

Supporting Information

Highly Diastereoselective 1,3-Dipolar Cycloadditions of Chiral Non-Racemic Nitrones to 1,2-Diaza-1,3-dienes: An Experimental and Computational Investigation

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Tentative assignments of the absolute configuration of compounds **13** and **14**.

Despite the absolute configuration of compounds **13** and **14** cannot be unambiguously assigned due to the rotation around the C α (sugar)-C $_3$ (isoxazolidine) bond, the observed NOE relationships extracted from NOESY experiments allow a tentative assignment on the basis of the observed results. The relative configuration at the isoxazolidine ring (Figure S1, blue arrows) corroborates that both isomers (in the case of **13b**, **13d** and **14b**) are epimeric at C-3 of the isoxazolidine ring, indicating a poor *endo/exo* selectivity but an excellent *Re/Si* diastereofacial selectivity.

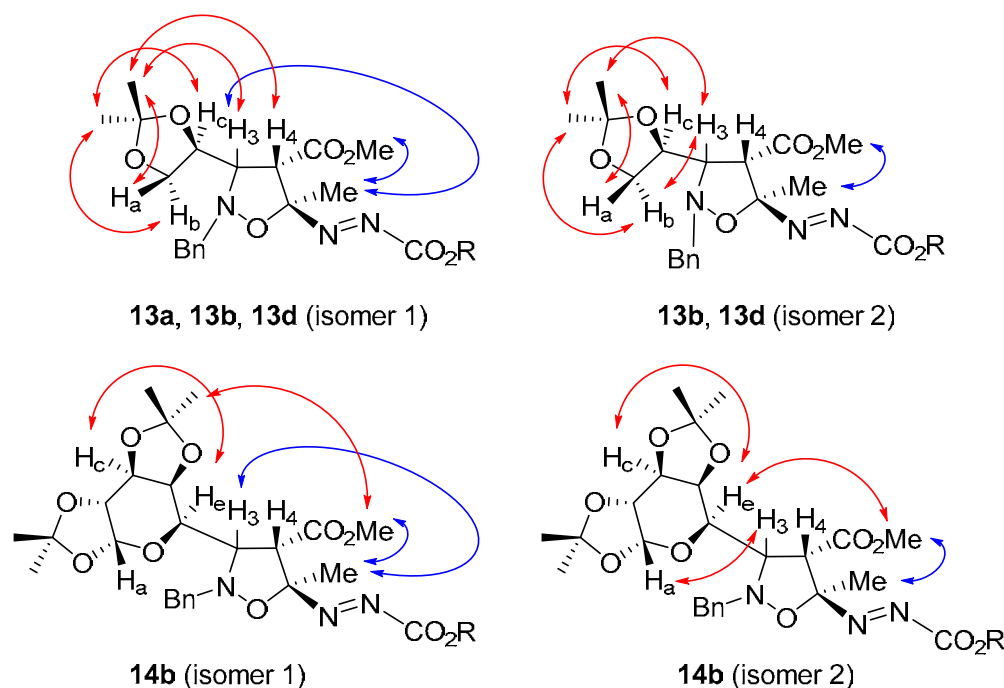


Figure S1. NOE relationships observed in NOESY experiments

In order to study the spatial relationships we have performed a simple conformational analysis for models of the four possible remaining isomers corresponding to compounds **13** and **14** (Figure S2). In the case of compounds **13** there are two possible configurations at C-3 for isomer 1 (Figure S2, Gly-**1A**/Gly-**2B** and Gly-**1B**/Gly-**2A**). The observed NOE between the glycerinaldehyde unit and the isoxazolidine ring in isomer 1 (Figure S1, red arrows) is more in agreement with the corresponding model Gly-**2A** thus indicating that a *Si* attack is favored, also in agreement with theoretical calculations. Similar NOE interactions between the glycerinaldehyde unit and the isoxazolidine ring were observed for isomer 2, which is in agreement with the same *Si* attack and, in consequence with Gly-**1B**.

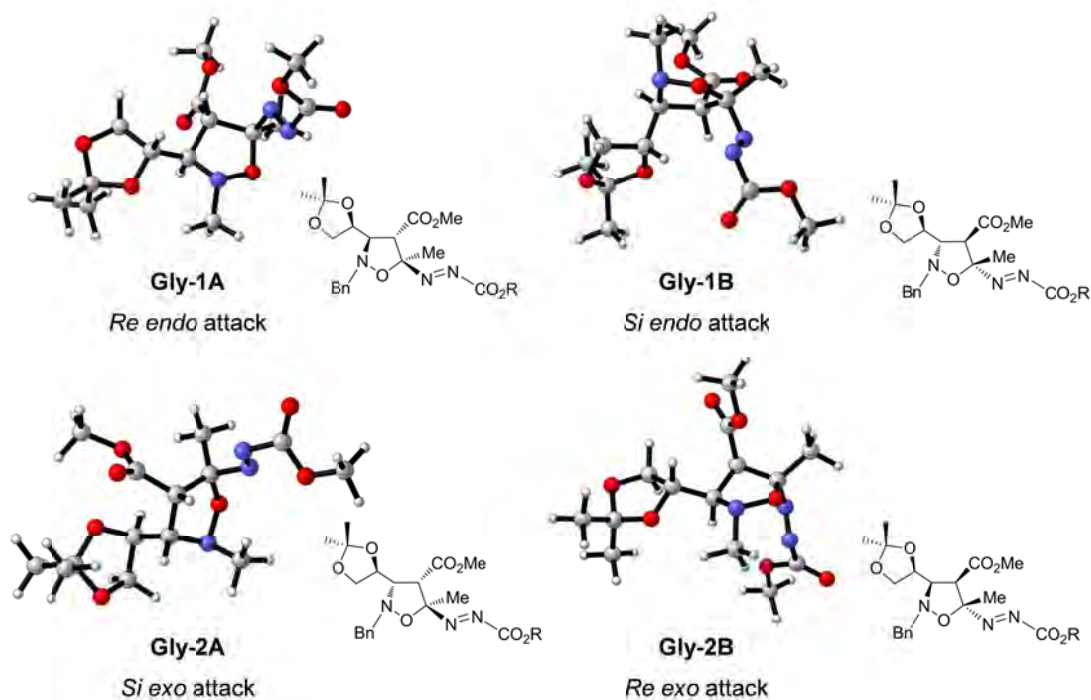


Figure S2. Possible configurations for compounds **13**

In a similar way, compound **14b** showed NOE relationships more in agreement with a *Si* attack. Thus, for isomer 1, NOESY results pointed out isomer **Gal-2A** and not **Gal-1A** (Figure S3) as the more plausible configuration. Following the same trend, for isomer 2 NOESY experiments are more in agreement with configuration of **Gal-1B**.

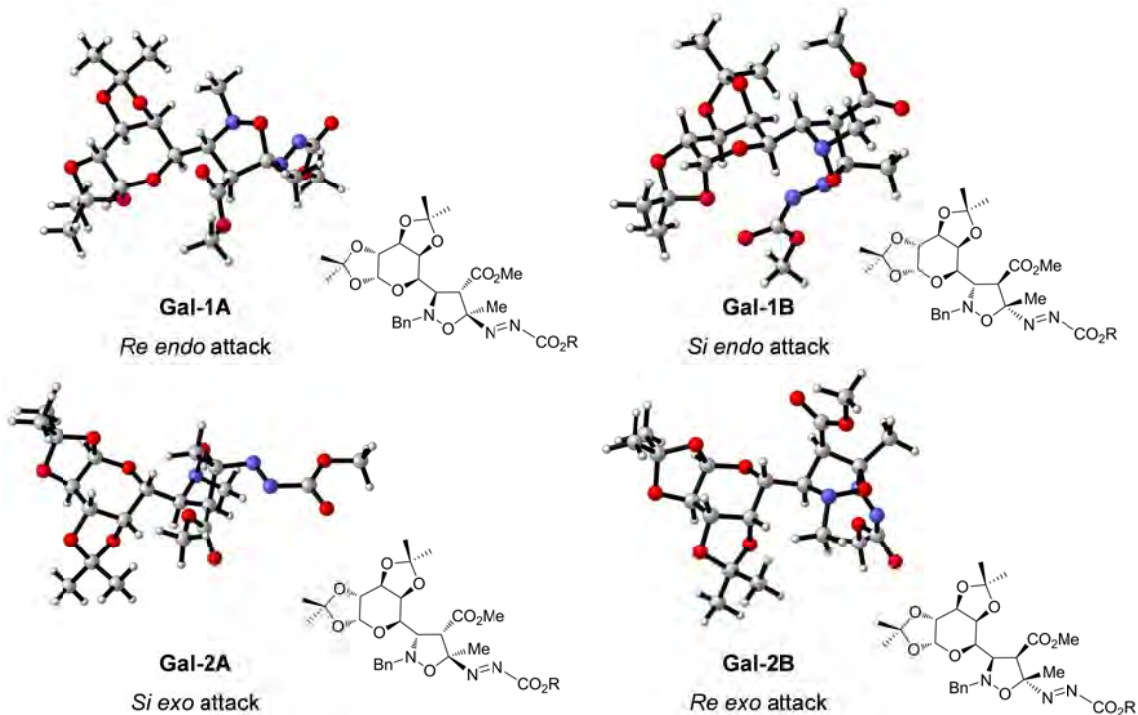


Figure S3. Possible configurations for compound **14b**

Reactivity Indices.

The electronic chemical potential μ , that is the negative of electronegativity χ , is associated with the charge transfer ability of the system in its ground state geometry and is the index pointing to the direction of the electronic flux during the cycloaddition. It can be approximated, using Koopmans' theorem, to the half value of the sum of the one-electron energies of HOMO and LUMO orbitals (Eq. 1).¹

$$\mu = \frac{\varepsilon_{\text{HOMO}} + \varepsilon_{\text{LUMO}}}{2} \quad (1)$$

The chemical hardness η (approximated to be the difference between LUMO and HOMO energies) is a measure of the stability of a system, the system having the maximum hardness being the most stable (Eq. 2).²

$$\eta = \varepsilon_{\text{HOMO}} - \varepsilon_{\text{LUMO}} \quad (2)$$

The chemical softness parameter S is strictly related to the chemical hardness and it is due to the inverse of 2η (Eq. 3).³

$$S = \frac{1}{2\eta} \quad (3)$$

The global electrophilicity power ω is a useful descriptor of reactivity that allows a quantitative classification of the global electrophilic character of a molecule,³ and it is extremely useful for evaluating both Diels-Alder reactions⁴ and 1,3-dipolar cycloaddition reactions.⁵ The ω index measures the stabilization in energy when the

¹ (a) Pearson, R. G. *J. Chem. Ed.* **1987**, *64*, 561–567. (b) Parr, R. G.; von Szentpály, L.; Liu, S. *J. Am. Chem. Soc.* **1999**, *121*, 1922–1924.

² Domingo, L. R.; Aurell, M. J.; Perez, P.; Contreras, R. *Tetrahedron* **2002**, *58*, 4417–4423.

³ Chattaraj, P. K.; Sarkar, U.; Roy, D. R. *Chem. Rev.* **2006**, *106*, 2065–2091.

⁴ (a) Chandra, A. K.; Nguyen, M. T. *J. Phys. Chem. A* **1998**, *102*, 6181–6185. (b) Chandra, A. K.; Nguyen, M. T. *J. Comput. Chem.* **1998**, *19*, 195–202. (c) Nguyen, T. L.; De Proft, F.; Chandra, A. K.; Uchimaru, T.; Nguyen, M. T.; Geerlings, P. *J. Org. Chem.* **2001**, *66*, 6096–6103. (d) Sengupta, D.; Chandra, A. K.; Nguyen, M. T. *J. Org. Chem.* **1997**, *62*, 6404–6406. (e) Damoun, S.; Van de Woude, G.; Mendez, F.; Geerlings, P. *J. Phys. Chem. A* **1997**, *101*, 886–893.

⁵ (a) Parr, R. G.; Pearson, R. G. *J. Am. Chem. Soc.* **1983**, *105*, 7512–7516. (b) Parr, R. G.; Yang, W. In *Density Functional Theory of Atoms and Molecules*; Oxford University, New York, 1989.

system acquires an additional electronic charge ΔN from the environment and it is defined as illustrated in Eq. 4.⁶

$$\omega = \frac{\mu^2}{2\eta} \quad (4)$$

The maximum amount of electronic charge that the electrophile system may accept is given by:

$$\Delta N_{\max} = -\frac{\mu}{\eta} \quad (5)$$

The Fukui function⁷ for electrophilic (f_k^-) and nucleophilic attack (f_k^+) can be expressed as indicated in Eqs. 6 and 7, respectively, where $\rho_k(N)$, $\rho_k(N-1)$ and $\rho_k(N+1)$ are the gross electronic population of the site k in neutral, cationic and anionic systems, respectively.

$$f_k^- = [\rho_k(N) - \rho_k(N-1)] \quad (6)$$

$$f_k^+ = [\rho_k(N+1) - \rho_k(N)] \quad (7)$$

The local electrophilicity index, ω_k condensed to atom k is obtained by projecting the global quantity on the corresponding atomic center k in the molecule by using the electrophilic Fukui function (Eq. 8).⁸

$$\omega_k = \omega f_k^+ \quad (8)$$

⁶ Perez, P.; Domingo, L. R.; Aurell, M. J.; Contreras, R. *Tetrahedron* **2003**, *59*, 3117–3125.

⁷ (a) Fukui, K. *Science* **1982**, *218*, 747-754. (b) Parr, R. G.; Yang, W. *J. Am. Chem. Soc.* **1984**, *106*, 4049-4050.

⁸ Domingo, L. R.; Aurell, M. J.; Perez, P. *J. Phys. Chem. A*, **2002**, *106*, 6871-6875.

Table S1. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the reaction between nitrene **N1** and diazadiene **D1** calculated at 2ζ and single point 3ζ levels

	B3LYP/6-31G(d)/PCM=MeCN				M06-2X/6-31G(d)/PCM=MeCN				PCM=MeCN/M06-2X/6-311+G(d,p) // M06-2X/6-31G(d)/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N1	-400.923426		-400.956252		-400.742372		-400.774806		-400.869673		-400.901815	
D1	-682.943672		-682.987153		-682.657710		-682.700079		-682.867038		-682.907969	
TS1a	-1083.842795	15.3	-1083.897251	29.0	-1083.390158	6.2	-1083.442762	20.2	-1083.720308	10.3	-1083.770573	24.6
TS2a	-1083.841825	15.9	-1083.895257	30.2	-1083.390662	5.9	-1083.441230	21.1	-1083.719563	10.8	-1083.768664	25.8
TS3a	-1083.850390	10.5	-1083.905523	23.8	-1083.395099	3.1	-1083.448508	16.6	-1083.725331	7.1	-1083.776232	21.1
TS4a	-1083.849864	10.8	-1083.903557	25.0	-1083.395455	2.9	-1083.447954	16.9	-1083.724332	7.8	-1083.775225	21.7
P1a	-1083.872659	-3.5	-1083.926630	10.5	-1083.439644	-24.8	-1083.490774	-10.0	-1083.765921	-18.3	-1083.815036	-3.3
P2a	-1083.865895	0.8	-1083.919127	15.2	-1083.435207	-22.0	-1083.485469	-6.6	-1083.760785	-15.1	-1083.808927	0.5
P3a	-1083.866209	0.6	-1083.919294	15.1	-1083.433342	-20.9	-1083.483885	-5.7	-1083.760101	-14.7	-1083.808915	0.6
P4a	-1083.881797	-9.2	-1083.935268	5.1	-1083.449114	-30.8	-1083.500763	-16.2	-1083.774519	-23.7	-1083.823764	-8.8

^a Referred to starting reagents. (**N1+D1**).

Table S2. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the reaction between nitrene **N1** and diazadiene **D2** calculated at 2ζ and single point 3ζ levels

	B3LYP/6-31G(d)/PCM=MeCN				M06-2X/6-31G(d)/PCM=MeCN				PCM=MeCN/M06-2X/6-311+G(d,p) // M06-2X/6-31G(d)/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N1	-400.923426		-400.956252		-400.742372		-400.774806		-400.869673		-400.901815	
D2	-623.794691		-623.836681		-623.533447		-623.575079		-623.730487		-623.770211	
TS1b	-1024.691931	16.4	-1024.744225	30.6	-1024.264948	6.8	-1024.315111	21.8	-1024.583316	10.6	-1024.631802	25.2
TS2b	-1024.690419	17.4	-1024.741931	32.0	-1024.265462	6.5	-1024.314744	22.1	-1024.582483	11.1	-1024.629999	26.4
TS3b	-1024.699049	12.0	-1024.751972	25.7	-1024.268376	4.7	-1024.319074	19.3	-1024.586543	8.5	-1024.635637	22.8
TS4b	-1024.698384	12.4	-1024.750645	26.5	-1024.269354	4.1	-1024.320352	18.5	-1024.586180	8.8	-1024.635334	23.0
P1b	-1024.724060	-3.7	-1024.774688	11.5	-1024.315311	-24.8	-1024.364022	-8.9	-1024.629218	-18.2	-1024.676329	-27.9
P2b	-1024.716485	1.0	-1024.766711	16.5	-1024.310371	-21.7	-1024.358990	-5.7	-1024.623589	-14.7	-1024.670256	-24.1
P3b	-1024.716737	0.9	-1024.767251	16.1	-1024.308198	-20.3	-1024.356525	-4.2	-1024.622776	-14.2	-1024.669388	-23.6
P4b	-1024.732475	-9.0	-1024.784279	5.4	-1024.324522	-30.6	-1024.375131	-15.8	-1024.637493	-23.4	-1024.685152	-33.5

^a Referred to starting reagents. (**N1+D2**).

Table S3. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the reaction between nitrene **N2** and diazadiene **D1** calculated at 2ζ and single point 3ζ levels.

	B3LYP/6-31G(d)/PCM=MeCN				M06-2X/6-31G(d)/PCM=MeCN				PCM=MeCN/M06-2X/6-311+G(d,p) // M06-2X/6-31G(d)/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N2	-554.718674		-554.757060		-554.475492		-554.512230		-554.647854		-554.684204	
D1	-682.943672		-682.987153		-682.657710		-682.700079		-682.867038		-682.907969	
TS5a	-1237.635330	17.0	-1237.694479	31.2	-1237.120121	8.2	-1237.177045	22.1	-1237.496105	11.8	-1237.550930	25.9
TS6a	-1237.637077	15.9	-1237.696405	30.0	-1237.121079	7.6	-1237.178556	21.9	-1237.496174	11.8	-1237.551485	25.5
TS7a	-1237.632438	18.8	-1237.691325	33.2	-1237.117996	9.5	-1237.173991	24.0	-1237.494037	13.1	-1237.547956	27.8
TS8a	-1237.638074	15.2	-1237.696930	29.7	-1237.125234	5.0	-1237.181058	19.6	-1237.499873	9.4	-1237.553896	24.0
P5a	-1237.683058	-13.0	-1237.742054	1.4	-1237.183526	-31.9	-1237.240574	-17.7	-1237.557012	-26.4	-1237.612008	-12.5
P6a	-1237.679757	-10.9	-1237.738278	3.7	-1237.178051	-28.1	-1237.234945	-14.2	-1237.550842	-22.6	-1237.605269	-8.2
P7a	-1237.676125	-8.7	-1237.735242	5.6	-1237.182544	-31.0	-1237.236708	-15.3	-1237.553043	-23.9	-1237.607130	-9.4
P8a	-1237.675015	-8.0	-1237.732215	7.5	-1237.180543	-29.7	-1237.236810	-15.4	-1237.553998	-24.5	-1237.606493	-9.0

^a Referred to starting reagents. (**N2+D1**).

Table S4. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the reaction between nitrene **N2** and diazadiene **D2** calculated at 2ζ and single point 3ζ levels.

	B3LYP/6-31G(d)/PCM=MeCN				M06-2X/6-31G(d)/PCM=MeCN				PCM=MeCN/M06-2X/6-311+G(d,p) // M06-2X/6-31G(d)/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N2	-554.718674		-554.757060		-554.475492		-554.512230		-554.647854		-554.684204	
D2	-623.794691		-623.836681		-623.533447		-623.575079		-623.730487		-623.770211	
TS5b	-1178.486519	16.9	-1178.543988	31.2	-1177.996088	8.1	-1178.051297	22.6	-1178.359736	11.7	-1178.412494	26.3
TS6b	-1178.488091	15.9	-1178.545562	30.2	-1177.996346	7.9	-1178.052047	22.1	-1178.359618	11.8	-1178.412804	26.1
TS7b	-1178.482536	19.4	-1178.538551	34.6	-1177.993644	9.6	-1178.047858	24.8	-1178.358069	12.7	-1178.410559	27.5
TS8b	-1178.488104	15.9	-1178.544308	31.0	-1178.000272	5.4	-1178.054230	20.8	-1178.363188	9.5	-1178.415124	24.7
P5b	-1178.534822	-13.5	-1178.592192	1.0	-1178.059631	-31.8	-1178.114936	-17.3	-1178.420160	-26.2	-1178.473215	-11.8
P6b	-1178.529849	-10.3	-1178.586697	4.4	-1178.053293	-27.8	-1178.107918	-12.9	-1178.413284	-21.9	-1178.465638	-7.0
P7b	-1178.528358	-9.4	-1178.584235	6.0	-1178.057060	-30.2	-1178.111871	-15.4	-1178.416188	-23.8	-1178.468762	-9.0
P8b	-1178.526037	-8.0	-1178.581153	7.9	-1178.058301	-31.0	-1178.110471	-14.5	-1178.417010	-24.3	-1178.467729	-8.4

^a Referred to starting reagents. (**N2+D2**).

Table S5. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the cycloaddition between nitrene **N1** and diazadiene **D1** calculated at 3 ζ levels.

	B3LYP-GD3BJ/6-311G(d,p)/PCM=MeCN				M06-2X/ccpVTZ/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N1	-400.904914		-400.934672		-400.904939		-400.937506	
D1	-682.965426		-683.000565		-682.929675		-682.972361	
C1a^b	-1084.237301	-7.5	-1084.293544	5.5	-1083.839661	-3.2	-1083.892845	10.7
C2a^c	-1084.239702	-9.0	-1084.295394	4.3	-1083.844284	-6.1	-1083.894624	9.6
C3a^d	-1084.238459	-8.2	-1084.294926	4.6	-1083.841989	-4.6	-1083.892823	10.7
C4a^e	-1084.240702	-9.6	-1084.297327	3.1	-1083.843231	-5.4	-1083.895478	9.0
TS1a	-1084.214376	6.9	-1084.269418	20.6	-1083.816437	11.4	-1083.868630	25.9
TS2a	-1084.214085	7.1	-1084.267601	21.8	-1083.815344	12.1	-1083.866330	27.3
TS3a	-1084.221543	2.4	-1084.277393	15.6	-1083.821499	8.2	-1083.874825	22.0
TS4a	-1084.221920	2.2	-1084.275609	16.7	-1083.820846	8.6	-1083.873403	22.9
P1a	-1084.242658	-10.8	-1084.296826	3.4	-1083.862469	-17.5	-1083.913799	-2.5
P2a	-1084.237541	-7.6	-1084.290265	7.5	-1083.857548	-14.4	-1083.908045	1.1
P3a	-1084.238123	-8.0	-1084.290905	7.1	-1083.856966	-14.0	-1083.908021	1.2
P4a	-1084.252623	-17.1	-1084.306508	-2.7	-1083.870862	-22.7	-1083.922089	-7.7

^a Referred to starting reagents. (**N2+D1**). ^b encounter complex previous to the formation of **TS1a**. ^c encounter complex previous to the formation of **TS2a**. ^d encounter complex previous to the formation of **TS3a**. ^e encounter complex previous to the formation of **TS4a**.

Table S6. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the cycloaddition between nitrene **N1** and diazadiene **D2** calculated at 3ζ levels.

	B3LYP-GD3BJ/6-311G(d,p)/PCM=MeCN				M06-2X/ccpVTZ/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N1	-400.904914		-400.934672		-400.904939		-400.937506	
D2	-623.816925		-623.852407		-623.785899		-623.828581	
C1b^b	-1025.074815	-7.5	-1025.127455	6.6	-1024.695859	-3.2	-1024.746127	12.5
C2b^c	-1025.076677	-8.7	-1025.130485	4.7	-1024.698060	-4.5	-1024.750889	9.5
C3b^d	-1025.075676	-8.1	-1025.130731	4.5	-1024.696374	-3.5	-1024.749485	10.4
C4b^e	-1025.077454	-9.2	-1025.129900	5.1	-1024.698597	-4.9	-1024.749139	10.6
TS1b	-1025.050246	7.9	-1025.103789	21.5	-1024.672299	11.6	-1024.722840	27.1
TS2b	-1025.049274	8.5	-1025.100601	23.5	-1024.671414	12.2	-1024.721385	28.1
TS3b	-1025.057147	3.6	-1025.110490	17.3	-1024.677215	8.5	-1024.728752	23.4
TS4b	-1025.057035	3.6	-1025.108983	18.2	-1024.675893	9.4	-1024.726466	24.9
P1b	-1025.080091	-10.8	-1025.131221	4.2	-1024.718428	-17.3	-1024.767394	-0.8
P2b	-1025.073876	-6.9	-1025.124373	8.5	-1024.718119	-17.1	-1024.764285	1.1
P3b	-1025.075403	-7.9	-1025.125581	7.8	-1024.713045	-13.9	-1024.762595	2.2
P4b	-1025.089144	-16.5	-1025.140523	-1.6	-1024.726705	-22.5	-1024.776517	-6.5

^a Referred to starting reagents. (**N2+D1**). ^b encounter complex previous to the formation of **TS1b**. ^c encounter complex previous to the formation of **TS2b**. ^d encounter complex previous to the formation of **TS3b**. ^e encounter complex previous to the formation of **TS4b**.

Table S7. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the cycloaddition between nitrene **N2** and diazadiene **D1** calculated at 3 ζ levels.

	B3LYP-GD3BJ/6-311G(d,p)/PCM=MeCN				M06-2X/ccpVTZ/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N2	-554.910259		-554.948318		-554.697990		-554.734824	
D1	-683.166216		-683.210346		-682.929675		-682.972361	
C5a^b	-1238.086428	-6.2	-1238.146966	7.3	-1237.629267	-1.0	-1237.686327	13.1
C6a^c	-1238.090042	-8.5	-1238.152181	4.1	-1237.632461	-3.0	-1237.686152	13.2
C7a^d	-1238.083672	-4.5	-1238.144146	9.1	-1237.627019	0.4	-1237.683416	14.9
C8a^e	-1238.091284	-9.3	-1238.151301	4.6	-1237.633952	-3.9	-1237.688901	11.5
TS5a	-1238.064334	7.6	-1238.124586	21.4	-1237.606874	13.0	-1237.664292	26.9
TS6a	-1238.066261	6.4	-1238.125416	20.9	-1237.603210	15.3	-1237.657486	31.2
TS7a	-1238.062661	8.7	-1238.122407	22.8	-1237.605148	14.1	-1237.661424	28.7
TS8a	-1238.068069	5.3	-1238.126109	20.4	-1237.611109	10.4	-1237.668002	24.6
P5a	-1238.107085	-19.2	-1238.166620	-5.0	-1237.668530	-25.6	-1237.726429	-12.1
P6a	-1238.105566	-18.3	-1238.165084	-4.0	-1237.666256	-24.2	-1237.723389	-10.2
P7a	-1238.103861	-17.2	-1238.163319	-2.9	-1237.664200	-22.9	-1237.721230	-8.8
P8a	-1238.104642	-17.7	-1238.159470	-0.5	-1237.664662	-23.2	-1237.719691	-7.8

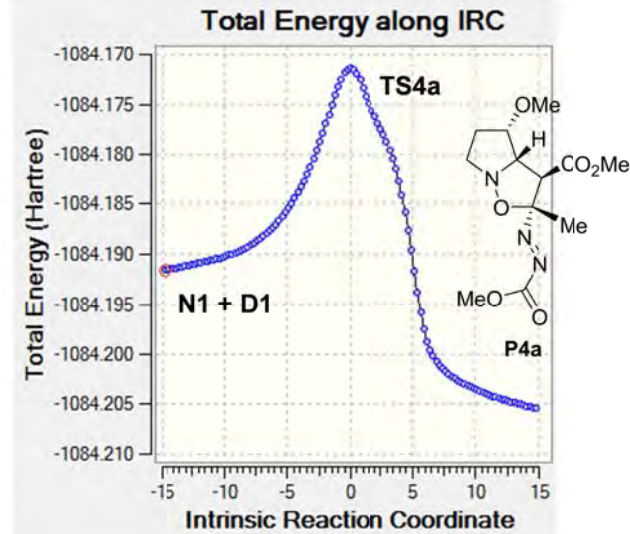
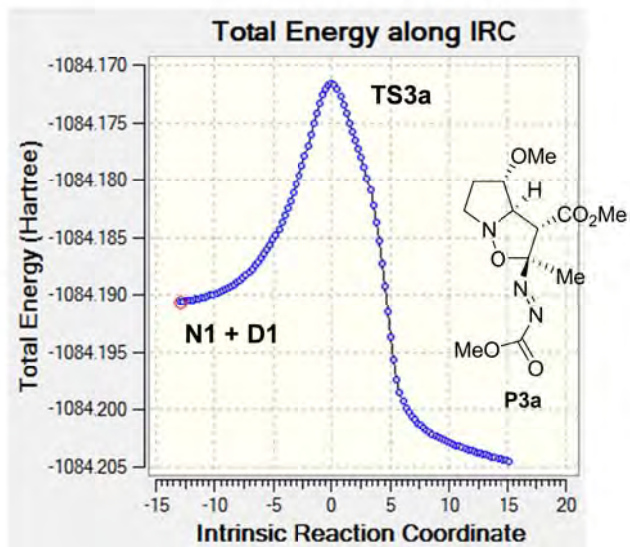
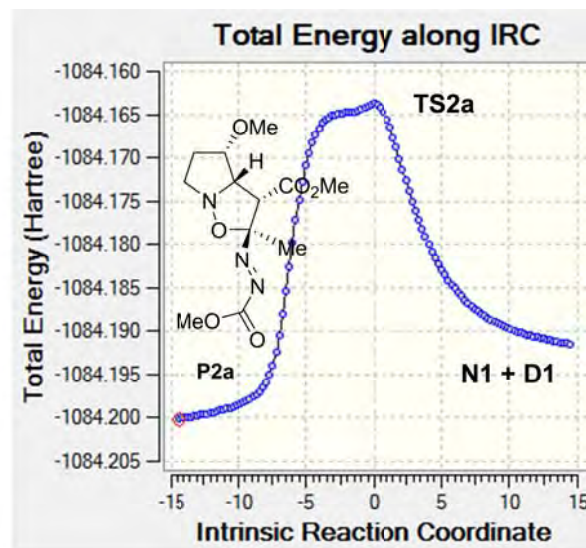
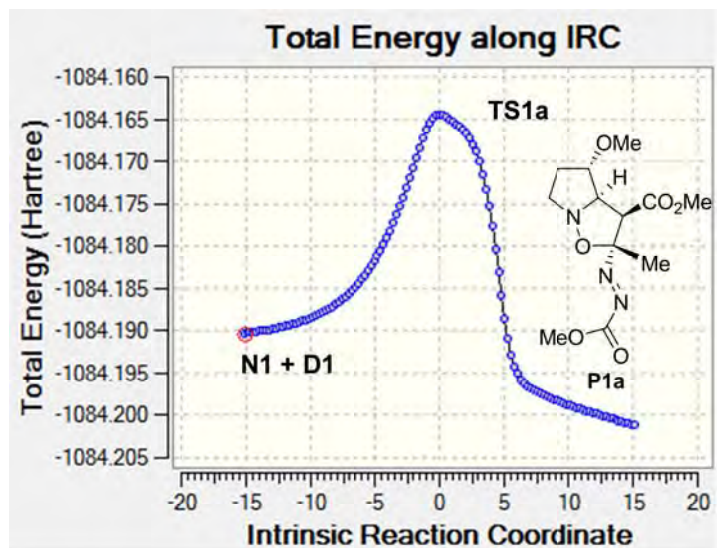
^a Referred to starting reagents. (**N2+D1**). ^b encounter complex previous to the formation of **TS5a**. ^c encounter complex previous to the formation of **TS6a**. ^d encounter complex previous to the formation of **TS7a**. ^e encounter complex previous to the formation of **TS8a**.

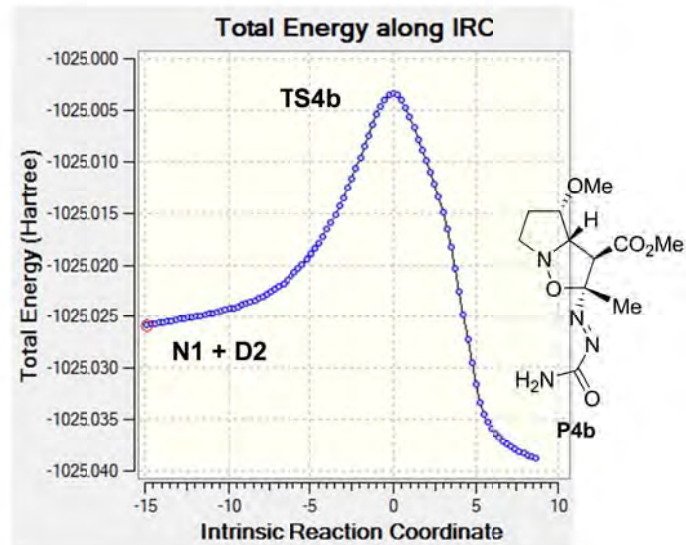
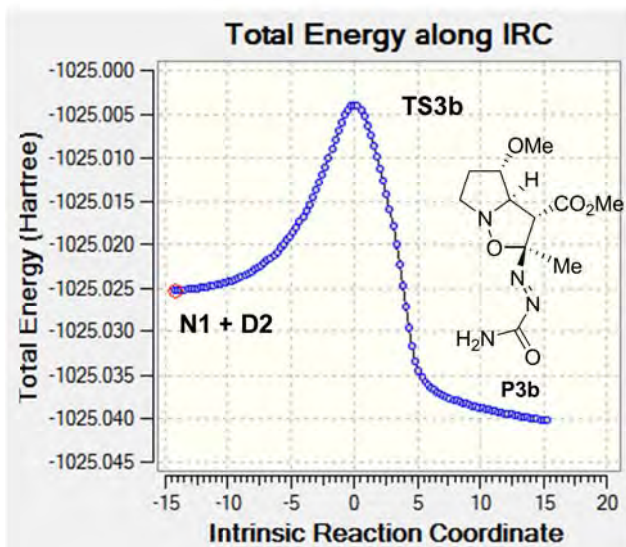
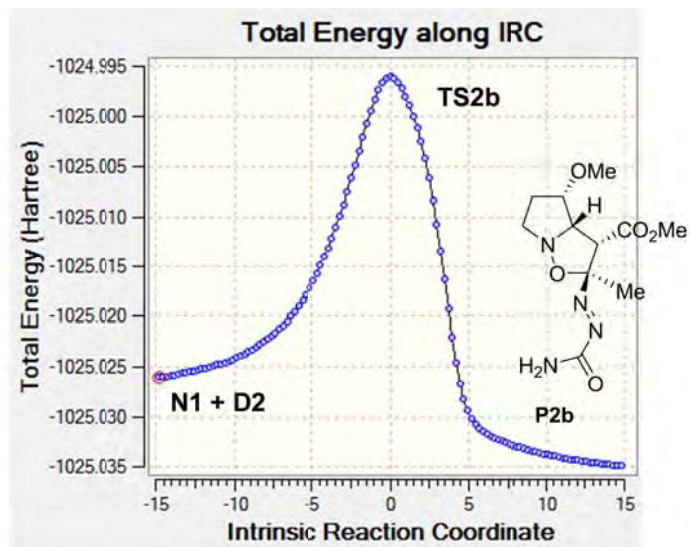
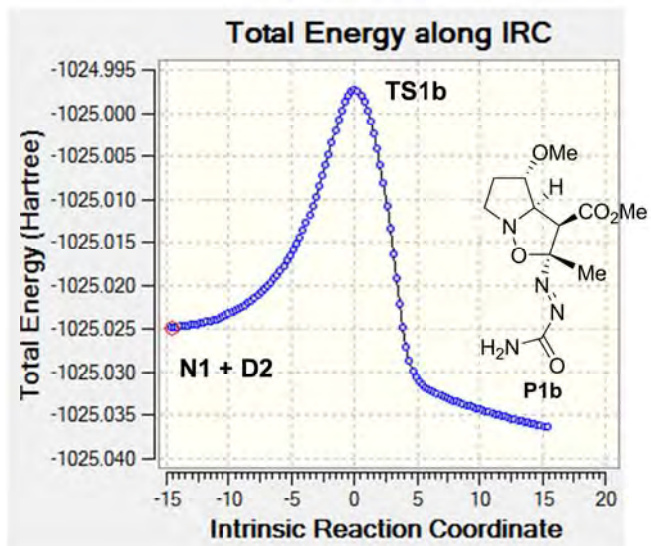
Table S8. Absolute (ΔE and ΔG , hartrees) and relative ($\Delta\Delta E$ and $\Delta\Delta G$, kcal/mol) electronic (E) and free (G) energies for the cycloaddition between nitrene **N2** and diazadiene **D2** calculated at 3 ζ levels.

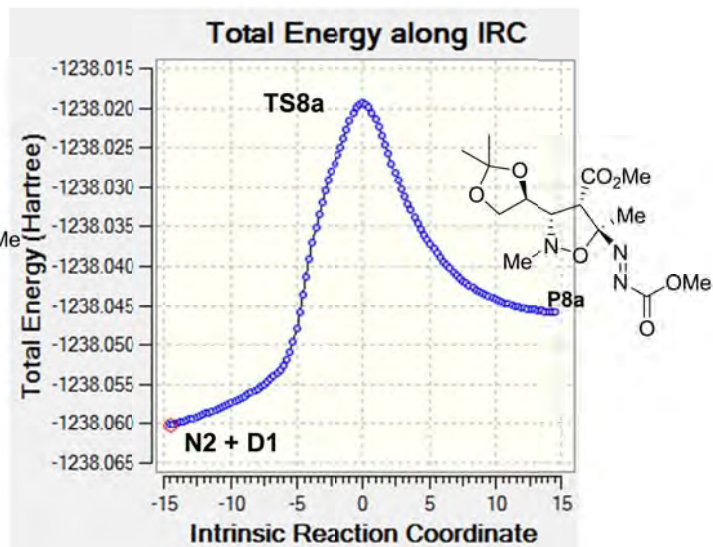
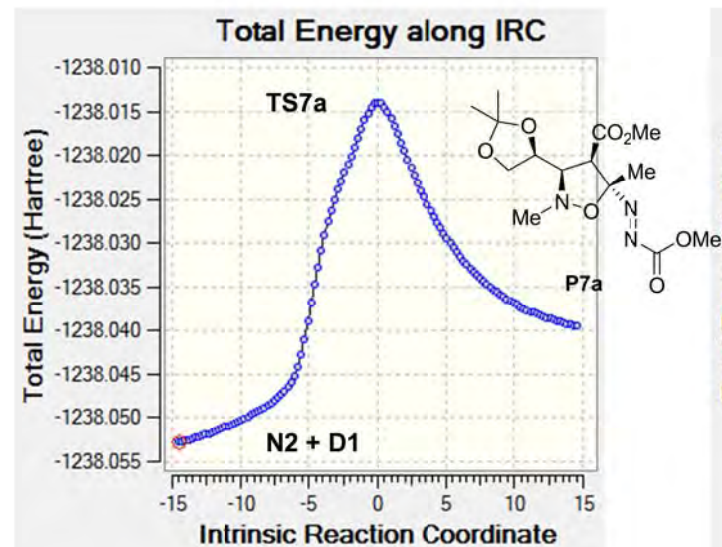
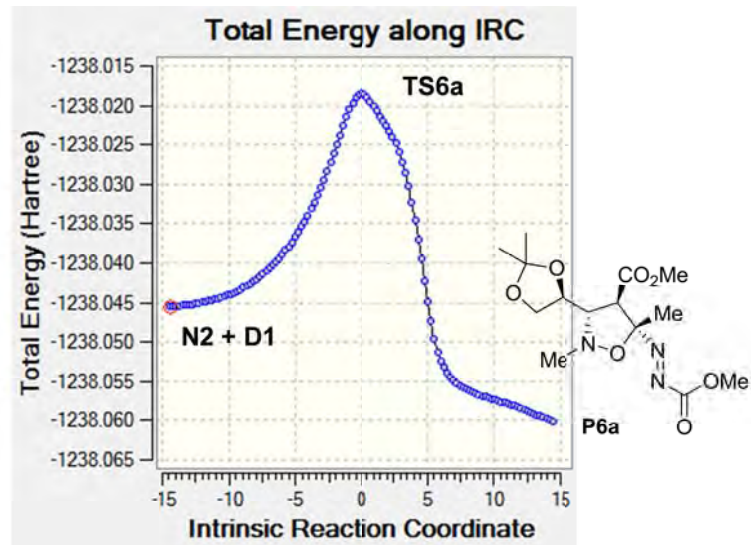
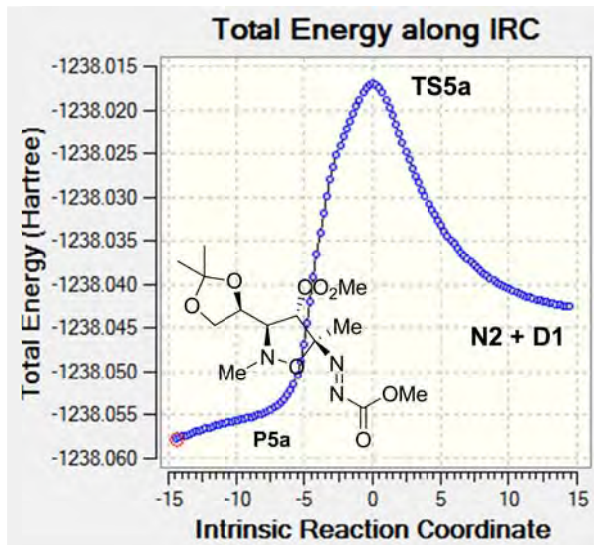
	B3LYP-GD3BJ/6-311G(d,p)/PCM=MeCN				M06-2X/ccpVTZ/PCM=MeCN			
	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$	ΔE	$\Delta\Delta E^a$	ΔG	$\Delta\Delta G^a$
N2	-554.910259		-554.948318		-554.697990		-554.734824	
D2	623.816925		-623.852407		-623.785899		-623.828581	
C5b^b	-1178.924454	-6.6	-1178.985012	5.9	-1178.485478	-1.0	-1178.541928	13.5
C6b^c	-1178.927452	-8.5	-1178.987226	4.5	-1178.488718	-3.0	-1178.545108	11.5
C7b^d	-1178.921413	-4.7	-1178.980877	8.5	-1178.483755	0.1	-1178.539856	14.8
C8b^e	-1178.928370	-9.1	-1178.986791	4.8	-1178.490201	-4.0	-1178.543609	12.4
TS5b	-1178.902118	7.4	-1178.959222	22.1	-1178.463018	13.1	-1178.517506	28.8
TS6b	-1178.903658	6.4	-1178.958722	22.4	-1178.463071	13.1	-1178.518166	28.4
TS7b	-1178.899959	8.8	-1178.954215	25.2	-1178.460901	14.4	-1178.514804	30.5
TS8b	-1178.905423	5.3	-1178.962195	20.2	-1178.466678	10.8	-1178.520479	26.9
P5b	-1178.944204	-19.0	-1178.999793	-3.4	-1178.523738	-25.0	-1178.579236	-9.9
P6b	-1178.942322	-17.8	-1178.998877	-2.8	-1178.521806	-23.8	-1178.577129	-8.6
P7b	-1178.940892	-16.9	-1178.995031	-0.4	-1178.519943	-22.6	-1178.574930	-7.2
P8b	-1178.941824	-17.5	-1178.994088	0.2	-1178.521224	-23.4	-1178.574580	-7.0

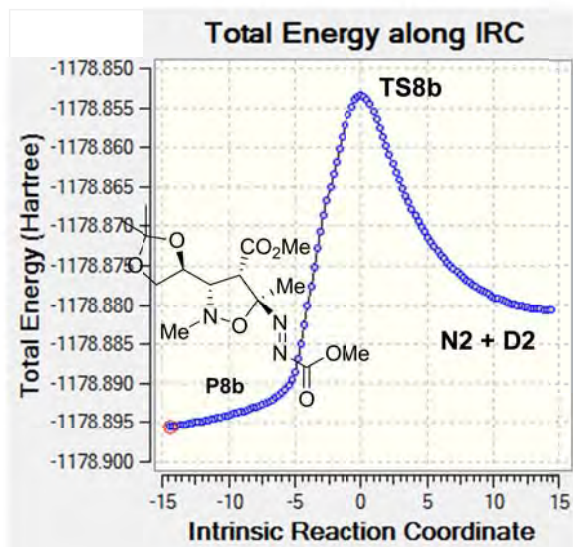
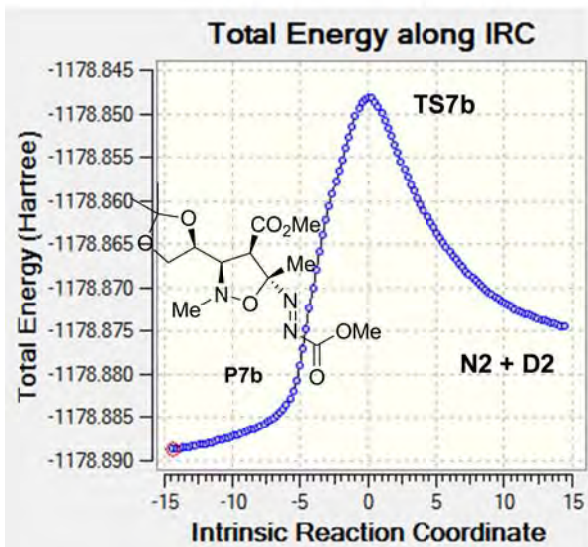
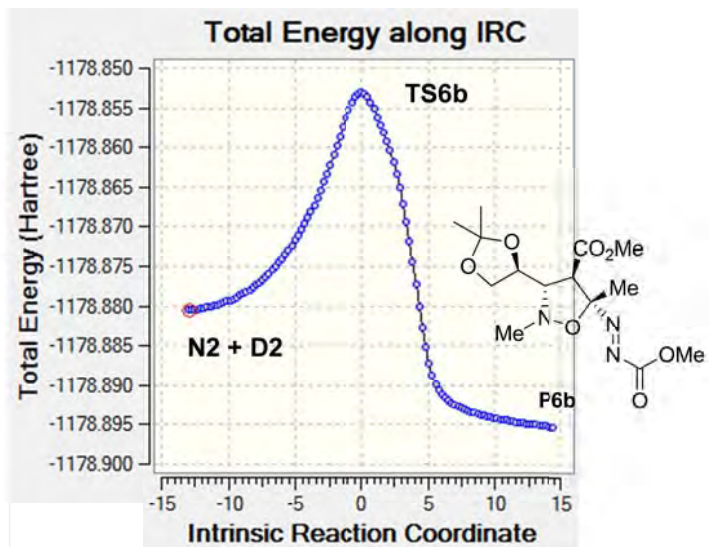
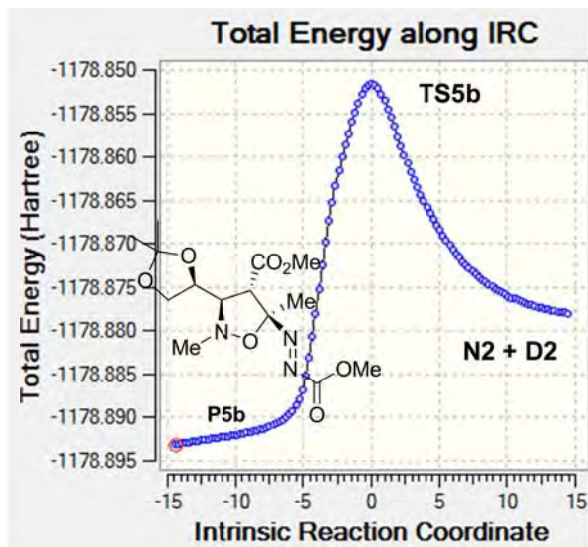
^a Referred to starting reagents. (**N2+D1**). ^b encounter complex previous to the formation of **TS5b**. ^c encounter complex previous to the formation of **TS6b**. ^d encounter complex previous to the formation of **TS7b**. ^e encounter complex previous to the formation of **TS8b**.

IRC Analyses









Calculations of the cycloaddition reaction between nitrone **9a** and DDs **D1** and **D2**

In order to evaluate the validity of the model we have calculated the stationary points corresponding to the reaction of the real nitrone **9a** with diazadienes **D1** and **D2**. Due to the increased size of the molecule we performed the calculations at the 3 ζ level B3LYP-GD3BJ/6-311G(d,p)/PCM=MeCN. The relative and absolute energy values are collected in Table S9 and the geometry of the transition structures in Figures S4 and S5.

Table S9. Absolute (ΔG , hartrees) and relative ($\Delta\Delta G$, kcal/mol) free energies for the cycloaddition between nitrone **9a** and diazadienes **D1** and **D2** calculated at B3LYP-GD3BJ/6-311G(d,p)/PCM=MeCN levels of theory.

	ΔG	$\Delta\Delta G^a$		ΔG	$\Delta\Delta G^b$
9a	-632.150612		9a	-632.150612	
D1	-683.210346		D2	-624.046052	
TS1a-OBn	-1315.360958	23.2	TS1b-OBn	-1256.163734	20.7
TS2a-OBn	-1315.337006	19.0	TS2b-OBn	-1256.159964	23.0
TS3a-OBn	-1315.330711	14.2	TS3b-OBn	-1256.174237	14.1
TS4a-OBn	-1315.323990	15.0	TS4b-OBn	-1256.170298	16.5
P1a-OBn	-1315.338356	5.2	P1b-OBn	-1256.189760	4.3
P2a-OBn	-1315.350610	5.4	P2b-OBn	-1256.184335	7.7
P3a-OBn	-1315.352697	6.5	P3b-OBn	-1256.185697	6.9
P4a-OBn	-1315.352325	-1.5	P4b-OBn	-1256.200062	-2.1

^aReferred to starting materials (**9a+D1**). ^bReferred to starting materials (**9a+D2**).

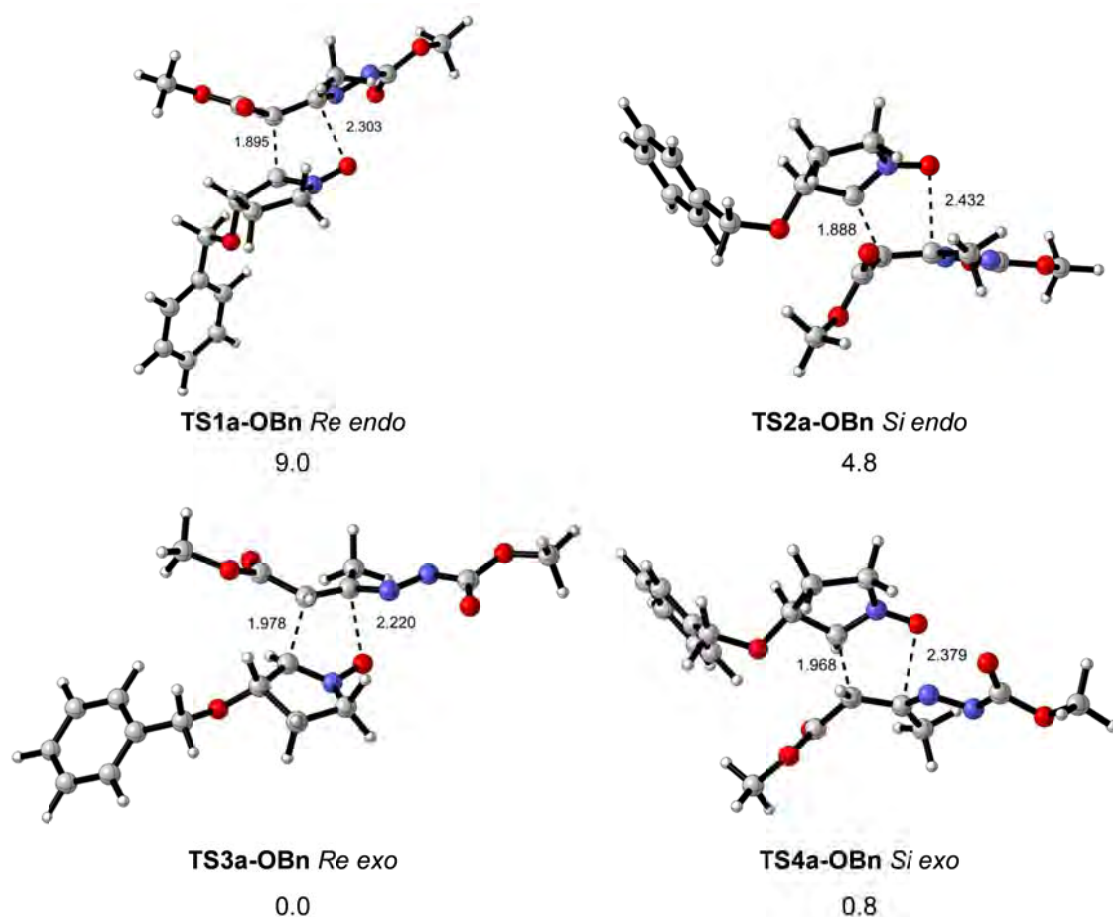


Figure S4. Transition structures (PCM=MeCN/ B3LYP-GD3BJ/6-311G(d,p)) corresponding to the reaction between **9a** and **D1**. **TS1a-OBn**, **TS2a-OBn**, **TS3a-OBn** and **TS4a-OBn** correspond to *Re endo*, *Si endo*, *Re exo* and *Si exo* approaches leading to **P1a-OBn**, **P2a-OBn**, **P3a-OBn** and **P4a-OBn**. Relative energy values between TSs referenced to isolated reagents are calculated at PCM=MeCN/ B3LYP-GD3BJ/6-311G(d,p) level on theory and given in kcal/mol. Bond distances are given in Å.

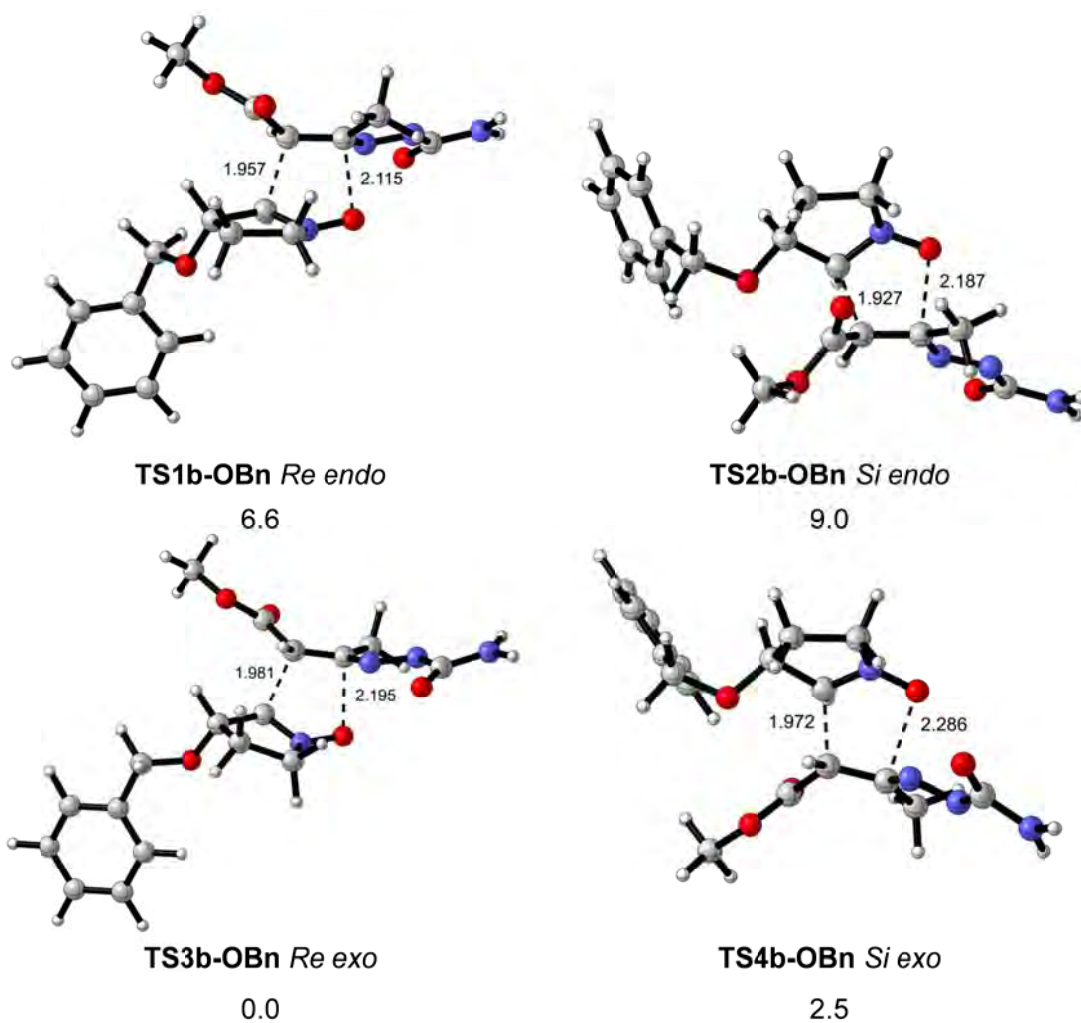


Figure S5. Transition structures (PCM=MeCN/ B3LYP-GD3BJ/6-311G(d,p)) corresponding to the reaction between **9a** and **D2**. **TS1b-OBn**, **TS2b-OBn**, **TS3b-OBn** and **TS4b-OBn** correspond to *Re endo*, *Si endo*, *Re exo* and *Si exo* approaches leading to **P1b-OBn**, **P2b-OBn**, **P3b-OBn** and **P4b-OBn**. Relative energy values between TSs referenced to isolated reagents are calculated at PCM=MeCN/ B3LYP-GD3BJ/6-311G(d,p) level on theory and given in kcal/mol. Bond distances are given in Å.

Cartesian Coordinates

N1

C	-1.30747400	1.19423100	-0.00025200
C	-0.55217000	-0.98347700	0.20388400
C	0.67371000	-0.15546200	0.41542700
C	0.21768800	1.25615800	-0.03260800
H	-1.81412800	1.63500300	-0.85904300
H	-1.74708200	1.59249900	0.91699500
H	-0.63056900	-2.06070200	0.26111700
H	0.61508600	2.05469500	0.59470400
N	-1.60725200	-0.26356900	-0.01624800
O	-2.80319400	-0.64045100	-0.18787800
H	0.96842900	-0.16113500	1.47783500
H	0.57070600	1.40252000	-1.05743000
C	2.96318700	-0.04579600	-0.06683700
H	3.72899000	-0.54666800	-0.66056500
H	2.94336700	1.01879100	-0.33436900
H	3.21279700	-0.13672300	0.99915400
O	1.73238500	-0.67795200	-0.35491500

N2

O	-2.59519500	-1.17300200	0.10566900
N	-2.40560000	0.08250300	-0.08288100
C	-3.57146000	0.94165000	0.16204600
C	-1.26785900	0.56386700	-0.46145600
C	-0.15112600	-0.40081900	-0.70553900
O	1.03852300	0.28343400	-1.05565900
C	0.23009200	-1.22734400	0.55423700
O	1.63511500	-1.06540100	0.64062800
C	1.94262600	0.17884700	0.04450800
C	3.35455600	0.12786100	-0.49545900
C	1.71970400	1.32763300	1.02282600
H	-3.32358900	1.98565800	-0.02168400

H	-3.87421700	0.78684100	1.19762100
H	-4.36525000	0.60490300	-0.50473700
H	-1.16110400	1.62937800	-0.61805800
H	-0.42898400	-1.06783300	-1.53125900
H	-0.27612100	-0.84709000	1.44936200
H	0.00751500	-2.28804300	0.44278000
H	3.44803900	-0.71358200	-1.18527000
H	3.58602900	1.05641000	-1.02284300
H	4.06411900	0.00378200	0.32614100
H	1.90111100	2.28315900	0.52407300
H	0.69242000	1.32482200	1.40067200
H	2.40248700	1.23366400	1.87128000

D1

O	-2.59519500	-1.17300200	0.10566900
N	-2.40560000	0.08250300	-0.08288100
C	-3.57146000	0.94165000	0.16204600
C	-1.26785900	0.56386700	-0.46145600
C	-0.15112600	-0.40081900	-0.70553900
O	1.03852300	0.28343400	-1.05565900
C	0.23009200	-1.22734400	0.55423700
O	1.63511500	-1.06540100	0.64062800
C	1.94262600	0.17884700	0.04450800
C	3.35455600	0.12786100	-0.49545900
C	1.71970400	1.32763300	1.02282600
H	-3.32358900	1.98565800	-0.02168400
H	-3.87421700	0.78684100	1.19762100
H	-4.36525000	0.60490300	-0.50473700
H	-1.16110400	1.62937800	-0.61805800
H	-0.42898400	-1.06783300	-1.53125900
H	-0.27612100	-0.84709000	1.44936200
H	0.00751500	-2.28804300	0.44278000
H	3.44803900	-0.71358200	-1.18527000
H	3.58602900	1.05641000	-1.02284300

H	4.06411900	0.00378200	0.32614100
H	1.90111100	2.28315900	0.52407300
H	0.69242000	1.32482200	1.40067200
H	2.40248700	1.23366400	1.87128000

D2

C	-0.00384100	0.40319700	0.00002000
C	1.07289400	-0.40059400	0.00001300
C	-0.04943100	1.89681300	0.00005800
H	-0.59993700	2.24759200	-0.87800900
H	0.95487000	2.31171600	0.00008100
H	-0.59995800	2.24754800	0.87812900
H	0.90986700	-1.47283400	-0.00001900
C	2.48890100	0.04313400	0.00004200
O	2.89929800	1.18351700	0.00009800
O	3.29548000	-1.02473400	-0.00000400
N	-1.22618800	-0.34579000	-0.00001800
N	-2.24022600	0.36816800	-0.00001600
C	-3.46881500	-0.45036100	-0.00005900
O	-3.49636700	-1.66187300	-0.00008900
N	-4.52497700	0.37691500	-0.00006100
H	-5.46168200	0.00031400	-0.00008600
H	-4.39170000	1.37735100	-0.00003100
C	4.69651100	-0.73486400	0.00001300
H	4.96303300	-0.16275100	0.89073600
H	5.19762200	-1.70057200	-0.00004300
H	4.96303300	-0.16264900	-0.89064500

TS1a

C	-1.84571600	-0.65815600	2.16979400
C	-1.30476300	-1.11143900	-0.06465500
C	-2.81583400	-1.04373700	-0.07110800
C	-3.17195000	-0.73818100	1.40481000
H	-1.79766200	-1.29026400	3.05746600

H	-1.57384300	0.36665600	2.43340600
H	-0.72543500	-1.62516400	-0.82289100
H	-3.72472000	0.19779900	1.48849500
C	-0.35290700	0.73627200	-0.49862000
H	-0.13385700	0.48025700	-1.52933000
C	0.74509000	0.68341400	0.39242300
N	-0.85546400	-1.14591500	1.19142500
O	0.40134000	-0.97615800	1.39616600
H	-3.16267000	-0.25605800	-0.75513300
H	-3.80140400	-1.55196000	1.76915500
C	-1.47925200	1.67243800	-0.32835800
O	-1.91177500	2.11450600	0.72000400
O	-2.05287500	1.94685700	-1.51271700
C	-3.20532800	2.79303500	-1.45347200
H	-2.93798600	3.76970800	-1.04571600
H	-3.55372400	2.88907600	-2.47983700
H	-3.97735600	2.33978900	-0.82721100
C	0.98139600	1.62216900	1.54465700
H	1.56833500	1.13179600	2.32148800
H	1.55021600	2.49042600	1.19247400
H	0.03523600	1.96843700	1.95533900
N	1.87502300	0.11039700	-0.27206900
N	2.95851000	0.31962500	0.30242400
C	4.04448600	-0.33092900	-0.41003800
O	3.94815000	-1.20316600	-1.23333300
C	-3.40625600	-2.48390600	-1.84179100
H	-2.39065100	-2.53918200	-2.25410800
H	-3.90952000	-3.43545500	-2.01756900
H	-3.95201500	-1.68202800	-2.35584400
O	-3.39847900	-2.27338600	-0.44297600
O	5.17918700	0.19130900	0.03532900
C	6.36659900	-0.34639700	-0.55910600
H	6.36111000	-0.16618400	-1.63563400
H	7.19497600	0.17574500	-0.08582300

H 6.42670700 -1.41934200 -0.36818000

TS2a

C 1.72077500 -2.06405600 1.31856700
C 1.11485400 -1.21791800 -0.79036500
C 2.61725900 -1.32986700 -0.86199800
C 3.02821600 -1.74454500 0.57768400
H 1.65375000 -3.09474000 1.67140400
H 1.51777500 -1.38119600 2.14678200
H 0.48741200 -1.23599800 -1.67334900
H 3.52225100 -0.89231300 1.04880100
C 0.36055100 0.64730500 -0.20907800
H 0.11993200 0.97680800 -1.21413300
C -0.74750900 0.25028600 0.57970700
N 0.67762800 -1.85775600 0.29614700
O -0.55494700 -1.72689400 0.62367500
H 3.71030900 -2.59543700 0.57246000
C 1.52370900 1.33435300 0.39630300
O 2.05895300 1.04031400 1.44861800
O 1.94063200 2.34966700 -0.36985300
C 3.15787000 2.96324900 0.05198000
H 3.03370200 3.43245000 1.03014200
H 3.39088800 3.71254000 -0.70266400
H 3.95031100 2.21264300 0.10826000
C -0.89395800 0.49668900 2.05691000
H -1.55693200 -0.24546100 2.50177500
H -1.33819100 1.48534400 2.22197800
H 0.07892300 0.46381800 2.54443200
N -1.91876700 0.16603400 -0.23010200
N -2.98432900 0.16737700 0.41478600
C -4.11857100 0.02253800 -0.47647200
O -4.10498200 -0.41576400 -1.59735900
H 2.89056100 -2.10830200 -1.59099900
C 4.53476200 -0.18783100 -1.57808800

H	4.84690700	0.79158300	-1.94334900
H	5.12009200	-0.44156700	-0.68503200
H	4.72334500	-0.94280800	-2.35276000
O	3.15394000	-0.10004400	-1.28613800
O	-5.19701300	0.42699600	0.18215200
C	-6.42466200	0.33071600	-0.54937000
H	-7.19517600	0.70997300	0.11804000
H	-6.36923700	0.93349200	-1.45760800
H	-6.62079000	-0.71013800	-0.81342900

TS3a

C	-0.34234900	-2.35303200	0.18530400
C	-1.66480800	-0.53148200	0.78048900
C	-2.51615700	-1.29112700	-0.20170600
C	-1.72811100	-2.61649000	-0.40592300
H	0.09644300	-3.19373500	0.72331200
H	0.38541700	-1.97223700	-0.54239800
H	-2.06748600	0.18727000	1.48681600
H	-1.67630100	-2.92335700	-1.45074200
C	-0.48103900	0.91296900	-0.22920500
C	0.68864100	0.91597800	0.55283100
N	-0.60288500	-1.25612900	1.13521200
O	0.36237500	-0.69119700	1.75113000
H	-0.40786900	0.40763600	-1.18832800
H	-2.24234600	-3.39437800	0.16565100
C	-1.49305800	1.98727300	-0.17716200
O	-1.67890000	2.77052800	0.73086500
O	-2.26157000	1.95426700	-1.27960000
C	-3.32527600	2.91027400	-1.31253000
H	-3.82879900	2.75834000	-2.26509900
H	-2.92549500	3.92388800	-1.24768200
H	-4.01363100	2.73866800	-0.48244800
C	0.98577000	1.88593300	1.65485100
H	1.35031400	2.83347200	1.24350300

H	1.75775500	1.47422900	2.30609700
H	0.08065600	2.08343400	2.22632000
N	1.74041200	0.23489500	-0.11434000
N	2.88666100	0.50388600	0.30143100
C	3.87150900	-0.27712300	-0.41138200
O	3.67602700	-1.28531100	-1.04142500
H	-2.59881800	-0.72177400	-1.13989400
C	-4.71024900	-2.00535100	-0.59465400
H	-4.40807600	-3.00582900	-0.93004900
H	-5.67951300	-2.07333700	-0.09959700
H	-4.79284700	-1.34818800	-1.47078200
O	-3.79789700	-1.47568800	0.34771100
O	5.05577900	0.29070900	-0.21596100
C	6.15781500	-0.38000300	-0.83758100
H	6.01640000	-0.41194900	-1.91950900
H	7.03973700	0.20309700	-0.58234600
H	6.24249600	-1.39720100	-0.45070200

TS4a

C	-0.13621000	-2.57404600	0.44391400
C	-1.55637100	-0.82208000	1.10585800
C	-2.43160600	-1.70074000	0.25267200
C	-1.41387700	-2.66862900	-0.40731500
H	0.06779900	-3.46943800	1.03430800
H	0.76222100	-2.30067400	-0.11902300
H	-1.94206200	-0.13452300	1.85189000
H	-1.22059000	-2.30756700	-1.42162900
C	-0.71243900	0.64761400	-0.03078500
C	0.52046900	0.88017000	0.60890100
N	-0.40931800	-1.45452600	1.36563400
O	0.53716000	-0.82118800	1.91988400
H	-0.64890400	0.13923600	-0.98885800
H	-1.78958300	-3.69008200	-0.47132800
C	-1.82248800	1.64093400	0.04724900

O	-2.29858600	2.09049600	1.06906700
O	-2.24906800	1.97715800	-1.17201900
C	-3.38180300	2.85023800	-1.20296500
H	-3.59468300	3.02106600	-2.25625700
H	-3.15262100	3.79117600	-0.69954600
H	-4.23194600	2.37207000	-0.71149900
C	0.76507600	1.92393700	1.65399500
H	1.13106900	2.84869700	1.19360600
H	1.52823900	1.57488200	2.35192300
H	-0.15767500	2.13745400	2.19298900
N	1.58519400	0.28139500	-0.08101000
N	2.72613000	0.69987900	0.23524400
C	3.73442200	-0.02729600	-0.48352100
O	3.61259700	-1.09743000	-1.02853300
H	-3.15165300	-2.24573000	0.88240400
C	-4.11001700	-1.60048000	-1.38502700
H	-4.59694200	-0.88452800	-2.04805700
H	-3.66141200	-2.40049400	-1.98723500
H	-4.85502200	-2.03888000	-0.70845900
O	-3.12750100	-0.88699100	-0.65886600
O	4.86735300	0.66778800	-0.41424300
C	5.98808100	0.06434300	-1.06730300
H	5.77691200	-0.07260600	-2.12968700
H	6.81775900	0.75396000	-0.92711300
H	6.20999600	-0.90370500	-0.61386500

TS1b

C	-1.42717400	-0.70576000	2.17900300
C	-1.00572400	-1.11420800	-0.08889200
C	-2.51186800	-1.00325600	-0.02216800
C	-2.79018900	-0.73609100	1.47753100
H	-1.35054800	-1.36577000	3.04423800
H	-1.12114700	0.30476000	2.45896600
H	-0.47205200	-1.61004300	-0.89088100

H	-3.31839800	0.20752800	1.61612100
C	-0.00654500	0.74164100	-0.52418200
H	0.15663200	0.50536600	-1.56966500
C	1.12042300	0.61646600	0.31990000
N	-0.49652200	-1.18356800	1.13916600
O	0.77484300	-1.04086300	1.28602600
H	-2.86416200	-0.18277700	-0.66363700
H	-3.41807200	-1.54842800	1.84783400
C	-1.10390600	1.68728200	-0.26918800
O	-1.47652800	2.10651000	0.81203100
O	-1.73671300	2.00507300	-1.41404900
C	-2.86949200	2.86557300	-1.26751800
H	-2.56292100	3.83013800	-0.85814700
H	-3.27891200	2.98835100	-2.26822400
H	-3.60931500	2.41207500	-0.60377900
C	1.43375100	1.51363700	1.48711300
H	2.06864800	0.99452200	2.20511300
H	1.97985300	2.39467100	1.13062600
H	0.51648900	1.84471600	1.96966300
N	2.21053400	0.03853600	-0.41769300
N	3.31943100	0.20228900	0.11135200
C	4.38537400	-0.43352300	-0.68156100
O	4.22710800	-0.99585200	-1.74491500
N	5.54930700	-0.27595200	-0.03055100
H	6.40095000	-0.65444100	-0.41843500
H	5.57767100	0.20529500	0.85602000
C	-3.23868800	-2.35669400	-1.80965300
H	-2.24854100	-2.41479400	-2.27952800
H	-3.77120600	-3.29062800	-1.99381300
H	-3.79463100	-1.52470000	-2.26143300
O	-3.14938000	-2.20178900	-0.40650000

TS2b

C	1.27781300	-2.11828800	1.26781700
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C	0.78832100	-1.20281200	-0.84052800
C	2.28882100	-1.34697100	-0.84792800
C	2.62395100	-1.79904500	0.59973500
H	1.17586300	-3.16037700	1.57649400
H	1.05040500	-1.46433200	2.11268900
H	0.19696200	-1.16716600	-1.74731900
H	3.10245900	-0.96230200	1.11284100
C	0.03274600	0.68707600	-0.22506500
H	-0.15967100	1.04911300	-1.22909900
C	-1.10733200	0.26845400	0.50180700
N	0.28688100	-1.85094500	0.20853500
O	-0.95665000	-1.68726600	0.48986200
H	3.29656400	-2.65741400	0.60948300
C	1.18807600	1.31730400	0.44446800
O	1.66738100	0.98289700	1.51278100
O	1.67712800	2.33317700	-0.27984700
C	2.89581600	2.88967800	0.20924600
H	2.74556000	3.34677700	1.18962900
H	3.19416000	3.64219500	-0.51900000
H	3.65549200	2.10789700	0.28792500
C	-1.30925200	0.47026900	1.97979700
H	-2.00827500	-0.26863400	2.37131800
H	-1.73552500	1.46423900	2.15937300
H	-0.35799200	0.39700800	2.50412400
N	-2.25421100	0.24969100	-0.35857800
N	-3.33930900	0.25103200	0.24293700
H	2.57913300	-2.11598700	-1.58070300
C	4.26136900	-0.23099600	-1.44473200
H	4.61045900	0.74782800	-1.77676900
H	4.79605600	-0.51120100	-0.52801600
H	4.47446200	-0.97673400	-2.22218900
O	2.86969400	-0.12039500	-1.22077500
C	-4.46885800	0.20447100	-0.69899200
O	-4.37557500	0.20879400	-1.90898100

N	-5.61001400	0.16190700	0.00872600
H	-6.49882200	0.11797700	-0.46763400
H	-5.58537500	0.15681900	1.01745700

TS3b

C	-0.10417700	-2.35851600	0.14607900
C	-1.36328600	-0.47143900	0.74897700
C	-2.25624100	-1.21661600	-0.20267700
C	-1.29207200	-2.26049600	-0.82358400
H	-0.07537000	-3.28361600	0.72503800
H	0.86750600	-2.19552900	-0.32935500
H	-1.73042500	0.24281800	1.47885500
H	-0.95102400	-1.91855600	-1.80292000
C	-0.16714400	0.95758900	-0.26645300
C	1.03243100	0.88488700	0.46719000
N	-0.31870600	-1.22990000	1.07415000
O	0.66638800	-0.69139800	1.68584200
H	-0.15676800	0.47553500	-1.23987500
H	-1.79843300	-3.21792100	-0.95759400
C	-1.11576300	2.08217000	-0.14720000
O	-1.24876100	2.82430500	0.80423400
O	-1.89510100	2.15604300	-1.24046400
C	-2.89631600	3.17659400	-1.20933100
H	-3.41808500	3.10722700	-2.16178800
H	-2.43348800	4.15869100	-1.09642100
H	-3.58656300	3.00526300	-0.38068000
C	1.44517200	1.83665800	1.54803200
H	1.84994600	2.75799700	1.11502300
H	2.22219000	1.37651600	2.15997800
H	0.58509500	2.09230200	2.16425800
N	2.00811400	0.12920900	-0.24234000
N	3.18705500	0.33565300	0.09736900
C	4.09782400	-0.53400000	-0.64895700
O	3.76145600	-1.50586200	-1.29718800

N	5.35833400	-0.10107300	-0.47420500
H	6.12470100	-0.58688400	-0.91609800
H	5.54624300	0.71076700	0.09489400
H	-2.67508900	-0.54060200	-0.96098800
C	-4.36984800	-2.24789600	-0.24640600
H	-4.04920600	-3.02079500	-0.95653700
H	-5.11520800	-2.67194400	0.42741100
H	-4.81673000	-1.41662900	-0.80747700
O	-3.29602500	-1.79627200	0.55575500

TS4b

C	0.22322300	-2.53551600	0.46288800
C	-1.19518400	-0.79856200	1.15059100
C	-2.09478500	-1.71446600	0.36709800
C	-1.08967000	-2.66859400	-0.32860300
H	0.46246900	-3.41384500	1.06556600
H	1.09069900	-2.26774300	-0.14835900
H	-1.55034300	-0.07399300	1.87611300
H	-0.95032400	-2.31276000	-1.35370700
C	-0.39144800	0.67826700	-0.09474500
C	0.87747100	0.87275800	0.48091600
N	-0.02539600	-1.39418300	1.36564600
O	0.94323000	-0.70368100	1.82565900
H	-0.40276800	0.14628400	-1.04150400
H	-1.44520800	-3.69869500	-0.36640900
C	-1.47991100	1.67666000	0.05356500
O	-1.84586100	2.18067300	1.09696600
O	-2.04658600	1.95160900	-1.12649700
C	-3.17430800	2.82832600	-1.07174300
H	-3.51926200	2.93177500	-2.09874800
H	-2.88489900	3.79919100	-0.66493100
H	-3.95688000	2.39226100	-0.44673900
C	1.22105400	1.95619600	1.45656800
H	1.54280300	2.85947600	0.92609600

H	2.04474400	1.63110700	2.09430600
H	0.35202600	2.19510500	2.06835500
N	1.89175400	0.24030300	-0.28117600
N	3.04704300	0.65943500	-0.07127100
C	4.01966500	-0.09516600	-0.85752600
O	3.79749200	-1.14712600	-1.42583200
N	5.20250400	0.54458700	-0.82429800
H	5.99704200	0.16267400	-1.31535400
H	5.30074300	1.41095800	-0.31655900
H	-2.76362900	-2.26461600	1.04758800
C	-3.85647700	-1.69348900	-1.18251100
H	-4.41141300	-1.00105100	-1.81667400
H	-3.41266500	-2.47729400	-1.80930300
H	-4.54279200	-2.15939700	-0.46321400
O	-2.86320800	-0.93758900	-0.51752300

TS5a

C	-0.03045400	-1.47440400	-0.55706600
C	1.18072000	-1.50337800	0.16210700
C	-0.94808700	-2.62295300	-0.68457800
O	-1.02933900	-3.58513100	0.05383600
O	-1.76517800	-2.44951600	-1.73739200
C	-2.74755800	-3.47189900	-1.92638200
H	-0.04890200	-0.79599300	-1.40231600
H	-3.40336000	-3.53190500	-1.05533800
H	-2.26472700	-4.43835100	-2.08204900
H	-3.31162000	-3.17965900	-2.80975200
C	-1.24089600	-0.25157300	0.73813100
O	-1.56445100	2.10619200	0.84062500
C	-1.49472900	1.22636600	-1.32554700
C	-2.54657900	2.72984200	0.01186500
O	-2.10053500	2.50186900	-1.31162200
C	-2.53128300	4.21932500	0.27955500
C	-3.91447400	2.09950600	0.24669100

C	-0.91676200	1.07882100	0.09979200
O	0.69542700	-0.46959700	1.81324300
N	-0.58270000	-0.63008500	1.83501900
C	-1.07974100	-1.70668000	2.69454800
H	-2.28351000	-0.56388800	0.70304500
H	-2.22125200	0.43148700	-1.54844200
H	-0.72391600	1.22563600	-2.09834400
H	-3.23869700	4.72389600	-0.38309300
H	-1.52666000	4.60867100	0.10182000
H	-2.81793300	4.41483500	1.31560800
H	-4.66621000	2.59686500	-0.37172200
H	-4.19515500	2.19959300	1.29803500
H	-3.90539200	1.03602100	-0.00963900
H	0.16227600	1.24856900	0.13234400
H	-0.64344000	-1.56282700	3.68217300
H	-0.77296200	-2.66938900	2.27919600
H	-2.16640200	-1.64897200	2.75056000
C	1.79626200	-2.71222400	0.81104100
H	1.02633100	-3.42529100	1.09858400
H	2.47176400	-3.19640300	0.09614200
H	2.38431400	-2.42255200	1.68202600
C	4.04038400	0.53071500	-0.36680400
O	5.14699800	0.33498700	-0.80052400
O	3.47437000	1.71535200	-0.18443600
C	4.28740500	2.83574500	-0.56300600
H	3.70243700	3.71849000	-0.31572400
H	5.22376900	2.82206200	-0.00264100
H	4.49899700	2.79828300	-1.63277700
N	2.03988400	-0.45061600	-0.28857700
N	3.21948200	-0.56010900	0.09075600

TS6a

C	1.28997900	0.52795500	1.07067600
O	0.25183200	2.10115800	-0.37978700

C	-0.27611600	2.39154400	1.81135200
C	-0.68775900	3.17226200	-0.32241000
O	-1.06348700	3.29275200	1.05300800
C	-1.92849500	2.82655100	-1.12959100
C	0.01079900	4.43444000	-0.78824400
C	0.04085200	1.31183300	0.77865200
O	0.18841600	-1.24606900	1.82559200
N	1.20528800	-0.46678500	1.96265300
C	2.39869100	-1.06860500	2.55918900
H	2.21969200	1.09388900	1.07416200
H	0.64408800	2.87140300	2.17278000
H	-0.86010200	2.02662800	2.65823400
H	-2.69524400	3.59178300	-0.98362400
H	-2.32525900	1.85976100	-0.80427300
H	-1.68081400	2.77120600	-2.19284700
H	-0.68185900	5.27887500	-0.75041800
H	0.36483800	4.31307400	-1.81528700
H	0.86455200	4.63954700	-0.13721400
H	-0.81318200	0.63841300	0.65065400
H	2.10673400	-1.49079800	3.52019100
H	3.15834300	-0.30058700	2.70117300
H	2.77201300	-1.85221900	1.89606300
C	1.23521500	-0.73714400	-0.60337000
C	0.41529400	-1.78489300	-0.13353600
C	2.67888900	-0.89536600	-0.88497900
O	3.43666000	-1.71401100	-0.40166400
O	3.09051000	0.04561600	-1.74846400
C	4.48635600	0.02459000	-2.05839700
H	4.76236200	-0.93399600	-2.50196100
H	5.07748800	0.18782400	-1.15475700
H	4.64329200	0.83341700	-2.76920600
C	-3.10234500	-2.06668200	-0.50673900
O	-3.86987400	-2.85726200	-0.99471300
O	-3.40768300	-0.83722300	-0.10978500

C	-4.77589300	-0.46025800	-0.31716300
H	-5.43747300	-1.15781000	0.19951000
H	-4.87051000	0.54052600	0.09843600
H	-5.00522000	-0.45886200	-1.38407700
N	-0.95130100	-1.48794100	-0.41362000
N	-1.73672300	-2.43809700	-0.23685100
H	0.74323400	0.00768600	-1.21970600
C	0.82121200	-3.21782900	0.07131500
H	0.62086900	-3.78217300	-0.84731100
H	1.88315000	-3.28807100	0.29697200
H	0.23710000	-3.66982200	0.87320300

TS7a

C	-0.41662200	1.01642300	0.72540100
C	-1.22576900	0.79583600	-0.40748300
C	0.53208400	2.13559800	0.91185900
O	1.00372800	2.42669800	1.99241600
O	0.82530900	2.81128200	-0.20999200
C	1.62906400	3.98271700	-0.03003200
H	-0.85967400	0.72594600	1.67346100
H	1.76759100	4.39897400	-1.02556000
H	2.59225100	3.72891100	0.41723100
H	1.11144800	4.69421500	0.61622300
C	0.88501200	-0.72163500	0.64745600
O	2.66736500	-1.36876300	-0.79991600
C	3.07993800	0.56921200	0.44468700
C	4.00613600	-1.36541300	-0.30345800
O	4.28190000	-0.00702300	-0.02261000
C	4.93141800	-1.82967500	-1.40742000
C	4.10528400	-2.22038800	0.95418300
C	1.97795500	-0.23714500	-0.28262900
O	-0.61953200	-1.06627200	-0.95602400
N	-0.09381200	-1.47209900	0.14359100
C	-0.95222800	-2.29602700	0.99308000

H	1.17742000	-0.98033900	1.66302400
H	2.98881400	0.48839600	1.53602500
H	3.08277700	1.62335400	0.16871600
H	5.96868700	-1.78699400	-1.06644200
H	4.80826100	-1.18167600	-2.27771600
H	4.69397700	-2.85948500	-1.68451600
H	5.13214400	-2.21678300	1.32879500
H	3.81173600	-3.24870100	0.72913000
H	3.44774700	-1.83746100	1.74017500
H	1.55084800	0.31084000	-1.12486400
H	-1.25550900	-3.16681000	0.41182600
H	-1.83605600	-1.70691900	1.25773300
H	-0.40072800	-2.60698600	1.87910000
C	-4.65728200	-0.11870200	-0.39577400
O	-5.70116700	0.36235400	-0.76010700
O	-4.53359300	-1.18997400	0.37944500
C	-5.77271000	-1.77437800	0.80106600
H	-6.36216000	-2.06928900	-0.06874200
H	-5.49988500	-2.64417600	1.39447100
H	-6.33890100	-1.05987200	1.40113100
N	-3.40475100	0.42003900	-0.85268300
N	-2.49393500	0.27956100	-0.01136400
C	-1.09218000	1.43857900	-1.75577300
H	-1.54685000	2.43477000	-1.74999900
H	-0.04632000	1.54186400	-2.03691000
H	-1.61281400	0.82929400	-2.49577100

TS8a

C	0.65059000	-0.95300500	-0.79874900
O	2.84332100	-0.18471400	-0.38160200
C	2.41143700	-2.22743400	0.51943200
C	4.02628300	-0.59036700	0.30492800
O	3.70320000	-1.83043200	0.94104100
C	4.38558400	0.41859700	1.38217900

C	5.11767900	-0.79431200	-0.72749800
C	1.76149800	-0.87905500	0.21086900
O	-0.92394500	-1.40143100	0.69989600
N	-0.45009200	-1.63425300	-0.47361100
C	-1.42256200	-2.04627200	-1.48339400
H	0.96538700	-1.01656000	-1.83751800
H	2.45650600	-2.85342900	-0.38214700
H	1.91781300	-2.77178100	1.32613200
H	5.21023800	0.03737700	1.99021200
H	3.51975100	0.59946100	2.02481100
H	4.69015700	1.36506900	0.92717800
H	6.04121000	-1.11010400	-0.23579600
H	5.30580600	0.13832000	-1.26642000
H	4.80672200	-1.56285900	-1.43983800
H	1.44066700	-0.39540100	1.14016100
H	-1.92181400	-2.94246400	-1.11523200
H	-0.91102800	-2.25613600	-2.42168100
H	-2.15595800	-1.24063500	-1.59732100
C	-0.30709900	0.93366200	-0.50052000
C	-1.17516700	0.64060500	0.56864800
C	0.88680100	1.79839800	-0.35057100
O	1.38052100	2.17980900	0.68990100
O	1.38410300	2.10989800	-1.55694800
C	2.60675500	2.84706300	-1.53625100
H	-0.76351500	0.97524400	-1.48513400
H	3.37610500	2.26383000	-1.02550800
H	2.46993800	3.80238900	-1.02560900
H	2.87355700	3.00811400	-2.57936000
C	-0.94100100	0.96508800	2.01320700
H	0.11764600	0.91412300	2.25688100
H	-1.29196900	1.98047500	2.22937700
H	-1.50686000	0.27237800	2.63811900
C	-4.70777100	0.34517500	0.46721900
O	-5.65461500	0.91180400	0.95382100

O	-4.76779300	-0.54435300	-0.51761100
C	-6.08653600	-0.80368400	-1.01562400
H	-5.96547700	-1.56353700	-1.78442900
H	-6.72597700	-1.16782600	-0.20948100
H	-6.51346800	0.10787800	-1.43733000
N	-2.50675800	0.45453600	0.10642600
N	-3.38496700	0.54609900	0.98985700

TS5b

C	-0.67497000	1.15682900	-0.55414100
C	-1.81257000	0.69243500	0.13462100
C	-0.28564600	2.57596500	-0.65218700
O	-0.59292700	3.47740300	0.10331400
O	0.53611300	2.76092200	-1.69990800
C	1.03346500	4.09195000	-1.86194600
H	-0.37145900	0.55368600	-1.40191700
H	1.61156100	4.38953300	-0.98473200
H	0.20778800	4.79160800	-2.00449100
H	1.66755900	4.06475400	-2.74579700
C	0.89816800	0.50423100	0.78099600
O	2.17298900	-1.50185100	0.87075400
C	1.73877100	-0.72917400	-1.29300000
C	3.31556200	-1.68364000	0.03228800
O	2.80477400	-1.65449500	-1.28694400
C	3.89637800	-3.05590600	0.29699900
C	4.32077900	-0.56053000	0.25839000
C	1.15570700	-0.83482100	0.13305800
O	-0.99639300	-0.08824000	1.78839600
N	0.10914900	0.57102400	1.85355200
C	0.10922100	1.73817900	2.73828500
H	1.72886300	1.20851600	0.78075600
H	2.08335300	0.29212800	-1.51137800
H	1.02987700	-1.03469100	-2.06493100
H	4.73729900	-3.24110900	-0.37575200

H	3.12590800	-3.81188700	0.13185100
H	4.25039000	-3.11837900	1.32880000
H	5.20353100	-0.71817900	-0.36684500
H	4.62665700	-0.54077700	1.30731500
H	3.88690800	0.41150300	0.00559800
H	0.24416300	-1.43637800	0.16780600
H	-0.25863200	1.40958300	3.70945300
H	-0.54652000	2.50567300	2.32138400
H	1.12543600	2.12020800	2.82982600
C	-2.86883400	1.55089700	0.77496800
H	-2.44901700	2.50244600	1.09448200
H	-3.66078200	1.74656200	0.04279500
H	-3.31890200	1.03477000	1.62311500
C	-3.64672000	-2.31287300	-0.53078500
O	-4.73808000	-2.76733700	-0.24791700
N	-2.19060000	-0.59685100	-0.35844100
N	-3.32217000	-0.97489700	-0.01669600
N	-2.70496000	-2.92161700	-1.26765600
H	-1.83457600	-2.45266100	-1.47437900
H	-2.89699800	-3.83300500	-1.65512700

TS6b

C	-0.81747000	0.69503600	1.07129000
O	-1.91413600	-0.80238600	-0.41370300
C	-1.95924700	-1.44806500	1.78707900
C	-2.83630000	-1.89261900	-0.27140800
O	-2.58457700	-2.45065000	1.01094500
C	-2.54371100	-2.95305600	-1.31415000
C	-4.24736500	-1.33442500	-0.35524100
C	-1.09176600	-0.74673900	0.73983000
O	1.24906600	0.33530100	1.80395100
N	0.14003700	0.97339300	1.96110500
C	0.24115400	2.28844900	2.59622400
H	-1.68936600	1.34619300	1.09185100

H	-2.69324300	-0.75454500	2.22095800
H	-1.38366300	-1.92007500	2.58418500
H	-3.20409000	-3.81218000	-1.17035700
H	-1.50490900	-3.28014700	-1.21873800
H	-2.70439900	-2.54698500	-2.31583500
H	-4.97653900	-2.14345900	-0.26393300
H	-4.39411300	-0.83137500	-1.31447000
H	-4.41179500	-0.61094100	0.44821000
H	-0.15516000	-1.29192800	0.58285600
H	0.72583800	2.15036100	3.56222800
H	-0.75734000	2.70258200	2.73249300
H	0.83831100	2.94543600	1.96036200
C	0.38264900	1.15355400	-0.60730600
C	1.66839200	0.82597000	-0.13090800
C	-0.06639400	2.53891900	-0.85941100
O	0.34757900	3.55280200	-0.33111400
O	-1.07212000	2.54901500	-1.74831400
C	-1.63228600	3.83493500	-2.02548500
H	-0.87056700	4.50223500	-2.43310800
H	-2.04453500	4.27268100	-1.11393800
H	-2.41958100	3.66302700	-2.75678300
C	3.42962700	-2.25097800	-0.61885800
O	4.56189500	-2.66603800	-0.46287400
N	1.98637800	-0.52676400	-0.45535900
N	3.17805600	-0.84096600	-0.29779000
N	2.38225700	-2.96855400	-1.05597400
H	2.52214600	-3.93362600	-1.31395700
H	1.48147800	-2.53053200	-1.18620200
H	-0.09544300	0.41009700	-1.23624000
C	2.79917500	1.78812100	0.11103300
H	3.42875800	1.83112500	-0.78544400
H	2.41800000	2.78623600	0.31694400
H	3.42271200	1.44710300	0.93778100

TS7b

C	-0.75522500	0.88801800	0.72362800
C	-1.55904900	0.51824400	-0.37196900
C	0.08951800	2.09674900	0.81507900
O	0.55073500	2.50172900	1.86350500
O	0.29996500	2.72153500	-0.35459300
C	0.98826300	3.97434500	-0.26757200
H	-1.14417700	0.61515900	1.70039500
H	1.07445900	4.33327700	-1.29100900
H	1.97647900	3.84548200	0.17850800
H	0.41103400	4.67483900	0.33892700
C	0.72171900	-0.74077300	0.70570400
O	2.52497300	-1.29466400	-0.74819700
C	2.75972600	0.75798000	0.35005300
C	3.86827900	-1.11541900	-0.29847000
O	4.00363800	0.28079400	-0.11920800
C	4.80866800	-1.55658300	-1.39915600
C	4.09216700	-1.86443700	1.00972700
C	1.73186800	-0.20682800	-0.28674000
O	-0.80069300	-1.30557100	-0.81939800
N	-0.20325400	-1.59703100	0.28126800
C	-0.95357500	-2.43923900	1.20965800
H	1.06908400	-0.91223600	1.72228300
H	2.70585700	0.74199300	1.44685500
H	2.64139600	1.78508400	0.00626200
H	5.84397600	-1.37885600	-1.09811600
H	4.59220000	-0.99002900	-2.30722500
H	4.67710800	-2.62305600	-1.59658200
H	5.12401900	-1.73168600	1.34501600
H	3.89827900	-2.93016800	0.86564800
H	3.42331300	-1.49436500	1.79239000
H	1.22906400	0.23420700	-1.14970600
H	-1.25687800	-3.33603700	0.67035400
H	-1.84275800	-1.88769900	1.53120100

H	-0.32592100	-2.70091200	2.06011600
C	-4.93564100	-0.66473100	-0.21499300
O	-5.83919600	-0.88522300	-0.99901800
N	-3.71250700	-0.06268700	-0.74697400
N	-2.78484300	-0.05855800	0.08209300
C	-1.50499100	1.08072200	-1.76138000
H	-2.04589000	2.03154800	-1.80781400
H	-0.47705800	1.25722400	-2.07044800
H	-1.98181300	0.38101900	-2.44875400
N	-4.96576000	-0.90976600	1.10552500
H	-4.16351600	-0.70575300	1.68338700
H	-5.78943600	-1.32982500	1.50878000

TS8b

C	0.45292700	-0.91269900	-0.93585400
O	2.58564500	-0.08684800	-0.35682600
C	2.22969900	-2.23223200	0.30840400
C	3.76626400	-0.50960700	0.32430300
O	3.48428100	-1.82207000	0.81903100
C	4.04681000	0.39430200	1.51211600
C	4.89592600	-0.55613300	-0.68607300
C	1.52205400	-0.89070600	0.11884700
O	-1.15997500	-1.57192500	0.44249000
N	-0.62909900	-1.66145100	-0.72824000
C	-1.53982100	-1.99924800	-1.81875400
H	0.80459100	-0.84892300	-1.96270300
H	2.33707800	-2.75426500	-0.65231600
H	1.73839200	-2.88386700	1.03292000
H	4.88349900	-0.00355700	2.09252600
H	3.16189800	0.44982000	2.15154000
H	4.30054800	1.40104400	1.16976400
H	5.81922300	-0.87772800	-0.19770200
H	5.05364000	0.43454200	-1.12137800
H	4.64553700	-1.26057200	-1.48355500

H	1.14572200	-0.52299600	1.07936500
H	-2.07179100	-2.90671800	-1.53536000
H	-0.97369300	-2.16023100	-2.73513300
H	-2.25532200	-1.17810500	-1.93638800
C	-0.61969700	0.90594900	-0.45858300
C	-1.50523900	0.44164300	0.53110100
C	0.52781000	1.78977000	-0.15616000
O	0.97017900	2.05455300	0.94249900
O	1.05032600	2.27583400	-1.29297400
C	2.23081900	3.06096200	-1.12654100
H	-1.04044600	1.04246800	-1.45040200
H	3.01400300	2.45056500	-0.67139200
H	2.02822000	3.92900800	-0.49596900
H	2.52116800	3.37620800	-2.12725200
C	-1.33455300	0.59615700	2.01235400
H	-0.28477100	0.54099000	2.29011900
H	-1.72216400	1.56904000	2.33434300
H	-1.90213200	-0.18112700	2.52577900
C	-5.05151200	0.06694000	0.24556300
O	-5.98304000	-0.19725000	0.98226400
N	-2.82173600	0.28570600	0.00659700
N	-3.73113700	0.22657000	0.85486600
N	-5.13095800	0.24579200	-1.08382000
H	-4.30047000	0.43591900	-1.62533700
H	-6.02048000	0.12323000	-1.54349400

Pla

C	-2.64661300	-1.99320900	0.47447200
C	-1.62893200	-0.32043100	-0.92440000
C	-2.91861300	0.24251500	-0.31670600
C	-3.12639300	-0.61307700	0.93555700
H	-3.47978300	-2.56538700	0.05741000
H	-2.17500400	-2.59561400	1.25315600
H	-1.64806700	-0.15994300	-2.00393000

H	-2.51722300	-0.20618700	1.74633500
C	-0.26626300	0.18409300	-0.36674300
H	0.38206800	0.39949500	-1.21696600
C	0.32154300	-1.05152300	0.35170100
N	-1.66770600	-1.77319600	-0.62680300
O	-0.35468400	-2.15194300	-0.25023800
H	-2.85003500	1.31694000	-0.09758800
H	-4.16818000	-0.62073500	1.26434600
C	-0.33930500	1.44624000	0.46287300
O	-0.83547600	1.53630900	1.56413100
O	0.18648500	2.48112600	-0.19263400
C	0.13388300	3.73717300	0.49534400
H	0.70639300	3.68005200	1.42284900
H	0.57439800	4.46313400	-0.18438200
H	-0.90132800	3.99854100	0.72182300
C	0.26781200	-1.12106000	1.87625900
H	0.70704400	-2.07293900	2.18627900
H	0.83192300	-0.29781500	2.31826000
H	-0.75983500	-1.07218300	2.23272900
N	1.73817200	-1.27743100	-0.00314500
N	2.41245500	-0.25306100	0.12353200
C	3.82217500	-0.51639300	-0.15386400
O	4.38648900	-1.55890900	0.03555100
C	-5.12976300	0.69599100	-1.00967300
H	-5.80852500	0.49462100	-1.83987500
H	-5.59672600	0.35091600	-0.07892300
H	-4.95850700	1.77857800	-0.93623900
O	-3.92518600	0.01314600	-1.28548300
O	4.35798400	0.60567300	-0.59829300
C	5.75693300	0.52400300	-0.91118000
H	5.92149300	-0.22942300	-1.68291000
H	6.03507100	1.51218100	-1.26916800
H	6.32071000	0.26244200	-0.01441700

P2a

C	1.30510900	-1.64233800	1.99737400
C	0.50279100	-1.08458500	-0.20674500
C	1.60757200	-2.15517100	-0.34284900
C	2.37099800	-2.10554200	0.98918300
H	1.00857100	-2.44084400	2.68158600
H	1.64426300	-0.78243700	2.57663400
H	-0.34106200	-1.36361100	-0.84698400
H	3.18800300	-1.38552500	0.95157800
C	0.68541500	0.43482500	-0.42123200
H	0.43030400	0.72594700	-1.44118800
C	-0.40772800	0.92063800	0.56812600
N	0.10476800	-1.24306600	1.20465100
O	-0.31764900	0.06039400	1.66149800
H	2.78348000	-3.08647800	1.23377900
C	1.99066300	1.09060500	-0.03667400
O	2.62363900	0.86966600	0.97083200
O	2.33051200	2.02428200	-0.92833500
C	3.52613000	2.75607100	-0.62756600
H	3.42152700	3.26610200	0.33180800
H	3.64297100	3.47440000	-1.43572800
H	4.38033700	2.07703200	-0.58812500
C	-0.31752300	2.35727800	1.05440600
H	-1.14602300	2.55603600	1.73874500
H	-0.38032200	3.04639600	0.20956500
H	0.62449000	2.50653800	1.58593900
N	-1.68468100	0.81573600	-0.19382500
N	-2.49541900	0.03351700	0.30483800
C	-3.69081300	-0.06573500	-0.51343000
O	-3.69087300	-0.25979800	-1.69947500
H	1.05872900	-3.10295700	-0.36762500
C	3.18421100	-1.07652800	-1.82216100
H	2.60433300	-0.22069500	-2.18821800
H	3.78891700	-0.76434400	-0.96253300

H	3.85786400	-1.39761700	-2.61868800
O	2.35895100	-2.18523400	-1.52830200
O	-4.74623600	0.01232600	0.27780800
C	-6.01305400	-0.11266100	-0.38726000
H	-6.08994700	-1.09630900	-0.85331400
H	-6.76395800	0.00623800	0.38993700
H	-6.11452700	0.66458600	-1.14606100

P3a

C	-0.18686700	1.87305100	-1.81490400
C	1.41915400	0.85805300	-0.34301500
C	0.59786700	1.91491200	0.41974000
C	0.17442600	2.86248400	-0.70594500
H	-0.14767600	2.31669800	-2.81217200
H	-1.18098000	1.44683200	-1.65909900
H	2.46504600	1.16987100	-0.41846300
H	-0.66190000	3.50865700	-0.43142700
C	1.32821900	-0.55798000	0.21811700
C	0.16118800	-1.15227000	-0.61392500
N	0.83830100	0.79906900	-1.70748300
O	0.21969500	-0.49282900	-1.84745400
H	-0.30252100	1.44347700	0.83458000
H	1.07618200	-0.54077300	1.27941300
H	1.01416400	3.49080700	-1.01972500
C	2.59472000	-1.34950200	-0.06084400
O	3.27722200	-1.14014500	-1.03402800
O	2.92272800	-2.35682200	0.75912800
C	2.25742800	-2.55837900	2.01055400
H	2.68623500	-3.47072900	2.42080300
H	2.45220800	-1.72474100	2.68909500
H	1.18114800	-2.69306100	1.88074700
C	0.18273800	-2.65003200	-0.89040500
H	0.09028200	-3.22673500	0.03212500
H	-0.66384000	-2.89230600	-1.53778200

H	1.10905100	-2.91564200	-1.40386600
N	-1.07026200	-0.90776900	0.19301900
N	-2.00672000	-0.43371100	-0.45097300
C	-3.14853100	-0.17325900	0.40448400
O	-3.09154600	0.48005700	1.41228700
C	2.27743700	3.39752700	1.26647100
H	2.80557300	3.56172100	2.20693400
H	2.99654100	3.04251900	0.51814800
H	1.85469100	4.34956500	0.92543100
O	1.26475500	2.44757100	1.53871600
O	-4.22781800	-0.68510700	-0.15494100
C	-5.45275700	-0.44794400	0.55944100
H	-5.63077800	0.62550200	0.63830400
H	-6.23064800	-0.92816300	-0.02889100
H	-5.39243400	-0.88837200	1.55562900

P4a

C	-0.56511000	1.82741600	1.68660700
C	1.52507400	0.94693100	0.90345700
C	1.23388800	2.29350600	0.22552900
C	-0.29555900	2.38124400	0.28704200
H	-0.47850800	2.62359700	2.43253100
H	-1.53494700	1.34554800	1.81137800
H	2.52989600	0.89687200	1.32625500
H	-0.72999400	1.74546700	-0.49590600
C	1.29597300	-0.24984600	-0.03500300
C	0.11534900	-1.00780800	0.62312600
N	0.51343300	0.83892800	1.98195600
O	0.02999000	-0.50220500	1.93226000
H	1.01679000	0.06314000	-1.04287500
H	-0.68071300	3.39533800	0.15949900
C	2.51989800	-1.13732500	-0.13466300
O	3.37814600	-1.23997200	0.71085200
O	2.50956300	-1.83870600	-1.26964900

C	3.58316500	-2.77595200	-1.42367300
H	3.43599800	-3.23574400	-2.39835900
H	3.53855700	-3.52714000	-0.63231400
H	4.54259900	-2.25778100	-1.38153100
C	0.22498700	-2.52316800	0.71298700
H	0.24022300	-2.96893000	-0.28364200
H	-0.63923400	-2.90240300	1.26412700
H	1.13905700	-2.79066100	1.24849600
N	-1.08702100	-0.74358200	-0.22487500
N	-2.11737300	-0.56742700	0.42669100
C	-3.24317400	-0.29109500	-0.44520200
O	-3.24046800	0.55244100	-1.30173400
H	1.67087700	3.10462300	0.83024500
C	1.64828500	3.54048100	-1.71951900
H	2.19588700	3.47163600	-2.66047500
H	0.59392100	3.75425500	-1.93288900
H	2.06212500	4.36129900	-1.11844400
O	1.80238500	2.30059000	-1.05833300
O	-4.25813900	-1.05100700	-0.07831400
C	-5.46770300	-0.85404000	-0.82877200
H	-6.18484200	-1.55873500	-0.41528100
H	-5.81566800	0.17250500	-0.70451000
H	-5.28754800	-1.05951000	-1.88486300

P1b

C	-2.29128300	-1.98345900	0.63291000
C	-1.36689200	-0.36454100	-0.88991400
C	-2.63477000	0.20957600	-0.24773600
C	-2.77381800	-0.59030400	1.04992000
H	-3.13291200	-2.58825600	0.28458300
H	-1.77391600	-2.53977600	1.41657300
H	-1.44486400	-0.25760600	-1.97354000
H	-2.13736200	-0.13647500	1.81325500
C	0.01631400	0.18103500	-0.43265500

H	0.61909900	0.35065200	-1.32565500
C	0.65433000	-1.00716000	0.32354900
N	-1.36858000	-1.80265700	-0.52242800
O	-0.03387500	-2.14510500	-0.19019600
H	-2.57318000	1.29324800	-0.07902400
H	-3.79930000	-0.59830900	1.42622000
C	-0.02110100	1.48588900	0.32906900
O	-0.49880800	1.64124700	1.43144200
O	0.51901000	2.47622600	-0.38242400
C	0.50392900	3.76351400	0.24634700
H	1.08661700	3.73646200	1.16889500
H	0.95201500	4.44715300	-0.47138300
H	-0.52193900	4.05983100	0.47250500
C	0.66593700	-0.99221300	1.84981700
H	1.12222500	-1.92442800	2.19301800
H	1.24837700	-0.14569400	2.21868300
H	-0.34380800	-0.92267400	2.25108700
N	2.05672300	-1.23449300	-0.08366800
N	2.71326300	-0.19416100	-0.06380300
C	4.13118600	-0.43620700	-0.42649800
O	4.61567000	-1.53129900	-0.60248200
N	4.74945100	0.74917100	-0.51107300
H	5.72702700	0.79247600	-0.76077700
H	4.24111900	1.60521200	-0.34326600
C	-4.89195500	0.57421600	-0.84449200
H	-5.59142800	0.35623200	-1.65313600
H	-5.31992200	0.21473100	0.09930400
H	-4.74828100	1.66106400	-0.77367300
O	-3.67910000	-0.07493600	-1.16118700

P2b

C	0.95623200	-1.77796500	1.87019500
C	0.18365000	-1.07448300	-0.29949300
C	1.28880300	-2.13470300	-0.49653600

C	2.03144600	-2.18530000	0.84744000
H	0.65594700	-2.61098400	2.51007800
H	1.29142000	-0.94822100	2.49441200
H	-0.64937400	-1.30358400	-0.97220700
H	2.85787300	-1.47497700	0.87118100
C	0.37007600	0.45662800	-0.39463800
H	0.13215200	0.82469300	-1.39373200
C	-0.74065800	0.87140800	0.60726600
N	-0.23728500	-1.33910200	1.08794900
O	-0.68577700	-0.07924100	1.62939700
H	2.42954000	-3.18554600	1.02957000
C	1.67087500	1.07940400	0.05551100
O	2.29608700	0.78018900	1.04771200
O	2.01924900	2.08094500	-0.75625400
C	3.21069800	2.78692100	-0.38620200
H	3.08830300	3.23546100	0.60134900
H	3.34509800	3.55477800	-1.14452700
H	4.06240100	2.10379600	-0.37384400
C	-0.63841100	2.25978500	1.21873200
H	-1.48328500	2.41682700	1.89395700
H	-0.66514600	3.01905500	0.43431500
H	0.28972800	2.34462700	1.78753900
N	-2.00297400	0.86571400	-0.18218300
N	-2.81615000	0.01881600	0.18167200
C	-4.05253600	0.07820700	-0.63978200
O	-4.26889400	0.89681000	-1.50558500
N	-4.86101800	-0.91551500	-0.24641000
H	-5.75886100	-1.04426900	-0.69017700
H	-4.57774000	-1.54225400	0.49248300
H	0.73923600	-3.07681800	-0.59950700
C	2.88053600	-0.94878700	-1.87320000
H	2.29713400	-0.06840800	-2.16804800
H	3.48631300	-0.70504700	-0.99222300
H	3.55338200	-1.20232900	-2.69436200

O 2.05978800 -2.08031300 -1.66892100

P3b

C -0.77572600 1.80686100 -1.70615700
C 1.03659500 0.93853300 -0.38741000
C 0.20232700 1.93145700 0.44509900
C -0.39815800 2.83202200 -0.63712200
H -0.87467600 2.24407300 -2.70200200
H -1.70772900 1.29475100 -1.45351600
H 2.04616600 1.32846700 -0.54725400
H -1.25635500 3.41035100 -0.28842900
C 1.09953300 -0.47799900 0.17665400
C -0.07143600 -1.16982800 -0.57012200
N 0.34916100 0.83215200 -1.69893800
O -0.15542200 -0.50959000 -1.80366000
H -0.61360200 1.38872600 0.94010100
H 0.91849000 -0.47553900 1.25242900
H 0.35457600 3.52467100 -1.02735100
C 2.40253700 -1.16945800 -0.18364600
O 3.01246700 -0.90509800 -1.19114200
O 2.84788000 -2.15719700 0.60501200
C 2.27296700 -2.41088900 1.89087400
H 2.77932400 -3.30006600 2.26222400
H 2.45903700 -1.57369500 2.56760100
H 1.20059600 -2.60719800 1.82428200
C 0.05602400 -2.65923200 -0.86345200
H 0.07127100 -3.24937800 0.05480000
H -0.80993600 -2.96413200 -1.45669100
H 0.96421900 -2.84604900 -1.44034000
N -1.25530700 -1.03355100 0.32818500
N -2.28122900 -0.66756800 -0.24123700
C -3.40009300 -0.54299400 0.71403500
O -3.25165300 -0.20784700 1.86911700
N -4.55366900 -0.79929500 0.08270800

H	-5.42494000	-0.76615500	0.59236300
H	-4.56324200	-1.05012200	-0.89540100
C	1.81761800	3.55938900	1.12936500
H	2.42073300	3.77419900	2.01281400
H	2.48615400	3.26259900	0.31194500
H	1.28288900	4.46962000	0.83393600
O	0.92188000	2.52792400	1.49751600

P4b

C	-1.26677400	1.48578400	1.65186500
C	0.99351100	1.05579000	0.97011600
C	0.49183300	2.36133400	0.33555100
C	-1.02839200	2.16720200	0.30314800
H	-1.37263500	2.23629600	2.44137300
H	-2.13414500	0.82654100	1.68690000
H	1.95997000	1.17747200	1.46211700
H	-1.29417900	1.51554800	-0.53954300
C	1.06350900	-0.11055400	-0.03085100
C	-0.02036200	-1.09294700	0.47854400
N	-0.04262300	0.69280000	1.96785800
O	-0.26891000	-0.70651500	1.80835300
H	0.82708000	0.20240900	-1.04939200
H	-1.58406500	3.10259800	0.20639400
C	2.42607700	-0.77143800	-0.03576300
O	3.21053600	-0.75983600	0.88418300
O	2.63799500	-1.42041000	-1.18245200
C	3.86317700	-2.16026700	-1.25546100
H	3.86947400	-2.62406000	-2.23950200
H	3.88971200	-2.91981100	-0.47119300
H	4.71525000	-1.48807500	-1.14069500
C	0.32660600	-2.57455700	0.48157100
H	0.48194100	-2.93724500	-0.53640700
H	-0.50223000	-3.12273600	0.93666200
H	1.23246000	-2.73887300	1.07054900

N	-1.19226400	-0.95391200	-0.44100600
N	-2.27612800	-1.04598800	0.13191800
C	-3.39184700	-0.89055000	-0.82102300
O	-3.33505200	-0.18014900	-1.80181000
N	-4.44569700	-1.59868700	-0.39244800
H	-5.29926800	-1.60814900	-0.93208800
H	-4.39298200	-2.13985000	0.45832400
H	0.73783600	3.20279200	1.00332700
C	0.79342700	3.78226800	-1.50960500
H	1.38904100	3.86046600	-2.42019400
H	-0.27052100	3.83585400	-1.77122700
H	1.03783300	4.62044700	-0.84336500
O	1.11815900	2.54522100	-0.90762900

P5a

C	-0.16452300	0.97541300	-0.10289500
C	-1.38273000	0.87866800	0.87503600
C	0.85714600	0.03770900	0.55068400
O	2.58730200	-1.62151500	0.15079200
C	2.52287000	0.13298500	-1.37656100
C	3.89753500	-1.34764300	-0.35430400
O	3.68725800	-0.64578500	-1.56533700
C	4.58826500	-2.65714200	-0.66984200
C	4.66297500	-0.49847800	0.65314900
C	1.64901400	-0.75727900	-0.47471100
O	-0.91607000	0.12752200	1.95032300
N	-0.00054400	-0.83362500	1.36861900
C	0.68184300	-1.42446900	2.51047200
C	0.33182600	2.39867700	-0.25298500
O	1.26983300	2.88005200	0.33980800
O	-0.43169900	3.07568400	-1.11046100
C	-0.10881000	4.46528300	-1.25954400
H	-0.47949000	0.61830900	-1.08936100
H	1.54236100	0.62399500	1.18394900

H	2.75589100	1.08758000	-0.88525600
H	2.07347400	0.33080800	-2.35128000
H	5.57427400	-2.46675800	-1.10101400
H	3.98366000	-3.22214800	-1.38273600
H	4.71109400	-3.24280000	0.24449800
H	5.67122400	-0.29398400	0.28325600
H	4.73480500	-1.02992600	1.60564700
H	4.15150100	0.45278000	0.82777100
H	0.95201200	-1.36567000	-1.06552500
H	-0.05469000	-1.95322400	3.11807600
H	1.18586400	-0.66143600	3.12101600
H	1.41772200	-2.13067100	2.12738800
H	0.91166800	4.57479200	-1.62996500
H	-0.20698900	4.97488700	-0.29898600
H	-0.82414400	4.85804600	-1.97840400
C	-1.94981600	2.18275000	1.41061000
H	-2.38553100	2.77031100	0.60084700
H	-2.72474500	1.95325200	2.14623000
H	-1.15587400	2.75687600	1.89506000
C	-4.03646900	-1.33998200	-0.10618500
O	-5.12894400	-1.47672000	0.37748800
O	-3.64346300	-1.73822600	-1.30358400
C	-4.65139900	-2.40265400	-2.08357700
H	-4.15707500	-2.69811600	-3.00592200
H	-5.02141800	-3.27611500	-1.54436600
H	-5.47472700	-1.71655600	-2.28721000
N	-2.94629900	-0.76835500	0.65145100
N	-2.47615200	0.22835800	0.09964200

P6a

C	1.15981300	-0.17907400	0.62110700
O	0.99738600	1.84340200	-0.68944800
C	1.35559300	2.16888200	1.59402700
C	1.80315600	3.00416800	-0.46878700

O	1.56726800	3.37153500	0.87750400
C	1.31384000	4.12114000	-1.36601000
C	3.27082600	2.66098700	-0.69574400
C	0.66516000	1.26332300	0.56451300
O	-0.53718800	-1.29447200	1.68080500
N	0.77121800	-0.75793000	1.90997000
C	1.61865600	-1.86949600	2.34042600
C	0.49483400	-1.05890200	-0.44737700
C	-0.74895200	-1.59575500	0.31327600
C	1.34984600	-2.13780400	-1.09446100
O	0.92493200	-2.89417700	-1.93624200
O	2.61666800	-2.13689600	-0.67839200
C	3.46872900	-3.10801100	-1.30152200
H	2.24913500	-0.18780700	0.53517900
H	2.30416900	1.73033900	1.93600700
H	0.73483300	2.38638300	2.46332300
H	1.88861400	5.03136000	-1.17709400
H	0.25778800	4.31132300	-1.16248900
H	1.43582400	3.83887100	-2.41458500
H	3.89241400	3.54532000	-0.53160100
H	3.41699900	2.30849400	-1.71989500
H	3.59570100	1.87259600	-0.01018800
H	-0.42403800	1.29265000	0.68780300
H	1.20900200	-2.26771200	3.26968900
H	2.61767700	-1.47109800	2.53289100
H	1.69082200	-2.67621400	1.60005400
H	0.15331000	-0.44613300	-1.28873100
H	3.52127100	-2.92215400	-2.37554300
H	3.08262600	-4.11274400	-1.12259300
H	4.44503400	-2.98099500	-0.83944300
C	-1.11370600	-3.06556200	0.15418900
H	-1.97094600	-3.27615100	0.79900200
H	-1.36710100	-3.29454700	-0.88115000
H	-0.27468400	-3.69296500	0.46354300

C	-3.59082400	0.59054200	-0.01289900
O	-3.55110300	1.78933100	-0.09668800
N	-2.50889100	-0.14978300	0.59070300
N	-1.91727300	-0.84714200	-0.23480200
O	-4.59007500	-0.20156000	-0.35384600
C	-5.74794600	0.47327600	-0.87582200
H	-5.48813700	0.99412500	-1.79832600
H	-6.47914300	-0.30862500	-1.06550300
H	-6.12381200	1.18607800	-0.14048800

P7a

C	0.14941100	1.18416500	-0.67927600
C	1.39543200	1.57328700	0.13851100
C	-0.39845000	0.06186600	0.21833400
O	-2.28481700	-1.31646800	0.81802400
C	-2.21277500	-0.69667300	-1.40544600
C	-3.12163200	-2.19161300	0.04912800
O	-3.33206100	-1.53188300	-1.18834500
C	-4.46197700	-2.34653100	0.73852300
C	-2.39289600	-3.51253600	-0.14909400
C	-1.87684600	-0.22412500	0.01037600
O	1.03277500	1.41272100	1.47527200
N	-0.13161500	0.54653400	1.57773700
C	0.21642500	-0.52196400	2.50696600
C	-0.84628700	2.30676400	-0.90684700
O	-1.36130100	2.52296400	-1.98019000
O	-1.12284300	2.99358500	0.20011400
C	-2.08853100	4.04409300	0.04818400
H	0.42824200	0.80918400	-1.66568400
H	0.16830100	-0.86072900	0.00262900
H	-1.37324000	-1.25608000	-1.84431200
H	-2.49713500	0.11467100	-2.07712300
H	-5.12287700	-2.97421100	0.13525500
H	-4.91833500	-1.36240000	0.86809200

H	-4.32747100	-2.81407700	1.71695400
H	-3.01132800	-4.19760800	-0.73479500
H	-2.17920200	-3.96859900	0.82113300
H	-1.44621700	-3.34958200	-0.67202400
H	-2.45948400	0.66720900	0.28128900
H	0.44545800	-0.07964300	3.47835100
H	1.07228800	-1.11459300	2.16007700
H	-0.66494300	-1.15874700	2.60006300
H	-3.03638700	3.63163700	-0.30202000
H	-1.72548900	4.78506700	-0.66601400
H	-2.20089900	4.48368400	1.03644300
C	1.97426400	2.96231800	-0.07469800
H	2.86627600	3.07682700	0.54675400
H	2.25517700	3.09611700	-1.12178000
H	1.23979700	3.71503300	0.21280100
C	3.86659700	-1.04750700	0.03281200
O	5.00285900	-1.00555900	0.42140900
O	3.34122700	-1.92393000	-0.80555300
C	4.25236600	-2.92841400	-1.28443600
H	4.66789800	-3.48347700	-0.44202900
H	3.65862400	-3.57854600	-1.92215300
H	5.05677100	-2.45760200	-1.85102600
N	2.85153000	-0.15244200	0.53650700
N	2.44677900	0.61822800	-0.33495100

P8a

C	0.75297800	-0.97534800	0.06601100
O	2.82893900	0.29170900	0.05711800
C	2.99906500	-1.89801100	0.71360200
C	3.78675500	-0.37099400	-0.77999900
O	3.58022000	-1.75917200	-0.57492200
C	5.17961500	0.04783100	-0.33491800
C	3.50655000	-0.04272900	-2.23356800
C	2.08111900	-0.68119700	0.77260800

O	-0.68775000	-1.06655000	1.80360100
N	-0.01523500	-1.91738300	0.88196400
C	-0.99668700	-2.69142500	0.12143000
C	-0.20294300	0.23759500	-0.10911900
C	-1.12769600	0.10579900	1.13276500
C	0.51722900	1.54194700	-0.38612800
O	0.68147600	1.96620400	-1.50652600
O	0.97019400	2.14848200	0.71031700
C	1.83046700	3.26593000	0.47344000
H	0.97526400	-1.43862800	-0.90083400
H	2.46455000	-2.84811000	0.75780700
H	3.76030700	-1.86148900	1.50272100
H	5.93421800	-0.42937500	-0.96559800
H	5.34724000	-0.24227900	0.70594800
H	5.28518700	1.13315600	-0.41577400
H	4.20299900	-0.57945500	-2.88317300
H	3.62336000	1.03170500	-2.39783500
H	2.48215900	-0.32560700	-2.48793500
H	1.90360700	-0.31716700	1.78880900
H	-1.60440400	-3.25862100	0.82765900
H	-0.44270800	-3.38769700	-0.51246100
H	-1.65920800	-2.08275600	-0.50995800
H	-0.80553500	0.07379000	-1.00412900
H	1.30631300	4.03651900	-0.09421000
H	2.71101700	2.92929700	-0.07826100
H	2.11062600	3.63750800	1.45723900
C	-4.31286300	0.46037000	-0.50049500
O	-5.07749100	1.38718200	-0.48832300
O	-4.57180400	-0.78165400	-0.86943600
C	-1.19448100	1.20970800	2.17996600
H	-0.22140200	1.32837000	2.65391200
H	-1.49570500	2.15253500	1.71977900
H	-1.93512200	0.92305500	2.93159000
C	-5.92468300	-1.01802400	-1.29472800

H	-6.16520700	-0.37237600	-2.14070000
H	-5.95915400	-2.06519300	-1.58517200
H	-6.61152800	-0.82072700	-0.47062200
N	-2.54874300	-0.12560400	0.73121000
N	-2.91654800	0.63515900	-0.16726500

P5b

C	-0.48365200	0.79636500	-0.04100200
C	-1.73974200	0.36660300	0.78891500
C	0.62220900	-0.06847600	0.56910400
O	2.68089000	-1.26240500	0.14572600
C	2.41185600	0.65460100	-1.09522600
C	3.93973500	-0.89387600	-0.43414200
O	3.63433600	0.04247800	-1.45523500
C	4.58071900	-2.10681500	-1.07783100
C	4.80189900	-0.26182800	0.64799400
C	1.64443600	-0.50729000	-0.46264500
O	-1.24828100	-0.51795600	1.74661800
N	-0.14608900	-1.20357800	1.10210800
C	0.52483600	-1.91436200	2.18061800
C	-0.21180900	2.28268700	0.05421100
O	0.59800700	2.79919500	0.78912600
O	-1.01401200	2.96296100	-0.76473000
C	-0.90078400	4.39117700	-0.69386700
H	-0.65917400	0.54804100	-1.09326600
H	1.12477800	0.48545100	1.37801000
H	2.56509200	1.46473300	-0.36830300
H	1.94282500	1.05611700	-1.99584700
H	5.51540400	-1.82209700	-1.56792500
H	3.89777900	-2.52621700	-1.82048600
H	4.79631600	-2.86223200	-0.31820200
H	5.77219500	0.02554400	0.23456400
H	4.95992600	-0.97446000	1.46165800
H	4.30866400	0.62571500	1.05441600

H	1.14418800	-1.11118200	-1.23344300
H	-0.16604700	-2.65357800	2.58960300
H	0.84998700	-1.23072500	2.97788100
H	1.39240000	-2.41877700	1.75534800
H	0.11417900	4.69917200	-0.94984300
H	-1.14499800	4.73447700	0.31337400
H	-1.61518800	4.77924100	-1.41620800
C	-2.50397800	1.46842100	1.50496800
H	-2.97046800	2.14098200	0.78314400
H	-3.27995000	1.01257300	2.12496200
H	-1.82091100	2.03340400	2.14427700
C	-4.03293900	-1.92134800	-0.86677000
O	-4.60726500	-2.94464700	-0.55843600
N	-3.06062200	-1.37661000	0.10888200
N	-2.68830400	-0.24131700	-0.18199700
N	-4.16568800	-1.24429500	-2.01567600
H	-3.71086400	-0.34956500	-2.13246700
H	-4.85732400	-1.54816300	-2.68498400

P6b

C	-0.65470000	0.59684100	0.65794000
O	-1.64864300	-1.15445400	-0.68943600
C	-2.12840700	-1.25976400	1.59445600
C	-2.98188500	-1.62539200	-0.47741900
O	-3.00123000	-2.09604600	0.85710300
C	-3.24128500	-2.79306800	-1.40522500
C	-3.97151900	-0.48240000	-0.67293400
C	-1.05138800	-0.87440300	0.56832200
O	1.39793800	0.48328200	1.65084600
N	0.03294000	0.80558900	1.93419900
C	-0.00120300	2.18759000	2.41120200
C	0.35928000	0.98792200	-0.42696500
C	1.71192700	0.70093900	0.28407300
C	0.24331000	2.38524300	-1.01624000

O	1.01031000	2.81396300	-1.84652500
O	-0.80918200	3.06806800	-0.56474000
C	-0.98439700	4.37411000	-1.13139200
H	-1.55127900	1.22008100	0.62301000
H	-2.64950900	-0.36971200	1.97548200
H	-1.73611000	-1.82543600	2.43992100
H	-4.23891300	-3.20088100	-1.22417500
H	-2.49432700	-3.56939200	-1.22578400
H	-3.17902700	-2.46475600	-2.44565500
H	-4.99370600	-0.84240500	-0.52906800
H	-3.87581800	-0.07692300	-1.68332800
H	-3.78186200	0.32368600	0.04208000
H	-0.15949400	-1.50214600	0.68245400
H	0.59647400	2.24505400	3.32199200
H	-1.03918200	2.43156700	2.64932500
H	0.37846400	2.91484500	1.68246200
H	0.26882800	0.32192700	-1.29198000
H	-1.10062200	4.29809900	-2.21360700
H	-0.12124600	4.99978800	-0.89868300
H	-1.88604900	4.77409800	-0.67313600
C	2.82540600	1.73495600	0.16496300
H	3.66514600	1.40032300	0.77968500
H	3.14821600	1.84557800	-0.87044100
H	2.47882000	2.70208300	0.53578600
C	2.95657300	-2.67016700	-0.30903200
O	2.78636300	-3.75179000	0.21290200
N	2.41284400	-1.49043200	0.39732200
N	2.26466200	-0.52507300	-0.35035900
N	3.62698900	-2.41942200	-1.44289100
H	3.58279700	-1.49960200	-1.85962800
H	3.95163000	-3.19913400	-1.99630300

P7b

C	0.56388500	1.00607000	-0.62465900
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C	1.87876300	0.95233100	0.17719100
C	-0.26948300	-0.00726400	0.17833200
O	-2.47966300	-0.81835000	0.75726100
C	-2.25441800	-0.03953900	-1.42787600
C	-3.33776000	-1.54749100	-0.12614100
O	-3.48164600	-0.72183500	-1.26659900
C	-4.69500000	-1.70652100	0.52537100
C	-2.68748100	-2.87847800	-0.48207500
C	-1.77437500	0.16782400	0.01969200
O	1.50106400	0.74757300	1.50359300
N	0.14806900	0.21709300	1.56757300
C	0.21089700	-1.01468500	2.34791600
C	-0.07837100	2.37901700	-0.70638700
O	-0.50273900	2.84781400	-1.73784300
O	-0.16254600	2.98891700	0.47512300
C	-0.79147700	4.27847800	0.45763100
H	0.71700100	0.67504000	-1.65344800
H	0.00321800	-1.02210600	-0.15949100
H	-1.53612800	-0.64154800	-2.00344200
H	-2.43694400	0.89689100	-1.95671400
H	-5.37514900	-2.23038000	-0.15105700
H	-5.10249100	-0.71967600	0.75579400
H	-4.60171400	-2.28432600	1.44801600
H	-3.33786600	-3.44938800	-1.14995700
H	-2.51398300	-3.45908300	0.42774900
H	-1.72523100	-2.71984900	-0.97758400
H	-2.05958900	1.15475100	0.40516900
H	0.56800800	-0.77420500	3.35124000
H	0.87013800	-1.76240800	1.89024800
H	-0.80863400	-1.39860500	2.41181800
H	-1.81168700	4.19093400	0.07978900
H	-0.22380300	4.96193900	-0.17619100
H	-0.79004500	4.61881700	1.49049100
C	2.80241000	2.15665600	0.08938900

H	3.70402700	1.96085800	0.67551100
H	3.08951700	2.33494200	-0.94931600
H	2.29842100	3.03544700	0.49250900
C	3.46504000	-2.28596900	-0.35970100
O	3.31009300	-3.39220900	0.11361400
N	2.74109300	-1.17316200	0.29049800
N	2.63792700	-0.18331400	-0.43128500
N	4.25523300	-1.95198800	-1.38930600
H	4.71857000	-2.68505200	-1.90645300
H	4.20582000	-1.02125600	-1.78033100

P8b

C	0.53286300	-0.99680200	-0.12072600
O	2.53919100	0.34181400	0.19575600
C	2.77489900	-1.91108600	0.55230800
C	3.58243900	-0.15568700	-0.65317900
O	3.43258700	-1.56619700	-0.65819300
C	4.91946800	0.25120700	-0.05297800
C	3.38234100	0.36268300	-2.06363900
C	1.79544900	-0.75252100	0.71352800
O	-1.01308400	-1.39322000	1.47942500
N	-0.23944900	-2.07569100	0.49817500
C	-1.13042000	-2.76987100	-0.43204900
C	-0.46932800	0.18937400	-0.19299700
C	-1.46197600	-0.15195600	0.95305000
C	0.20253100	1.54722800	-0.24007100
O	0.41864400	2.12625400	-1.27934000
O	0.55362300	2.01572300	0.95689100
C	1.37493600	3.18668300	0.93214100
H	0.84023800	-1.30889600	-1.12430700
H	2.28655800	-2.87800900	0.42282100
H	3.47881500	-1.95957100	1.39235100
H	5.73815200	-0.09721400	-0.68805200
H	5.03234200	-0.18060700	0.94514500

H	4.97442000	1.34003700	0.03054500
H	4.14580500	-0.04861600	-2.72908900
H	3.45538700	1.45335900	-2.07003200
H	2.39213600	0.07556900	-2.42618900
H	1.53308800	-0.54307600	1.75470600
H	-1.77824800	-3.42861400	0.14765300
H	-0.50721500	-3.37472600	-1.09462100
H	-1.75346900	-2.10008500	-1.04132700
H	-1.00684600	0.12897300	-1.14069000
H	0.85189400	4.00794700	0.43974000
H	2.30175800	2.96213200	0.39982700
H	1.57654400	3.42847100	1.97381300
C	-4.59765600	0.32950800	-0.81981400
O	-5.13311100	1.27598900	-1.35625900
C	-1.63527200	0.78724700	2.13946100
H	-0.69559500	0.87157500	2.68319200
H	-1.95214000	1.77425900	1.79851400
H	-2.40219200	0.36943700	2.79739000
N	-2.83975000	-0.36919000	0.42331300
N	-3.21026800	0.51848900	-0.34478200
N	-5.11266300	-0.89606500	-0.64663900
H	-6.07672300	-1.05842400	-0.89865600
H	-4.62425100	-1.57565700	-0.07964600

N1-OBn

C	-3.73025000	0.95284800	-0.17723300
C	-2.51685200	-1.00779500	0.10246100
C	-1.62495400	0.05004800	0.65669900
C	-2.30733200	1.36601900	0.19430300
H	-4.10814700	1.36483500	-1.11107800
H	-4.46090100	1.13219700	0.61232200
H	-2.32705800	-2.07028000	0.08700000
H	-2.28446300	2.14599700	0.95332100
N	-3.64280700	-0.53316700	-0.34926500

O	-4.62881200	-1.15968900	-0.84005800
H	-1.57992100	-0.01250200	1.75450500
H	-1.77061700	1.71824500	-0.68802400
C	0.66237000	0.68325400	0.81546900
H	0.48372900	1.74632900	0.61897700
H	0.57285200	0.52064300	1.89859000
O	-0.31018500	-0.12258900	0.14135600
C	2.02986200	0.28593100	0.33334000
C	2.50943900	-1.00446600	0.58228400
C	2.83136600	1.18194900	-0.37455500
C	3.76967700	-1.38814600	0.13575000
H	1.88805000	-1.70673900	1.12658700
C	4.09788400	0.80235800	-0.81931200
H	2.46324500	2.18154500	-0.57883500
C	4.56854600	-0.48331000	-0.56558800
H	4.13249300	-2.38963400	0.33632600
H	4.71217300	1.50859200	-1.36569200
H	5.55165200	-0.78098100	-0.91123500

TS1a-OBn

C	-0.15940400	1.59185900	2.47079400
C	-0.19467600	0.35226000	0.44181500
C	-1.48213500	1.15697700	0.42039600
C	-1.40681300	2.03599500	1.69576600
H	-0.35513000	1.26422800	3.49105800
H	0.62829000	2.34526200	2.47809100
H	-0.17849300	-0.63481500	-0.00169500
H	-1.34303400	3.08933000	1.43461700
C	1.23560800	1.08115300	-0.56539200
H	1.06891200	0.49471700	-1.46106000
C	2.47250300	0.74177400	0.08288700
N	0.32961000	0.42219600	1.70369200
O	1.43147900	-0.14050400	1.93828300
H	-1.56297100	1.75854200	-0.48961800

H	-2.31854600	1.87149200	2.26731700
C	0.88541700	2.52270200	-0.76014000
O	0.95052200	3.39261700	0.08164300
O	0.43597800	2.73121800	-2.00588600
C	0.03407400	4.08479200	-2.31855400
H	0.87057300	4.76749800	-2.17350600
H	-0.26779600	4.06051600	-3.36152900
H	-0.79937300	4.38379300	-1.68298800
C	3.35657500	1.69551400	0.83173800
H	3.88893400	1.17095600	1.62243900
H	4.11105900	2.10803400	0.15074900
H	2.78498300	2.51967900	1.24632900
N	2.92333100	-0.49327300	-0.31897500
N	4.10837100	-0.78861000	0.04160700
C	4.45404000	-2.11044200	-0.36396900
O	3.73894800	-2.95956100	-0.84213700
C	-3.00657400	-0.27058400	-0.73806500
H	-2.20912100	-0.91184800	-1.12952400
H	-3.18082700	0.53588000	-1.46184700
O	-2.61666300	0.30628100	0.51746400
O	5.75850100	-2.27727400	-0.09933600
C	6.29816200	-3.56890300	-0.43560900
H	6.19168400	-3.75899400	-1.50428400
H	7.34801800	-3.52727700	-0.15826900
H	5.78465100	-4.35182800	0.12367500
C	-4.25775800	-1.07145100	-0.51520800
C	-5.48164400	-0.42065100	-0.33175700
C	-4.21212100	-2.46467500	-0.44786000
C	-6.64089400	-1.15155100	-0.09007900
H	-5.52191100	0.66203900	-0.38036500
C	-5.37201100	-3.20044100	-0.20916300
H	-3.26489700	-2.97511200	-0.58405100
C	-6.58776700	-2.54460000	-0.02923400
H	-7.58537400	-0.63797400	0.04720700

H	-5.32566700	-4.28220700	-0.16297700
H	-7.49076000	-3.11469700	0.15551400

TS2a-OBn

C	0.42312900	1.18568600	2.68728600
C	0.15459400	-0.21237700	0.76918900
C	1.63194100	0.11330000	0.82002100
C	1.76210500	1.18916000	1.93752300
H	0.49355200	0.84071000	3.71908200
H	-0.09740900	2.14261500	2.66253200
H	-0.15995200	-1.19575300	0.44409400
H	1.92580700	2.15852400	1.47259500
C	-0.86606000	0.75755800	-0.48828600
H	-0.74460800	0.05540800	-1.30449800
C	-2.22305000	0.82552100	-0.02227800
N	-0.39831600	0.19542500	1.95010200
O	-1.61088500	-0.00286500	2.18082600
H	2.59590600	0.96895500	2.60162900
C	-0.16921900	2.06151200	-0.74767100
O	0.05127000	2.91494600	0.08419200
O	0.13811600	2.18335800	-2.04207200
C	0.85646600	3.38049600	-2.40714800
H	0.27682900	4.26616200	-2.14812000
H	1.00030900	3.31504300	-3.48191200
H	1.81664100	3.40516800	-1.89139200
C	-2.88370800	2.05745300	0.52576000
H	-3.64825500	1.78108800	1.24885300
H	-3.38439200	2.60167100	-0.28476300
H	-2.15792800	2.72337500	0.98391900
N	-2.92649600	-0.29926000	-0.33443300
N	-4.18538100	-0.25318900	-0.10066100
C	-4.80732500	-1.48933200	-0.41055600
O	-4.30561300	-2.50362100	-0.84069400
H	2.18157200	-0.79388600	1.09210100

C	3.46799300	0.70664000	-0.59420900
H	3.59996500	1.12635300	-1.59268600
H	3.83913700	1.43847400	0.13113000
O	2.05131900	0.54521400	-0.46247500
O	-6.11775700	-1.35535500	-0.13802900
C	-6.92343600	-2.51993600	-0.38946700
H	-7.93695700	-2.23863900	-0.11559500
H	-6.87539400	-2.79686600	-1.44349800
H	-6.58202800	-3.35856600	0.21889000
C	4.21896200	-0.59620700	-0.45476300
C	3.86407900	-1.69406300	-1.24604100
C	5.25933700	-0.72967200	0.46515100
C	4.54299000	-2.90151200	-1.12145300
H	3.04713200	-1.59782900	-1.95226300
C	5.94659800	-1.93739300	0.58740500
H	5.53090700	0.11373500	1.09095500
C	5.58893600	-3.02498200	-0.20499800
H	4.26070100	-3.74636400	-1.73893600
H	6.75368800	-2.02914300	1.30488000
H	6.11853200	-3.96558200	-0.10885400

TS3a-OBn

C	0.92060800	-2.34545000	0.15343700
C	-0.13966300	-0.30827500	0.66002800
C	-1.05066700	-0.97102700	-0.34345800
C	-0.46932100	-2.40916700	-0.48288000
H	1.20758200	-3.22833600	0.72127900
H	1.72165900	-2.09894500	-0.55129200
H	-0.53753300	0.37671300	1.39800300
H	-0.43182900	-2.74596600	-1.51693400
C	1.07876700	0.95927200	-0.24511300
C	2.28753000	0.97169300	0.50555100
N	0.79754600	-1.19762100	1.08092700
O	1.78262200	-0.78824500	1.76176600

H	1.17302100	0.45976600	-1.20176300
H	-1.11545900	-3.08187200	0.08318000
C	0.16169800	2.13285100	-0.28509700
O	0.00558300	2.96055200	0.58404700
O	-0.54493900	2.11685700	-1.43023700
C	-1.54318300	3.15083500	-1.57312400
H	-2.03232000	2.94955400	-2.52188600
H	-1.06900100	4.13201200	-1.58525800
H	-2.25795300	3.09920800	-0.75198400
C	2.59307500	1.91170600	1.62555900
H	3.01405000	2.84418600	1.23395300
H	3.33422700	1.46408800	2.28526400
H	1.68967600	2.15712100	2.17659400
N	3.27236400	0.20567000	-0.10067800
N	4.44949400	0.37041300	0.34546400
C	5.36855900	-0.50415500	-0.30312300
O	5.12099800	-1.47794000	-0.97550100
H	-1.00869500	-0.43378900	-1.29663100
C	-3.36609200	-1.20391500	-0.84550700
H	-3.37889300	-2.27171900	-1.09052600
H	-3.11191800	-0.65239000	-1.76155400
O	-2.37664000	-0.92617500	0.14991400
O	6.60402500	-0.08077700	-0.00393900
C	7.67927900	-0.86143500	-0.55990700
H	7.62476100	-0.86235100	-1.64908500
H	8.59299000	-0.37886600	-0.22384800
H	7.63034300	-1.88751300	-0.19373000
C	-4.70882300	-0.76501100	-0.32792200
C	-4.87294300	0.53119800	0.17174400
C	-5.80422400	-1.62826000	-0.34994200
C	-6.11285000	0.95551400	0.63783300
H	-4.02016100	1.19920500	0.20165800
C	-7.05061500	-1.20272700	0.10992300
H	-5.68282300	-2.63843200	-0.72577400

C	-7.20685700	0.08903400	0.60567400
H	-6.22884000	1.96158700	1.02413800
H	-7.89432500	-1.88265800	0.08786500
H	-8.17323000	0.41988100	0.96789200

TS4a-OBn

C	0.77150300	-2.62985400	0.01714600
C	-0.35460800	-0.66427400	0.71586900
C	-1.30059100	-1.33467700	-0.24970700
C	-0.41535500	-2.40849300	-0.93349200
H	0.72344800	-3.56918700	0.56881000
H	1.75258500	-2.54091100	-0.45223900
H	-0.71168500	-0.03902500	1.52370100
H	-0.07177900	-2.00023000	-1.88427400
C	0.68086300	0.74168800	-0.19268900
C	1.89203800	0.88892600	0.53222600
N	0.65592700	-1.51925000	0.99374100
O	1.62147600	-1.15936700	1.71094100
H	0.81615900	0.30409700	-1.17366600
H	-0.96099700	-3.32895100	-1.13116600
C	-0.33014600	1.85073100	-0.18145700
O	-0.94089300	2.23813100	0.79160800
O	-0.46175300	2.37270900	-1.40332200
C	-1.44585800	3.42127700	-1.54169600
H	-1.37156300	3.75047400	-2.57417200
H	-1.22688800	4.24026000	-0.85750000
H	-2.44046300	3.02459200	-1.33668600
C	2.07188500	1.80028200	1.70366300
H	2.58503300	2.71747900	1.39502300
H	2.69889100	1.31853600	2.45367700
H	1.11189100	2.06778100	2.13888000
N	2.94747400	0.23382500	-0.05518800
N	4.10040400	0.50427000	0.42548600
C	5.10377500	-0.28158800	-0.19150400

O	4.96763400	-1.25609200	-0.89817300
H	-2.12645400	-1.78744700	0.30866100
C	-3.12057300	-0.63531700	-1.64321000
H	-3.26929200	0.09529900	-2.44125100
H	-3.16887900	-1.63296700	-2.09378400
O	-1.80724900	-0.36619600	-1.15263500
O	6.29532500	0.21853300	0.17849500
C	7.44524700	-0.47818000	-0.33349500
H	7.45294000	-0.45361700	-1.42398200
H	8.30756900	0.05001800	0.06484900
H	7.44303800	-1.51551700	0.00369500
C	-4.18993400	-0.48538300	-0.58319000
C	-5.30589800	-1.32411000	-0.58347600
C	-4.08523400	0.50911700	0.39477100
C	-6.31249200	-1.16512000	0.36783100
H	-5.38702000	-2.10793300	-1.32925300
C	-5.08625800	0.66274000	1.35030100
H	-3.21391400	1.15222100	0.41639700
C	-6.20439700	-0.17095600	1.33788600
H	-7.17352300	-1.82334900	0.35698600
H	-4.99347300	1.43397500	2.10641500
H	-6.98236400	-0.05008200	2.08263500

TS1b-OBn

C	0.40103600	1.23264300	2.50998400
C	0.03981600	0.18313800	0.42518700
C	-1.08539500	1.19284300	0.53120000
C	-0.82420700	1.90982800	1.88072800
H	0.24819500	0.89272700	3.53332700
H	1.29312400	1.85712000	2.46587100
H	-0.10261000	-0.73124000	-0.13508300
H	-0.64601700	2.97195300	1.72964700
C	1.61080600	0.78818700	-0.57213500
H	1.36098600	0.29363900	-1.50251500

C	2.73918400	0.19812100	0.08783100
N	0.61852300	0.04619400	1.65051800
O	1.69320700	-0.64669900	1.72066400
H	-1.07661400	1.88719500	-0.31373600
H	-1.71421400	1.78898500	2.49631600
C	1.46693300	2.26559600	-0.65380100
O	1.71194800	3.06730600	0.22410600
O	0.96285700	2.62083800	-1.84959500
C	0.73537200	4.03313300	-2.04873800
H	1.67069000	4.58302800	-1.94755400
H	0.34494500	4.12171300	-3.05858300
H	0.01190400	4.40514900	-1.32310800
C	3.79182500	0.94725500	0.85279100
H	4.22814600	0.30797800	1.61730200
H	4.59855500	1.24004200	0.17038200
H	3.38195200	1.84476700	1.30447300
N	3.02389000	-1.06302500	-0.45981800
N	4.14073500	-1.54114600	-0.14713400
C	4.34109500	-2.86987800	-0.72121400
O	3.53686500	-3.48460400	-1.39431800
N	5.57131300	-3.30081000	-0.37500300
H	5.89483900	-4.20483800	-0.67778000
H	6.16632600	-2.71942900	0.19192700
C	-2.87048400	0.17787100	-0.68958000
H	-2.13763200	-0.44135400	-1.22243400
H	-3.05170300	1.07650100	-1.29082400
O	-2.35403800	0.55006100	0.59424300
C	-4.14417300	-0.59314800	-0.48112900
C	-5.36703100	-0.09905500	-0.93530700
C	-4.11240900	-1.81982900	0.19083500
C	-6.54268700	-0.82182200	-0.73203000
H	-5.40076600	0.85485900	-1.45015200
C	-5.28382200	-2.53990000	0.40051100
H	-3.16502700	-2.20430600	0.55175200

C	-6.50294600	-2.04245800	-0.06311200
H	-7.48662500	-0.42907700	-1.09166100
H	-5.24848600	-3.48954200	0.92176100
H	-7.41537800	-2.60470600	0.09780200

TS2b-OBn

C	-0.10185600	0.75708200	2.68466800
C	-0.08267300	-0.47816100	0.65648200
C	1.33605200	0.02020300	0.81707800
C	1.27135200	0.98750000	2.03386300
H	-0.04704600	0.38067900	3.70611500
H	-0.74236500	1.63865200	2.66065500
H	-0.25927600	-1.43196400	0.17631100
H	1.34150300	2.01007900	1.66896400
C	-1.23856000	0.54491800	-0.49780700
H	-1.11498800	-0.06826600	-1.38206200
C	-2.55703600	0.44224300	0.06193600
N	-0.72287400	-0.29381000	1.84451900
O	-1.96250200	-0.57223300	1.90542200
H	2.08724900	0.80261800	2.73056500
C	-0.64663600	1.90709500	-0.66110800
O	-0.52511800	2.73674800	0.21620800
O	-0.28431700	2.11922400	-1.93336500
C	0.37576300	3.37364500	-2.19385800
H	-0.27984700	4.20877400	-1.94706300
H	0.60430800	3.36651000	-3.25610700
H	1.29036900	3.43987500	-1.60411600
C	-3.31548900	1.57043800	0.69940000
H	-4.00964800	1.18609000	1.44369900
H	-3.90863700	2.09199000	-0.06173600
H	-2.63772600	2.28516700	1.15624500
N	-3.21973600	-0.68832800	-0.40974900
N	-4.45763500	-0.72455700	-0.17827200
H	1.98754900	-0.83332500	1.03488200

C	3.14334400	0.97024200	-0.42340600
H	3.26847600	1.51638500	-1.35992000
H	3.38757600	1.65147900	0.39881900
O	1.75503600	0.62527100	-0.39452600
C	-5.06058000	-1.96239200	-0.64896000
O	-4.47079900	-2.90649300	-1.14093700
N	-6.39325500	-1.89642900	-0.44066800
H	-6.98436300	-2.66870400	-0.70036600
H	-6.79606500	-1.07618400	-0.01869600
C	4.04742000	-0.23915600	-0.38547300
C	5.05830400	-0.35085900	0.56949800
C	3.87118600	-1.27054100	-1.31425000
C	5.89234200	-1.46892400	0.59163200
H	5.19284600	0.43969500	1.30011700
C	4.69686200	-2.38946700	-1.29053700
H	3.07798500	-1.19357900	-2.04938200
C	5.71253800	-2.48986300	-0.33792800
H	6.67490600	-1.54408900	1.33767300
H	4.55260300	-3.18295900	-2.01467900
H	6.35669600	-3.36121100	-0.32051500

TS3b--OBn

C	0.45971800	-1.91157600	-0.53356200
C	0.06758600	0.19529400	0.46940800
C	-0.92620800	0.11784100	-0.65720100
C	-0.41407100	-1.08699300	-1.49084900
H	0.00804900	-2.85033300	-0.21342000
H	1.46493200	-2.10344100	-0.91291500
H	-0.14065700	0.77773300	1.35801500
H	0.18064500	-0.73068700	-2.33192600
C	1.72329800	1.12619400	-0.09286400
C	2.78098700	0.52225000	0.64542800
N	0.60971400	-1.03425200	0.65335300
O	1.60144300	-1.15051600	1.43808400

H	1.73170300	0.86610200	-1.14406300
H	-1.24997000	-1.65921700	-1.88985400
C	1.29583400	2.52980000	0.15536300
O	1.28132700	3.10513300	1.22088200
O	0.85473200	3.08176300	-0.99055000
C	0.34508300	4.42883000	-0.88835700
H	0.03285900	4.69565100	-1.89407900
H	1.12714000	5.10184400	-0.53738600
H	-0.50049300	4.45990100	-0.20118100
C	3.30803800	1.01938700	1.95211100
H	4.07286100	1.78647100	1.78766600
H	3.77444900	0.19798700	2.49358100
H	2.51009700	1.45982400	2.54323500
N	3.48556700	-0.39821600	-0.12936300
N	4.60237200	-0.76550700	0.32773800
C	5.21361000	-1.77578500	-0.51239000
O	4.65789700	-2.40005000	-1.40024800
N	6.49846400	-1.94607000	-0.13207700
H	7.07898900	-2.62095800	-0.60169600
H	6.87624500	-1.39887200	0.62355100
H	-0.94173700	1.04299900	-1.24036900
C	-3.28972200	0.16029500	-0.95706600
H	-3.12796700	-0.35670900	-1.91291300
H	-3.34279300	1.23533900	-1.16765600
O	-2.20295200	-0.11043300	-0.07142600
C	-4.57107100	-0.32010300	-0.32951700
C	-5.74182300	0.43062400	-0.44866000
C	-4.61167800	-1.54054700	0.35121800
C	-6.93977400	-0.03483200	0.09161600
H	-5.71722900	1.38458000	-0.96451000
C	-5.80530600	-2.00245800	0.89853600
H	-3.70136600	-2.11732300	0.45779900
C	-6.97428600	-1.25256200	0.76742100
H	-7.84174800	0.55784800	-0.00792200

H	-5.82435600	-2.94847700	1.42742100
H	-7.90334300	-1.61307900	1.19332800

TS4b-OBn

C	1.06350500	-2.64399000	0.08172500
C	-0.06950700	-0.67474500	0.74207200
C	-1.01670000	-1.35928900	-0.21061900
C	-0.13917600	-2.46111900	-0.86055700
H	1.04916400	-3.58352600	0.63455100
H	2.03472000	-2.52811900	-0.40284500
H	-0.42579800	-0.02105700	1.52758500
H	0.19105900	-2.09340000	-1.83233000
C	1.00124100	0.68982300	-0.19513800
C	2.22693300	0.78506200	0.51518200
N	0.92954000	-1.53028000	1.05136800
O	1.91205900	-1.12289500	1.73497000
H	1.10617000	0.24372800	-1.17607200
H	-0.68795600	-3.38859000	-1.01244600
C	0.03743700	1.83502100	-0.17766200
O	-0.53379400	2.26357700	0.80323300
O	-0.11780900	2.33779000	-1.40696200
C	-1.07340200	3.41257400	-1.53566200
H	-1.02176900	3.72038800	-2.57621300
H	-0.80954200	4.23762400	-0.87486700
H	-2.07326900	3.05154700	-1.29301700
C	2.47382200	1.72154000	1.65403100
H	2.98061700	2.62576600	1.29944600
H	3.12810800	1.24990100	2.38656900
H	1.53708000	2.01008700	2.12507700
N	3.25952800	0.10565100	-0.11321100
N	4.42391600	0.36135700	0.31263400
C	5.42147600	-0.43943200	-0.35878800
O	5.20723400	-1.38339900	-1.10169600
N	6.65094100	0.00432600	-0.01173600

H	7.47233900	-0.44678600	-0.37850000
H	6.74496000	0.78170000	0.62044000
H	-1.85270800	-1.78766400	0.35173700
C	-2.82234000	-0.66872200	-1.62571900
H	-2.95654700	0.03368100	-2.45140300
H	-2.88970900	-1.68169100	-2.03866500
O	-1.50651800	-0.40679600	-1.14161400
C	-3.89209800	-0.45801600	-0.57602600
C	-3.75856500	0.55180700	0.38235200
C	-5.03820600	-1.25508400	-0.56812400
C	-4.76033400	0.76165500	1.32653200
H	-2.86456800	1.16318400	0.39768300
C	-6.04520500	-1.04002700	0.37144200
H	-5.14277300	-2.05076700	-1.29828100
C	-5.90813300	-0.03061200	1.32202800
H	-4.64471600	1.54444700	2.06748000
H	-6.92959400	-1.66662800	0.36700000
H	-6.68661200	0.13389600	2.05782400

P1a-OBn

C	-0.74002300	-2.03321700	-1.63735300
C	-0.21350400	-0.02335100	-0.41106100
C	-1.34187100	-0.77222100	0.30691300
C	-1.18260800	-2.21689900	-0.18110400
H	-1.60576000	-2.00630500	-2.30101900
H	-0.05719900	-2.79870200	-2.00148500
H	-0.51207700	1.01353300	-0.55386200
H	-0.42038700	-2.70926900	0.42344500
C	1.20902900	-0.04912300	0.23196400
H	1.59669800	0.96597000	0.19897900
C	2.06107700	-0.88569100	-0.75044700
N	-0.07377000	-0.69852300	-1.72789600
O	1.32987800	-0.81730000	-1.98810900
H	-1.28362100	-0.68212100	1.39576500

H	-2.10524000	-2.78979500	-0.08987200
C	1.23430000	-0.47254600	1.68199000
O	1.10621000	-1.60220500	2.09700800
O	1.37685400	0.59574000	2.47693000
C	1.37224300	0.33506700	3.89831900
H	2.20596600	-0.31553800	4.16185100
H	1.48024900	1.30777900	4.36951100
H	0.43343600	-0.13392900	4.19220600
C	2.42959300	-2.32346700	-0.39343800
H	2.99829000	-2.74189600	-1.22548000
H	3.03879900	-2.35248000	0.50903800
H	1.54122400	-2.92746700	-0.23295400
N	3.34363200	-0.22033100	-1.08820300
N	3.91799000	0.23396900	-0.09442800
C	5.21178500	0.79921100	-0.37644800
O	6.22639100	0.21152700	-0.11461000
C	-3.70782800	-0.57632600	0.58590400
H	-3.93158100	-1.63585800	0.42146400
H	-3.51131900	-0.43985700	1.65928300
O	-2.55379400	-0.17589900	-0.15179200
O	5.08298300	2.02848400	-0.84416600
C	6.31980400	2.75768200	-1.05967600
H	6.90169500	2.27204700	-1.84184300
H	6.01268100	3.75229500	-1.36749100
H	6.89315400	2.79530100	-0.13446500
C	-4.87595200	0.26904800	0.15390300
C	-6.05977200	-0.32048200	-0.29019500
C	-4.78772200	1.66438000	0.20097200
C	-7.14543600	0.46759800	-0.67265600
H	-6.13329300	-1.40152100	-0.33894600
C	-5.86628800	2.45308500	-0.18620900
H	-3.86751400	2.12722100	0.53792000
C	-7.05014800	1.85578600	-0.62245500
H	-8.05963700	-0.00311500	-1.01513800

H	-5.78705700	3.53338400	-0.14624700
H	-7.89072100	2.47054200	-0.92260300

P2a-OBn

C	0.42793500	-0.92992100	2.90526900
C	0.56829900	0.37643400	0.88431300
C	-0.73944200	0.75646800	1.61495800
C	-0.98620800	-0.39244400	2.60809300
H	0.74213000	-0.73357600	3.93080400
H	0.49352900	-1.99877300	2.70880400
H	1.05842700	1.28924300	0.54146600
H	-1.59382400	-1.17818100	2.16499800
C	0.68863000	-0.61653900	-0.30321800
H	0.66565700	-0.08147800	-1.24943600
C	2.13454100	-1.11976500	-0.02228800
N	1.35848000	-0.20598000	1.98390000
O	2.25305400	-1.18618000	1.37387700
H	-1.49401600	-0.02633700	3.50032900
C	-0.25305800	-1.79508500	-0.40508400
O	-0.55833000	-2.54841000	0.49072900
O	-0.68072800	-1.93675900	-1.66782100
C	-1.57556800	-3.04379000	-1.91853500
H	-1.10184900	-3.98246900	-1.63371500
H	-1.77215400	-3.01778800	-2.98631600
H	-2.49918000	-2.91041500	-1.35494900
C	2.54983000	-2.45494500	-0.62049600
H	3.58309300	-2.66424700	-0.33935700
H	2.48264200	-2.41808200	-1.70775300
H	1.91144000	-3.24987200	-0.23839700
N	3.01982600	-0.09400100	-0.66476300
N	3.72213100	0.53303600	0.13149800
C	4.50644500	1.56230600	-0.49518900
O	4.11794400	2.69801200	-0.56991200
H	-0.47378600	1.64198800	2.19620100

C	-2.47811400	0.29701000	-0.03866900
H	-1.92777200	0.21263500	-0.98015900
H	-2.52746000	-0.69805700	0.41495300
O	-1.82918900	1.21233200	0.83818700
O	5.68802700	1.08688400	-0.84995700
C	6.62422900	2.05629600	-1.38915300
H	6.79108100	2.85210800	-0.66449300
H	7.53770200	1.49840400	-1.57020600
H	6.23290100	2.47106600	-2.31715900
C	-3.87979400	0.77522000	-0.32161900
C	-4.62610800	1.43795800	0.65510600
C	-4.46329800	0.51331800	-1.56326200
C	-5.93777500	1.82741300	0.39405100
H	-4.16933500	1.65346300	1.61260600
C	-5.77783900	0.89552100	-1.82282700
H	-3.88509700	0.00951700	-2.33084800
C	-6.51899600	1.55499700	-0.84387100
H	-6.50738000	2.34422700	1.15804300
H	-6.21873500	0.68665000	-2.79070300
H	-7.53956300	1.85885000	-1.04546700

P3a-OBn

C	-1.25608700	-1.18339700	2.52711100
C	0.10585800	0.28232800	1.18453600
C	0.24984500	-1.16902300	0.68399500
C	-0.09768700	-1.98923400	1.93115700
H	-1.38892000	-1.35138400	3.59595700
H	-2.19142700	-1.40749000	2.01378300
H	1.05231000	0.63727800	1.59117400
H	-0.38573900	-3.01322100	1.69318000
C	-0.41839200	1.27832600	0.15036500
C	-1.94272300	1.31340600	0.46521000
N	-0.89074900	0.24357100	2.28755300
O	-2.05779500	0.98949100	1.82812500

H	-0.49881400	-1.37001100	-0.08431700
H	-0.26363600	0.89719000	-0.85556900
H	0.74729500	-2.01931600	2.62230600
C	0.20501900	2.65564300	0.31735200
O	0.53920000	3.09202100	1.39200800
O	0.35062800	3.43214300	-0.77034100
C	0.10171900	2.94587000	-2.10726300
H	0.24701600	3.80815800	-2.75220700
H	0.81745400	2.16661100	-2.37135000
H	-0.91822600	2.57846800	-2.21818800
C	-2.68615000	2.62438300	0.23709600
H	-2.68240200	2.90509600	-0.81558900
H	-3.72157200	2.49669400	0.55604800
H	-2.22943500	3.41490700	0.83117200
N	-2.55575800	0.33524900	-0.49188300
N	-3.20507400	-0.56798200	0.03762100
C	-3.71504600	-1.52624000	-0.90773400
O	-3.09553000	-2.51802900	-1.19039300
C	2.65353600	-1.46410700	0.84430300
H	2.56594600	-0.76613800	1.68497300
H	2.78758400	-2.46600500	1.26597100
O	1.48122800	-1.42519400	0.02951000
O	-4.93191500	-1.19149900	-1.29209600
C	-5.60776700	-2.13864200	-2.16201500
H	-5.66794600	-3.11015600	-1.67370600
H	-6.59704800	-1.72105700	-2.32039600
H	-5.06724200	-2.22389000	-3.10362600
C	3.85047400	-1.08624500	0.00914900
C	3.77635100	-0.02766500	-0.90105100
C	5.06064100	-1.76451900	0.16319400
C	4.89587200	0.34909700	-1.63737700
H	2.83576300	0.49145800	-1.03594300
C	6.18459200	-1.38527900	-0.56948000
H	5.12419600	-2.59537500	0.85780500

C	6.10489200	-0.32716200	-1.47207500
H	4.82590700	1.17091100	-2.34084100
H	7.11776800	-1.92139200	-0.44076500
H	6.97602400	-0.03390200	-2.04625000

P4a-OBn

C	1.95037600	-1.27882900	2.19378800
C	0.59181900	0.64387900	1.68137700
C	-0.29965900	-0.60029100	1.81959600
C	0.66268200	-1.75845300	1.51786100
H	1.97282100	-1.58411200	3.24250300
H	2.86363100	-1.62328700	1.71491800
H	0.22835900	1.48283800	2.27107300
H	0.78594900	-1.85275400	0.43558800
C	0.77579700	1.08497500	0.21739200
C	2.29941000	0.92190100	-0.03616900
N	1.92464200	0.21788600	2.17599100
O	2.88333900	0.76239000	1.24446700
H	0.23498500	0.43586100	-0.46672500
H	0.31806500	-2.71632800	1.90772200
C	0.28974100	2.49963200	-0.02368000
O	0.20238100	3.36586300	0.81498700
O	-0.01933400	2.67593500	-1.31422700
C	-0.44699700	4.00349200	-1.69261300
H	-0.64890500	3.94847500	-2.75846400
H	0.34362400	4.72492600	-1.48683800
H	-1.34728800	4.27762600	-1.14326100
C	3.02413900	2.06425400	-0.73491100
H	2.64883600	2.19493400	-1.74919700
H	4.08905100	1.83073500	-0.77602300
H	2.88235700	2.98714300	-0.17241700
N	2.43259400	-0.26062600	-0.94860100
N	3.30554500	-1.06340800	-0.62263500
C	3.35896800	-2.22059500	-1.52988400

O	2.36409100	-2.81414200	-1.89041800
N	4.63535300	-2.53176300	-1.80220900
H	4.84522100	-3.31213100	-2.40397700
H	5.39066800	-1.98978500	-1.41416800
H	-0.66188600	-0.67542300	2.85353400
C	-2.39391500	-1.48111300	1.09522900
H	-2.00817300	-2.45338000	0.76971200
H	-2.66025200	-1.56730200	2.15873100
O	-1.40109400	-0.46943300	0.94265100
C	-3.60291900	-1.10160200	0.28128400
C	-4.08235700	0.21184100	0.30245900
C	-4.27126200	-2.05588100	-0.48684500
C	-5.21285900	0.56144000	-0.42997700
H	-3.55725000	0.95714400	0.88715100
C	-5.40914800	-1.70952200	-1.21474400
H	-3.89866400	-3.07406600	-0.51961300
C	-5.88189300	-0.39962400	-1.18880000
H	-5.57370600	1.58339900	-0.40914600
H	-5.91851900	-2.46007800	-1.80800400
H	-6.76246300	-0.12700100	-1.75878100

P1b-OBn

C	-0.45354500	-2.31919900	1.04893300
C	0.00836700	-0.36352800	-0.28737300
C	-1.03822500	-0.01250900	0.77600600
C	-0.82077000	-1.07245400	1.86213500
H	-1.34758600	-2.89612800	0.80667100
H	0.25641400	-2.98403100	1.53769100
H	-0.36273700	-0.04982100	-1.26135400
H	-0.00660800	-0.74742800	2.51036800
C	1.45833900	0.18437200	-0.10624100
H	1.78152100	0.56957400	-1.06966200
C	2.31380800	-1.07284000	0.18051300
N	0.12862600	-1.84510300	-0.24317900

O	1.52336500	-2.15359000	-0.35000100
H	-0.93238400	1.00895700	1.15262100
H	-1.70576700	-1.21900100	2.48121500
C	1.58614700	1.32135500	0.87937800
O	1.51608800	1.22897100	2.08427600
O	1.75050600	2.48511400	0.23629300
C	1.84246100	3.66199600	1.06943400
H	2.70998400	3.58937500	1.72518800
H	1.95054300	4.49489700	0.38058100
H	0.93833000	3.77093400	1.66809700
C	2.76830300	-1.36159000	1.61032600
H	3.32595800	-2.29952200	1.60317800
H	3.41113300	-0.56340700	1.97896000
H	1.91832900	-1.46127200	2.27897100
N	3.54343800	-1.11774700	-0.64087900
N	4.13646600	-0.03855800	-0.66163400
C	5.39712200	-0.10034500	-1.44632200
O	5.87607000	-1.11367400	-1.90159100
N	5.88331400	1.14708400	-1.53738700
H	6.73457500	1.32476500	-2.04622300
H	5.38751800	1.91294500	-1.11009100
C	-3.39556400	0.38602200	0.88157300
H	-3.54428600	-0.17901100	1.80785400
H	-3.16929900	1.42648700	1.15095100
O	-2.30333400	-0.15019900	0.12987900
C	-4.62954600	0.31479700	0.02566500
C	-5.59481500	-0.67001000	0.24084200
C	-4.80144300	1.21552500	-1.02986500
C	-6.71945000	-0.75141700	-0.57940800
H	-5.46524500	-1.37549100	1.05451100
C	-5.92123300	1.13646200	-1.85214000
H	-4.05317500	1.98115800	-1.20362700
C	-6.88382500	0.15150400	-1.62741900
H	-7.46414500	-1.51835800	-0.40081200

H	-6.04659800	1.84226400	-2.66508600
H	-7.75774400	0.09053700	-2.26551000

P2b-OBn

C	-0.91615700	-0.11730200	2.91942400
C	-0.85792300	-0.72626300	0.58860300
C	0.42834100	-1.25984200	1.25933200
C	0.54452200	-0.47073800	2.57469400
H	-1.27360000	-0.63911400	3.80767700
H	-1.03963400	0.95538200	3.05905100
H	-1.26646600	-1.50621800	-0.05593000
H	1.12120000	0.44109300	2.44046300
C	-0.97417900	0.58191900	-0.23738800
H	-0.86341400	0.37313700	-1.29859900
C	-2.46417000	0.91089200	0.07653200
N	-1.74552000	-0.55459400	1.75283500
O	-2.66419900	0.52802700	1.41401700
H	1.02584700	-1.07442300	3.34408000
C	-0.10380000	1.77073500	0.10183800
O	0.11243200	2.20988400	1.20798000
O	0.37518000	2.32748200	-1.02011400
C	1.21399400	3.49172800	-0.84709200
H	0.67718600	4.26512700	-0.29917200
H	1.45346200	3.82503400	-1.85262400
H	2.12122600	3.21919800	-0.30721300
C	-2.91530500	2.35461000	-0.09212600
H	-3.97294500	2.42920900	0.16531900
H	-2.78270000	2.67233400	-1.12605800
H	-2.34382500	3.00284700	0.57028100
N	-3.24671400	0.12474700	-0.92562100
N	-3.94958700	-0.76159400	-0.44345200
C	-4.70252000	-1.50306900	-1.49190500
O	-4.74789800	-1.19780500	-2.66233100
N	-5.30965000	-2.54245000	-0.89785900

H	-5.86870700	-3.18268000	-1.43870200
H	-5.20061100	-2.68714200	0.09303800
H	0.18752400	-2.29355200	1.51638200
C	2.22860400	-0.23176700	-0.03335800
H	1.71538400	0.14008500	-0.92504400
H	2.21418800	0.56153900	0.72111600
O	1.58683200	-1.40215300	0.46104600
C	3.66106800	-0.54785700	-0.38322200
C	4.38207600	-1.51471200	0.31992300
C	4.29592500	0.16922400	-1.40025100
C	5.71930500	-1.75683300	0.01247400
H	3.88680100	-2.07947800	1.09920500
C	5.63520400	-0.06622900	-1.70274400
H	3.73807500	0.91374000	-1.95877600
C	6.35110300	-1.03207200	-0.99698100
H	6.26879000	-2.51250000	0.56226900
H	6.11593000	0.49703500	-2.49427000
H	7.39127500	-1.22143400	-1.23511300

P3b--OBn

C	-1.53624600	-1.75077700	2.09635500
C	-0.23515200	0.01503800	1.09770700
C	0.07587200	-1.32211500	0.39531300
C	-0.27517500	-2.35625100	1.46998800
H	-1.71253100	-2.09279500	3.11635900
H	-2.41493100	-1.96789400	1.48919400
H	0.64555600	0.37652100	1.62794900
H	-0.45724900	-3.34705700	1.05353800
C	-0.77999600	1.11583200	0.18795300
C	-2.31848600	0.96606000	0.37120500
N	-1.29502000	-0.27753200	2.09858300
O	-2.49565300	0.42666000	1.65778600
H	-0.59728100	-1.46005400	-0.45170600
H	-0.51536200	0.91681200	-0.84716700

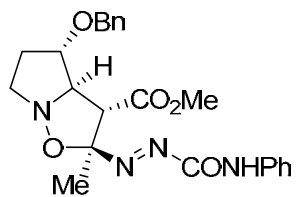
H	0.52423200	-2.43395600	2.21033700
C	-0.30969900	2.49574500	0.61988700
O	-0.10529800	2.78123600	1.77481200
O	-0.15449300	3.44683200	-0.31833700
C	-0.25008400	3.16348300	-1.73094400
H	-0.13409600	4.12682300	-2.22008000
H	0.55305500	2.49541900	-2.04420900
H	-1.21997800	2.74014800	-1.99076400
C	-3.16950600	2.22677600	0.27648200
H	-3.11334300	2.66754400	-0.71830300
H	-4.20858200	1.96228100	0.47833800
H	-2.84107100	2.95172700	1.02019100
N	-2.75987400	0.09570500	-0.76896000
N	-3.32552500	-0.94717700	-0.43760900
C	-3.64089900	-1.80057400	-1.57475600
O	-2.91466600	-2.74982600	-1.79565900
N	-4.76829700	-1.46627200	-2.21417500
H	-5.10990700	-2.05247000	-2.96035000
H	-5.29493900	-0.64606500	-1.95988500
C	2.47937500	-1.45003700	0.70447300
H	2.27290800	-0.90073500	1.63037900
H	2.66872500	-2.49312800	0.97911500
O	1.36767900	-1.36912800	-0.18897900
C	3.69417200	-0.85885300	0.03598000
C	3.60016900	0.34578600	-0.66751600
C	4.93568000	-1.48758700	0.14105000
C	4.73006300	0.91292500	-1.24940300
H	2.63642100	0.83015400	-0.76363600
C	6.07017500	-0.91828700	-0.43627400
H	5.01575100	-2.42859800	0.67480300
C	5.96988700	0.28326100	-1.13359100
H	4.64471900	1.84649000	-1.79370900
H	7.02808100	-1.41773200	-0.34808600
H	6.84937700	0.72475700	-1.58761400

P4b-OBn

C	1.64045400	-0.64053600	2.63530200
C	0.17082700	1.04071300	1.73246100
C	-0.62566200	-0.24301400	2.00477700
C	0.45251100	-1.33708100	1.96427200
H	1.62216400	-0.79395400	3.71651700
H	2.60886900	-0.95633100	2.25636600
H	-0.31493100	1.92858000	2.13247500
H	0.67334800	-1.58882800	0.92347300
C	0.45802900	1.24256600	0.23342500
C	2.00847000	1.30519600	0.15215000
N	1.47531600	0.82871600	2.39854100
O	2.46799600	1.35234800	1.49082100
H	0.11105400	0.39642400	-0.35510000
H	0.15751200	-2.25107800	2.47959100
C	-0.22147500	2.47563200	-0.32685300
O	-0.55939700	3.44368400	0.31307300
O	-0.38970100	2.35712400	-1.64925600
C	-0.99545100	3.48507800	-2.32020300
H	-1.05627500	3.19908500	-3.36627800
H	-0.37370400	4.37188700	-2.19860200
H	-1.98867300	3.67268100	-1.91317600
C	2.62338300	2.48280800	-0.59236000
H	2.34842800	2.45504900	-1.64612800
H	3.70955200	2.42991000	-0.50579800
H	2.27413700	3.41525700	-0.14897200
N	2.42014800	0.08641500	-0.61577400
N	3.24589500	-0.62861900	-0.04524500
C	3.57075700	-1.81886800	-0.78521700
O	3.01685300	-2.86471000	-0.56920600
H	-1.07304700	-0.19255100	3.00589900
C	-2.58948800	-1.38585400	1.27802100
H	-2.11519700	-2.36982000	1.18914400

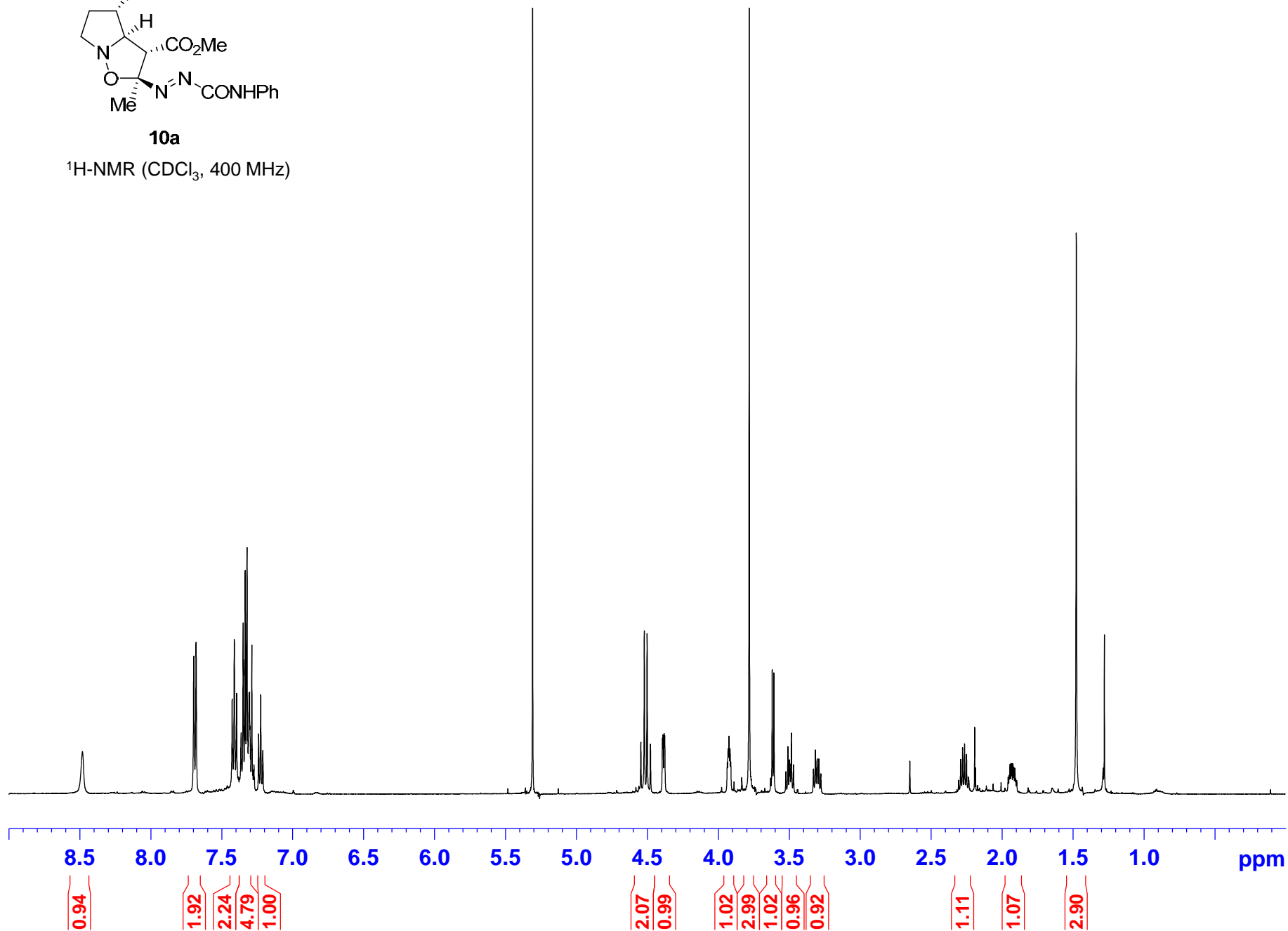
H	-2.97072600	-1.29376800	2.30576200
O	-1.64638700	-0.34894900	1.03280800
O	4.58060300	-1.59199900	-1.60564300
C	5.08301400	-2.74717800	-2.32807300
H	5.92639300	-2.37721300	-2.90264100
H	5.39851600	-3.51507000	-1.62312600
H	4.30697000	-3.13713100	-2.98524200
C	-3.72048900	-1.26564400	0.28922400
C	-4.14965700	-0.01174000	-0.15454500
C	-4.37158600	-2.41023700	-0.17512200
C	-5.21462100	0.09310600	-1.04575700
H	-3.63820600	0.87629300	0.19445200
C	-5.44329700	-2.30594900	-1.05985200
H	-4.03619200	-3.38834400	0.15329100
C	-5.86706300	-1.05305600	-1.49883000
H	-5.53579600	1.07063600	-1.38698100
H	-5.93947700	-3.20252100	-1.41307300
H	-6.69589600	-0.97041600	-2.19219400

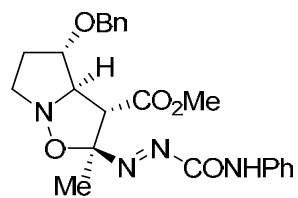
Spectra of compounds



10a

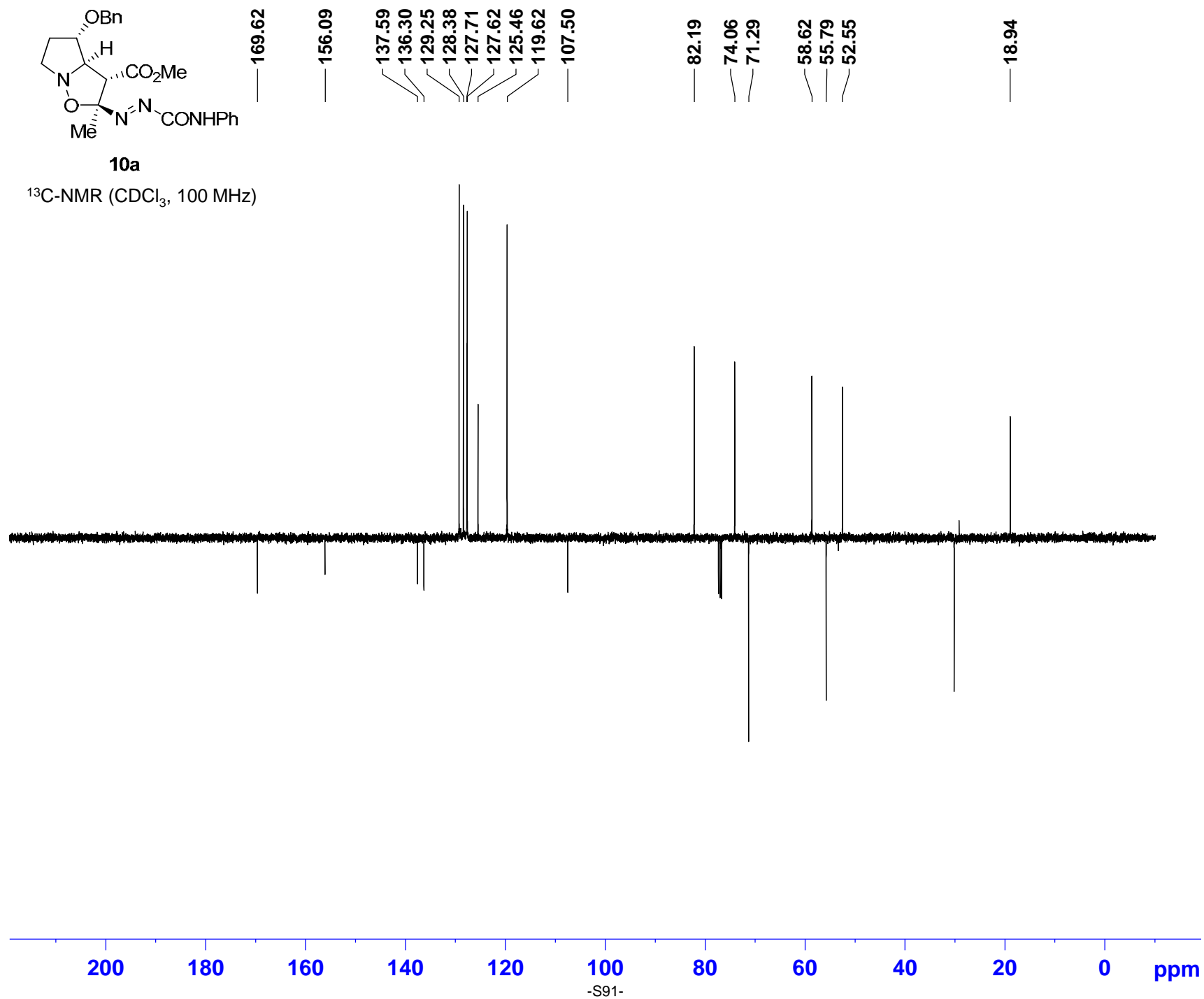
¹H-NMR (CDCl₃, 400 MHz)

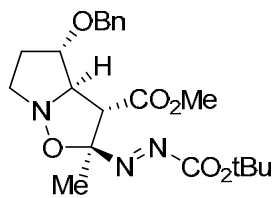




10a

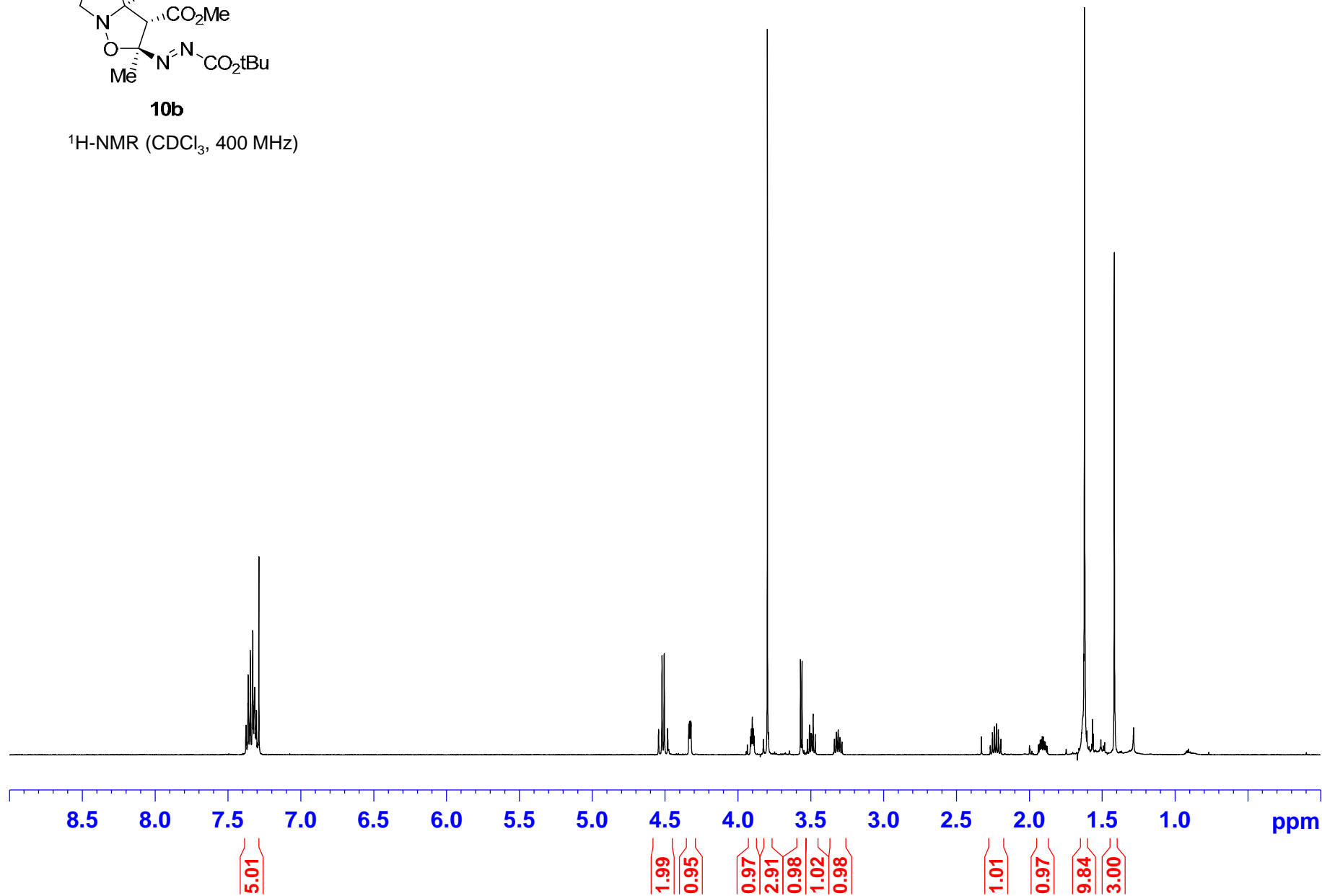
¹³C-NMR (CDCl₃, 100 MHz)

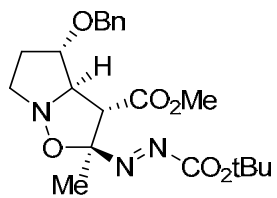




10b

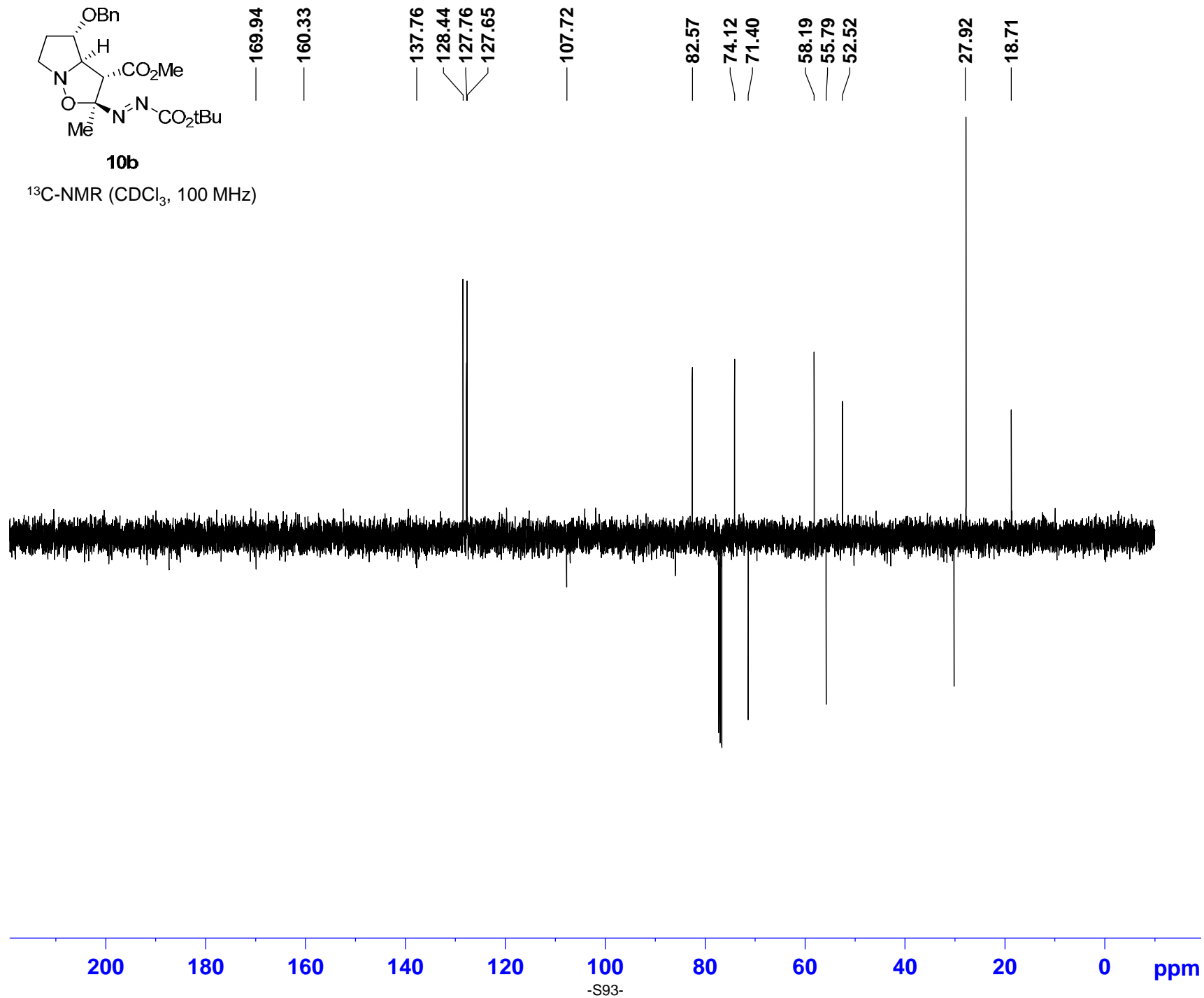
¹H-NMR (CDCl₃, 400 MHz)

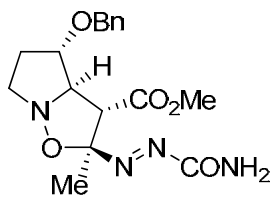




10b

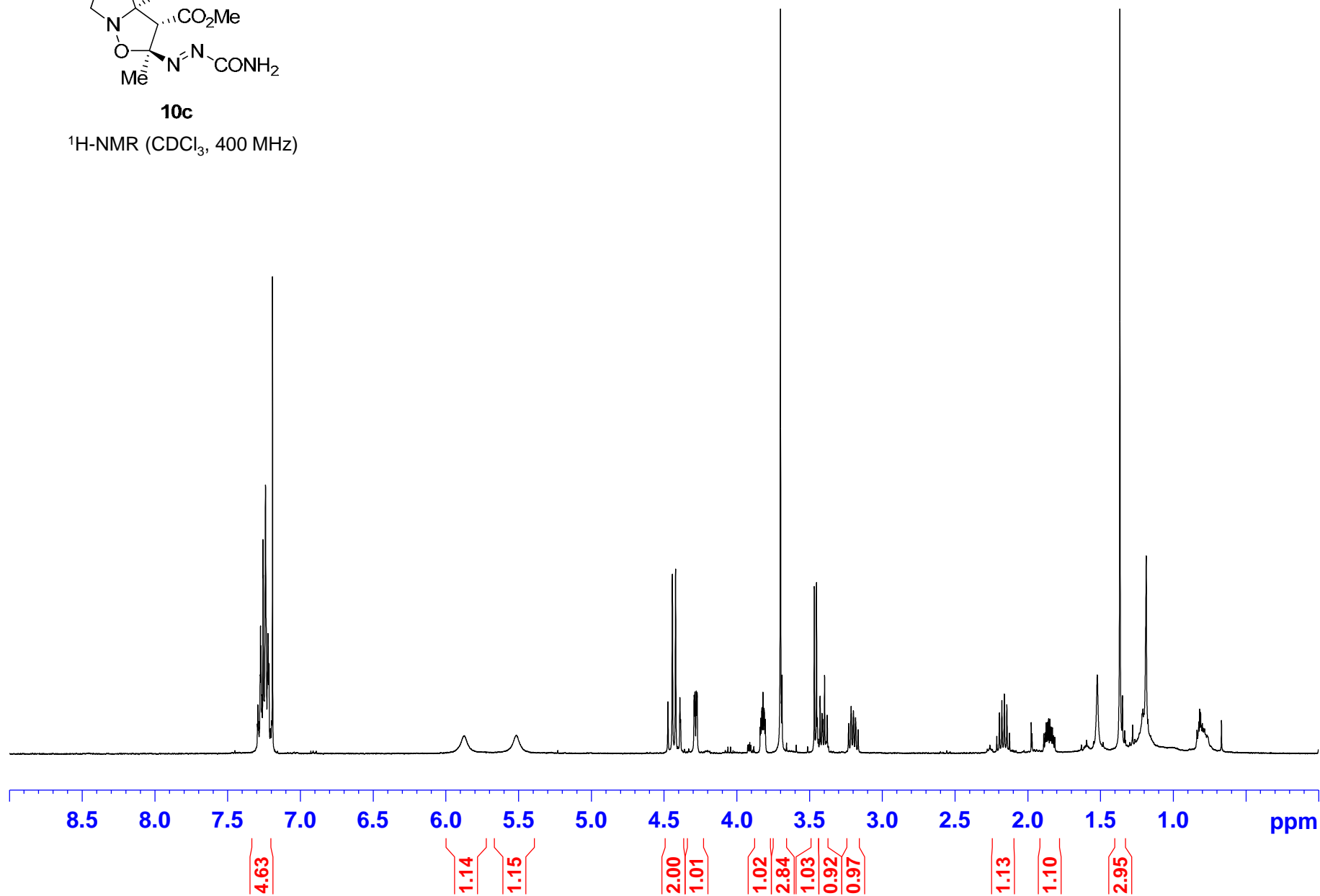
¹³C-NMR (CDCl₃, 100 MHz)

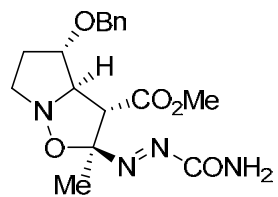




10c

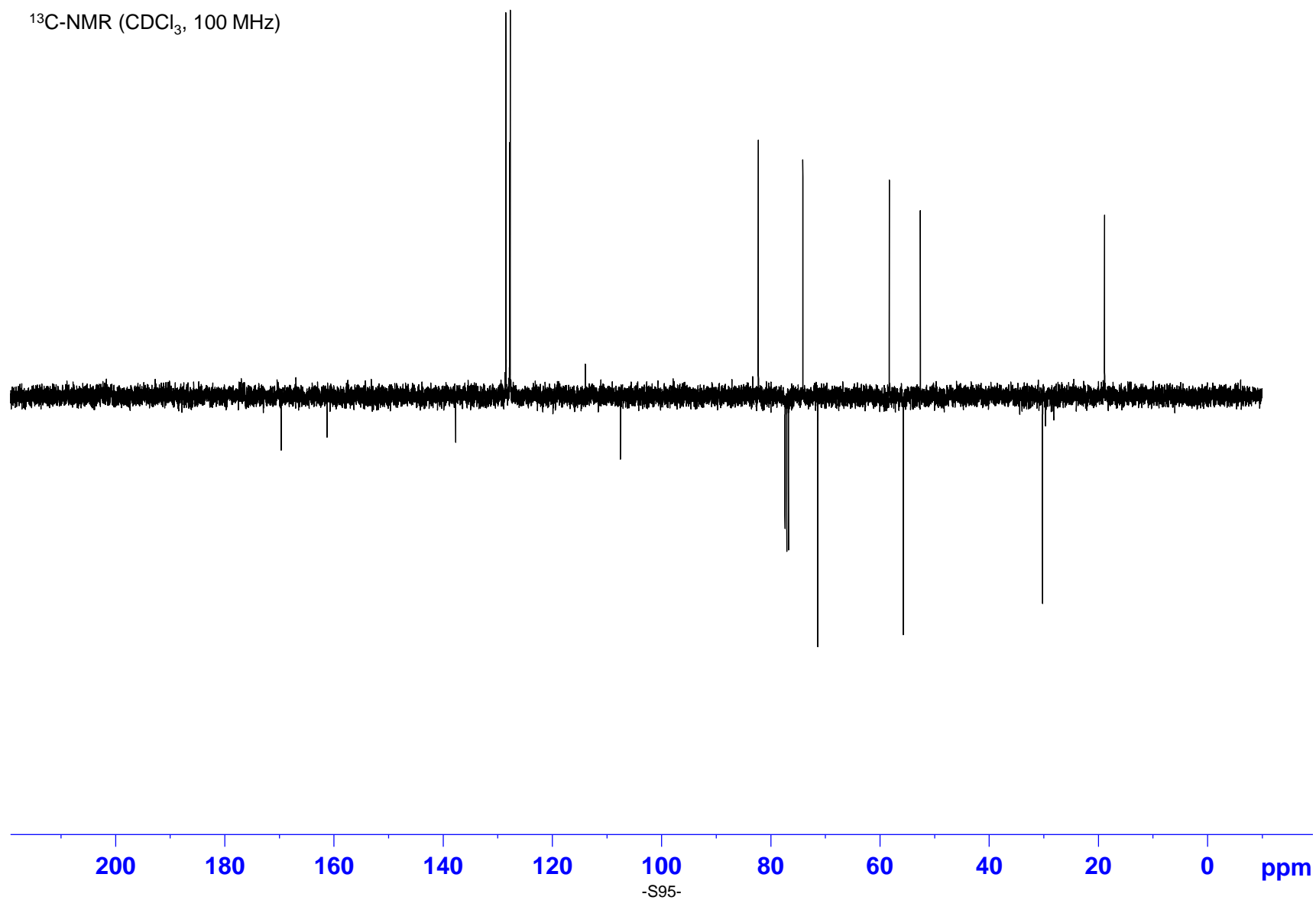
¹H-NMR (CDCl₃, 400 MHz)

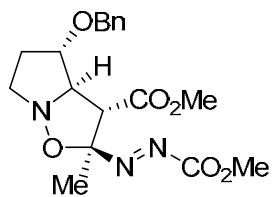




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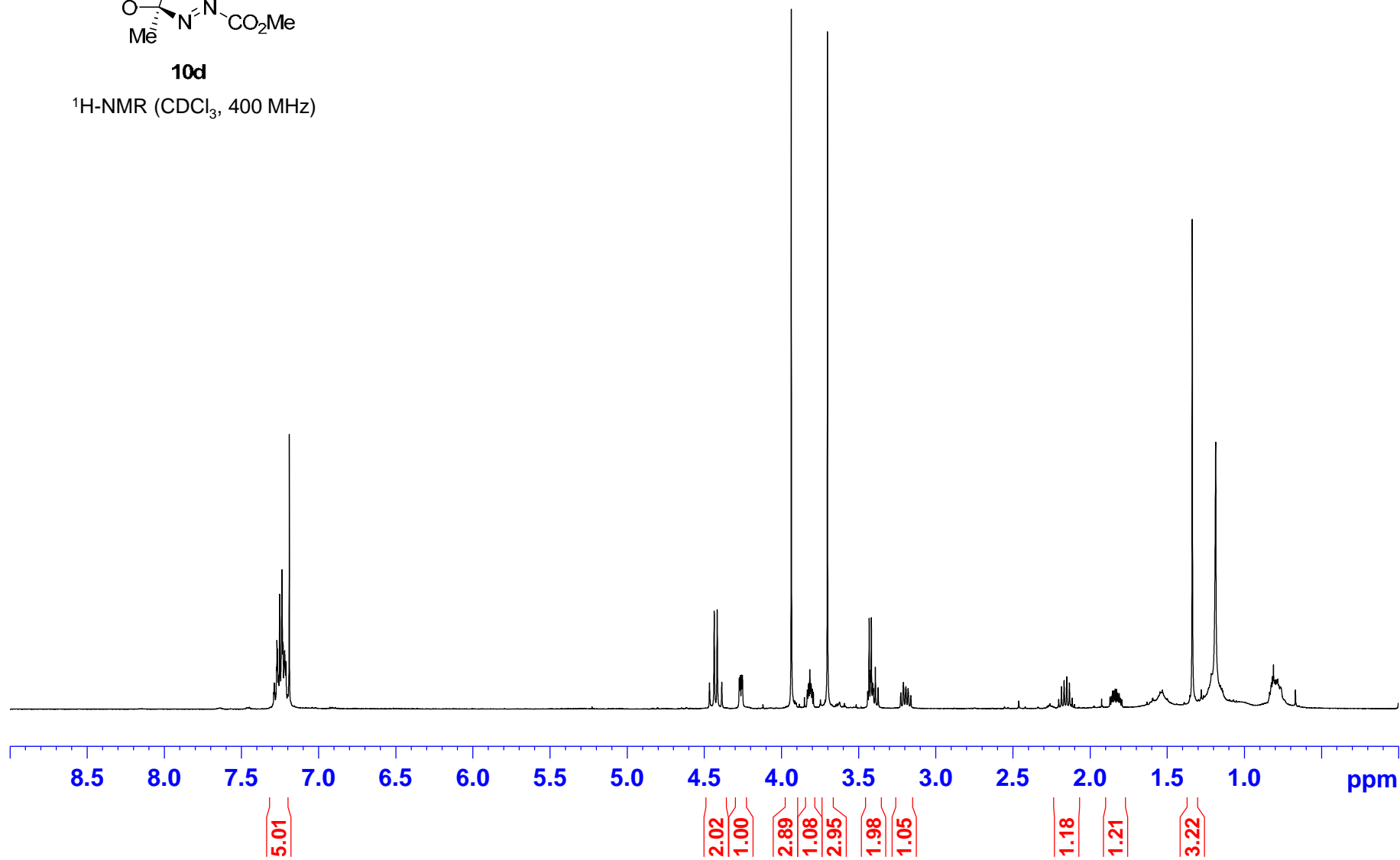
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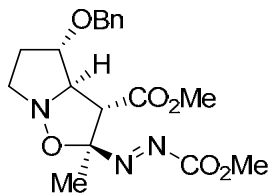




10d

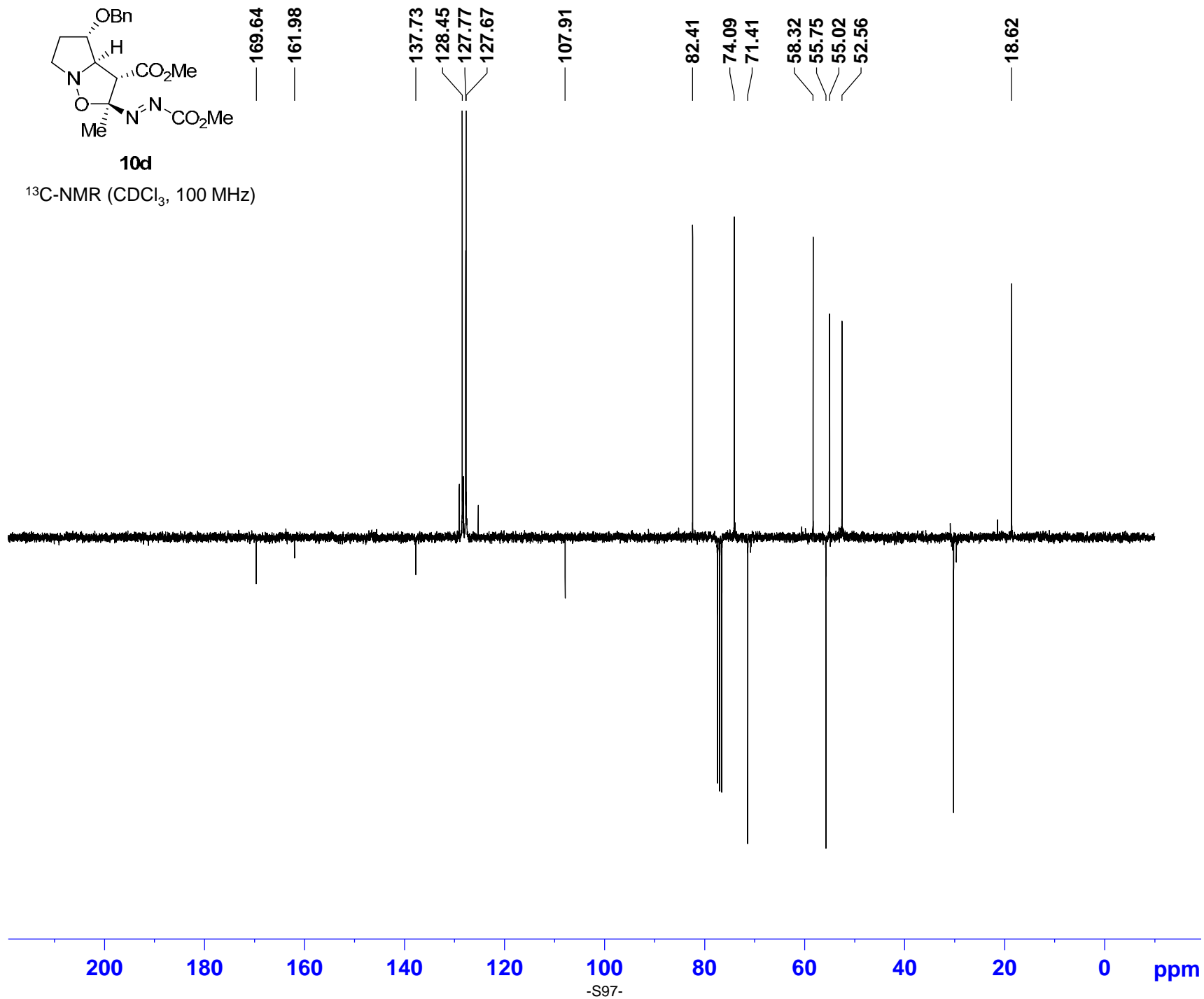
¹H-NMR (CDCl₃, 400 MHz)

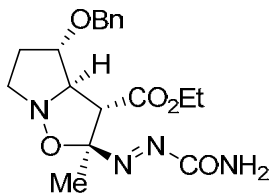




10d

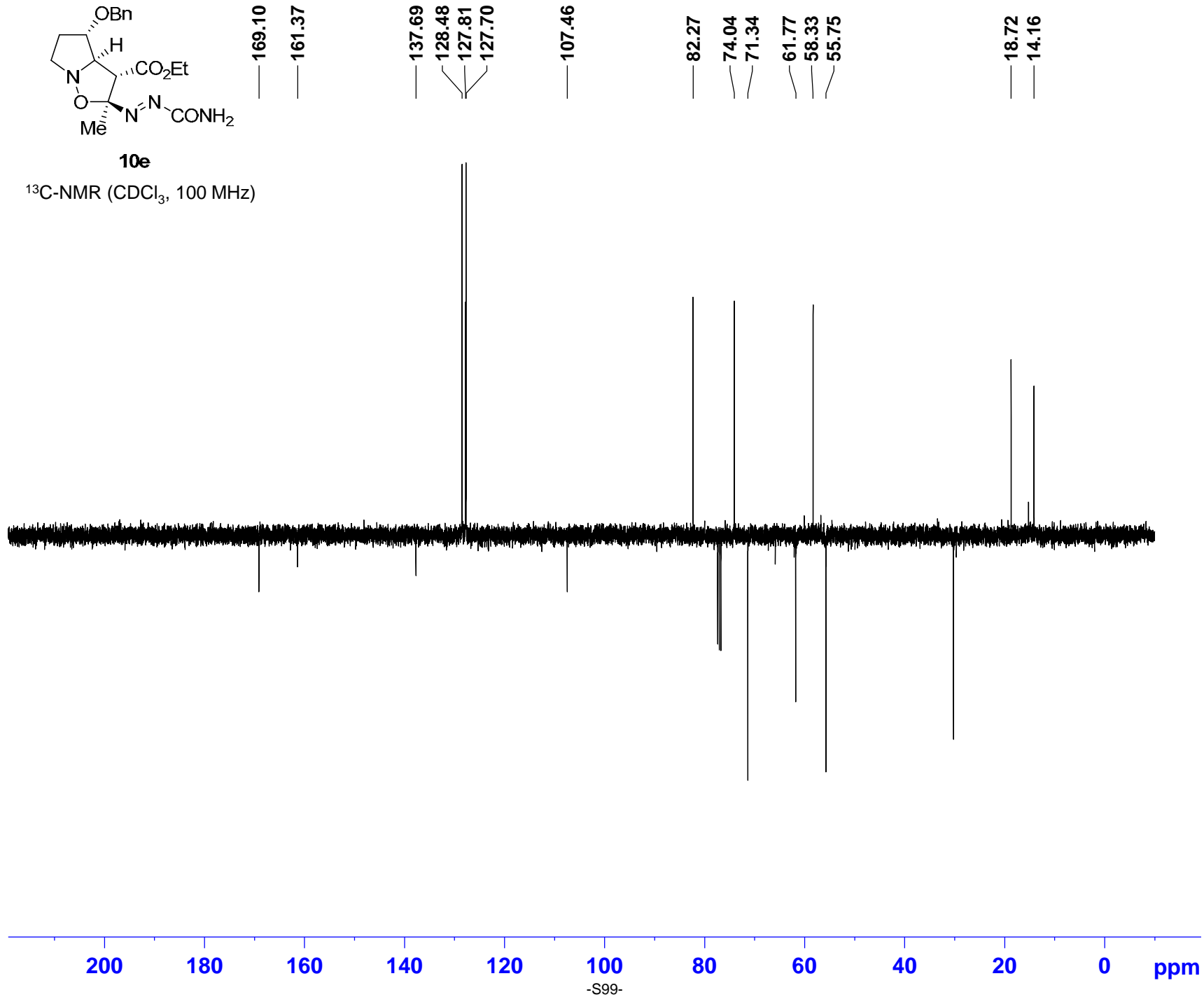
¹³C-NMR (CDCl₃, 100 MHz)

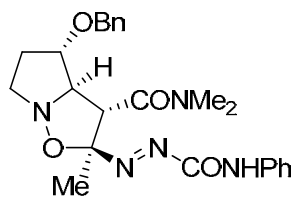




10e

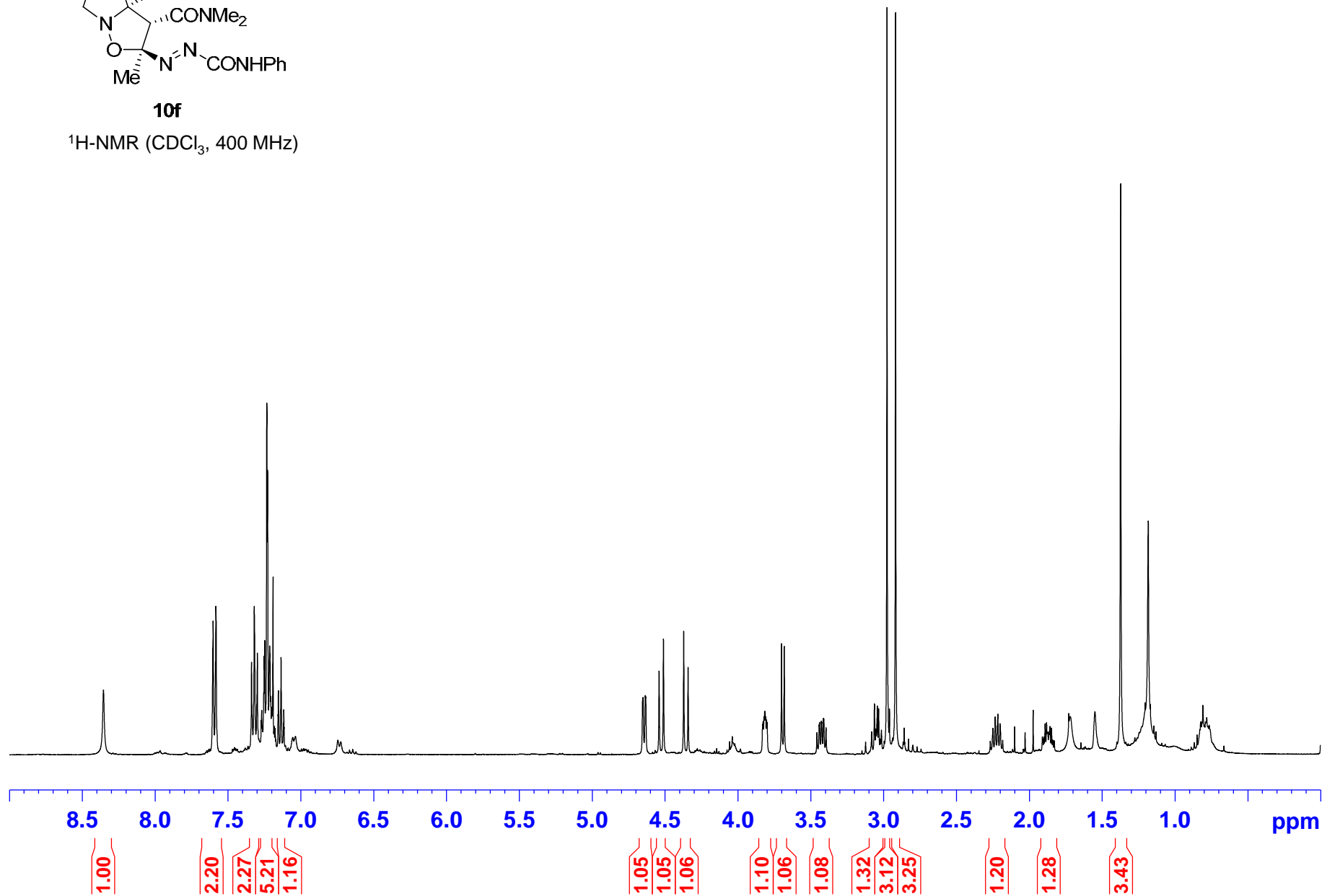
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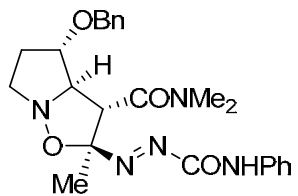




10f

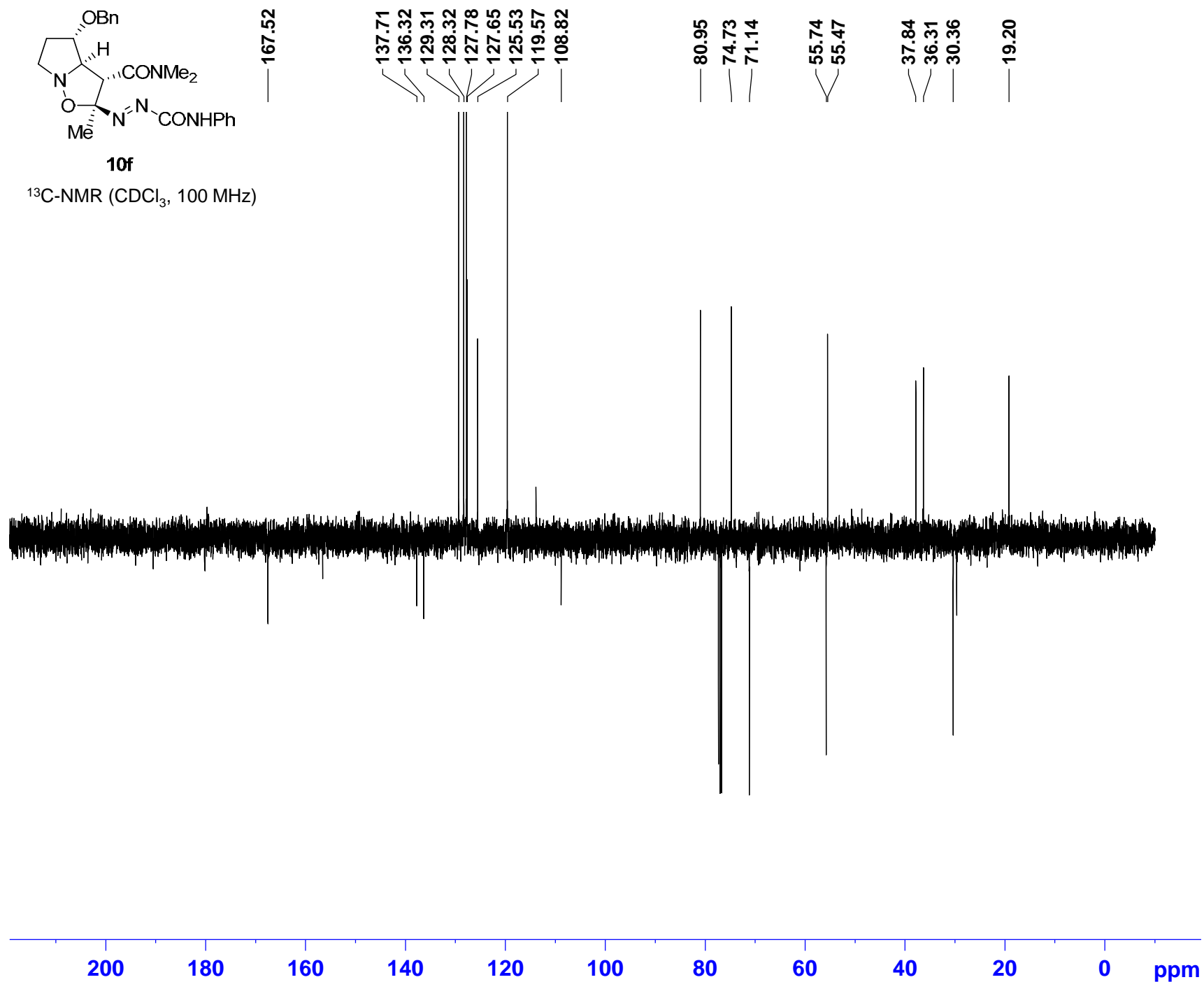
¹H-NMR (CDCl₃, 400 MHz)

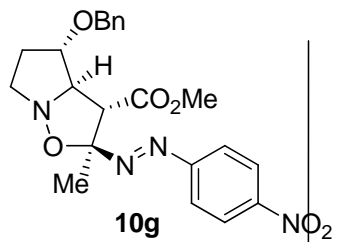




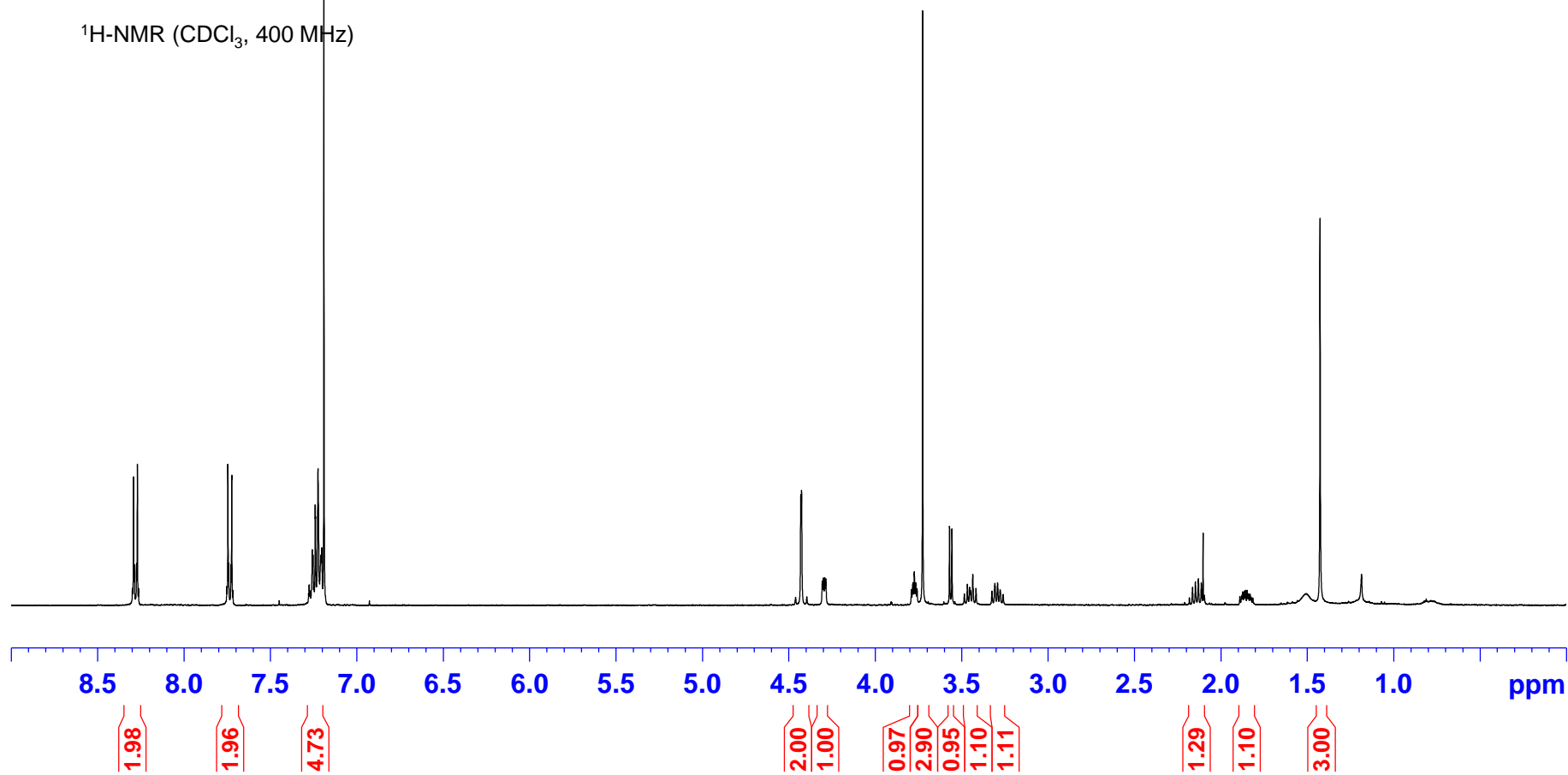
10f

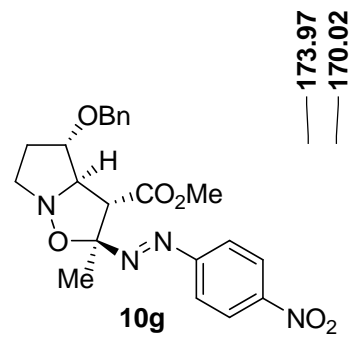
¹³C-NMR (CDCl₃, 100 MHz)



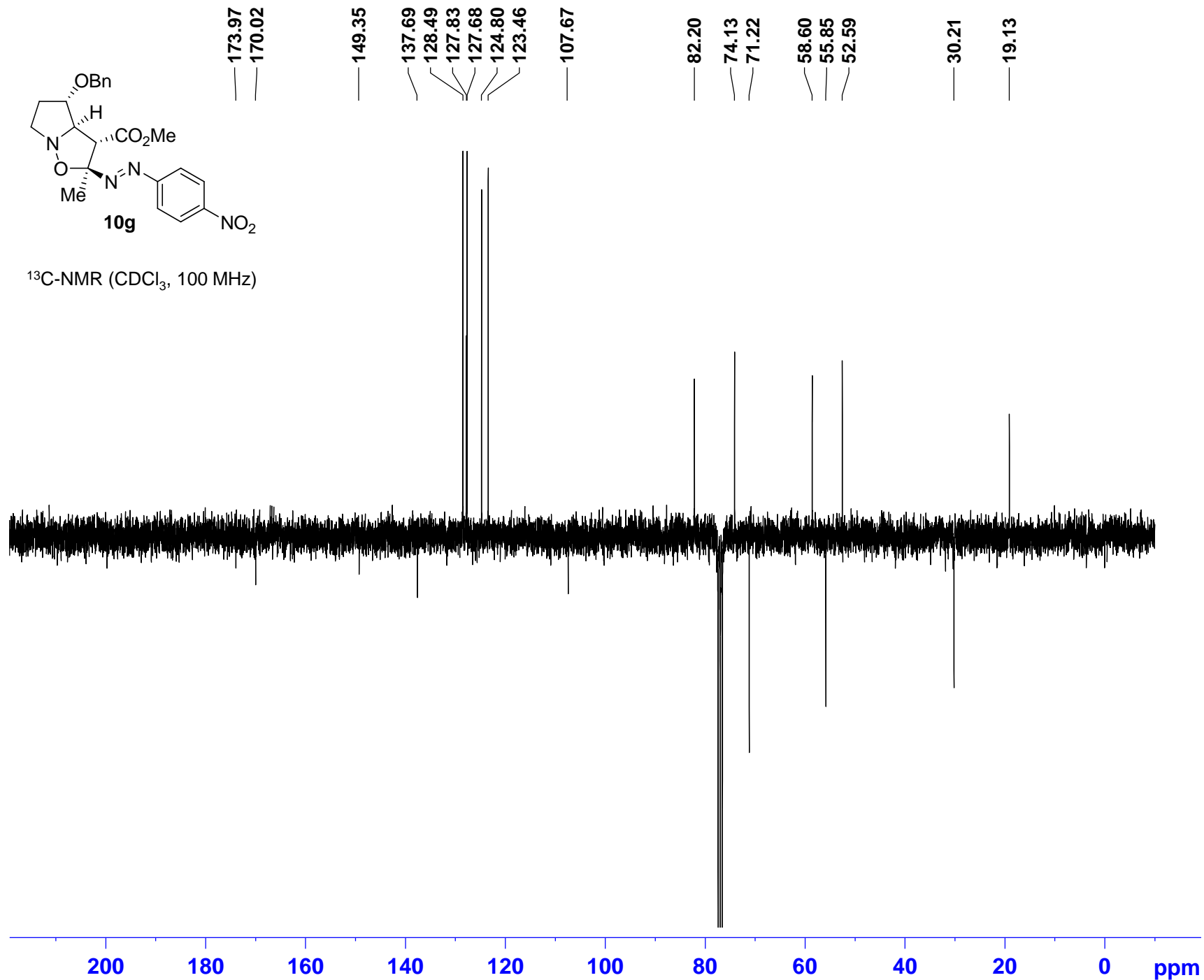


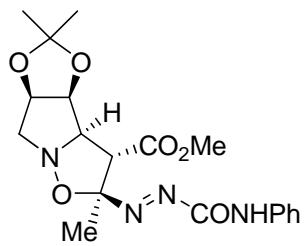
$^1\text{H-NMR}$ (CDCl_3 , 400 MHz)





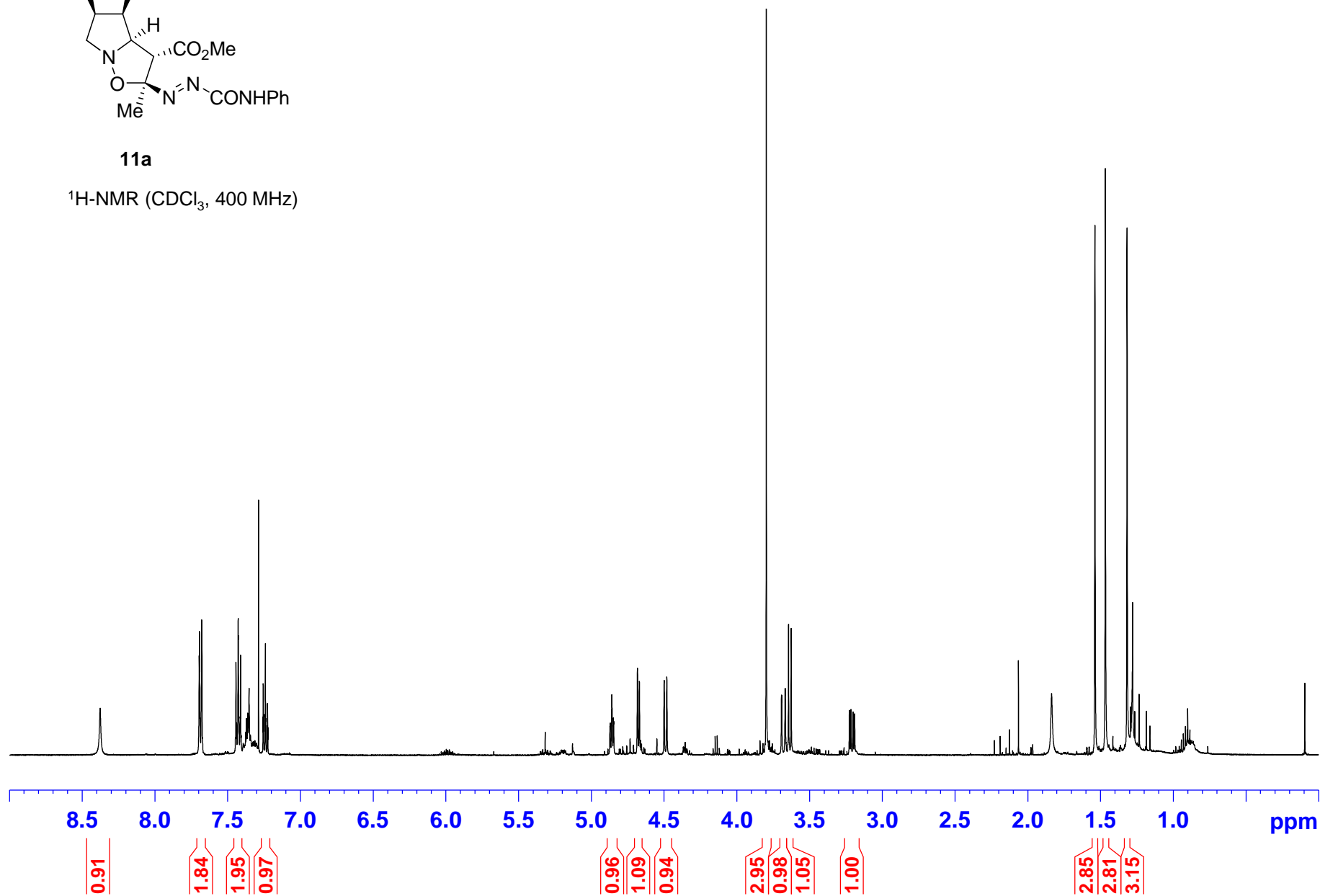
$^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz)

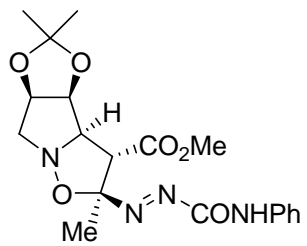




11a

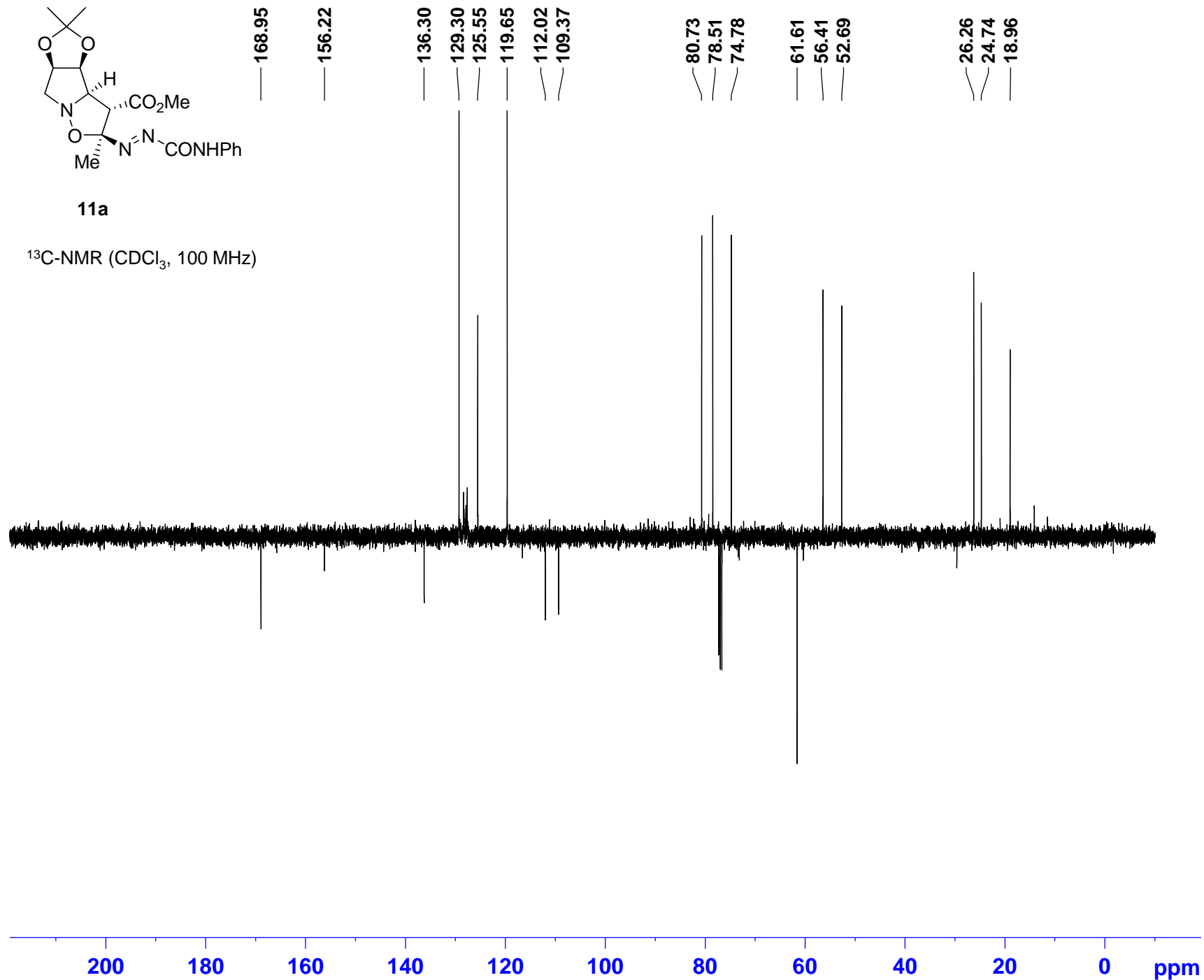
¹H-NMR (CDCl₃, 400 MHz)

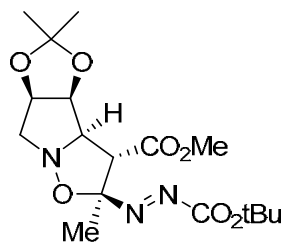




11a

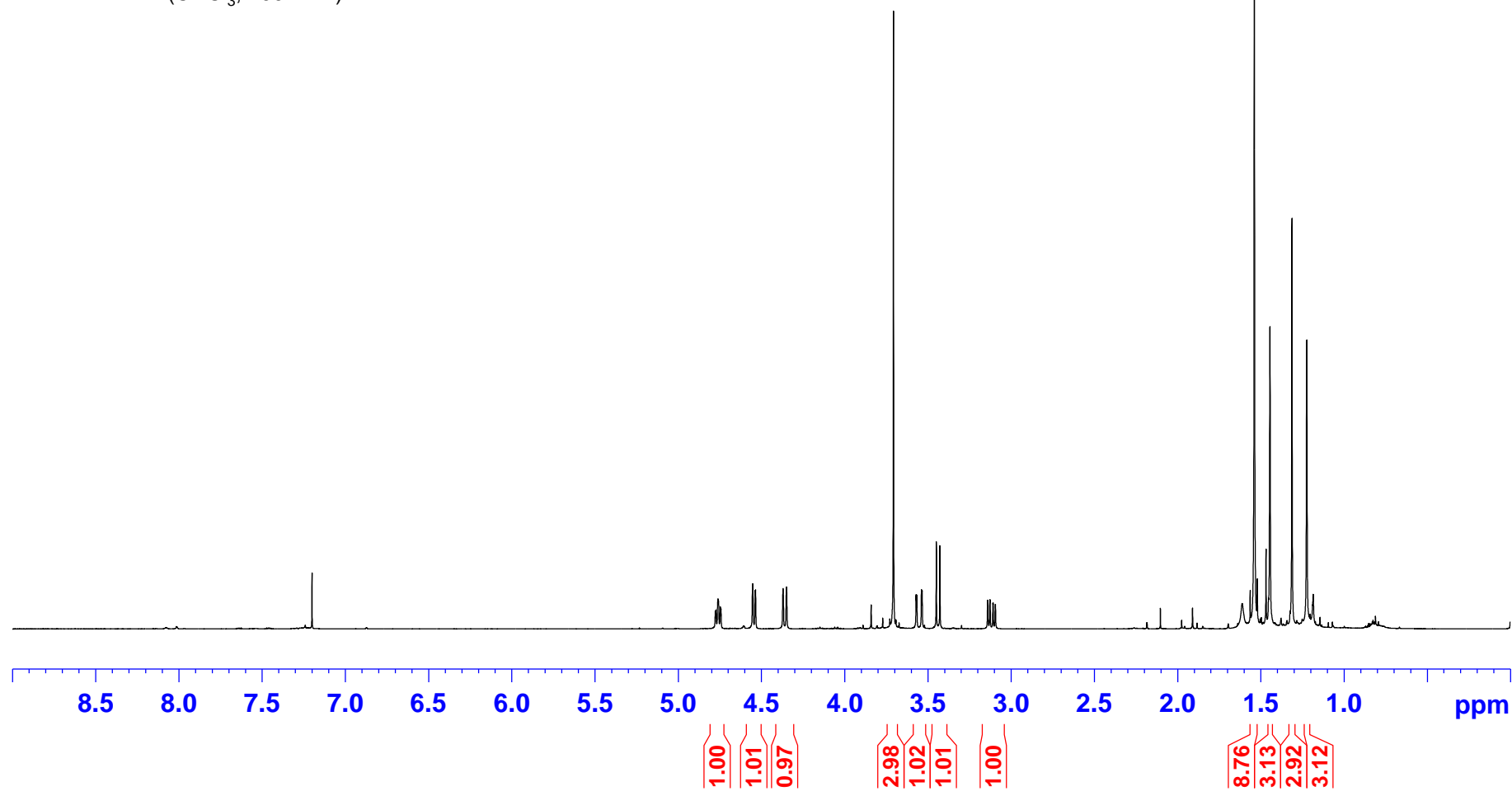
¹³C-NMR (CDCl₃, 100 MHz)

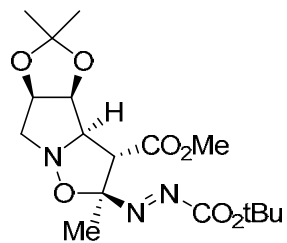




11b

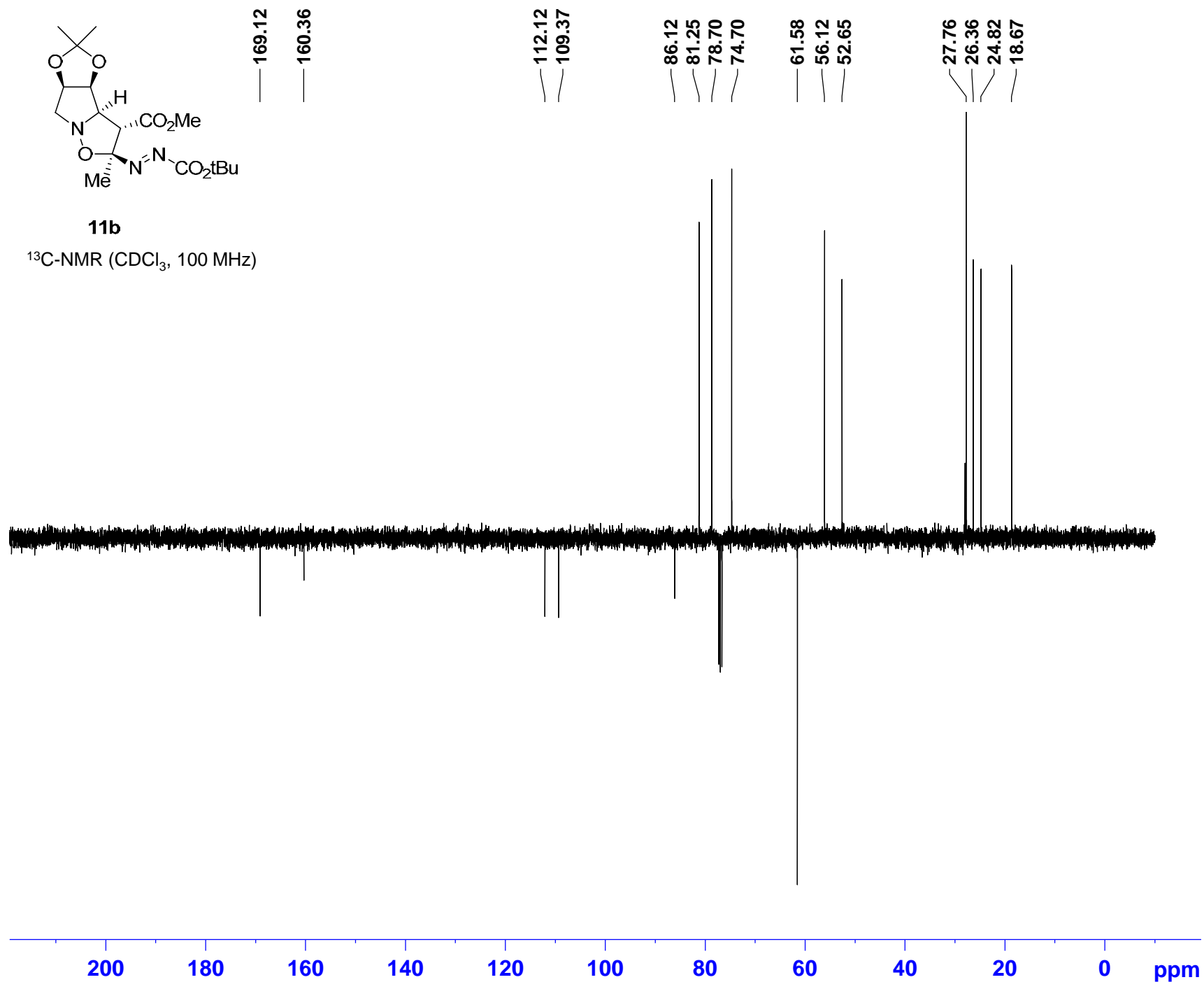
¹H-NMR (CDCl₃, 400 MHz)

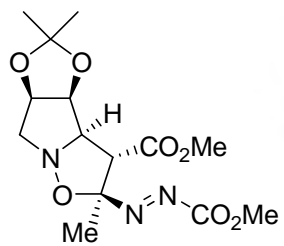




11b

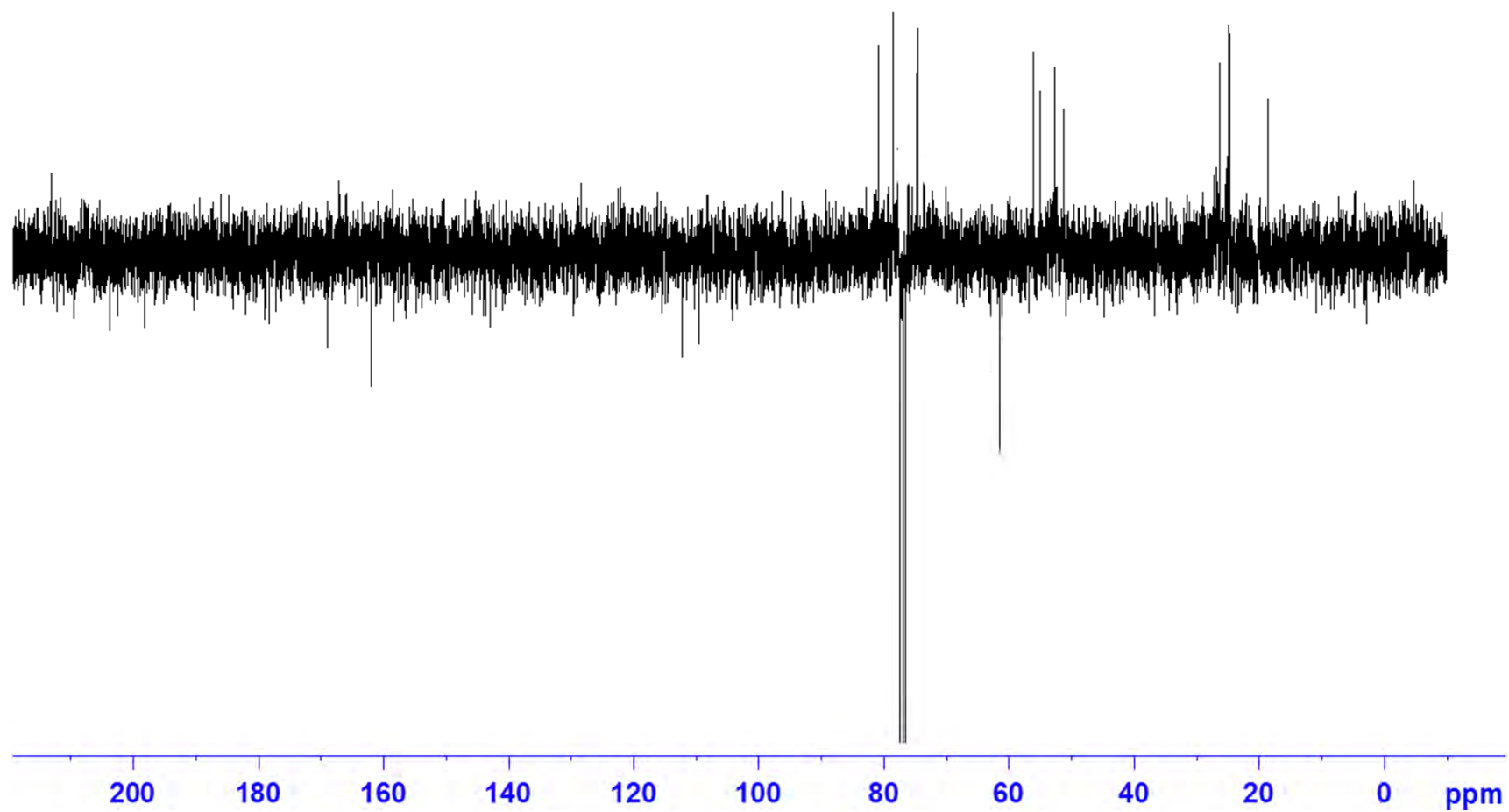
¹³C-NMR (CDCl₃, 100 MHz)

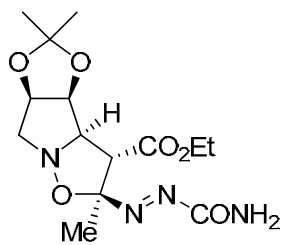




11d

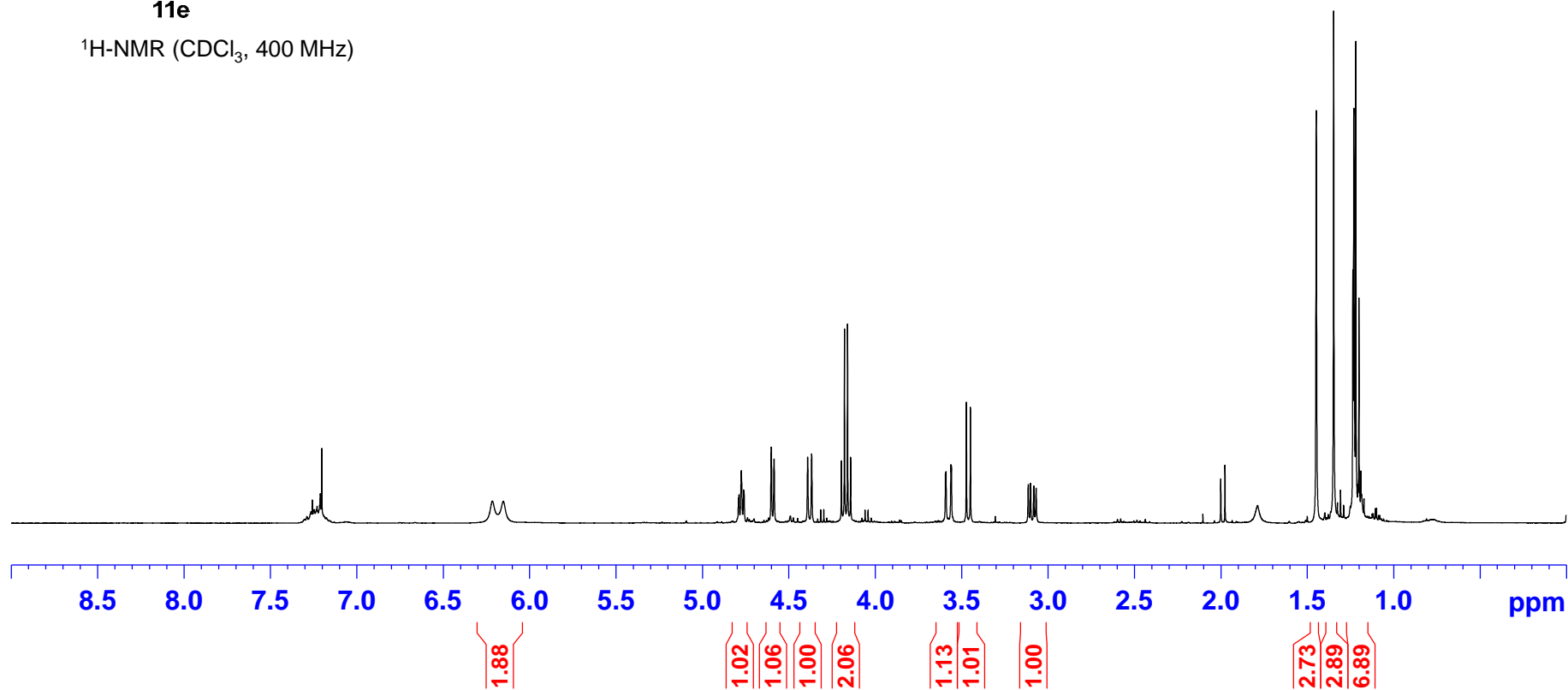
¹³C-NMR (CDCl₃, 100 MHz)

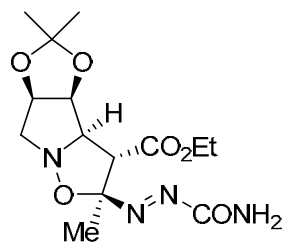




11e

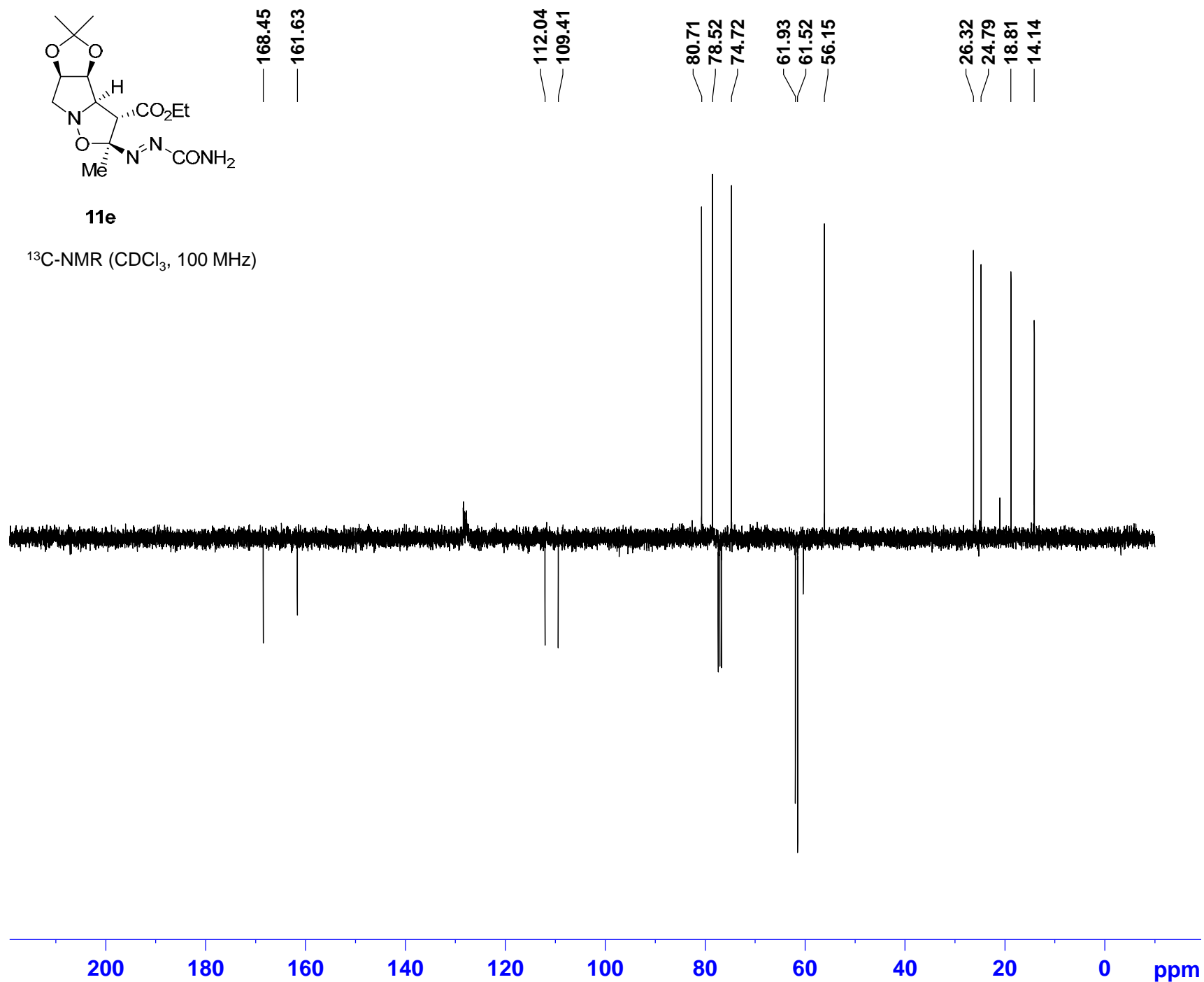
¹H-NMR (CDCl₃, 400 MHz)

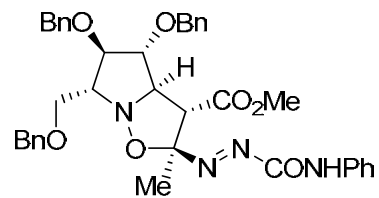




11e

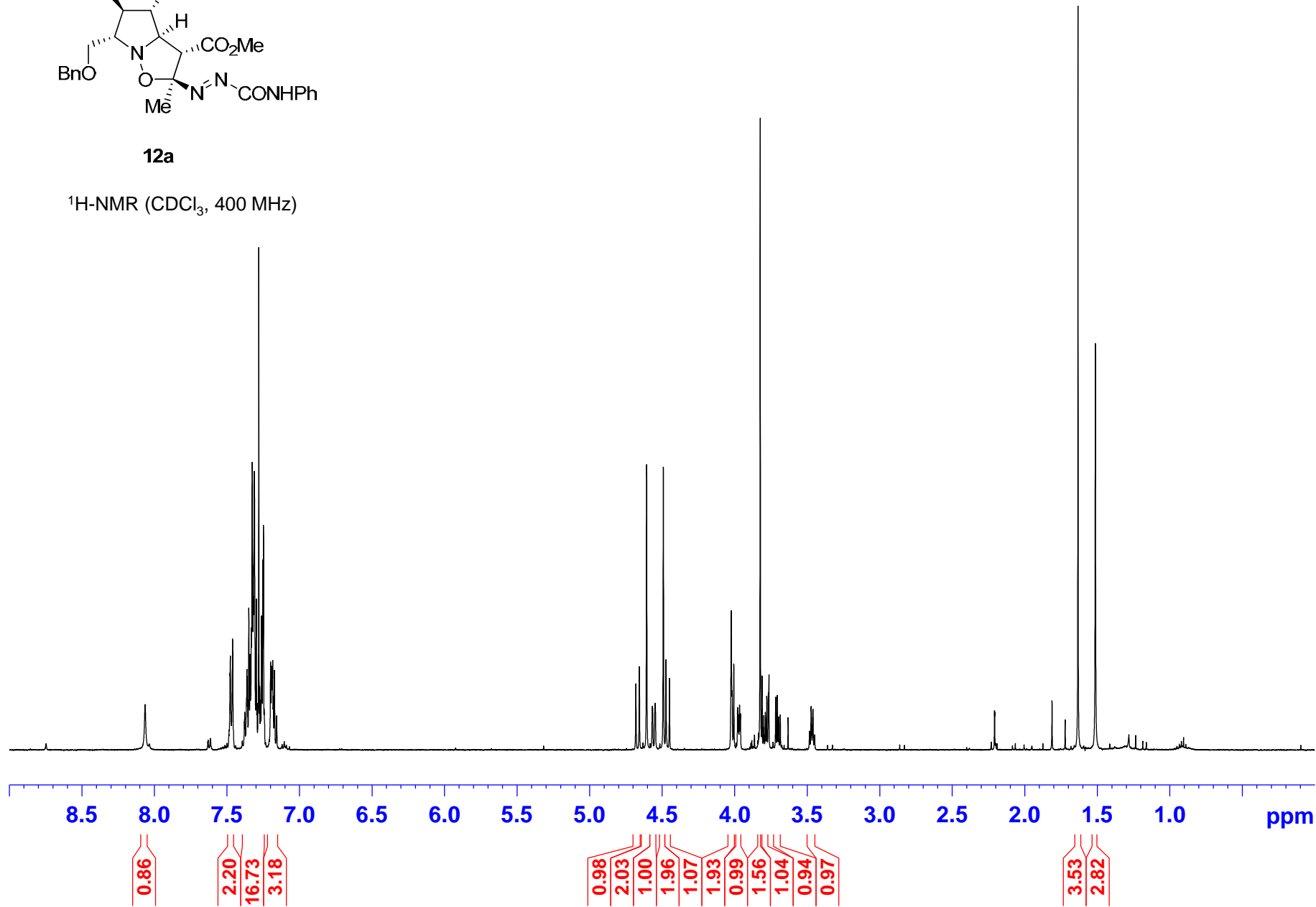
^{13}C -NMR (CDCl_3 , 100 MHz)

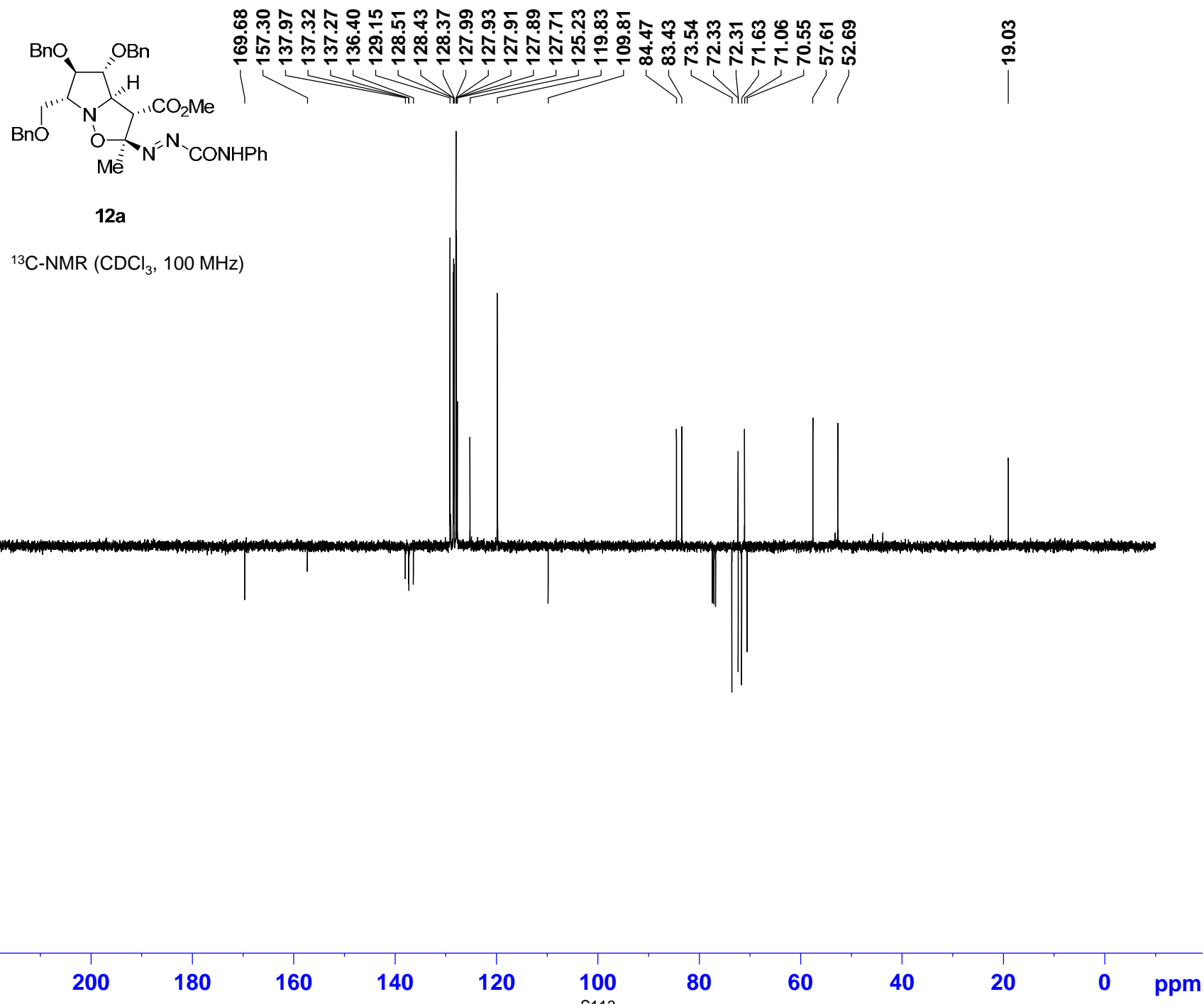


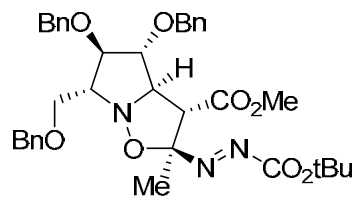


12a

¹H-NMR (CDCl₃, 400 MHz)

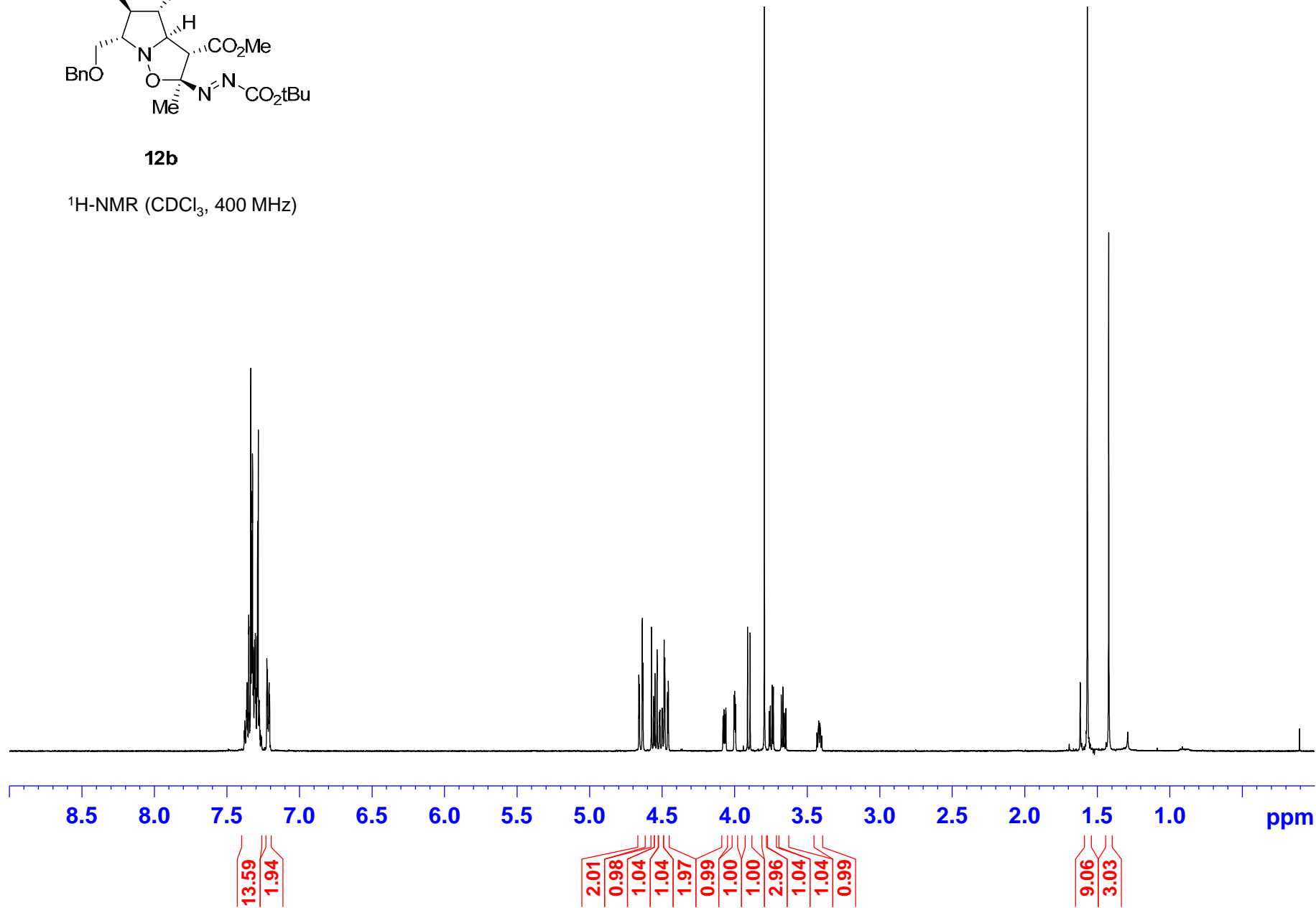


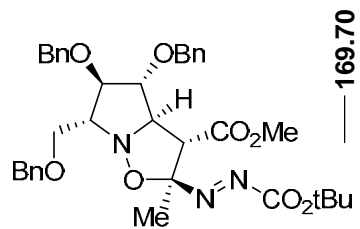




12b

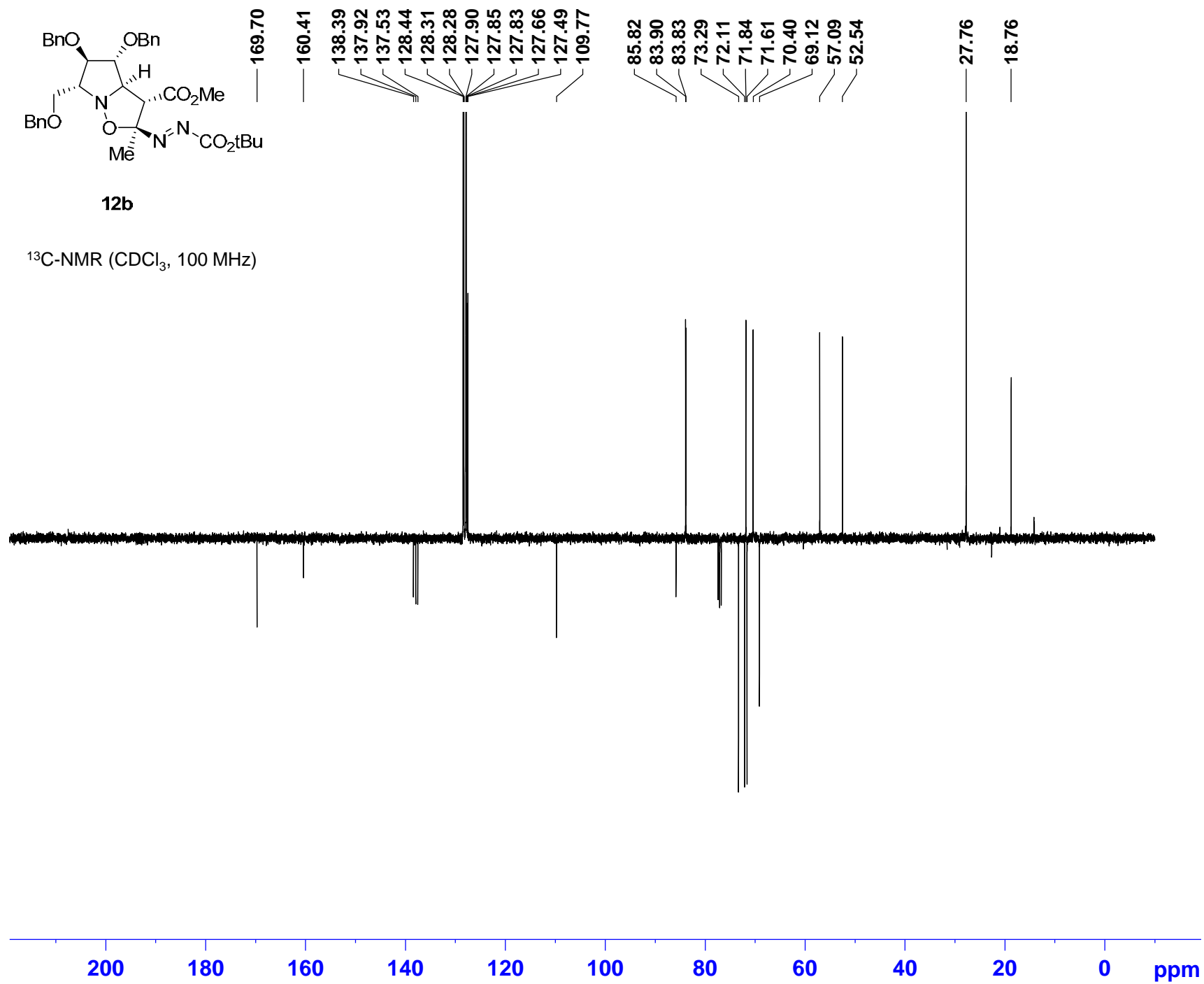
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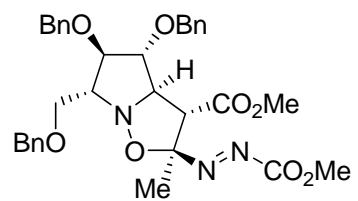




12b

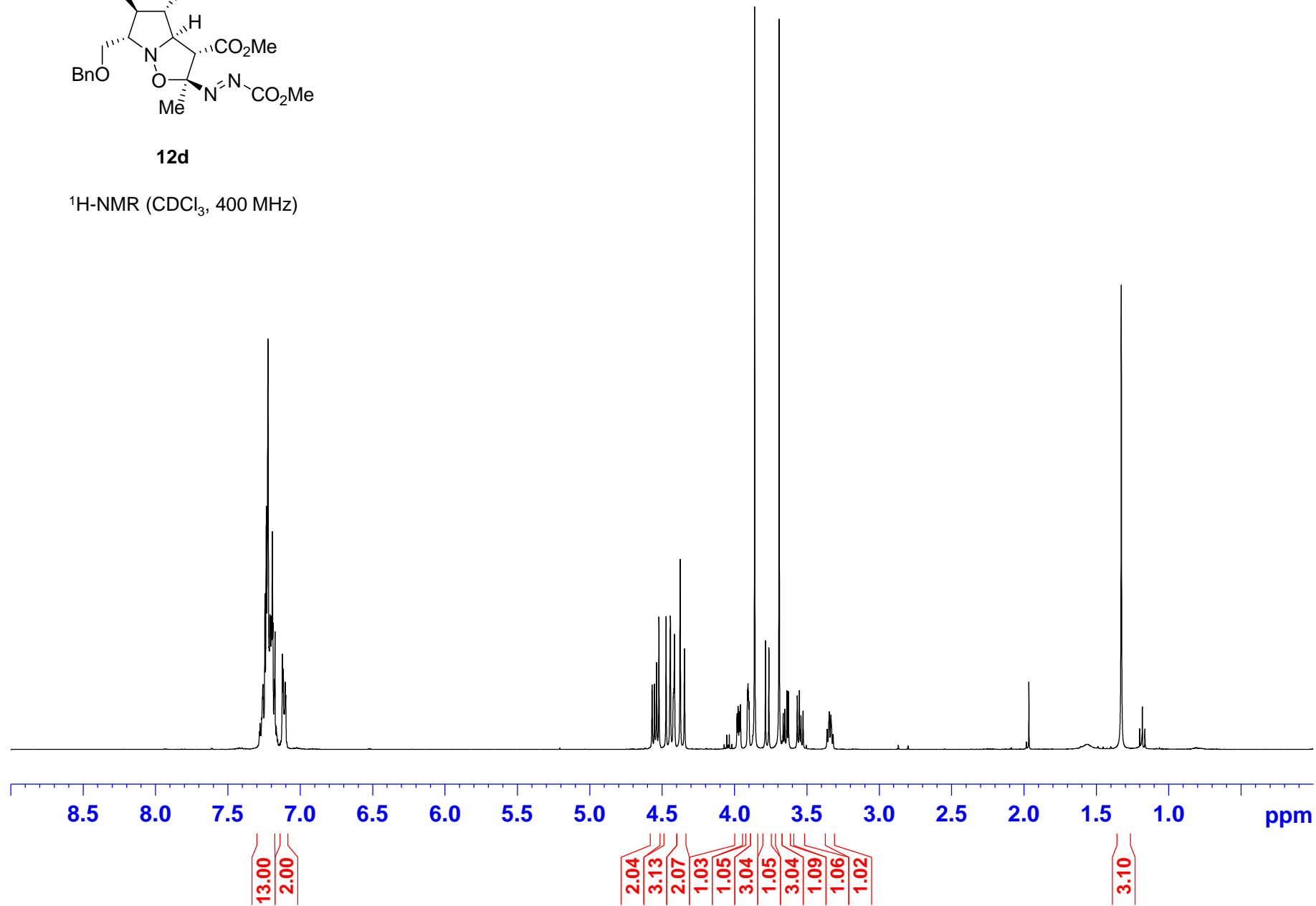
¹³C-NMR (CDCl₃, 100 MHz)

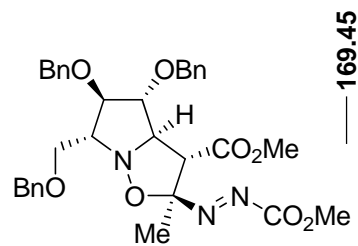




12d

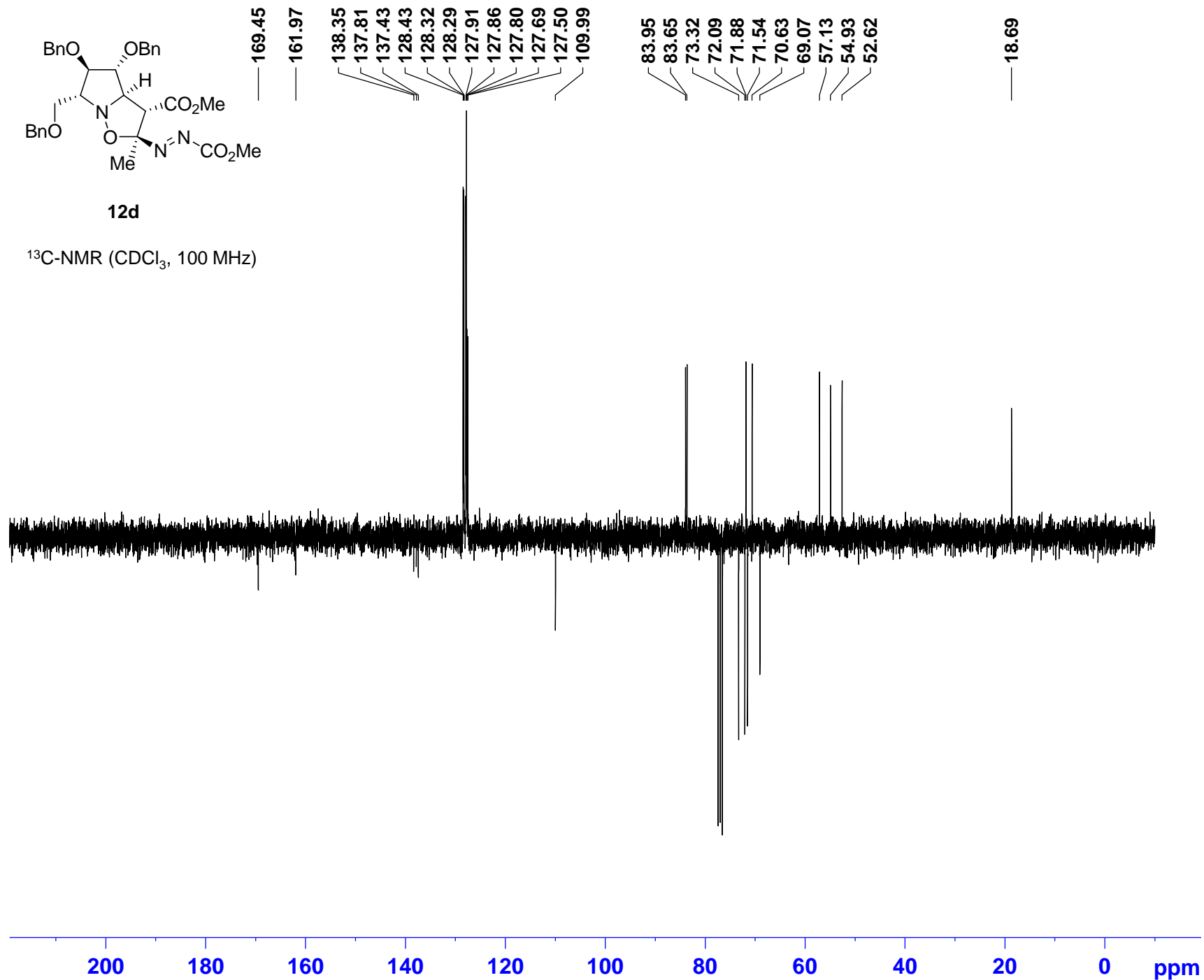
¹H-NMR (CDCl₃, 400 MHz)

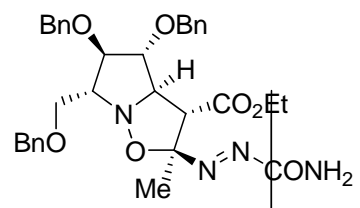




12d

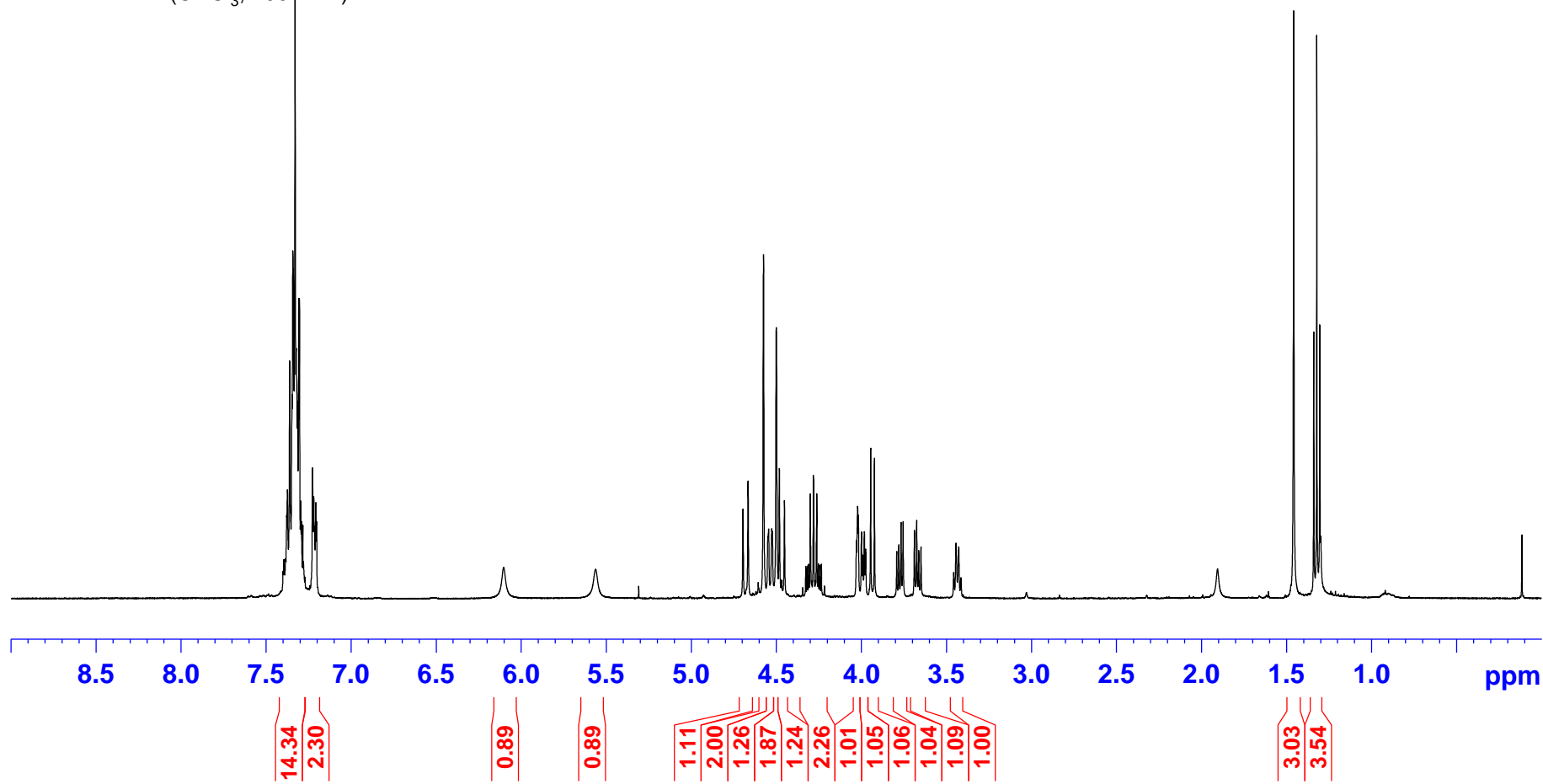
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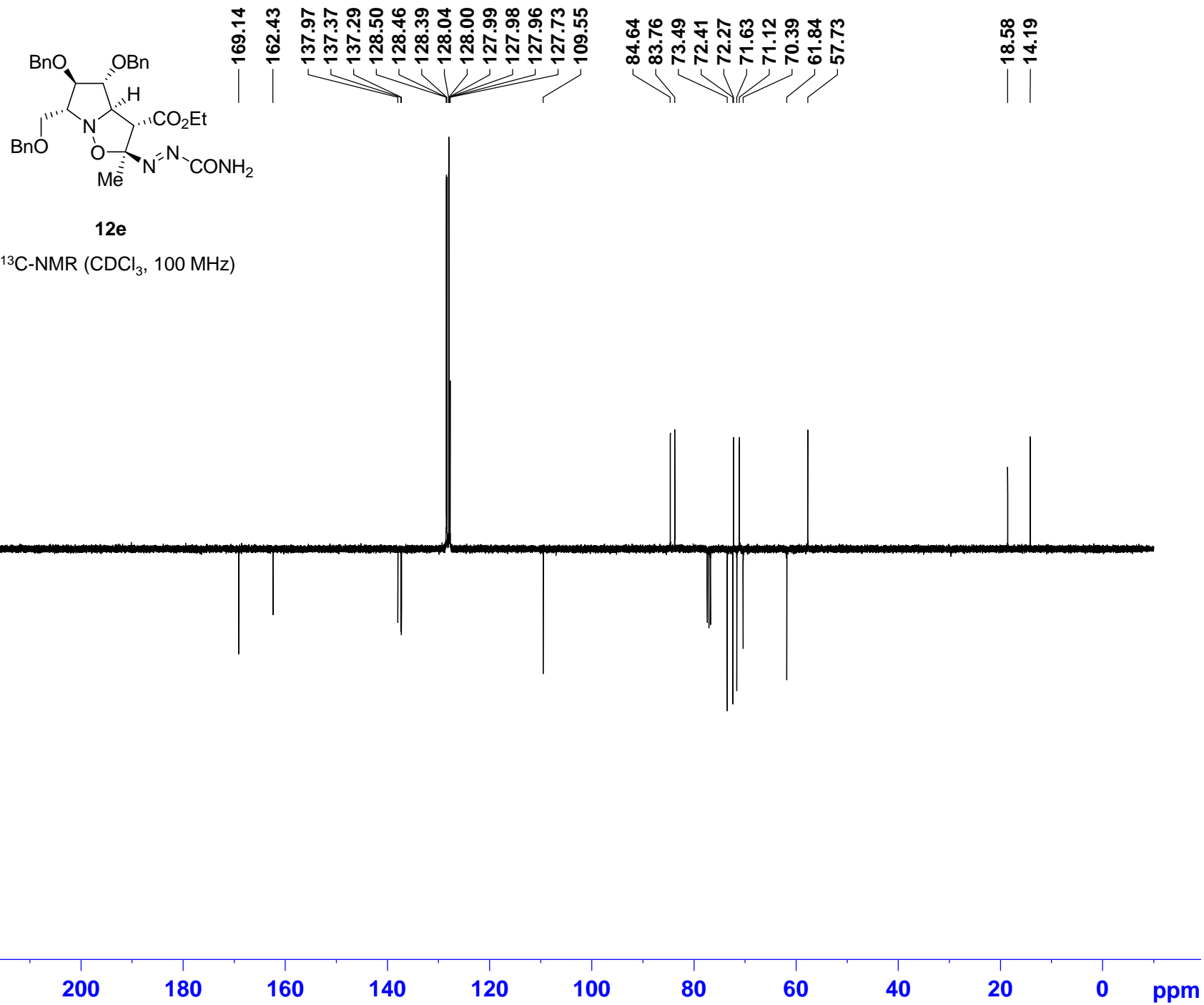


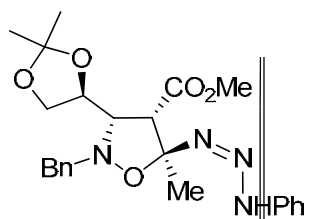


12e

¹H-NMR (CDCl₃, 400 MHz)

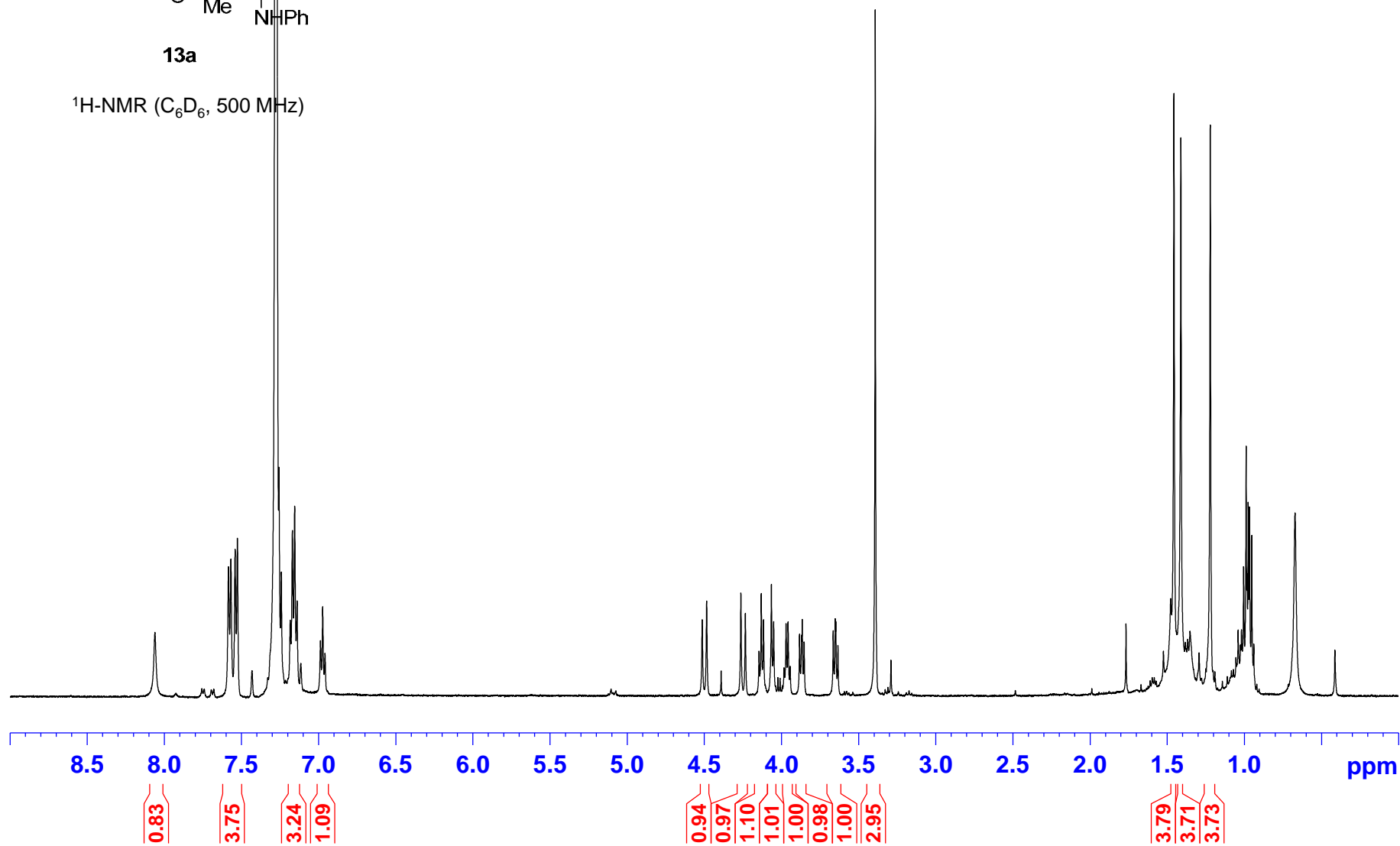


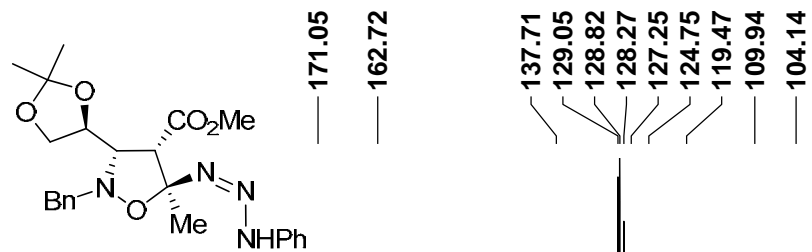




13a

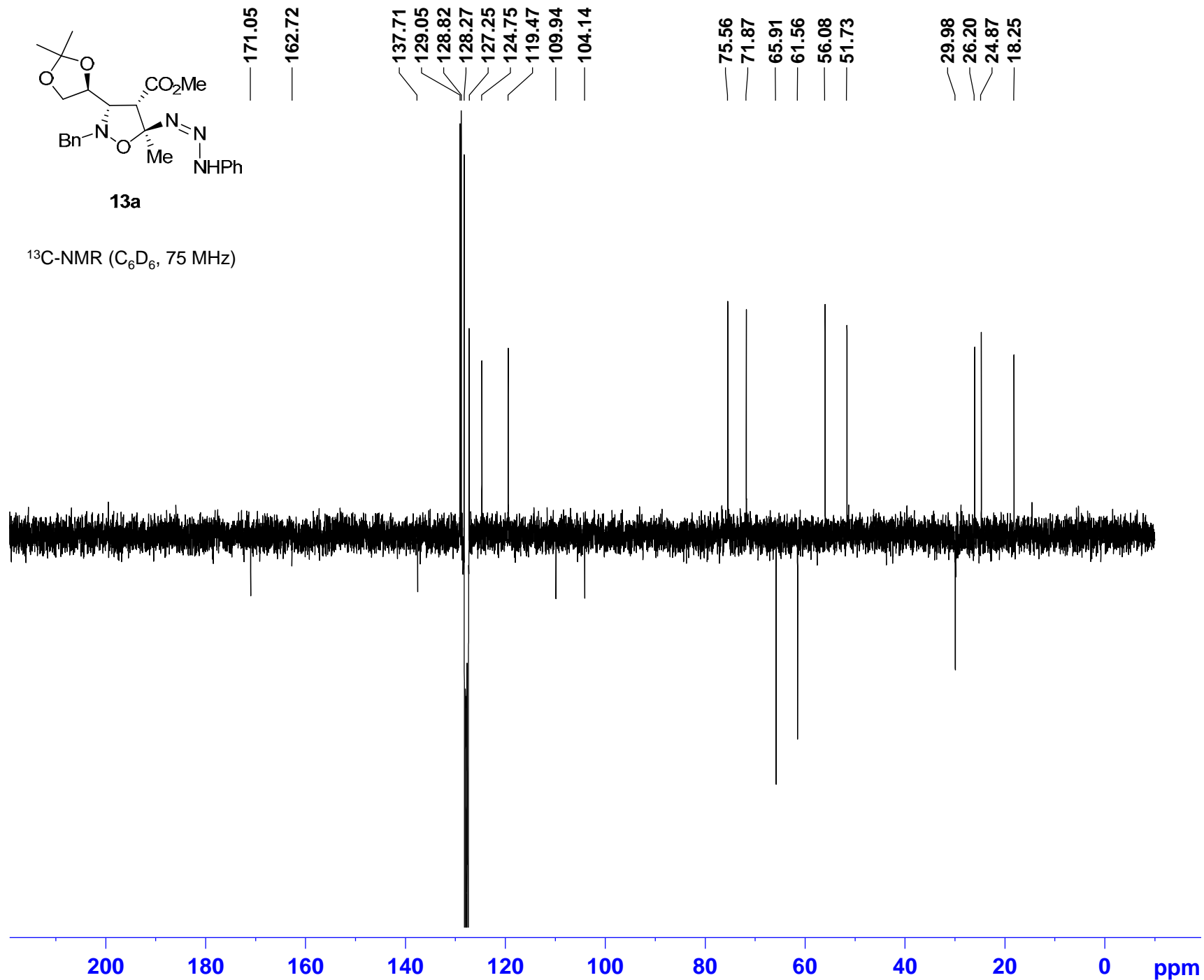
¹H-NMR (C₆D₆, 500 MHz)

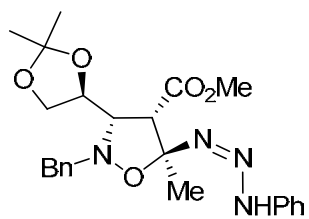




13a

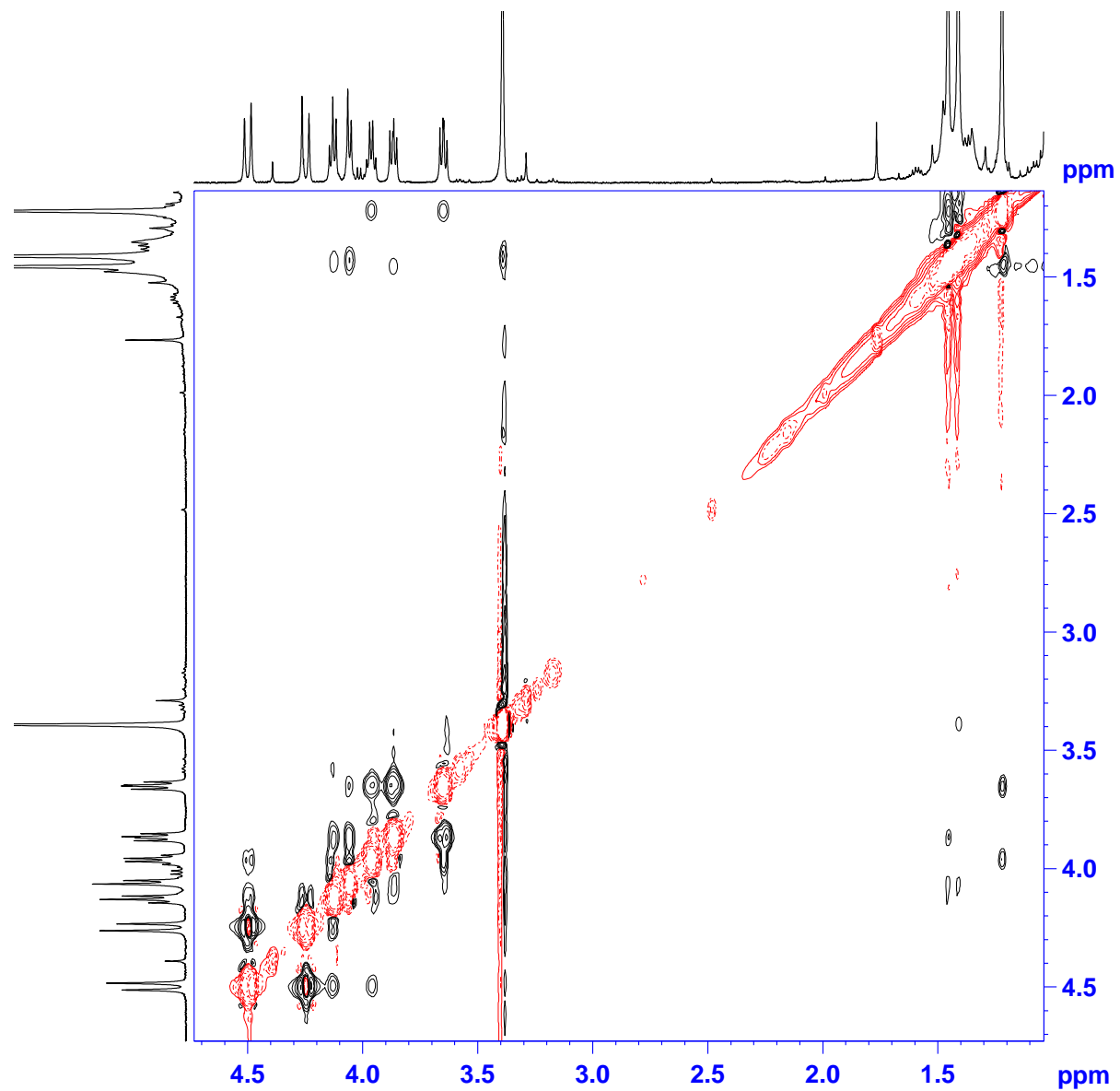
^{13}C -NMR (C_6D_6 , 75 MHz)

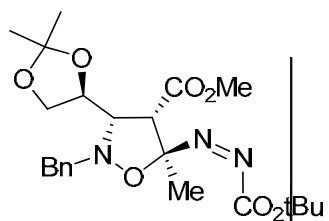




13a

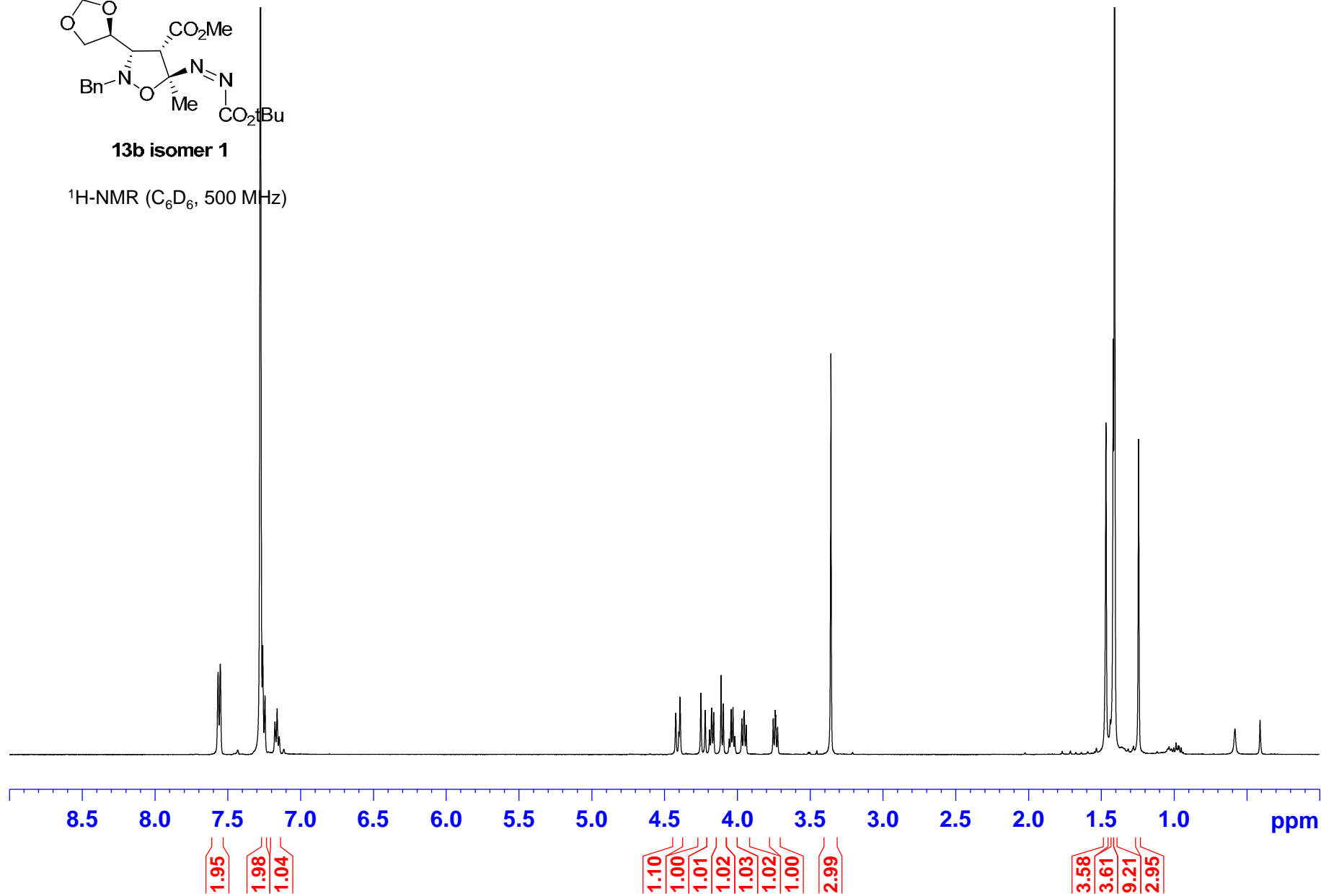
NOESY (C₆D₆, 500 MHz)

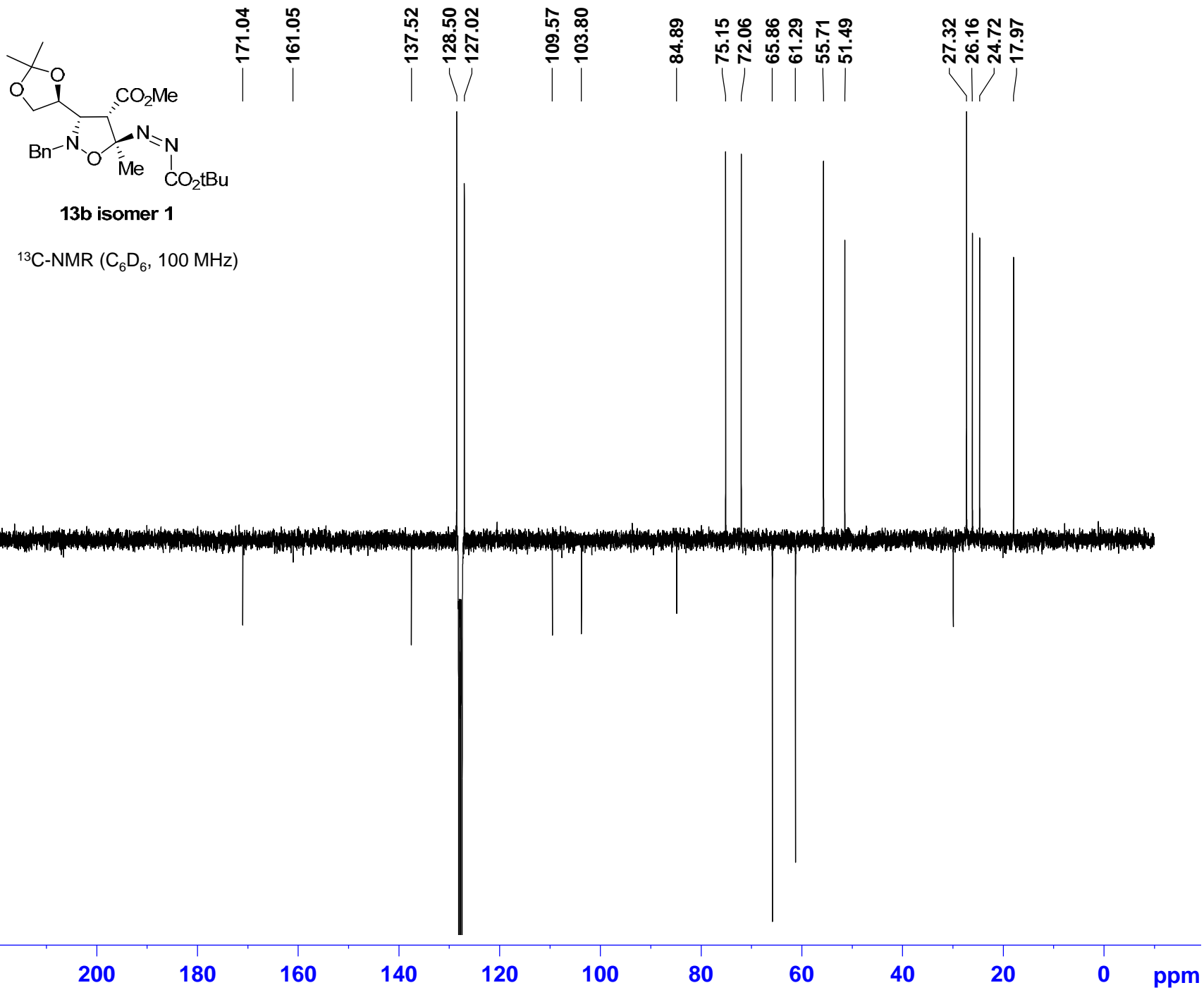


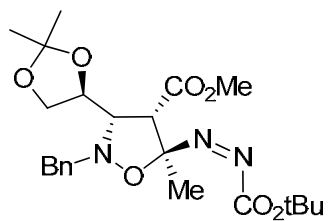


13b isomer 1

¹H-NMR (C₆D₆, 500 MHz)

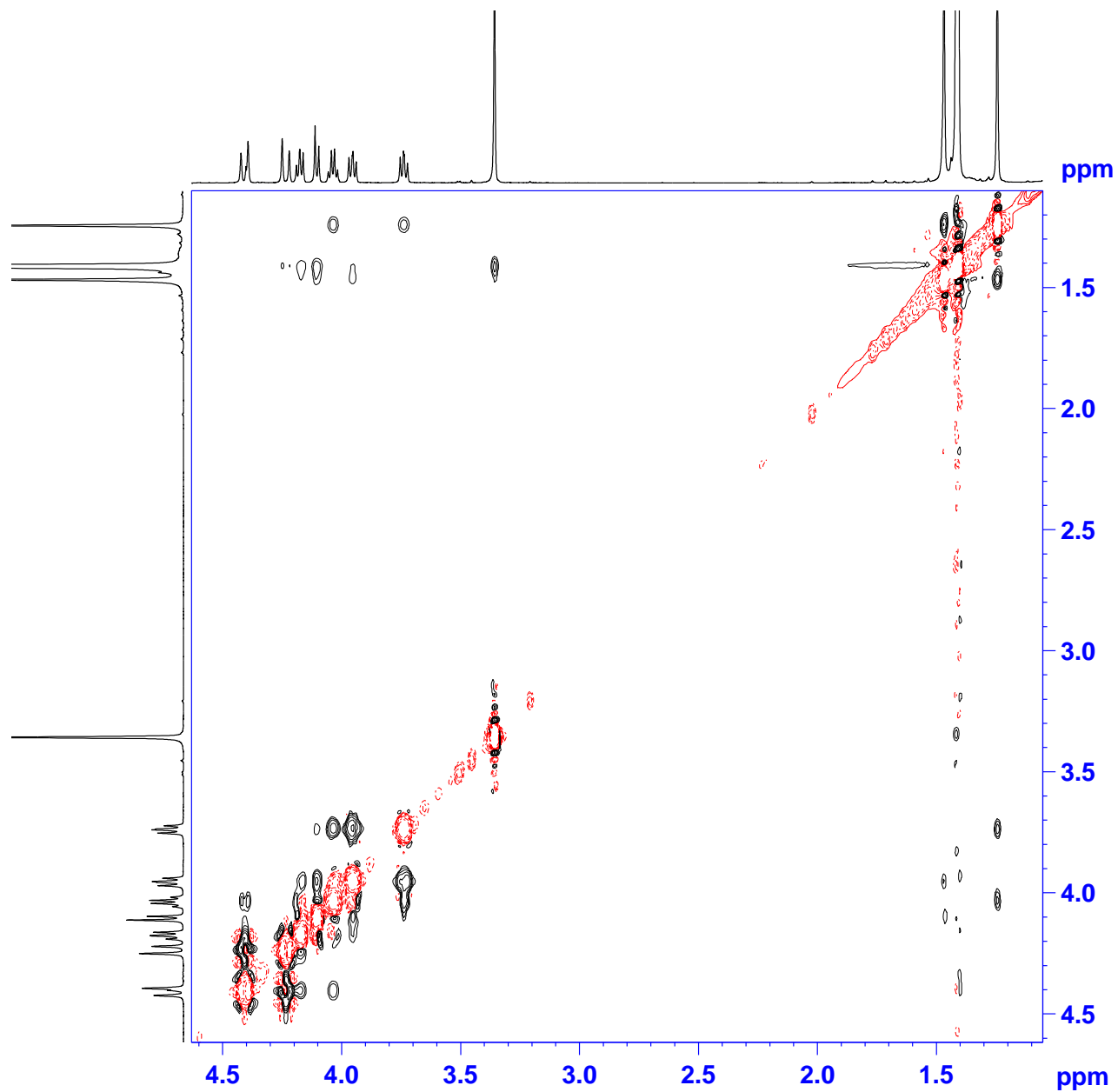


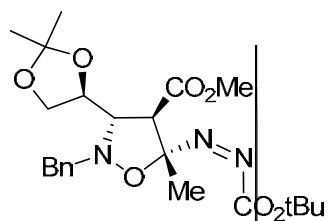




13b isomer 1

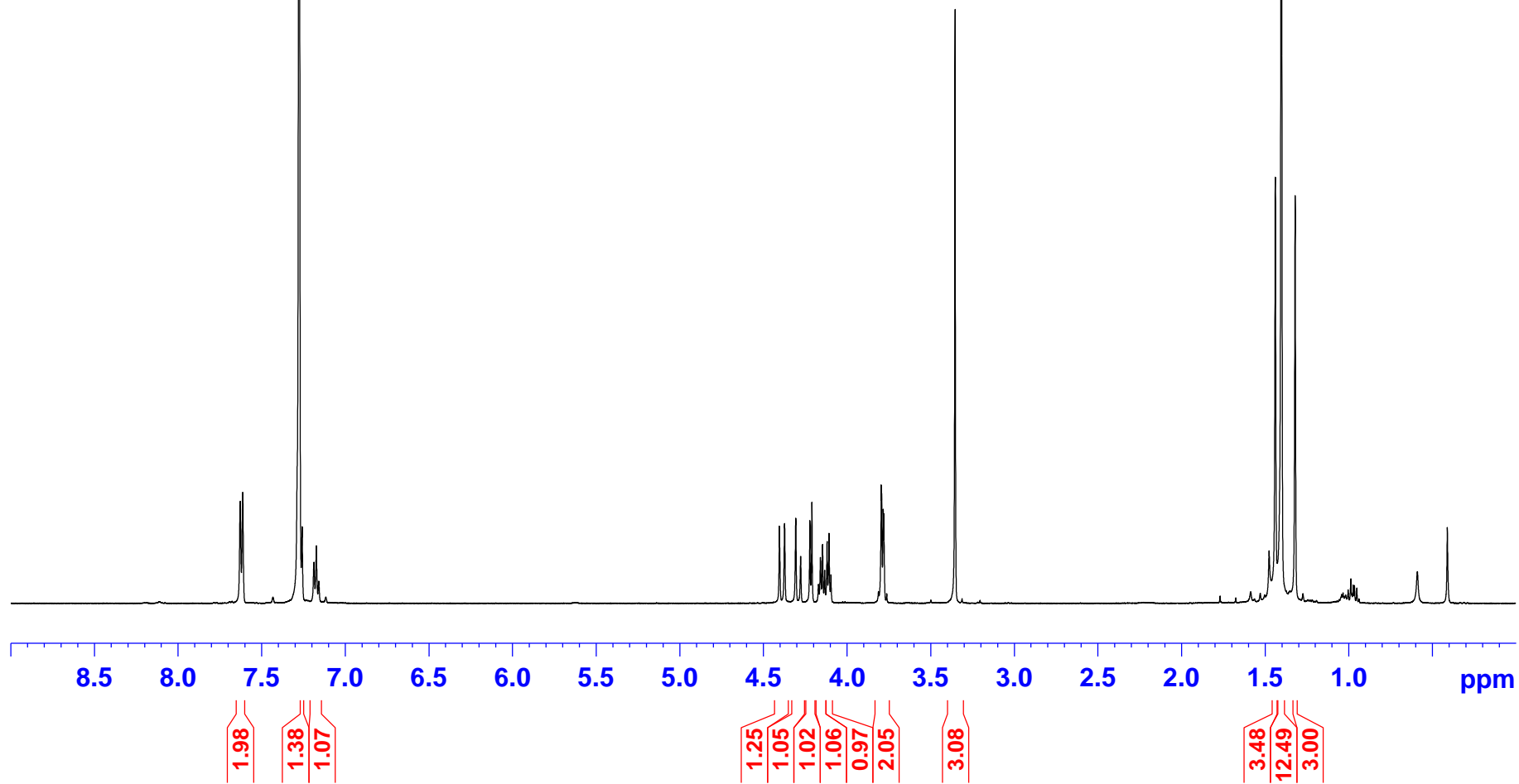
NOESY (C₆D₆, 500 MHz)

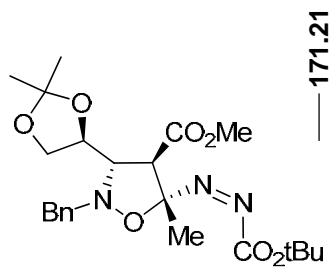




13b isomer 2

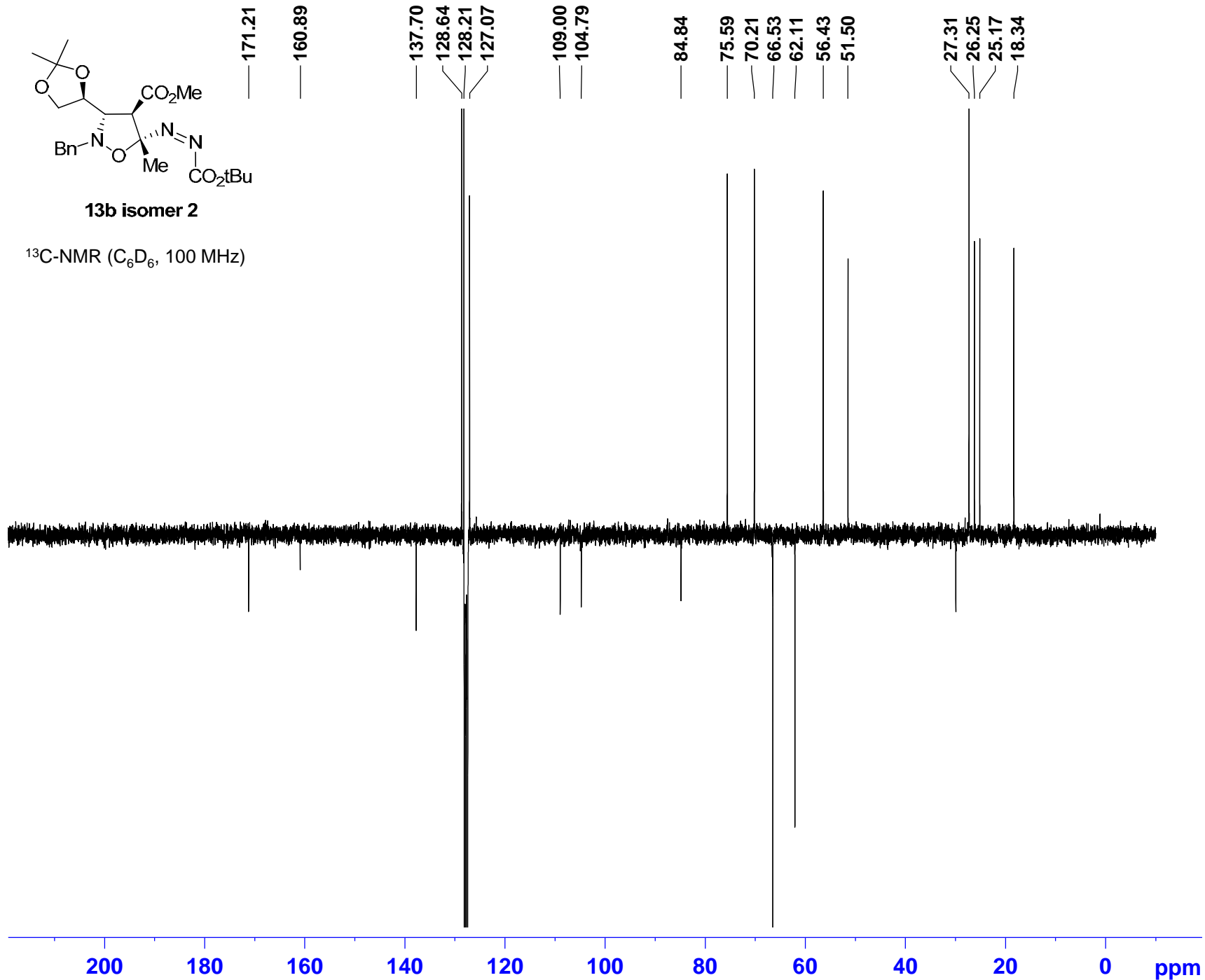
$^1\text{H-NMR}$ (C_6D_6 , 500 MHz)

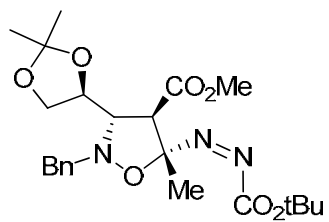




13b isomer 2

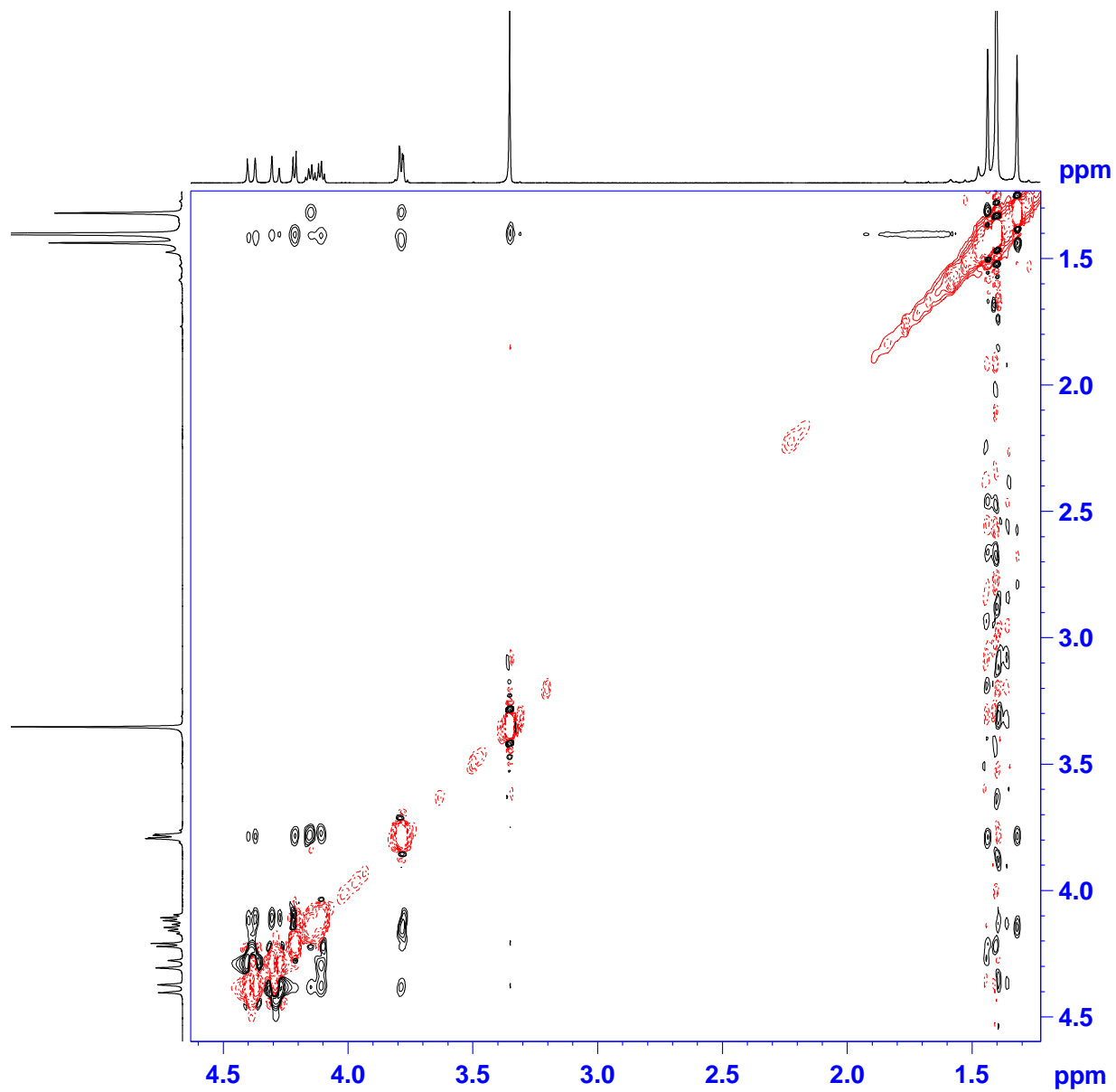
¹³C-NMR (C₆D₆, 100 MHz)

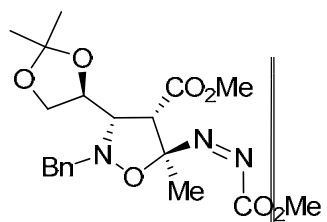




13b isomer 2

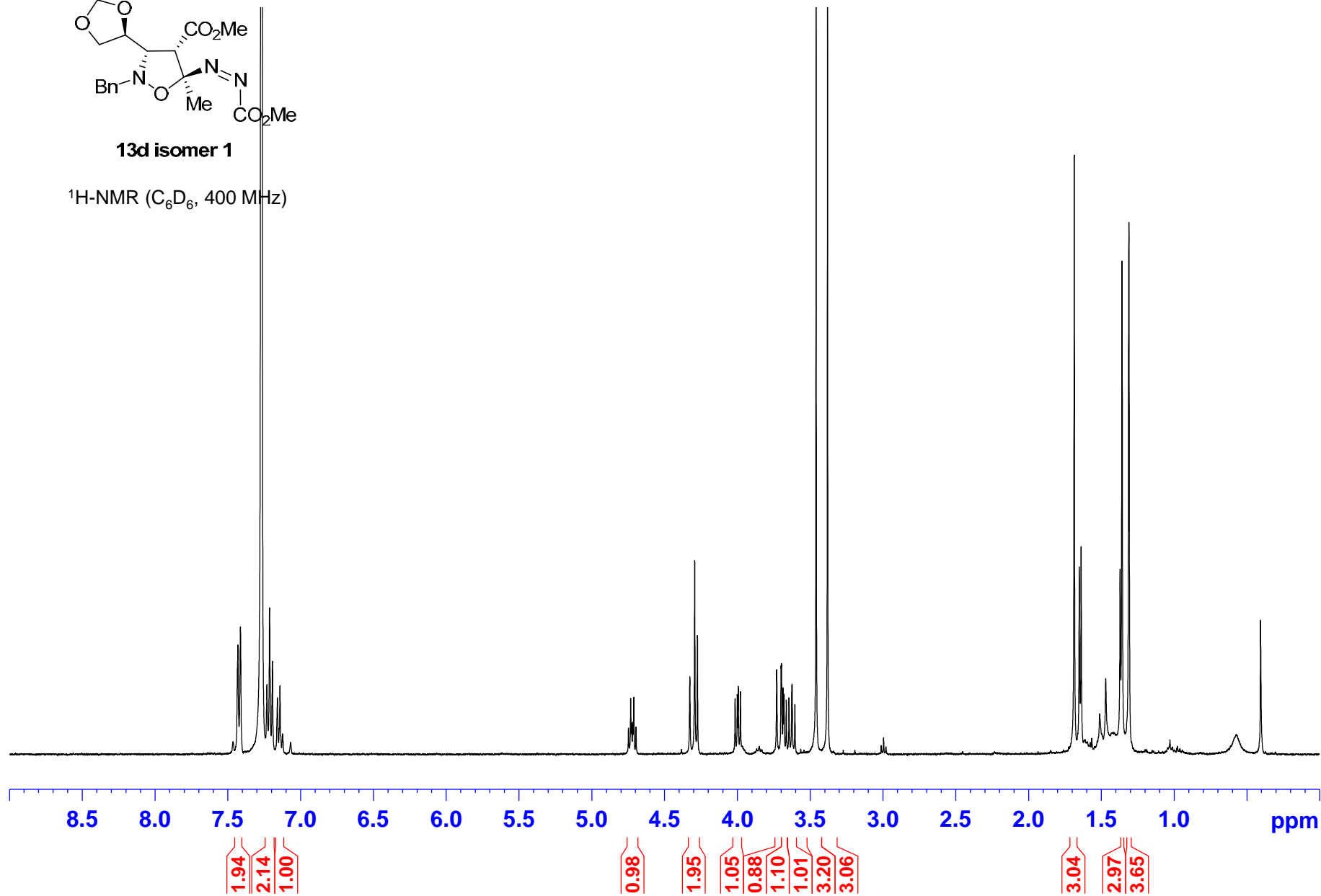
NOESY (C₆D₆, 500 MHz)

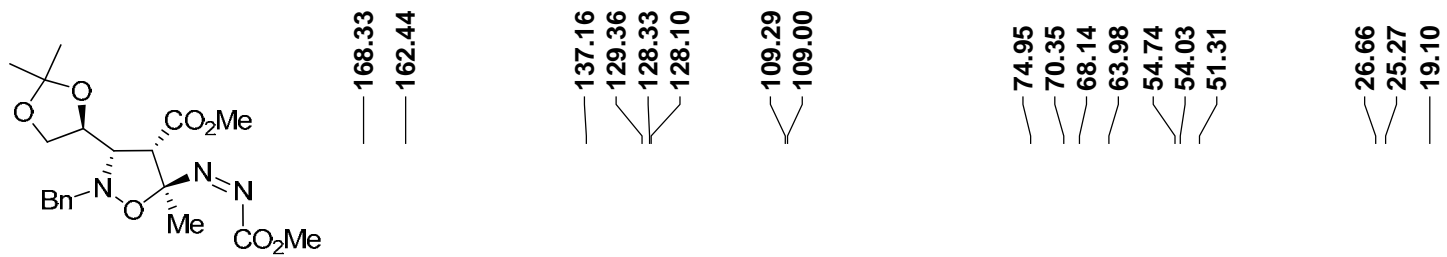




13d isomer 1

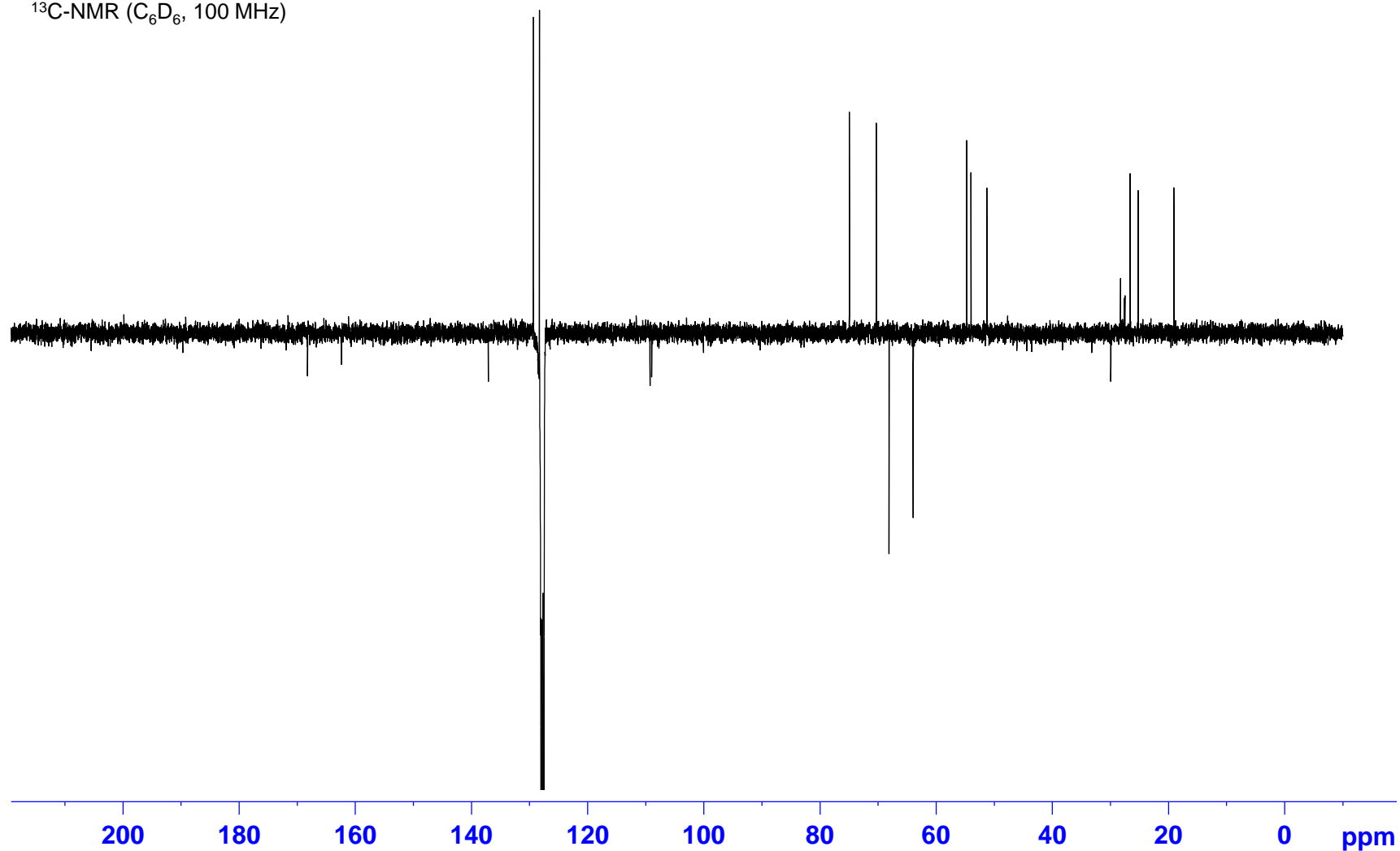
¹H-NMR (C₆D₆, 400 MHz)

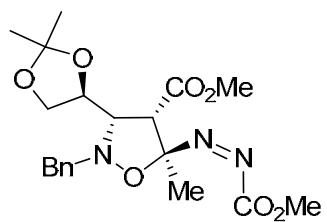




13d isomer 1

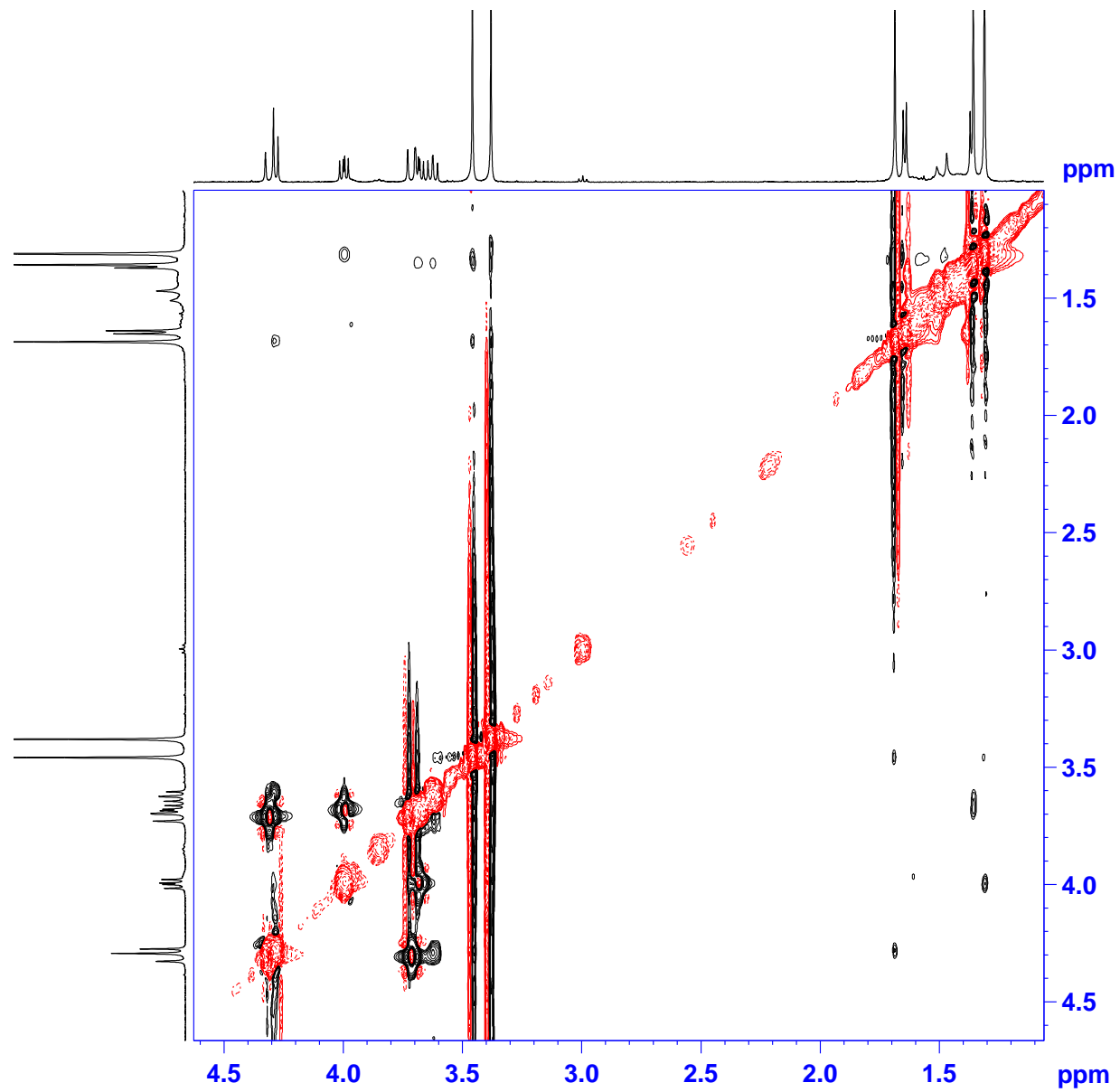
$^{13}\text{C-NMR}$ (C_6D_6 , 100 MHz)

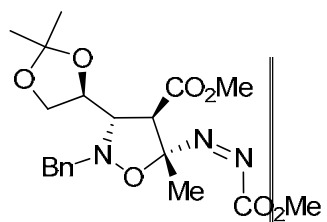




13d isomer 1

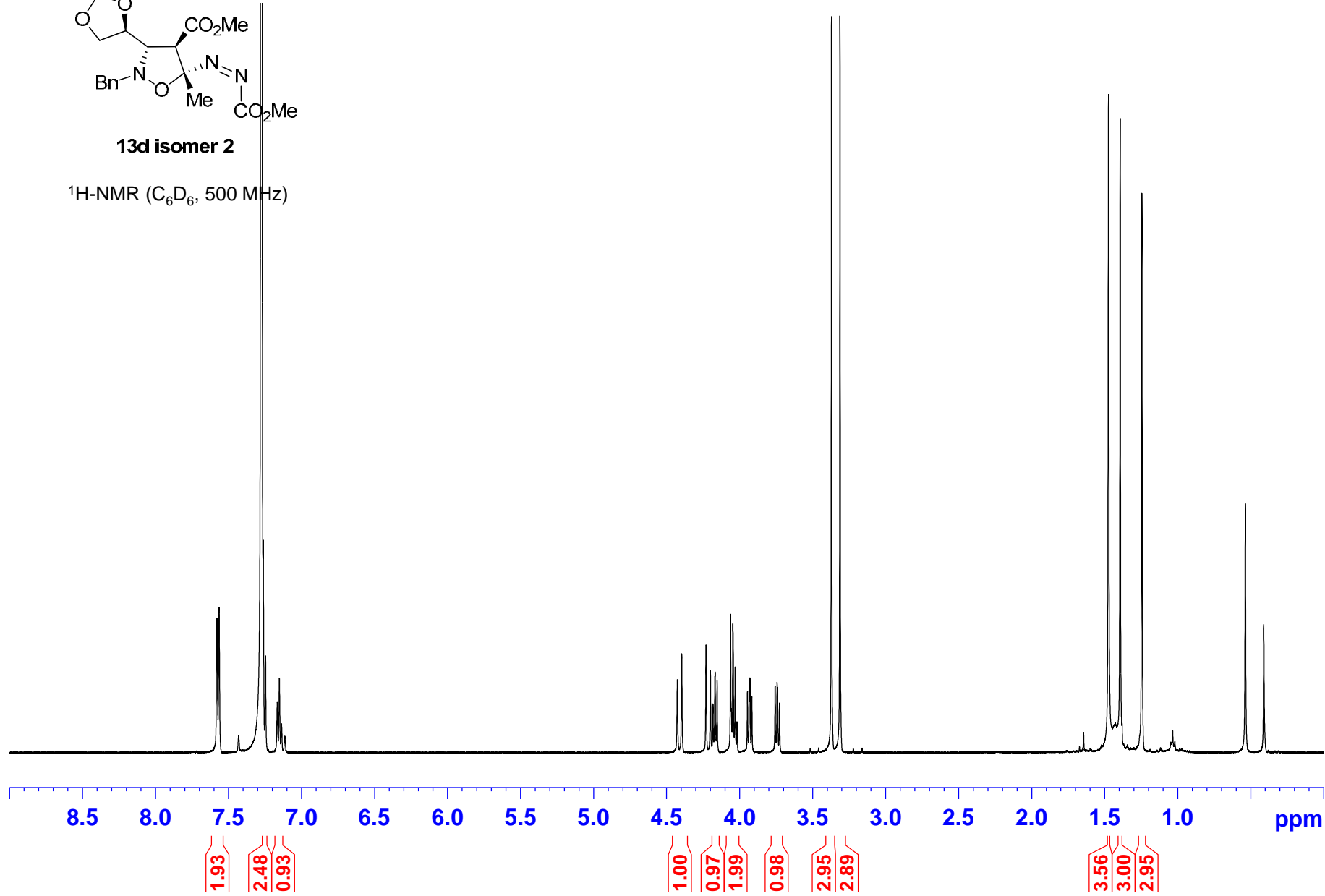
NOESY (C₆D₆, 400 MHz)

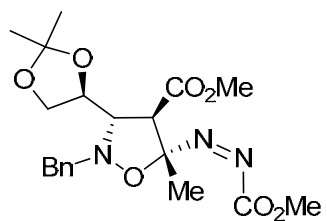




13d isomer 2

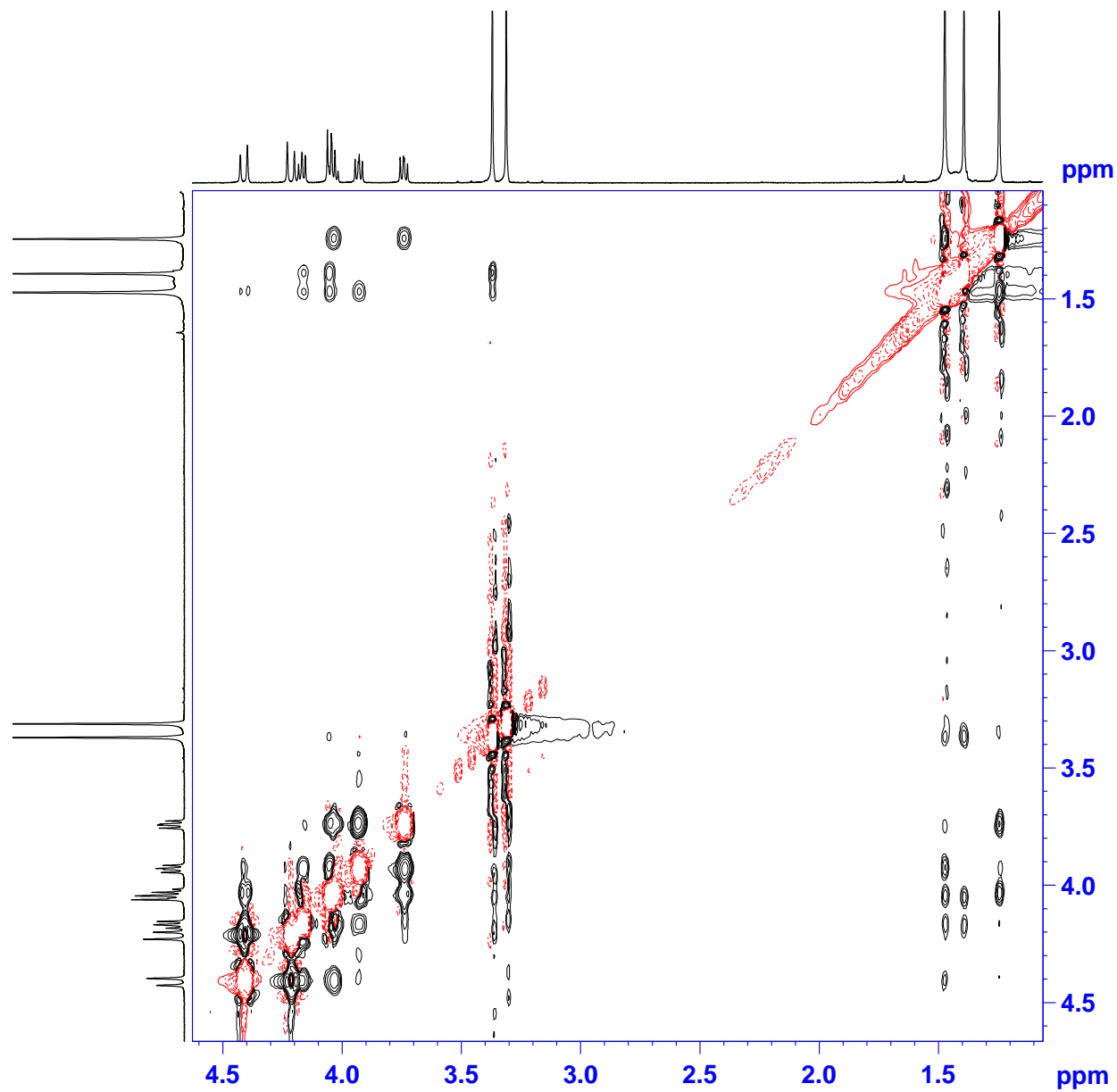
¹H-NMR (C₆D₆, 500 MHz)

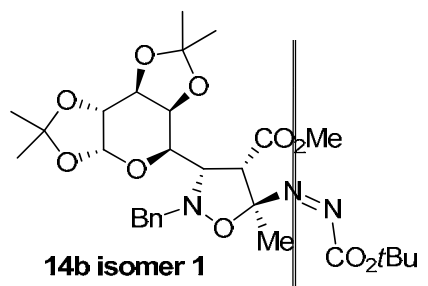




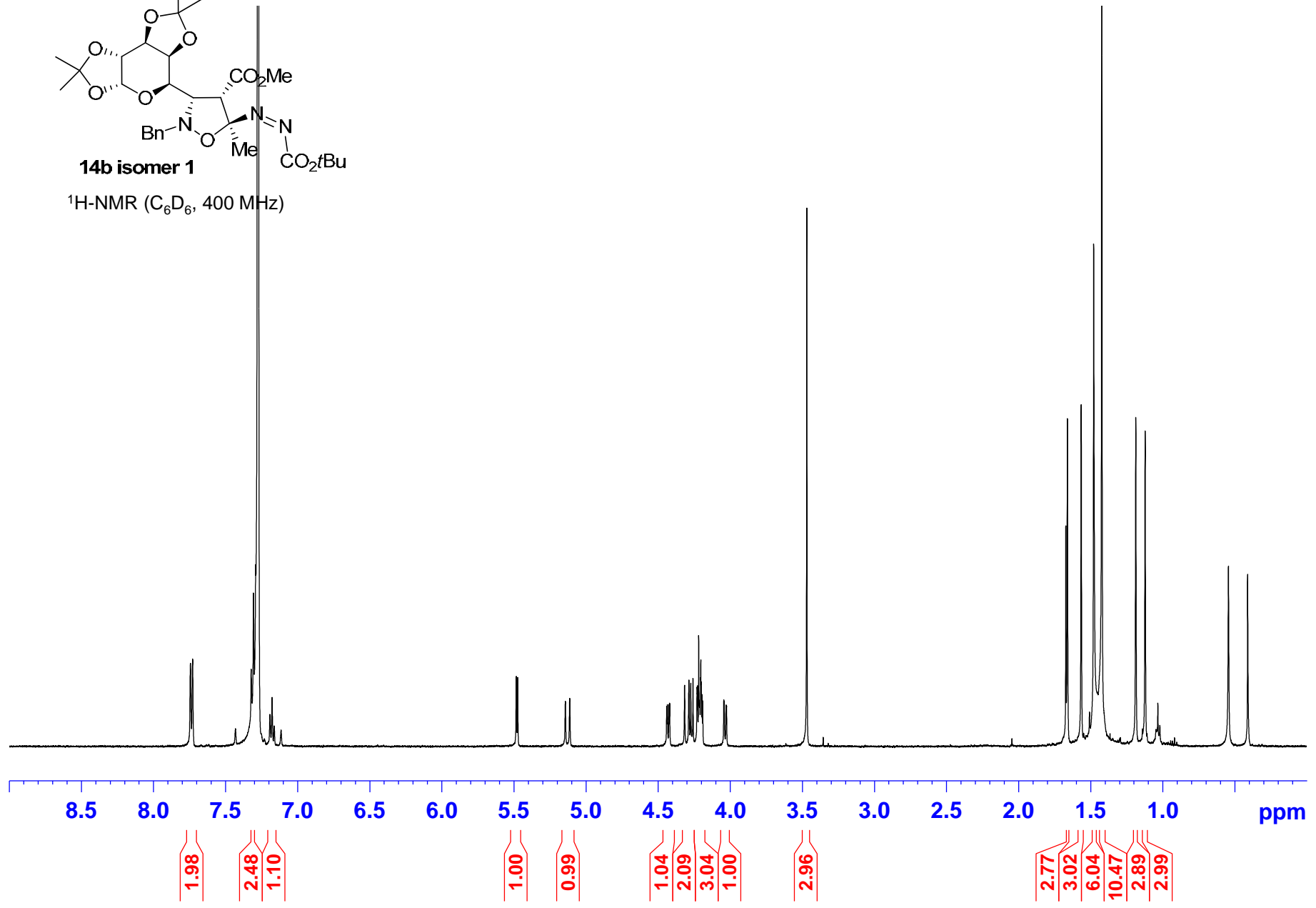
13d isomer 2

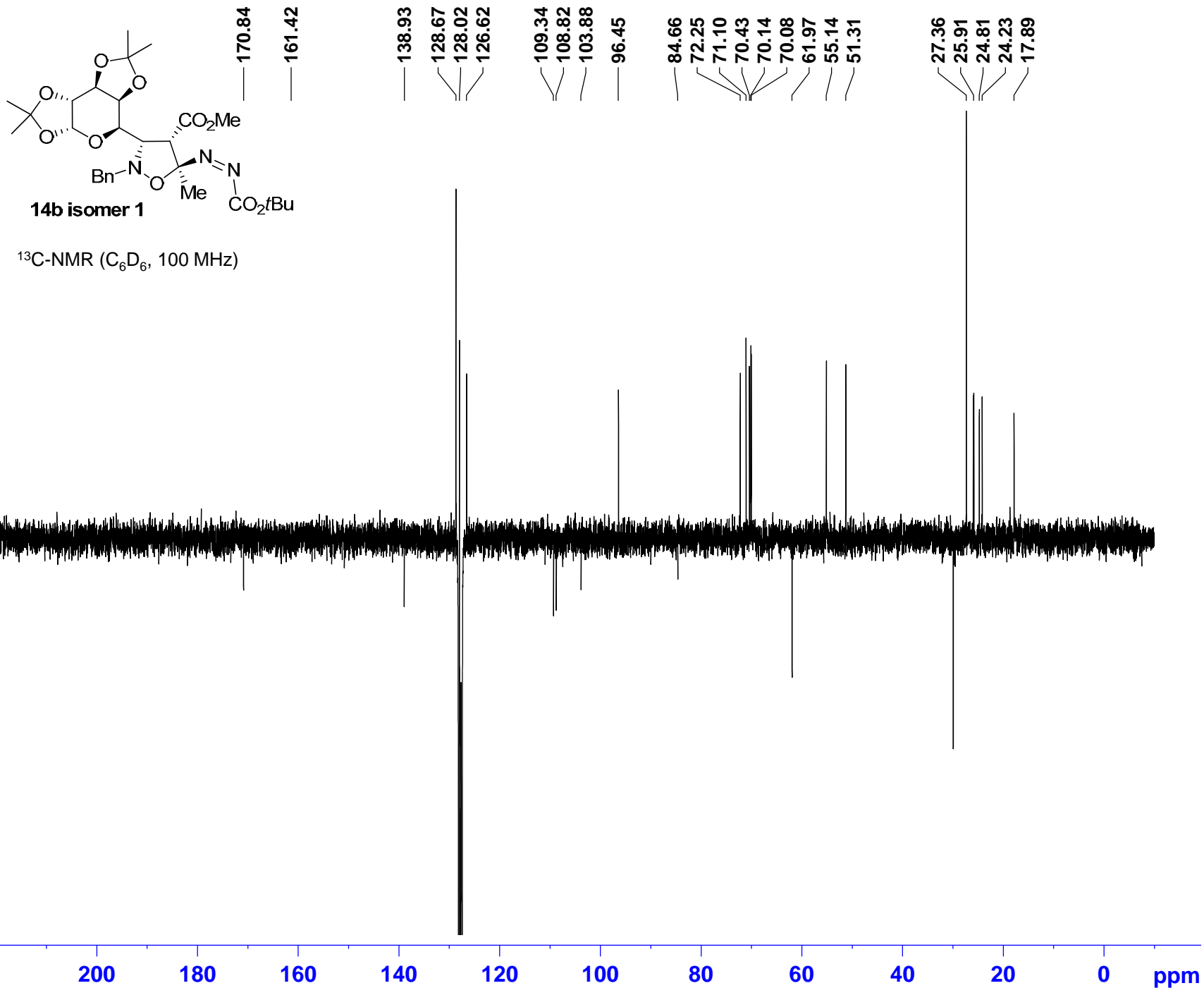
NOESY (C₆D₆, 500 MHz)

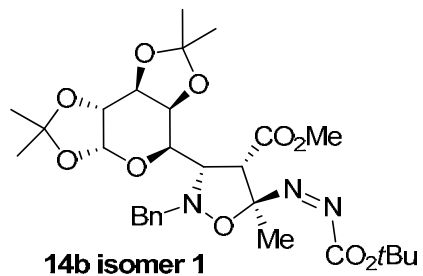




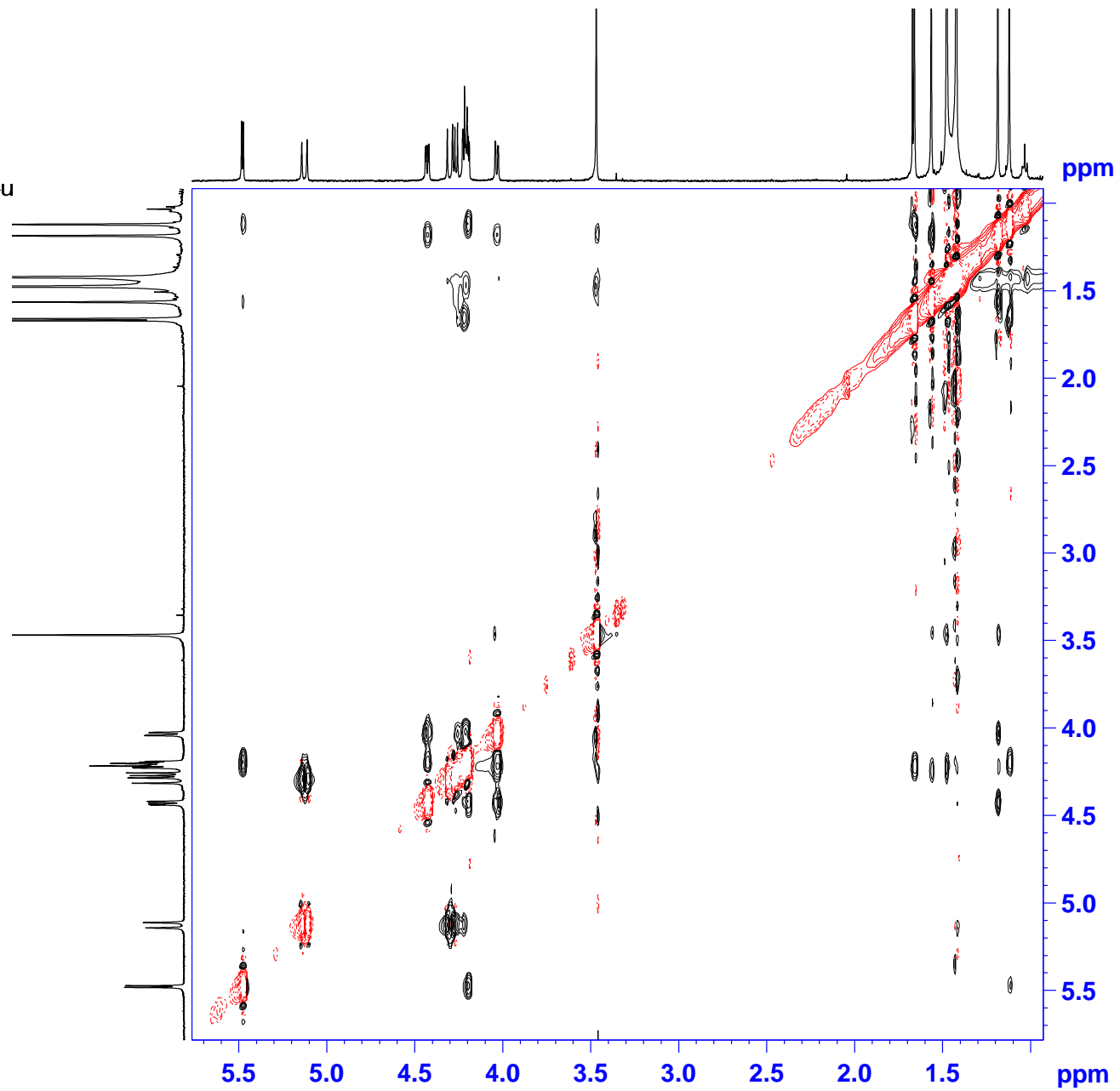
¹H-NMR (C₆D₆, 400 MHz)

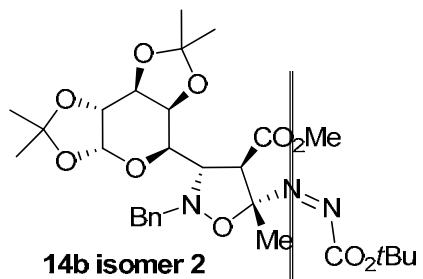




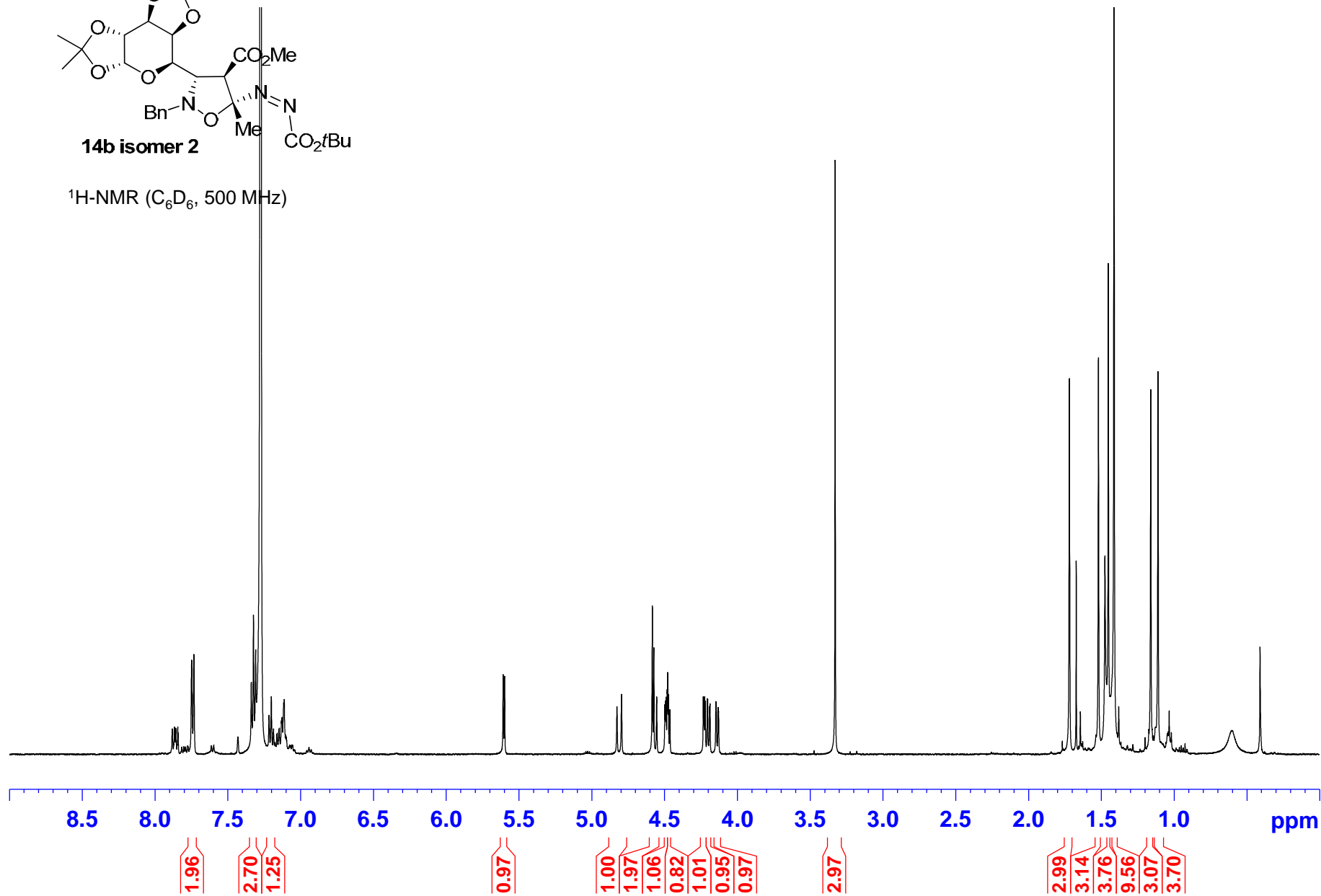


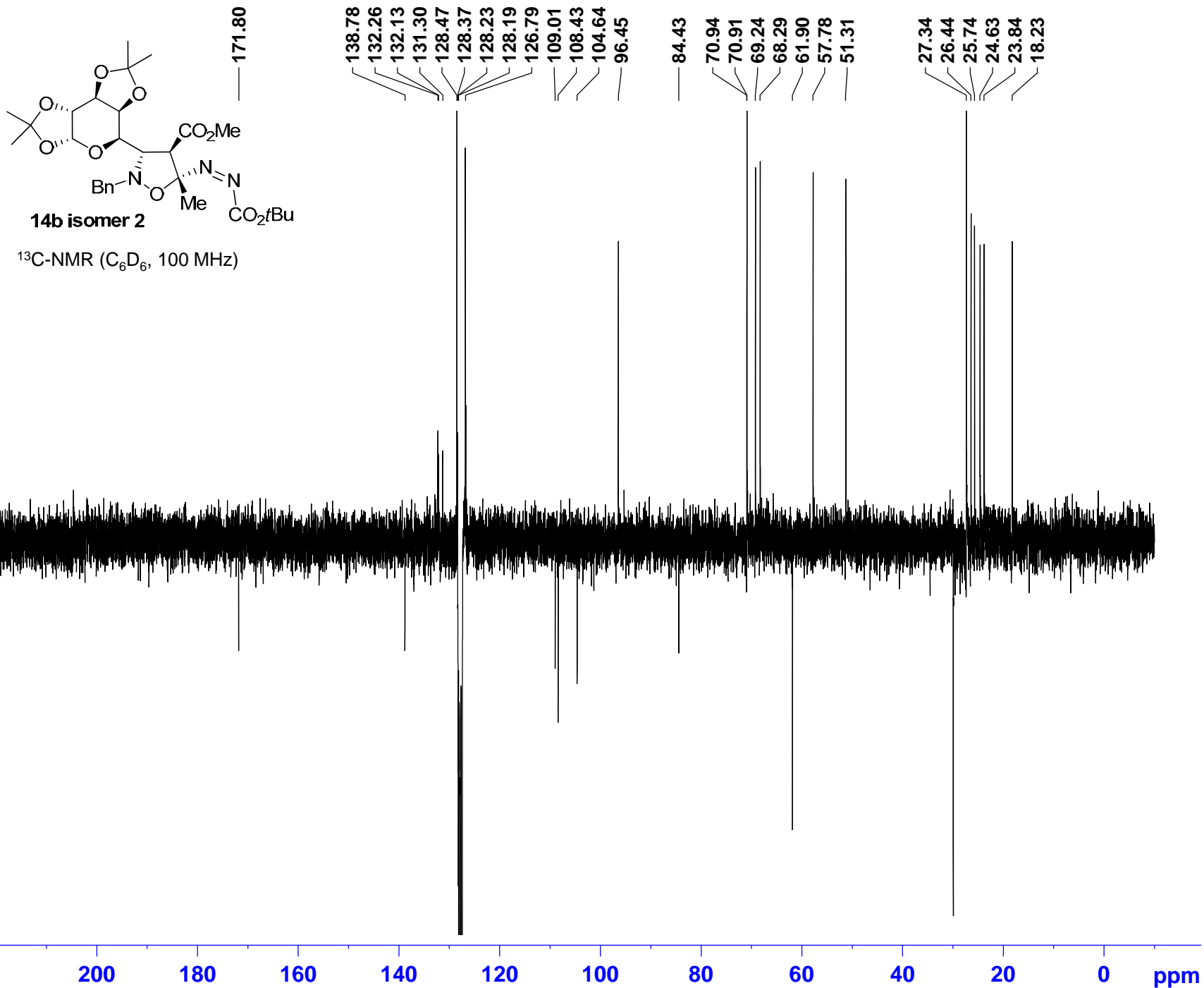
NOESY (C₆D₆, 500 MHz)

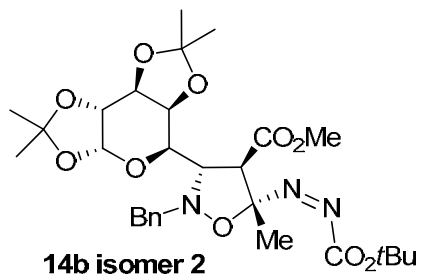




$^1\text{H-NMR}$ (C_6D_6 , 500 MHz)







NOESY (C₆D₆, 500 MHz)

