Supplementary Information

for

Measuring the Distance between Two Mercapto Groups with an Optical Molecular Ruler at the Nanometer Scale

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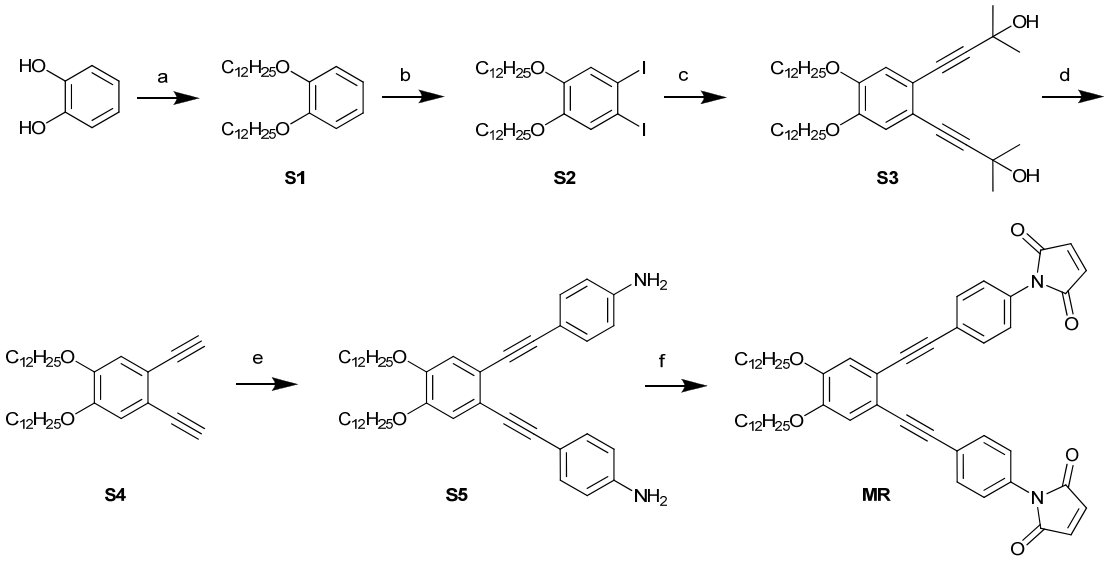
1. Syntheses

1.1 Syntheses of MR



a. n-$C_{12}H_{25}Br$, K_2CO_3, DMF b. I_2, HIO_3, HOAc, H_2SO_4 c. $Pd(PPh_3)_4$, CuI, Et_3N, 

d. KOH, Tol. t-BuOH e. $Pd(PPh_3)_4$, CuI, Et_3N, 

f. 1) THF,  2) Ac_2O, AcONa

Scheme S1. Syntheses of **MR**

1.2 Thiol-ene Reaction

Table S1. High Resolution ESI Mass of **1-9**

	species	formula	cala'd	found	error(ppm)
1	$(1+H)^+$	$C_{62}H_{85}N_2O_6S_2$	1017.58436	1017.58248	2
2	$(2+H)^+$	$C_{56}H_{71}N_2O_6S_2$	931.47481	931.47531	-1
3	$(3+H)^+$	$C_{57}H_{73}N_2O_6S_2$	945.49046	945.48802	2
4	$(4+H)^+$	$C_{58}H_{75}N_2O_6S_2$	959.50611	959.50377	2
5	$(5+H)^+$	$C_{59}H_{77}N_2O_6S_2$	973.52176	973.51970	2
6	$(6+H)^+$	$C_{60}H_{79}N_2O_6S_2$	987.53741	987.53756	0
7	$(7+H)^+$	$C_{58}H_{75}N_2O_7S_2$	975.50102	975.50075	0
8	$(8+H)^+$	$C_{60}H_{79}N_2O_8S_2$	1019.52724	1019.52577	1
9	$(9+H)^+$	$C_{62}H_{83}N_2O_9S_2$	1063.55345	1063.55224	1

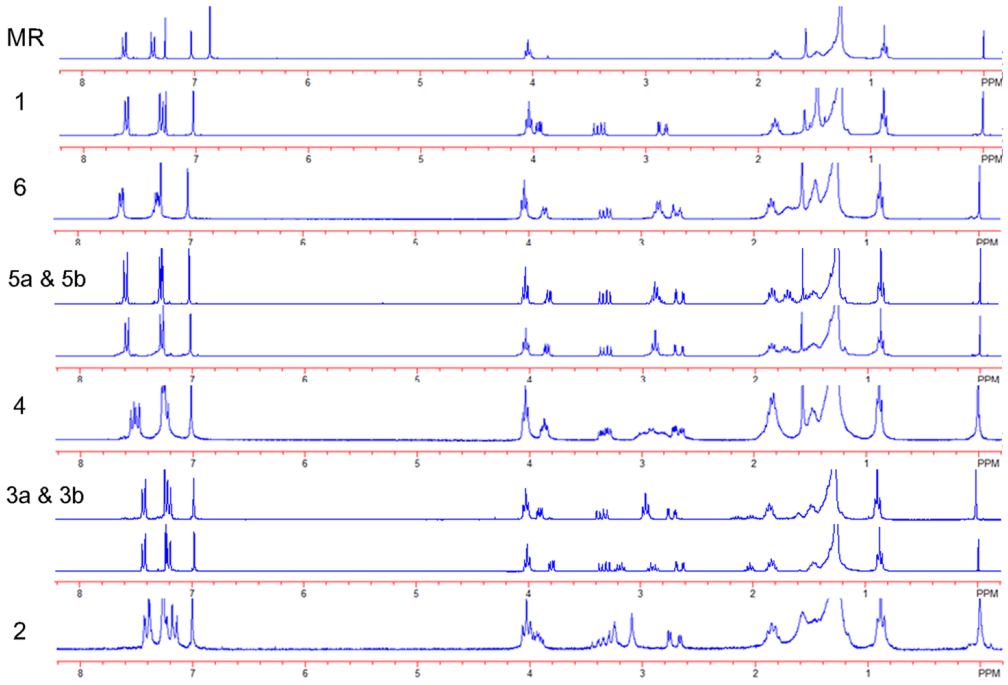
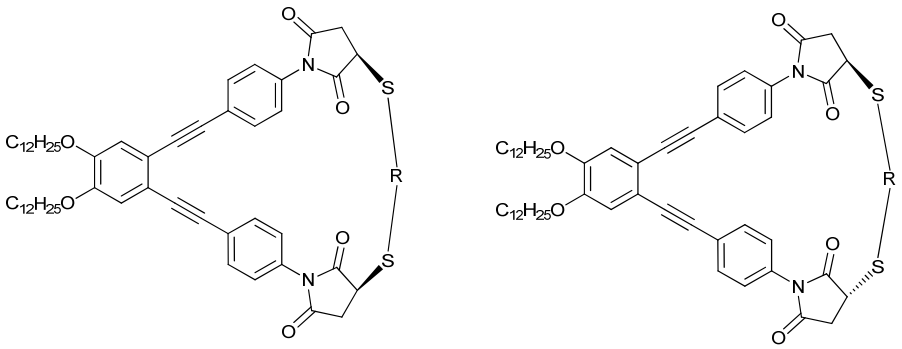


Figure S1 ^{1}H NMR spectra of **MR**, **1**-**6**. **2**, **4**, **6** are mixtures of two diastereoisomers. **3a**,**b** and **5a**,**b** are two seperated diastereoisomers.

1.3 Diastereoisomers



Scheme S2. Two diastereoisomers of the cyclic molecule

2. UV & FL spectra

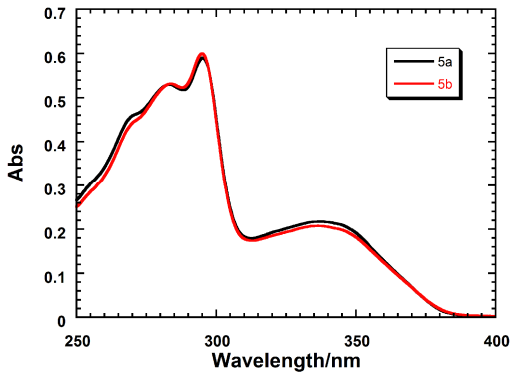


Figure S2. UV spectra of the two diastereoisomers of **5** (1×10^{-5} mol/L, chloroform).

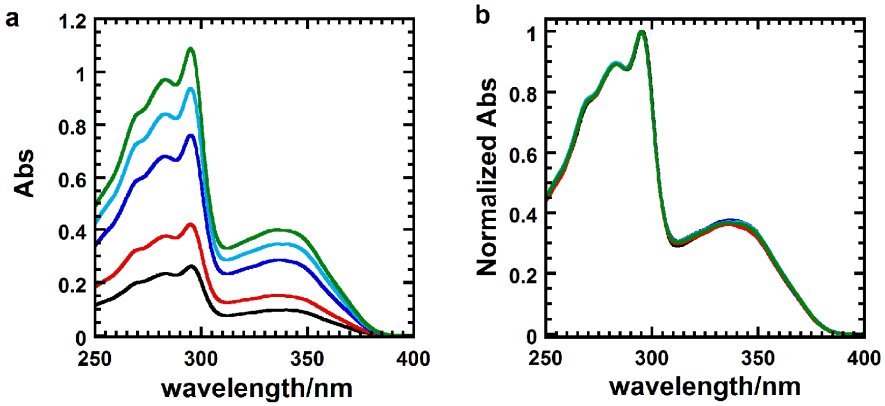


Figure S3. UV spectra and normalized UV spectra of **5** in chloroform at different concentration (from 5×10^{-6} mol/L to 2×10^{-5} mol/L)

Table S2. Fluorescence quantum yield of **2-7**

	$d_{S\text{-}S}$/Å [a]	φ_f [b]
2	4.6	45%
3	5.0	51%
4	5.9	61%
5	7.4	72%
6	8.3	76%
7	5.3	56%

[a] the distance of the two S atoms of **2-7;** [b] calculated with 9,10-Diphenylanthracene as standard.

3. DFT Calculation

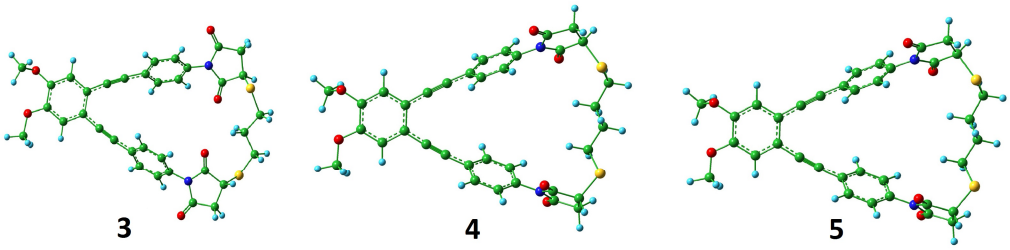


Figure S4. DFT optimized geometry of **3-5**. Dodecanoxy groups were replaced by methoxy groups in calculation.

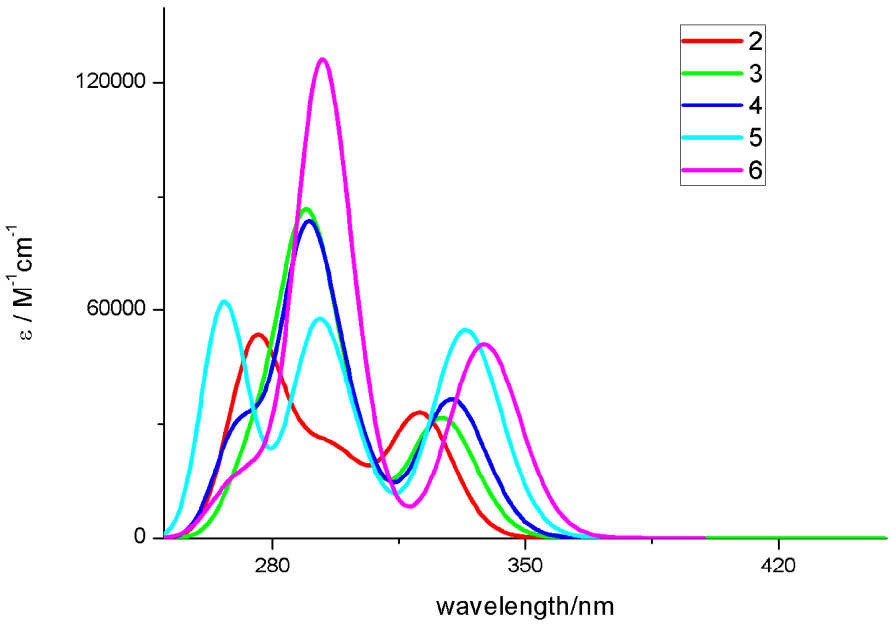


Figure S5. TD-DFT calculated absorption spectra of **2-6** at PBE0 level.

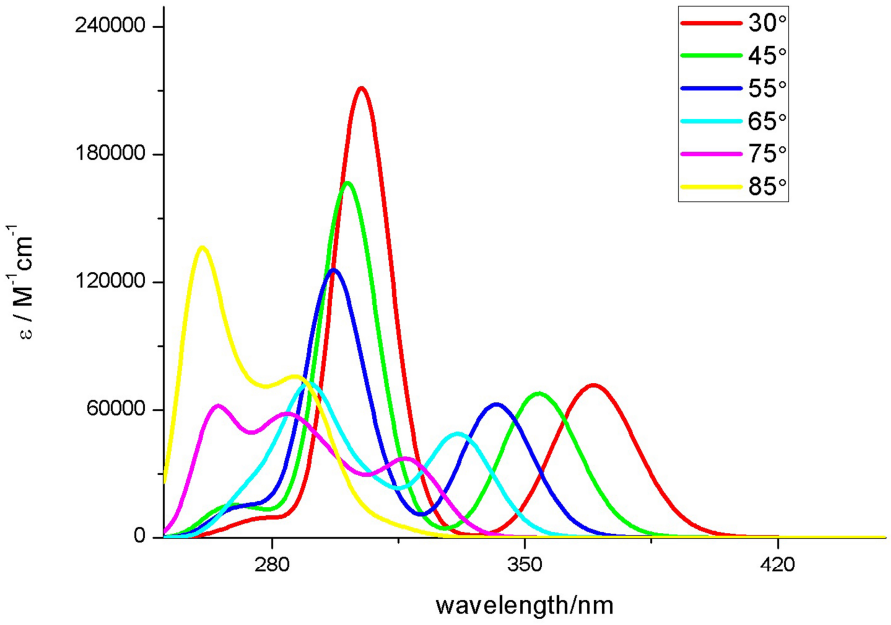


Figure S6. TD-DFT calculated absorption spectra of **1** with no bond bending and the dihedral angle of ring A and B adjusted from 15°to 90° at PBE0 level.

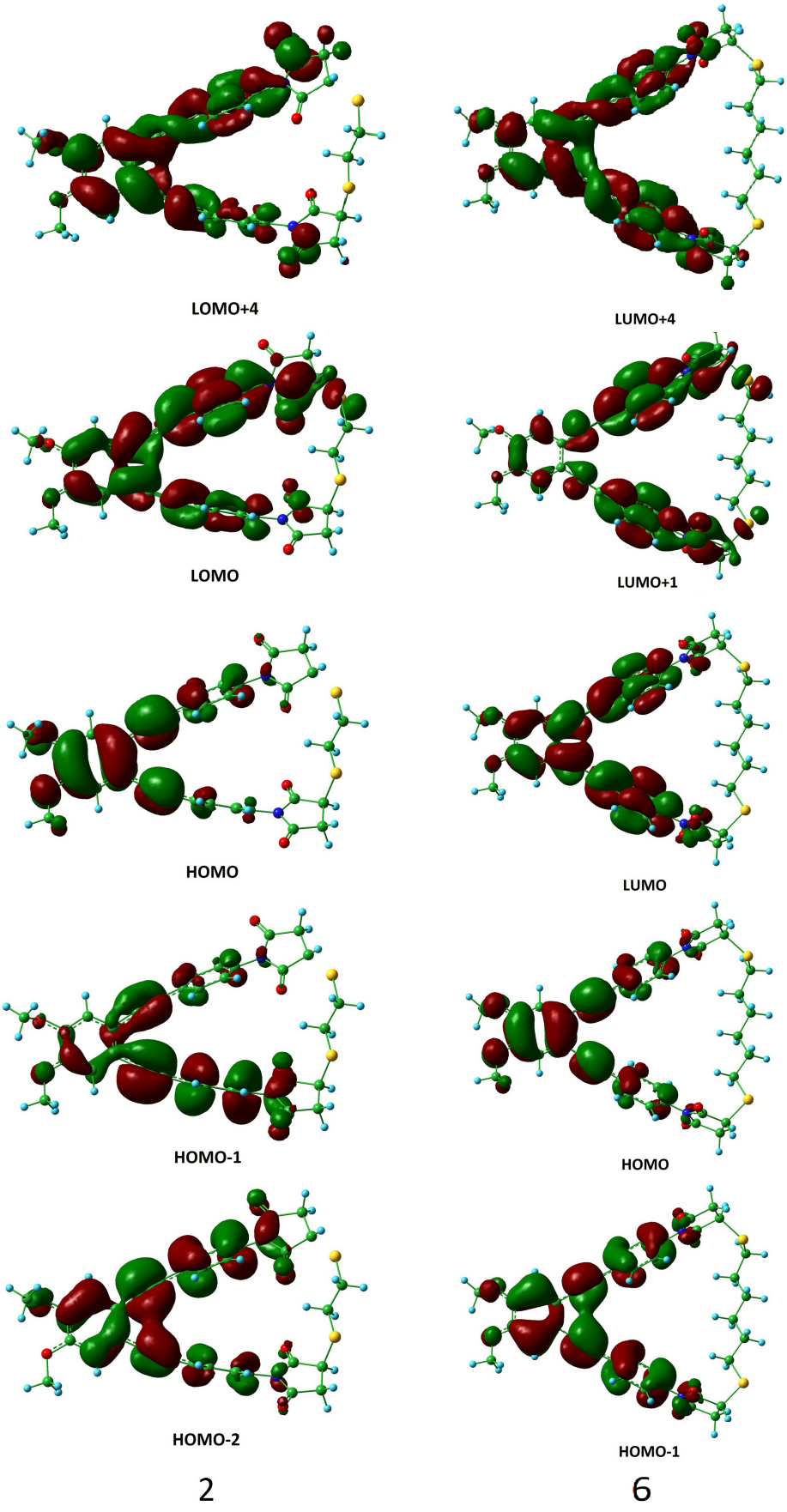


Figure S7. Isodensity surface plots for selected orbitals of **2** and **6**.

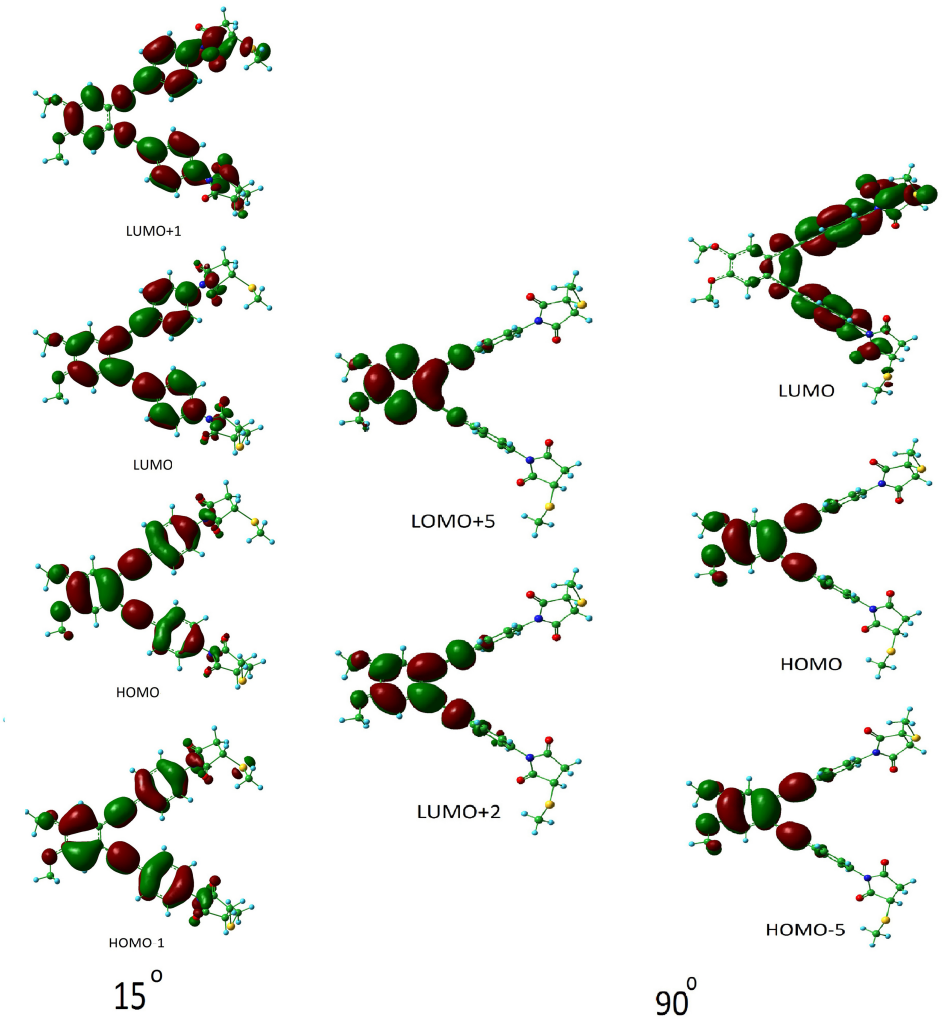


Figure S8. Isodensity surface plots for selected orbitals of **1** at the different torsion angle.

Table S3. Transitions corresponding to major peaks for the molecular **2**, **4**, **6.**

Compound	Excited state no.	Wavelength/nm	Oscillator strength	CI description
2	1	333.17	0.2478	H→L (0.66)
	4	296.43	0.1148	H-2→L (0.37) H-1→L (-0.36)
	10	279.64	0.1690	H-2→L (0.32) H→L+4 (0.40)
4	1	341.90	0.2944	H→L (0.67)
	4	298.90	0.5985	H-1→L (0.63)
	10	277.26	0.2171	H-5→L (0.28) H→L+4 (0.47)
6	1	350.78	0.4276	H→L (0.67)
	3	302.89	0.9324	H-1→L (0.60)
	10	275.58	0.1085	H-1→L+1 (-0.35) H→L+4 (0.46)

Table S4. Transitions corresponding to major peaks for molecular **1** at the different torsion angle.

Torsion angle	Excited state no.	Wavelength/nm	Oscillator strength	CI description
15	1	391.72	0.6371	H→L (0.67)
	3	316.34	1.9583	H-1→L (0.48) H→L+1 (-0.44)
	9	281.37	0.0619	H-1→L+1 (0.50)
55	1	354.53	0.5272	H→L (0.67)
	3	306.24	0.9127	H-1→L (0.61)
	10	277.89	0.1243	H-1→L+1 (-0.42) H→L+4 (0.43)
90	1	323.13	0.0001	H→L (0.68)
	4	295.31	0.6041	H→L+2 (0.52)
	8	281.25	0.3107	H-5→ L+2 (0.40) H→L+5 (0.44)

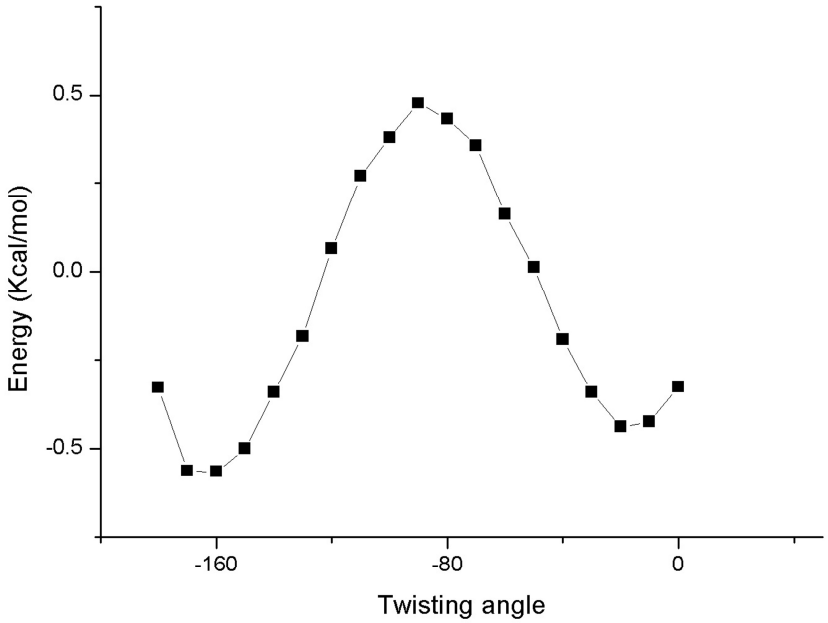


Figure S9. Ground-state rotational potential for the phenyl ring **A** and **B** in compound **1.**

4. Monitoring Conformation Transition

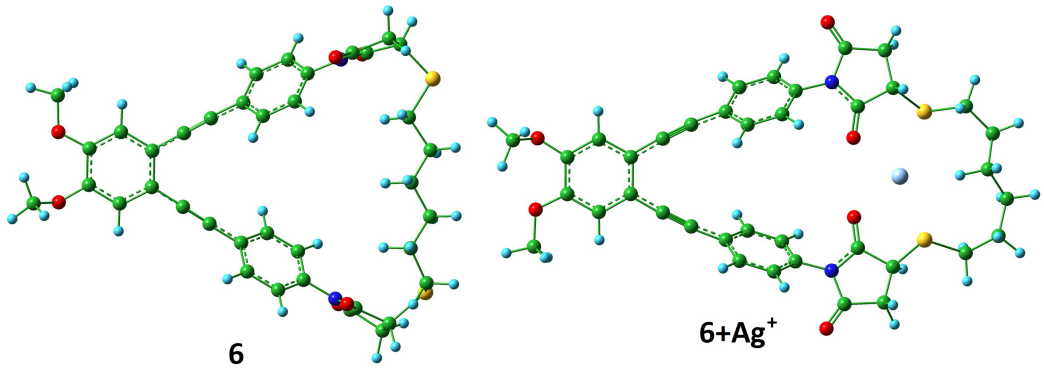


Figure S10. DFT optimized geometry of **6** before and after interacts with Ag^+. Sulfur atoms are brought closer by the Ag^+.

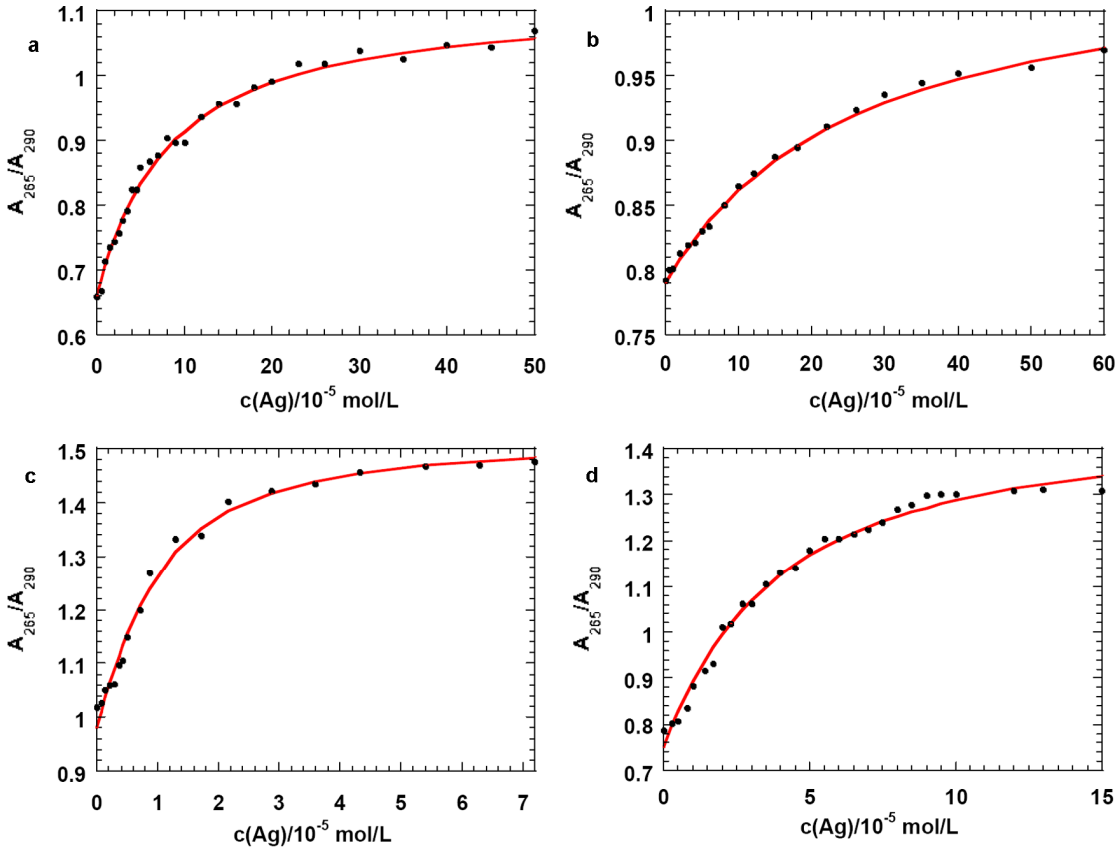


Figure S11. Ag^+ titration experiments and of a) **1**, b) **6**, c) **8** and d) **9,** x axis is the concentration of the Ag^+ ion and y axis is the A_{295}/A_{269} ratio. The solid line represents the best fit corresponding to a stoichiometry of the complex of 1:1 using the following equation.

$$y = y_0 + \frac{y_{lim} - y_0}{2c_0}\left[c_0 + x + \frac{1}{K} - \sqrt{(c_0 + x + \frac{1}{K})^2 - 4c_0x}\right]$$

c_0, concentration of **1**, **6**, **8** or **9;** x, concentration of Ag^+**;** K, binding constant.

Appendix I: ^{1}H & ^{13}C NMR of S5, MR and 1

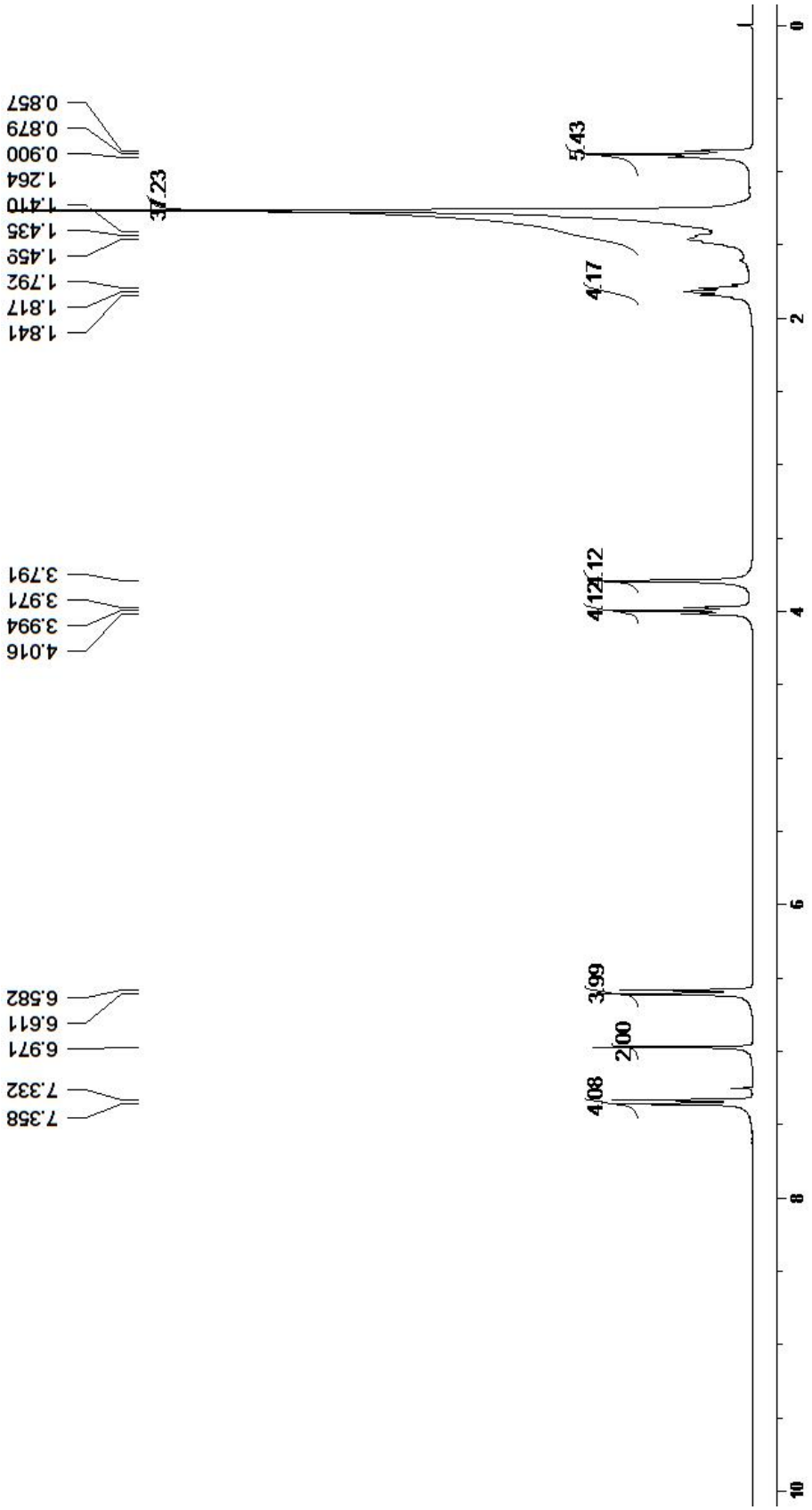


Figure A1. ^{1}H NMR of **S5**

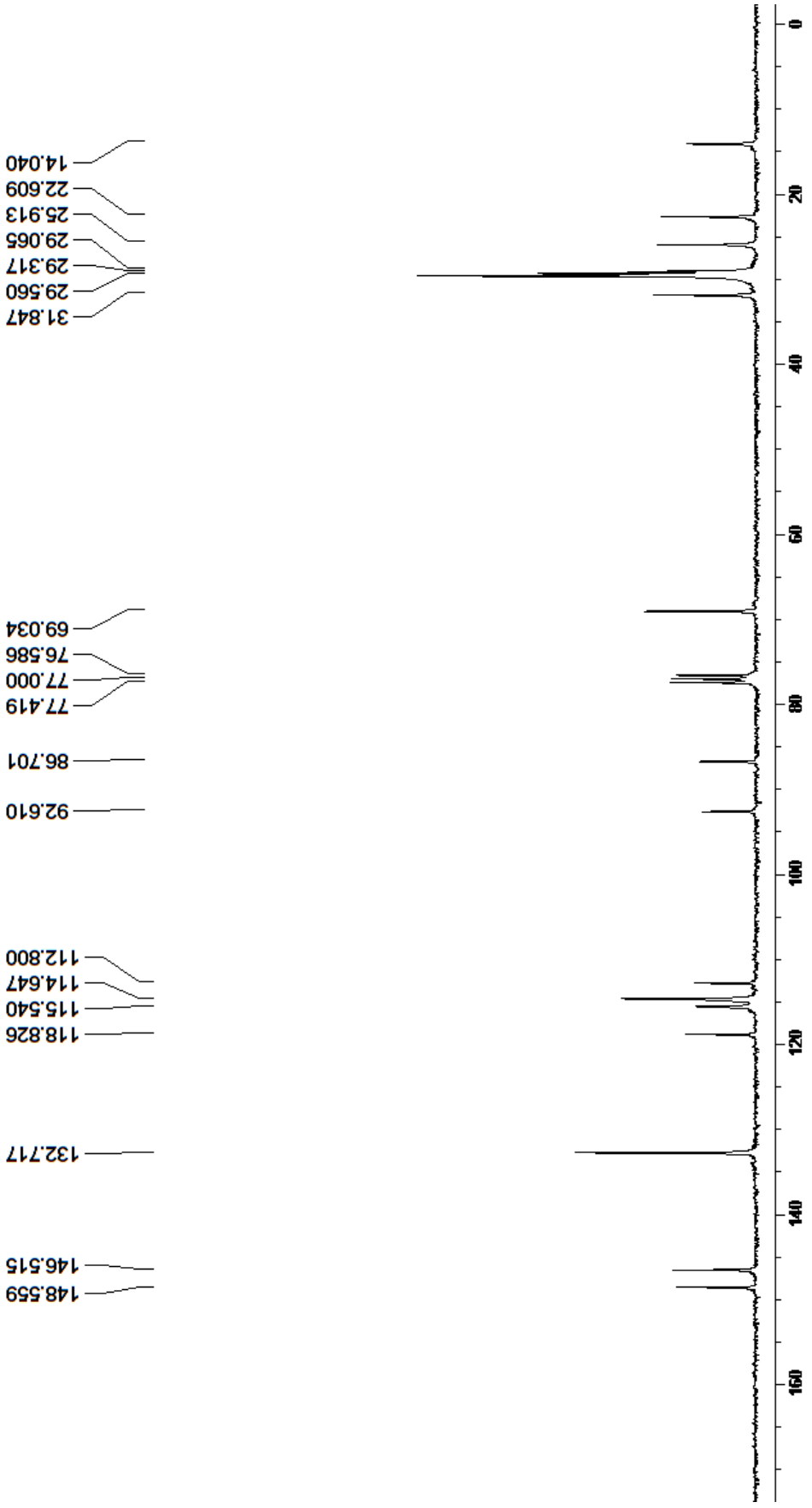


Figure A2. ^{13}C NMR of **S5**

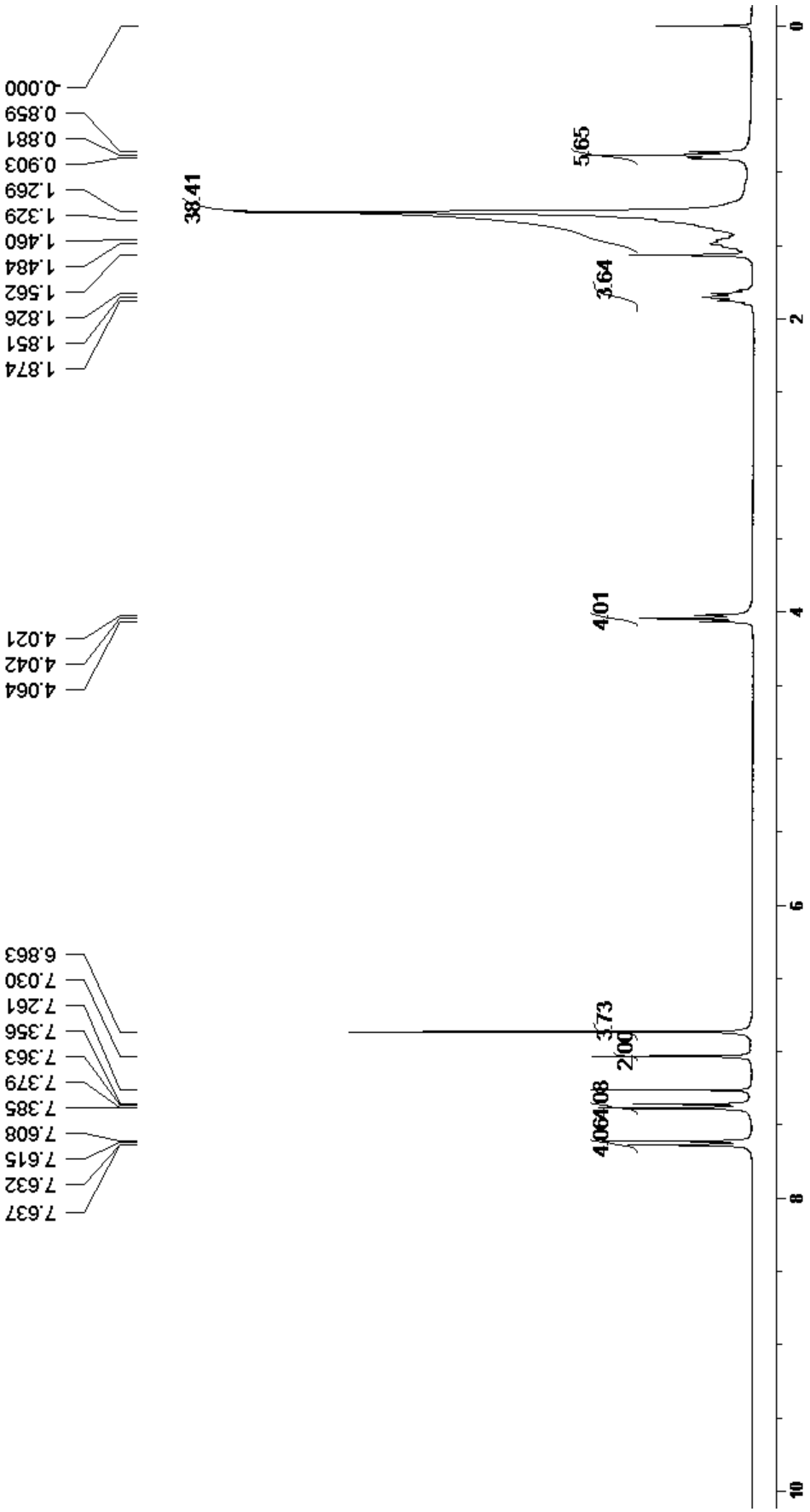


Figure A3. ^{1}H NMR of **MR**

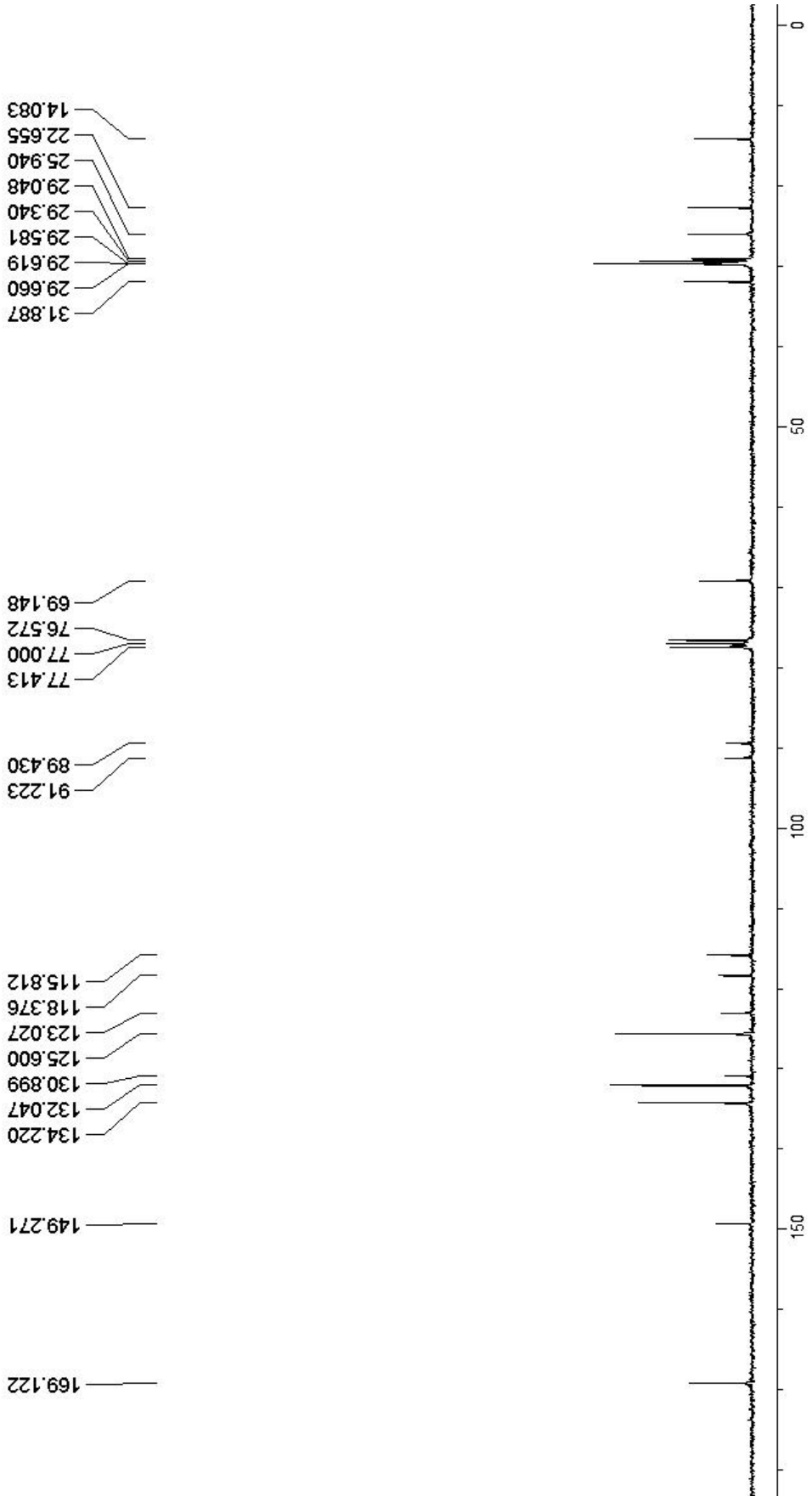


Figure A4. ^{13}C NMR of **MR**

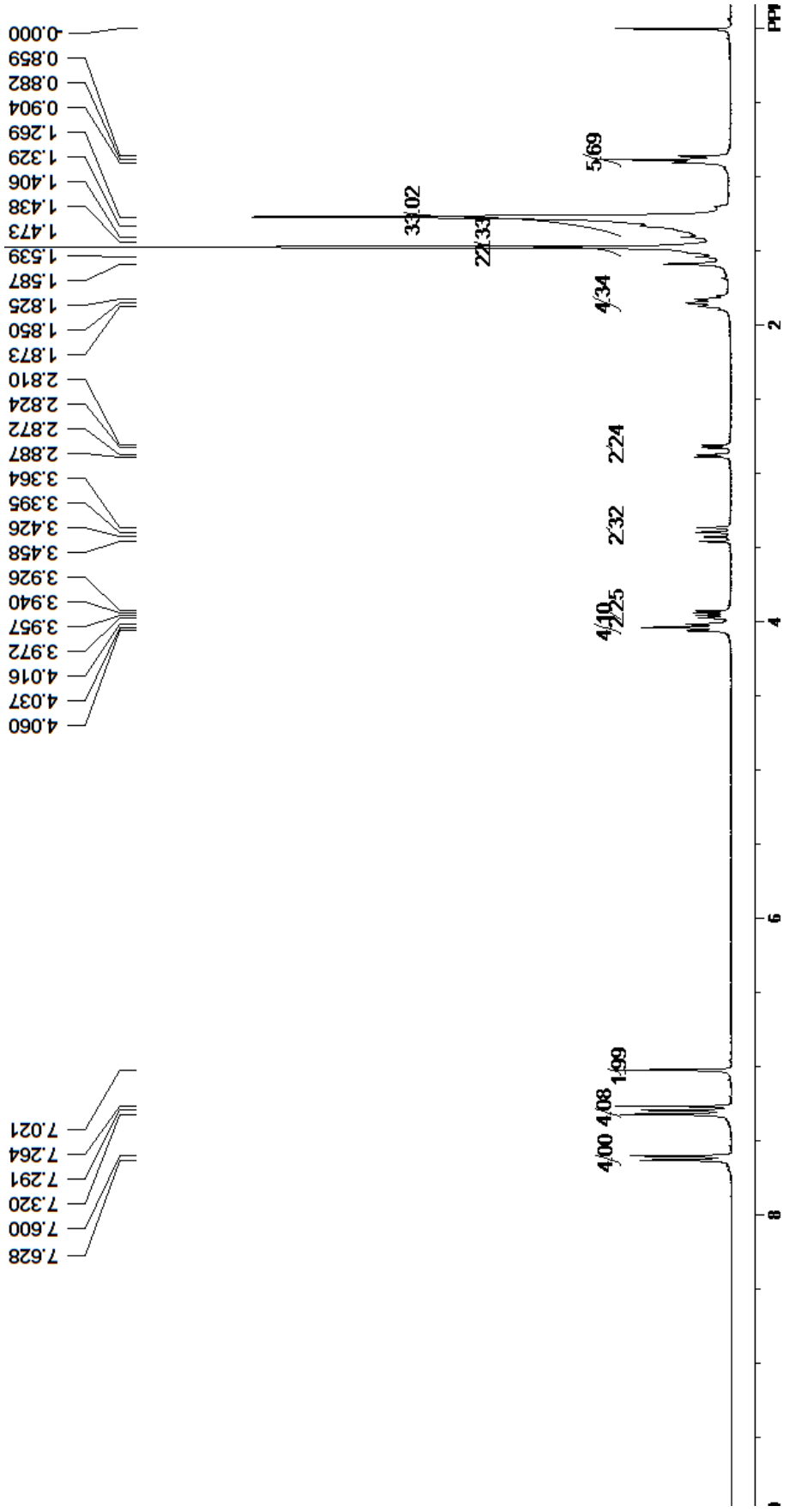


Figure A5. ^{1}H NMR of **1**

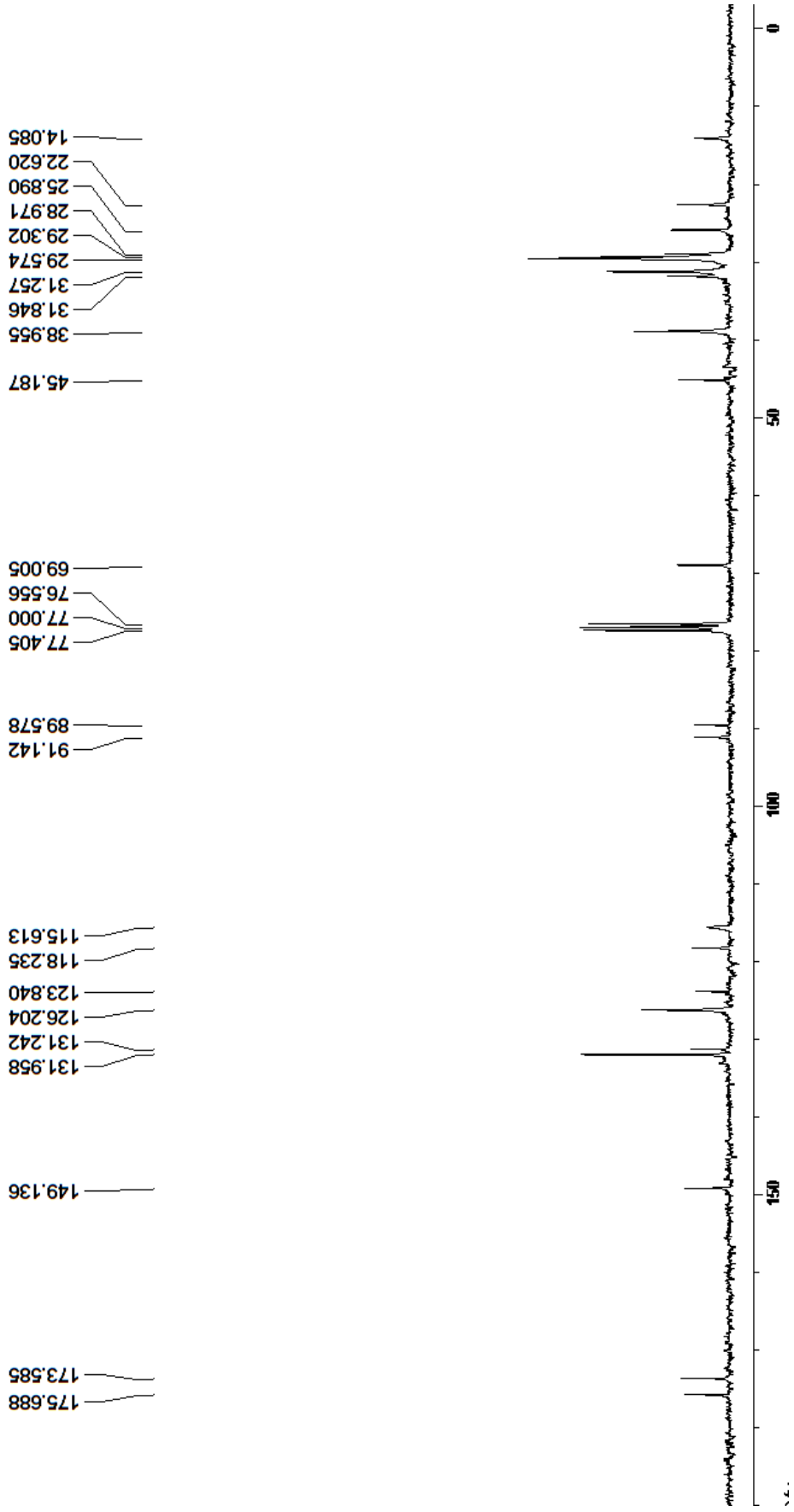


Figure A6. ^{13}C NMR of **1**

Appendix II: Optimized Cartesian Coordinates for 2-7

Optimized Cartesian Coordinates for **2**

Atomic	Coordinates (Angstroms)		
No.	X	Y	Z
C	7.02862500	-0.71475500	1.53901400
C	7.17364600	-1.65932300	0.49345500
C	6.31246200	-1.61621700	-0.59427100
C	5.28783700	-0.65825400	-0.68925300
C	5.13736700	0.28286900	0.36505800
C	6.01259600	0.23683800	1.46491400
C	4.11922700	1.27716000	0.28374000
C	4.39275400	-0.63400100	-1.79721000
C	3.22882700	2.08670400	0.10931500
C	3.57902300	-0.54383300	-2.69657000
C	2.19021500	3.00490100	-0.23060400
C	2.54501000	-0.38511400	-3.66685100
C	0.89622800	2.88292300	0.30901500
C	-0.13921000	3.69906500	-0.13168400
C	0.10785400	4.66532800	-1.11408900
C	1.40048100	4.83791600	-1.62125700
C	2.42791700	4.01020800	-1.18646800
C	1.20096900	-0.56679600	-3.28758700
C	0.16832100	-0.35107200	-4.19030300
C	0.46015300	0.06683100	-5.49382900
C	1.79029500	0.23441800	-5.89612400
C	2.82063500	0.00243400	-4.99121500
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N	-0.60876600	0.33832700	-6.40947000
C	-1.13252900	5.71027000	-3.01166200
C	-2.50976800	6.33182300	-3.22025900
C	-2.96117800	6.72402700	-1.80916100
C	-2.02955700	5.96689100	-0.86898400
C	-1.80238500	0.97644400	-6.04056700
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S	-2.92341400	2.92108600	-7.73468200
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H	1.59086800	5.58681700	-2.37790600
H	3.42331000	4.12073100	-1.60244400
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H	-0.85910400	-0.47846900	-3.87737200
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H	-2.43392100	5.33793500	-5.98320100
H	-1.92185800	3.88843800	-5.09791700
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H	-4.13116100	2.79014900	-5.64373900
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O	8.19039300	-2.57840900	0.48955900
C	8.12570100	-3.59606900	1.49448600
H	8.97498200	-4.25604000	1.30855100
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H	7.98533400	1.16807000	3.24021400
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H	8.66221900	-0.10007000	4.29700300
H	-1.69829000	1.05210300	-9.27142400
H	-3.65106000	0.70149700	-7.08331000

Optimized Cartesian Coordinates for **3**

Atomic	Coordinates (Angstroms)		
No.	X	Y	Z
C	6.48170100	-1.55363900	-0.14279600
C	5.26205300	-0.85445000	-0.12172100
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C	6.53253000	1.23092900	-0.05747100
C	7.73204600	0.52225000	-0.09688800
C	7.70241500	-0.89361500	-0.12649500
H	6.48692300	-2.63687700	-0.18620100
H	6.53096000	2.31273700	-0.02386200
C	4.07393100	1.30008000	-0.00252200
C	4.01467900	-1.54045000	-0.16477300
C	2.99098700	1.84977400	0.05985900
C	2.91051100	-2.04842600	-0.20555900
C	1.67761800	2.39760700	0.16320600
C	0.88365800	2.11151000	1.28987000
C	1.12305300	3.18016300	-0.86661900
C	-0.42568200	2.56799200	1.37649800
H	1.30064600	1.51412500	2.09311200
C	-0.19112000	3.62653200	-0.79367700
H	1.72304600	3.41334200	-1.73967500
C	-0.97356100	3.31037800	0.32409300
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C	1.01884100	-3.32048900	0.75384400
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C	-2.81720600	4.96271900	-0.09474200

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S	-5.59630600	-2.62461100	1.04643100
O	8.85119000	-1.63570900	-0.21830800
O	8.96829700	1.09581000	-0.11701300
C	9.05200000	2.51462500	-0.13576900
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H	10.53625200	-2.28804700	0.69583700
H	10.10474300	-0.60603600	1.11022800
H	9.18535700	-1.96980900	1.81744300

Optimized Cartesian Coordinates for **4**

Atomic	Coordinates (Angstroms)		
No.	X	Y	Z
C	7.48320600	-0.13631900	-1.77308600
C	7.21656200	-1.02154600	-0.69952400
C	6.67040100	-0.52749800	0.47671700
C	6.36182300	0.83533400	0.63446200
C	6.60459500	1.71723900	-0.45213100
C	7.16677500	1.21435300	-1.64017700
C	6.26439400	3.09564100	-0.33961100
C	5.83131500	1.33227000	1.85945500
C	5.93781500	4.25579800	-0.17861800
C	5.39001000	1.81501700	2.88457300
C	5.48582200	5.58202600	0.08718000
C	4.91383900	2.45449500	4.06795600
C	4.13846500	5.80399400	0.43393000
C	3.68917100	7.07559300	0.76373000
C	4.58138200	8.15344400	0.74895500
C	5.91717900	7.95714000	0.38406900
C	6.36354300	6.68140400	0.05662400
C	5.73730500	3.36759800	4.75554600
C	5.27301800	4.03877300	5.87963200
C	3.97347400	3.80351400	6.33991000
C	3.14629700	2.88809900	5.68169300
C	3.61381000	2.22166300	4.55440500
N	4.12609300	9.45136100	1.14258200
N	3.48786400	4.51522900	7.48281600
C	2.91230100	10.02267000	0.71045800
C	2.80140200	11.40527300	1.33595700
C	3.93897700	11.48394300	2.36296800
C	4.82605400	10.27345000	2.04983500
C	4.21913200	4.66977400	8.67979400
C	3.34046300	5.43141300	9.66369500
C	2.15398500	5.93877600	8.83597900
C	2.24195100	5.15616400	7.52794400
O	5.92056100	10.03574600	2.50412800
O	2.11883100	9.49559300	-0.03610100
O	1.39001700	5.10375200	6.66447500
O	5.33180400	4.24216200	8.87828300
S	2.35067200	7.75496600	8.54144900
C	2.60225600	9.87971000	4.32180200
C	2.15256300	9.69611600	5.77505500
C	1.33870000	8.40805400	5.95964300
C	0.93360200	8.13605600	7.41180000

H	6.49643700	-1.22235000	1.29046200
H	7.35192800	1.90731500	-2.45071600
H	3.45336300	4.96383800	0.45848700
H	2.65211300	7.23441400	1.03053700
H	6.60559800	8.79243200	0.38198400
H	7.40308100	6.52514500	-0.21057000
H	6.74097900	3.55410900	4.38992400
H	5.91353500	4.73972600	6.39991800
H	2.13896700	2.71502500	6.03893700
H	2.96995300	1.51968200	4.03562100
H	2.91757600	12.14895200	0.53991300
H	4.54503700	12.38752800	2.26395200
H	3.01923200	4.73572600	10.44608900
H	3.92530800	6.21691000	10.14803200
H	1.18278500	5.76004700	9.30206400
H	1.73888100	9.83013000	3.64924900
H	3.30363500	9.08552400	4.04739800
H	3.03610000	9.67479700	6.42372500
H	1.54744700	10.55742100	6.08719800
H	0.41566000	8.47534200	5.36671400
H	1.89143700	7.54513000	5.57418200
H	0.42982600	9.00539900	7.84617500
H	0.24854200	7.28770400	7.45879000
O	8.05137400	-0.69156700	-2.88010500
O	7.55737900	-2.34744400	-0.75886900
C	8.38184700	0.16210900	-3.96773200
H	7.49014800	0.63991300	-4.39206000
H	9.09743400	0.93636900	-3.66589500
H	8.84058500	-0.47897900	-4.72124800
C	6.82301700	-3.14773900	-1.69165400
H	7.19539600	-4.16665100	-1.57120700
H	5.75001000	-3.12568000	-1.46280900
H	6.98590200	-2.81700300	-2.72086000
H	1.80530200	11.54261300	1.76119400
S	3.43379500	11.51252900	4.13545400

Optimized Cartesian Coordinates for **5**

Atomic	Coordinates (Angstroms)		
No.	X	Y	Z
C	-6.59875800	-1.55728700	0.27831100
C	-5.38397200	-0.85285000	0.20244300
C	-5.42542700	0.55780200	0.04613300
C	-6.67127600	1.21021100	-0.02396900
C	-7.86531000	0.49762100	0.06268900
C	-7.82485600	-0.91098300	0.20997300
H	-6.59544400	-2.63490300	0.39632200
H	-6.67749700	2.28720000	-0.13055300
C	-4.21885800	1.31035100	-0.01290100
C	-4.13798000	-1.54277100	0.24173600
C	-3.16623000	1.91850100	-0.04436100
C	-3.05777000	-2.10102600	0.24982500
C	-1.89636900	2.56503800	-0.01914700
C	-1.55418900	3.56113400	-0.95294100
C	-0.94489100	2.19367400	0.95169900
C	-0.30147900	4.16411900	-0.92204300
H	-2.27633000	3.85362900	-1.70754900
C	0.30664100	2.79344200	0.98505700
H	-1.19821300	1.42457400	1.67280600
C	0.63082700	3.77858200	0.04621400
H	-0.03998900	4.91791600	-1.65401600
H	1.02840400	2.50624400	1.73930700
C	-1.76893200	-2.71181500	0.19304700
C	-1.09274100	-2.81398200	-1.03839100
C	-1.13487400	-3.19853900	1.35126700
C	0.17783300	-3.36993700	-1.10919200
H	-1.57151000	-2.44157100	-1.93731500
C	0.13542100	-3.76142900	1.28447700
H	-1.64481900	-3.12747700	2.30594900
C	0.79512900	-3.84169800	0.05414300
H	0.68829400	-3.44332000	-2.06099600
H	0.62127000	-4.11997700	2.18305700
N	2.11245900	-4.39532700	-0.02326000
C	2.51740400	-5.31016600	-1.01742300
C	3.15734400	-4.05439500	0.85124800
C	3.97129400	-5.67428200	-0.74808100
C	4.44441000	-4.68018400	0.31777700
H	4.53872000	-5.64261800	-1.68105600
N	1.92822500	4.38048700	0.07752300
C	2.74179600	4.53434400	-1.06244800
C	2.53422100	4.85996400	1.25647900

C	4.09607600	5.08703900	-0.59921700
C	3.88720000	5.44295000	0.87948200
H	4.65850900	5.04291300	1.54124300
O	1.81486800	-5.73706300	-1.90387700
O	3.04789500	-3.36277800	1.84259000
O	2.04353600	4.81266100	2.36161200
O	2.41539400	4.25723400	-2.19305600
H	3.85209900	6.52524300	1.04327300
H	4.00492500	-6.70589300	-0.38210500
C	5.44953500	-0.04366400	0.34402800
H	4.75713800	-0.45744500	-0.39846500
H	4.86891700	0.08834000	1.26712600
C	5.96604600	1.31923600	-0.14011100
H	6.43742300	1.20191100	-1.12422200
H	6.74513600	1.68939900	0.53800000
C	6.57938000	-1.04623900	0.61280900
H	7.23638600	-1.12090600	-0.26420600
H	7.21043600	-0.66828400	1.42787000
O	-8.96694700	-1.65330000	0.35801400
O	-9.10557100	1.06106500	0.03180100
C	-9.20054200	2.47593800	-0.06775300
H	-10.26667500	2.70485500	-0.05477200
H	-8.71286700	2.97076300	0.78078500
H	-8.76132400	2.84603800	-1.00245400
C	-9.82839500	-1.72446100	-0.78352200
H	-10.64496900	-2.39172300	-0.50188700
H	-10.23096400	-0.74238500	-1.04549000
H	-9.29731400	-2.14716200	-1.64568000
C	6.08927300	-2.44331200	1.01765400
H	5.26116000	-2.37716000	1.72787300
H	6.90002200	-3.01992200	1.47268200
C	4.84134900	2.35535900	-0.22546200
H	4.44972800	2.55635200	0.77751600
H	4.02175200	1.98425400	-0.84870800
H	5.00299100	-5.13970100	1.13598600
H	4.33575200	5.95662400	-1.21600700
S	5.47800300	3.92140200	-0.95745700
S	5.49266600	-3.37216400	-0.46304500

Optimized Cartesian Coordinates for **6**

Atomic	Coordinates (Angstroms)		
No.	X	Y	Z
C	7.40875800	-0.00504800	-1.64486000
C	7.09619100	-0.88197500	-0.57668100
C	6.54204500	-0.37111000	0.58786000
C	6.26871400	1.00097700	0.74154900
C	6.55549800	1.87398000	-0.33993000
C	7.12720100	1.35323800	-1.51699200
C	6.25181200	3.26264300	-0.25637400
C	5.73249800	1.49361100	1.96522400
C	5.96895000	4.44327300	-0.18711600
C	5.29489200	1.91080500	3.02048900
C	5.57065000	5.80691200	-0.06537400
C	4.82139400	2.43234400	4.26079600
C	4.24247800	6.12133200	0.28382000
C	3.84134800	7.44173400	0.43643900
C	4.76339000	8.47632100	0.24033200
C	6.08258900	8.18479300	-0.12079700
C	6.48063900	6.86071200	-0.27106700
C	5.54766600	3.43545400	4.93246700
C	5.09723200	3.95222500	6.14089200
C	3.90965100	3.47149600	6.70213100
C	3.17464600	2.47533500	6.05154400
C	3.62736100	1.96309600	4.84078600
N	4.35418500	9.83139500	0.44614400
N	3.44920800	4.00551500	7.94742100
C	3.14343300	10.36822600	-0.03634200
C	3.08094500	11.82662100	0.39381500
C	4.22163000	12.00089000	1.40532000
C	5.09274600	10.75484200	1.21569800
C	4.27654400	4.17880400	9.07789500
C	3.40051300	4.68691900	10.21570300
C	2.07705000	5.08648800	9.55344800
C	2.13022500	4.42167200	8.18023600
O	6.19949100	10.56211400	1.66180400
O	2.32070200	9.76307800	-0.68571600
O	1.20130000	4.28528700	7.41093600
O	5.45874400	3.93223700	9.12260100
S	2.01739600	6.92995800	9.40487100
C	2.91053800	10.55687300	3.48885900
C	2.47506800	10.45151300	4.95344900
C	1.76645900	9.11655900	5.22745700
C	1.44121300	8.88401700	6.70782900

C	0.71673500	7.55370000	6.94503400
C	0.47603400	7.21689000	8.41945100
H	6.33334300	-1.05985300	1.39856600
H	7.34581400	2.04055400	-2.32395600
H	3.53280300	5.31696200	0.44295900
H	2.81719300	7.67261700	0.70082400
H	6.79471700	8.98789300	-0.26039300
H	7.50623100	6.63261200	-0.54053500
H	6.46815900	3.80535400	4.49446000
H	5.66706800	4.71717700	6.65329100
H	2.25015400	2.11555500	6.48534100
H	3.05747500	1.19233600	4.33321700
H	3.22712000	12.45036700	-0.49525500
H	4.83296700	12.88745700	1.22396100
H	3.26093300	3.86859200	10.93042700
H	3.90908100	5.49713600	10.74311300
H	1.18994300	4.74384900	10.08998700
H	2.04355300	10.43769700	2.82966900
H	3.62882300	9.76230900	3.26432600
H	3.35637300	10.54379800	5.59968000
H	1.80829800	11.28521000	5.20728700
H	2.39993200	8.29223700	4.87208100
H	0.84241000	9.06791300	4.63472500
H	0.82610100	9.71182600	7.08866100
H	2.37480400	8.89979600	7.28519300
H	-0.26421600	7.58115200	6.44946500
H	1.27073000	6.73325400	6.47742100
H	-0.04376300	8.03487400	8.92869000
H	-0.13766900	6.31850300	8.51288400
O	7.98210800	-0.57601100	-2.74092200
O	7.39979300	-2.21704500	-0.62884600
C	8.35466600	0.26767800	-3.82272000
H	7.48369000	0.76880600	-4.26287900
H	9.08521500	1.02275200	-3.50838500
H	8.80935800	-0.38599600	-4.56781700
C	6.66297000	-2.99652600	-1.57729100
H	7.00106600	-4.02607000	-1.44663600
H	5.58616500	-2.94112600	-1.37337000
H	6.85968500	-2.67315300	-2.60290500
H	2.09108000	12.05687600	0.79237300
S	3.70802300	12.18589500	3.16872900

Optimized Cartesian Coordinates for **7**

Atomic	Coordinates (Angstroms)		
No.	X	Y	Z
C	8.04208500	0.54309700	0.05972800
C	8.05461300	-0.87355700	0.09804800
C	6.85394800	-1.56860700	0.11168900
C	5.61365100	-0.90665800	0.08163300
C	5.60087000	0.51489800	0.03320600
C	6.82279400	1.21564100	0.02182600
C	4.36849800	1.22292900	0.02143100
C	4.39250500	-1.63576700	0.07960900
C	3.29239200	1.79130400	0.03025100
C	3.31495200	-2.20005500	0.07358000
C	1.98553500	2.35568800	0.05525600
C	1.99102900	-2.72653900	0.03486300
C	1.76446200	3.74033200	-0.07262200
C	0.47619400	4.26355400	-0.03831300
C	-0.62000400	3.40668400	0.11603900
C	-0.41843000	2.02637500	0.23745700
C	0.86866900	1.50959100	0.21331100
C	1.54151700	-3.69541400	0.95068500
C	0.21409300	-4.11346800	0.95185500
C	-0.68933000	-3.56402800	0.03619200
C	-0.25061400	-2.62684200	-0.90751100
C	1.07545000	-2.21944900	-0.91034500
N	-1.95176300	3.92778500	0.14889900
N	-2.07854700	-3.89889200	0.09246700
C	-2.41668900	4.97299400	-0.67466500
C	-3.87508300	5.23763900	-0.32012200
C	-4.27466900	4.10926100	0.63748200
C	-2.95303400	3.44101600	1.00830400
C	-2.81195900	-3.99974300	1.29198200
C	-4.26437300	-4.27301700	0.92426000
C	-4.35618100	-3.98306200	-0.57728500
C	-2.89741600	-4.01854700	-1.04646000
O	-2.78984000	2.61861400	1.88442600
O	-1.75604500	5.56748800	-1.49528700
O	-2.50968600	-4.08352000	-2.18985000
O	-2.35273400	-3.91370400	2.40758100
S	-4.91430800	-2.26848700	-0.99992100
C	-5.57497200	1.60769600	1.04431900
C	-6.76389300	0.71362900	0.72800200
H	6.89085300	-2.65138700	0.14991400
H	6.78975400	2.29711100	-0.00305100

H	2.61206900	4.40583400	-0.19681800
H	0.31954900	5.32858800	-0.14836800
H	-1.26389700	1.36277200	0.36299900
H	1.02279300	0.44118500	0.31282600
H	2.23492600	-4.10160200	1.67909500
H	-0.12744600	-4.83371000	1.68371700
H	-0.94393700	-2.21750100	-1.63113300
H	1.41411100	-1.48469200	-1.63258200
H	-3.94162600	6.22050300	0.15780200
H	-4.76922100	4.45675500	1.54776400
H	-4.48012300	-5.32625900	1.14114500
H	-4.91584300	-3.66845300	1.55645300
H	-4.94411300	-4.70917000	-1.14264900
O	9.26078500	1.15224900	0.07747600
O	9.22414400	-1.58105800	0.19448700
C	9.30386700	2.57313200	0.08720600
H	8.85310900	2.99763900	-0.81842100
H	8.79668700	2.98315500	0.96887800
H	10.36085800	2.83912800	0.12277700
C	10.08679400	-1.53500700	-0.94735300
H	10.92976500	-2.18765900	-0.71312300
H	9.57224100	-1.91511300	-1.83888300
H	10.44945400	-0.52118600	-1.13680600
H	-4.46664500	5.28385700	-1.23783200
S	-5.37877800	2.91526600	-0.24130900
C	-6.63186100	-2.27319400	-0.34443100
H	-6.62154800	-2.31327300	0.74935600
H	-7.16949000	-3.15255800	-0.71551900
C	-7.33803300	-1.00578100	-0.84427400
H	-8.34642900	-0.95556700	-0.40510800
H	-7.44397700	-1.05094900	-1.93196600
O	-6.59856900	0.17232400	-0.57445300
H	-6.79933400	-0.07853100	1.49136100
H	-7.70840300	1.27649000	0.78278000
H	-4.66037300	1.01615500	1.09693800
H	-5.73088600	2.08821300	2.01454700