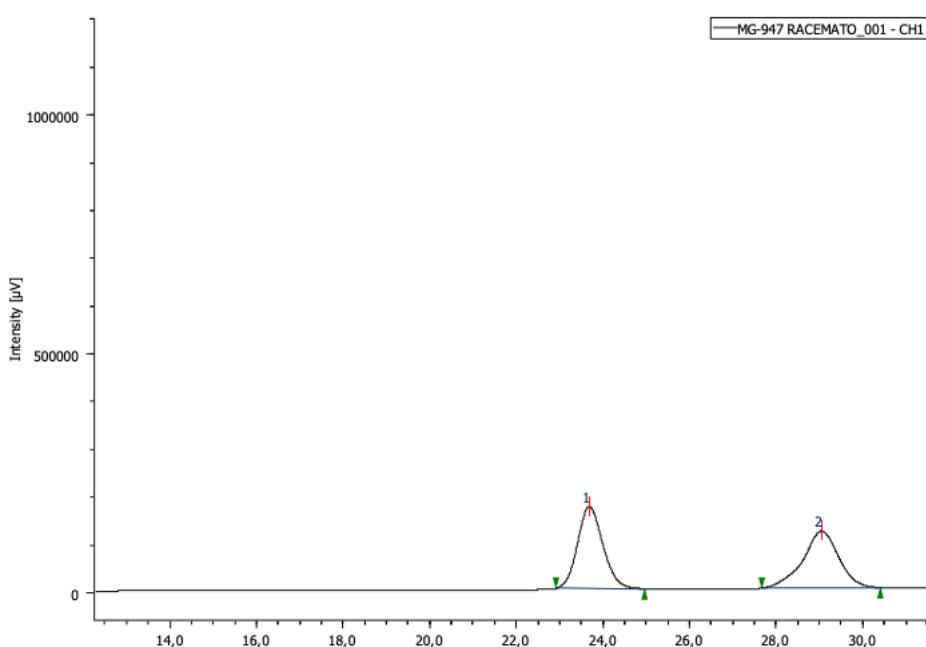
ORTEP Syngle Crystal X-Ray Diffraction of **3ac**. The ellipsoids are shown at 50% probability. CCDC 2110499.

Crystal data and structure refinement for 3ac	
Identification code	3ac
Empirical formula	C ₂₄ H ₁₇ CIN ₂ O ₃
Formula weight	416.84
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	10.0795(6)
b/Å	13.8030(9)
c/Å	14.5673(11)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	2026.7(2)
Z	4
ρcalcg/cm ³	1.366
μ/mm ⁻¹	1.908
F(000)	864.0
Crystal size/mm ³	1.401 × 1.214 × 0.9
Radiation	CuKα ($\lambda = 1.54184$)
2θ range for data collection/°	8.826 to 149.654
Index ranges	-10 ≤ h ≤ 12, -16 ≤ k ≤ 12, -18 ≤ l ≤ 15
Reflections collected	6218
Independent reflections	3944 [R _{int} = 0.0533, R _{sigma} = 0.0550]
Data/restraints/parameters	3944/0/271
Goodness-of-fit on F ²	1.040
Final R indexes [>=2σ (I)]	R ₁ = 0.0735, wR ₂ = 0.1866
Final R indexes [all data]	R ₁ = 0.0806, wR ₂ = 0.1984
Largest diff. peak/hole / e Å ⁻³	0.34/-0.43
Flack parameter	-0.05(3)

Datablock mgo-enant - ellipsoid plot

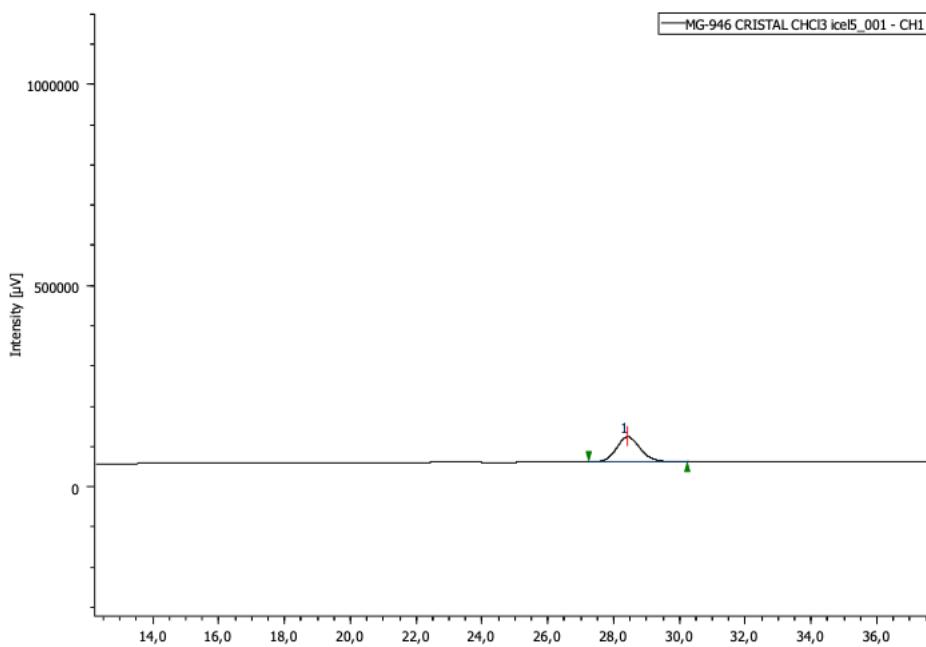


HPLC profile of racemic **3ac**



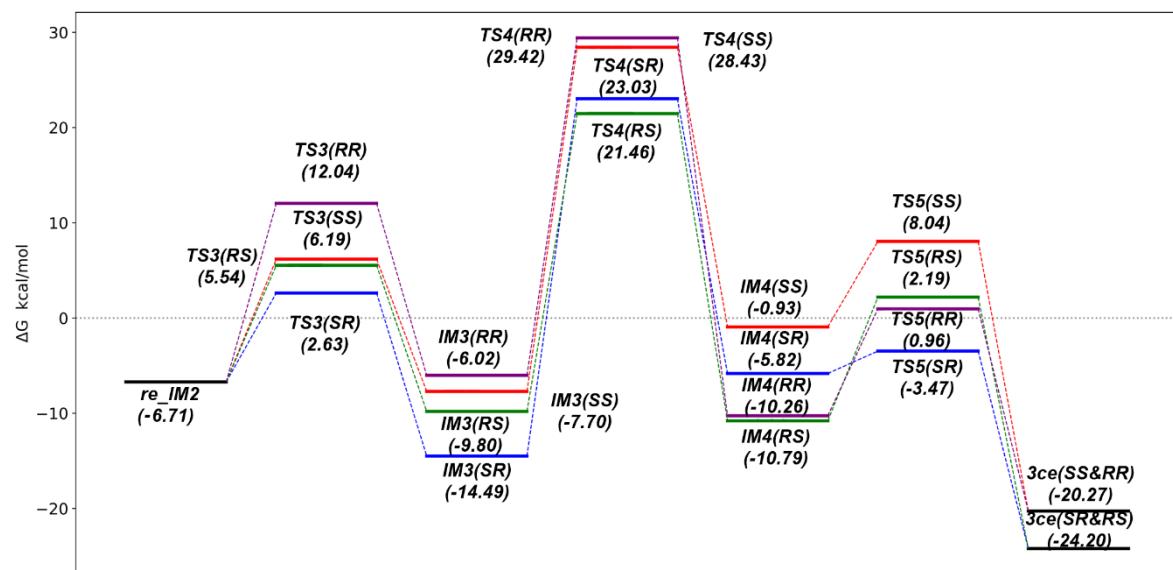
	Time	Area	Area%
1	23,667	6943416	50,308
2	29,025	6858408	49,692

HPLC profile of **3ac** after recrystallization from chloroform



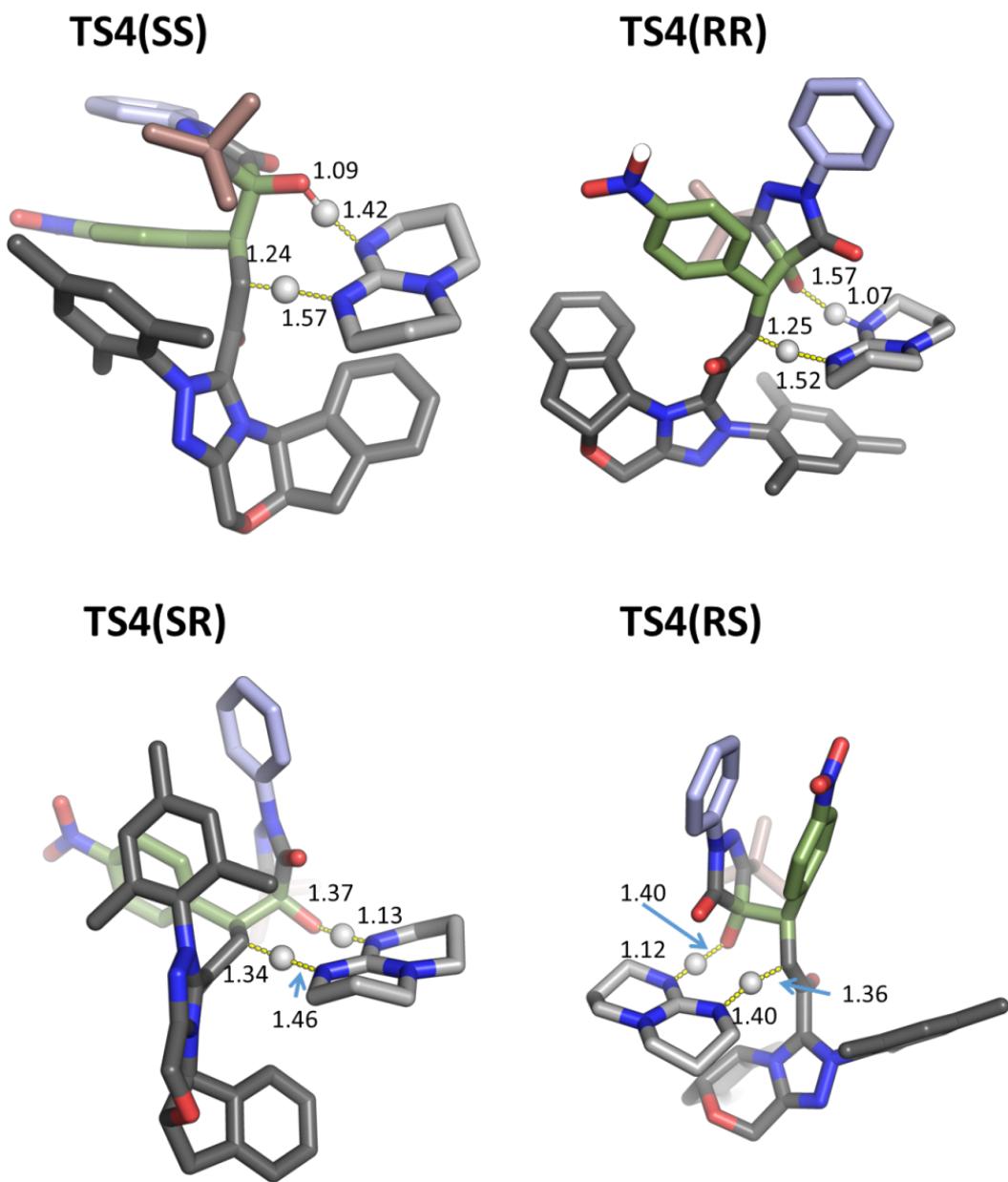
	Time	Area	Area%
1	28,400	3124913	100,000

Scheme S5. Free-energy profile of the second stage of the reaction (complete).



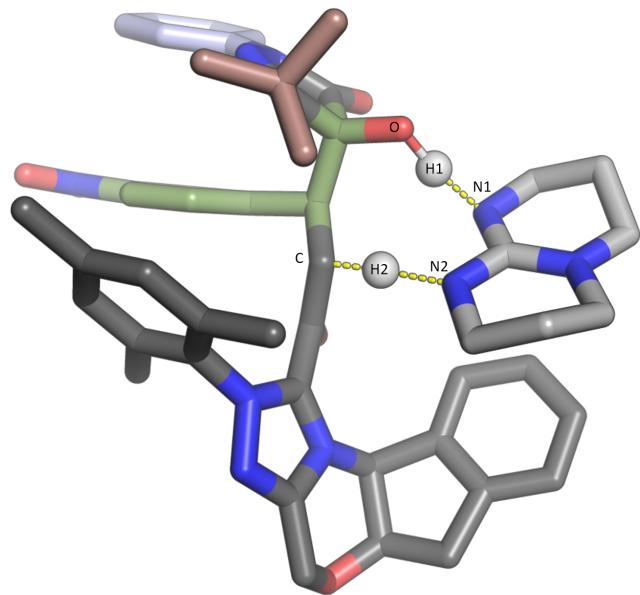
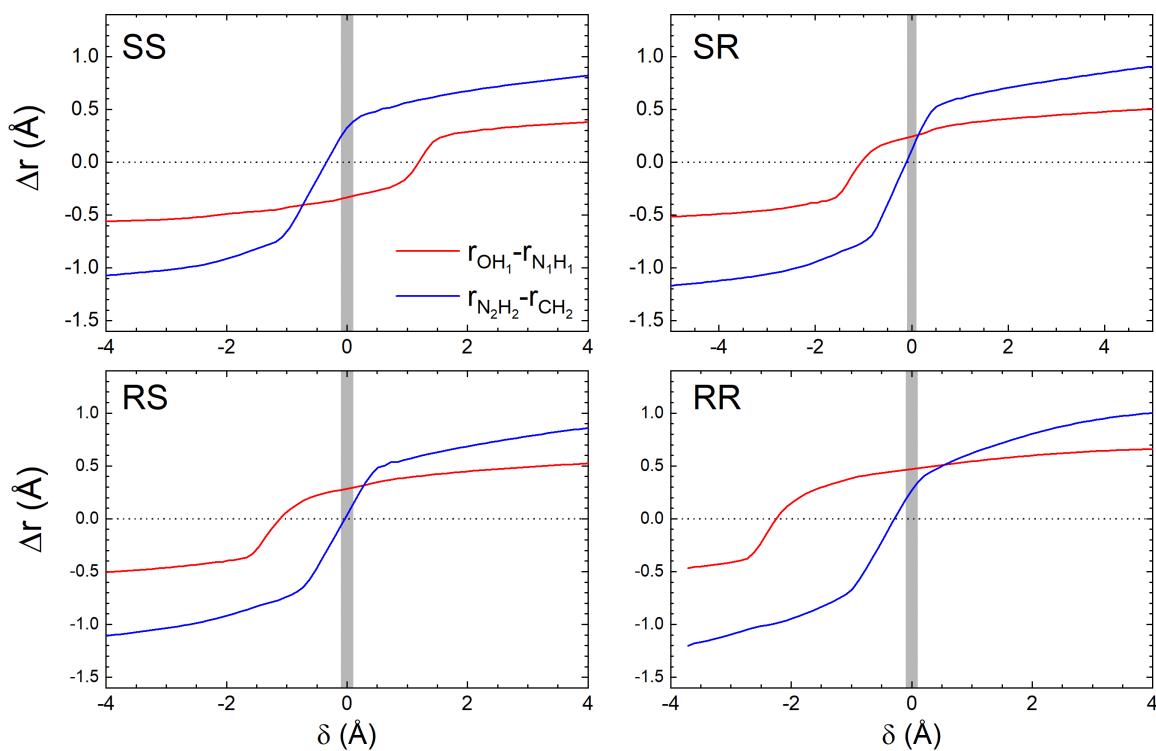
The solvation-corrected relative free-energies at the SMD(toluene)/M06-2X/maug-cc-pVTZ level are given in kcal mol^{-1}

Scheme S6. TS4 detailed structures, with the most relevant distances marked (in Angstroms)



Structures of the four **TS4**. The relevant rOH, rCH and rNH distances are shown. Colour scheme corresponds to that used in Scheme 3. Hydrogens other than those transferred in the reaction are not shown.

Scheme S7. Synchronicity at TS4



Evolution of the proton transfer coordinates as a function of the Intrinsic Reaction Coordinate (δ). Proton transfer coordinates are defined as $r_{\text{OH}1}-r_{\text{N}1\text{H}1}$ for the proton transfer from a hydroxyl group at C4-position of the pyrazoldione moiety to TBD (red line), and as $r_{\text{N}2\text{H}2}-r_{\text{CH}2}$ for the proton transfer from TBD to the α -carbon atom of the homoenolate intermediate (blue line). The TS

region (around $\delta=0$) is shaded. The figure shows how for (SR) and (RS) pathways both proton transfer steps are more concerted. O, H1, N1, N2 and H2 labels are shown in the bottom panel.

Table S3. Energy distortion-interaction analysis

	$\Delta\Delta G$	$\Delta\Delta E_{\text{distortion}}$	$\Delta\Delta E_{\text{interaction}}$	$\Delta\Delta E_{\text{total}}$
TS4(RS)	0.00	0.00	0.00	0.00
TS4(SR)	1.57	-5.02	5.90	0.87
TS4(SS)	6.97	-34.87	35.37	0.50

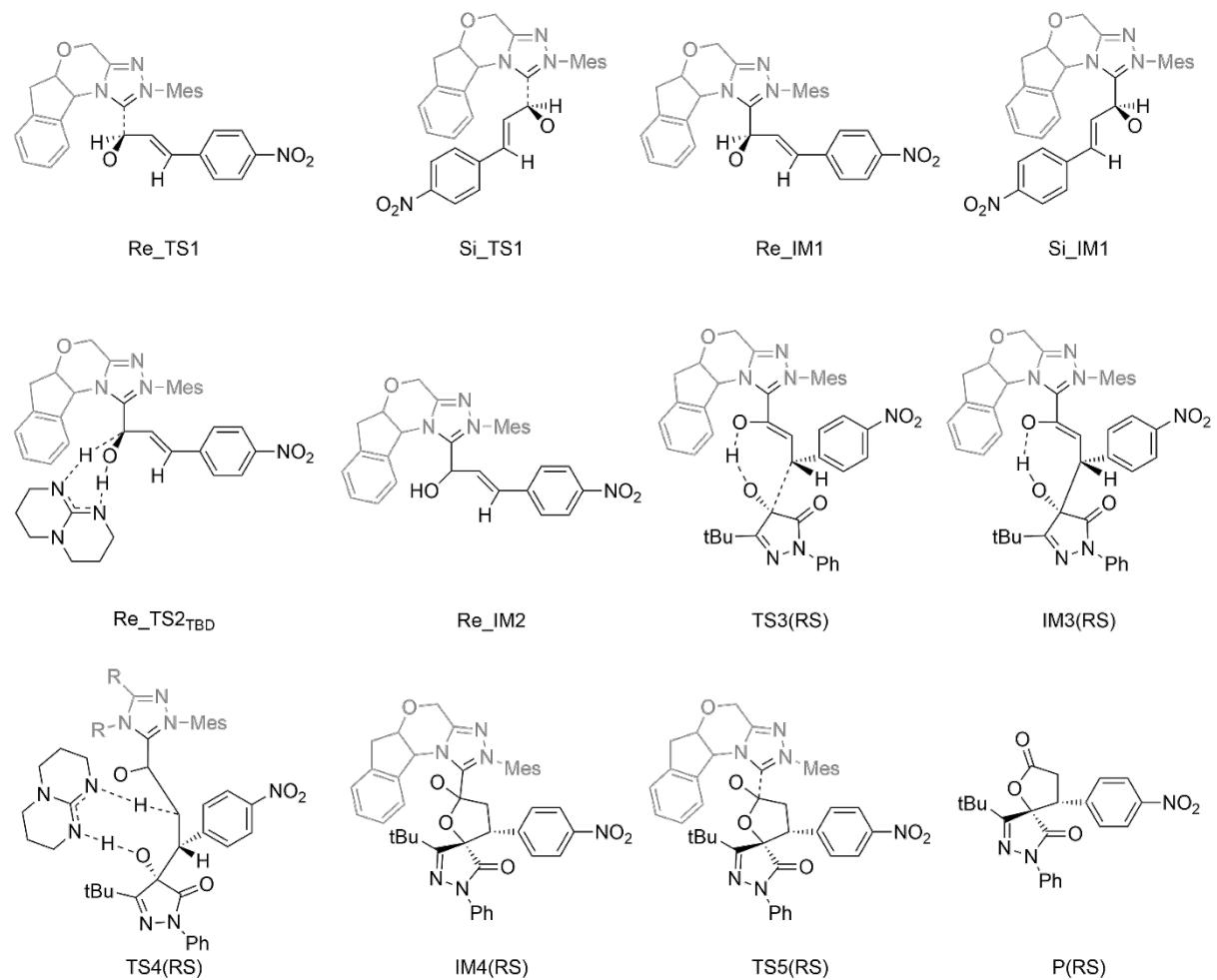
Table S3. Energy distortion-interaction analysis at the SMD(toluene)/M06-2X/maug-cc-pVTZ level (kcal/mol). Results for the (RR) pathway are not shown, as **TS4(RR)** is very high in energy, and its structure is considerably different to **TS4(RS)**, **TS4(SR)**, and **TS4(SS)**, and it would require the definition of different fragments than for the other three structures.

Table S4. Energy decomposition analysis

	Pauli	Electrostatic	Dispersion	Polarization	Chg. Transfer	Total
TS4(RS)	258.13	-157.7	-29.41	-91.81	-98.53	-119.32
TS4(SR)	279.21	-184.23	-23.86	-83.31	-98.23	-110.42
TS4(SS)	205.08	-121.14	-25.27	-61.13	-76.56	-79.04

Table S4. Energy decomposition analysis at the M06-2X/6-31G level (kcal/mol).

Optimized structures for the NHC-catalyzed cycloaddition reaction.



Cartesian coordinates for all the optimized structures.

The following stationary points (minima and saddle points) were optimized at the M06-2X/6-31G(d,p) level of theory using Gaussian16. Solvation effects were included using the SMD continuum solvation model, with the default parameters for toluene.

NHC-1

O	2.7644270000	-1.9385130000	1.0746420000
N	0.8351930000	-0.7285800000	-0.4185190000
N	-1.1936880000	-0.4574300000	-0.0475280000
N	-0.7956240000	-1.3935880000	0.8872240000
C	0.4651850000	-1.5348470000	0.6266410000
C	2.9518690000	0.6104820000	-0.5322140000
C	4.2768130000	0.2923750000	-0.2311090000
C	-2.5638430000	-0.0424620000	-0.0399870000
C	-3.5460550000	-0.9647700000	-0.4172670000
C	2.2018540000	-0.6490520000	-0.9136830000
H	2.1688530000	-0.7578190000	-2.0029260000
C	-0.2348070000	-0.0071810000	-0.8835240000
C	5.1729220000	1.2946450000	0.1189220000
H	6.2043620000	1.0567440000	0.3627560000
C	3.0808090000	-1.7674330000	-0.2988490000
H	2.9647310000	-2.7226360000	-0.8291000000
C	-2.8776020000	1.2597360000	0.3595580000
C	3.3937060000	2.9241260000	-0.1318830000
H	3.0583140000	3.9552600000	-0.0840870000
C	-4.8753770000	-0.5472900000	-0.3948510000
H	-5.6512870000	-1.2494020000	-0.6914030000
C	2.4938330000	1.9194780000	-0.4890580000

H	1.4578870000	2.1446380000	-0.7243120000
C	-3.1747370000	-2.3603020000	-0.8404870000
H	-2.3719820000	-2.3437390000	-1.5840930000
H	-4.0366950000	-2.8719980000	-1.2735770000
H	-2.8148130000	-2.9451130000	0.0109810000
C	-1.8047030000	2.2320650000	0.7696900000
H	-1.0910670000	1.7678390000	1.4569610000
H	-2.2455380000	3.1011370000	1.2626090000
H	-1.2387730000	2.5781370000	-0.0999130000
C	4.5019200000	-1.1977010000	-0.3544690000
H	5.1143940000	-1.6208750000	0.4454200000
H	4.9719660000	-1.4468100000	-1.3127820000
C	-5.2321450000	0.7457440000	-0.0090400000
C	4.7205270000	2.6139180000	0.1671320000
H	5.4071490000	3.4068350000	0.4469740000
C	-4.2220960000	1.6332500000	0.3603250000
H	-4.4846170000	2.6438540000	0.6645370000
C	-6.6795440000	1.1613390000	0.0355920000
H	-7.2591320000	0.6628440000	-0.7456640000
H	-6.7869590000	2.2409850000	-0.0941260000
H	-7.1303850000	0.8973420000	0.9983800000
C	1.4629780000	-2.4449450000	1.2731000000
H	1.2868520000	-2.5011460000	2.3484860000
H	1.3711260000	-3.4578240000	0.8522730000
R1			
C	-1.4452680000	1.4127920000	0.0000090000

C	0.0840270000	1.6431090000	-0.0001270000
C	-1.5742460000	-0.0772860000	-0.0000190000
N	-0.4059670000	-0.6080560000	-0.0000970000
N	0.5965240000	0.3698760000	-0.0002300000
C	1.9481910000	-0.0551730000	-0.0000940000
C	2.9826060000	0.8857750000	0.0000860000
C	2.2347720000	-1.4230670000	-0.0001650000
C	4.3010380000	0.4416750000	0.0002160000
H	2.7583420000	1.9433760000	0.0001240000
C	3.5598260000	-1.8425930000	-0.0000340000
H	1.4256490000	-2.1417820000	-0.0003040000
C	4.5999920000	-0.9172930000	0.0001530000
H	5.1007250000	1.1753920000	0.0003640000
H	3.7758560000	-2.9061990000	-0.0000890000
H	5.6317670000	-1.2520710000	0.0002530000
O	-2.2800780000	2.2755580000	0.0001690000
O	0.6501240000	2.7102490000	-0.0001750000
C	-2.8593710000	-0.8584630000	0.0000540000
C	-3.6578920000	-0.4706800000	-1.2559820000
H	-3.8746520000	0.6009410000	-1.2735910000
H	-3.1099350000	-0.7322810000	-2.1663330000
H	-4.6093790000	-1.0111950000	-1.2633760000
C	-2.5663020000	-2.3582500000	0.0000390000
H	-1.9934790000	-2.6498500000	-0.8849020000
H	-1.9933010000	-2.6498490000	0.8848670000
H	-3.5092870000	-2.9126670000	0.0001340000

C	-3.6578330000	-0.4706470000	1.2561060000
H	-4.6093170000	-1.0111750000	1.2635830000
H	-3.1098580000	-0.7321840000	2.1664730000
H	-3.8746290000	0.6009690000	1.2736840000

R2

C	2.1908230000	0.6130040000	0.0000240000
H	2.4792540000	1.6647010000	0.0000380000
C	0.7449860000	0.3622250000	0.0000120000
C	-0.1252500000	1.4611430000	-0.0000020000
C	0.2059000000	-0.9340510000	0.0000140000
C	-1.5017590000	1.2840070000	-0.0000140000
H	0.2845450000	2.4665090000	-0.0000040000
C	-1.1653640000	-1.1296450000	0.0000030000
H	0.8620810000	-1.7975640000	0.0000250000
C	-1.9942340000	-0.0129540000	-0.0000110000
H	-2.1859880000	2.1230790000	-0.0000250000
H	-1.5978340000	-2.1222020000	0.0000060000
C	3.1708390000	-0.3014080000	0.0000190000
H	2.9953570000	-1.3735300000	0.0000030000
C	4.5741120000	0.1405990000	0.0000290000
H	4.7191870000	1.2413320000	0.0000590000
O	5.5196820000	-0.6158480000	0.0000030000
N	-3.4497140000	-0.2144290000	-0.0000220000
O	-4.1582500000	0.7763190000	-0.0000370000
O	-3.8625470000	-1.3603270000	-0.0000150000

re_IM1

O	5.0790140000	0.8661750000	1.7945860000
N	2.6321330000	0.1337810000	0.8844440000
N	0.8697230000	1.2816030000	0.5782880000
N	1.7211220000	2.0996810000	1.2688560000
C	2.7848190000	1.3763160000	1.4440020000
C	4.4455530000	-1.1075350000	-0.3666270000
C	5.7810070000	-1.3603820000	-0.0439060000
C	-0.4074530000	1.7824060000	0.1395770000
C	-0.4760090000	2.3975320000	-1.1102420000
C	3.6664580000	-0.9071160000	0.9189080000
H	3.1815840000	-1.8362940000	1.2361970000
C	1.4000370000	0.0811060000	0.3355210000
C	6.7023110000	-1.6288600000	-1.0470410000
H	7.7441830000	-1.8200330000	-0.8069980000
C	4.7684550000	-0.5121030000	1.9334550000
H	4.4770670000	-0.7290460000	2.9699530000
C	-1.5116980000	1.6202440000	0.9807030000
C	4.9319430000	-1.3702530000	-2.6834780000
H	4.6133250000	-1.3684120000	-3.7210530000
C	-1.7375420000	2.8164200000	-1.5394290000
H	-1.8269250000	3.2861220000	-2.5156990000
C	3.9947150000	-1.1062000000	-1.6816550000
H	2.9515900000	-0.8887720000	-1.9339350000
C	0.7530130000	2.5710490000	-1.9551540000
H	1.5247020000	3.1278890000	-1.4128340000
H	0.5159220000	3.1172790000	-2.8702910000

H	1.1431200000	1.5777640000	-2.2075390000
C	-1.3777760000	0.9574790000	2.3232420000
H	-2.2990770000	1.0655910000	2.8985520000
H	-0.5559770000	1.3904880000	2.9017040000
H	-1.1770040000	-0.1135660000	2.2078260000
C	5.9945800000	-1.2898460000	1.4510690000
H	6.9117620000	-0.7733570000	1.7439760000
H	6.0064470000	-2.2899240000	1.8994020000
C	-2.8769820000	2.6408030000	-0.7559260000
C	6.2656890000	-1.6319850000	-2.3723610000
H	6.9746630000	-1.8317970000	-3.1699300000
C	-2.7455430000	2.0514230000	0.5051040000
H	-3.6288140000	1.9087870000	1.1239120000
C	-4.2319980000	3.0798570000	-1.2435060000
H	-4.2145580000	3.3166540000	-2.3096890000
H	-4.5711930000	3.9714690000	-0.7059560000
H	-4.9773050000	2.2961380000	-1.0757010000
C	4.0319040000	1.7111880000	2.2037880000
H	4.3293750000	2.7411950000	2.0013390000
H	3.8374660000	1.6090340000	3.2819180000
C	0.8463300000	-1.0096020000	-0.6295200000
H	1.5035440000	-1.8940110000	-0.4042150000
O	0.9285620000	-0.5276390000	-1.8571760000
C	-0.5458070000	-1.3941590000	-0.1310340000
C	-1.6165480000	-1.0841070000	-0.8635010000
H	-0.6154830000	-1.8980110000	0.8340730000

H	-1.4104370000	-0.5751960000	-1.8043430000
C	-3.0227370000	-1.2779300000	-0.4929040000
C	-4.0147620000	-0.6974530000	-1.3005910000
C	-3.4240960000	-1.9774800000	0.6576460000
C	-5.3596380000	-0.7966270000	-0.9767660000
H	-3.7147240000	-0.1502390000	-2.1895290000
C	-4.7623730000	-2.0851200000	0.9998680000
H	-2.6804870000	-2.4487850000	1.2917640000
C	-5.7112940000	-1.4881960000	0.1763320000
H	-6.1297090000	-0.3523060000	-1.5955410000
H	-5.0811860000	-2.6213320000	1.8850790000
N	-7.1258990000	-1.5937930000	0.5355830000
O	-7.4128760000	-2.2071190000	1.5503160000
O	-7.9420470000	-1.0603470000	-0.1972380000

re_TS1

O	4.7051850000	-0.1885280000	2.2793040000
N	2.3829590000	-0.0827640000	0.8739440000
N	0.9095920000	1.4094350000	0.7515670000
N	1.7266330000	1.8079340000	1.7834130000
C	2.6206720000	0.8684040000	1.8339640000
C	4.1839850000	-1.2260980000	-0.4765990000
C	5.3810570000	-1.8375390000	-0.0961150000
C	-0.2119660000	2.2271680000	0.3837300000
C	-1.4349020000	2.0053620000	1.0210650000
C	3.2181190000	-1.2685400000	0.6914970000
H	2.5464710000	-2.1304080000	0.6105900000

C	1.2702450000	0.2590320000	0.1761480000
C	6.4205470000	-1.9674070000	-1.0072160000
H	7.3571500000	-2.4346790000	-0.7170300000
C	4.1613340000	-1.4461000000	1.9070390000
H	3.6524680000	-1.9049490000	2.7656570000
C	-0.0307230000	3.1984400000	-0.6040770000
C	5.0495070000	-0.8554900000	-2.6684710000
H	4.9322960000	-0.4677050000	-3.6753690000
C	-2.5158900000	2.7961540000	0.6313100000
H	-3.4800730000	2.6423520000	1.1112560000
C	3.9970090000	-0.7263830000	-1.7592510000
H	3.0706300000	-0.2372930000	-2.0618560000
C	-1.5790440000	0.9266660000	2.0589110000
H	-1.4112970000	-0.0606600000	1.6134200000
H	-2.5804410000	0.9383240000	2.4937570000
H	-0.8488570000	1.0547360000	2.8641610000
C	1.3060830000	3.3804880000	-1.2660690000
H	2.0996650000	3.5012670000	-0.5219720000
H	1.2986030000	4.2623780000	-1.9095650000
H	1.5338530000	2.4981470000	-1.8747640000
C	5.3197950000	-2.2760390000	1.3494970000
H	6.2362230000	-2.0787900000	1.9107780000
H	5.0917880000	-3.3450420000	1.4312340000
C	-2.3876000000	3.7742670000	-0.3577080000
C	6.2449160000	-1.4707950000	-2.2994340000
H	7.0506790000	-1.5572120000	-3.0218570000

C	-1.1428600000	3.9602030000	-0.9620700000
H	-1.0323790000	4.7174280000	-1.7344530000
C	-3.5611440000	4.6359460000	-0.7431370000
H	-4.5090110000	4.1321580000	-0.5389750000
H	-3.5301850000	4.8948900000	-1.8043150000
H	-3.5549100000	5.5723450000	-0.1750890000
C	3.7449500000	0.6948980000	2.8088670000
H	4.2362460000	1.6512180000	2.9956280000
H	3.3449370000	0.3172240000	3.7617170000
C	0.6195700000	-0.3886440000	-1.6032640000
H	1.0919040000	-1.3874980000	-1.4619320000
O	1.0507070000	0.3923400000	-2.4769090000
C	-0.8551970000	-0.4223000000	-1.3092230000
C	-1.4804030000	-1.5310230000	-0.9000570000
H	-1.3833620000	0.5082570000	-1.5101660000
H	-0.8919760000	-2.4409000000	-0.7725070000
C	-2.9135450000	-1.6553810000	-0.6001920000
C	-3.4708390000	-2.9313100000	-0.4297570000
C	-3.7456130000	-0.5323360000	-0.4548410000
C	-4.8171780000	-3.0953890000	-0.1381460000
H	-2.8364160000	-3.8063210000	-0.5333390000
C	-5.0919140000	-0.6768580000	-0.1629870000
H	-3.3297770000	0.4651790000	-0.5560940000
C	-5.6065870000	-1.9602670000	-0.0102530000
H	-5.2572190000	-4.0762700000	-0.0089500000
H	-5.7425040000	0.1811410000	-0.0464100000

N	-7.0282410000	-2.1195260000	0.3057510000
O	-7.4595470000	-3.2525420000	0.4355600000
O	-7.7020230000	-1.1099750000	0.4226410000

si_IM1

O	0.4300750000	3.7131950000	-1.7027630000
N	1.0302290000	1.2116960000	-0.7831200000
N	2.9108740000	0.2492620000	-0.5366730000
N	3.1891620000	1.4217810000	-1.1807230000
C	2.0277920000	1.9847700000	-1.3219120000
C	-0.9662690000	2.2007700000	0.4305760000
C	-1.8685410000	3.2058590000	0.0745470000
C	3.9841640000	-0.6415070000	-0.1810710000
C	4.3943210000	-1.5897130000	-1.1194210000
C	-0.3879140000	1.5990120000	-0.8333310000
H	-0.9542710000	0.7123990000	-1.1344030000
C	1.6109620000	0.0933820000	-0.2880540000
C	-2.5797580000	3.8824800000	1.0559930000
H	-3.2803070000	4.6691200000	0.7913830000
C	-0.5857670000	2.7345150000	-1.8666650000
H	-0.5908370000	2.3641400000	-2.9007300000
C	4.5832160000	-0.4852430000	1.0718080000
C	-1.4457770000	2.5509920000	2.7373740000
H	-1.2802000000	2.3131970000	3.7836650000
C	5.4539020000	-2.4228330000	-0.7647400000
H	5.7957530000	-3.1709940000	-1.4753170000
C	-0.7324440000	1.8575690000	1.7556170000

H	-0.0187220000	1.0664610000	2.0039470000
C	3.7062930000	-1.7074670000	-2.4523170000
H	2.6763810000	-2.0624590000	-2.3327740000
H	4.2313720000	-2.4162940000	-3.0949320000
H	3.6672130000	-0.7415170000	-2.9650850000
C	4.0879680000	0.5576230000	2.0329480000
H	4.1482760000	1.5569610000	1.5880370000
H	4.6856100000	0.5522070000	2.9464070000
H	3.0377900000	0.3486320000	2.2767640000
C	-1.8970070000	3.3886280000	-1.4260170000
H	-1.9289620000	4.4331930000	-1.7445910000
H	-2.7485010000	2.8658160000	-1.8764130000
C	6.0820520000	-2.3147950000	0.4770290000
C	-2.3615920000	3.5448960000	2.3929560000
H	-2.9027440000	4.0714170000	3.1732680000
C	5.6384000000	-1.3432450000	1.3767190000
H	6.1258110000	-1.2485340000	2.3439030000
C	7.2061240000	-3.2431380000	0.8541720000
H	7.6541200000	-3.7051850000	-0.0284680000
H	6.8406270000	-4.0462530000	1.5027620000
H	7.9900200000	-2.7124550000	1.4007720000
C	1.7054400000	3.2477470000	-2.0623530000
H	2.4317050000	4.0227360000	-1.8117710000
H	1.7666910000	3.0501840000	-3.1431420000
C	1.0349340000	-1.0267760000	0.6181820000
H	1.6888570000	-1.9001900000	0.3543460000

O	1.1084380000	-0.6109580000	1.8737240000
C	-0.3503800000	-1.4070650000	0.1008530000
C	-1.4074030000	-1.3404840000	0.9124130000
H	-0.4370100000	-1.7445740000	-0.9349940000
H	-1.2162550000	-0.9726960000	1.9189670000
C	-2.7947890000	-1.6507270000	0.5428020000
C	-3.8397670000	-1.0174300000	1.2337050000
C	-3.1150810000	-2.5476010000	-0.4892660000
C	-5.1651850000	-1.2472400000	0.8960320000
H	-3.5998730000	-0.3254020000	2.0353070000
C	-4.4336570000	-2.7904510000	-0.8399530000
H	-2.3199290000	-3.0757590000	-1.0052900000
C	-5.4388740000	-2.1304380000	-0.1412730000
H	-5.9789560000	-0.7581340000	1.4167250000
H	-4.6943120000	-3.4838460000	-1.6298550000
N	-6.8343390000	-2.3811970000	-0.5078910000
O	-7.7028970000	-1.8068220000	0.1266660000
O	-7.0522400000	-3.1486050000	-1.4305960000

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O	-0.3038810000	3.2340540000	-1.8795340000
N	0.8042370000	0.9638860000	-0.8390810000
N	2.8144440000	0.3731150000	-0.6549250000
N	2.8490580000	1.4971320000	-1.4449960000
C	1.5990650000	1.8344010000	-1.5402440000
C	-1.1866340000	1.7091190000	0.5111570000
C	-2.2894900000	2.5086710000	0.2038450000

C	4.0502890000	-0.2771690000	-0.3144660000
C	4.6183530000	-1.1511490000	-1.2446590000
C	-0.6492160000	1.1060340000	-0.7676220000
H	-1.0887190000	0.1169380000	-0.9356770000
C	1.5876600000	0.0106420000	-0.2695380000
C	-3.0108610000	3.1212170000	1.2199450000
H	-3.8705680000	3.7449810000	0.9929850000
C	-1.1515620000	2.0951620000	-1.8437620000
H	-1.2085470000	1.6366130000	-2.8403320000
C	4.6423780000	0.0188810000	0.9158850000
C	-1.4768640000	2.1575930000	2.8357520000
H	-1.1611430000	2.0374420000	3.8673200000
C	5.8252060000	-1.7583730000	-0.9034570000
H	6.2884450000	-2.4422410000	-1.6103830000
C	-0.7552290000	1.5279070000	1.8179880000
H	0.1024170000	0.8961640000	2.0505210000
C	3.9442400000	-1.4180890000	-2.5632530000
H	2.9554930000	-1.8658790000	-2.4169520000
H	4.5400260000	-2.1032620000	-3.1689530000
H	3.8039340000	-0.4909280000	-3.1273130000
C	3.9927850000	0.9759090000	1.8764490000
H	3.7237840000	1.9119080000	1.3760650000
H	4.6707110000	1.2093570000	2.6998240000
H	3.0786070000	0.5289130000	2.2848000000
C	-2.5033980000	2.5586020000	-1.2926240000
H	-2.7549290000	3.5521020000	-1.6711450000

H	-3.2918140000	1.8621880000	-1.6019270000
C	6.4493940000	-1.5061230000	0.3197800000
C	-2.5959980000	2.9370840000	2.5408000000
H	-3.1426840000	3.4179910000	3.3461390000
C	5.8489430000	-0.6156540000	1.2107610000
H	6.3327770000	-0.4040950000	2.1610750000
C	7.7359820000	-2.1999710000	0.6823750000
H	8.3636950000	-1.5660300000	1.3134710000
H	8.3064160000	-2.4711600000	-0.2092260000
H	7.5333680000	-3.1211070000	1.2392290000
C	0.9905810000	2.9406830000	-2.3495820000
H	1.5922790000	3.8468040000	-2.2619320000
H	0.9665610000	2.6405140000	-3.4078600000
C	1.2481900000	-1.3762610000	1.1083040000
H	2.0589690000	-2.0159370000	0.7008230000
O	1.3605960000	-0.8877450000	2.2550000000
C	-0.1093820000	-1.7762980000	0.5865820000
C	-1.2083300000	-1.5721980000	1.3167250000
H	-0.1573790000	-2.1692420000	-0.4300200000
H	-1.0773490000	-1.1396500000	2.3060750000
C	-2.5813690000	-1.7349930000	0.8195870000
C	-3.5655040000	-0.8315180000	1.2533340000
C	-2.9281810000	-2.7177740000	-0.1205180000
C	-4.8568600000	-0.8883760000	0.7496690000
H	-3.3009830000	-0.0647840000	1.9771100000
C	-4.2165660000	-2.7933840000	-0.6277340000

H	-2.1824610000	-3.4395820000	-0.4382400000
C	-5.1587560000	-1.8712090000	-0.1856970000
H	-5.6217220000	-0.1902470000	1.0664560000
H	-4.5020150000	-3.5507990000	-1.3470980000
N	-6.5198930000	-1.9409380000	-0.7238200000
O	-7.3305270000	-1.1191030000	-0.3312840000
O	-6.7668490000	-2.8146510000	-1.5379020000

re_IM2

O	-5.5344600000	0.8782750000	-0.1074310000
N	-2.8727460000	0.5294450000	-0.6450930000
N	-1.2177430000	1.8138490000	-0.1086180000
N	-2.3665400000	2.5521270000	0.1031230000
C	-3.3259530000	1.7593480000	-0.2312640000
C	-3.9039790000	-1.6178950000	0.1766580000
C	-5.2262200000	-2.0651810000	0.2234540000
C	0.0545120000	2.4099100000	0.1384510000
C	0.8271740000	2.8343430000	-0.9496800000
C	-3.7693620000	-0.5882620000	-0.9287940000
H	-3.4342160000	-1.0661800000	-1.8515600000
C	-1.4912520000	0.5432420000	-0.5528160000
C	-5.6039190000	-3.0474310000	1.1295560000
H	-6.6320770000	-3.3947790000	1.1730730000
C	-5.2237710000	-0.0873810000	-1.0993980000
H	-5.3977300000	0.3342830000	-2.0986550000
C	0.4953740000	2.5171480000	1.4604210000
C	-3.3294030000	-3.1043540000	1.9633020000

H	-2.5983630000	-3.5049390000	2.6582180000
C	2.0934270000	3.3483700000	-0.6824260000
H	2.7162770000	3.6721950000	-1.5130860000
C	-2.9458630000	-2.1243490000	1.0461270000
H	-1.9264860000	-1.7466230000	1.0431800000
C	0.3116190000	2.6956050000	-2.3547600000
H	0.2899360000	1.6422400000	-2.6565860000
H	0.9497900000	3.2372200000	-3.0553340000
H	-0.7074060000	3.0850520000	-2.4386020000
C	-0.3722410000	2.0432880000	2.5942380000
H	-1.3177430000	2.5929710000	2.6209370000
H	0.1350450000	2.1759690000	3.5515550000
H	-0.6185770000	0.9817210000	2.4815340000
C	-6.0680710000	-1.3273470000	-0.7928570000
H	-7.0541060000	-1.0380220000	-0.4217150000
H	-6.2053580000	-1.9232900000	-1.7023360000
C	2.5808490000	3.4583840000	0.6231550000
C	-4.6438850000	-3.5673310000	1.9984680000
H	-4.9261400000	-4.3291500000	2.7181700000
C	1.7668600000	3.0492200000	1.6805130000
H	2.1316770000	3.1372130000	2.7008610000
C	3.9674020000	3.9918710000	0.8707540000
H	4.1175490000	4.9483770000	0.3618940000
H	4.7227770000	3.2978000000	0.4874950000
H	4.1536920000	4.1386990000	1.9367200000
C	-4.7914780000	2.0638890000	-0.2698950000

H	-5.0507700000	2.7439210000	0.5426080000
H	-5.0386850000	2.5497560000	-1.2259740000
C	-0.6234710000	-0.4939760000	-0.8750580000
O	-1.1925220000	-1.5800690000	-1.5317910000
C	0.7628140000	-0.5208050000	-0.5859850000
C	1.6119090000	-1.5220700000	-0.9540180000
H	1.1521870000	0.3063420000	-0.0029500000
H	1.2316540000	-2.3385770000	-1.5624670000
C	3.0217300000	-1.5701940000	-0.6280530000
C	3.7972630000	-2.6541770000	-1.0958690000
C	3.6829450000	-0.5797940000	0.1362290000
C	5.1492310000	-2.7551440000	-0.8259210000
H	3.3134850000	-3.4266120000	-1.6863390000
C	5.0332340000	-0.6670380000	0.4125600000
H	3.1319520000	0.2733580000	0.5195840000
C	5.7580870000	-1.7560790000	-0.0706570000
H	5.7394180000	-3.5881770000	-1.1876750000
H	5.5386040000	0.0920450000	0.9972720000
H	-1.0736030000	-2.3653970000	-0.9754960000
N	7.1774610000	-1.8497430000	0.2202640000
O	7.6906130000	-0.9574450000	0.8809580000
O	7.7914720000	-2.8160160000	-0.2093190000

re_TS2

C	-1.0973530000	-0.5317430000	0.4658840000
C	-0.4061370000	-0.4234690000	1.6172310000
C	0.9549710000	0.0762720000	1.7807330000

H	-0.8561680000	-0.7241210000	2.5618740000
H	1.1624200000	0.6414470000	2.7861450000
O	1.7941850000	-0.5501190000	2.7800840000
C	-2.4966420000	-0.9214720000	0.3275130000
C	-3.3333030000	-1.2138210000	1.4217880000
C	-3.0454110000	-1.0018200000	-0.9657900000
C	-4.6534780000	-1.5825250000	1.2335130000
C	-4.3658480000	-1.3642770000	-1.1723830000
H	-2.4136210000	-0.7717540000	-1.8193340000
C	-5.1541360000	-1.6524420000	-0.0639880000
H	-5.3018420000	-1.8107570000	2.0704020000
H	-4.7906890000	-1.4271740000	-2.1665050000
H	-2.9475520000	-1.1468550000	2.4330700000
C	2.7736680000	-4.2901010000	-0.9060940000
C	3.8357630000	-3.5247360000	-1.3848260000
C	4.1291190000	-2.3175530000	-0.7583590000
C	2.3194890000	-2.6593560000	0.8297350000
C	2.0233950000	-3.8622390000	0.1908660000
H	2.5329100000	-5.2333150000	-1.3870650000
H	4.4250980000	-3.8667190000	-2.2307930000
H	1.7803590000	-2.3106660000	1.7089730000
H	1.2067690000	-4.4772970000	0.5556640000
C	3.3717340000	-1.8940800000	0.3357290000
C	3.8657640000	-0.5596520000	0.8513270000
C	5.2438740000	-0.4065040000	0.1447720000
H	3.9086350000	-0.5184030000	1.9387500000

C	5.2073080000	-1.3221230000	-1.1001510000
H	5.9952950000	-0.7869150000	0.8397680000
H	4.9451430000	-0.7669770000	-2.0077120000
H	6.1808170000	-1.7847760000	-1.2805330000
N	2.9896880000	0.5525290000	0.4238600000
O	5.6166470000	0.9374730000	-0.0933380000
C	3.3404920000	1.5043410000	-0.4969260000
C	4.7577270000	1.6319950000	-0.9662350000
H	4.8443190000	1.2824630000	-2.0025410000
H	5.0532540000	2.6828040000	-0.9428520000
N	2.3284020000	2.2359790000	-0.8422180000
C	1.6659960000	0.7187280000	0.6972520000
N	1.2830040000	1.7455380000	-0.1024010000
C	-0.0080430000	2.3522070000	-0.2226970000
C	-0.6909020000	2.1903040000	-1.4392560000
C	-0.5438630000	3.0702280000	0.8467760000
C	-1.9677710000	2.7286470000	-1.5411990000
C	-1.8340540000	3.5871130000	0.6933780000
C	-2.5632650000	3.4164580000	-0.4785560000
H	-2.5186250000	2.6026140000	-2.4705140000
H	-2.2719620000	4.1432120000	1.5187800000
C	-0.0652670000	1.4584850000	-2.5966110000
H	-0.8116070000	1.2533870000	-3.3668020000
H	0.7361400000	2.0535650000	-3.0447710000
H	0.3825090000	0.5079020000	-2.2869930000
C	0.2067470000	3.3038160000	2.1293750000

H	1.2888120000	3.2660660000	1.9819770000
H	-0.0466670000	4.2855980000	2.5361570000
H	-0.0601780000	2.5525160000	2.8788930000
C	-3.9652490000	3.9480220000	-0.6121280000
H	-4.2308260000	4.5880890000	0.2318660000
H	-4.0814870000	4.5272060000	-1.5326570000
H	-4.6854510000	3.1242100000	-0.6507740000
H	-0.5911960000	-0.3069630000	-0.4694860000
N	-6.5482790000	-2.0337860000	-0.2661790000
O	-7.2235650000	-2.2801750000	0.7204120000
O	-6.9668010000	-2.0862350000	-1.4119630000

re_TS2_{2w}

C	-1.6907710000	-1.5007330000	0.5187480000
C	-0.9620740000	-0.4116120000	0.7958070000
C	0.5117390000	-0.4492680000	1.0017720000
H	-1.4502040000	0.5421470000	0.9721990000
O	1.0614940000	-1.7347280000	0.8692690000
C	-3.1508700000	-1.5224790000	0.3722950000
C	-3.7992610000	-2.7582760000	0.2176400000
C	-3.9335030000	-0.3533050000	0.3585930000
C	-5.1751760000	-2.8394200000	0.0629510000
C	-5.3076450000	-0.4145030000	0.2052780000
H	-3.4614080000	0.6189970000	0.4562500000
C	-5.9099030000	-1.6608590000	0.0596920000
H	-5.6801060000	-3.7903470000	-0.0534090000
H	-5.9168590000	0.4809310000	0.1936420000

H	-3.2077530000	-3.6686600000	0.2226930000
C	5.3503110000	-3.0294430000	-2.2964150000
C	6.1348980000	-2.2355720000	-1.4632750000
C	5.5078190000	-1.4172690000	-0.5270940000
C	3.3268990000	-2.2017750000	-1.2520900000
C	3.9574760000	-3.0150370000	-2.1903730000
H	5.8259430000	-3.6682750000	-3.0340410000
H	7.2178170000	-2.2517480000	-1.5450890000
H	2.2474350000	-2.1972340000	-1.1362430000
H	3.3620610000	-3.6468300000	-2.8416500000
C	4.1181690000	-1.4025730000	-0.4321630000
C	3.6586950000	-0.4398760000	0.6419460000
C	4.9661650000	0.3301400000	1.0689600000
H	3.2322080000	-0.9542710000	1.5044620000
C	6.1360790000	-0.4935200000	0.4838330000
H	5.0150080000	0.3848410000	2.1569930000
H	6.8866360000	0.1778980000	0.0547450000
H	6.6290260000	-1.0647150000	1.2771400000
N	2.6555540000	0.5054720000	0.1290770000
O	5.0051830000	1.6869900000	0.6486970000
C	3.0336100000	1.6232960000	-0.5660170000
C	4.4952790000	1.9103760000	-0.6515660000
H	4.9830970000	1.2741580000	-1.4025280000
H	4.6586440000	2.9574560000	-0.9076680000
N	2.0101660000	2.3397050000	-0.9124200000
C	1.3042250000	0.5106440000	0.2000080000

N	0.9367440000	1.6289230000	-0.4406260000
C	-0.3838140000	2.1773590000	-0.5794170000
C	-1.1482650000	1.8108200000	-1.6866600000
C	-0.8469600000	3.0149980000	0.4393730000
C	-2.4431360000	2.3236520000	-1.7622740000
C	-2.1484650000	3.4983830000	0.3187560000
C	-2.9558980000	3.1655730000	-0.7735740000
H	-3.0693040000	2.0465580000	-2.6065280000
H	-2.5441810000	4.1433550000	1.0993640000
C	-0.6122700000	0.8522700000	-2.7131880000
H	0.3984450000	1.1275730000	-3.0278540000
H	-0.5707540000	-0.1623370000	-2.2997760000
H	-1.2564120000	0.8309380000	-3.5938570000
C	0.0112550000	3.3161080000	1.6388430000
H	0.1998360000	2.4145880000	2.2391570000
H	0.9821440000	3.7203130000	1.3345020000
H	-0.4771280000	4.0496980000	2.2825220000
C	-4.3566010000	3.7077940000	-0.8799280000
H	-4.9793340000	3.0734720000	-1.5151440000
H	-4.8275540000	3.7818660000	0.1037110000
H	-4.3504780000	4.7119110000	-1.3171340000
O	2.1953330000	-1.8523270000	3.1905860000
O	1.2867250000	0.4113180000	3.4106270000
H	0.7727300000	0.0098790000	2.1233680000
H	1.4407570000	-1.9708390000	1.7681250000
H	1.9015140000	-2.4589280000	3.8774740000

H	1.8308240000	-0.8657720000	3.4315900000
H	2.0187700000	1.0264150000	3.2723570000
H	-1.1726020000	-2.4484950000	0.3982340000
N	-7.3611600000	-1.7298410000	-0.1077950000
O	-7.8709400000	-2.8314280000	-0.2283220000
O	-7.9847920000	-0.6810360000	-0.1193610000

re_TS2_{TBD}

C	-1.9941210000	0.8687640000	0.9446100000
C	-1.2336990000	0.2697850000	0.0158770000
H	-1.6772660000	-0.0840470000	-0.9134810000
C	-3.4441290000	1.0482110000	0.8529200000
C	-4.0882790000	1.9129720000	1.7539510000
C	-4.2342470000	0.3601910000	-0.0880580000
C	-5.4602690000	2.1075310000	1.7151390000
C	-5.6049220000	0.5443880000	-0.1435880000
H	-3.7709560000	-0.3451590000	-0.7710920000
C	-6.2004190000	1.4196890000	0.7610110000
H	-5.9595180000	2.7771640000	2.4043970000
H	-6.2183940000	0.0182250000	-0.8648190000
H	-3.4939100000	2.4430380000	2.4917880000
C	5.3199330000	-1.7643930000	3.5260060000
C	5.9801820000	-1.5521010000	2.3174460000
C	5.2389330000	-1.1590190000	1.2064370000
C	3.1948680000	-1.1767610000	2.5200330000
C	3.9397560000	-1.5753210000	3.6279560000
H	5.8847250000	-2.0769140000	4.3988980000

H	7.0543980000	-1.6952530000	2.2432950000
H	2.1255690000	-0.9950610000	2.5822210000
H	3.4444920000	-1.7352560000	4.5804090000
C	3.8608580000	-0.9832870000	1.3139000000
C	3.2698170000	-0.5537370000	-0.0122040000
C	4.4351790000	-0.7565080000	-1.0443230000
H	2.9392530000	0.4878620000	0.0043400000
C	5.7183650000	-0.8484870000	-0.1894570000
H	4.4591730000	0.0840570000	-1.7390640000
H	6.3906970000	-1.6064810000	-0.6027630000
H	6.2532250000	0.1071280000	-0.2085810000
N	2.1239290000	-1.3814260000	-0.3931600000
O	4.2727630000	-1.8990650000	-1.8796180000
C	2.2911360000	-2.6336410000	-0.9136490000
C	3.6905020000	-3.0281400000	-1.2551650000
H	4.2438460000	-3.3374000000	-0.3582760000
H	3.6884940000	-3.8480370000	-1.9739650000
N	1.1518470000	-3.2088940000	-1.1502710000
C	0.7972370000	-1.1480830000	-0.2999940000
N	0.2257690000	-2.2799040000	-0.7426090000
C	-1.1644910000	-2.6321690000	-0.6903670000
C	-1.7606760000	-2.7768600000	0.5677730000
C	-1.8599900000	-2.7857400000	-1.8908710000
C	-3.1235370000	-3.0634140000	0.5946580000
C	-3.2208770000	-3.0847290000	-1.8076960000
C	-3.8672020000	-3.2197030000	-0.5781200000

H	-3.6188960000	-3.1644390000	1.5571710000
H	-3.7887530000	-3.2030460000	-2.7270780000
C	-0.9677540000	-2.6068930000	1.8361090000
H	-0.0385360000	-3.1853880000	1.8008000000
H	-0.7042150000	-1.5558370000	2.0048630000
H	-1.5498710000	-2.9496270000	2.6934400000
C	-1.1690360000	-2.6133410000	-3.2163290000
H	-0.6451700000	-1.6528950000	-3.2696660000
H	-0.4222350000	-3.3968030000	-3.3743970000
H	-1.8915820000	-2.6538040000	-4.0332680000
C	-5.3399240000	-3.5235930000	-0.5038580000
H	-5.5080150000	-4.5581780000	-0.1871250000
H	-5.8355960000	-2.8749300000	0.2239530000
H	-5.8246030000	-3.3873080000	-1.4732230000
H	-1.5006640000	1.2523500000	1.8341040000
N	-7.6475530000	1.6119160000	0.7116890000
O	-8.1511540000	2.3789830000	1.5161770000
O	-8.2781870000	0.9946190000	-0.1319300000
C	0.2333420000	0.1431320000	0.1270380000
O	0.7802660000	0.5135060000	1.3595020000
H	0.7640990000	0.9243490000	-0.7288530000
C	2.0529900000	2.8686250000	-0.6430370000
N	2.4119760000	4.1104450000	-1.1491230000
N	1.5888030000	1.9083890000	-1.4531200000
C	2.4654280000	4.3261200000	-2.5843030000
C	1.4128900000	2.1204150000	-2.8738050000

C	1.3136800000	3.5931460000	-3.2519990000
H	2.3973870000	5.4047660000	-2.7615740000
H	0.5067410000	1.5883410000	-3.1979600000
H	1.3548700000	3.7238510000	-4.3376460000
N	2.1306000000	2.5930980000	0.6561050000
H	1.3399820000	1.3824010000	1.1659420000
C	2.7022840000	3.5507970000	1.5817600000
H	2.2148820000	3.4242750000	2.5559140000
H	3.7730530000	3.3434380000	1.7503840000
C	2.5578530000	4.9923280000	1.1110360000
H	3.1049150000	5.6782890000	1.7649040000
H	1.5014730000	5.2815410000	1.1161830000
C	3.0901960000	5.0825310000	-0.3089450000
H	2.9079390000	6.0762610000	-0.7332160000
H	4.1811970000	4.9226740000	-0.3136300000
H	2.2451960000	1.6708730000	-3.4420930000
H	0.3688440000	4.0123110000	-2.8902130000
H	3.4254790000	3.9866970000	-3.0080050000

si_IM2

O	1.4169640000	4.2899870000	-0.7089630000
N	1.3550100000	1.5620940000	-0.6561110000
N	2.9655380000	0.1370480000	-0.4059380000
N	3.5582530000	1.3821760000	-0.5245930000
C	2.5747070000	2.1982170000	-0.6796510000
C	-0.6786250000	2.5590480000	0.4442470000
C	-1.3007530000	3.8034250000	0.3205460000

C	3.7712750000	-0.9567150000	0.0328930000
C	4.7480110000	-1.4548220000	-0.8385940000
C	0.0943700000	2.2631290000	-0.8294240000
H	-0.5153900000	1.6904330000	-1.5403020000
C	1.5976610000	0.2046190000	-0.5222340000
C	-2.0975330000	4.2928690000	1.3466080000
H	-2.5799240000	5.2618880000	1.2589750000
C	0.3348320000	3.6831160000	-1.3962680000
H	0.5303050000	3.6704020000	-2.4768910000
C	3.5891670000	-1.4712140000	1.3195110000
C	-1.6031880000	2.3004680000	2.6369860000
H	-1.7141240000	1.7279860000	3.5520270000
C	5.5468940000	-2.5020950000	-0.3905380000
H	6.3081910000	-2.9035050000	-1.0558270000
C	-0.8060990000	1.8040270000	1.6036120000
H	-0.2907540000	0.8530560000	1.7118660000
C	4.9020520000	-0.8833050000	-2.2208590000
H	3.9493810000	-0.9189840000	-2.7591490000
H	5.6422050000	-1.4484360000	-2.7906660000
H	5.2157330000	0.1638540000	-2.1829220000
C	2.5567530000	-0.9014200000	2.2557560000
H	2.5599270000	0.1928910000	2.2296370000
H	2.7550090000	-1.2196240000	3.2812160000
H	1.5425610000	-1.2275710000	1.9938140000
C	-0.9296780000	4.4472430000	-0.9962550000
H	-0.7247340000	5.5174040000	-0.9187590000

H	-1.7125920000	4.3005650000	-1.7490650000
C	5.3860820000	-3.0589990000	0.8813490000
C	-2.2503100000	3.5280580000	2.5042290000
H	-2.8654790000	3.9008940000	3.3169660000
C	4.4043950000	-2.5332420000	1.7180770000
H	4.2752470000	-2.9464150000	2.7156490000
C	6.2595710000	-4.2030330000	1.3254220000
H	7.3192560000	-3.9423360000	1.2458410000
H	6.0942900000	-5.0864200000	0.7004060000
H	6.0553410000	-4.4802460000	2.3619580000
C	2.6491020000	3.6655360000	-0.9809730000
H	3.4114350000	4.1393000000	-0.3604750000
H	2.9285900000	3.7973630000	-2.0370660000
C	0.7269080000	-0.8763120000	-0.5834380000
O	1.3351890000	-2.1099220000	-0.7566280000
C	-0.6889290000	-0.8307500000	-0.5110310000
C	-1.4977340000	-1.9198090000	-0.6451060000
H	-1.1502460000	0.1271150000	-0.2982880000
H	-1.0479700000	-2.8711880000	-0.9152190000
C	-2.9377640000	-1.9029770000	-0.4959840000
C	-3.6804510000	-3.0470510000	-0.8624700000
C	-3.6552540000	-0.7958770000	0.0135890000
C	-5.0577840000	-3.0877620000	-0.7520830000
H	-3.1508880000	-3.9128260000	-1.2486170000
C	-5.0320810000	-0.8203910000	0.1250260000
H	-3.1241370000	0.0902730000	0.3476330000

C	-5.7240150000	-1.9673290000	-0.2616730000
H	-5.6243810000	-3.9650930000	-1.0391570000
H	-5.5808840000	0.0273670000	0.5165950000
H	1.2385580000	-2.6280050000	0.0567360000
N	-7.1712860000	-1.9978290000	-0.1400130000
O	-7.7341710000	-1.0023230000	0.2929780000
O	-7.7563080000	-3.0170520000	-0.4771280000

si_TS2

O	1.6555480000	4.3565200000	-0.1459080000
N	1.4979480000	1.6590400000	-0.5506040000
N	2.9515910000	0.1111770000	-0.2239160000
N	3.6032060000	1.3045120000	0.0014370000
C	2.7082190000	2.2102640000	-0.2117440000
C	-0.6616690000	2.6275090000	0.3242330000
C	-1.2038130000	3.9142970000	0.2702840000
C	3.6399750000	-1.1020300000	0.1134580000
C	4.8420490000	-1.3785760000	-0.5400260000
C	0.3137560000	2.4609260000	-0.8293550000
H	-0.1752740000	2.0340170000	-1.7138160000
C	1.6655620000	0.2996500000	-0.5972320000
C	-2.1551760000	4.3124720000	1.1993750000
H	-2.5765330000	5.3127870000	1.1661890000
C	0.7170000000	3.9264210000	-1.1190200000
H	1.1263880000	4.0550400000	-2.1297760000
C	3.1218150000	-1.9211060000	1.1224990000
C	-1.9760210000	2.1415110000	2.2641040000

H	-2.2720670000	1.4602520000	3.0549270000
C	5.5421130000	-2.5201400000	-0.1482470000
H	6.4779470000	-2.7563860000	-0.6488390000
C	-1.0236840000	1.7363330000	1.3265150000
H	-0.5789870000	0.7462170000	1.3890280000
C	5.3647720000	-0.4952730000	-1.6412360000
H	5.7741000000	0.4376680000	-1.2437620000
H	4.5680260000	-0.2297980000	-2.3431660000
H	6.1519040000	-1.0090910000	-2.1967890000
C	1.8087420000	-1.6157470000	1.7884840000
H	1.7389070000	-0.5627230000	2.0822690000
H	1.6852550000	-2.2252020000	2.6860780000
H	0.9919760000	-1.8503970000	1.0962250000
C	-0.5736090000	4.7048350000	-0.8545380000
H	-0.3516190000	5.7413330000	-0.5909940000
H	-1.2046880000	4.7042830000	-1.7506270000
C	5.0687470000	-3.3637040000	0.8544160000
C	-2.5434000000	3.4127760000	2.1934830000
H	-3.2816140000	3.7125030000	2.9303960000
C	3.8590110000	-3.0474900000	1.4759720000
H	3.4747700000	-3.6990660000	2.2573450000
C	5.8240370000	-4.6069030000	1.2449980000
H	6.8520170000	-4.5803480000	0.8762850000
H	5.3429650000	-5.4989940000	0.8302500000
H	5.8528460000	-4.7272430000	2.3315700000
C	2.8956200000	3.6981920000	-0.2400000000

H	3.5095620000	4.0168000000	0.6039780000
H	3.4156530000	3.9693470000	-1.1708240000
C	0.7905990000	-0.7216620000	-1.1332090000
O	1.3419270000	-2.0237460000	-1.2132080000
C	-0.6563130000	-0.6262840000	-0.9175930000
C	-1.4189760000	-1.7354750000	-0.8709400000
H	-1.1161190000	0.3501670000	-0.8139310000
H	-0.9156690000	-2.6880640000	-1.0111470000
C	-2.8643330000	-1.7589170000	-0.6563450000
C	-3.5498190000	-2.9803870000	-0.7852630000
C	-3.6094990000	-0.6152300000	-0.3066040000
C	-4.9187810000	-3.0676160000	-0.5902460000
H	-2.9888800000	-3.8724590000	-1.0464750000
C	-4.9771670000	-0.6837020000	-0.1092820000
H	-3.1103960000	0.3389670000	-0.1684140000
C	-5.6158700000	-1.9122430000	-0.2562520000
H	-5.4495000000	-4.0061180000	-0.6921720000
H	-5.5539780000	0.1914360000	0.1632340000
H	1.1719220000	-1.0557340000	-2.1834190000
N	-7.0582130000	-1.9899210000	-0.0447600000
O	-7.5977170000	-3.0775460000	-0.1704060000
O	-7.6502520000	-0.9626110000	0.2466630000

si_TS2_{2w}

O	-1.6927700000	4.3819150000	-0.4631060000
N	-1.4491160000	1.7126210000	0.0438330000
N	-2.7225580000	0.0606770000	-0.4101810000

N	-3.3682450000	1.1741210000	-0.8873340000
C	-2.5801220000	2.1589060000	-0.5878440000
C	0.7670120000	2.8627770000	-0.3609090000
C	1.1823550000	4.1866230000	-0.1855910000
C	-3.3224610000	-1.2284300000	-0.6428210000
C	-4.4862860000	-1.5492310000	0.0580370000
C	-0.4116720000	2.6050050000	0.5620220000
H	-0.1171590000	2.2098430000	1.5445430000
C	-1.5621610000	0.3681130000	0.1765970000
C	2.2763320000	4.6763190000	-0.8843400000
H	2.6002400000	5.7046360000	-0.7542530000
C	-0.9953620000	4.0258730000	0.7240520000
H	-1.6490860000	4.1124230000	1.6018640000
C	-2.7278770000	-2.0790840000	-1.5741000000
C	2.4957250000	2.5282070000	-1.9842770000
H	3.0009830000	1.8914520000	-2.7032570000
C	-5.0838520000	-2.7738860000	-0.2337360000
H	-5.9890600000	-3.0533970000	0.2996590000
C	1.3987400000	2.0313910000	-1.2759110000
H	1.0492340000	1.0176810000	-1.4544030000
C	-5.0246400000	-0.6457770000	1.1336360000
H	-4.3211740000	-0.6060210000	1.9752650000
H	-5.9762950000	-1.0280860000	1.5081540000
H	-5.1852880000	0.3705860000	0.7639140000
C	-1.4243290000	-1.7210520000	-2.2321200000
H	-1.4469510000	-0.7100020000	-2.6523050000

H	-1.1952410000	-2.4195620000	-3.0389730000
H	-0.6064300000	-1.7681900000	-1.5023510000
C	0.2546810000	4.9063720000	0.7686780000
H	0.0218680000	5.9289570000	0.4637650000
H	0.6596000000	4.9298600000	1.7866090000
C	-4.5442950000	-3.6510240000	-1.1762020000
C	2.9380770000	3.8332830000	-1.7793070000
H	3.7913140000	4.2051100000	-2.3374610000
C	-3.3635020000	-3.2928630000	-1.8277880000
H	-2.9210420000	-3.9763850000	-2.5479690000
C	-5.2338510000	-4.9518510000	-1.4928820000
H	-4.5282280000	-5.6917220000	-1.8779960000
H	-6.0082140000	-4.8046730000	-2.2534800000
H	-5.7190270000	-5.3683190000	-0.6065580000
C	-2.8572220000	3.6303950000	-0.6973950000
H	-3.2177080000	3.8775680000	-1.6974930000
H	-3.6462270000	3.8814730000	0.0267400000
C	-0.7499040000	-0.4818180000	1.0890700000
O	-1.3121380000	-1.7459710000	1.2295370000
C	0.7070610000	-0.5123610000	0.7971250000
C	1.4250160000	-1.6433420000	0.7823070000
H	1.1954520000	0.4493770000	0.6700390000
H	0.8982450000	-2.5799100000	0.9464790000
C	2.8737960000	-1.7309000000	0.5671030000
C	3.4856470000	-2.9935930000	0.6227190000
C	3.6804280000	-0.6111460000	0.2929370000

C	4.8481880000	-3.1477690000	0.4163970000
H	2.8755050000	-3.8664050000	0.8336570000
C	5.0419270000	-0.7460300000	0.0821190000
H	3.2416680000	0.3799760000	0.2366470000
C	5.6069320000	-2.0161600000	0.1475050000
H	5.3247700000	-4.1191220000	0.4602030000
H	5.6690800000	0.1106710000	-0.1313960000
O	-1.2917930000	1.0350550000	3.2354630000
O	-2.5309650000	-1.1170920000	3.4679030000
H	-1.8307430000	-1.7037350000	2.0816790000
H	-0.9195220000	0.2124650000	2.0965960000
H	-2.0213410000	1.6123110000	2.9712230000
H	-2.0265670000	-0.1946320000	3.5183120000
H	-2.2952560000	-1.6139960000	4.2580990000
N	7.0447970000	-2.1634000000	-0.0768160000
O	7.6910280000	-1.1566280000	-0.3161910000
O	7.5206570000	-3.2847870000	-0.0139240000

si_TS2_{TBD}

O	-0.8387830000	4.0762600000	-2.0048780000
N	-0.7138690000	1.4789880000	-1.1836690000
N	-1.9241270000	-0.2188140000	-1.6429610000
N	-2.4519250000	0.8278580000	-2.3591350000
C	-1.7115580000	1.8427950000	-2.0475440000
C	1.5512490000	2.6061990000	-1.3079400000
C	1.9365510000	3.9456670000	-1.1935660000
C	-2.5165990000	-1.5185240000	-1.8118220000

C	-3.824470000	-1.6574330000	-1.5485580000
C	0.2203220000	2.4293360000	-0.5958610000
H	0.3552640000	2.1385750000	0.4536250000
C	-0.8750750000	0.1612230000	-0.8982880000
C	3.1460040000	4.3741560000	-1.7215450000
H	3.4477850000	5.4141200000	-1.6394760000
C	-0.3719230000	3.8526810000	-0.6807500000
H	-1.1751220000	4.0134460000	0.0502210000
C	-1.7259590000	-2.5683660000	-2.2921580000
C	3.5534330000	2.1261560000	-2.5304710000
H	4.1814620000	1.4251720000	-3.0705620000
C	-4.4512110000	-2.9137150000	-1.7669540000
H	-5.5103320000	-3.0469290000	-1.5600560000
C	2.3390540000	1.6912550000	-1.9938290000
H	2.0226960000	0.6600360000	-2.1270860000
C	-4.7209190000	-0.5183540000	-1.0335590000
H	-4.2022590000	-0.0059900000	-0.2166630000
H	-5.6747450000	-0.8973210000	-0.6586180000
H	-4.9263640000	0.2105320000	-1.8220350000
C	-0.2579050000	-2.3962160000	-2.5627450000
H	-0.0533320000	-1.4748440000	-3.1180150000
H	0.1210130000	-3.2346310000	-3.1505780000
H	0.2971580000	-2.3608430000	-1.6193890000
C	0.8553330000	4.7483330000	-0.5029020000
H	0.6891090000	5.7312900000	-0.9492390000
H	1.0709260000	4.8839880000	0.5633030000

C	-3.7035520000	-3.9920230000	-2.2350330000
C	3.9579250000	3.4513730000	-2.3837950000
H	4.9036320000	3.7741620000	-2.8071820000
C	-2.3457650000	-3.7981480000	-2.4947200000
H	-1.7491310000	-4.6284620000	-2.8649970000
C	-4.3325130000	-5.3449470000	-2.4393130000
H	-5.4229340000	-5.2809810000	-2.4390780000
H	-4.0371160000	-6.0334630000	-1.6407280000
H	-4.0150600000	-5.7888700000	-3.3869820000
C	-1.9476830000	3.2900130000	-2.3679720000
H	-2.1140390000	3.4260870000	-3.4381240000
H	-2.8530490000	3.6094750000	-1.8315140000
C	1.2213400000	-0.5891800000	0.2751790000
C	1.9109430000	-1.6553090000	0.7081940000
H	1.7442590000	0.3209020000	-0.0030920000
H	1.3457620000	-2.5378200000	0.9965170000
C	3.3695220000	-1.7335620000	0.8238100000
C	3.9448020000	-2.9255890000	1.2953990000
C	4.2290250000	-0.6746930000	0.4739570000
C	5.3182330000	-3.0695260000	1.4165200000
H	3.2949650000	-3.7507550000	1.5698540000
C	5.6024830000	-0.8009640000	0.5865660000
H	3.8224250000	0.2616250000	0.1044590000
C	6.1293120000	-2.0004340000	1.0574850000
H	5.7645330000	-3.9866390000	1.7803640000
H	6.2687660000	0.0093840000	0.3178720000

N	7.5793110000	-2.1390080000	1.1754610000
O	8.2727550000	-1.1894900000	0.8480370000
O	8.0205580000	-3.1968170000	1.5939000000
C	-0.2579490000	-0.5485700000	0.2517820000
O	-0.8627930000	-1.7620800000	0.5043960000
H	-0.6248410000	0.2436120000	1.1457220000
C	-2.5319850000	0.3849680000	2.4927000000
N	-3.4014970000	0.8934600000	3.4599000000
N	-1.4013200000	1.0349770000	2.1910290000
C	-2.9733080000	1.9418220000	4.3708380000
C	-0.9122780000	2.0941280000	3.0436840000
C	-2.0414040000	2.9083020000	3.6624060000
H	-3.8705300000	2.4591560000	4.7301920000
H	-0.2598120000	2.7554190000	2.4544920000
H	-1.6586710000	3.6506000000	4.3698450000
N	-2.8382600000	-0.7057200000	1.7930640000
H	-1.7061070000	-1.4708960000	1.0495110000
C	-4.0057340000	-1.4946020000	2.1322120000
H	-4.3573390000	-2.0004460000	1.2233210000
H	-3.7413770000	-2.2992420000	2.8398940000
C	-5.1260030000	-0.6671200000	2.7442120000
H	-5.9480250000	-1.3028050000	3.0875950000
H	-5.5225020000	0.0355570000	2.0018140000
C	-4.5428260000	0.1133110000	3.9084470000
H	-5.2804980000	0.8107870000	4.3220560000
H	-4.2597440000	-0.5772820000	4.7203590000

H	-0.2796220000	1.7010990000	3.8587860000
H	-2.5950710000	3.4334490000	2.8757990000
H	-2.4698320000	1.5179070000	5.2559510000

IM3(SS)

O	-6.4547250000	0.8941310000	-2.0217260000
N	-4.0267230000	0.5120380000	-0.9307920000
N	-2.8276050000	2.0541080000	-0.0698810000
N	-4.1124860000	2.4959860000	0.0287490000
C	-4.8167660000	1.5383730000	-0.4947820000
C	-4.8074210000	-1.7788850000	-0.4317660000
C	-6.1509680000	-2.1279790000	-0.3152670000
C	-1.7692040000	2.8703860000	0.4599280000
C	-1.4853100000	2.7588790000	1.8225910000
C	-4.6000480000	-0.7315500000	-1.5029480000
H	-3.8988350000	-1.0561900000	-2.2669550000
C	-2.7456020000	0.8473760000	-0.6504180000
C	-6.5480550000	-3.0667970000	0.6348720000
H	-7.5933590000	-3.3463550000	0.7301350000
C	-6.0424220000	-0.4615810000	-2.0812760000
H	-6.0273440000	-0.6884770000	-3.1471830000
C	-1.0514200000	3.6873350000	-0.4146080000
C	-4.2353590000	-3.3049550000	1.3196340000
H	-3.4922400000	-3.7807400000	1.9517050000
C	-0.4049310000	3.4936290000	2.3088190000
H	-0.1481980000	3.4144810000	3.3625280000
C	-3.8325540000	-2.3745180000	0.3661240000

H	-2.7827590000	-2.1408370000	0.2192340000
C	-2.2876580000	1.8410240000	2.7034110000
H	-1.9265930000	1.8819710000	3.7325110000
H	-2.2118920000	0.8029180000	2.3578850000
H	-3.3470020000	2.1158740000	2.6967380000
C	-1.3786670000	3.7275740000	-1.8807890000
H	-1.0762170000	2.7896280000	-2.3605000000
H	-0.8475560000	4.5448150000	-2.3713050000
H	-2.4515430000	3.8612930000	-2.0479220000
C	-7.0049220000	-1.4118670000	-1.3269590000
H	-7.8232800000	-0.8439330000	-0.8712090000
H	-7.4658360000	-2.1172280000	-2.0245230000
C	0.3563120000	4.3157900000	1.4735110000
C	-5.5843070000	-3.6430830000	1.4574650000
H	-5.8816370000	-4.3728560000	2.2040320000
C	0.0165260000	4.4045890000	0.1214890000
H	0.6058270000	5.0379660000	-0.5365450000
C	1.5127860000	5.1069190000	2.0239650000
H	2.2837010000	5.2604380000	1.2650630000
H	1.9661650000	4.6026200000	2.8808530000
H	1.1786360000	6.0941120000	2.3605490000
C	-6.2849580000	1.4712260000	-0.7468930000
H	-6.7859830000	0.8924220000	0.0414520000
H	-6.7055730000	2.4771740000	-0.7643760000
C	-1.5581020000	-0.0089590000	-0.9686810000
O	-1.8297500000	-1.0568740000	-1.6663230000

C	-0.3274040000	0.3517200000	-0.4997090000
C	0.8641440000	-0.4487860000	-0.9444850000
H	-0.1726200000	1.2379190000	0.0950660000
H	0.6735450000	-0.7777010000	-1.9769930000
C	2.1582990000	0.3442710000	-0.9461510000
C	3.0428890000	0.2267440000	-2.0267460000
C	2.5126530000	1.1749810000	0.1227490000
C	4.2539060000	0.9055530000	-2.0415150000
H	2.7856750000	-0.4236360000	-2.8565640000
C	3.7170960000	1.8664670000	0.1267340000
H	1.8404050000	1.2930480000	0.9645490000
C	4.5682580000	1.7164950000	-0.9591770000
H	4.9468890000	0.8124330000	-2.8682350000
H	4.0004960000	2.5088190000	0.9512210000
H	-0.7724310000	-2.1374460000	-1.0182180000
C	0.9929750000	-1.8516600000	-0.2127470000
C	2.2454740000	-2.4584710000	-0.8688610000
C	1.4700080000	-1.7596260000	1.2338890000
N	2.7307450000	-1.9842370000	1.3252590000
N	3.2414330000	-2.3316560000	0.0733720000
C	4.6355320000	-2.4622620000	-0.0849900000
C	5.1731980000	-3.0330270000	-1.2444090000
C	5.4819360000	-1.9797810000	0.9192520000
C	6.5554430000	-3.1098320000	-1.3847800000
H	4.5149180000	-3.4057640000	-2.0166500000
C	6.8590840000	-2.0730680000	0.7601720000

H	5.0516800000	-1.5342940000	1.8073550000
C	7.4059850000	-2.6354220000	-0.3907080000
H	6.9671400000	-3.5526950000	-2.2863820000
H	7.5085310000	-1.6949300000	1.5435490000
H	8.4821300000	-2.7013020000	-0.5113230000
O	-0.1452050000	-2.6143640000	-0.4069550000
O	2.3433730000	-2.8446800000	-2.0145290000
C	0.6754050000	-1.5170160000	2.5143290000
N	5.8403990000	2.4463500000	-0.9653700000
O	6.0979500000	3.1496550000	-0.0026440000
O	6.5684460000	2.3146860000	-1.9333400000
C	-0.8015050000	-1.8844890000	2.3303400000
H	-1.2616010000	-1.2632020000	1.5583140000
H	-0.9193400000	-2.9294400000	2.0331310000
H	-1.3302710000	-1.7220700000	3.2765910000
C	0.7715330000	-0.0422900000	2.9375530000
H	0.2614330000	0.0938550000	3.8981170000
H	1.8156460000	0.2641470000	3.0571950000
H	0.2879310000	0.6137350000	2.2079260000
C	1.2720860000	-2.3832360000	3.6338960000
H	2.3136270000	-2.1187940000	3.8290100000
H	0.6963330000	-2.2375260000	4.5537070000
H	1.2366960000	-3.4439620000	3.3688890000

TS3(SS)

O	-6.44203300	0.75153600	-1.97589200
N	-3.95876100	0.50401000	-0.99683500

N	-2.78040200	2.12081400	-0.22862900
N	-4.08024200	2.51138800	-0.08442800
C	-4.76618400	1.51540100	-0.55000700
C	-4.68056400	-1.74333300	-0.28817600
C	-6.00714200	-2.13945200	-0.13458800
C	-1.73304700	3.00217200	0.20264700
C	-1.48848500	3.10268600	1.57395000
C	-4.52330300	-0.78732900	-1.44886400
H	-3.85387600	-1.16707400	-2.21565300
C	-2.67434600	0.89009400	-0.77184300
C	-6.36006600	-3.00584500	0.89763000
H	-7.39144500	-3.32188900	1.02454100
C	-5.98505000	-0.58991400	-2.00913400
H	-5.98731800	-0.84636100	-3.06832600
C	-0.99337100	3.69224700	-0.76362900
C	-4.03802900	-3.07285600	1.59126300
H	-3.27455900	-3.45174400	2.26334400
C	-0.41117800	3.89582400	1.97268900
H	-0.19033600	3.98493300	3.03323200
C	-3.67704200	-2.21330200	0.55689100
H	-2.63166100	-1.95179300	0.40358300
C	-2.36121500	2.39706600	2.57603300
H	-1.88189900	2.37826400	3.55660900
H	-2.57171800	1.36580600	2.27709900
H	-3.32313000	2.91085700	2.67366800
C	-1.30923100	3.56510400	-2.22796900

H	-0.97665800	2.59558900	-2.61549100
H	-0.79974500	4.34546200	-2.79569900
H	-2.38422700	3.65041100	-2.41263200
C	-6.89249300	-1.54787600	-1.19909000
H	-7.74922900	-1.00097500	-0.79078300
H	-7.29883800	-2.32695700	-1.85088000
C	0.38439300	4.57040600	1.04571500
C	-5.36923700	-3.46089800	1.76337800
H	-5.63150000	-4.13312000	2.57431300
C	0.06997500	4.46905700	-0.31279500
H	0.67222900	5.00610800	-1.04138100
C	1.57126800	5.38386300	1.48721600
H	1.57772500	5.52633000	2.56974300
H	1.57301000	6.36777800	1.01032500
H	2.50359700	4.88339200	1.20566400
C	-6.24071300	1.37590500	-0.72779300
H	-6.67635800	0.79637000	0.09845500
H	-6.70854100	2.36054800	-0.75300100
C	-1.48100100	0.12988600	-1.08092900
O	-1.70102800	-0.91953700	-1.93019800
C	-0.23882900	0.47163800	-0.63197700
C	0.93265000	-0.24927800	-1.03410700
H	-0.13329400	1.29009100	0.06950900
H	0.80733100	-0.76364200	-1.98667100
C	2.25692400	0.35384400	-0.85563300
C	3.23376300	0.18485300	-1.85565600

C	2.61887600	1.03164400	0.32300900
C	4.52076900	0.66750100	-1.69430700
H	2.97476400	-0.36330500	-2.75679800
C	3.90386200	1.52111300	0.50052100
H	1.88928800	1.15324400	1.11944800
C	4.83745000	1.33043300	-0.51261400
H	5.28316900	0.51532300	-2.44838700
H	4.19846200	2.02259200	1.41430100
H	-1.24212300	-1.69444600	-1.50535700
C	0.68657800	-2.06927100	-0.00972600
C	1.88434000	-2.55966700	-0.82138400
C	1.30256300	-1.79983000	1.32599000
N	2.58050900	-1.95374800	1.29742800
N	2.96347300	-2.37506400	0.02712800
C	4.33931900	-2.38145200	-0.28633800
C	4.79712300	-2.93154800	-1.48853400
C	5.24154900	-1.77902200	0.59761200
C	6.14972500	-2.84297300	-1.80583400
H	4.09744000	-3.40140000	-2.16574500
C	6.58797900	-1.70214800	0.26140400
H	4.87408300	-1.35333200	1.52290900
C	7.05124300	-2.22473900	-0.94420500
H	6.49688700	-3.26446500	-2.74425300
H	7.27669300	-1.21473800	0.94533300
H	8.10125400	-2.15061100	-1.20670000
O	-0.51396600	-2.41196300	-0.20327000

O	1.90348700	-2.95844200	-1.97091300
N	6.20949100	1.77674900	-0.30013300
O	7.00675000	1.64006600	-1.21367400
O	6.49271700	2.26181300	0.78534100
C	0.56679500	-1.57093900	2.62379200
C	-0.48648700	-0.46824200	2.47594400
C	-0.14628700	-2.89532200	2.95855800
C	1.54711000	-1.20830000	3.74014800
H	-0.02587700	0.51036900	2.29403000
H	-1.16805900	-0.69195400	1.65008000
H	-1.06888700	-0.39649200	3.40114800
H	0.58251500	-3.69591400	3.11802700
H	-0.73801700	-2.78046400	3.87362900
H	-0.80753100	-3.18849200	2.13799200
H	0.99916500	-1.05579500	4.67562500
H	2.28415900	-2.00021700	3.89365700
H	2.09145800	-0.28831400	3.50308200

IM3(SR)

O	-6.4901300000	0.5336250000	0.6565400000
N	-3.9944290000	0.8726840000	-0.3560900000
N	-2.6078250000	2.4604790000	-0.0228570000
N	-3.8052580000	2.9168200000	0.4444760000
C	-4.6290680000	1.9343720000	0.2277620000
C	-4.3131160000	-1.5332630000	0.3097980000
C	-5.4688670000	-2.2713760000	0.5735160000
C	-1.4374960000	3.2907120000	0.0879960000

C	-0.7711800000	3.3146190000	1.3174210000
C	-4.6565280000	-0.4129270000	-0.6500680000
H	-4.3805500000	-0.6775120000	-1.6717230000
C	-2.6985900000	1.2179050000	-0.5103870000
C	-5.4143470000	-3.3866190000	1.3991900000
H	-6.3107050000	-3.9614600000	1.6133700000
C	-6.1884320000	-0.2625780000	-0.4825850000
H	-6.6621140000	0.1702030000	-1.3737570000
C	-1.0064410000	3.9929020000	-1.0356790000
C	-3.0378430000	-3.0079220000	1.6879780000
H	-2.0859060000	-3.2953940000	2.1222090000
C	0.3902530000	4.0779060000	1.3941230000
H	0.9379960000	4.1087660000	2.3329110000
C	-3.0856250000	-1.8921740000	0.8519110000
H	-2.1698770000	-1.3433880000	0.6553680000
C	-1.2618470000	2.4902000000	2.4763890000
H	-2.3040080000	2.7190010000	2.7177480000
H	-0.6539330000	2.6753270000	3.3634650000
H	-1.2016670000	1.4198830000	2.2433450000
C	-1.7507430000	3.9039630000	-2.3388780000
H	-1.6063100000	2.9187150000	-2.7965790000
H	-1.3894720000	4.6577130000	-3.0404990000
H	-2.8251970000	4.0530540000	-2.1950440000
C	-6.6548880000	-1.6832210000	-0.1562260000
H	-7.5731650000	-1.6548860000	0.4352990000
H	-6.8601560000	-2.2329780000	-1.0816440000

C	0.8759320000	4.7883990000	0.2917830000
C	-4.1879270000	-3.7482610000	1.9580960000
H	-4.1301940000	-4.6136320000	2.6111000000
C	0.1632190000	4.7426070000	-0.9060420000
H	0.5280750000	5.2965290000	-1.7670350000
C	2.1629500000	5.5621140000	0.3986450000
H	3.0202580000	4.8802620000	0.4016000000
H	2.2013340000	6.1388520000	1.3265910000
H	2.2855930000	6.2503830000	-0.4402600000
C	-6.1000350000	1.8735340000	0.5008110000
H	-6.3277590000	2.4072080000	1.4248900000
H	-6.6437490000	2.3555040000	-0.3254120000
C	-1.6699450000	0.3360100000	-1.1378390000
O	-2.1428650000	-0.5564110000	-1.9410760000
C	-0.3819460000	0.5017250000	-0.7400440000
C	0.7221230000	-0.3369260000	-1.3291720000
H	-0.1220340000	1.2510260000	-0.0078870000
H	0.5693420000	-0.3993890000	-2.4134780000
C	2.0807790000	0.2866070000	-1.0635480000
C	3.0160240000	0.4157550000	-2.0945460000
C	2.4290770000	0.7343780000	0.2185270000
C	4.2694830000	0.9705010000	-1.8666360000
H	2.7573790000	0.0895960000	-3.0968830000
C	3.6769900000	1.2861230000	0.4717370000
H	1.7228730000	0.6363330000	1.0388370000
C	4.5749750000	1.3981060000	-0.5823750000

H	4.9971810000	1.0791070000	-2.6611250000
H	3.9585000000	1.6186920000	1.4632450000
H	-1.2211510000	-1.7533680000	-1.5529960000
C	0.6320750000	-1.8508550000	-0.8464860000
C	0.9050390000	-1.8220300000	0.6655190000
C	1.8540700000	-2.6187850000	-1.3191720000
N	2.7329300000	-2.7523990000	-0.3948760000
N	2.2115620000	-2.2343130000	0.7996050000
O	-0.5689640000	-2.4378940000	-1.1945680000
O	0.1651890000	-1.4232820000	1.5458630000
N	5.8885900000	2.0003220000	-0.3310520000
O	6.1031570000	2.4540440000	0.7798550000
O	6.6914660000	2.0190300000	-1.2481220000
C	2.0195640000	-3.3083410000	-2.6557740000
C	1.3053550000	-2.5585450000	-3.7867300000
C	3.5055020000	-3.4702760000	-2.9863700000
C	1.3645610000	-4.6959520000	-2.5010000000
H	0.2489350000	-2.4013930000	-3.5541510000
H	1.7712150000	-1.5909120000	-3.9952990000
H	1.3678640000	-3.1534440000	-4.7035460000
H	4.0218930000	-4.0428780000	-2.2123510000
H	3.6158620000	-3.9956420000	-3.9403880000
H	3.9975990000	-2.4954660000	-3.0687780000
H	1.4380330000	-5.2460410000	-3.4454080000
H	1.8705420000	-5.2734250000	-1.7217180000
H	0.3096540000	-4.5944590000	-2.2328180000

C	3.0622430000	-2.1038290000	1.9144650000
C	2.5380250000	-1.9383880000	3.2010050000
C	4.4467020000	-2.1014300000	1.7109630000
C	3.4104180000	-1.7689090000	4.2723200000
H	1.4672230000	-1.9419860000	3.3509770000
C	5.2993780000	-1.9390170000	2.7958920000
H	4.8337760000	-2.2221560000	0.7062890000
C	4.7889740000	-1.7694820000	4.0812310000
H	3.0000870000	-1.6422840000	5.2693850000
H	6.3721840000	-1.9371090000	2.6306890000
H	5.4596640000	-1.6390050000	4.9239750000

TS3(SR)

O	6.4220060000	-1.2786650000	-0.6179340000
N	3.7231680000	-0.9333900000	-0.9630310000
N	2.1317560000	-2.3184710000	-0.5693080000
N	3.2851490000	-3.0409840000	-0.4714650000
C	4.2266750000	-2.1855090000	-0.7206400000
C	4.7920630000	1.1317080000	0.0238580000
C	6.1167200000	1.5733710000	0.0438800000
C	0.8802490000	-2.9377050000	-0.2295230000
C	0.1184490000	-3.5098350000	-1.2502820000
C	4.5965150000	0.2366680000	-1.1851670000
H	4.1865910000	0.7970510000	-2.0259780000
C	2.3670020000	-1.0268090000	-0.8784280000
C	6.5521270000	2.4389410000	1.0384440000
H	7.5819600000	2.7831440000	1.0615740000

C	6.0397820000	-0.2299660000	-1.4964810000
H	6.1571920000	-0.5520990000	-2.5399090000
C	0.4561910000	-2.8602200000	1.0997260000
C	4.3247090000	2.3971370000	1.9925210000
H	3.6278590000	2.7226240000	2.7581870000
C	-1.1483000000	-3.9816260000	-0.9112680000
H	-1.7755730000	-4.4094890000	-1.6891440000
C	3.8790920000	1.5364440000	0.9883760000
H	2.8414460000	1.2160540000	0.9688170000
C	0.6246640000	-3.5249900000	-2.6658580000
H	0.6565680000	-2.5064370000	-3.0707120000
H	-0.0297860000	-4.1211870000	-3.3038320000
H	1.6359550000	-3.9383760000	-2.7218180000
C	1.3304410000	-2.2389190000	2.1525680000
H	2.3329940000	-2.6776610000	2.1393860000
H	0.8990900000	-2.3942440000	3.1434580000
H	1.4201480000	-1.1599010000	1.9855090000
C	6.8908090000	0.9816750000	-1.1118550000
H	7.9054220000	0.6689680000	-0.8542220000
H	6.9493320000	1.6835640000	-1.9514480000
C	-1.6367310000	-3.8911400000	0.3951470000
C	5.6445670000	2.8460340000	2.0167730000
H	5.9704990000	3.5160850000	2.8062310000
C	-0.8200410000	-3.3428860000	1.3872540000
H	-1.1920010000	-3.2682740000	2.4063200000
C	-3.0183840000	-4.3822110000	0.7365310000

H	-2.9916300000	-5.4354640000	1.0362320000
H	-3.6923930000	-4.2998030000	-0.1195950000
H	-3.4401080000	-3.8129280000	1.5692820000
C	5.6947020000	-2.4581720000	-0.8360900000
H	5.9940510000	-3.1909850000	-0.0852670000
H	5.9017410000	-2.8754120000	-1.8332250000
C	1.4290720000	0.0521840000	-1.1281680000
O	2.0330350000	1.2321840000	-1.3782720000
C	0.0808040000	-0.1448070000	-1.1341850000
C	-0.9020290000	0.8559230000	-1.4400090000
H	-0.2949200000	-1.1106850000	-0.8279630000
H	-0.6101350000	1.6054760000	-2.1730290000
C	-2.2948640000	0.4085320000	-1.5109270000
C	-3.1583530000	0.8888420000	-2.5143630000
C	-2.8190250000	-0.4958270000	-0.5677620000
C	-4.4859860000	0.5007000000	-2.5749020000
H	-2.7633360000	1.5485860000	-3.2794260000
C	-4.1460770000	-0.8942530000	-0.6119170000
H	-2.1833380000	-0.8882510000	0.2205830000
C	-4.9647830000	-0.3845220000	-1.6128730000
H	-5.1477050000	0.8596160000	-3.3535610000
H	-4.5523300000	-1.5783280000	0.1235170000
H	1.4746700000	2.0069850000	-1.0117980000
C	-0.4947830000	2.4789270000	-0.0259190000
C	-0.3732950000	1.4837160000	1.0995000000
C	-1.8923850000	2.9583640000	0.1161880000

N	-2.5356880000	2.2723880000	1.0039770000
N	-1.6629080000	1.3495830000	1.5770780000
C	-2.1506220000	0.4613350000	2.5564640000
C	-1.2738280000	-0.2065890000	3.4184530000
C	-3.5291550000	0.2320600000	2.6427080000
C	-1.7860090000	-1.1099580000	4.3469630000
H	-0.2119800000	-0.0102050000	3.3630250000
C	-4.0193510000	-0.6727210000	3.5765710000
H	-4.1954520000	0.7634440000	1.9740590000
C	-3.1536330000	-1.3554240000	4.4301050000
H	-1.1005160000	-1.6181120000	5.0192970000
H	-5.0897460000	-0.8448260000	3.6338830000
H	-3.5426890000	-2.0600590000	5.1576580000
O	0.4838080000	3.0656680000	-0.5677660000
O	0.6429520000	0.9345220000	1.5031250000
N	-6.3622520000	-0.8024850000	-1.6665060000
O	-6.7527030000	-1.6038540000	-0.8320890000
O	-7.0675300000	-0.3315790000	-2.5444250000
C	-2.4760040000	4.1896400000	-0.5313910000
C	-1.8620100000	5.3913360000	0.2124870000
C	-2.0786290000	4.2766590000	-2.0102330000
C	-3.9981320000	4.2012800000	-0.3884080000
H	-2.1294280000	5.3692580000	1.2733630000
H	-0.7711250000	5.3807650000	0.1264660000
H	-2.2345910000	6.3264150000	-0.2192880000
H	-2.5675630000	3.4951460000	-2.5956370000

H	-2.3992820000	5.2422250000	-2.4152610000
H	-0.9956560000	4.1917340000	-2.1305340000
H	-4.4056650000	5.1038710000	-0.8550450000
H	-4.4410810000	3.3269120000	-0.8763460000
H	-4.2979560000	4.1877800000	0.6626650000

IM3(RS)

O	6.6333820000	-1.4446560000	-1.0449180000
N	4.0294720000	-0.9243140000	-0.4637730000
N	2.4058160000	-2.2682190000	-0.1356380000
N	3.5320040000	-3.0387500000	-0.0876670000
C	4.5039310000	-2.1970810000	-0.2940590000
C	4.7010470000	1.3618500000	0.2791430000
C	5.7333600000	1.2820790000	1.2195340000
C	1.0983030000	-2.8707290000	-0.0830920000
C	0.3785230000	-2.9753460000	-1.2783800000
C	4.8597720000	0.2706620000	-0.7570170000
H	4.6030110000	0.5794040000	-1.7703520000
C	2.6899940000	-0.9874530000	-0.3631410000
C	5.8098010000	2.2035420000	2.2576210000
H	6.6142890000	2.1517500000	2.9852590000
C	6.3420070000	-0.1461430000	-0.5716390000
H	6.9373760000	0.5252820000	-1.1943570000
C	0.6189580000	-3.3108320000	1.1504150000
C	3.8206860000	3.2864100000	1.3921620000
H	3.0856040000	4.0816520000	1.4638160000
C	-0.8942320000	-3.5370800000	-1.1971150000

H	-1.4867430000	-3.6213400000	-2.1049030000
C	3.7403800000	2.3683900000	0.3463150000
H	2.9555840000	2.4339210000	-0.4009090000
C	0.9563630000	-2.4983670000	-2.5824330000
H	1.0575980000	-1.4085020000	-2.5975460000
H	0.3017860000	-2.7801680000	-3.4089940000
H	1.9411530000	-2.9461460000	-2.7562610000
C	1.4437410000	-3.1604240000	2.3996910000
H	2.3636070000	-3.7500030000	2.3376230000
H	0.8803110000	-3.4911990000	3.2736150000
H	1.7346730000	-2.1159560000	2.5585060000
C	6.6620930000	0.1357290000	0.9109750000
H	6.4260030000	-0.7264720000	1.5458820000
H	7.7177020000	0.3728790000	1.0606100000
C	-1.4245530000	-3.9940980000	0.0132350000
C	4.8415870000	3.2026650000	2.3399220000
H	4.8894890000	3.9313310000	3.1432360000
C	-0.6566310000	-3.8763720000	1.1728700000
H	-1.0616120000	-4.2200080000	2.1212850000
C	-2.8050640000	-4.5957420000	0.0532430000
H	-3.5269790000	-3.9480680000	-0.4546400000
H	-3.1459050000	-4.7480760000	1.0802220000
H	-2.8214910000	-5.5656310000	-0.4546080000
C	5.9718090000	-2.4858340000	-0.3649300000
H	6.3731290000	-2.6420080000	0.6442550000
H	6.1328690000	-3.4019430000	-0.9360520000

C	1.7593560000	0.1461740000	-0.6282650000
O	2.0594940000	0.7580790000	-1.7283060000
C	0.8069400000	0.3361590000	0.3175740000
C	-0.2954920000	1.3663170000	0.4017160000
H	0.8229820000	-0.3606490000	1.1514380000
H	0.0450580000	2.2154500000	1.0077410000
C	-1.5119070000	0.7535840000	1.0848650000
C	-2.3497260000	1.5303410000	1.8920410000
C	-1.8493110000	-0.5860170000	0.8537140000
C	-3.5128700000	1.0019440000	2.4382580000
H	-2.0955990000	2.5691550000	2.0839250000
C	-3.0049200000	-1.1349600000	1.3911140000
H	-1.2195110000	-1.1921130000	0.2080070000
C	-3.8193180000	-0.3262660000	2.1714320000
H	-4.1777740000	1.5993310000	3.0496960000
H	-3.2907490000	-2.1602920000	1.1906290000
H	1.1021570000	1.8479320000	-1.7980460000
C	-0.6854380000	2.0149520000	-1.0021830000
C	-1.4267930000	0.8900350000	-1.7454700000
C	-1.8262380000	3.0000250000	-0.8198220000
N	-2.9656340000	2.4918370000	-1.1141380000
N	-2.7703870000	1.1981250000	-1.6090830000
C	-3.8538390000	0.2978100000	-1.6078670000
C	-3.7596280000	-0.9325610000	-2.2675100000
C	-5.0003290000	0.6136950000	-0.8698280000
C	-4.8066730000	-1.8445060000	-2.1581120000

H	-2.8760490000	-1.1657610000	-2.8452990000
C	-6.0328770000	-0.3114740000	-0.7724540000
H	-5.0562100000	1.5676730000	-0.3594260000
C	-5.9412920000	-1.5488750000	-1.4072320000
H	-4.7298850000	-2.7971060000	-2.6745480000
H	-6.9106530000	-0.0647390000	-0.1826510000
H	-6.7473240000	-2.2698970000	-1.3215860000
O	0.3921630000	2.5831380000	-1.6441940000
O	-0.9569010000	-0.1121020000	-2.2410190000
C	-1.6983130000	4.4691400000	-0.4781440000
N	-5.0719940000	-0.8833240000	2.6884320000
O	-5.2747500000	-2.0753220000	2.5316890000
O	-5.8472590000	-0.1230760000	3.2442060000
C	-1.3859780000	5.2004450000	-1.7993980000
H	-0.4617190000	4.8205170000	-2.2406950000
H	-2.2004280000	5.0579390000	-2.5158600000
H	-1.2752470000	6.2735180000	-1.6089410000
C	-3.0168180000	4.9944780000	0.0964330000
H	-2.9212620000	6.0624170000	0.3168130000
H	-3.8379150000	4.8575570000	-0.6109380000
H	-3.2822900000	4.4741050000	1.0227900000
C	-0.5517630000	4.7285730000	0.5070870000
H	-0.7434060000	4.2858810000	1.4905010000
H	0.3901270000	4.3350910000	0.1155210000
H	-0.4416250000	5.8083010000	0.6510440000

TS3(RS)

O	-6.76349600	0.95930600	-0.29833000
N	-4.06204900	0.69850100	-0.49734900
N	-2.55346600	2.22033500	-0.46815100
N	-3.73772900	2.87671400	-0.62885500
C	-4.63147300	1.93645600	-0.64663800
C	-5.00276000	-1.14960500	0.94096200
C	-6.30177000	-1.64220500	1.07890900
C	-1.32088700	2.96200600	-0.46034700
C	-0.49026200	2.88615400	-1.58228400
C	-4.85028000	-0.54693300	-0.44055800
H	-4.37980900	-1.25537800	-1.12377800
C	-2.72332600	0.89100300	-0.37663900
C	-6.68879000	-2.28141800	2.24959000
H	-7.69953800	-2.66168600	2.36410100
C	-6.31475700	-0.26459400	-0.86093000
H	-6.43352800	-0.24003900	-1.95203400
C	-0.99437900	3.66919100	0.70041700
C	-4.46301700	-1.92128500	3.13803600
H	-3.75163400	-2.03269500	3.94979200
C	0.73701100	3.54184200	-1.49887700
H	1.41955600	3.47020100	-2.34077700
C	-4.06850800	-1.28882600	1.95899600
H	-3.05420900	-0.91742900	1.85139200
C	-0.86762200	2.08264300	-2.79417800
H	-0.66206300	1.01728000	-2.62824400
H	-0.27130400	2.39769000	-3.65214500

H	-1.92560500	2.21267700	-3.04387900
C	-1.92645600	3.69617700	1.88162800
H	-2.87995400	4.16632500	1.62347200
H	-1.48009200	4.25216800	2.70763200
H	-2.14640600	2.68292200	2.23606700
C	-7.10639000	-1.37842000	-0.17245300
H	-8.13183200	-1.05377300	0.01879300
H	-7.14107400	-2.26705900	-0.81250800
C	1.12034600	4.25001100	-0.35849500
C	-5.75961100	-2.41425700	3.28107000
H	-6.04899200	-2.90362600	4.20564900
C	0.24177200	4.31233400	0.72618100
H	0.52997300	4.86043000	1.61945000
C	2.46718300	4.92170300	-0.30618900
H	2.48841900	5.80337200	-0.95504500
H	3.25205700	4.24278800	-0.65296000
H	2.71388300	5.24420300	0.70774600
C	-6.10874200	2.07299300	-0.84991100
H	-6.46950600	2.96960600	-0.34364100
H	-6.31983600	2.16821700	-1.92541900
C	-1.72407300	-0.15152100	-0.21517800
O	-2.16298900	-1.40254100	-0.55475400
C	-0.47936900	0.10187600	0.25478500
C	0.54266100	-0.90981100	0.39637300
H	-0.22654100	1.12536100	0.49925200
H	0.15435400	-1.88770200	0.68454400

C	1.78693700	-0.52432500	1.08069300
C	2.56745600	-1.50074000	1.72649300
C	2.28355600	0.79553000	1.03397300
C	3.80032200	-1.19101200	2.27909300
H	2.20233300	-2.52089700	1.77962800
C	3.50816200	1.12065300	1.59169700
H	1.73723200	1.56733400	0.50005000
C	4.25826200	0.11894000	2.19896600
H	4.41477700	-1.94688500	2.75255900
H	3.90554800	2.12657300	1.53260000
H	-1.51817600	-1.65500900	-1.28405000
C	0.84306200	-1.43289400	-1.57861200
C	1.96855300	-0.42838800	-1.77101500
C	1.59649300	-2.69571300	-1.27933800
N	2.86189800	-2.47407800	-1.19188000
N	3.11702900	-1.12638600	-1.45877200
C	4.40457200	-0.62016200	-1.18233800
C	4.72375500	0.71456300	-1.46237400
C	5.34940500	-1.44935100	-0.56769500
C	5.96194100	1.21529700	-1.07213800
H	3.99505200	1.34871600	-1.94772700
C	6.58169100	-0.92958500	-0.18841900
H	5.09414400	-2.48054400	-0.36030800
C	6.89179600	0.40814300	-0.42227400
H	6.19502100	2.25650500	-1.27414800
H	7.29645200	-1.57467900	0.31277900

H	7.84549300	0.81470900	-0.10278500
O	-0.25302200	-1.33333100	-2.21054900
O	1.86804200	0.74763800	-2.07468500
N	5.58555000	0.43884300	2.70988700
O	6.26749800	-0.47533500	3.14681500
O	5.94997500	1.60359400	2.67404200
C	1.07169600	-4.11835600	-1.17551800
C	1.58956600	-4.88568700	-2.40440000
C	1.61028300	-4.78246300	0.09904700
C	-0.45956000	-4.16852300	-1.16659800
H	1.25018100	-4.41233900	-3.33121100
H	2.68262800	-4.90822100	-2.41182500
H	1.21551000	-5.91500600	-2.38836300
H	1.16436200	-4.33494500	0.99391100
H	1.35387200	-5.84708800	0.09927500
H	2.69737400	-4.68623000	0.16443200
H	-0.77945500	-5.21045400	-1.06105100
H	-0.88725000	-3.60497200	-0.33135300
H	-0.87479000	-3.77123600	-2.09543100

IM3(RR)

O	3.7281840000	-4.7170610000	-0.8156870000
N	1.6492930000	-3.0072650000	-0.6048570000
N	-0.2452900000	-3.2156400000	0.3439040000
N	0.3164820000	-4.4602480000	0.3751480000
C	1.4672580000	-4.3045890000	-0.2133230000
C	3.8379980000	-1.7943920000	-0.3573580000

C	5.1357460000	-2.1542270000	-0.7266340000
C	-1.5866580000	-2.9992680000	0.8215950000
C	-2.6108570000	-2.9158760000	-0.1213150000
C	2.8532510000	-2.4960250000	-1.2724890000
H	2.5009900000	-1.8385670000	-2.0743620000
C	0.5469420000	-2.3242710000	-0.2503760000
C	6.2269760000	-1.6246530000	-0.0512940000
H	7.2391900000	-1.9031360000	-0.3291460000
C	3.6843610000	-3.6903860000	-1.8018430000
H	3.2964890000	-4.0884180000	-2.7479810000
C	-1.7905660000	-2.8751930000	2.1981430000
C	4.6996550000	-0.3843720000	1.3665830000
H	4.5387000000	0.3097770000	2.1857170000
C	-3.8972500000	-2.6753910000	0.3617740000
H	-4.7188030000	-2.5895250000	-0.3461580000
C	3.6013900000	-0.9023390000	0.6780260000
H	2.5910550000	-0.5942800000	0.9310310000
C	-2.3331900000	-3.0674040000	-1.5926030000
H	-1.6581550000	-2.2863250000	-1.9610490000
H	-3.2629450000	-3.0150710000	-2.1624000000
H	-1.8624630000	-4.0345480000	-1.8018960000
C	-0.6409930000	-2.9955240000	3.1613670000
H	-0.1899340000	-3.9914980000	3.1125480000
H	-0.9771800000	-2.8204740000	4.1846660000
H	0.1484570000	-2.2702750000	2.9342110000
C	5.1050320000	-3.1292670000	-1.8817390000

H	5.8401050000	-3.9336440000	-1.8048440000
H	5.2536560000	-2.6142290000	-2.8373640000
C	-4.1525120000	-2.5135220000	1.7225960000
C	5.9983450000	-0.7398150000	1.0033610000
H	6.8406650000	-0.3261380000	1.5492810000
C	-3.0919570000	-2.6282580000	2.6271030000
H	-3.2818210000	-2.5147590000	3.6916860000
C	-5.5415650000	-2.1880530000	2.2048350000
H	-6.2823300000	-2.3402310000	1.4154190000
H	-5.6041200000	-1.1420400000	2.5250830000
H	-5.8209170000	-2.8078500000	3.0615170000
C	2.4898010000	-5.3369130000	-0.5795100000
H	2.6188860000	-6.0506890000	0.2356900000
H	2.1374540000	-5.8814600000	-1.4681530000
C	0.2219480000	-0.9194520000	-0.6568500000
O	0.3388520000	-0.7487450000	-1.9313550000
C	-0.1637360000	-0.0857000000	0.3403060000
C	-0.7412810000	1.3032000000	0.1550510000
H	-0.2261160000	-0.4879210000	1.3473160000
H	-0.5695050000	1.8605750000	1.0837680000
C	-2.2380920000	1.1116250000	0.0112190000
C	-3.0947860000	1.5111210000	1.0404670000
C	-2.7654330000	0.4200100000	-1.0909080000
C	-4.4521350000	1.2116560000	0.9981370000
H	-2.6918210000	2.0466270000	1.8951580000
C	-4.1157850000	0.1236620000	-1.1555200000

H	-2.0991420000	0.1097190000	-1.8885390000
C	-4.9340220000	0.5072940000	-0.0956760000
H	-5.1245350000	1.4943680000	1.7990650000
H	-4.5373820000	-0.4222380000	-1.9911430000
H	0.0456590000	0.7225090000	-2.2595610000
C	-0.0636040000	2.1669910000	-0.9869570000
C	1.4121860000	2.2218610000	-0.5436970000
C	-0.4303780000	3.6332200000	-0.7970600000
N	0.4382160000	4.2490270000	-0.0781650000
N	1.5114810000	3.3913130000	0.1915820000
C	2.6129440000	3.8906460000	0.9156380000
C	3.8023840000	3.1563700000	1.0095460000
C	2.4986310000	5.1227420000	1.5693090000
C	4.8586850000	3.6643520000	1.7592280000
H	3.8966880000	2.2098160000	0.4948180000
C	3.5686120000	5.6116270000	2.3096260000
H	1.5756000000	5.6825600000	1.4890670000
C	4.7544590000	4.8888200000	2.4130130000
H	5.7781790000	3.0893020000	1.8213360000
H	3.4686240000	6.5691380000	2.8114260000
H	5.5857220000	5.2763670000	2.9925540000
O	-0.2576100000	1.6953370000	-2.2677430000
O	2.2706240000	1.3936060000	-0.7428110000
C	-1.4947170000	4.4414850000	-1.5186680000
N	-6.3315270000	0.0781960000	-0.0918140000
O	-6.6835550000	-0.7258490000	-0.9420840000

O	-7.0680510000	0.5235180000	0.7720300000
C	-0.8367940000	4.8580560000	-2.8518320000
H	0.0500340000	5.4718250000	-2.6685380000
H	-0.5394160000	3.9756680000	-3.4255850000
H	-1.5482230000	5.4400800000	-3.4475050000
C	-1.8503020000	5.6908080000	-0.7072450000
H	-2.2947760000	5.4180980000	0.2554220000
H	-0.9686750000	6.3057050000	-0.5133440000
H	-2.5778620000	6.2908740000	-1.2628370000
C	-2.7661400000	3.6527340000	-1.8404590000
H	-2.5316290000	2.7438600000	-2.3981750000
H	-3.3230510000	3.3822800000	-0.9396180000
H	-3.4166090000	4.2796910000	-2.4593710000

TS3(RR)

O	-5.8626050000	-1.9221530000	-0.6130900000
N	-3.3059380000	-0.9650380000	-0.9201460000
N	-2.6737860000	0.9655780000	-1.6169210000
N	-4.0129050000	0.8964080000	-1.8747580000
C	-4.3651810000	-0.2767390000	-1.4537340000
C	-3.5288680000	-2.3178840000	1.2032520000
C	-4.4631470000	-3.2742580000	1.6064610000
C	-1.9834800000	2.1925930000	-1.9025830000
C	-1.3837380000	2.3448910000	-3.1527010000
C	-3.4719490000	-2.3009040000	-0.3114840000
H	-2.6645560000	-2.9333760000	-0.6801160000
C	-2.2085160000	-0.1597790000	-1.0348510000

C	-4.6815650000	-3.5145540000	2.9563500000
H	-5.4093600000	-4.2542180000	3.2768910000
C	-4.8419090000	-2.9042190000	-0.7079110000
H	-4.8290170000	-3.3357600000	-1.7177890000
C	-1.9205220000	3.1575190000	-0.8925890000
C	-3.0332190000	-1.8178420000	3.4837380000
H	-2.4781440000	-1.2488320000	4.2226830000
C	-0.6705170000	3.5220680000	-3.3769940000
H	-0.1823090000	3.6653080000	-4.3374940000
C	-2.8024130000	-1.5807370000	2.1278560000
H	-2.0667690000	-0.8413850000	1.8252700000
C	-1.4621220000	1.2494460000	-4.1794480000
H	-0.9156990000	0.3628810000	-3.8374200000
H	-1.0223020000	1.5728900000	-5.1241790000
H	-2.4989870000	0.9524970000	-4.3636580000
C	-2.5673200000	2.9126530000	0.4420090000
H	-3.6149460000	2.6178950000	0.3250010000
H	-2.5292470000	3.8151480000	1.0549880000
H	-2.0427740000	2.1131770000	0.9792680000
C	-5.1131690000	-3.9194960000	0.4041040000
H	-6.1872090000	-4.0861670000	0.5147630000
H	-4.6394050000	-4.8778490000	0.1630450000
C	-0.5558320000	4.5059500000	-2.3932010000
C	-3.9590640000	-2.7760950000	3.8942860000
H	-4.1235150000	-2.9462540000	4.9537500000
C	-1.1887660000	4.3108930000	-1.1621220000

H	-1.0951510000	5.0666110000	-0.3859350000
C	0.2228550000	5.7690580000	-2.6472470000
H	0.8915630000	5.6599460000	-3.5037850000
H	0.8210070000	6.0387620000	-1.7726180000
H	-0.4536820000	6.6049720000	-2.8539400000
C	-5.7180010000	-0.9089040000	-1.5721290000
H	-6.4907410000	-0.1581940000	-1.3994740000
H	-5.8380400000	-1.3057670000	-2.5915980000
C	-0.8559950000	-0.5181120000	-0.6635590000
O	-0.7828770000	-1.7782140000	-0.1514140000
C	0.1956330000	0.3453510000	-0.8079120000
C	1.5961490000	0.1693090000	-0.5697790000
H	-0.0755230000	1.3755490000	-1.0056420000
H	2.1209690000	1.1226820000	-0.5384360000
C	2.4384660000	-0.8901940000	-1.1014850000
C	3.7768000000	-0.5526620000	-1.4181930000
C	2.0166230000	-2.2114450000	-1.3546700000
C	4.6510230000	-1.4699950000	-1.9657950000
H	4.1147960000	0.4642040000	-1.2389850000
C	2.8918330000	-3.1463500000	-1.8885000000
H	0.9983850000	-2.5059240000	-1.1421260000
C	4.1945610000	-2.7686770000	-2.1922410000
H	5.6702730000	-1.2045060000	-2.2183990000
H	2.5744910000	-4.1641150000	-2.0802120000
H	-0.1339190000	-1.7960110000	0.6072240000
C	1.6163370000	-0.6302450000	1.6741930000

C	0.7793670000	0.6089640000	1.8915030000
C	2.9982110000	-0.1521820000	1.9497140000
N	3.0081310000	1.1327120000	2.1161710000
N	1.7116720000	1.6200560000	2.0502240000
C	1.4931190000	3.0108900000	2.0239100000
C	0.2605900000	3.5419060000	2.4180400000
C	2.5181250000	3.8556900000	1.5871150000
C	0.0628660000	4.9184180000	2.3578920000
H	-0.5199440000	2.8812120000	2.7720670000
C	2.3036590000	5.2282970000	1.5417080000
H	3.4693620000	3.4264540000	1.2945830000
C	1.0758870000	5.7684560000	1.9201510000
H	-0.8920960000	5.3286230000	2.6736010000
H	3.1044940000	5.8791320000	1.2047720000
H	0.9145650000	6.8409090000	1.8846840000
O	1.1754710000	-1.7889860000	1.5877210000
O	-0.4381740000	0.6886980000	1.9657000000
N	5.1025960000	-3.7490500000	-2.7704280000
O	4.6800110000	-4.8777920000	-2.9703510000
O	6.2429730000	-3.3931220000	-3.0275230000
C	4.2208350000	-0.9883060000	2.2706530000
C	4.1893590000	-1.2049350000	3.7969620000
C	4.1894060000	-2.3590890000	1.5850960000
C	5.4982600000	-0.2345930000	1.8900990000
H	4.2406730000	-0.2488440000	4.3262890000
H	3.2725400000	-1.7210140000	4.1010730000

H	5.0417960000	-1.8211130000	4.1019040000
H	4.2398500000	-2.2694420000	0.4991840000
H	5.0600320000	-2.9357820000	1.9149790000
H	3.2846280000	-2.9133800000	1.8403980000
H	6.3731830000	-0.8151920000	2.1993730000
H	5.5541160000	-0.0865150000	0.8073500000
H	5.5417930000	0.7437570000	2.3755570000

IM4(SS)

O	-5.8218970000	0.2086890000	-1.3866700000
N	-3.3295330000	0.4642470000	-0.4644180000
N	-2.5594570000	2.3797170000	0.0264250000
N	-3.8924130000	2.4322330000	0.3487710000
C	-4.3284890000	1.2467970000	0.0411810000
C	-3.7189860000	-1.9192390000	0.1097890000
C	-4.8810360000	-2.6707920000	-0.0537510000
C	-1.7327060000	3.5450270000	0.1686160000
C	-1.3680620000	3.9569540000	1.4506450000
C	-3.5899560000	-0.8813200000	-0.9855150000
H	-2.7741130000	-1.0887950000	-1.6838190000
C	-2.2029550000	1.1977350000	-0.4779780000
C	-5.1884320000	-3.6878320000	0.8459310000
H	-6.0936270000	-4.2759290000	0.7255520000
C	-4.9900570000	-0.9034000000	-1.7048370000
H	-4.8524890000	-0.8352160000	-2.7841220000
C	-1.3351040000	4.2114950000	-0.9984610000
C	-3.1477610000	-3.1903390000	2.0551920000

H	-2.4718000000	-3.4067330000	2.8765720000
C	-0.4878760000	5.0378260000	1.5449360000
H	-0.1743880000	5.3724810000	2.5305490000
C	-2.8358200000	-2.1755690000	1.1537060000
H	-1.9191200000	-1.6017540000	1.2364950000
C	-1.9440590000	3.3209340000	2.6871490000
H	-1.2665890000	3.4460520000	3.5345220000
H	-2.1443060000	2.2558400000	2.5556300000
H	-2.8954900000	3.8001630000	2.9407710000
C	-1.8655320000	3.8090420000	-2.3503600000
H	-1.6056120000	2.7804480000	-2.6267270000
H	-1.4785540000	4.4796030000	-3.1199780000
H	-2.9589980000	3.8780590000	-2.3598580000
C	-5.6396210000	-2.2377410000	-1.2817740000
H	-6.7108080000	-2.0947610000	-1.1109860000
H	-5.5321290000	-2.9796200000	-2.0803520000
C	-0.0105780000	5.6953210000	0.4128310000
C	-4.3176790000	-3.9380100000	1.9042870000
H	-4.5474520000	-4.7257330000	2.6149310000
C	-0.4579210000	5.2813570000	-0.8466440000
H	-0.1225690000	5.8142780000	-1.7331560000
C	0.9550130000	6.8447220000	0.5298610000
H	1.9112380000	6.5988160000	0.0574170000
H	1.1487830000	7.0980910000	1.5740970000
H	0.5646690000	7.7352310000	0.0284790000
C	-5.7129930000	0.6979710000	-0.0621060000

H	-5.8913600000	-0.0842120000	0.6872670000
H	-6.4478700000	1.4930280000	0.0645360000
C	-0.9287280000	0.7010430000	-1.2132660000
O	-1.2527950000	0.4284630000	-2.4173870000
C	0.3788520000	1.4975700000	-1.0154470000
C	1.3957850000	0.3720960000	-1.1907190000
H	0.4705120000	2.2567090000	-1.7935300000
H	1.2795090000	0.0245050000	-2.2270900000
C	2.8494280000	0.6970560000	-0.9605890000
C	3.7971340000	-0.3277460000	-0.8331710000
C	3.2861880000	2.0259570000	-0.9031690000
C	5.1403820000	-0.0419210000	-0.6316540000
H	3.4928990000	-1.3686840000	-0.8929960000
C	4.6254330000	2.3331550000	-0.7040850000
H	2.5695940000	2.8356070000	-0.9983500000
C	5.5300870000	1.2895490000	-0.5664840000
H	5.8777010000	-0.8280930000	-0.5268950000
H	4.9720680000	3.3576500000	-0.6512960000
C	0.7658030000	-0.7774250000	-0.3438960000
C	1.0274190000	-2.1345700000	-1.0336530000
C	1.3053400000	-1.0761060000	1.0583500000
N	1.7526880000	-2.2753630000	1.1421820000
N	1.6299730000	-2.9284720000	-0.0817730000
C	2.0655510000	-4.2695120000	-0.1788800000
C	1.8713480000	-5.0017140000	-1.3559430000
C	2.7043460000	-4.8591530000	0.9175580000

C	2.3215180000	-6.3166630000	-1.4198860000
H	1.3771360000	-4.5448290000	-2.2015480000
C	3.1435990000	-6.1747570000	0.8308190000
H	2.8482150000	-4.2840420000	1.8230470000
C	2.9574400000	-6.9127780000	-0.3351120000
H	2.1674280000	-6.8781210000	-2.3360500000
H	3.6378120000	-6.6232750000	1.6869850000
H	3.3039650000	-7.9389570000	-0.3970840000
O	-0.6134510000	-0.5184130000	-0.3250170000
O	0.7727350000	-2.4150140000	-2.1824760000
C	1.2968680000	-0.2116020000	2.3104590000
H	0.4640980000	1.9718760000	-0.0317190000
N	6.9458480000	1.6043700000	-0.3482230000
O	7.2658250000	2.7796850000	-0.2971730000
O	7.7235480000	0.6739360000	-0.2284070000
C	1.6726640000	-1.0714180000	3.5237500000
H	2.6840410000	-1.4742930000	3.4283400000
H	1.6290840000	-0.4551020000	4.4269280000
H	0.9856310000	-1.9137920000	3.6424570000
C	-0.0969100000	0.3895760000	2.5430300000
H	-0.4088050000	1.0248730000	1.7103130000
H	-0.8541480000	-0.3877360000	2.6840910000
H	-0.0695300000	1.0031060000	3.4498820000
C	2.3110450000	0.9392730000	2.2005760000
H	3.3126590000	0.5706370000	1.9583630000
H	2.0214790000	1.6719070000	1.4440430000

H 2.3598880000 1.4597470000 3.1628680000

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O 4.6507710000 -4.0827360000 -2.0942390000
N 2.8806220000 -2.3911170000 -0.8778110000
N 1.4522750000 -2.9051140000 0.6306120000
N 2.3768350000 -3.9010510000 0.6494350000
C 3.2346350000 -3.5673480000 -0.2728510000
C 4.1658970000 -0.4605800000 -1.9211890000
C 5.5536190000 -0.5616650000 -1.7532110000
C 0.2496980000 -3.0673320000 1.4161090000
C 0.2783750000 -2.7014780000 2.7615210000
C 3.5594270000 -1.8363570000 -2.0894760000
H 2.8109610000 -1.8826760000 -2.8803930000
C 1.7382150000 -1.9881550000 -0.2898200000
C 6.3404780000 0.5804690000 -1.6836750000
H 7.4172400000 0.5031890000 -1.5657860000
C 4.8122030000 -2.7122340000 -2.3882460000
H 4.9575780000 -2.6672250000 -3.4698340000
C -0.8605930000 -3.6448840000 0.7914330000
C 4.3432130000 1.9251030000 -1.9581460000
H 3.8699020000 2.8980330000 -2.0394210000
C -0.8863810000 -2.9139150000 3.4999040000
H -0.9043900000 -2.6126710000 4.5442530000
C 3.5474530000 0.7825760000 -2.0214710000
H 2.4760680000 0.8836280000 -2.1530510000
C 1.4866370000 -2.0397810000 3.3624280000

H	1.3808580000	-1.9588750000	4.4455920000
H	1.6039810000	-1.0252010000	2.9616000000
H	2.4018120000	-2.5981420000	3.1433060000
C	-0.8509230000	-3.9912680000	-0.6725110000
H	0.0054770000	-4.6235350000	-0.9286280000
H	-0.8048590000	-3.0877720000	-1.2923950000
H	-1.7624630000	-4.5273060000	-0.9418420000
C	5.9948480000	-1.9997950000	-1.7067210000
H	6.1275730000	-2.3236090000	-0.6676310000
H	6.9332240000	-2.1894430000	-2.2322440000
C	-2.0235680000	-3.4886100000	2.9295690000
C	5.7232540000	1.8270860000	-1.7914560000
H	6.3256770000	2.7303130000	-1.7541560000
C	-1.9897500000	-3.8521720000	1.5803590000
H	-2.8684660000	-4.3025050000	1.1251550000
C	-3.2659890000	-3.7192280000	3.7477470000
H	-4.1611150000	-3.4191940000	3.1959740000
H	-3.2352320000	-3.1571180000	4.6835300000
H	-3.3736040000	-4.7805560000	3.9944510000
C	4.4201490000	-4.3547480000	-0.7331320000
H	5.2936850000	-4.1336780000	-0.1083020000
H	4.1949580000	-5.4183170000	-0.6394090000
C	0.8732540000	-0.8240960000	-0.7610920000
O	0.7934440000	-0.7317820000	-1.9765960000
C	0.3308850000	0.0674180000	0.2484070000
C	-0.7955650000	0.9260390000	-0.3247710000

H	0.0861500000	-0.4774730000	1.1607480000
H	-0.3638260000	1.4799310000	-1.1672120000
C	-1.9273380000	0.0670710000	-0.8601980000
C	-2.3954270000	0.2341610000	-2.1685820000
C	-2.5554050000	-0.8720700000	-0.0320790000
C	-3.4914800000	-0.4811940000	-2.6345550000
H	-1.9143900000	0.9628590000	-2.8133630000
C	-3.6532920000	-1.5960530000	-0.4765640000
H	-2.1929040000	-1.0266550000	0.9821660000
C	-4.1063560000	-1.3791780000	-1.7723480000
H	-3.8834790000	-0.3353700000	-3.6334260000
H	-4.1695100000	-2.2984140000	0.1664970000
C	-1.3415960000	2.1039970000	0.5984980000
C	-2.3507200000	2.7479590000	-0.3874290000
C	-2.3175310000	1.6727710000	1.6881410000
N	-3.5447610000	1.7738580000	1.3265350000
N	-3.5974290000	2.3306330000	0.0435830000
C	-4.7594190000	2.1504900000	-0.7300050000
C	-4.9227680000	2.8273710000	-1.9445100000
C	-5.7182070000	1.2200980000	-0.3112040000
C	-6.0269510000	2.5381860000	-2.7412580000
H	-4.1841050000	3.5516440000	-2.2588480000
C	-6.8147880000	0.9489530000	-1.1209850000
H	-5.5776260000	0.7020200000	0.6295670000
C	-6.9728070000	1.5971870000	-2.3444150000
H	-6.1431010000	3.0596670000	-3.6864260000

H	-7.5436910000	0.2124340000	-0.7960340000
H	-7.8244060000	1.3724720000	-2.9778520000
O	-0.3610920000	2.9195810000	1.0785270000
O	-2.0939060000	3.3599120000	-1.4022400000
H	0.5309230000	2.9526550000	0.4608010000
C	-1.9942700000	1.4177620000	3.1471910000
C	-3.0877250000	0.5578870000	3.7891360000
C	-0.6346560000	0.7418550000	3.3312260000
C	-1.9565820000	2.8040020000	3.8207420000
H	-4.0659660000	1.0391000000	3.7203000000
H	-3.1566150000	-0.4200270000	3.2972500000
H	-2.8533970000	0.3929480000	4.8464480000
H	0.1562690000	1.2802800000	2.7997120000
H	-0.3860100000	0.7138200000	4.3985720000
H	-0.6764760000	-0.2937730000	2.9834320000
H	-1.7202470000	2.6915900000	4.8847990000
H	-1.1947420000	3.4307180000	3.3507770000
H	-2.9271760000	3.3008000000	3.7300130000
C	1.8474770000	4.5197240000	-0.7295020000
C	2.7851910000	2.6818970000	0.5421660000
C	4.1062470000	4.7519200000	0.2134070000
C	2.7606420000	5.4418310000	0.0657070000
H	2.1991470000	4.5006100000	-1.7762990000
C	5.0693590000	2.8913100000	1.5183890000
H	4.7635210000	5.3204010000	0.8810860000
H	2.8849830000	6.4081740000	-0.4327770000

C	4.6336160000	1.7659440000	2.4403510000
C	3.7902280000	0.7996620000	1.6190980000
H	5.8438440000	2.5213410000	0.8267810000
H	5.5138270000	1.2759400000	2.8688660000
H	3.4444520000	-0.0279540000	2.2526730000
N	3.9363180000	3.4251030000	0.7808210000
N	1.7776470000	3.1788960000	-0.1824200000
N	2.6464360000	1.4490080000	1.0249430000
H	1.3322370000	0.7207720000	0.5753400000
H	0.8279040000	4.9216740000	-0.7619250000
H	2.3351060000	5.6196100000	1.0592310000
H	4.6123090000	4.7034660000	-0.7665510000
H	5.5157270000	3.7111440000	2.0941950000
H	4.0275330000	2.1680810000	3.2590220000
H	4.4431960000	0.3478750000	0.8453510000
N	-5.3049890000	-2.0878560000	-2.2254530000
O	-5.8877100000	-2.7953540000	-1.4186050000
O	-5.6588160000	-1.9355900000	-3.3813660000

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O	-6.4828100000	1.1676890000	-0.6787850000
N	-3.7590310000	0.8796910000	-0.7944830000
N	-2.2380760000	2.2158970000	-0.1262020000
N	-3.3988800000	2.9307340000	-0.0794190000
C	-4.3049000000	2.0969120000	-0.4931090000
C	-4.8682820000	-1.2954820000	-0.1672820000
C	-6.1823630000	-1.7434180000	-0.3040710000

C	-1.0486520000	2.8713790000	0.3594540000
C	-0.3551550000	3.7074220000	-0.5147340000
C	-4.5843770000	-0.2642990000	-1.2386770000
H	-4.0609500000	-0.7184720000	-2.0797140000
C	-2.4275980000	0.9696310000	-0.5633720000
C	-6.6811200000	-2.7208700000	0.5478550000
H	-7.7037780000	-3.0732470000	0.4495260000
C	-6.0028290000	0.2210850000	-1.6248440000
H	-6.0366250000	0.6518450000	-2.6346270000
C	-0.7438720000	2.7515210000	1.7174160000
C	-4.5344670000	-2.7770090000	1.6742860000
H	-3.8986890000	-3.1848350000	2.4541540000
C	0.7371780000	4.4024550000	0.0027130000
H	1.3055110000	5.0529760000	-0.6573390000
C	-4.0265770000	-1.8077100000	0.8096580000
H	-2.9967540000	-1.4707660000	0.8767840000
C	-0.7962410000	3.8824340000	-1.9434050000
H	-0.8191050000	2.9304940000	-2.4837120000
H	-0.1188520000	4.5546550000	-2.4731180000
H	-1.8040890000	4.3083090000	-1.9885610000
C	-1.5521710000	1.8655400000	2.6231170000
H	-2.6196670000	2.1032740000	2.5643770000
H	-1.2337530000	1.9866830000	3.6600980000
H	-1.4226520000	0.8172570000	2.3353870000
C	-6.8657570000	-1.0303310000	-1.4483310000
H	-7.9028440000	-0.7528390000	-1.2455600000

H	-6.8431780000	-1.6361200000	-2.3612100000
C	1.0990250000	4.2993360000	1.3452700000
C	-5.8474460000	-3.2311220000	1.5429900000
H	-6.2249640000	-3.9874910000	2.2241310000
C	0.3407800000	3.4847940000	2.1877010000
H	0.6085710000	3.4085940000	3.2388590000
C	2.2959120000	5.0355360000	1.8852970000
H	2.6756100000	5.7645300000	1.1659750000
H	3.1040430000	4.3326260000	2.1136720000
H	2.0512470000	5.5622350000	2.8121370000
C	-5.7616500000	2.3698130000	-0.7088200000
H	-6.1372370000	3.0161160000	0.0863540000
H	-5.8901770000	2.8891840000	-1.6705860000
C	-1.4332940000	-0.1849430000	-0.9131470000
O	-2.0638550000	-1.1857380000	-1.3942450000
C	-0.1909650000	0.2625850000	-1.7199330000
C	0.7496960000	-0.8825040000	-1.3477820000
H	-0.4217200000	0.2838700000	-2.7867540000
H	0.2972070000	-1.8077410000	-1.7125390000
C	2.1866790000	-0.8275180000	-1.7964500000
C	2.9120140000	-2.0237800000	-1.8676940000
C	2.8350680000	0.3772920000	-2.0934820000
C	4.2564800000	-2.0287800000	-2.2111270000
H	2.4133030000	-2.9626850000	-1.6436320000
C	4.1781580000	0.3924180000	-2.4470900000
H	2.2927320000	1.3146260000	-2.0310110000

C	4.8647730000	-0.8132640000	-2.4953710000
H	4.8293400000	-2.9460290000	-2.2621470000
H	4.6942120000	1.3158960000	-2.6780070000
C	0.5532590000	-0.8665140000	0.2269290000
C	1.6310420000	0.1010460000	0.7412360000
C	1.0029130000	-2.1533450000	0.8914700000
N	2.1713940000	-2.0330370000	1.4086890000
N	2.6042250000	-0.7106890000	1.2756860000
C	3.8879350000	-0.3634170000	1.7468220000
C	4.4326740000	0.8951730000	1.4649300000
C	4.6241860000	-1.2989030000	2.4807710000
C	5.7062710000	1.2048460000	1.9311720000
H	3.8618230000	1.6118780000	0.8910880000
C	5.8954290000	-0.9684880000	2.9348190000
H	4.1966330000	-2.2728630000	2.6814030000
C	6.4447870000	0.2827740000	2.6672160000
H	6.1244340000	2.1814420000	1.7072860000
H	6.4601540000	-1.7013720000	3.5025850000
H	7.4380720000	0.5340440000	3.0238500000
O	-0.7598330000	-0.4466490000	0.4463810000
O	1.6725110000	1.3041330000	0.5870960000
C	0.2175830000	-3.4344730000	1.0653650000
H	0.2099440000	1.2208340000	-1.3797260000
N	6.2841780000	-0.8032250000	-2.8665450000
O	6.8016680000	0.2735050000	-3.1091730000
O	6.8674790000	-1.8722260000	-2.9143580000

C	-0.5733120000	-3.7906630000	-0.1980790000
H	-1.2398390000	-2.9802800000	-0.5128090000
H	0.0994340000	-4.0358390000	-1.0287870000
H	-1.1795760000	-4.6806840000	0.0021800000
C	1.1594400000	-4.5838960000	1.4350000000
H	1.7027240000	-4.3773060000	2.3602750000
H	0.5753620000	-5.4994180000	1.5717120000
H	1.8962880000	-4.7610330000	0.6451710000
C	-0.7629980000	-3.1926370000	2.2299020000
H	-1.4155800000	-2.3416620000	2.0206540000
H	-1.3807760000	-4.0848880000	2.3781380000
H	-0.2173320000	-2.9908540000	3.1570990000

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O	-5.6994100000	-2.8942320000	-0.7118370000
N	-3.1448630000	-2.2390660000	-0.2364840000
N	-1.4534020000	-2.1325580000	-1.5447100000
N	-2.4373570000	-2.7377110000	-2.2654480000
C	-3.4561740000	-2.7842620000	-1.4538530000
C	-4.6367350000	-1.0076620000	1.4379340000
C	-5.9667280000	-1.2415660000	1.7956280000
C	-0.0966790000	-2.1086680000	-2.0517020000
C	0.7421410000	-3.1541130000	-1.6566960000
C	-4.0244750000	-2.3066250000	0.9540120000
H	-3.4219500000	-2.7646240000	1.7420180000
C	-1.8725990000	-1.8112250000	-0.3227680000
C	-6.7429910000	-0.2181930000	2.3245690000

H	-7.7787410000	-0.3965830000	2.5979480000
C	-5.2577250000	-3.1813880000	0.6075220000
H	-5.0395330000	-4.2531830000	0.7016610000
C	0.3082760000	-1.0720540000	-2.8979080000
C	-4.8397810000	1.2694030000	2.1448390000
H	-4.3996750000	2.2526910000	2.2757600000
C	2.0519840000	-3.1331980000	-2.1322940000
H	2.7292700000	-3.9292040000	-1.8324810000
C	-4.0536900000	0.2395190000	1.6284910000
H	-3.0225140000	0.4475040000	1.3625700000
C	0.2770610000	-4.2249220000	-0.7069940000
H	0.1779350000	-3.8266060000	0.3103620000
H	1.0000260000	-5.0414140000	-0.6706830000
H	-0.6907300000	-4.6401430000	-1.0061420000
C	-0.6216450000	0.0405080000	-3.2881890000
H	-1.6080010000	-0.3442380000	-3.5655600000
H	-0.2136130000	0.5902530000	-4.1385930000
H	-0.7380370000	0.7518580000	-2.4600410000
C	-6.3451510000	-2.6840730000	1.5598610000
H	-7.3322030000	-2.8190180000	1.1110140000
H	-6.3152880000	-3.2529620000	2.4956000000
C	2.5247160000	-2.0919710000	-2.9315010000
C	-6.1714690000	1.0429340000	2.4903250000
H	-6.7683590000	1.8550220000	2.8933640000
C	1.6387400000	-1.0807020000	-3.3118290000
H	1.9953540000	-0.2657890000	-3.9362780000

C	3.9781450000	-2.0116740000	-3.3094850000
H	4.4671240000	-2.9854760000	-3.2278600000
H	4.4985550000	-1.3121860000	-2.6432000000
H	4.1081080000	-1.6386560000	-4.3288230000
C	-4.8140180000	-3.3704770000	-1.6916990000
H	-5.1873980000	-3.0604050000	-2.6692370000
H	-4.7453440000	-4.4678360000	-1.6756140000
C	-1.1176730000	-1.1162750000	0.8012590000
O	-1.3278010000	-1.5794420000	1.9178970000
C	-0.3507470000	0.0381090000	0.4176790000
C	0.7099040000	0.3891360000	1.4648860000
H	0.0670800000	-0.0786350000	-0.5826790000
H	0.2135420000	0.4793590000	2.4344780000
C	1.7277410000	-0.7318550000	1.5561990000
C	1.8937940000	-1.4448700000	2.7522560000
C	2.5071560000	-1.1002860000	0.4494720000
C	2.8358920000	-2.4586200000	2.8681310000
H	1.2539330000	-1.2136570000	3.5974540000
C	3.4694960000	-2.0948660000	0.5488770000
H	2.3552680000	-0.6210560000	-0.5151340000
C	3.6198250000	-2.7574190000	1.7607340000
H	2.9633720000	-3.0159360000	3.7879570000
H	4.0893680000	-2.3658010000	-0.2975030000
C	1.3264770000	1.8362840000	1.2409310000
C	1.8639510000	1.8512470000	-0.2132200000
C	2.6608820000	1.9615040000	1.9817480000

N	3.6862830000	1.9035040000	1.2137210000
N	3.2391440000	1.7864110000	-0.1130400000
C	4.1776790000	1.5404910000	-1.1280140000
C	3.8643380000	1.7754410000	-2.4742590000
C	5.4396780000	1.0382740000	-0.7833880000
C	4.8199540000	1.5178980000	-3.4533540000
H	2.8894550000	2.1632680000	-2.7352860000
C	6.3810680000	0.7936010000	-1.7772530000
H	5.6667180000	0.8568460000	0.2602010000
C	6.0810100000	1.0319210000	-3.1171480000
H	4.5724490000	1.7119540000	-4.4930760000
H	7.3575750000	0.4105970000	-1.4971900000
H	6.8200320000	0.8402340000	-3.8881400000
O	0.4323120000	2.7884760000	1.5655320000
O	1.2246190000	1.8357670000	-1.2517120000
C	2.8251500000	2.3591950000	3.4333140000
H	-1.2246340000	0.9912390000	0.0585160000
N	4.6095360000	-3.8307780000	1.8595070000
O	4.7713300000	-4.3623070000	2.9452240000
O	5.2165120000	-4.1435800000	0.8476520000
C	1.6642090000	1.8544090000	4.2957780000
H	0.7111550000	2.1916790000	3.8808250000
H	1.6642190000	0.7631640000	4.3670060000
H	1.7703280000	2.2501410000	5.3116310000
C	2.8048660000	3.9005570000	3.4453680000
H	1.8761120000	4.2570400000	2.9918930000

H	2.8701830000	4.2681300000	4.4757950000
H	3.6515140000	4.2993650000	2.8781150000
C	4.1575400000	1.8442640000	3.9829320000
H	4.9991000000	2.2218260000	3.3968970000
H	4.2819000000	2.1706440000	5.0209710000
H	4.1914370000	0.7496910000	3.9587280000
C	-2.1172710000	3.1535590000	-0.7301500000
C	-4.0130330000	3.2447810000	-2.3038930000
C	-3.6088470000	1.8294530000	-2.6729700000
C	-3.2082770000	1.1146680000	-1.3907820000
H	-4.9370430000	3.2319890000	-1.7043980000
H	-4.2130250000	3.8408140000	-3.2003520000
H	-4.4390550000	1.3114800000	-3.1623790000
H	-2.7637940000	1.8672480000	-3.3690360000
H	-4.1148260000	0.9479020000	-0.7896710000
H	-2.8168430000	0.1192950000	-1.6376370000
C	-2.9293460000	5.3367500000	-1.5297750000
C	-1.5186690000	5.8518820000	-1.2942470000
H	-3.6037970000	5.7027210000	-0.7397700000
H	-3.3204110000	5.6987040000	-2.4858660000
C	-0.9946630000	5.2222550000	-0.0150440000
H	-1.5213010000	6.9426000000	-1.2182730000
H	-0.8863160000	5.5656480000	-2.1407340000
H	0.0777440000	5.4033950000	0.1075290000
H	-1.4960100000	5.6837170000	0.8494460000
N	-2.1956030000	1.8275460000	-0.6356340000

N	-2.9256850000	3.8817360000	-1.5820750000
N	-1.1971990000	3.7895380000	-0.0137090000
H	-0.4865980000	3.2110790000	0.6409630000

IM4(RS)

O	4.3921050000	-0.8348230000	3.0376570000
N	3.1743040000	0.1013030000	0.8572190000
N	2.4643310000	2.0952600000	0.6925590000
N	3.5459410000	2.1663270000	1.5299720000
C	3.9586620000	0.9380110000	1.6041250000
C	4.6011490000	-1.5840150000	-0.2491820000
C	5.6085290000	-2.3622570000	0.3161470000
C	1.7659170000	3.3019960000	0.3380580000
C	0.7993420000	3.7899400000	1.2231210000
C	3.4904870000	-1.3285870000	0.7473360000
H	2.5616720000	-1.8318700000	0.4798180000
C	2.2146920000	0.8510950000	0.2842920000
C	6.7226400000	-2.7129090000	-0.4420310000
H	7.5164470000	-3.3170360000	-0.0122770000
C	4.0582070000	-1.8637250000	2.1162680000
H	3.2934770000	-2.4449360000	2.6317770000
C	2.0876550000	3.9148760000	-0.8724310000
C	5.7839840000	-1.4962040000	-2.3195510000
H	5.8636000000	-1.1676180000	-3.3509520000
C	0.1224250000	4.9457580000	0.8452320000
H	-0.6390730000	5.3499380000	1.5080190000
C	4.6637300000	-1.1452110000	-1.5690530000

H	3.8426230000	-0.5590300000	-1.9801080000
C	0.4897290000	3.0659280000	2.5053020000
H	0.0691710000	2.0710820000	2.3116600000
H	-0.2356110000	3.6280670000	3.0962550000
H	1.3928480000	2.9291240000	3.1078280000
C	3.1309930000	3.3278050000	-1.7832030000
H	4.0823920000	3.2017080000	-1.2551980000
H	3.3007010000	3.9803590000	-2.6414880000
H	2.8153960000	2.3401700000	-2.1426600000
C	5.2841020000	-2.7278750000	1.7416690000
H	6.1037580000	-2.5331080000	2.4404460000
H	5.0364860000	-3.7913610000	1.8240090000
C	0.3974940000	5.5955630000	-0.3627690000
C	6.8039890000	-2.2703490000	-1.7606430000
H	7.6697970000	-2.5319390000	-2.3612380000
C	1.3786280000	5.0715110000	-1.2034870000
H	1.6011100000	5.5712550000	-2.1424440000
C	-0.3570200000	6.8446750000	-0.7343700000
H	-0.1760430000	7.6398340000	-0.0045410000
H	-1.4350770000	6.6586950000	-0.7523250000
H	-0.0585590000	7.2126870000	-1.7181200000
C	5.0044280000	0.3015540000	2.4586940000
H	5.8920860000	0.0379280000	1.8676930000
H	5.2980770000	0.9762000000	3.2630940000
C	1.2229950000	0.3925740000	-0.8192880000
O	1.8489680000	0.2398590000	-1.9294270000

C	-0.0894130000	1.2137520000	-0.8475680000
C	-1.0905830000	0.1632970000	-1.3090350000
H	-0.3515280000	1.5797380000	0.1478360000
H	-0.8411590000	-0.1135220000	-2.3356140000
C	-2.5630010000	0.4800080000	-1.2323570000
C	-3.4519760000	-0.2688320000	-2.0148180000
C	-3.0776160000	1.4482100000	-0.3623660000
C	-4.8233480000	-0.0776180000	-1.9265320000
H	-3.0603840000	-1.0169900000	-2.6983980000
C	-4.4471380000	1.6586960000	-0.2637670000
H	-2.4082650000	2.0418520000	0.2508120000
C	-5.2950310000	0.8869990000	-1.0460100000
H	-5.5199210000	-0.6548480000	-2.5213090000
H	-4.8597250000	2.4014660000	0.4072450000
C	-0.6486630000	-1.0427260000	-0.3895290000
C	-1.4533210000	-0.9139330000	0.9098520000
C	-1.1523150000	-2.3710170000	-0.9020980000
N	-2.1866190000	-2.7621160000	-0.2513560000
N	-2.4288800000	-1.8756980000	0.8092940000
C	-3.5807990000	-2.0669010000	1.6024480000
C	-3.7816070000	-1.3138570000	2.7649290000
C	-4.5368590000	-3.0044680000	1.1976840000
C	-4.9409110000	-1.5097930000	3.5087930000
H	-3.0409370000	-0.5899880000	3.0740130000
C	-5.6850150000	-3.1861590000	1.9591950000
H	-4.3723370000	-3.5759800000	0.2933750000

C	-5.8966940000	-2.4423640000	3.1171440000
H	-5.0918700000	-0.9221540000	4.4089300000
H	-6.4222170000	-3.9147330000	1.6368070000
H	-6.7967580000	-2.5866090000	3.7053060000
O	0.7212870000	-0.9145900000	-0.2133920000
O	-1.3023970000	-0.0799700000	1.7825600000
C	-0.5286690000	-3.2233130000	-1.9849300000
H	-0.0045140000	2.0490210000	-1.5444430000
N	-6.7429190000	1.1032390000	-0.9449660000
O	-7.1379150000	1.9625990000	-0.1762960000
O	-7.4704730000	0.4130670000	-1.6375690000
C	-0.0766970000	-2.3778520000	-3.1836330000
H	-0.9269740000	-1.9096350000	-3.6925840000
H	0.6387350000	-1.6019070000	-2.8871240000
H	0.4155220000	-3.0334170000	-3.9096350000
C	0.7173170000	-3.8947720000	-1.3733700000
H	1.4686060000	-3.1449760000	-1.1135130000
H	0.4557210000	-4.4675500000	-0.4781070000
H	1.1546910000	-4.5811390000	-2.1059260000
C	-1.5190230000	-4.2993280000	-2.4371940000
H	-2.4307450000	-3.8519790000	-2.8458160000
H	-1.0574180000	-4.9130210000	-3.2167550000
H	-1.8078900000	-4.9502050000	-1.6080990000

TS4(RS)

O	-4.6803110000	-1.0037420000	-2.0550640000
N	-3.3295610000	0.4376700000	-0.2979540000

N	-2.7342140000	2.4579780000	-0.6069050000
N	-3.8957470000	2.3093240000	-1.3139850000
C	-4.2340130000	1.0680010000	-1.1063750000
C	-4.4745210000	-1.0074750000	1.3201720000
C	-5.4987230000	-1.9167280000	1.0669720000
C	-2.1119820000	3.7487380000	-0.4506360000
C	-1.3472650000	4.2697480000	-1.4969790000
C	-3.5026100000	-0.9482400000	0.1601360000
H	-2.5068990000	-1.3389740000	0.4026440000
C	-2.3815170000	1.3292790000	-0.0004440000
C	-6.4996730000	-2.1184030000	2.0140090000
H	-7.3033600000	-2.8244240000	1.8261610000
C	-4.1900050000	-1.7933020000	-0.9741040000
H	-3.4568910000	-2.4536230000	-1.4351530000
C	-2.3385820000	4.4284470000	0.7511550000
C	-5.4212820000	-0.4912190000	3.4531370000
H	-5.3982210000	0.0553320000	4.3903100000
C	-0.7756440000	5.5252390000	-1.2995760000
H	-0.1754420000	5.9566430000	-2.0964630000
C	-4.4157140000	-0.2896470000	2.5112310000
H	-3.5935780000	0.3959970000	2.6989140000
C	-1.1263400000	3.5082820000	-2.7752260000
H	-2.0510520000	3.0516290000	-3.1387880000
H	-0.3909710000	2.7088940000	-2.6296810000
H	-0.7431410000	4.1740520000	-3.5507140000
C	-3.2011530000	3.8394090000	1.8354770000

H	-2.7102510000	2.9827750000	2.3096880000
H	-4.1616680000	3.4974380000	1.4357110000
H	-3.4008270000	4.5849250000	2.6067850000
C	-5.3191640000	-2.5814600000	-0.2731880000
H	-6.2238020000	-2.5748550000	-0.8894720000
H	-5.0197170000	-3.6274490000	-0.1478410000
C	-0.9518280000	6.2362800000	-0.1114340000
C	-6.4555340000	-1.3969140000	3.2045560000
H	-7.2321190000	-1.5416240000	3.9491230000
C	-1.7385630000	5.6773080000	0.8970200000
H	-1.8971130000	6.2288940000	1.8199690000
C	-0.2887710000	7.5727520000	0.0869790000
H	0.7016170000	7.4443700000	0.5363460000
H	-0.8739710000	8.2105570000	0.7534800000
H	-0.1552640000	8.0947490000	-0.8632960000
C	-5.3085700000	0.2087060000	-1.6893530000
H	-6.1207610000	0.0540470000	-0.9662390000
H	-5.7156620000	0.6667630000	-2.5910880000
C	-1.1737000000	1.0258860000	0.8802930000
O	-1.4105660000	0.9383500000	2.0777890000
C	0.0134690000	0.7176970000	0.1373080000
C	1.2005070000	0.3633680000	1.0171840000
H	-0.4675450000	-0.2767520000	-0.6605470000
H	0.9955280000	0.7307990000	2.0267920000
C	2.5236520000	0.9290590000	0.5696550000
C	3.5031350000	1.2471210000	1.5222040000

C	2.8505210000	1.0543370000	-0.7888990000
C	4.7824020000	1.6265560000	1.1422310000
H	3.2610420000	1.1676190000	2.5782130000
C	4.1234080000	1.4362660000	-1.1897890000
H	2.1158660000	0.7897010000	-1.5423750000
C	5.0750930000	1.7024910000	-0.2143000000
H	5.5535120000	1.8400860000	1.8720660000
H	4.3952340000	1.4965510000	-2.2363160000
C	1.2066930000	-1.2770600000	1.1980730000
C	2.1289640000	-1.7284140000	0.0432040000
C	2.1224310000	-1.5959960000	2.3710040000
N	3.3239540000	-1.8756350000	2.0182000000
N	3.3803110000	-1.8956180000	0.6142410000
C	4.6374970000	-1.7747410000	-0.0062740000
C	4.7652700000	-1.8523850000	-1.3998230000
C	5.7623640000	-1.4929360000	0.7801040000
C	5.9978090000	-1.5855640000	-1.9882710000
H	3.8991890000	-2.0841180000	-2.0034420000
C	6.9853560000	-1.2360240000	0.1719740000
H	5.6541970000	-1.4405850000	1.8560310000
C	7.1101840000	-1.2632760000	-1.2154580000
H	6.0829790000	-1.6253260000	-3.0701340000
H	7.8433320000	-0.9923710000	0.7908820000
H	8.0613510000	-1.0381370000	-1.6863360000
O	-0.0447560000	-1.7533040000	1.2606270000
O	1.8648530000	-1.8107100000	-1.1421830000

C	1.6869060000	-1.7331560000	3.8113720000
H	0.1895970000	1.4612500000	-0.6498130000
N	6.4405260000	2.0241680000	-0.6270140000
O	6.6683190000	2.1334980000	-1.8206040000
O	7.2826410000	2.1670670000	0.2445050000
C	0.9808610000	-3.1001770000	3.9119110000
H	1.6786070000	-3.9102350000	3.6758120000
H	0.6082640000	-3.2513050000	4.9313720000
H	0.1452730000	-3.1363680000	3.2090640000
C	2.8951260000	-1.7053100000	4.7494200000
H	3.4326900000	-0.7539190000	4.6757780000
H	2.5596680000	-1.8297520000	5.7844500000
H	3.6004730000	-2.5062530000	4.5140600000
C	0.6876800000	-0.6358920000	4.1954280000
H	1.1633040000	0.3516230000	4.2196350000
H	-0.1486060000	-0.6050220000	3.4923110000
H	0.3002470000	-0.8363210000	5.2005000000
C	-0.9980180000	-2.2887250000	-1.8561270000
C	-1.1595710000	-2.1291920000	-4.2939740000
C	-1.8631010000	-0.8066180000	-4.0488480000
C	-1.1846480000	-0.1145940000	-2.8764280000
H	-0.1294140000	-1.9607880000	-4.6436400000
H	-1.6776740000	-2.7105030000	-5.0634710000
H	-1.8225230000	-0.1822160000	-4.9458900000
H	-2.9128750000	-0.9947070000	-3.7995430000
H	-0.1908690000	0.2487170000	-3.1884630000

H	-1.7621280000	0.7762140000	-2.5919720000
C	-0.8421880000	-4.3317800000	-3.2309690000
C	-1.1858370000	-5.1089900000	-1.9714540000
H	0.2251660000	-4.4536140000	-3.4703380000
H	-1.4151800000	-4.7034030000	-4.0868900000
C	-0.5152270000	-4.4277700000	-0.7911330000
H	-0.8489290000	-6.1441920000	-2.0712430000
H	-2.2722140000	-5.1138000000	-1.8273170000
H	-0.8103010000	-4.8941260000	0.1530960000
H	0.5772870000	-4.5296140000	-0.8781520000
N	-1.0680200000	-0.9746770000	-1.7160900000
N	-1.1652160000	-2.9175580000	-3.0701090000
N	-0.8959330000	-3.0288440000	-0.7380730000
H	-0.5031010000	-2.4600490000	0.1398210000

IM4(RR)

O	4.3933990000	-0.8339240000	3.0373130000
N	3.1745880000	0.1014940000	0.8570430000
N	2.4647400000	2.0954680000	0.6920610000
N	3.5467690000	2.1667050000	1.5289240000
C	3.9594110000	0.9383750000	1.6032690000
C	4.6009020000	-1.5844430000	-0.2490860000
C	5.6081970000	-2.3628180000	0.3162150000
C	1.7662120000	3.3021560000	0.3376160000
C	0.8001200000	3.7903790000	1.2230660000
C	3.4905480000	-1.3284700000	0.7476390000
H	2.5616100000	-1.8317670000	0.4805740000

C	2.2147940000	0.8511990000	0.2843040000
C	6.7220690000	-2.7139090000	-0.4421030000
H	7.5158200000	-3.3181320000	-0.0123790000
C	4.0585840000	-1.8631500000	2.1166010000
H	3.2938200000	-2.4437350000	2.6327650000
C	2.0876990000	3.9149940000	-0.8729510000
C	5.7833360000	-1.4973860000	-2.3197090000
H	5.8628300000	-1.1690450000	-3.3511970000
C	0.1235100000	4.9464850000	0.8455320000
H	-0.6373870000	5.3510650000	1.5087690000
C	4.6633210000	-1.1459400000	-1.5690600000
H	3.8422860000	-0.5596260000	-1.9800730000
C	0.4909650000	3.0665620000	2.5054710000
H	0.0699370000	2.0718660000	2.3120840000
H	-0.2338510000	3.6289860000	3.0967910000
H	1.3943580000	2.9294500000	3.1075140000
C	3.1307870000	3.3278260000	-1.7839470000
H	4.0824120000	3.2020580000	-1.2562690000
H	3.3000470000	3.9801380000	-2.6425040000
H	2.8152130000	2.3400290000	-2.1429720000
C	5.2839000000	-2.7280480000	1.7418730000
H	6.1038080000	-2.5336940000	2.4404610000
H	5.0356420000	-3.7913760000	1.8243640000
C	0.3982190000	5.5961610000	-0.3626270000
C	6.8032590000	-2.2716580000	-1.7608330000
H	7.6688870000	-2.5335860000	-2.3615410000

C	1.3789320000	5.0718910000	-1.2036830000
H	1.6013440000	5.5716720000	-2.1426350000
C	-0.3581420000	6.8438560000	-0.7352340000
H	-0.2043900000	7.6297020000	0.0106050000
H	-1.4335390000	6.6477320000	-0.7842910000
H	-0.0381300000	7.2289160000	-1.7055830000
C	5.0055670000	0.3021020000	2.4574900000
H	5.8928310000	0.0380740000	1.8660810000
H	5.2998070000	0.9770470000	3.2614250000
C	1.2228540000	0.3925500000	-0.8189810000
O	1.8487190000	0.2398060000	-1.9291980000
C	-0.0895530000	1.2137270000	-0.8471940000
C	-1.0906890000	0.1632190000	-1.3086240000
H	-0.3516230000	1.5797650000	0.1482070000
H	-0.8412230000	-0.1136130000	-2.3351900000
C	-2.5631250000	0.4798540000	-1.2320030000
C	-3.4520040000	-0.2689500000	-2.0146070000
C	-3.0778530000	1.4479510000	-0.3619600000
C	-4.8233880000	-0.0777640000	-1.9264530000
H	-3.0603250000	-1.0170400000	-2.6982090000
C	-4.4473900000	1.6584070000	-0.2634900000
H	-2.4085780000	2.0415160000	0.2513740000
C	-5.2951820000	0.8867820000	-1.0459140000
H	-5.5198900000	-0.6549550000	-2.5213520000
H	-4.8600610000	2.4011090000	0.4075460000
C	-0.6486990000	-1.0427750000	-0.3891130000

C	-1.4533750000	-0.9139780000	0.9102580000
C	-1.1523300000	-2.3710650000	-0.9017090000
N	-2.1866500000	-2.7621570000	-0.2509850000
N	-2.4289170000	-1.8757540000	0.8096750000
C	-3.5810180000	-2.0667380000	1.6026080000
C	-3.7813240000	-1.3144920000	2.7656850000
C	-4.5377510000	-3.0032570000	1.1970090000
C	-4.9408320000	-1.5101500000	3.5093070000
H	-3.0401340000	-0.5914130000	3.0753770000
C	-5.6860930000	-3.1847050000	1.9582940000
H	-4.3735810000	-3.5741390000	0.2922350000
C	-5.8972900000	-2.4416800000	3.1168290000
H	-5.0914010000	-0.9231400000	4.4099190000
H	-6.4238340000	-3.9124520000	1.6352690000
H	-6.7975050000	-2.5857230000	3.7048080000
O	0.7212480000	-0.9145440000	-0.2129810000
O	-1.3025090000	-0.0799960000	1.7829550000
C	-0.5286790000	-3.2233830000	-1.9845320000
H	-0.0046830000	2.0489500000	-1.5441240000
N	-6.7430790000	1.1030310000	-0.9450610000
O	-7.4705460000	0.4128670000	-1.6377720000
O	-7.1381720000	1.9623990000	-0.1764530000
C	-1.5190820000	-4.2993010000	-2.4369100000
H	-1.0574200000	-4.9130930000	-3.2163600000
H	-1.8081800000	-4.9501020000	-1.6078380000
H	-2.4306750000	-3.8518610000	-2.8457220000

C	-0.0765750000	-2.3779040000	-3.1831730000
H	-0.9268070000	-1.9097010000	-3.6922080000
H	0.6388010000	-1.6019350000	-2.8865900000
H	0.4157320000	-3.0334540000	-3.9091300000
C	0.7172080000	-3.8949470000	-1.3729070000
H	0.4554380000	-4.4680410000	-0.4778990000
H	1.1548130000	-4.5810330000	-2.1055860000
H	1.4683870000	-3.1451920000	-1.1126080000

TS4(RR)

O	-6.6602530000	-0.3631870000	-0.3446320000
N	-4.0687780000	0.4434980000	-0.5049370000
N	-3.1334330000	2.2802370000	0.0454970000
N	-4.4753290000	2.4917280000	0.1671510000
C	-5.0210250000	1.3611980000	-0.1672010000
C	-4.2638920000	-1.9634040000	0.1910550000
C	-5.2699340000	-2.9163070000	0.0123690000
C	-2.2440590000	3.4096750000	0.1963320000
C	-2.1637770000	4.2773680000	-0.9012920000
C	-4.3753430000	-0.9321960000	-0.9135350000
H	-3.7189550000	-1.1700450000	-1.7550190000
C	-2.8690460000	1.0377050000	-0.3707350000
C	-5.3524760000	-4.0057210000	0.8682160000
H	-6.1311550000	-4.7520100000	0.7428200000
C	-5.8654240000	-1.0360640000	-1.3120500000
H	-6.0648500000	-0.6384710000	-2.3151980000
C	-1.5588520000	3.6144540000	1.3938220000

C	-3.4449950000	-3.1479700000	2.1002240000
H	-2.7432100000	-3.2410760000	2.9228060000
C	-1.3333760000	5.3822680000	-0.7780050000
H	-1.2337150000	6.0626820000	-1.6210080000
C	-3.3580130000	-2.0506540000	1.2406160000
H	-2.5965080000	-1.2884430000	1.4024480000
C	-2.9194640000	4.0017350000	-2.1738860000
H	-2.6792560000	3.0101810000	-2.5745670000
H	-2.6583440000	4.7385480000	-2.9358070000
H	-4.0021010000	4.0452290000	-2.0152470000
C	-1.6048330000	2.6715030000	2.5651070000
H	-2.3961840000	1.9223350000	2.4749060000
H	-1.7753530000	3.2275000000	3.4909580000
H	-0.6380510000	2.1564710000	2.6477790000
C	-6.1597520000	-2.5298410000	-1.1496280000
H	-7.2233540000	-2.6935390000	-0.9627960000
H	-5.8819600000	-3.0683530000	-2.0625820000
C	-0.6030760000	5.6193050000	0.3892710000
C	-4.4269980000	-4.1180980000	1.9077230000
H	-4.4821860000	-4.9642370000	2.5849890000
C	-0.7413090000	4.7438870000	1.4603480000
H	-0.1635210000	4.9108560000	2.3647240000
C	0.3708020000	6.7636770000	0.4498910000
H	1.2627230000	6.5142830000	-0.1387280000
H	0.6885050000	6.9635640000	1.4758310000
H	-0.0569480000	7.6806990000	0.0341980000

C	-6.4754960000	1.0298270000	-0.3229590000
H	-7.0441870000	1.4315110000	0.5172130000
H	-6.8417700000	1.4993870000	-1.2478630000
C	-1.5497910000	0.4021350000	-0.8519930000
O	-1.6346980000	-0.0813700000	-1.9732250000
C	-0.4218560000	0.5137700000	0.0308880000
C	0.8297330000	-0.3176870000	-0.2319390000
H	-0.7068830000	0.5936740000	1.0797660000
H	1.4064750000	0.2269000000	-0.9897150000
C	0.6770150000	-1.7325700000	-0.7348640000
C	1.7221470000	-2.3241730000	-1.4613410000
C	-0.4569230000	-2.5019840000	-0.4693340000
C	1.6677440000	-3.6556730000	-1.8473270000
H	2.5945480000	-1.7328360000	-1.7257000000
C	-0.5451710000	-3.8315500000	-0.8528290000
H	-1.2941010000	-2.0342990000	0.0288370000
C	0.5334500000	-4.3935910000	-1.5258520000
H	2.4811470000	-4.1211900000	-2.3904130000
H	-1.4259450000	-4.4259130000	-0.6414610000
C	1.7767940000	-0.1919210000	1.1288460000
C	3.1856160000	-0.1468330000	0.4683040000
C	1.9132240000	-1.5374980000	1.8570950000
N	2.9882900000	-2.1707750000	1.5657610000
N	3.7365620000	-1.3941530000	0.6681400000
C	4.8905230000	-1.9625000000	0.0980950000
C	5.8583050000	-1.1696830000	-0.5318660000

C	5.0479170000	-3.3540160000	0.1442810000
C	6.9688170000	-1.7802880000	-1.1076450000
H	5.7320930000	-0.0968320000	-0.5654740000
C	6.1674290000	-3.9413400000	-0.4319290000
H	4.2892220000	-3.9536620000	0.6319010000
C	7.1343580000	-3.1616350000	-1.0627420000
H	7.7163220000	-1.1599640000	-1.5928390000
H	6.2789980000	-5.0205200000	-0.3901140000
H	8.0056190000	-3.6257090000	-1.5131550000
O	1.4365230000	0.8265250000	1.9223500000
O	3.6749550000	0.7574810000	-0.1898900000
H	1.7693980000	2.2731750000	1.4007550000
C	1.0950890000	-2.0000270000	3.0467890000
C	1.7335850000	-1.3278100000	4.2785320000
C	-0.3633870000	-1.5499150000	2.9470380000
C	1.1608010000	-3.5233260000	3.1849280000
H	2.7636030000	-1.6728470000	4.4110810000
H	1.7395890000	-0.2434950000	4.1405010000
H	1.1628580000	-1.5786380000	5.1800440000
H	-0.8575300000	-2.0412730000	2.1057720000
H	-0.8963760000	-1.8280920000	3.8635900000
H	-0.4131390000	-0.4648560000	2.8273560000
H	0.5957650000	-3.8395440000	4.0684860000
H	0.7297740000	-4.0126760000	2.3047470000
H	2.1923140000	-3.8672010000	3.2917140000
C	3.4988450000	3.4327790000	1.6065230000

C	2.0132210000	3.2634330000	-0.3133870000
C	4.1784740000	4.4725760000	-0.5159690000
C	4.0841640000	4.6881540000	0.9843010000
H	3.3808950000	3.5478630000	2.6876680000
C	2.9036120000	3.8667350000	-2.5255390000
H	4.9992540000	3.7746530000	-0.7410790000
H	3.4240350000	5.5332640000	1.2048210000
C	2.1017680000	2.6621310000	-2.9873300000
C	0.7596240000	2.7035310000	-2.2636180000
H	2.4816600000	4.7934510000	-2.9405610000
H	1.9719110000	2.6908490000	-4.0725950000
H	0.1593690000	1.8192860000	-2.5149270000
N	2.9354840000	3.9446220000	-1.0673150000
N	2.1831050000	3.1863010000	1.0374510000
N	0.9284370000	2.7305200000	-0.8242640000
H	0.0552980000	1.6493630000	-0.2006150000
H	4.1699970000	2.5803720000	1.4292880000
H	5.0769470000	4.9154550000	1.3819830000
H	4.3985430000	5.4152120000	-1.0322960000
H	3.9393040000	3.7931610000	-2.8763850000
H	2.6407100000	1.7462230000	-2.7198280000
H	0.1874740000	3.5817930000	-2.6092790000
N	0.4609580000	-5.7973600000	-1.9308450000
O	1.4112510000	-6.2716120000	-2.5307050000
O	-0.5483470000	-6.4235820000	-1.6492710000

TS5(SS)

O	6.0968940000	-0.1996690000	-1.5592490000
N	3.6265110000	-0.4137100000	-0.5329910000
N	2.7594010000	-2.2346260000	0.0341540000
N	4.1098880000	-2.4275370000	0.2116240000
C	4.6085890000	-1.2818010000	-0.1374960000
C	3.9769820000	1.9300680000	0.1610030000
C	5.1959550000	2.5987930000	0.2195320000
C	1.8450390000	-3.3147240000	0.2511080000
C	1.4751660000	-3.6410750000	1.5570860000
C	3.9295320000	0.9470790000	-0.9856000000
H	3.1577050000	1.1990980000	-1.7165210000
C	2.4155980000	-1.0198840000	-0.4230900000
C	5.4238100000	3.5420240000	1.2198120000
H	6.3718720000	4.0693130000	1.2761720000
C	5.3717320000	1.0188380000	-1.6237900000
H	5.2782740000	1.2162920000	-2.6917420000
C	1.3464070000	-3.9875190000	-0.8710320000
C	3.1889730000	3.1368220000	2.0699930000
H	2.4081740000	3.3641740000	2.7893270000
C	0.4939400000	-4.6215820000	1.7216070000
H	0.1771270000	-4.8835300000	2.7282720000
C	2.9587880000	2.1964870000	1.0698580000
H	2.0048020000	1.6872610000	0.9723210000
C	2.1556170000	-3.0070000000	2.7397940000
H	1.5381950000	-3.0932810000	3.6366900000
H	2.3790890000	-1.9517610000	2.5671200000

H	3.1083310000	-3.5108520000	2.9346380000
C	1.8800880000	-3.6935180000	-2.2490680000
H	1.8169940000	-2.6326700000	-2.5103160000
H	1.3347320000	-4.2667360000	-3.0017020000
H	2.9377550000	-3.9722540000	-2.3086740000
C	6.1089030000	2.1745700000	-0.9004710000
H	7.0881120000	1.8311730000	-0.5497530000
H	6.2927990000	3.0022730000	-1.5924660000
C	-0.0841560000	-5.2692590000	0.6298670000
C	4.4167140000	3.8003540000	2.1464270000
H	4.5834370000	4.5317660000	2.9311150000
C	0.3698140000	-4.9576070000	-0.6558390000
H	-0.0416230000	-5.4891990000	-1.5108950000
C	-1.1833940000	-6.2798620000	0.8254560000
H	-2.1654720000	-5.8111400000	0.6968920000
H	-1.1533140000	-6.7117470000	1.8282930000
H	-1.1097050000	-7.0920980000	0.0979260000
C	6.0244880000	-0.8429950000	-0.3011100000
H	6.3276170000	-0.1737240000	0.5168740000
H	6.6937210000	-1.7036470000	-0.3201800000
C	0.8475170000	-0.2145490000	-1.5536880000
O	1.4371320000	0.0528690000	-2.5851150000
C	-0.3028590000	-1.2078430000	-1.4469190000
C	-1.4767940000	-0.2312740000	-1.4345070000
H	-0.3145500000	-1.8754760000	-2.3086280000
H	-1.5320300000	0.2145020000	-2.4379570000

C	-2.8419180000	-0.7807520000	-1.1028820000
C	-3.9104900000	0.0877800000	-0.8462140000
C	-3.0710490000	-2.1604280000	-1.0786160000
C	-5.1728080000	-0.4028650000	-0.5417150000
H	-3.7657670000	1.1638880000	-0.8819280000
C	-4.3268450000	-2.6711940000	-0.7779300000
H	-2.2557480000	-2.8497320000	-1.2749940000
C	-5.3551800000	-1.7792440000	-0.5075270000
H	-6.0039180000	0.2593450000	-0.3336980000
H	-4.5143500000	-3.7373330000	-0.7470950000
C	-0.9223000000	0.9275580000	-0.5392510000
C	-1.3756460000	2.2776210000	-1.1366540000
C	-1.4148580000	1.0821270000	0.9022840000
N	-2.0145190000	2.2044210000	1.0645790000
N	-2.0261500000	2.9345400000	-0.1208330000
C	-2.6425230000	4.2081440000	-0.1267880000
C	-2.5558860000	5.0368300000	-1.2506290000
C	-3.3472370000	4.6270790000	1.0063230000
C	-3.1819560000	6.2791240000	-1.2261570000
H	-2.0086440000	4.7108700000	-2.1239860000
C	-3.9620910000	5.8734820000	1.0083690000
H	-3.4035720000	3.9777290000	1.8705500000
C	-3.8860790000	6.7066620000	-0.1045920000
H	-3.1116190000	6.9180830000	-2.1007300000
H	-4.5066220000	6.1915260000	1.8918610000
H	-4.3693690000	7.6778730000	-0.0971540000

O	0.4887640000	0.8448430000	-0.6457060000
O	-1.2073050000	2.6355080000	-2.2804850000
C	-1.2376640000	0.1671270000	2.1036980000
H	-0.2487620000	-1.7850850000	-0.5205230000
N	-6.6833640000	-2.3095230000	-0.1769480000
O	-7.5744500000	-1.5096060000	0.0469580000
O	-6.8188420000	-3.5202170000	-0.1429170000
C	-1.9954480000	-1.1583550000	1.9321580000
H	-3.0605650000	-0.9943990000	1.7416410000
H	-1.5868500000	-1.7660360000	1.1218310000
H	-1.8962660000	-1.7387500000	2.8555960000
C	0.2513180000	-0.1463820000	2.3005700000
H	0.6845780000	-0.6392680000	1.4240790000
H	0.8252640000	0.7625070000	2.5050390000
H	0.3583590000	-0.8120780000	3.1628820000
C	-1.7700180000	0.8676830000	3.3594480000
H	-1.6050320000	0.2193070000	4.2252600000
H	-1.2587250000	1.8179990000	3.5336710000
H	-2.8409880000	1.0718120000	3.2789380000

TS5(SR)

O	-5.8896910000	-0.0776540000	0.9650620000
N	-3.4698970000	0.7598250000	0.0512570000
N	-2.3846380000	2.5208000000	0.3802450000
N	-3.6151870000	2.7571180000	0.9550150000
C	-4.2576090000	1.6511700000	0.7297140000
C	-3.4701110000	-1.7145520000	0.4942150000

C	-4.4891540000	-2.6652860000	0.5596760000
C	-1.3717980000	3.5346000000	0.4059840000
C	-1.2046840000	4.3361540000	-0.7280860000
C	-3.9253040000	-0.5588080000	-0.3695230000
H	-3.5957110000	-0.6918740000	-1.4063060000
C	-2.2532550000	1.3173370000	-0.1883520000
C	-4.2851300000	-3.8573250000	1.2439250000
H	-5.0716520000	-4.6041130000	1.3046290000
C	-5.4628130000	-0.6548180000	-0.2631710000
H	-5.9733400000	-0.1690230000	-1.1053080000
C	-0.5758870000	3.6544250000	1.5463720000
C	-2.0582630000	-3.0972990000	1.8391770000
H	-1.1197090000	-3.2654830000	2.3590790000
C	-0.1705110000	5.2696850000	-0.7076790000
H	-0.0128340000	5.9003140000	-1.5795950000
C	-2.2602790000	-1.9039130000	1.1447300000
H	-1.5089330000	-1.1213940000	1.1330990000
C	-2.1153610000	4.1842170000	-1.9171720000
H	-2.0699720000	3.1763390000	-2.3447860000
H	-1.8527500000	4.9035550000	-2.6954670000
H	-3.1564890000	4.3596100000	-1.6258640000
C	-0.8132940000	2.7736430000	2.7414860000
H	-1.8382160000	2.8844300000	3.1084740000
H	-0.1265840000	3.0298450000	3.5507720000
H	-0.6625760000	1.7227710000	2.4772650000
C	-5.7214420000	-2.1622830000	-0.1612050000

H	-6.6538210000	-2.3587120000	0.3737540000
H	-5.8037560000	-2.5957320000	-1.1645350000
C	0.6618970000	5.4173750000	0.4054120000
C	-3.0581270000	-4.0704470000	1.8749980000
H	-2.8881280000	-4.9947190000	2.4184450000
C	0.4426490000	4.6090570000	1.5215060000
H	1.0798310000	4.7200570000	2.3954490000
C	1.7552890000	6.4537410000	0.4038340000
H	1.3388190000	7.4563320000	0.5471420000
H	2.2951380000	6.4579270000	-0.5470420000
H	2.4746950000	6.2743650000	1.2059730000
C	-5.6899760000	1.3164910000	1.0243940000
H	-5.9619110000	1.6481810000	2.0279410000
H	-6.3348620000	1.8367490000	0.3004540000
C	-1.2554970000	0.5836810000	-1.8659600000
O	-2.1174510000	0.7150820000	-2.7203550000
C	0.1022470000	1.2941870000	-1.8433370000
C	1.0772640000	0.1214950000	-1.9726100000
H	0.1675090000	1.9971620000	-2.6748100000
H	1.0512230000	-0.2507900000	-3.0003470000
C	2.5188550000	0.3242830000	-1.5750320000
C	3.4716440000	-0.5868170000	-2.0484000000
C	2.9248930000	1.3421140000	-0.7051960000
C	4.8008890000	-0.5020600000	-1.6599860000
H	3.1631650000	-1.3772800000	-2.7272630000
C	4.2530450000	1.4474890000	-0.3105830000

H	2.2064510000	2.0586850000	-0.3228810000
C	5.1648530000	0.5195930000	-0.7930930000
H	5.5454040000	-1.2036900000	-2.0143060000
H	4.5834690000	2.2297970000	0.3610610000
C	0.3198920000	-0.9467020000	-1.0951350000
C	0.7828980000	-0.7180500000	0.3524190000
C	0.7598640000	-2.3724870000	-1.3109510000
N	1.5179640000	-2.7802270000	-0.3606390000
N	1.6081080000	-1.7812590000	0.6174710000
C	2.3891890000	-2.0274300000	1.7708100000
C	2.6876910000	-0.9874600000	2.6571540000
C	2.8736560000	-3.3172920000	2.0051690000
C	3.4655280000	-1.2552340000	3.7788940000
H	2.3122270000	0.0091940000	2.4694970000
C	3.6524000000	-3.5613020000	3.1304580000
H	2.6431840000	-4.1094900000	1.3043660000
C	3.9513300000	-2.5363430000	4.0241220000
H	3.6957830000	-0.4457520000	4.4642040000
H	4.0274640000	-4.5645680000	3.3060310000
H	4.5592940000	-2.7335190000	4.9006860000
O	-1.0358740000	-0.7316860000	-1.3564420000
O	0.5479870000	0.2452010000	1.0573900000
C	0.2900320000	-3.3026560000	-2.4062480000
H	0.2313050000	1.8163010000	-0.8957880000
N	6.5689460000	0.6263590000	-0.3766960000
O	6.8691720000	1.5323980000	0.3806480000

O	7.3547260000	-0.1959970000	-0.8133390000
C	0.1251730000	-2.5684400000	-3.7429080000
H	-0.5793490000	-1.7349170000	-3.6608770000
H	1.0822620000	-2.1940650000	-4.1226320000
H	-0.2699820000	-3.2677410000	-4.4862140000
C	1.2728960000	-4.4657870000	-2.5637930000
H	1.3753560000	-5.0273330000	-1.6322500000
H	0.9105730000	-5.1457830000	-3.3407000000
H	2.2665480000	-4.1095650000	-2.8540370000
C	-1.0838860000	-3.8467570000	-1.9611180000
H	-1.4630170000	-4.5374870000	-2.7218040000
H	-0.9977500000	-4.3860570000	-1.0131030000
H	-1.8065590000	-3.0367360000	-1.8321540000

TS5(RS)

O	-2.9892100000	-0.8935630000	-2.9330610000
N	-2.2084430000	0.6657870000	-0.8766450000
N	-1.1643780000	2.4806230000	-1.0072500000
N	-1.7953120000	2.3544940000	-2.2230630000
C	-2.4322270000	1.2309970000	-2.1029650000
C	-4.0632790000	-0.3261870000	0.4067320000
C	-5.2141590000	-0.8476240000	-0.1789420000
C	-0.3491090000	3.6329570000	-0.7556750000
C	0.8834620000	3.7304610000	-1.4130110000
C	-2.8425850000	-0.5825530000	-0.4455010000
H	-2.0851360000	-1.1431420000	0.1039910000
C	-1.3746580000	1.4633980000	-0.1615360000

C	-6.4436560000	-0.7072340000	0.4613620000
H	-7.3480700000	-1.1116110000	0.0157120000
C	-3.3824270000	-1.4076980000	-1.6715280000
H	-2.9286740000	-2.3992610000	-1.6377360000
C	-0.8067410000	4.5942410000	0.1478490000
C	-5.3358040000	0.4893750000	2.2565390000
H	-5.3959080000	1.0104690000	3.2066950000
C	1.6801510000	4.8358720000	-1.1236880000
H	2.6454760000	4.9313240000	-1.6158340000
C	-4.1026700000	0.3485420000	1.6247250000
H	-3.1959460000	0.7589240000	2.0677700000
C	1.3319440000	2.6647830000	-2.3769180000
H	1.1982980000	1.6607750000	-1.9588630000
H	2.3851090000	2.7986970000	-2.6333520000
H	0.7446980000	2.7057160000	-3.2996960000
C	-2.1440830000	4.4568300000	0.8233400000
H	-2.9258600000	4.2105710000	0.0979520000
H	-2.4166340000	5.3910360000	1.3187560000
H	-2.1141590000	3.6587010000	1.5726130000
C	-4.9187580000	-1.5145730000	-1.4970800000
H	-5.4374040000	-1.0268420000	-2.3299260000
H	-5.2331290000	-2.5620120000	-1.5057000000
C	1.2701490000	5.8191290000	-0.2186820000
C	-6.4955640000	-0.0361070000	1.6802570000
H	-7.4478520000	0.0815720000	2.1882660000
C	0.0302970000	5.6827160000	0.4038010000

H	-0.3014780000	6.4431260000	1.1064090000
C	2.1436160000	7.0161900000	0.0514400000
H	1.8627900000	7.5110990000	0.9838510000
H	2.0539990000	7.7507300000	-0.7559480000
H	3.1971410000	6.7312140000	0.1172580000
C	-3.2583460000	0.4858960000	-3.0970170000
H	-4.3253660000	0.7092380000	-2.9598490000
H	-2.9730400000	0.7650080000	-4.1118640000
C	-0.5286570000	1.1957210000	1.7031070000
O	-1.1954590000	1.8098360000	2.5208360000
C	0.9444810000	1.4887440000	1.3728850000
C	1.6660230000	0.1744880000	1.6914900000
H	1.0758090000	1.7298810000	0.3190070000
H	1.8456530000	0.1254460000	2.7715820000
C	2.9833510000	-0.0335470000	0.9765440000
C	3.5038770000	-1.3205040000	0.7879170000
C	3.7170410000	1.0641030000	0.5121490000
C	4.7212340000	-1.5149420000	0.1494250000
H	2.9571860000	-2.1916990000	1.1369260000
C	4.9387020000	0.8905710000	-0.1251190000
H	3.3326450000	2.0700940000	0.6441390000
C	5.4181840000	-0.4003000000	-0.2951790000
H	5.1276940000	-2.5061090000	-0.0078890000
H	5.5137390000	1.7330470000	-0.4885910000
C	0.5623350000	-0.8625330000	1.3700010000
C	0.5283230000	-1.2498990000	-0.1213450000

C	0.5720110000	-2.2392770000	2.0167510000
N	0.4524180000	-3.1725690000	1.1455860000
N	0.4016000000	-2.6153090000	-0.1364850000
C	0.2008690000	-3.4657290000	-1.2486220000
C	-0.3273750000	-2.9522090000	-2.4372330000
C	0.5075940000	-4.8232740000	-1.1347800000
C	-0.5403090000	-3.8127850000	-3.5099220000
H	-0.5766060000	-1.9014470000	-2.5200020000
C	0.2865250000	-5.6657300000	-2.2183670000
H	0.9034530000	-5.2045680000	-0.2013080000
C	-0.2349040000	-5.1674050000	-3.4099810000
H	-0.9581300000	-3.4114700000	-4.4277270000
H	0.5254610000	-6.7204610000	-2.1268080000
H	-0.4051450000	-5.8304780000	-4.2516190000
O	-0.6590380000	-0.2368750000	1.7120240000
O	0.5667400000	-0.4967740000	-1.0742210000
C	0.6611740000	-2.5523700000	3.4956980000
H	1.2761760000	2.3302510000	1.9831230000
N	6.7074320000	-0.5941500000	-0.9697100000
O	7.2974640000	0.3970930000	-1.3622810000
O	7.1155460000	-1.7350260000	-1.0970460000
C	-0.1260540000	-1.5197830000	4.3171620000
H	0.2524920000	-0.5016710000	4.1914960000
H	-1.1821140000	-1.5092880000	4.0368260000
H	-0.0481660000	-1.7810260000	5.3772620000
C	2.1426430000	-2.5397310000	3.9205100000

H	2.6253290000	-1.5742740000	3.7427160000
H	2.2127950000	-2.7534430000	4.9918730000
H	2.7067240000	-3.3085950000	3.3829900000
C	0.0899360000	-3.9500340000	3.7598270000
H	0.6397830000	-4.7169360000	3.2089430000
H	0.1603090000	-4.1732300000	4.8286610000
H	-0.9608620000	-4.0069300000	3.4623280000

TS5(RR)

O	-4.5985470000	-1.5076420000	-3.0181320000
N	-2.9406440000	-0.0021020000	-1.4845320000
N	-3.3206560000	1.4916910000	-0.0683210000
N	-4.5422800000	1.2566990000	-0.6635440000
C	-4.2675870000	0.3309910000	-1.5322170000
C	-2.0370480000	-2.3274280000	-1.7425260000
C	-2.2510360000	-3.3286750000	-2.6894340000
C	-3.2022500000	2.5036370000	0.9401530000
C	-2.8688950000	3.8003890000	0.5403150000
C	-2.3232900000	-0.9815090000	-2.3679080000
H	-1.4028010000	-0.5283650000	-2.7538760000
C	-2.3133220000	0.7486390000	-0.5394540000
C	-1.9785560000	-4.6540590000	-2.3715490000
H	-2.1407240000	-5.4443320000	-3.0989210000
C	-3.2793910000	-1.3464580000	-3.5245670000
H	-3.2739820000	-0.5945740000	-4.3249510000
C	-3.3988300000	2.1457880000	2.2756090000
C	-1.3402540000	-3.9533220000	-0.1364210000

H	-1.0043230000	-4.2098650000	0.8639660000
C	-2.7244040000	4.7634810000	1.5381340000
H	-2.4609320000	5.7798010000	1.2550190000
C	-1.6035550000	-2.6215310000	-0.4584650000
H	-1.4993120000	-1.8296180000	0.2761900000
C	-2.6661080000	4.1231900000	-0.9157070000
H	-1.8564990000	3.5255370000	-1.3504680000
H	-2.4278620000	5.1807190000	-1.0460500000
H	-3.5722270000	3.9020740000	-1.4894470000
C	-3.7349560000	0.7268820000	2.6437890000
H	-4.6075970000	0.3739090000	2.0857590000
H	-3.9502910000	0.6461410000	3.7110850000
H	-2.8974090000	0.0623680000	2.4076160000
C	-2.7940860000	-2.7312760000	-3.9698610000
H	-3.6147580000	-3.3041910000	-4.4085930000
H	-2.0076380000	-2.6258960000	-4.7260590000
C	-2.9116070000	4.4535770000	2.8868370000
C	-1.5127910000	-4.9574310000	-1.0909120000
H	-1.3020230000	-5.9893760000	-0.8279150000
C	-3.2463930000	3.1443180000	3.2372760000
H	-3.3898600000	2.8916540000	4.2850590000
C	-2.7837700000	5.5201210000	3.9429610000
H	-2.4427470000	5.0998820000	4.8923040000
H	-3.7503530000	6.0024580000	4.1241460000
H	-2.0796530000	6.2982530000	3.6383560000
C	-5.1635910000	-0.3013070000	-2.5559130000

H	-6.1361520000	-0.5355140000	-2.1197150000
H	-5.3161730000	0.4044220000	-3.3860550000
C	-0.2730510000	1.1591220000	-0.9389420000
O	-0.3821620000	1.6521490000	-2.0505860000
C	0.2158890000	1.8628360000	0.3259680000
C	1.5099770000	1.1079140000	0.6579740000
H	0.3591650000	2.9287460000	0.1450390000
H	1.6928380000	1.1021200000	1.7361590000
C	2.7653840000	1.6207170000	-0.0100470000
C	4.0028070000	1.2086420000	0.5015470000
C	2.7333410000	2.4858970000	-1.1073990000
C	5.1919020000	1.6394340000	-0.0693410000
H	4.0322010000	0.5390610000	1.3573210000
C	3.9141500000	2.9331730000	-1.6890400000
H	1.7845230000	2.7878230000	-1.5391490000
C	5.1210340000	2.5004650000	-1.1582130000
H	6.1556460000	1.3288980000	0.3145510000
H	3.9076680000	3.5987540000	-2.5431870000
C	1.0671380000	-0.3482180000	0.2163970000
C	0.4737180000	-0.9326360000	1.5151010000
C	2.1513750000	-1.3643540000	-0.0729300000
N	2.3454500000	-2.1347550000	0.9345400000
N	1.4163460000	-1.8368320000	1.9401850000
C	1.4479040000	-2.6005680000	3.1314300000
C	0.4422650000	-2.4700740000	4.0960380000
C	2.5124660000	-3.4836390000	3.3397880000

C	0.5166480000	-3.2283980000	5.2603670000
H	-0.3812700000	-1.7893360000	3.9339350000
C	2.5642630000	-4.2319920000	4.5096320000
H	3.2840400000	-3.5768650000	2.5866670000
C	1.5702810000	-4.1109940000	5.4770730000
H	-0.2669070000	-3.1232570000	6.0041280000
H	3.3936980000	-4.9152370000	4.6622680000
H	1.6164710000	-4.6976740000	6.3883680000
O	0.1824020000	-0.1824650000	-0.8541020000
O	-0.5338000000	-0.5703470000	2.0899180000
C	2.7656950000	-1.7201450000	-1.4158380000
H	-0.5034190000	1.7187340000	1.1312930000
N	6.3720120000	2.9695130000	-1.7690170000
O	7.4199990000	2.5717760000	-1.2913190000
O	6.2907790000	3.7288860000	-2.7179930000
C	4.1088950000	-2.4242320000	-1.1998970000
H	4.8192100000	-1.7599560000	-0.6966900000
H	3.9961450000	-3.3275030000	-0.5961340000
H	4.5306130000	-2.7048080000	-2.1698650000
C	2.9589330000	-0.5266610000	-2.3564210000
H	3.7757020000	0.1193730000	-2.0266620000
H	3.2225030000	-0.9101420000	-3.3474170000
H	2.0468480000	0.0682220000	-2.4582500000
C	1.7663730000	-2.7019290000	-2.0686290000
H	2.1651870000	-3.0331490000	-3.0332730000
H	1.6100730000	-3.5793430000	-1.4344060000

H 0.7974270000 -2.2225650000 -2.2381650000

P(ss)

N -2.4367090000 -0.1117040000 0.0078030000
N -1.5684740000 -0.7353520000 0.9110350000
C -0.5336150000 -0.0013470000 1.1059090000
C 0.3621680000 -0.2708940000 2.3023880000
C -0.5635370000 1.2035690000 0.1923470000
C -2.0248650000 1.1646820000 -0.2886910000
C -3.6597750000 -0.7520120000 -0.3085410000
C -3.8647420000 -2.0676180000 0.1171610000
C -4.6404930000 -0.0881850000 -1.0526810000
C -5.0540370000 -2.7122640000 -0.2018210000
H -3.0976600000 -2.5699850000 0.6922670000
C -5.8220220000 -0.7547000000 -1.3618870000
H -4.4823150000 0.9311150000 -1.3761490000
C -6.0387740000 -2.0635110000 -0.9418820000
H -5.2068500000 -3.7331600000 0.1333810000
H -6.5814470000 -0.2348510000 -1.9371760000
H -6.9647760000 -2.5723460000 -1.1875480000
O -2.6007540000 2.0403410000 -0.8956480000
C 0.3508410000 2.6191160000 -1.4730850000
C 0.3208700000 3.2932520000 -0.1177600000
O -0.2087840000 2.4237350000 0.8014850000
O 0.6724860000 4.3907080000 0.1931540000
H 1.2289180000 2.9205550000 -2.0429700000
H -0.5433320000 2.9472560000 -2.0095640000

C	0.2649280000	1.1261220000	-1.1535920000
C	1.5892500000	0.4054850000	-1.0405570000
C	2.8014610000	1.0772570000	-0.8644680000
C	1.5868240000	-0.9932820000	-1.1144340000
C	3.9948990000	0.3713900000	-0.7608810000
H	2.8315960000	2.1596270000	-0.7895360000
C	2.7666730000	-1.7162030000	-1.0099310000
H	0.6464870000	-1.5200880000	-1.2543650000
C	3.9527310000	-1.0130230000	-0.8362100000
H	4.9421640000	0.8769810000	-0.6211260000
H	2.7804790000	-2.7974000000	-1.0677910000
H	-0.3371030000	0.5925040000	-1.8939610000
N	5.2110410000	-1.7661210000	-0.7297810000
O	5.1497760000	-2.9806560000	-0.7952590000
O	6.2395190000	-1.1314820000	-0.5816920000
C	1.7965750000	0.2395890000	2.1442350000
H	2.3675050000	-0.3660380000	1.4376990000
H	1.8280090000	1.2861880000	1.8290990000
H	2.2952850000	0.1719220000	3.1159610000
C	0.3833880000	-1.7718620000	2.6064390000
H	1.0012600000	-1.9527280000	3.4910490000
H	-0.6204120000	-2.1563110000	2.7997820000
H	0.8117620000	-2.3318210000	1.7687440000
C	-0.2997800000	0.4861310000	3.4749310000
H	-1.3214700000	0.1311570000	3.6365500000
H	0.2782040000	0.3150600000	4.3885970000

H -0.3290770000 1.5632920000 3.2854270000

P(SR)

N -0.1510510000 1.3550430000 -0.4507940000
N -0.7982590000 1.4897980000 0.7821700000
C -1.8611980000 0.7719060000 0.7932760000
C -2.8806600000 0.8742330000 1.9042610000
C -1.9477980000 -0.0671840000 -0.4547290000
C -0.8650390000 0.5780530000 -1.3254060000
C 1.1053490000 1.9769260000 -0.6384740000
C 1.8119300000 2.4234700000 0.4813990000
C 1.6421240000 2.1178950000 -1.9213960000
C 3.0579380000 3.0145220000 0.3105020000
H 1.3819120000 2.3023320000 1.4678780000
C 2.8942990000 2.7068190000 -2.0678180000
H 1.0881720000 1.7726620000 -2.7835480000
C 3.6072290000 3.1581120000 -0.9611810000
H 3.6039970000 3.3594080000 1.1826620000
H 3.3099960000 2.8158060000 -3.0643890000
H 4.5818790000 3.6171960000 -1.0877800000
O -0.6572420000 0.3412650000 -2.4968120000
C -1.5273000000 -1.5719780000 -0.2506400000
O -3.2042240000 -0.1200630000 -1.0900520000
C -3.3541960000 -1.3081130000 -1.7620740000
C -2.1477530000 -2.1888690000 -1.5023920000
H -2.0774680000 -1.9322020000 0.6221770000
C -0.0507810000 -1.7424960000 0.0175790000

C	0.8827610000	-1.9729340000	-0.9978000000
C	0.3992180000	-1.5784710000	1.3334780000
C	2.2409980000	-2.0307560000	-0.7098680000
H	0.5622540000	-2.0931050000	-2.0262690000
C	1.7517070000	-1.6278220000	1.6397690000
H	-0.3221810000	-1.4052010000	2.1276060000
C	2.6482410000	-1.8524200000	0.6041930000
H	2.9767430000	-2.2031940000	-1.4851470000
H	2.1137080000	-1.4975660000	2.6518040000
H	-2.4565020000	-3.2268900000	-1.3810110000
H	-1.5014060000	-2.1091480000	-2.3804740000
O	-4.3233010000	-1.5286620000	-2.4219260000
N	4.0836920000	-1.9077770000	0.9136490000
O	4.8537090000	-2.1215420000	-0.0050270000
O	4.4195820000	-1.7383220000	2.0723020000
C	-3.9912240000	1.8193550000	1.4028500000
H	-3.5822480000	2.8089140000	1.1798340000
H	-4.4705050000	1.4295880000	0.5008140000
H	-4.7548120000	1.9274010000	2.1797980000
C	-3.4999310000	-0.4900630000	2.2317900000
H	-3.9888960000	-0.9344350000	1.3587760000
H	-2.7569750000	-1.1941020000	2.6217630000
H	-4.2639980000	-0.3582900000	3.0036300000
C	-2.2293320000	1.4663020000	3.1565670000
H	-1.4195730000	0.8266120000	3.5218980000
H	-1.8127480000	2.4560040000	2.9563000000

H -2.9796940000 1.5584450000 3.9473020000

P(RS)

N 0.1990560000 1.4712800000 -0.2887710000
N 0.9326560000 1.4548230000 0.9009220000
C 1.9036150000 0.6225880000 0.8094680000
C 2.8918700000 0.4468860000 1.9514380000
C 1.8500110000 -0.1129460000 -0.5090050000
C 0.7689240000 0.6794480000 -1.2503380000
C -0.9001660000 2.3559560000 -0.4040650000
C -1.1373750000 3.2874810000 0.6094780000
C -1.7484440000 2.2814380000 -1.5129550000
C -2.2256750000 4.1457710000 0.5058010000
H -0.4748890000 3.3290080000 1.4645090000
C -2.8293640000 3.1529490000 -1.5975260000
H -1.5583000000 1.5598570000 -2.2958130000
C -3.0759770000 4.0863520000 -0.5951040000
H -2.4063090000 4.8675130000 1.2959050000
H -3.4853800000 3.0941620000 -2.4600830000
H -3.9228940000 4.7600100000 -0.6703380000
O 0.4842730000 0.5572200000 -2.4231600000
C 1.9797240000 -2.1645970000 -1.7126700000
C 3.1638420000 -1.2625090000 -1.9935530000
O 3.0529720000 -0.1208080000 -1.2478620000
O 4.0885880000 -1.4389510000 -2.7275590000
H 2.3021380000 -3.2038770000 -1.6506010000
H 1.2907630000 -2.0623330000 -2.5554620000

C	1.4060490000	-1.6146110000	-0.4066000000
H	1.9659650000	-2.0433110000	0.4308680000
C	-0.0721280000	-1.8038520000	-0.1380540000
C	-1.0245230000	-1.7967720000	-1.1649580000
C	-0.5051810000	-1.9465180000	1.1842960000
C	-2.3775680000	-1.9225340000	-0.8797090000
H	-0.7208950000	-1.6707830000	-2.1975470000
C	-1.8539460000	-2.0736570000	1.4899780000
H	0.2226410000	-1.9616570000	1.9881570000
C	-2.7660350000	-2.0586860000	0.4456740000
H	-3.1238830000	-1.9156580000	-1.6642170000
H	-2.1988600000	-2.1847750000	2.5102580000
N	-4.1963480000	-2.1978220000	0.7535410000
O	-4.5150190000	-2.3111210000	1.9236310000
O	-4.9791580000	-2.1933690000	-0.1792180000
C	4.2298830000	-0.1023880000	1.4405480000
H	4.1205580000	-1.0946670000	0.9900050000
H	4.6847730000	0.5576150000	0.6982120000
H	4.9180720000	-0.1974640000	2.2859500000
C	3.1178690000	1.8131540000	2.6141830000
H	3.8428450000	1.7076210000	3.4268010000
H	3.5082610000	2.5383430000	1.8945950000
H	2.1874900000	2.2095300000	3.0275980000
C	2.3187760000	-0.5206830000	3.0018400000
H	1.3269810000	-0.1986940000	3.3329540000
H	2.2524780000	-1.5444800000	2.6205830000

H 2.9825660000 -0.5413180000 3.8721770000

P(RR)

N 2.5141830000 -0.1298550000 -0.0424430000
N 1.6975980000 -0.8459290000 0.8319920000
C 0.6153190000 -0.2019760000 1.0773380000
C -0.3243130000 -0.7303420000 2.1601310000
C 0.5733660000 1.0825370000 0.2620820000
C 2.0162780000 1.1251040000 -0.2776680000
C 3.7907140000 -0.6552560000 -0.3651690000
C 4.1755360000 -1.8871160000 0.1707960000
C 4.6459500000 0.0410300000 -1.2250030000
C 5.4196780000 -2.4148930000 -0.1541030000
H 3.5035400000 -2.4166690000 0.8334330000
C 5.8870860000 -0.5061230000 -1.5346650000
H 4.3481080000 0.9960780000 -1.6348680000
C 6.2827390000 -1.7308530000 -1.0056940000
H 5.7130150000 -3.3712740000 0.2668090000
H 6.5490250000 0.0393290000 -2.1996440000
H 7.2529930000 -2.1476880000 -1.2538270000
O 2.5265200000 2.0616460000 -0.8523200000
C -0.3252010000 1.1671140000 -1.0323000000
O 0.2832850000 2.2407920000 1.0169270000
C -0.2423780000 3.2230900000 0.2235850000
C -0.4129690000 2.6916540000 -1.1835700000
H -1.3516990000 3.0437870000 -1.6118430000
H 0.4166780000 3.0795420000 -1.7788790000

O	-0.5068850000	4.3029680000	0.6601620000
C	-1.6725300000	0.4913200000	-0.9503550000
C	-2.7499500000	1.0743880000	-0.2725610000
C	-1.8565380000	-0.7333310000	-1.5995600000
C	-3.9836100000	0.4374360000	-0.2217910000
H	-2.6404780000	2.0375690000	0.2190500000
C	-3.0846490000	-1.3812270000	-1.5694070000
H	-1.0270330000	-1.1851860000	-2.1355290000
C	-4.1246310000	-0.7809440000	-0.8733380000
H	-4.8261640000	0.8714940000	0.3018730000
H	-3.2429960000	-2.3285170000	-2.0696180000
H	0.2261340000	0.7152550000	-1.8600290000
C	-1.0721570000	0.4165010000	2.8507310000
H	-0.3849470000	1.1270620000	3.3168020000
H	-1.7100770000	0.9663020000	2.1548920000
H	-1.7138260000	-0.0052260000	3.6306340000
C	0.5284520000	-1.4633490000	3.2095140000
H	1.0150050000	-2.3437060000	2.7836560000
H	1.3038480000	-0.8090340000	3.6176590000
H	-0.1181950000	-1.7880990000	4.0299950000
C	-1.3410390000	-1.7343500000	1.5894830000
H	-2.1150030000	-1.2440780000	0.9981950000
H	-0.8464910000	-2.4901460000	0.9717940000
H	-1.8352730000	-2.2448670000	2.4223050000
N	-5.4292790000	-1.4577110000	-0.8294400000
O	-5.5363950000	-2.5169620000	-1.4203340000

O -6.3246000000 -0.9196890000 -0.2037440000