Mechanistic insight into the acid-catalyzed isomerization of biomass-derived polysubstituted pyrrolidines: an experimental and DFT study.

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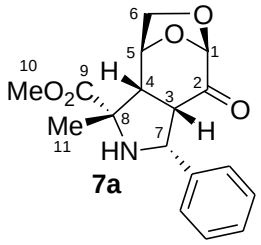
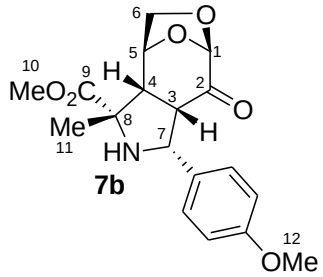
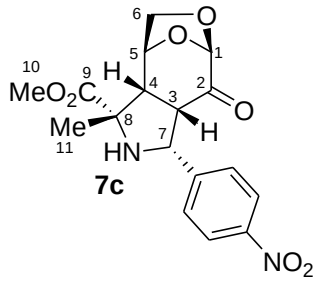
Spectroscopic and analytic data for all compounds



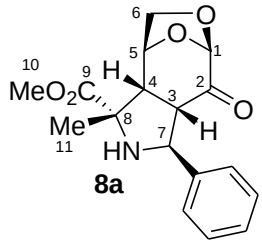
Adduct **7a**: Colorless oil; $[\alpha]_D$ -116.7 (*c* 1.66, $CHCl_3$); IR (film) ν_{max} 3344, 3061, 3028, 2954, 2904, 1738, 1732, 1450, 1433, 1261, 1240, 1152, 1119, 988, 910 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.37-7.21 (m, 5H, arom), 4.79 (d, *J* = 5.4 Hz, 1H, H-5), 4.71 (s, 1H, H-1), 4.47 (d, *J* = 7.5 Hz, 1H, H-7), 3.90 (dd, *J* = 7.7 *J*z, *J* = 5.3 Hz, 1H, H-6*exo*), 3.87-3.84 (m, 4H, H-6*endo* and H-10), 3.50 (dd, *J* = 8.1 Hz, *J* = 7.5 Hz, 1H, H-3), 3.30 (bs, 1H, NH), 2.55 (d, *J* = 8.1 Hz, 1H, H-4), 1.53 (s, 3H, H-11); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.2 (C, C-2), 174.0 (C, C-9), 137.2 (C, arom), 128.0 (CH, 2C, arom), 127.0 (CH, arom), 126.5 (CH, 2C, arom), 100.1 (CH, C-1), 72.9 (CH, C-5), 68.6 (CH_2, C-6), 67.8 (C, C-8), 62.4 (CH, C-7), 56.6 (CH, C-4), 52.6 (CH_3, C-10), 51.0 (CH, C-3), 26.3 (CH_3, C-11); HRMS calc. for $C_{17}H_{19}NO_5Na$ $[M+Na]^+$ 340.11554. Found 340.11526.



Adduct **7b**: Yellowish oil; $[\alpha]_D$ -69.0 (*c* 1.08, $CHCl_3$); IR (film) ν_{max} , 3368, 3057, 2955, 2905, 2839, 1746, 1732, 1614, 1514, 1445, 1252, 1113, 1034, 988 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.4 Hz, 2H, arom), 6.85 (d, *J* = 8.7 Hz, 2H, arom), 4.75 (d, *J* = 5.4 Hz, 1H, H-5), 4.71 (s, 1H, H-1), 4.50 (d, *J* = 8.1 Hz, 1H, H-7), 3.91 (dd, *J* = 7.5 Hz, *J* = 5.7 Hz, 1H, H-6*exo*), 3.88-3.75 (m, 7H, H-6*endo,* H-10 and H-12), 3.44 (dd, *J* = 8.1 Hz, *J* = 8.1 Hz, 1H, H-3), 3.08 (s, 1H, NH), 2.52 (d, *J* = 8.1 Hz, 1H, H-4), 1.54 (s, 3H, H-11); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6 (C, C-2), 174.1 (C, C-9), 158.6 (C, arom), 129.0 (C, arom), 127.8 (CH, 2C arom), 113.5 (CH, 2C arom), 100.0 (CH, C-1), 73.0 (CH, C-5), 68.7 (CH_2, C-6), 68.5 (C, C-8), 62.6 (CH, C-7), 55.8 (CH, C-4), 55.0 (CH_3, C-12), 52.7 (CH_3, C-10), 51.1 (CH, C-3), 26.1 (CH_3, C-11); HRMS calc. for $C_{18}H_{21}NNaO_6$ $[M+Na]^+$ 370.12666. Found 370.12537.

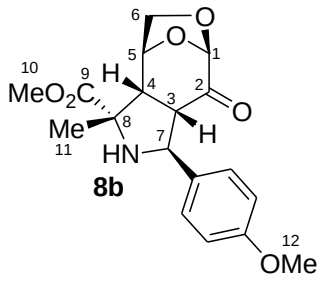


Adduct **7c**: Yellowish oil; $[\alpha]_D$ -68.4 (*c* 0.988, $CHCl_3$); IR (film) ν_{max} 2957, 2924, 2853, 1738, 1732, 1601, 1520, 1514, 1344, 1263, 1242, 1153, 1113, 988 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 9.0 Hz, 2H, arom), 7.55 (d, *J* = 8.4 Hz, 2H, arom), 5.00-4.94 (m, 1H, H-5), 4.81 (s, 1H, H-1), 4.48 (d, *J* = 6.3 Hz, 1H, H-7), 4.03-3.97 (m, 2H, H-6), 3.83 (s, 3H, H-10), 3.64 (dd, *J* = 7.4 Hz, *J* = 6.3 Hz, 1H, H-3), 2.71 (d, *J* = 7.4 Hz, 1H, H-4), 1.58 (s, 3H, H-11); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.1 (C, C-2), 174.1 (C, C-9), 146.7 (C, arom), 146.0 (C, arom), 127.3 (CH, 2C arom), 123.2 (CH, 2C arom), 100.7 (CH, C-1), 72.9 (CH, C-5), 68.6 (CH_2, C-6), 66.5 (C, C-8), 61.0 (CH, C-7), 58.3 (CH, C-4), 53.0 (CH_3, C-10), 50.6 (CH, C-3), 27.1 (CH_3, C-11); HRMS calc. for $C_{17}H_{18}N_2NaO_7$ $[M+Na]^+$ 385.10062. Found 385.09924.



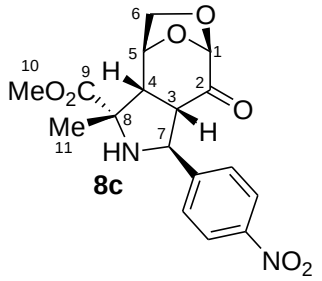
Adduct **8a**: White crystalline solid; mp 184-185 ºC (hexane/$CHCl_3$); $[\alpha]_D$ -110.2 (*c* 1.27, $CHCl_3$); IR (KBr) ν_{max} 3356, 3028, 2953, 2906, 1738, 1732, 1454, 1231, 1113, 1042, 982, 754 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.54-7.47 (m, 2H, arom), 7.36-7.19 (m, 3H, arom), 5.15 (d, *J* = 4.5 Hz, 1H, H-7), 5.10 (s, 1H, H-1), 4.90 (d, *J* = 4.5 Hz, 1H, H-5), 3.95 (dd, *J* = 6.9 Hz, *J* = 4.9 Hz, 1H, H-6*exo*), 3.89 (d, *J* = 6.9 Hz, 1H, H-6*endo*), 3.69 (s, 3H, H-10), 3.00 (dd, *J* = 10.2 Hz, *J* = 4.2 Hz, 1H, H-3), 2.53 (d, *J*=10.2 Hz, 1H, H-4), 2.22 (bs, 1H, NH), 1.60 (s, 3H, H-11); ^{13}C NMR

(75 MHz, $CDCl_3$) δ 198.2 (C, C-2), 176.1 (C, C-9), 145.2 (C, arom), 128.3 (CH, 2C, arom), 126.9 (CH, arom), 126.3 (CH, 2C, arom), 100.7 (CH, C-1), 71.9 (CH, C-5), 68.8 (CH_2, C-6), 66.4 (C, C-8), 60.1 (CH, C-7), 54.9 (CH, C-4), 53.3 (CH, C-3), 52.2 (CH_3, C-10), 25.0 (CH_3, C-11); HRMS calc. for $C_{17}H_{19}NO_5Na$ $[M+Na]^+$ 340.11554. Found 340.11514.



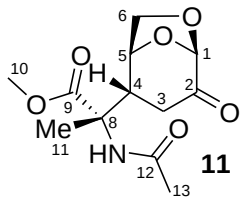
8b

Adduct **8b**: white solid; mp = 152-153 ºC (Hex/CH_2Cl_2); $[\alpha]_D$ -96.9 (*c* 1.27, $CHCl_3$); IR (KBr)) ν_{max} 3358, 2953, 2849, 1738, 1732, 1614, 1510, 1246, 1165, 1111, 1036, 982 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.7 Hz, 2H, arom), 6.86 (d, *J* = 8.6 Hz, 2H, arom), 5.09-5.07 (m, 2H, H-1 and H-7), 4.90 (d, *J* = 4.8 Hz, 1H, H-5), 3.95 (dd, *J* = 7.3 Hz, *J* = 4.9 Hz, 1H, H-6*exo*), 3.89 (dd, *J* = 7.3 Hz, *J* = 0.8 Hz, 1H, H-6*endo*), 3.79 (s, 3H, H-12), 3.68 (s, 3H, H-10), 2.96 (dd, *J* = 4.5 Hz, *J* = 10.2 Hz, 1H, H-3), 2.52 (d, *J* = 10.2 Hz, 1H, H-4), 2.21 (s, 1H, NH), 1.58 (s, 3H, H-11); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.4 (C, C-2), 176.0 (C, C-9), 158.5 (C, arom), 137.2 (C, arom), 127.4 (CH,2C arom), 113.7 (CH, 2C arom), 100.7 (CH, C-1), 71.9 (CH, C-5), 68.8 (CH_2, C-6), 66.4 (C, C-8), 59.9 (CH, C-7), 55.2 (CH_3, C-12), 54.9 (CH, C-4), 53.2 (CH, C-3), 52.2 (CH3, C-10), 25.0 (CH_3, C-11); HRMS calc. for $C_{18}H_{21}NNaO_6$ $[M+Na]^+$ 370.12666. Found 370.12644.



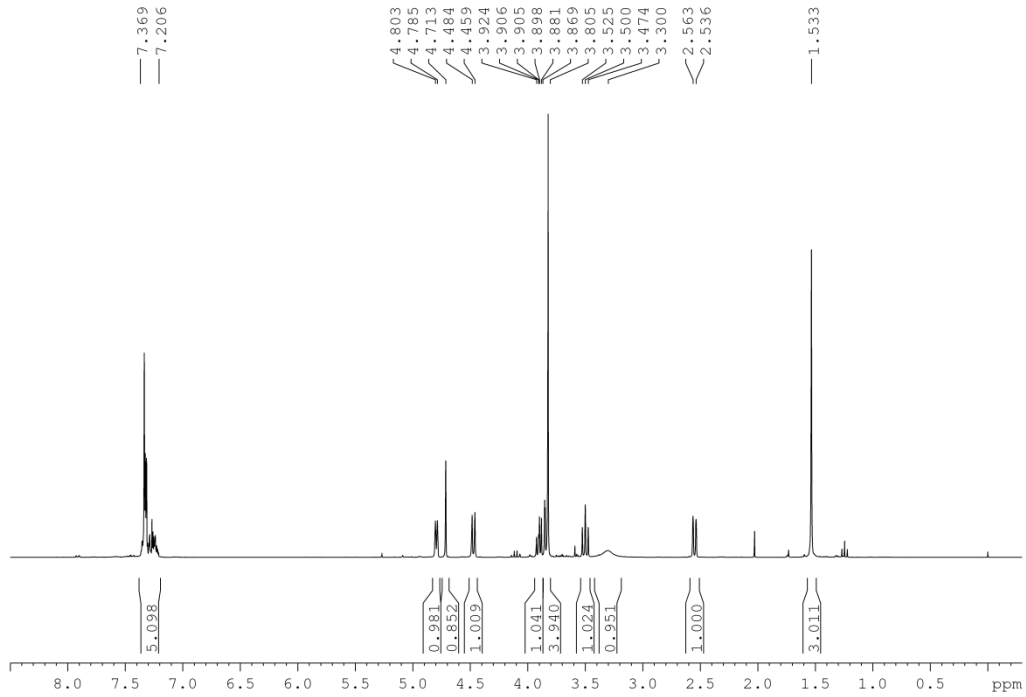
8c

Adduct **8c**: yellow solid; mp = 76-77°C (Hex/CH_2Cl_2); $[\alpha]_D$ -48.1 (*c* 1.15, $CHCl_3$); IR (KBr) ν_{max} 3350, 2916, 2849, 1734, 1728, 1599, 1516, 1346, 1227, 1167, 1126, 1111, 982 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.7 Hz, 2H, arom), 7.72 (d, *J* = 8.7 Hz, 2H, arom), 5.25 (d, *J* = 4.5 Hz, 1H, H-7), 5.14 (s, 1H, H-1), 4.93 (d, *J* = 4.8 Hz 1H, H-5), 3.98 (dd, *J* = 7.5 Hz, *J* = 4.8 Hz, 1H, H-6*exo*), 3.91 (d, *J* = 7.2 Hz, 1H, H-6*endo*), 3.71 (s, 3H, H-10), 2.93 (dd, *J* = 10.2 Hz, *J* = 4.5 Hz, 1H, H-3), 2.54 (d, *J* = 10.2 Hz, 1H, H-4), 1.62 (s, 3H, H-11); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.7 (C, C-2), 176.0 (C, C-9), 152.8 (C, arom), 146.9 (C, arom), 127.2 (CH, 2C arom), 123.6 (CH, 2C arom), 100.6 (CH, C-1), 71.8 (CH, C-5), 68.8 (CH_2, C-6), 66.5 (C, C-8), 59.5 (CH, C-7), 54.5 (CH, C-4), 52.9 (CH, C-3), 52.4 (CH_3, C-10), 24.9 (CH_3, C-11); HRMS calc. for $C_{17}H_{19}N_2O_7$ $[M+H]^+$ 363.11868. Found 363.11965.

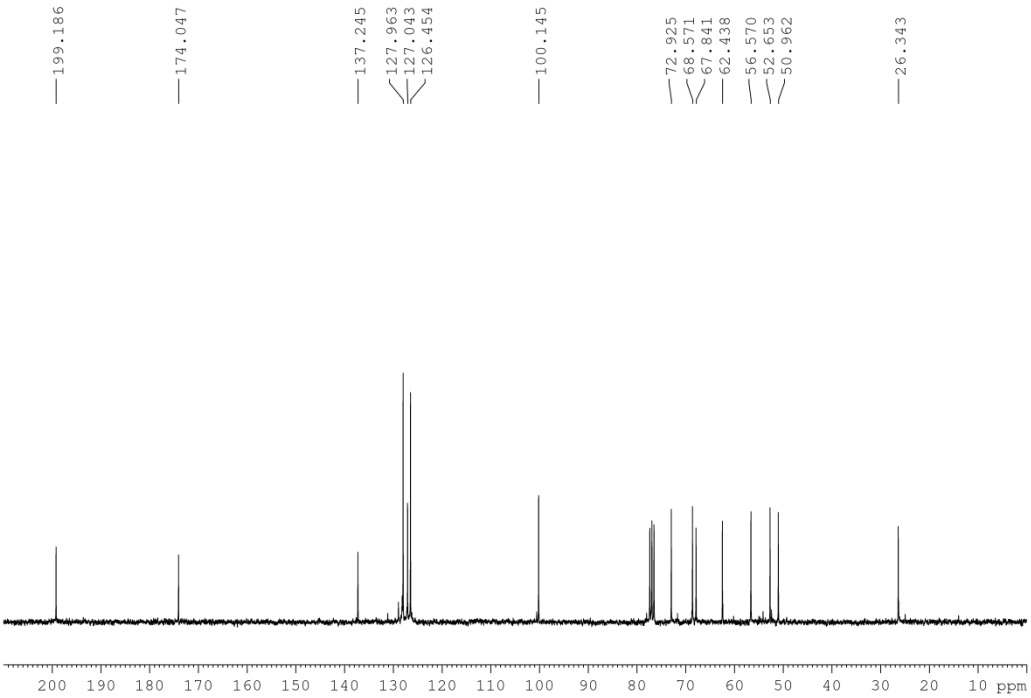


11

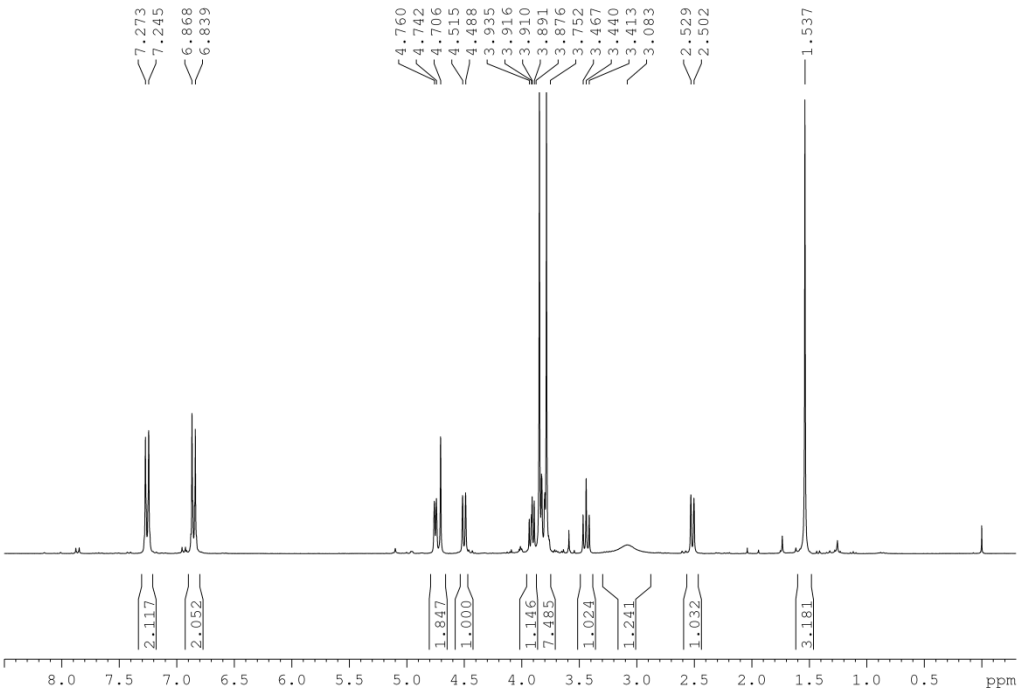
Compound **11**: Yellowish oil; $[\alpha]_D$ -90.6 (*c* 0.39, $CHCl_3$); IR (film) ν_{max} 3360, 3280, 2953, 1738, 1732, 1661, 1537, 1435, 1258, 1232, 1119, 984, 910, 756 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 6.16 (bs, 1H, NH) 5.07 (s, 1H, H-1), 4.83 (s, 1H, H-5), 4.01-3.97 (m, 2H, H-6), 3.74 (s, 3H, H-10), 3.10 (d, *J* = 7.8 Hz, 1H, H-4), 2.75 (dd, *J* = 17.9 Hz, *J* = 8.5 Hz, 1H, H-3*ax*), 2.62 (d, *J* = 18.0, 1H, H-3*eq*), 2.01 (s, 3H, H-13), 1.67 (s, 3H, H-11); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6 (C, C-2), 172.9 (C, C-9), 170.0 (C, C-12), 100.8 (CH, C-1), 73.7(CH, C-5), 68.7 (CH_2, C-6), 61.5 (C, C-8), 52.9 (CH_3, C-10), 44.3 (CH, C-4), 32.6 (CH_2, C-3), 23.5 (CH_3, C-13), 21.0 (CH_3, C-11); HRMS calc. for $C_{12}H_{17}NNaO_6$ $[M+Na]^+$ 294.09481. Found 294.09578.



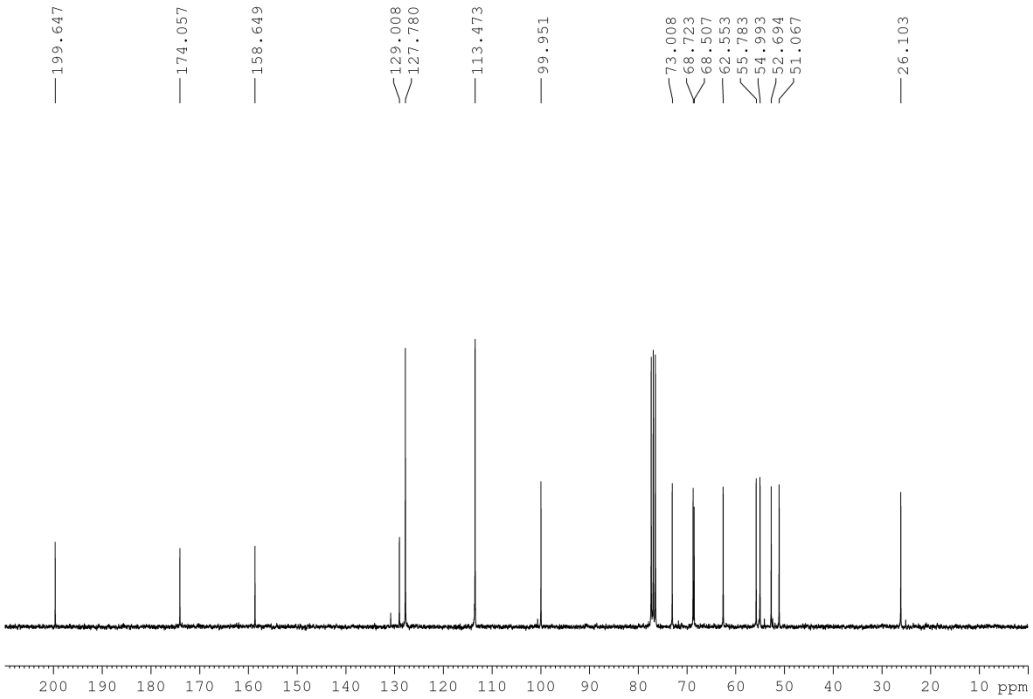
^{1}H NMR spectrum of a **7a** ($CDCl_3$, 300 MHz)



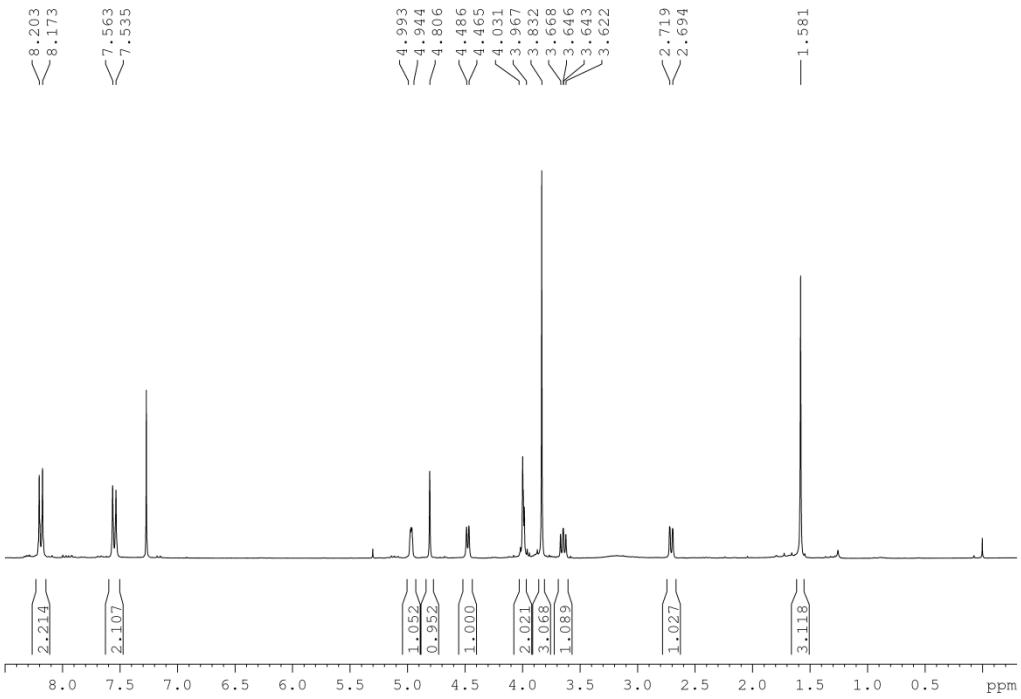
^{13}C NMR spectrum of a **7a** ($CDCl_3$, 75 MHz)



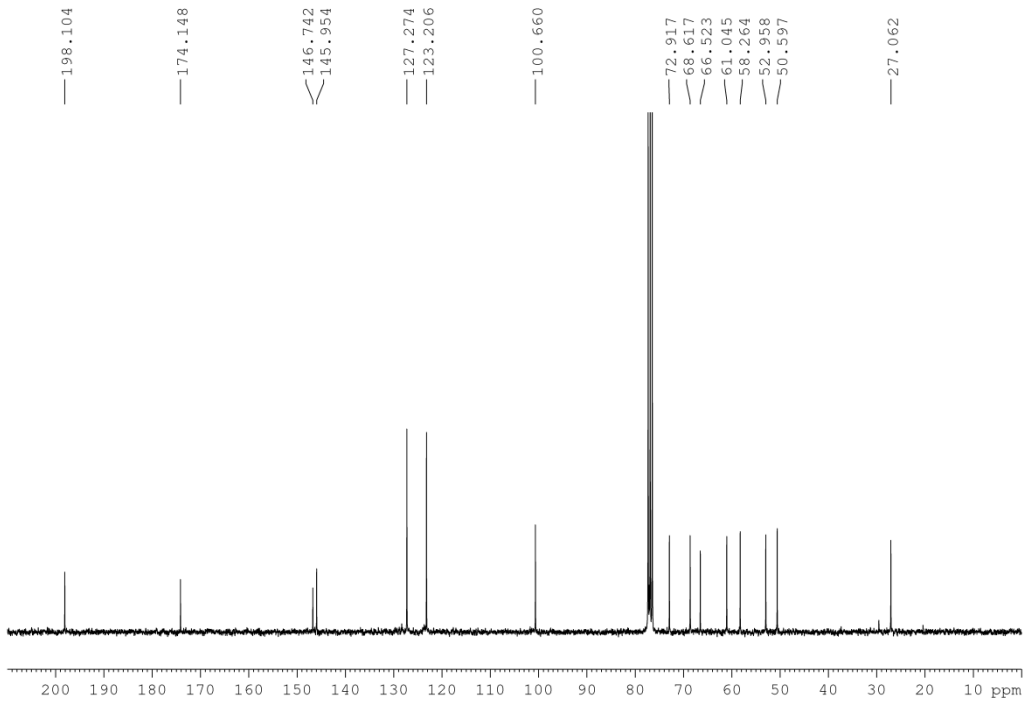
^{1}H NMR spectrum of a **7b** ($CDCl_3$, 300 MHz)



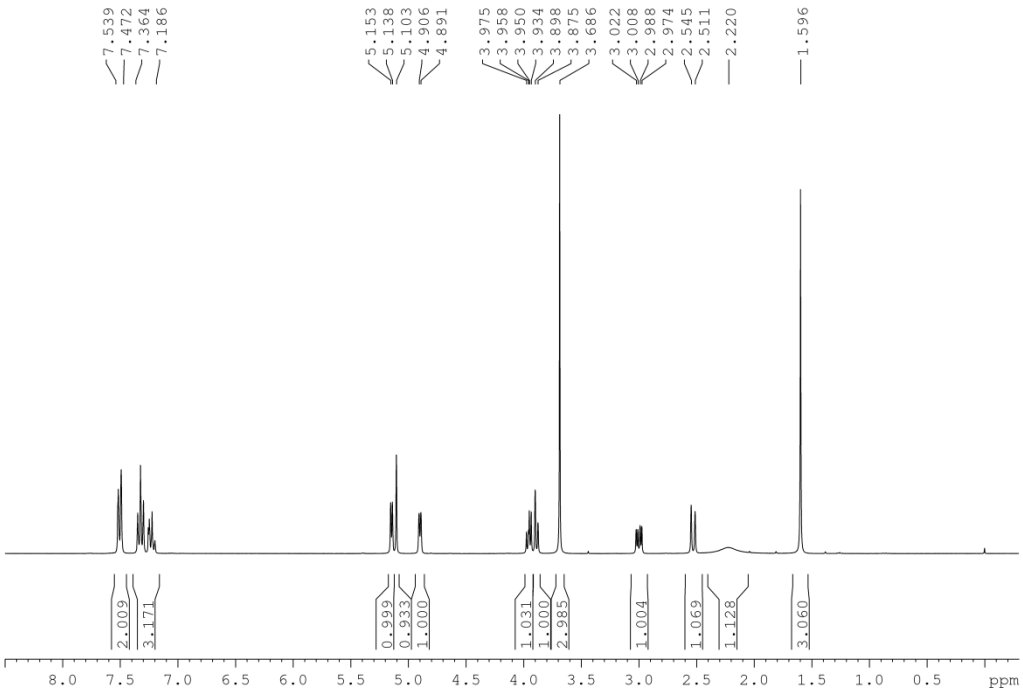
^{13}C NMR spectrum of a **7b** ($CDCl_3$, 75 MHz)



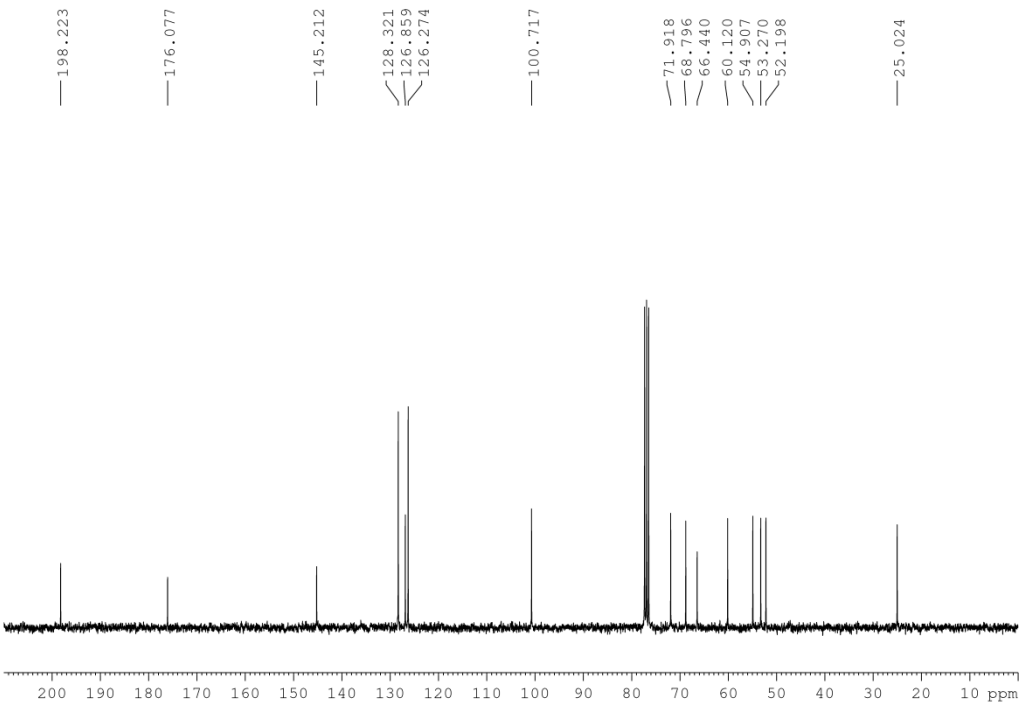
^{1}H NMR spectrum of a **7c** ($CDCl_3$, 300 MHz)



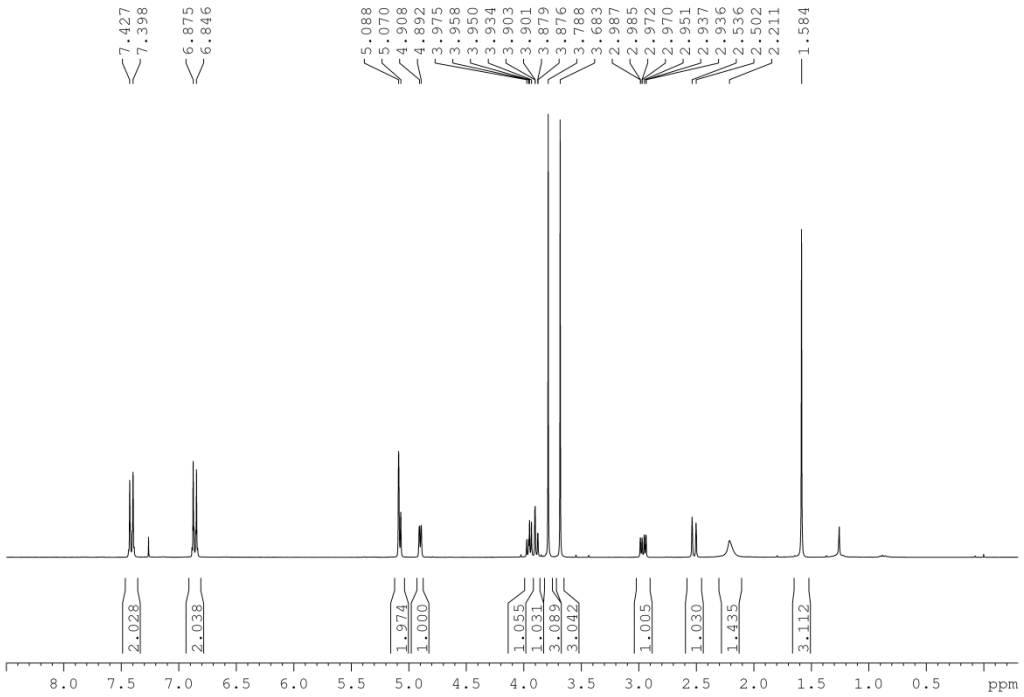
^{13}C NMR spectrum of a **7c** ($CDCl_3$, 75 MHz)



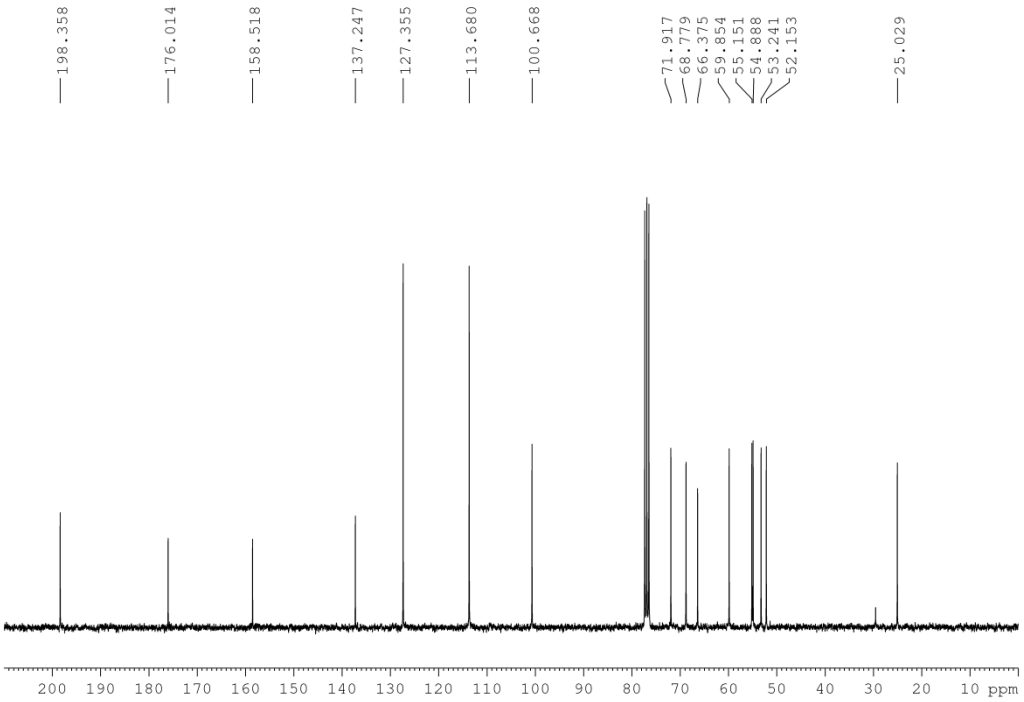
^{1}H NMR spectrum of a **8a** ($CDCl_3$, 300 MHz)



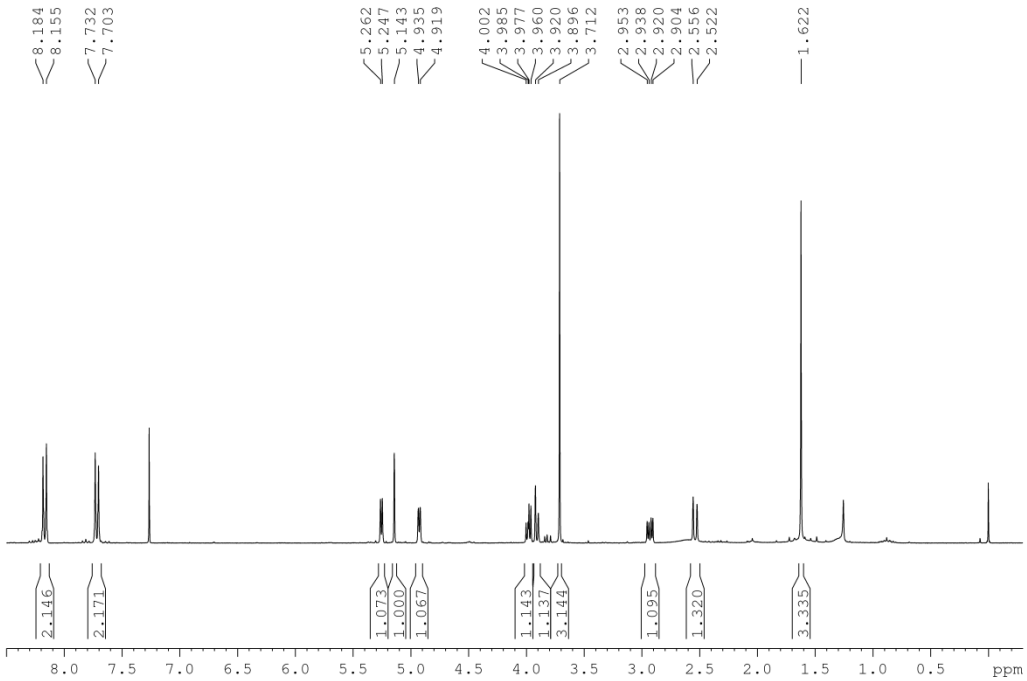
^{13}C NMR spectrum of a **8a** ($CDCl_3$, 75 MHz)



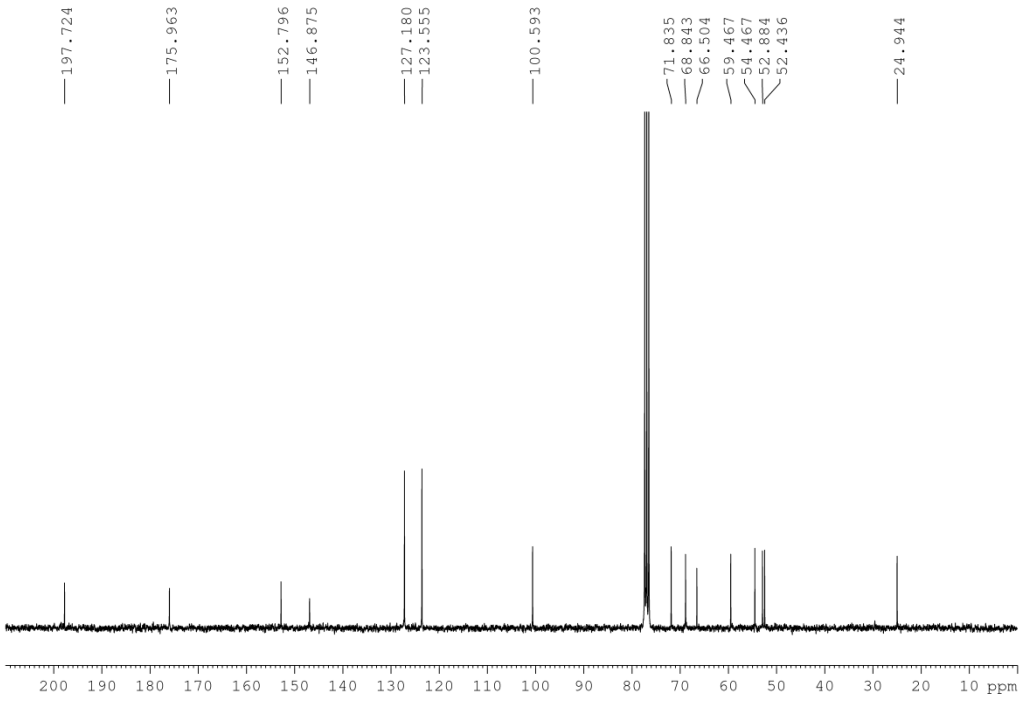
^{1}H NMR spectrum of a **8b** ($CDCl_3$, 300 MHz)



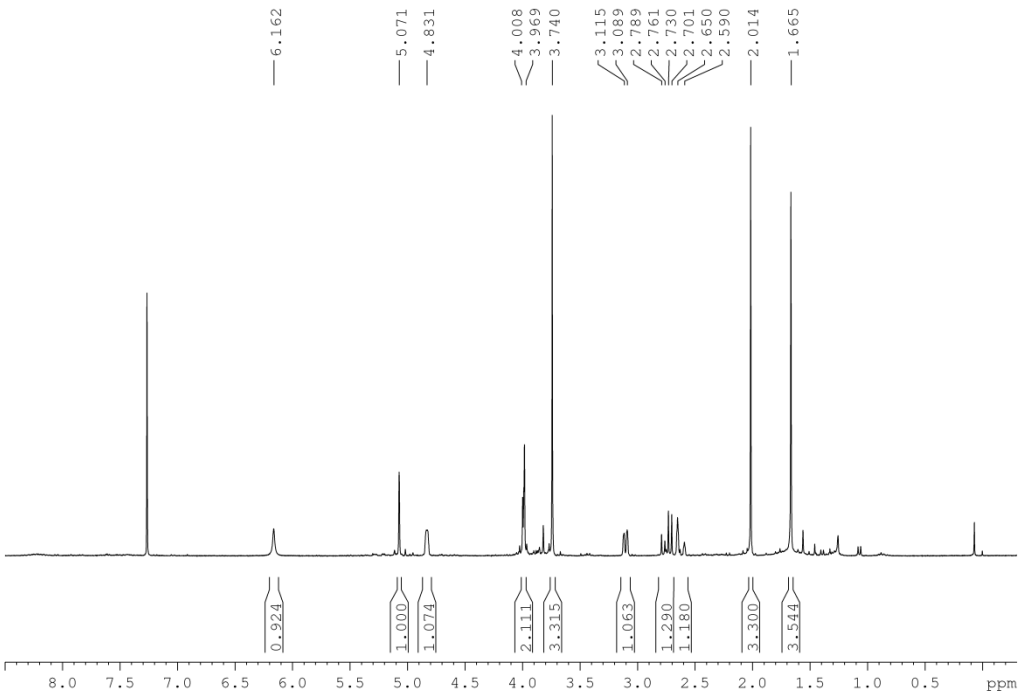
^{13}C NMR spectrum of a **8b** ($CDCl_3$, 75 MHz)



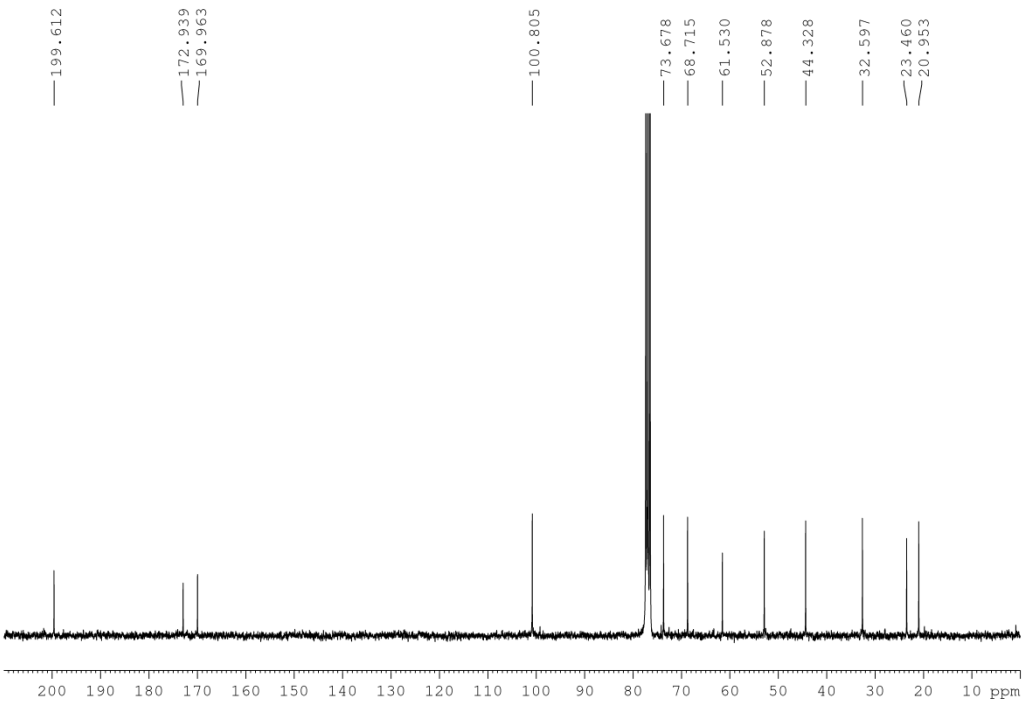
^{1}H NMR spectrum of a **8c** ($CDCl_3$, 300 MHz)



^{13}C NMR spectrum of a **8c** ($CDCl_3$, 75 MHz)



^{1}H NMR spectrum of a **11** ($CDCl_3$, 300 MHz)



^{13}C NMR spectrum of a **11** ($CDCl_3$, 75 MHz)

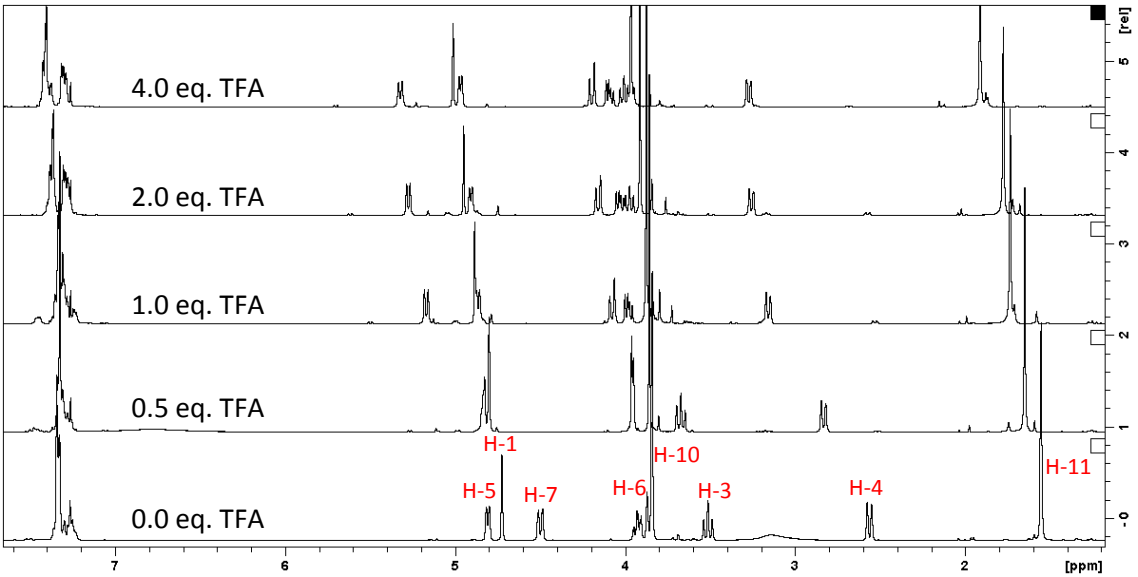


Figure S1. ^{1}H NMR Spectra of **7a** ($CDCl_3$, 300 MHz) recorded after the addition of increasing amounts of TFA.

Table S1. Selected ^{1}H NMR chemical shift (ppm) for **7a** after the addition of increasing amounts of TFA (see Figure S1).

	Nº Equivalents of TFA				
	0.0	**0.5**	**1.0**	**2.0**	**4.0**
H1	4.72	4.80	4.89	4.95	5.00
H3	3.51	3.67	3.86	3.97	4.00
H4	2.56	2.83	3.16	3.26	3.27
H5	4.80	4.84	4.87	4.91	4.96
H6*endo*	3.86	3.95	4.08	4.16	4.19
H6*exo*	3.92	3.96	3.98	4.03	4.09
H7	4.50	4.82	5.17	5.28	5.32
H10	3.86	3.86	3.88	3.91	3.96
H11	1.55	1.65	1.74	1.77	1.90

Table S2. Changes in the ^{1}H NMR chemical shifts ($\Delta\delta$, ppm) of selected protons of **7a** observed after the addition of increasing amounts of TFA (see Figures S1 and Table S1).

	Nº Equivalents of TFA				
	0.0	**0.5**	**1.0**	**2.0**	**4.0**
H1	-	0.08	0.17	0.23	0.28
H3	-	0.16	0.35	0.46	0.49
H4	-	0.27	0.60	0.70	0.71
H5	-	0.04	0.07	0.11	0.16
H6*endo*	-	0.09	0.22	0.30	0.33
H6*exo*	-	0.04	0.06	0.11	0.17
H7	-	0.32	0.67	0.78	0.82
H10	-	0.00	0.02	0.05	0.10
H11	-	0.10	0.19	0.22	0.35

Procedure for the ^{1}H NMR Kinetics Experiments

The corresponding pyrrolidine **7a-c** (0.048 mmol) was quantitatively transferred to an NMR tube and dissolved in $CDCl_3$ (500 mL). After the first ^{1}H NMR spectrum was taken, 100 μL of a TFA solution (480 mM in $CDCl_3$) was quickly added, affording a final concentration of **7a-c** and TFA of 80 mM. The NMR tube was immediately placed into the spectrometer with an internal temperature of 60 ºC, and series of spectra were taken at regular intervals of time (20-40 min depending on the sample) until significant conversion towards **8a-c** was noted. The different chemical shifts in the H11 signals exhibited by the starting material (**7a-c**) and the corresponding isomerized product (**8a-c**) allowed the determination of the progress of the reaction by integration of those signals in each ^{1}H NMR spectrum. With the integral values we calculated the concentration of the starting pyrolidine (**7a-c**), and plotted them over time.

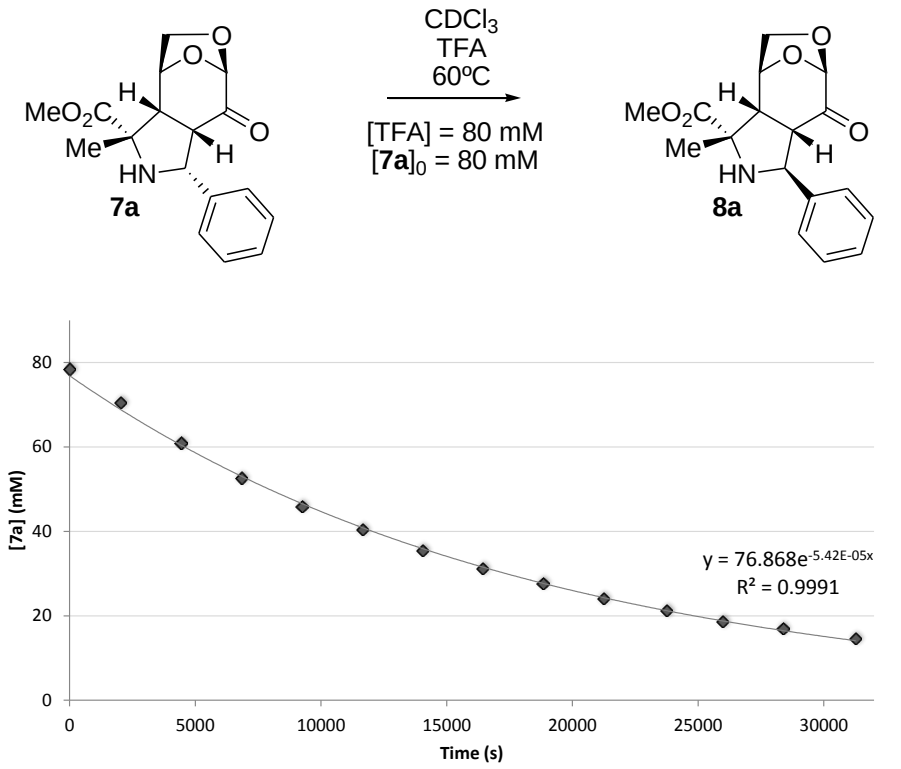


Figure S2. Concentration *versus* Time plot for **7a** obtained by integration of the ^{1}H NMR spectrum (80 mM TFA, 300 MHz, $CDCl_3$) recorded at 60ºC.

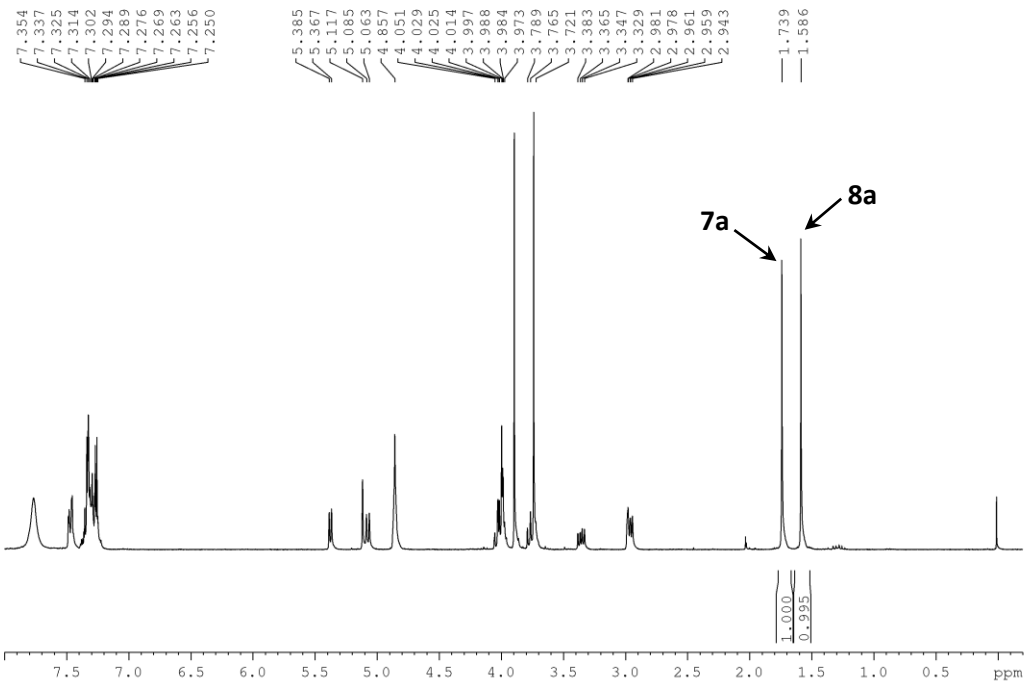


Figure S3. Representative ^{1}H NMR spectrum of a **7a**/**8a** mixture (80 mM TFA, $CDCl_3$, 300 MHz), recorded at 60ºC. The isomeric ratio was determined by integration of the signals at δ 1.74 ppm (H11 of **7a**) and 1.59 ppm (H11 of **8a**).

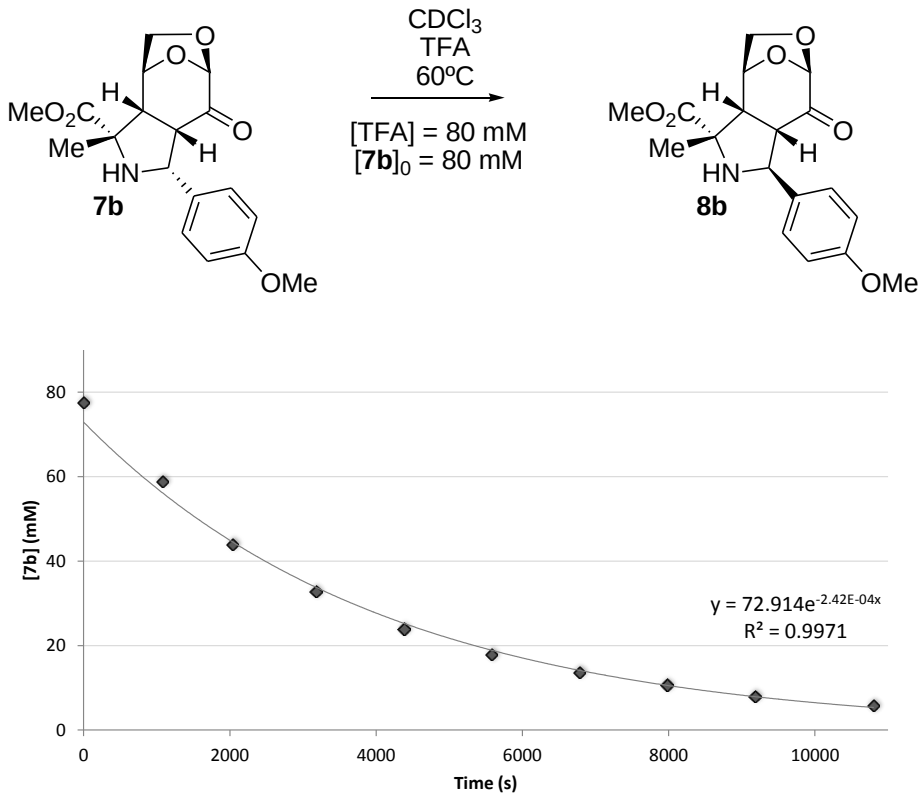


Figure S4. Concentration *versus* Time plot for **7b** obtained by integration of the ^{1}H NMR spectrum (80 mM TFA, 300 MHz, $CDCl_3$) recorded at 60ºC.

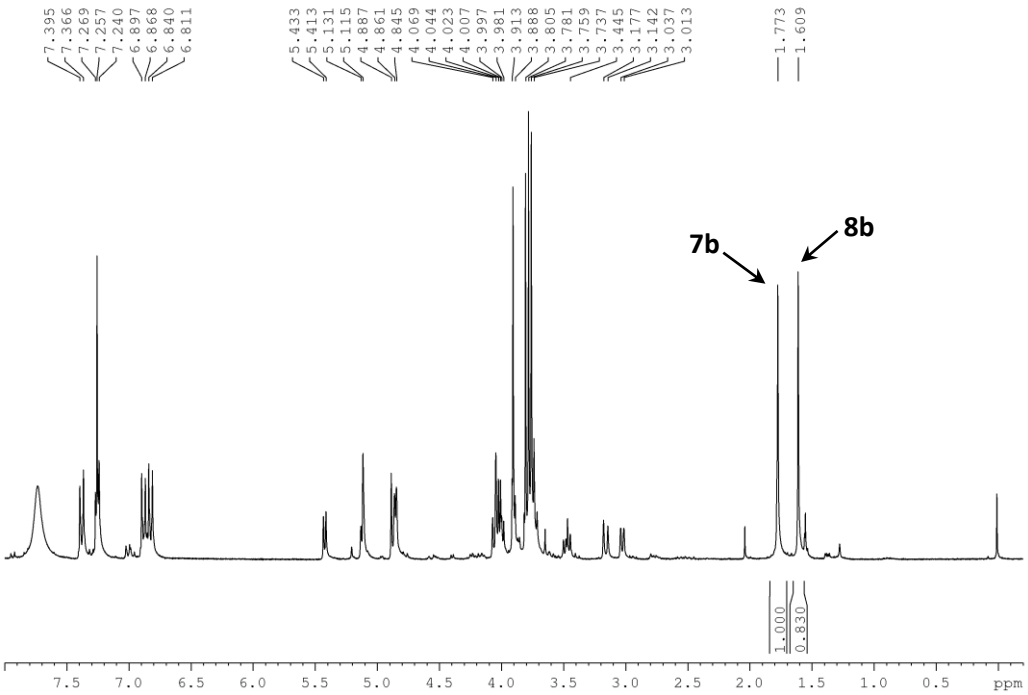


Figure S5. Representative ^{1}H NMR spectrum of a **7b**/**8b** mixture (80 mM TFA, $CDCl_3$, 300 MHz), recorded at 60ºC. The isomeric ratio was determined by integration of the signals at δ 1.77 ppm (H11 of **7b**) and 1.61 ppm (H11 of **8b**).

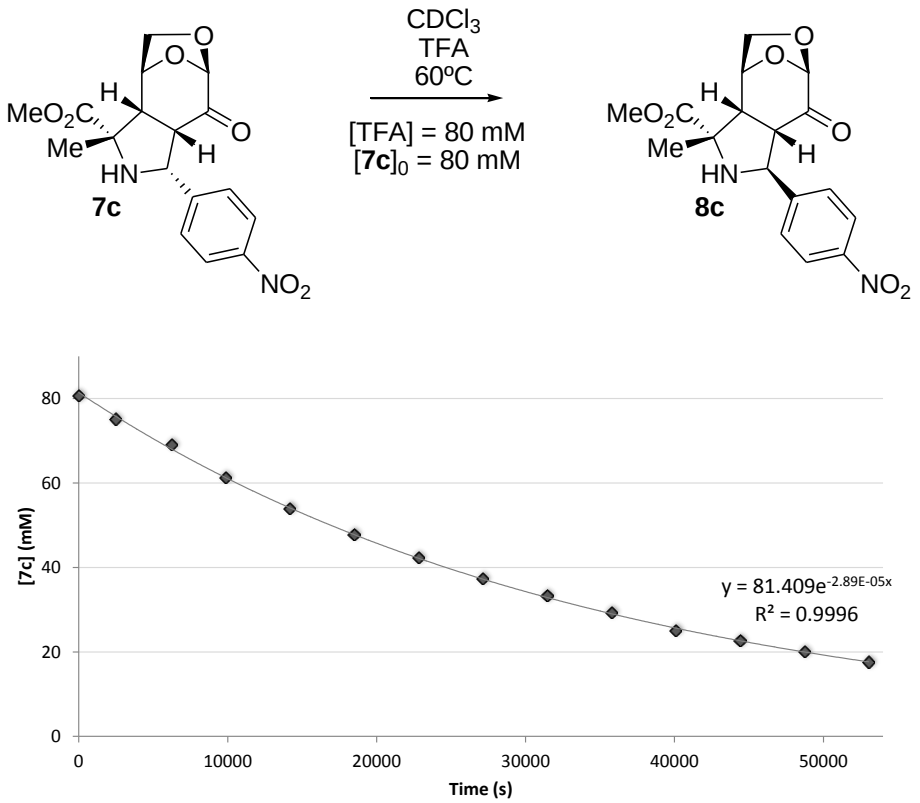


Figure S6. Concentration *versus* Time plot for **7c** obtained by integration of the ^{1}H NMR spectrum (80 mM TFA, 300 MHz, $CDCl_3$) recorded at 60ºC.

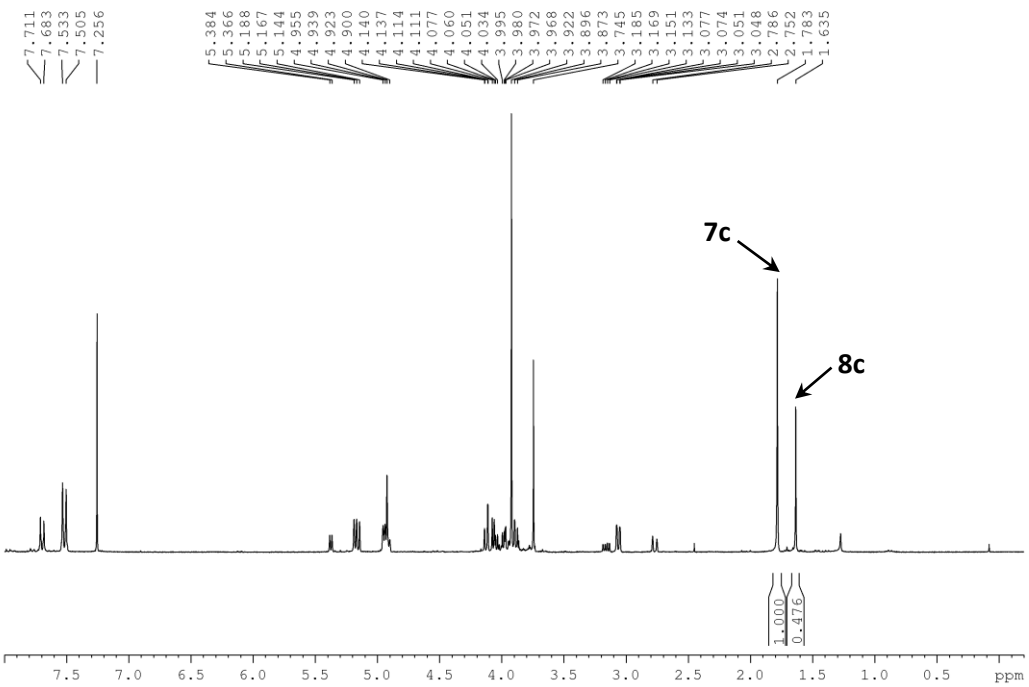


Figure S7. Representative ^{1}H NMR spectrum of a **7c**/**8c** mixture (80 mM TFA, $CDCl_3$, 300 MHz), recorded at 60ºC. The isomeric ratio was determined by integration of the signals at δ 1.78 ppm (H11 of **7c**) and 1.64 ppm (H11 of **8c**).

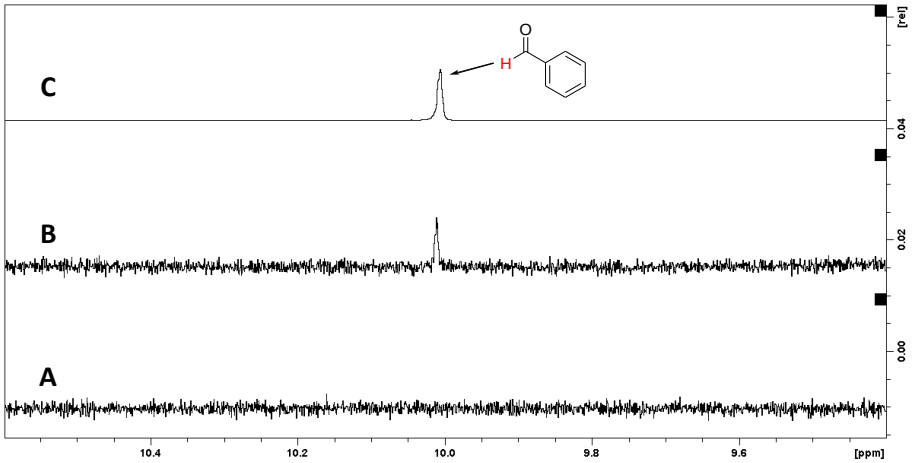


Figure S8. Expansion of low-field sections of the ^{1}H NMR spectra (300 MHz, $CDCl_3$) of: A) **7a** before the addition of TFA. B) **7a** after the addition of TFA. C) Pure analytical sample of benzaldehyde.

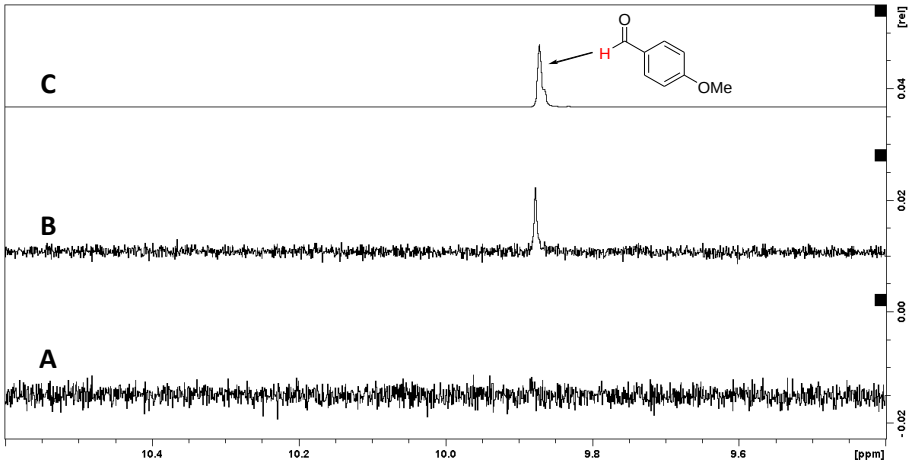


Figure S9. Expansion of low-field sections of the ^{1}H NMR spectra (300 MHz, $CDCl_3$) of: A) **7b** before the addition of TFA. B) **7b** after the addition of TFA. C) Pure analytical sample of *p*-anisaldehyde.

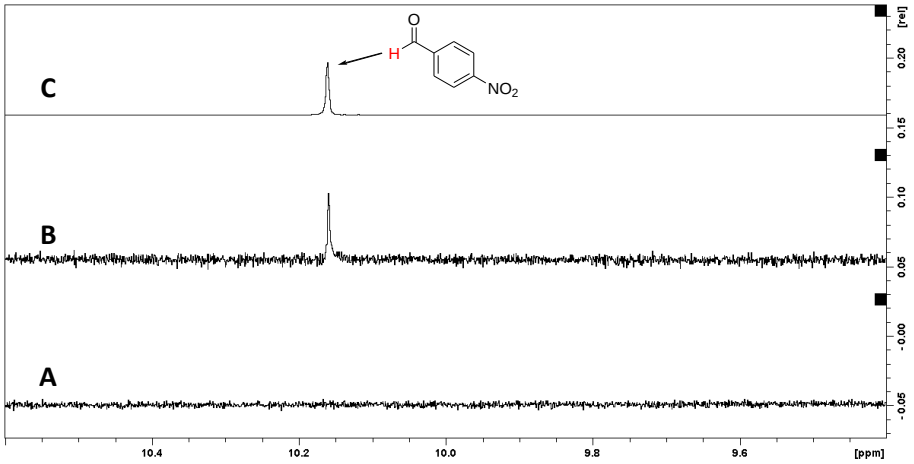


Figure S10. Expansion of low-field sections of the ^{1}H NMR spectra (300 MHz, $CDCl_3$) of: A) **7c** before the addition of TFA. B) **7c** after the addition of TFA. C) Pure analytical sample of *p*-nitrobenzaldehyde.

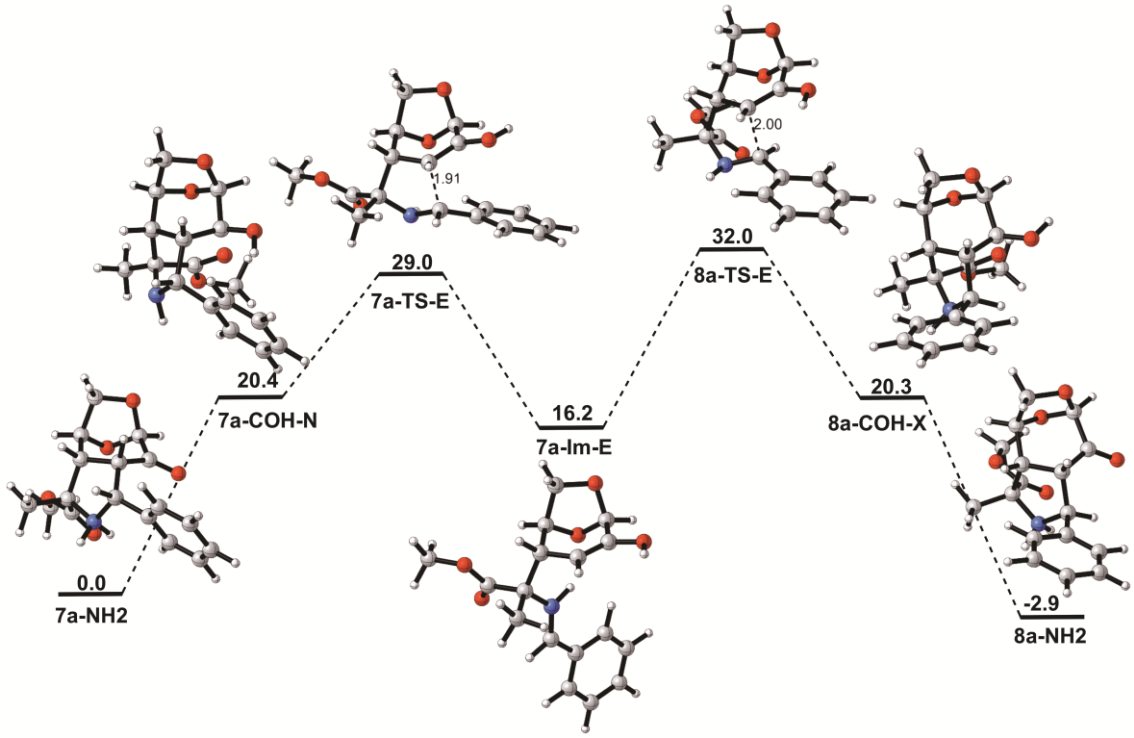


Figure S11. Full reaction coordinate diagram of the isomerization of **7a** (path E) computed at the ωB97XD/6-311+G** level of theory. Relative enthalpies are given in kcal/mol. Optimized structures and relevant bond-forming and bond-breaking distances are also shown.

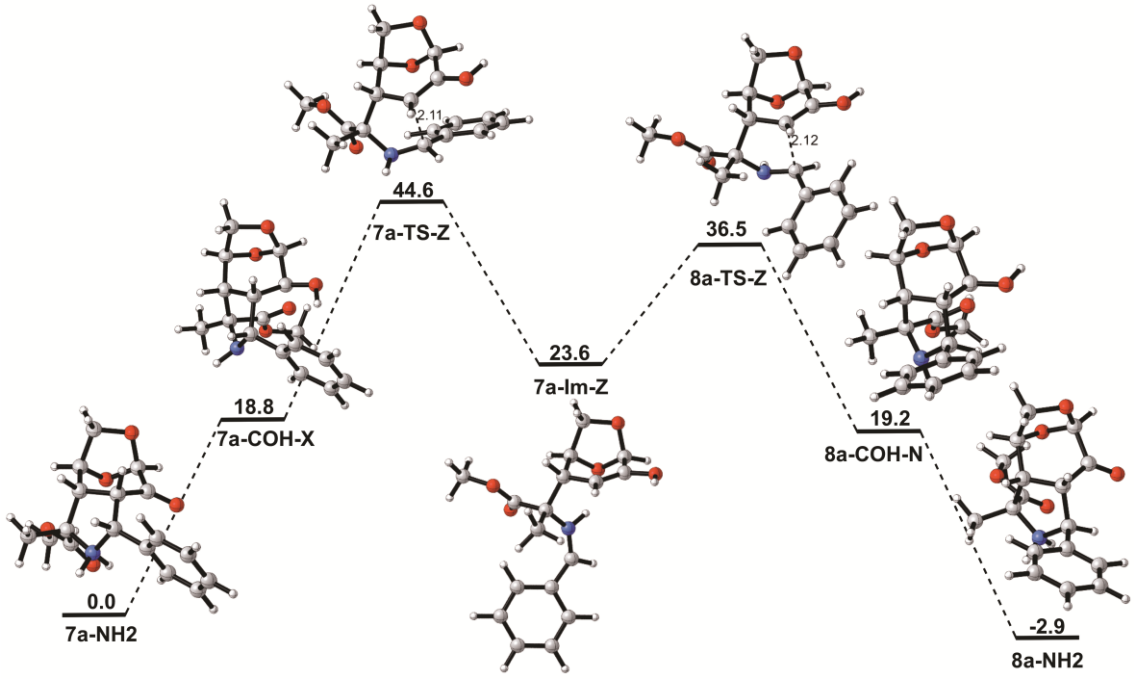


Figure S12. Full reaction coordinate diagram of the isomerization of **7a** (path Z) computed at the ωB97XD/6-311+G** level of theory. Relative enthalpies are given in kcal/mol. Optimized structures and relevant bond-forming and bond-breaking distances are also shown.

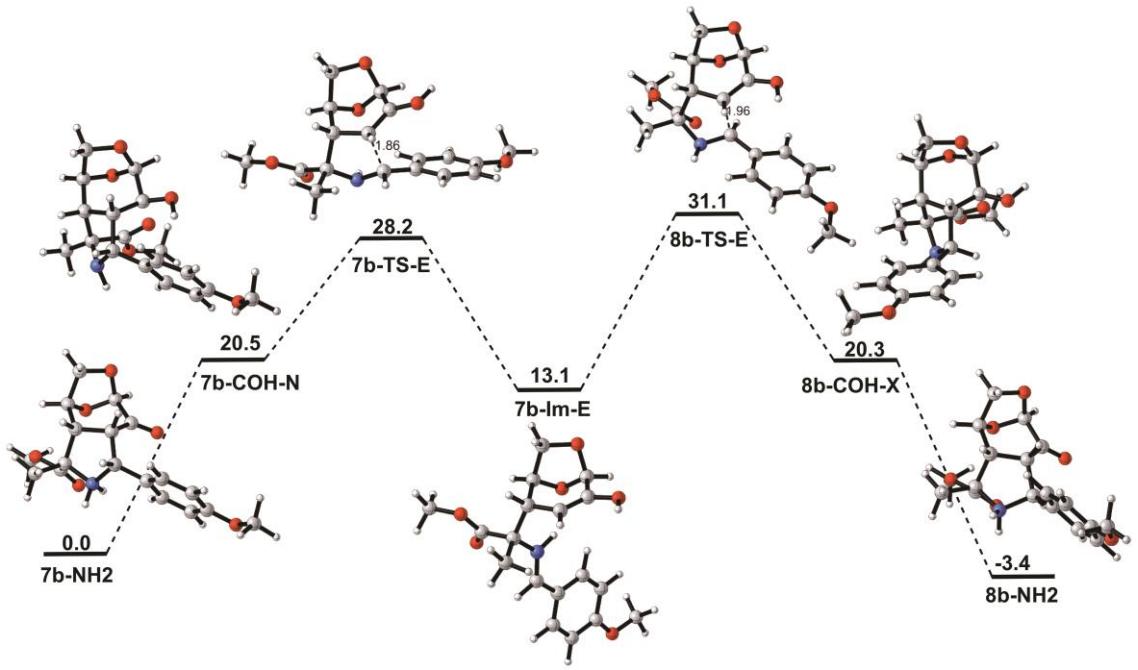


Figure S13. Full reaction coordinate diagram of the isomerization of **7b** (path E) computed at the ωB97XD/6-311+G** level of theory. Relative enthalpies are given in kcal/mol. Optimized structures and relevant bond-forming and bond-breaking distances are also shown.

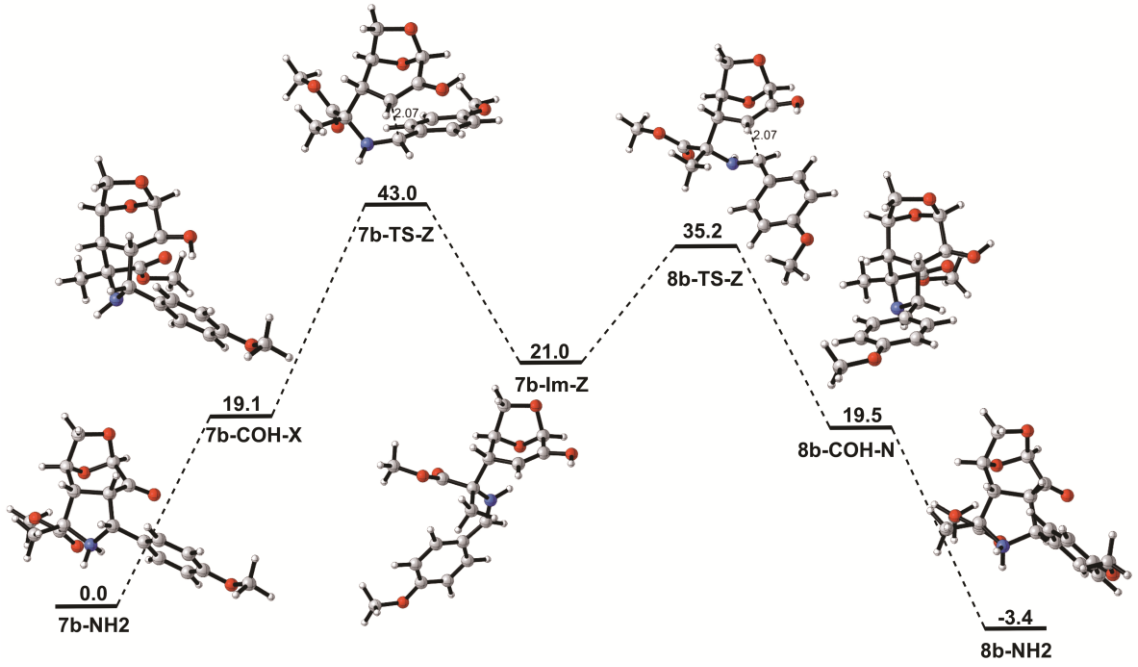


Figure S14. Full reaction coordinate diagram of the isomerization of **7b** (path Z) computed at the ωB97XD/6-311+G** level of theory. Relative enthalpies are given in kcal/mol. Optimized structures and relevant bond-forming and bond-breaking distances are also shown.

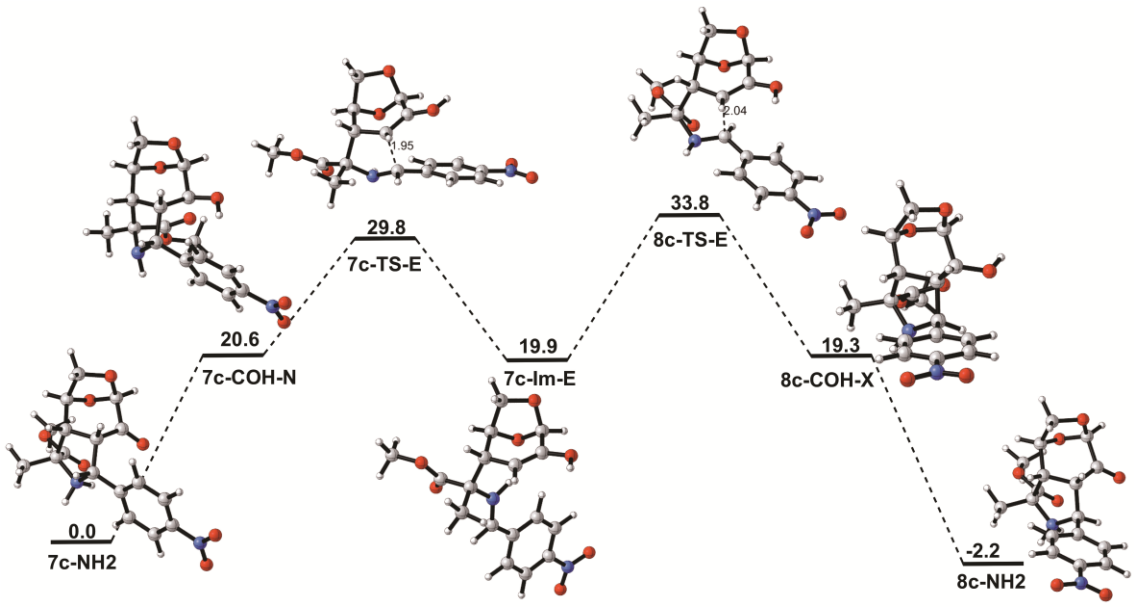


Figure S15. Full reaction coordinate diagram of the isomerization of **7c** (path E) computed at the ωB97XD/6-311+G** level of theory. Relative enthalpies are given in kcal/mol. Optimized structures and relevant bond-forming and bond-breaking distances are also shown.

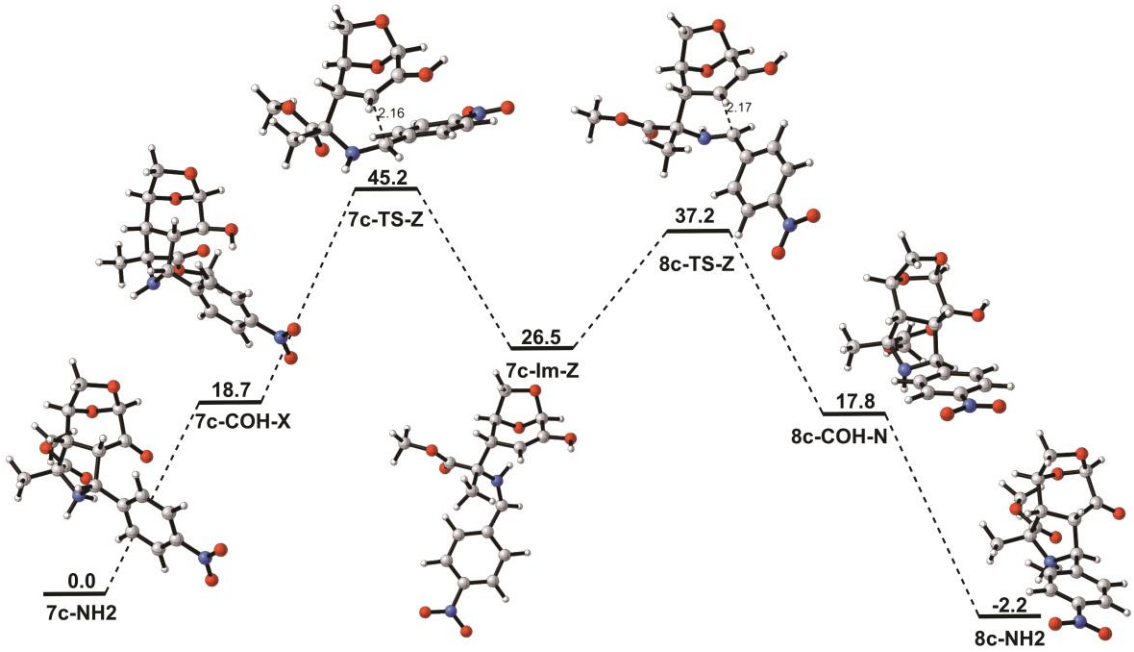


Figure S16. Full reaction coordinate diagram of the isomerization of **7c** (path Z) computed at the ωB97XD/6-311+G** level of theory. Relative enthalpies are given in kcal/mol. Optimized structures and relevant bond-forming and bond-breaking distances are also shown.

7a-NH2

ωB97XD/6-311+G(d,p) geometry

C	-1.886044	-1.586065	-0.376464
O	-3.179066	-1.552751	-0.171208
O	-1.342135	-1.940059	-1.396143
C	-1.095665	-1.171060	0.876929
C	-4.024256	-1.886944	-1.291781
C	-1.109572	0.362538	1.190494
N	0.345871	-1.457026	0.528218
C	0.247523	0.903186	0.675380
C	-2.295126	1.143537	0.631962
C	1.187833	-0.280097	0.931116
O	-2.211048	1.155089	-0.797056
C	0.153031	1.490772	-0.735043
C	-2.206285	2.634950	0.958336
C	-1.217022	2.115475	-1.040521
O	-1.446373	3.168990	-0.135602
O	1.059135	1.531379	-1.524281
C	2.583878	-0.322229	0.358434
C	2.879825	-0.828954	-0.905522
C	3.617738	0.169314	1.154462
C	4.927233	0.172566	0.688570
C	5.216734	-0.337347	-0.571504
C	4.190972	-0.841022	-1.364270
C	-1.520466	-2.000191	2.083250
H	-3.832825	-2.912283	-1.608064
H	-3.840421	-1.193278	-2.112282
H	-5.041262	-1.783813	-0.922292
H	-1.125873	0.458567	2.278635
H	0.374372	-1.618394	-0.490465
H	0.568207	1.742106	1.300607
H	-3.246795	0.702120	0.915948
H	1.271677	-0.361291	2.016904
H	-1.694136	2.840445	1.899917
H	-3.192406	3.101473	0.963458
H	-1.270110	2.466266	-2.070519
H	2.100333	-1.201188	-1.561453
H	3.398476	0.554697	2.145503
H	5.720598	0.562288	1.316256
H	6.238107	-0.345549	-0.935000
H	4.408811	-1.240075	-2.348361
H	-1.516487	-3.068373	1.853347
H	-2.528002	-1.712282	2.384818
H	-0.841505	-1.808146	2.917669
H	0.682049	-2.315878	0.969196

Number of imaginary frequencies = 0

Enthalpy = -1090.143456

ZPE Energy = -1090.169701

7a-COH-N

ωB97XD/6-311+G(d,p) geometry

C	0.810332	1.447720	-0.272275
O	0.931151	2.662076	-0.631765
C	1.142330	1.089450	1.174395
C	0.469878	3.072614	-1.954125
C	1.599344	-0.377823	1.241388
N	-0.162394	0.988354	1.820507
C	0.316770	-1.056475	0.721497
C	2.848787	-0.736987	0.443868
C	-0.794483	-0.302260	1.500456
O	2.669890	-0.301386	-0.913379
C	0.341755	-0.866527	-0.796737
C	2.977235	-2.244429	0.241814
C	1.735696	-1.230054	-1.385960
O	2.133514	-2.481832	-0.902711
C	2.060048	2.098830	1.829280
H	-0.600829	2.891271	-2.032728
H	1.021839	2.516320	-2.710076
H	0.693719	4.133704	-2.003181
H	1.756322	-0.623500	2.293381
H	-0.747445	1.811574	1.768696
H	0.279283	-2.127655	0.914130
H	3.744524	-0.264950	0.840811
H	-0.937938	-0.851904	2.435544
H	2.616014	-2.828277	1.089245
H	4.000016	-2.533175	-0.004931
H	1.704207	-1.220641	-2.475303
H	1.596297	3.085643	1.872926
H	3.003518	2.181286	1.285152
H	2.265211	1.765751	2.848039
O	-0.616151	-1.453905	-1.534894
H	-1.465543	-1.454038	-1.070594
O	0.245471	0.633412	-1.077338
C	-2.150421	-0.243809	0.817224
C	-4.642838	-0.302588	-0.463959
C	-2.929371	-1.406326	0.819229
C	-2.646656	0.891298	0.179248
C	-3.885737	0.862056	-0.454077
C	-4.160561	-1.440005	0.176536
H	-2.563016	-2.292569	1.329025
H	-2.081774	1.816767	0.166746
H	-4.258875	1.756378	-0.940586
H	-4.746173	-2.352387	0.184425
H	-5.606256	-0.323122	-0.960390

Number of imaginary frequencies = 0

Enthalpy = -1090.110902

ZPE Energy = -1090.136089

7a-COH-X

ωB97XD/6-311+G(d,p) geometry

C	0.929829	1.437091	-0.269913
O	1.204914	2.622944	-0.628889
C	1.170633	1.042534	1.184305
C	0.847559	3.075350	-1.969702
C	1.539052	-0.450364	1.261148
N	-0.218471	1.102165	1.654414
C	0.232625	-1.038419	0.702719
C	2.784388	-0.881223	0.492040
C	-0.841373	-0.219967	1.465086
O	2.662347	-0.417084	-0.862939
C	0.300752	-0.833374	-0.812547
C	2.823558	-2.390384	0.270026
C	1.683546	-1.279922	-1.370971
O	1.988015	-2.559309	-0.892416
C	2.100515	1.991414	1.906840
H	1.218667	4.094366	-2.020009
H	-0.234884	3.042977	-2.081494
H	1.341052	2.438916	-2.702665

H	1.650364	-0.711776	2.315869
H	-0.272928	1.435992	2.607955
H	0.115060	-2.106465	0.880430
H	3.698193	-0.469238	0.913999
H	-0.961835	-0.711996	2.435199
H	2.411109	-2.961663	1.102428
H	3.830534	-2.740199	0.037294
H	1.682519	-1.256588	-2.460541
H	1.705140	3.008263	1.913321
H	3.084286	2.003000	1.433995
H	2.214031	1.650019	2.938090
O	-0.675375	-1.349966	-1.577974
H	-1.532354	-1.304495	-1.129645
O	0.310651	0.675127	-1.084544
C	-2.204305	-0.172181	0.798162
C	-4.691567	-0.198026	-0.483182
C	-2.982151	-1.334481	0.778301
C	-2.692162	0.978087	0.183160
C	-3.929709	0.964227	-0.453506
C	-4.215056	-1.349602	0.136544
H	-2.616755	-2.233373	1.266572
H	-2.103596	1.887215	0.211679
H	-4.300557	1.867381	-0.925683
H	-4.805211	-2.259154	0.126113
H	-5.654749	-0.206593	-0.980768

Number of imaginary frequencies = 0
Enthalpy = -1090.113524
ZPE Energy = -1090.139015

7a-TS-(E)

ωB97XD/6-311+G(d,p) geometry

C	-2.672307	-1.184125	-0.394018
O	-3.853663	-0.784825	0.047412
O	-2.465317	-1.632119	-1.494015
C	-1.584470	-0.967943	0.654855
C	-4.959269	-0.906505	-0.865969
C	-1.308628	0.571139	0.893558
N	-0.342875	-1.495515	0.120064
C	0.125295	0.641551	1.403608
C	-1.459360	1.432182	-0.367418
C	0.759252	-1.055652	0.813563
O	-0.314151	1.209943	-1.209935
C	1.006107	1.494499	0.740559
C	-1.366463	2.945791	-0.094573
C	0.635850	2.038782	-0.633514
O	0.008389	3.267954	-0.387225
O	2.124454	1.835423	1.294847
C	2.086169	-1.073364	0.141135
C	2.234229	-0.883203	-1.235329
C	3.221937	-1.249965	0.933140
C	4.487955	-1.243078	0.360417
C	4.628528	-1.058412	-1.010135
C	3.500047	-0.880026	-1.805602
C	-1.971186	-1.653455	1.968445
H	-5.121624	-1.954845	-1.118343
H	-4.768524	-0.328511	-1.771121
H	-5.819439	-0.507279	-0.333954
H	-1.997761	0.942220	1.653623
H	-0.294097	-1.415603	-0.889248
H	0.278434	0.562251	2.474513
H	-2.349218	1.188035	-0.942723
H	0.819141	-1.429927	1.831434
H	-1.596758	3.200625	0.940943
H	-1.994836	3.521944	-0.772207
H	1.496811	2.161820	-1.291831
H	2.706600	2.324158	0.689211
H	1.372043	-0.729053	-1.874685
H	3.111079	-1.395274	2.002749
H	5.363016	-1.386374	0.983897
H	5.614580	-1.055314	-1.460789
H	3.606308	-0.736704	-2.874822
H	-2.109176	-2.724147	1.804397
H	-2.898647	-1.232008	2.356232
H	-1.197629	-1.517710	2.727273

Number of imaginary frequencies = 1 (-299.4327)
Enthalpy = -1090.097223
ZPE Energy = -1090.123548

7a-TS-(Z)

ωB97XD/6-311+G(d,p) geometry

C	-2.356015	-1.072714	0.031990
O	-3.260370	-0.403181	-0.673654
O	-2.140657	-2.249270	-0.096709
C	-1.715085	-0.168055	1.091719
C	-3.981708	-1.148720	-1.670405
C	-1.055942	1.178138	0.551044
N	-0.701192	-0.874707	1.881569
C	0.257438	1.385224	1.273911
C	-0.851447	1.354500	-0.965994
C	0.630455	-0.647384	1.706644
O	0.379753	0.747608	-1.369231
C	1.359483	1.755292	0.546318
C	-0.605589	2.827691	-1.353977
C	1.314315	1.692812	-0.975618
O	0.829055	2.938026	-1.412555
O	2.450048	2.168411	1.141084
C	1.489167	-1.229324	0.663582
C	1.014009	-2.002795	-0.395124
C	2.870725	-1.034186	0.806363
C	3.754586	-1.563348	-0.120527
C	3.270081	-2.317327	-1.186740
C	1.904208	-2.545440	-1.311746
C	-2.851426	0.194858	2.067488
H	-4.525211	-1.971316	-1.204774
H	-3.292122	-1.533916	-2.422859
H	-4.675137	-0.439895	-2.116941
H	-1.741020	1.971899	0.855588
H	-0.934672	-0.800602	2.863610
H	0.232841	1.666185	2.321431
H	-1.652281	0.912817	-1.547718
H	1.157797	-0.525088	2.650199
H	-1.003653	3.535928	-0.625756
H	-0.999848	3.050052	-2.345306
H	2.287063	1.479594	-1.421734
H	-0.043849	-2.199202	-0.492007
H	3.249578	-0.471404	1.653376
H	4.820436	-1.405680	-0.001968
H	1.527359	-3.151786	-2.127519

H	-3.277880	-0.706656	2.515343
H	-3.641944	0.732501	1.545304
H	-2.458869	0.836872	2.860900
H	3.173577	2.314783	0.513337
H	3.960010	-2.740228	-1.908546

Number of imaginary frequencies = 1 (-387.7370)

Enthalpy = -1090.072366

ZPE Energy = -1090.098882

7a-(E)-Im-a

ωB97XD/6-311+G(d,p) geometry

C	0.873886	2.333600	-0.177412
O	2.082451	2.855461	-0.067747
C	0.727211	1.108576	0.748622
C	2.351054	4.039264	-0.842931
C	1.902612	0.109207	0.542171
N	-0.517085	0.416678	0.368786
C	1.768331	-1.111746	1.425122
C	2.049507	-0.340616	-0.920113
C	-1.711436	0.845746	0.583627
O	1.023970	-1.311379	-1.199941
C	1.622083	-2.318626	0.875506
C	3.335234	-1.156115	-1.170952
C	1.588483	-2.475233	-0.634380
O	2.891441	-2.520245	-1.150470
O	1.549471	-3.502119	1.515255
C	0.661525	1.609155	2.196778
H	2.233344	3.826679	-1.905993
H	3.382472	4.300861	-0.619526
H	1.678343	4.843365	-0.543211
H	2.808755	0.656569	0.811874
H	1.830327	-0.993942	2.501807
H	1.934064	0.477365	-1.630022
H	-1.813376	1.774597	1.136424
H	4.087401	-0.984793	-0.397608
H	3.762472	-0.956799	-2.153271
H	1.031718	-3.355372	-0.951805
H	-0.049611	2.430013	2.308211
H	1.644534	1.974486	2.495973
H	0.366102	0.797586	2.863048
H	1.669008	-3.380577	2.464759
C	-2.925175	0.192645	0.155763
C	-5.347753	-0.919306	-0.625867
C	-4.127138	0.864958	0.417005
C	-2.947745	-1.051669	-0.495583
C	-4.156306	-1.599757	-0.881345
C	-5.334927	0.310270	0.022246
H	-4.106119	1.823847	0.923401
H	-2.034069	-1.598986	-0.699185
H	-4.177330	-2.560078	-1.382186
H	-6.262653	0.833594	0.219651
H	-6.290632	-1.356337	-0.934845
H	-0.370569	-0.426025	-0.194730
O	-0.007489	2.767668	-0.872575

Number of imaginary frequencies = 0

Enthalpy = -1090.117669

ZPE Energy = -1090.145548

7a-(Z)-Im-a

ωB97XD/6-311+G(d,p) geometry

C	-0.273623	1.884016	-0.161440
O	-0.012686	2.836155	0.714854
C	0.026005	0.504019	0.441175
C	-0.215575	4.192716	0.275066
C	1.569804	0.403363	0.701761
N	-0.287418	-0.523250	-0.577355
C	1.957464	-0.942628	1.271544
C	2.421780	0.686370	-0.545819
C	-1.368383	-1.141016	-0.910884
O	2.383791	-0.478222	-1.390893
C	2.780955	-1.742245	0.590992
C	3.927351	0.798870	-0.224072
C	3.333419	-1.308397	-0.755272
O	4.455179	-0.486359	-0.579447
O	3.267689	-2.934113	0.986340
C	-0.738453	0.284013	1.752931
H	0.068236	4.815034	1.120309
H	-1.264310	4.350870	0.021372
H	0.417547	4.406252	-0.586724
H	1.786861	1.186466	1.432375
H	1.585869	-1.227424	2.250044
H	2.060317	1.531875	-1.129042
H	4.106768	1.009655	0.832581
H	4.422386	1.548092	-0.840992
H	3.585165	-2.150043	-1.398164
H	-1.764935	0.642163	1.708428
H	-0.231355	0.828583	2.549884
H	-0.750538	-0.776740	2.006286
H	2.983888	-3.131379	1.887115
H	0.551211	-0.837467	-1.077772
O	-0.675604	2.065324	-1.282542
H	-1.195118	-1.950961	-1.616073
C	-2.745016	-0.957047	-0.494166
C	-5.425591	-0.823968	0.231472
C	-3.337452	0.284436	-0.229251
C	-3.521666	-2.124477	-0.439041
C	-4.849031	-2.058922	-0.047935
C	-4.675470	0.344579	0.123653
H	-2.776633	1.201493	-0.345788
H	-3.072752	-3.080661	-0.685338
H	-5.437566	-2.966026	0.018881
H	-5.138794	1.306500	0.307694
H	-6.470376	-0.767912	0.515604

Number of imaginary frequencies = 0

Enthalpy = -1090.105872

ZPE Energy = -1090.133555

8a-TS-(E)

ωB97XD/6-311+G(d,p) geometry

C	-1.937118	-1.615406	-0.517537
O	-3.247296	-1.566409	-0.317157
O	-1.426374	-1.888261	-1.572123
C	-1.163331	-1.311299	0.782299
C	-4.084835	-1.796471	-1.462872
C	-1.172285	0.248560	1.164889
N	0.230333	-1.657803	0.561188
C	0.223813	0.798759	0.926473
C	-2.202822	1.109328	0.424098
C	0.916098	-0.735110	-0.160700

O	-1.722184	1.322452	-0.913620
C	0.373919	1.867726	0.069259
C	-2.304348	2.550152	0.958509
C	-0.814591	2.361953	-0.736667
O	-1.454240	3.310202	0.080124
O	1.476395	2.534327	-0.127092
C	2.385577	-0.679744	-0.169229
C	3.162094	-1.084661	0.922233
C	3.011072	-0.156133	-1.303654
C	4.395870	-0.052889	-1.355441
C	5.161191	-0.466296	-0.272094
C	4.543073	-0.983238	0.865533
C	-1.726447	-2.152902	1.924794
H	-3.905476	-2.792176	-1.869595
H	-3.894241	-1.040531	-2.226039
H	-5.104954	-1.715221	-1.094531
H	-1.394076	0.302681	2.232469
H	0.694316	-2.012383	1.389167
H	0.958721	0.687707	1.717447
H	-3.173865	0.628515	0.364984
H	0.442712	-0.482070	-1.102472
H	-1.960336	2.645220	1.990031
H	-3.315774	2.944196	0.865283
H	-0.529015	2.801197	-1.690840
H	2.696990	-1.472994	1.822482
H	2.409599	0.161679	-2.149002
H	4.873704	0.350122	-2.240714
H	5.141786	-1.302020	1.710977
H	-1.721069	-3.215015	1.669460
H	-2.751089	-1.853753	2.144165
H	-1.122927	-2.000362	2.823551
H	2.188958	2.242631	0.464470
H	6.241716	-0.385266	-0.310028

Number of imaginary frequencies = 1 (-382.3339)

Enthalpy = -1090.092499

ZPE Energy = -1090.119041

8a-TS-(Z)

ωB97XD/6-311+G(d,p) geometry

C	1.923400	-1.938806	0.329120
O	2.665403	-2.318024	-0.696240
O	2.204783	-2.118739	1.487362
C	0.669710	-1.195068	-0.137490
C	3.896516	-2.998172	-0.389435
C	1.049806	0.196933	-0.795587
N	-0.075817	-0.835075	1.064874
C	-0.184428	1.063412	-0.715680
C	2.233154	0.906323	-0.122646
C	-1.070817	0.074629	0.937402
O	1.781867	1.469233	1.120890
C	-0.095282	2.284829	-0.091352
C	2.705318	2.160510	-0.885460
C	1.162281	2.638188	0.696590
O	2.040431	3.246834	-0.211756
O	-1.038980	3.185217	-0.221712
C	-2.415238	-0.276363	0.406894
C	-3.313139	0.723589	0.022524
C	-2.837931	-1.606520	0.427047
C	-4.129860	-1.934173	0.032692
C	-5.008368	-0.940402	-0.379425
C	-4.597714	0.390784	-0.378761
C	-0.099136	-2.054127	-1.141470
H	4.371596	-3.180741	-1.350293
H	3.687006	-3.940813	0.117187
H	4.530736	-2.369005	0.236278
H	1.302391	0.012698	-1.841697
H	0.560264	-0.624236	1.826611
H	-0.963952	0.925884	-1.454675
H	3.061673	0.236636	0.095630
H	-1.105345	0.793360	1.754047
H	2.424197	2.142814	-1.939750
H	3.779042	2.314684	-0.786846
H	0.964075	3.298671	1.541667
H	-3.006272	1.762820	0.026866
H	-2.165115	-2.379826	0.775275
H	-4.449088	-2.969884	0.056634
H	-6.015923	-1.197339	-0.686396
H	-5.284144	1.171821	-0.685137
H	-0.419806	-2.989568	-0.679981
H	0.553035	-2.285630	-1.983467
H	-0.975502	-1.531609	-1.523955
H	-0.875813	3.965211	0.329755

Number of imaginary frequencies = 1 (-332.4481)

Enthalpy = -1090.085264

ZPE Energy = -1090.111537

8a-COH_N

ωB97XD/6-311+G(d,p) geometry

C	-1.817087	-1.178995	-0.245397
O	-2.669759	-2.120794	-0.294692
C	-0.778327	-1.203590	0.871831
C	-3.575064	-2.224873	-1.433842
C	-0.365631	0.237288	1.211573
N	0.429846	-1.677479	0.203362
C	0.217102	0.650564	-0.149828
C	-1.476870	1.163167	1.696475
C	1.021891	-0.594643	-0.599240
O	-2.557677	1.119637	0.747522
C	-0.977800	0.938813	-1.045582
C	-1.074774	2.632968	1.598536
C	-2.021951	1.842837	-0.324453
O	-1.370243	2.951904	0.222025
C	-1.193956	-2.065829	2.043520
H	-2.994865	-2.432885	-2.331642
H	-4.136818	-1.297165	-1.529652
H	-4.227363	-3.056616	-1.186557
H	0.424174	0.186656	1.963446
H	0.339203	-2.565053	-0.276028
H	0.829640	1.549356	-0.115125
H	-1.867489	0.875230	2.669627
H	-0.016259	2.807263	1.793510
H	-1.686589	3.264258	2.244255
H	-2.817791	2.152689	-1.004298
H	-1.330962	-3.105993	1.743267
H	-2.126395	-1.705349	2.483446
H	-0.405963	-2.021998	2.797270
O	-0.605659	1.344199	-2.273844
H	-1.352290	1.721075	-2.758498

O	-1.748055	-0.368983	-1.233771
H	0.868262	-0.759909	-1.670417
C	2.509874	-0.429573	-0.354400
C	5.238438	-0.000272	0.078846
C	3.279924	0.244667	-1.303445
C	3.118315	-0.889467	0.809988
C	4.477461	-0.676671	1.024770
C	4.635226	0.460775	-1.088529
H	2.813871	0.603348	-2.216720
H	2.527233	-1.426430	1.542702
H	4.941645	-1.045035	1.933248
H	5.223133	0.984620	-1.834377
H	6.297217	0.163590	0.246162

Number of imaginary frequencies = 0

Enthalpy = -1090.112840

ZPE Energy = -1090.138310

8a-COH_X

ωB97XD/6-311+G(d,p) geometry

C	-1.807547	-1.202763	-0.196192
O	-2.669089	-2.133767	-0.163024
C	-0.716685	-1.175916	0.869489
C	-3.621060	-2.279498	-1.258631
C	-0.325124	0.281516	1.170377
N	0.378803	-1.693048	0.044291
C	0.204604	0.669449	-0.216606
C	-1.441263	1.197388	1.666435
C	1.027548	-0.569783	-0.660036
O	-2.549515	1.100124	0.753220
C	-1.023712	0.904240	-1.083154
C	-1.081719	2.673493	1.515037
C	-2.065710	1.805508	-0.355094
O	-1.424796	2.944882	0.139872
C	-1.038644	-2.036863	2.069216
H	-3.078453	-2.537174	-2.166878
H	-4.176492	-1.350469	-1.375819
H	-4.272391	-3.090394	-0.948005
H	0.485004	0.269515	1.901892
H	1.009796	-2.281927	0.572587
H	0.799000	1.580951	-0.232204
H	-1.794333	0.927962	2.659148
H	-0.023108	2.879829	1.675349
H	-1.691520	3.307216	2.160481
H	-2.890272	2.076650	-1.017140
H	-1.193156	-3.078667	1.784942
H	-1.937416	-1.675392	2.572436
H	-0.203009	-1.983955	2.770611
O	-0.697184	1.279256	-2.333286
H	-1.466141	1.623491	-2.807246
O	-1.779309	-0.422645	-1.209186
H	0.917671	-0.703924	-1.739031
C	2.504579	-0.410322	-0.364182
C	5.230981	0.011123	0.111629
C	3.343813	0.037911	-1.385222
C	3.048426	-0.649238	0.897757
C	4.403902	-0.440816	1.133424
C	4.696383	0.250327	-1.150573
H	2.930942	0.219678	-2.372803
H	2.421868	-1.004185	1.709715
H	4.814072	-0.632914	2.118729
H	5.335554	0.596095	-1.955535
H	6.287289	0.171608	0.295928

Number of imaginary frequencies = 0

Enthalpy = -1090.111177

ZPE Energy = -1090.136549

8a-NH2

ωB97XD/6-311+G(d,p) geometry

C	-1.929221	-1.498936	-0.520698
O	-3.000172	-1.693037	0.208003
O	-1.891305	-1.463686	-1.728007
C	-0.665017	-1.355555	0.344701
C	-4.260911	-1.727851	-0.491107
C	-0.501180	0.063562	0.952569
N	0.486278	-1.464266	-0.633127
C	0.292164	0.868838	-0.097615
C	-1.797188	0.770526	1.349164
C	1.193188	-0.130842	-0.826055
O	-2.549301	1.082135	0.170328
C	-0.615586	1.661554	-1.037712
C	-1.533817	2.165289	1.917599
C	-1.873842	2.200029	-0.349078
O	-1.516216	3.000274	0.749070
O	-0.374731	1.847112	-2.201588
C	2.623977	-0.182104	-0.347432
C	3.628096	0.254115	-1.209583
C	2.966214	-0.615825	0.935653
C	4.293753	-0.611852	1.345297
C	5.290501	-0.168577	0.481574
C	4.955656	0.264743	-0.795634
C	-0.584653	-2.458361	1.391778
H	-4.260614	-2.533495	-1.225213
H	-4.432243	-0.767593	-0.978015
H	-5.010008	-1.907843	0.275656
H	0.107762	-0.045088	1.853263
H	0.098901	-1.764114	-1.536788
H	0.903101	1.624257	0.404527
H	-2.417657	0.153025	1.994353
H	1.179851	0.073380	-1.896203
H	-0.578815	2.246112	2.439011
H	-2.344313	2.488067	2.572662
H	-2.514220	2.743712	-1.042573
H	3.371047	0.589279	-2.209116
H	2.204646	-0.962435	1.627505
H	4.549073	-0.951896	2.342599
H	6.325649	-0.164121	0.803767
H	5.727330	0.607186	-1.475693
H	-0.710509	-3.444535	0.939453
H	-1.371927	-2.312946	2.131949
H	0.380842	-2.414533	1.900844
H	1.149155	-2.181466	-0.333082

Number of imaginary frequencies = 0

Enthalpy = -1090.148070

ZPE Energy = -1090.174424

7b-NH2

ωB97XD/6-311+G(d,p) geometry

C	-2.466529	-1.604983	-0.410087
O	-3.767318	-1.589386	-0.254937
O	-1.880490	-1.954432	-1.407583
C	-1.728853	-1.175141	0.869874
C	-4.560641	-1.938981	-1.408192
C	-1.782439	0.358148	1.181470
N	-0.271856	-1.434170	0.573359
C	-0.415016	0.922333	0.722152
C	-2.958076	1.116373	0.572272
C	0.536949	-0.245142	1.011846
O	-2.814090	1.126838	-0.852008
C	-0.461609	1.516568	-0.686822
C	-2.912657	2.609984	0.899159
C	-1.830931	2.106945	-1.055350
O	-2.122885	3.158744	-0.166049
O	0.480154	1.592403	-1.430678
C	1.950759	-0.278961	0.493206
C	2.294000	-0.723835	-0.786981
C	2.966549	0.149743	1.338826
C	4.297462	0.160457	0.932420
C	4.625562	-0.290137	-0.345158
C	3.611518	-0.737165	-1.200129
C	-2.180509	-2.013774	2.059827
H	-4.358517	-2.970215	-1.697643
H	-4.335278	-1.260457	-2.230993
H	-5.594003	-1.826497	-1.090383
H	-1.846664	0.454634	2.267700
H	-0.201161	-1.587303	-0.444412
H	-0.132985	1.763728	1.362634
H	-3.912306	0.657341	0.816704
H	0.577743	-0.326444	2.100321
H	-2.440787	2.826126	1.859305
H	-3.907388	3.056447	0.865752
H	-1.845532	2.453783	-2.087911
H	1.536650	-1.053541	-1.490237
H	2.725968	0.487487	2.342259
H	5.057131	0.506459	1.620667
H	3.877298	-1.084192	-2.191903
H	-2.139607	-3.081600	1.831572
H	-3.206834	-1.752447	2.319261
H	-1.541207	-1.803893	2.920757
H	0.063427	-2.290108	1.020387
O	5.879089	-0.339280	-0.840613
C	6.950138	0.109573	-0.022027
H	7.854009	-0.021988	-0.614472
H	6.835059	1.167860	0.232111
H	7.028232	-0.487118	0.892128

Number of imaginary frequencies = 0

Enthalpy = -1204.630125

ZPE Energy = -1204.659425

7b-COH-N

ωB97XD/6-311+G(d,p) geometry

C	1.482488	1.396471	-0.313148
O	1.687052	2.590758	-0.701171
C	1.887743	1.025319	1.111006
C	1.154334	3.035484	-1.984905
C	2.217775	-0.475741	1.167287
N	0.628736	1.050843	1.849870
C	0.844233	-1.041289	0.757324
C	3.366299	-0.947754	0.281327
C	-0.134554	-0.186674	1.606241
O	3.117868	-0.510931	-1.064593
C	0.765979	-0.868512	-0.759377
C	3.350350	-2.462037	0.092637
C	2.072332	-1.359355	-1.447945
O	2.396804	-2.636009	-0.974739
C	2.936483	1.954903	1.681843
H	0.069731	2.940480	-1.974922
H	1.596679	2.435670	-2.778441
H	1.458044	4.074889	-2.060324
H	2.432400	-0.725501	2.208192
H	0.113736	1.920812	1.812731
H	0.726239	-2.103380	0.967809
H	4.326912	-0.548989	0.598974
H	-0.242983	-0.711776	2.559750
H	3.013127	-3.006077	0.975696
H	4.320332	-2.839953	-0.234185
H	1.957089	-1.358474	-2.531681
H	2.568240	2.980642	1.737598
H	3.844070	1.943741	1.073920
H	3.180313	1.618034	2.690894
O	-0.297446	-1.377126	-1.406475
H	-1.098309	-1.300046	-0.868508
O	0.781503	0.630768	-1.057061
C	-1.532364	-0.016423	1.037154
C	-4.126505	0.128680	-0.043398
C	-2.447842	-1.052797	1.213393
C	-1.952722	1.110289	0.324147
C	-3.227653	1.186172	-0.207859
C	-3.730613	-0.998487	0.677284
H	-2.157178	-1.932150	1.780666
H	-1.288845	1.954435	0.174866
H	-3.547342	2.064825	-0.756409
H	-4.406416	-1.828157	0.837847
C	-6.308421	-0.739568	-0.438974
H	-6.535481	-0.904516	0.618887
H	-7.204713	-0.391528	-0.949608
H	-5.970815	-1.674495	-0.897290
O	-5.343286	0.290481	-0.603432

Number of imaginary frequencies = 0

Enthalpy = -1204.597492

ZPE Energy = -1204.625992

7b-COH-X

ωB97XD/6-311+G(d,p) geometry

C	1.567515	1.390627	-0.321602
O	1.876702	2.556851	-0.716790
C	1.909196	0.994960	1.111664
C	1.410114	3.025622	-2.017528
C	2.177961	-0.519393	1.183745
N	0.571708	1.159454	1.693286
C	0.791050	-1.018486	0.748317
C	3.319017	-1.048683	0.319823
C	-0.156879	-0.118469	1.583335
O	3.115179	-0.591905	-1.027633
C	0.743486	-0.839066	-0.769590
C	3.231807	-2.559370	0.120579

C	2.037917	-1.387540	-1.436410
O	2.292592	-2.680865	-0.965884
C	2.958225	1.885303	1.738183
H	1.817043	4.028065	-2.107545
H	0.321414	3.039640	-2.021600
H	1.802301	2.369532	-2.792841
H	2.359042	-0.776239	2.229951
H	0.619209	1.514534	2.639589
H	0.614070	-2.073263	0.954334
H	4.293098	-0.700270	0.655523
H	-0.223624	-0.589869	2.568579
H	2.851055	-3.091016	0.993360
H	4.188244	-2.983022	-0.189665
H	1.944057	-1.374868	-2.522111
H	2.639010	2.928429	1.752923
H	3.901339	1.815847	1.192857
H	3.125686	1.554117	2.765507
O	-0.331299	-1.296051	-1.434562
H	-1.136017	-1.182085	-0.908607
O	0.835534	0.661687	-1.070354
C	-1.564651	0.022727	1.034357
C	-4.153343	0.165515	-0.046490
C	-2.464981	-1.029509	1.185897
C	-1.991113	1.161856	0.347338
C	-3.264774	1.235521	-0.187995
C	-3.749280	-0.973489	0.650897
H	-2.165011	-1.920919	1.729392
H	-1.317370	2.003652	0.242160
H	-3.594253	2.122018	-0.718137
H	-4.418223	-1.812385	0.791264
O	-5.371644	0.327381	-0.606326
C	-6.331539	-0.708494	-0.453710
H	-7.230391	-0.358082	-0.958375
H	-5.991232	-1.636374	-0.924423
H	-6.556285	-0.888204	0.602388

Number of imaginary frequencies = 0

Enthalpy = -1204.599648

ZPE Energy = -1204.628252

7b-TS-(E)

ωB97XD/6-311+G(d,p) geometry

C	-3.052605	-1.377844	-0.499726
O	-4.311979	-1.039011	-0.276009
O	-2.654115	-1.912577	-1.504281
C	-2.150668	-0.962469	0.658911
C	-5.256526	-1.331301	-1.321234
C	-2.006235	0.608735	0.740133
N	-0.813203	-1.451631	0.381221
C	-0.666634	0.832566	1.435646
C	-2.016364	1.307485	-0.626280
C	0.142213	-0.823913	1.162077
O	-0.739306	1.099364	-1.257698
C	0.239865	1.698846	0.814547
C	-2.077363	2.843048	-0.535611
C	0.047812	2.064358	-0.650276
O	-0.697813	3.252267	-0.634471
O	1.228851	2.187592	1.482831
C	1.549004	-0.814690	0.679798
C	1.887310	-0.794553	-0.672040
C	2.580113	-0.777841	1.625301
C	3.903841	-0.724626	1.235276
C	4.232300	-0.706462	-0.124522
C	3.214676	-0.746037	-1.080517
C	-2.689766	-1.514497	1.981320
O	5.546003	-0.650884	-0.413776
C	5.944863	-0.609164	-1.778086
H	-6.210790	-0.954483	-0.960813
H	-5.311201	-2.407564	-1.487835
H	-4.969148	-0.824444	-2.243392
H	-2.818589	1.014187	1.344875
H	-0.616976	-1.467443	-0.613164
H	-0.682968	0.901700	2.518477
H	-2.782473	0.920903	-1.294034
H	0.086843	-1.095800	2.212999
H	-2.503979	3.194723	0.404656
H	-2.613592	3.277783	-1.378125
H	0.988907	2.196377	-1.186283
H	1.860939	2.669627	0.922829
H	1.121846	-0.809320	-1.440472
H	2.338616	-0.791452	2.683314
H	4.700323	-0.700503	1.969813
H	3.439916	-0.739220	-2.138780
H	-2.732128	-2.604904	1.941833
H	-3.689879	-1.126097	2.173466
H	-2.048724	-1.224418	2.816649
H	5.542688	0.276566	-2.279417
H	5.632407	-1.513488	-2.308997
H	7.032246	-0.555164	-1.767220

Number of imaginary frequencies = 1 (-279.1872)

Enthalpy = -1204.585250

ZPE Energy = -1204.615227

7b-TS-(Z)

ωB97XD/6-311+G(d,p) geometry

C	2.105512	-1.865412	-0.181347
O	2.965875	-1.856867	0.831706
O	1.437140	-2.818540	-0.485238
C	2.167905	-0.539926	-0.949219
C	3.050005	-3.056767	1.619452
C	1.974255	0.763860	-0.063794
N	1.202425	-0.480601	-2.052538
C	1.151757	1.742080	-0.875198
C	1.396786	0.645325	1.363827
C	0.100584	0.332734	-1.963801
O	-0.032377	0.709701	1.336642
C	0.186078	2.476156	-0.228912
C	1.732429	1.880397	2.225030
C	-0.262484	2.065036	1.167613
O	0.579395	2.731985	2.075658
O	-0.356426	3.520291	-0.798748
C	-1.145536	-0.041814	-1.291600
C	-1.320902	-1.250697	-0.624650
C	-2.236972	0.838982	-1.383277
C	-3.437186	0.545194	-0.777061
C	-3.592508	-0.665225	-0.083709
C	-2.532268	-1.570963	-0.027953
C	3.569601	-0.495696	-1.589589
H	3.361188	-3.896420	0.997127

H	2.086101	-3.271417	2.083196
H	3.799199	-2.850942	2.380423
H	2.977056	1.178436	0.056370
H	1.695646	-0.295659	-2.916249
H	1.612695	2.195329	-1.746705
H	1.680339	-0.278123	1.855732
H	-0.064180	0.924524	-2.861737
H	2.627407	2.407287	1.892256
H	1.822499	1.619631	3.279580
H	-1.309322	2.304272	1.361733
H	-0.513452	-1.969109	-0.588018
H	-2.137153	1.764573	-1.941349
H	-4.279523	1.223915	-0.843656
H	-2.638397	-2.525146	0.470447
H	3.704383	-1.334845	-2.277229
H	4.341124	-0.544925	-0.822149
H	3.687154	0.440535	-2.142091
H	-1.085143	3.882936	-0.271678
O	-4.797883	-0.868921	0.473411
C	-5.038420	-2.095514	1.154295
H	-6.060456	-2.033416	1.523699
H	-4.947995	-2.945517	0.471490
H	-4.353766	-2.219401	1.998493

Number of imaginary frequencies = 1 (-437.5716)

Enthalpy = -1204.561525

ZPE Energy = -1204.591251

7b-(E)-Im-b

ωB97XD/6-311+G(d,p) geometry

C	1.823929	2.209053	-0.332723
O	3.104213	2.538517	-0.341551
C	1.558881	1.076041	0.679884
C	3.484907	3.630697	-1.198788
C	2.541105	-0.111312	0.458587
N	0.193510	0.582690	0.443399
C	2.279111	-1.247022	1.422902
C	2.512267	-0.655504	-0.978307
C	-0.895224	1.210203	0.750133
O	1.330075	-1.459868	-1.135387
C	1.904574	-2.440779	0.959789
C	3.633973	-1.681653	-1.247954
C	1.739374	-2.667719	-0.532161
O	2.980473	-2.952214	-1.122344
O	1.692642	-3.563117	1.675657
C	1.703651	1.660065	2.091565
H	3.267920	3.386446	-2.239213
H	4.555124	3.753918	-1.051670
H	2.953872	4.537732	-0.907666
H	3.539977	0.294372	0.635701
H	2.433884	-1.085041	2.484523
H	2.480082	0.131554	-1.730436
H	-0.784754	2.145851	1.289311
H	4.449097	-1.595600	-0.525691
H	4.027558	-1.602931	-2.260963
H	1.028663	-3.460372	-0.759433
H	1.161809	2.602014	2.197431
H	2.757467	1.855834	2.292107
H	1.325425	0.952976	2.831170
H	1.902426	-3.414888	2.605445
C	-2.224564	0.780301	0.451152
C	-4.878336	0.092654	-0.086215
C	-3.282688	1.609282	0.874481
C	-2.528600	-0.402616	-0.244473
C	-3.835345	-0.747888	-0.512175
C	-4.588982	1.274354	0.613453
H	-3.061239	2.527065	1.408863
H	-1.746952	-1.072024	-0.585796
H	-4.043022	-1.663348	-1.048974
H	-5.406916	1.908272	0.933041
H	0.146147	-0.282136	-0.099064
O	0.970003	2.741598	-0.993148
O	-6.169124	-0.153703	-0.302387
C	-6.548949	-1.320236	-1.032560
H	-6.231330	-2.227365	-0.511998
H	-7.635443	-1.291213	-1.082755
H	-6.135137	-1.297179	-2.043991

Number of imaginary frequencies = 0

Enthalpy = -1204.609185

ZPE Energy = -1204.640121

7b-(Z)-Im-b

ωB97XD/6-311+G(d,p) geometry

C	0.050037	1.524144	-0.209549
O	-0.063708	2.629949	0.505859
C	0.726944	0.408483	0.604577
C	-0.625803	3.775447	-0.161178
C	2.275939	0.649834	0.476916
N	0.430019	-0.887252	-0.026304
C	3.088298	-0.255685	1.376518
C	2.802310	0.521933	-0.963807
C	-0.679407	-1.493615	-0.330521
O	2.943141	-0.875043	-1.275163
C	3.980714	-1.097931	0.852083
C	4.253250	1.028990	-1.112068
C	4.169795	-1.175344	-0.651182
O	5.045024	-0.166688	-1.084159
O	4.832795	-1.897797	1.521541
C	0.319680	0.396040	2.081821
H	-0.630372	4.567266	0.583856
H	-1.641861	3.555704	-0.491182
H	-0.006748	4.056038	-1.014041
H	2.426792	1.686385	0.793852
H	2.983409	-0.162704	2.451885
H	2.131891	0.958798	-1.699977
H	4.541650	1.699830	-0.299639
H	4.416705	1.518893	-2.071557
H	4.532362	-2.147930	-0.979968
H	-0.760228	0.366903	2.217930
H	0.704331	1.286802	2.578471
H	0.738900	-0.487333	2.563401
H	4.754452	-1.753715	2.472202
H	1.269930	-1.387317	-0.318813
O	-0.288437	1.411490	-1.359900
H	-0.495336	-2.458017	-0.796579
C	-2.064680	-1.165082	-0.196122
C	-4.848973	-0.794912	-0.130290
C	-2.628276	0.015566	0.324380
C	-2.951177	-2.156330	-0.681250

C	-4.311384	-1.982222	-0.649906
C	-3.991878	0.204394	0.359761
H	-2.018322	0.813922	0.717800
H	-2.546345	-3.074696	-1.092359
H	-4.984921	-2.743492	-1.023768
H	-4.386499	1.125402	0.766410
O	-6.175210	-0.701925	-0.142326
C	-6.804884	0.479122	0.355887
H	-6.497492	1.356174	-0.219707
H	-7.872380	0.314748	0.226428
H	-6.581922	0.622219	1.416251

Number of imaginary frequencies = 0

Enthalpy = -1204.596663

ZPE Energy = -1204.627255

8b-TS-(E)

ωB97XD/6-311+G(d,p) geometry

C	-2.476286	-1.689800	-0.510306
O	-3.781381	-1.754396	-0.276257
O	-1.974414	-1.898061	-1.583632
C	-1.694585	-1.343012	0.772956
C	-4.624515	-2.040265	-1.405144
C	-1.794485	0.210596	1.157069
N	-0.288153	-1.605282	0.519956
C	-0.424173	0.827177	0.925023
C	-2.864979	1.020012	0.414714
C	0.335175	-0.609446	-0.179347
O	-2.384419	1.286497	-0.913518
C	-0.331205	1.928201	0.095688
C	-3.059223	2.442397	0.971712
C	-1.540473	2.372457	-0.708071
O	-2.238038	3.265815	0.123432
O	0.736424	2.650378	-0.082505
C	1.796621	-0.489887	-0.210164
C	2.612336	-0.878416	0.854834
C	2.397473	0.067902	-1.347244
C	3.768052	0.208823	-1.427673
C	4.576868	-0.204946	-0.363204
C	3.989880	-0.747165	0.786487
C	-2.178409	-2.216325	1.928288
H	-4.355336	-3.001048	-1.844779
H	-4.535754	-1.249342	-2.151648
H	-5.636351	-2.075956	-1.007982
H	-2.024162	0.253048	2.223372
H	0.206078	-1.938760	1.338873
H	0.307327	0.747859	1.723041
H	-3.805634	0.484230	0.336200
H	-0.157080	-0.378024	-1.117635
H	-2.740951	2.538767	2.011164
H	-4.090305	2.778019	0.864997
H	-1.273586	2.846707	-1.650933
H	2.181852	-1.287561	1.763273
H	1.778058	0.380455	-2.181624
H	4.235437	0.630072	-2.309738
O	5.898771	-0.040877	-0.530257
H	4.595323	-1.063822	1.625301
H	-2.106821	-3.276813	1.676330
H	-3.216132	-1.985937	2.167865
H	-1.568547	-2.020290	2.814490
H	1.462303	2.378555	0.502699
C	6.783213	-0.491548	0.489981
H	7.786753	-0.290216	0.119914
H	6.622912	0.057370	1.422656
H	6.668433	-1.565737	0.662777

Number of imaginary frequencies = 1 (-385.1564)

Enthalpy = -1204.580511

ZPE Energy = -1204.609980

8b-TS-(Z)

ωB97XD/6-311+G(d,p) geometry

C	2.414610	-2.071479	0.365969
O	3.137492	-2.484790	-0.661398
O	2.688533	-2.270427	1.522788
C	1.201636	-1.261730	-0.099652
C	4.338753	-3.215793	-0.353627
C	1.658984	0.081060	-0.788728
N	0.488311	-0.836698	1.103092
C	0.461944	1.001167	-0.729991
C	2.872795	0.758491	-0.131708
C	-0.390480	0.210264	0.987405
O	2.442584	1.440287	1.057254
C	0.634209	2.274177	-0.229308
C	3.446177	1.918475	-0.967796
C	1.903425	2.613595	0.536872
O	2.825700	3.090299	-0.406972
O	-0.195341	3.272701	-0.370247
C	-1.807352	0.066905	0.607815
C	-2.621879	1.211106	0.631914
C	-2.400985	-1.161822	0.327014
C	-3.753031	-1.254078	0.023776
C	-4.538385	-0.099607	-0.001604
C	-3.961060	1.137184	0.317354
C	0.374675	-2.099212	-1.075505
H	5.000351	-2.609887	0.266727
H	4.803658	-3.424245	-1.314210
H	4.091295	-4.145580	0.159593
H	1.904535	-0.137078	-1.830144
H	1.156369	-0.677692	1.849755
H	-0.339093	0.838251	-1.443088
H	3.648231	0.051156	0.152731
H	-0.249100	0.956788	1.767498
H	3.203901	1.835555	-2.028594
H	4.523575	2.014933	-0.837242
H	1.735155	3.349082	1.321941
H	-2.202562	2.168123	0.924375
H	-1.819944	-2.072281	0.384874
H	-4.184888	-2.226758	-0.170147
H	-4.589116	2.020185	0.336270
H	0.006428	-3.003113	-0.586608
H	0.999139	-2.390776	-1.920108
H	-0.474147	-1.535220	-1.462610
H	-0.922107	3.055874	-0.975748
O	-5.850735	-0.078244	-0.288047
C	-6.504483	-1.302248	-0.601703
H	-6.072431	-1.761525	-1.495920
H	-6.456906	-2.003148	0.237017
H	-7.543698	-1.043097	-0.796010

Number of imaginary frequencies = 1 (-391.1853)

Enthalpy = -1204.573966
ZPE Energy = -1204.603553

8b-COH_N

ωB97XD/6-311+G(d,p) geometry

C	-2.432834	-1.183360	-0.164915
O	-3.288020	-2.124659	-0.159254
C	-1.343886	-1.190546	0.904591
C	-4.246411	-2.243733	-1.252214
C	-0.917924	0.256118	1.200813
N	-0.163574	-1.673857	0.194556
C	-0.400955	0.646437	-0.193247
C	-2.006600	1.188143	1.723376
C	0.377038	-0.608264	-0.667506
O	-3.130727	1.127381	0.826849
C	-1.636247	0.923772	-1.035149
C	-1.615107	2.657356	1.584065
C	-2.648756	1.835531	-0.280020
O	-1.975020	2.954436	0.218200
C	-1.708935	-2.032872	2.107126
H	-3.709714	-2.465182	-2.173432
H	-4.811742	-1.316964	-1.334888
H	-4.887464	-3.070960	-0.963775
H	-0.093374	0.218016	1.915119
H	-0.271101	-2.573643	-0.258082
H	0.216369	1.542580	-0.201340
H	-2.350247	0.915052	2.718401
H	-0.549633	2.837961	1.729028
H	-2.199632	3.296197	2.247435
H	-3.477733	2.132573	-0.925534
H	-1.858937	-3.077878	1.830841
H	-2.622069	-1.664173	2.579548
H	-0.890663	-1.977093	2.827251
O	-1.321050	1.311763	-2.284672
H	-2.088092	1.685289	-2.738954
O	-2.410448	-0.389135	-1.168312
H	0.151789	-0.794037	-1.722854
C	1.875647	-0.447735	-0.528061
C	4.635808	-0.008176	-0.293195
C	2.603186	0.114967	-1.581251
C	2.552654	-0.786059	0.635214
C	3.924996	-0.574184	0.763405
C	3.963435	0.335471	-1.470832
H	2.095053	0.381985	-2.503360
H	2.008808	-1.236969	1.457694
H	4.420318	-0.855912	1.683555
H	4.526954	0.767587	-2.290003
O	5.966293	0.238456	-0.277670
C	6.703403	-0.113259	0.882547
H	6.645595	-1.189041	1.077881
H	7.737453	0.157349	0.674160
H	6.353780	0.440663	1.759801

Number of imaginary frequencies = 0
Enthalpy = -1204.598984
ZPE Energy = -1204.627696

8b-COH_X

ωB97XD/6-311+G(d,p) geometry

C	2.428487	-1.198970	0.111456
O	3.284611	-2.131311	0.017257
C	1.257168	-1.176050	-0.864636
C	4.304010	-2.283397	1.049318
C	0.840615	0.280052	-1.138433
N	0.234658	-1.690131	0.050885
C	0.421983	0.672753	0.284994
C	1.912486	1.193965	-1.725462
C	-0.368201	-0.563662	0.791297
O	3.089788	1.099349	-0.903392
C	1.715829	0.908820	1.050397
C	1.564935	2.670400	-1.550190
C	2.696035	1.808407	0.237809
O	2.017665	2.946408	-0.208081
C	1.480164	-2.043070	-2.082510
H	3.817801	-2.525018	1.993019
H	4.879728	-1.362286	1.122728
H	4.921348	-3.106733	0.704140
H	-0.024153	0.264863	-1.804085
H	-0.431389	-2.292660	-0.414981
H	-0.168449	1.584904	0.344629
H	2.184288	0.921718	-2.742792
H	0.496554	2.875757	-1.625496
H	2.120349	3.302801	-2.244200
H	3.571848	2.082387	0.829767
H	1.656665	-3.083747	-1.806571
H	2.334979	-1.685187	-2.659620
H	0.589770	-1.993025	-2.713173
O	1.489071	1.288642	2.321520
H	2.292166	1.635818	2.732128
O	2.478156	-0.415670	1.121489
H	-0.185577	-0.690637	1.861365
C	-1.861202	-0.416196	0.593329
C	-4.626290	-0.019387	0.295174
C	-2.643026	0.033518	1.662487
C	-2.493110	-0.664052	-0.619940
C	-3.864400	-0.472407	-0.780129
C	-4.003155	0.233694	1.521503
H	-2.175023	0.227047	2.622877
H	-1.926960	-1.021016	-1.474467
H	-4.318841	-0.680443	-1.739916
H	-4.605783	0.577777	2.354404
O	-5.959931	0.196960	0.252246
C	-6.649902	-0.074721	-0.958104
H	-6.552517	-1.127452	-1.242199
H	-7.697411	0.148026	-0.761093
H	-6.291429	0.564817	-1.771135

Number of imaginary frequencies = 0
Enthalpy = -1204.597817
ZPE Energy = -1204.626815

8b-NH2

ωB97XD/6-311+G(d,p) geometry

C	2.439955	-1.581989	0.202395
O	3.649318	-1.643479	-0.305197
O	2.148496	-1.781544	1.356453
C	1.395909	-1.233598	-0.865788
C	4.727577	-1.839855	0.629692
C	1.246101	0.292923	-1.067765

N	0.056955	-1.588331	-0.275635
C	0.357363	0.772926	0.103907
C	2.552953	1.078624	-1.168418
C	-0.477962	-0.433431	0.566323
O	3.186294	1.124924	0.114852
C	1.146110	1.400973	1.249207
C	2.305681	2.562958	-1.436925
C	2.436120	2.093711	0.803132
O	2.143058	3.112504	-0.120744
O	0.791329	1.355568	2.397985
C	-1.970809	-0.326028	0.424190
C	-2.798867	-0.712089	1.480507
C	-2.557913	0.143502	-0.747914
C	-3.938611	0.231511	-0.878259
C	-4.754836	-0.154259	0.188116
C	-4.174374	-0.627213	1.368927
C	1.622065	-1.997817	-2.161542
H	4.628441	-2.811551	1.114106
H	4.720384	-1.042534	1.373022
H	5.636774	-1.800891	0.034930
H	0.699016	0.426159	-2.005397
H	0.111964	-2.437351	0.293075
H	-0.294546	1.576378	-0.249604
H	3.246681	0.624544	-1.873166
H	-0.224537	-0.676993	1.596520
H	1.406299	2.752412	-2.024503
H	3.168727	3.030184	-1.913975
H	3.000065	2.480670	1.651033
H	-2.359368	-1.075928	2.403597
H	-1.937304	0.456180	-1.583505
H	-4.362322	0.607018	-1.800248
H	-4.819430	-0.919304	2.189436
H	1.692091	-3.072618	-1.981569
H	2.551973	-1.663513	-2.621492
H	0.801968	-1.800700	-2.856372
H	-0.596833	-1.781261	-1.038309
O	-6.101283	-0.104528	0.171664
C	-6.753382	0.373229	-0.996984
H	-6.525837	-0.256043	-1.863245
H	-7.819881	0.319738	-0.784739
H	-6.479194	1.411694	-1.207058

Number of imaginary frequencies = 0

Enthalpy = -1204.635602

ZPE Energy = -1204.665255

7c-NH2

ωB97XD/6-311+G(d,p) geometry

C	-2.618826	-1.558400	-0.396127
O	-3.925913	-1.545780	-0.351514
O	-1.943094	-1.904090	-1.336813
C	-1.994631	-1.109268	0.937034
C	-4.619719	-1.872323	-1.574667
C	-2.025045	0.436051	1.165830
N	-0.519153	-1.426052	0.781981
C	-0.624177	0.922046	0.728377
C	-3.139688	1.200383	0.452780
C	0.279043	-0.222685	1.178665
O	-2.949598	1.097220	-0.963240
C	-0.615827	1.255966	-0.762517
C	-3.014113	2.708637	0.664884
C	-1.889947	1.994187	-1.200650
O	-2.122933	3.113658	-0.386974
O	0.247338	0.936030	-1.536534
C	1.716228	-0.241551	0.716183
C	2.305297	-1.340801	0.098206
C	2.484051	0.895211	0.978618
C	3.816185	0.946663	0.611286
C	4.373394	-0.158784	-0.015390
C	3.641601	-1.303511	-0.276298
C	-2.581501	-1.880009	2.110266
H	-4.405509	-2.902971	-1.856994
H	-4.312700	-1.186285	-2.363827
H	-5.675324	-1.748154	-1.347551
H	-2.132829	0.599561	2.240596
H	-0.379831	-1.665424	-0.214707
H	-0.364229	1.842268	1.256784
H	-4.125132	0.810148	0.694503
H	0.271725	-0.221681	2.271930
H	-2.584012	2.974903	1.631776
H	-3.973467	3.210919	0.532499
H	-1.853114	2.268246	-2.254194
H	1.748830	-2.246315	-0.113443
H	2.039287	1.754730	1.467006
H	4.413643	1.827115	0.806089
H	4.104397	-2.152121	-0.761622
H	-2.562622	-2.956799	1.926890
H	-3.615811	-1.571044	2.263844
H	-2.015836	-1.656967	3.018063
H	-0.257941	-2.249763	1.327795
N	5.788911	-0.114466	-0.411075
O	6.427537	0.880754	-0.127480
O	6.246440	-1.074994	-1.000028

Number of imaginary frequencies = 0

Enthalpy = -1294.632526

ZPE Energy = -1294.661907

7c-COH-N

ωB97XD/6-311+G(d,p) geometry

C	1.573004	1.430578	-0.278468
O	1.716196	2.640884	-0.638724
C	2.045524	1.034476	1.119769
C	1.136045	3.098362	-1.898013
C	2.445085	-0.450142	1.116618
N	0.818404	0.973997	1.905153
C	1.085164	-1.068441	0.733060
C	3.584842	-0.838586	0.180929
C	0.102103	-0.281527	1.644730
O	3.272671	-0.366887	-1.139586
C	0.950181	-0.850429	-0.775403
C	3.631965	-2.344424	-0.059672
C	2.257021	-1.250597	-1.520587
O	2.654232	-2.525847	-1.103866
C	3.071333	1.993794	1.682745
H	0.056511	2.961826	-1.865585
H	1.582369	2.536636	-2.716719
H	1.398543	4.150252	-1.951383
H	2.705572	-0.721376	2.141593
H	0.275048	1.824932	1.957736

H	1.023739	-2.140303	0.915517
H	4.535029	-0.405750	0.484450
H	0.038910	-0.842862	2.581767
H	3.347226	-2.932375	0.813952
H	4.607184	-2.666168	-0.427878
H	2.104863	-1.216866	-2.599129
H	2.655912	2.996790	1.793878
H	3.949671	2.050765	1.035897
H	3.377783	1.631716	2.665655
O	-0.098117	-1.396102	-1.417388
H	-0.888536	-1.416803	-0.862131
O	0.875941	0.655930	-1.019300
C	-1.319083	-0.163323	1.122838
C	-3.908680	-0.117850	0.151197
C	-2.137485	-1.294497	1.221669
C	-1.836515	0.996349	0.547658
C	-3.135272	1.027101	0.060295
C	-3.431958	-1.285482	0.728799
H	-1.752577	-2.196136	1.686466
H	-1.242113	1.898455	0.468693
H	-3.540130	1.925698	-0.385661
H	-4.061166	-2.162701	0.797232
N	-5.281157	-0.092257	-0.377755
O	-5.950105	-1.102006	-0.273244
O	-5.672596	0.936519	-0.894783

Number of imaginary frequencies = 0
Enthalpy = -1294.599765
ZPE Energy = -1294.628369

7c-COH-X

ωB97XD/6-311+G(d,p) geometry

C	1.674896	1.424417	-0.304219
O	1.937781	2.604072	-0.688204
C	2.060227	1.015900	1.114881
C	1.435977	3.074099	-1.976602
C	2.397356	-0.486114	1.149124
N	0.729662	1.106961	1.728841
C	1.025243	-1.040301	0.727813
C	3.545643	-0.937495	0.251928
C	0.064495	-0.199834	1.609933
O	3.291441	-0.454036	-1.077512
C	0.939096	-0.824478	-0.785268
C	3.528526	-2.444197	0.013197
C	2.247485	-1.291856	-1.487914
O	2.571932	-2.582242	-1.056317
C	3.081837	1.938377	1.740306
H	1.822090	4.084598	-2.066385
H	0.347452	3.067039	-1.957909
H	1.825156	2.431016	-2.764094
H	2.609536	-0.757485	2.185769
H	0.781822	1.444284	2.681477
H	0.899954	-2.105959	0.913769
H	4.506963	-0.549364	0.580262
H	0.041609	-0.695663	2.585202
H	3.193516	-3.016650	0.879113
H	4.497089	-2.812154	-0.328732
H	2.130970	-1.255237	-2.570832
H	2.715533	2.964991	1.788122
H	4.014432	1.926266	1.173018
H	3.287414	1.590343	2.754968
O	-0.116647	-1.322463	-1.452610
H	-0.925873	-1.282456	-0.925830
O	0.947223	0.682435	-1.047045
C	-1.364340	-0.121369	1.107502
C	-3.951532	-0.086450	0.144836
C	-2.160049	-1.269930	1.175299
C	-1.894304	1.046673	0.564460
C	-3.194890	1.072571	0.081726
C	-3.456612	-1.264185	0.686768
H	-1.760119	-2.179299	1.611659
H	-1.288240	1.942841	0.527671
H	-3.614643	1.976209	-0.339845
H	-4.074013	-2.151324	0.730823
N	-5.327078	-0.067117	-0.375423
O	-5.943040	-1.115558	-0.395813
O	-5.776572	0.995808	-0.759347

Number of imaginary frequencies = 0
Enthalpy = -1294.602798
ZPE Energy = -1294.631417

7c-TS-(E)

ωB97XD/6-311+G(d,p) geometry

C	-3.253821	-1.393021	-0.479280
O	-4.510828	-1.082402	-0.217108
O	-2.866523	-1.896656	-1.504070
C	-2.328457	-0.985370	0.664994
C	-5.475728	-1.360155	-1.249320
C	-2.206173	0.591110	0.768393
N	-0.992571	-1.440198	0.328146
C	-0.871999	0.851621	1.447919
C	-2.250489	1.305191	-0.589434
C	-0.023458	-0.869143	1.098876
O	-0.982575	1.116347	-1.243846
C	0.025806	1.705931	0.818796
C	-2.325410	2.839387	-0.476359
C	-0.196570	2.086730	-0.639276
O	-0.954444	3.264912	-0.610507
O	1.034586	2.192683	1.471646
C	1.373269	-0.813149	0.593747
C	1.677311	-0.788455	-0.769799
C	2.402418	-0.740596	1.533557
C	3.724271	-0.646436	1.127880
C	3.993631	-0.624957	-0.230601
C	2.994459	-0.698917	-1.189339
C	-2.818041	-1.572540	1.990079
N	5.395433	-0.519003	-0.673423
O	5.610321	-0.451913	-1.867763
O	6.259756	-0.501819	0.180651
H	-5.524829	-2.433112	-1.437030
H	-5.211410	-0.830567	-2.165524
H	-6.424761	-0.999084	-0.860531
H	-3.021764	0.964882	1.389427
H	-0.829898	-1.458238	-0.672420
H	-0.851141	0.864129	2.532251
H	-3.024786	0.919137	-1.248064
H	-0.075050	-1.119160	2.153797
H	-2.728817	3.172852	0.480897
H	-2.891328	3.279451	-1.296254

H	0.733857	2.232934	-1.190129
H	1.649086	2.681082	0.899168
H	0.900099	-0.826847	-1.523850
H	2.169665	-0.757618	2.592172
H	4.528257	-0.592554	1.849427
H	3.240656	-0.680755	-2.242334
H	-2.837372	-2.662714	1.931804
H	-3.822202	-1.211135	2.210466
H	-2.166744	-1.280881	2.816625

Number of imaginary frequencies = 1 (-322.1469)
Enthalpy = -1294.585035
ZPE Energy = -1294.614849

7c-TS-(Z)

ωB97XD/6-311+G(d,p) geometry

C	2.397083	-1.762899	-0.139658
O	3.272522	-1.717621	0.854964
O	1.743228	-2.733323	-0.420983
C	2.412577	-0.452952	-0.935784
C	3.404962	-2.906423	1.655900
C	2.143442	0.875827	-0.093640
N	1.459433	-0.472402	-2.050300
C	1.229649	1.778626	-0.890801
C	1.627291	0.752547	1.354486
C	0.290208	0.203835	-2.023515
O	0.201031	0.646522	1.363433
C	0.182452	2.387833	-0.251765
C	1.839394	2.052611	2.158237
C	-0.190696	1.962542	1.163886
O	0.581479	2.744066	2.039392
O	-0.498639	3.343509	-0.834916
C	-0.945694	-0.172200	-1.313953
C	-1.050210	-1.272209	-0.465271
C	-2.080596	0.602860	-1.590858
C	-3.291383	0.320118	-0.986429
C	-3.353935	-0.763865	-0.122421
C	-2.261255	-1.574421	0.136334
C	3.814064	-0.360300	-1.569622
H	3.722998	-3.744557	1.035218
H	2.456946	-3.138150	2.143211
H	4.165951	-2.670806	2.395823
H	3.119510	1.359922	-0.021972
H	1.947520	-0.289540	-2.918153
H	1.615189	2.251192	-1.787860
H	2.033861	-0.110589	1.869468
H	0.086146	0.725652	-2.956077
H	2.644547	2.674215	1.764103
H	2.009443	1.846150	3.214631
H	-1.254429	2.083670	1.374842
H	-0.195656	-1.906560	-0.283559
H	-2.015664	1.429893	-2.288987
H	-4.172450	0.912842	-1.191333
H	-2.352623	-2.425016	0.798070
H	4.001746	-1.219951	-2.218354
H	4.577058	-0.336036	-0.792825
H	3.888178	0.557128	-2.159861
H	-1.251781	3.631121	-0.297010
N	-4.639886	-1.075103	0.527159
O	-4.701843	-2.073446	1.217128
O	-5.568708	-0.313110	0.339965

Number of imaginary frequencies = 1 (-373.4321)
Enthalpy = -1294.560458
ZPE Energy = -1294.590364

7c-(E)-Im-c

ωB97XD/6-311+G(d,p) geometry

C	2.042964	2.227028	-0.306203
O	3.322504	2.548609	-0.325376
C	1.787730	1.081388	0.695969
C	3.700301	3.652171	-1.171638
C	2.767487	-0.105392	0.465825
N	0.421259	0.585171	0.442326
C	2.494277	-1.248737	1.418410
C	2.736486	-0.634030	-0.976631
C	-0.664980	1.190130	0.755719
O	1.541178	-1.419852	-1.140843
C	2.104091	-2.433097	0.942869
C	3.843440	-1.673562	-1.253418
C	1.934837	-2.642202	-0.551613
O	3.169834	-2.935261	-1.146185
O	1.880367	-3.559978	1.645559
C	1.917861	1.652309	2.113251
H	3.476795	3.419618	-2.213231
H	4.771403	3.771050	-1.028536
H	3.171965	4.555484	-0.865108
H	3.766657	0.295974	0.650180
H	2.654922	-1.100471	2.481082
H	2.716266	0.160210	-1.721528
H	-0.580790	2.118988	1.310716
H	4.656014	-1.608376	-0.526269
H	4.242815	-1.589030	-2.263506
H	1.212735	-3.421823	-0.787447
H	1.373360	2.592198	2.223421
H	2.970239	1.848607	2.320212
H	1.538975	0.936885	2.844424
H	2.098327	-3.428255	2.576086
C	-2.001410	0.723768	0.430756
C	-4.583788	-0.013111	-0.121076
C	-3.063235	1.543306	0.826705
C	-2.252017	-0.477454	-0.246309
C	-3.552708	-0.851714	-0.523407
C	-4.370677	1.178983	0.547551
H	-2.866175	2.471743	1.350021
H	-1.450689	-1.134983	-0.561332
H	-3.768222	-1.775737	-1.042357
H	-5.201625	1.804646	0.843016
H	0.389260	-0.274437	-0.117098
O	1.179385	2.770093	-0.944712
N	-5.975512	-0.414529	-0.422626
O	-6.857373	0.383803	-0.181594
O	-6.152946	-1.519350	-0.893250

Number of imaginary frequencies = 0
Enthalpy = -1294.600770
ZPE Energy = -1294.631545

7c-(Z)-Im-c

ωB97XD/6-311+G(d,p) geometry

C	0.684740	1.996476	-0.194052
O	1.028634	2.868503	0.733147
C	0.837089	0.563170	0.339044
C	0.910237	4.263373	0.388945
C	2.324338	0.308943	0.759107
N	0.565105	-0.365018	-0.786405
C	2.525100	-1.103273	1.260403
C	3.334586	0.595257	-0.362807
C	-0.505140	-0.912546	-1.230993
O	3.286376	-0.496909	-1.299686
C	3.341588	-1.931299	0.606187
C	4.798596	0.535469	0.121828
C	4.079192	-1.461601	-0.635202
O	5.242989	-0.768639	-0.277206
O	3.668966	-3.191220	0.949757
C	-0.095786	0.338232	1.536346
H	1.229179	4.804911	1.276025
H	-0.126478	4.500686	0.148510
H	1.558737	4.496895	-0.455879
H	2.519074	1.018110	1.567249
H	2.023832	-1.417766	2.169669
H	3.118870	1.512340	-0.909480
H	4.879165	0.656298	1.204362
H	5.425293	1.271845	-0.380098
H	4.323668	-2.276431	-1.314060
H	-1.068583	0.808179	1.404240
H	0.366714	0.776101	2.421130
H	-0.241767	-0.728712	1.710449
H	3.263068	-3.427852	1.792543
H	1.430047	-0.659525	-1.260195
O	0.294556	2.272762	-1.299876
H	-0.334836	-1.652151	-2.010248
C	-1.894581	-0.708881	-0.821060
C	-4.520068	-0.490479	-0.076387
C	-2.472628	0.555492	-0.696404
C	-2.656887	-1.863326	-0.619747
C	-3.977753	-1.757636	-0.219039
C	-3.802793	0.668253	-0.326784
H	-1.899140	1.447748	-0.910617
H	-2.212019	-2.842179	-0.755930
H	-4.576317	-2.638654	-0.031662
H	-4.273023	1.637359	-0.230277
N	-5.929861	-0.370203	0.347990
O	-6.348763	0.740109	0.605697
O	-6.586654	-1.388906	0.420275

Number of imaginary frequencies = 0

Enthalpy = -1294.590226

ZPE Energy = -1294.621056

8c-TS-(E)

ωB97XD/6-311+G(d,p) geometry

C	-2.684676	-1.648360	-0.575475
O	-3.998830	-1.667695	-0.405887
O	-2.134435	-1.871732	-1.621802
C	-1.956367	-1.338099	0.749246
C	-4.795387	-1.919465	-1.576853
C	-2.029535	0.216786	1.156854
N	-0.546359	-1.631939	0.558357
C	-0.646225	0.822501	1.002287
C	-3.049661	1.054438	0.374939
C	0.128056	-0.688955	-0.129536
O	-2.505228	1.308726	-0.930107
C	-0.489218	1.912658	0.177124
C	-3.233713	2.480546	0.927449
C	-1.649219	2.378431	-0.686003
O	-2.369885	3.287478	0.106620
O	0.594354	2.629896	0.058408
C	1.597460	-0.591335	-0.102734
C	2.359524	-1.019325	0.988967
C	2.226656	-0.008728	-1.204745
C	3.605985	0.133760	-1.232880
C	4.332665	-0.312871	-0.142838
C	3.736164	-0.888134	0.970993
C	-2.514647	-2.216614	1.865534
H	-4.549829	-2.894477	-1.998442
H	-4.630112	-1.137241	-2.319198
H	-5.826983	-1.904106	-1.232935
H	-2.308609	0.242654	2.211896
H	-0.091891	-2.018721	1.377040
H	0.064129	0.699550	1.814007
H	-3.998645	0.541666	0.256128
H	-0.338944	-0.401512	-1.063967
H	-2.948690	2.569529	1.977320
H	-4.253764	2.836660	0.787831
H	-1.327052	2.844243	-1.615675
H	1.891863	-1.450202	1.866690
H	1.636568	0.327166	-2.049784
H	4.104027	0.577990	-2.083898
H	4.339170	-1.218577	1.805827
H	-2.468484	-3.273704	1.594277
H	-3.553152	-1.954468	2.065440
H	-1.937187	-2.057818	2.780178
H	1.276064	2.369285	0.698255
N	5.800710	-0.167721	-0.161060
O	6.299838	0.426271	-1.095741
O	6.428423	-0.650909	0.760254

Number of imaginary frequencies = 1 (-377.4779)

Enthalpy = -1294.578636

ZPE Energy = -1294.608477

8c-TS-(Z)

ωB97XD/6-311+G(d,p) geometry

C	2.446503	-2.121896	0.287194
O	3.024060	-2.640262	-0.780318
O	2.808708	-2.299109	1.423285
C	1.269267	-1.219994	-0.098080
C	4.167892	-3.485211	-0.551489
C	1.783856	0.099991	-0.819241
N	0.689957	-0.742002	1.153720
C	0.703590	1.140885	-0.666671
C	3.109125	0.635788	-0.261644
C	-0.189492	0.273896	1.105186
O	2.846534	1.253328	1.009495
C	1.008263	2.331021	-0.053129
C	3.682475	1.812570	-1.076448
C	2.364759	2.499990	0.626275
O	3.242634	2.979426	-0.355558
O	0.193508	3.358680	-0.118040

C	-1.598491	0.109579	0.654536
C	-2.358902	1.221239	0.283457
C	-2.201682	-1.145645	0.740736
C	-3.540533	-1.302142	0.415378
C	-4.259118	-0.188698	0.015813
C	-3.693124	1.076733	-0.050077
C	0.308610	-1.972979	-1.017108
H	4.493131	-3.803560	-1.538915
H	3.881043	-4.347145	0.051566
H	4.957997	-2.923607	-0.051492
H	1.918183	-0.137368	-1.876285
H	1.410035	-0.617909	1.858377
H	-0.146468	1.111696	-1.337231
H	3.854151	-0.141455	-0.109182
H	-0.079746	0.991733	1.916260
H	3.305922	1.837971	-2.100416
H	4.771774	1.811935	-1.077989
H	2.335490	3.178972	1.479442
H	-1.907792	2.204329	0.239834
H	-1.632227	-2.000254	1.081563
H	-4.017110	-2.271062	0.477177
H	-4.287278	1.928906	-0.351244
H	-0.109905	-2.843227	-0.509430
H	0.855482	-2.312538	-1.896355
H	-0.505736	-1.333186	-1.356641
H	0.509312	4.106510	0.411145
N	-5.679170	-0.350352	-0.339651
O	-6.283728	0.632368	-0.722489
O	-6.169185	-1.457560	-0.233474

Number of imaginary frequencies = 1 (-306.1795)

Enthalpy = -1294.573288

ZPE Energy = -1294.602982

8c-COH_N

ωB97XD/6-311+G(d,p) geometry

C	-2.663276	-1.131290	-0.278867
O	-3.539526	-2.047758	-0.356393
C	-1.598307	-1.242650	0.809959
C	-4.470236	-2.078455	-1.479850
C	-1.140397	0.166818	1.216143
N	-0.417491	-1.708866	0.087872
C	-0.580672	0.640414	-0.135564
C	-2.216797	1.090266	1.778273
C	0.174801	-0.600797	-0.674831
O	-3.319040	1.123141	0.854706
C	-1.788539	1.006204	-0.984957
C	-1.783887	2.553852	1.752745
C	-2.792327	1.893719	-0.188411
O	-2.099742	2.954206	0.401707
C	-2.008375	-2.155955	1.944618
H	-3.911414	-2.236830	-2.400876
H	-5.025883	-1.142690	-1.508008
H	-5.123705	-2.918350	-1.265874
H	-0.335752	0.056213	1.945474
H	-0.541494	-2.567996	-0.434277
H	0.057188	1.519538	-0.067886
H	-2.591324	0.755198	2.742587
H	-0.718271	2.696388	1.934552
H	-2.369068	3.161509	2.444034
H	-3.597016	2.258629	-0.829784
H	-2.170068	-3.176848	1.594676
H	-2.925713	-1.801134	2.419311
H	-1.206850	-2.163179	2.685181
O	-1.432343	1.468982	-2.197081
H	-2.178408	1.891740	-2.643269
O	-2.594655	-0.270773	-1.224053
H	-0.008322	-0.705534	-1.748843
C	1.671635	-0.480435	-0.466531
C	4.384748	-0.142051	-0.100113
C	2.425251	0.231956	-1.401568
C	2.300059	-1.024668	0.650203
C	3.664418	-0.858515	0.842382
C	3.786961	0.409115	-1.225583
H	1.942050	0.653590	-2.276799
H	1.720086	-1.590296	1.368400
H	4.160553	-1.278571	1.707135
H	4.378050	0.959302	-1.945426
N	5.829179	0.041385	0.097804
O	6.442690	0.684034	-0.733590
O	6.339262	-0.457269	1.083664

Number of imaginary frequencies = 0

Enthalpy = -1294.604105

ZPE Energy = -1294.632856

8c-COH_X

ωB97XD/6-311+G(d,p) geometry

C	-2.671529	-1.137903	-0.243482
O	-3.560148	-2.042467	-0.241037
C	-1.518283	-1.243389	0.750244
C	-4.570364	-2.075400	-1.293024
C	-1.055021	0.165544	1.158551
N	-0.499522	-1.709304	-0.194452
C	-0.591819	0.663984	-0.216861
C	-2.107284	1.066749	1.799812
C	0.167277	-0.552122	-0.810117
O	-3.266190	1.089745	0.947631
C	-1.858157	1.010444	-0.987637
C	-1.703127	2.538398	1.762406
C	-2.819267	1.878523	-0.119039
O	-2.105910	2.944055	0.436929
C	-1.790982	-2.207092	1.882240
H	-4.079164	-2.235606	-2.251319
H	-5.127203	-1.140032	-1.281056
H	-5.206781	-2.915238	-1.032144
H	-0.206393	0.059889	1.837182
H	0.108936	-2.417449	0.192878
H	0.029127	1.557354	-0.185570
H	-2.414328	0.715860	2.782314
H	-0.631329	2.698599	1.883643
H	-2.256655	3.129015	2.493699
H	-3.669526	2.237339	-0.702768
H	-1.984355	-3.214313	1.510168
H	-2.651965	-1.879856	2.468342
H	-0.915500	-2.232983	2.534721
O	-1.584982	1.485354	-2.216352
H	-2.363718	1.896338	-2.614999
O	-2.670887	-0.270826	-1.184375
H	0.026472	-0.575391	-1.893667

C	1.655853	-0.453884	-0.541769
C	4.365266	-0.138081	-0.104625
C	2.454541	0.195087	-1.485939
C	2.243030	-0.944551	0.623640
C	3.603756	-0.792350	0.849593
C	3.812128	0.363655	-1.274315
H	2.007339	0.575074	-2.398110
H	1.647584	-1.451768	1.374415
H	4.064612	-1.173503	1.751035
H	4.433700	0.867058	-2.002720
N	5.806396	0.031654	0.130023
O	6.449715	0.650448	-0.696189
O	6.281520	-0.454125	1.139254

Number of imaginary frequencies = 0

Enthalpy = -1294.601782

ZPE Energy = -1294.630513

8c-NH2

ωB97XD/6-311+G(d,p) geometry

C	-2.774587	-1.468494	-0.534782
O	-3.793369	-1.712699	0.249480
O	-2.816384	-1.357432	-1.737573
C	-1.453784	-1.374455	0.250490
C	-5.097107	-1.717674	-0.367575
C	-1.244900	0.002747	0.934958
N	-0.375849	-1.415807	-0.813379
C	-0.535083	0.878876	-0.118322
C	-2.510648	0.674250	1.468960
C	0.305395	-0.069061	-0.977124
O	-3.345644	1.055006	0.368677
C	-1.509535	1.723999	-0.939162
C	-2.214849	2.031636	2.105321
C	-2.713564	2.208725	-0.125421
O	-2.271367	2.937305	0.991906
O	-1.350204	1.982943	-2.102628
C	1.768516	-0.124335	-0.608995
C	2.687885	0.457812	-1.479499
C	2.213905	-0.697888	0.583412
C	3.562058	-0.695360	0.903636
C	4.450967	-0.104768	0.018688
C	4.039358	0.475678	-1.169725
C	-1.304122	-2.540749	1.217296
H	-5.151363	-2.508529	-1.115628
H	-5.288263	-0.746259	-0.823498
H	-5.797695	-1.907055	0.441515
H	-0.567759	-0.160818	1.777169
H	-0.833999	-1.656452	-1.702669
H	0.111119	1.604743	0.383106
H	-3.081562	0.011772	2.115518
H	0.209661	0.201744	-2.028110
H	-1.229984	2.086667	2.571231
H	-2.984512	2.307928	2.827337
H	-3.404503	2.793455	-0.731377
H	2.347529	0.903107	-2.407376
H	1.517560	-1.154839	1.277647
H	3.918523	-1.139853	1.823045
H	4.759416	0.923594	-1.841308
H	-1.446111	-3.498036	0.710872
H	-2.053447	-2.451796	2.004173
H	-0.314339	-2.518961	1.678210
H	0.303801	-2.151798	-0.612224
N	5.885416	-0.098631	0.353928
O	6.648606	0.437333	-0.425066
O	6.228303	-0.630354	1.392154

Number of imaginary frequencies = 0

Enthalpy = -1294.636016

ZPE Energy = -1294.665532