OBC

Organic & Biomolecular Chemistry

Supporting Information

Novel pyrrolobenzodiazepine and pyrroloquinazoline scaffolds synthesized by a simple and highly selective Ugi/cyclization sequence

Pablo Pertejo,[a] Pablo Peña-Calleja,[a] Israel Carreira-Barral,[a] Roberto Quesada,[a] Nicolás Cordero,[b] Francisco Rodríguez[c] and María García-Valverde*[a]

Contents

5-Benzoyl-5-(*N*-cyclohexylcarbamoyl)-1-(2-nitrobenzyl)-2-pyrrolidinone. 5a

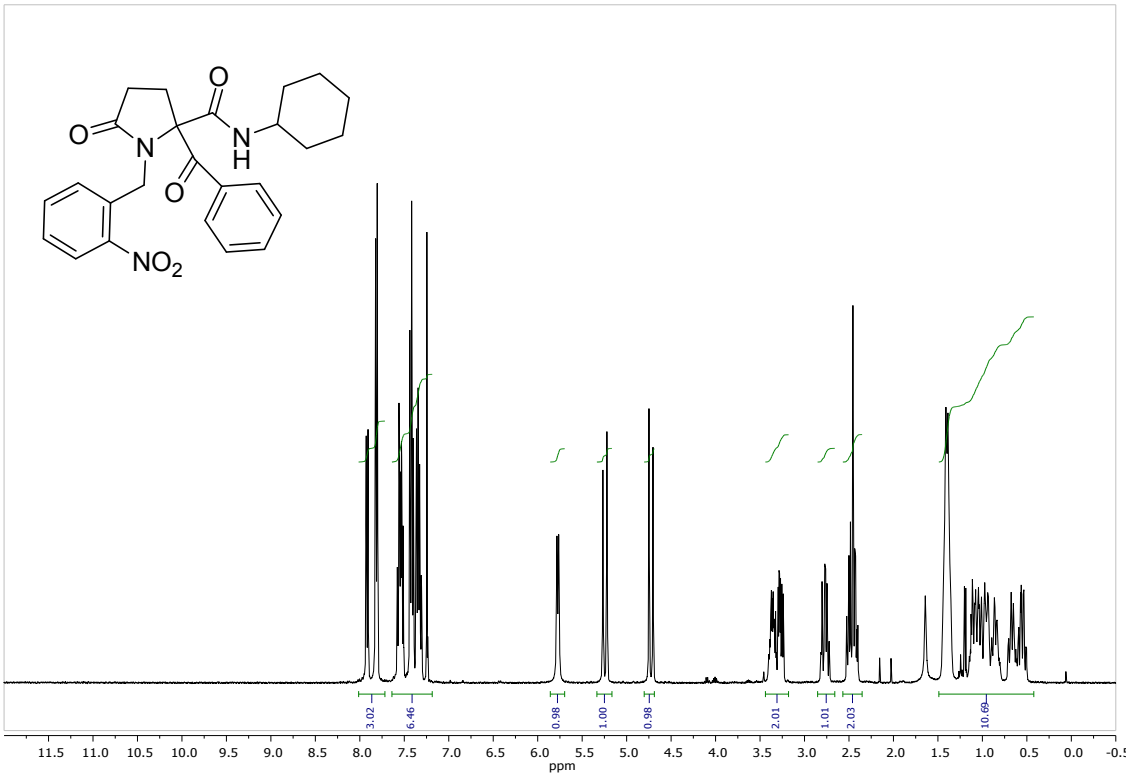

Figure S1. ^{1}H NMR spectrum of **5a** (400 MHz, $CDCl_3$)

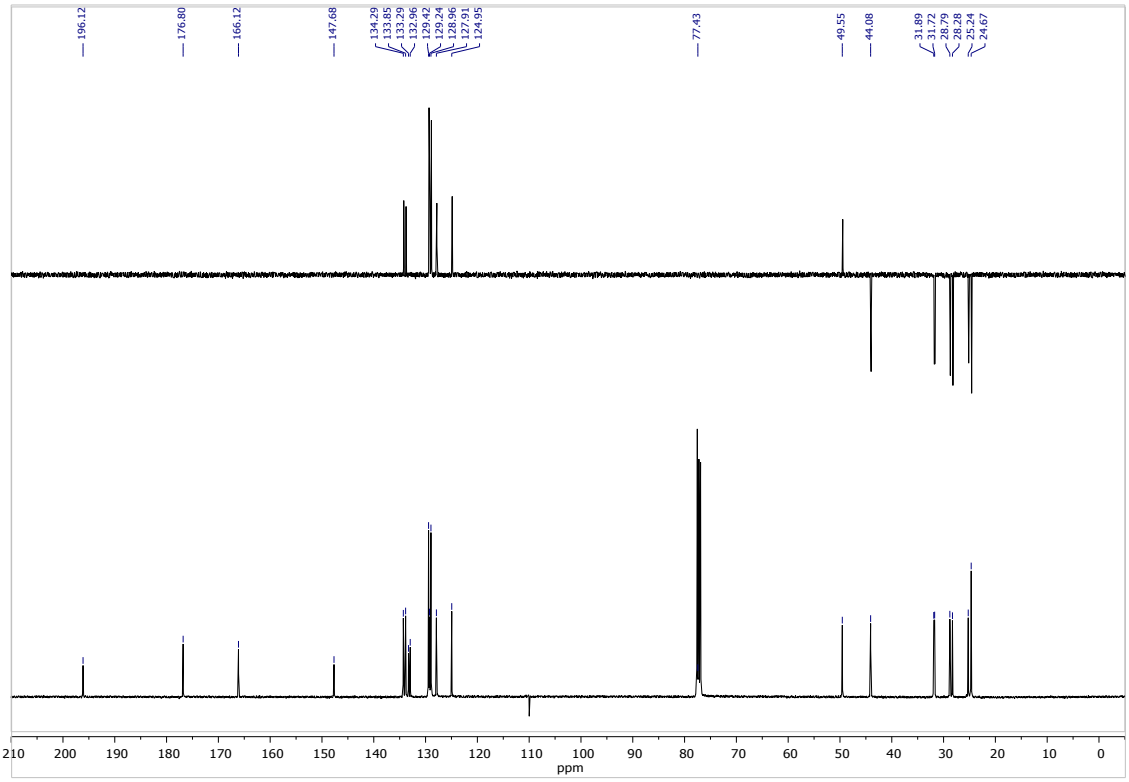

Figure S2. ^{13}C and DEPT NMR spectra of **5a** (100 MHz, $CDCl_3$)

5-Benzoyl-5-(*N*-butylcarbamoyl)-1-(2-nitrobenzyl)-2-pyrrolidinone. 5b

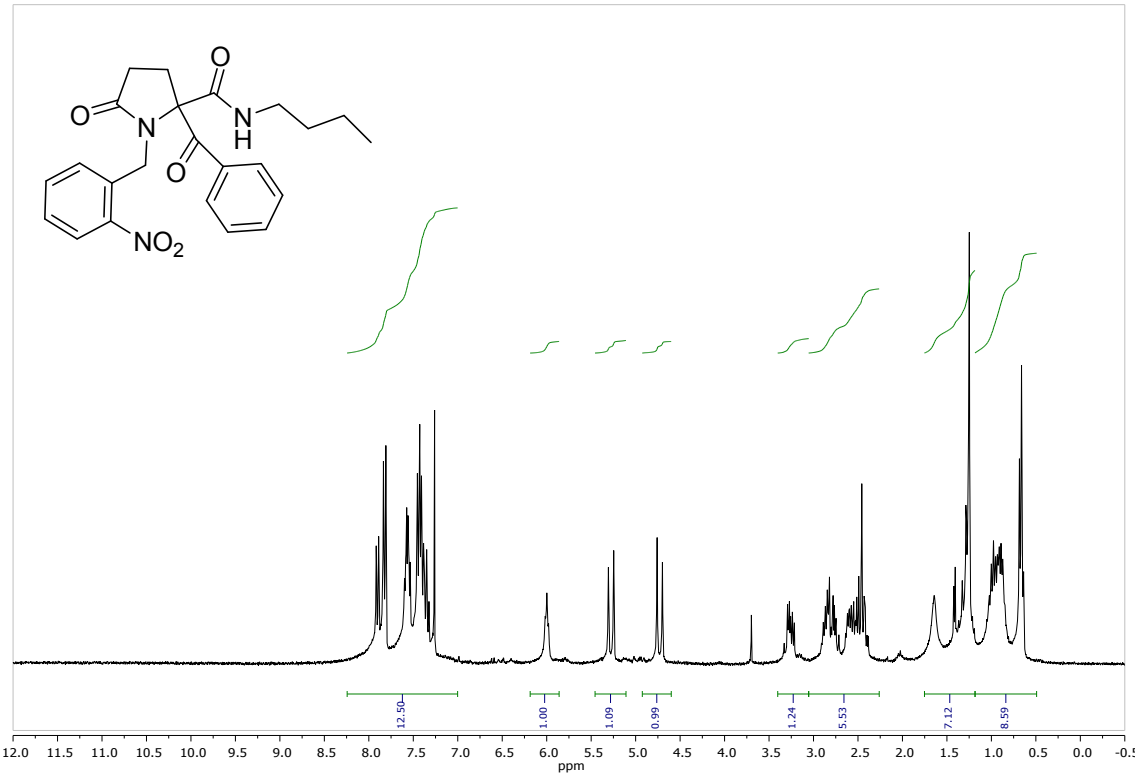

Figure S3. ^{1}H NMR spectrum of **5b** (400 MHz, $CDCl_3$)

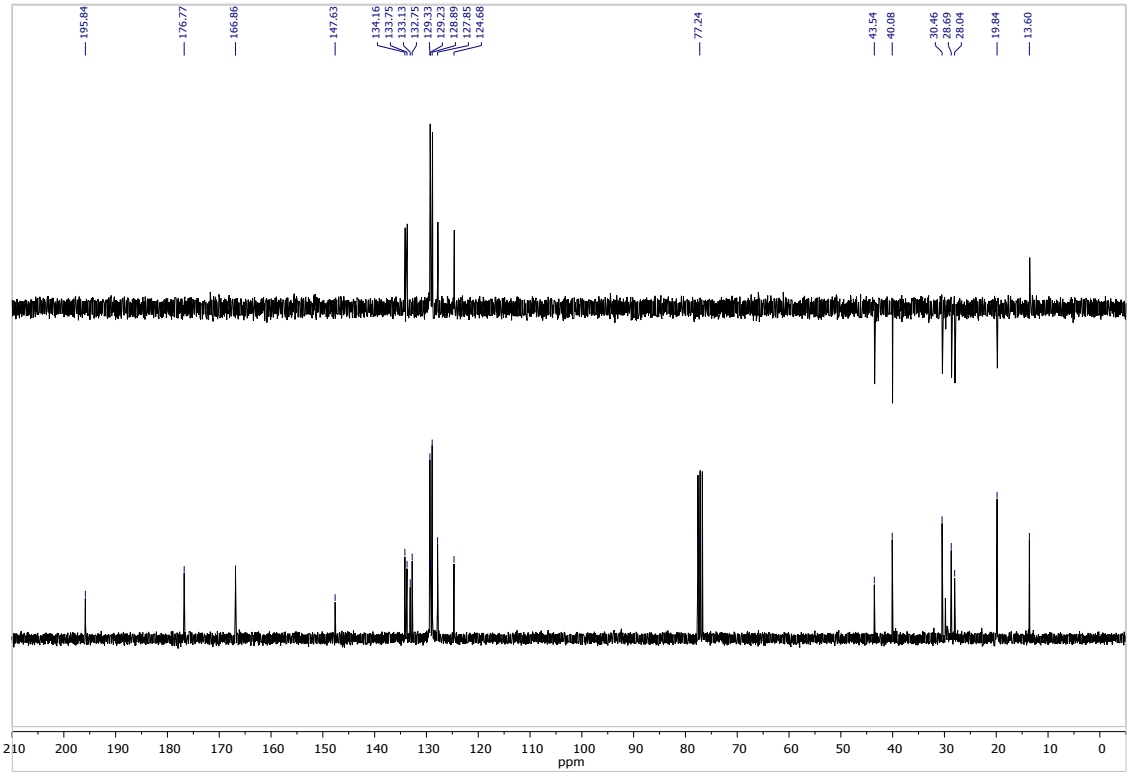

Figure S4. ^{13}C and DEPT NMR spectra of **5b** (100 MHz, $CDCl_3$)

5-Benzoyl-1-(2-nitrobenzyl)-5-(*N*-tertbutylcarbamoyl)-2-pyrrolidinone. 5c

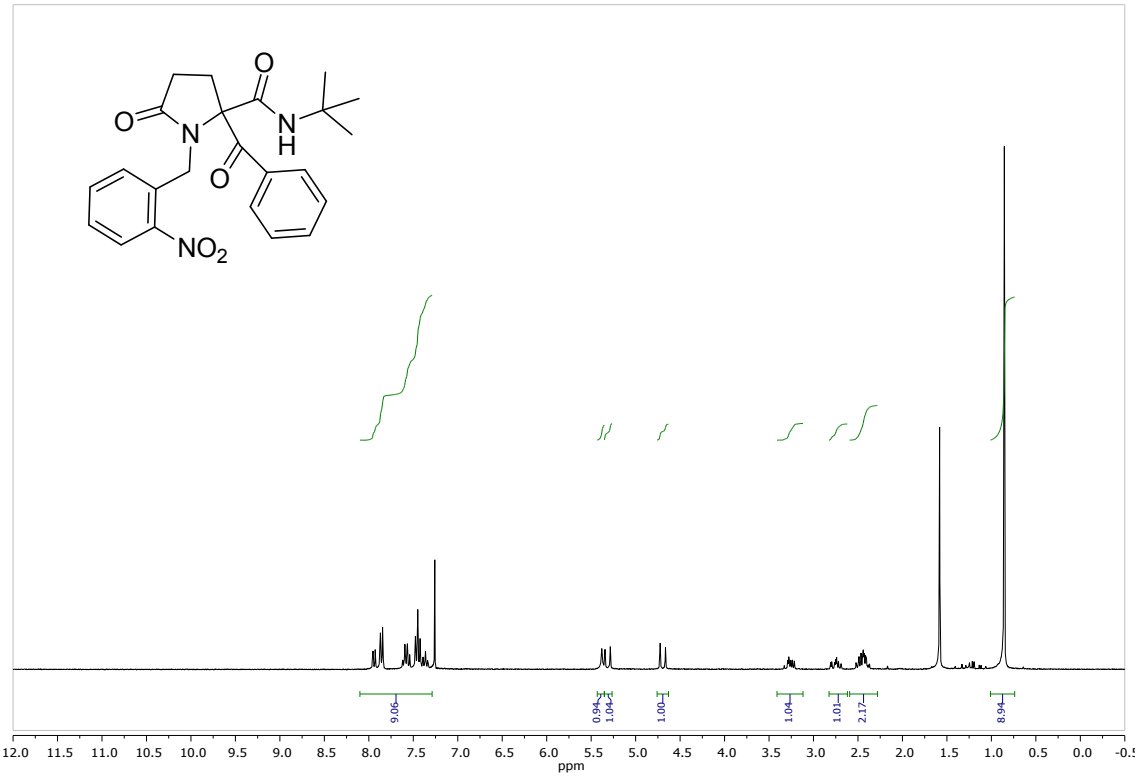

Figure S5. ^{1}H NMR spectrum of **5c** (300 MHz, $CDCl_3$)

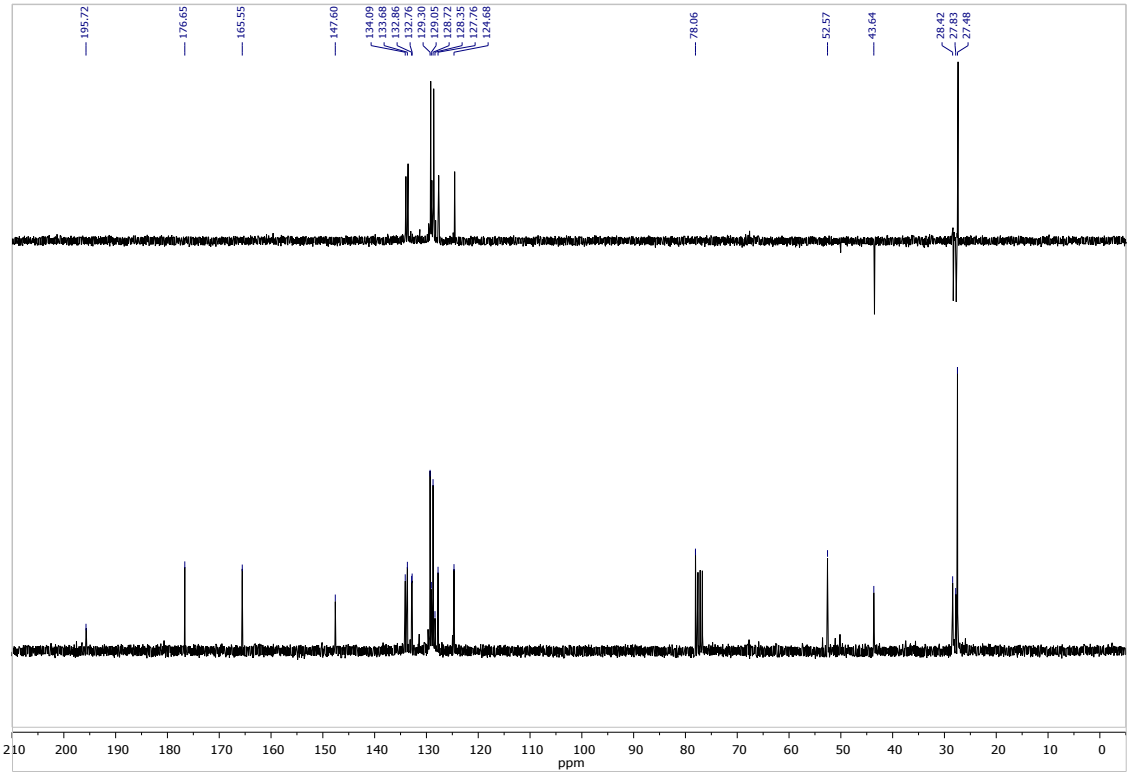

Figure S6. ^{13}C and DEPT NMR spectra of **5c** (75 MHz, $CDCl_3$)

5-Benzoyl-5-(*N*-benzylcarbamoyl)-1-(2-nitrobenzyl)-2-pyrrolidinone. 5d

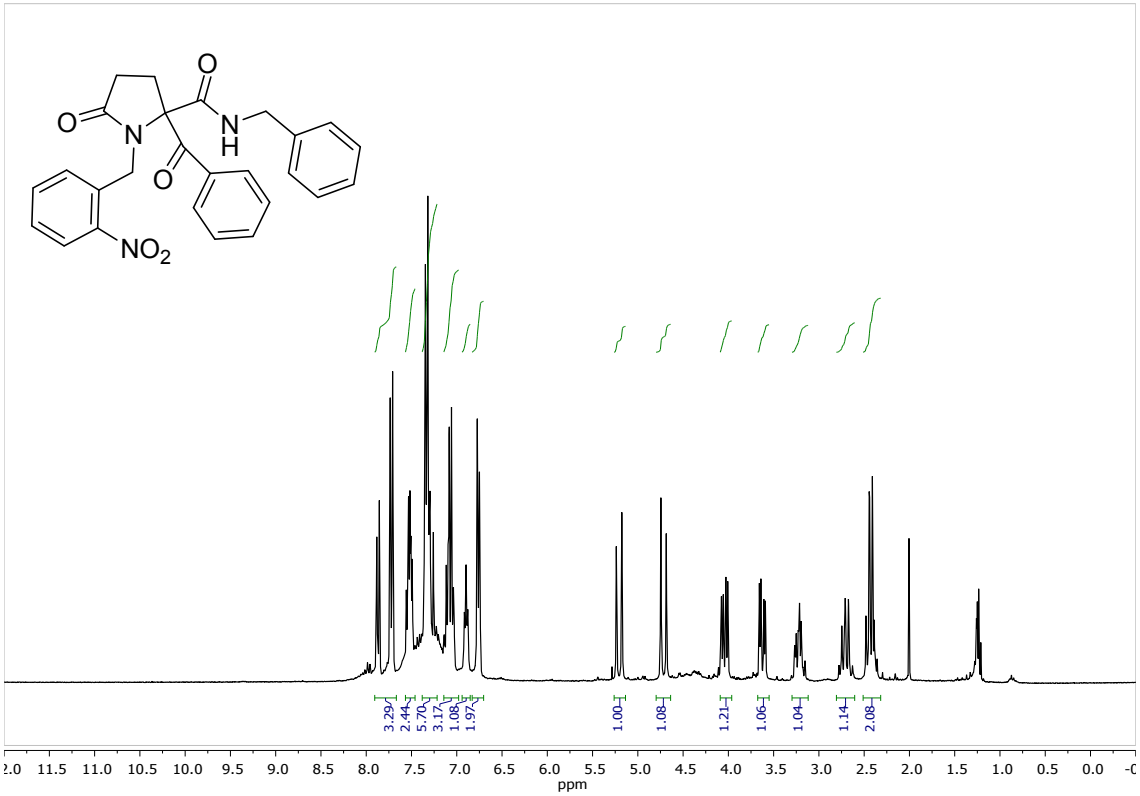

Figure S7. ^{1}H NMR spectrum of **5d** (300 MHz, $CDCl_3$)

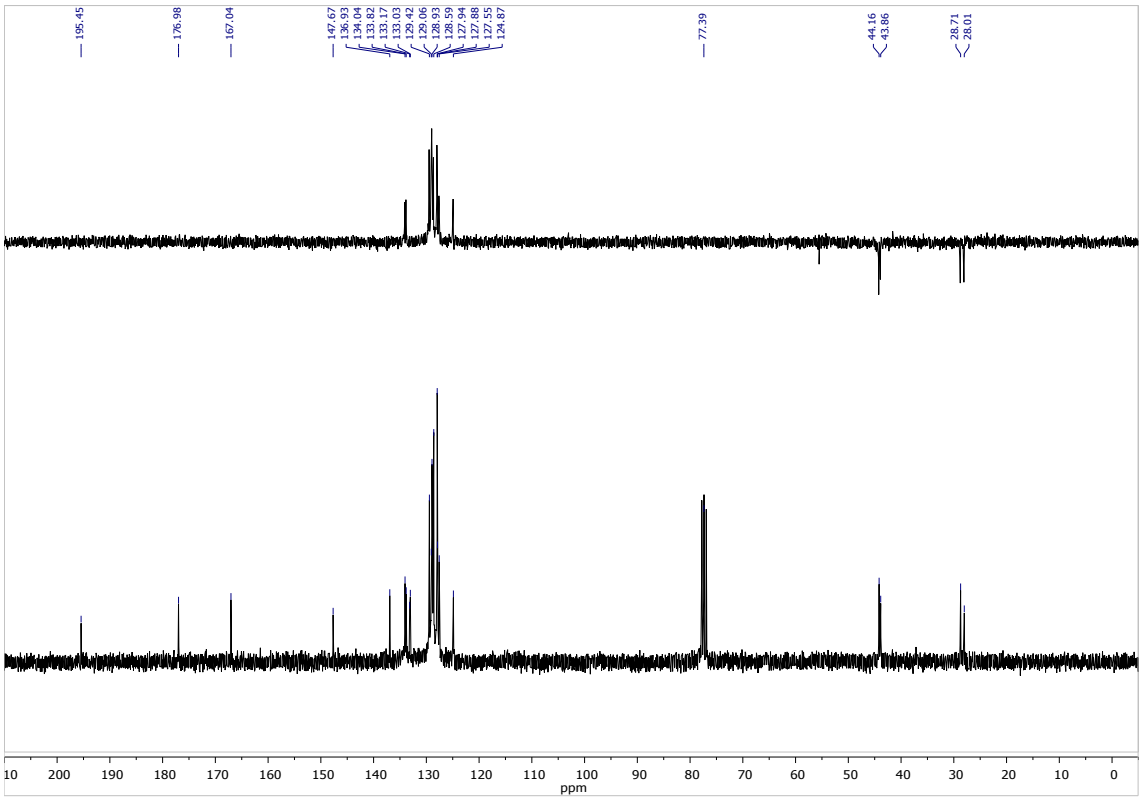

Figure S8. ^{13}C and DEPT NMR spectra of **5d** (75 MHz, $CDCl_3$)

5-(*N*-Cyclohexylcarbamoyl)-5-(4-methylbenzoyl)-1-(2-nitrobenzyl)-2-pyrrolidinone. 5e

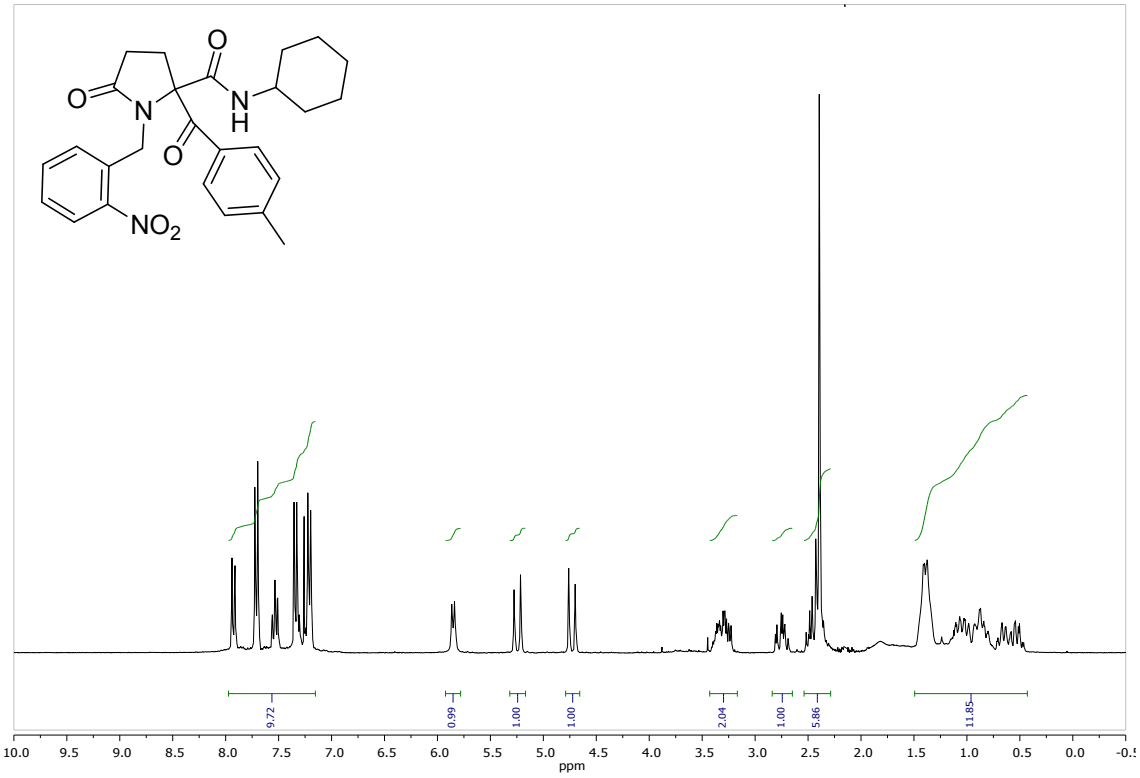

Figure S9. ^{1}H NMR spectrum of **5e** (300 MHz, $CDCl_3$)

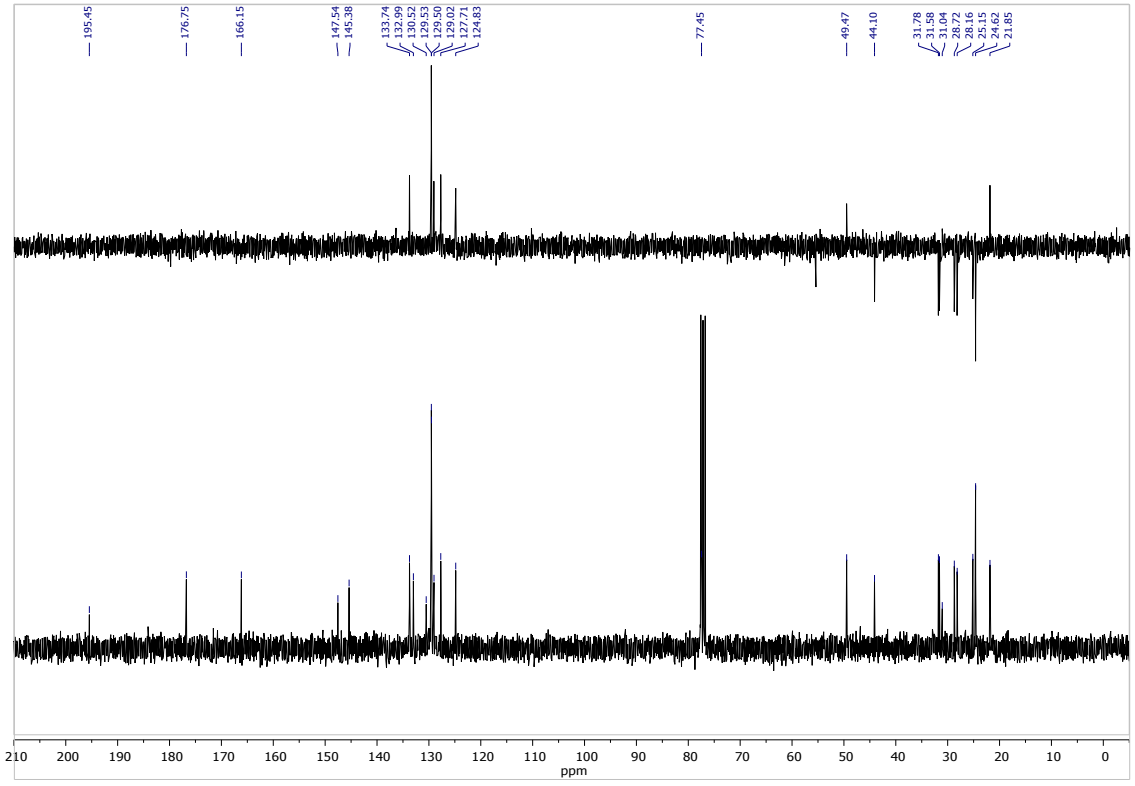

Figure S10. ^{13}C and DEPT NMR spectra of **5e** (75 MHz, $CDCl_3$)

5-(4-Chlorobenzoyl)-5-(*N*-cyclohexylcarbamoyl)-1-(2-nitrobenzyl)-2-pyrrolidinone. 5f

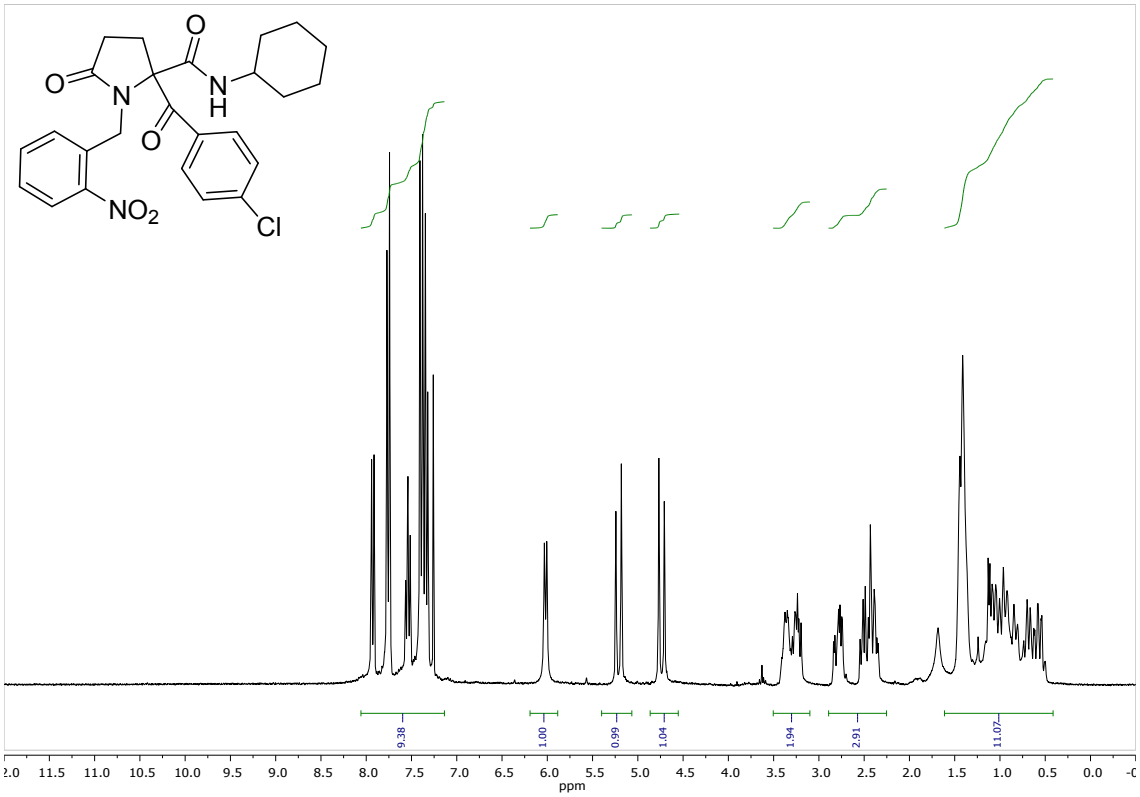

Figure S11. ^{1}H NMR spectrum of **5f** (300 MHz, $CDCl_3$)

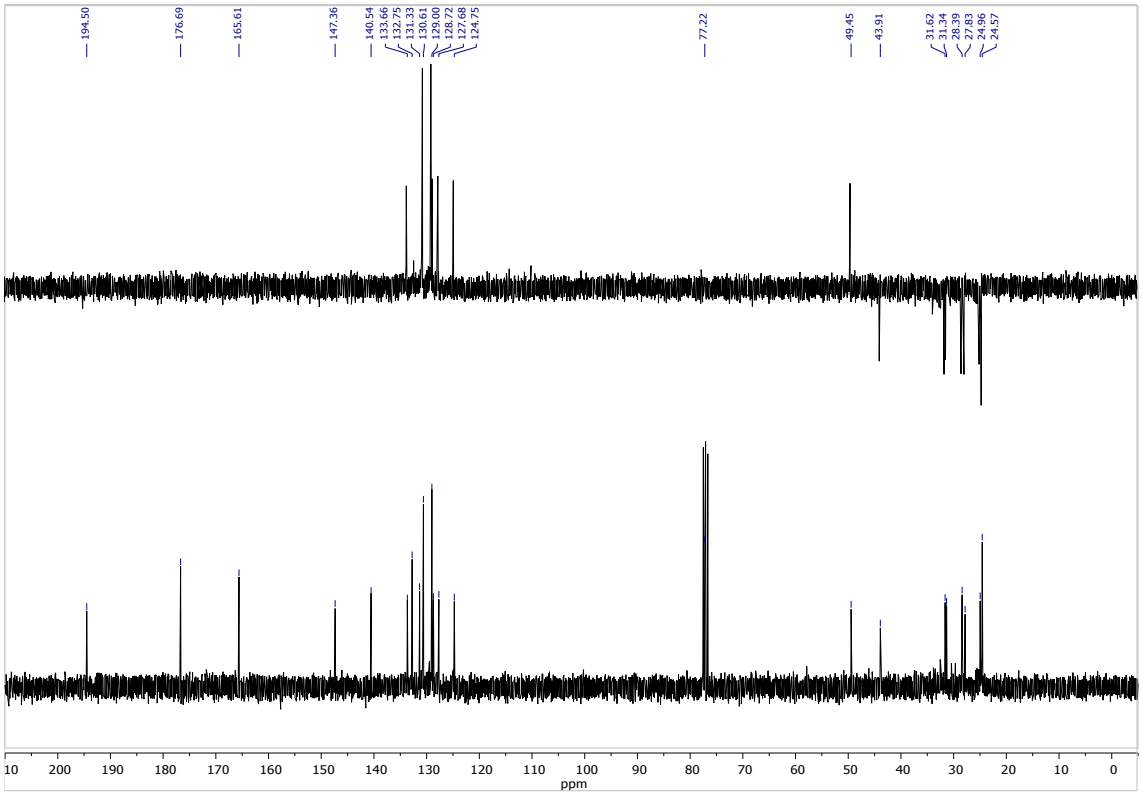

Figure S12. ^{13}C and DEPT NMR spectra of **5f** (75 MHz, $CDCl_3$)

5-Acetyl-5-(*N*-cyclohexylcarbamoyl)-1-(2-nitrobenzyl)-2-pyrrolidinone. 5g

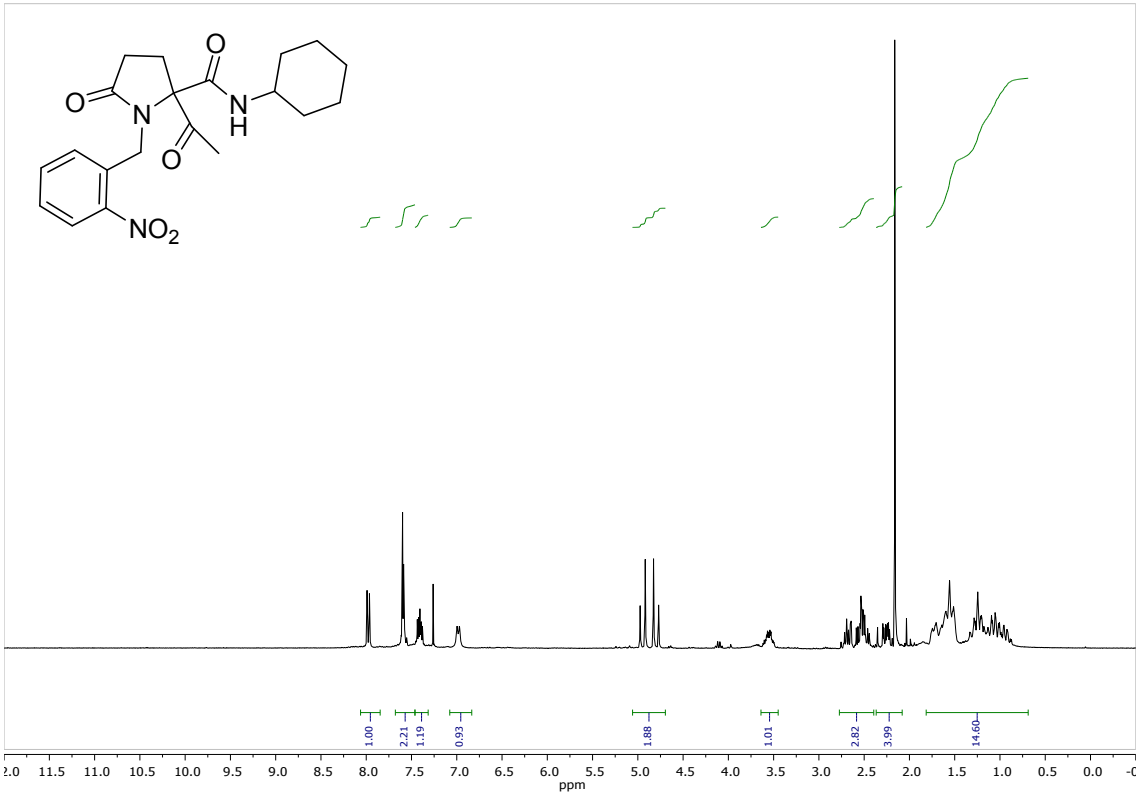

Figure S13. ^{1}H NMR spectrum of **5g** (300 MHz, $CDCl_3$)

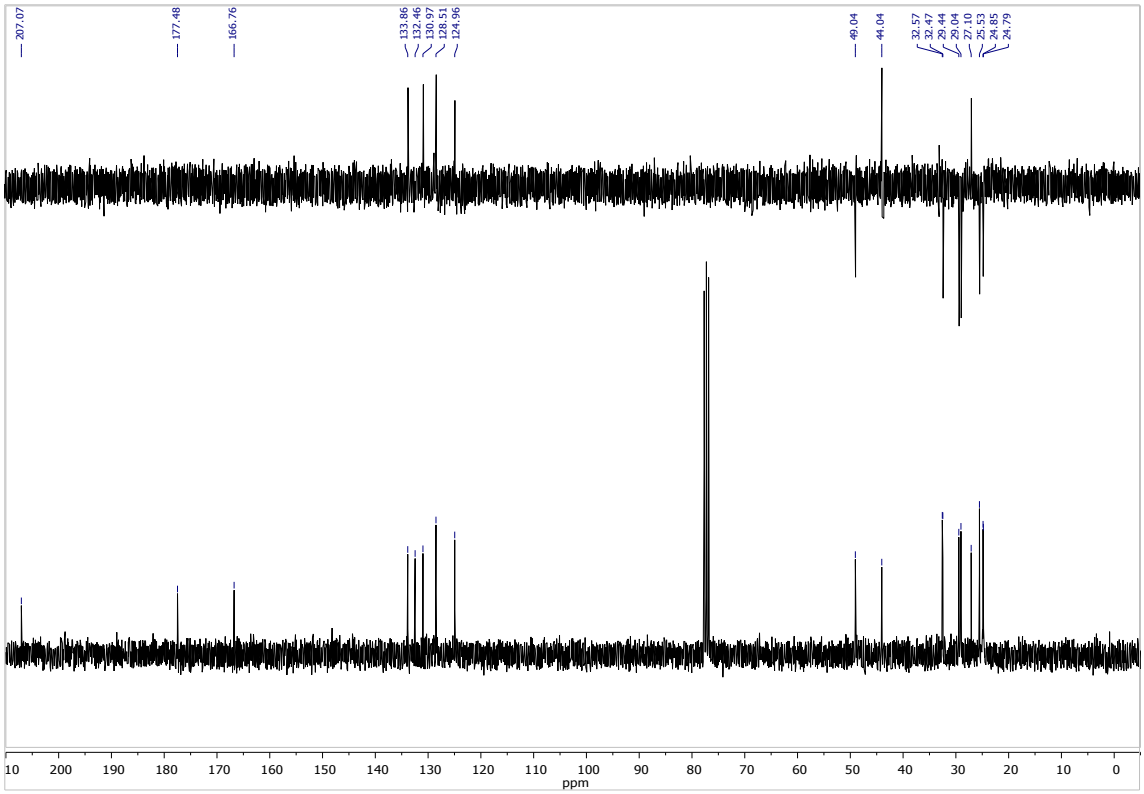

Figure S14. ^{13}C and DEPT NMR spectra of **5g** (75 MHz, $CDCl_3$)

11a-(*N*-Cyclohexylcarbamoyl)-11-phenyl-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6a

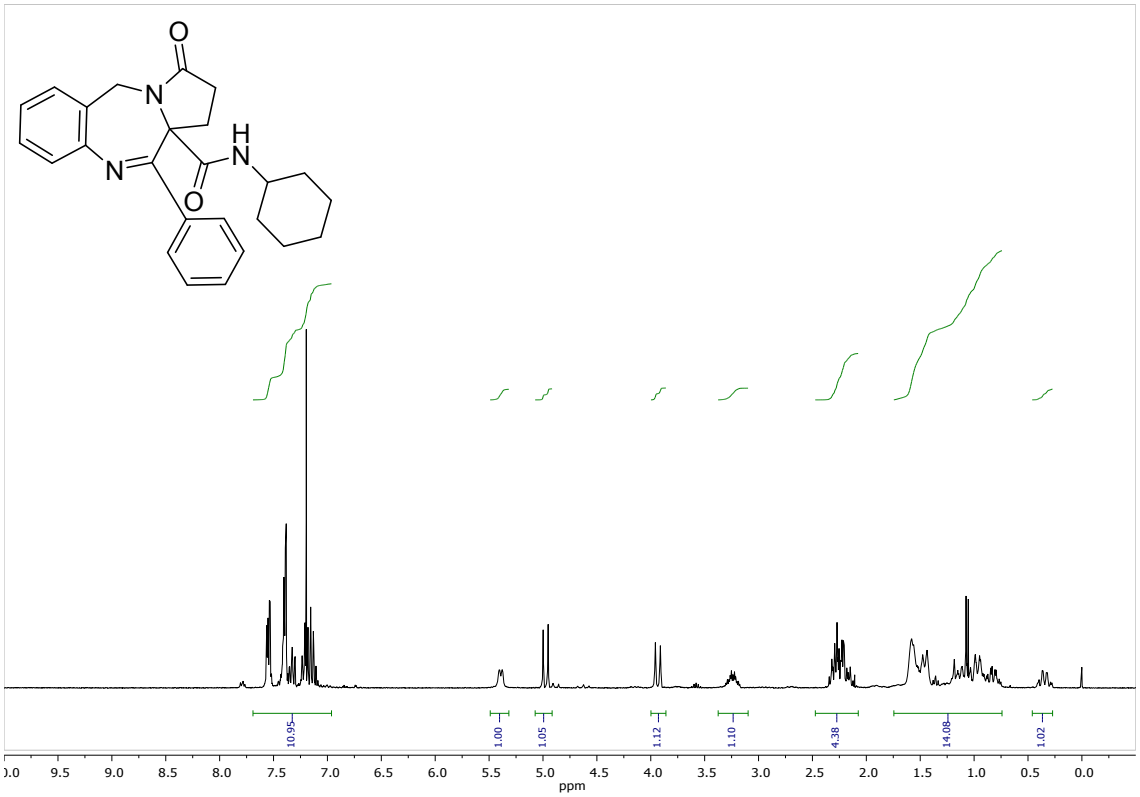

Figure S15. ^{1}H NMR spectrum of **6a** (400 MHz, $CDCl_3$)

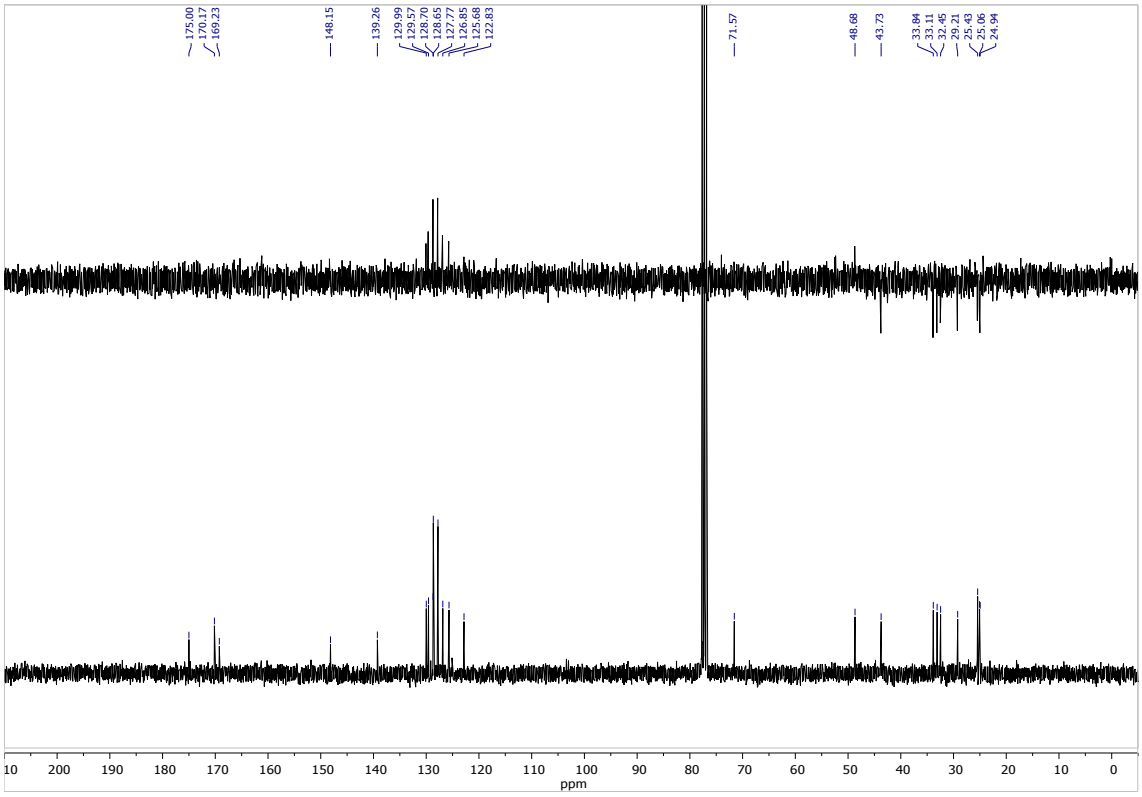

Figure S16. ^{13}C and DEPT NMR spectra of **6a** (100 MHz, $CDCl_3$)

11a-(*N*-Butylcarbamoyl)-11-phenyl-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6b

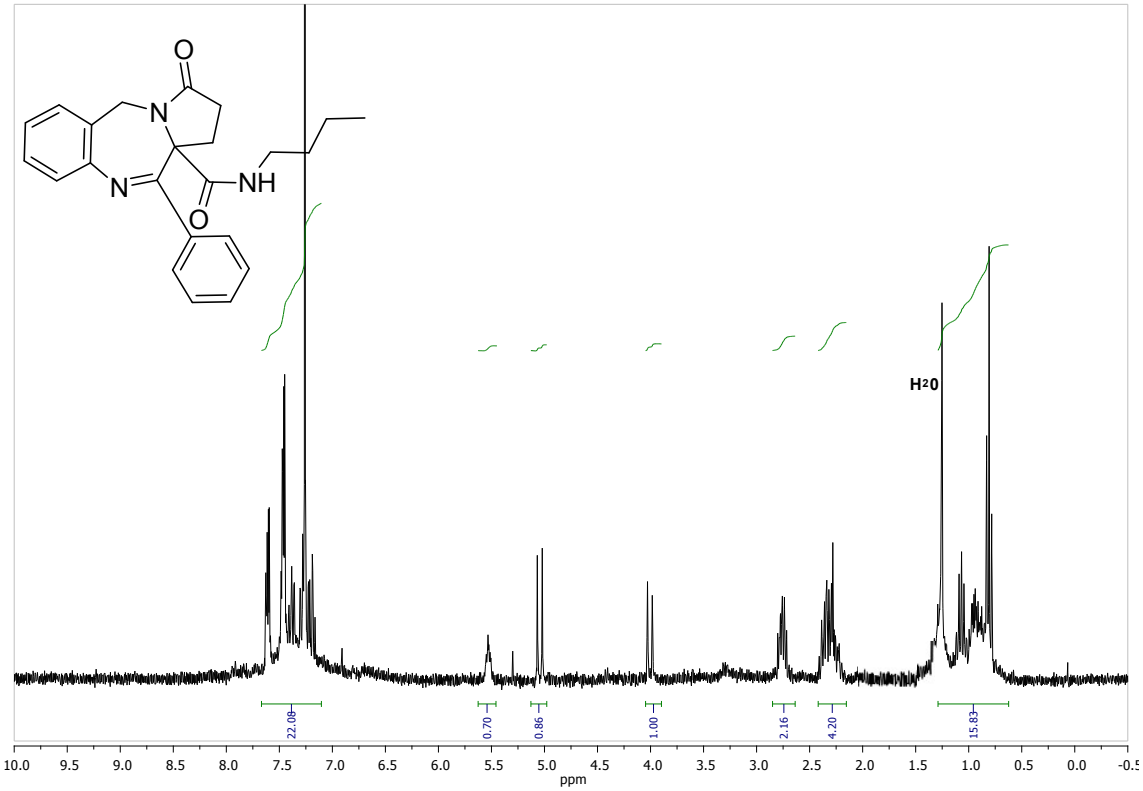

Figure S17. ^{1}H NMR spectrum of **6b** (300 MHz, $CDCl_3$)

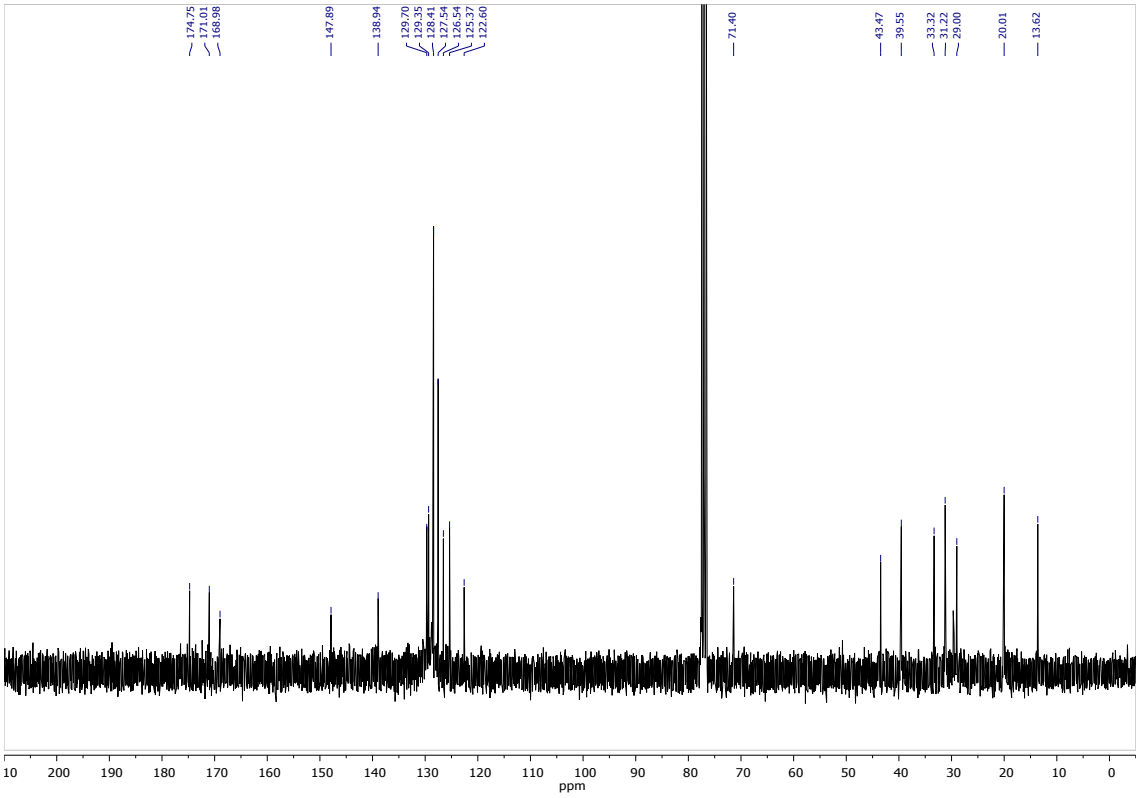

Figure S18. ^{13}C and DEPT NMR spectra of **6b** (75 MHz, $CDCl_3$)

11-Phenyl-11a-(*N*-tertbutylcarbamoyl)-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6c

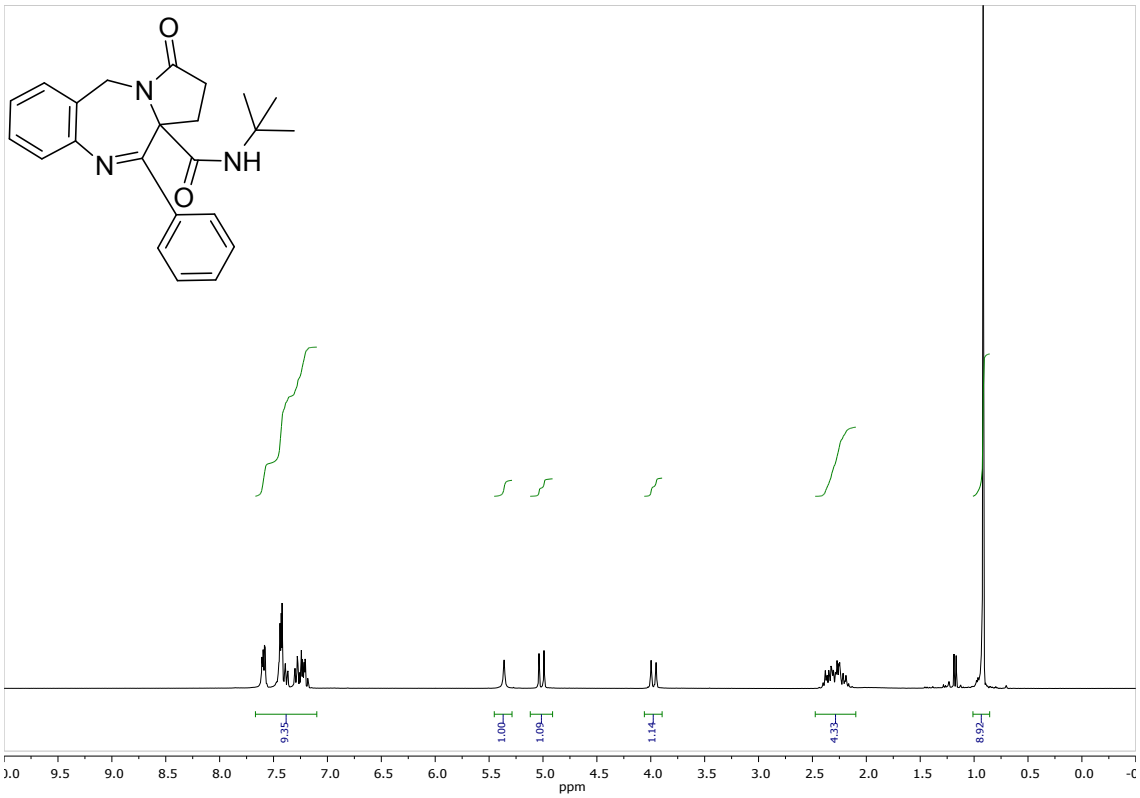

Figure S19. ^{1}H NMR spectrum of **6c** (300 MHz, $CDCl_3$)

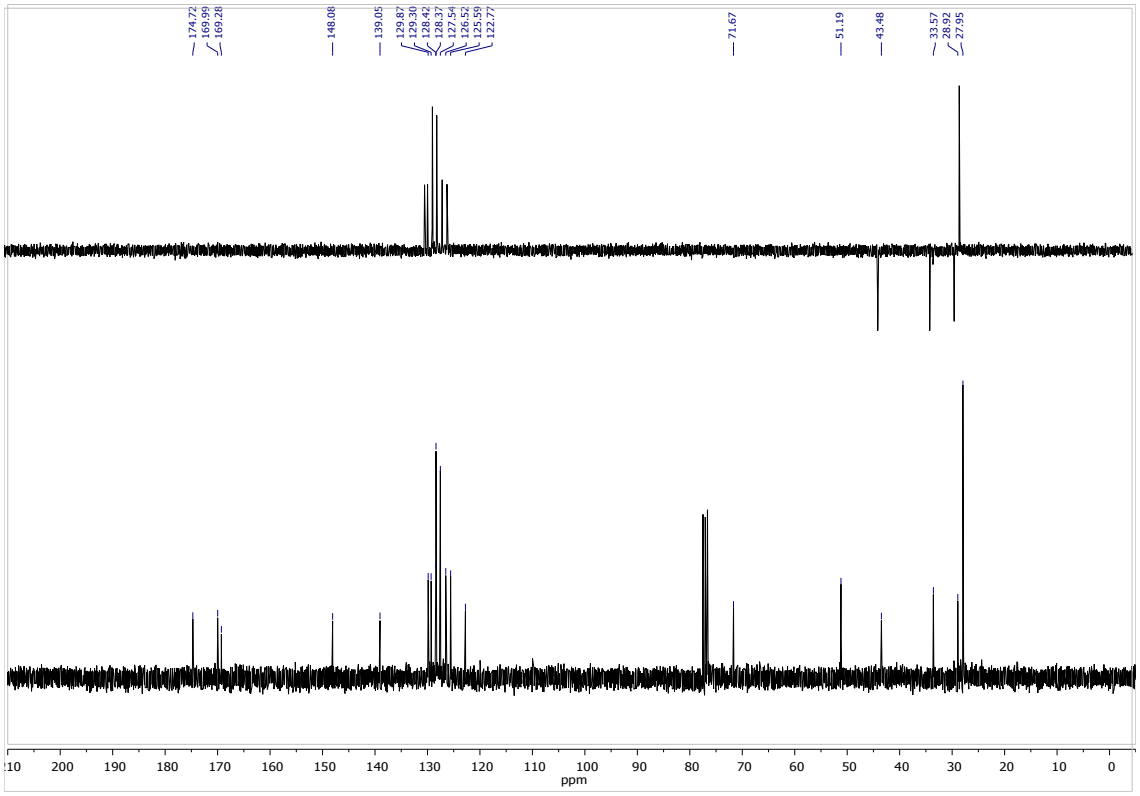

Figure S20. ^{13}C and DEPT NMR spectra of **6c** (75 MHz, $CDCl_3$)

11a-(*N*-Benzylcarbamoyl)-11-phenyl-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6d

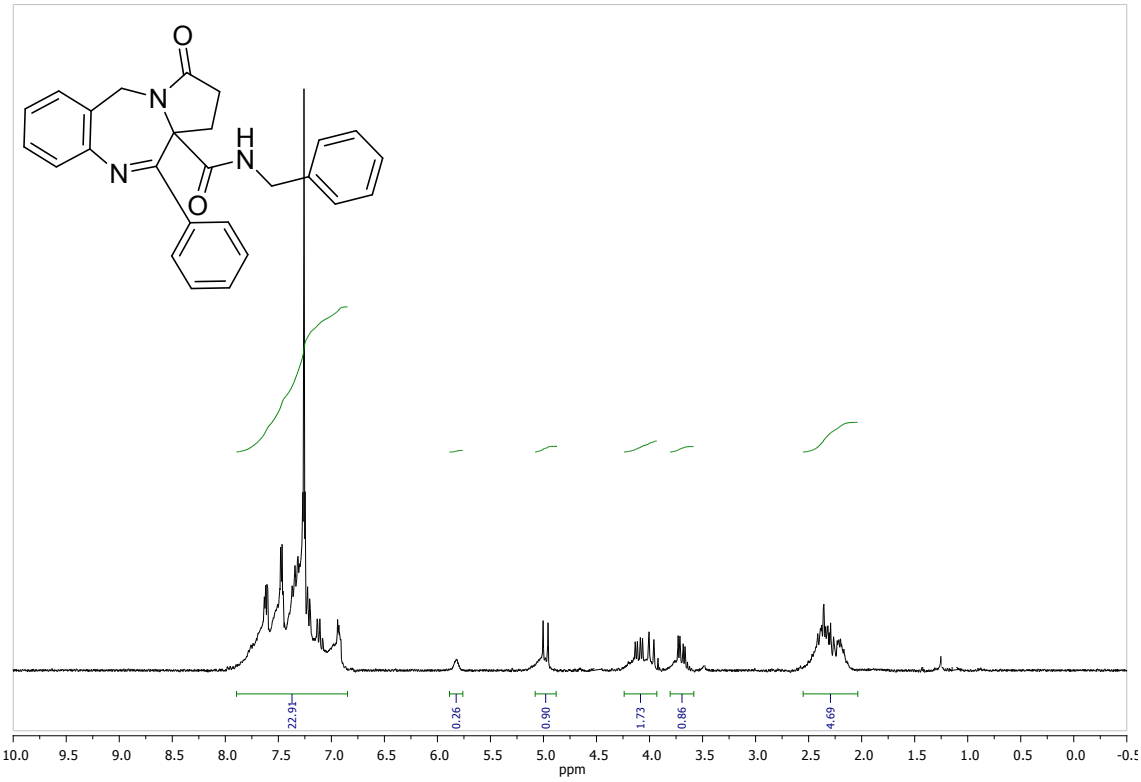

Figure S21. ^{1}H NMR spectrum of **6d** (300 MHz, $CDCl_3$)

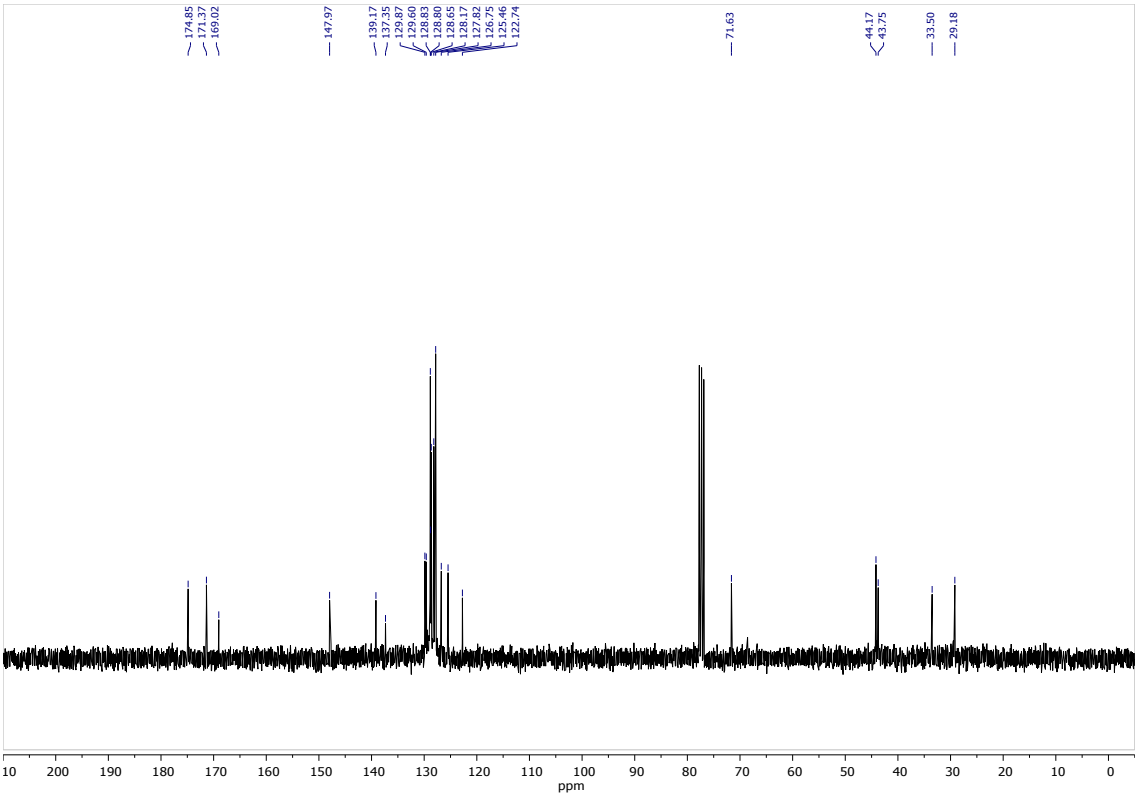

Figure S22. ^{13}C and DEPT NMR spectra of **6d** (75 MHz, $CDCl_3$)

11a-(*N*-Cyclohexylcarbamoyl)-11-tolyl-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6e

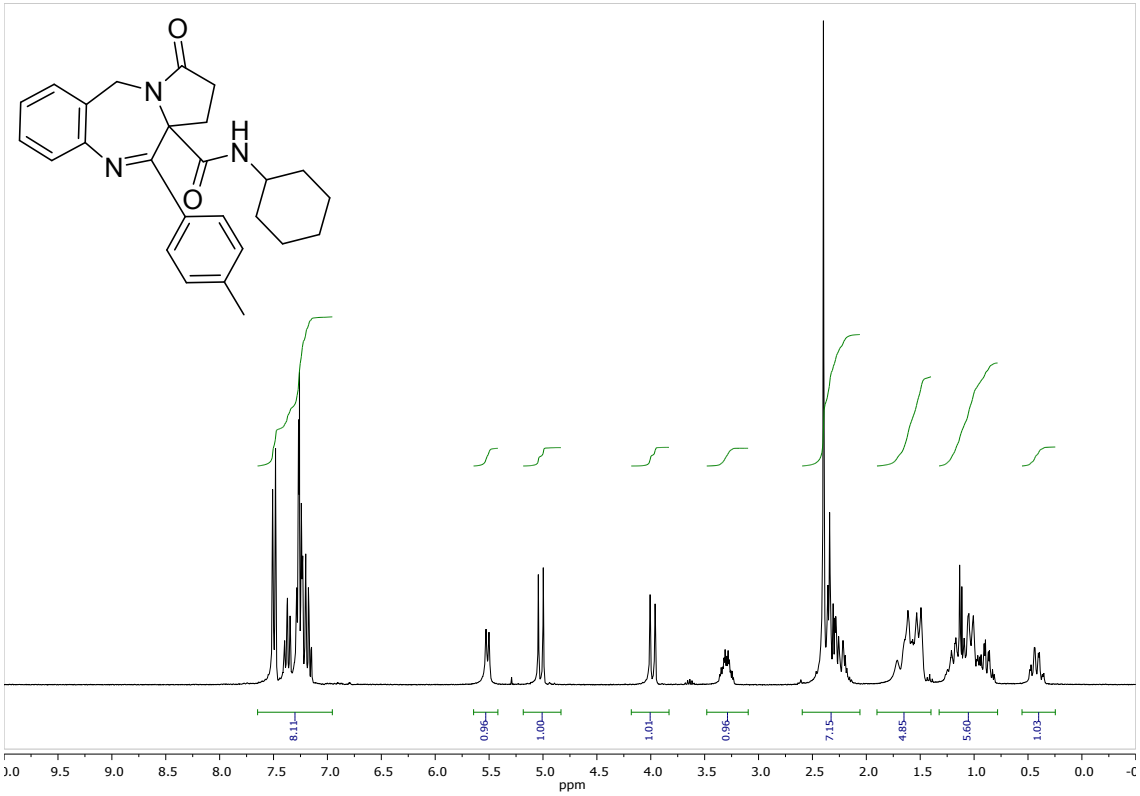

Figure S23. ^{1}H NMR spectrum of **6e** (300 MHz, $CDCl_3$)

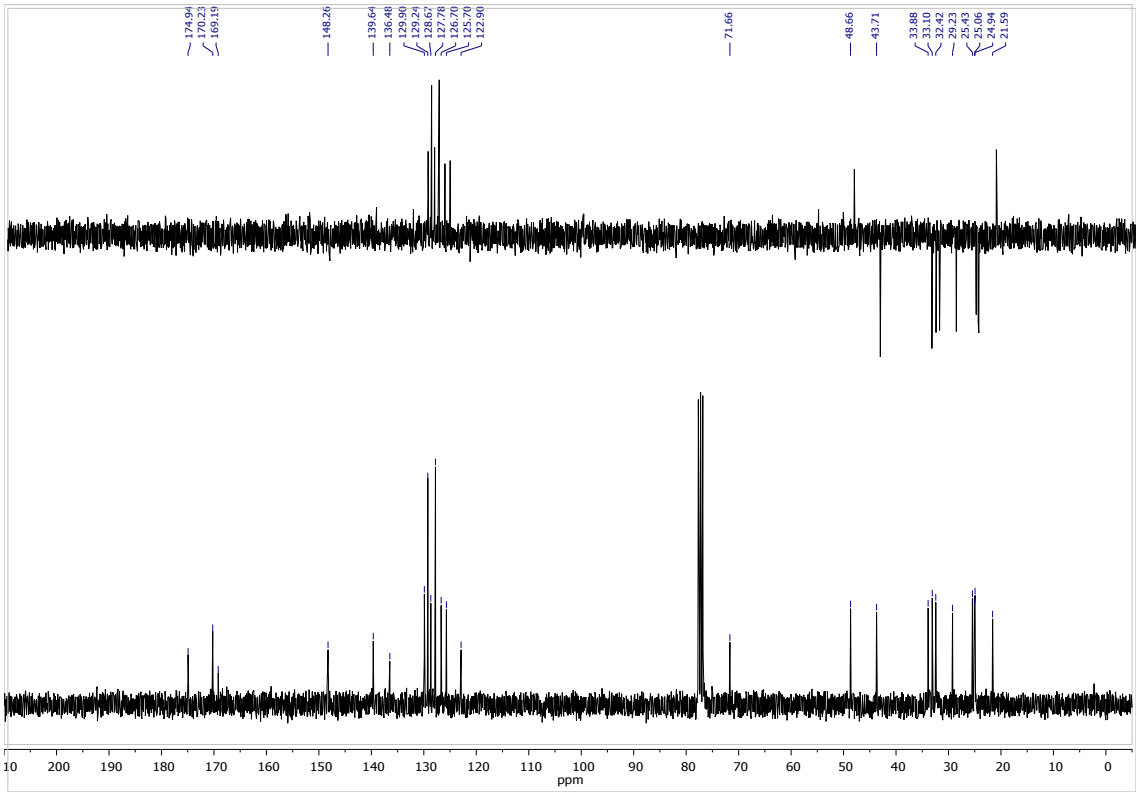

Figure S24. ^{13}C and DEPT NMR spectra of **6e** (75 MHz, $CDCl_3$)

11-(4-Chlorophenyl)-11a-(*N*-cyclohexylcarbamoyl)-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6f

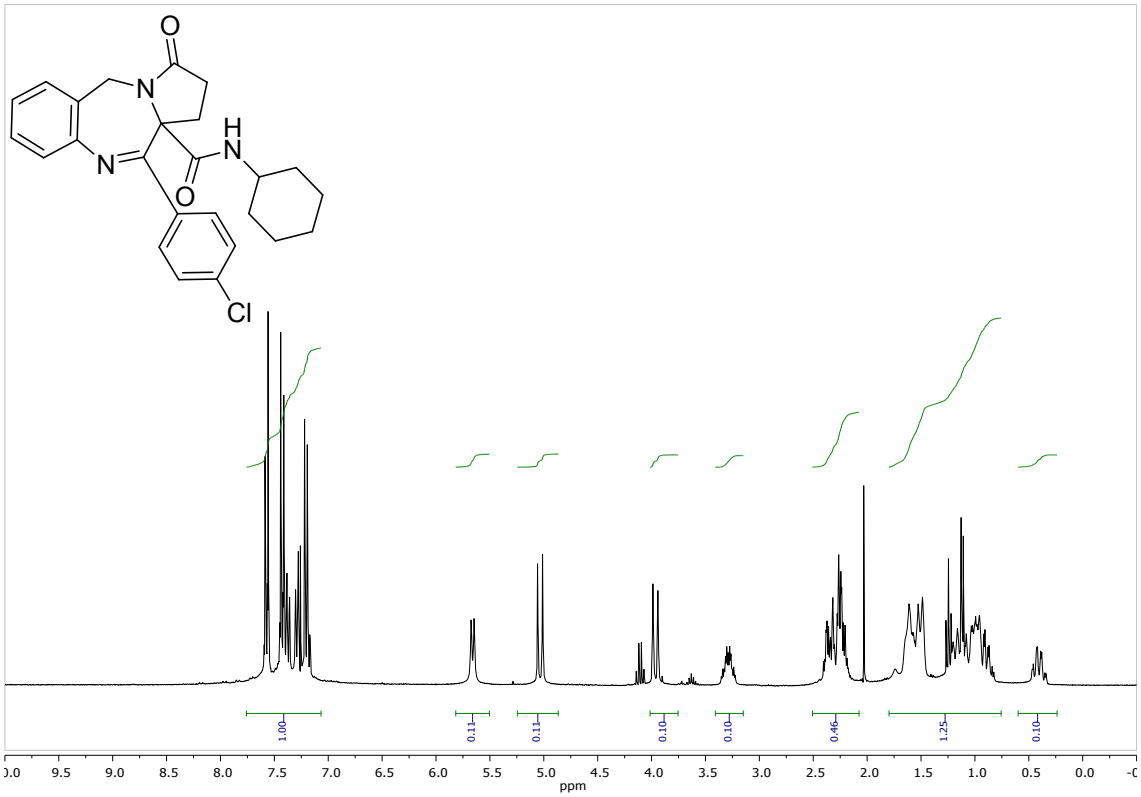

Figure S25. ^{1}H NMR spectrum of **6f** (300 MHz, $CDCl_3$)

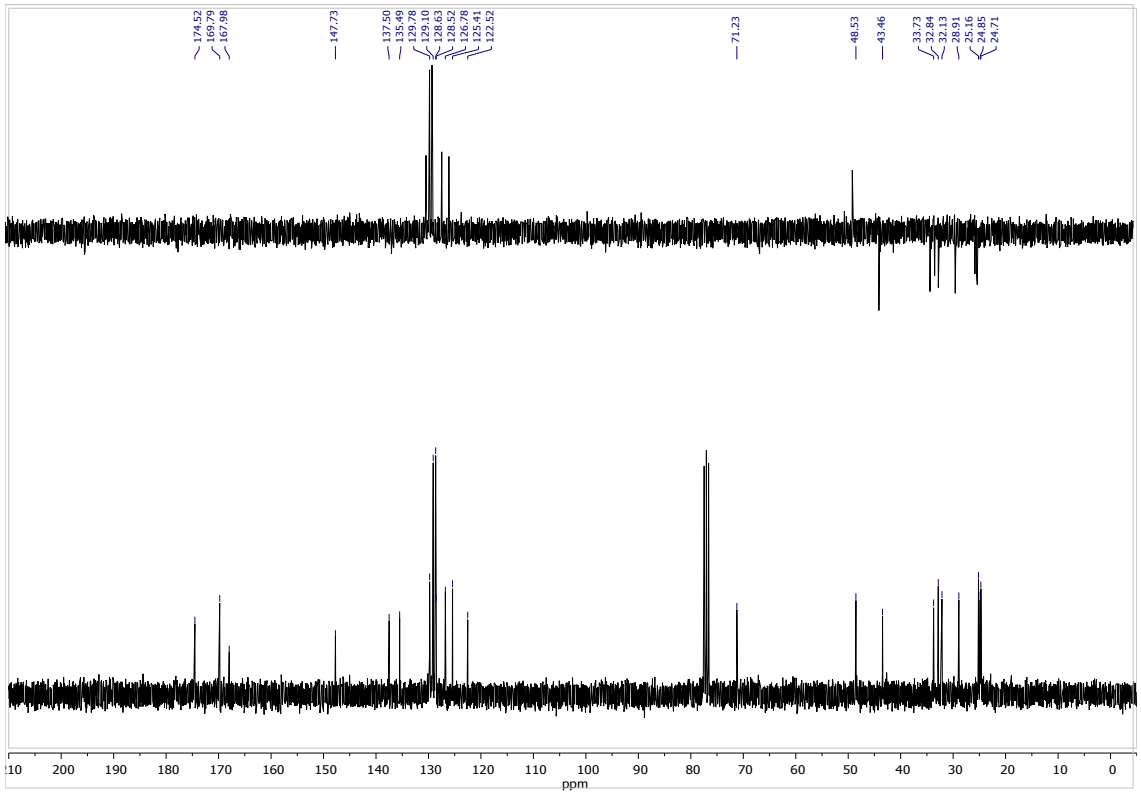

Figure S26. ^{13}C and DEPT NMR spectra of **6f** (75 MHz, $CDCl_3$)

11a-(*N*-Cyclohexylcarbamoyl)-11-methyl-2,3,5,11a-tetrahydro-1*H*-pyrrolo[2,1c][1,4]benzodiazepin-3-one. 6g

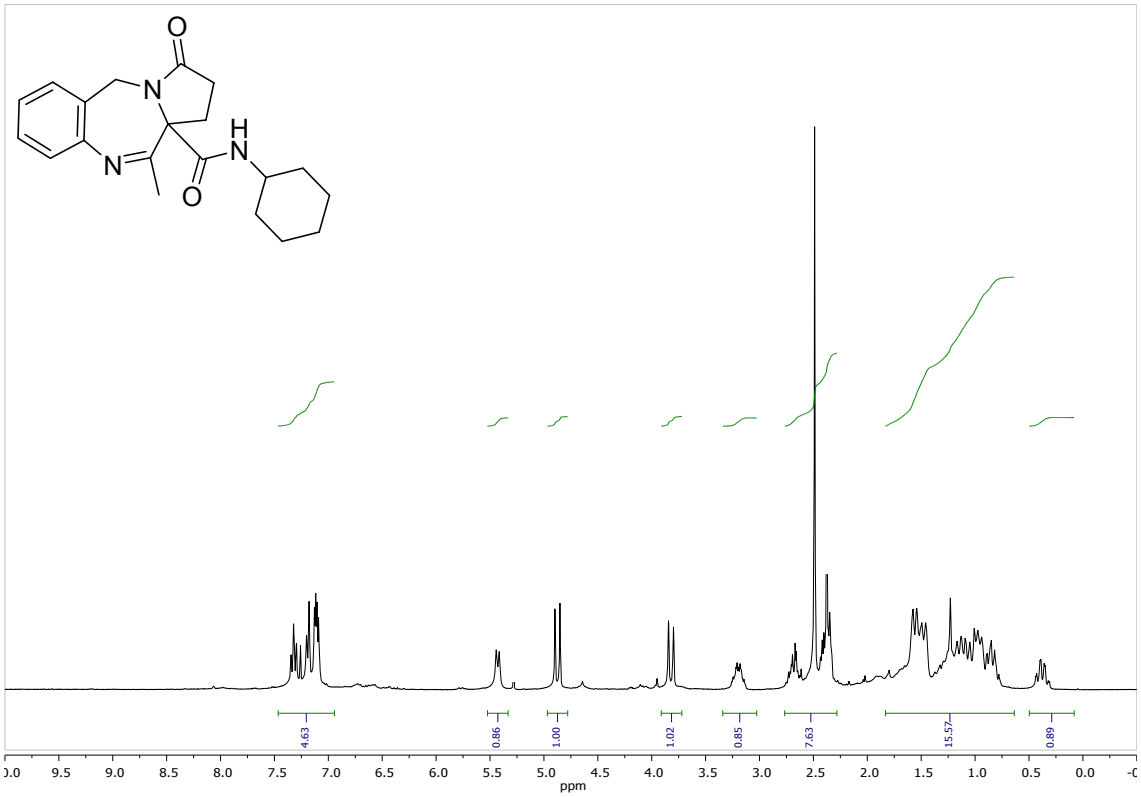

Figure S27. ^{1}H NMR spectrum of **6g** (300 MHz, $CDCl_3$)

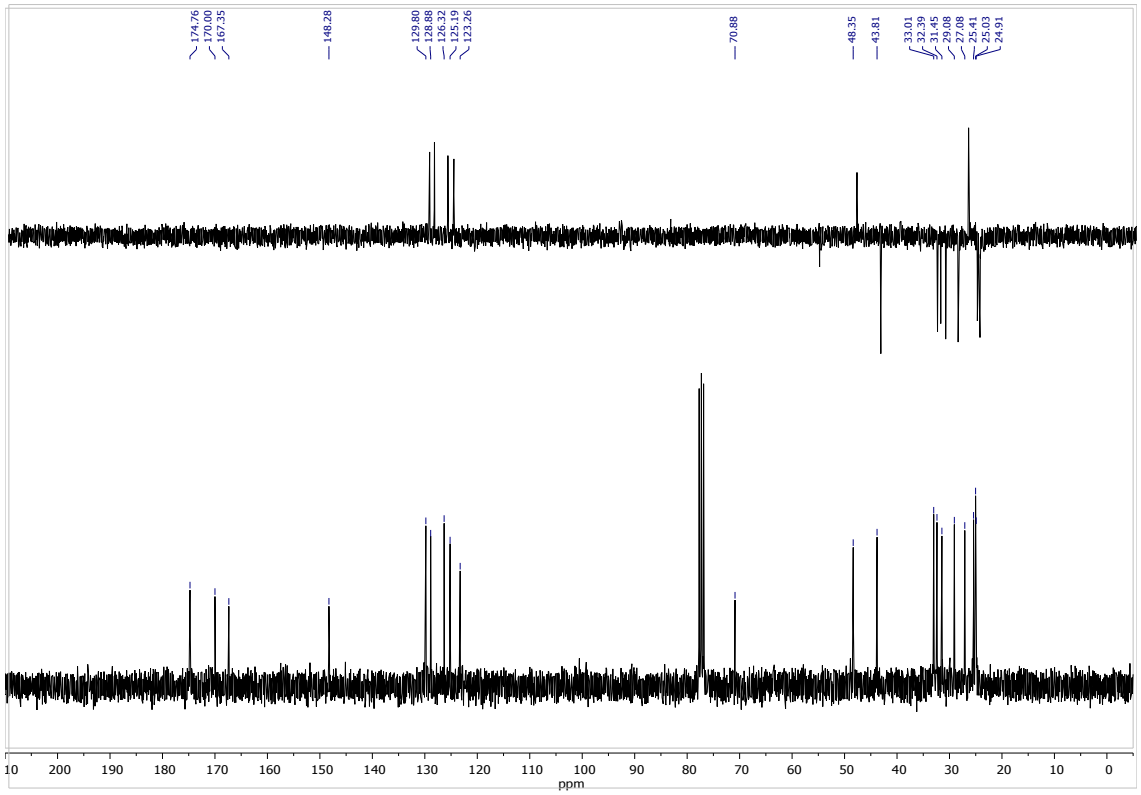

Figure S28. ^{13}C and DEPT NMR spectra of **6g** (75 MHz, $CDCl_3$)

1-Benzoyl-1-(*N*-cyclohexylcarbamoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7a

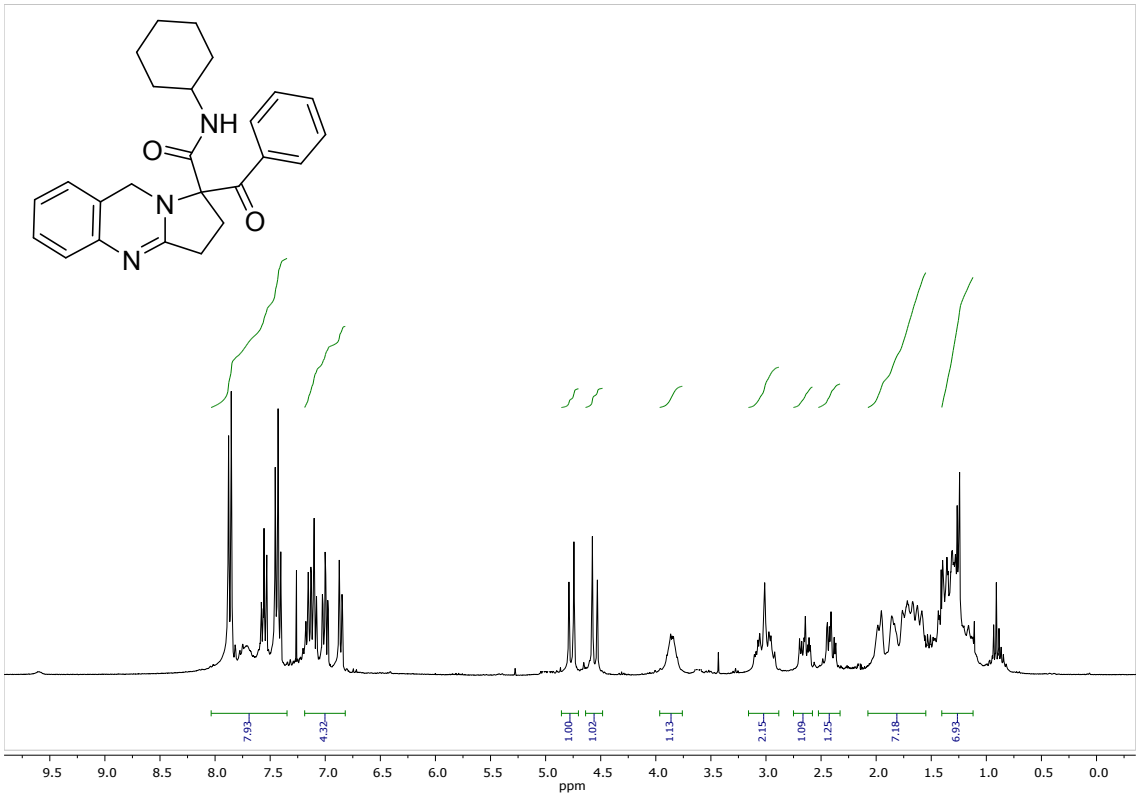

Figure S29. ^{1}H NMR spectrum of **7a** (300 MHz, $CDCl_3$)

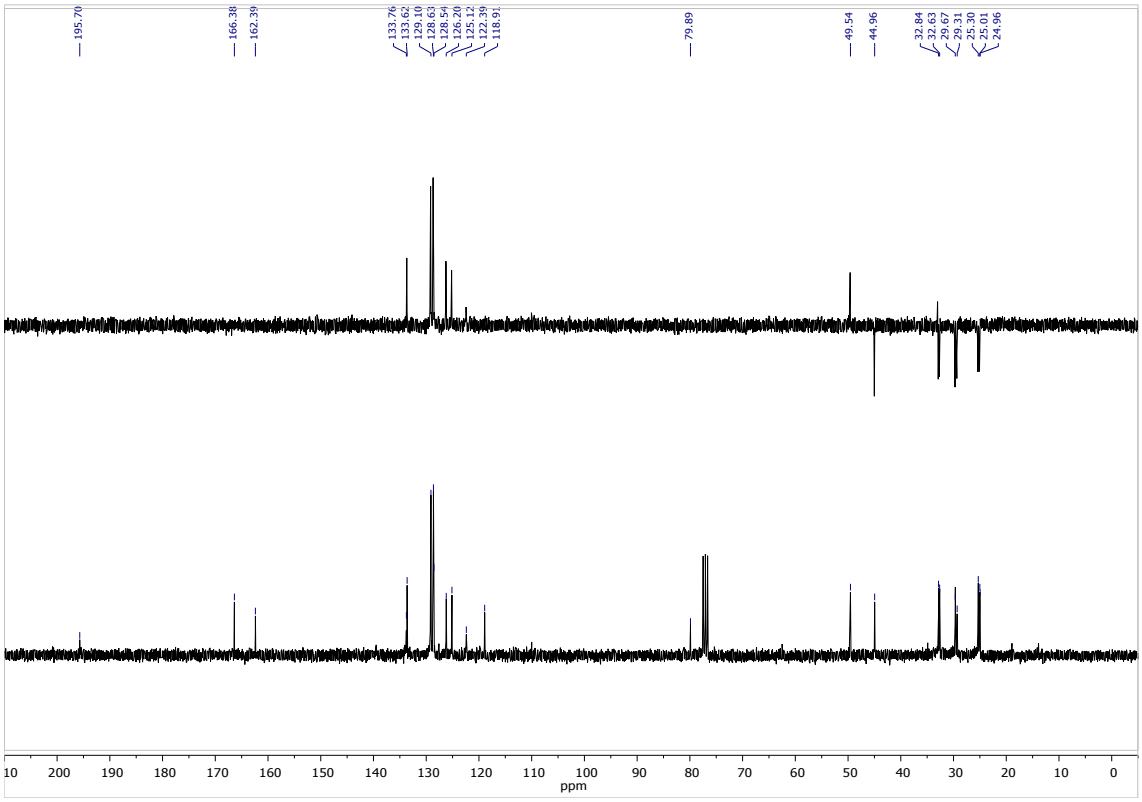

Figure S30. ^{13}C and DEPT NMR spectra of **7a** (75 MHz, $CDCl_3$)

1-Benzoyl-1-(*N*-butylcarbamoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7b

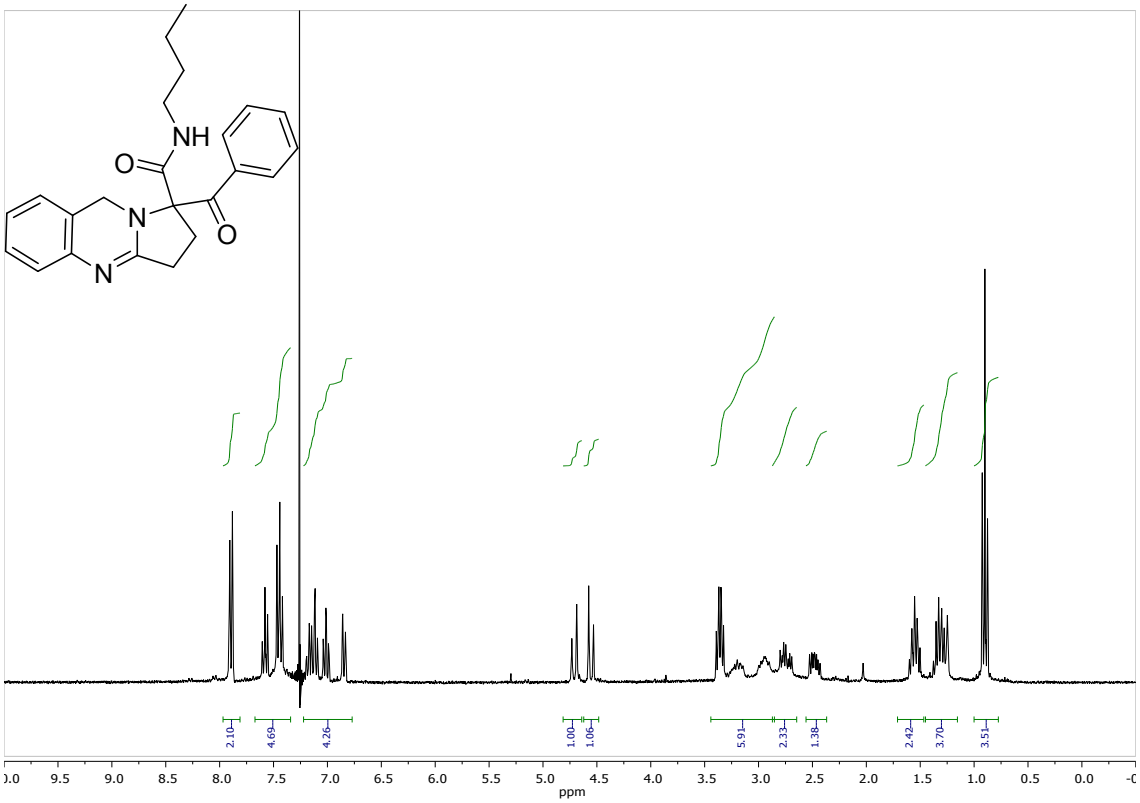

Figure S31. ^{1}H NMR spectrum of **7b** (300 MHz, $CDCl_3$)

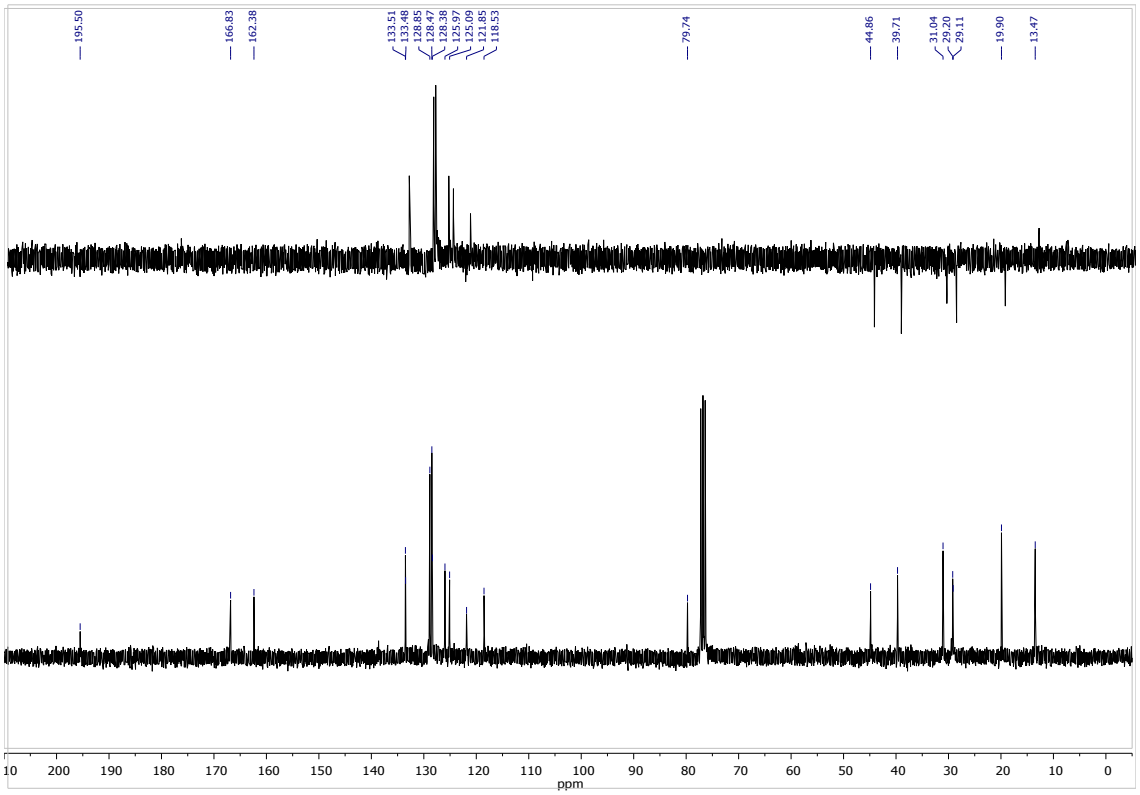

Figure S32. ^{13}C and DEPT NMR spectra of **7b** (75 MHz, $CDCl_3$)

1-Benzoyl-1-(*N*-tertbutylcarbamoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7c

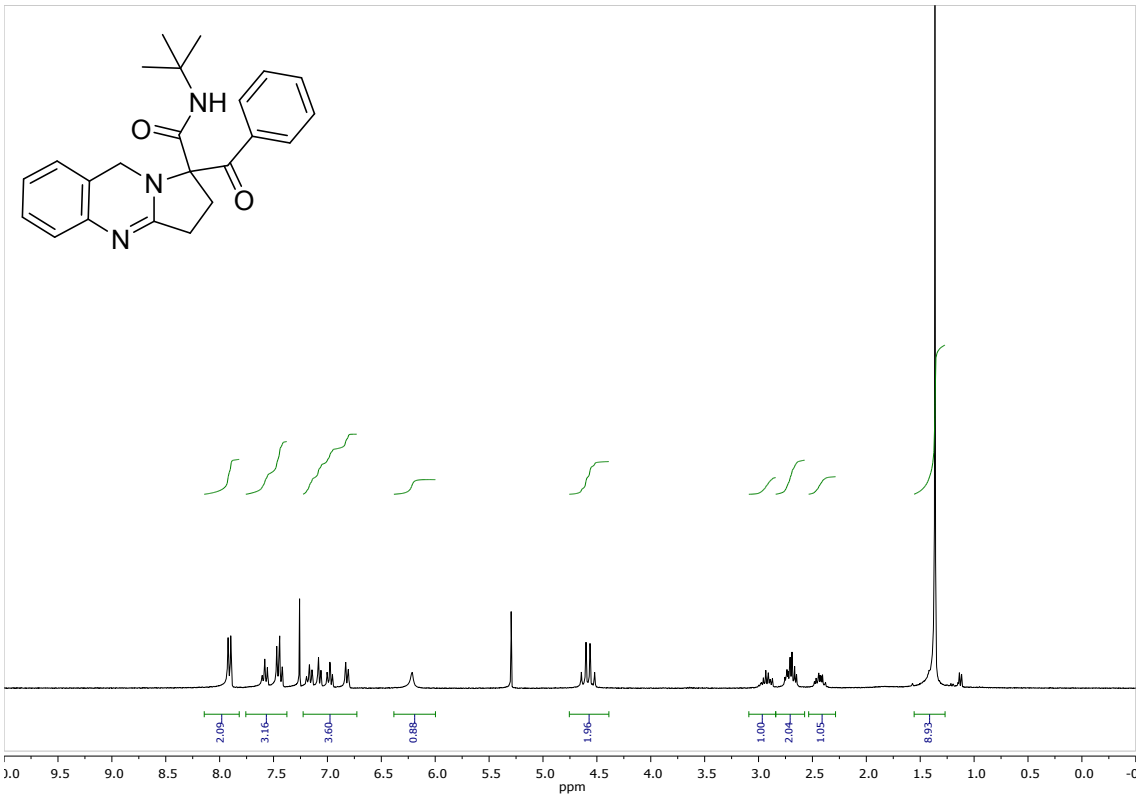

Figure S33. ^{1}H NMR spectrum of **7c** (300 MHz, $CDCl_3$)

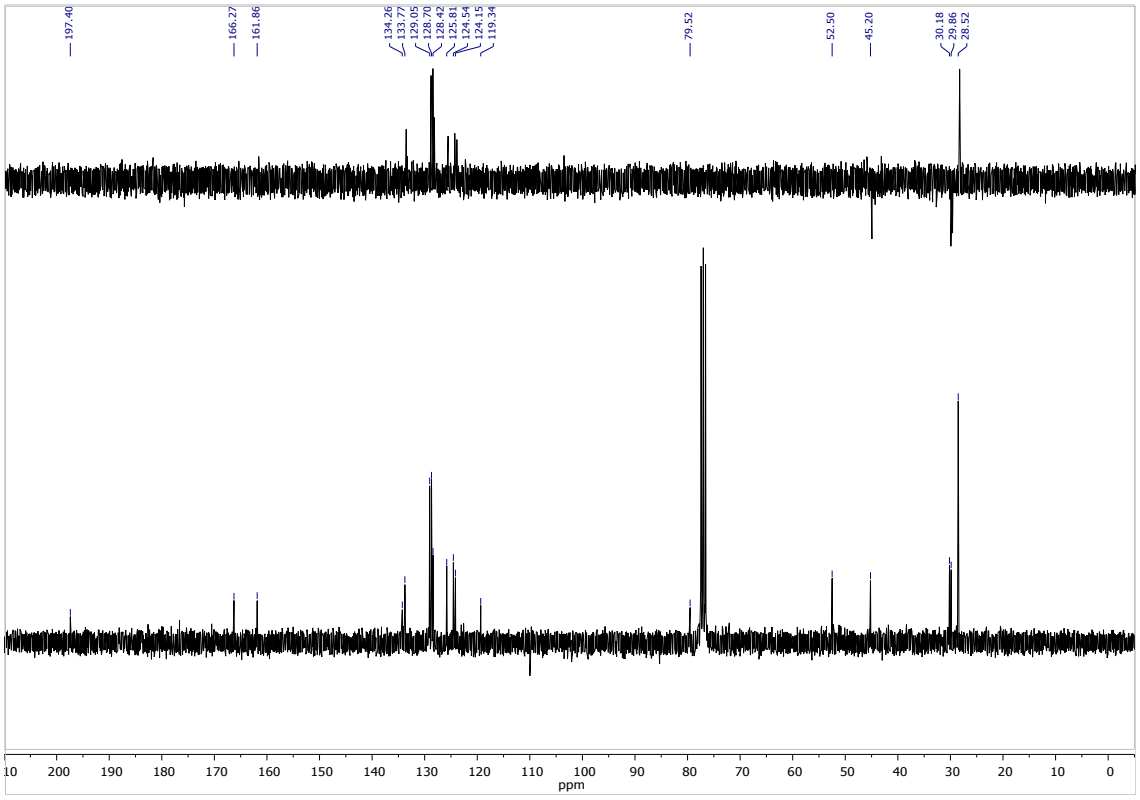

Figure S34. ^{13}C and DEPT NMR spectra of **7c** (75 MHz, $CDCl_3$)

1-Benzoyl-1-(*N*-benzylcarbamoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7d

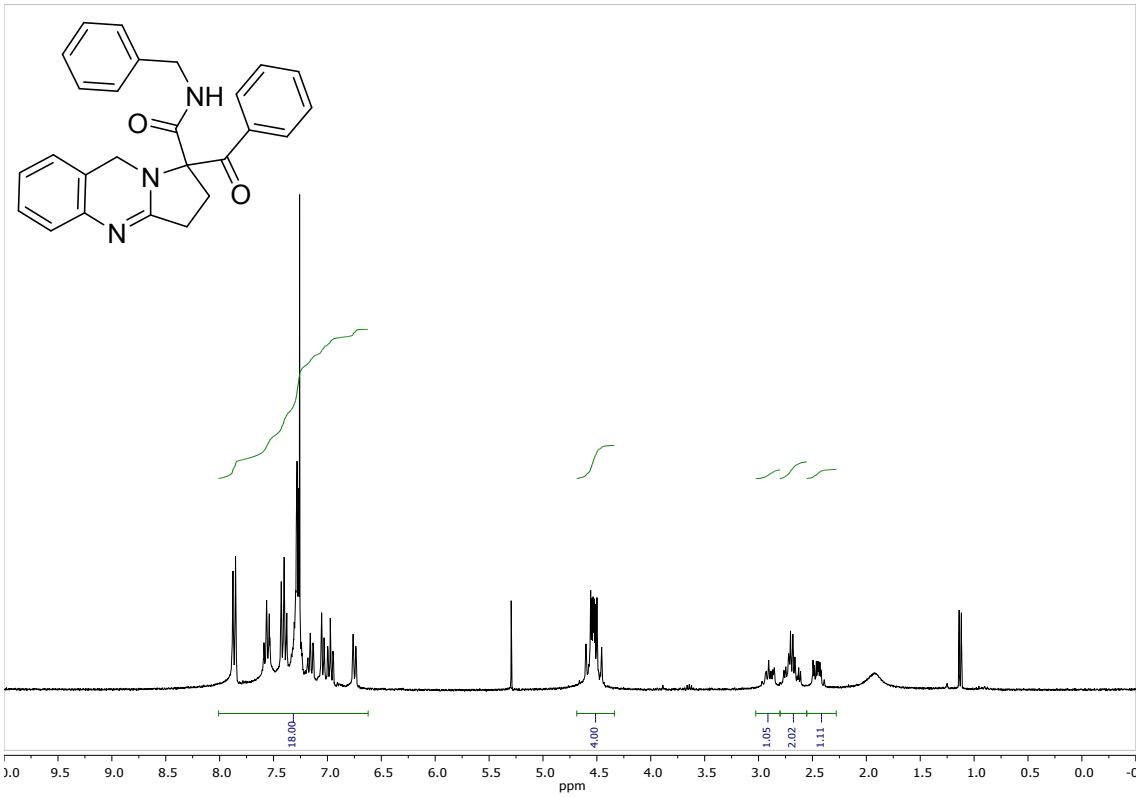

Figure S35. ^{1}H NMR spectrum of **7d** (300 MHz, $CDCl_3$)

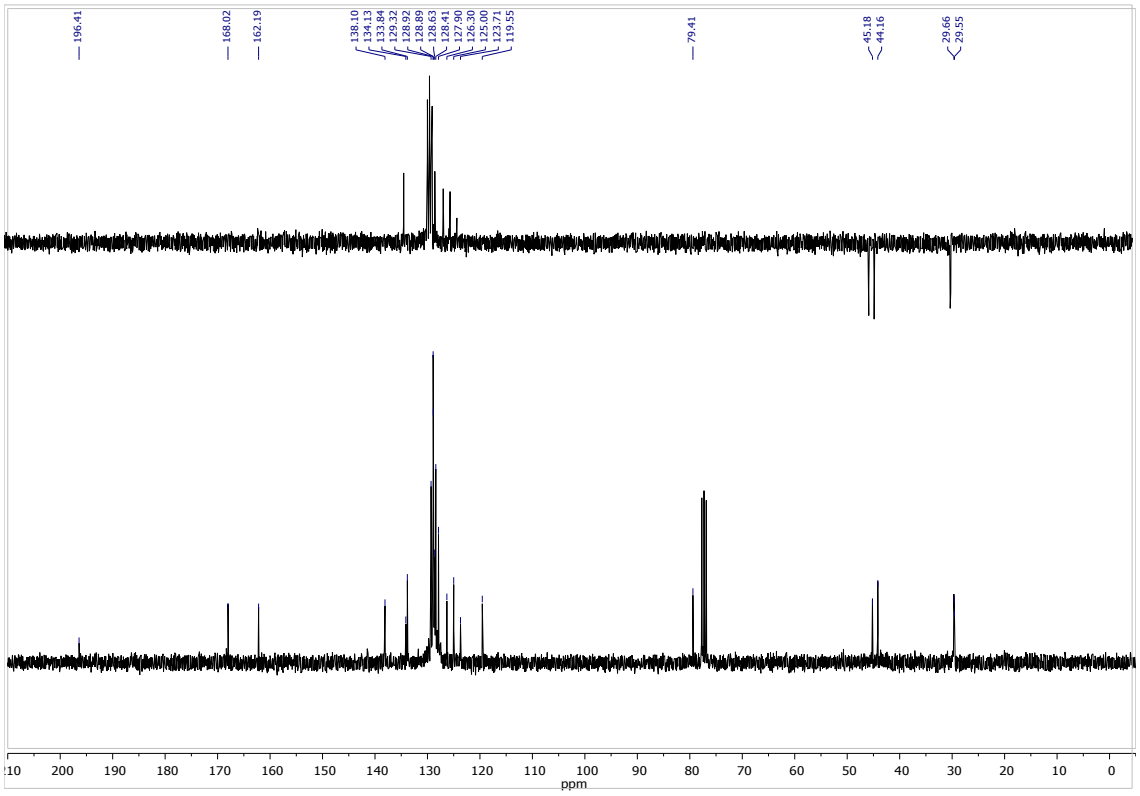

Figure S36. ^{13}C and DEPT NMR spectra of **7d** (75 MHz, $CDCl_3$)

1-(*N*-Cyclohexylcarbamoyl)-1-(4-methylbenzoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7e

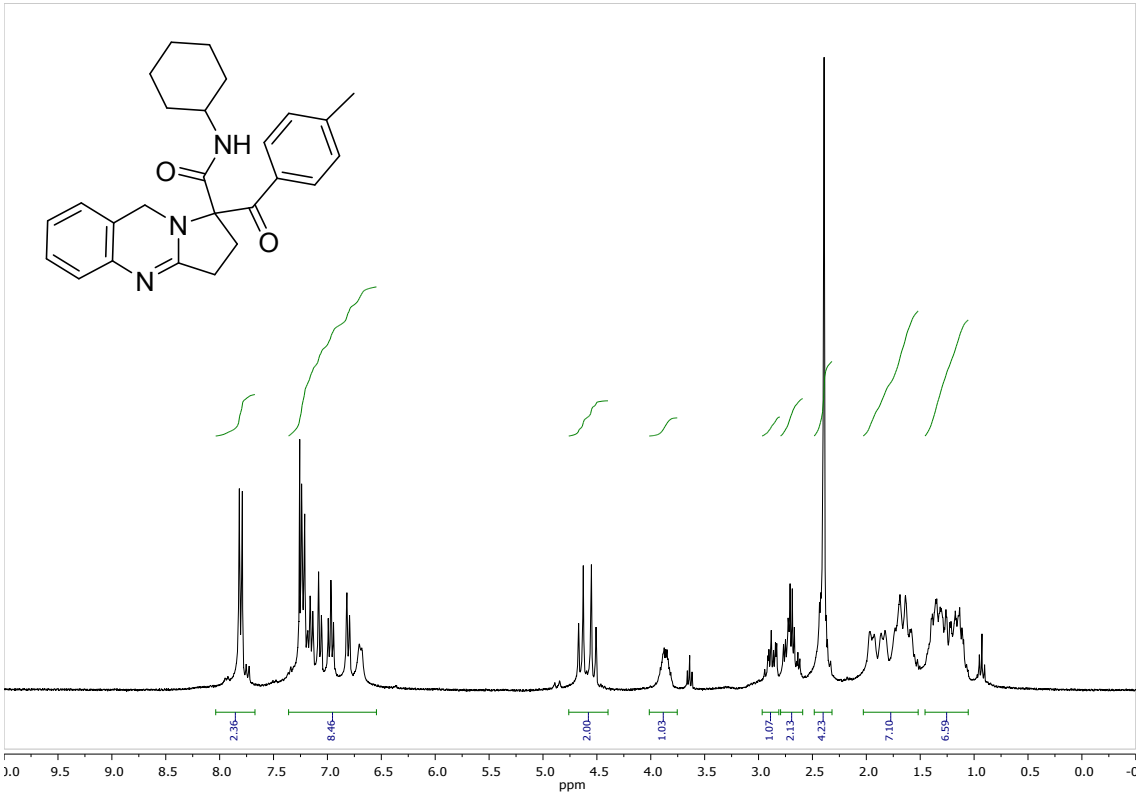

Figure S37. ^{1}H NMR spectrum of **7e** (300 MHz, $CDCl_3$)

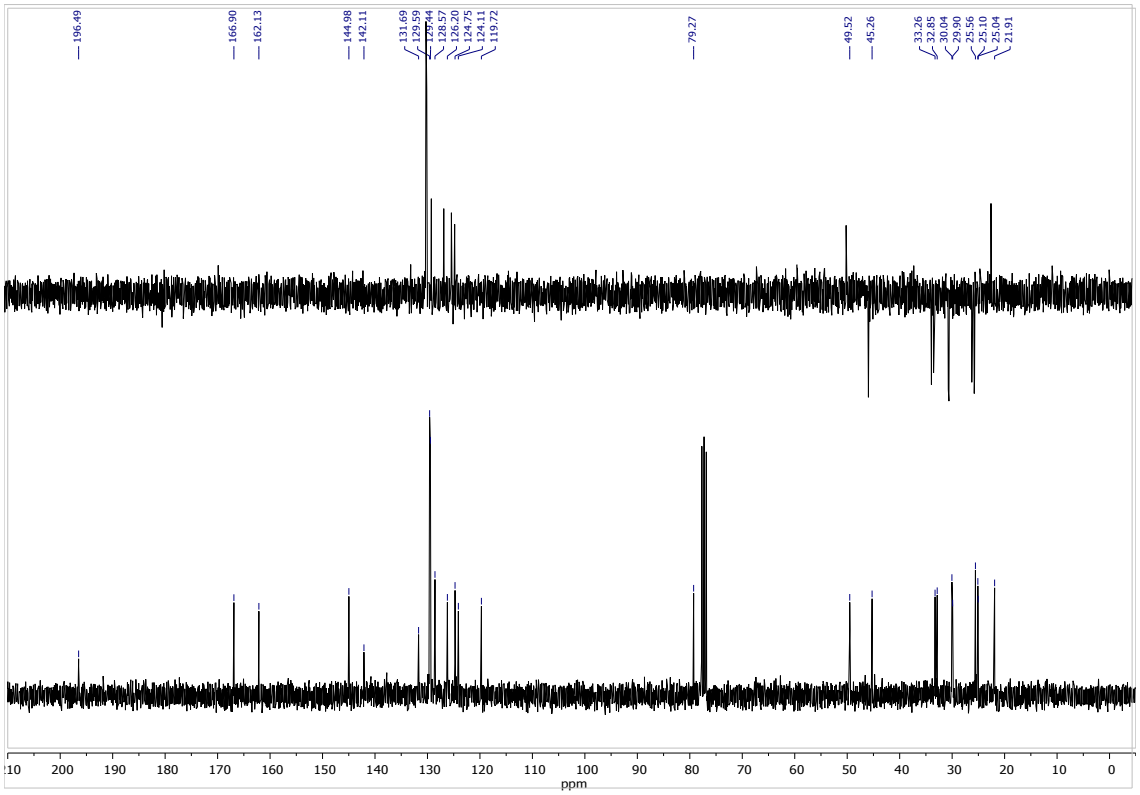

Figure S38. ^{13}C and DEPT NMR spectra of **7e** (75 MHz, $CDCl_3$)

1-(4-Chlorobenzoyl)-1-(*N*-cyclohexylcarbamoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7f

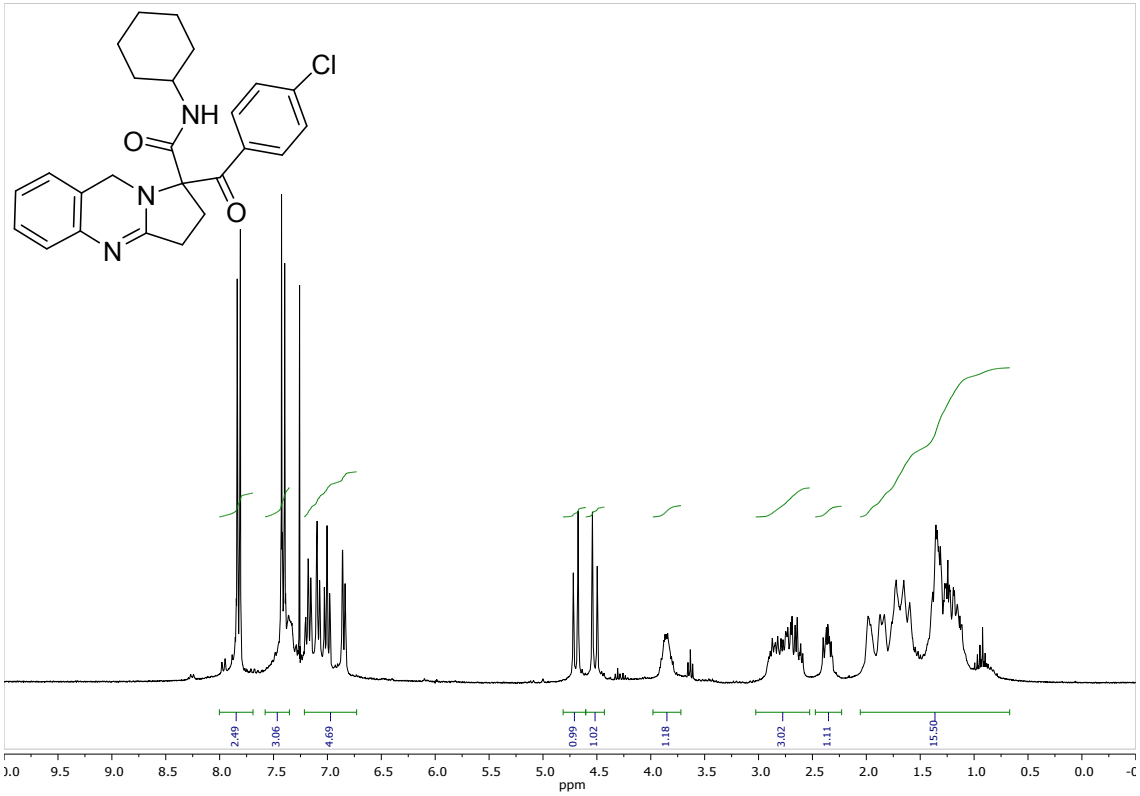

Figure S39. ^{1}H NMR spectrum of **7f** (300 MHz, $CDCl_3$)

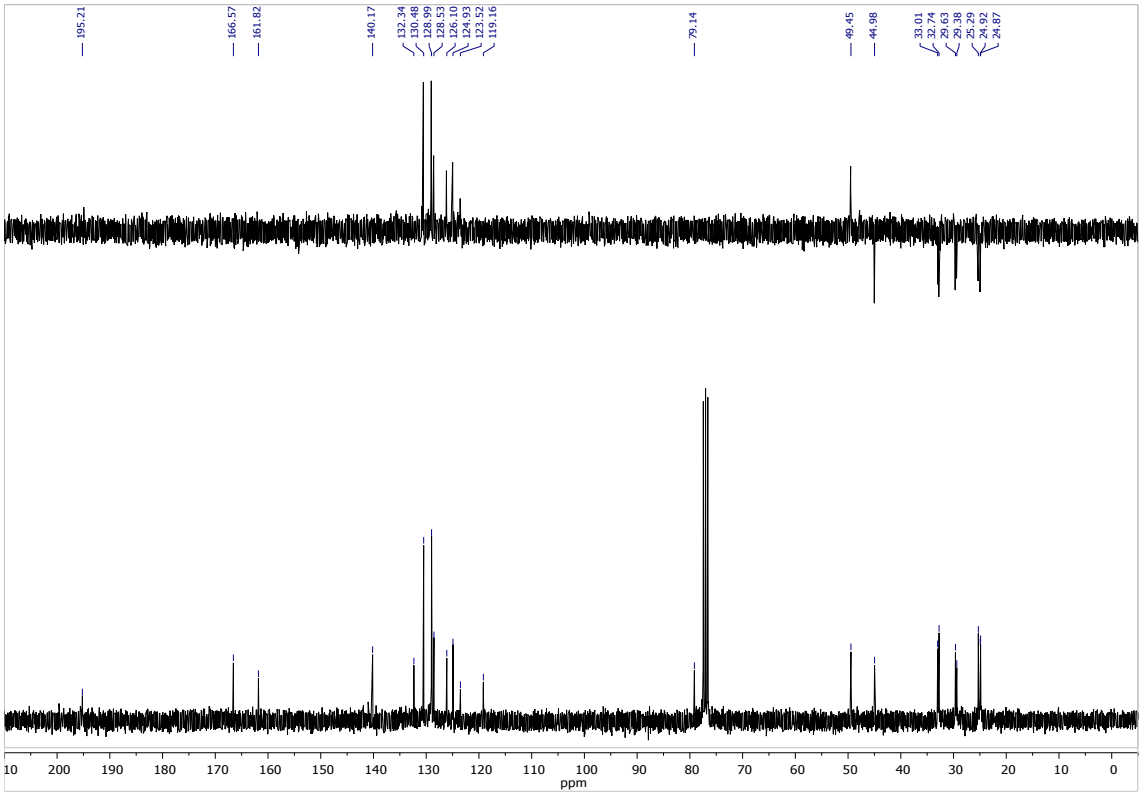

Figure S40. ^{13}C and DEPT NMR spectra of **7f** (75 MHz, $CDCl_3$)

1-Acetyl-1-(*N*-cyclohexylcarbamoyl)-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 7g

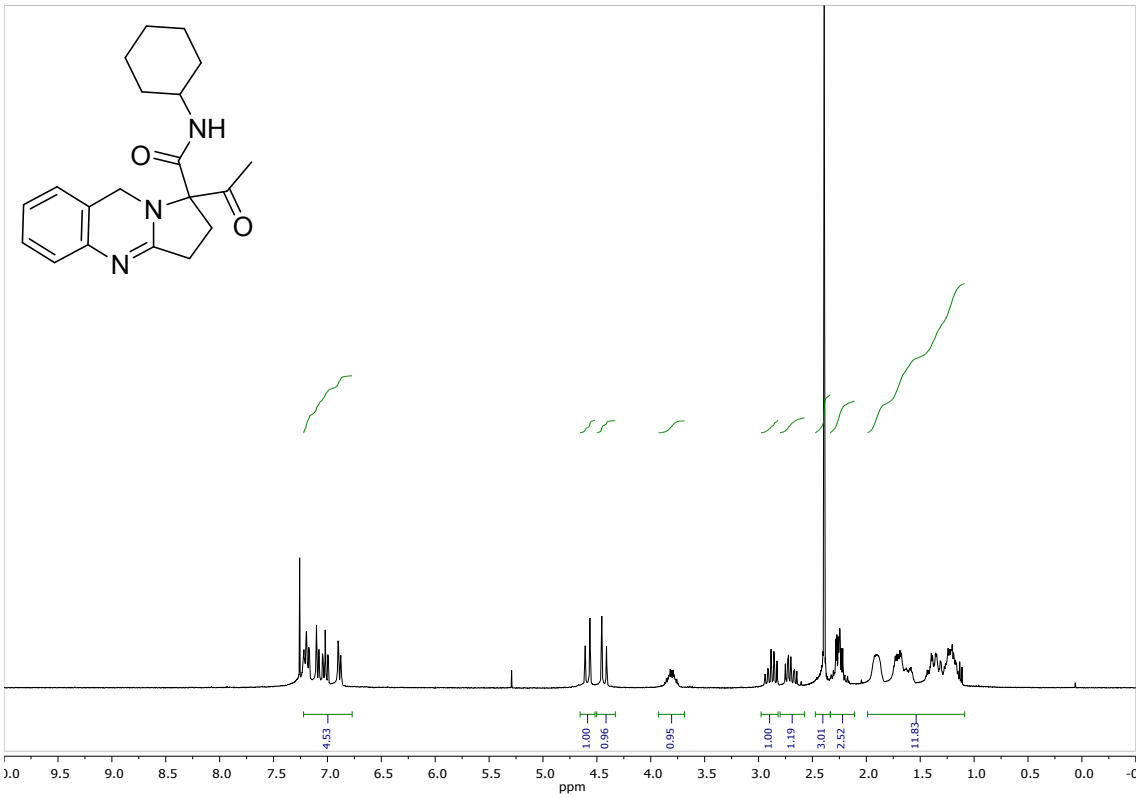

Figure S41. ^{1}H NMR spectrum of **7g** (300 MHz, $CDCl_3$)

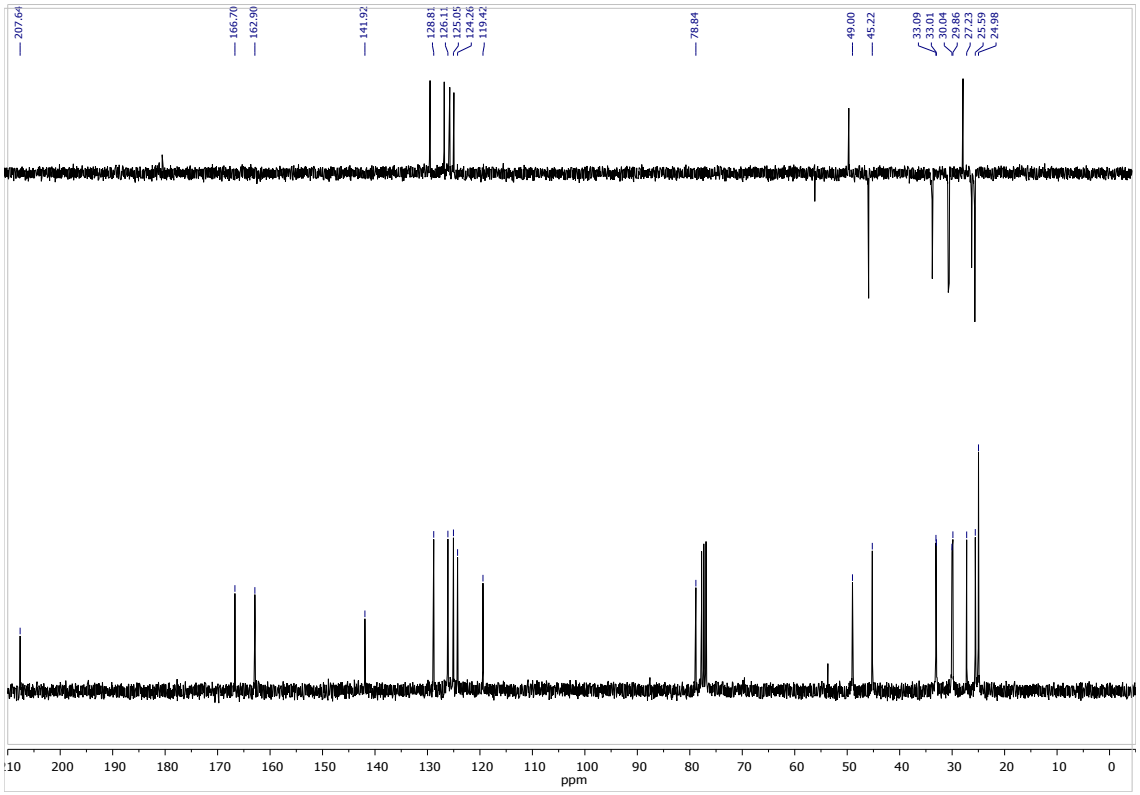

Figure S42. ^{13}C and DEPT NMR spectra of **7g** (75 MHz, $CDCl_3$)

N-Cyclohexylcarbamoyl-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazoline. 8a

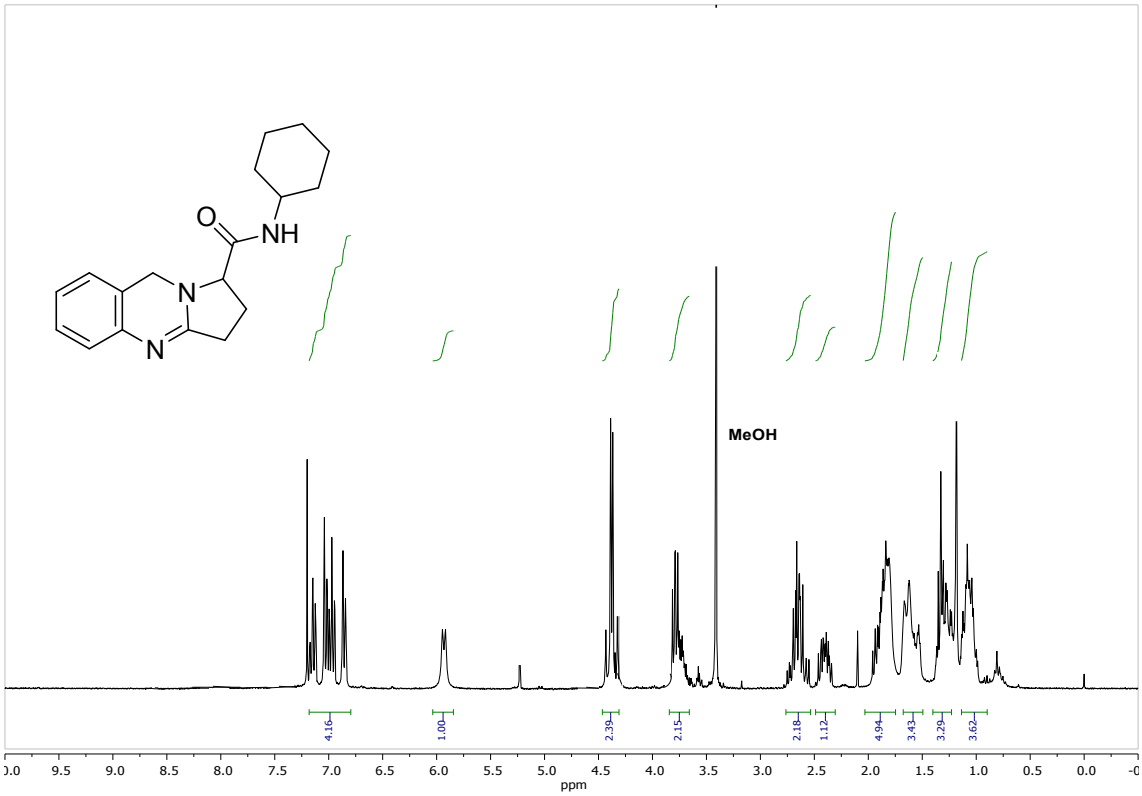

Figure S43. ^{1}H NMR spectrum of **8a** (300 MHz, $CDCl_3$)

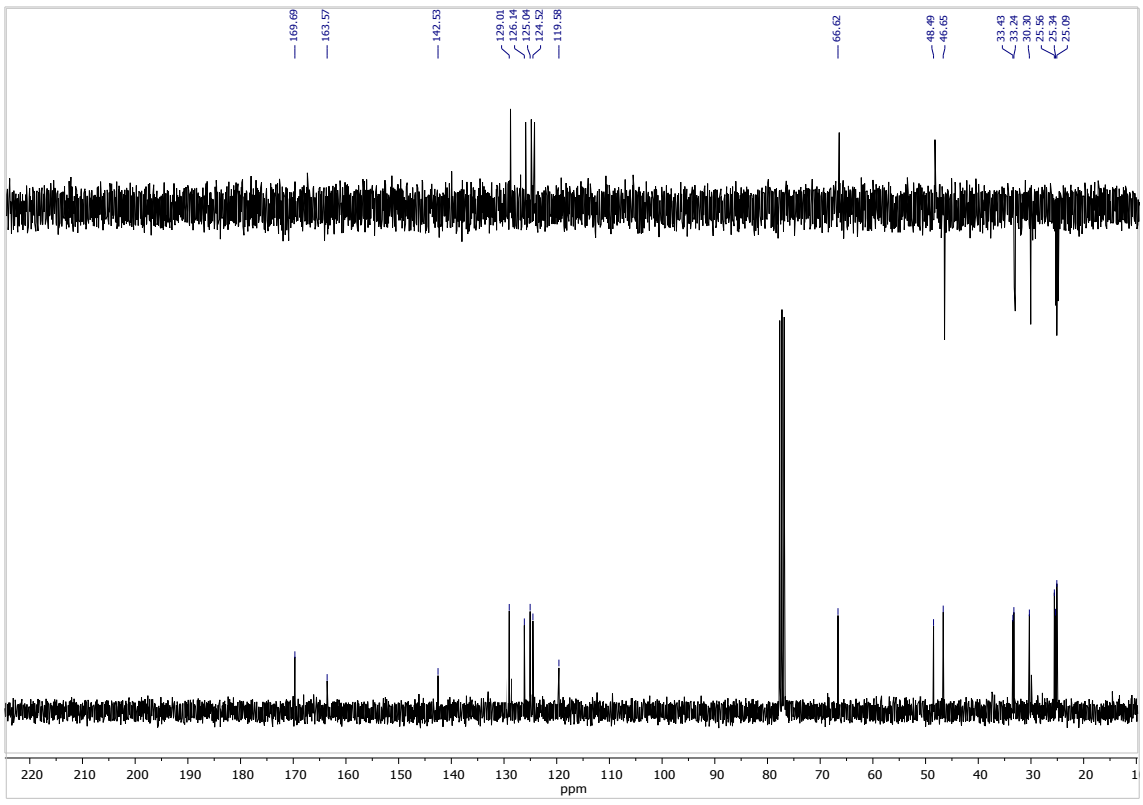

Figure S44. ^{13}C and DEPT NMR spectra of **8a** (75 MHz, $CDCl_3$)

Table S1. Crystal data and refinement details for **6c** and **7g**.

	6c	**7g**
formula	$C_{23}H_{25}N_3O_2$	$C_{20}H_{25}N_3O_2$
MW	375.46	339.43
crystal system	Monoclinic	Triclinic
space group	Pc	P-1
T/K	100(2)	100(2)
a/Å	9.1046(8)	9.9552(5)
b/Å	15.0988(14)	10.5626(5)
c/Å	14.5408(15)	10.5690(5)
α/deg	90	69.563(3)
β/deg	93.271(6)	62.162(3)
γ/deg	90	69.785(3)
V/Å^3	1995.6(3)	898.28(8)
F(000)	800	364
Z	4	2
λ, Å (MoK_α)	0.71073	0.71073
D_{calc}/g cm^{-3}	1.250	1.255
μ/mm^{-1}	0.081	0.082
θ range/deg	1.95 – 26.37	2.11 – 26.73
R_{int}	0.1179	0.0346
reflections measured	63009	35725
unique reflections	8051	3816
reflections observed	6180	3021
GOF on F^2	1.044	1.039
$R1$[a]	0.0618	0.0405
$wR2$[b]	0.1561	0.1078
Largest ≠ peak & hole/eÅ^{-3}	0.234 and -0.491	0.309 and -0.232

[a] $R1 = \sum \| \|F_0\| - \|Fc\| \| / \sum |F_0|$. [b] $wR2$ (all data) $= \{\sum[w(\|\|F_0|^2 - |Fc|^2)^2]/\sum[w(F_0^4)]\}^{1/2}$

X-ray diffraction studies. Single crystals were obtained from solutions of the isolated compounds (slow diffusion of diethyl ether into a solution of the compound in methanol, in the case of 6c, and slow evaporation of a solution of the compound in a dichloromethane-diisopropyl ether mixture, for 7g). Three dimensional X-ray data were collected on a BRUKER KAPPA APEXII CCD diffractometer. Data were corrected for Lorentz and polarization effects and for absorption by semiempirical methods[1] based on symmetry-equivalent reflections. Complex scattering factors were taken from the program SHELX-97[2] running under the WinGX program system[3] as implemented on a Pentium computer. The structure of 6c was solved with SUPERFLIP,[4] while that of 7g was solved employing SIR92.[5] Both structures were refined by full-matrix least-squares on F^2. For the two compounds all hydrogen atoms, except that of 7g corresponding to the NH fragment of the amide group, which was refined freely, were included in calculated positions and refined in riding mode. Refinement converged with anisotropic displacement parameters for all non-hydrogen atoms for both crystals. Crystal data and details on data collection and refinement are summarized in Table S1.

[1] SADABS 2016/2: L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst.*, 2015, **48**, 3.

[2] G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112.

[3] L. J. Farrugia, *J. Appl. Cryst.*, 1999, **32**, 837.

[4] SUPERFLIP: L. Palatinus, G. Chapuis, *J. Appl. Cryst.*, 2007, **40**, 786.

[5] SIR92: A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. C. Burla, G. Polidori, M. Camalli, *J. Appl. Cryst.*, 1994, **27**, 435.

Cartesian coordinates of the computational study

Electronic and thermal Free Energies in Hartree (gas phase and ethanol), number of imaginary frequencies and Cartesian coordinates (gas phase) in Ångströms. Images of structures are reported in the main manuscript (Figures 3 and 4).

B_6H$^+$

-1360,078217 (gas phase), -1360,140971 (ethanol)

0

C	-0.8335610	-0.4917790	2.5103860
C	0.4811130	2.2076570	-0.8833370
C	0.1609280	2.1293100	0.4884310
C	1.6439440	2.8810210	-1.2781720
C	2.4883130	3.4584870	-0.3294780
C	2.1801630	3.3802670	1.0292790
C	1.0145610	2.7239030	1.4264180
H	1.8824560	2.9597640	-2.3358450
H	3.3797160	3.9838120	-0.6582240
H	2.8272730	3.8394600	1.7689460
H	0.7527050	2.6663910	2.4796170
N	-0.9725070	-0.0245880	1.1988510
N	-0.3322470	1.5340610	-1.8307330
C	-0.9912030	-1.0765540	0.2016920
C	-2.1115190	-1.0429640	-0.8771890
C	0.3948230	-1.2750340	-0.4595210
N	1.4803700	-0.8725630	0.1441020
H	1.3613910	-0.2149620	0.9091570
O	-1.8753630	-1.6359870	-1.9415720
O	0.5009970	-2.0051780	-1.5230810
C	-3.4525630	-0.4662930	-0.6590580
C	-3.9832930	-0.1235840	0.6025060
C	-4.2637030	-0.3194720	-1.8060300
C	-5.2859280	0.3539620	0.7058710
H	-3.3960180	-0.2403570	1.5031540
C	-5.5557820	0.1770450	-1.6955130
H	-3.8610180	-0.6006110	-2.7721780
C	-6.0703390	0.5125070	-0.4393510
H	-5.6895810	0.6027410	1.6816190
H	-6.1661570	0.2966810	-2.5844580
H	-7.0829870	0.8936830	-0.3525510
C	2.8665350	-1.2485380	-0.2498870
C	3.4052940	-0.3781460	-1.3960590
C	3.7602760	-1.1711570	0.9955300
H	2.8030550	-2.2868790	-0.5929960
C	4.8492680	-0.7853420	-1.7366420
H	3.3766240	0.6729210	-1.0864800
H	2.7575830	-0.4804010	-2.2726050
C	5.2074880	-1.5603540	0.6510120
H	3.7400460	-0.1420490	1.3825430
H	3.3659700	-1.8235390	1.7836170
C	5.7622120	-0.7148160	-0.5041980
H	5.2282230	-0.1366170	-2.5329970
H	4.8545210	-1.8067800	-2.1407020
H	5.8316930	-1.4528800	1.5436530
H	5.2379670	-2.6231580	0.3761170
H	6.7713070	-1.0515950	-0.7626910
H	5.8549910	0.3302370	-0.1787870
C	-1.0974470	1.4300390	0.9564270
H	-1.3955400	1.8374820	1.9242980
H	-1.9312870	1.5897900	0.2705490
C	-0.7649130	-2.0133360	2.4705760
H	0.2685620	-2.3236570	2.6579020
H	-1.3787650	-2.4342480	3.2687320

C	-1.2486160	-2.3862260	1.0689510
H	-0.7523800	-3.2528880	0.6292850
H	-2.3223170	-2.5898090	1.0718520
H	-1.3100060	1.8061270	-1.7830080
O	-0.7644690	0.2267260	3.4845040
H	-0.0114100	1.6847310	-2.7817880
H	-0.4515600	-2.0498690	-1.9159570

$TS1_6$

-1360,065785 (gas phase), -1360,131795 (ethanol)

1

C	0.7013430	-1.4637990	2.1739980
C	0.4957770	2.4209770	-0.1661460
C	0.0031100	2.0279230	1.0869110
C	-0.1791320	3.3461280	-0.9610300
C	-1.3542080	3.9255470	-0.4823470
C	-1.8389990	3.5808040	0.7800470
C	-1.1651530	2.6340190	1.5547740
H	0.2157260	3.6267420	-1.9335240
H	-1.8786550	4.6550080	-1.0902480
H	-2.7410660	4.0474020	1.1617420
H	-1.5485460	2.3627200	2.5341030
N	0.7188680	-0.3652760	1.3095240
N	1.7269640	1.8167450	-0.6138040
C	0.6962150	-0.7112950	-0.1038520
C	1.8354300	-0.1000920	-0.9856450
C	-0.7055760	-0.4718980	-0.7552640
N	-1.7706190	-0.5745150	0.0349250
H	-1.6197860	-0.6593770	1.0307360
O	1.5940540	-0.1533780	-2.2746110
O	-0.8071910	-0.3121200	-1.9935050
C	3.2846340	-0.3099280	-0.6441350
C	3.7771030	-0.3739500	0.6736910
C	4.1906480	-0.4315010	-1.7135840
C	5.1390720	-0.5546960	0.9072260
H	3.1116180	-0.3062070	1.5235410
C	5.5505020	-0.6099880	-1.4709490
H	3.8206460	-0.3971860	-2.7307680
C	6.0295300	-0.6704600	-0.1616460
H	5.5019670	-0.6096760	1.9283980
H	6.2346940	-0.7066520	-2.3076450
H	7.0890790	-0.8119200	0.0259070
C	-3.1635240	-0.5587120	-0.4623120
C	-3.6040290	-1.9615520	-0.9157310
C	-4.0907870	0.0018900	0.6236090
H	-3.1678660	0.1102380	-1.3289070
C	-5.0661950	-1.9501330	-1.3900400
H	-3.4954670	-2.6560390	-0.0708450
H	-2.9416390	-2.3119650	-1.7144420
C	-5.5543440	0.0030310	0.1515700
H	-4.0030740	-0.6218020	1.5263030
H	-3.7727080	1.0142100	0.8969280
C	-6.0039990	-1.3905110	-0.3108630
H	-5.3666780	-2.9643170	-1.6726030
H	-5.1460160	-1.3381730	-2.2987470
H	-6.1970930	0.3663930	0.9601070
H	-5.6631460	0.7158430	-0.6770400
H	-7.0307930	-1.3463390	-0.6885560
H	-6.0173830	-2.0729510	0.5500810
C	0.7451880	0.9891590	1.8931400
H	1.7900000	1.3003880	2.0488930
H	0.3180410	0.8885710	2.8929760
C	0.6125230	-2.7278430	1.3344860

H	1.3122180	-3.4752600	1.7129990
H	-0.3942820	-3.1445150	1.4441660
C	0.9173620	-2.2812050	-0.0992820
H	1.9567880	-2.4949330	-0.3525250
H	0.2906740	-2.7591080	-0.8533670
H	0.5579940	-0.2115410	-2.3998550
O	0.7174900	-1.3670980	3.3830230
H	2.4957870	1.9843550	0.0372340
H	2.0126850	2.1667000	-1.5285710

6int$_1$H$^+$

-1360,070605 (gas phase), -1360,135368 (ethanol)

0

C	0.4646540	-0.2644160	2.3887990
C	1.8623900	1.7139260	-1.0229870
C	1.3350860	2.2393730	0.1644080
C	2.9916830	2.2523650	-1.6338570
C	3.6170490	3.3614190	-1.0650980
C	3.1106470	3.9086770	0.1119810
C	1.9864420	3.3458230	0.7183200
H	3.3837620	1.8147900	-2.5482960
H	4.4946850	3.7863730	-1.5397350
H	3.5938080	4.7673400	0.5659890
H	1.6076180	3.7656320	1.6451000
N	0.1758940	0.2240110	1.1140590
N	1.2260930	0.5567510	-1.6738220
C	-0.0593270	-0.7920020	0.1051090
C	1.0946270	-0.9014390	-0.9716410
C	-1.4091670	-0.4603440	-0.6203620
N	-2.4999400	-0.4012220	0.1429360
H	-2.3968940	-0.5651990	1.1368580
O	0.7153600	-1.7110180	-2.0197700
O	-1.4241380	-0.2140340	-1.8487100
C	2.4655940	-1.3403820	-0.4777640
C	3.1632980	-0.6807900	0.5498480
C	3.0571450	-2.4632550	-1.0817010
C	4.4153620	-1.1396810	0.9591590
H	2.7533910	0.1904140	1.0408240
C	4.3089740	-2.9148690	-0.6666630
H	2.5330170	-2.9852170	-1.8714750
C	4.9926090	-2.2562880	0.3548390
H	4.9367110	-0.6181620	1.7553700
H	4.7460710	-3.7859480	-1.1441350
H	5.9662550	-2.6101120	0.6785980
C	-3.8607180	-0.0969080	-0.3470820
C	-4.7754920	-1.3208990	-0.1749350
C	-4.4236590	1.1378700	0.3747420
H	-3.7432360	0.1228890	-1.4115420
C	-6.2073640	-1.0077430	-0.6399440
H	-4.7914410	-1.6082190	0.8865590
H	-4.3633670	-2.1700330	-0.7313910
C	-5.8575090	1.4426640	-0.0908980
H	-4.4253800	0.9502260	1.4586000
H	-3.7695330	2.0000970	0.2002040
C	-6.7774540	0.2248980	0.0759150
H	-6.8445240	-1.8814680	-0.4691930
H	-6.2034010	-0.8327130	-1.7242520
H	-6.2468700	2.2997170	0.4680850
H	-5.8359960	1.7431680	-1.1471230
H	-7.7764790	0.4543640	-0.3088280
H	-6.8987060	0.0028000	1.1450280
C	0.1119000	1.6579530	0.8521370
H	-0.0037420	2.1322180	1.8289940

H	-0.7945920	1.8766580	0.2717910
C	0.4292080	-1.7837220	2.3225300
H	1.4471940	-2.1535920	2.4722040
H	-0.1799340	-2.1720760	3.1419070
C	-0.1236780	-2.1266600	0.9288370
H	0.4434760	-2.9091900	0.4248340
H	-1.1575400	-2.4725870	0.9879440
H	0.2476800	0.7446120	-1.9633780
O	0.7015620	0.4438180	3.3440110
H	1.7369700	0.3317410	-2.5320810
H	-0.1894160	-1.4388660	-2.2860640

$TS2_6$

-1360,056683 (gas phase), -1360,123294 (ethanol)

1

C	0.1606060	0.4945500	2.6163510
C	2.1136090	1.3335580	-1.2366190
C	1.8681640	2.1516060	-0.1234250
C	3.2540860	1.5195380	-2.0193910
C	4.1600020	2.5334320	-1.7126180
C	3.9356210	3.3484190	-0.6048410
C	2.8017920	3.1477230	0.1819210
H	3.4390550	0.8692200	-2.8708510
H	5.0397260	2.6737990	-2.3316840
H	4.6390690	4.1340610	-0.3504470
H	2.6283130	3.7805580	1.0473530
N	0.3635910	0.6731090	1.2438520
N	1.1671980	0.2992120	-1.6252440
C	-0.0490160	-0.4655630	0.4335900
C	0.9541950	-0.8967600	-0.7108370
C	-1.3712930	-0.0616930	-0.2752580
N	-2.5442570	-0.3170680	0.2487610
H	-2.5671220	-0.8972760	1.0780990
O	0.1856680	-1.8403050	-1.4489120
O	-1.3177780	0.6546290	-1.3533020
C	2.2656630	-1.5387090	-0.2624040
C	3.0937510	-0.9581810	0.7137330
C	2.6797010	-2.7297640	-0.8772740
C	4.3047300	-1.5581160	1.0575680
H	2.8053910	-0.0413570	1.2102160
C	3.8952210	-3.3212810	-0.5337050
H	2.0411390	-3.2017590	-1.6135060
C	4.7118480	-2.7381240	0.4344010
H	4.9303700	-1.0972710	1.8153680
H	4.1971840	-4.2433250	-1.0203230
H	5.6556810	-3.2008070	0.7048590
C	-3.8579780	0.1290610	-0.2854580
C	-4.4738690	-0.9612820	-1.1785060
C	-4.7776230	0.4977380	0.8874470
H	-3.6525410	1.0187370	-0.8869440
C	-5.8589480	-0.5243880	-1.6840370
H	-4.5693280	-1.8873600	-0.5951840
H	-3.8017850	-1.1751170	-2.0165780
C	-6.1652810	0.9220520	0.3769990
H	-4.8865270	-0.3781060	1.5447170
H	-4.3232750	1.2967780	1.4836980
C	-6.7922900	-0.1525170	-0.5229050
H	-6.2939250	-1.3285380	-2.2858800
H	-5.7435320	0.3384360	-2.3537030
H	-6.8130970	1.1361810	1.2326860
H	-6.0692870	1.8615640	-0.1832620
H	-7.7529690	0.1997320	-0.9117450
H	-7.0072560	-1.0491850	0.0741480

C	0.6178560	2.0186360	0.7178170
H	0.6981510	2.6522230	1.6031150
H	-0.2571120	2.3664550	0.1516400
C	-0.3499530	-0.9208540	2.8405950
H	0.2349380	-1.4088150	3.6227320
H	-1.3767010	-0.8500170	3.2180220
C	-0.2315450	-1.6114950	1.4741370
H	0.6615500	-2.2349520	1.4456320
H	-1.0646630	-2.2687030	1.2175710
H	-0.2941840	0.6929290	-1.6505220
O	0.3450630	1.3545880	3.4492780
H	1.5078820	-0.0841590	-2.5081320
H	0.0512080	-1.5575100	-2.3628790

6int$_2$H$^+$

-1360,065329 (gas phase), -1360,130523 (ethanol)

0

C	1.2709490	-1.2419310	2.1033640
C	0.3949130	2.3450440	-0.2799330
C	-0.2326030	2.0458950	0.9445000
C	-0.1323910	3.3300880	-1.1207370
C	-1.2826390	4.0249520	-0.7476220
C	-1.9216840	3.7230070	0.4559490
C	-1.3989880	2.7344040	1.2914850
H	0.3667340	3.5580860	-2.0583000
H	-1.6801100	4.7969650	-1.3984980
H	-2.8150610	4.2640250	0.7501330
H	-1.8799760	2.5201760	2.2420960
N	0.6418470	-0.2748990	1.3118070
N	1.6166790	1.6817360	-0.5817360
C	0.6617590	-0.5694530	-0.1059140
C	1.7486320	0.2992510	-0.8916260
C	-0.7673050	-0.4347900	-0.6858740
N	-1.7909910	-0.6604280	0.0929890
H	-1.5666840	-0.8118790	1.0720200
O	1.4298600	-0.0073420	-2.3117940
O	-0.9819090	-0.2283750	-1.9467430
C	3.1926450	-0.1398010	-0.6338200
C	3.8849650	0.3539930	0.4826240
C	3.8478300	-1.0349150	-1.4949660
C	5.1957160	-0.0481190	0.7387850
H	3.4030690	1.0614770	1.1467020
C	5.1615420	-1.4288020	-1.2396990
H	3.3371660	-1.4204260	-2.3702080
C	5.8373580	-0.9407830	-0.1206720
H	5.7146440	0.3410830	1.6087940
H	5.6560180	-2.1155690	-1.9192730
H	6.8586100	-1.2500550	0.0774040
C	-3.2135250	-0.7180010	-0.3280040
C	-3.6008260	-2.1517200	-0.7304550
C	-4.0971590	-0.1823630	0.8064000
H	-3.2982100	-0.0621920	-1.1995330
C	-5.0885740	-2.2212270	-1.1139280
H	-3.4061920	-2.8231230	0.1170060
H	-2.9712340	-2.4856740	-1.5625630
C	-5.5841890	-0.2651600	0.4222080
H	-3.9220360	-0.7845080	1.7104720
H	-3.8138960	0.8493320	1.0406110
C	-5.9871600	-1.6885530	0.0113320
H	-5.3500790	-3.2552960	-1.3598000
H	-5.2540930	-1.6330310	-2.0265970
H	-6.1934040	0.0806420	1.2632420
H	-5.7793700	0.4263600	-0.4083100

H	-7.0348160	-1.7038580	-0.3056890
H	-5.9149050	-2.3543200	0.8820490
C	0.4204830	1.0704490	1.8915590
H	1.3898560	1.4667860	2.2173910
H	-0.1790070	0.9424690	2.7958370
C	1.6426430	-2.4177370	1.2140480
H	2.7334470	-2.4661720	1.1574000
H	1.2944710	-3.3529150	1.6578890
C	0.9986970	-2.1126810	-0.1452720
H	1.6370360	-2.3452350	-0.9951210
H	0.0734350	-2.6815320	-0.2630790
H	-0.0772910	-0.0625740	-2.3799750
O	1.4689490	-1.1012090	3.2898220
H	2.3531220	2.2624970	-0.9618700
H	2.0042670	0.5227140	-2.8843060

$TS3_6$

-1360,051725 (gas phase), -1360,118813 (ethanol)

1

C	-5.6991920	-1.3020840	-0.3752220
C	-5.2249280	-2.5703470	-0.7076890
C	-3.8519220	-2.7843740	-0.7919470
C	-4.7986460	-0.2686270	-0.1434300
H	-6.7644120	-1.1138740	-0.2931330
H	-5.9151610	-3.3879820	-0.8848600
H	-3.4757750	-3.7759160	-1.0265500
H	-5.1710440	0.7198110	0.1162290
C	-3.4168070	-0.4832810	-0.2424660
C	-2.9268030	-1.7592660	-0.5668790
C	-1.3029550	0.9479910	-0.2607000
C	-0.2533990	-0.0313830	0.3711940
C	-0.5660830	-2.0255410	1.6646080
N	-0.7130670	-1.4095610	0.4251590
O	-0.8801920	-3.1714150	1.8987400
C	0.0544130	-1.0107740	2.6172710
H	1.0957570	-1.2936870	2.8107970
H	-0.4609720	-1.0448200	3.5786330
C	-0.1128540	0.3323830	1.8905220
H	0.6771540	1.0640830	2.0677110
H	-1.0475880	0.7934760	2.2120810
C	-1.4480580	-2.0712440	-0.6456130
H	-1.2946240	-3.1438420	-0.5123360
H	-1.0215350	-1.7876240	-1.6117080
N	-2.6149000	0.6859040	-0.0128980
C	-0.9472390	2.4150300	-0.1105660
C	0.1114280	2.9957290	-0.8311290
C	-1.6590190	3.2158900	0.8008340
C	0.4254260	4.3437640	-0.6627040
H	0.6941130	2.4096200	-1.5317290
C	-1.3393010	4.5629400	0.9643980
H	-2.4511410	2.7898010	1.4079980
C	-0.2994870	5.1328830	0.2304460
H	1.2376650	4.7763470	-1.2377830
H	-1.9025100	5.1624500	1.6720460
H	-0.0530420	6.1819970	0.3566100
C	1.1149160	-0.0422790	-0.3928880
N	2.2350150	-0.1692400	0.3077520
H	2.1799840	-0.2109410	1.3152020
C	3.5742210	-0.3728020	-0.2913470
C	4.6315500	0.3169000	0.5815190
C	3.8739300	-1.8704400	-0.4760860
H	3.5384320	0.1074870	-1.2733890
C	6.0418880	0.1003880	0.0075210

H	4.5877230	-0.1033830	1.5979440
H	4.4081300	1.3867030	0.6652730
C	5.2845510	-2.0757330	-1.0523340
H	3.7974290	-2.3720320	0.4986630
H	3.1181080	-2.3178640	-1.1301980
C	6.3526650	-1.3905890	-0.1879570
H	6.7785570	0.5644750	0.6711510
H	6.1202510	0.6208340	-0.9564670
H	5.4889990	-3.1476920	-1.1390870
H	5.3210120	-1.6688680	-2.0720090
H	7.3407030	-1.5102410	-0.6441660
H	6.3998860	-1.8842150	0.7924040
O	1.1482870	-0.0332970	-1.6544180
O	-1.1126880	0.6193310	-2.0156410
H	-0.0693990	0.3256780	-2.0678270
H	-1.2727120	1.4435640	-2.5027760
H	-3.1863460	1.5191830	-0.0844090

6aH$^+$

-1360,083393 (gas phase), -1360,148792 (ethanol)

0

C	3.3745290	3.6975840	-1.4414750
C	2.4369140	4.5717790	-0.8917200
C	1.3357240	4.0603490	-0.2094190
C	3.1981440	2.3280870	-1.3019450
H	4.2428590	4.0771180	-1.9688630
H	2.5647190	5.6451010	-0.9847490
H	0.6143360	4.7426100	0.2302080
H	3.9300180	1.6434080	-1.7178480
C	2.0789700	1.8132770	-0.6186730
C	1.1242520	2.6859110	-0.0629310
C	1.3517030	-0.5666020	-0.0071110
C	0.0622530	-0.3106910	0.8030480
C	0.3901330	1.0321530	2.7603810
N	0.0351300	1.0065350	1.4085050
O	0.5007870	2.0467710	3.4126990
C	0.5901960	-0.4112020	3.1989800
H	0.1314960	-0.5799120	4.1747860
H	1.6654310	-0.5949020	3.3090410
C	-0.0327210	-1.2369850	2.0674640
H	-1.0908250	-1.4198770	2.2688150
H	0.4426920	-2.2022610	1.9081670
C	-0.1249330	2.2325300	0.6525230
H	-0.4188400	2.9993180	1.3732420
H	-0.9490910	2.1114110	-0.0601630
N	2.0685890	0.3818560	-0.5605320
C	1.9401730	-1.9262230	-0.1009120
C	1.2064170	-3.0481990	-0.5282100
C	3.2848770	-2.0904330	0.2925070
C	1.8188370	-4.2982710	-0.5776560
H	0.1850850	-2.9191450	-0.8630570
C	3.8816600	-3.3492520	0.2554210
H	3.8498120	-1.2395420	0.6625650
C	3.1504860	-4.4548730	-0.1844670
H	1.2525790	-5.1545720	-0.9294210
H	4.9097910	-3.4673560	0.5827730
H	3.6147240	-5.4354860	-0.2147020
C	-1.1219870	-0.5314430	-0.1897990
N	-2.3329640	-0.1558730	0.2637460
H	-2.3921260	0.2659760	1.1821250
C	-3.5827240	-0.3090290	-0.5016630
C	-4.5231850	-1.3106180	0.1898270
C	-4.2640690	1.0534940	-0.7055210

H	-3.2772470	-0.7106280	-1.4722870
C	-5.8459290	-1.4545770	-0.5805520
H	-4.7318310	-0.9573410	1.2104790
H	-4.0212300	-2.2802630	0.2837570
C	-5.5886960	0.9039620	-1.4719940
H	-4.4619450	1.5052310	0.2780080
H	-3.5849510	1.7294890	-1.2383480
C	-6.5303750	-0.0957940	-0.7854250
H	-6.5085530	-2.1428470	-0.0454360
H	-5.6444740	-1.9130960	-1.5582470
H	-6.0695130	1.8832980	-1.5665240
H	-5.3756900	0.5619240	-2.4939030
H	-7.4438050	-0.2188850	-1.3767380
H	-6.8410630	0.3061480	0.1889160
O	-0.8993070	-1.0194000	-1.2976150
O	3.9622090	-0.6071990	-2.4354350
H	3.6271760	-0.6728970	-3.3400790
H	4.3830840	-1.4577570	-2.2514360
H	2.8286780	-0.0028870	-1.1543690

B_7H$^+$

-1360,061197 (gas phase), -1360,129459 (ethanol)

0

C	2.9680530	0.5811030	-2.0526090
C	2.7419930	-1.9001450	1.3012170
C	1.7816410	-2.0076330	0.2673100
C	2.5067600	-2.5675970	2.5138590
C	1.3521000	-3.3194060	2.7054580
C	0.3954740	-3.4179930	1.6921340
C	0.6236430	-2.7679260	0.4824110
H	3.2440680	-2.4922840	3.3087020
H	1.1987500	-3.8305530	3.6509910
H	-0.4977390	-4.0173540	1.8325840
H	-0.0874710	-2.8808180	-0.3312590
N	2.0378560	-0.0589190	-1.4078860
N	3.9292170	-1.1915710	1.0718020
C	0.8871600	0.8447640	-1.0744750
C	1.1325940	1.4243620	0.3554100
C	-0.4171320	0.0507600	-1.4359770
N	-1.3319010	-0.1660880	-0.4783930
H	-1.1741070	0.1845300	0.4556280
O	2.2440330	1.2647770	0.8439950
O	-0.5063420	-0.3537340	-2.5913920
C	0.1119510	2.2521900	1.0535900
C	-1.0299670	2.7972510	0.4325950
C	0.3594670	2.5480480	2.4090970
C	-1.8963410	3.6158010	1.1526870
H	-1.2524980	2.5944820	-0.6084220
C	-0.5180490	3.3516730	3.1268220
H	1.2456880	2.1354470	2.8773560
C	-1.6455030	3.8897340	2.4992870
H	-2.7660630	4.0409970	0.6626980
H	-0.3234660	3.5640160	4.1729470
H	-2.3270060	4.5233140	3.0582550
C	-2.5868990	-0.8999890	-0.7340520
C	-3.1530170	-1.4190270	0.5941190
C	-3.6139750	-0.0288260	-1.4790950
H	-2.3239990	-1.7482000	-1.3774380
C	-4.4660460	-2.1862780	0.3693400
H	-3.3427170	-0.5620560	1.2581450
H	-2.4130890	-2.0540220	1.0947190
C	-4.9221570	-0.8023270	-1.7073230
H	-3.8149520	0.8683570	-0.8768440

H	-3.1881490	0.3006820	-2.4320090
C	-5.4981070	-1.3382200	-0.3887850
H	-4.8692270	-2.5111370	1.3342380
H	-4.2538750	-3.0998630	-0.2025160
H	-5.6490950	-0.1549200	-2.2090070
H	-4.7305760	-1.6404700	-2.3912110
H	-6.3993880	-1.9295330	-0.5821320
H	-5.8088150	-0.4940490	0.2425470
C	2.0981200	-1.5370190	-1.1283820
H	3.1165030	-1.8285050	-1.3907320
H	1.4012140	-1.9776490	-1.8447540
C	2.6252650	2.0096770	-2.3332570
H	3.1660390	2.6519990	-1.6270090
H	2.9109250	2.3032620	-3.3478460
C	1.1050540	2.0047140	-2.0991400
H	0.7348920	2.9622640	-1.7352240
H	0.5830760	1.7335210	-3.0193990
H	4.6732900	0.5647680	-2.8899350
O	4.0789930	-0.0249870	-2.4006330
H	4.5603030	-1.2166970	1.8643540
H	3.7553070	-0.2280860	0.8047120

$TS1_7$

-1360,046112 (gas phase), -1360,112485 (ethanol)

1

C	-2.5019510	0.5307950	1.4516930
C	-4.2578750	-0.1581000	-0.2333410
C	-3.3153410	-1.0415580	-0.7560030
C	-5.6212160	-0.2588890	-0.4922130
C	-6.0711960	-1.2814840	-1.3229360
C	-5.1529510	-2.1826190	-1.8676300
C	-3.7951480	-2.0665830	-1.5799500
H	-6.3226870	0.4471100	-0.0553870
H	-7.1298390	-1.3757450	-1.5378670
H	-5.4984900	-2.9837200	-2.5124280
H	-3.0916900	-2.7820040	-1.9960790
N	-1.5527710	0.1188030	0.5168730
N	-3.7759500	0.9404530	0.6364270
C	-0.2238240	0.6905550	0.7039710
C	0.0484950	1.7103670	-0.4492570
C	0.7283080	-0.5423830	0.9111070
N	1.7054110	-0.7670840	0.0109320
H	1.9257930	-0.0479610	-0.6649610
O	-0.8861770	1.9710910	-1.1980900
O	0.4589010	-1.3011280	1.8410760
C	1.3598380	2.4055890	-0.5987520
C	2.3991580	2.3368380	0.3501580
C	1.5350540	3.2052160	-1.7449310
C	3.5794280	3.0503680	0.1527940
H	2.2988200	1.7350680	1.2463300
C	2.7185390	3.9067030	-1.9426280
H	0.7260050	3.2597890	-2.4645830
C	3.7419720	3.8322230	-0.9929350
H	4.3703720	2.9984620	0.8939210
H	2.8451370	4.5146560	-2.8325930
H	4.6642770	4.3843600	-1.1445840
C	2.6520410	-1.8908510	0.1260910
C	3.0757470	-2.3634300	-1.2716380
C	3.8699570	-1.5047120	0.9846500
H	2.1030240	-2.6905370	0.6330090
C	4.0924970	-3.5139370	-1.1833110
H	3.5312460	-1.5201740	-1.8128370
H	2.1927670	-2.6700140	-1.8443020

C	4.8821550	-2.6579120	1.0679820
H	4.3509310	-0.6238560	0.5356500
H	3.5292970	-1.2155540	1.9849680
C	5.3095400	-3.1319060	-0.3282490
H	4.4060290	-3.8033680	-2.1919030
H	3.6018300	-4.3936410	-0.7451180
H	5.7540730	-2.3416230	1.6504730
H	4.4302890	-3.4958800	1.6160430
H	5.9928750	-3.9838090	-0.2463590
H	5.8689320	-2.3299800	-0.8299170
C	-1.8376700	-0.9364340	-0.4424750
H	-1.2978160	-0.7050360	-1.3673120
H	-1.4740500	-1.9111270	-0.0855210
C	-1.8883040	1.7552140	2.1403890
H	-2.1301660	2.6735730	1.5930720
H	-2.2555390	1.8513030	3.1633810
C	-0.3835080	1.4582780	2.0551050
H	0.2173530	2.3665340	2.1016400
H	-0.0807310	0.7880230	2.8624230
H	-3.4915740	1.7432240	0.0636560
O	-3.0149640	-0.4488010	2.3079210
H	-2.2774060	-1.0420480	2.5264590
H	-4.5204410	1.2313870	1.2776860

7int$_1$H$^+$

-1360,052761 (gas phase), -1360,119277 (ethanol)

0

C	2.3420340	-0.6530710	1.4353560
C	4.3161410	0.0592150	-0.0002550
C	3.3997160	0.7032020	-0.8260600
C	5.6927120	0.2443300	-0.0956520
C	6.1847540	1.1124150	-1.0660430
C	5.2936700	1.7736920	-1.9155100
C	3.9215960	1.5724540	-1.7926200
H	6.3719990	-0.2778660	0.5732250
H	7.2536230	1.2710480	-1.1563950
H	5.6714050	2.4503460	-2.6747540
H	3.2368880	2.0959940	-2.4534480
N	1.5887030	-0.5799330	0.2252420
N	3.8081300	-0.8998710	1.0169080
C	0.1778970	-0.9248130	0.4905330
C	-0.3821540	-1.7199010	-0.7307730
C	-0.5765660	0.4119340	0.8202380
N	-1.6348530	0.7701750	0.0813930
H	-2.0000630	0.1184320	-0.6009030
O	0.3012170	-1.7833710	-1.7403510
O	-0.1129290	1.1276140	1.7235150
C	-1.7167100	-2.3944730	-0.6697030
C	-2.5924370	-2.3337920	0.4316910
C	-2.1002250	-3.1385820	-1.8023750
C	-3.8152500	-3.0007900	0.3969350
H	-2.3390990	-1.7629490	1.3177140
C	-3.3191340	-3.8055720	-1.8315350
H	-1.4204830	-3.1790630	-2.6460070
C	-4.1790980	-3.7387370	-0.7312840
H	-4.4824790	-2.9465720	1.2510580
H	-3.6015990	-4.3776760	-2.7093930
H	-5.1311140	-4.2599610	-0.7532480
C	-2.3653530	2.0403310	0.2467400
C	-2.5380860	2.7198590	-1.1209240
C	-3.7200490	1.8221340	0.9425210
H	-1.7318750	2.6606480	0.8866900
C	-3.3139610	4.0400050	-0.9894040

H	-3.0867890	2.0412490	-1.7910990
H	-1.5557740	2.8914320	-1.5757560
C	-4.4923900	3.1457260	1.0693900
H	-4.3119900	1.1050060	0.3558570
H	-3.5561650	1.3735830	1.9287920
C	-4.6663490	3.8337090	-0.2923730
H	-3.4555760	4.4817310	-1.9813650
H	-2.7113640	4.7550620	-0.4130060
H	-5.4666600	2.9582930	1.5328890
H	-3.9482880	3.8152100	1.7494040
H	-5.1753990	4.7950510	-0.1663690
H	-5.3146760	3.2183900	-0.9314680
C	1.9060210	0.5305390	-0.6741350
H	1.4648720	0.3008000	-1.6459100
H	1.4835740	1.4819260	-0.3159680
C	1.7615520	-1.8755970	2.1526280
H	2.1956900	-2.8024720	1.7618860
H	1.9498990	-1.8242720	3.2261490
C	0.2634450	-1.7947980	1.7981420
H	-0.1599510	-2.7871150	1.6456260
H	-0.2906370	-1.3103330	2.6033900
H	3.8786730	-1.8574060	0.6593620
O	2.4481440	0.4929310	2.2052270
H	1.5394820	0.8922840	2.2115740
H	4.3778820	-0.8273070	1.8663720

$TS2_7$

-1360,024943 (gas phase), -1360,086982 (ethanol)

1

C	1.2106480	-1.6028940	-1.3588290
C	3.2343990	-1.9253160	0.1592040
C	2.5881620	-1.2062100	1.1691460
C	4.5744540	-2.2934320	0.2588620
C	5.2886630	-1.9481250	1.4049210
C	4.6619580	-1.2365540	2.4295280
C	3.3242330	-0.8625690	2.3054630
H	5.0529940	-2.8529540	-0.5405950
H	6.3314850	-2.2332040	1.4933240
H	5.2175940	-0.9640820	3.3204880
H	2.8445620	-0.2936490	3.0965930
N	0.8975500	-0.5830580	-0.4412540
N	2.4581600	-2.3639390	-0.9869070
C	-0.2500560	0.1836640	-0.9295480
C	-0.1662360	1.7097680	-0.6113230
C	-1.5771790	-0.5078800	-0.4292030
N	-2.6910570	0.1951070	-0.3180830
H	-2.5994150	1.1985260	-0.4766150
O	-1.2096030	2.3547750	-0.6672910
O	-1.5488450	-1.7460510	-0.1956590
C	1.1054040	2.4239020	-0.3021370
C	2.3953470	1.9963940	-0.6681580
C	0.9619400	3.6695730	0.3443460
C	3.5042130	2.7933700	-0.3935420
H	2.5356600	1.0525470	-1.1739400
C	2.0739290	4.4494220	0.6365600
H	-0.0335190	4.0078570	0.6076460
C	3.3490670	4.0143570	0.2648430
H	4.4921520	2.4604960	-0.6952700
H	1.9481470	5.3994190	1.1456900
H	4.2179790	4.6271870	0.4838510
C	-3.9871230	-0.3705550	0.1023780
C	-4.1585460	-0.2751660	1.6292280
C	-5.1234140	0.3483560	-0.6390550

H	-3.9696980	-1.4260110	-0.1861440
C	-5.5317360	-0.8110300	2.0643330
H	-4.0594950	0.7770020	1.9302500
H	-3.3521200	-0.8301940	2.1211290
C	-6.4949300	-0.1868070	-0.1959720
H	-5.0664580	1.4252930	-0.4231840
H	-4.9944600	0.2318000	-1.7211590
C	-6.6743720	-0.0985480	1.3265920
H	-5.6428510	-0.6966590	3.1478380
H	-5.5804610	-1.8891480	1.8589500
H	-7.2859420	0.3695420	-0.7095020
H	-6.5936090	-1.2333380	-0.5150490
H	-7.6381400	-0.5299270	1.6169490
H	-6.7006830	0.9573420	1.6291870
C	1.1397640	-0.8108920	0.9876810
H	0.9481740	0.1272160	1.5142490
H	0.4556320	-1.5651190	1.4033790
C	1.0601430	-0.9551210	-2.7244000
H	1.9597460	-0.3817830	-2.9656370
H	0.8865800	-1.6951890	-3.5069460
C	-0.1559440	-0.0232510	-2.5014850
H	-0.0395820	0.9304940	-3.0180610
H	-1.0738010	-0.4830530	-2.8715810
H	3.0465740	-2.5575960	-1.7972330
O	0.3752240	-2.8291320	-1.2547160
H	-0.4996700	-2.5276700	-0.7302860
H	1.4891300	-3.2253830	-0.8498940

7int$_2$H$^+$

-1360,064741 (gas phase), -1360,122841 (ethanol)

0

C	-1.5389170	-0.9195540	1.5460420
C	-3.2439760	-1.9380180	0.1495480
C	-2.4126650	-1.8250410	-0.9760170
C	-4.4273990	-2.6848590	0.0768930
C	-4.7819340	-3.3169610	-1.1099620
C	-3.9588120	-3.2159510	-2.2348850
C	-2.7839800	-2.4736920	-2.1585710
H	-5.0677460	-2.7607570	0.9518270
H	-5.7014800	-3.8913510	-1.1553710
H	-4.2319830	-3.7091950	-3.1613050
H	-2.1410910	-2.3893000	-3.0312400
N	-0.9944890	-0.3305170	0.3593220
N	-2.9008340	-1.2642080	1.3469370
C	0.1495530	0.5200190	0.6358820
C	0.1160800	1.8692860	-0.1653770
C	1.4678120	-0.2936700	0.4593290
N	2.5392400	0.1755170	-0.1100710
H	2.4239170	1.1360540	-0.4622340
O	1.1703680	2.3037810	-0.6301220
O	1.5080450	-1.5033190	0.9386410
C	-1.1155140	2.6994930	-0.2676300
C	-2.4290680	2.2859920	0.0380600
C	-0.9109690	4.0253170	-0.7123710
C	-3.4921250	3.1767540	-0.0928160
H	-2.6309510	1.2710720	0.3461400
C	-1.9758090	4.9072780	-0.8348730
H	0.0963260	4.3452170	-0.9503950
C	-3.2718160	4.4854620	-0.5239980
H	-4.4985490	2.8418380	0.1366380
H	-1.7982360	5.9234840	-1.1714260
H	-4.1059130	5.1734980	-0.6215030
C	3.8306250	-0.5365240	-0.2534140

C	4.4674580	-0.1610630	-1.5996350
C	4.7580290	-0.2031880	0.9294670
H	3.6029360	-1.6061810	-0.2400470
C	5.8335930	-0.8478390	-1.7618780
H	4.5994250	0.9294660	-1.6413200
H	3.7961510	-0.4361280	-2.4207900
C	6.1217770	-0.8915120	0.7575730
H	4.8954890	0.8854570	0.9756790
H	4.2844830	-0.5116340	1.8680460
C	6.7707230	-0.5324970	-0.5871170
H	6.2840410	-0.5352670	-2.7092450
H	5.6850030	-1.9339000	-1.8312670
H	6.7762210	-0.6096260	1.5886690
H	5.9882400	-1.9798800	0.8219380
H	7.7150760	-1.0736320	-0.7050190
H	7.0203510	0.5372130	-0.5972000
C	-1.1269880	-1.0216610	-0.9227860
H	-0.2655580	-1.6836970	-1.1198520
H	-1.1296520	-0.2658250	-1.7182640
C	-1.2787870	0.1247780	2.6305310
H	-2.1212840	0.8179730	2.6438490
H	-1.1817330	-0.3369770	3.6140640
C	0.0141120	0.8359640	2.1817240
H	-0.0327140	1.9124180	2.3532310
H	0.8859490	0.4609090	2.7220170
H	-1.1274580	-2.9100810	1.5160300
O	-0.7373020	-2.1331680	1.9483850
H	-3.3715460	-1.5978010	2.1790890
H	0.6299630	-1.8171450	1.3683930

TS3$_7$

-1360,064617 (gas phase), -1360,121892 (ethanol)

1

C	-1.5189780	-0.9511550	1.5972550
C	-3.1941630	-1.9357180	0.1401790
C	-2.3986530	-1.6706980	-0.9830090
C	-4.3817310	-2.6646440	0.0156490
C	-4.7775410	-3.1344170	-1.2328870
C	-3.9931230	-2.8802650	-2.3605710
C	-2.8135600	-2.1517850	-2.2282540
H	-4.9920010	-2.8556210	0.8943520
H	-5.6994760	-3.6991950	-1.3238650
H	-4.2998470	-3.2448000	-3.3348460
H	-2.2021370	-1.9501480	-3.1039900
N	-0.9663480	-0.3195730	0.4869170
N	-2.8017900	-1.4322930	1.4040360
C	0.1725780	0.5272030	0.8303680
C	0.1353440	1.9209980	0.1147880
C	1.4967380	-0.2836650	0.6182360
N	2.6007950	0.2838440	0.1955140
H	2.5071760	1.2754340	-0.0416330
O	1.2102650	2.4655260	-0.1302800
O	1.4904890	-1.5241940	0.9233790
C	-1.1290650	2.6482530	-0.1926240
C	-2.4300760	2.2601690	0.1873050
C	-0.9684710	3.8592010	-0.9022220
C	-3.5242660	3.0609040	-0.1313410
H	-2.6024720	1.3364440	0.7178290
C	-2.0647680	4.6473890	-1.2249290
H	0.0307950	4.1637170	-1.1890780
C	-3.3481390	4.2512380	-0.8380230
H	-4.5190460	2.7501330	0.1711220
H	-1.9211040	5.5716700	-1.7749200

H	-4.2065130	4.8674590	-1.0869850
C	3.8980360	-0.4053190	0.0317400
C	4.0761370	-0.8940640	-1.4169480
C	5.0319300	0.5407800	0.4535670
H	3.8739800	-1.2714430	0.6995420
C	5.4481910	-1.5624680	-1.6012660
H	3.9886860	-0.0340700	-2.0949230
H	3.2689760	-1.5901990	-1.6709560
C	6.4019250	-0.1301990	0.2617950
H	4.9839470	1.4526850	-0.1589640
H	4.8938420	0.8467840	1.4966650
C	6.5924980	-0.6304070	-1.1773500
H	5.5673200	-1.8678950	-2.6460030
H	5.4843940	-2.4823230	-1.0018470
H	7.1930180	0.5768710	0.5314660
H	6.4896900	-0.9753600	0.9579240
H	7.5529640	-1.1478650	-1.2705570
H	6.6341180	0.2296730	-1.8597480
C	-1.1047310	-0.8917000	-0.8551140
H	-1.0955180	-0.0650600	-1.5748210
H	-0.2447740	-1.5376790	-1.0934710
C	-1.2514760	-0.0492760	2.7908230
H	-2.1122170	0.6119580	2.9166870
H	-1.1158180	-0.6252260	3.7063760
C	0.0112090	0.7440650	2.3899280
H	-0.0864650	1.8048360	2.6255550
H	0.8961850	0.3775080	2.9129030
H	-3.2702190	-1.8061780	2.2178950
O	-0.5308460	-2.2862130	1.9681040
H	0.5170220	-1.9589160	1.4423260
H	-0.8974390	-3.0645090	1.5184770

7aH$^+$

-1360,099057 (gas phase), -1360,161549 (ethanol)

0

C	2.4911820	-1.1734520	0.8682720
C	4.2867220	0.0466860	-0.1585000
C	3.3678270	0.8431190	-0.8467260
C	5.6617710	0.2337010	-0.2923120
C	6.1332590	1.2406280	-1.1315340
C	5.2320220	2.0470290	-1.8280210
C	3.8589530	1.8455320	-1.6833300
H	6.3544900	-0.4007280	0.2535000
H	7.2017490	1.3922780	-1.2397440
H	5.5957010	2.8314770	-2.4828390
H	3.1607010	2.4758610	-2.2269660
N	1.5768300	-0.4610350	0.2411080
N	3.7878390	-0.9764450	0.6889710
C	0.1918040	-0.9095370	0.5370720
C	-0.3155700	-1.7416620	-0.6852260
C	-0.6065540	0.3930890	0.8951720
N	-1.5817250	0.7807140	0.0565140
H	-1.8805130	0.1519990	-0.6773730
O	0.4454400	-1.8784620	-1.6317090
O	-0.2468640	1.0504990	1.8740710
C	-1.6616940	-2.3828800	-0.6736160
C	-2.5732560	-2.2970030	0.3974130
C	-2.0159730	-3.1308340	-1.8135820
C	-3.8038150	-2.9452060	0.3255430
H	-2.3393740	-1.7261250	1.2891750
C	-3.2456400	-3.7749140	-1.8805870
H	-1.3067990	-3.1935210	-2.6312640
C	-4.1410870	-3.6843970	-0.8107400

H	-4.4982300	-2.8759460	1.1564490
H	-3.5079710	-4.3488220	-2.7633750
H	-5.1006060	-4.1895050	-0.8618480
C	-2.3464760	2.0310280	0.2175030
C	-2.5261190	2.7012440	-1.1531660
C	-3.6999920	1.7861310	0.9074330
H	-1.7327360	2.6688740	0.8603150
C	-3.3303490	4.0051290	-1.0312790
H	-3.0576000	2.0086820	-1.8232210
H	-1.5456700	2.8924400	-1.6045770
C	-4.4998280	3.0941420	1.0257890
H	-4.2727450	1.0544450	0.3200880
H	-3.5302670	1.3453000	1.8960770
C	-4.6813040	3.7736460	-0.3393170
H	-3.4766420	4.4388970	-2.0260050
H	-2.7453580	4.7354640	-0.4559850
H	-5.4722900	2.8884900	1.4852730
H	-3.9731070	3.7770680	1.7061520
H	-5.2100880	4.7249900	-0.2191980
H	-5.3142980	3.1433840	-0.9791790
C	1.8739390	0.6355450	-0.6957700
H	1.4168800	0.3861340	-1.6579690
H	1.4013760	1.5460750	-0.3095630
C	1.8879600	-2.2352510	1.7286960
H	2.0332090	-3.2106320	1.2493250
H	2.3557800	-2.2476430	2.7145120
C	0.4068570	-1.8145940	1.7897930
H	-0.2634770	-2.6724420	1.7947920
H	0.2416300	-1.2142440	2.6847040
H	4.4372510	-1.5030590	1.2565030
O	2.1908870	0.3961130	3.1924700
H	1.3692750	0.8089670	2.8707170
H	2.3955850	0.8425050	4.0228310