Supporting Information

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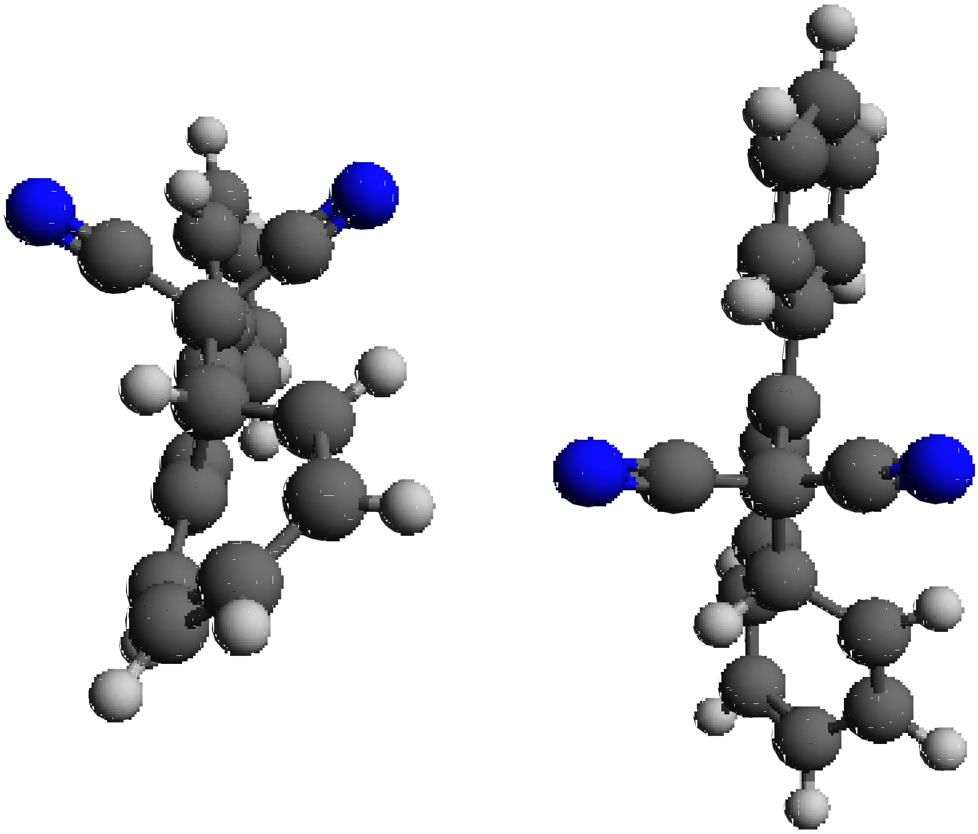
Two different views of the calculated geometries for DHA **1**, showing the different steric hindrances of the two CN



SUPPORTING INFORMATION

Table S1: Optimization of hydrolysis conditions. Amide **10a** is the only diastereomer formed and imidate **11** is formed as single diastereomer **11b** or mixture. When the second diastereoisomer **11a** (minor) was also formed, the ratio **11b**/**11a** is reported in brackets.

Conditions	**amide 10a**	**imidate 11**
CsF/THF-MeOH reflux 16h	65%	31% (11b)
KF/THF-MeOH reflux 16h	61%	32% (mix 19/1 11b/11a)
CsF/THF-MeOH r.t. 2d	50%	37% (mix 10/1 of 11b/11a)
Aq.NH_3/THF-MeOH 70°C 24h	46%	18% (11b)
KF 40% on Al_2O_3, *t*BuOH 80 °C 12h	not found	-

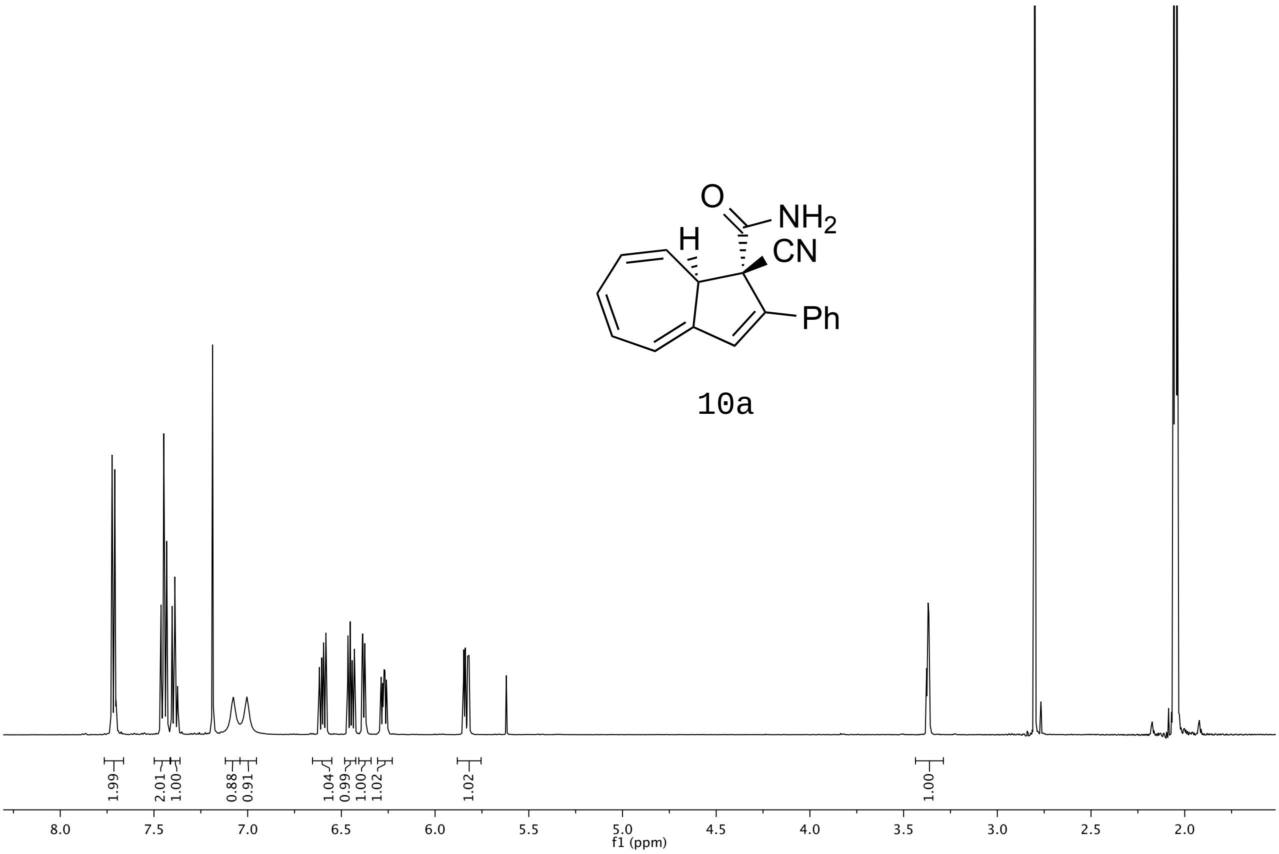
2-Phenylazulene-1-carboxamide; R_f = 0.18 (2% acetone/CH_2Cl_2). M.p. = 195-198 °C. IR: 3375, 3171, 1685, 1634, 1618sh, 1604 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 9.39 (d, *J* = 9.7 Hz, 1H), 8.40 (d, *J* = 9.7 Hz, 1H), 7.75–7.67 (m, 3H), 7.50–7.47 (m, 3H), 7.44–7.40 (m, 1H), 7.37 (dd, *J* = 9.7, 9.7 Hz, 1H), 7.33 (s, 1H), 5.69 (br s, 1H), 5.49 (br s, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ = 168.77, 150.13, 141.94, 140.99, 138.64, 137.90, 137.73, 136.83, 129.99, 128.89, 128.48, 127.29, 126.33, 118.40, 118.35 ppm. HRMS (ESP+) calcd for $C_{17}H_{13}NO$ ($[M+H]^+$): *m/z* = 248.10699; exp 248.10834.

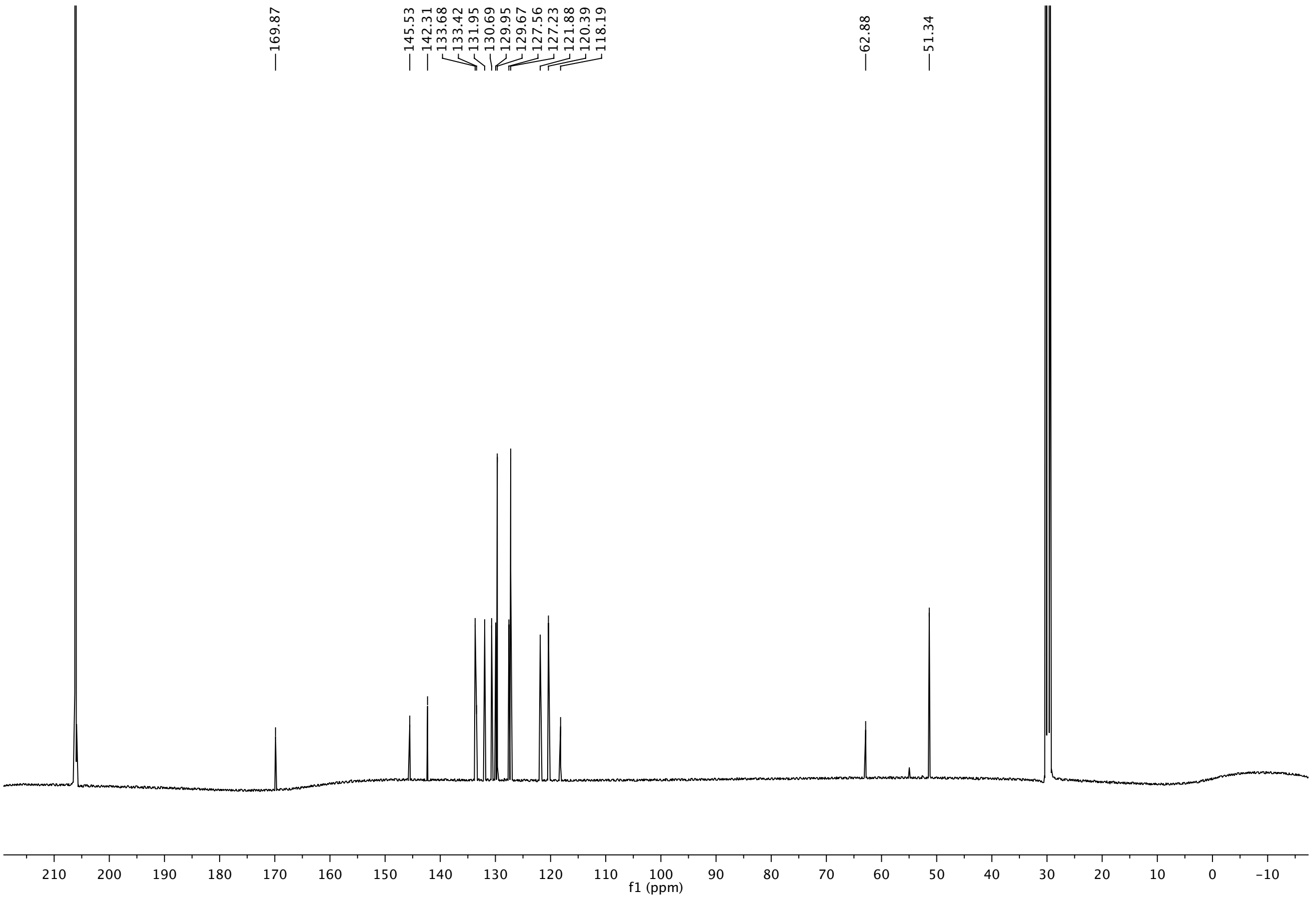
Table S2. Chemical shift for H-8 and H-8a in different solvents for the two isomers of compounds **10-19**. The values for **1** and **7** are reported for comparison.

compound	chemical shift MAJOR isomer isolated		chemical shift minor isomer isolated	
	H-8	H-8a	H-8	H-8a
10 CD3CN	5.8	3.34	5.38	3.92
12 CD3CN	5.83	3.34	5.43	3.93
14 CDCl3	5.84	3.33	5.39	3.94
15 CDCl3	5.76	3.35	5.35	3.83
16 CD3CN	5.7	3.09	4.23	3.79
16 CDCl3	5.82	3.31	n.d	n.d.
17 CD3CN	5.78	3.33	5.31	3.91
18 CDCl3	6.05	3.44	4.75	4.39
7 CDCl3	5.93	3.41	4.58	4.19
19 CD3CN	5.74	3.29	5.14	4.06
11 CDCl3	5.09 (11b)	3.77 (11b)	5.88 (11a)	3.28 (11a)
13 CDCl3	5.07 (13b)	3.82 (13b)	n.d.	n.d
1 CD3CN	5.73	3.83		

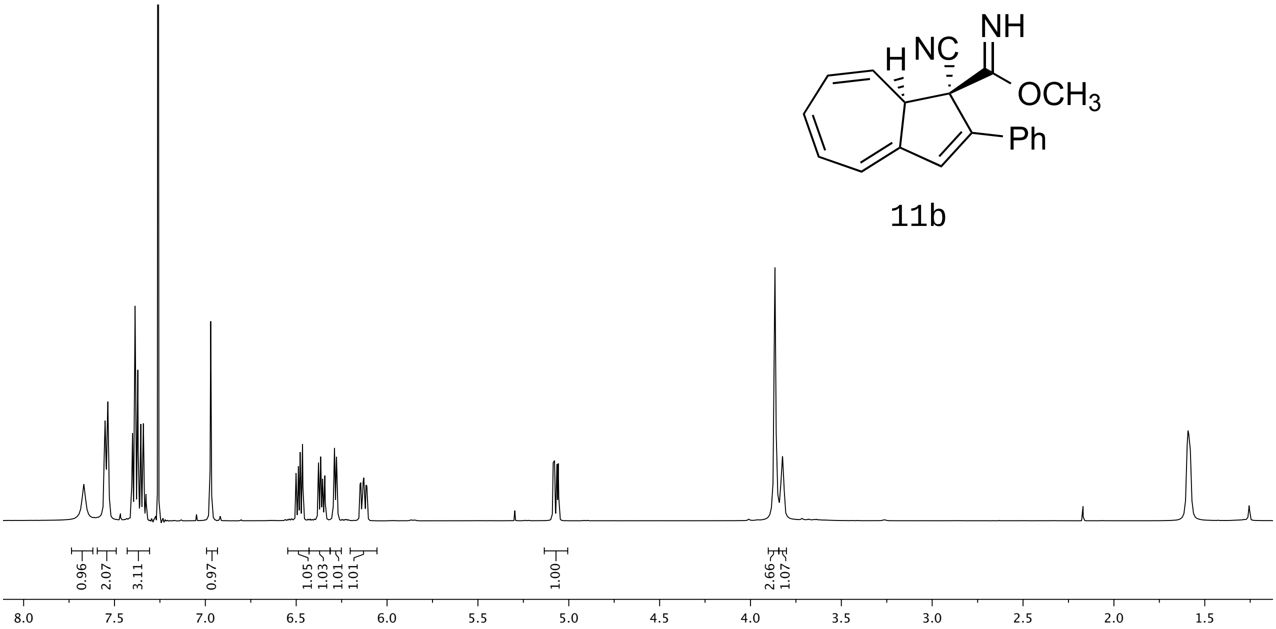
Table S2 shows that the chemical shifts of H-8a and H-8 change by up to 0.6 ppm between the MAJOR and the minor stereoisomer, depending more on the stereochemistry than on the substituents at C-1. The chemical shift of H-8a is diagnostic of the relative stereochemistry between C-1 and C-8a; indeed when the chemical shift for H-8a is ca. 3.3 ppm, the substituent is on the same side of H-8a, while if it is at ca. 3.9 ppm, it is on the opposite side. A similar analogy is observed also on the chemical shift of H-8. As for imidates **11** and **13**, the major isomers isolated **11b** and **13b** are indeed the minor isomers formed as discussed in the manuscript, and having H-8a on the side of the remaining CN group.

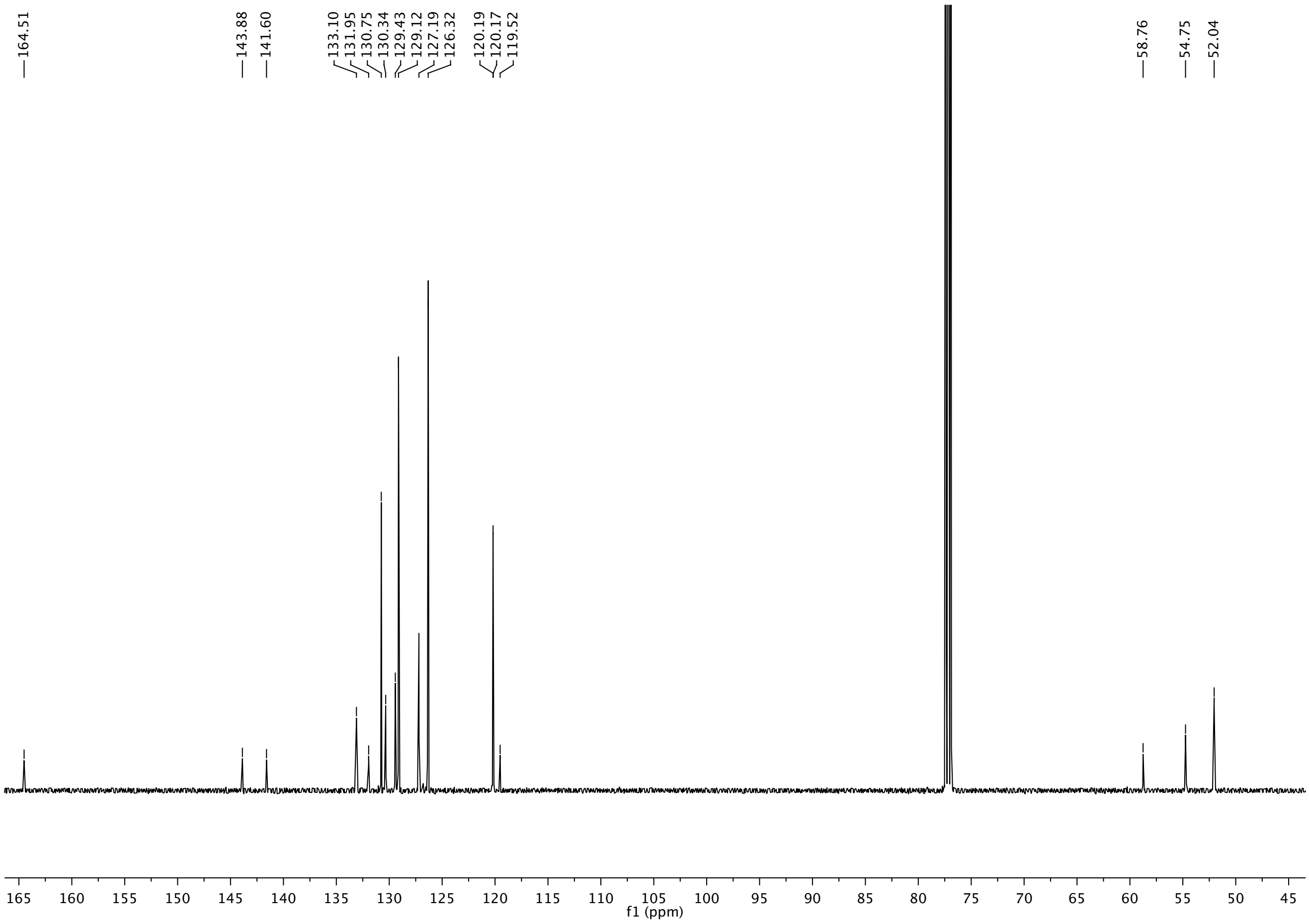
^{1}H and ^{13}C NMR spectra of **10a** in acetone-d_6:



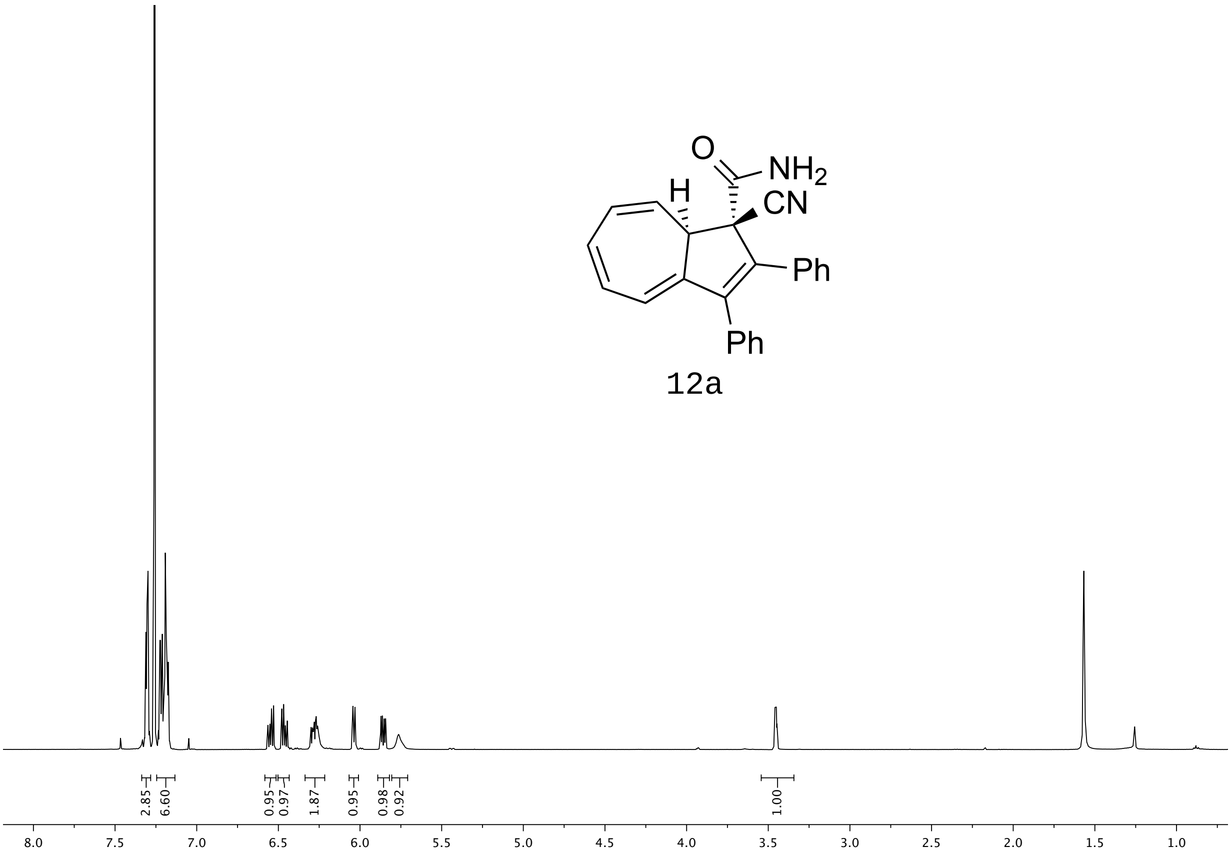


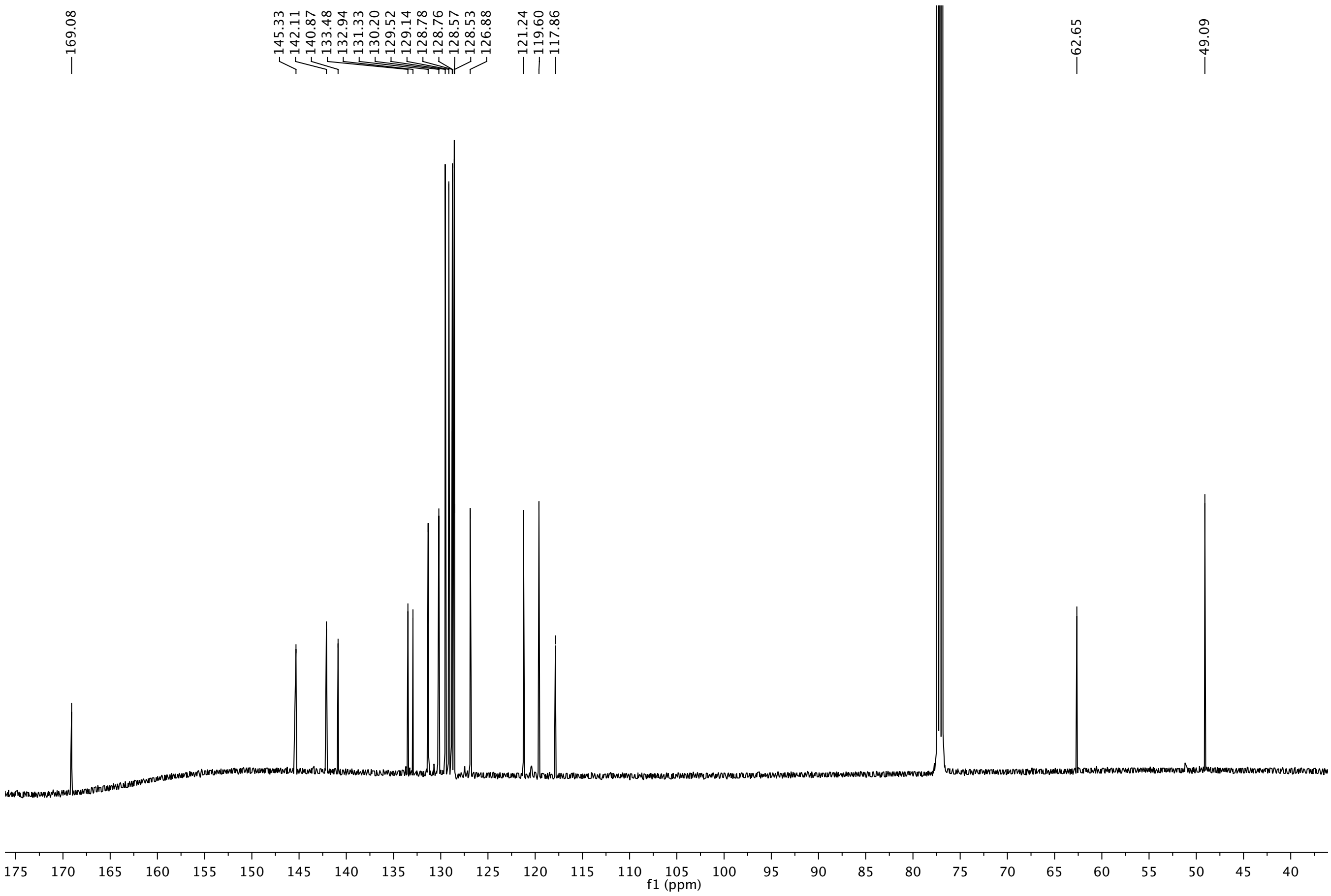
^{1}H and ^{13}C NMR spectra of **11b** in $CDCl_3$:



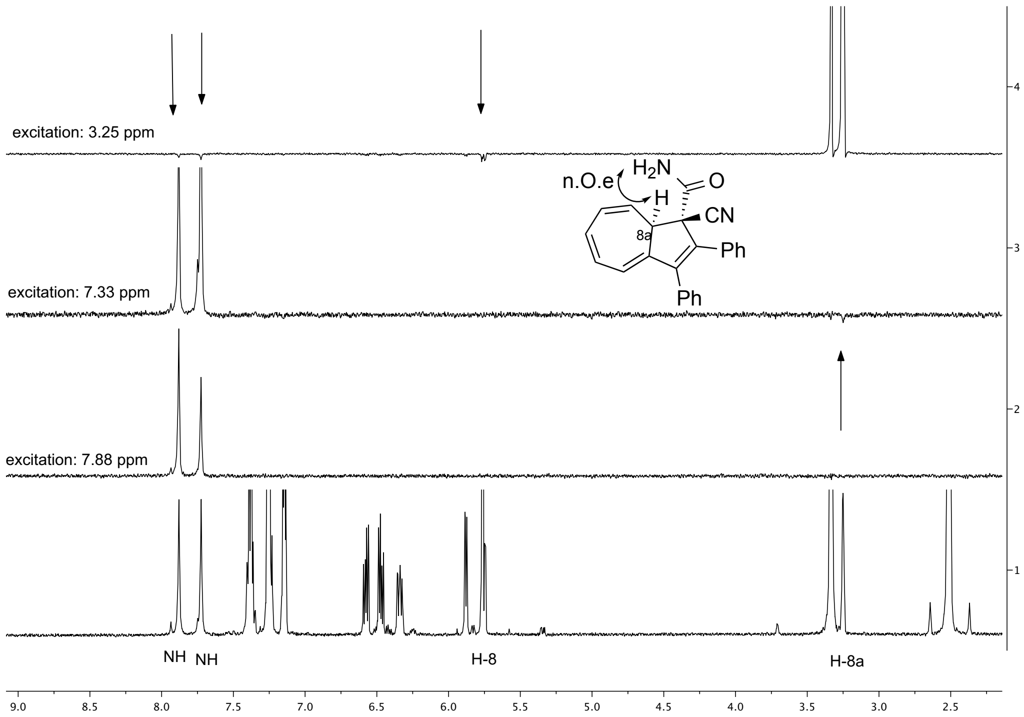


^{1}H and ^{13}C NMR spectra of **12a** in $CDCl_3$:

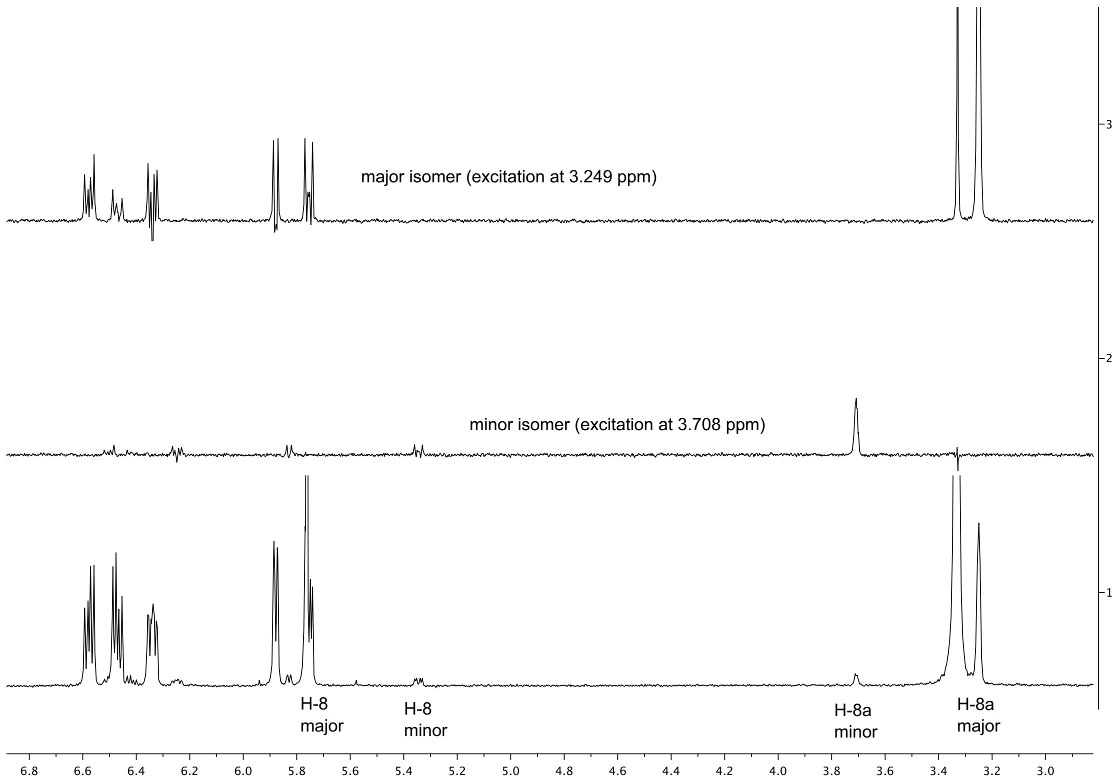




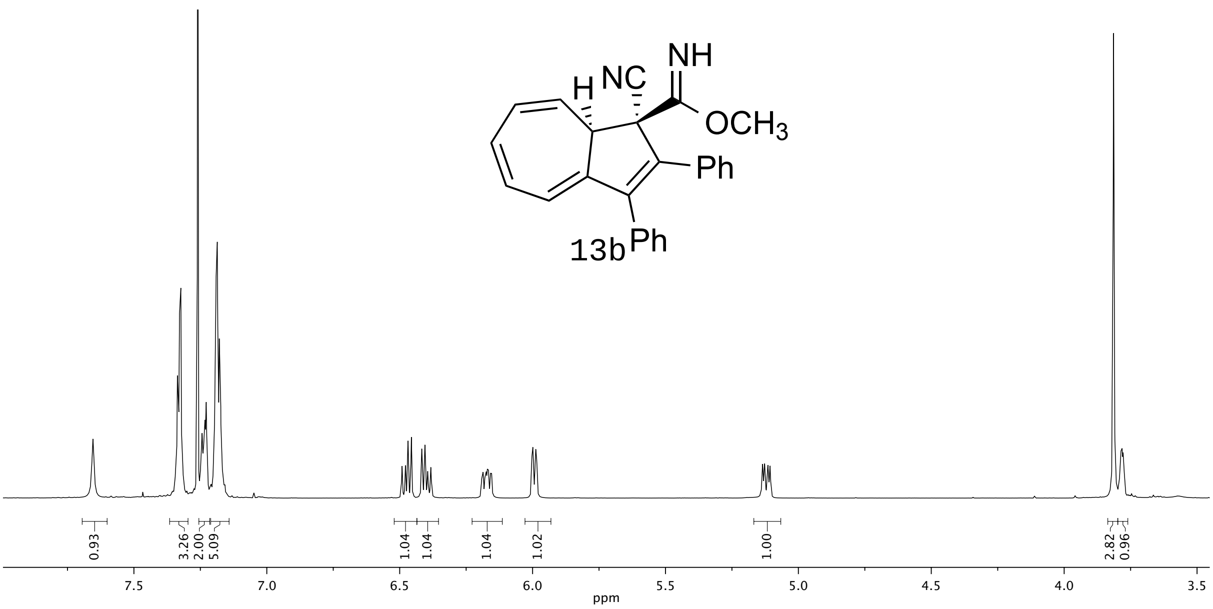
NOESY-1D experiment on **12a** in dmso-d_6 (mix = 500 ms, selective excitation on the two NHs (middle) and H-8a (top)), showing n.O.e. on the two NHs when H-8a is excited and viceversa.

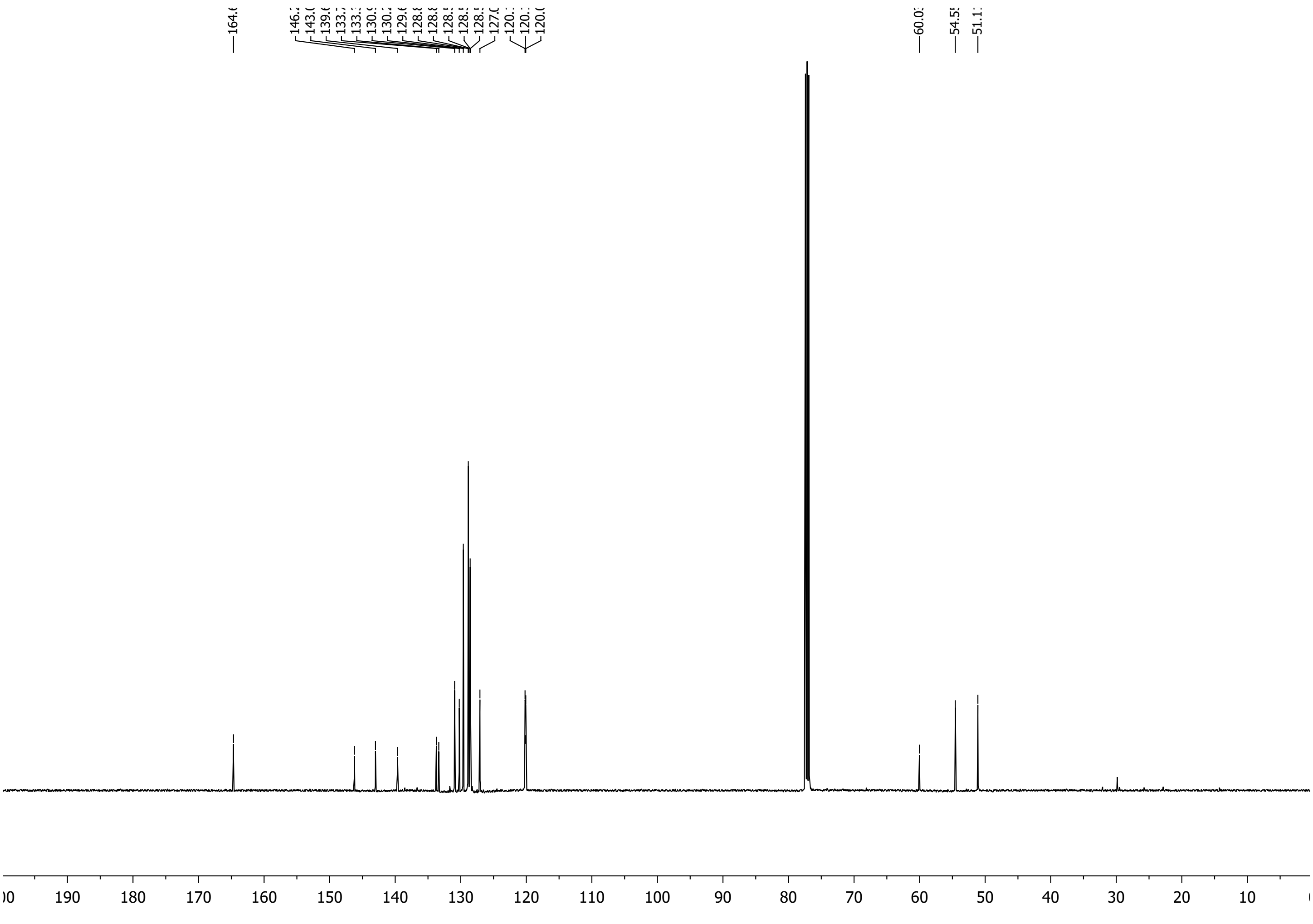


TOCSY-1D experiments on a mixture of diastereomers **12a** and **12b** in dmso-d_6 showing the two different spin system for the seven membered rings (middle: minor isomer; top: major isomer).

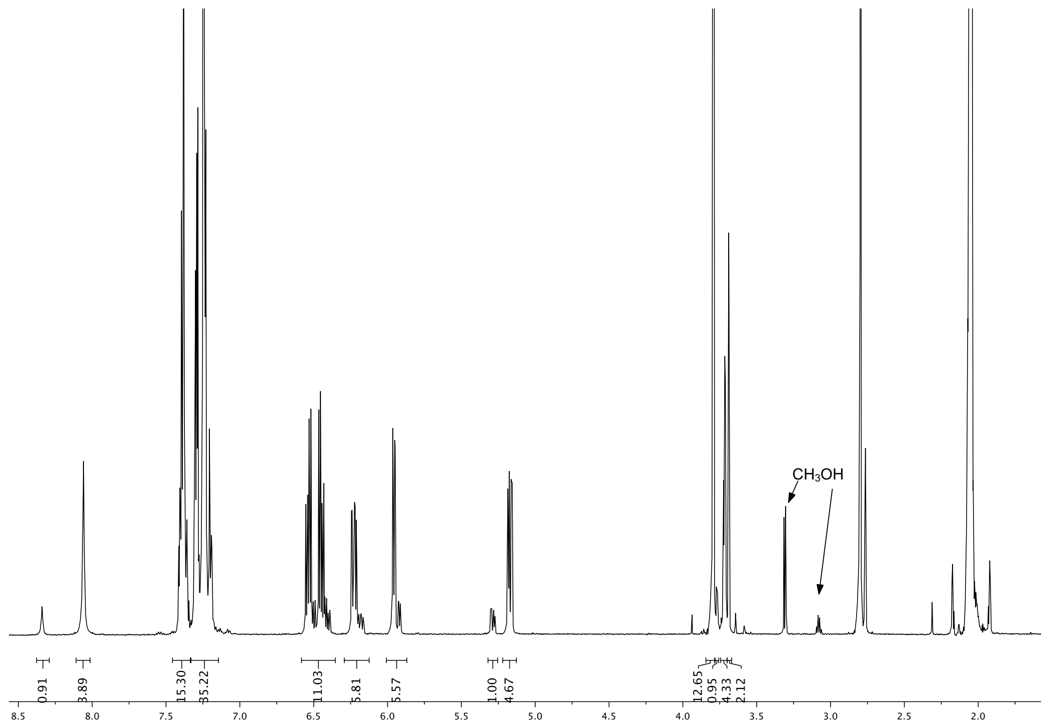


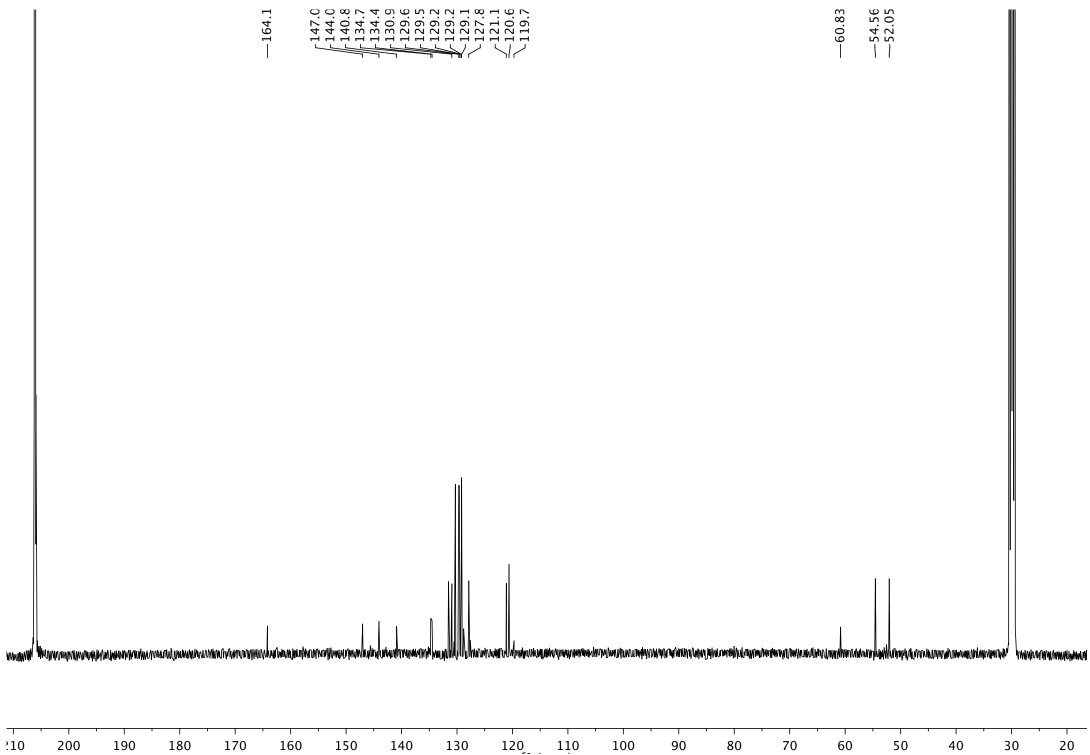
[1]H and [13]C NMR spectra of **13b** in $CDCl_3$:

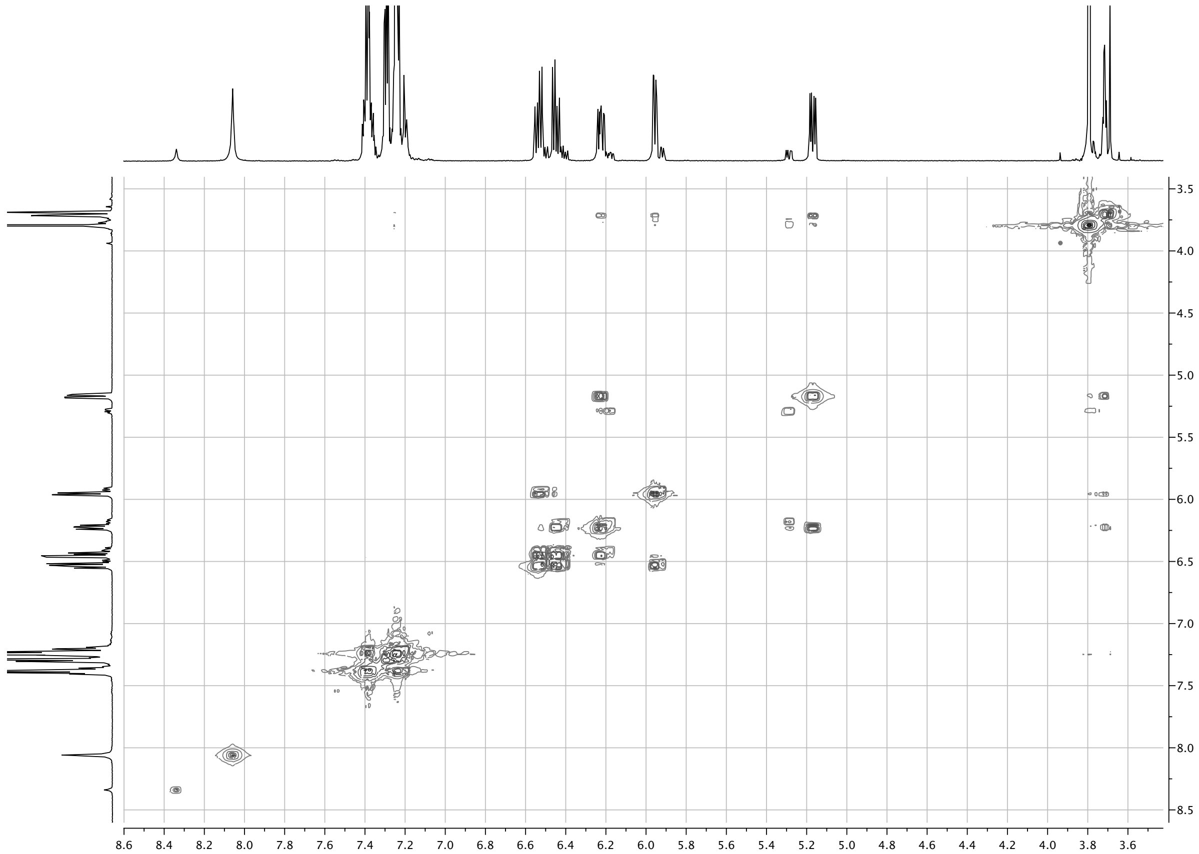




[1]H, [13]C, gCOSY and gHSQC NMR spectra of compound **13b** (isomeric mixture C=NH *E/Z*) in acetone-d_6:



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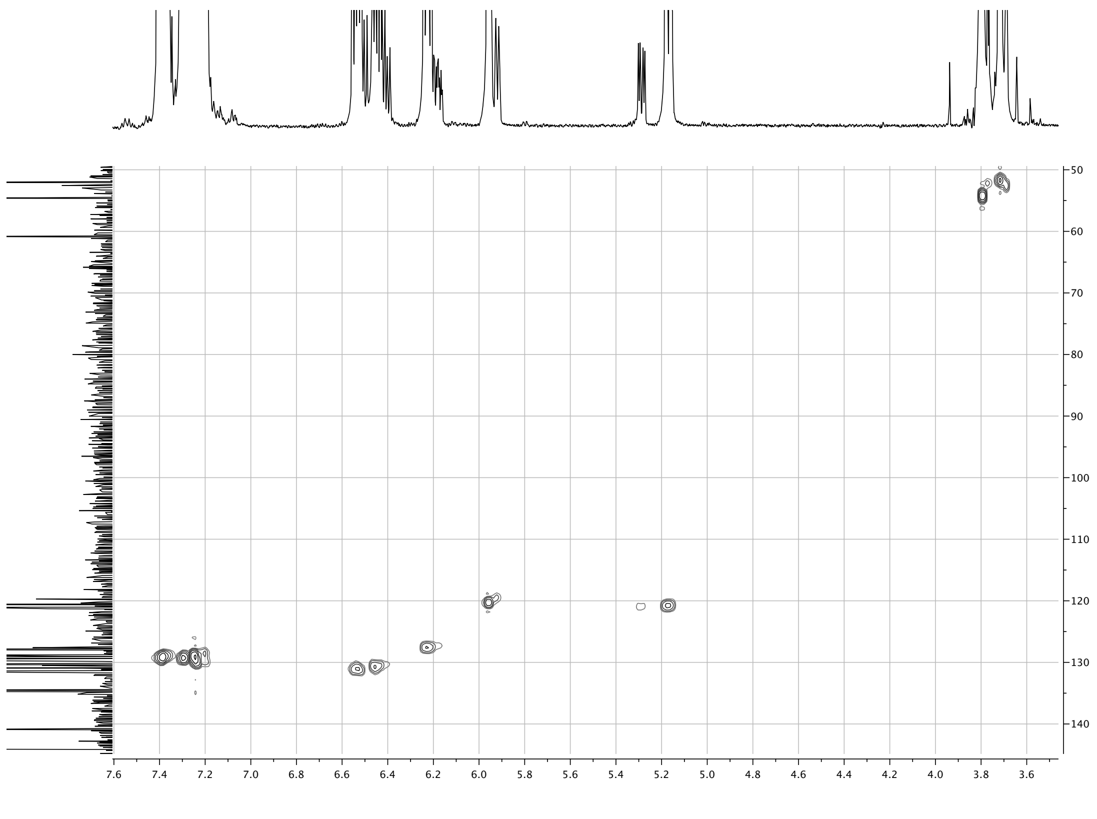
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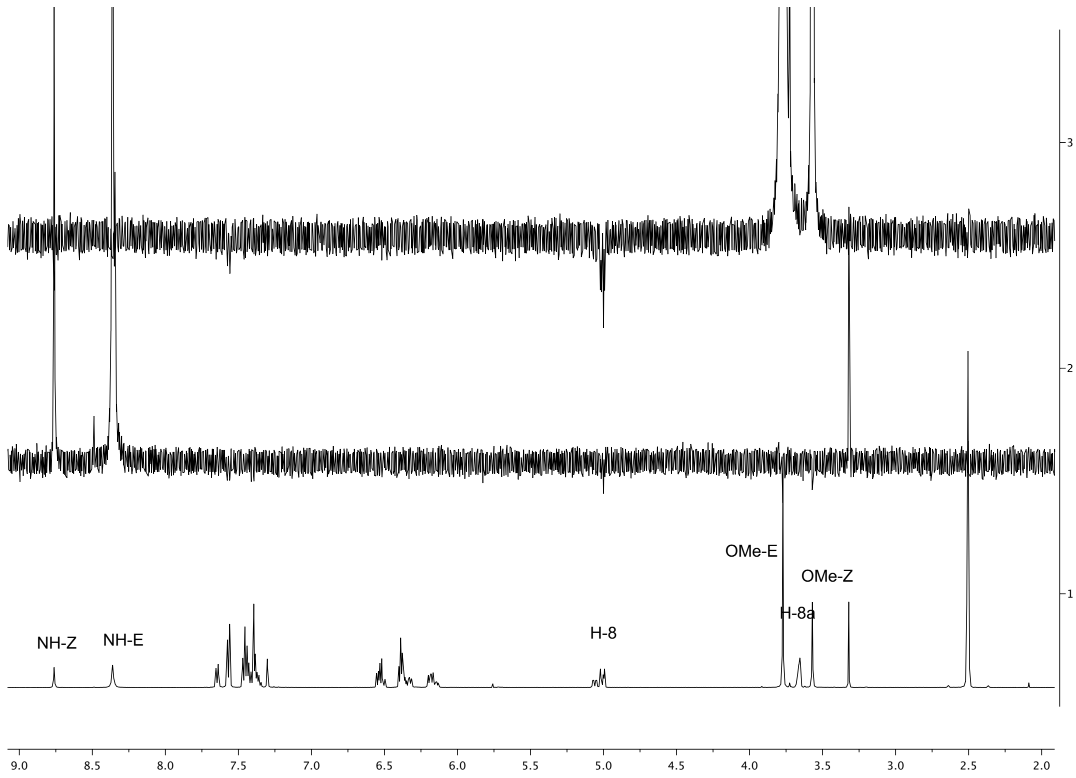
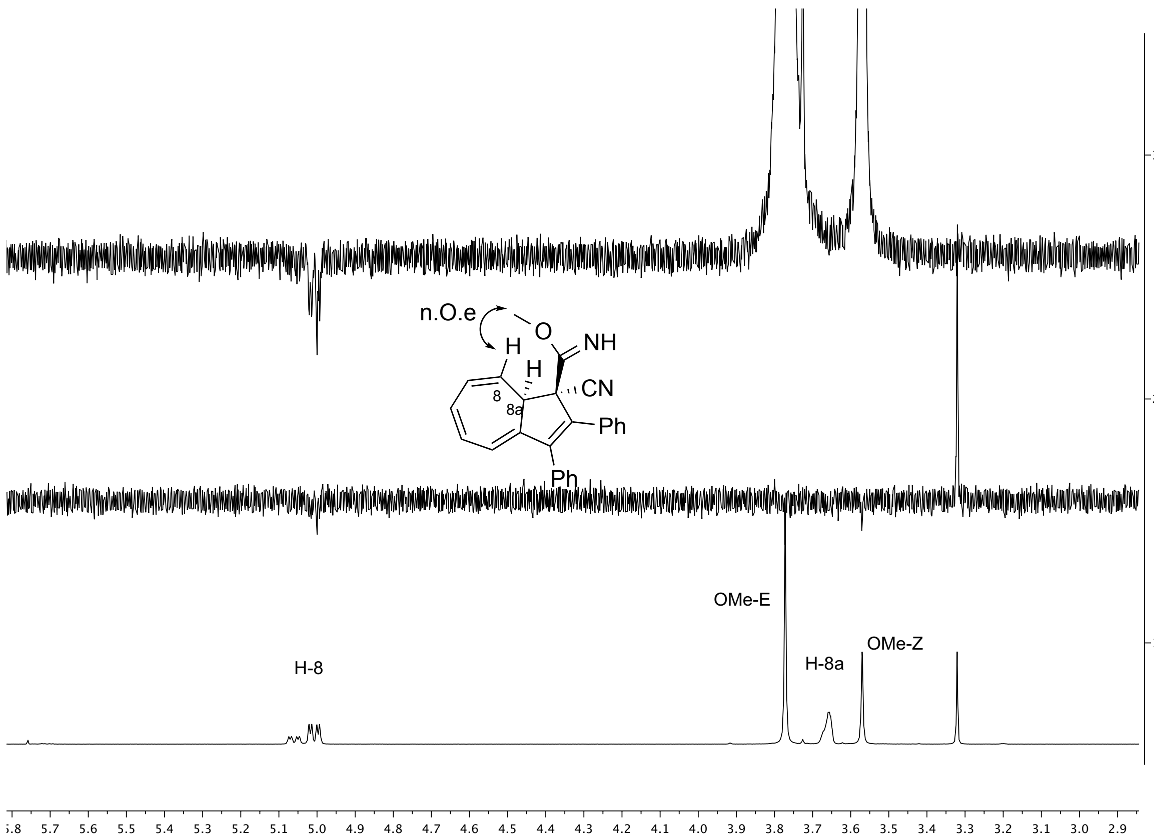
50 60 70 80 90 100 110 120 130 140

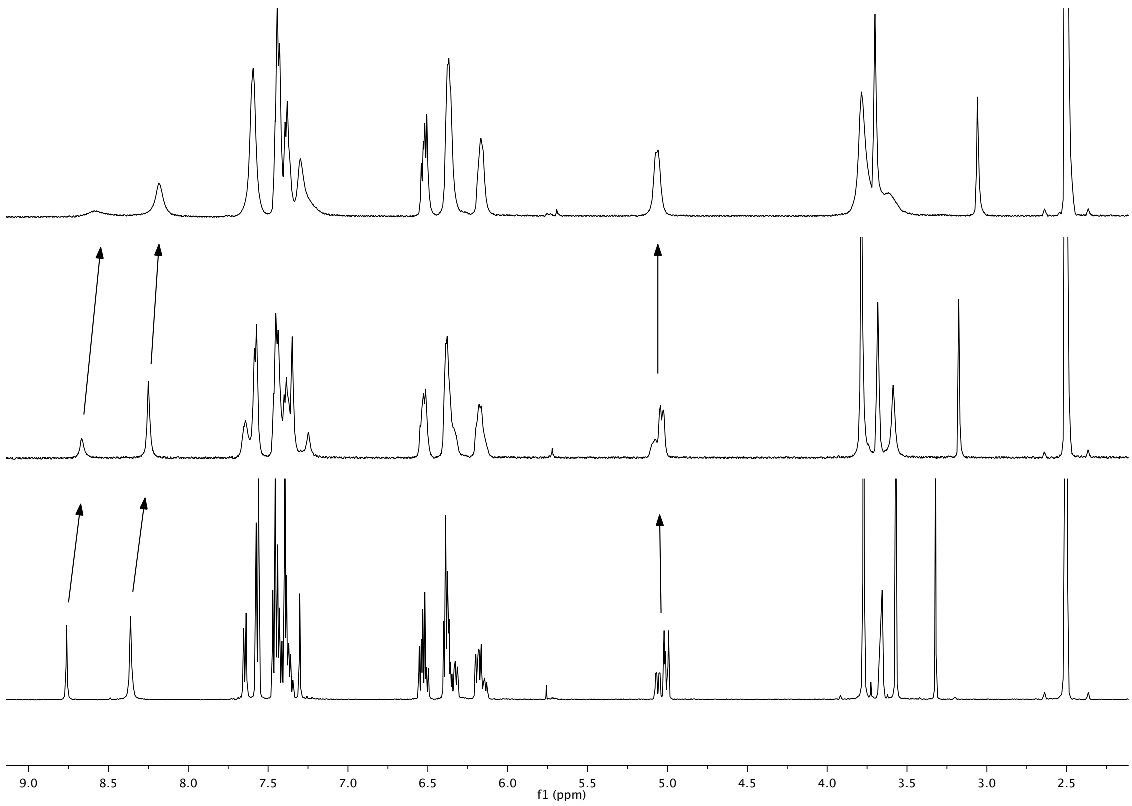
ROESY-1D experiment on 1*R*,8a*R* isomer of **13b** (racemic mixture at C-1 and C-8a, but isomeric mixture C=NH *E/Z*) in dmso-d_6 (mix = 200 ms, selective excitation on NH-*E* isomer (middle) and OMe-*E* isomer (top))



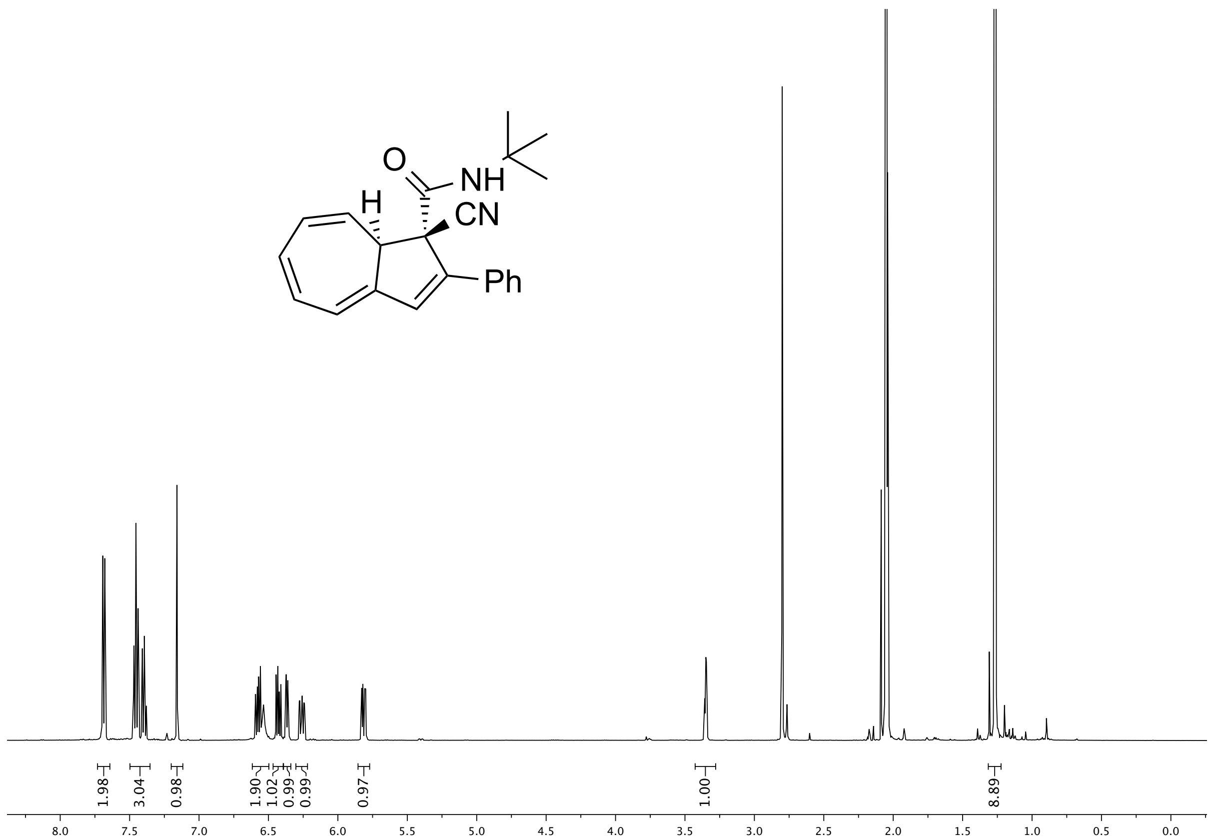
Expansion of the ROESY-1D experiment showing n.O.e. on H-8 when OMe is excited. No effect is detected on H-8a.

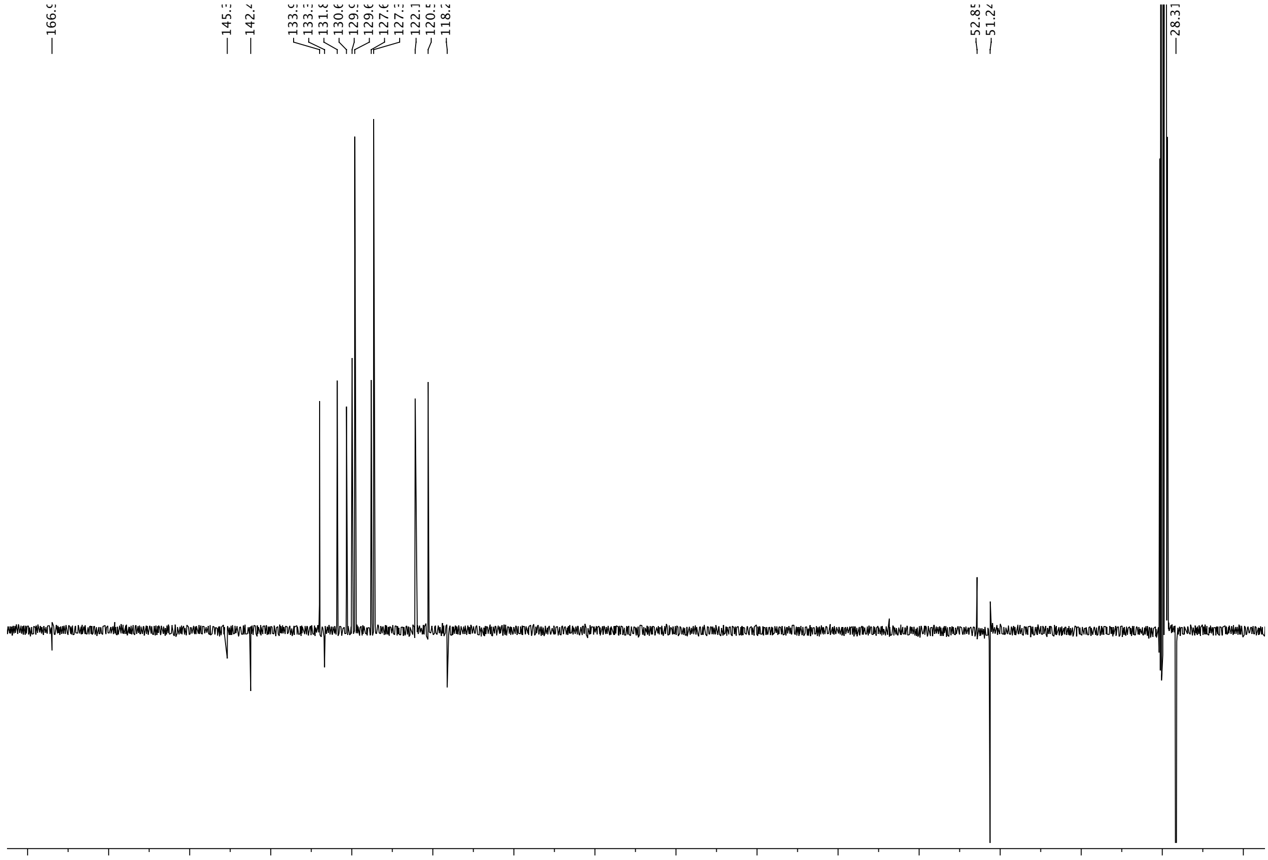


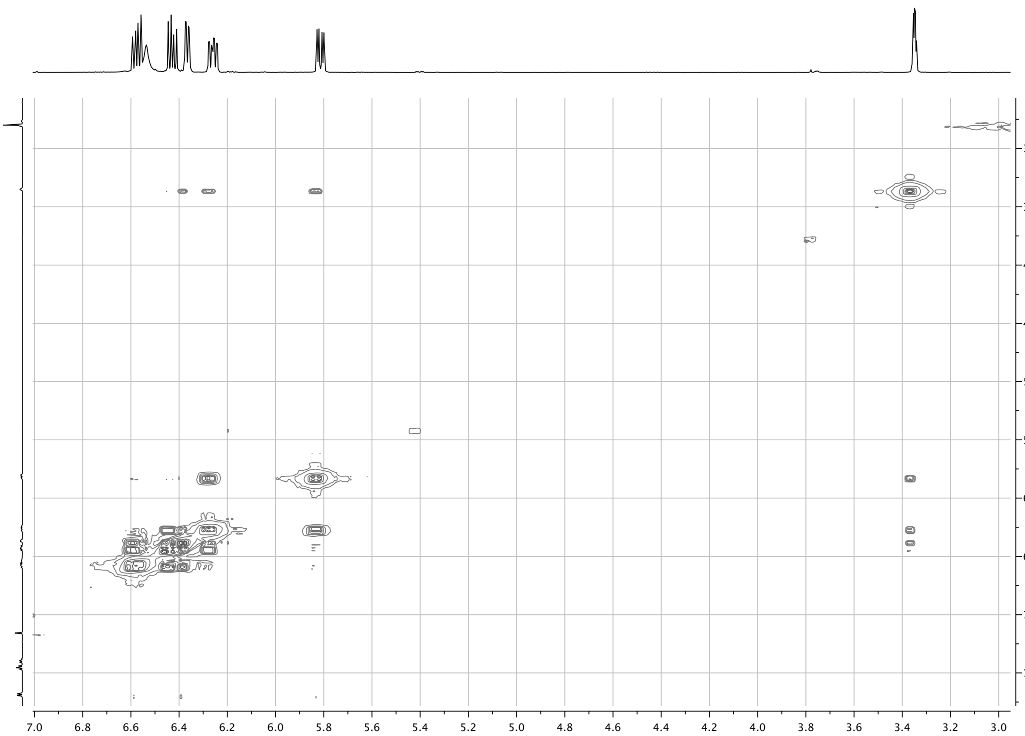
^{1}H NMR spectra of **13b** (isomeric mixture C=NH *E/Z*) in dmso-d_6 at 298, 330 and 350 K (bottom to top):

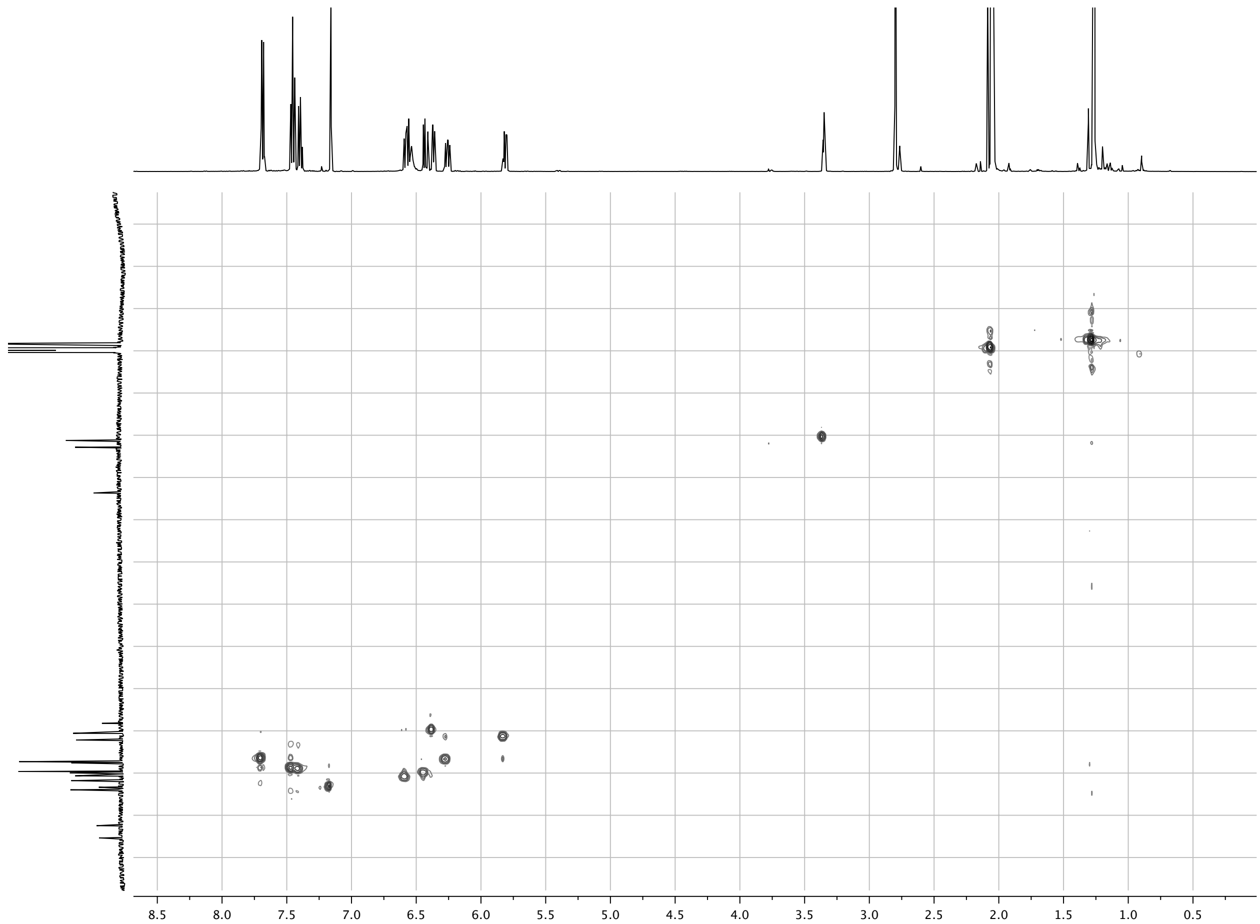


^{1}H, APT, gCOSY (expansion) and gHSQC NMR spectra of **14** in acetone-d_6:

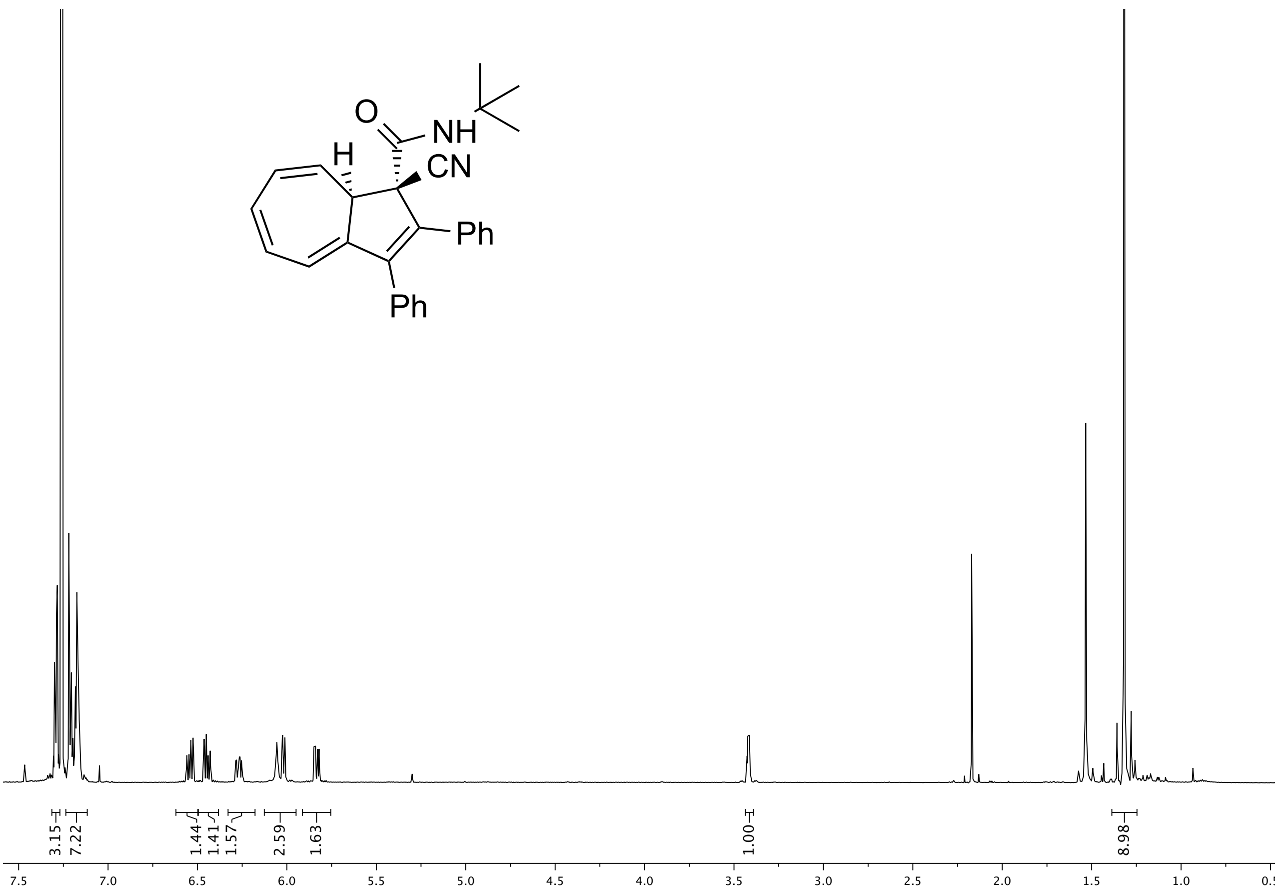


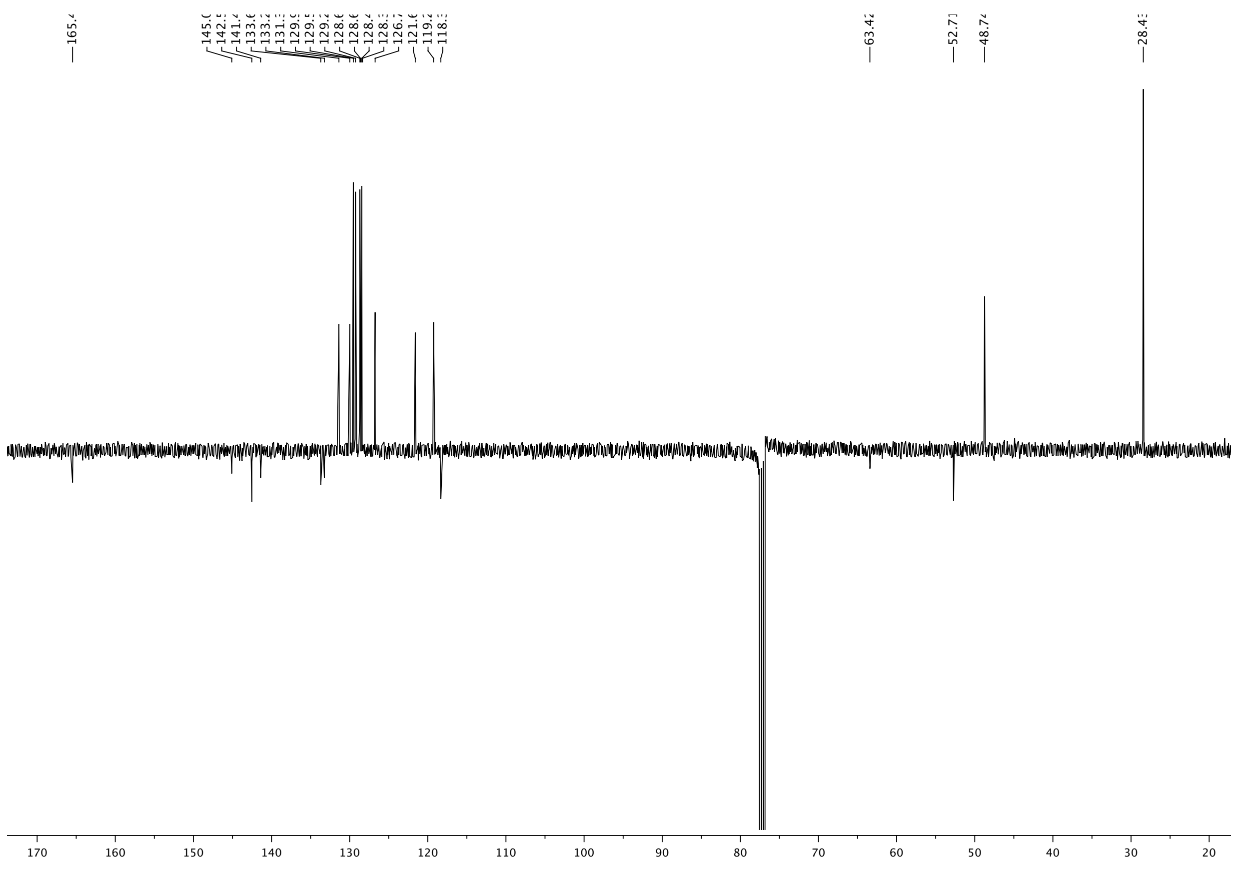


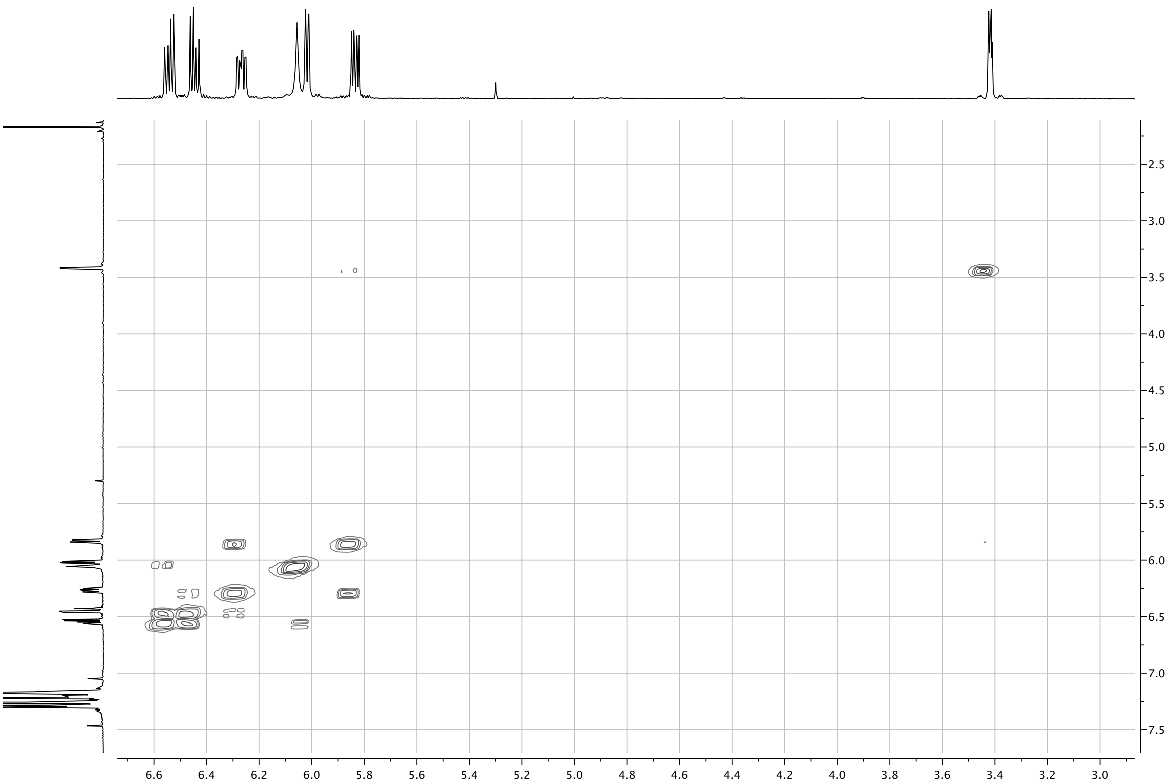




^{1}H, APT, gCOSY (expansion) and gHSQC NMR spectra of **15** in $CDCl_3$:



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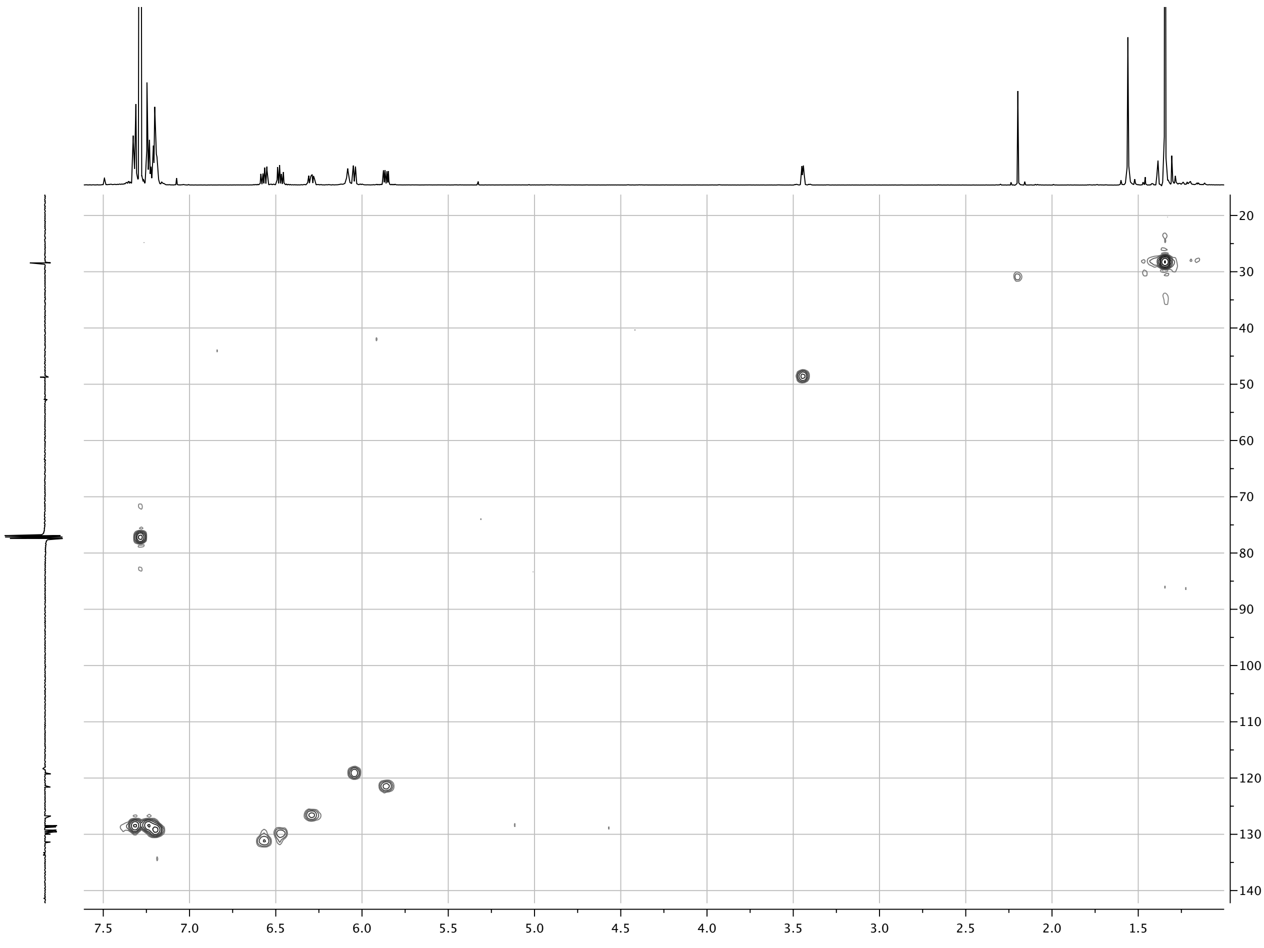
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2.5
2.0
1.5
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50
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100
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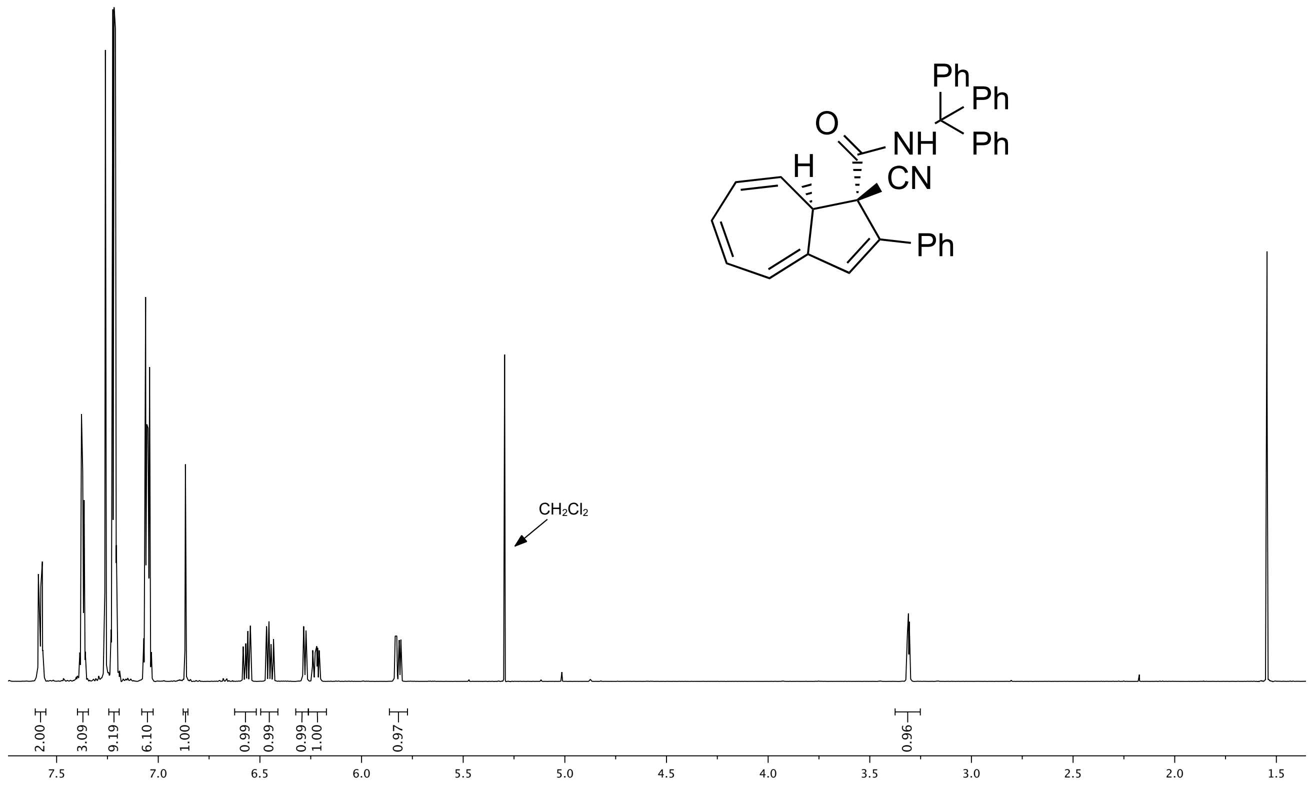
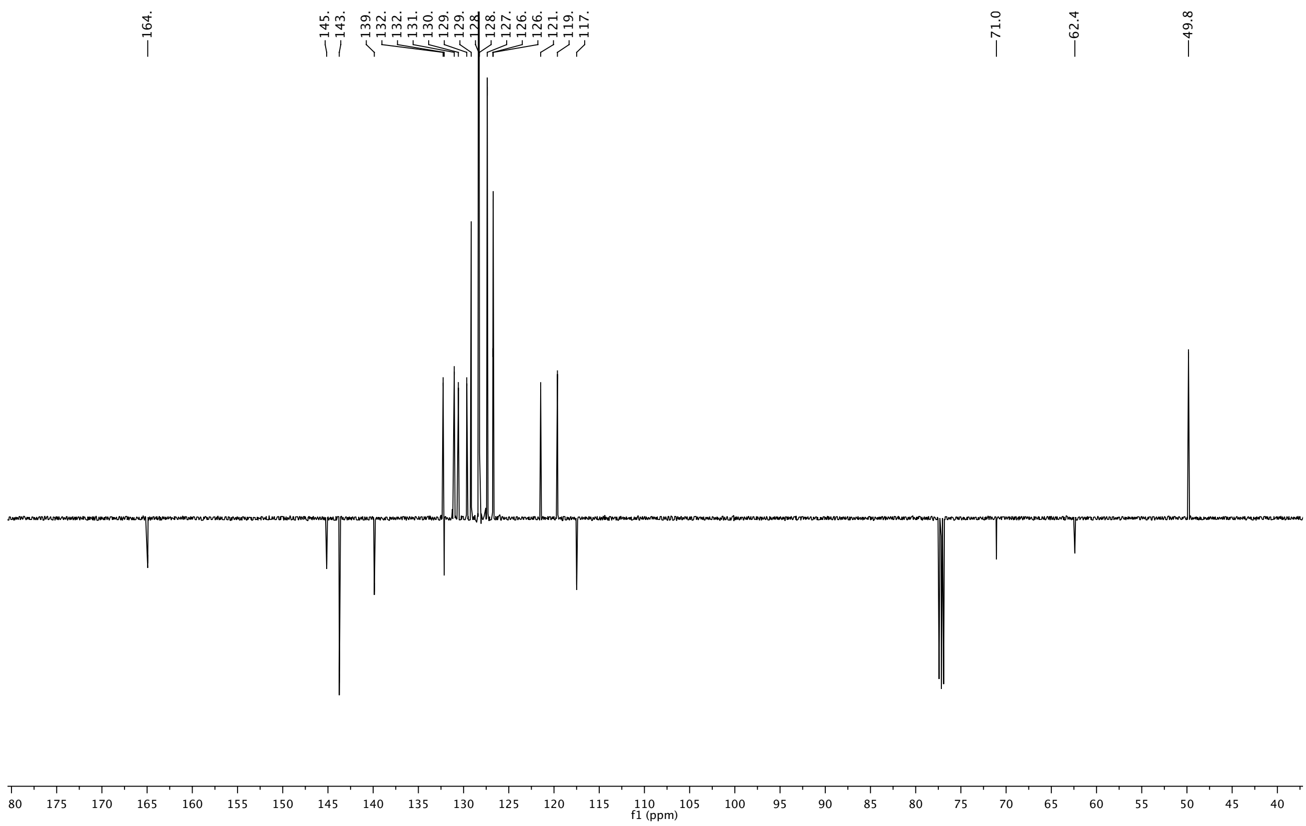
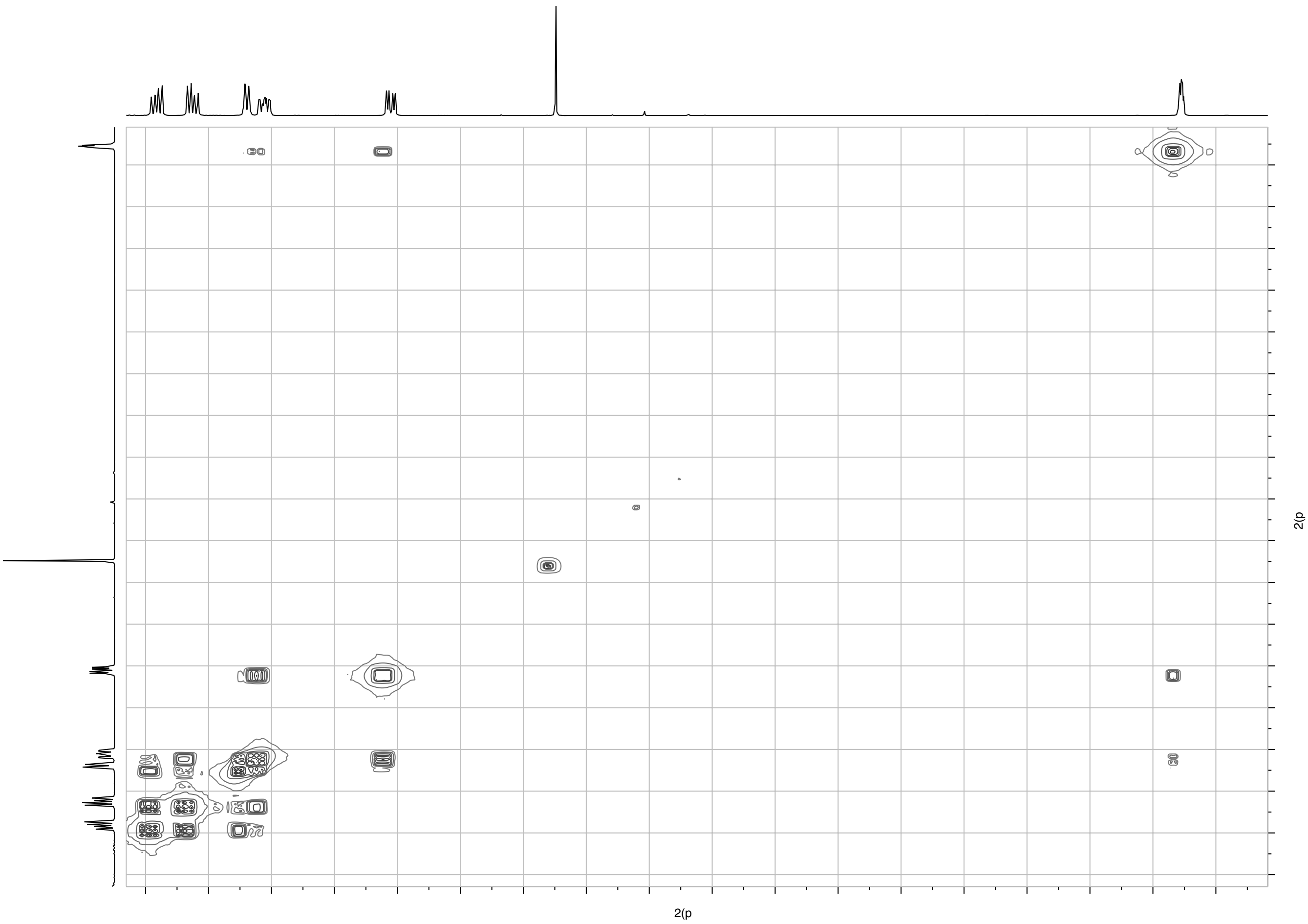
120
130
140

^{1}H, APT, gCOSY (expansion) and gHSQC NMR spectra of **16** in $CDCl_3$:



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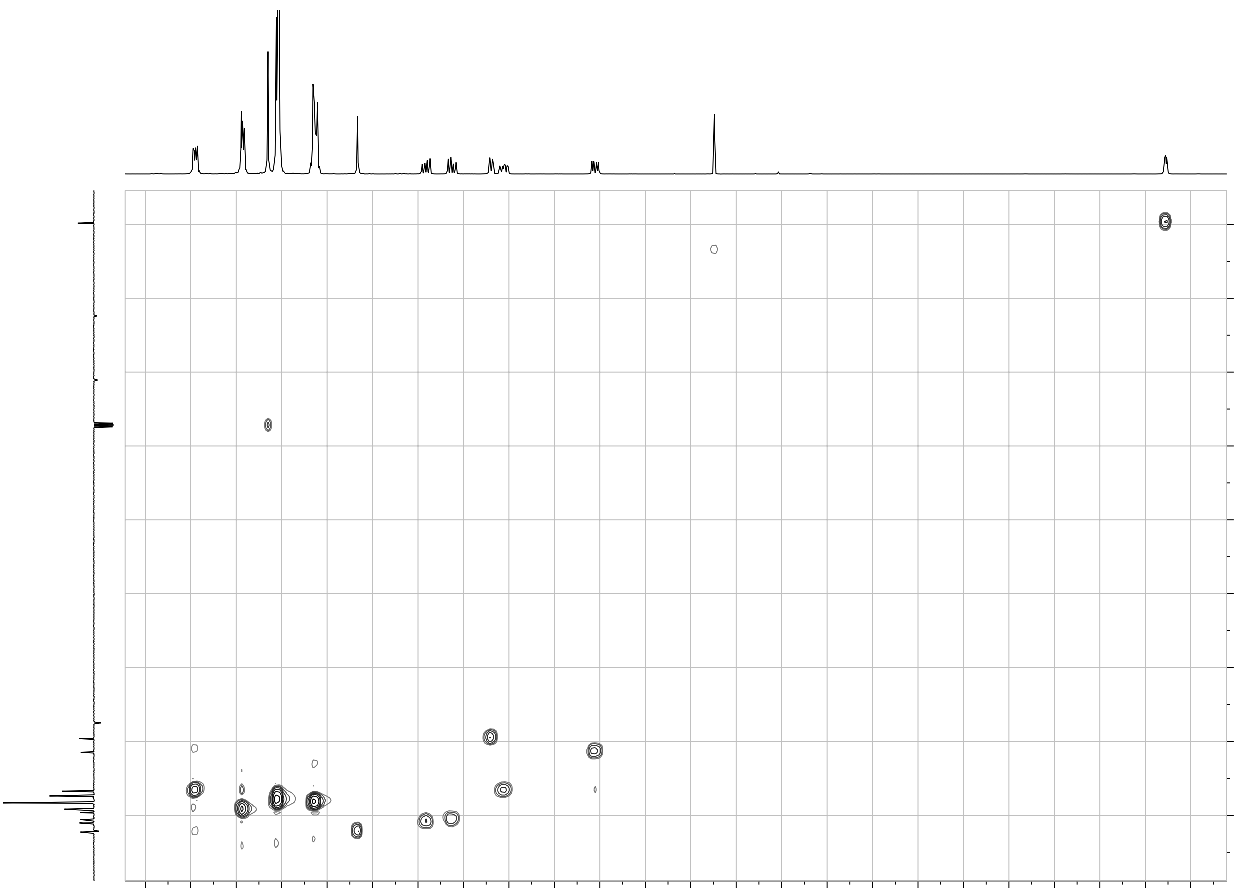
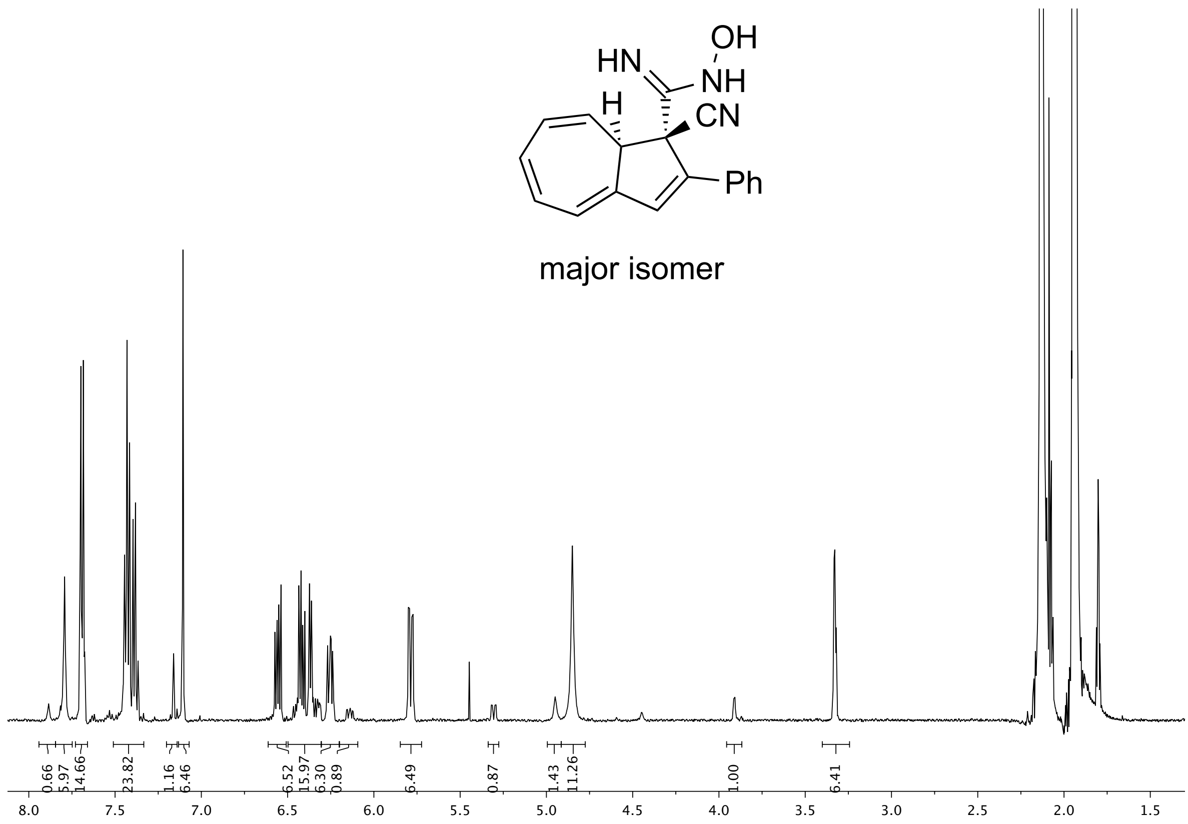
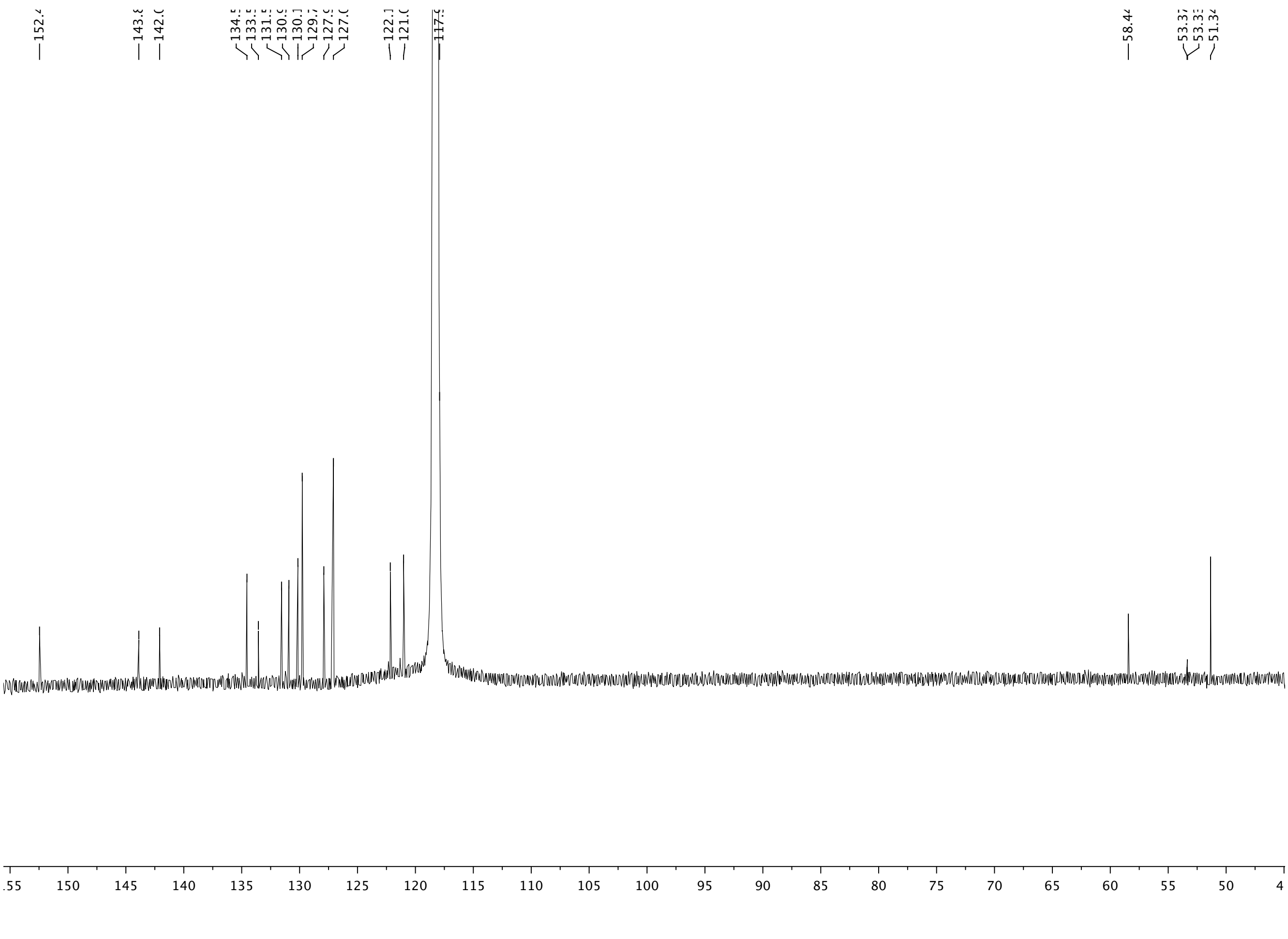
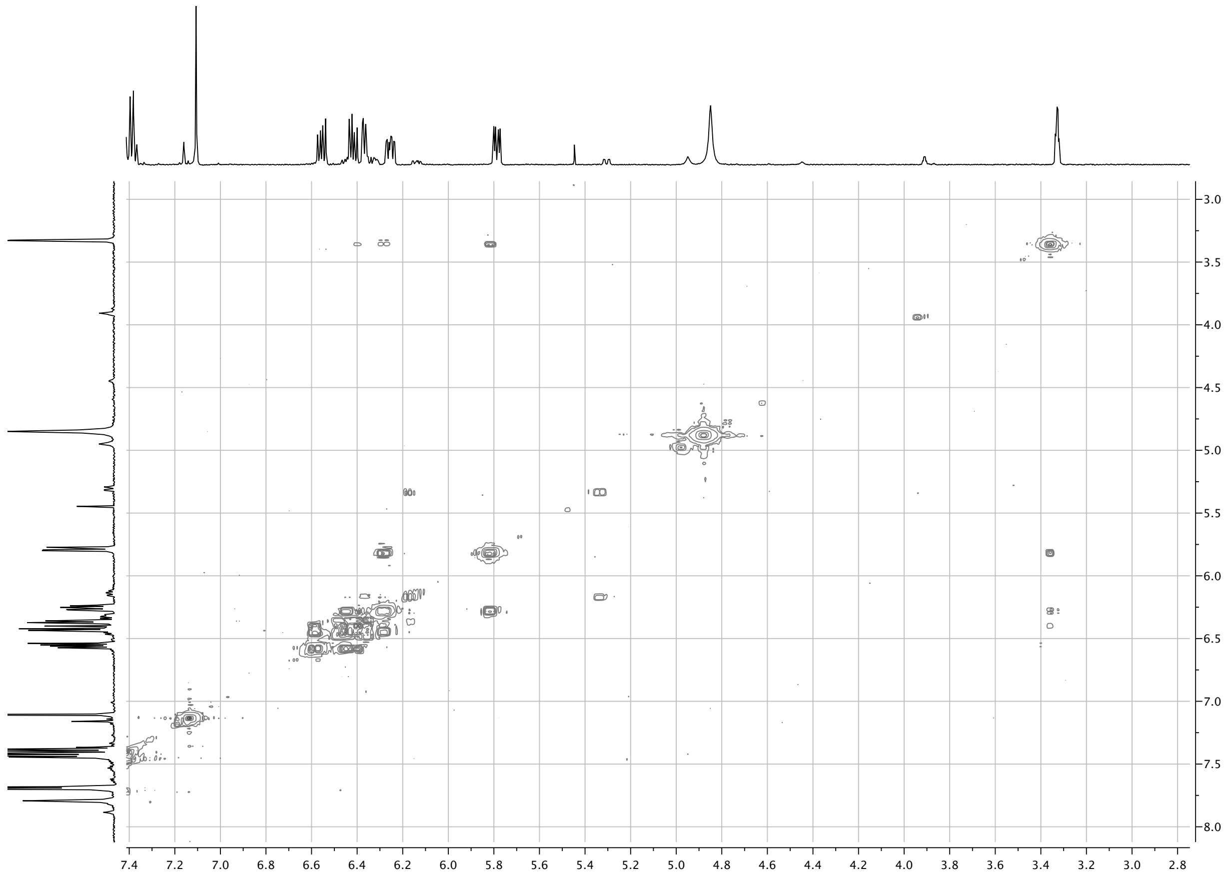


^{1}H, ^{13}C, gCOSY (expansion) and gHSQC NMR spectra of **17** in CD_3CN:



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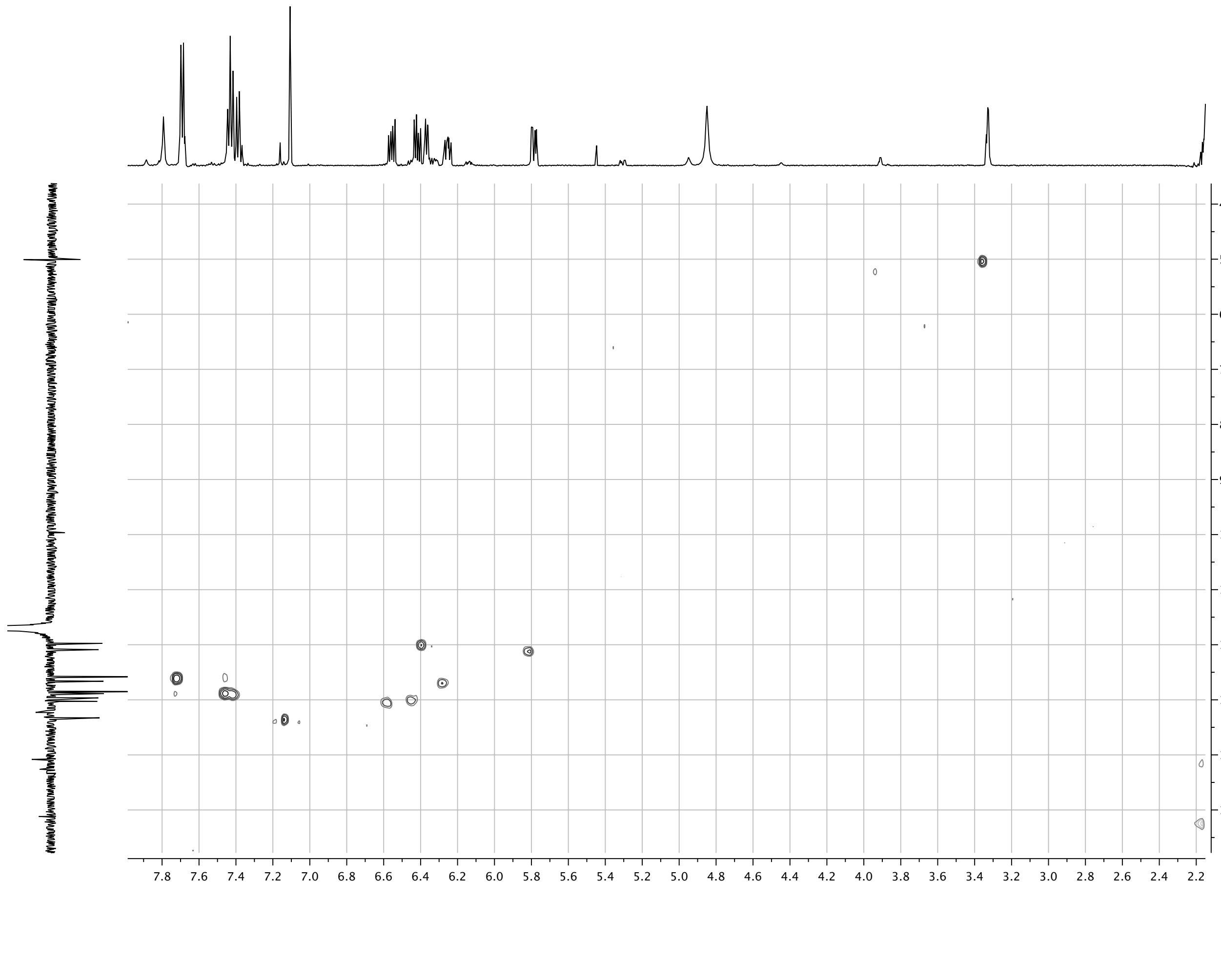
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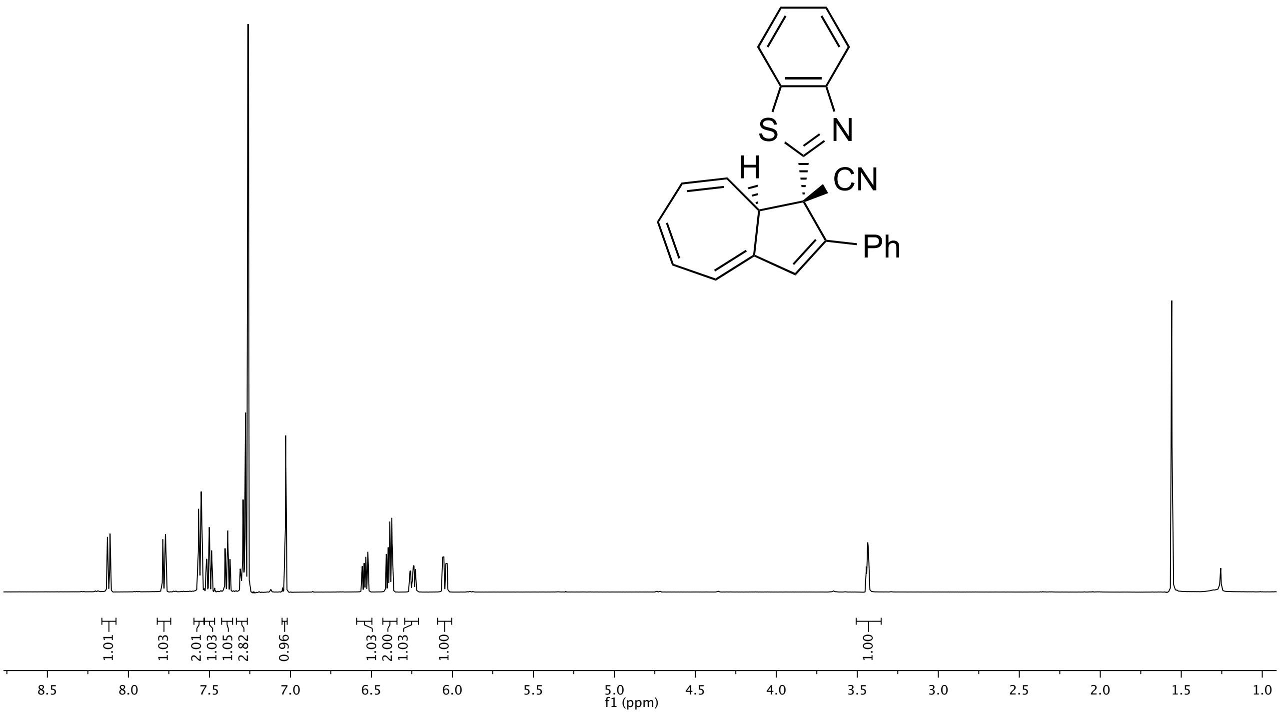
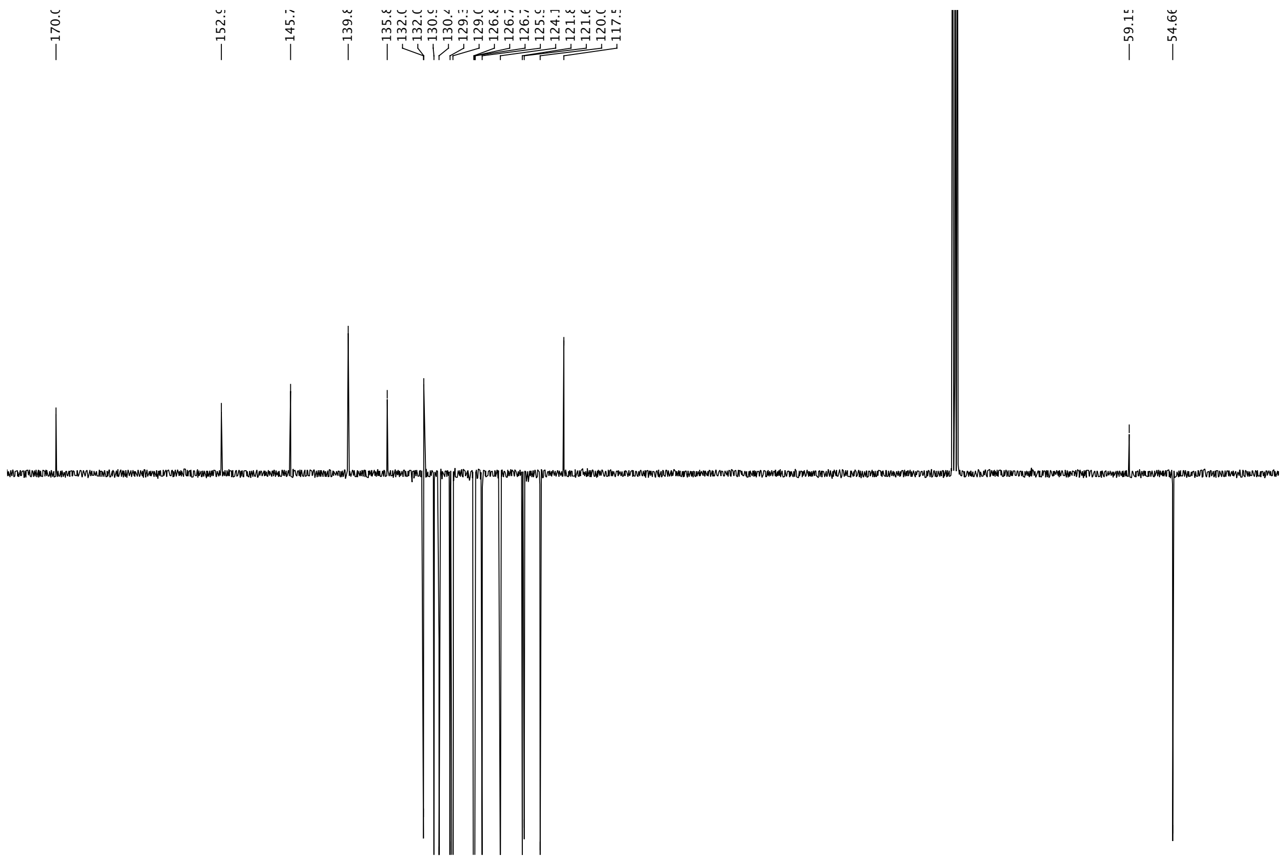
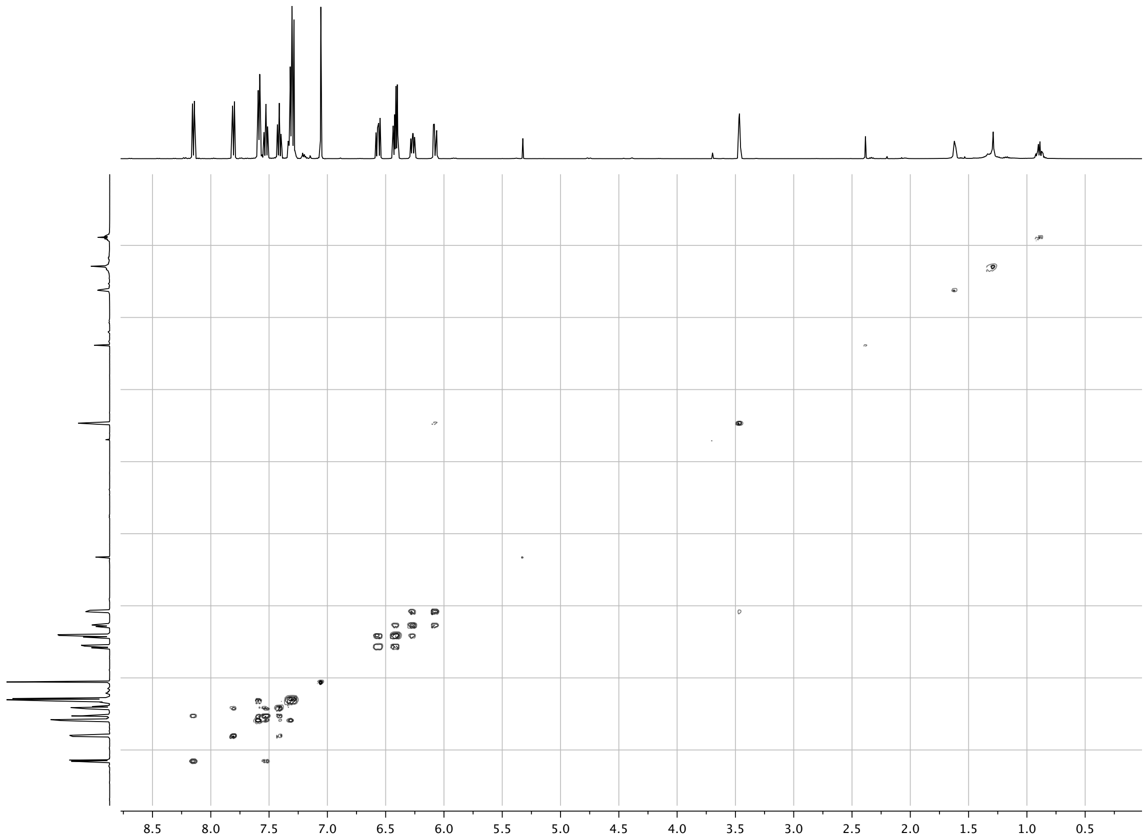
[1]H, APT, gCOSY and gHSQC NMR of **18** in $CDCl_3$:







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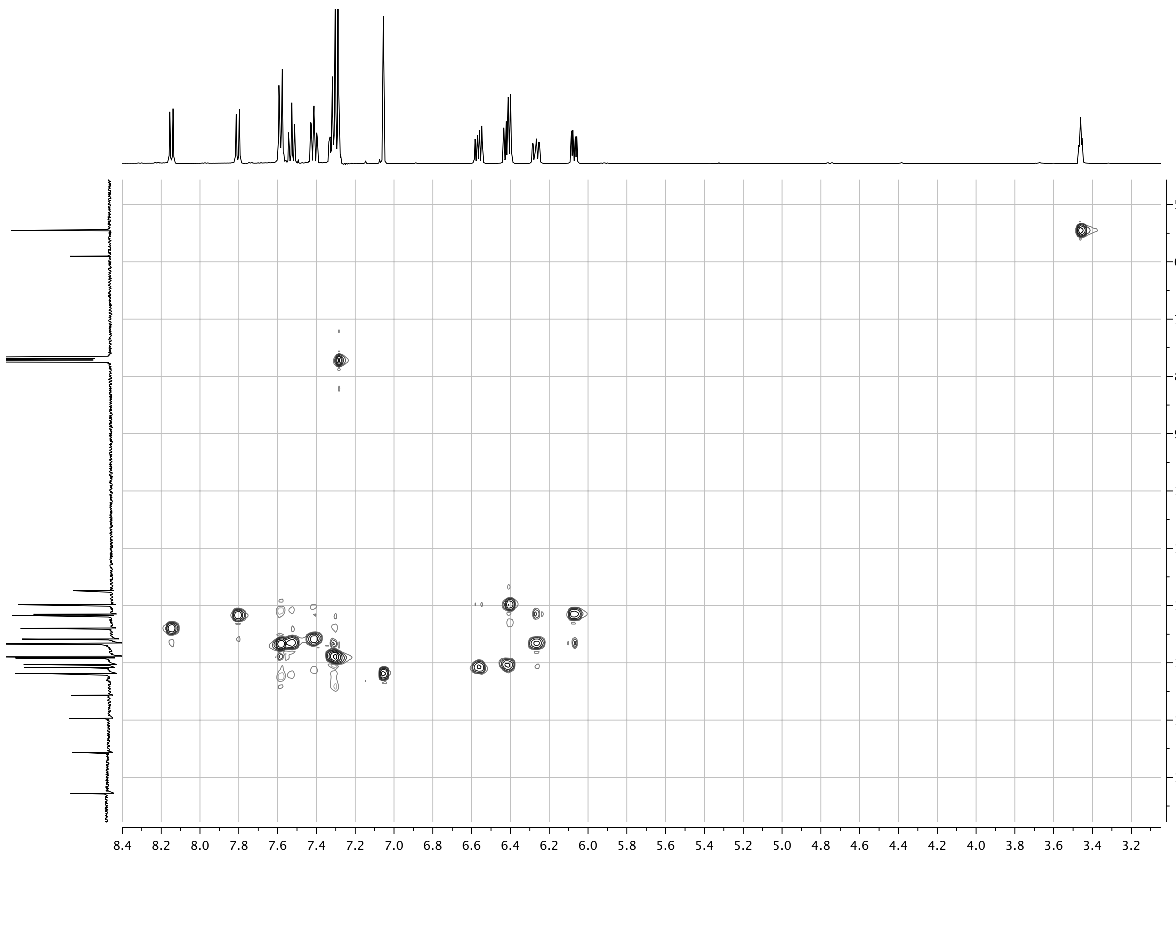

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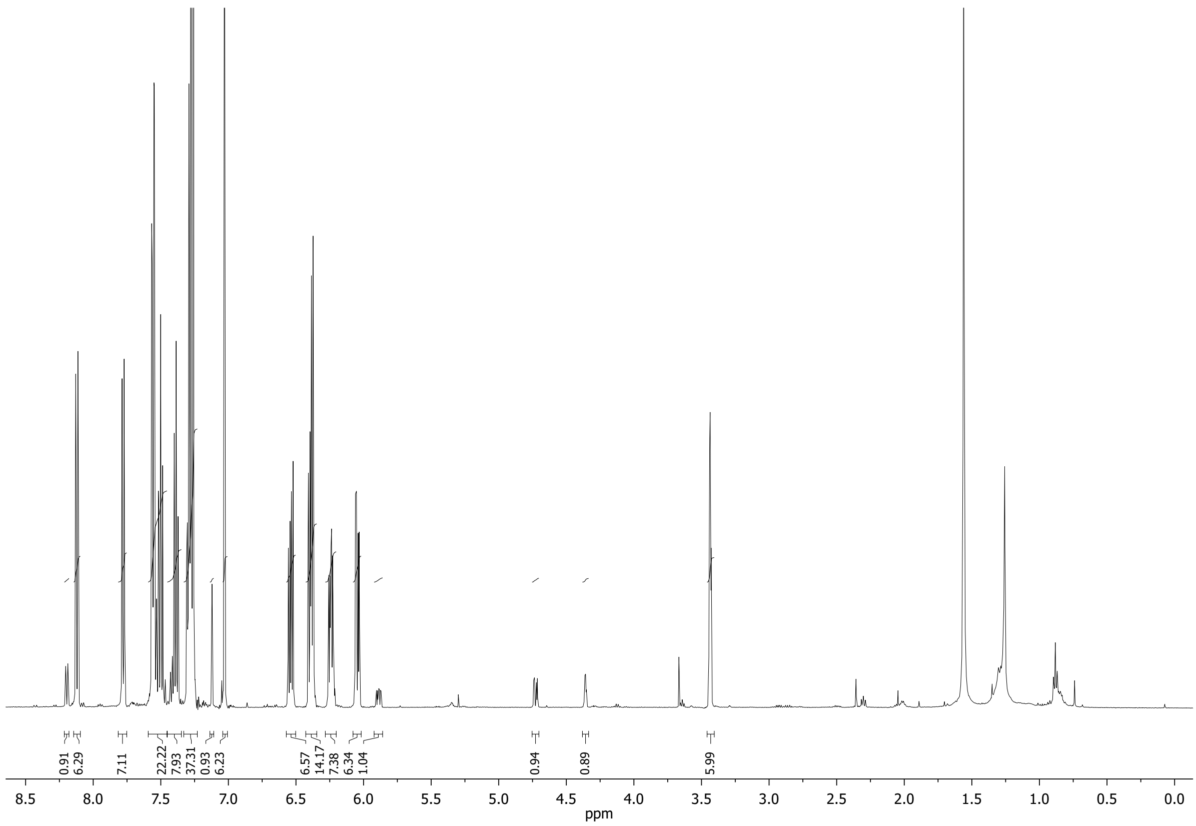
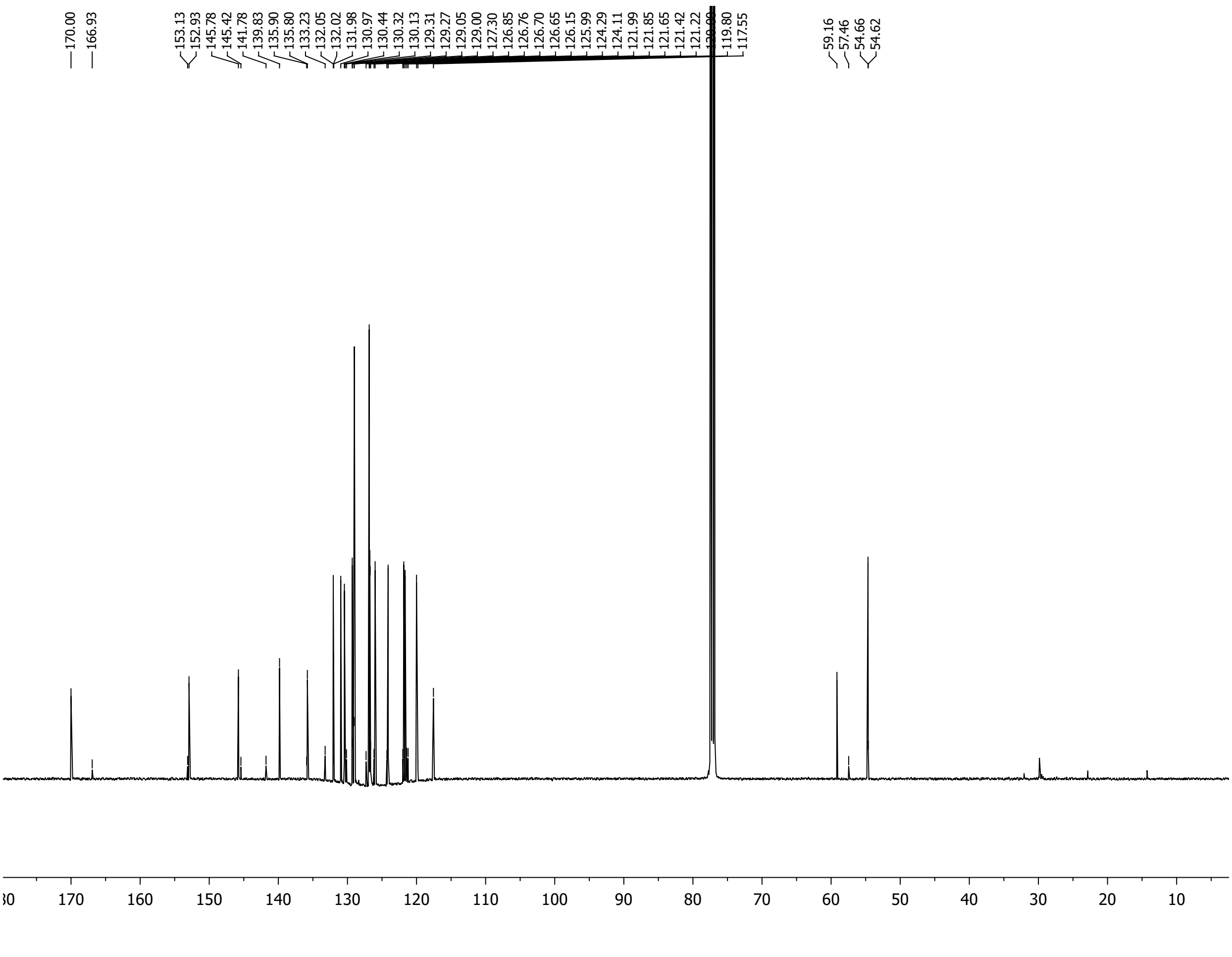
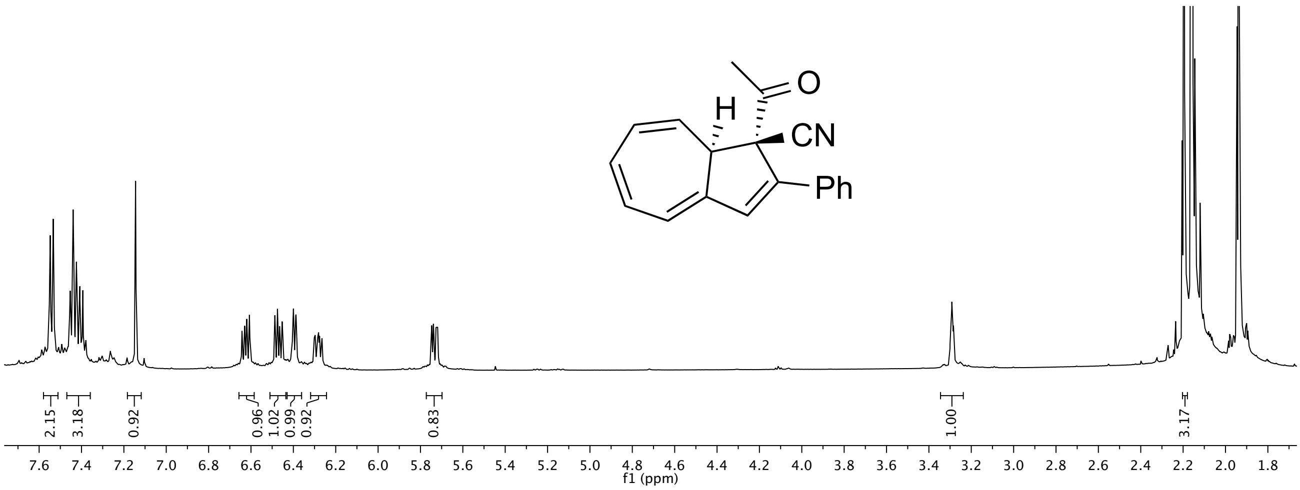
50 60 70 80 90 100 110 120 130 140 150

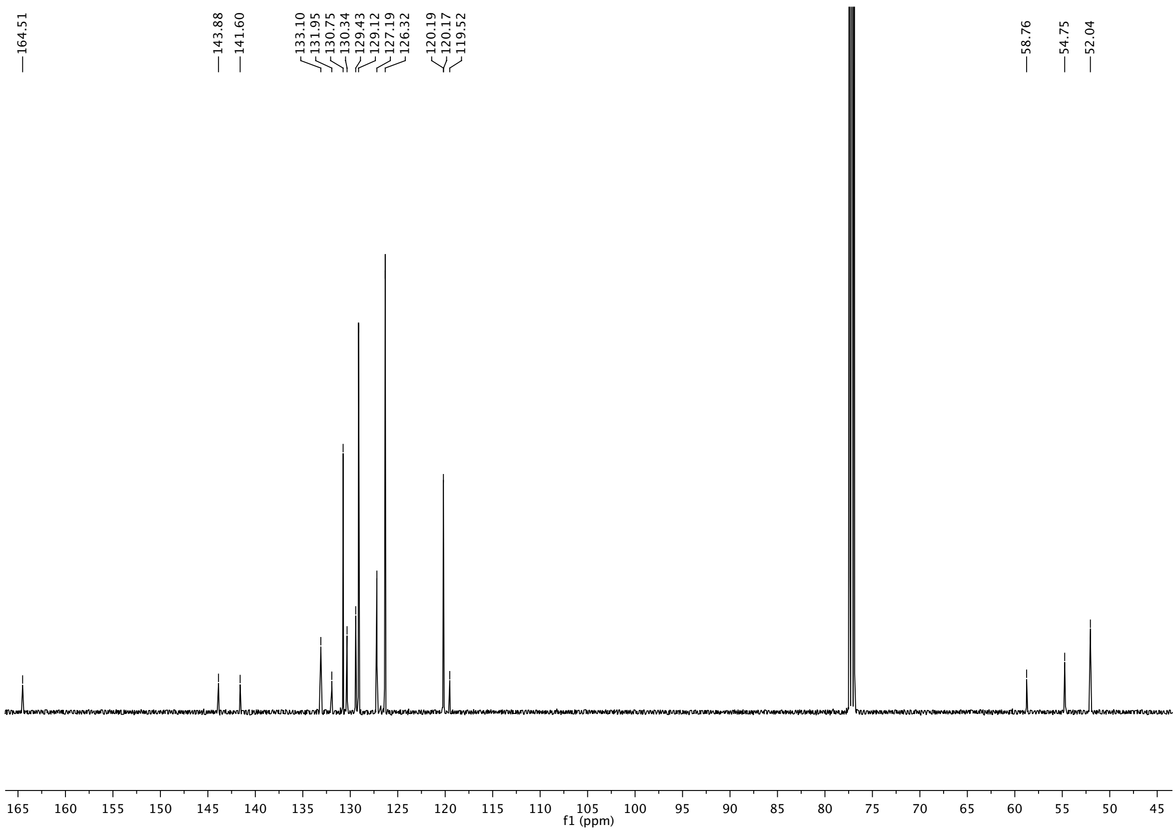
[1]H and [13]C NMR spectra of **18** (mixture of isomers) in $CDCl_3$:

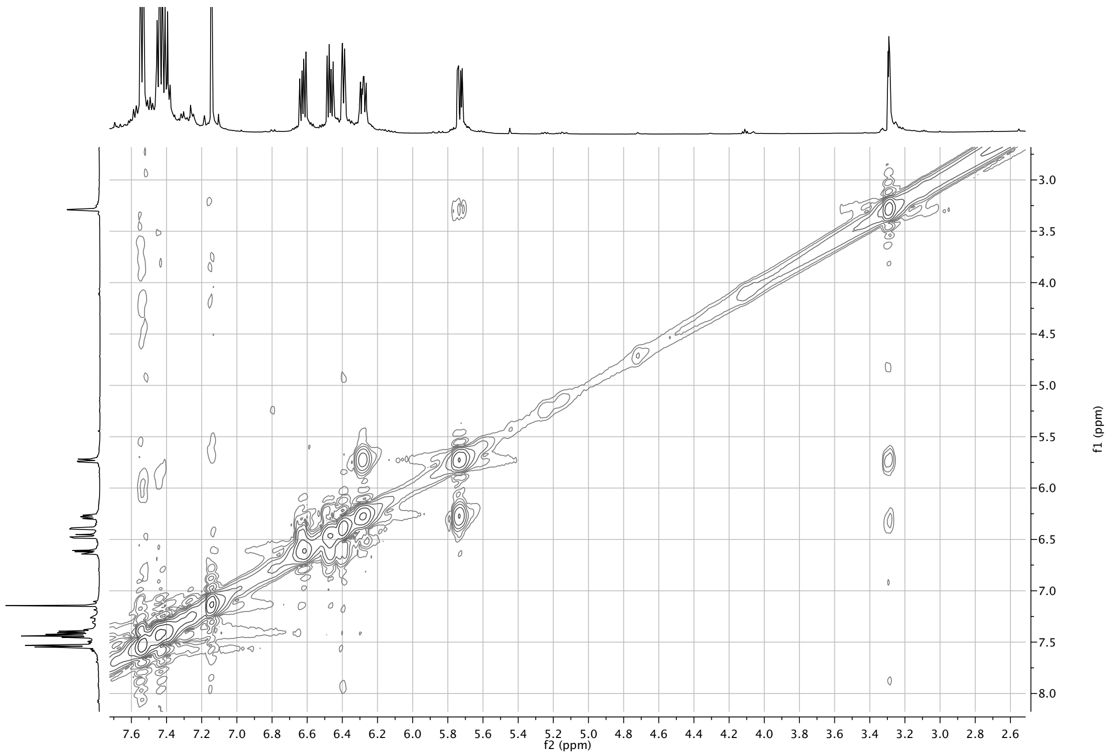




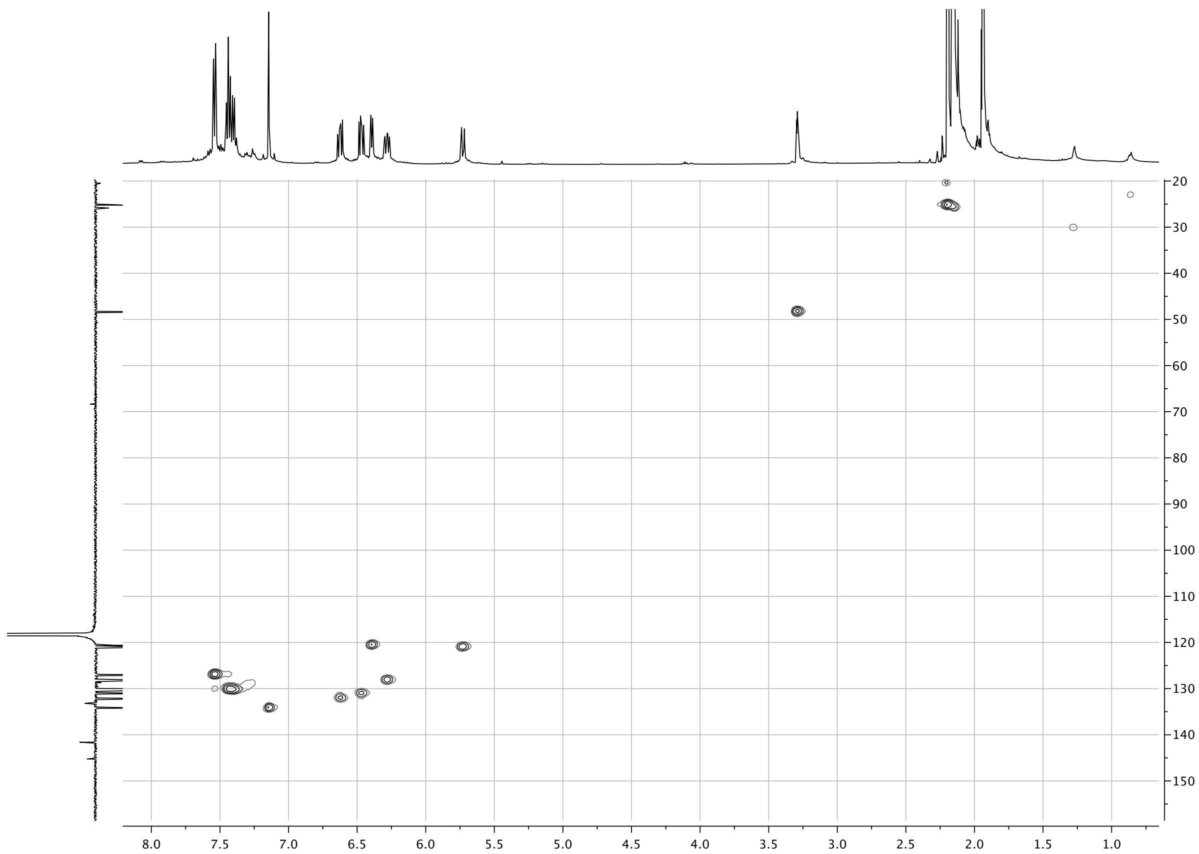
^{1}H, ^{13}C, gCOSY and gHSQC NMR of **19** in CD_3CN:



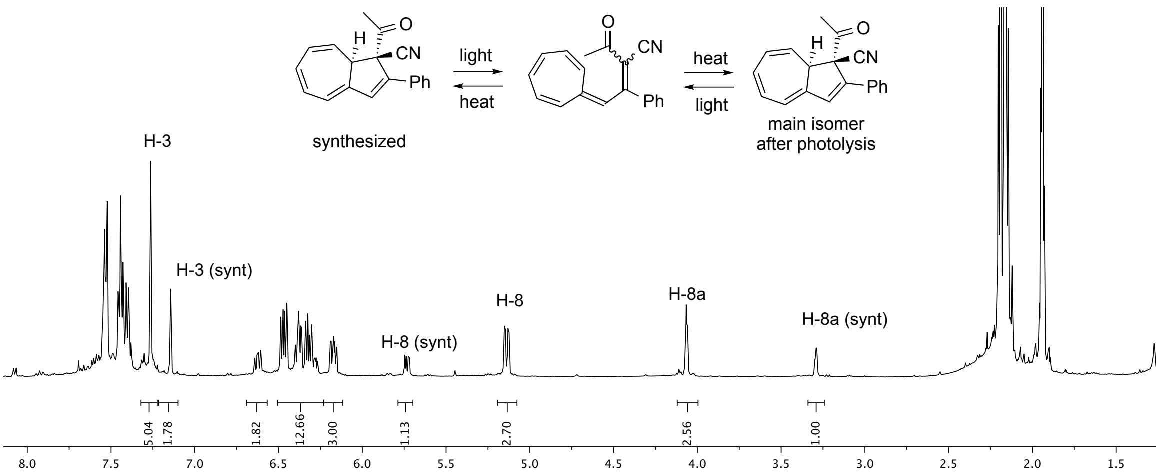




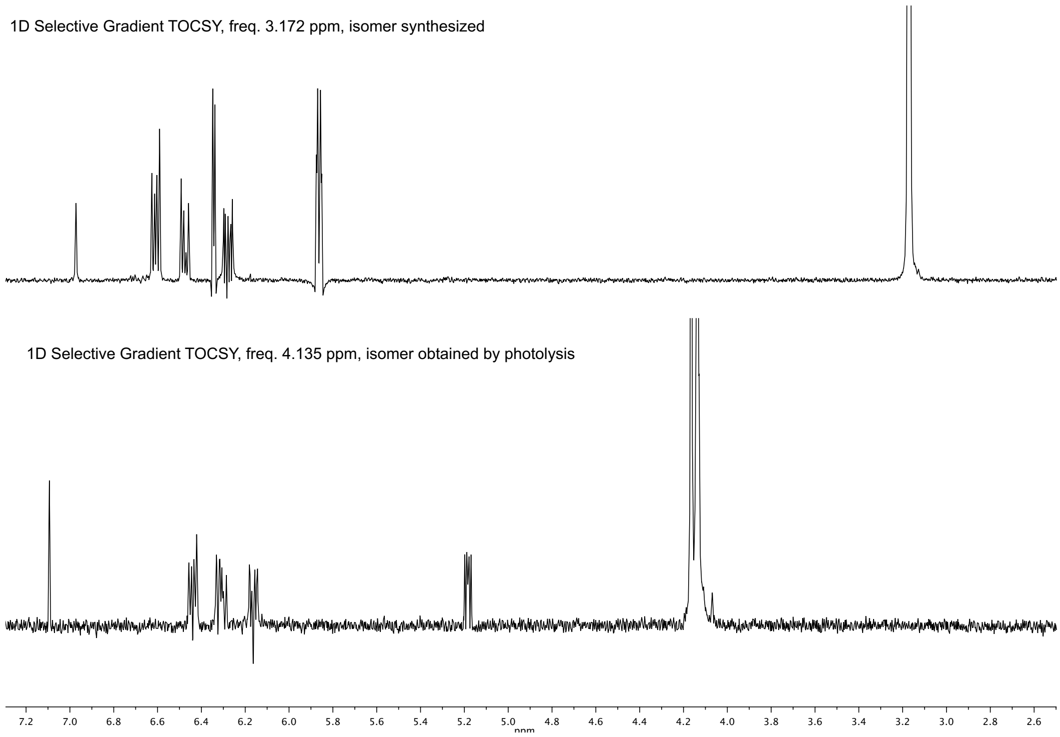
f1 (ppm)
f2 (ppm)



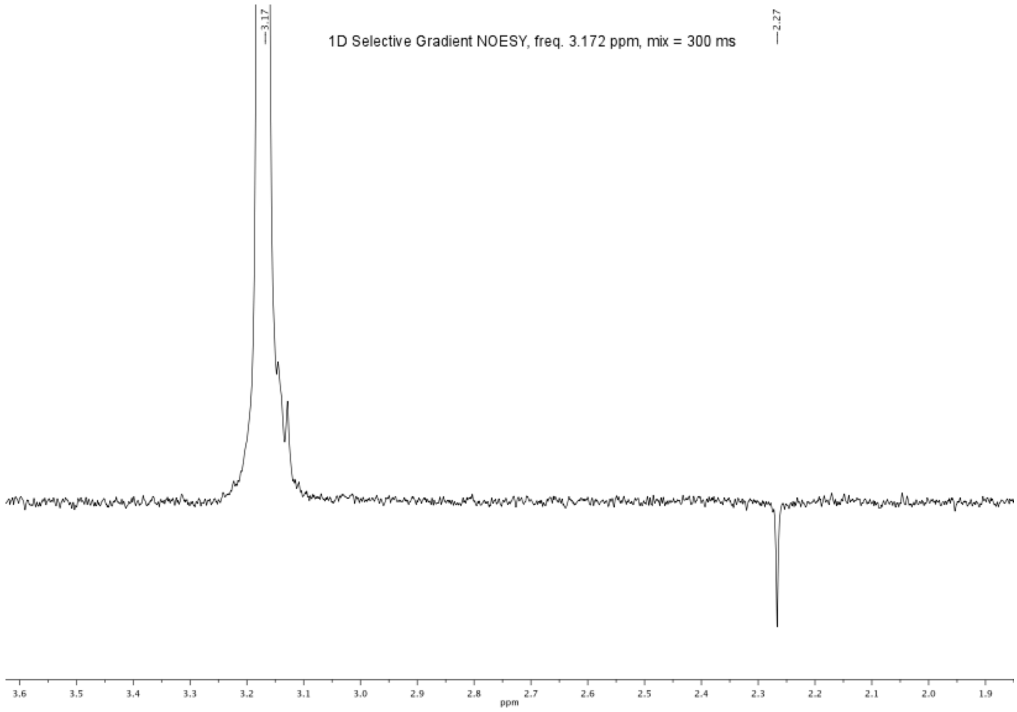
^{1}H NMR spectrum of **19** in CD_3CN after photolysis, showing the presence of a new main diastereomer. The more significant signals are highlighted to distinguish between the initial diastereomer (synt) and the second, which is the result of the photolysis ring closure.

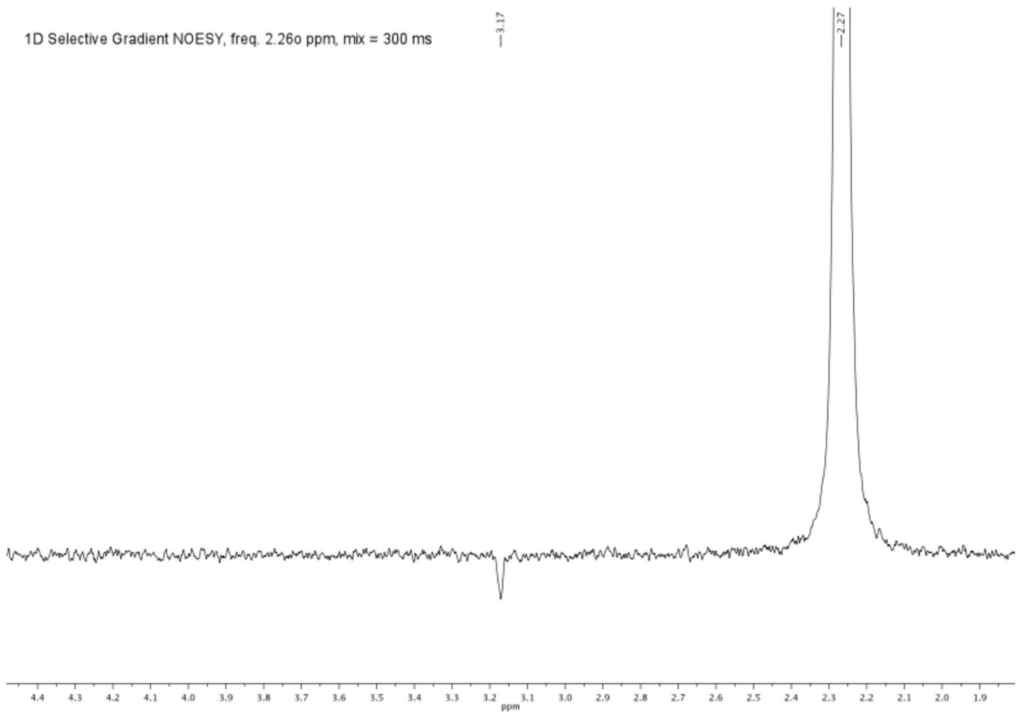


TOCSY-1D experiments of **19** isomers in CD_3CN, showing the different spin systems of dihydroazulene in the two diastereomers (excitation on H-8a; top: isomer synthesized, bottom: main isomer obtained after photolysis).

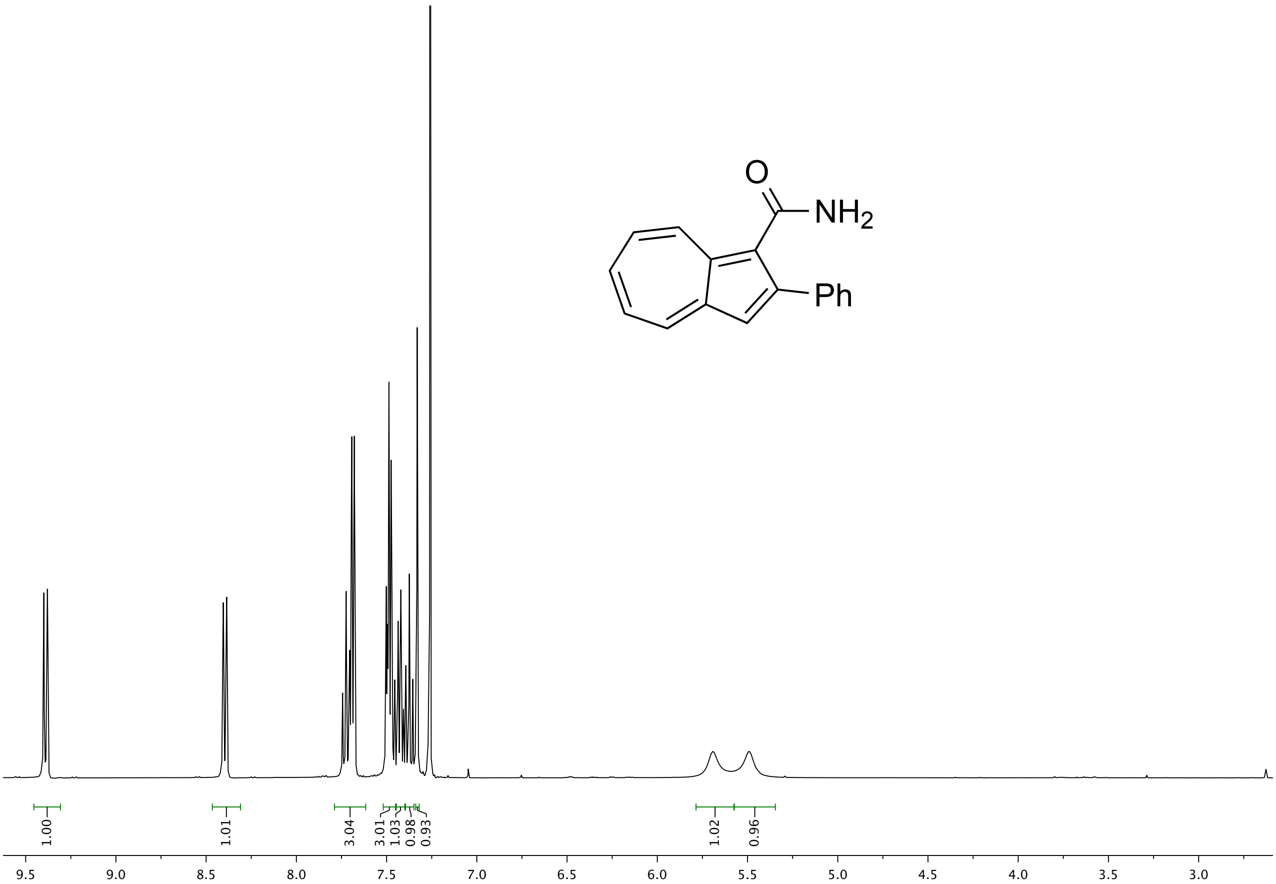


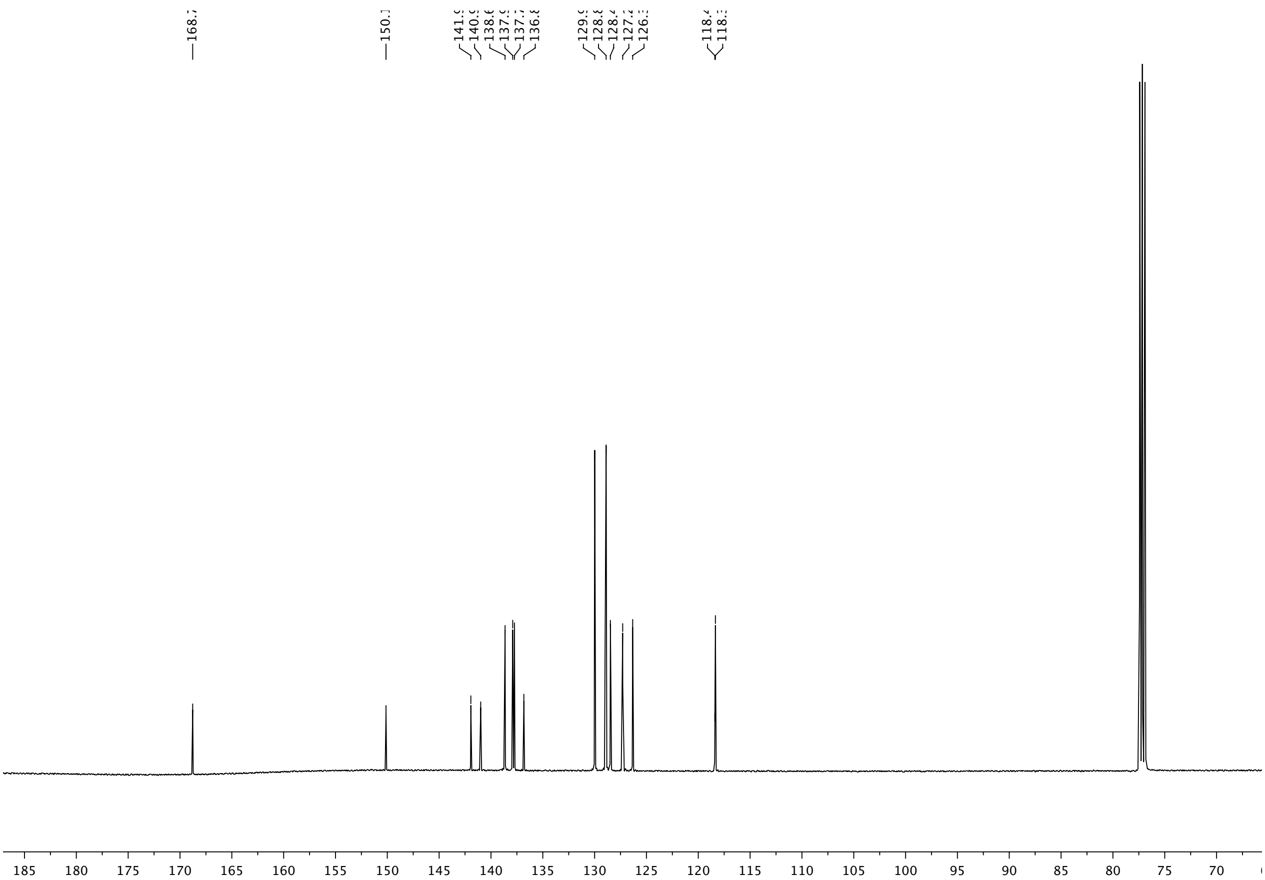
NOESY-1D experiments in CD_3CN on **19** diastereomer synthesized, showing n.O.e. between the acetyl group and H-8a (bottom) and viceversa (top).



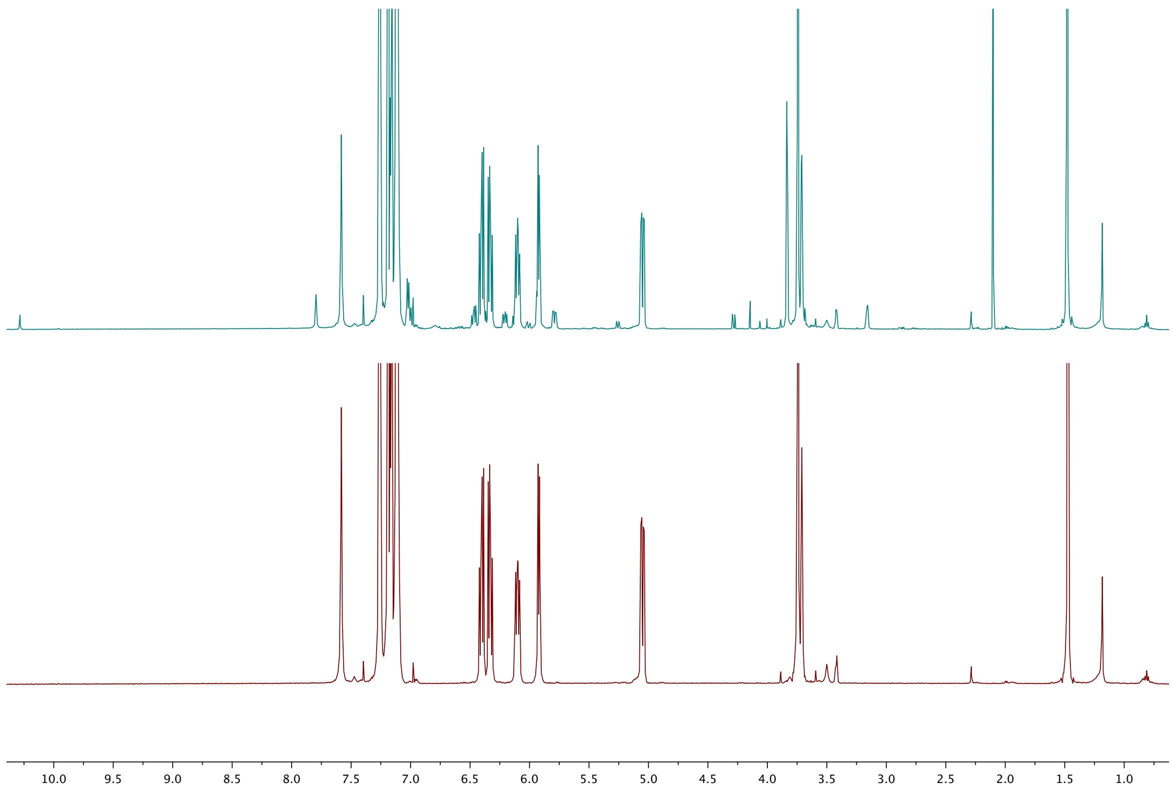


¹H and ¹³C NMR spectra of **2-Ph-azulene-amide** in $CDCl_3$:

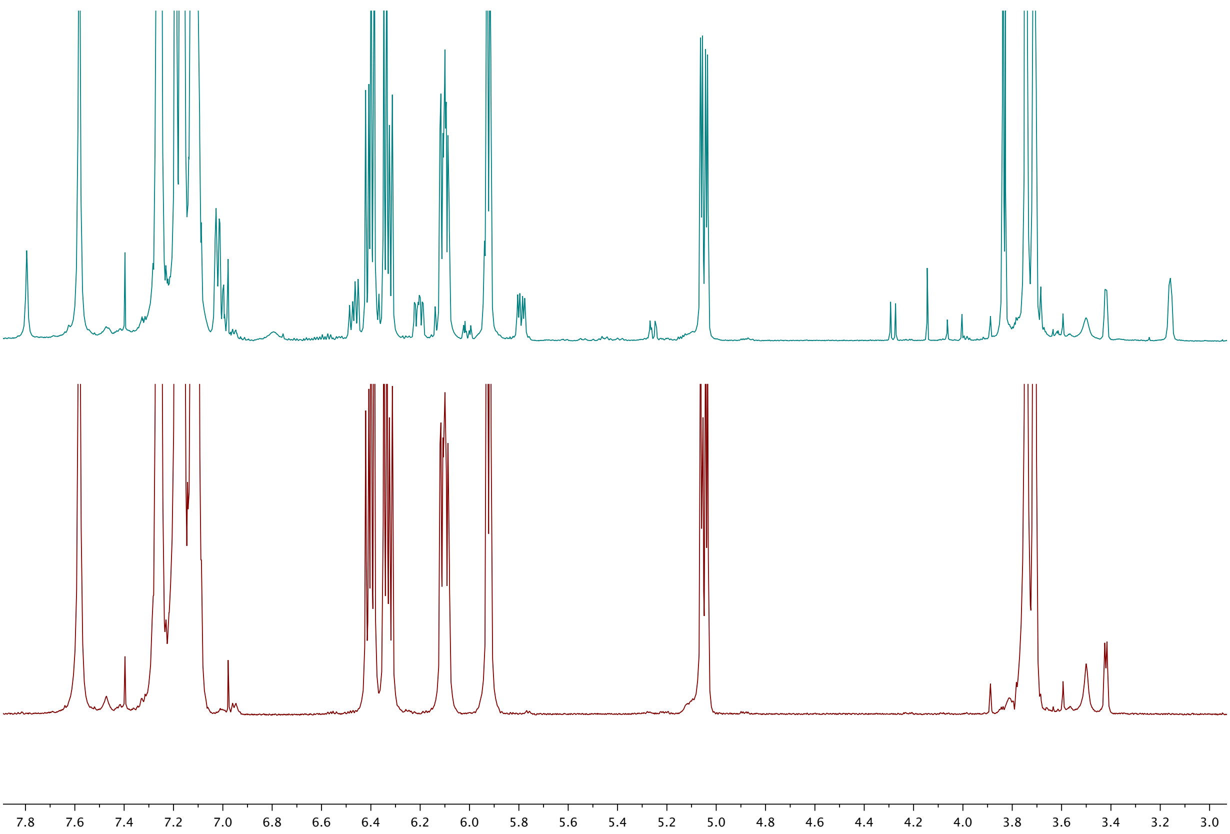




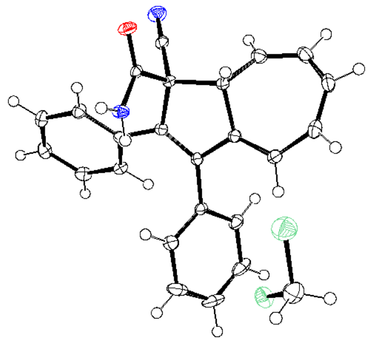
^{1}H-NMR spectra at 500 MHz in $CDCl_3$ of compound **13b** before (bottom) and after 1 h of irradiation (top).



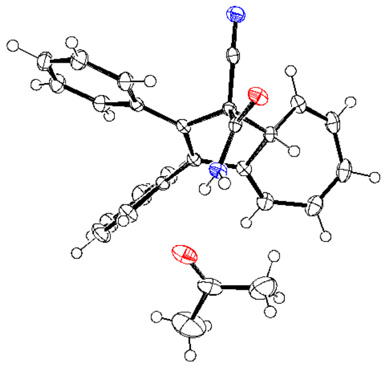
Expansion:



Molecular structure of **12a**, crystals grown from CH_2Cl_2; CCDC 1454795.

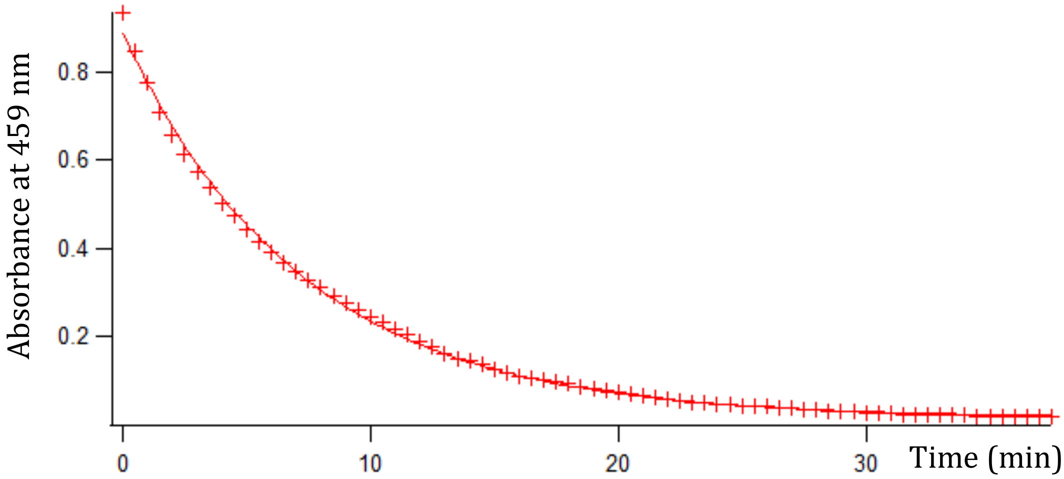


Molecular structure of **12a** co-crystallized with one molecule of acetone (crystals grown from CH_2Cl_2/acetone); CCDC 1454796.

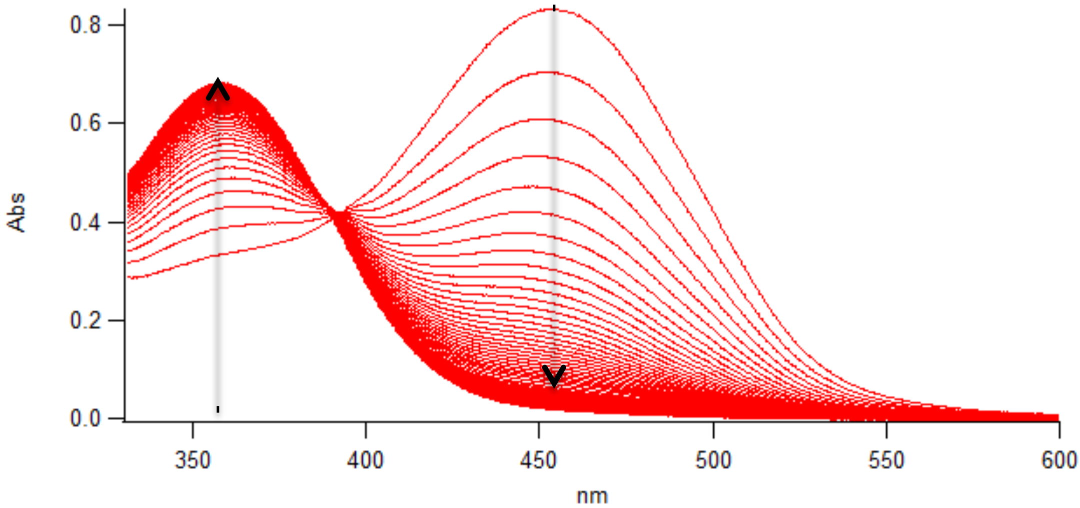


Kinetics Experiments – VHF to DHA conversions

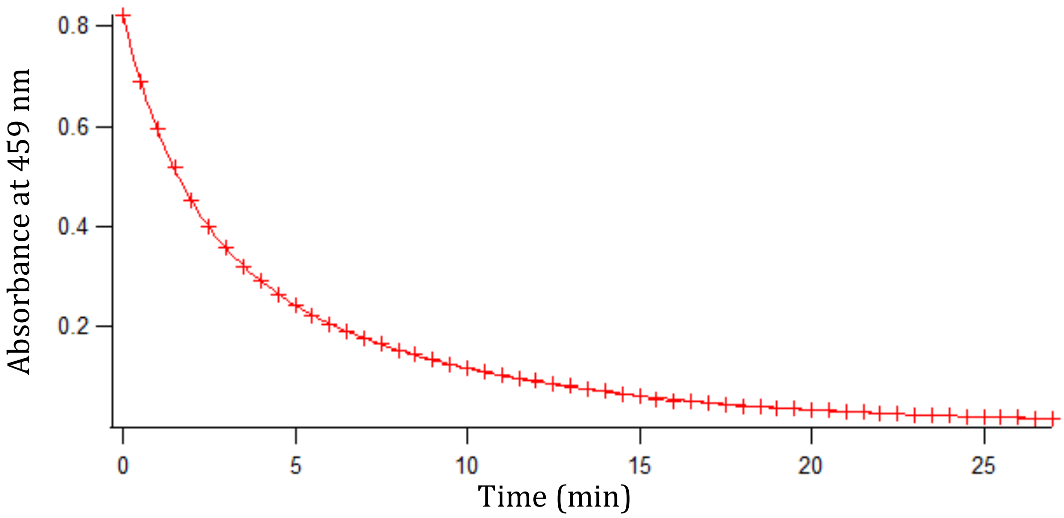
Fit with exponential decay of VHF of **19** formed after the 1st DHA to VHF conversion in cyclohexane at 25 °C



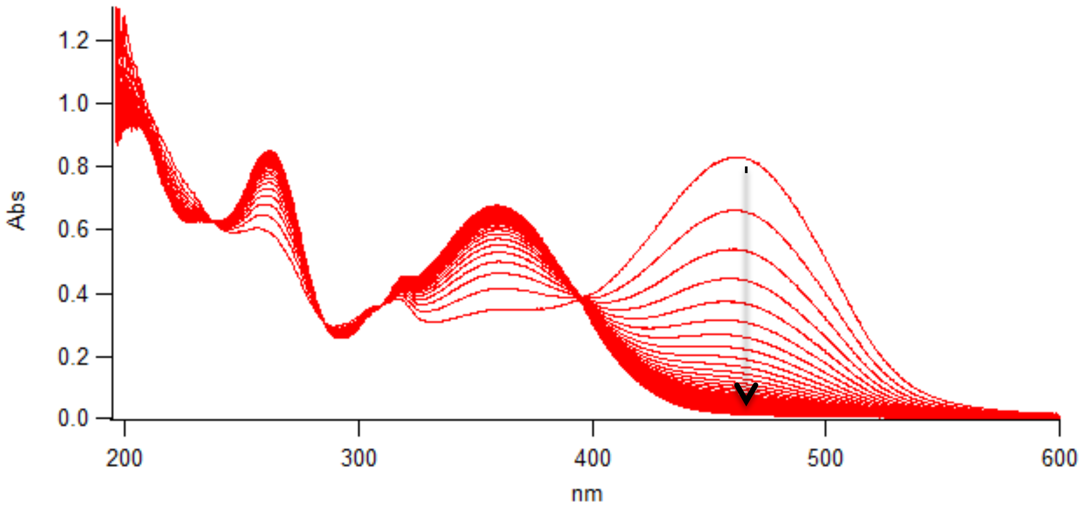
UV-Vis absorption spectra showing conversion of VHF to DHA **19** in 2nd cycle in cyclohexane at 25 °C.



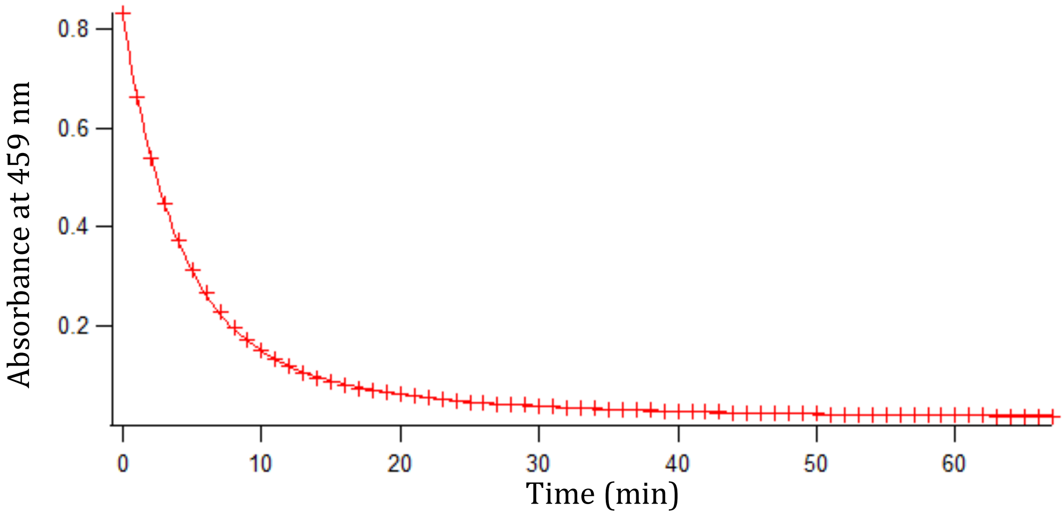
Fit with double-exponential decay of of VHF of **19** formed after the 2nd DHA to VHF conversion:



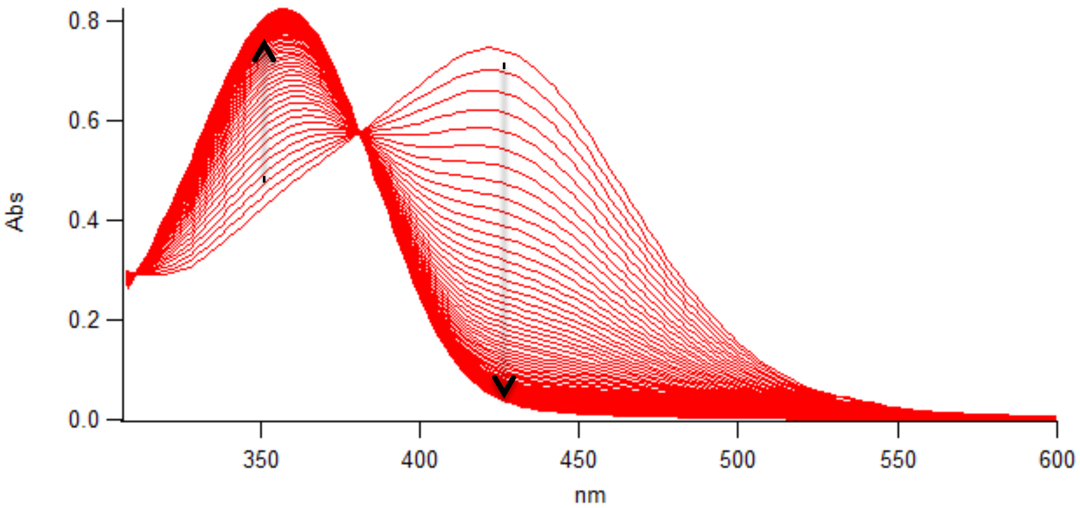
UV-Vis absorption spectra showing conversion of VHF to DHA **19** in 6th cycle in cyclohexane at 25 °C.



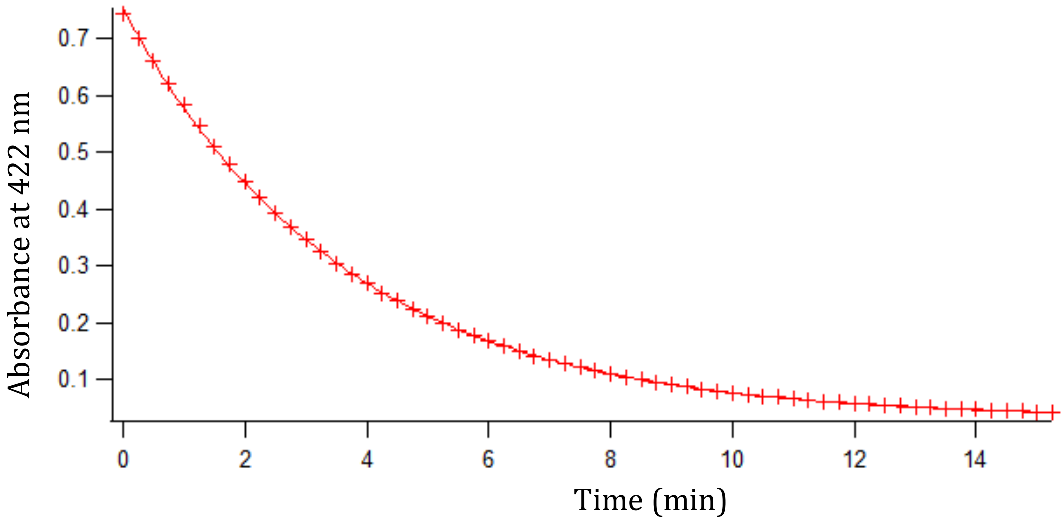
Fit with double-exponential decay of of VHF of **19** formed after the 6th DHA to VHF conversion:



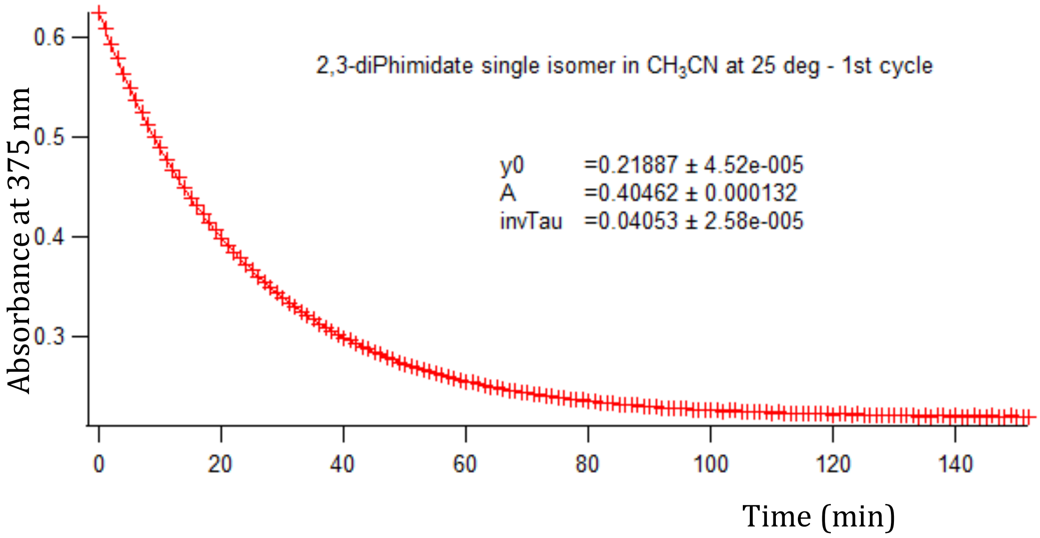
UV-Vis absorption spectra showing conversion of VHF to DHA **10** in CH_3CN at 25 °C (starting from a diastereomerically pure sample of **10a**).



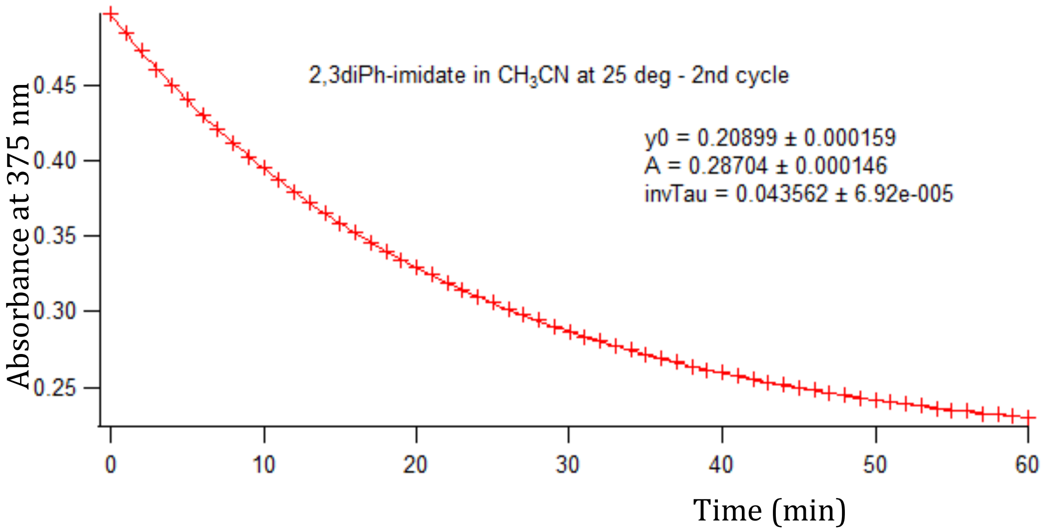
Fit with exponential decay of VHF of **10a** formed after the 1st DHA to VHF conversion.



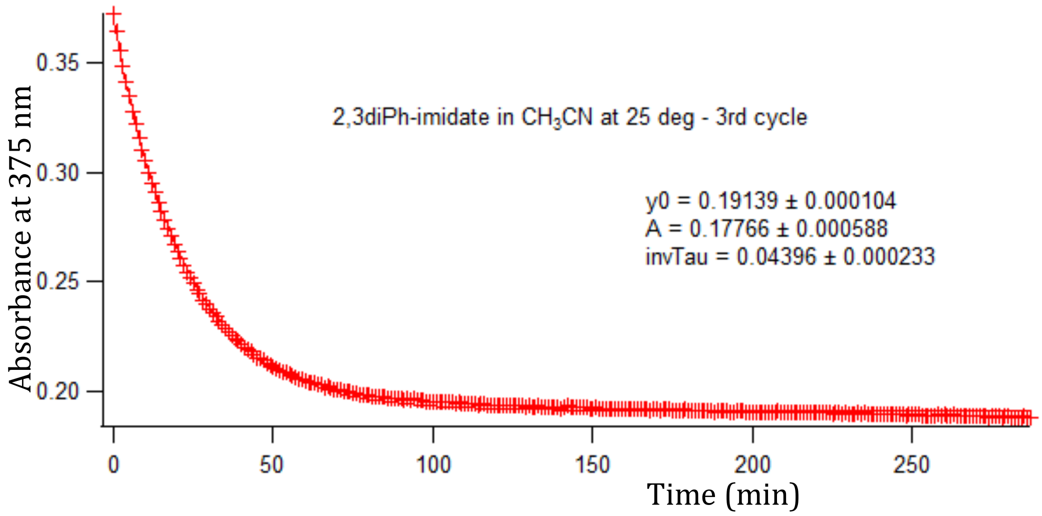
Fit with exponential decay of VHF of **13** in CH_3CN at 25 °C formed after the 1st DHA to VHF conversion (starting from a diastereomerically pure sample of **13b**)



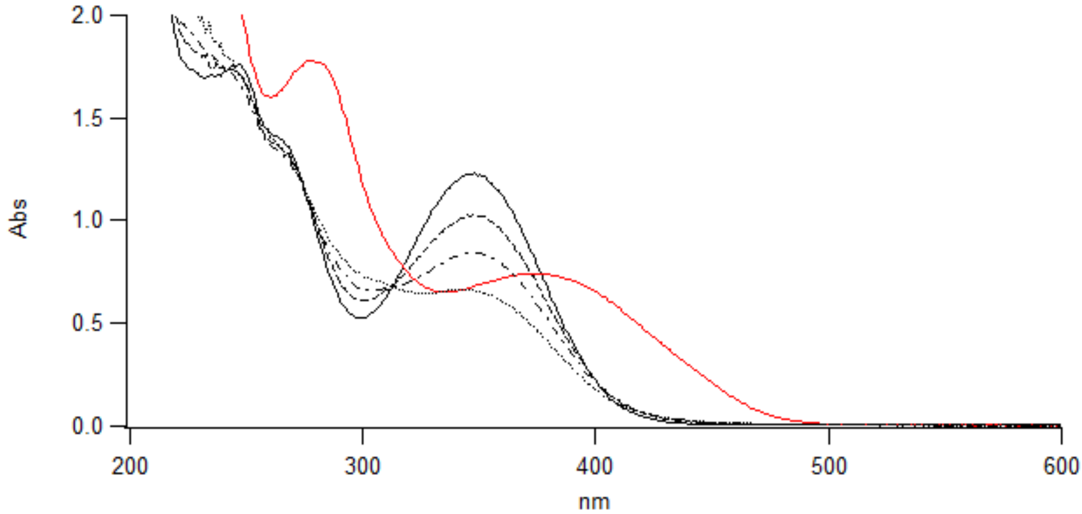
Fit with exponential decay of VHF of **13** in CH_3CN at 25 °C formed after the 2nd DHA to VHF conversion



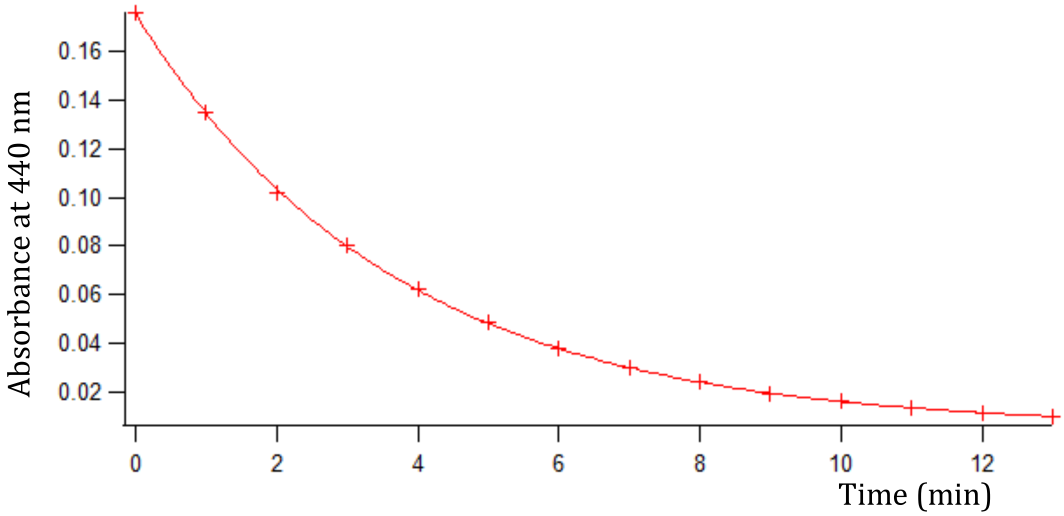
Fit with exponential decay of VHF of **13** in CH_3CN at 25 °C formed after the 3rd DHA to VHF conversion.



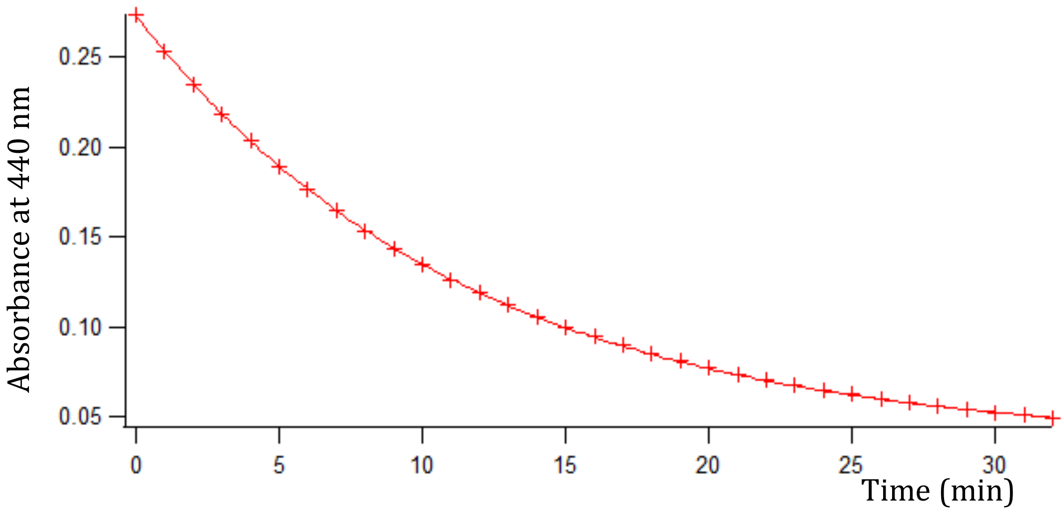
UV-Vis absorption spectra of VHF (red) and DHA (black, full line: before 1st cycle, ---: after 1st cycle, -·-·: after 2nd cycle, ·····: after 3rd cycle) **13** in CH_3CN at 25 °C, showing the fatigue resistance and the not complete reversibility of the switching (initial solution prepared with a diastereomerically pure sample of **13b**).



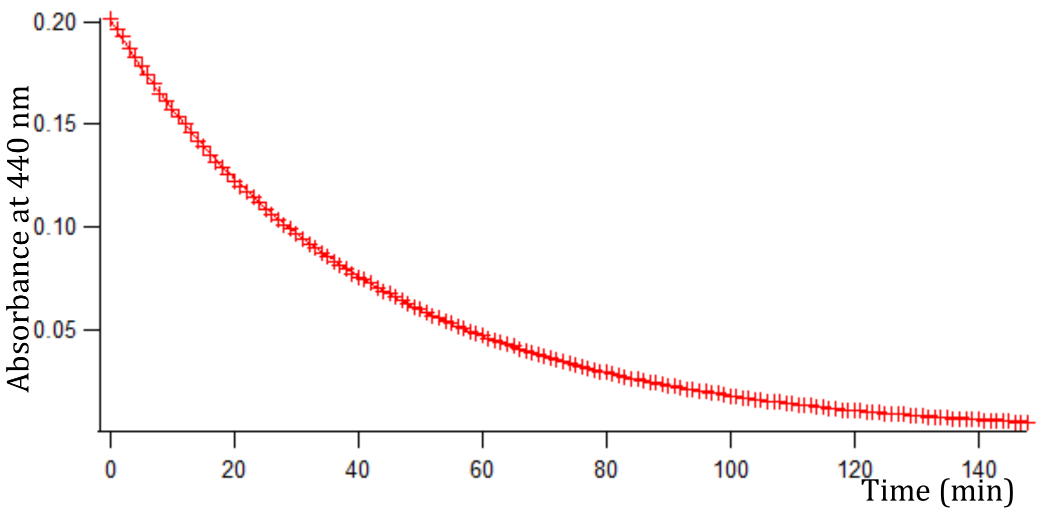
Fit with exponential decay of VHF of **12** in CH_2Cl_2 at -30 °C



Fit with exponential decay of VHF of **12** in CH_2Cl_2 at -40 °C

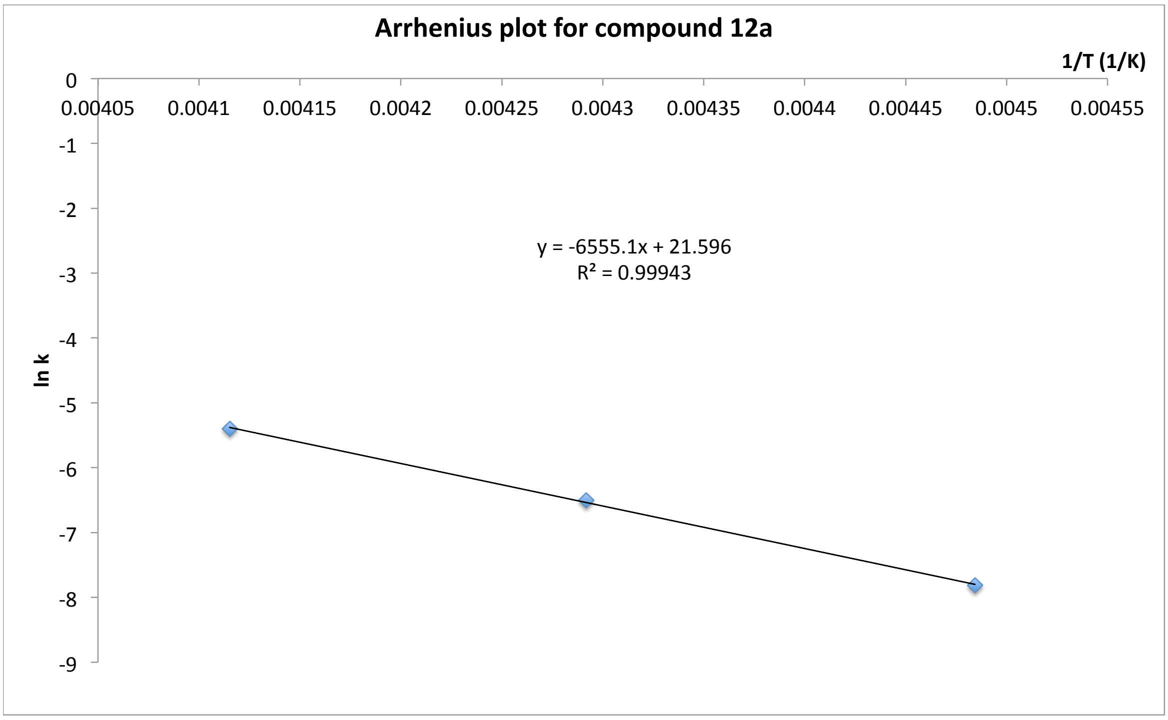


Fit with exponential decay of VHF of **12** in CH_2Cl_2 at -50 °C



Arrhenius Plot for compound **12a** (kinetic constants evaluated at -30, -40 and -50 °C). [k]: s^{-1}

Temp Celsius	Temp Kelvin	x=1/T	y=ln k	k (1/s)
-30	243	0.00411523	-5.3971632	0.00452941
-40	233	0.00429185	-6.5041786	0.00149717
-50	223	0.0044843	-7.8150863	0.0004036



DHA stereoisomers

The Gibbs free energy difference between the lowest identified (R,R)-DHA and (R,S)-DHA isomers. Values are presented in kJ/mol using M06-2X/6-311+G(d) in vacuum. In all cases were the (R,S) isomer most stable.

Ketone	5.8
Amide	6.5
Imidate	3.9

VHF s-cis/s-trans conformations

The Gibbs free energy difference between the lowest identified *s-cis* and *s-trans* VHF conformations. Values are presented in kJ/mol using M06-2X/6-311+G(d) in vacuum.

	Lowest conf	Gibbs diff
Ketone	*s-trans*	11.4
Amide	*s-trans*	12.7
Imidate	*s-trans*	2.9

Dipole moments

The dipole moments for all species calculated using M06-2X/6-311+G(d).

	DHA	*s-trans*	*s-cis*	TS
ketone	5.9	6.1	5.1	6.5
Amide	0.4	4.6	3.9	4.3
Imidate	3.3	7.1	4.6	6.0

Energy storage

The Gibbs free energy difference between the lowest identified DHA and VHF conformations. The corresponding enthalpies are given in the parenthsis. Values are presented in kJ/mol calculated using M06-2X/6-311+G(d).

sub	ketone	Amide	Imidate
vacuum	-46.9 (-55.2)	-46.6 (-54.6)	-55.2 (-62.8)
ch	-46.1 (-54.3)	-47.8 (-55.0)	-53.3 (-61.5)
an	-42.9 (-52.0)	-47.1 (-57.3)	-51.6 (-59.8)

Thermal back reaction (TBR)

The Gibbs free energy reaction barrier from the lowest identified s-cis conformation to the transition state. Values are presented in kJ/mol using PBE0/6-311+G(d).

	parent	-H	ketone	Amide	Imidate
vacuum	105.9	112.0	77.6	80.8	88.5
ch	102.2	110.9	70.6	77.1	85.7
an	93.5	109.7	62.9	70.4	78.3

Molecular geometries

The lowest identified free energy structures, presented at the M06-2X/6-311+G(d) level of theory in vacuum.

C1 - ketone - DHA

C	-4.57841900	-0.42518300	-0.29150300
C	-4.10755200	-1.37854700	0.55207400
C	-2.75406400	-1.88190200	0.58540200
C	-1.66852700	-1.15189200	0.25548800
C	-1.73023800	0.33302800	-0.01656400
C	-2.51221100	0.53821300	-1.28669600
C	-3.81940100	0.23859400	-1.33509600
C	-0.28712900	-1.58053500	0.17230200
C	0.55669600	-0.54982100	-0.02111600
C	-0.21988000	0.77291100	-0.03249100
C	0.12443900	1.58892100	-1.19862500
N	0.39122000	2.20032400	-2.13328000
C	0.03400800	1.59871500	1.26382800
C	-0.00109000	0.81826700	2.55424000
H	-2.61457000	-2.91758100	0.88433300
H	-2.01569200	0.95570500	-2.15639900
C	2.01949000	-0.60266300	-0.13507000
C	2.80281100	0.54989600	0.00450000
C	2.66771400	-1.82386100	-0.37248700
C	4.18993400	0.47725400	-0.06667900
H	2.34264200	1.51950300	0.15978100
C	4.04966000	-1.89325900	-0.44359600
H	2.08327400	-2.72433200	-0.52360400
C	4.81845000	-0.74162500	-0.28636700
H	4.77625000	1.38232800	0.04225400
H	4.53052800	-2.84650000	-0.63208900
H	5.89945400	-0.79532400	-0.34733300
H	-4.36891800	0.49785600	-2.23590300
H	-2.26661100	0.83940300	0.79627800
H	-4.83132200	-1.89130500	1.17930400
H	-5.64762900	-0.23385200	-0.27769700
H	-0.80985000	0.08458400	2.57200300
H	-0.09413400	1.51284300	3.38635600
H	0.93805700	0.26442800	2.64952400
O	0.22749400	2.78082700	1.21759900
H	0.01190000	-2.61570600	0.28607200

C1 - ketone - s-trans-VHF

C	4.42702700	0.04832900	-0.33356400

C	3.21125300	0.52016500	-0.94501400
C	1.95009400	0.04356900	-0.84868100
C	1.43906600	-1.08635800	-0.07692500
C	2.32730300	-2.19221600	0.26065800
C	3.67116400	-2.21546300	0.40822200
C	4.62960100	-1.15214300	0.25268900
C	0.11087400	-1.26149500	0.21906200
C	-0.95825400	-0.30115600	0.09856500
C	-2.28166400	-0.68171400	0.03789600
C	-3.31216700	0.30914700	0.14226300
N	-4.18245200	1.06059800	0.22412100
C	-2.76538200	-2.08892600	-0.11210200
C	-4.26032300	-2.30409200	-0.04934200
H	1.20498900	0.57650000	-1.42760100
H	1.80979000	-3.12545900	0.46800900
H	4.09021200	-3.16544800	0.72780800
C	-0.62840900	1.15042800	0.14655000
C	0.19919700	1.64328800	1.15862900
C	-1.11320600	2.02721800	-0.82679800
C	0.53379400	2.99034900	1.19717900
H	0.57960100	0.96285900	1.91281900
C	-0.76155500	3.37094600	-0.79798500
H	-1.75383000	1.65120000	-1.61704500
C	0.06129800	3.85530600	0.21399600
H	1.16808900	3.36462100	1.99264400
H	-1.13595100	4.04096500	-1.56338500
H	0.32940400	4.90568700	0.23970300
H	5.63207400	-1.36915300	0.60879300
H	3.32726500	1.40457500	-1.56558400
H	5.28099000	0.71421700	-0.41224800
H	-4.66933200	-1.92362600	0.88967900
H	-4.46389900	-3.36828100	-0.14336600
H	-4.76149500	-1.75800100	-0.85243600
O	-2.00778800	-3.01873000	-0.28582900
H	-0.17668600	-2.23608900	0.58820000

C1 - ketone - s-cis-VHF

C	-4.62932100	-0.23882300	0.80280100
C	-3.37818500	0.30654100	1.24710000
C	-2.11807800	0.06448000	0.81522000
C	-1.63292000	-0.84026100	-0.20789400
C	-2.47182000	-1.88842600	-0.75461000
C	-3.81386600	-2.06605200	-0.69446500
C	-4.82046700	-1.27785500	-0.04345700
C	-0.31179600	-0.83905500	-0.59705200
C	0.76344100	0.03551300	-0.21687800
C	0.70217500	1.40394800	-0.02000400
C	1.82558400	2.07903700	0.56358800
N	2.68133100	2.67540200	1.05472400
C	-0.38048400	2.30164600	-0.51244700
C	-0.10849900	3.78952400	-0.45514600
H	-1.33506900	0.62003500	1.32164300
H	-1.92987600	-2.62440200	-1.34315500
H	-4.19308600	-2.92267200	-1.24469200
C	2.07740400	-0.65888900	-0.08432100
C	2.15472900	-1.85157100	0.64053300
C	3.22945800	-0.16377100	-0.70073600
C	3.36486200	-2.52192200	0.77010500
H	1.26115100	-2.24019800	1.11773100
C	4.43493600	-0.84371100	-0.58576100
H	3.17813000	0.74997800	-1.28218700
C	4.50695600	-2.01955900	0.15478000

H	3.41526400	-3.43580800	1.35119900
H	5.32030900	-0.45281100	-1.07376800
H	5.45143700	-2.54341500	0.25039700
H	-5.84617900	-1.57464400	-0.23953700
H	-3.46326100	1.04746900	2.03696700
H	-5.51626300	0.22202300	1.22665300
H	0.03075200	4.11437700	0.57925600
H	-0.95390800	4.31201600	-0.89716900
H	0.80939600	4.04580400	-0.98870100
O	-1.42168600	1.87749400	-0.96695100
H	0.01073300	-1.69027400	-1.19022800

C1 - ketone - TS

C	4.47931500	-1.25614500	0.52021700
C	3.66412300	-2.27248600	0.07708800
C	2.36051800	-2.19182600	-0.43150200
C	1.58315600	-1.07949900	-0.68502500
C	2.04331800	0.28110700	-0.73036600
C	3.21345900	0.79164400	-0.15693500
C	4.25442100	0.12533400	0.45197800
C	0.16126400	-1.23736400	-0.84611900
C	-0.66098400	-0.29610000	-0.32535600
C	-0.12036800	0.98638800	0.19700800
C	-0.17587700	1.12438900	1.60724000
N	-0.15810400	1.21049300	2.75900600
H	1.86676800	-3.14709600	-0.58987300
H	1.55740100	0.89552700	-1.47545300
H	3.32292900	1.86998100	-0.23132500
H	-0.23184100	-2.18883000	-1.18754900
C	-2.10192900	-0.57870900	-0.13724900
C	-3.03629200	0.44793700	-0.29026400
C	-2.56335500	-1.85779600	0.18535300
C	-4.39237500	0.19732800	-0.15038400
H	-2.69541500	1.44303000	-0.54773400
C	-3.91832400	-2.10606300	0.33535100
H	-1.85238900	-2.65734300	0.35901500
C	-4.83784600	-1.07949000	0.16315900
H	-5.10416600	1.00386400	-0.28574600
H	-4.25743000	-3.10096000	0.60190600
H	-5.89812300	-1.27282100	0.28245800
H	5.04776400	0.74986200	0.85048600
C	-0.05039700	2.18205600	-0.61221000
H	4.05057000	-3.27926500	0.20057100
H	5.42399300	-1.55909800	0.96028100
O	-0.10214600	2.14097400	-1.84050900
C	0.13054700	3.50634700	0.09950600
H	0.32894500	4.27936800	-0.64053000
H	0.94273300	3.47040100	0.82896200
H	-0.77208500	3.76982300	0.65661400

C1 - Amide - DHA

C	4.56927500	-0.49055500	0.29305200
C	4.11550100	-1.35822800	-0.64671700
C	2.76290700	-1.85265000	-0.76114300
C	1.66939500	-1.15276200	-0.39833600
C	1.72981000	0.29794000	0.01811600
C	2.47793100	0.37368900	1.32190000
C	3.78400400	0.07014300	1.37687000
C	0.28655700	-1.58255000	-0.38294900
C	-0.55791800	-0.57742300	-0.09804400
C	0.21900900	0.73501700	0.04010400

C	-0.15120600	1.45482900	1.26081600
N	-0.43499000	2.06404600	2.19363900
C	-0.00433000	1.62019100	-1.22251200
H	2.63033800	-2.85259100	-1.16553600
H	1.95894500	0.69344000	2.22023200
C	-2.01743000	-0.64823500	0.03156900
C	-2.82204500	0.48583900	-0.12525600
C	-2.63888700	-1.87082300	0.32054500
C	-4.20491100	0.39532400	-0.01990900
H	-2.37802200	1.45156700	-0.34105600
C	-4.01853200	-1.96027900	0.42384400
H	-2.03190900	-2.75337000	0.48939000
C	-4.80874800	-0.82652100	0.25111600
H	-4.81031700	1.28525200	-0.14902500
H	-4.47974600	-2.91474600	0.65120100
H	-5.88727400	-0.89490300	0.33737000
H	4.30703300	0.23375600	2.31527700
H	2.27550900	0.87334000	-0.73823800
H	4.85237100	-1.80882800	-1.30591400
H	5.63847700	-0.30108100	0.32166600
O	0.02609400	1.11415600	-2.31656600
H	-0.01655600	-2.59890000	-0.60465200
N	-0.16094100	2.94868400	-1.00732500
H	-0.24723200	3.54826000	-1.81289100
H	-0.19114200	3.35877200	-0.08788500

C1 - Amide - s-trans-VHF

C	4.61974300	-1.10511000	0.26990900
C	3.67885900	-2.18984600	0.39052200
C	2.33699300	-2.18494400	0.23022000
C	1.43645100	-1.08153900	-0.08861300
C	1.93811000	0.05746000	-0.85607900
C	3.19191000	0.55431900	-0.93396500
C	4.40536100	0.09915000	-0.30331100
C	0.11443600	-1.26849800	0.21550400
C	-0.96379300	-0.31311300	0.09753100
C	-2.28170800	-0.69357400	0.03982300
C	-3.31791000	0.28861400	0.13799300
N	-4.22091600	1.00188000	0.21635800
C	-2.74995500	-2.11395800	-0.10238400
H	1.83072000	-3.13023800	0.40898300
H	1.19195400	0.57652900	-1.44634200
H	3.30399700	1.44095300	-1.55217200
C	-0.64434000	1.14173800	0.14360100
C	0.17489600	1.64215200	1.15851700
C	-1.13166700	2.01306200	-0.83302500
C	0.49725900	2.99213900	1.19744500
H	0.55940300	0.96486500	1.91343200
C	-0.79317700	3.36041900	-0.80304300
H	-1.76216600	1.62984800	-1.62813500
C	0.02063900	3.85264300	0.21222200
H	1.12598900	3.37226000	1.99455800
H	-1.16919600	4.02640000	-1.57119400
H	0.27974700	4.90526500	0.23821300
H	5.24783200	0.78193500	-0.35780700
H	4.11187600	-3.13963100	0.69161400
H	5.61949400	-1.30834300	0.64173700
O	-1.99243300	-3.05061700	-0.27276400
H	-0.16742500	-2.24492000	0.58408900
N	-4.09731100	-2.28943900	-0.03448500
H	-4.44612100	-3.22736700	-0.14431300
H	-4.75170600	-1.53639300	0.09913600

C1 - Amide - s-cis-VHF

C	-4.59941300	-0.21509700	0.72392200
C	-3.35514300	0.34749600	1.17816000
C	-2.08703900	0.06882600	0.80262000
C	-1.57859700	-0.89900300	-0.15388600
C	-2.40364100	-2.00486900	-0.61307700
C	-3.74461700	-2.17669000	-0.56976400
C	-4.76937300	-1.32002600	-0.03510900
C	-0.26769000	-0.89821300	-0.55575800
C	0.79132100	0.03451100	-0.24879700
C	0.67338500	1.39603300	-0.11119600
C	1.75558000	2.16017900	0.43063100
N	2.55436300	2.86149500	0.87906000
C	-0.50863400	2.20488200	-0.56759200
H	-1.31685700	0.65167400	1.30002300
H	-1.84610100	-2.79560200	-1.10898300
H	-4.11236000	-3.08549400	-1.03791300
C	2.13016500	-0.60120200	-0.08912000
C	2.25695600	-1.75886300	0.68392000
C	3.26020200	-0.08406100	-0.72766800
C	3.49384400	-2.37241900	0.83770400
H	1.38017600	-2.16504500	1.17738600
C	4.49359300	-0.70730900	-0.58612900
H	3.16964900	0.79914800	-1.35026800
C	4.61450100	-1.84784600	0.20119400
H	3.58200500	-3.25981100	1.45428600
H	5.36160100	-0.30035500	-1.09194400
H	5.57981300	-2.32816400	0.31631700
H	-5.78969500	-1.62254700	-0.25001800
H	-3.45763400	1.13495900	1.91960400
H	-5.49529700	0.29310400	1.06740900
O	-1.35893500	1.76992400	-1.31465500
H	0.06658500	-1.76705400	-1.11554100
N	-0.57094500	3.47392100	-0.06668100
H	-1.26993400	4.07923300	-0.46710600
H	0.20321100	3.90067500	0.41701000

C1 - Amide - TS

C	4.13487200	-1.54629300	0.85719400
C	3.53588300	-2.33253600	-0.11468500
C	2.38011000	-2.06552200	-0.85467300
C	1.60204700	-0.91342300	-0.86426100
C	2.09536300	0.40679800	-0.48611100
C	3.03018600	0.66811900	0.51880300
C	3.85737900	-0.21693200	1.19303800
C	0.21669300	-1.00702700	-1.15956700
C	-0.62818800	-0.15200000	-0.48971900
C	-0.11947800	1.09598600	0.04756300
C	-0.40821600	1.38090300	1.41410700
N	-0.55444100	1.64867800	2.52912700
H	1.97786500	-2.90491700	-1.41868300
H	1.93189800	1.17863500	-1.22415200
H	3.14232100	1.71943100	0.77439100
H	-0.16888300	-1.91007200	-1.62180600
C	-2.01196400	-0.56981500	-0.17574500
C	-3.02499700	0.39226300	-0.08905300
C	-2.34169900	-1.91380000	0.03741700
C	-4.33382700	0.01891500	0.18504100
H	-2.78167400	1.43541900	-0.26025800
C	-3.65036600	-2.28681000	0.31201400
H	-1.55965700	-2.66510500	0.02521700

C	-4.65047600	-1.32122200	0.38395600
H	-5.10847500	0.77503000	0.24371200
H	-3.88805000	-3.33009700	0.48711100
H	-5.67179400	-1.61162500	0.60378300
H	4.46647700	0.20908700	1.98418700
C	0.10117900	2.26489900	-0.83348700
H	3.95155700	-3.32727800	-0.24258200
H	4.94220200	-2.01476300	1.41206400
O	0.15371100	2.17758900	-2.04895200
N	0.33074800	3.45826000	-0.19350000
H	0.07210800	3.58703100	0.77266900
H	0.32325400	4.27493700	-0.78442300

C1 - Imidate - DHA

C	4.50229100	-0.95911600	0.24851600
C	4.04119100	-1.52537200	-0.89546000
C	2.67224700	-1.90861300	-1.15299300
C	1.60087200	-1.27832900	-0.62989100
C	1.70544900	0.01047500	0.15060000
C	2.42255600	-0.29274200	1.43849700
C	3.71253900	-0.66244200	1.42933200
C	0.20356500	-1.65140900	-0.72532100
C	-0.61150000	-0.72295100	-0.19109100
C	0.20959000	0.49026800	0.25956200
C	-0.15492200	0.90272800	1.62047200
N	-0.44089100	1.18354800	2.69676700
C	0.04717000	1.67371000	-0.71026300
H	2.50811600	-2.76934400	-1.79628200
H	1.89495700	-0.18444700	2.38083200
C	-2.07409300	-0.78599900	-0.06968500
C	-2.84297300	0.36422700	0.14397000
C	-2.73397700	-2.01978100	-0.16417100
C	-4.22711000	0.28423300	0.24005400
H	-2.36831800	1.33462300	0.23568000
C	-4.11484700	-2.09726800	-0.07164400
H	-2.15797800	-2.93028000	-0.28581100
C	-4.86872000	-0.94335000	0.12860800
H	-4.80284400	1.18731000	0.40669100
H	-4.60445200	-3.06196100	-0.14340000
H	-5.94823000	-1.00410400	0.20768200
H	4.21924500	-0.76946100	2.38463100
H	2.29274600	0.74583100	-0.41045800
H	4.77696400	-1.82611000	-1.63609400
H	5.57764000	-0.83732300	0.34448700
H	-0.12711200	-2.57540700	-1.18524600
O	0.46408100	2.80255900	-0.12763600
C	0.45974100	3.96976800	-0.94687900
H	-0.54741000	4.16967900	-1.31311400
H	0.80763500	4.77594600	-0.30679500
H	1.12512000	3.83319600	-1.79992900
N	-0.33517300	1.63228100	-1.91085800
H	-0.62068600	0.69236400	-2.17643100

C1 - Imidate - s-trans-VHF

C	4.61918600	0.88870300	0.18998600
C	3.35251200	1.06616200	0.85683700
C	2.23933300	0.30372600	0.81434600
C	1.98508500	-0.92501800	0.06135400
C	3.10095800	-1.80424200	-0.27831700
C	4.40476900	-1.51190200	-0.47386700
C	5.08222000	-0.24200900	-0.38485600
C	0.73080200	-1.39191300	-0.21570700

C	-0.54561500	-0.72007600	-0.05844600
C	-1.69626500	-1.45144000	0.03040700
C	-1.63016700	-2.87390800	0.15845200
N	-1.58620200	-4.01981000	0.27355500
C	-3.07858700	-0.88630400	0.03851000
H	1.41156700	0.64698100	1.42437700
H	2.81542600	-2.84081700	-0.44047600
H	5.03157500	-2.34484500	-0.77947400
C	-0.60404600	0.76539900	-0.02855500
C	-1.26934000	1.42545200	1.00686400
C	0.02921100	1.51222200	-1.02183200
C	-1.29491000	2.81386400	1.05078000
H	-1.75847500	0.84612000	1.78434200
C	-0.01007500	2.90041000	-0.98546400
H	0.54965800	0.99891400	-1.82342500
C	-0.66637600	3.55462500	0.05348500
H	-1.80527400	3.31793100	1.86402300
H	0.47675400	3.47243600	-1.76733600
H	-0.68832000	4.63812300	0.08597300
H	6.09118500	-0.22003200	-0.78526100
H	3.28485400	1.95815700	1.47385400
H	5.28732300	1.74415900	0.21654400
H	0.66918600	-2.40091600	-0.61370600
O	-3.21005100	0.11358200	-0.84291900
C	-4.44972200	0.81135100	-0.81442900
H	-4.36242600	1.58914700	-1.56905200
H	-5.27453300	0.13601900	-1.04258000
H	-4.61284900	1.24723500	0.17296700
N	-4.04991100	-1.27450400	0.75354800
H	-3.77628900	-2.04767800	1.35555500

C1 - Imidate - s-cis-VHF

C	4.88052400	0.49714300	0.73424000
C	3.55139000	0.81756800	1.18908000
C	2.36391000	0.27920100	0.83764400
C	2.06114000	-0.79386900	-0.09882100
C	3.08239200	-1.76954200	-0.46252000
C	4.42901800	-1.68003600	-0.41041400
C	5.26441200	-0.59525300	0.04038800
C	0.78740300	-1.03006000	-0.54519200
C	-0.40343800	-0.22393000	-0.35923800
C	-0.42190200	1.14345600	-0.41341000
C	0.70086300	1.88033800	-0.89549600
N	1.58251500	2.50879900	-1.29153100
C	-1.60746100	1.98830700	-0.07569300
H	1.49097800	0.71354000	1.31671400
H	2.68465100	-2.69069900	-0.88170300
H	4.96916100	-2.53922100	-0.79837900
C	-1.66890600	-0.99314000	-0.21080300
C	-1.71691700	-2.09912100	0.63932900
C	-2.80624000	-0.65278100	-0.94895400
C	-2.89039600	-2.83225400	0.77569000
H	-0.83425800	-2.36946600	1.20984000
C	-3.97341200	-1.39324300	-0.82359400
H	-2.76959900	0.19124900	-1.63067500
C	-4.02051800	-2.48120500	0.04461600
H	-2.92110000	-3.67969900	1.45121100
H	-4.84663300	-1.12467000	-1.40769700
H	-4.93381200	-3.05708700	0.14413900
H	6.32242900	-0.69859200	-0.17987600
H	3.49872500	1.63696000	1.90004200
H	5.65570400	1.19933600	1.02507100

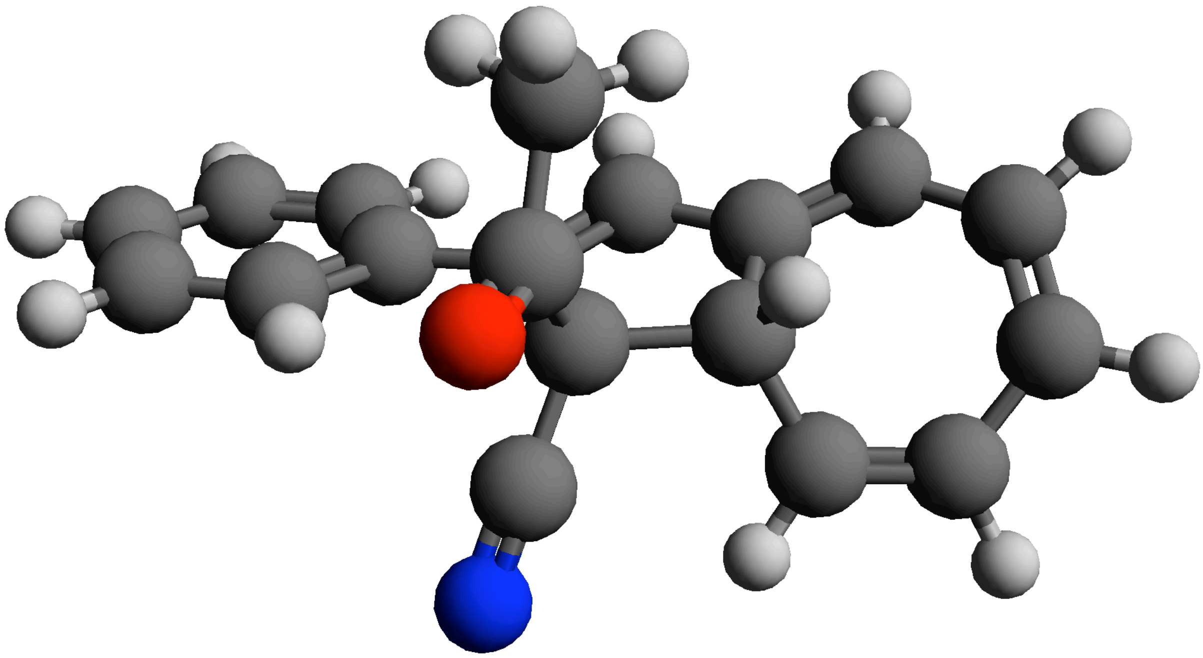
H	0.61490700	-1.96650000	-1.06868800
O	-2.25521400	1.51659200	0.99932700
C	-3.48946800	2.15145000	1.31095000
H	-3.87331700	1.63020000	2.18440600
H	-3.33337200	3.20903200	1.52421700
H	-4.18132700	2.05891500	0.47150300
N	-1.99047100	3.03710000	-0.67452800
H	-1.38009200	3.25448700	-1.45913800

C1 - Imidate - TS

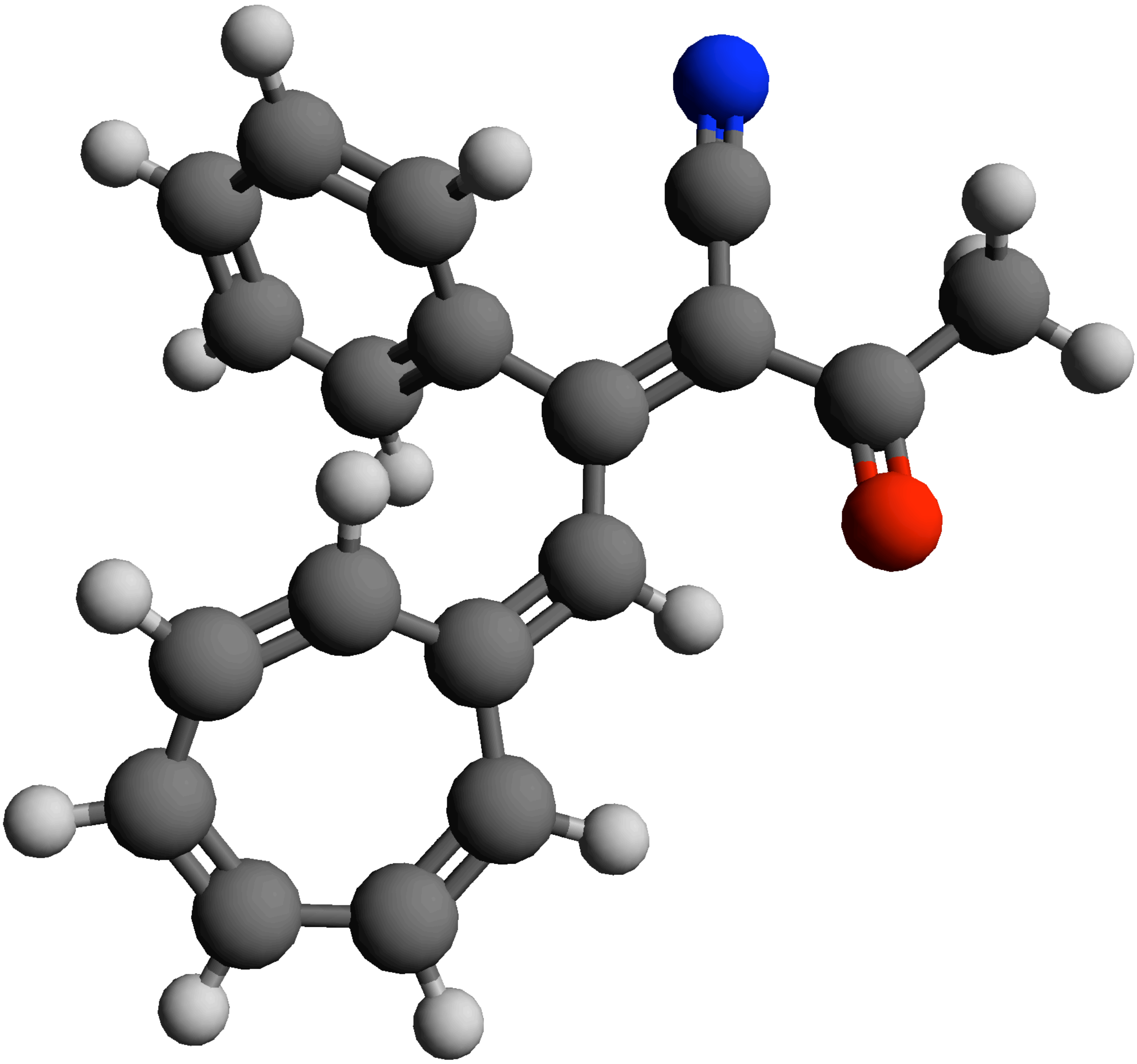
C	3.92643900	-2.13544600	0.60183600
C	3.44090600	-2.45793200	-0.65928000
C	2.36397100	-1.88956400	-1.34081600
C	1.57960500	-0.80263900	-0.95752200
C	2.07582900	0.27495600	-0.09414900
C	2.88941700	0.09355400	1.02404800
C	3.61625800	-1.02947000	1.39719400
C	0.21227600	-0.76122200	-1.30505600
C	-0.64193500	-0.13837900	-0.41222500
C	-0.12340500	0.88600200	0.46118900
C	-0.44629600	0.79877800	1.84944800
N	-0.60488600	0.73466700	2.99137100
H	2.01726400	-2.43534800	-2.21644800
H	2.05268100	1.26678400	-0.52070200
H	2.99473000	0.96972400	1.66116000
H	-0.17277800	-1.46390600	-2.03732700
C	-2.02041100	-0.63781100	-0.22548700
C	-3.02882300	0.24816300	0.17327600
C	-2.35382000	-1.98051900	-0.44434400
C	-4.33569900	-0.19140800	0.33313300
H	-2.78359300	1.29145200	0.34210600
C	-3.66137000	-2.41909500	-0.28619200
H	-1.57574700	-2.69062200	-0.70219300
C	-4.65623100	-1.52536000	0.10056100
H	-5.10536100	0.50800000	0.63886700
H	-3.90232000	-3.46365100	-0.44880400
H	-5.67599700	-1.87069500	0.22823500
H	4.12859300	-0.97052100	2.35233100
C	0.17314500	2.26083200	0.00237300
H	3.87231100	-3.34055900	-1.12114400
H	4.66338500	-2.81949000	1.01192700
O	0.22636900	2.33471900	-1.34351900
C	0.51535000	3.61916600	-1.88473700
H	1.48629400	3.97416500	-1.53654700
H	0.51567500	3.48644400	-2.96402200
H	-0.24567500	4.33909800	-1.58305000
N	0.38499900	3.29228400	0.71414300
H	0.30755000	3.07706700	1.70567300

Molecular structures

Ketone DHA



Ketone s-trans-vhf



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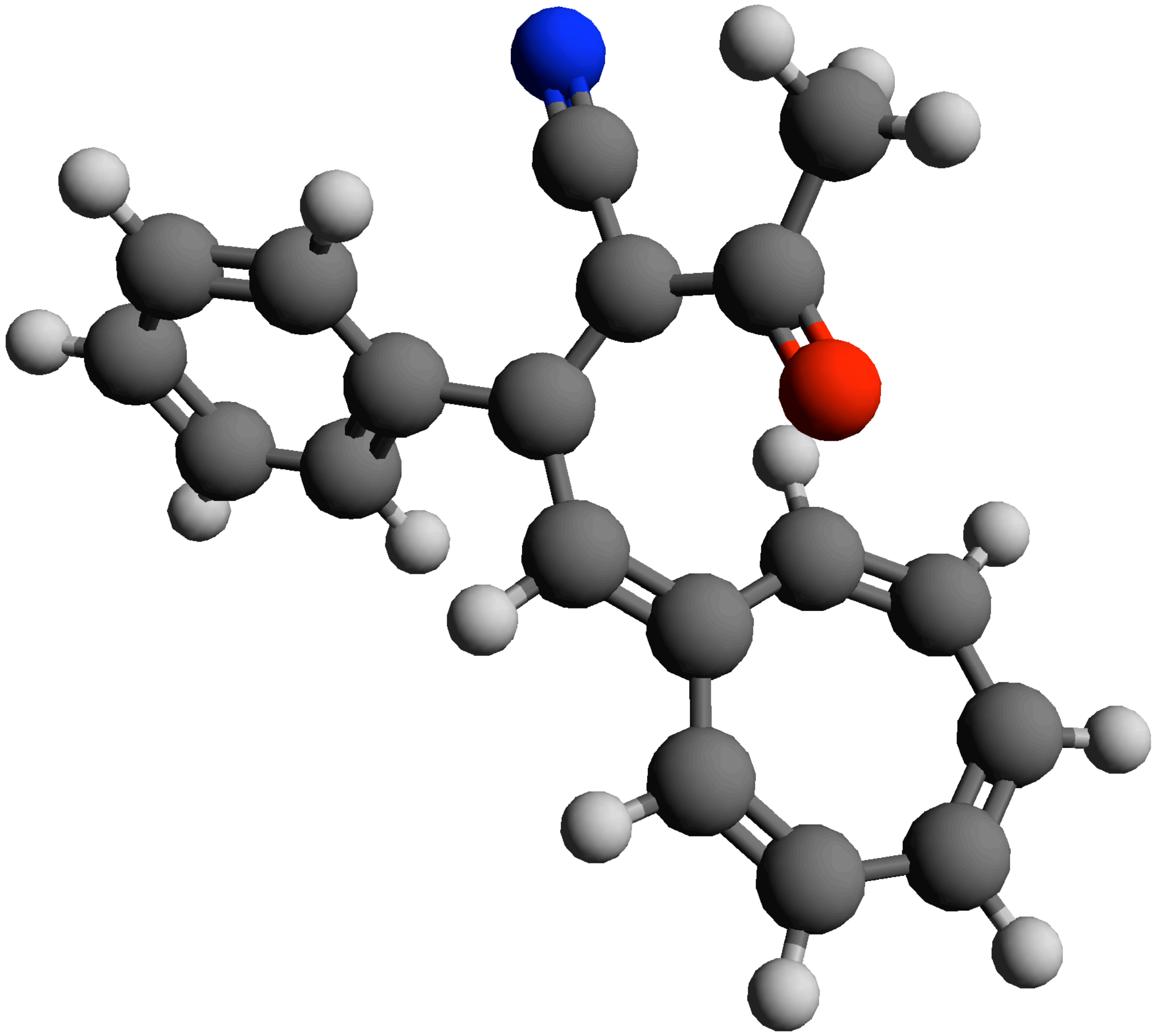

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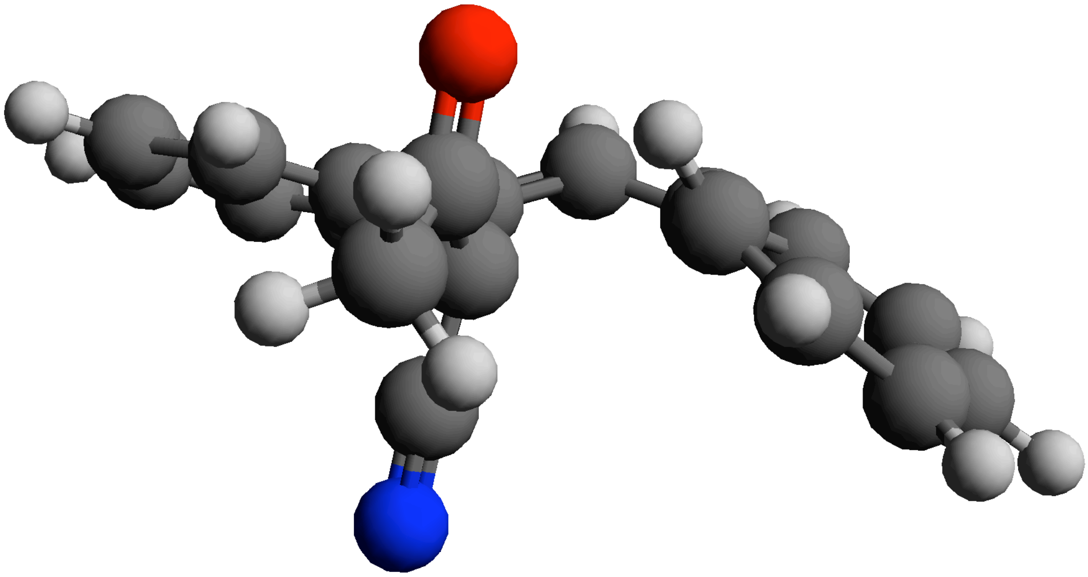

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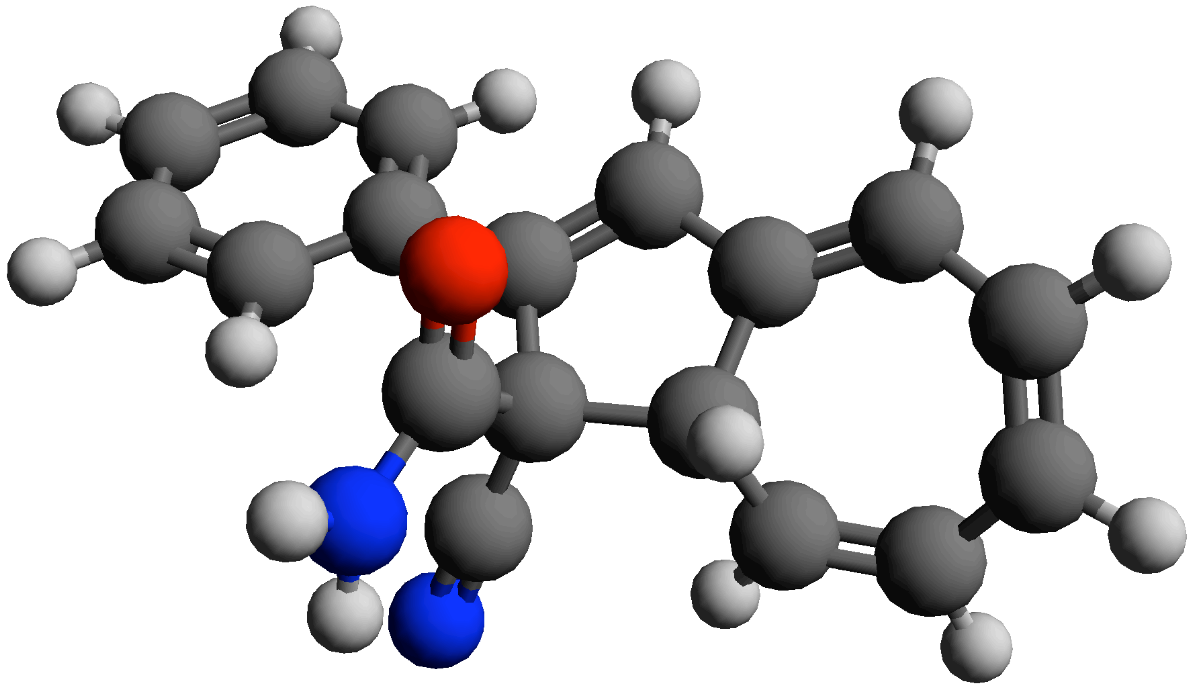

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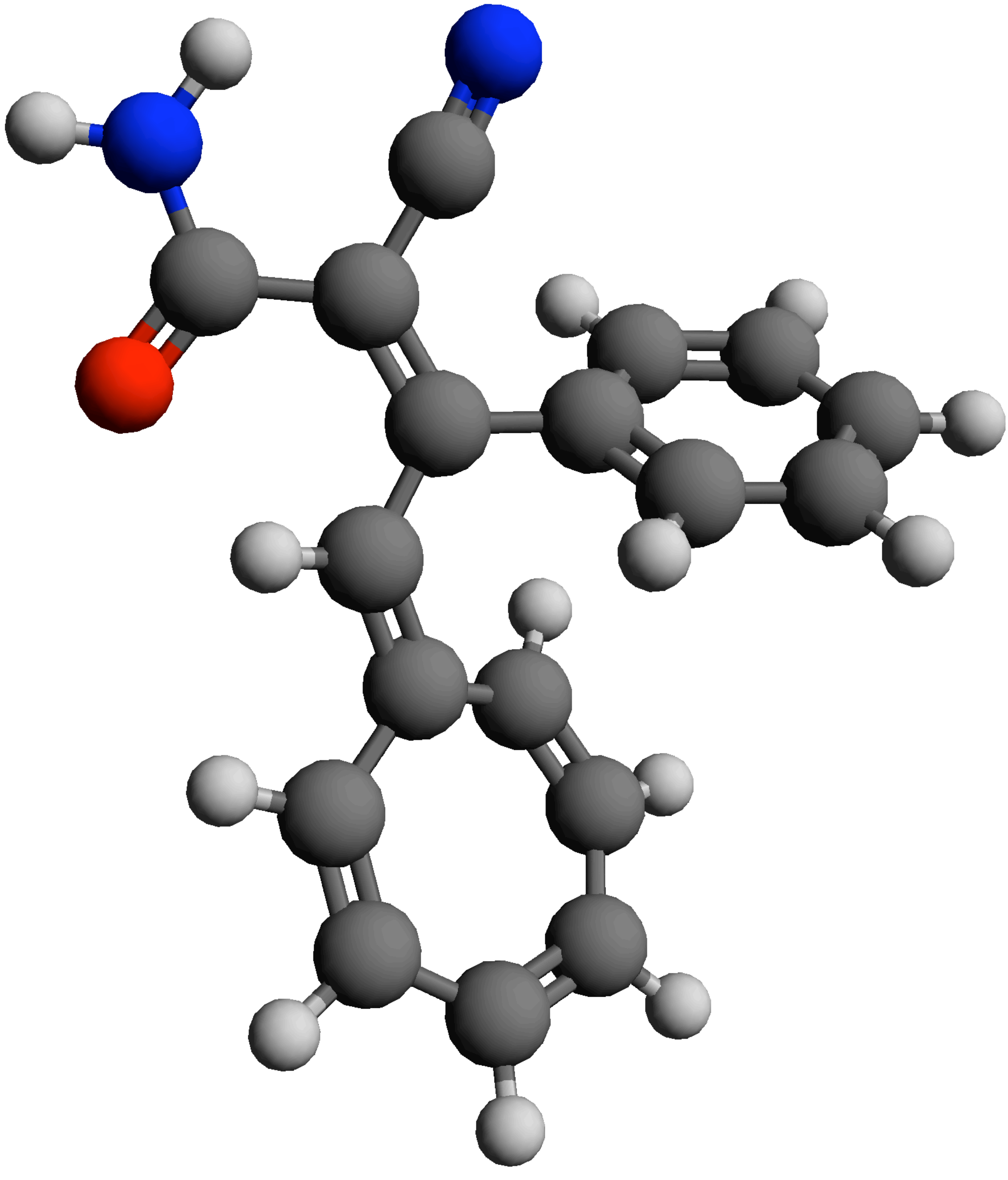

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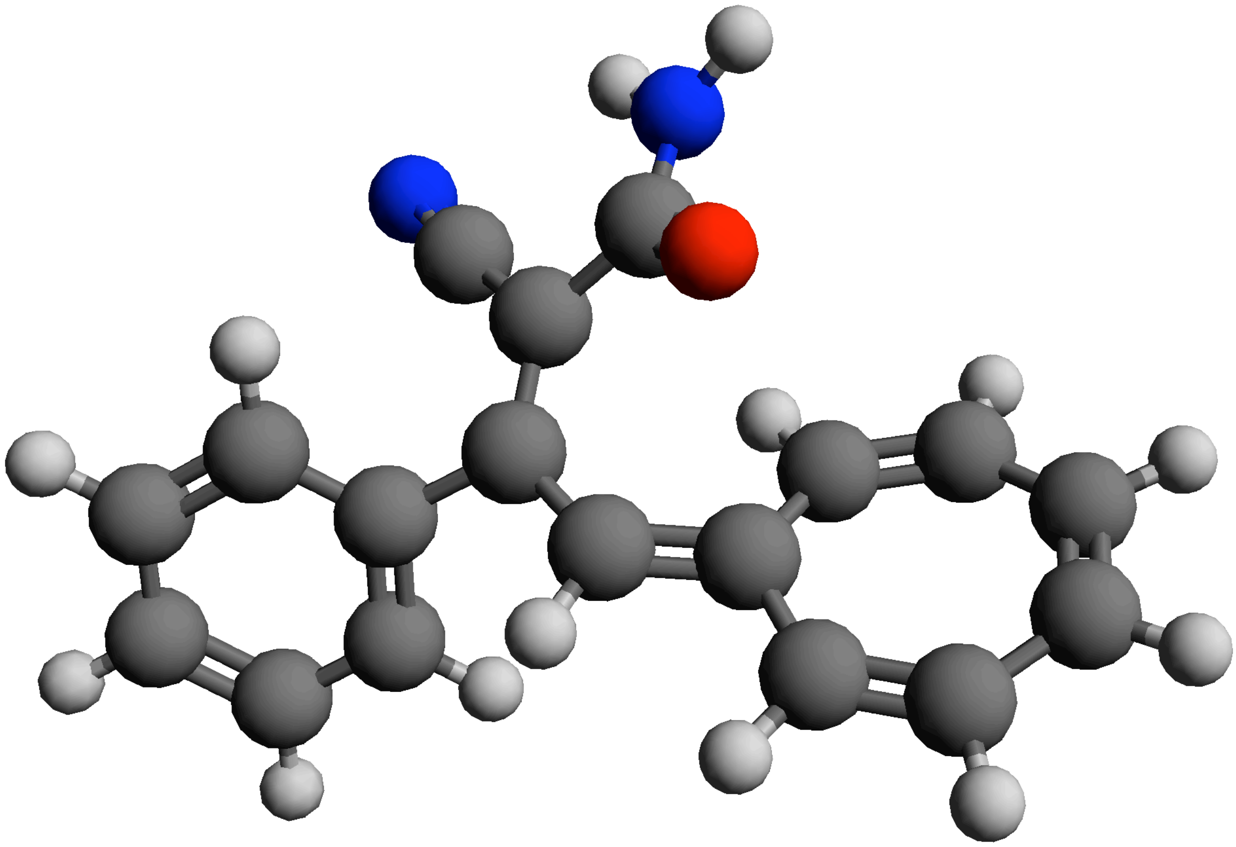

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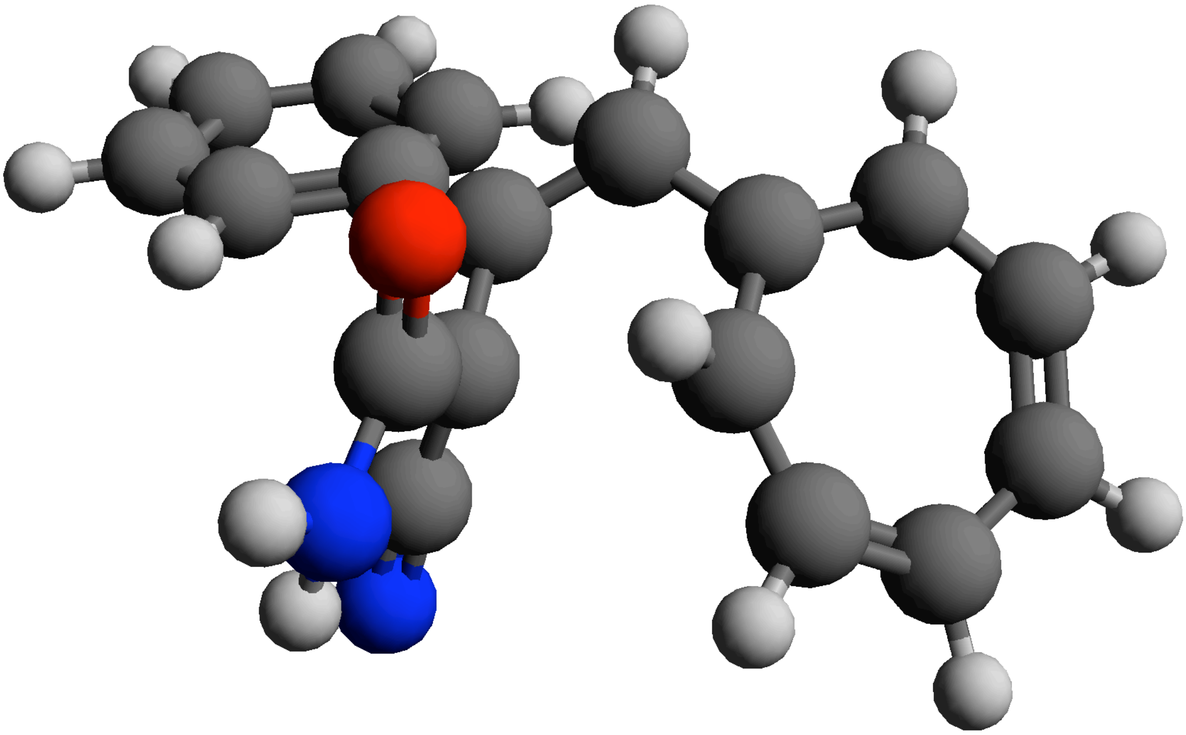
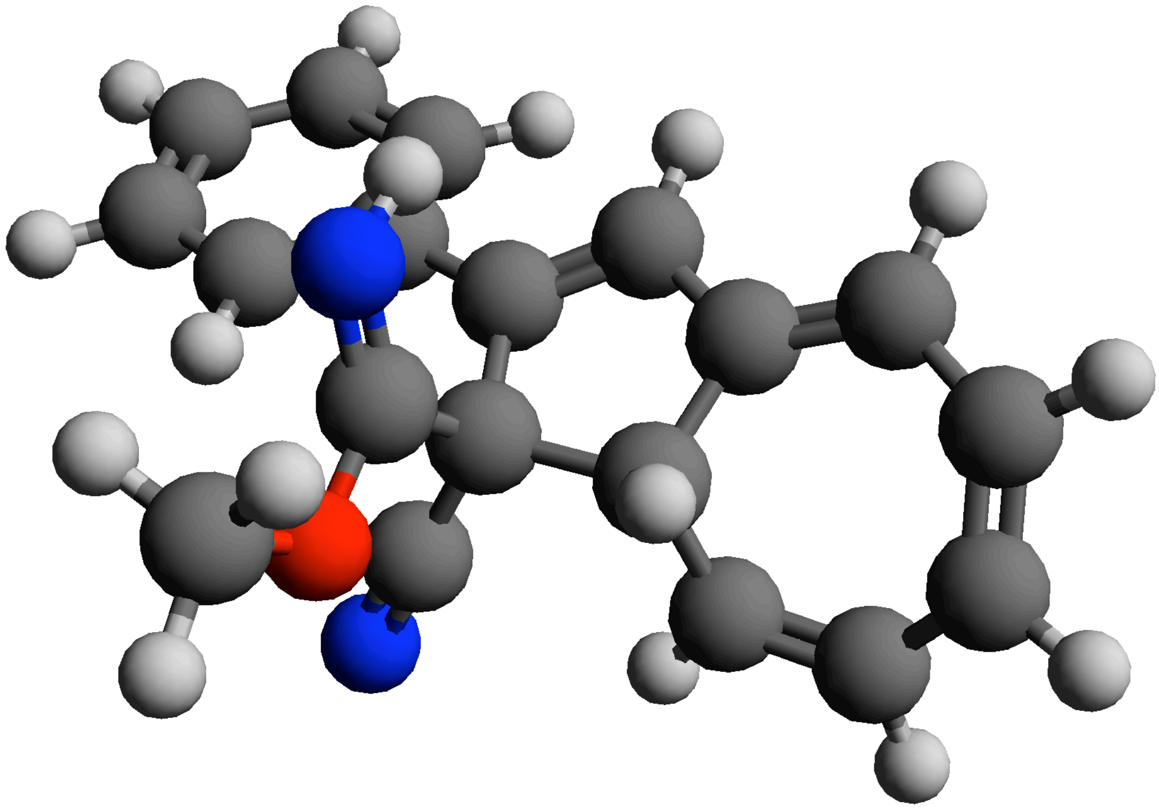


Imidate DHA



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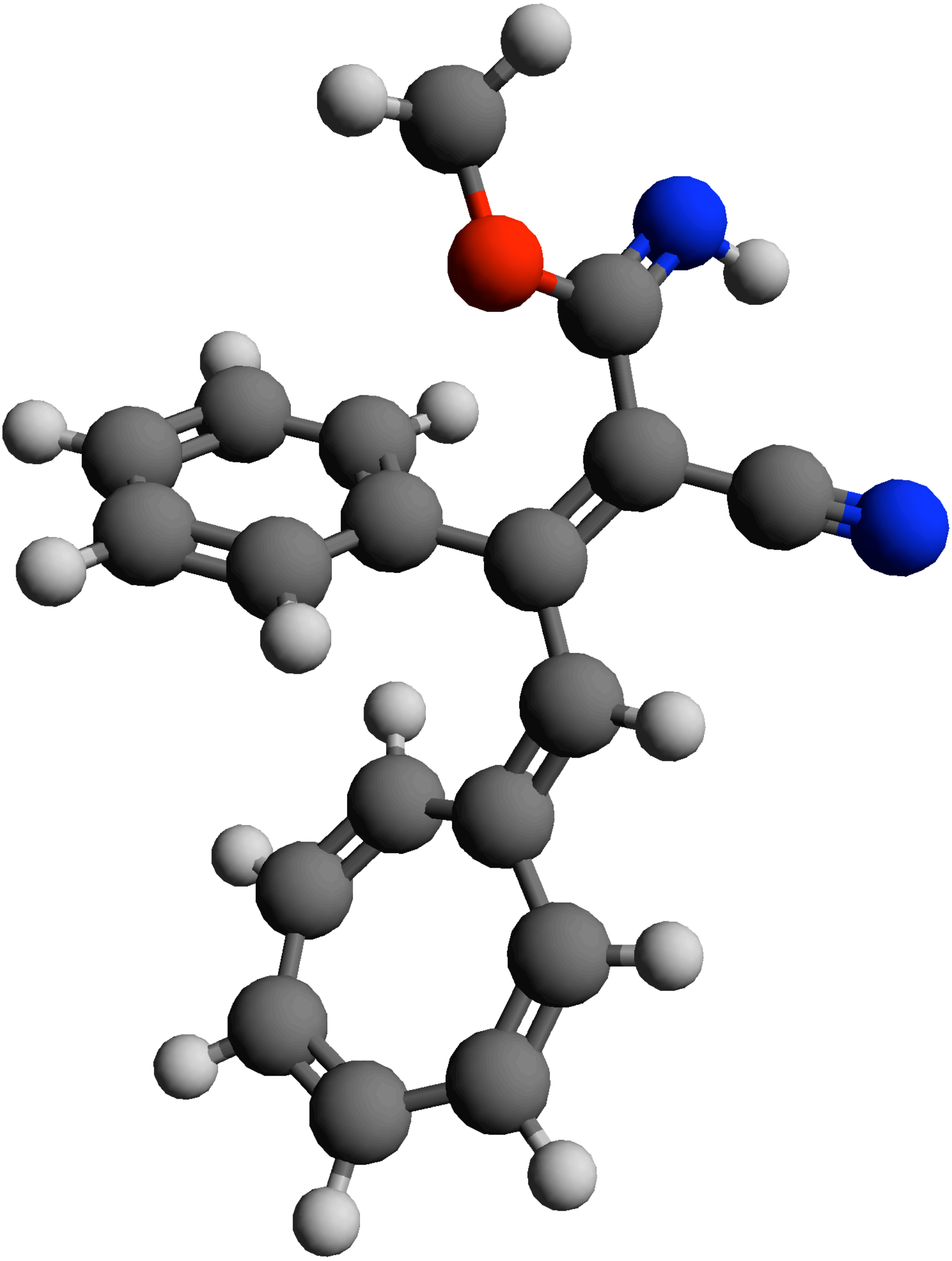

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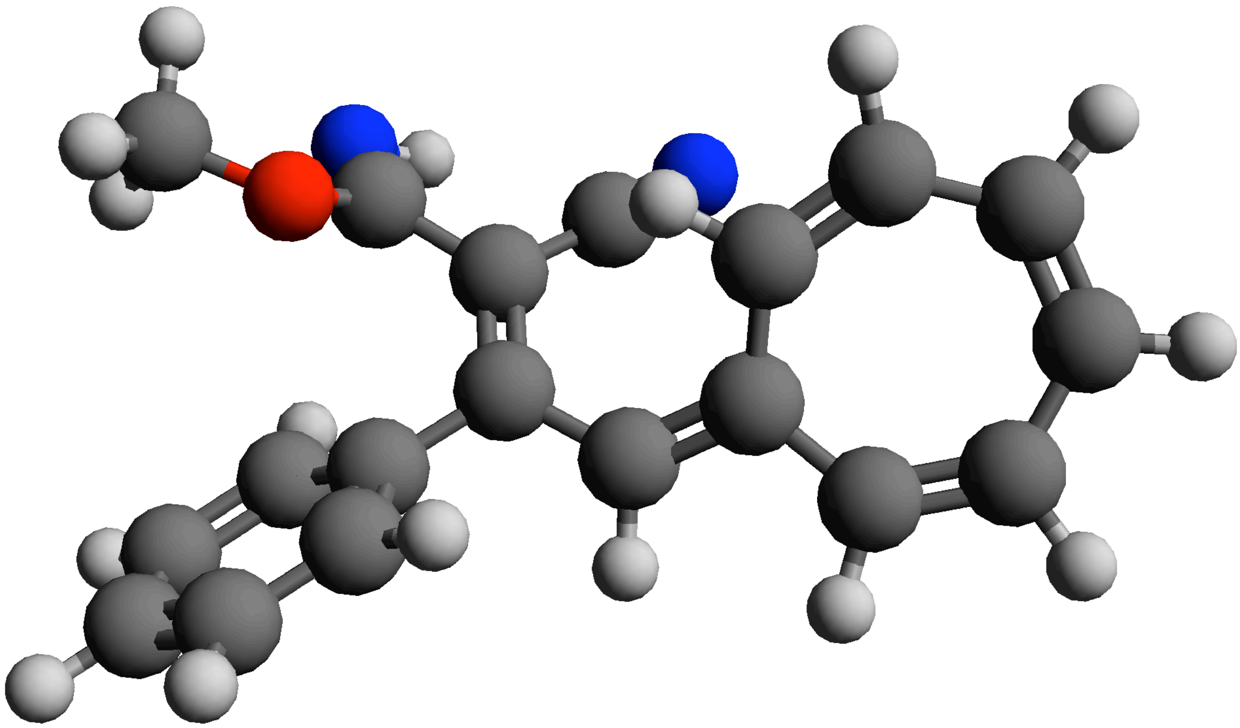

Imidate TS