Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

On the scope of oxidation of tertiary amines: Meisenheimer Rearrangements *versus* Cope Elimination in 2-(cyanoethyl)-2-azanorbornanes

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Supplementary data

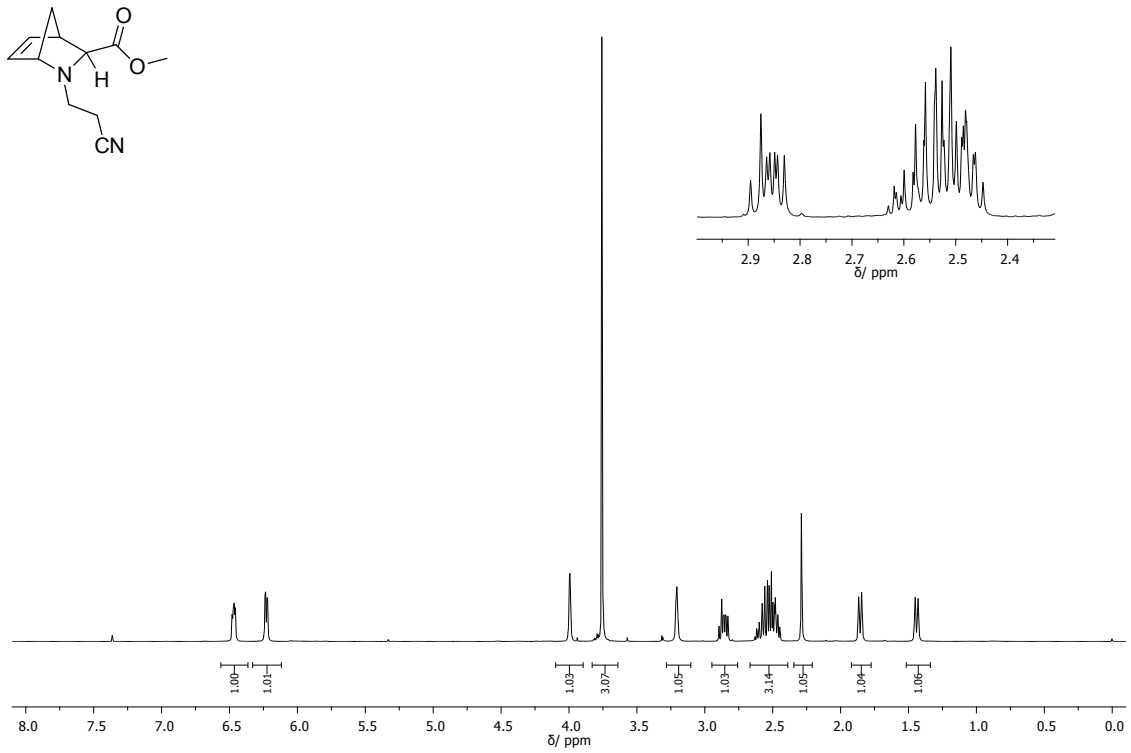


Fig. S1. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **1**.

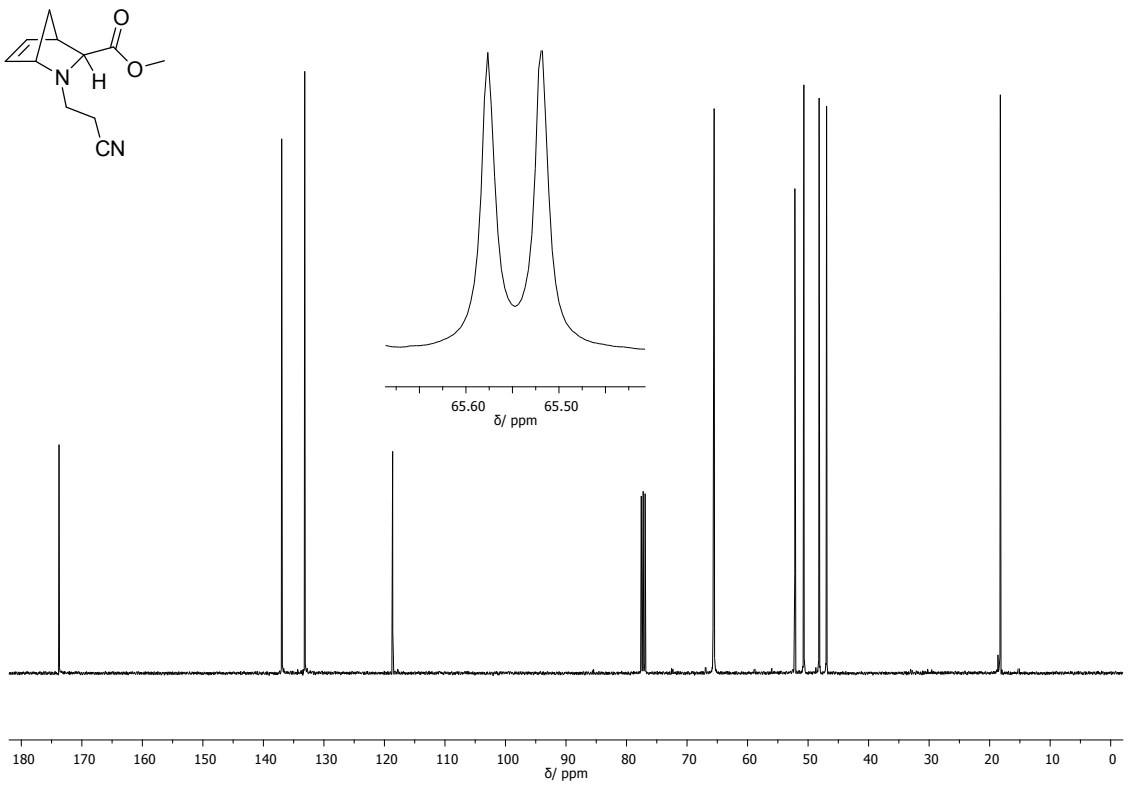


Fig. S2. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **1**.

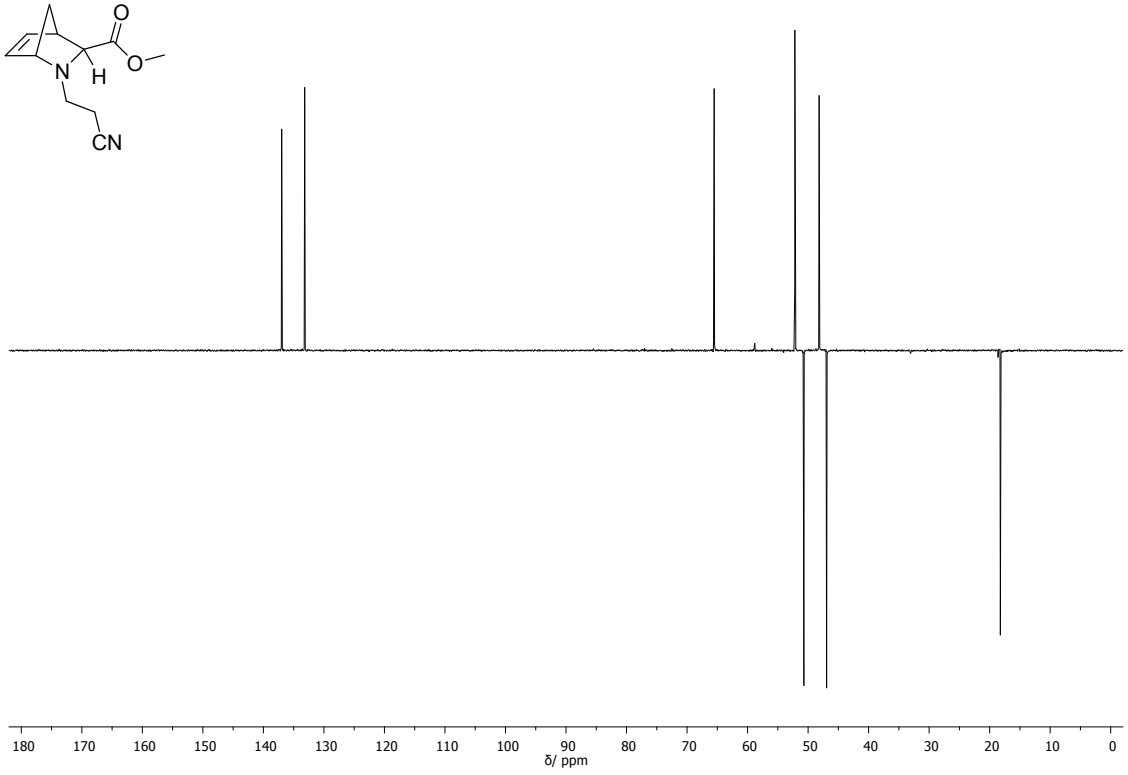


Fig. S3. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **1**.

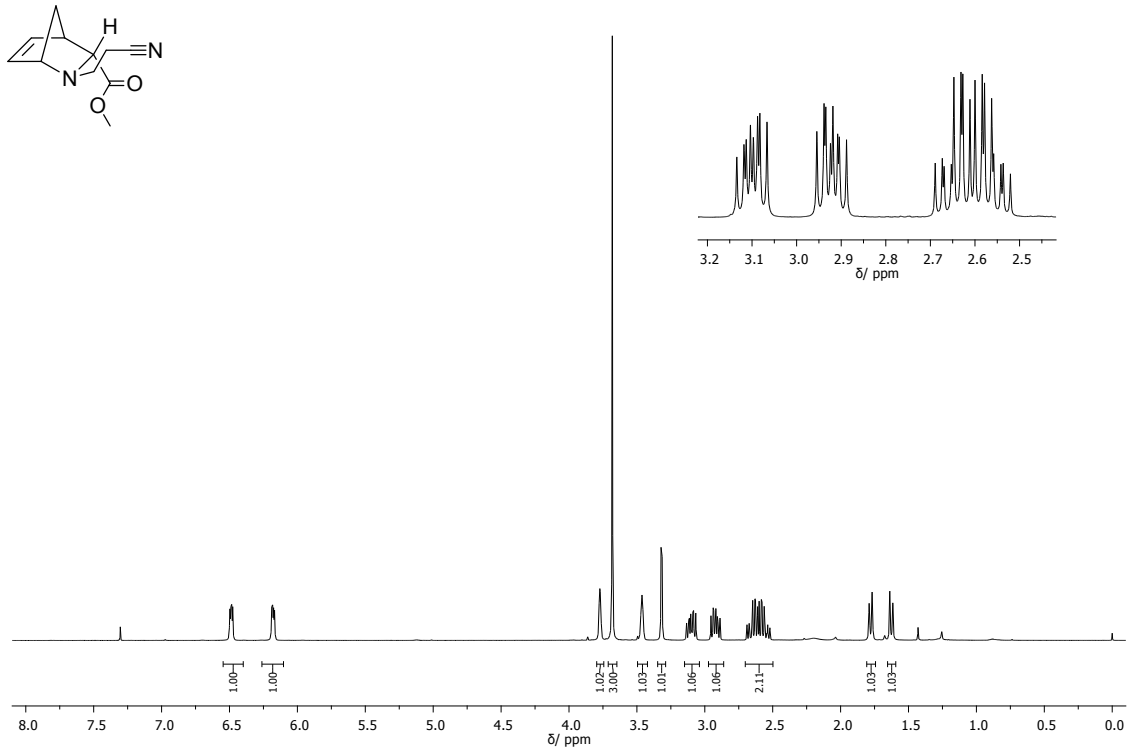


Fig. S4. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **2**.

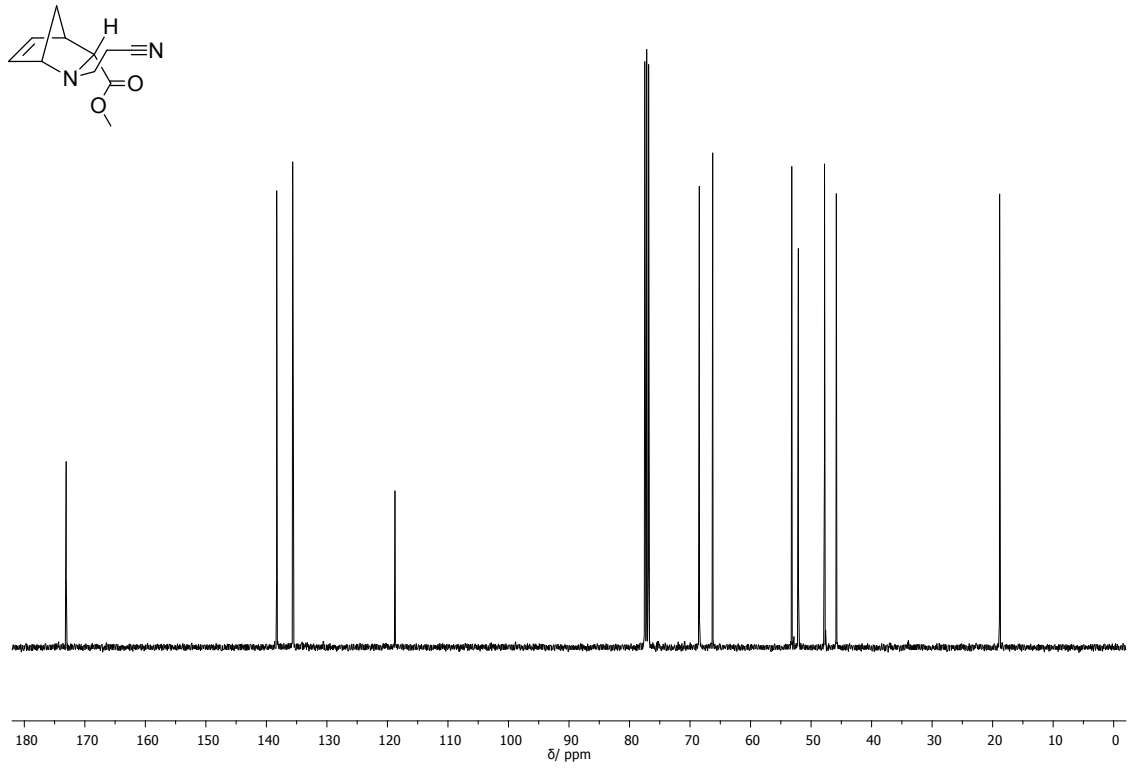


Fig. S5. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **2**.

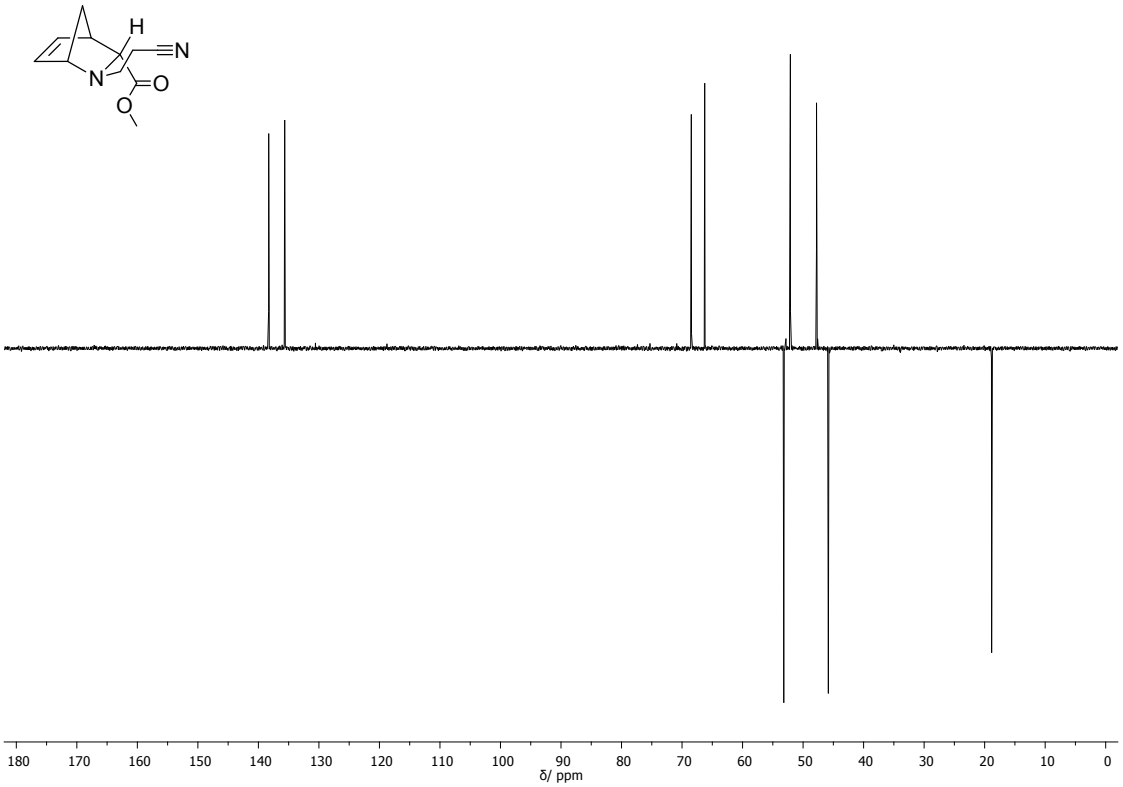


Fig. S6. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **2**.

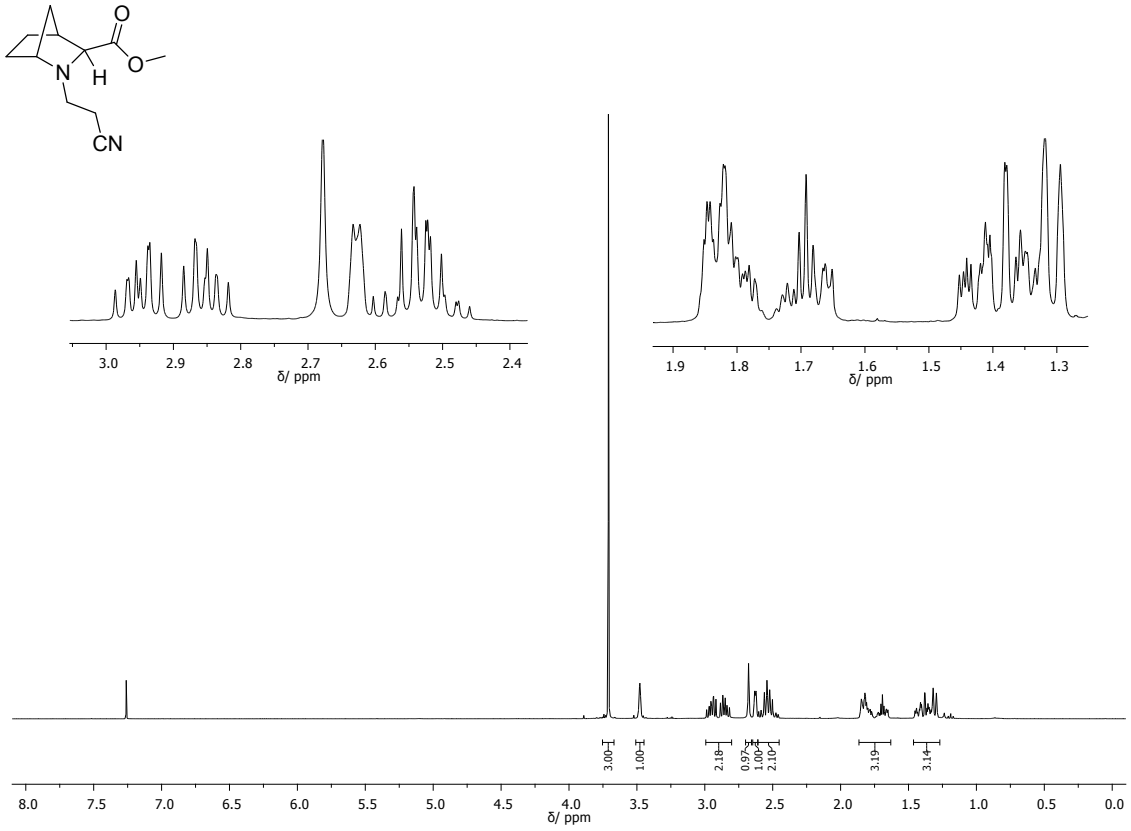


Fig. S7. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **5**.

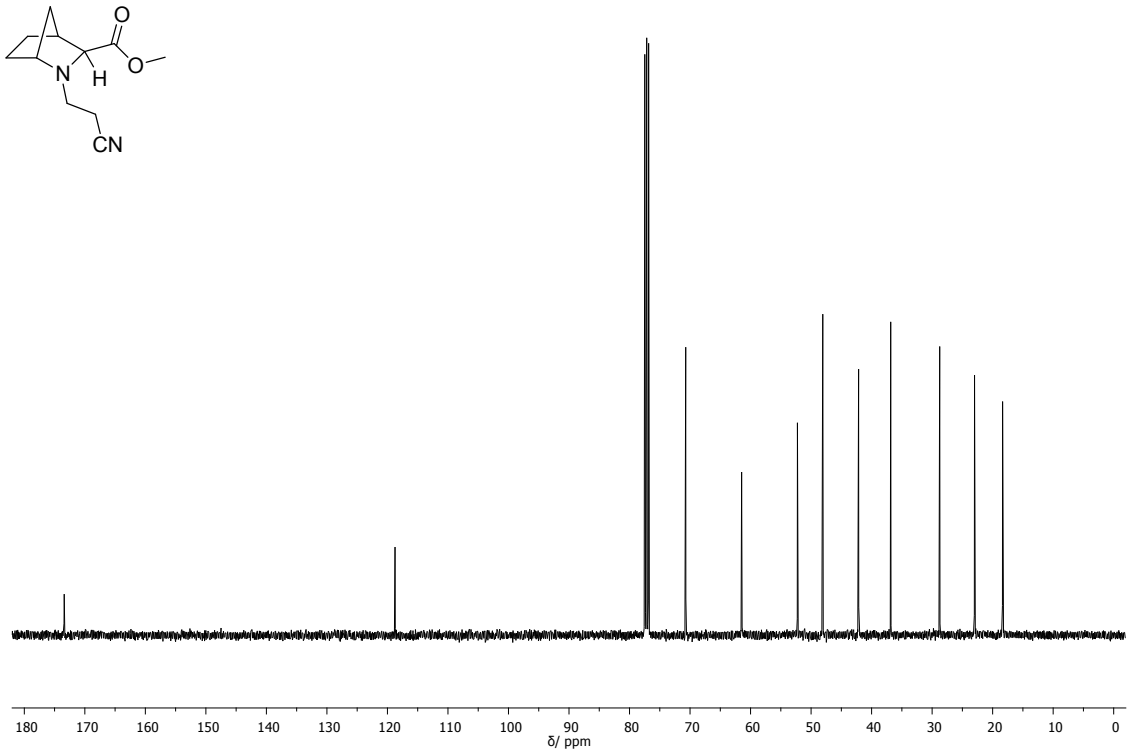


Fig. S8. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **5**.

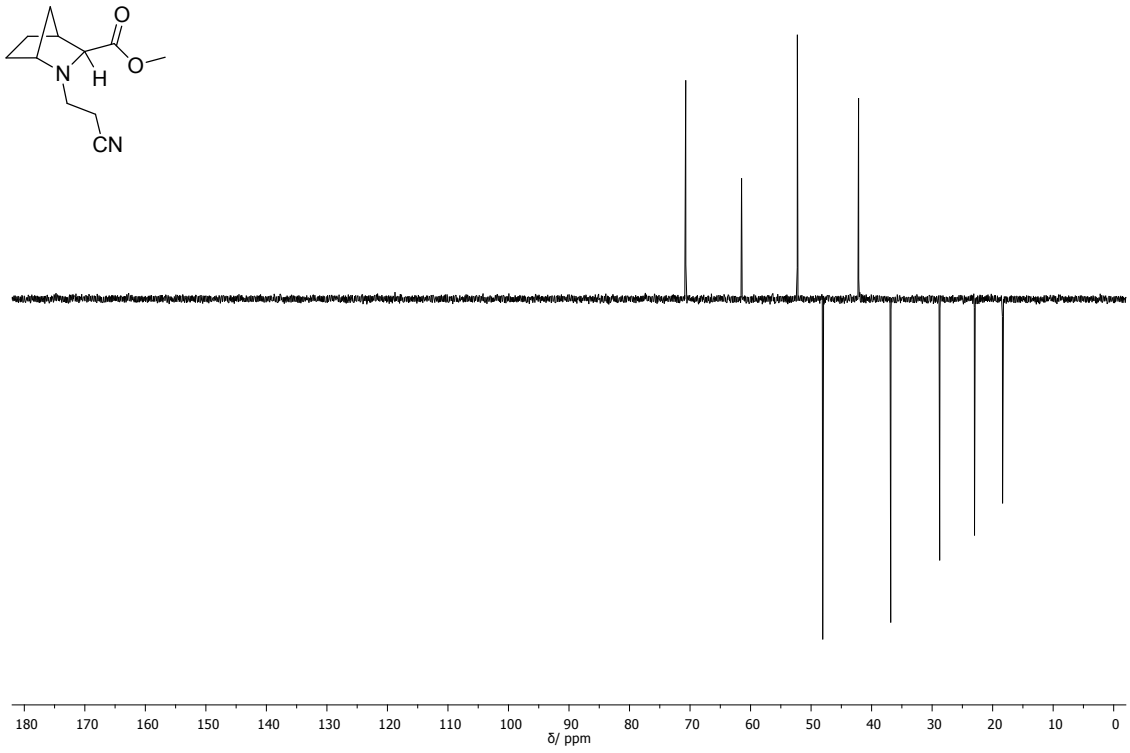


Fig. S9. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **5**.

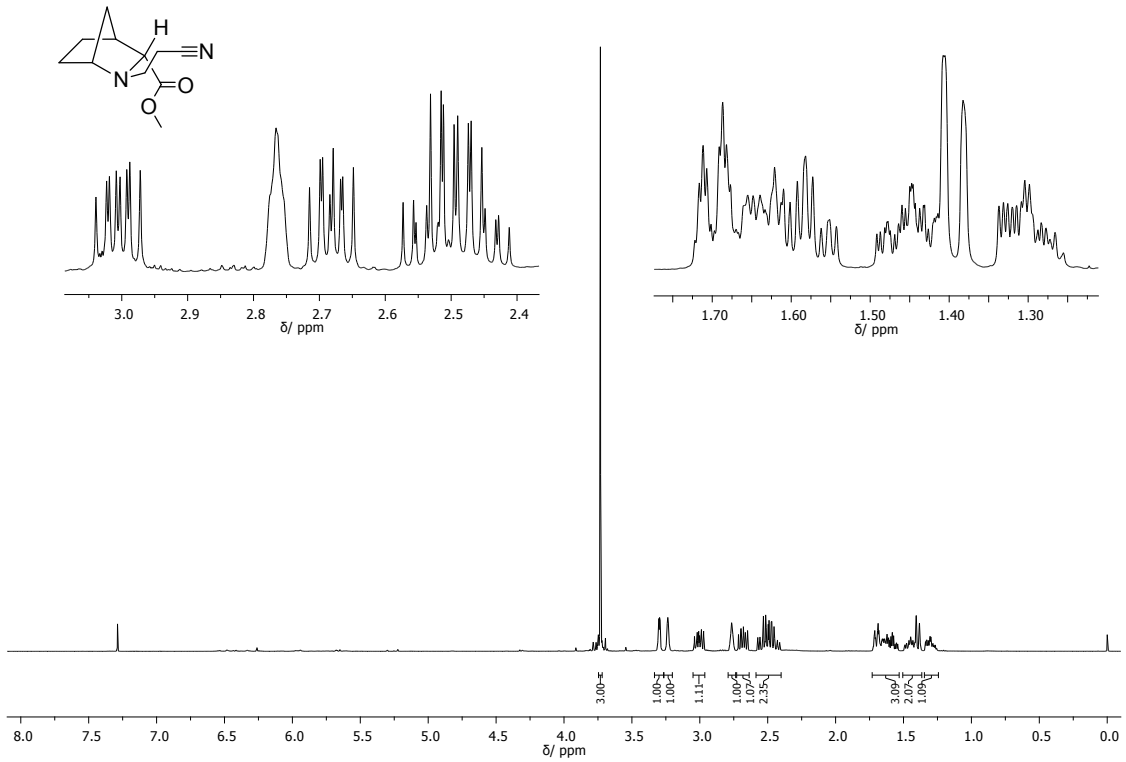


Fig. S10. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **6**.

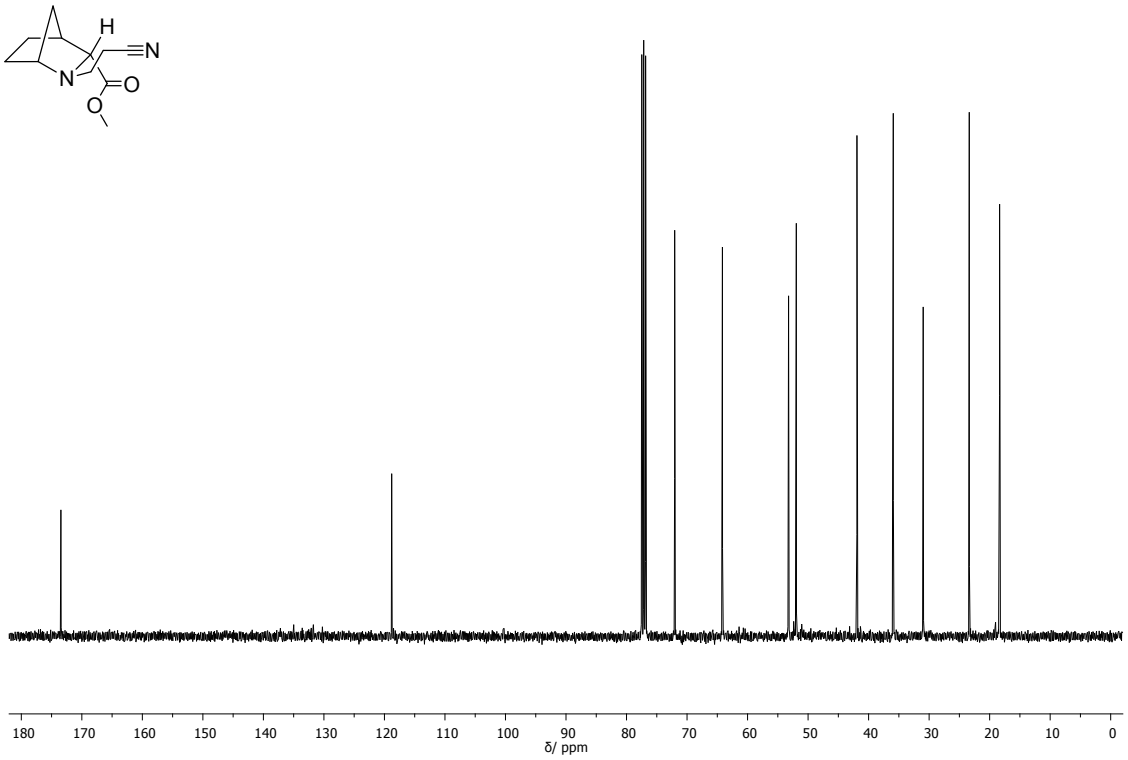


Fig. S11. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **6**.

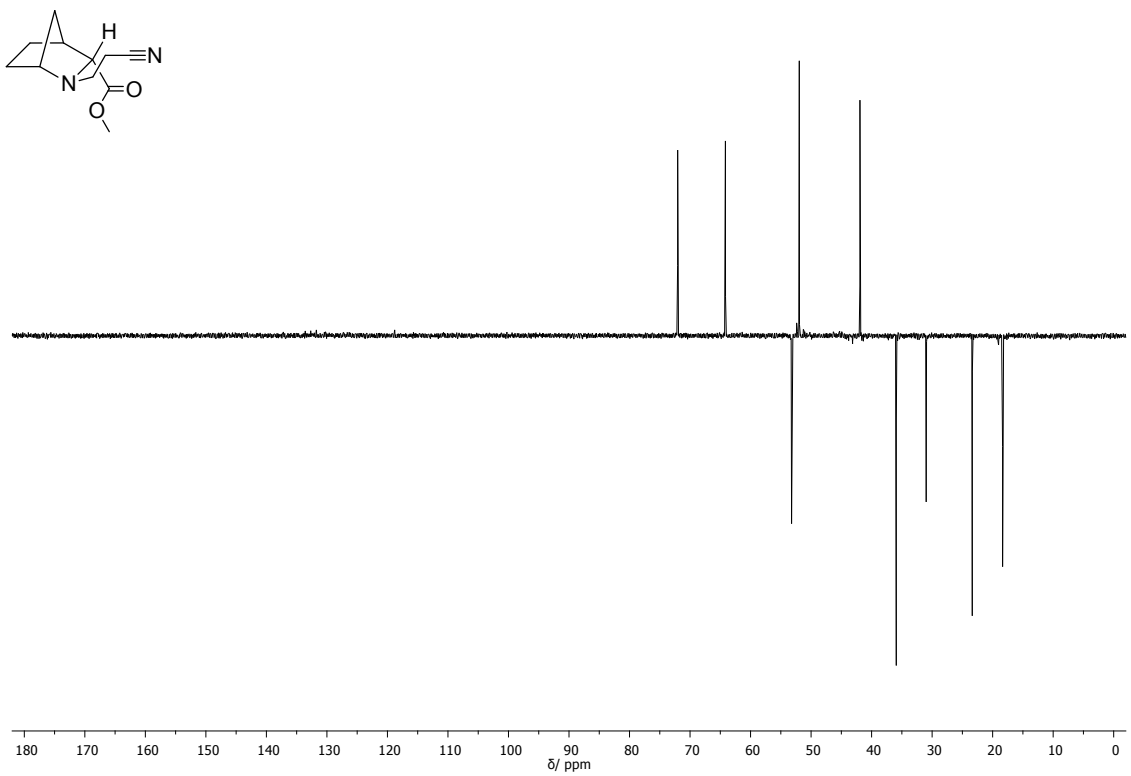


Fig. S12. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **6**.

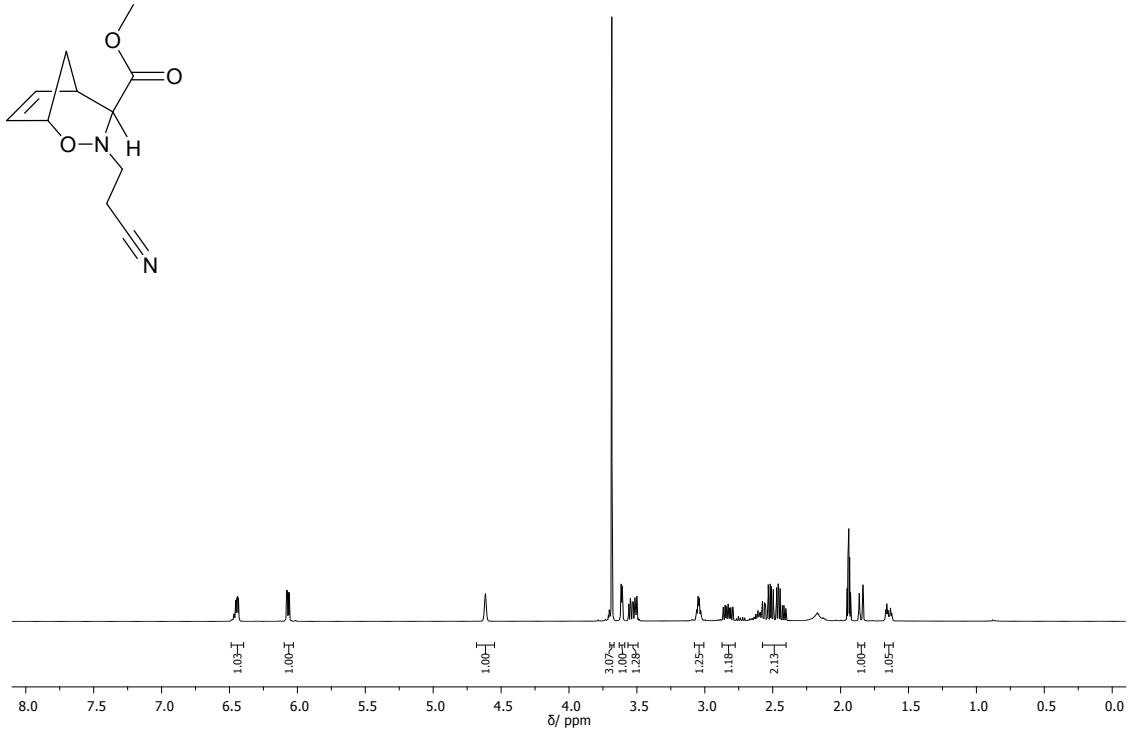


Fig. S13. ^{1}H-NMR spectrum (CD_3CN, 400 MHz) of compound **11**.

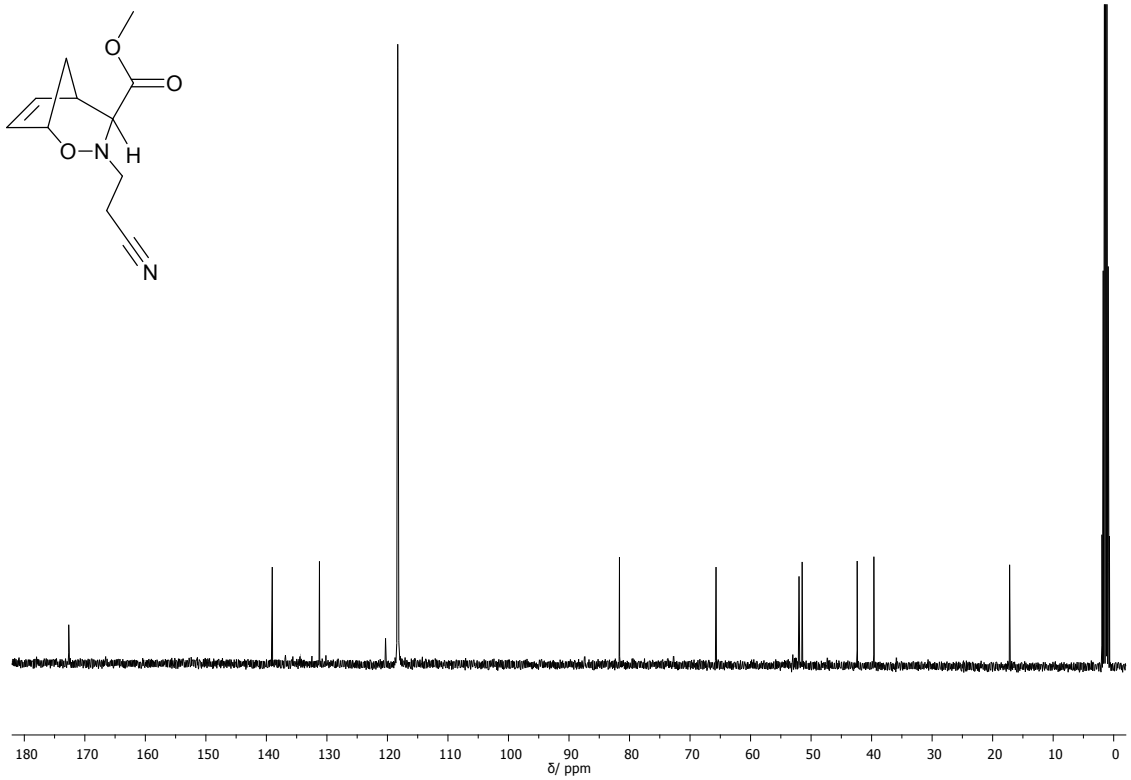


Fig. S14. ^{13}C-NMR spectrum (CD_3CN, 101 MHz) of compound **11**.

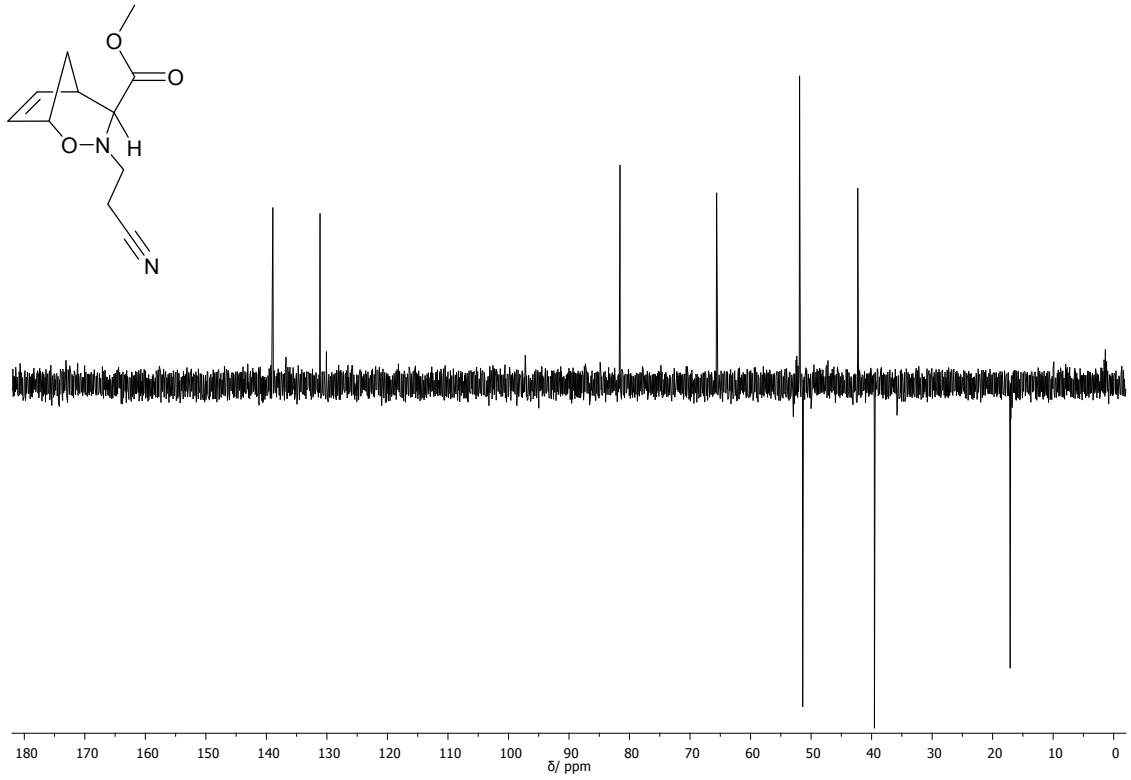


Fig. S15. DEPT-135 spectrum (CD_3CN, 101 MHz) of compound **11**.

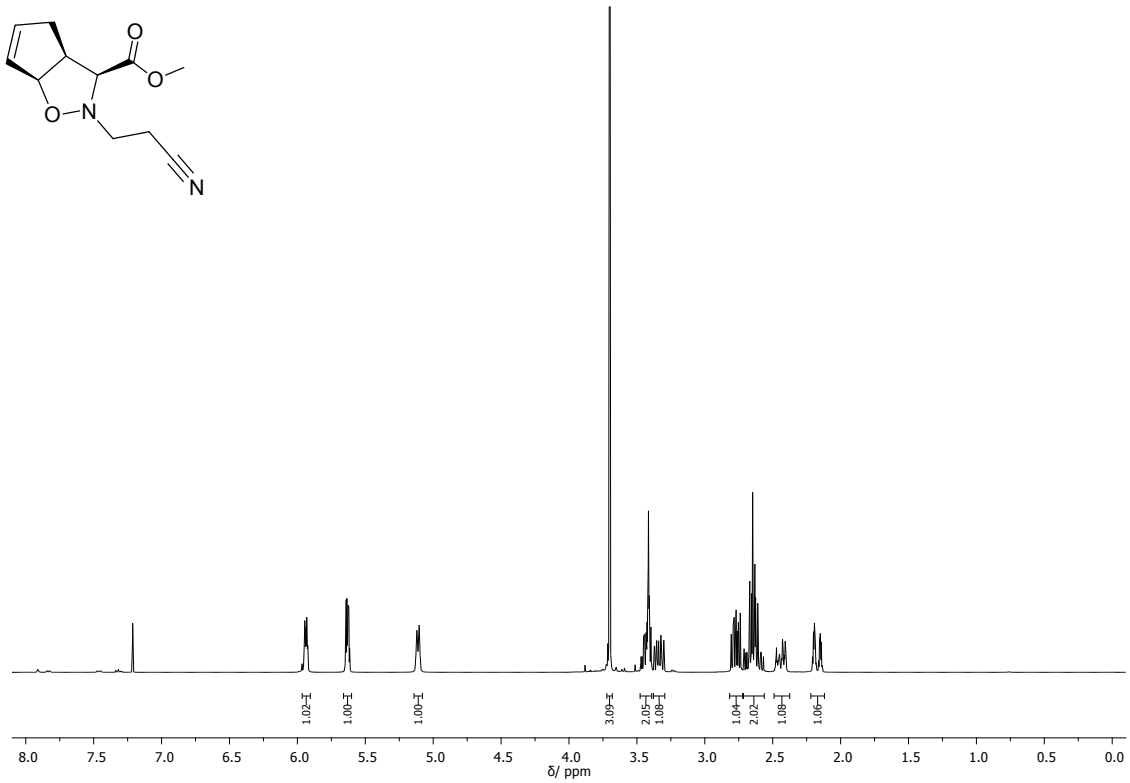


Fig. S16. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **12**.

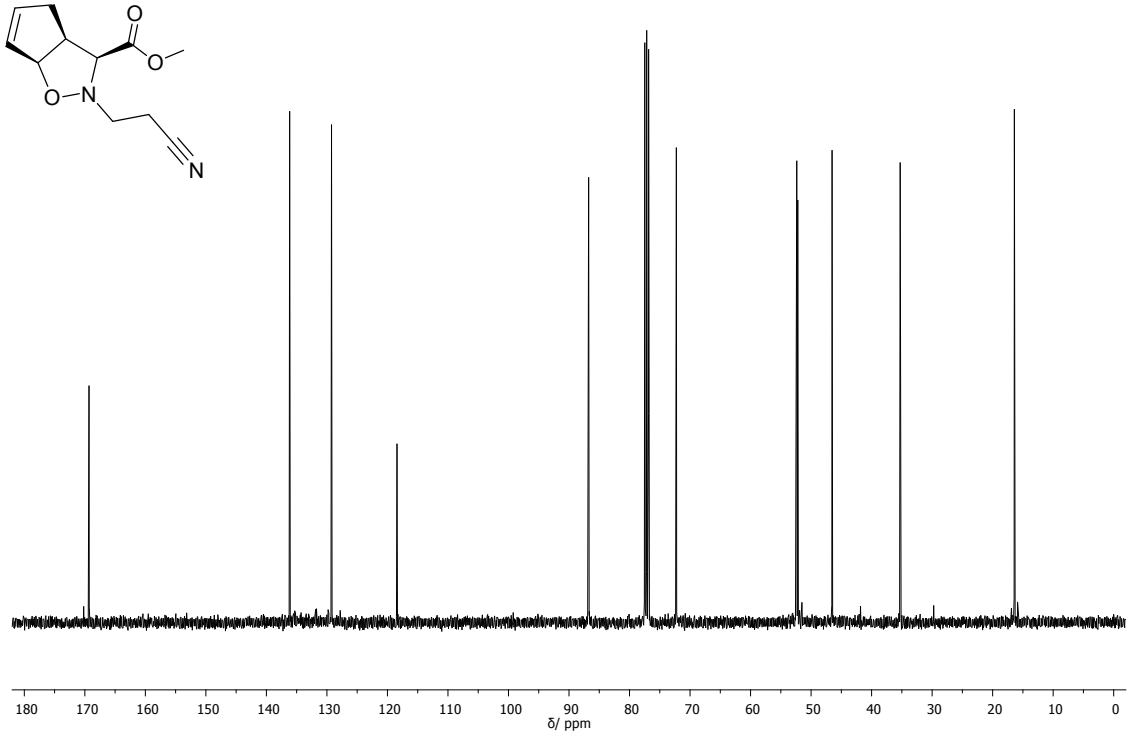


Fig. S17. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **12**.

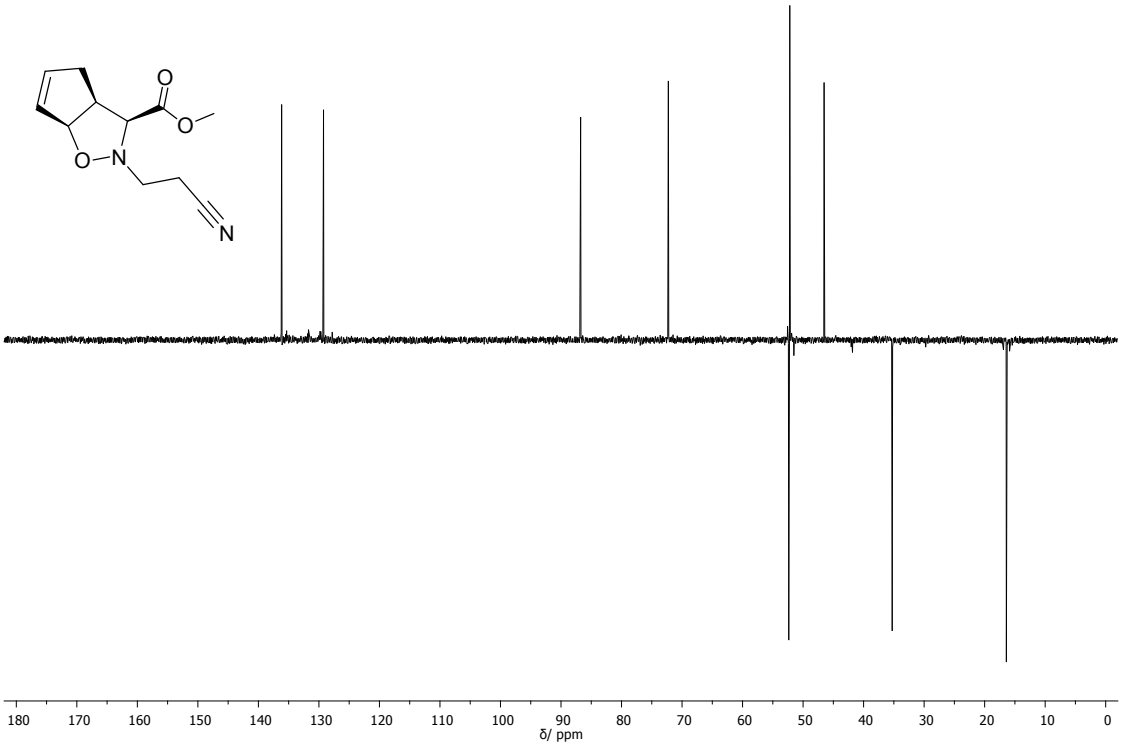


Fig. S18. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **12**.

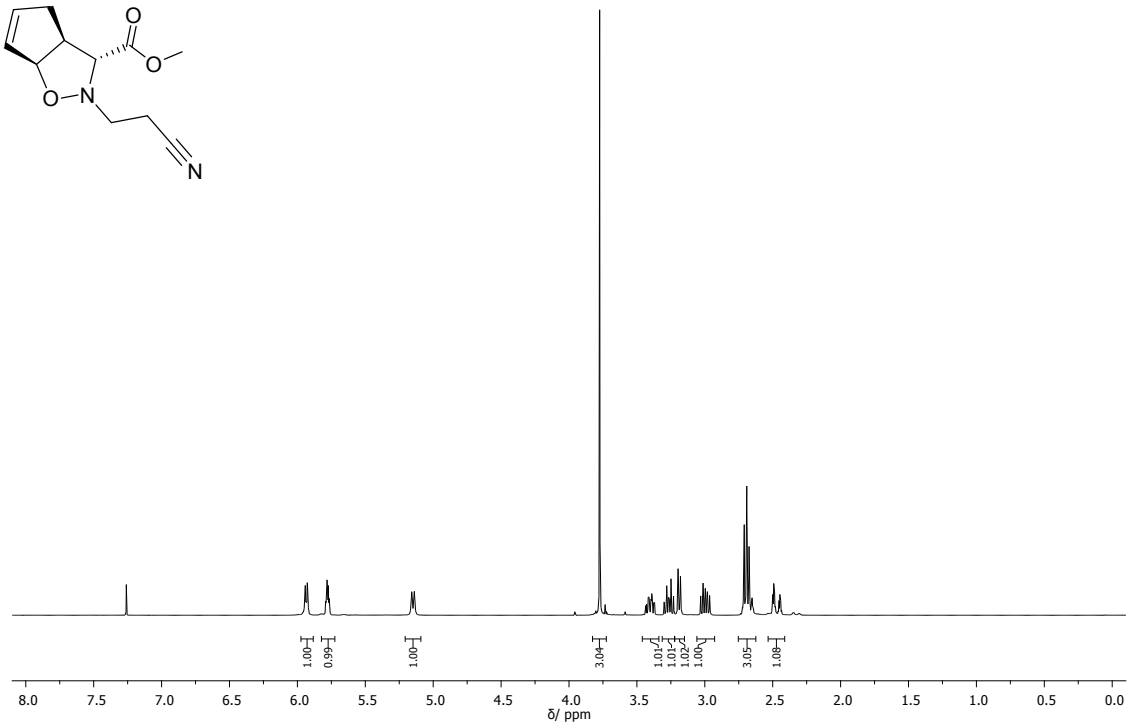


Fig. S19. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **13**.

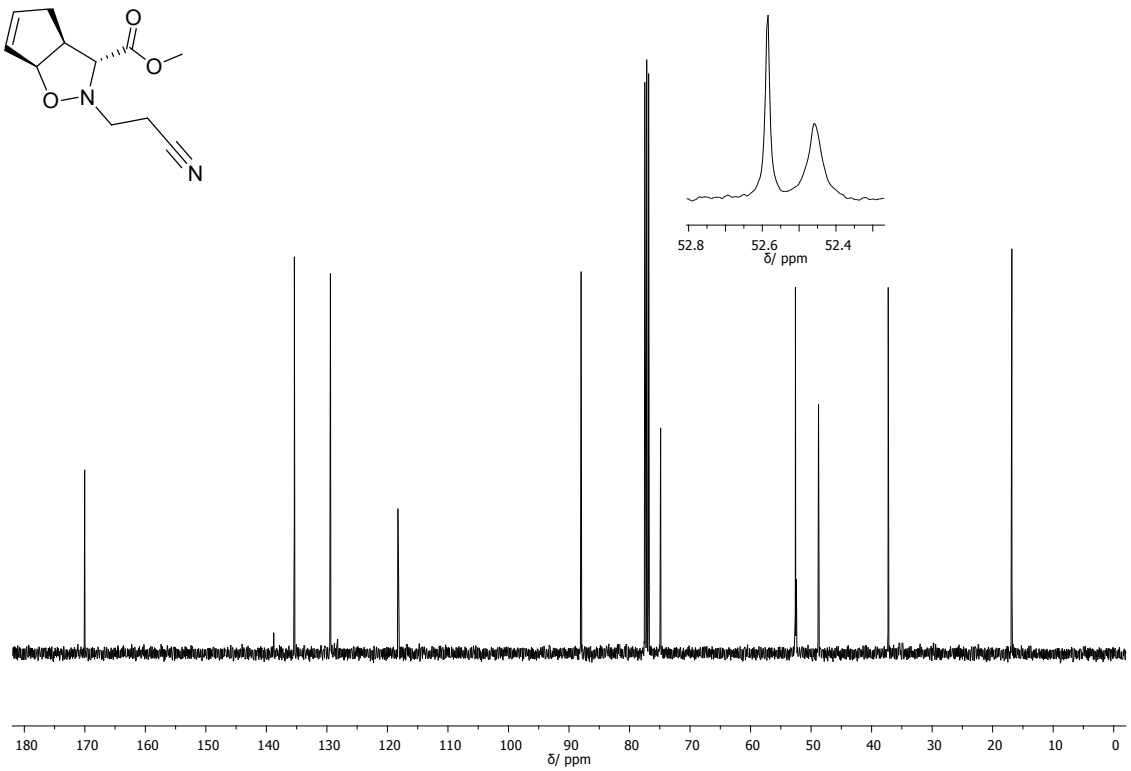


Fig. S20. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **13**.

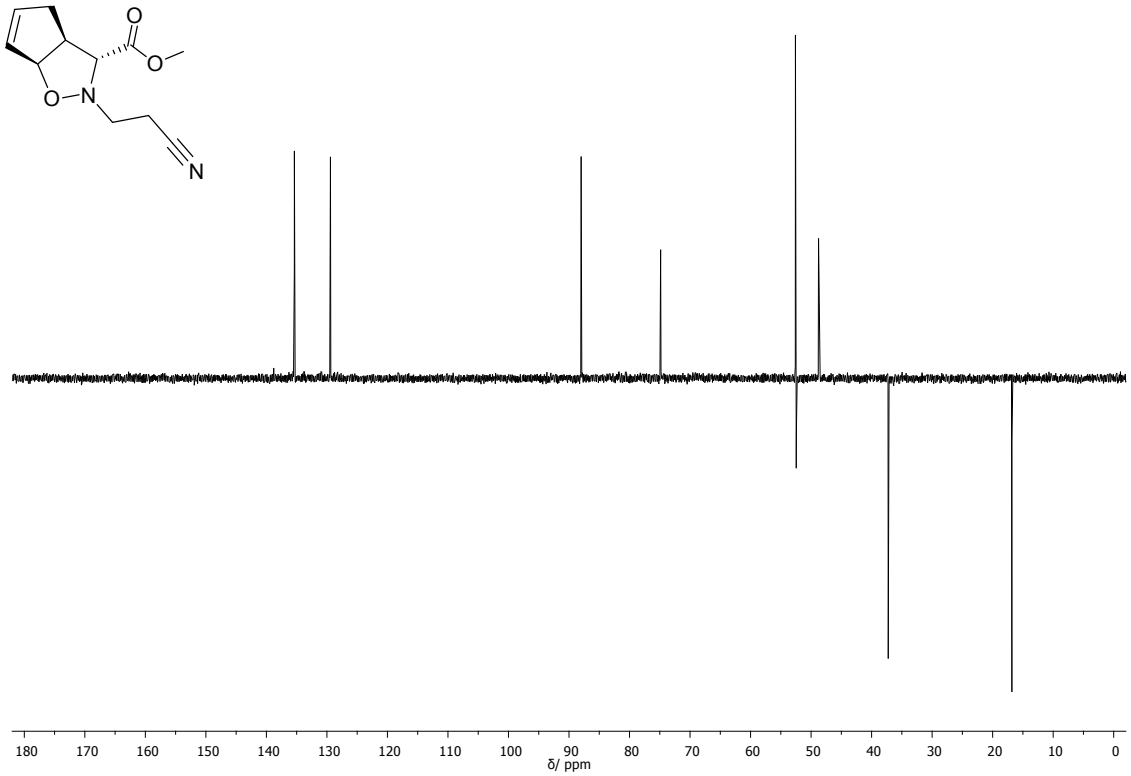


Fig. S21. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **13**.

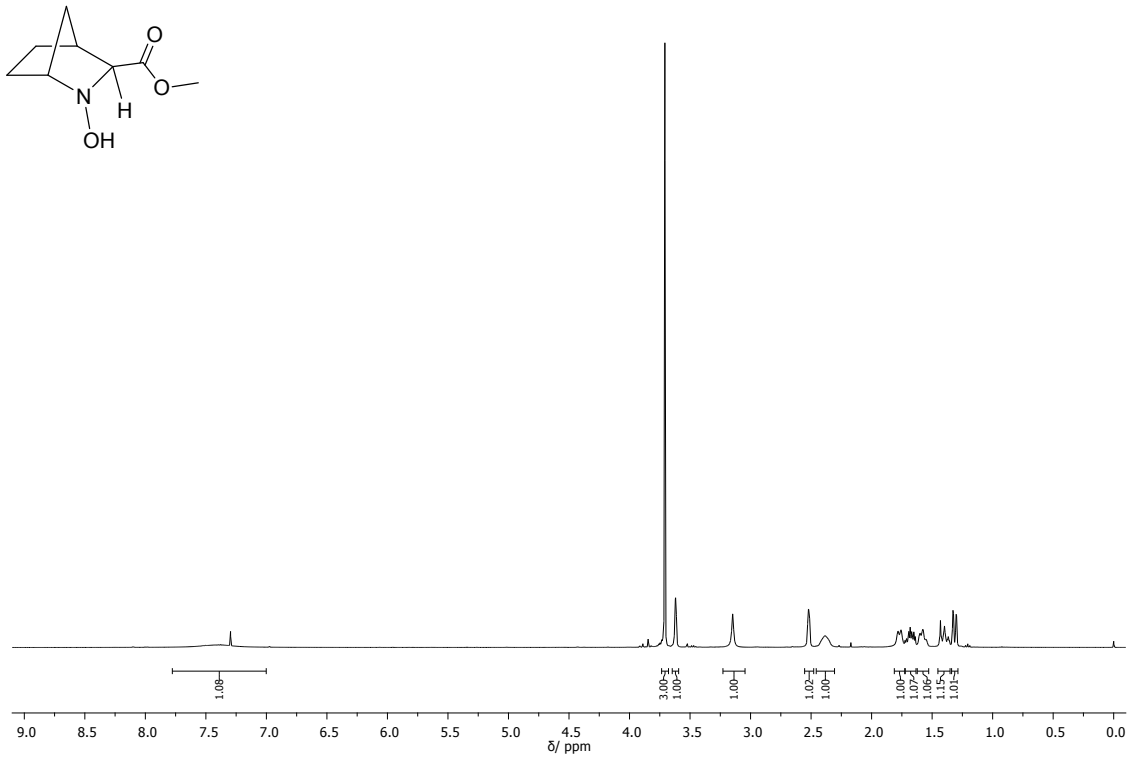


Fig. S22. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **15**.

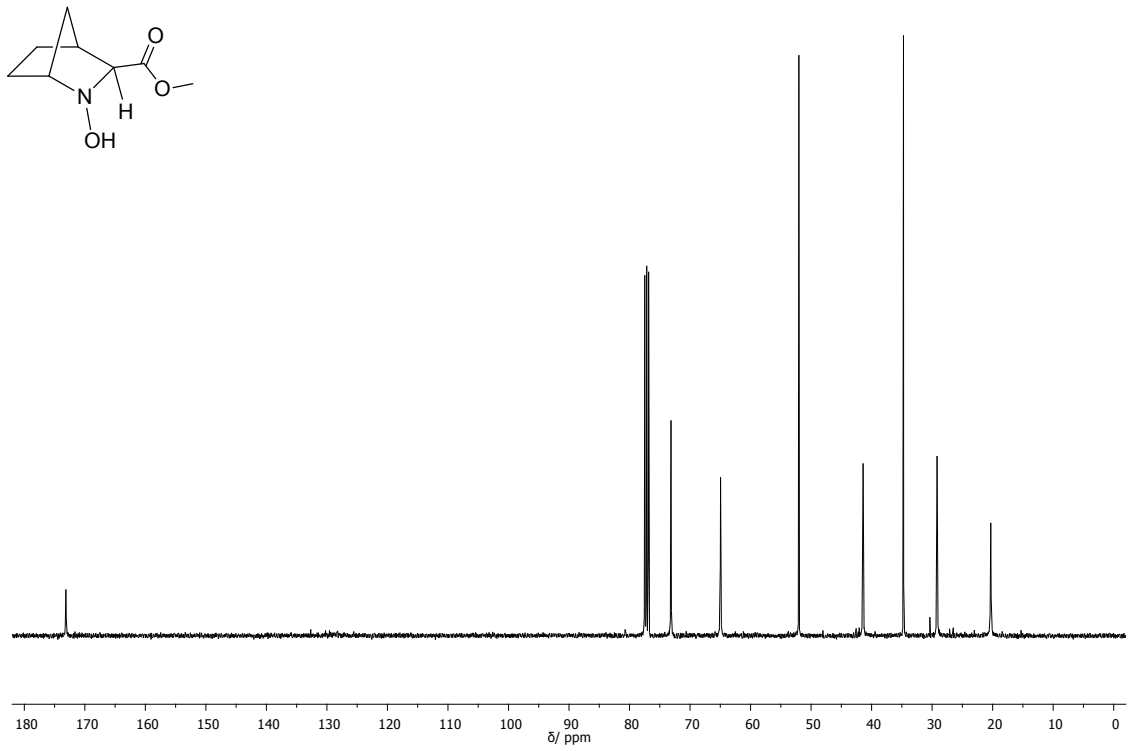


Fig. S23. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **15**.

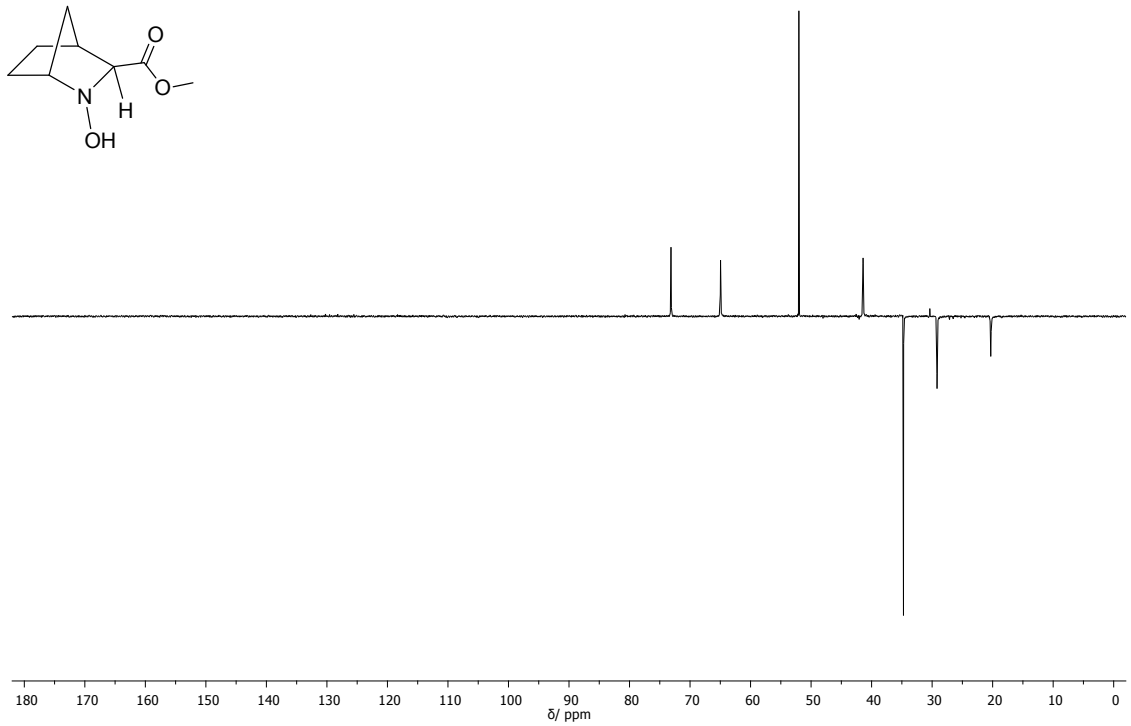


Fig. S24. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **15**.

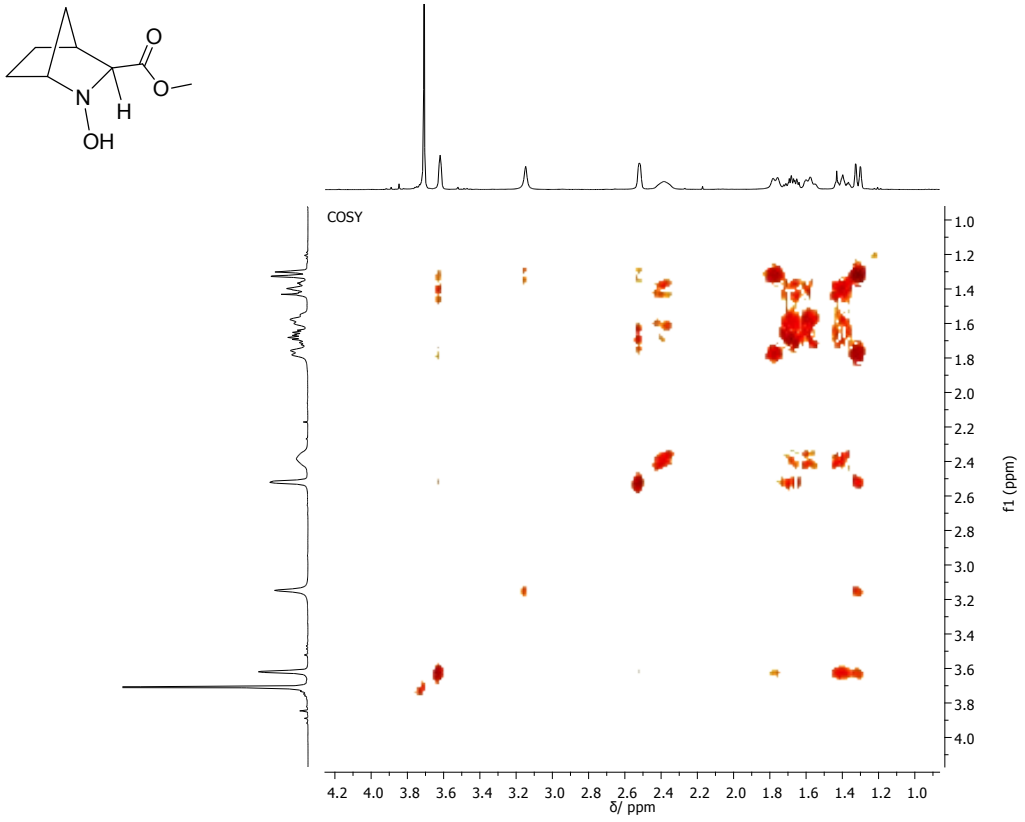


Fig. S25. COSY spectrum ($CDCl_3$, 101 MHz) of compound **15**.

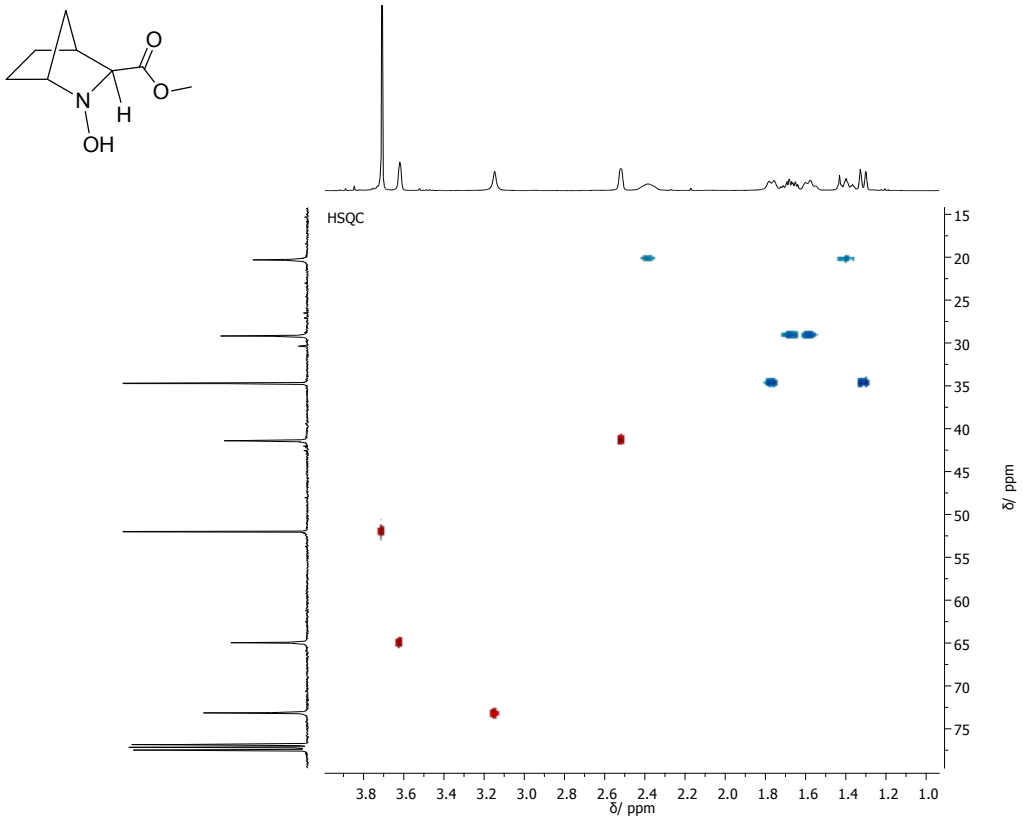


Fig. S26. HSQC spectrum ($CDCl_3$, 101 MHz) of compound **15**.

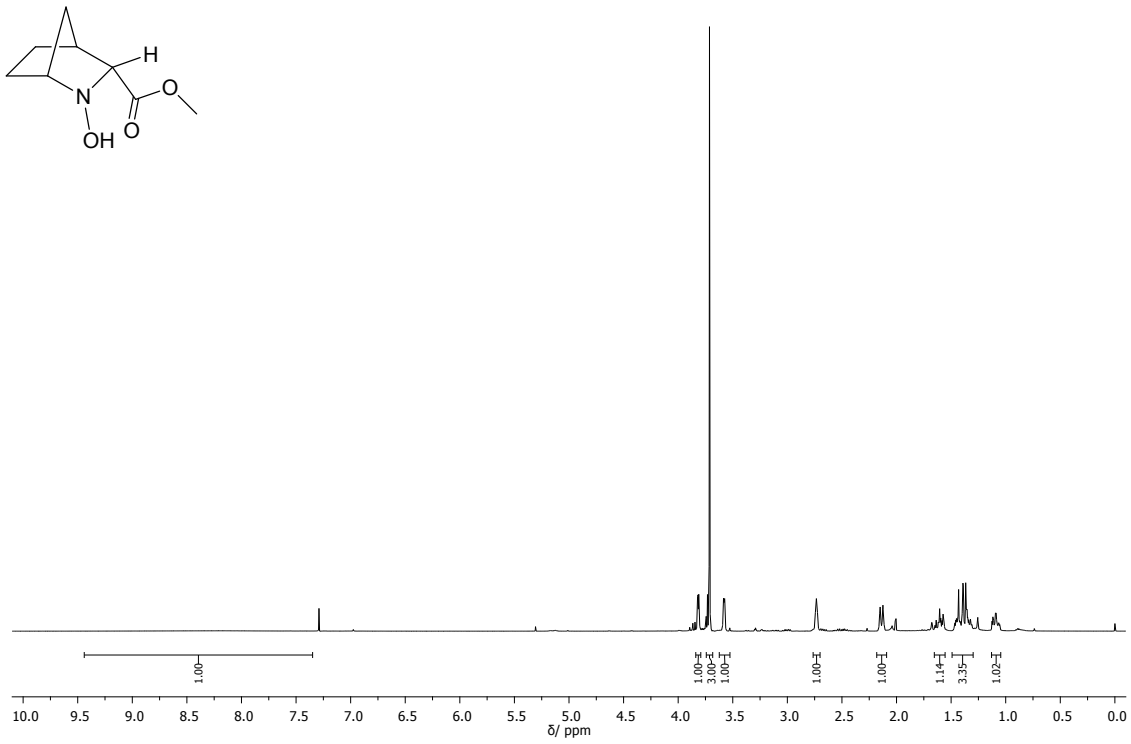


Fig. S27. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **16**.

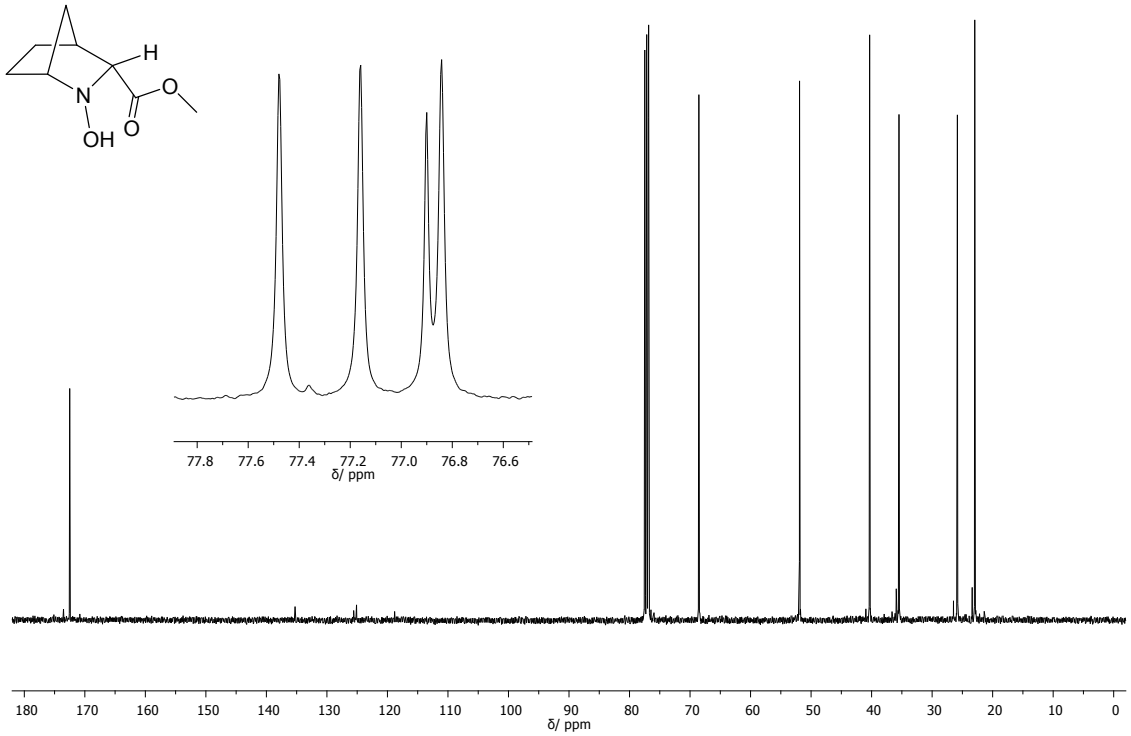


Fig. S28. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **16**.

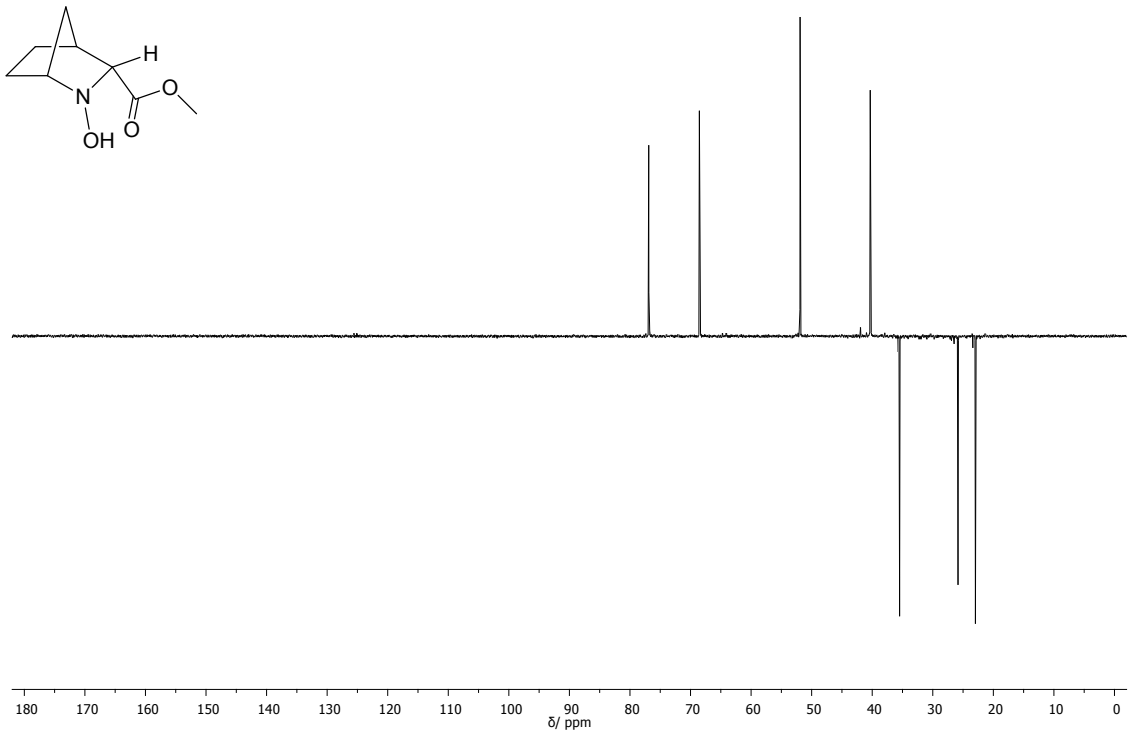


Fig. S29. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **16**.

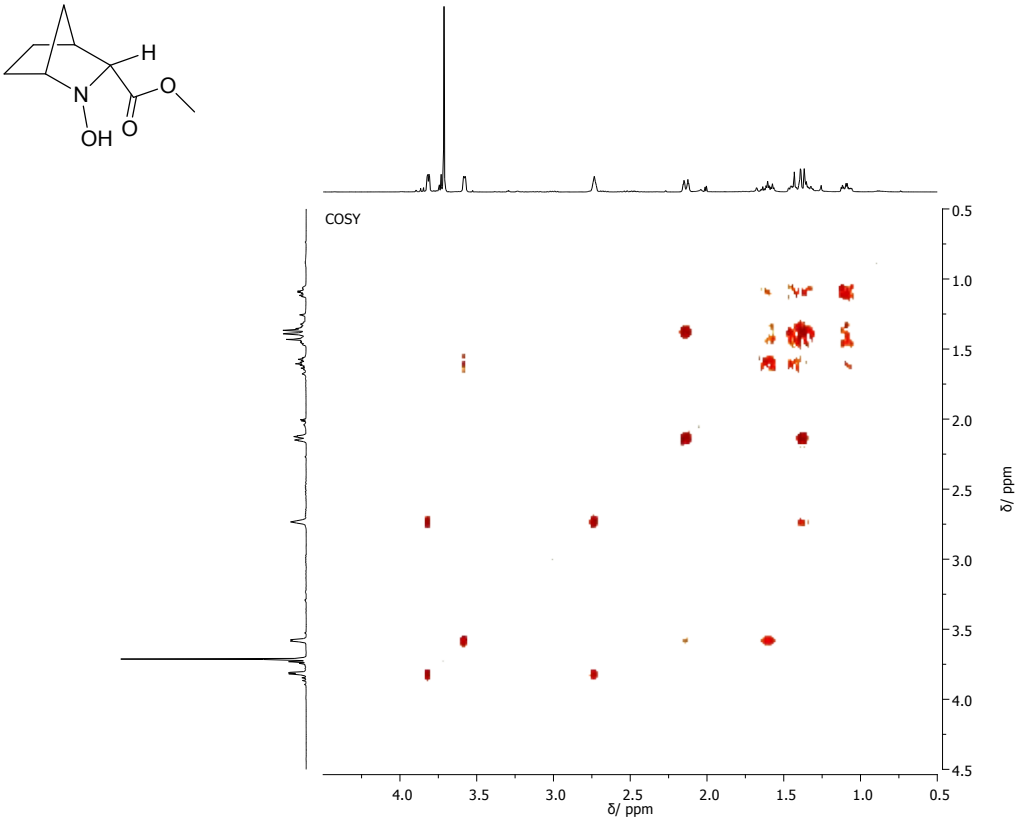


Fig. S30. COSY spectrum ($CDCl_3$, 101 MHz) of compound **16**.

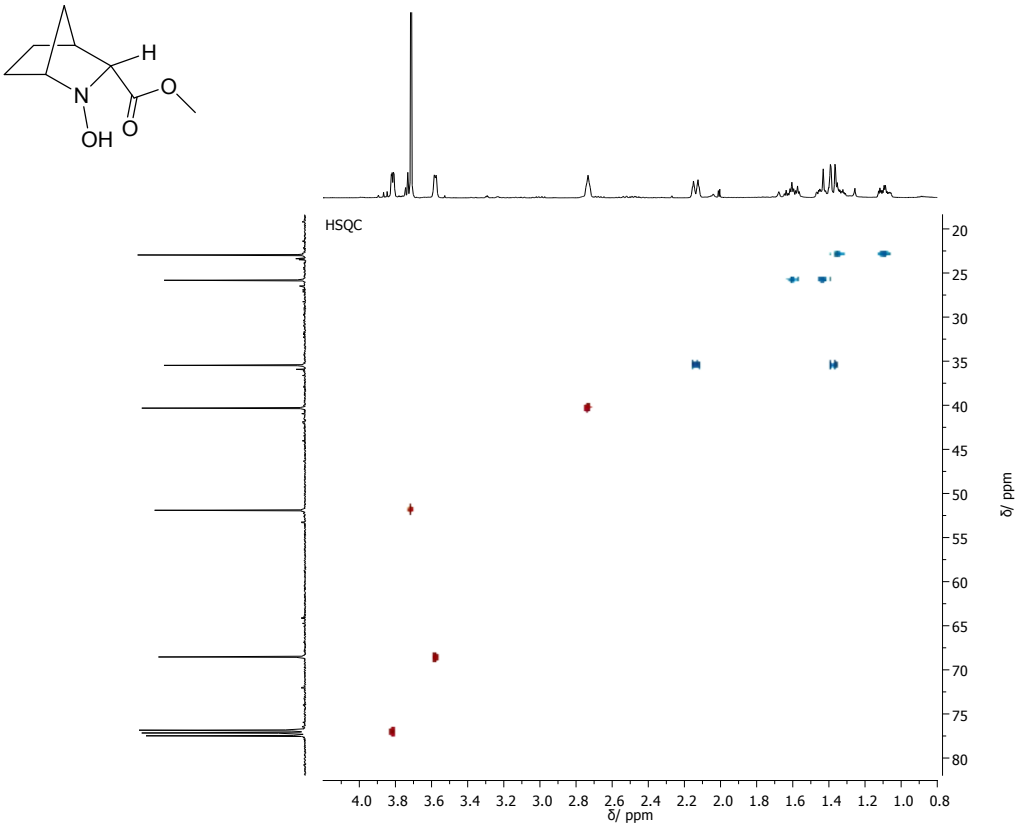


Fig. S31. HSQC spectrum ($CDCl_3$, 101 MHz) of compound **16**.

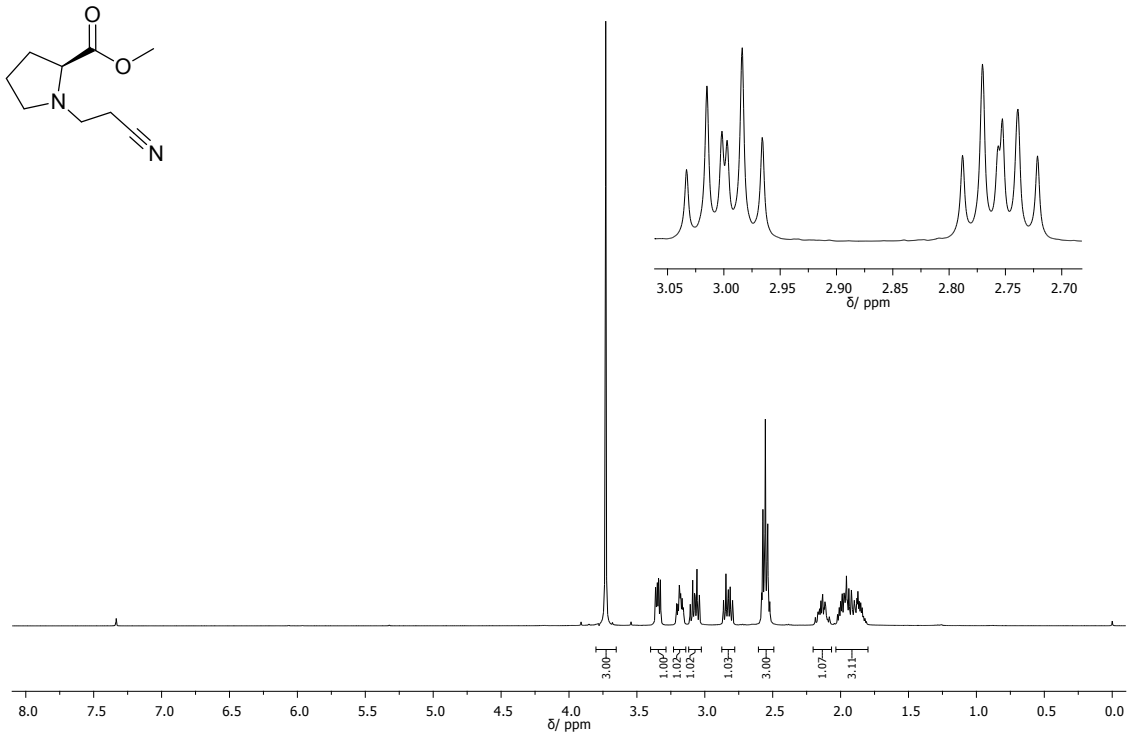


Fig. S32. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **20**.

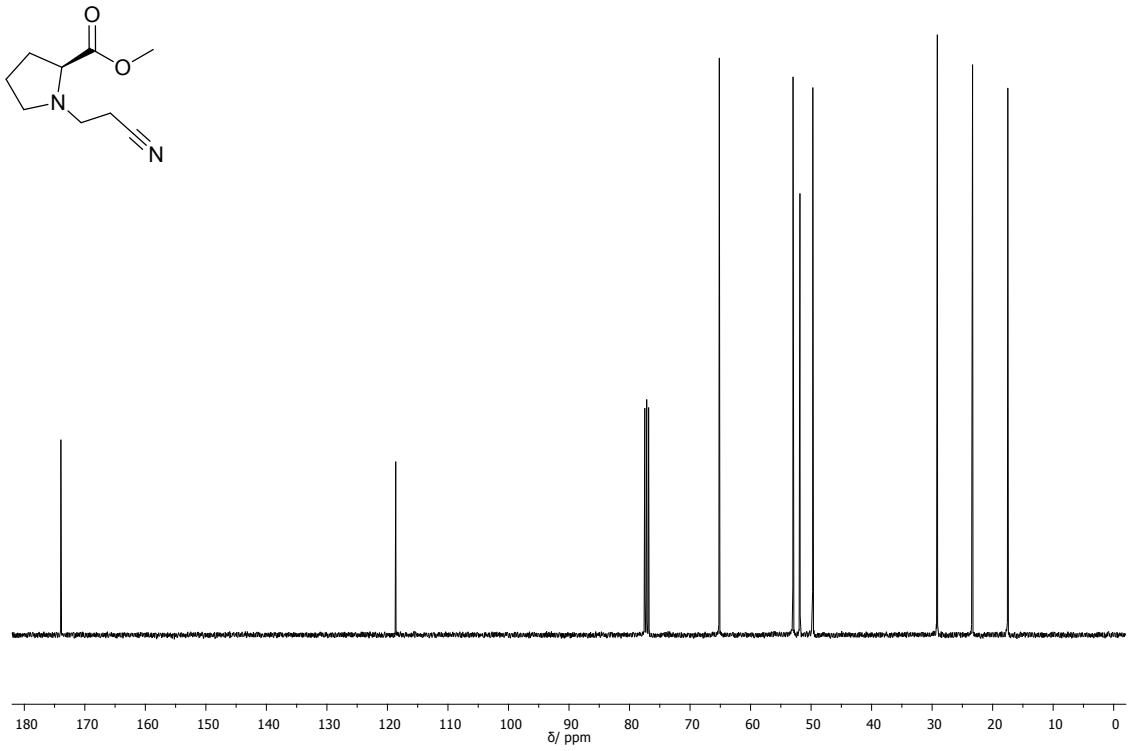


Fig. S33. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **20**.

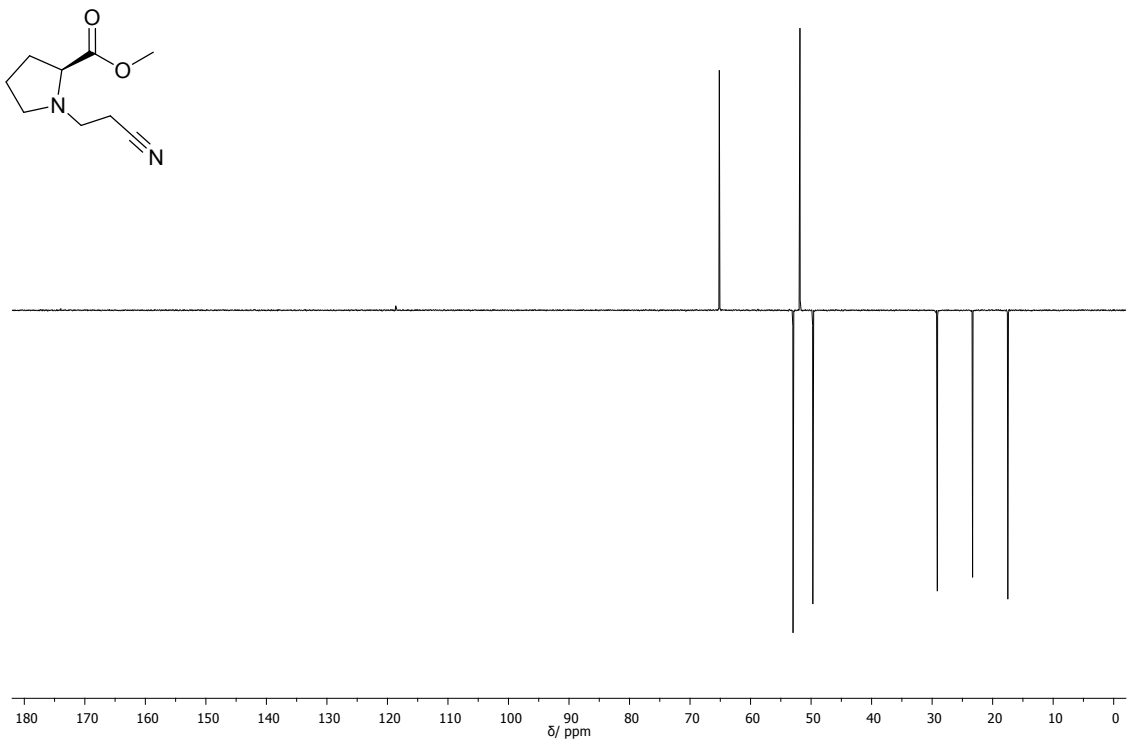


Fig. S34. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **20**.

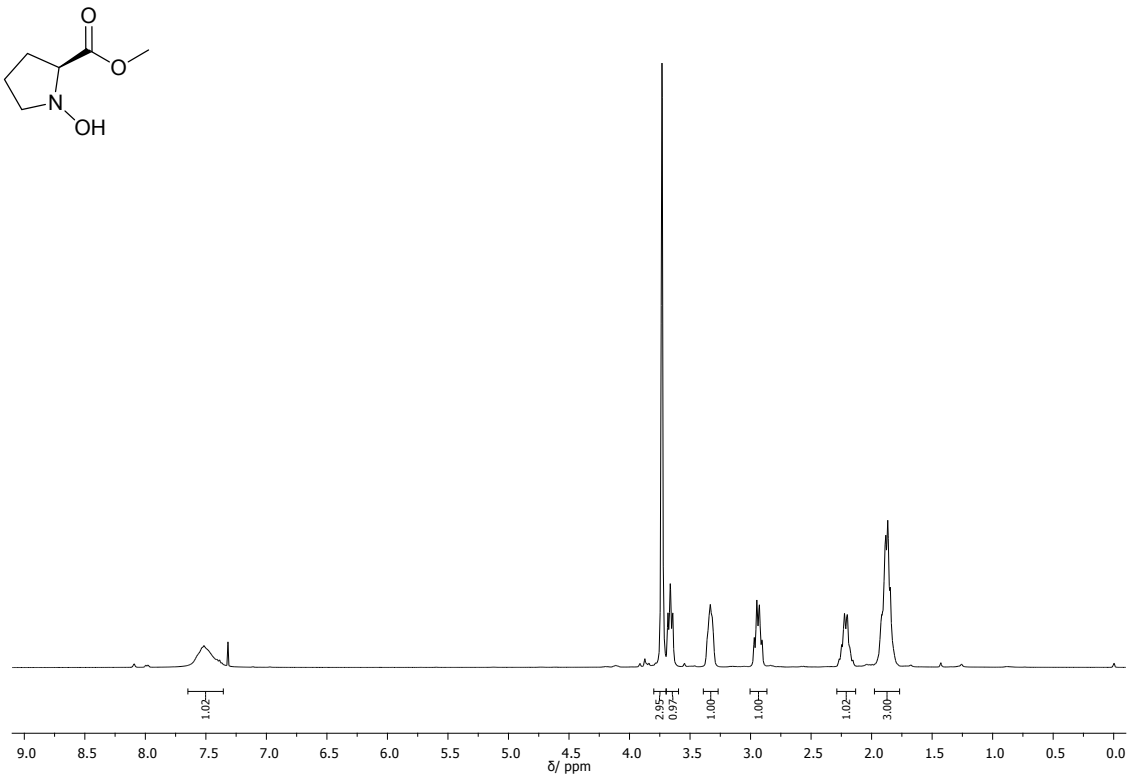


Fig. S35. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **21**.

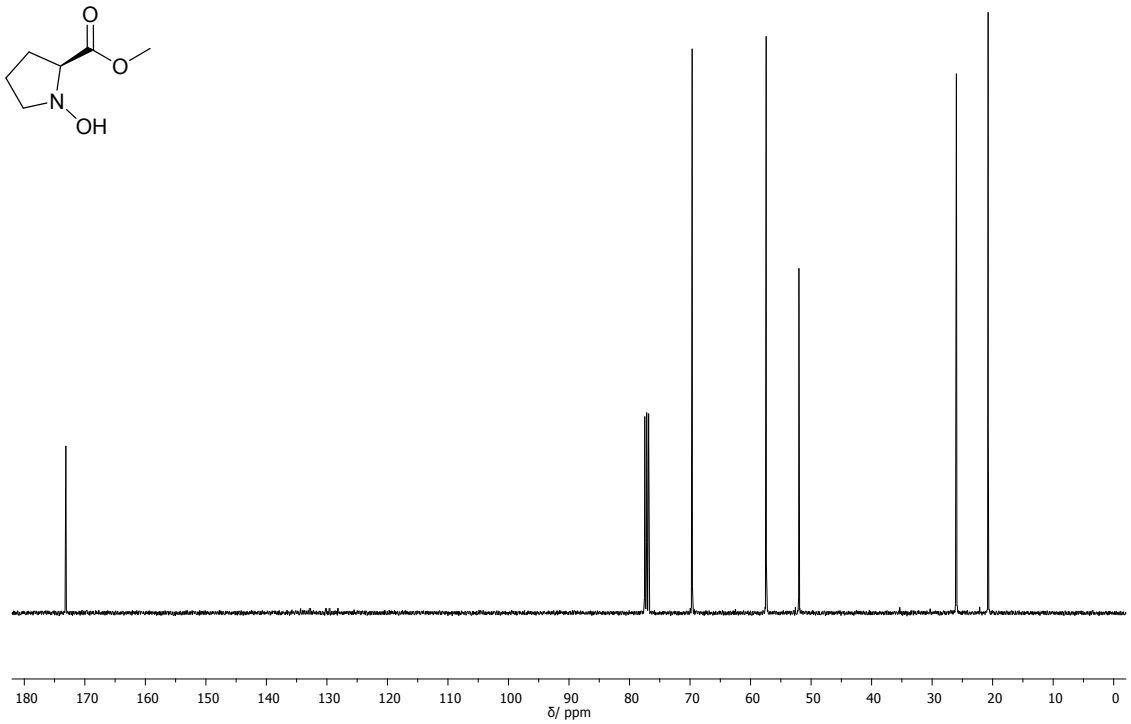


Fig. S36. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **21**.

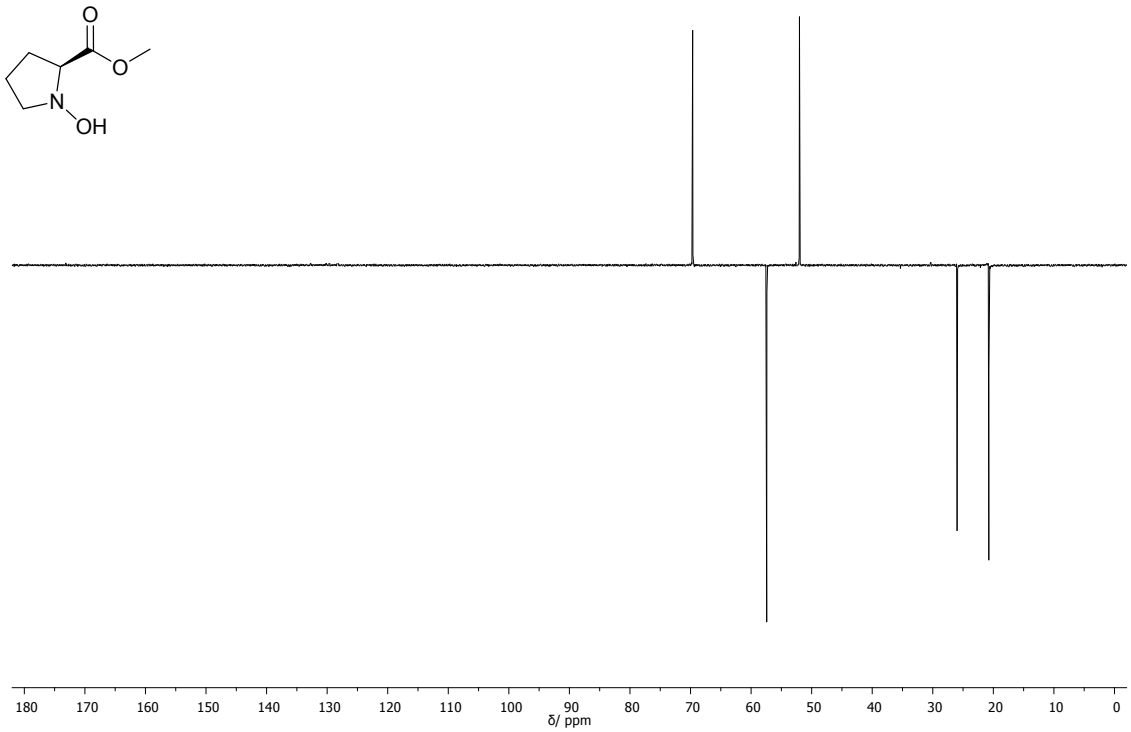


Fig. S37. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **21**.

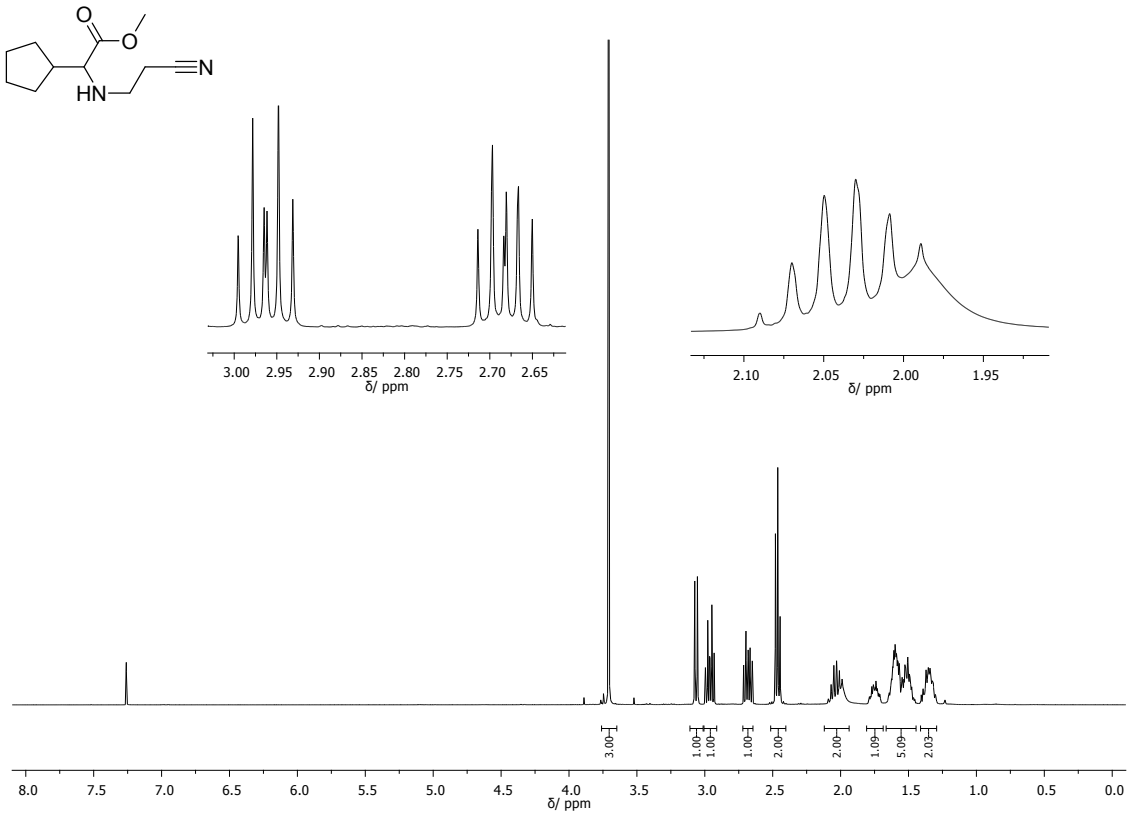


Fig. S38. ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of compound **23**.

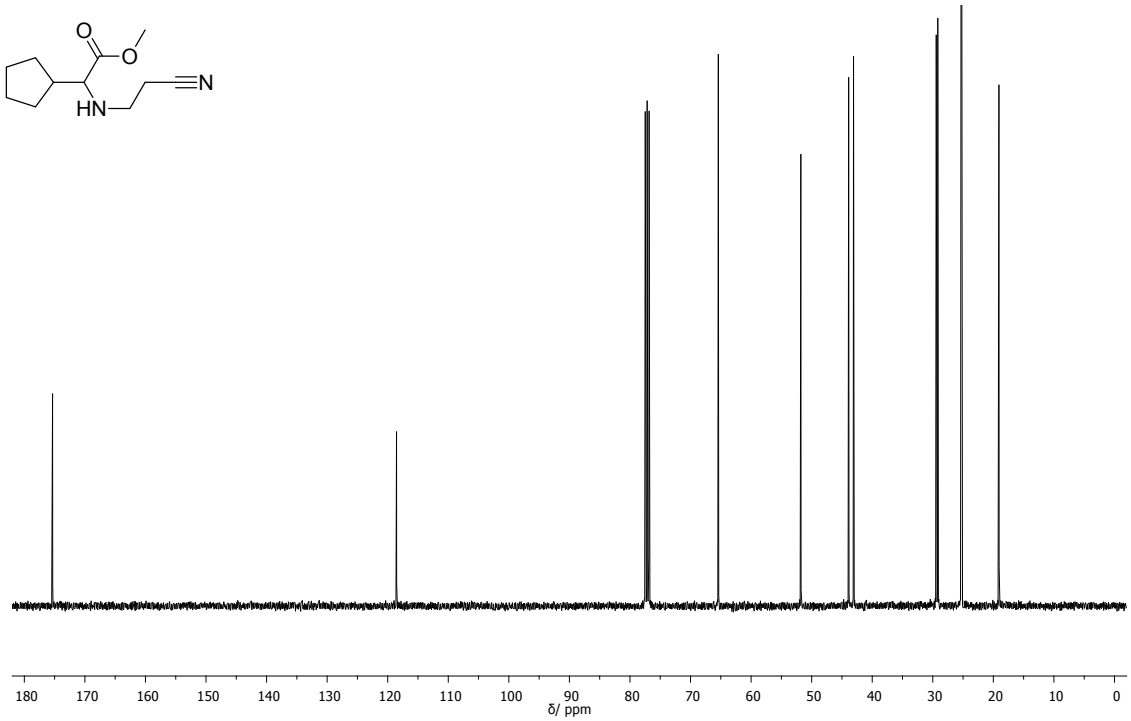


Fig. S39. ^{13}C-NMR spectrum ($CDCl_3$, 101 MHz) of compound **23**.

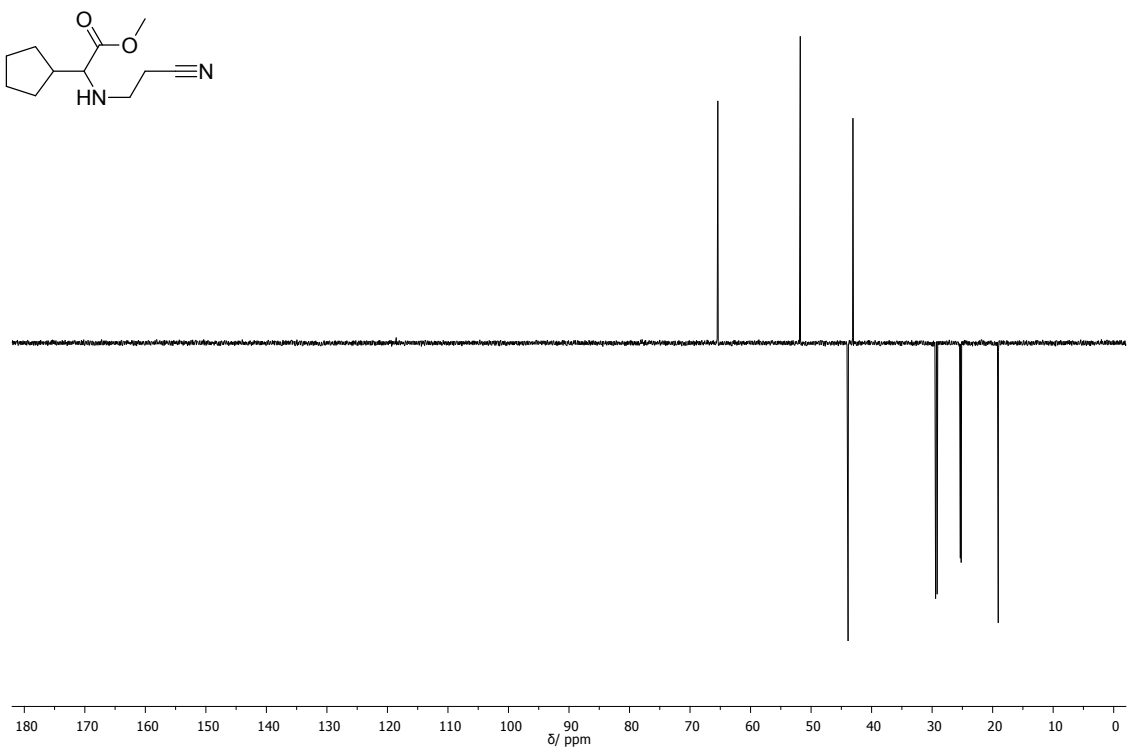


Fig. S40. DEPT-135 spectrum ($CDCl_3$, 101 MHz) of compound **23**.

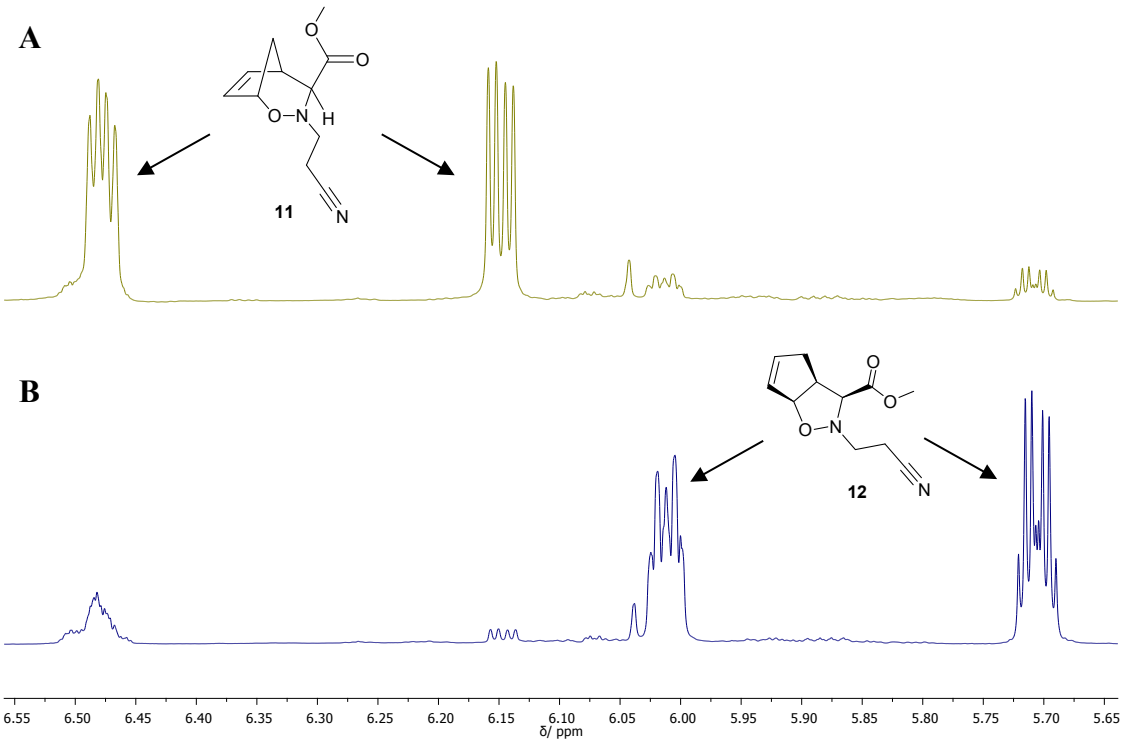


Fig. S41. Part of ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) between 5.65 – 6.55 ppm depicting the signals corresponding to the double bonds of **11** and **12**: **A)** 15 min after the addiction of $CDCl_3$ (**11**:**12** ratio of

87:13); **B**) 2 h after the addiction of $CDCl_3$ (**11**:**12** ratio of 7:93). This demonstrates the conversion of compound **11** into isoxazolidine **12**.

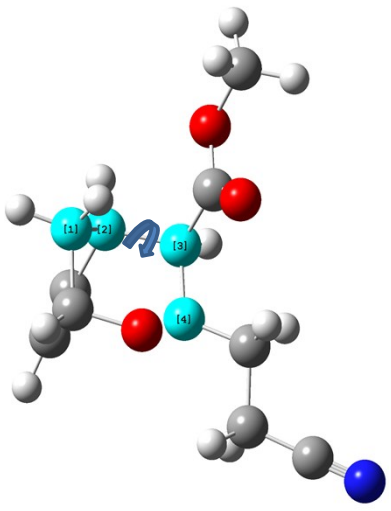
Table S1. Calculated electronic energies, E_{el}, at T = 0 K, and unscaled enthalpies, at T = 298.15 K, H_{298}, at the B3LYP/6-311++G(d,p) level of theory for the relevant molecular species.

Molecular species	E_{el} / hartree	H_{298} / hartree
1 (*anti*-cyanoethyl)	-687.681021	---
1 (*syn*-cyanoethyl)	-687.673302	---
2 (*anti*-cyanoethyl)	-687.674548	---
2 (*syn*-cyanoethyl)	-687.676328	---
10 (*anti*-cyanoethyl)	-762.853225	-762.352561
10 (*syn*-cyanoethyl)	-762.846228	---
11	-762.878234	-762.377281
$\mathbf{11}_{endo}$	-762.879427	-762.378466
12	-762.890877	-762.389742
13	-762.896831	-762.395845
14 (*anti*-cyanoethyl)	-762.849869	---
14 (*syn*-cyanoethyl)	-762.848028	-762.347618
H radical	-0.502257	---
methyl 2-(cyclopent-2-enyl)acetate [a]	-462.649202	---
methyl 2-(cyclopent-2-enyl)acetate radical [a]	-462.007891	---
methyl 2-cyclopentylacetate [a]	-463.877965	---
methyl 2-cyclopentylacetate radical [a]	-463.216034	---

[a] See scheme 8 of the main article for the molecular structure of these species.

Table S2. Rotational barrier calculations, at the B3LYP/6-311++G(d,p) level of theory, for the hindered internal rotation around the $C(H_2)$−C(H)−$C(H)(COOCH_3)$−N dihedral angle in **11**.

Dihedral angle / º	E_{el} (0 K) / hartree	$\Delta_{rel}E_{el}$ / kJ·mol^{-1}
61.2	-762.878234	33.2
70	-762.876447	37.9
80	-762.868824	57.9
90	-762.854209	96.3
100	-762.886393	11.8
110	-762.888276	6.8
120	-762.889847	2.7
130	-762.890673	0.5
136.7	-762.890877	0.0
140	-762.890798	0.2
150	-762.889487	3.6
160	-762.885967	12.9



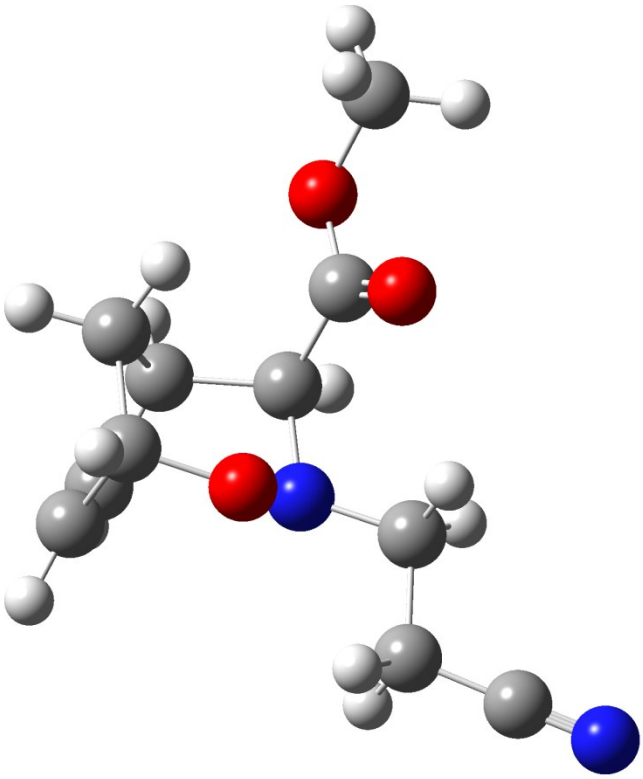


Fig. S42. Optimized structure of the transition state (dihedral angle = 90 º) for the hindered internal rotation around the $C(H_2)$−C(H)−C(H)($COOCH_3$)−N dihedral angle in **11**.

Table S3. Optimized geometries in Cartesian coordinates for the molecular systems considered, obtained at the B3LYP/6-311++G(d,p) level of theory.

A) 1 (*anti*-cyanoethyl)

1	6	0	1.536608	-2.484779	0.378679
2	6	0	1.202026	-1.670865	-0.870744
3	6	0	2.228238	-0.289115	0.540261
4	6	0	2.141883	-1.642720	1.226523
5	6	0	2.411700	-0.731534	-0.935982
6	1	0	2.296772	0.076741	-1.656203
7	1	0	3.351042	-1.262026	-1.090426
8	6	0	0.749739	0.227397	0.483104
9	1	0	0.258589	0.138838	1.458606
10	1	0	0.929527	-2.219013	-1.770901
11	1	0	2.934760	0.431062	0.946745
12	1	0	2.432823	-1.835025	2.251685
13	1	0	1.232617	-3.505799	0.571461
14	6	0	0.660319	1.686613	0.037131
15	8	0	1.458023	2.264550	-0.657349
16	8	0	-0.449044	2.276062	0.537557
17	6	0	-0.655266	3.655673	0.168300
18	1	0	-0.746473	3.749252	-0.914486
19	1	0	-1.578552	3.953339	0.660195
20	1	0	0.178822	4.267781	0.512711
21	6	0	-1.151376	-1.273294	-0.129120
22	1	0	-1.305701	-2.164371	-0.742890
23	1	0	-1.162531	-1.597627	0.922578
24	6	0	-2.326688	-0.303189	-0.372899
25	1	0	-2.198356	0.606667	0.218116
26	1	0	-2.340182	-0.005912	-1.425335
27	6	0	-3.611616	-0.907707	-0.031900
28	7	0	-4.617083	-1.402901	0.240731
29	7	0	0.121598	-0.676766	-0.518393

B) 1 (*syn*-cyanoethyl)

1	6	0	-2.585439	-1.798675	-0.582289
2	6	0	-1.533586	-1.633004	0.510257
3	6	0	-2.248350	0.405555	-0.000405
4	6	0	-3.003777	-0.567620	-0.893538
5	6	0	-2.111305	-0.438891	1.291930
6	1	0	-1.416495	-0.023784	2.021788
7	1	0	-3.079387	-0.641975	1.751013
8	6	0	-0.748342	0.364047	-0.511347
9	1	0	-0.709518	0.544301	-1.587345
10	1	0	-1.248765	-2.526666	1.061023
11	1	0	-2.652933	1.413074	0.083102
12	1	0	-3.667517	-0.277317	-1.697968
13	1	0	-2.827201	-2.728063	-1.081109
14	6	0	0.047547	1.472019	0.166618
15	8	0	0.362072	1.521706	1.332491
16	8	0	0.346677	2.446185	-0.720311
17	6	0	1.037790	3.595516	-0.189444
18	1	0	1.993936	3.298216	0.242641
19	1	0	1.188570	4.259149	-1.037653
20	1	0	0.433290	4.081384	0.577533
21	6	0	0.966556	-1.305963	0.369040
22	1	0	0.970585	-2.351337	0.684515
23	1	0	1.218401	-0.696291	1.246477
24	6	0	2.058204	-1.125854	-0.710042
25	1	0	2.076412	-0.094414	-1.075421
26	1	0	1.829258	-1.764261	-1.567877
27	6	0	3.389982	-1.455712	-0.209981
28	7	0	4.433919	-1.728353	0.197604
29	7	0	-0.347391	-1.029311	-0.192313

C) 2 (*anti*-cyanoethyl)

1	6	0	0.147830	-1.939053	1.383013
2	6	0	-0.522959	-1.962244	0.011031
3	6	0	1.629995	-1.521495	-0.334774
4	6	0	1.440929	-1.669607	1.165939
5	6	0	0.602906	-2.559923	-0.848583
6	1	0	0.399055	-2.498891	-1.919388
7	1	0	0.869422	-3.577091	-0.562552
8	6	0	0.867978	-0.198315	-0.763562
9	1	0	-1.503224	-2.430555	-0.054325
10	1	0	2.647521	-1.569796	-0.717064
11	1	0	2.201819	-1.467449	1.908352
12	1	0	-0.354443	-2.007248	2.339191
13	1	0	1.061891	-0.015716	-1.825031
14	6	0	1.406453	1.006385	-0.003975
15	8	0	0.990307	1.462183	1.031837
16	8	0	2.479303	1.507203	-0.658642
17	6	0	3.139973	2.621900	-0.029079
18	1	0	3.960981	2.884679	-0.692278
19	1	0	2.450665	3.459997	0.080369
20	1	0	3.516191	2.337027	0.954483
21	6	0	-1.496628	0.373646	0.011445
22	1	0	-1.213081	1.384529	-0.279417
23	1	0	-1.521860	0.364766	1.108429
24	6	0	-2.910291	0.088146	-0.547553
25	1	0	-3.237212	-0.920969	-0.280916
26	1	0	-2.886800	0.139543	-1.639525
27	6	0	-3.904915	1.032990	-0.046324
28	7	0	-4.678134	1.789346	0.354224
29	7	0	-0.544070	-0.571131	-0.552990

D) 2 (*syn*-cyanoethyl)

1	6	0	1.291159	-2.078387	1.247604
2	6	0	0.044348	-2.166269	0.376559
3	6	0	1.599842	-1.140225	-0.835353
4	6	0	2.224975	-1.461183	0.517604
5	6	0	0.681435	-2.372992	-1.014739
6	1	0	-0.033034	-2.280008	-1.837746
7	1	0	1.242581	-3.302903	-1.110849
8	6	0	0.494320	-0.054178	-0.562603
9	1	0	-0.732558	-2.853567	0.703996
10	1	0	2.276186	-0.877400	-1.644444
11	1	0	3.208266	-1.140264	0.835267
12	1	0	1.340867	-2.359401	2.291126
13	6	0	-1.878029	-0.646152	-0.128059
14	1	0	-2.433902	-1.475774	0.314383
15	1	0	-2.010704	-0.716793	-1.221339
16	6	0	-2.503674	0.674895	0.370680
17	1	0	-1.957370	1.536808	-0.018606
18	1	0	-2.419471	0.726788	1.458712
19	6	0	-3.906907	0.788236	-0.017662
20	7	0	-5.014003	0.854279	-0.335136
21	1	0	0.044654	0.229687	-1.526718
22	6	0	1.007215	1.245872	0.050952
23	8	0	0.461934	1.887460	0.911948
24	8	0	2.150510	1.633713	-0.555986
25	6	0	2.702456	2.891753	-0.119821
26	1	0	3.603702	3.034183	-0.711887
27	1	0	1.993039	3.700881	-0.298306
28	1	0	2.941994	2.853110	0.943437
29	7	0	-0.486945	-0.758985	0.287180

E) 10 (*anti*-cyanoethyl)

1	6	0	0.948050	2.732756	-0.354601
2	6	0	0.927907	1.830437	0.859804
3	6	0	2.072707	0.749190	-0.726247
4	6	0	1.639984	2.090988	-1.303314
5	6	0	2.284108	1.133342	0.762044
6	1	0	2.375280	0.283539	1.434009
7	1	0	3.112739	1.828676	0.891474
8	6	0	0.780938	-0.103824	-0.626508
9	1	0	0.175660	-0.063167	-1.531044
10	1	0	0.588971	2.217247	1.815429
11	1	0	2.886624	0.229892	-1.226141
12	7	0	-0.003785	0.580535	0.554877
13	1	0	0.429644	3.678540	-0.439890
14	1	0	1.797579	2.404965	-2.327547
15	6	0	-1.384953	1.051614	0.156886
16	1	0	-1.689055	1.746548	0.940235
17	1	0	-1.327795	1.582684	-0.793402
18	6	0	-2.365978	-0.122738	0.100616
19	1	0	-2.330037	-0.639164	1.062299
20	1	0	-2.077194	-0.847342	-0.664016
21	6	0	-3.718864	0.347369	-0.175939
22	7	0	-4.783701	0.730041	-0.400017
23	6	0	1.038993	-1.562584	-0.259218
24	8	0	2.094715	-1.996681	0.120487
25	8	0	-0.045315	-2.312121	-0.512483
26	6	0	0.045654	-3.699009	-0.124077
27	1	0	-0.904560	-4.143864	-0.410121
28	1	0	0.872237	-4.184850	-0.643209
29	1	0	0.196639	-3.769401	0.953342
30	8	0	-0.075101	-0.214145	1.641733

F) 10 (*syn*-cyanoethyl)

1	6	0	-2.956538	-1.190453	-0.360430
2	6	0	-1.759439	-1.385385	0.539670
3	6	0	-2.108445	0.815890	0.394232
4	6	0	-3.176859	0.124468	-0.433257
5	6	0	-1.898161	-0.224852	1.523996
6	1	0	-1.020771	-0.034390	2.140506
7	1	0	-2.780417	-0.325457	2.155503
8	6	0	-0.770059	0.653273	-0.402257
9	1	0	-0.876236	0.828554	-1.466814
10	1	0	-1.551661	-2.388914	0.898331
11	1	0	-2.306148	1.843823	0.695100
12	1	0	-3.892176	0.636383	-1.063521
13	1	0	-3.443801	-1.978473	-0.913880
14	7	0	-0.520079	-0.922260	-0.338233
15	6	0	0.315798	1.543890	0.164635
16	8	0	0.703318	1.556816	1.310977
17	8	0	0.770325	2.385339	-0.781166
18	6	0	1.754645	3.352546	-0.353476
19	1	0	1.986298	3.936404	-1.240658
20	1	0	1.343878	3.987025	0.432424
21	1	0	2.645513	2.846989	0.020500
22	6	0	0.759320	-1.339504	0.372715
23	1	0	0.870178	-0.796773	1.308381
24	1	0	0.632700	-2.402845	0.570831
25	6	0	1.966382	-1.143953	-0.550554
26	1	0	1.747992	-1.645064	-1.496333
27	1	0	2.140420	-0.088450	-0.775400
28	6	0	3.176823	-1.692615	0.050625
29	7	0	4.130020	-2.130175	0.530492
30	8	0	-0.546913	-1.458606	-1.565584

G) 11

1	6	0	0.445995	-2.972911	0.360399
2	6	0	0.443669	-2.216672	-0.959700
3	6	0	1.790624	-1.069729	0.548938
4	6	0	1.216767	-2.311326	1.224339
5	6	0	1.815063	-1.530529	-0.925190
6	1	0	1.887416	-0.724623	-1.656224
7	1	0	2.620917	-2.248650	-1.088983
8	6	0	0.743901	0.089989	0.659094
9	1	0	0.646221	0.374507	1.711592
10	1	0	0.223632	-2.802211	-1.851521
11	1	0	2.747765	-0.732126	0.945987
12	1	0	1.357670	-2.544174	2.272843
13	1	0	-0.164384	-3.842116	0.567421
14	6	0	1.242594	1.331181	-0.088704
15	8	0	0.859383	1.730272	-1.159223
16	8	0	2.197140	1.949511	0.642400
17	6	0	2.771109	3.138656	0.061355
18	1	0	1.998591	3.890787	-0.102228
19	1	0	3.503024	3.490506	0.784649
20	1	0	3.251128	2.903823	-0.889429
21	8	0	-0.558419	-1.164635	-0.979912
22	7	0	-0.575962	-0.431941	0.276783
23	6	0	-1.642900	0.546834	0.142209
24	1	0	-1.559649	1.224404	0.996555
25	1	0	-1.547778	1.138465	-0.774297
26	6	0	-3.007452	-0.167458	0.180709
27	1	0	-3.080900	-0.853181	-0.666128
28	1	0	-3.086423	-0.763827	1.093922
29	6	0	-4.121161	0.774427	0.129651
30	7	0	-4.991368	1.530865	0.099091

H) 11*endo*

1	6	0	0.855833	-2.458374	1.201924
2	6	0	0.291868	-2.653835	-0.195841
3	6	0	1.887123	-0.971520	-0.273902
4	6	0	1.770811	-1.489273	1.156393
5	6	0	1.477293	-2.227632	-1.068792
6	1	0	1.183349	-2.029621	-2.101241
7	1	0	2.273993	-2.973969	-1.049595
8	6	0	0.772211	0.101668	-0.536707
9	1	0	-0.140159	-3.630152	-0.412787
10	1	0	2.858032	-0.556126	-0.542489
11	1	0	2.287415	-1.054571	2.002733
12	1	0	0.482846	-2.958363	2.085880
13	8	0	-0.791730	-1.725402	-0.475081
14	7	0	-0.500978	-0.382327	0.024196
15	6	0	-1.657108	0.399303	-0.390831
16	1	0	-1.421833	1.447556	-0.205888
17	1	0	-1.868787	0.268645	-1.461825
18	6	0	-2.885640	0.001141	0.446693
19	1	0	-3.090617	-1.063187	0.314368
20	1	0	-2.670912	0.169120	1.505373
21	6	0	-4.072211	0.763214	0.070571
22	7	0	-5.000684	1.374156	-0.237736
23	6	0	1.154463	1.427671	0.115956
24	8	0	0.702227	1.890816	1.131342
25	8	0	2.124001	2.020364	-0.611879
26	6	0	2.629290	3.268995	-0.096371
27	1	0	3.385614	3.590345	-0.808548
28	1	0	1.826262	4.003673	-0.029417
29	1	0	3.067175	3.123492	0.891875
30	1	0	0.719659	0.265975	-1.623280

I) 12

1	6	0	-2.899199	-0.649697	-0.259896
2	6	0	-2.891831	-1.695079	0.827067
3	6	0	-1.793274	-2.448110	0.827228
4	6	0	-0.844591	-2.050690	-0.264416
5	6	0	-1.549174	-0.865484	-0.997458
6	6	0	-0.469785	0.257238	-0.950909
7	1	0	-3.743844	-0.789235	-0.942427
8	1	0	-3.016571	0.355195	0.157830
9	1	0	-3.711504	-1.798938	1.529395
10	1	0	-1.578137	-3.252687	1.518992
11	1	0	-0.372717	0.737481	-1.925361
12	8	0	0.367645	-1.509461	0.279849
13	7	0	0.758572	-0.521371	-0.711963
14	6	0	1.921125	0.181196	-0.186947
15	1	0	1.757558	0.535875	0.835811
16	1	0	2.086479	1.046250	-0.835039
17	6	0	3.145566	-0.750386	-0.242300
18	1	0	2.973916	-1.614285	0.404003
19	1	0	3.278701	-1.124490	-1.261203
20	6	0	4.368382	-0.074308	0.179893
21	7	0	5.328588	0.474899	0.506236
22	1	0	-0.588051	-2.867601	-0.949386
23	1	0	-1.724205	-1.119308	-2.042313
24	6	0	-0.769323	1.358154	0.070258
25	8	0	-0.548739	1.325302	1.253801
26	8	0	-1.321181	2.423041	-0.557287
27	6	0	-1.666423	3.543760	0.282549
28	1	0	-2.089321	4.288645	-0.387462
29	1	0	-2.396049	3.245184	1.036499
30	1	0	-0.777018	3.932604	0.779423

J) 13

1	6	0	3.104070	-0.080093	-0.728609
2	6	0	3.389986	-1.558587	-0.817049
3	6	0	2.615869	-2.291875	-0.017166
4	6	0	1.649865	-1.440847	0.754613
5	6	0	1.962887	0.017250	0.317680
6	6	0	0.605774	0.515970	-0.203102
7	1	0	3.988809	0.480059	-0.409548
8	1	0	2.819831	0.330490	-1.705188
9	1	0	4.153677	-1.960958	-1.473696
10	1	0	2.650287	-3.369660	0.081732
11	8	0	0.299868	-1.692685	0.318221
12	7	0	-0.365406	-0.401099	0.449946
13	6	0	-1.629834	-0.548989	-0.260829
14	1	0	-1.469400	-0.956704	-1.268906
15	1	0	-2.064759	0.445934	-0.358450
16	6	0	-2.572695	-1.463545	0.540055
17	1	0	-2.130674	-2.457871	0.634284
18	1	0	-2.698629	-1.064394	1.550413
19	6	0	-3.882884	-1.581943	-0.092607
20	7	0	-4.914383	-1.660610	-0.602443
21	1	0	1.697672	-1.580122	1.840096
22	1	0	2.259002	0.625549	1.170433
23	6	0	0.304057	1.961723	0.195945
24	8	0	0.852260	2.573354	1.076389
25	8	0	-0.671319	2.476494	-0.577577
26	6	0	-1.067593	3.833690	-0.283404
27	1	0	-0.219541	4.507957	-0.405768
28	1	0	-1.852258	4.066755	-0.999076
29	1	0	-1.441448	3.905073	0.738359
30	1	0	0.542463	0.426023	-1.296634

K) 14 (*anti*-cyanoethyl)

1	6	0	1.831265	-1.205594	1.481848
2	6	0	1.696305	-1.655598	0.049455
3	6	0	2.297617	0.496202	-0.007760
4	6	0	2.189537	0.082881	1.454674
5	6	0	2.775880	-0.830586	-0.648631
6	1	0	2.693256	-0.864781	-1.733938
7	1	0	3.777514	-1.107089	-0.321433
8	6	0	0.852545	0.562175	-0.594257
9	1	0	1.596196	-2.711127	-0.181085
10	1	0	2.874476	1.394427	-0.224823
11	1	0	2.288951	0.753064	2.296851
12	1	0	1.582273	-1.800162	2.350245
13	7	0	0.409365	-0.963601	-0.590311
14	1	0	0.869241	0.781040	-1.656949
15	6	0	-0.041423	1.558116	0.111884
16	8	0	-0.354041	1.542149	1.279527
17	8	0	-0.422136	2.523718	-0.746257
18	6	0	-1.226483	3.586305	-0.190644
19	1	0	-0.676939	4.105188	0.595508
20	1	0	-1.433310	4.254622	-1.022732
21	1	0	-2.152277	3.184430	0.222273
22	6	0	-0.812877	-1.294540	0.243740
23	1	0	-0.773225	-2.374454	0.386267
24	1	0	-0.751661	-0.789979	1.205186
25	6	0	-2.090248	-0.930328	-0.519582
26	1	0	-2.170862	0.148139	-0.680248
27	1	0	-2.043495	-1.400900	-1.504113
28	8	0	0.242773	-1.390764	-1.851555
29	6	0	-3.275378	-1.378581	0.203193
30	7	0	-4.208414	-1.738677	0.777703

L) 14 (*syn*-cyanoethyl)

1	6	0	2.169373	-1.547928	1.050886
2	6	0	0.874284	-2.019375	0.439950
3	6	0	1.895238	-0.766610	-1.103474
4	6	0	2.789822	-0.809228	0.127416
5	6	0	1.259041	-2.177945	-1.034050
6	1	0	0.419867	-2.330224	-1.716598
7	1	0	1.992127	-2.969870	-1.181979
8	6	0	0.647133	0.092243	-0.762307
9	1	0	0.319351	-2.799584	0.952576
10	1	0	2.366041	-0.474098	-2.040781
11	1	0	3.693042	-0.230105	0.245557
12	1	0	2.449172	-1.695173	2.082616
13	7	0	-0.048344	-0.722982	0.396450
14	6	0	-1.457825	-1.146792	0.023678
15	1	0	-1.467137	-1.579175	-0.977809
16	1	0	-1.726698	-1.913715	0.749296
17	6	0	-2.431758	0.029033	0.141063
18	1	0	-2.334727	0.443622	1.146854
19	1	0	-2.182645	0.827226	-0.561393
20	6	0	-3.801523	-0.409437	-0.102344
21	7	0	-4.879670	-0.766889	-0.303393
22	8	0	-0.065424	-0.074401	1.572707
23	1	0	-0.039577	0.131560	-1.608650
24	6	0	0.933767	1.514471	-0.299747
25	8	0	2.021789	1.938740	-0.010267
26	8	0	-0.180674	2.260854	-0.349869
27	6	0	-0.057034	3.610266	0.146346
28	1	0	0.684063	4.161159	-0.433439
29	1	0	-1.043551	4.053298	0.031749
30	1	0	0.238138	3.590452	1.195523

M) methyl 2-(cyclopent-2-enyl)acetate

1	6	0	2.512298	1.114640	0.608439
2	6	0	3.141309	-0.258451	0.601182
3	6	0	1.009653	-0.191573	-0.677512
4	6	0	1.376391	1.156048	-0.087469
5	6	0	2.312620	-1.018919	-0.468103
6	1	0	2.108481	-2.053686	-0.181959
7	1	0	2.871656	-1.050210	-1.406388
8	6	0	-0.209226	-0.822944	0.019024
9	1	0	-0.046723	-0.912787	1.097253
10	1	0	4.207029	-0.230881	0.352995
11	1	0	0.769414	-0.098232	-1.740527
12	1	0	2.940563	1.953209	1.146605
13	1	0	0.743781	2.027110	-0.208161
14	6	0	-1.505179	-0.075265	-0.211099
15	8	0	-1.693721	0.777679	-1.044597
16	8	0	-2.467243	-0.505890	0.635726
17	6	0	-3.763619	0.101647	0.482706
18	1	0	-4.393977	-0.366407	1.235622
19	1	0	-3.702652	1.178105	0.648422
20	1	0	-4.157481	-0.084434	-0.517535
21	1	0	-0.368390	-1.843191	-0.351282
22	1	0	3.070522	-0.724002	1.592915

N) methyl 2-(cyclopent-2-enyl)acetate radical

1	6	0	2.719039	-1.082375	-0.531306
2	6	0	3.291546	0.170313	-0.360711
3	6	0	1.038332	0.227857	0.538423
4	6	0	1.424528	-1.117316	-0.033514
5	6	0	2.312792	1.102562	0.303376
6	1	0	2.095561	1.974122	-0.328751
7	1	0	2.706167	1.505687	1.244264
8	6	0	-0.218617	0.835091	-0.106742
9	1	0	-0.105669	0.911682	-1.192027
10	1	0	0.836763	0.125185	1.610973
11	1	0	3.221155	-1.926988	-0.988597
12	1	0	0.771448	-1.978973	-0.013074
13	6	0	-1.491089	0.072422	0.194880
14	8	0	-1.627975	-0.767264	1.051459
15	8	0	-2.495388	0.471834	-0.616549
16	6	0	-3.773955	-0.153097	-0.396379
17	1	0	-4.441864	0.285316	-1.134553
18	1	0	-3.700432	-1.232188	-0.537657
19	1	0	-4.130640	0.051981	0.614036
20	1	0	-0.372713	1.858811	0.256714
21	1	0	4.291673	0.456049	-0.658763

O) methyl 2-cyclopentylacetate

1	6	0	2.300342	1.340609	-0.105178
2	6	0	2.908356	0.224609	0.795209
3	6	0	0.974693	-0.704051	-0.411257
4	6	0	1.371816	0.614518	-1.108319
5	6	0	2.286084	-1.103491	0.297080
6	1	0	2.133658	-1.827366	1.102760
7	1	0	2.950159	-1.575139	-0.434036
8	6	0	-0.179159	-0.521828	0.585381
9	1	0	0.010668	0.287964	1.295082
10	1	0	0.671158	-1.456157	-1.142650
11	1	0	1.733709	2.053137	0.500587
12	1	0	0.511037	1.216415	-1.408832
13	6	0	-1.521139	-0.279427	-0.073173
14	8	0	-1.815563	-0.563374	-1.208794
15	8	0	-2.393708	0.280904	0.796383
16	6	0	-3.727570	0.499406	0.300556

17	1	0	-4.275798	0.944166	1.128229
18	1	0	-3.711056	1.174720	-0.555982
19	1	0	-4.183847	-0.445410	0.001471
20	1	0	-0.297280	-1.428644	1.191941
21	1	0	3.998846	0.199027	0.737485
22	1	0	1.923247	0.375658	-2.023235
23	1	0	3.070327	1.919108	-0.620504
24	1	0	2.658793	0.400214	1.845177

P) methyl 2-cyclopentylacetate radical

1	6	0	2.353398	-1.318055	-0.272976
2	6	0	2.974988	-0.035099	-0.730234
3	6	0	1.017095	0.581451	0.530856
4	6	0	1.404168	-0.879031	0.867801
5	6	0	2.317394	1.151460	-0.095792
6	1	0	2.127858	1.971088	-0.800420
7	1	0	2.953759	1.582508	0.695009
8	6	0	-0.154198	0.661711	-0.458111
9	1	0	0.029048	0.066479	-1.357043
10	1	0	0.735513	1.125062	1.434477
11	1	0	1.794518	-1.807479	-1.087471
12	1	0	0.535947	-1.530888	0.985171
13	6	0	-1.484638	0.250820	0.136630
14	8	0	-1.758659	0.227954	1.312134
15	8	0	-2.372341	-0.066129	-0.833889
16	6	0	-3.698113	-0.410230	-0.390197
17	1	0	-4.258197	-0.634070	-1.295496
18	1	0	-3.667320	-1.279926	0.267490
19	1	0	-4.151163	0.425976	0.144492
20	1	0	-0.282643	1.694454	-0.805791
21	1	0	3.814268	0.027511	-1.411733
22	1	0	1.945278	-0.893802	1.818679
23	1	0	3.090576	-2.059677	0.058808