

SUPPORTING INFORMATION

Asymmetric Synthesis of 2nd Generation Light-Driven Molecular Motors

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NMR spectra

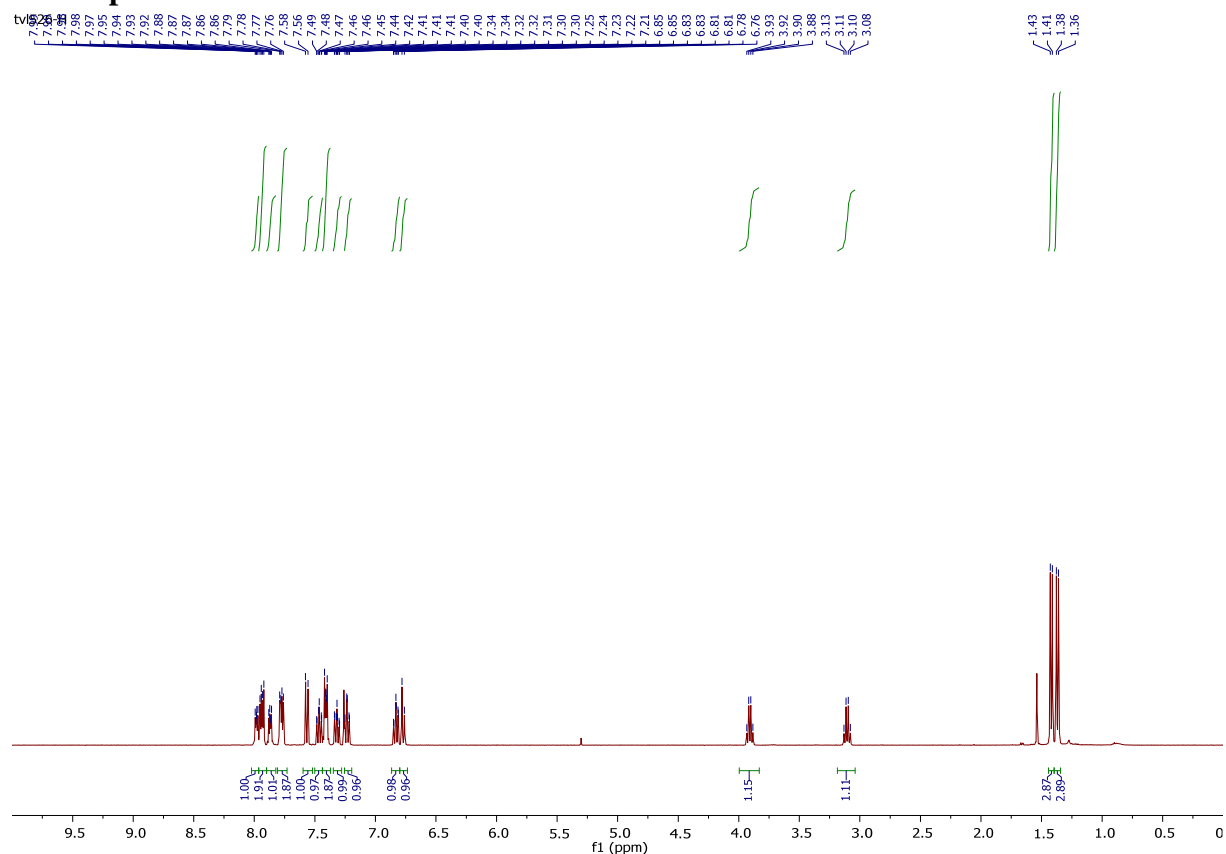


Figure S 1: ^1H -NMR of **2**.

tv1526-C

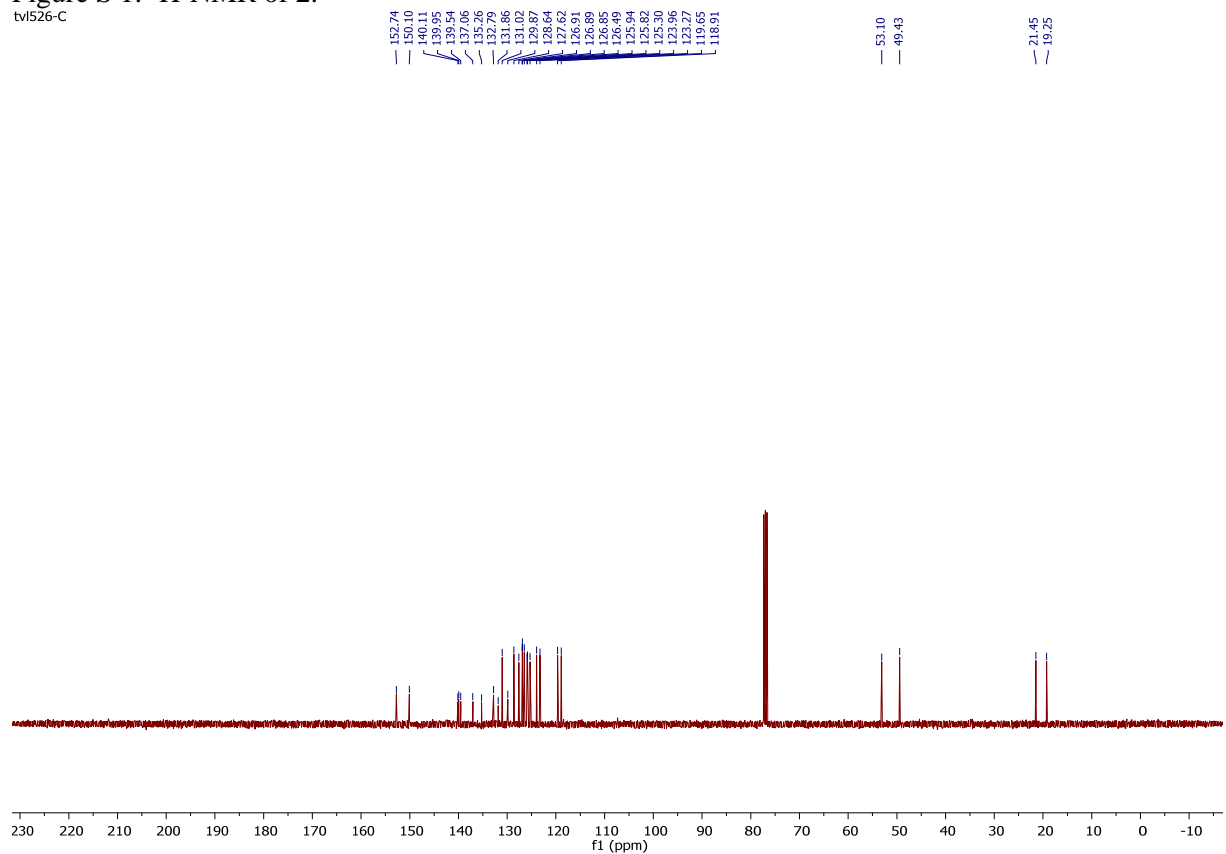


Figure S 2: ^{13}C -NMR of **2**.

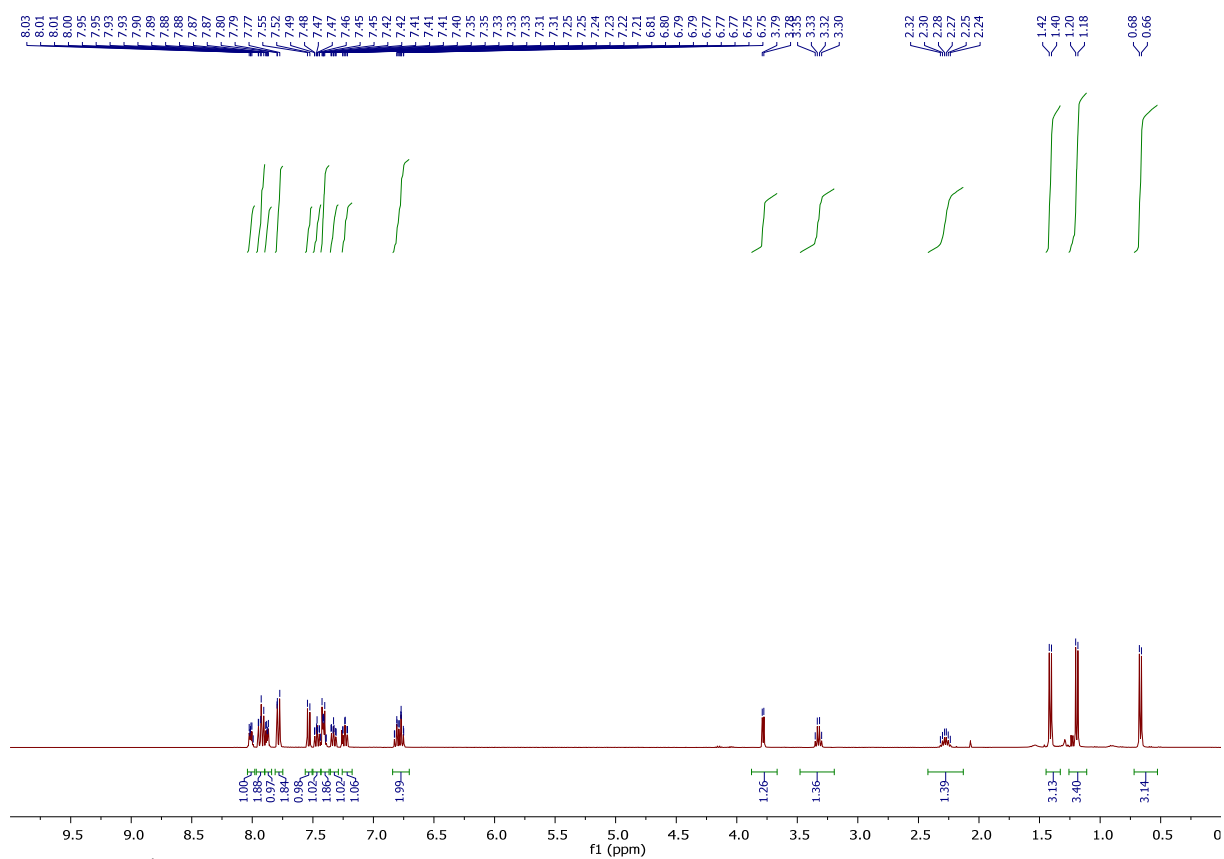


Figure S 3: ¹H-NMR of **3**.

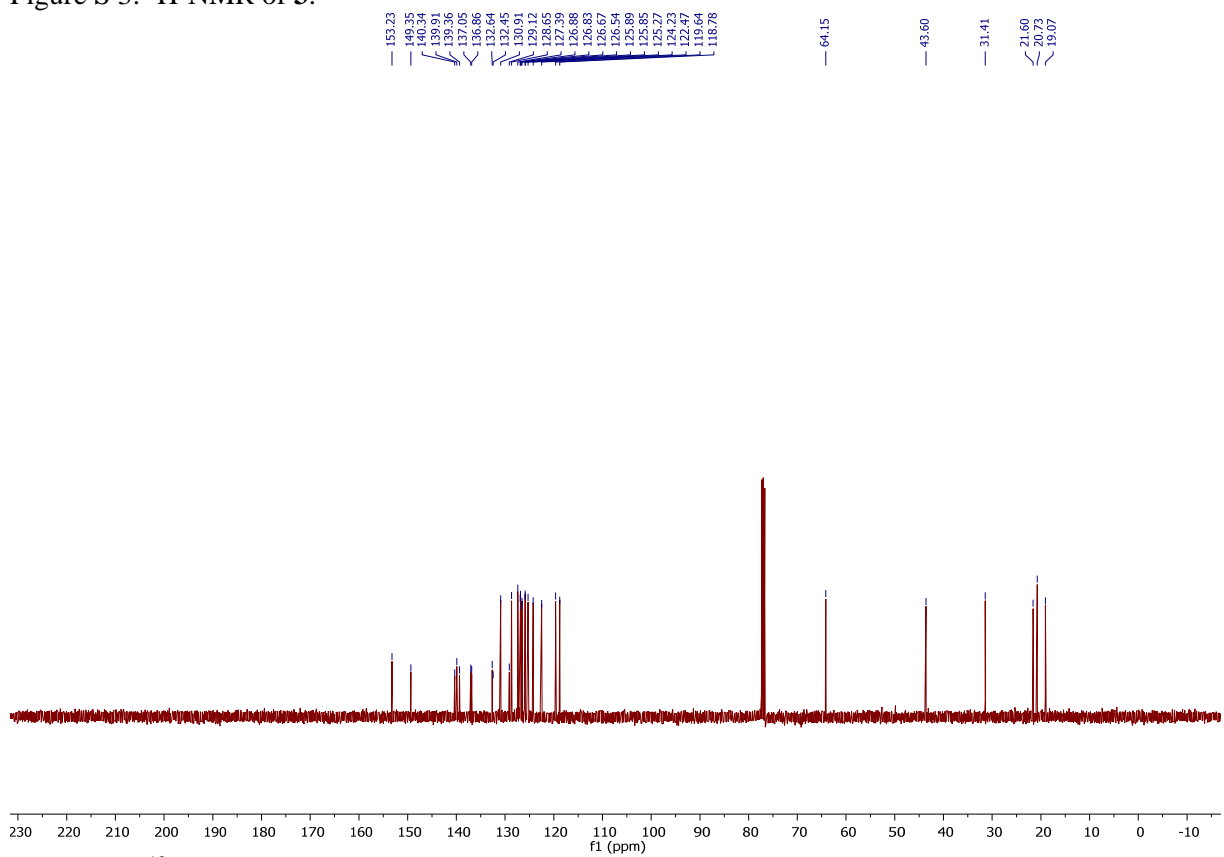


Figure S 4: ¹³C-NMR of **3**.

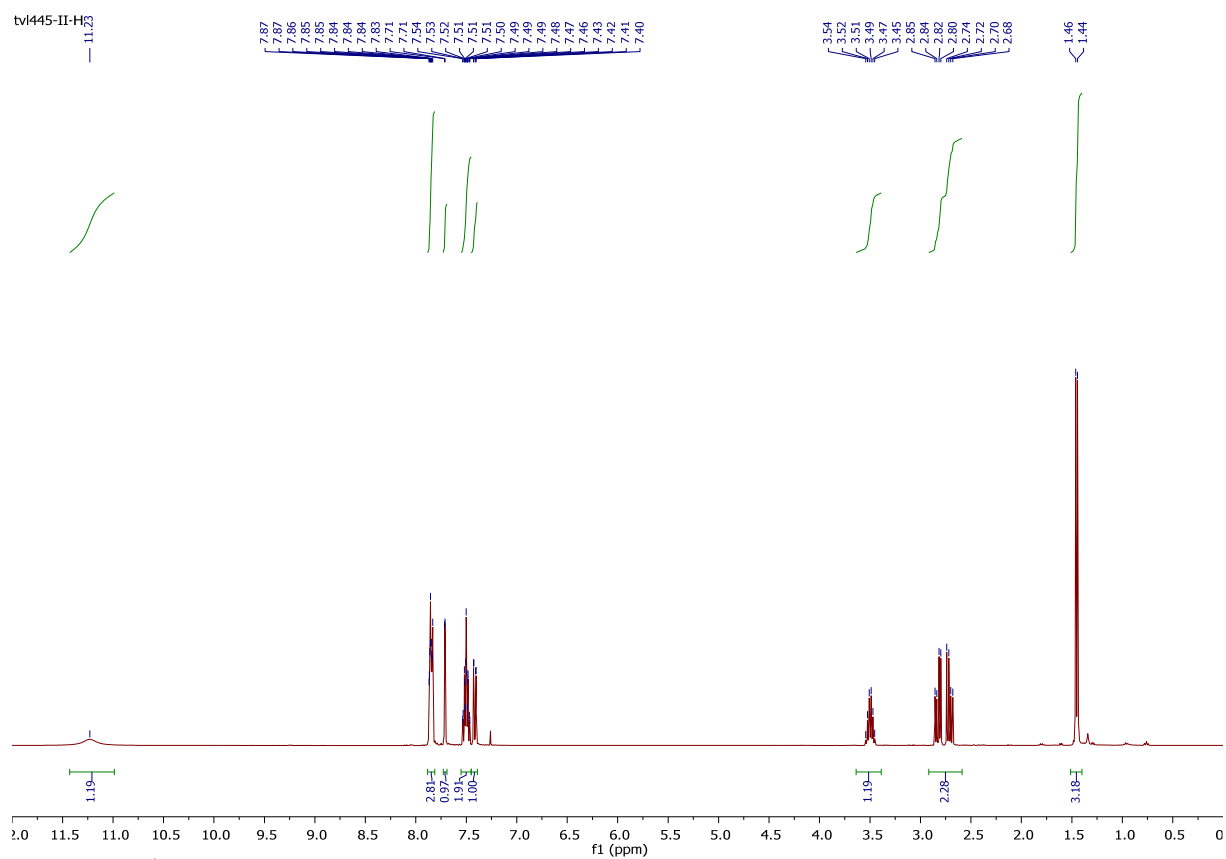


Figure S 5: ^1H -NMR of **8**.

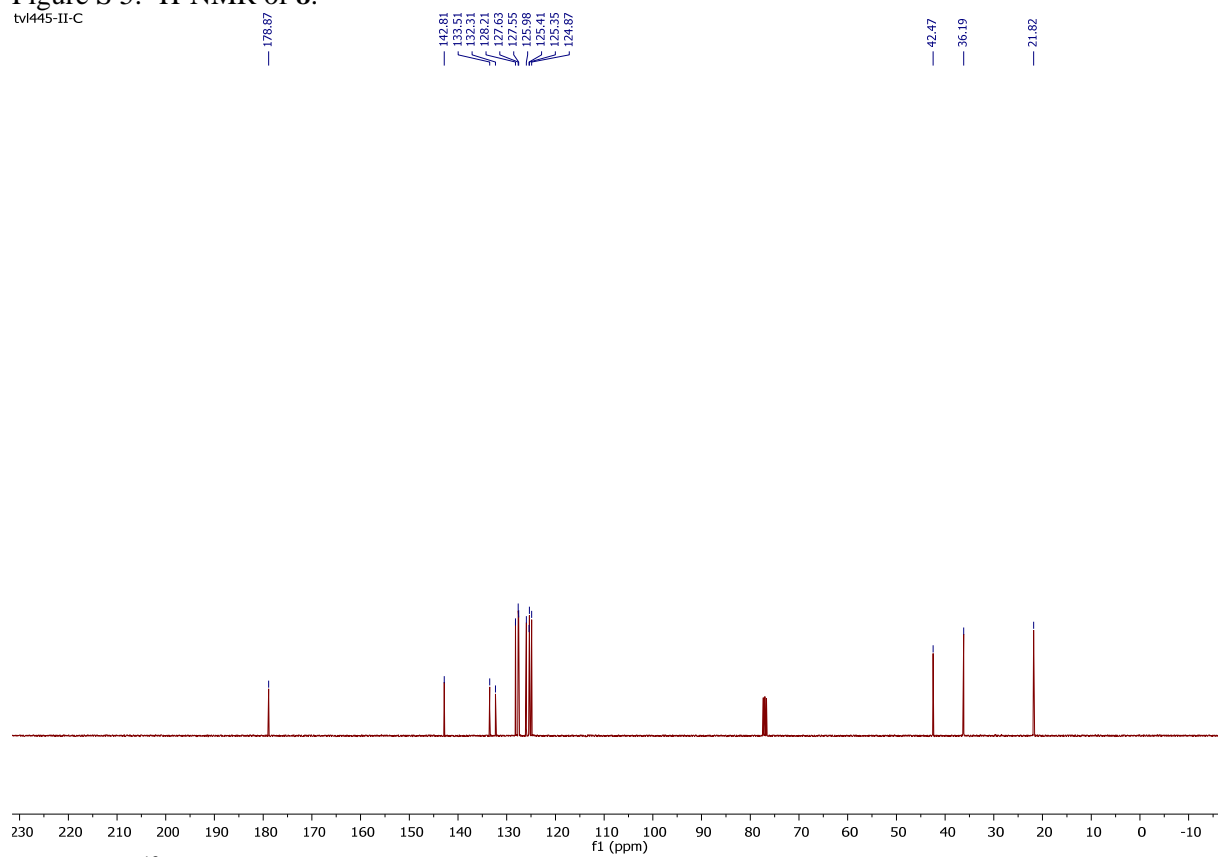


Figure S 6: ^{13}C -NMR of **8**.

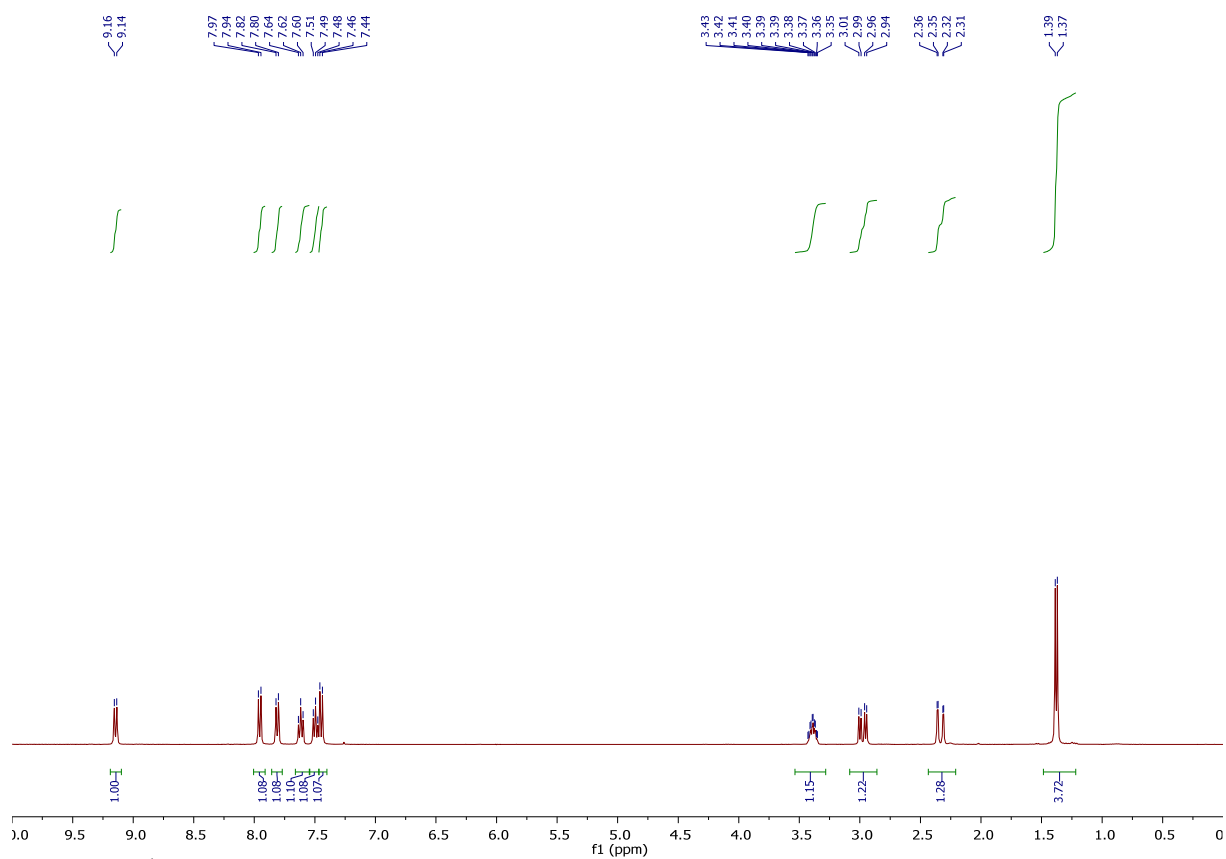


Figure S 7: ¹H-NMR of **9**.

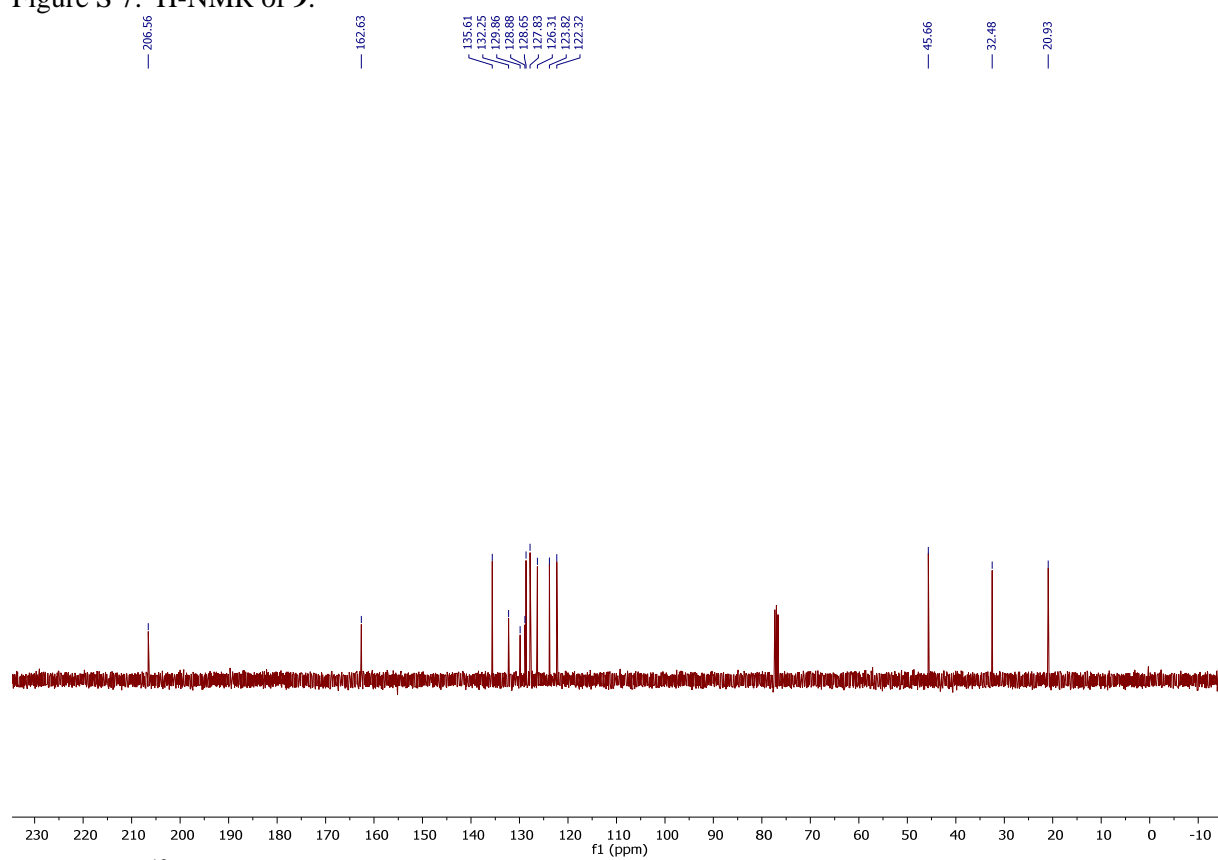


Figure S 8: ¹³C-NMR of **9**.

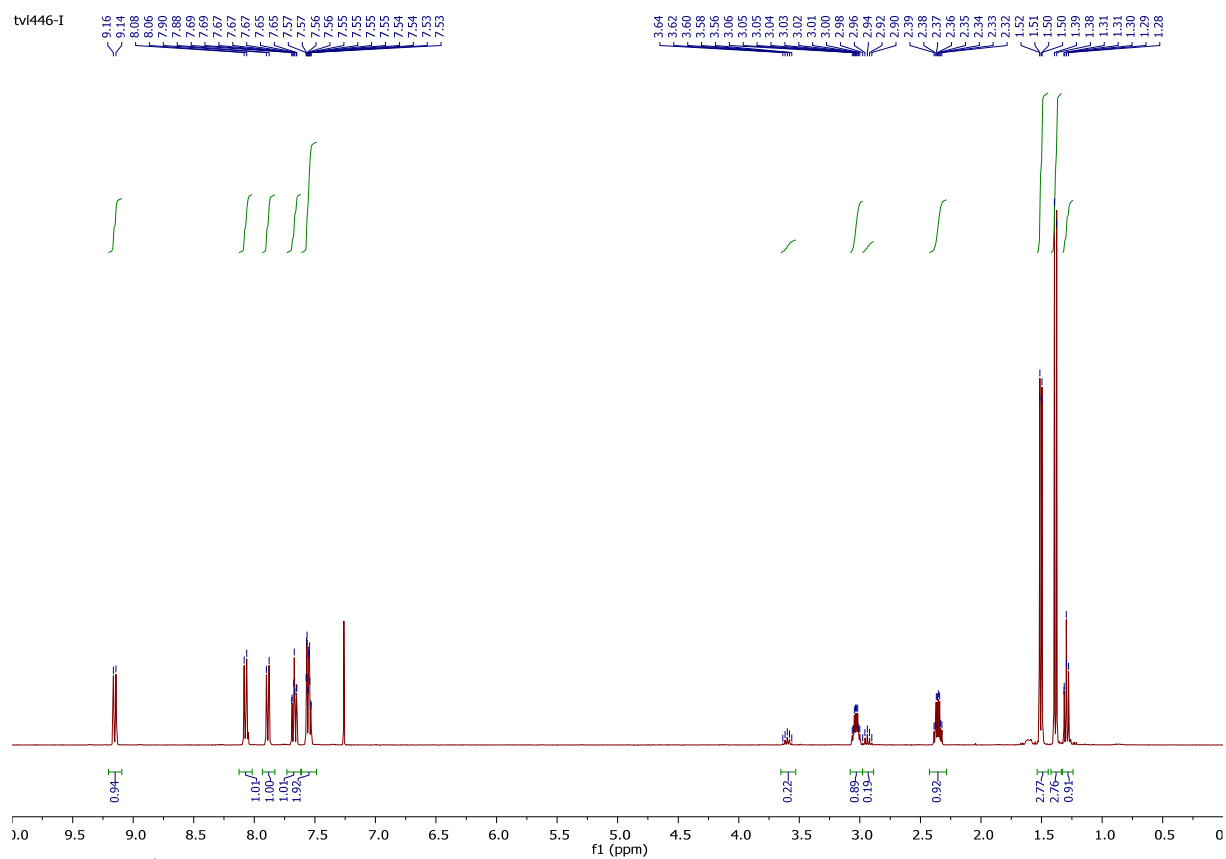


Figure S 9: ^1H -NMR of **10**.

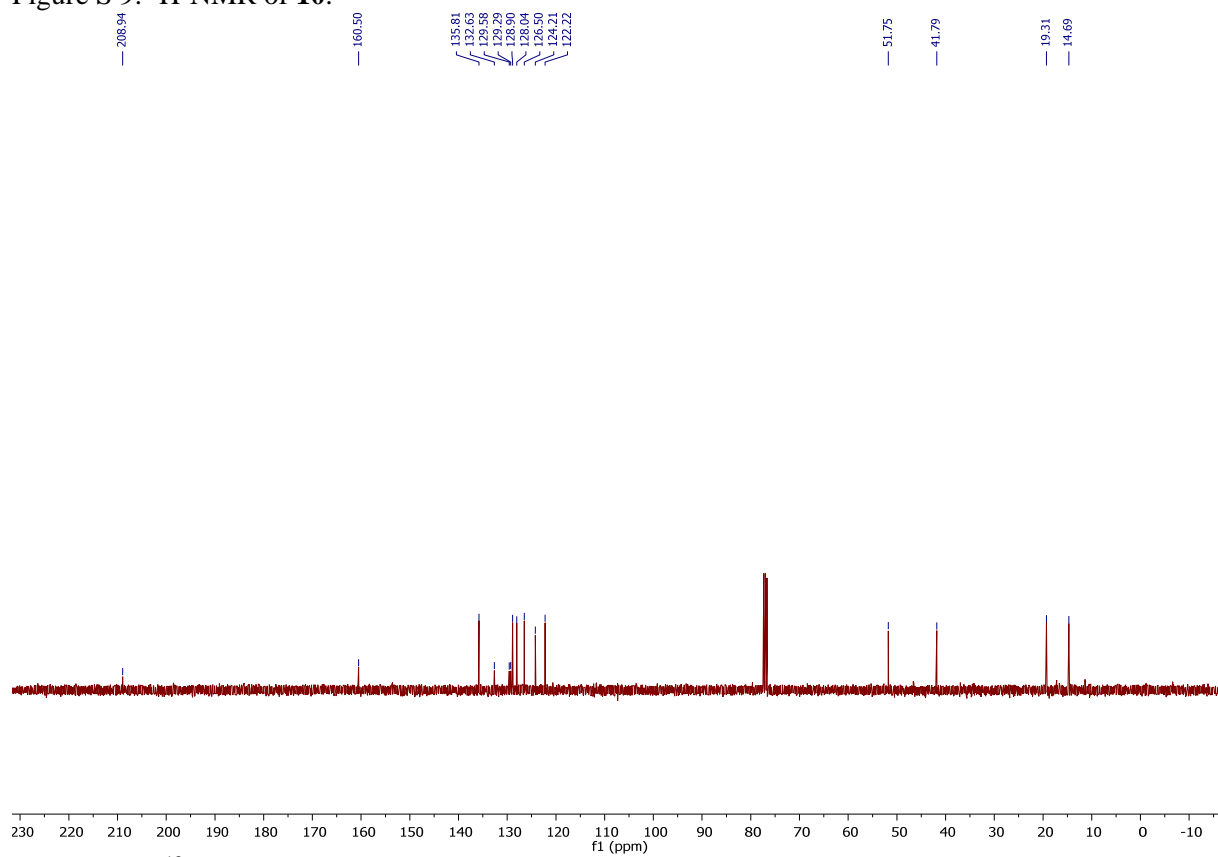


Figure S 10: ^{13}C -NMR of **10**.

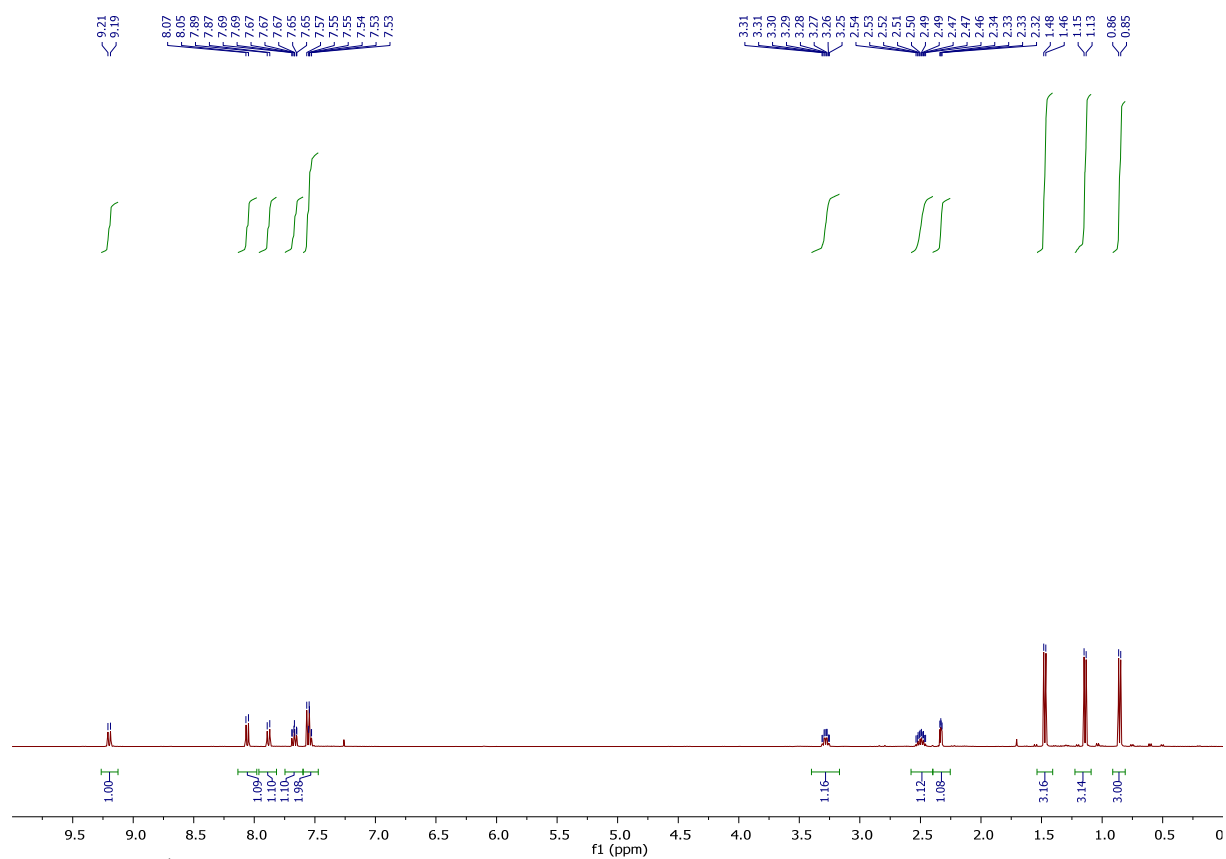


Figure S 11: ¹H-NMR of **11**.

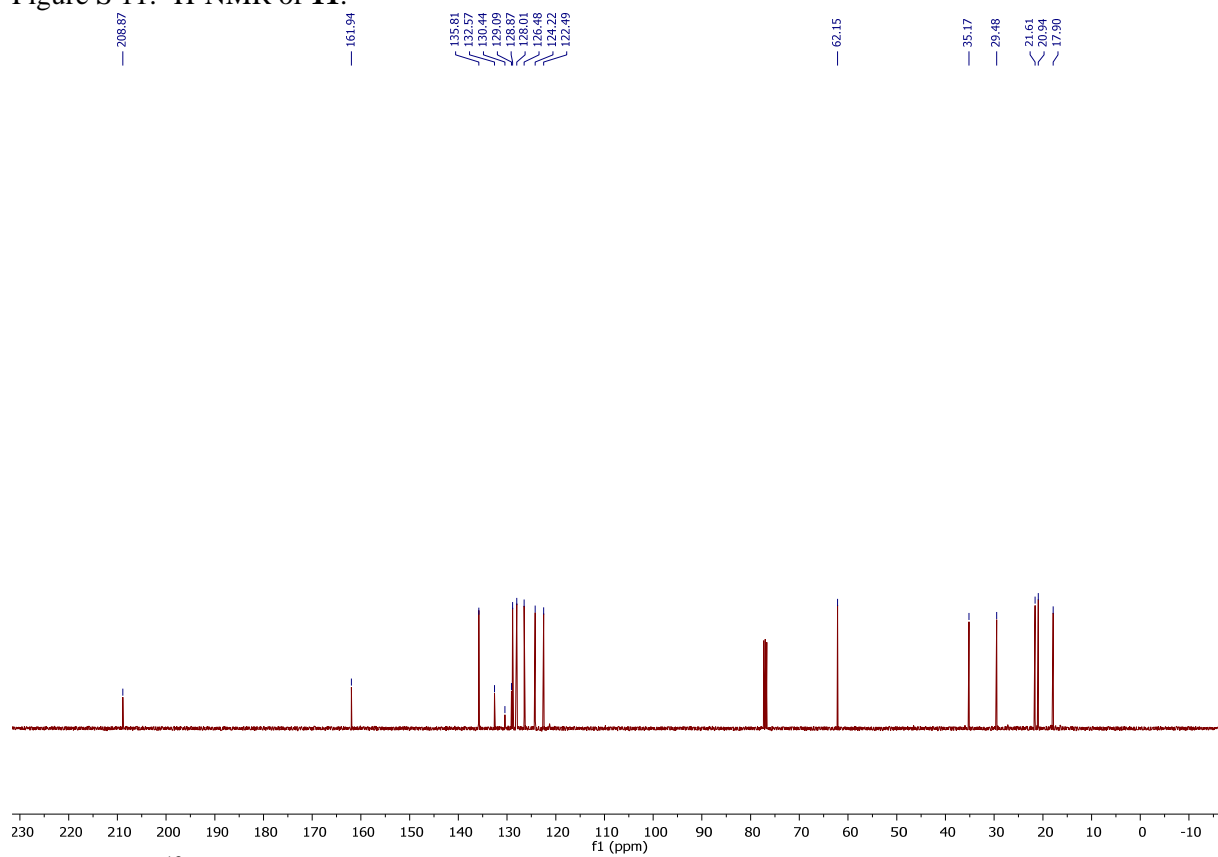


Figure S 12: ¹³C-NMR of **11**.

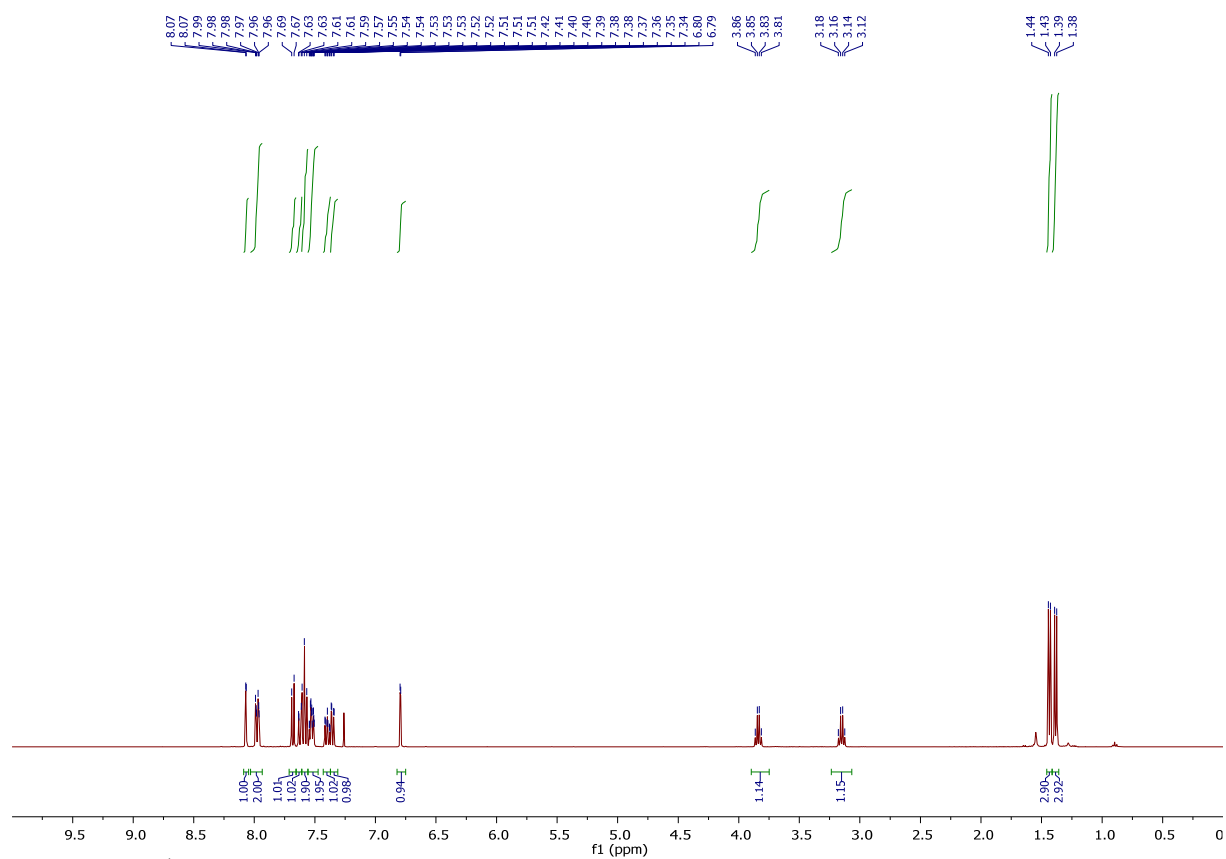


Figure S 13: ¹H-NMR of **15**.

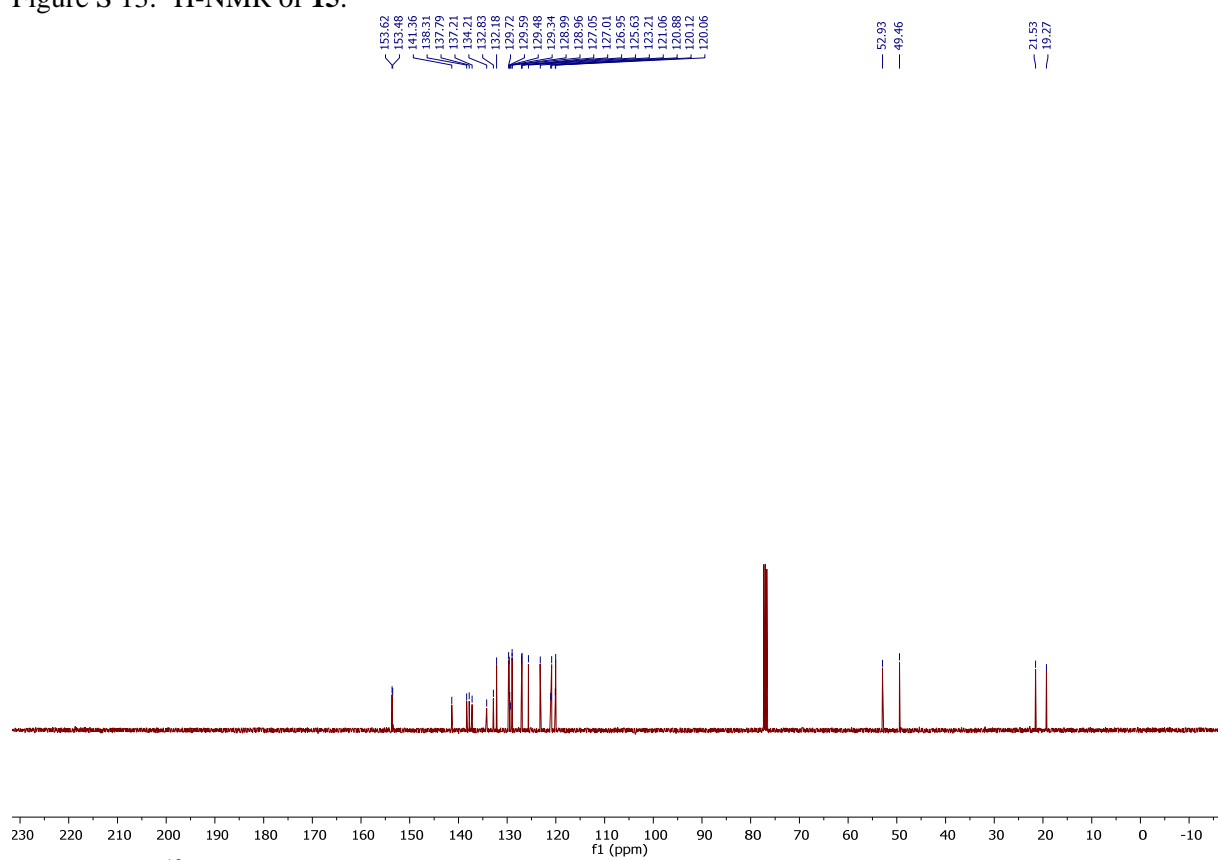


Figure S 14: ¹³C-NMR of **15**.

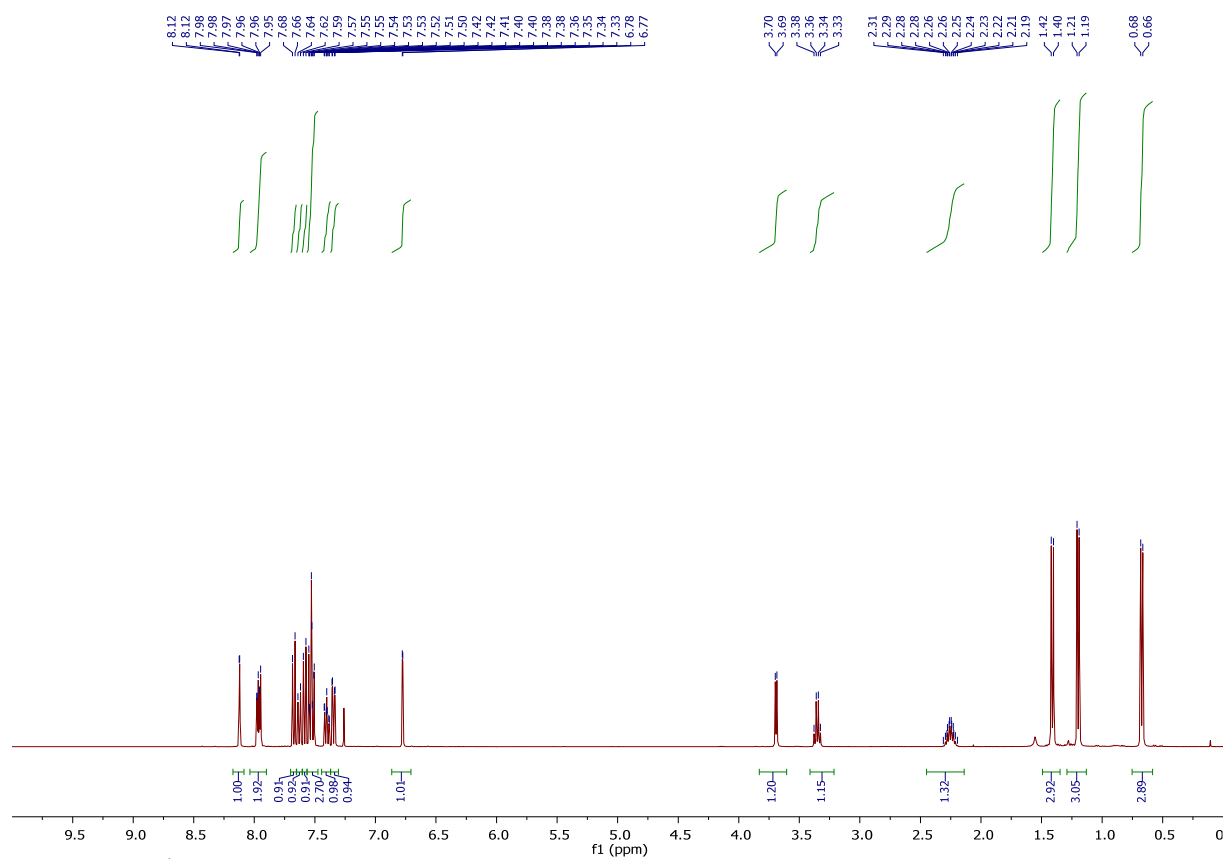


Figure S 15: ^1H -NMR of **17**.

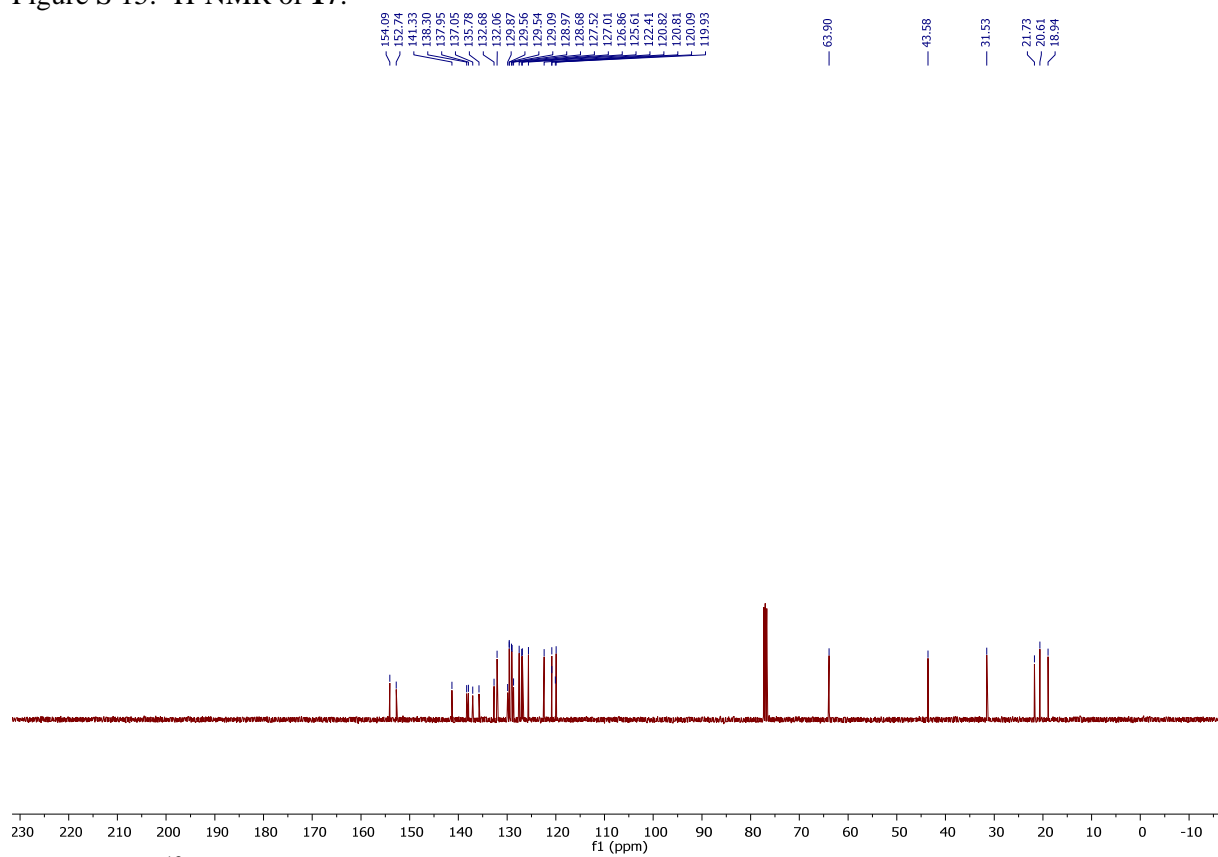


Figure S 16: ^{13}C -NMR of **17**.

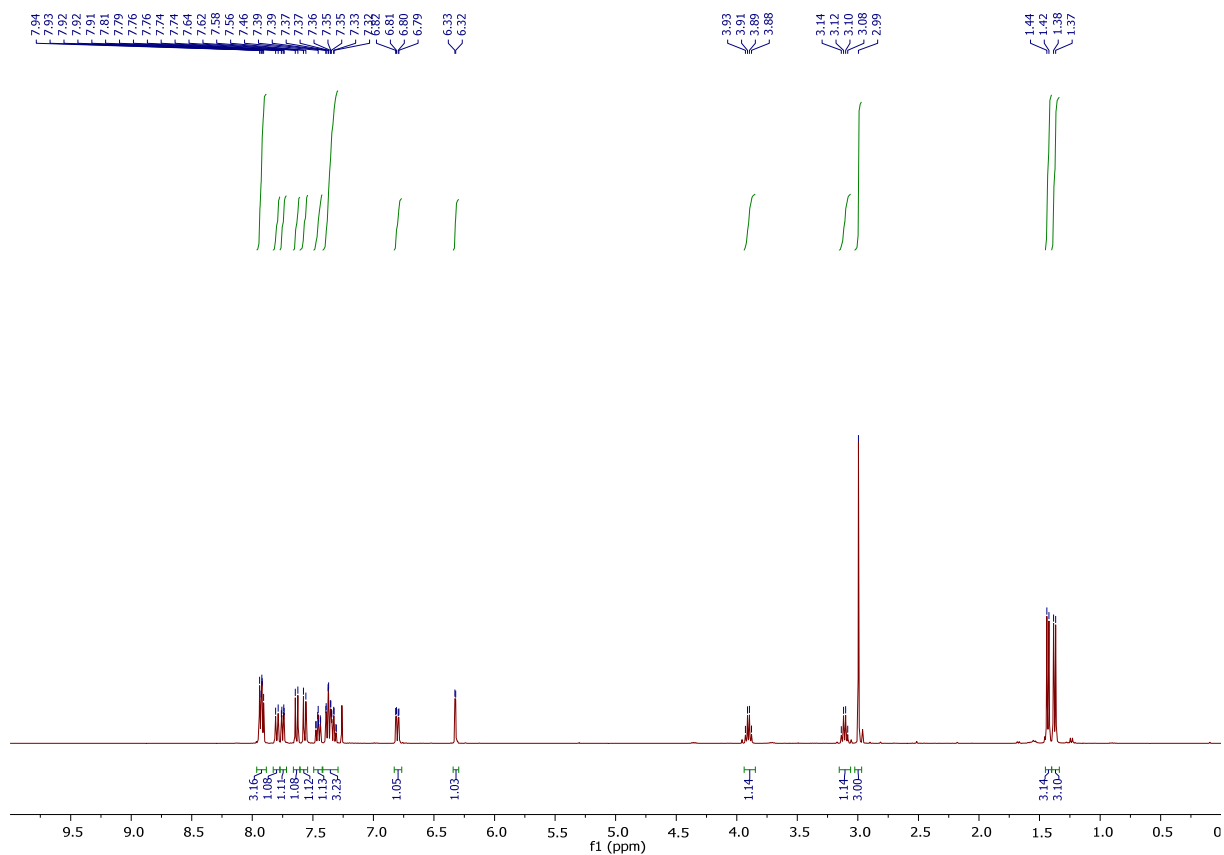


Figure S 17: ¹H-NMR of **18**.

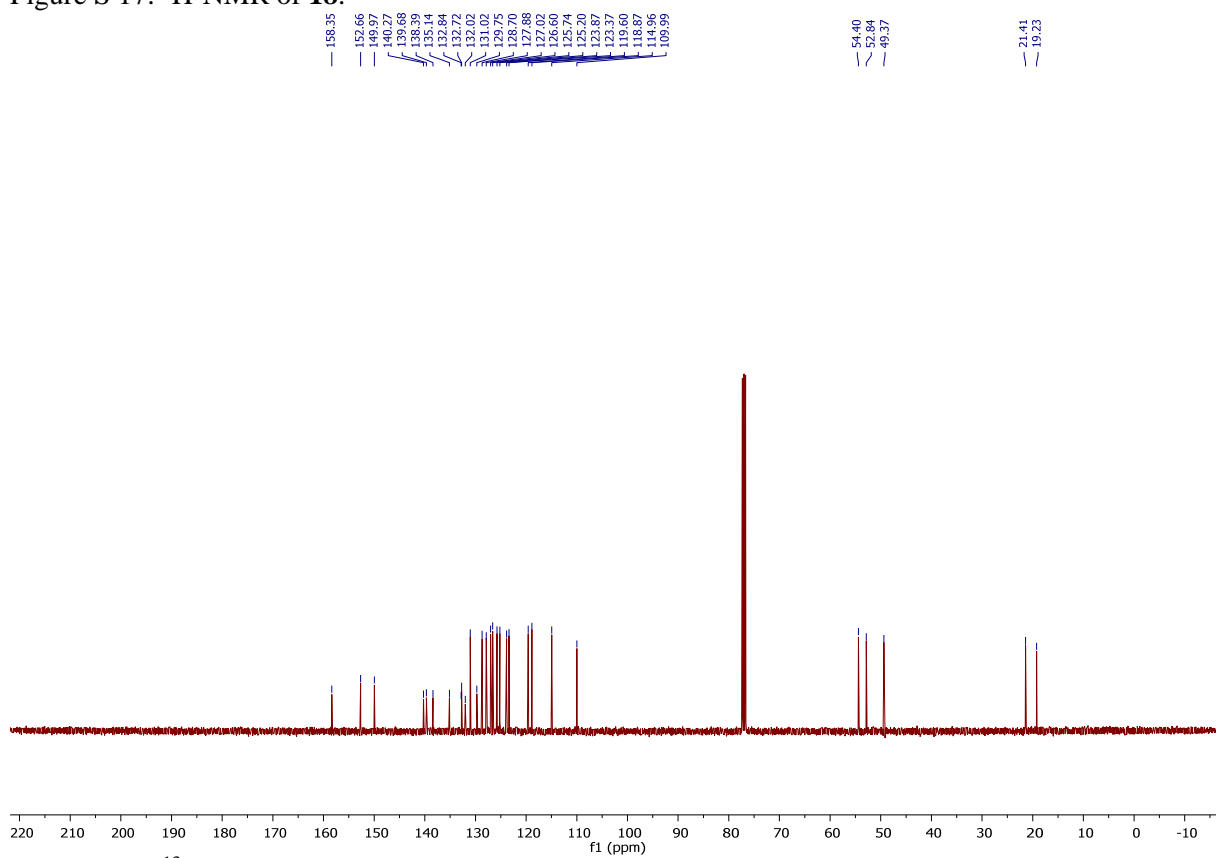


Figure S 18: ¹³C-NMR of **18**.

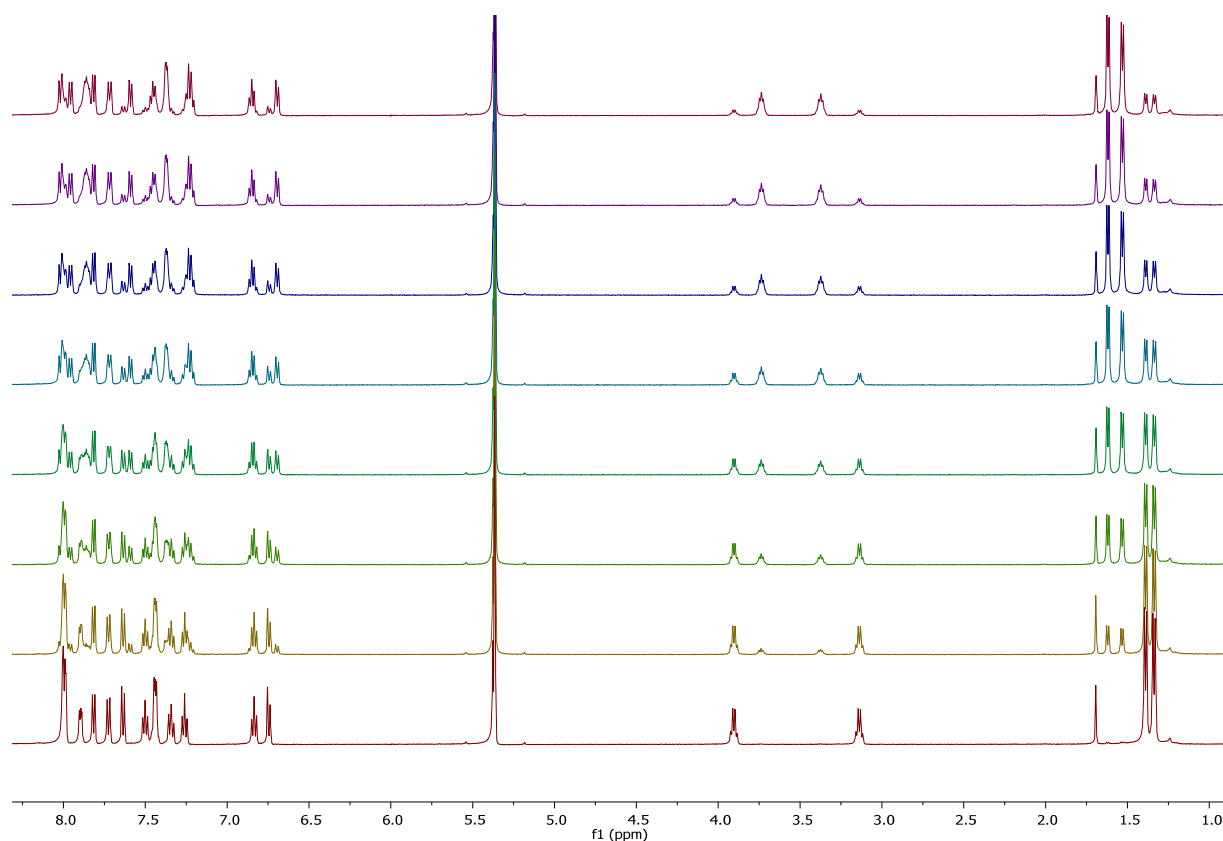


Figure S 19: ^1H -NMR of **2** in CD_2Cl_2 upon irradiation at 365 nm. Initial state (bottom spectrum), PSS (top spectrum). NMR irradiation experiments were performed at -40°C with a Thorlab model M365F1 LED coupled to a 600 mm optical fiber, which guided the light into the NMR tube inside the spectrometer.¹

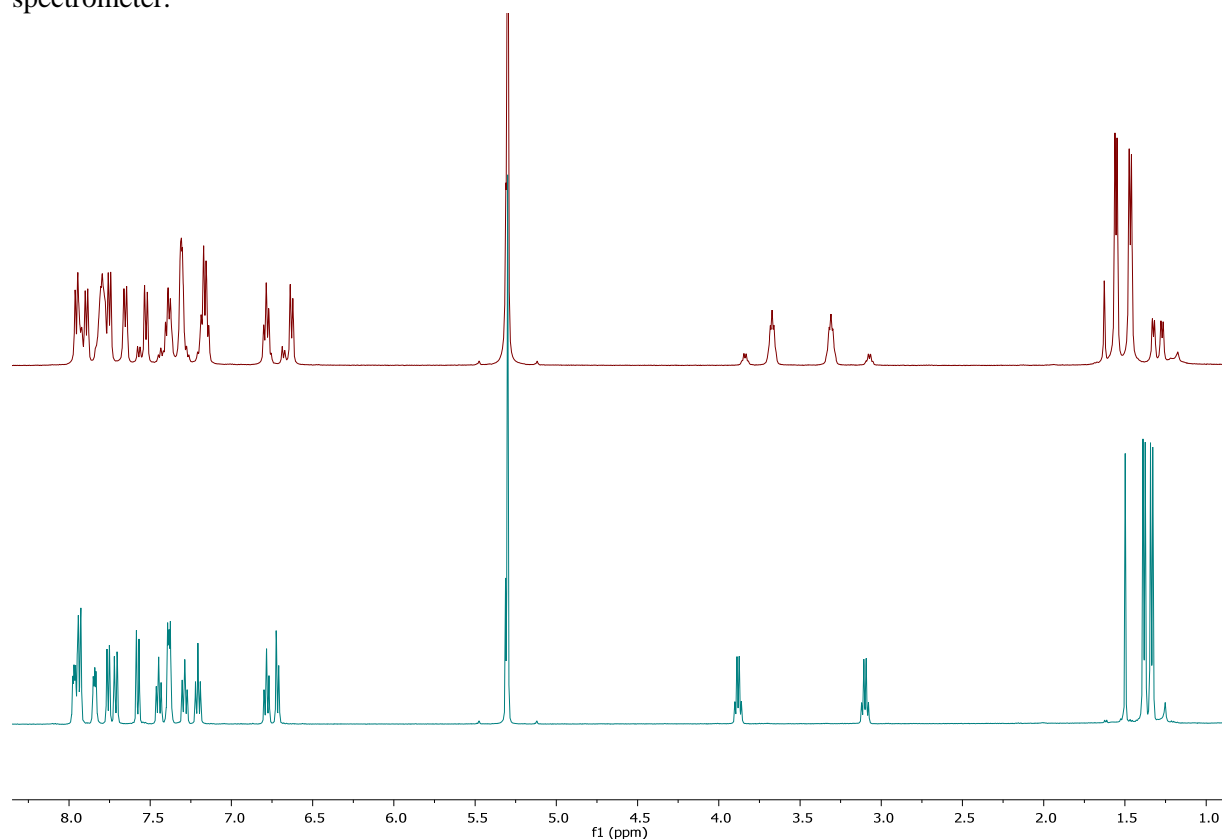


Figure S 20: ^1H -NMR of **2** in CD_2Cl_2 after irradiation at 365 nm at -40°C (top). Heating of PSS at 30°C (bottom).

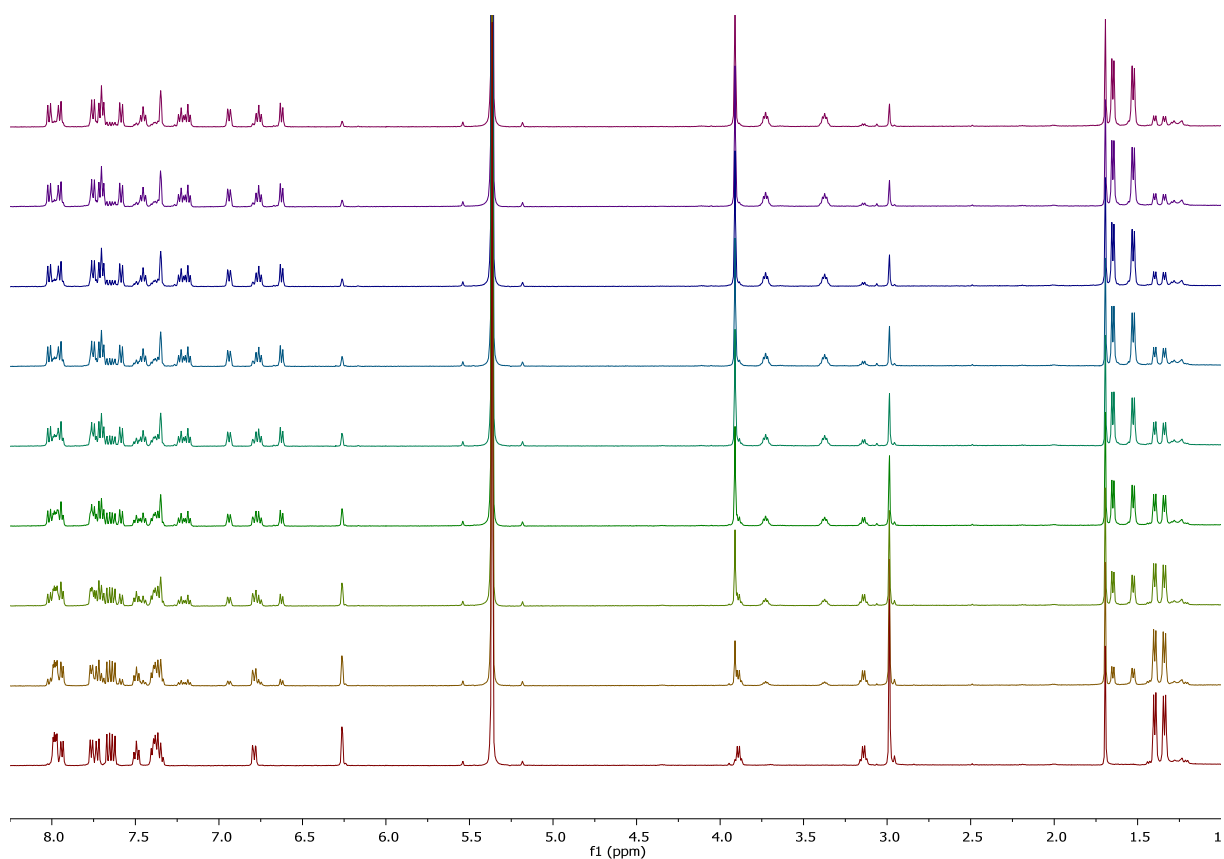


Figure S 21 ^1H -NMR of **18** in CD_2Cl_2 upon irradiation at 365 nm at $-40\text{ }^\circ\text{C}$. Initial state (bottom spectrum), PSS (top spectrum).

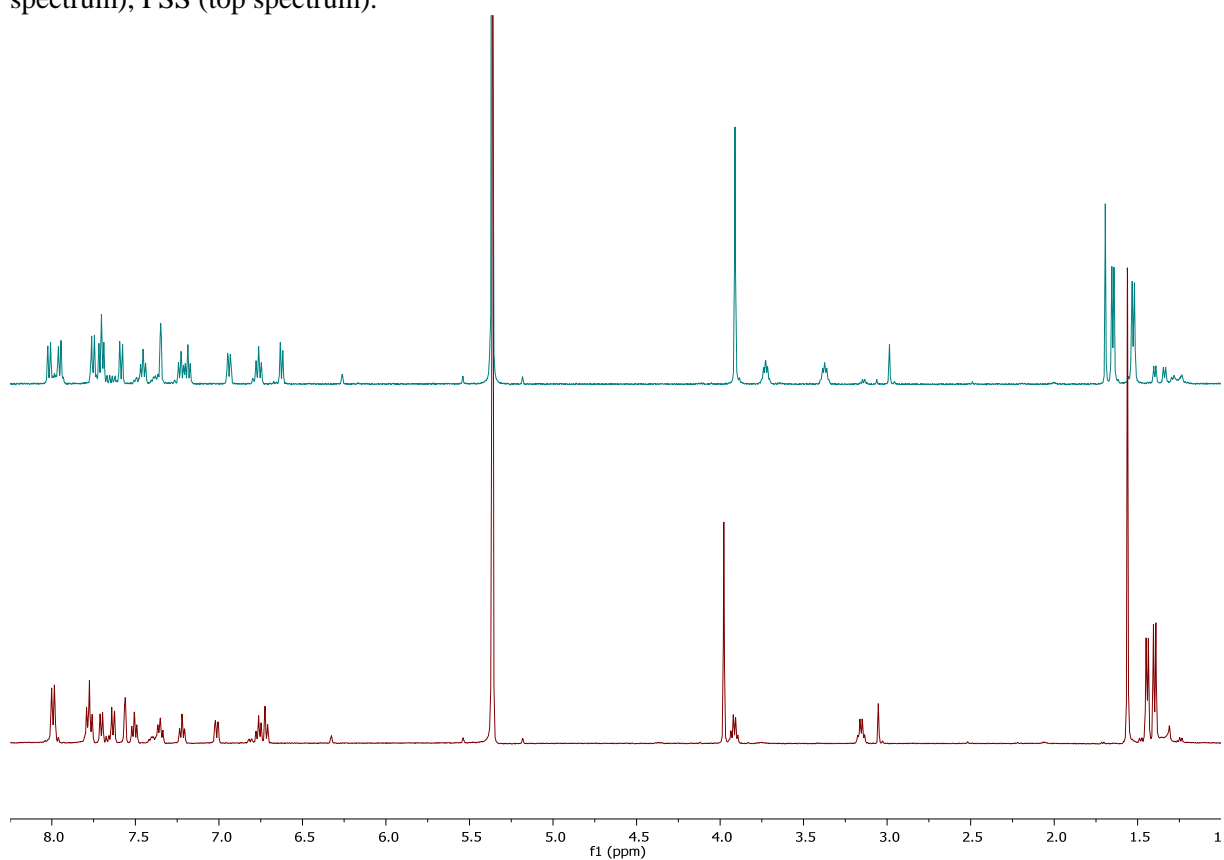


Figure S 22: ^1H -NMR of **18** in CD_2Cl_2 after irradiation at 365 nm at $-40\text{ }^\circ\text{C}$ (top). Heating of PSS at $30\text{ }^\circ\text{C}$ (bottom).

UV/Vis and CD spectra

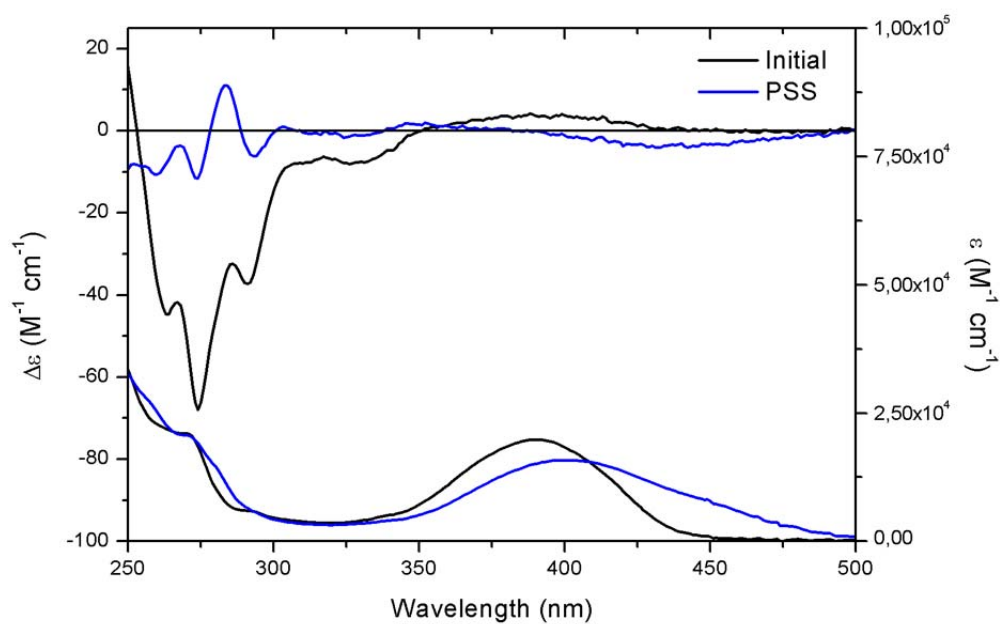


Figure S 23: UV/Vis and CD spectra of a solution of **2** in CH_2Cl_2 at 20 °C.

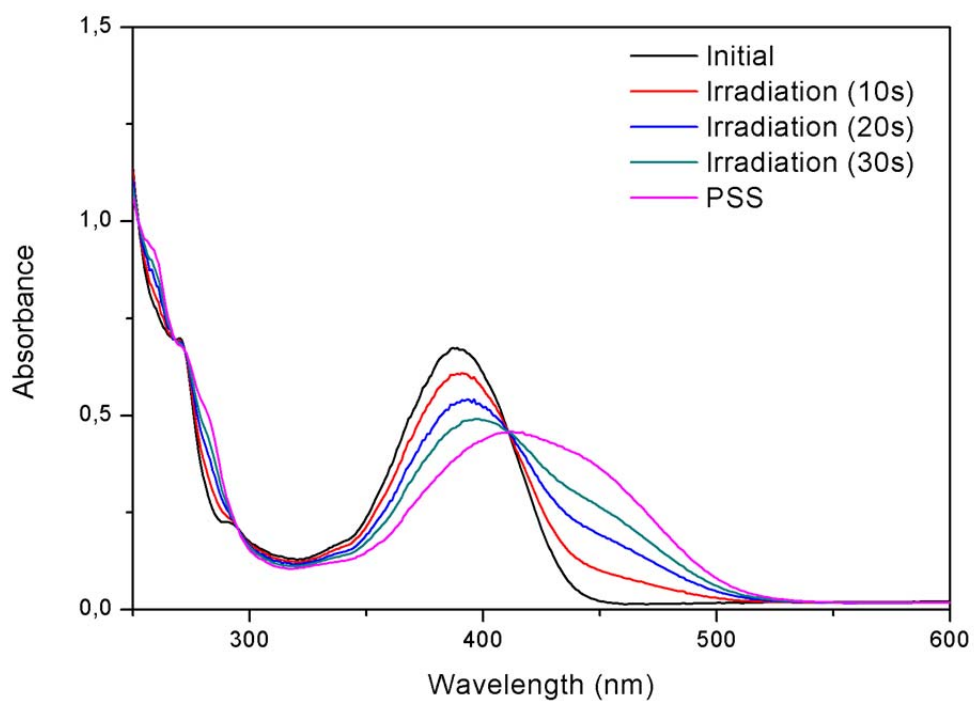


Figure S 24: Changes in UV/Vis spectrum of a solution of **3** in CH_2Cl_2 at 20 °C upon irradiation.

HRMS spectra

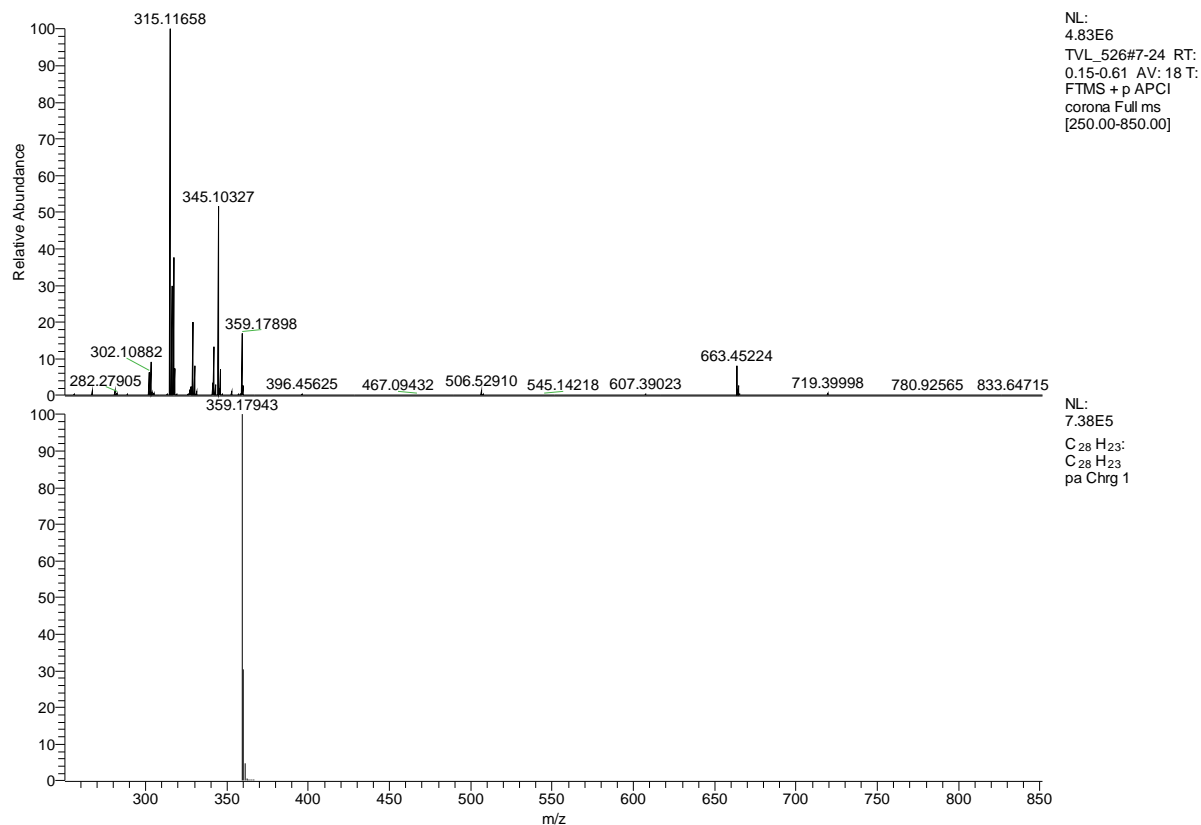


Figure S 25: HRMS of **2**. (top: measured, bottom: calcd.)

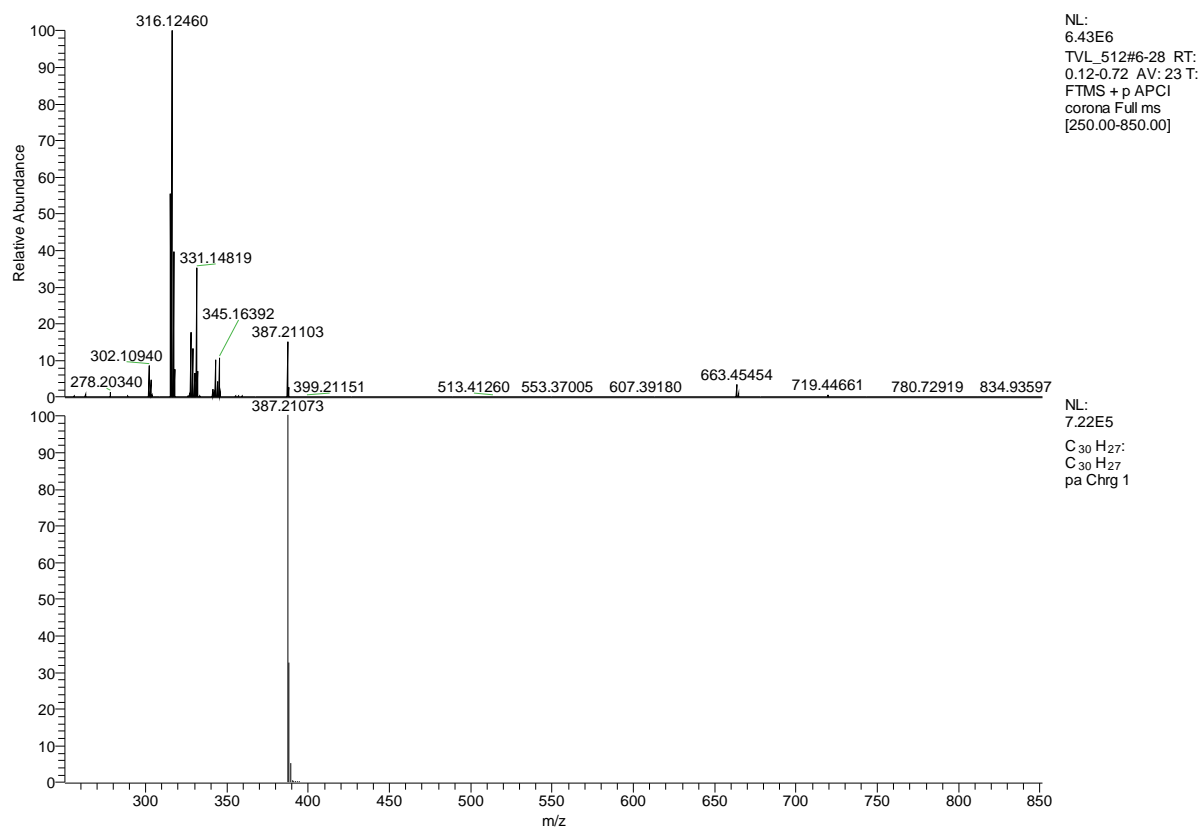


Figure S 26 HRMS of **3**. (top: measured, bottom: calcd.)

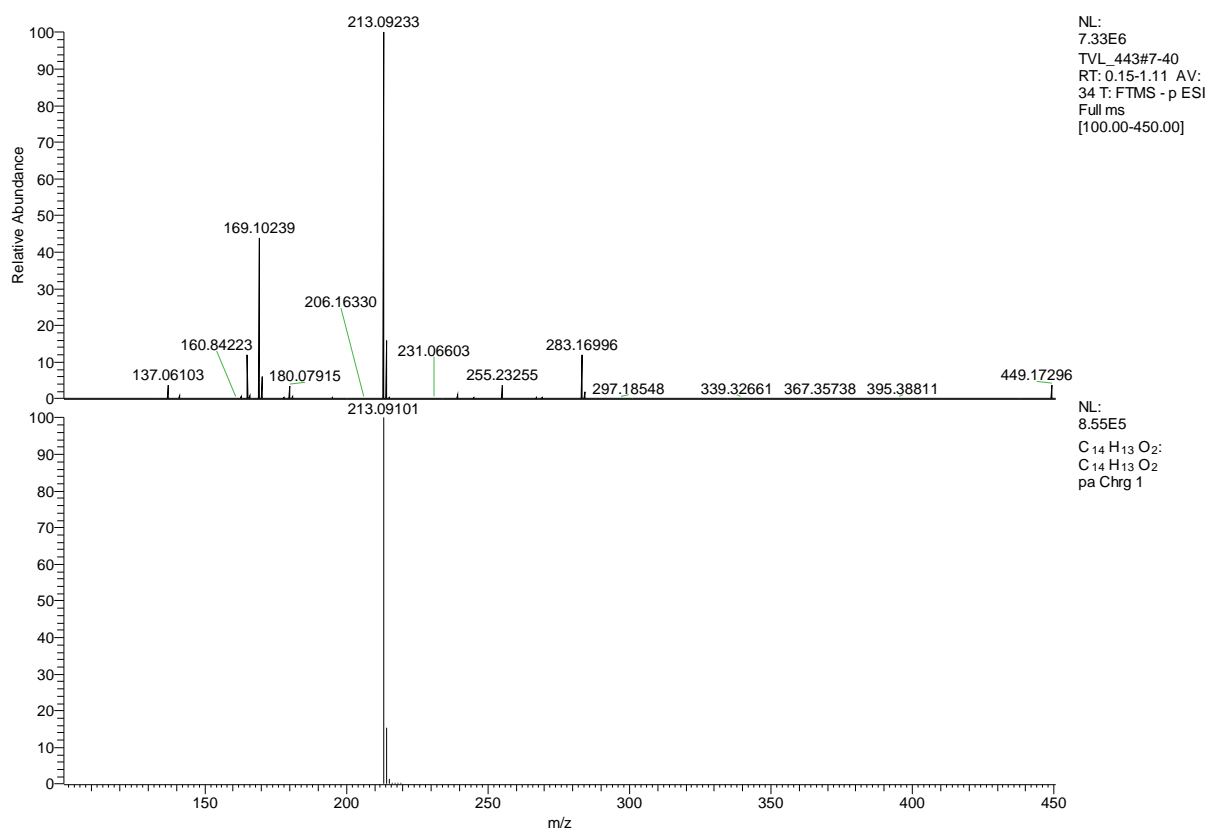


Figure S 27: HRMS of **8**. (top: measured, bottom: calcd.)

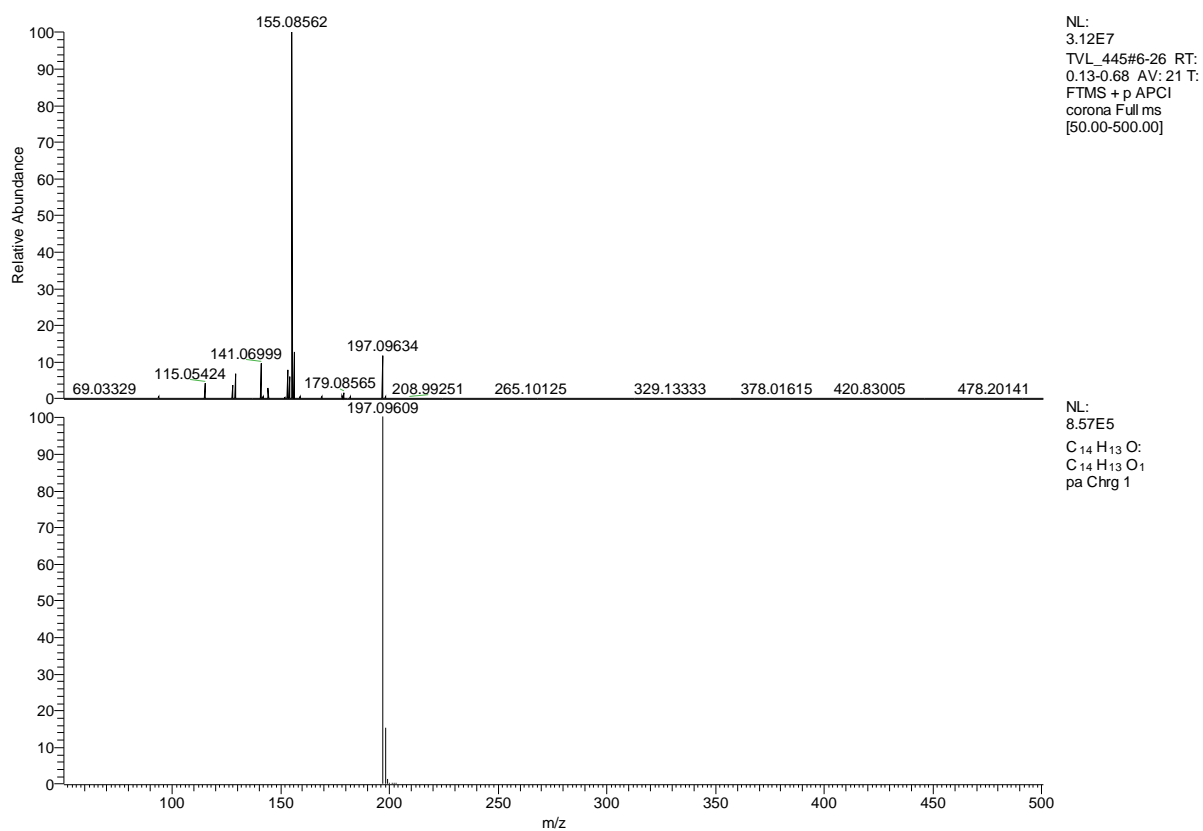


Figure S 28 HRMS of **9**. (top: measured, bottom: calcd.)

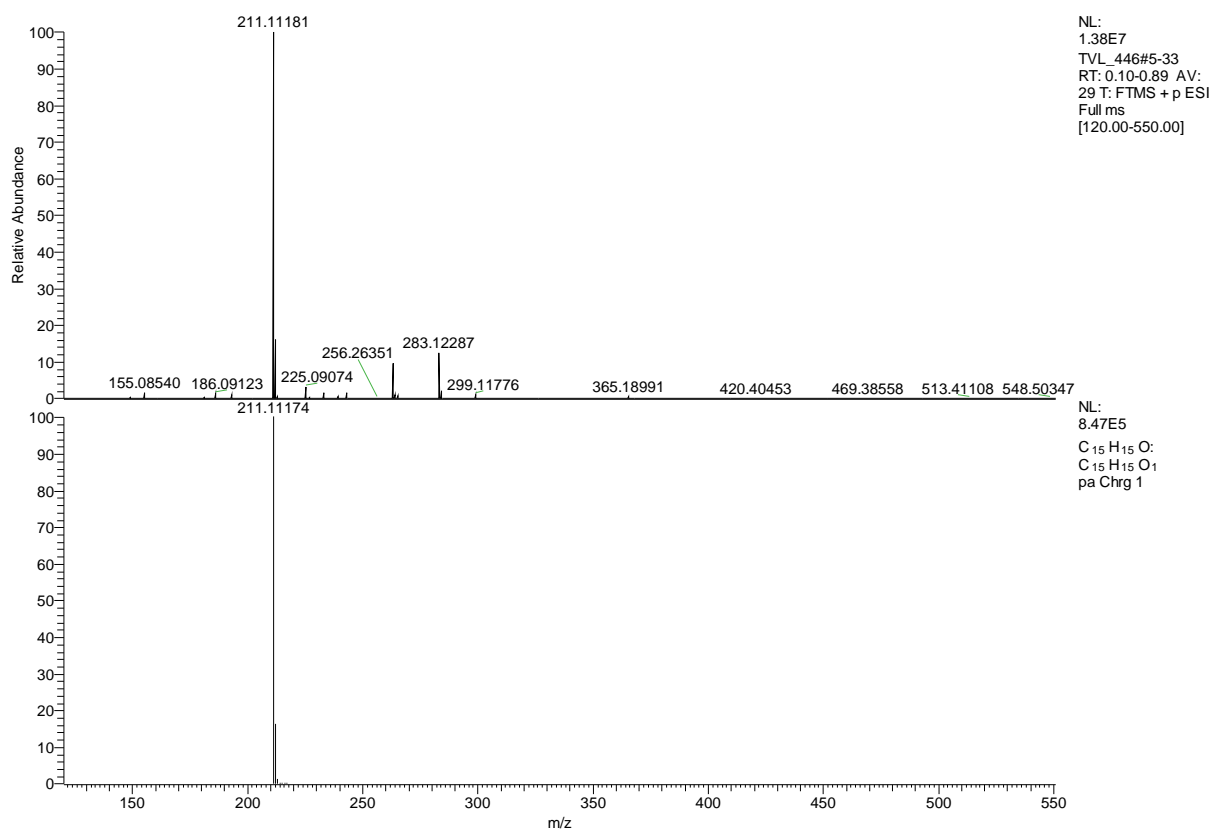


Figure S 29 HRMS of **10**. (top: measured, bottom: calcd.)

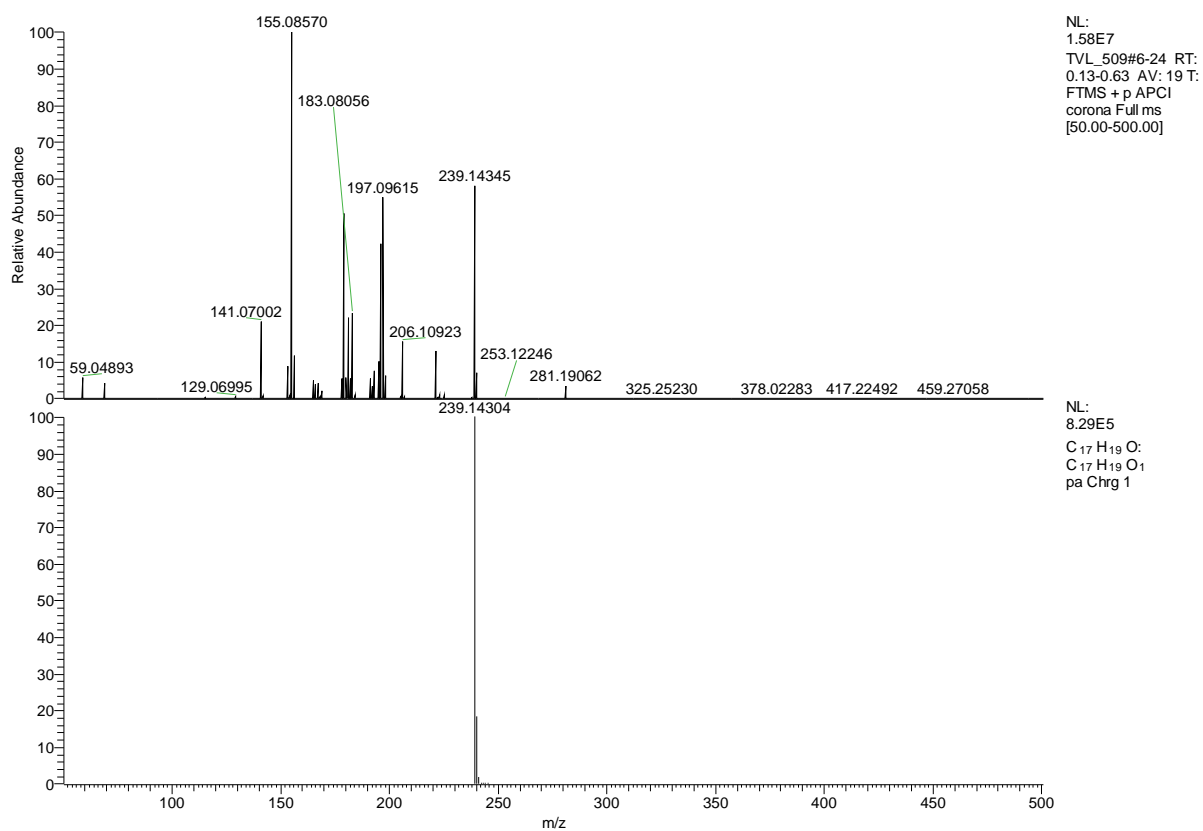


Figure S 30 Figure S 31 HRMS of **11**. (top: measured, bottom: calcd.)

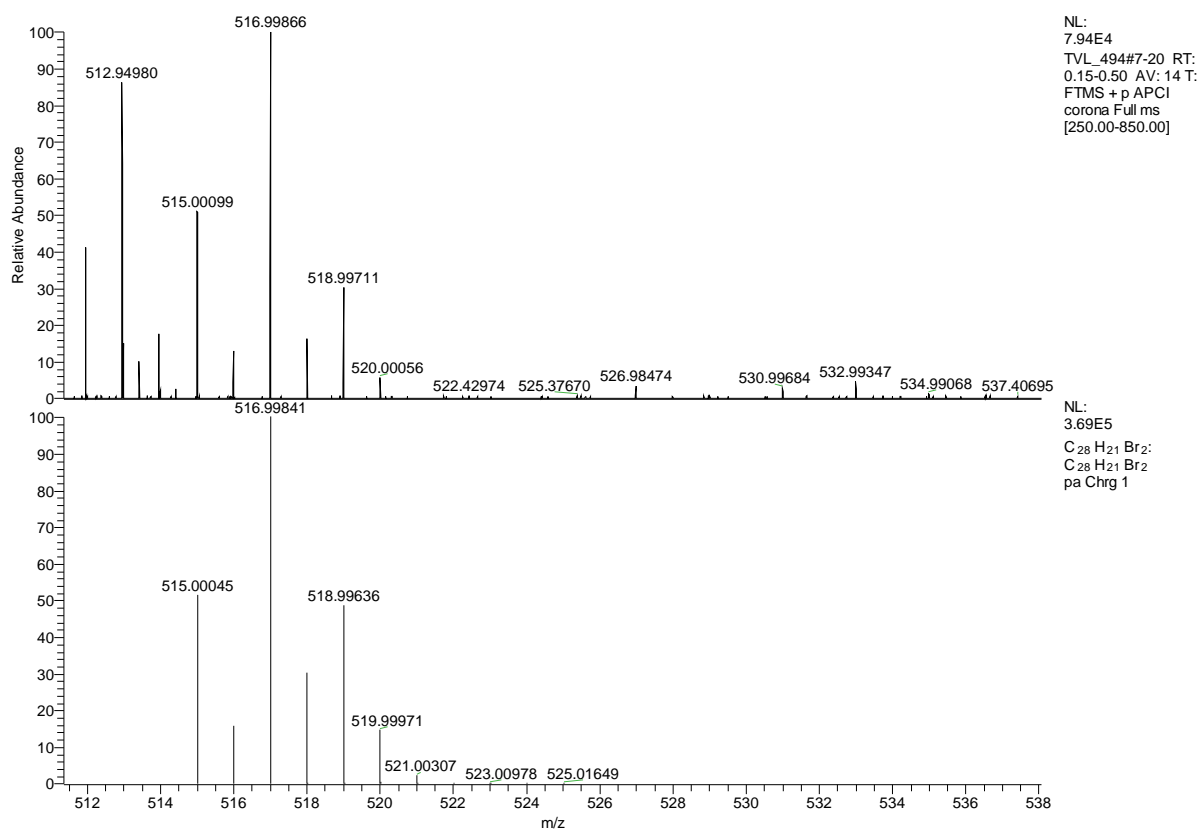


Figure S 32: HRMS of **15**. (top: measured, bottom: calcd.)

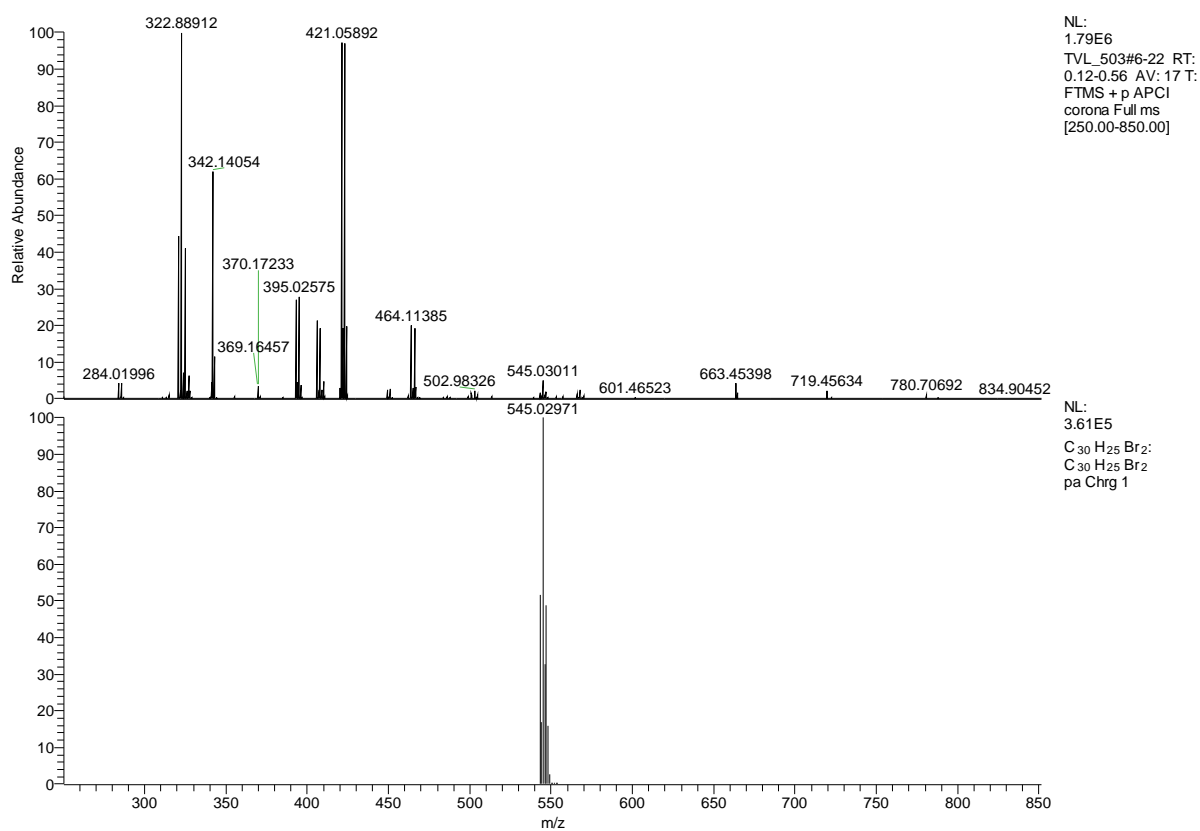


Figure S 33: HRMS of **17**. (top: measured, bottom: calcd.)

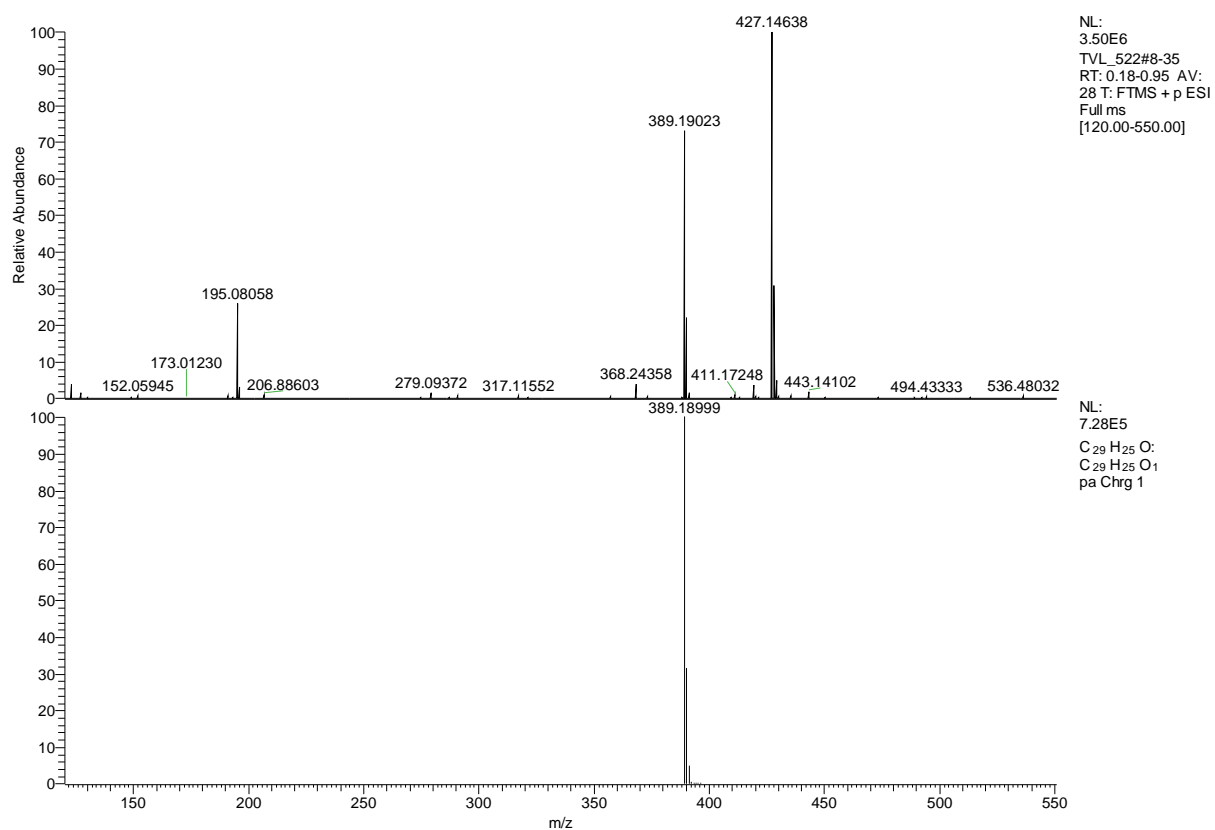
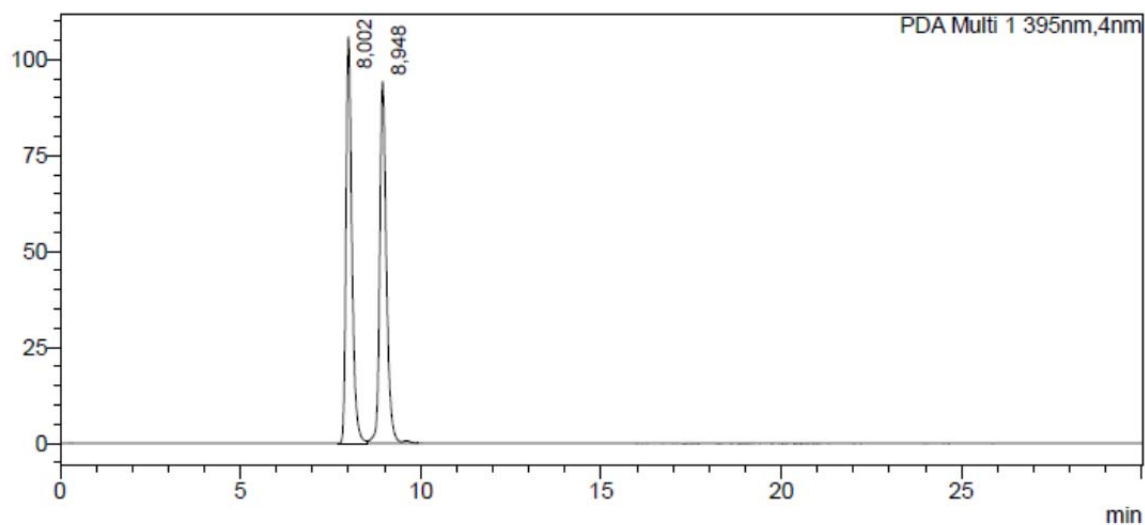


Figure S 34: HRMS of **18**. (top: measured, bottom: calcd.)

HPLC chromatograms

<Chromatogram>

mAU



<Peak Table>

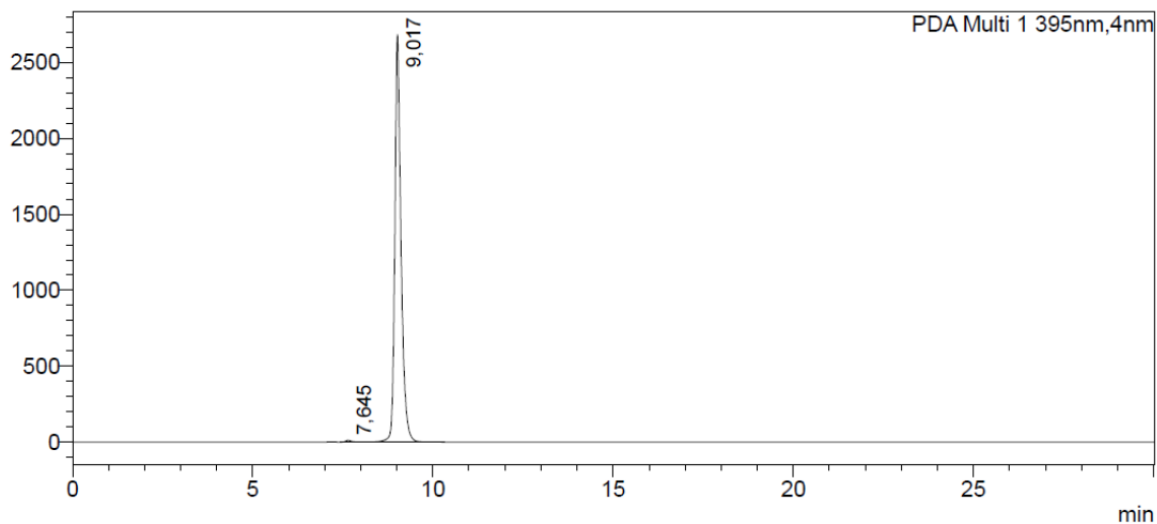
PDA Ch1 395nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8,002	1205904	106109	49,846			
2	8,948	1213372	94529	50,154		SV	
Total		2419275	200638				

Figure S 35: HPLC chromatogram of (±)-**15**.

<Chromatogram>

mAU



<Peak Table>

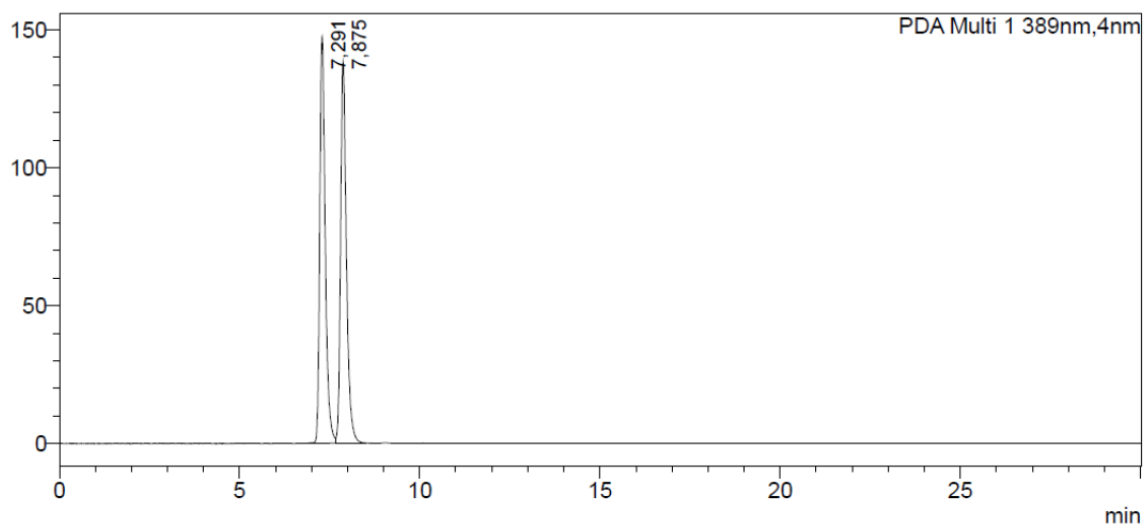
PDA Ch1 395nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7,645	137742	12124	0,428		V	
2	9,017	32045339	2683467	99,572		V	
Total		32183080	2695592				

Figure S 36: HPLC chromatogram of (S,S)-**15**.

<Chromatogram>

mAU



<Peak Table>

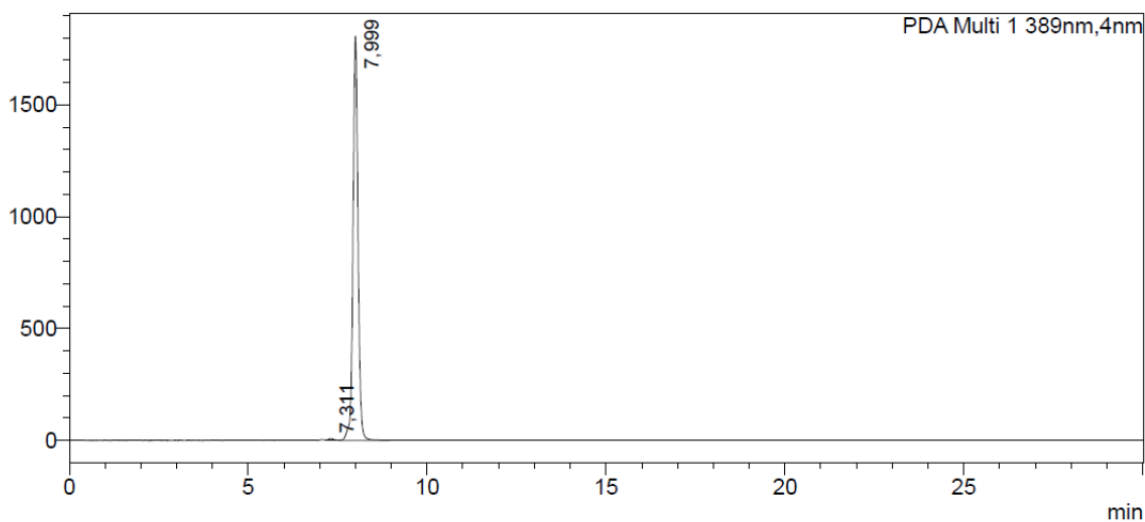
PDA Ch1 389nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7,291	1561290	147480	49,977			
2	7,875	1562740	138337	50,023		V	
Total		3124030	285817				

Figure S 37: HPLC chromatogram of (±)-**17**.

<Chromatogram>

mAU



<Peak Table>

PDA Ch1 389nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7,311	86553	8364	0,489		V	
2	7,999	17620059	1807282	99,511		V	
Total		17706612	1815646				

Figure S 38: HPLC chromatogram of (S,S)-**17**.

Eyring Plots

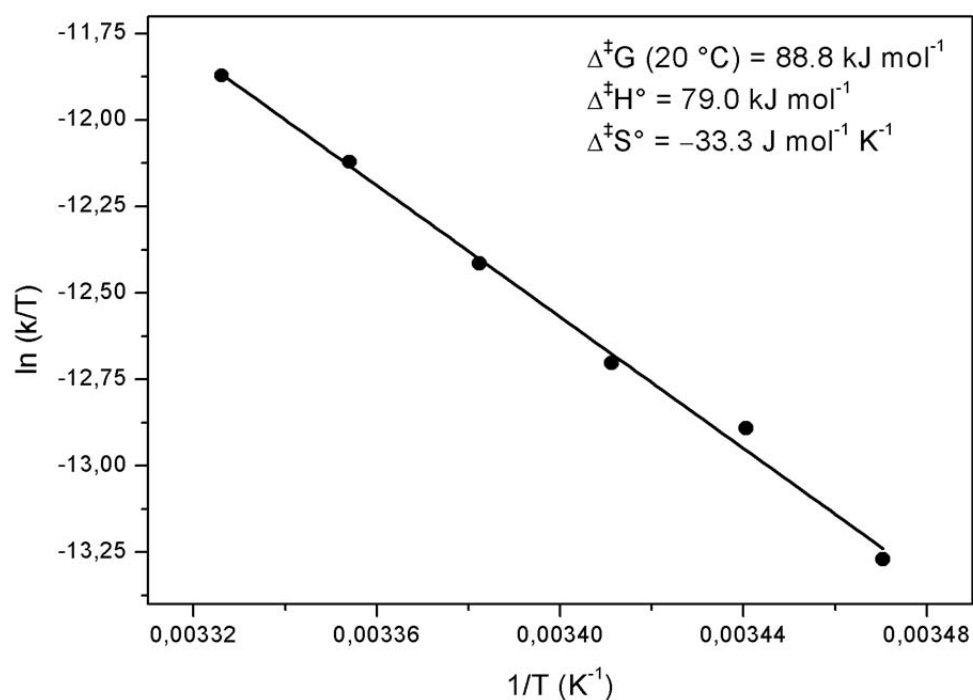


Figure S 39: Eyring plot of the THI of **2**. A solution of **2** in CH₂Cl₂ (~3 × 10⁻⁵ M) in a 1cm cuvette was irradiated to PSS at 365 nm. The rate of the thermal relaxation was followed by monitoring the absorbance at 450 nm at 6 different temperatures (15, 17.5, 20, 22.5, 25 and 27.5 °C). The Eyring equation gave the thermodynamic parameters of the process.

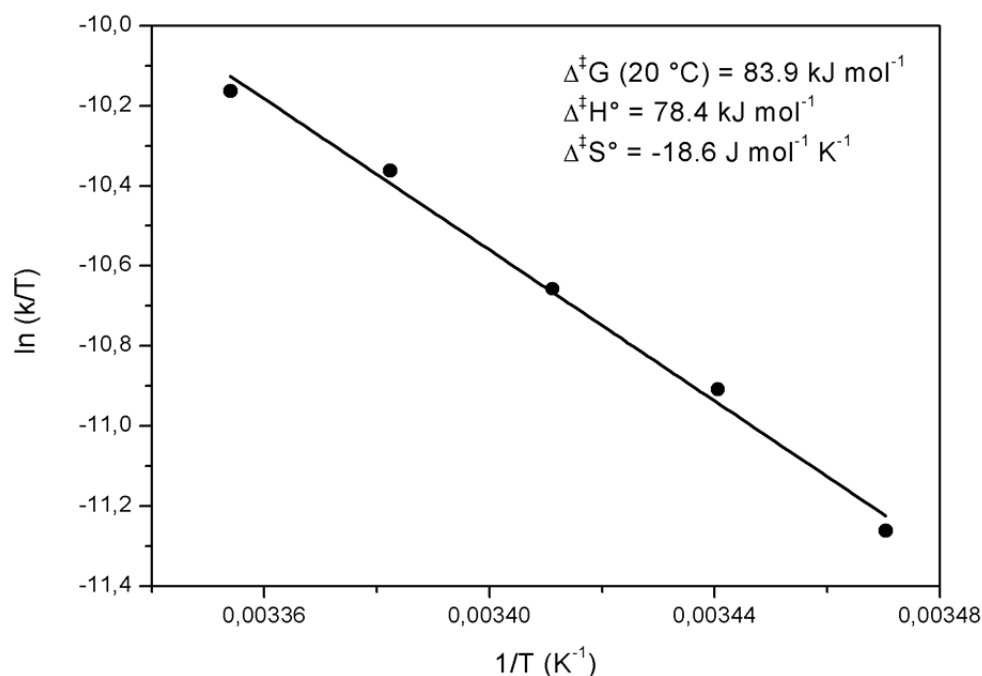


Figure S 40: Eyring Plot of the THI of **3**. A solution of **3** in CH₂Cl₂ (~1 × 10⁻⁵ M) in a 1cm cuvette was irradiated to PSS at 365 nm. The rate of the thermal relaxation was followed by monitoring the absorbance at 455 nm at 5 different temperatures (15, 17.5, 20, 22.5 and 25 °C). The Eyring equation gave the thermodynamic parameters of the process.

Crystallographic data

A single crystal of compound **2**, obtained by recrystallization from heptane, was mounted on top of a cryoloop and transferred into the cold nitrogen stream (100 K) of a Bruker-AXS D8 Venture diffractometer. Data collection and reduction was done using the Bruker software suite APEX3.² The final unit cell was obtained from the xyz centroids of 9368 reflections after integration. A multiscan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular settings (*SADABS*). The structures were solved by direct methods using *SHELXT*³ and refinement of the structure was performed using *SHLELXL*.⁴ The hydrogen atoms were generated by geometrical considerations, constrained to idealised geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms. Crystal data and details on data collection and refinement are presented in Table S1

chem formula	C ₂₈ H ₂₀ Br ₂
M _r	516.26
cryst syst	orthorhombic
color, habit	yellow, block
size (mm)	0.25 x 0.25 x 0.25
space group	P2 ₁ 2 ₁ 2 ₁
a (Å)	7.2152(3)
b (Å)	14.0726(7)
c (Å)	20.7911(10)
V (Å ³)	2111.06(17)
Z	4
ρ _{calc} , g.cm ⁻³	1.624
μ(Mo K α), cm ⁻¹	3.853
F(000)	1032
temp (K)	100(2)
θ range (deg)	2.895 – 28.735
data collected (h,k,l)	-9:9, -18:18, -28:27
no. of rflns collected	41974
no. of indepndt rflns	5424
observed rflns	5215 (F _o ≥ 2 σ(F _o))
R(F) (%)	1.57
wR(F ²) (%)	3.95
GooF	1.084
Weighting a,b	0.0182, 0.2190
params refined	273
restraints	0
min, max resid dens	-0.434, 0.247
Flack x	0.008(2)

Table S1. Crystallographic data for (*M*)-(*S,S*)-**15**

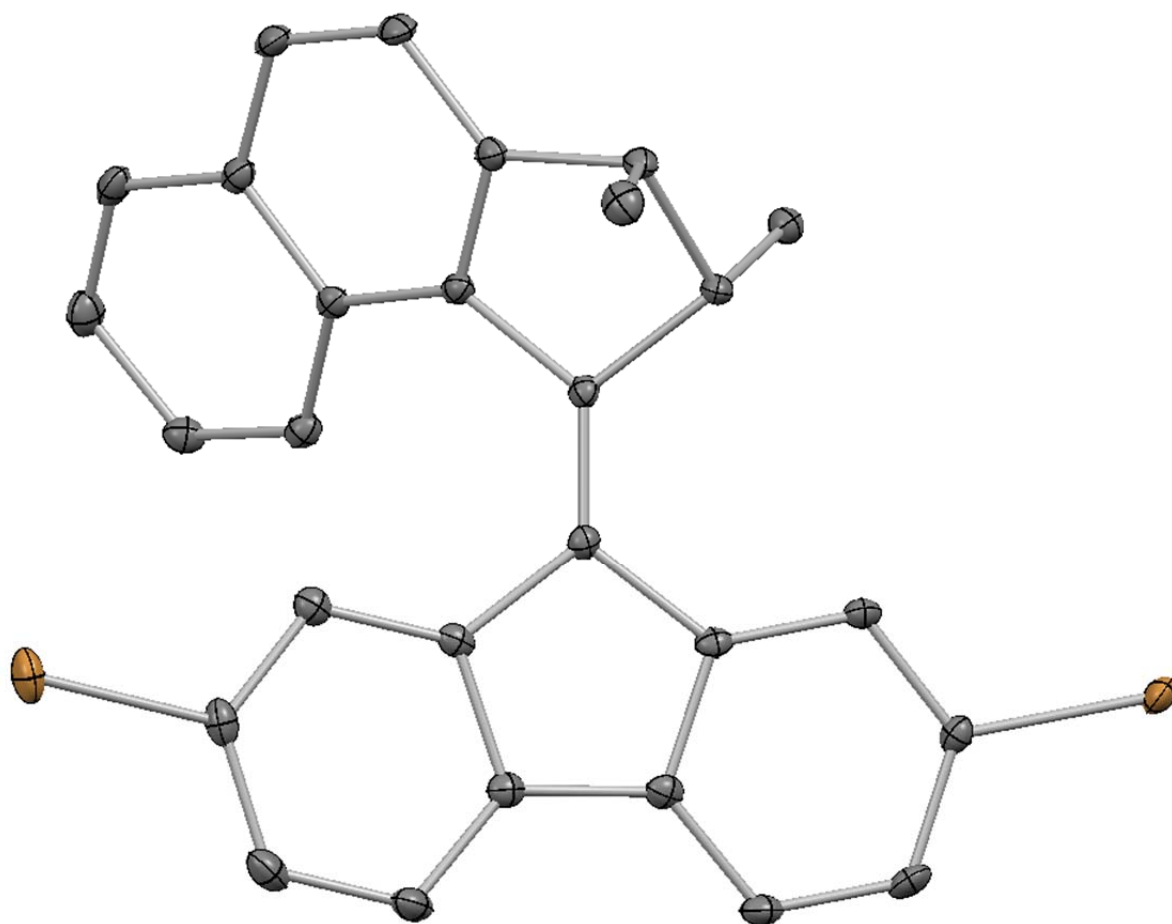


Figure S 41: Thermal Ellipsoid Plot (50% probability) of (*S,S*)-**15**. Hydrogens are omitted for clarity.

Computational Details

SCF energy in Hartree, number of imaginary frequencies and Cartesian coordinates in Ångströms.

(P)-(R)-1

-1040.97380111

0

C	-5.288702000	-3.700928000	3.502823000
C	-4.425014000	-4.597377000	2.916847000
C	-3.571282000	-4.172681000	1.872358000
C	-3.619281000	-2.875872000	1.408880000
C	-4.520643000	-1.932147000	1.968257000
C	-5.347510000	-2.349484000	3.067574000
C	-4.603966000	-0.562093000	1.554167000
C	-5.341412000	0.347132000	2.312833000
C	-6.152618000	-0.069548000	3.384580000
C	-6.173895000	-1.402655000	3.732704000
C	-3.888987000	0.178550000	0.495036000
C	-3.766550000	1.610485000	1.027329000
C	-5.091018000	1.755461000	1.834272000
C	-3.565239000	-0.199868000	-0.780701000
C	-4.086078000	-1.353491000	-1.562458000
C	-3.512888000	-1.328079000	-2.859079000
C	-2.615850000	-0.177830000	-2.947466000
C	-2.667835000	0.529566000	-1.718321000
C	-5.085227000	-2.293149000	-1.285646000
C	-5.447236000	-3.223858000	-2.262723000
C	-4.837355000	-3.221813000	-3.521184000
C	-3.873309000	-2.261211000	-3.829700000
C	-1.807535000	0.249919000	-3.998696000
C	-1.031746000	1.398477000	-3.835619000
C	-1.061545000	2.096786000	-2.625178000
C	-1.864806000	1.666243000	-1.565458000
C	-2.546392000	1.818741000	1.945400000
H	-5.928963000	-4.009608000	4.325153000
H	-4.384412000	-5.625403000	3.264356000
H	-2.868729000	-4.874751000	1.433174000
H	-2.956789000	-2.560681000	0.612262000
H	-6.745415000	0.655239000	3.935736000
H	-6.794213000	-1.744820000	4.556971000
H	-3.737226000	2.329541000	0.206028000
H	-5.010633000	2.473371000	2.658023000
H	-5.899378000	2.102039000	1.176389000
H	-5.591464000	-2.307045000	-0.330019000
H	-6.217626000	-3.955842000	-2.038373000
H	-5.129168000	-3.956154000	-4.266364000
H	-3.425259000	-2.230872000	-4.819058000
H	-1.777649000	-0.304515000	-4.932552000
H	-0.398354000	1.745650000	-4.646670000
H	-0.448636000	2.984711000	-2.499970000
H	-1.840289000	2.222908000	-0.638562000
H	-2.507970000	2.853618000	2.302778000
H	-1.607023000	1.601136000	1.429801000
H	-2.603656000	1.160699000	2.818150000

(M)-(R)-1

-1040.96809153

0

C	-9.648643000	2.928445000	-3.369824000
C	-9.214578000	2.370964000	-4.550526000
C	-7.898075000	1.867847000	-4.642038000
C	-7.058463000	1.884948000	-3.547902000
C	-7.484795000	2.411387000	-2.301166000
C	-8.799218000	2.990492000	-2.233170000
C	-6.658415000	2.481000000	-1.121350000
C	-7.082071000	3.259326000	-0.042582000
C	-8.364306000	3.835850000	0.008854000
C	-9.220218000	3.667506000	-1.055725000
C	-5.287121000	2.008691000	-0.884447000
C	-4.722608000	2.833798000	0.290811000
C	-5.999569000	3.390929000	0.987205000
C	-4.618788000	0.969223000	-1.493250000
C	-5.188785000	-0.283093000	-2.046949000
C	-4.128374000	-1.116489000	-2.489533000
C	-2.868429000	-0.402005000	-2.293507000
C	-3.153546000	0.836452000	-1.661632000
C	-6.493511000	-0.789581000	-2.038358000
C	-6.733679000	-2.078002000	-2.519292000
C	-5.686362000	-2.878027000	-2.990913000
C	-4.374305000	-2.403216000	-2.966781000
C	-1.565829000	-0.742545000	-2.655439000
C	-0.532846000	0.162544000	-2.406464000
C	-0.809667000	1.405722000	-1.825822000
C	-2.113152000	1.752692000	-1.464853000
C	-3.862276000	2.065028000	1.303920000
H	-10.646188000	3.353505000	-3.294492000
H	-9.870467000	2.337096000	-5.415318000
H	-7.539311000	1.466957000	-5.585406000
H	-6.050678000	1.505233000	-3.643756000
H	-8.670355000	4.406698000	0.881164000
H	-10.220295000	4.092334000	-1.031036000
H	-4.151816000	3.689239000	-0.100394000
H	-6.228492000	2.787709000	1.876765000
H	-5.879190000	4.423485000	1.333910000
H	-7.318348000	-0.196860000	-1.662062000
H	-7.748945000	-2.463946000	-2.522645000
H	-5.893854000	-3.877918000	-3.360828000
H	-3.555356000	-3.035136000	-3.299383000
H	-1.357367000	-1.692640000	-3.139613000
H	0.486874000	-0.090298000	-2.681731000
H	-0.003221000	2.114258000	-1.660505000
H	-2.304074000	2.734750000	-1.046038000
H	-3.627407000	2.715033000	2.154227000
H	-2.922366000	1.702840000	0.890051000
H	-4.414259000	1.199844000	1.685380000

TS (R)-1

-1040.93506681

1

C	4.670596000	1.130710000	-0.774936000
C	4.414326000	2.360819000	-0.215463000
C	3.232253000	2.536775000	0.530922000
C	2.322271000	1.508010000	0.653427000
C	2.507067000	0.246226000	0.048936000
C	3.760445000	0.049793000	-0.637394000
C	1.575858000	-0.861835000	0.144699000
C	2.048431000	-2.110206000	-0.282114000
C	3.290096000	-2.300779000	-0.920690000
C	4.116544000	-1.230465000	-1.134652000
C	0.119724000	-1.023720000	0.508266000
C	-0.092001000	-2.538981000	0.669451000
C	1.077377000	-3.221602000	-0.050067000
C	-1.002401000	-0.212423000	0.503331000
C	-1.183688000	1.269990000	0.403386000
C	-2.306581000	1.538227000	-0.422189000
C	-3.031121000	0.283224000	-0.617088000
C	-2.367738000	-0.736897000	0.120324000
C	-0.656034000	2.338596000	1.130933000
C	-1.064828000	3.649129000	0.859660000
C	-2.041649000	3.906388000	-0.103760000
C	-2.700657000	2.840346000	-0.720516000
C	-4.255185000	0.060764000	-1.240723000
C	-4.885908000	-1.175854000	-1.086268000
C	-4.302649000	-2.150397000	-0.277650000
C	-3.056857000	-1.938640000	0.327579000
C	-0.169217000	-2.919354000	2.159713000
H	5.594878000	0.954613000	-1.319059000
H	5.123373000	3.176074000	-0.323290000
H	3.035745000	3.485361000	1.022278000
H	1.448851000	1.655564000	1.253557000
H	3.567008000	-3.296823000	-1.255262000
H	5.064877000	-1.348696000	-1.651784000
H	-1.016108000	-2.840103000	0.183521000
H	1.524125000	-4.028551000	0.544339000
H	0.761287000	-3.673054000	-0.999670000
H	0.008072000	2.167408000	1.968122000
H	-0.635062000	4.468824000	1.427755000
H	-2.341473000	4.928225000	-0.316565000
H	-3.549004000	3.024351000	-1.373712000
H	-4.729520000	0.850906000	-1.816061000
H	-5.846037000	-1.361023000	-1.558559000
H	-4.824696000	-3.085131000	-0.094805000
H	-2.686226000	-2.698786000	1.002443000
H	-0.336088000	-3.996454000	2.274775000
H	-0.980378000	-2.387775000	2.666157000
H	0.765010000	-2.666057000	2.672920000

(P)-(2R,3R)-2

-1080.29094131

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C	-9.816498000	-1.192209000	1.469305000
C	-9.490050000	-2.513831000	1.270036000
C	-8.156844000	-2.871215000	0.961585000
C	-7.184367000	-1.904853000	0.823605000

C	-7.491918000	-0.528646000	0.990191000
C	-8.834583000	-0.170879000	1.358802000
C	-6.525475000	0.525466000	0.887715000
C	-6.861378000	1.815856000	1.295727000
C	-8.179402000	2.159644000	1.649572000
C	-9.152360000	1.183657000	1.651733000
C	-5.084725000	0.495756000	0.563252000
C	-4.481188000	1.658876000	1.355778000
C	-5.639976000	2.709326000	1.319893000
C	-4.406972000	-0.233328000	-0.377507000
C	-4.958352000	-0.989446000	-1.534233000
C	-3.884924000	-1.546200000	-2.274634000
C	-2.630306000	-1.175873000	-1.623060000
C	-2.928777000	-0.355244000	-0.504434000
C	-6.256729000	-1.097703000	-2.044451000
C	-6.476048000	-1.805414000	-3.228959000
C	-5.414845000	-2.395000000	-3.923168000
C	-4.108195000	-2.255406000	-3.453596000
C	-1.317360000	-1.505773000	-1.952976000
C	-0.275272000	-1.018917000	-1.162633000
C	-0.555326000	-0.221887000	-0.049046000
C	-1.871473000	0.104691000	0.289796000
C	-4.128943000	1.285640000	2.808560000
C	-5.557374000	3.644386000	0.099842000
H	-10.831987000	-0.909331000	1.734382000
H	-10.248487000	-3.285202000	1.365095000
H	-7.896344000	-3.917931000	0.835528000
H	-6.165696000	-2.190431000	0.592348000
H	-8.421687000	3.181298000	1.929715000
H	-10.175964000	1.428978000	1.922694000
H	-3.596500000	2.056399000	0.852414000
H	-5.632267000	3.322541000	2.230575000
H	-7.095584000	-0.634530000	-1.542940000
H	-7.487464000	-1.893094000	-3.614936000
H	-5.605725000	-2.944897000	-4.840172000
H	-3.276378000	-2.677814000	-4.010513000
H	-1.106247000	-2.136795000	-2.811865000
H	0.753499000	-1.265600000	-1.408200000
H	0.258771000	0.146998000	0.568151000
H	-2.044517000	0.705359000	1.172504000
H	-3.712596000	2.150364000	3.336956000
H	-3.398149000	0.473569000	2.855412000
H	-5.022030000	0.956467000	3.348939000
H	-5.518673000	3.068444000	-0.830175000
H	-4.662263000	4.273257000	0.149633000
H	-6.430215000	4.303413000	0.051110000

(M)-(2R,3R)-2

-1080.28561537

0

C	-7.503852000	4.503844000	-1.689565000
C	-6.985951000	4.290076000	-2.946178000
C	-5.977268000	3.318297000	-3.129591000
C	-5.538730000	2.548445000	-2.072752000
C	-6.079337000	2.709942000	-0.770731000

C	-7.052591000	3.749550000	-0.573699000
C	-5.656903000	1.957777000	0.384411000
C	-6.052479000	2.380144000	1.655074000
C	-6.998774000	3.406124000	1.836993000
C	-7.516381000	4.050181000	0.735982000
C	-4.683968000	0.865274000	0.504728000
C	-4.209644000	0.847901000	1.969798000
C	-5.334086000	1.616973000	2.738242000
C	-4.309697000	-0.059499000	-0.445319000
C	-5.127546000	-0.614333000	-1.551264000
C	-4.376011000	-1.612704000	-2.224842000
C	-3.047841000	-1.677402000	-1.617765000
C	-3.013884000	-0.771346000	-0.525966000
C	-6.473754000	-0.433459000	-1.888527000
C	-7.032683000	-1.193818000	-2.917343000
C	-6.272393000	-2.148573000	-3.602774000
C	-4.940584000	-2.370639000	-3.249945000
C	-1.919925000	-2.413929000	-1.977116000
C	-0.735823000	-2.236983000	-1.259617000
C	-0.678362000	-1.310838000	-0.211552000
C	-1.804508000	-0.568723000	0.149949000
C	-3.997282000	-0.539434000	2.593658000
C	-4.815164000	2.483264000	3.891630000
H	-8.254144000	5.272979000	-1.525443000
H	-7.332722000	4.878830000	-3.790184000
H	-5.537509000	3.177835000	-4.112563000
H	-4.757725000	1.818078000	-2.233431000
H	-7.317852000	3.685315000	2.836856000
H	-8.259489000	4.834153000	0.856213000
H	-3.285536000	1.439415000	2.066314000
H	-6.019224000	0.865236000	3.159112000
H	-7.088327000	0.285925000	-1.361187000
H	-8.074318000	-1.042255000	-3.185212000
H	-6.725642000	-2.730032000	-4.400358000
H	-4.358242000	-3.135289000	-3.756735000
H	-1.955006000	-3.105013000	-2.814806000
H	0.150034000	-2.805169000	-1.527845000
H	0.254962000	-1.159909000	0.323093000
H	-1.724384000	0.165654000	0.944061000
H	-3.813010000	-0.437318000	3.669026000
H	-3.158514000	-1.085064000	2.164027000
H	-4.894781000	-1.152572000	2.463180000
H	-4.164409000	3.281757000	3.519768000
H	-4.240331000	1.878225000	4.600647000
H	-5.634369000	2.948555000	4.449048000

TS (2R,3R)-2

-1080.25206554

1

C	4.583395000	1.627460000	-0.639859000
C	4.195934000	2.868245000	-0.190887000
C	2.960125000	2.996601000	0.474052000
C	2.132989000	1.904779000	0.630504000
C	2.456512000	0.621367000	0.140836000
C	3.756692000	0.485618000	-0.469253000

C	1.615073000	-0.552200000	0.275362000
C	2.196260000	-1.780760000	-0.067170000
C	3.482085000	-1.906806000	-0.630043000
C	4.238516000	-0.789263000	-0.861398000
C	0.170001000	-0.814888000	0.629970000
C	0.097823000	-2.328189000	0.890333000
C	1.297338000	-2.959065000	0.163571000
C	-1.019722000	-0.109322000	0.569679000
C	-1.336622000	1.338328000	0.351767000
C	-2.468173000	1.433323000	-0.500199000
C	-3.075348000	0.105851000	-0.591143000
C	-2.331173000	-0.783677000	0.232412000
C	-0.921922000	2.506775000	0.993894000
C	-1.445740000	3.747519000	0.613020000
C	-2.426542000	3.834030000	-0.376206000
C	-2.975351000	2.664623000	-0.907823000
C	-4.269951000	-0.277921000	-1.193390000
C	-4.791640000	-1.546417000	-0.929061000
C	-4.133451000	-2.389600000	-0.034740000
C	-2.915504000	-2.016440000	0.548578000
C	0.103851000	-2.614336000	2.403547000
C	0.897554000	-3.669145000	-1.143347000
H	5.547956000	1.492351000	-1.122314000
H	4.841174000	3.731282000	-0.324572000
H	2.655457000	3.959398000	0.874189000
H	1.212863000	2.022863000	1.162559000
H	3.854829000	-2.894035000	-0.888497000
H	5.223166000	-0.862502000	-1.315191000
H	-0.811163000	-2.742361000	0.462891000
H	1.802481000	-3.690694000	0.809608000
H	-0.258459000	2.466844000	1.848080000
H	-1.102418000	4.646680000	1.115953000
H	-2.815788000	4.802856000	-0.674800000
H	-3.827467000	2.715254000	-1.579707000
H	-4.807386000	0.413297000	-1.836624000
H	-5.727909000	-1.856204000	-1.383604000
H	-4.574330000	-3.345583000	0.232357000
H	-2.484328000	-2.676629000	1.289611000
H	0.034337000	-3.691697000	2.592736000
H	-0.734655000	-2.121177000	2.904732000
H	1.027562000	-2.249535000	2.865890000
H	0.359342000	-2.983450000	-1.805916000
H	0.245402000	-4.524297000	-0.936021000
H	1.774909000	-4.038838000	-1.683491000

(P)-(2R,3R)-3

-1158.91920121

0

C	-9.765384000	-0.888139000	1.539084000
C	-9.539549000	-2.234332000	1.365291000
C	-8.240812000	-2.695298000	1.048009000
C	-7.202707000	-1.805870000	0.873728000
C	-7.406448000	-0.407465000	1.013141000
C	-8.712974000	0.055370000	1.393965000
C	-6.365805000	0.569719000	0.877343000

C	-6.595551000	1.884399000	1.276399000
C	-7.880030000	2.333342000	1.638109000
C	-8.924508000	1.435130000	1.665808000
C	-4.938467000	0.430080000	0.522652000
C	-4.221330000	1.553025000	1.279207000
C	-5.308930000	2.679639000	1.296632000
C	-4.354010000	-0.347201000	-0.444053000
C	-5.013952000	-1.075477000	-1.563089000
C	-4.022678000	-1.728057000	-2.338311000
C	-2.714014000	-1.436135000	-1.758637000
C	-2.894518000	-0.570360000	-0.648339000
C	-6.337105000	-1.086853000	-2.018684000
C	-6.663262000	-1.794955000	-3.178116000
C	-5.684641000	-2.482835000	-3.902266000
C	-4.352147000	-2.439656000	-3.490653000
C	-1.447316000	-1.860561000	-2.154464000
C	-0.329776000	-1.420516000	-1.444139000
C	-0.491058000	-0.571077000	-0.346372000
C	-1.761079000	-0.151640000	0.059619000
C	-3.693119000	1.165148000	2.698551000
C	-5.178049000	3.638810000	0.098755000
H	-10.753195000	-0.525849000	1.811942000
H	-10.350935000	-2.945592000	1.487842000
H	-8.059239000	-3.760812000	0.942847000
H	-6.211366000	-2.170208000	0.633921000
H	-8.040317000	3.374053000	1.907003000
H	-9.923191000	1.761682000	1.943894000
H	-3.358943000	1.893904000	0.699171000
H	-5.250384000	3.273649000	2.216849000
H	-7.114048000	-0.546528000	-1.496017000
H	-7.693925000	-1.805012000	-3.520598000
H	-5.958594000	-3.032227000	-4.798281000
H	-3.580624000	-2.935834000	-4.072885000
H	-1.329990000	-2.525732000	-3.005484000
H	0.664403000	-1.740632000	-1.741836000
H	0.380626000	-0.232235000	0.206005000
H	-1.837009000	0.491822000	0.924789000
H	-3.065171000	0.276506000	2.557984000
H	-5.189586000	3.086075000	-0.846078000
H	-4.242018000	4.204454000	0.151861000

(M)-(2R,3R)-3

-1158.91421070

0

C	-10.165350000	0.219074000	0.049176000
C	-10.118748000	-0.398690000	-1.179795000
C	-8.870999000	-0.613342000	-1.804499000
C	-7.695763000	-0.261308000	-1.173130000
C	-7.700813000	0.334512000	0.113977000
C	-8.976113000	0.628781000	0.707952000
C	-6.513843000	0.750659000	0.824461000
C	-6.650494000	1.619431000	1.909760000
C	-7.905711000	1.907679000	2.479656000
C	-9.042815000	1.378201000	1.914842000
C	-5.094158000	0.566595000	0.513156000

C	-4.295947000	1.586621000	1.351947000
C	-5.336964000	2.235215000	2.316758000
C	-4.498099000	-0.393505000	-0.279880000
C	-4.953401000	-1.780882000	-0.538435000
C	-4.002914000	-2.434913000	-1.365111000
C	-2.943339000	-1.483279000	-1.689095000
C	-3.206299000	-0.270861000	-0.997921000
C	-6.000650000	-2.529564000	0.012802000
C	-6.127476000	-3.880880000	-0.314144000
C	-5.211971000	-4.504314000	-1.170000000
C	-4.135284000	-3.784508000	-1.689327000
C	-1.836481000	-1.612435000	-2.526736000
C	-0.979488000	-0.524039000	-2.694336000
C	-1.243482000	0.685200000	-2.041115000
C	-2.352873000	0.820844000	-1.204504000
C	-3.076694000	0.965943000	2.100783000
C	-5.374618000	3.772193000	2.241274000
H	-11.119665000	0.430266000	0.524666000
H	-11.035520000	-0.696704000	-1.679692000
H	-8.833655000	-1.055945000	-2.795480000
H	-6.752677000	-0.424273000	-1.675612000
H	-7.971827000	2.543719000	3.357915000
H	-10.018336000	1.573069000	2.352583000
H	-3.906862000	2.381274000	0.699894000
H	-5.100141000	1.959998000	3.352485000
H	-6.711740000	-2.076086000	0.692227000
H	-6.948001000	-4.454833000	0.106566000
H	-5.328776000	-5.556234000	-1.413872000
H	-3.399985000	-4.275495000	-2.320919000
H	-1.648052000	-2.544667000	-3.052132000
H	-0.111938000	-0.611428000	-3.341774000
H	-0.580085000	1.532623000	-2.187813000
H	-2.538984000	1.776746000	-0.728625000
H	-2.432463000	0.517882000	1.339625000
H	-5.618548000	4.105439000	1.226961000
H	-4.404265000	4.197802000	2.515629000
H	-6.125937000	4.189066000	2.919813000
C	-3.459531000	-0.159851000	3.074915000
H	-4.036662000	-0.944237000	2.578209000
H	-2.555840000	-0.622426000	3.485350000
H	-4.045844000	0.207588000	3.924698000
C	-2.248056000	2.047988000	2.810657000
H	-1.928393000	2.832952000	2.115755000
H	-2.807789000	2.527872000	3.621724000
H	-1.347111000	1.610806000	3.253996000

TS (2R,3R)-3

-1158.88237783

0

C	4.503709000	1.925789000	-0.752563000
C	4.179427000	3.076448000	-0.072299000
C	3.005708000	3.100275000	0.707337000
C	2.164607000	2.008112000	0.738280000
C	2.415014000	0.828914000	0.003742000
C	3.667892000	0.778883000	-0.708323000

C	1.558015000	-0.340704000	-0.000256000
C	2.104904000	-1.516855000	-0.529660000
C	3.352803000	-1.567091000	-1.183768000
C	4.101700000	-0.427929000	-1.314744000
C	0.118211000	-0.626176000	0.343295000
C	0.000421000	-2.157206000	0.381110000
C	1.216866000	-2.717688000	-0.380728000
C	-1.049577000	0.119600000	0.373486000
C	-1.306536000	1.593355000	0.392983000
C	-2.420541000	1.875433000	-0.439535000
C	-3.068454000	0.606659000	-0.767460000
C	-2.371628000	-0.439635000	-0.099858000
C	-0.853800000	2.619376000	1.224835000
C	-1.325781000	3.925787000	1.056762000
C	-2.291591000	4.216449000	0.091581000
C	-2.876834000	3.176798000	-0.634822000
C	-4.257253000	0.376571000	-1.453325000
C	-4.821030000	-0.901235000	-1.435021000
C	-4.208072000	-1.913432000	-0.698067000
C	-2.996617000	-1.690932000	-0.030207000
C	-0.167553000	-2.687592000	1.838688000
C	0.833374000	-3.364038000	-1.724909000
H	5.427998000	1.863612000	-1.321056000
H	4.832675000	3.943039000	-0.109133000
H	2.762888000	3.979315000	1.297350000
H	1.300015000	2.034677000	1.368948000
H	3.701322000	-2.509905000	-1.595593000
H	5.051395000	-0.438997000	-1.842738000
H	-0.889892000	-2.462917000	-0.165731000
H	1.743615000	-3.475128000	0.215205000
H	-0.200907000	2.409201000	2.061843000
H	-0.954199000	4.713410000	1.705543000
H	-2.640701000	5.236318000	-0.040066000
H	-3.717037000	3.374120000	-1.294619000
H	-4.756919000	1.189550000	-1.972737000
H	-5.753529000	-1.093432000	-1.957206000
H	-4.680354000	-2.888447000	-0.620648000
H	-2.605819000	-2.488465000	0.586674000
H	-1.049179000	-2.173570000	2.245370000
H	0.286623000	-2.654509000	-2.354686000
H	0.194115000	-4.238576000	-1.564894000
H	1.717440000	-3.693643000	-2.279821000
C	1.013419000	-2.350634000	2.760946000
H	1.181324000	-1.272047000	2.823171000
H	0.821403000	-2.718948000	3.774321000
H	1.944508000	-2.814378000	2.416400000
C	-0.461843000	-4.196129000	1.852324000
H	-1.322877000	-4.448872000	1.223002000
H	0.392651000	-4.779170000	1.491055000
H	-0.681260000	-4.537702000	2.869406000

(P)-(S)-4

-1040.97610051

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C	-9.898419000	-1.108500000	1.445297000
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C	-9.540192000	-2.420630000	1.238187000
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C	-7.253828000	-1.750549000	0.779048000
C	-7.595187000	-0.383002000	0.950294000
C	-8.943158000	-0.062627000	1.332520000
C	-6.656110000	0.696932000	0.845127000
C	-7.021300000	1.977445000	1.265567000
C	-8.345470000	2.282091000	1.632932000
C	-9.292633000	1.281326000	1.635555000
C	-5.224437000	0.696402000	0.497241000
C	-4.640266000	1.902926000	1.219644000
C	-5.825467000	2.907221000	1.274310000
C	-4.521201000	-0.061667000	-0.401485000
C	-5.021433000	-0.849720000	-1.556431000
C	-3.912170000	-1.390067000	-2.257478000
C	-2.686844000	-0.990881000	-1.566514000
C	-3.042386000	-0.166970000	-0.467588000
C	-6.302347000	-0.996237000	-2.099770000
C	-6.470732000	-1.724454000	-3.280015000
C	-5.375433000	-2.294314000	-3.937340000
C	-4.085829000	-2.117324000	-3.433793000
C	-1.355799000	-1.306746000	-1.831143000
C	-0.359612000	-0.808169000	-0.989508000
C	-0.700761000	-0.020331000	0.114348000
C	-2.034855000	0.294201000	0.387531000
C	-5.765444000	3.884975000	2.450237000
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H	-7.912898000	-3.781387000	0.791260000
H	-6.229805000	-2.010968000	0.543419000
H	-8.616600000	3.294088000	1.918973000
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H	-3.767552000	2.320159000	0.714573000
H	-4.348086000	1.647532000	2.249347000
H	-5.817488000	3.487308000	0.338651000
H	-7.165205000	-0.548121000	-1.624793000
H	-7.468382000	-1.844186000	-3.692361000
H	-5.526959000	-2.859617000	-4.852322000
H	-3.229212000	-2.526680000	-3.962207000
H	-1.094782000	-1.939405000	-2.674987000
H	0.682465000	-1.044028000	-1.184549000
H	0.079132000	0.347367000	0.774915000
H	-2.266586000	0.878650000	1.269388000
H	-6.595707000	4.598220000	2.426948000
H	-4.836149000	4.463660000	2.422638000
H	-5.805194000	3.351947000	3.406279000

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-1040.97529079

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C	-7.209920000	1.967108000	-3.614223000
C	-7.587995000	2.448033000	-2.333119000

C	-8.915695000	2.974782000	-2.170811000
C	-6.698679000	2.520330000	-1.208619000
C	-7.080806000	3.231609000	-0.070726000
C	-8.383622000	3.741293000	0.081154000
C	-9.291589000	3.586179000	-0.943440000
C	-5.294065000	2.098209000	-1.059646000
C	-4.709544000	3.025775000	-0.000409000
C	-5.930633000	3.368612000	0.902457000
C	-4.623756000	1.021511000	-1.578231000
C	-5.169019000	-0.242460000	-2.135697000
C	-4.088824000	-1.103896000	-2.459946000
C	-2.836532000	-0.415600000	-2.149416000
C	-3.149970000	0.849556000	-1.589005000
C	-6.476544000	-0.731323000	-2.230116000
C	-6.694528000	-2.027982000	-2.702149000
C	-5.624237000	-2.852259000	-3.064914000
C	-4.311857000	-2.396086000	-2.932460000
C	-1.514773000	-0.815786000	-2.334433000
C	-0.484845000	0.052885000	-1.968106000
C	-0.782179000	1.314156000	-1.442553000
C	-2.106343000	1.722702000	-1.261064000
C	-6.052970000	2.418780000	2.108744000
H	-10.827557000	3.305714000	-3.124674000
H	-10.130203000	2.385044000	-5.313295000
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H	-6.196469000	1.618498000	-3.766493000
H	-8.664301000	4.260289000	0.993720000
H	-10.302991000	3.971684000	-0.844656000
H	-4.323425000	3.949259000	-0.453909000
H	-3.897575000	2.562395000	0.563011000
H	-5.867962000	4.397813000	1.276806000
H	-7.322721000	-0.124062000	-1.936516000
H	-7.711904000	-2.399572000	-2.783110000
H	-5.814471000	-3.856542000	-3.432245000
H	-3.476731000	-3.046650000	-3.177111000
H	-1.285953000	-1.786504000	-2.765560000
H	0.550294000	-0.246326000	-2.104256000
H	0.025006000	1.991152000	-1.178174000
H	-2.300976000	2.718899000	-0.883394000
H	-6.972840000	2.613181000	2.669627000
H	-5.207317000	2.545695000	2.792632000
H	-6.073235000	1.374673000	1.780175000

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-1040.93557733

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C	4.297609000	1.742607000	-1.127799000
C	3.997578000	2.973146000	-0.591462000
C	2.939643000	3.081690000	0.335957000
C	2.166533000	1.983122000	0.644208000
C	2.383289000	0.716020000	0.053614000
C	3.540118000	0.587915000	-0.795511000
C	1.603453000	-0.463056000	0.338099000
C	2.150598000	-1.706879000	-0.021505000
C	3.307700000	-1.822691000	-0.815936000

C	3.959573000	-0.692170000	-1.242201000
C	0.207704000	-0.751559000	0.812580000
C	0.321686000	-2.163899000	1.369454000
C	1.322467000	-2.881670000	0.457334000
C	-1.036460000	-0.201012000	0.552553000
C	-1.526870000	1.197883000	0.475949000
C	-2.822781000	1.214330000	-0.103499000
C	-3.224676000	-0.157478000	-0.374621000
C	-2.203948000	-1.032659000	0.082827000
C	-1.071742000	2.383436000	1.063752000
C	-1.795880000	3.568399000	0.923293000
C	-3.015362000	3.586600000	0.240059000
C	-3.549062000	2.395161000	-0.249190000
C	-4.387407000	-0.626836000	-0.985973000
C	-4.557344000	-1.996565000	-1.168653000
C	-3.545398000	-2.873472000	-0.767834000
C	-2.374751000	-2.404066000	-0.169350000
C	2.123807000	-3.996618000	1.137468000
H	5.146198000	1.625502000	-1.796706000
H	4.591863000	3.845232000	-0.846913000
H	2.741023000	4.032019000	0.822615000
H	1.410708000	2.067199000	1.404401000
H	3.660230000	-2.807209000	-1.109668000
H	4.831885000	-0.762127000	-1.886349000
H	-0.621346000	-2.674760000	1.534219000
H	0.781652000	-2.047846000	2.363372000
H	0.784319000	-3.310355000	-0.401818000
H	-0.192271000	2.393666000	1.686304000
H	-1.414145000	4.480422000	1.372836000
H	-3.568057000	4.515613000	0.135841000
H	-4.534054000	2.382073000	-0.707248000
H	-5.146245000	0.072393000	-1.325927000
H	-5.459188000	-2.379647000	-1.636692000
H	-3.660980000	-3.941288000	-0.930272000
H	-1.614428000	-3.132842000	0.072488000
H	2.828400000	-4.471169000	0.447214000
H	1.454327000	-4.778264000	1.512214000
H	2.695972000	-3.604577000	1.985152000

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