Chemistry–A European Journal

Supporting Information

Geländer Molecules with Orthogonal Joints: Synthesis of Macrocyclic Dimers

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CONTENTS

HPLC CHROMATOGRAMS OF MACROCYCLES 1 AND 2

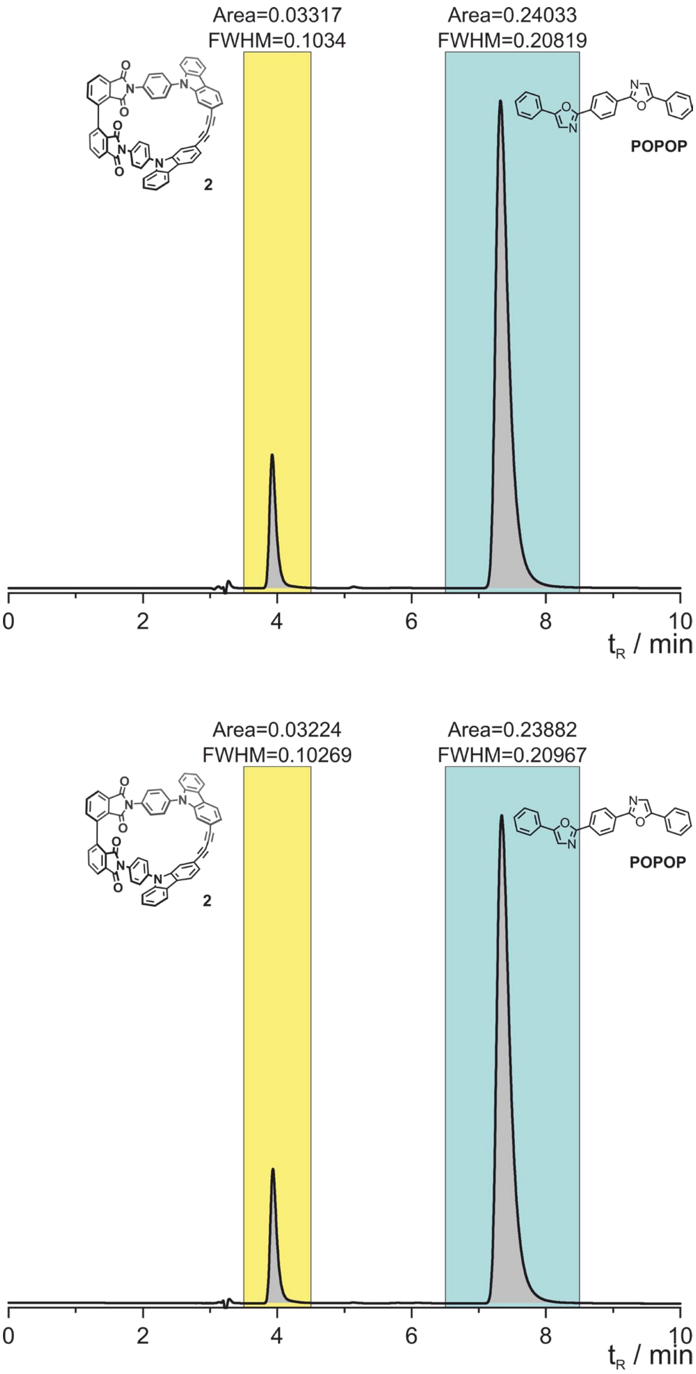


Figure S1. A solution (*P*)-**2** and 1,4-Bis(5-phenyloxazol-2-yl)-benzene (**POPOP**) were separated on an analytical chiral HPLC before (top) heat treatment and after (bottom) 20 h at 120 °C.

POPOP was chosen as adequate internal standard due to a similar absorption spectrum to macrocycle **2**. The ratio of the area **POPOP** to the area (*P*)-**2** before heat treatment (0.1380) and after 20 h at 120 °C (0.1350) differ by 2%. No formation of (*M*)-**2** was observed.

ENANTIOPURE TRANSFORMATION FROM 2 TO 1

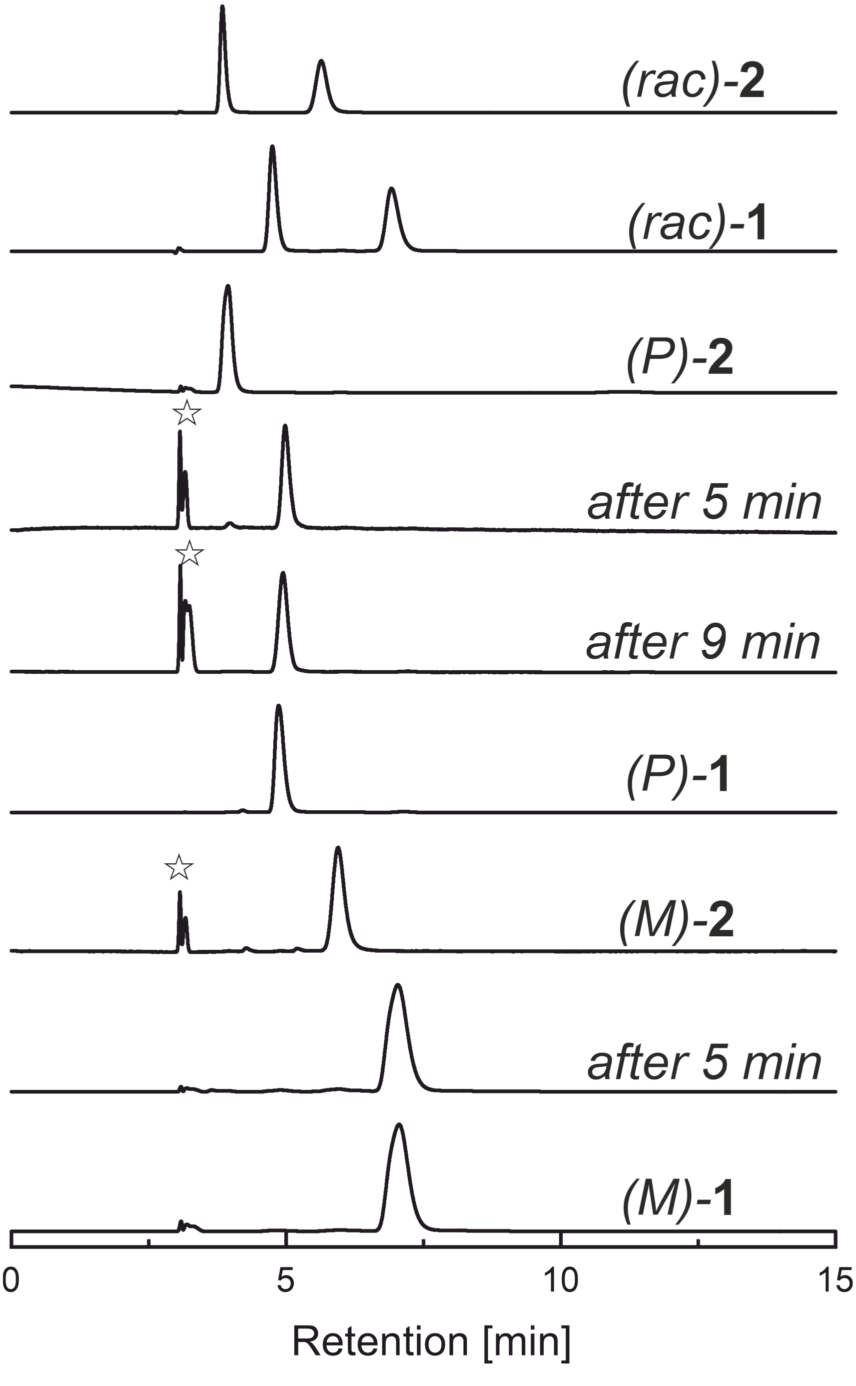
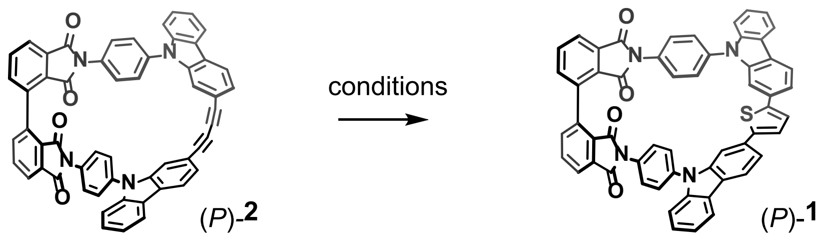


Figure S2. Synthesis of *(P)*-**1** and *(M)*-**1** from enantiomeric pure starting material using analytical chiral HPLC. * marks the injection peak (more visible at lower concentrations).



Scheme S1. Conditions: S_8, NaHS, DMF, 25 °C, 10 min

In Figure S1 chromatorgrams are shown of racemic mixtures of **1** and **2** as well as enantiopure samples of the same compounds. Enantiopure samples of (*P*)-**2** and (*M*)-**2** were submitted to the reaction conditions to (*P*)-**1** and (*M*)-**1**. Aliquots of the reaction mixtures were diluted in CH_2Cl_2, filtered and submitted to the analytical chiral HPLC. For the reaction of (*P*)-**2** to (*P*)-**1** traces of (*P*)-**2** were still observed after 5 minutes under reyction conditions. After 9 minutes no starting material was detected anymore. The same experiment was conducted for the reaction of (*M*)-**2** to (*M*)-**1** but no starting material was observed after 5 minutes.

CIRCULAR DICHROISM MEASUREMENTS:

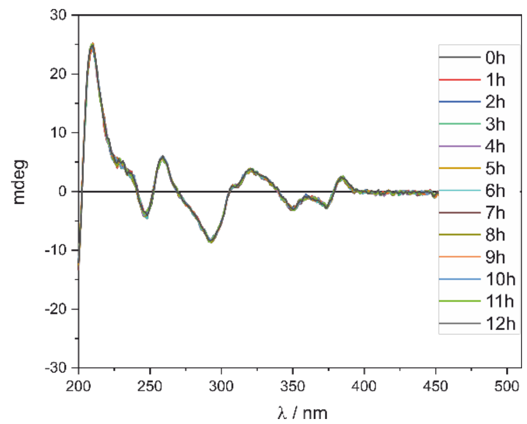


Figure S3. Raw data from CD measurments of *(P)*-**2**. Every hour a spectrum was measured for 12h. Concentration is 10^{-6} M in acetonitrile and at 25 °C.

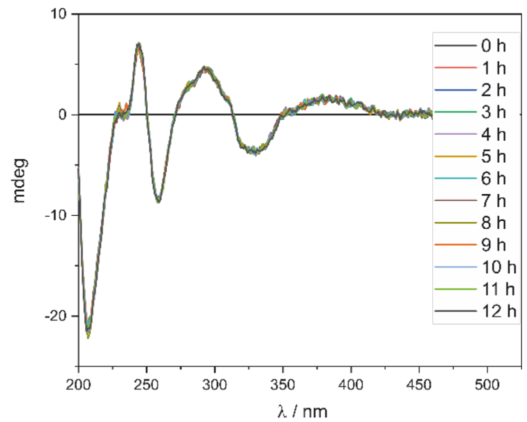


Figure S4. Raw data from CD measurments of *(M)*-**1**. Every hour a spectrum was measured for 12 h. Concentration is 10^{-6} M in acetonitrile and at 25 °C.

In Figure S2 and Figure S3 spectra of time course experiments are shown. The same sample was measured every hour over a period of 12 h and no change in the CD signal was observed.

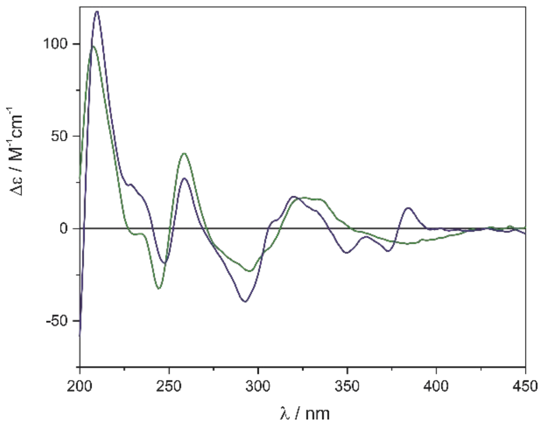


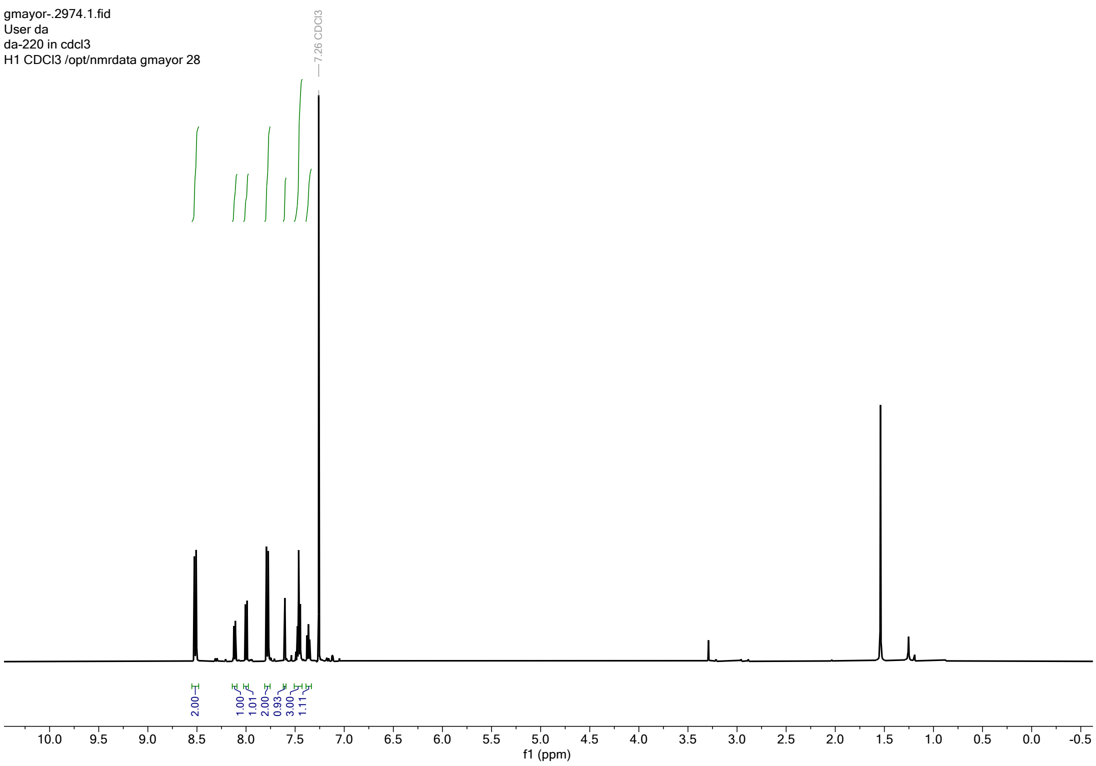
Figure S5: CD spectrum of *(P)*-**1** (green) and *(P)*-**2** (blue) over layered. Concentration is 10^{-6} M in acetonitrile and at 25 °C.

Overlaying the CD spectrum of (*P*)-**1** and (*P*)-**2** (Figure S4**)** visualizes the similarity of the chiroptical activity of both compounds, the cotton bands are found with similar wavelength.

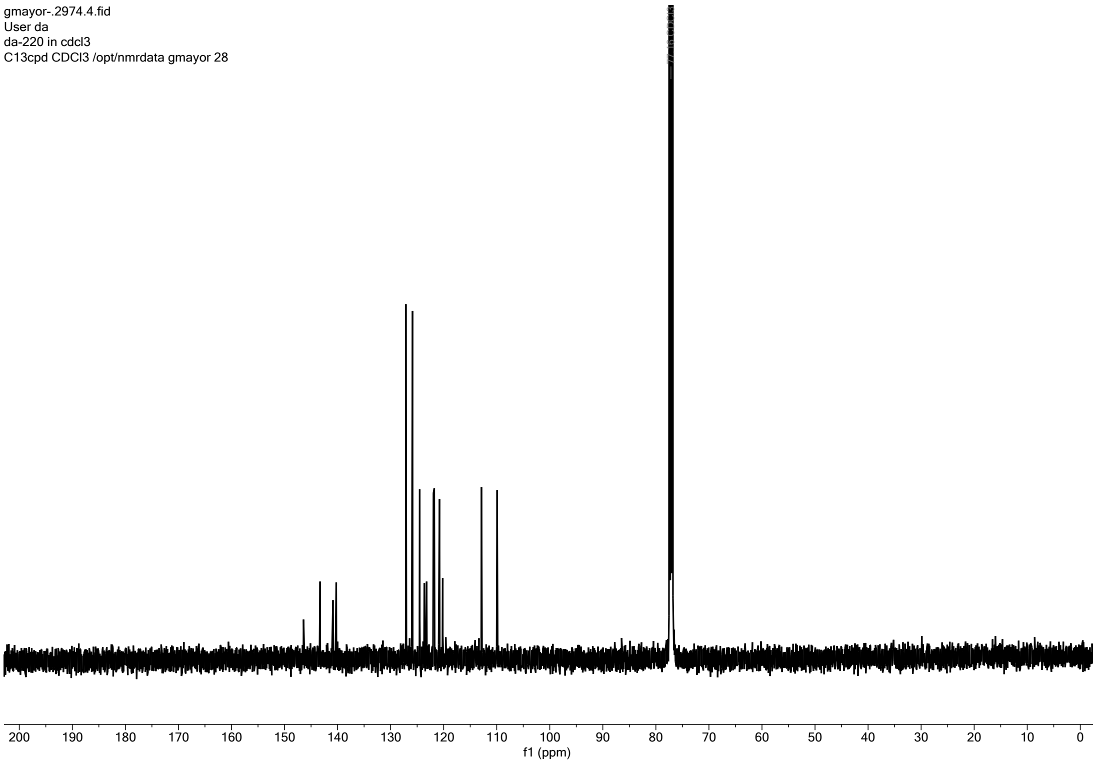
NMR AND HR-MS SPECTRA

2-bromo-9-(4-nitrophenyl)-9H-carbazole 3:

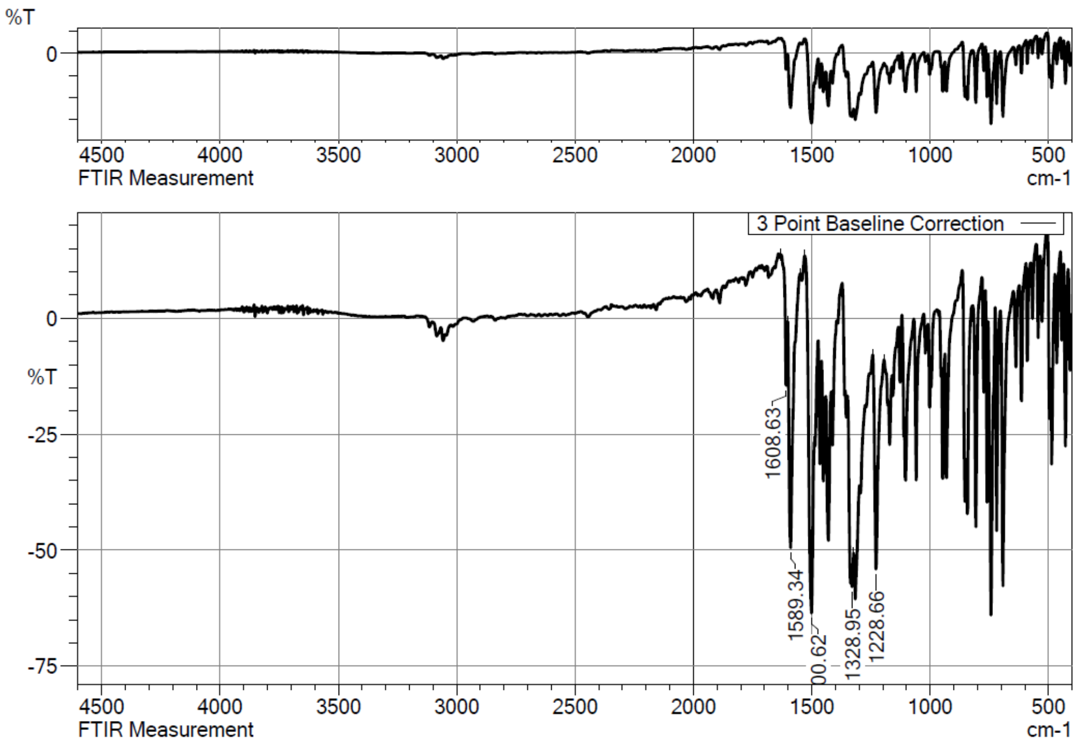
^{1}H NMR (500 MHz, $CDCl_3$):



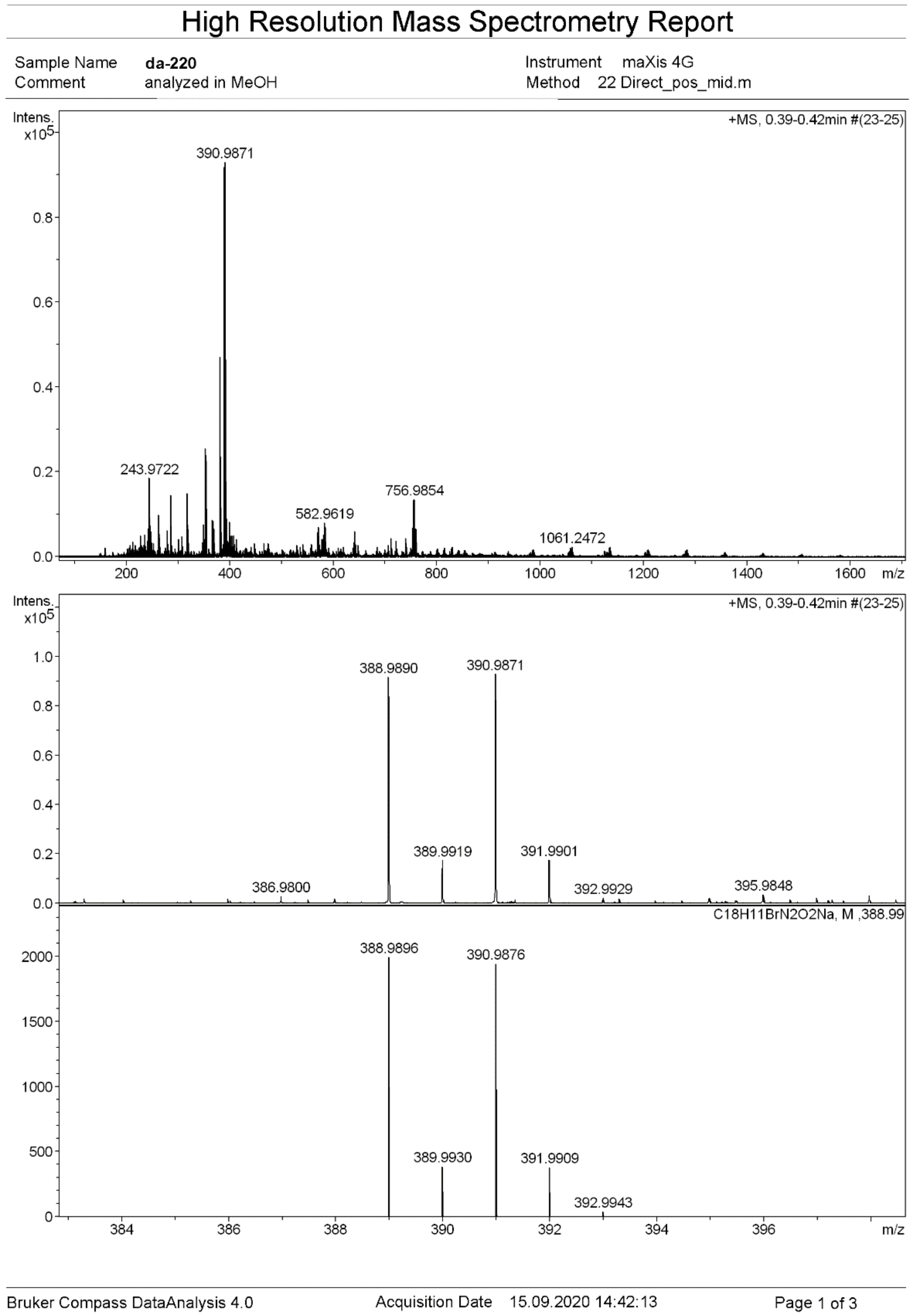
^{13}C NMR (126 MHz, CDCl3):



FT-IR (neat)



HRMS (ESIToF):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Bruker Compass DataAnalysis 4.0
Acquisition Date 15.09.2020 14:42:13
Page 1 of 3

High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

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22	264.1229	4.9	4546
23	279.2288	6.7	6256
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27	286.9942	3.0	2814
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Acquisition Parameter

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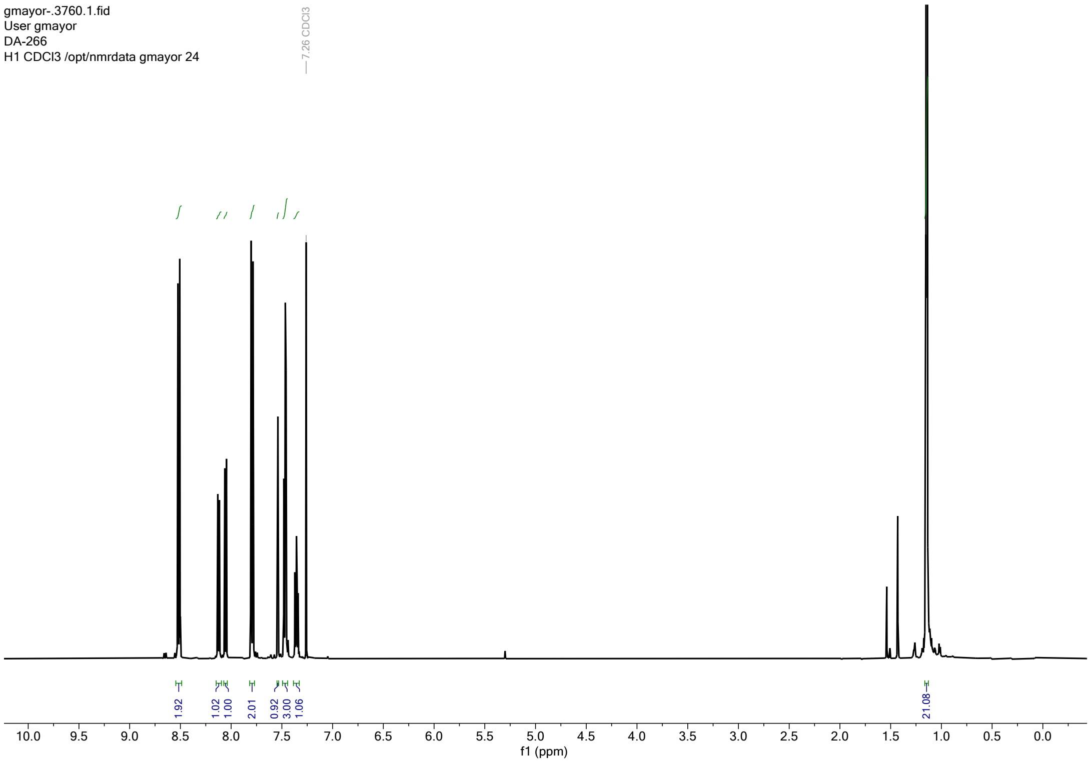
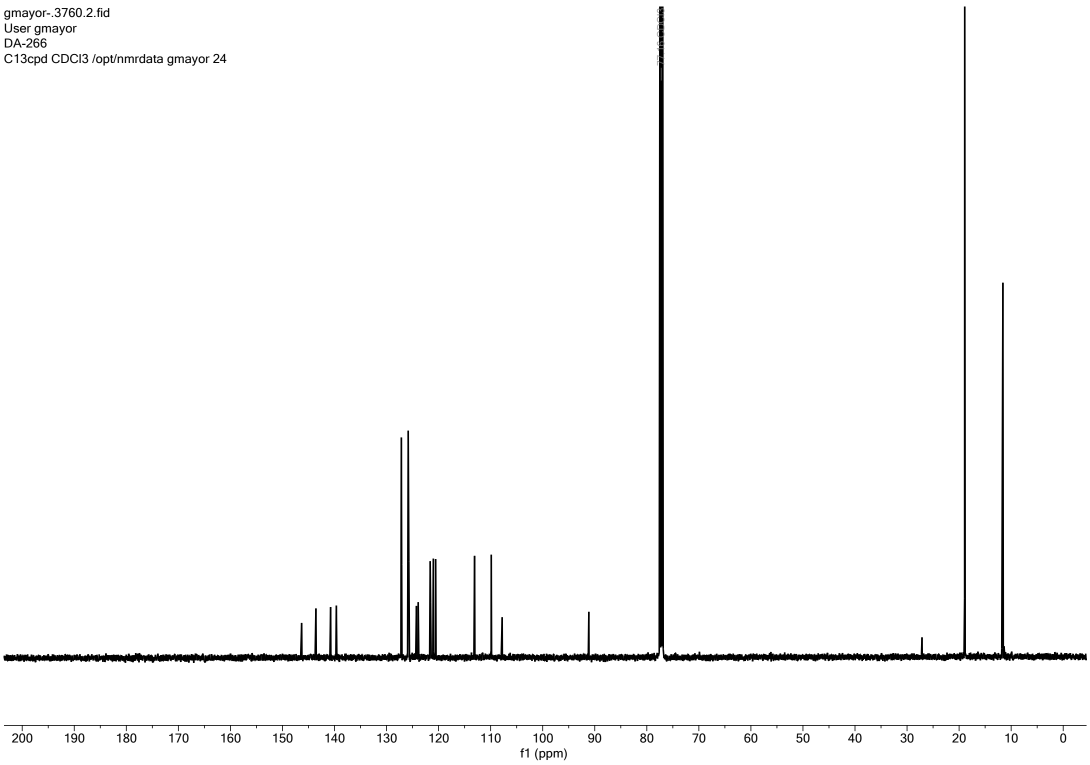
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	350.0 Vpp		
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

9-(4-nitrophenyl)-2-((triisopropylsilyl)ethynyl)-carbazole 4:

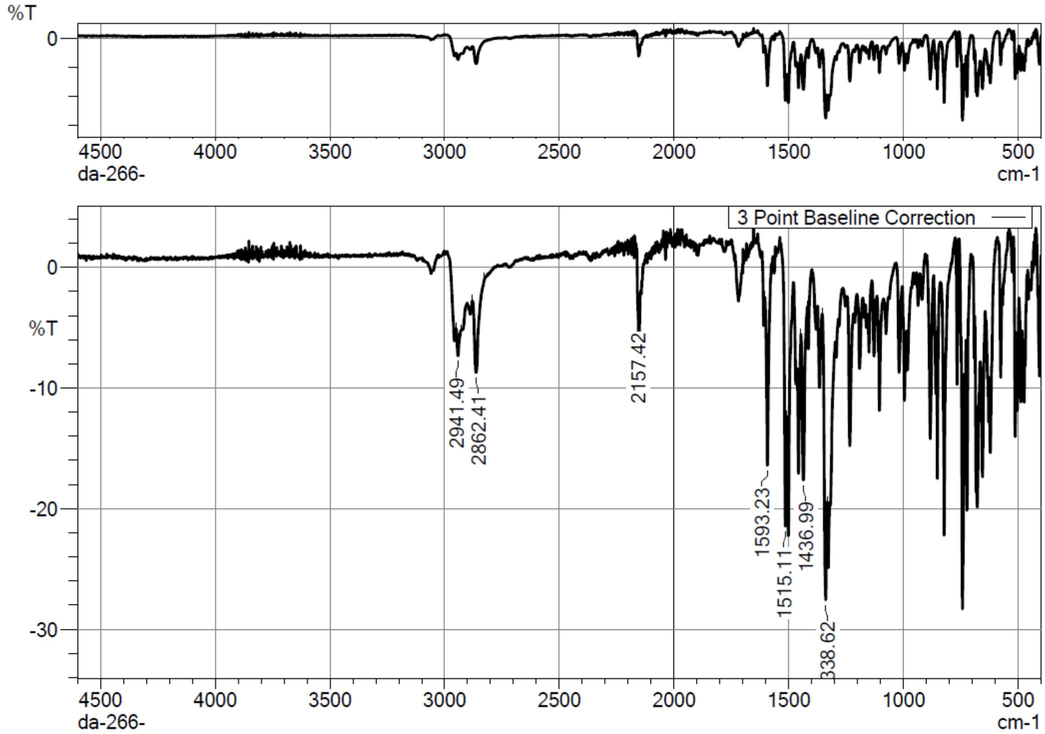
^{1}H NMR (500 MHz, $CDCl_3$):



^{13}C NMR (126 MHz, $CDCl_3$):



FT-IR (neat)



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High Resolution Mass Spectrometry Report

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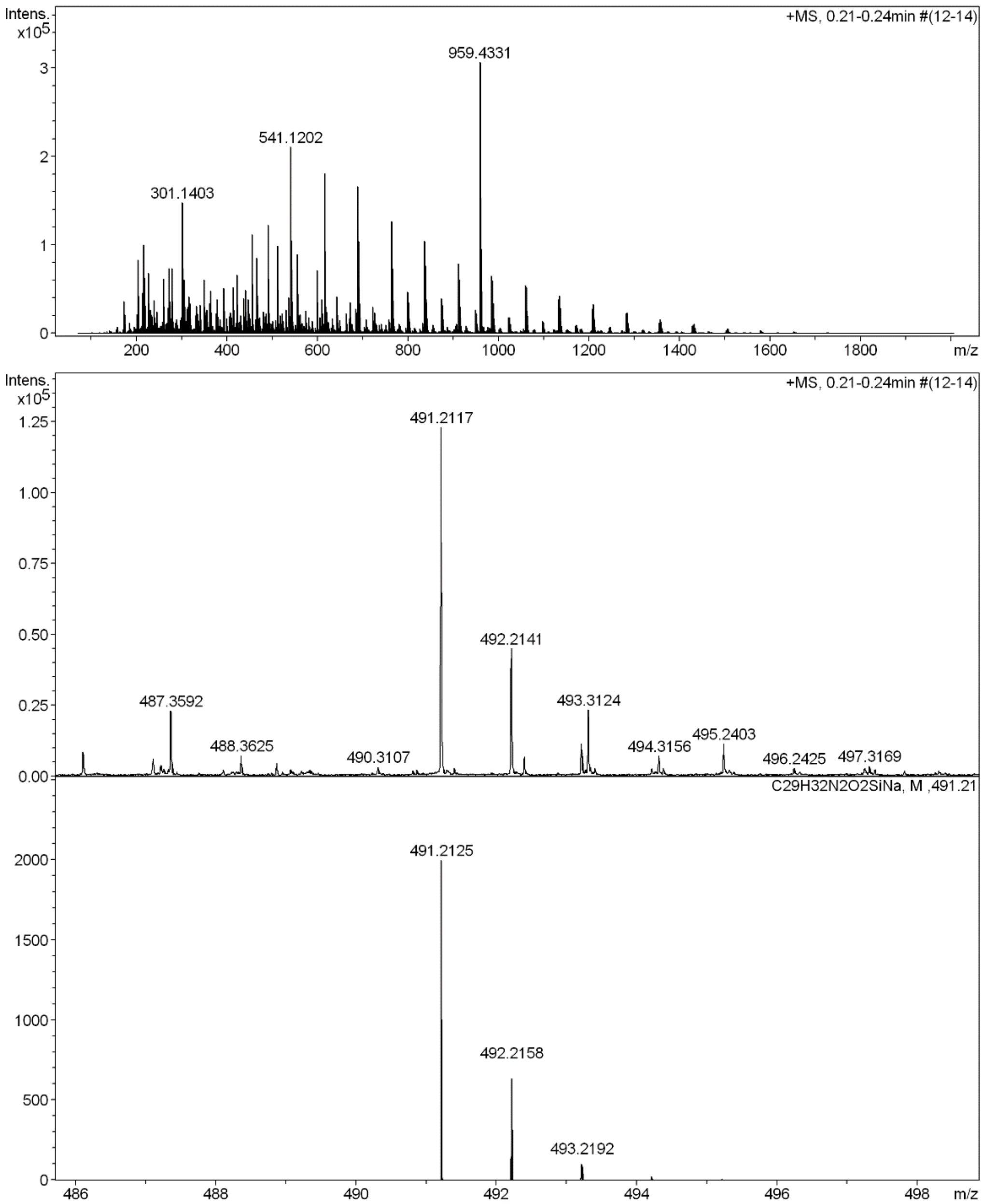

High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

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Mass list

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23	333.1683	10.1	31095
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43	531.3854	8.7	26572
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70	802.2657	9.8	30116
71	837.1938	34.2	104816
72	838.1946	25.1	77079
73	839.1924	21.9	67130
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75	874.2844	12.9	39575
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77	876.2830	9.0	27728
78	911.2117	25.8	78987
79	912.2127	22.7	69583
80	913.2106	20.1	61540
81	914.2097	12.0	36735
82	959.4331	100.0	306485
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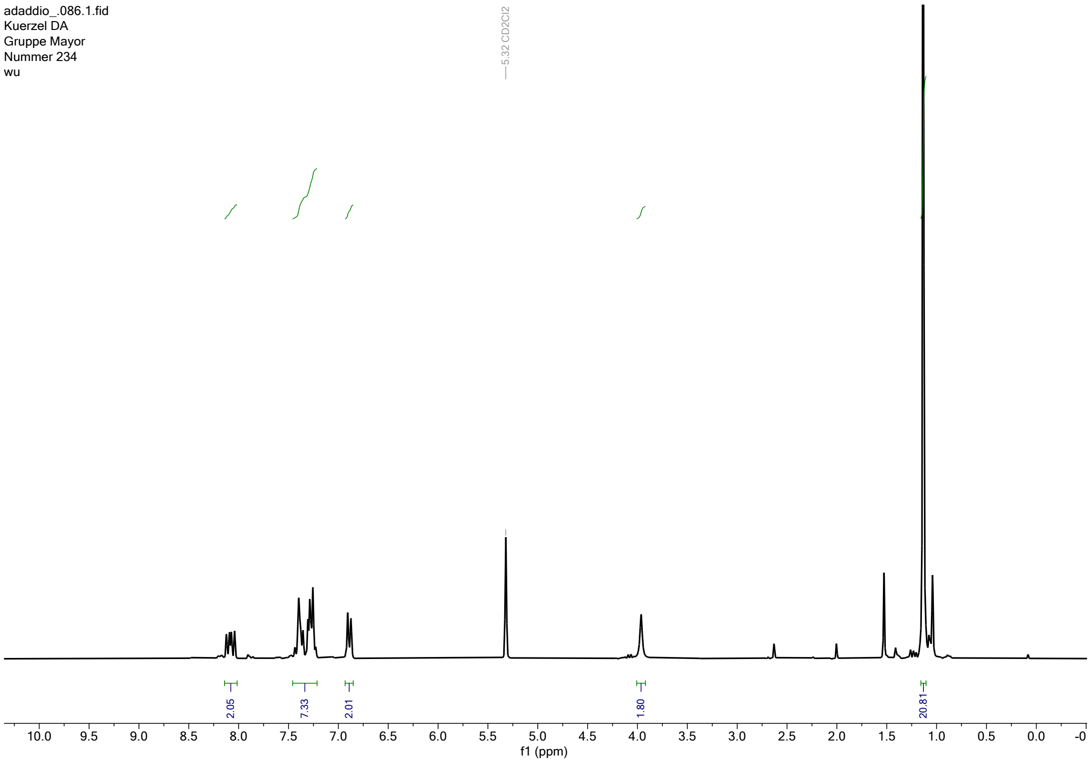
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	600.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

4-(2-((triisopropylsilyl)ethynyl)-carbazol-9-yl)aniline 5:

^{1}H NMR (500 MHz, CD_2Cl_2):



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High Resolution Mass Spectrometry Report

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Comment

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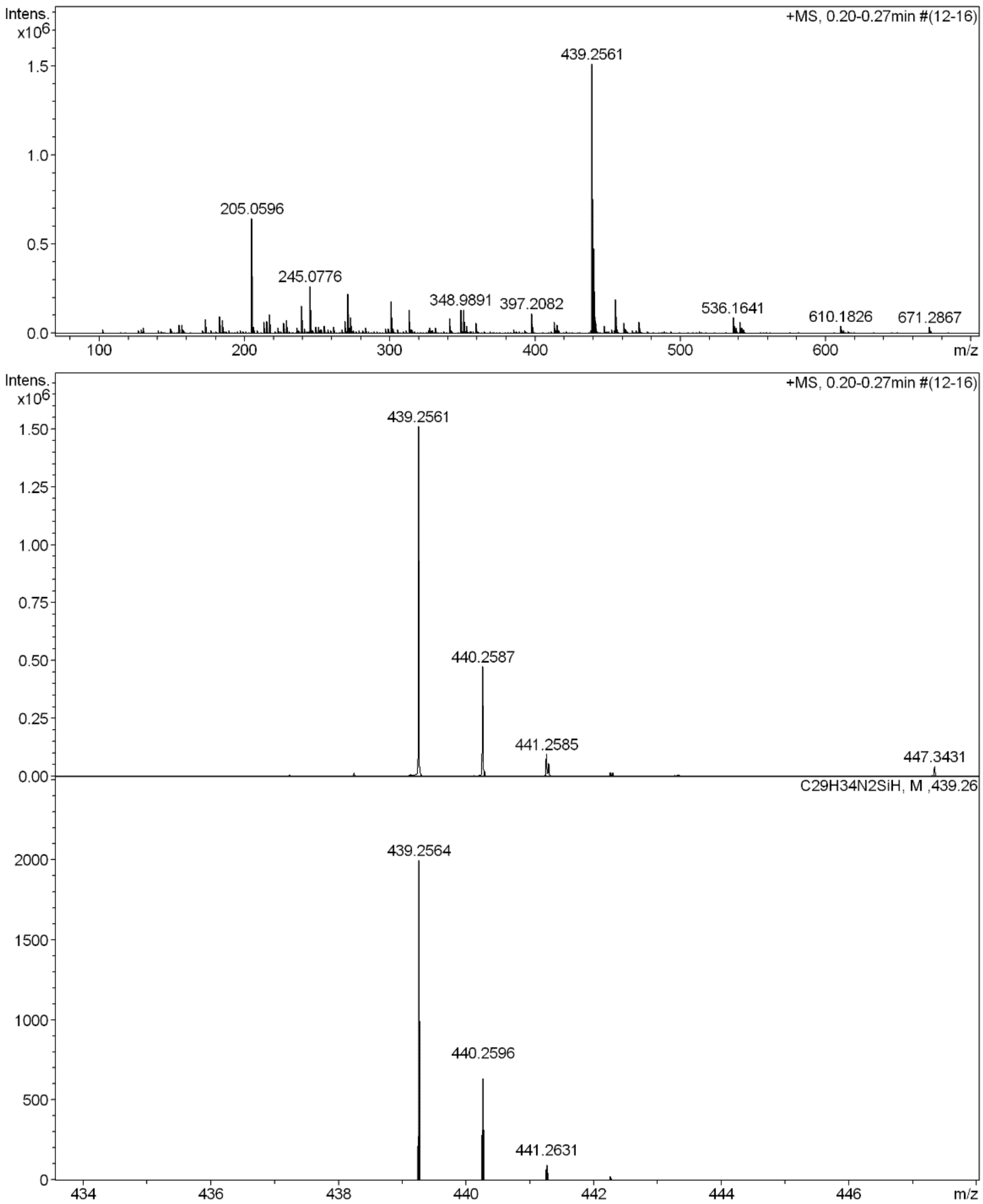

Bruker Compass DataAnalysis 4.0 Acquisition Date 22.09.2020 10:14:04 Page 1 of 2

High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z

Mass list

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Acquisition Parameter

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	Set Dry Heater	200 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	350.0 Vpp	55.0 Vpp	
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Monomer 6:

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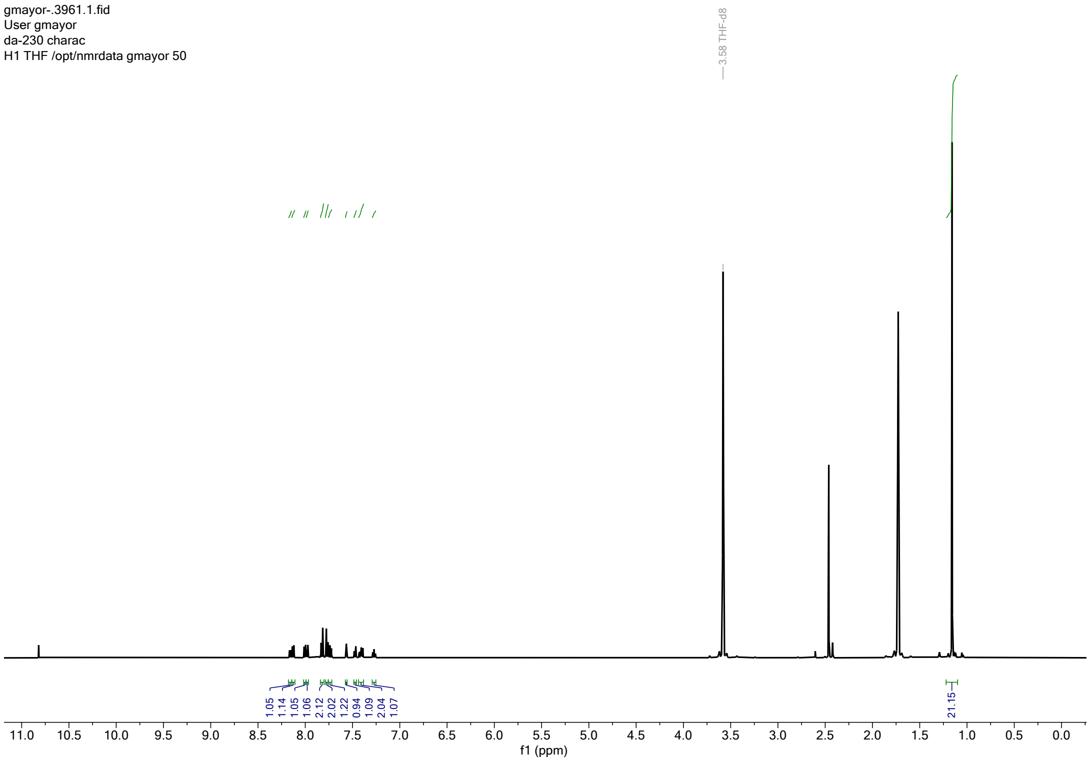
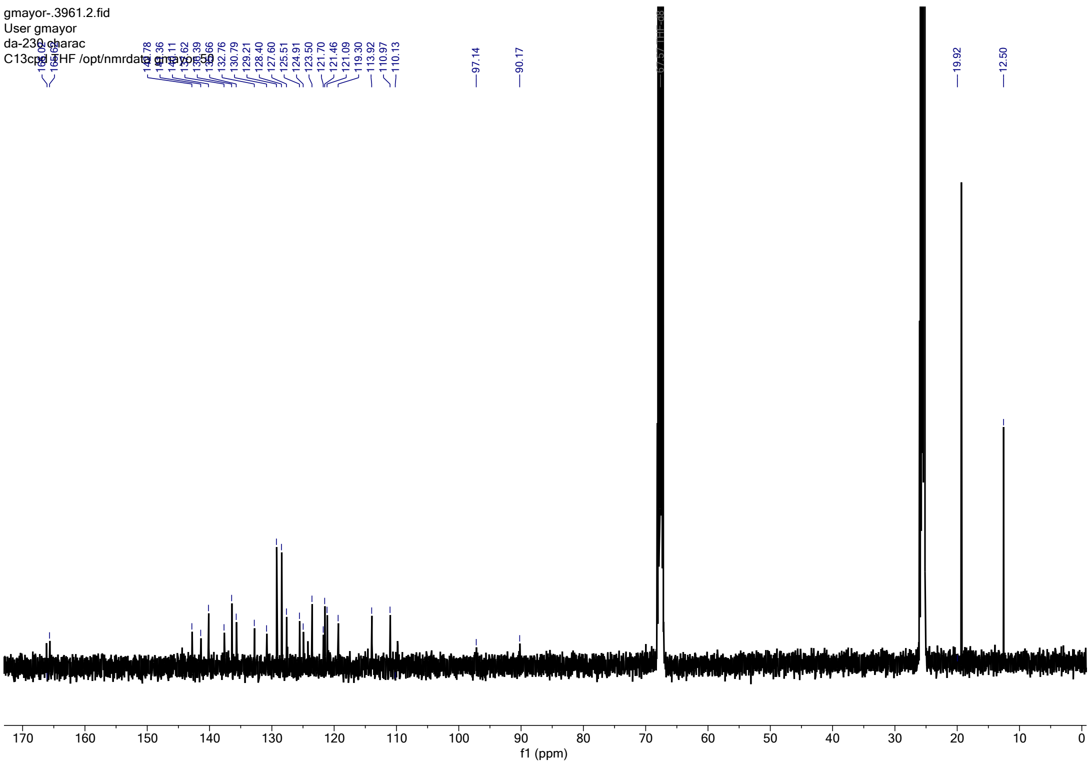
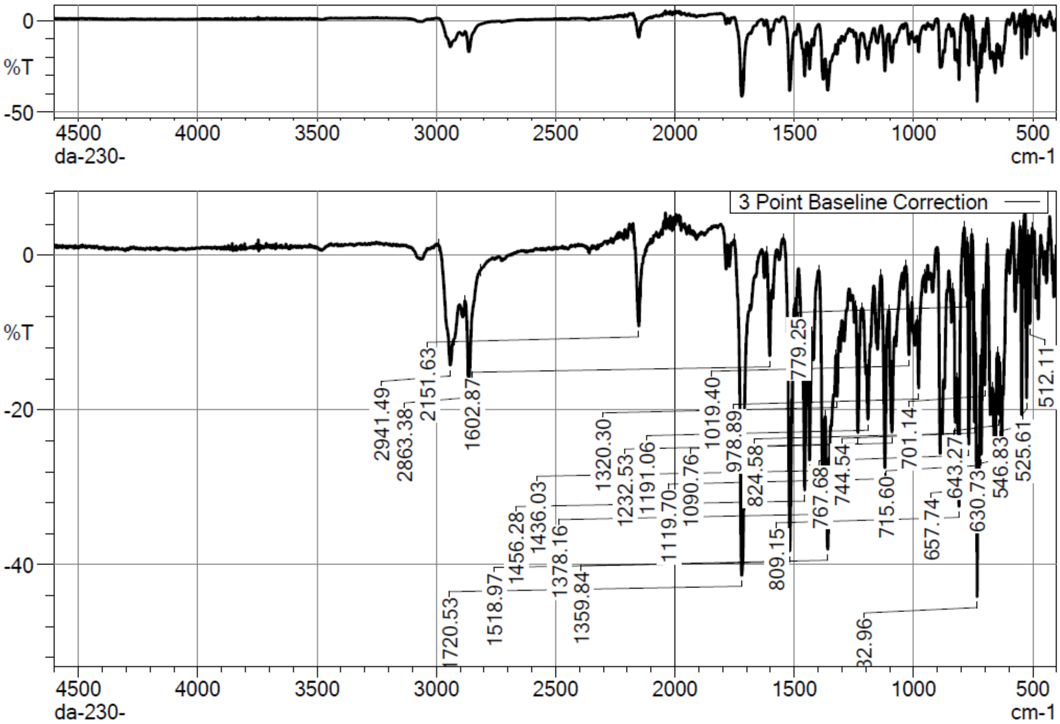


^{13}C NMR (126 MHz, THF-d8):



FT-IR (neat)



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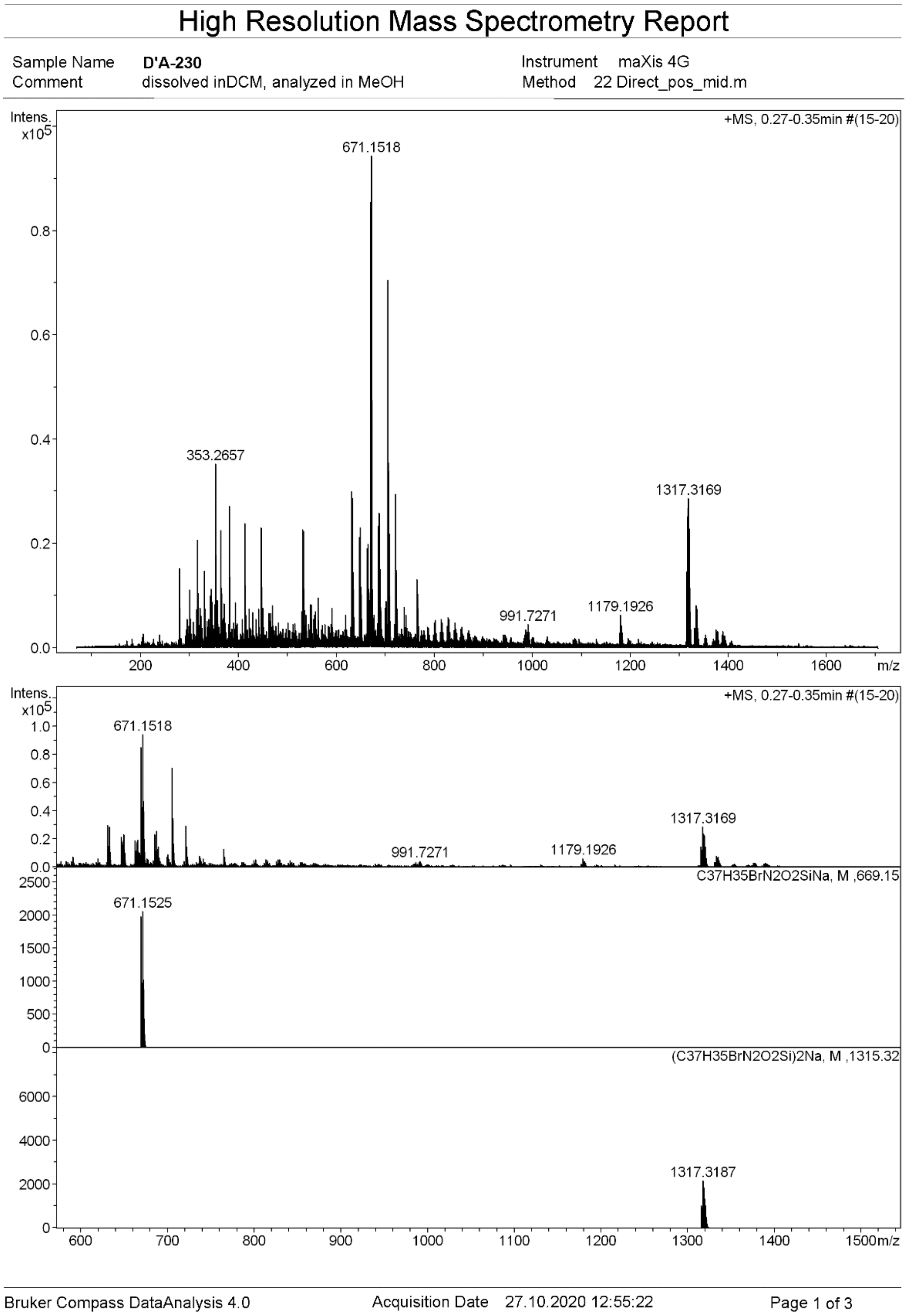
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Page 1 of 3

High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	z
669.1530	1	C 37 H 35 Br N 2 Na O 2 Si	100.00	669.1543	1.3	2.0	5.9	21.5	even	1+
1315.3173	1	C 74 H 70 Br 2 N 4 Na O 4 Si 2	100.00	1315.3195	2.2	1.7	41.1	42.5	even	

Mass list

#	m/z	I %	I
1	279.0929	16.2	15319
2	279.2293	8.1	7676
3	301.0749	11.8	11173
4	315.1922	7.8	7395
5	317.0513	21.9	20725
6	319.2237	8.3	7857
7	321.2394	8.1	7644
8	331.1875	15.7	14810
9	343.0632	10.7	10100
10	344.0626	12.0	11360
11	347.2914	9.4	8866
12	352.0683	8.8	8313
13	353.0678	11.2	10616
14	353.2657	37.4	35340
15	354.2689	7.9	7434
16	357.1463	9.7	9156
17	363.5763	23.2	21882
18	364.0777	11.3	10681
19	364.5758	24.0	22675
20	365.0769	11.1	10436
21	371.1623	9.0	8500
22	381.2970	28.8	27153
23	382.3000	7.4	6972
24	393.2969	9.3	8761
25	413.2653	25.4	23946
26	421.3281	8.1	7620
27	429.2391	7.3	6887
28	441.2969	7.9	7464
29	447.3437	24.5	23114
30	448.3473	7.4	7020
31	449.3619	7.6	7213
32	463.3175	7.2	6761
33	465.3687	7.1	6737
34	469.3277	8.6	8159
35	529.4939	7.4	6986
36	531.0306	24.0	22707
37	532.0339	8.0	7557
38	533.0285	23.7	22399
39	534.0318	7.7	7313
40	547.0042	8.8	8351
41	549.0024	8.9	8358
42	557.5246	7.4	7032
43	562.2381	10.3	9692
44	591.4941	8.2	7735
45	619.5253	6.8	6419
46	631.0855	31.8	30021
47	632.0888	13.0	12319
48	633.0856	30.4	28675
49	634.0882	11.9	11266
50	647.1708	22.6	21298
51	648.1733	10.6	9965
52	649.1694	24.5	23122
53	650.1719	10.9	10313
54	663.0576	20.3	19161
55	663.4521	8.9	8391
56	664.0607	8.8	8312
57	665.0579	21.1	19943
58	666.0602	8.7	8255
59	667.1444	11.4	10761
60	667.1784	7.2	6786
61	667.6451	9.7	9178

High Resolution Mass Spectrometry Report

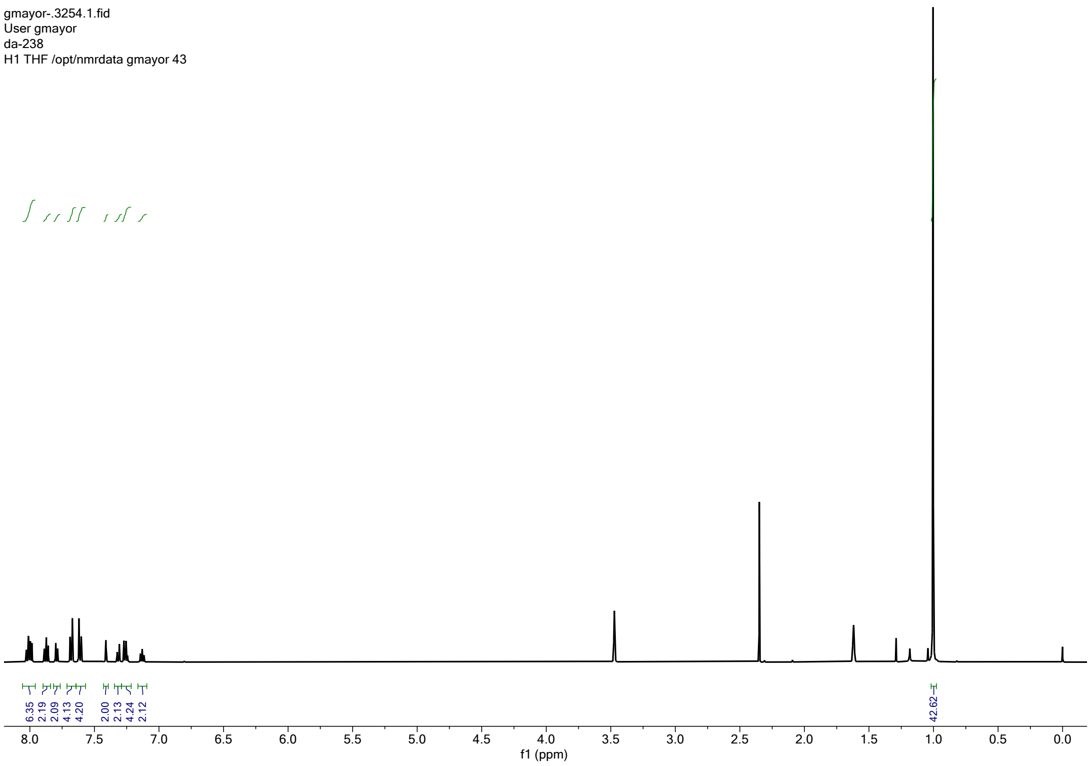
#	m/z	I %	I
62	668.1443	9.4	8907
63	668.6447	6.9	6561
64	669.1530	90.6	85535
65	670.1558	41.9	39523
66	671.1518	100.0	94424
67	672.1542	42.3	39940
68	673.1549	12.1	11397
69	685.1270	24.9	23499
70	685.4339	19.2	18117
71	686.1296	12.1	11463
72	686.4371	9.1	8615
73	687.1255	27.4	25831
74	687.1616	14.5	13687
75	688.1278	12.2	11528
76	688.1634	7.3	6934
77	689.1614	16.0	15087
78	690.1636	7.6	7137
79	699.5936	8.2	7699
80	700.6250	9.6	9091
81	705.5812	74.8	70583
82	706.5843	36.1	34084
83	707.5848	11.3	10712
84	721.1472	14.9	14049
85	721.5721	31.3	29515
86	722.5751	15.5	14677
87	737.5516	8.3	7851
88	764.5723	14.0	13190
89	765.5753	8.1	7634
90	1179.1926	6.8	6376
91	1315.3173	15.5	14654
92	1316.3195	13.4	12634
93	1317.3169	30.4	28681
94	1318.3196	25.3	23935
95	1319.3167	24.4	22999
96	1320.3180	15.6	14746
97	1321.3189	7.5	7036
98	1333.2905	8.6	8124
99	1334.2948	7.4	6970
100	1335.2945	8.0	7573

Acquisition Parameter

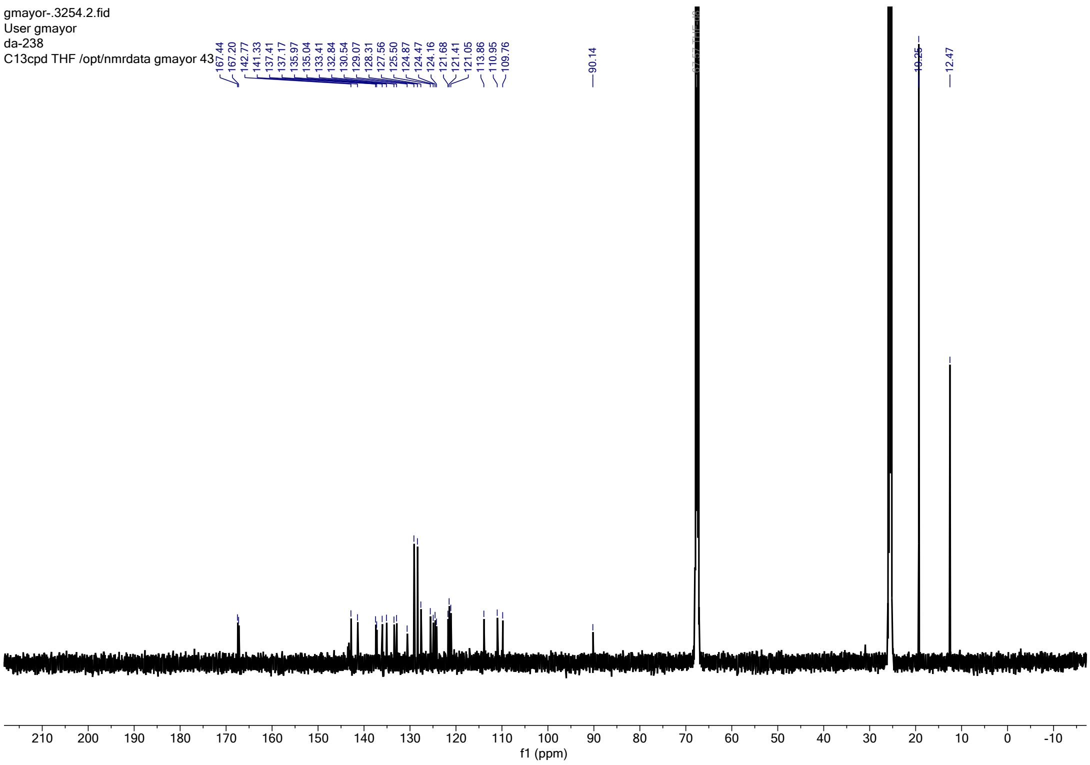
General	Fore Vacuum	2.48e+000 mBar	High Vacuum	1.21e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	1700 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV			100.0 Vpp	
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	350.0 Vpp		
Ion Cooler	Set Ion Cooler Transfer Time	75.0 µs	Set Ion Cooler Pre Pulse Storage Time	10.0 µs		

Dimer 7:

^{1}H NMR (500 MHz, THF-d8):



^{13}C NMR (126 MHz, THF-d8):



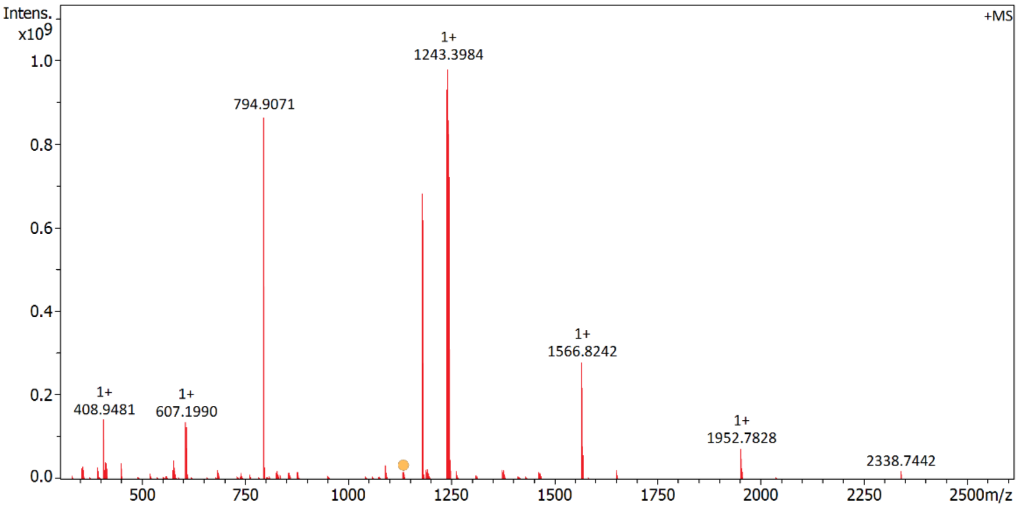
HRMS (MALDI-ToF):

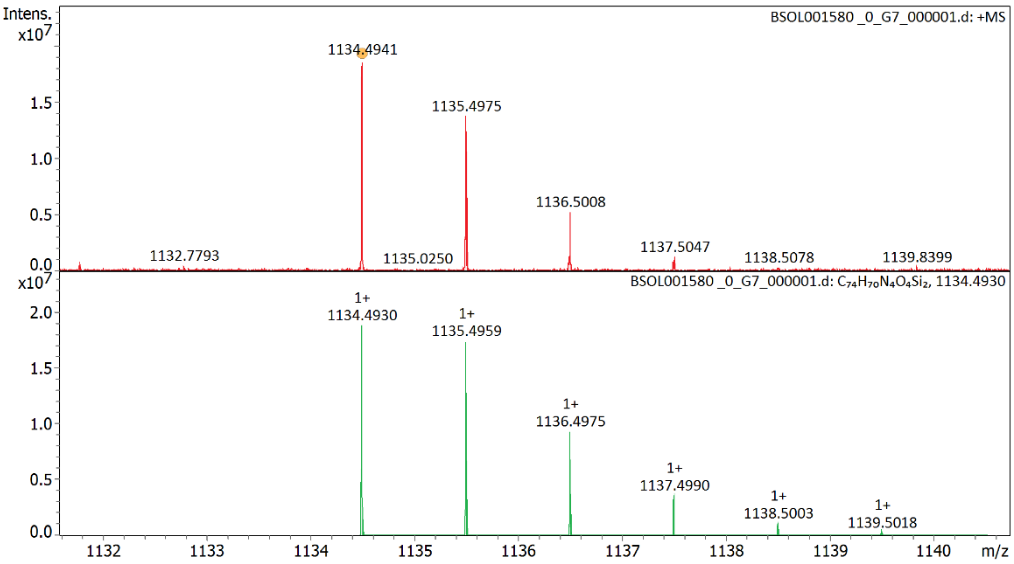
BSOL001580 Adriano D'Addio/ - DA-337-M3-P4 - DCM - DCTB+Ag 1:10:1

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Acquisition Parameter

Method:	MALDI_MS_POS_300-2600_2M_16AvScans			Acquisition Date:	17.12.2021 15:09:38
File Name:	D:\Data\ETH Data\BSOL0015xx\BSOL001580 _0_G7_000001.d			Operator:	Daniel Wirz
Source	Dual (MALDI/ESI)	Polarity	Positive	Nebulizer Gas	1.3 bar
Broadband Low Mass	303.1 m/z			Drying Gas Flow Rate	3.7 L/min
Broadband High Mass	2600.0 m/z	Laser Power	34.0 lp	Capillary	4500.0 V
No. of Cell Fills	1			Drying Gas	200.0 °C
Apodization	Full-Sine	Time of Flight to Detector	0.001 sec	Temperature	





BSOL001580 Adriano D'Addio/ - DA-337-M3-P4 - DCM - DCTB+Ag 1:10:1

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C74H70N4O4Si2	M	1134.4930	1+	1134.4941	88.5	ok	-1.1	-1.0

Calibration Info:

Internal calibration

Date: 17.12.2021 15:10:59
Polarity: Positive
Calibration spectrum: +MS: Scan
Reference mass list: MALDI: DCTB Matrix + Na-PFHA Cluster (pos)
Calibration mode: Quadratic
Standard deviation: 0.604 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
250.1464			
251.1543			
273.1362			
332.2009			
408.9481	408.9481	143402448	-0.013
500.2934			
501.3013			
523.2832			
750.4404			
751.4483			
773.4302			
794.9069	794.9071	871369152	0.205
1000.5874			
1001.5953			
1023.5772			
1180.8657	1180.8654	681921536	-0.291
1566.8246	1566.8242	281248256	-0.247
1952.7834	1952.7828	74977648	-0.344
2338.7423	2338.7442	20150266	0.827
2724.7011			
3110.6599			
3496.6188			
3882.5776			
4268.5365			
4654.4953			
5040.4541			
5426.4130			
5812.3718			
6198.3307			
6584.2895			
6970.2483			
7356.2072			
7742.1660			
8128.1249			
8514.0837			
8900.0425			
9286.0014			
9671.9602			

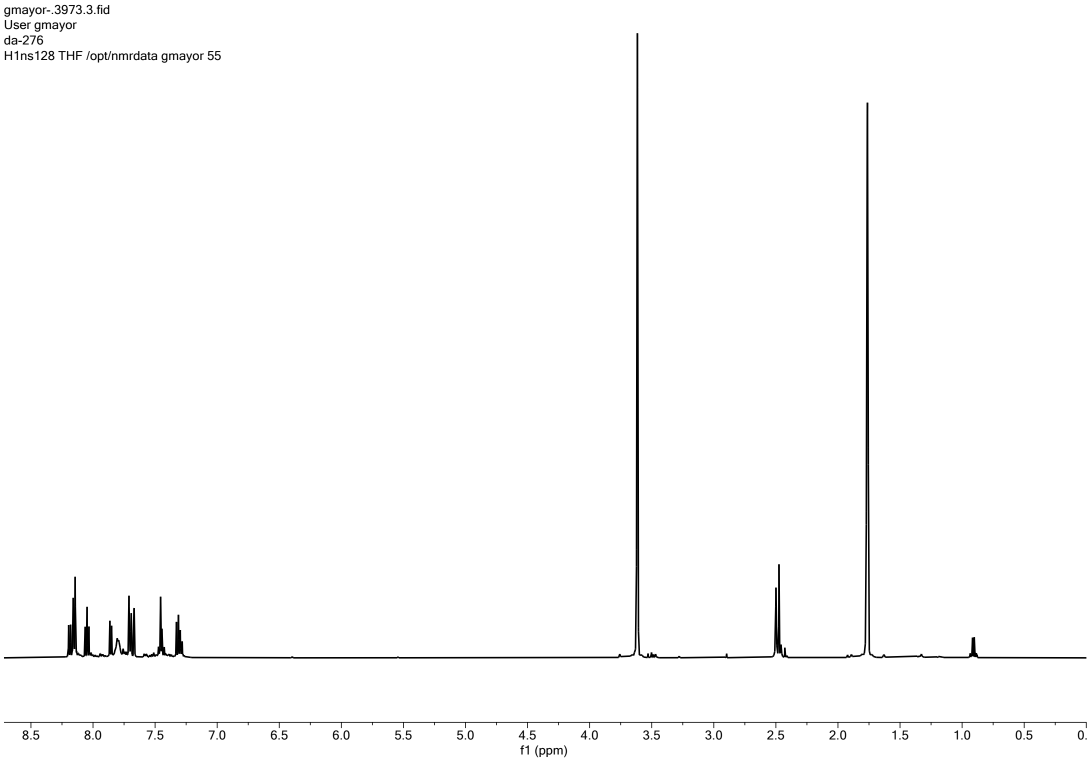
Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	357.0515	558651	1121.4	2.8	0.0006
2	359.0512	559389	1344.2	3.3	0.0006
3	408.9481	450815	5664.6	14.5	0.0009
4	449.9749	419844	1459.2	3.9	0.0011
5	576.9423	332643	772.2	2.3	0.0017
6	578.9419	332803	1535.7	4.5	0.0017
7	580.9416	323088	668.9	2.0	0.0018
8	607.1990	320205	4608.1	14.0	0.0019
9	608.2025	314428	1549.8	4.7	0.0019
10	609.1967	473404	589.8	1.8	0.0013
11	609.1988	319543	4205.6	12.7	0.0019
12	610.2021	314910	1442.7	4.4	0.0019
13	685.4364	284836	719.0	2.3	0.0024
14	794.9071	244104	24668.5	88.1	0.0033
15	795.9109	244115	2880.8	10.3	0.0033
16	829.0892	231134	567.4	2.1	0.0036
17	878.8902	215888	489.9	1.8	0.0041
18	1091.4393	179518	837.9	3.6	0.0061
19	1092.4425	184266	583.1	2.5	0.0059
20	1134.4941	169930	431.6	1.9	0.0067
21	1180.8654	165277	14309.4	68.9	0.0071
22	1181.8692	165073	2631.8	12.7	0.0072
23	1193.1622	163421	530.6	2.6	0.0073
24	1241.3972	160357	18579.9	94.0	0.0077
25	1242.4004	161191	16528.9	83.6	0.0077
26	1243.3984	160643	19776.5	100.0	0.0077
27	1244.4005	163449	16480.4	83.3	0.0076
28	1245.3947	185537	919.4	4.7	0.0067
29	1245.4036	165467	5847.7	29.6	0.0075
30	1246.3972	179882	579.7	2.9	0.0069
31	1246.4074	149567	1045.7	5.3	0.0083
32	1376.3065	147642	483.9	2.4	0.0093
33	1377.3104	140792	376.8	1.9	0.0098
34	1463.2877	132522	362.0	1.8	0.0110
35	1464.2916	125042	323.2	1.6	0.0117
36	1566.8242	123877	5479.5	28.4	0.0126
37	1567.8283	119579	1424.2	7.4	0.0131
38	1952.7828	92751	1334.2	7.6	0.0211
39	1953.7866	90698	473.5	2.7	0.0215
40	2338.7442	78443	319.1	2.0	0.0298

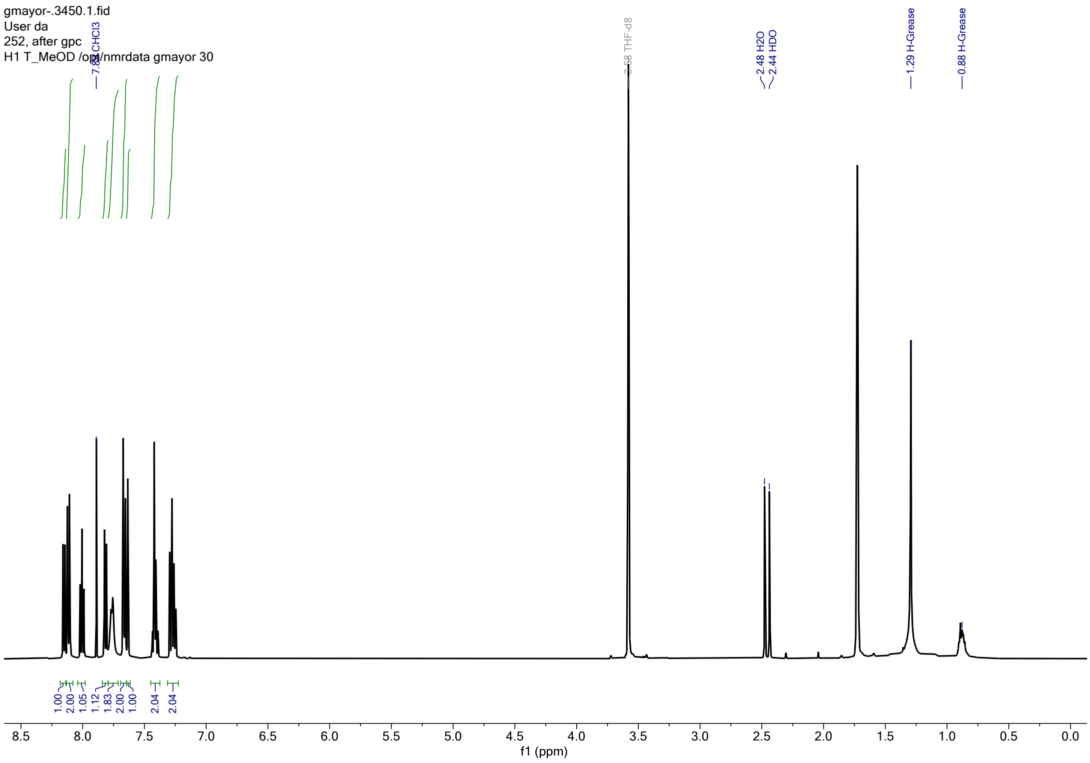
#	m/z	Res.	S/N	I %	FWHM
1	1134.4930	169930		100.0	0.0067
2	1135.4959	170080		92.6	0.0067
3	1136.4975	170230		49.7	0.0067
4	1137.4990	170380		19.2	0.0067
5	1138.5003	170530		5.8	0.0067
6	1139.5018	170680		1.4	0.0067
7	1140.5033	170830		0.3	0.0067

Butadiyne macrocycle 2:

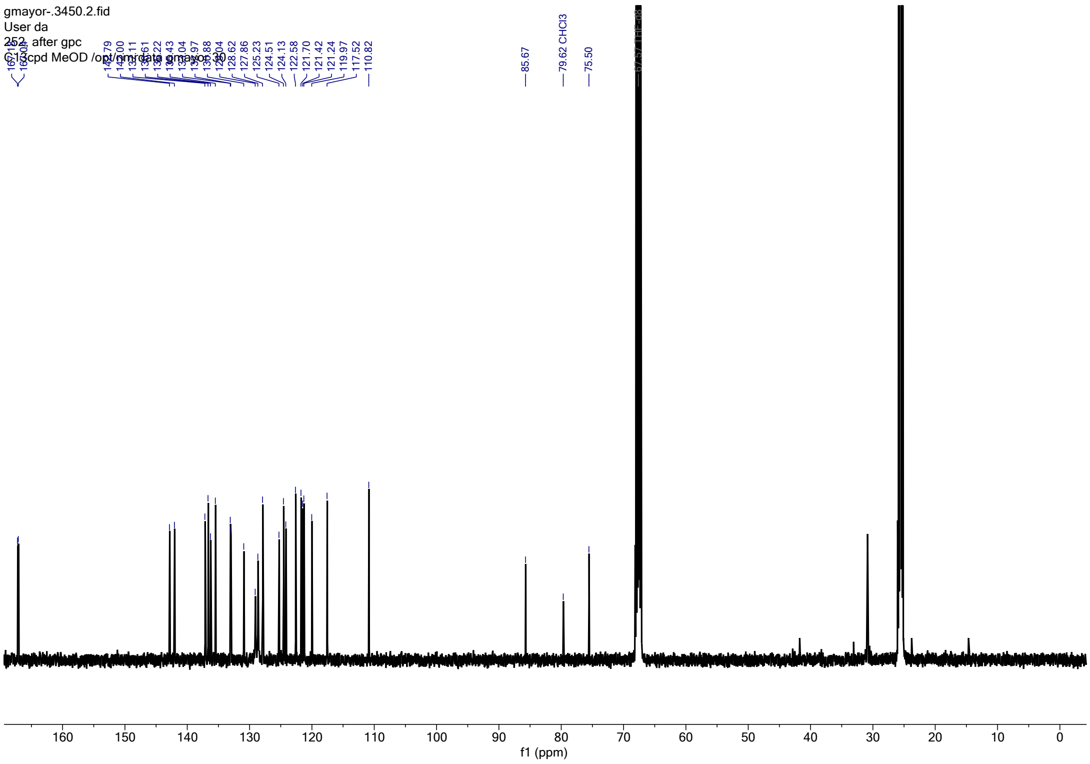
^{1}H NMR (500 MHz, THF-d8): as used for further synthesis



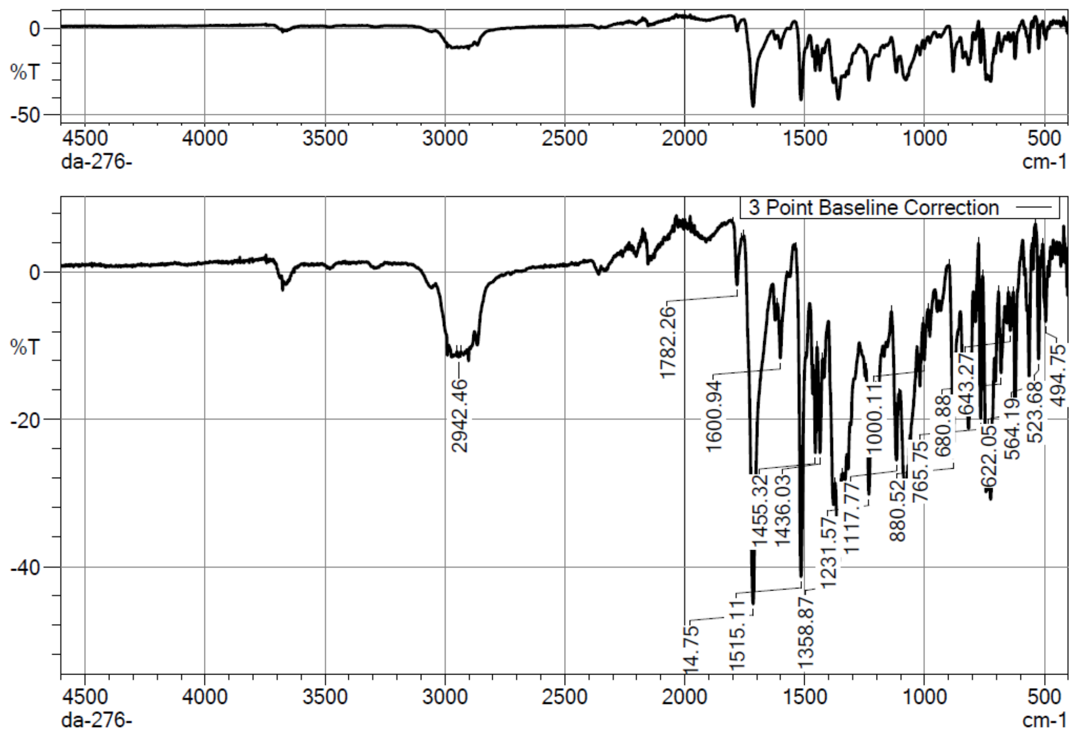
^{1}H NMR (500 MHz, THF-d8): after GPC



^{13}C NMR (126 MHz, THF-d8):



FT-IR (neat)



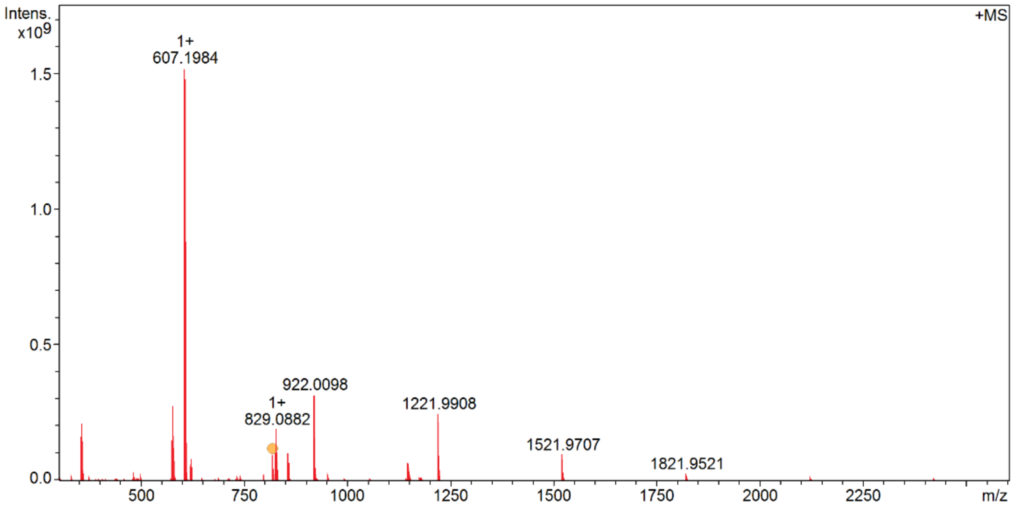
HRMS (MALDI-ToF):

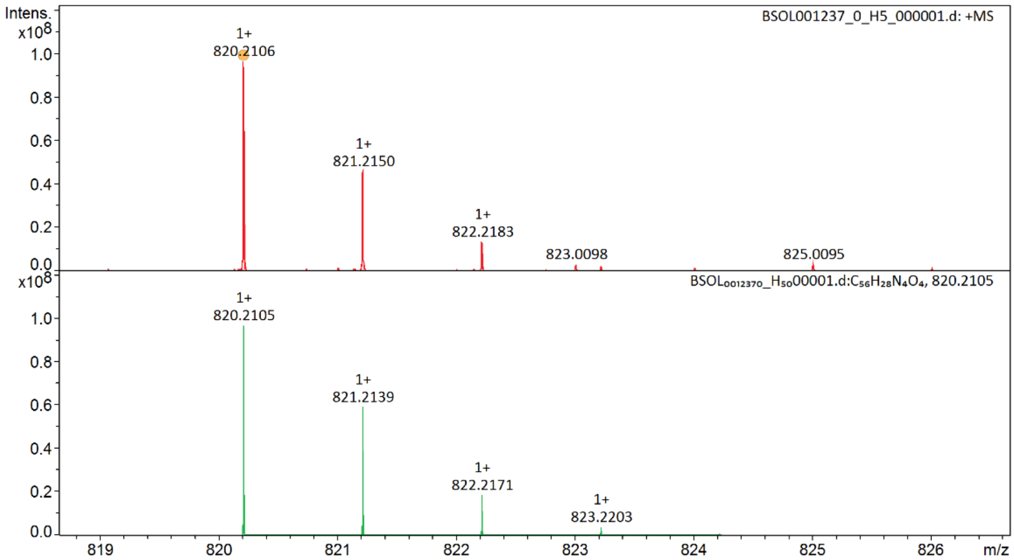
BSOL001237 Adriano D'Addio/ - DA-252 - DCM - DCTB+Ag 1:10:1

ETH Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Acquisition Parameter

Method:	MALDI_MS_POS_300-2600_2M_16AvScans			Acquisition Date:	27.01.2021 07:56:13
File Name:	D:\ETH\Data\BSOL0012xx\BSOL001237_0_H5_000001.d			Operator:	Michael Meier
Source	Dual (MALDI/ESI)	Polarity	Positive	Nebulizer Gas	1.3 bar
Broadband Low Mass	303.1 m/z	n/a	n/a	Drying Gas Flow Rate	3.7 L/min
Broadband High Mass	2600.0 m/z	Laser Power	35.0 lp	Capillary	3000.0 V
No. of Cell Fills	1	n/a	n/a	Drying Gas	200.0 °C
Apodization	Full-Sine	Time of Flight to Detector	0.001 sec	Temperature	





BSOL001237 Adriano D'Addio/ - DA-252 - DCM - DCTB+Ag 1:10:1

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C56H28N4O4	M	820.2105	1+	820.2106	59.8	ok	-0.1	-0.1

Calibration Info:

Date: 27.01.2021 07:57:51
Polarity: Positive
Calibration spectrum: +MS: Scan
Reference mass list: MALDI: DCTB+Ag Matrix + HP-Mix (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
106.9045			
118.0863			
250.1464			
251.1543			
273.1362			
322.0481	322.0482	214019	0.368
332.2009	332.2009	15808783	-0.006
357.0515	357.0513	164832720	-0.649
500.2934			
501.3013			
523.2832	523.2837	1404337	0.918
607.1985	607.1984	1522726784	-0.197
622.0290	622.0286	79968880	-0.608
750.4404			
751.4483			
773.4302			
857.3455			
922.0098	922.0098	319618944	-0.023
1000.5874			
1001.5953			
1023.5772			
1107.4925	1107.4933	2420207	0.683
1221.9906	1221.9908	248277472	0.171
1521.9715	1521.9707	98525208	-0.541
1821.9523	1821.9521	27006852	-0.095
2121.9332	2121.9328	14298138	-0.186
2421.9140			
2721.8948			

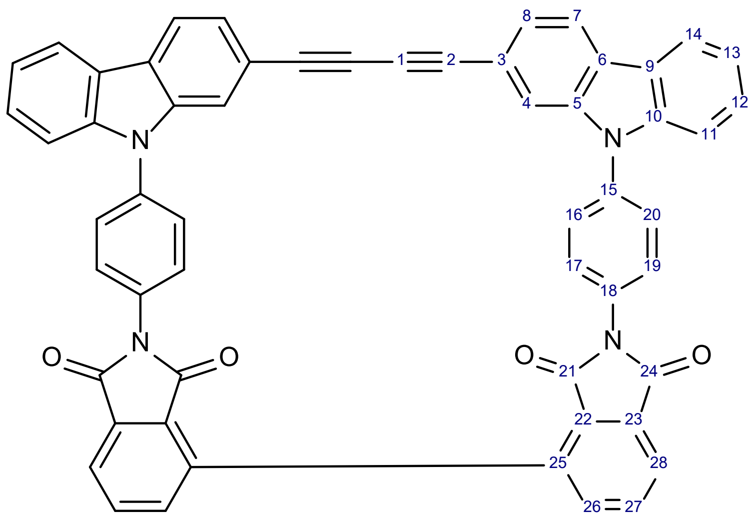
Standard deviation: 0.554

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	357.0513	554839	6694.8	10.8	0.0006
2	359.0510	566548	8532.8	13.8	0.0006
3	359.0518	567191	3669.1	5.9	0.0006
4	576.9421	351471	4728.3	9.9	0.0016
5	576.9439	407711	2148.6	4.5	0.0014
6	578.9417	322079	8632.2	18.1	0.0018
7	578.9433	348406	4146.0	8.7	0.0017
8	579.9453	332571	1777.2	3.8	0.0017
9	580.9416	295407	3729.7	7.9	0.0020
10	580.9433	351769	1700.0	3.6	0.0017
11	607.1950	300260	2655.5	5.8	0.0020
12	607.1964	383989	3540.9	7.7	0.0016
13	607.1984	319817	46103.1	100.0	0.0019
14	608.2023	288424	19038.3	41.3	0.0021
15	609.1940	412863	1890.9	4.1	0.0015
16	609.1951	353732	2489.3	5.4	0.0017
17	609.1963	417428	2379.1	5.2	0.0015
18	609.1983	339598	44876.8	97.3	0.0018
19	609.2051	406026	2383.0	5.2	0.0015
20	610.2020	284792	18860.7	40.9	0.0021
21	611.2055	254361	1489.2	3.3	0.0024
22	622.0286	193950	2358.8	5.3	0.0032
23	820.2106	240736	2344.9	6.3	0.0034
24	820.2139	224757	2236.6	6.1	0.0036
25	827.0888	192202	2513.7	6.8	0.0043
26	827.0920	330211	1946.5	5.3	0.0025
27	829.0882	236534	4645.2	12.6	0.0035
28	829.0919	258057	3665.6	9.9	0.0032
29	830.0925	188239	1517.2	4.1	0.0044
30	831.0887	239377	1792.7	4.9	0.0035
31	831.0930	287835	1354.8	3.7	0.0029
32	857.3457	228233	1438.6	4.0	0.0038
33	857.3489	210308	2507.0	6.9	0.0041
34	859.3463	256942	1570.6	4.4	0.0033
35	859.3503	291941	1588.7	4.4	0.0029
36	922.0098	183914	7394.5	21.0	0.0050
37	922.0149	253375	2830.7	8.0	0.0036
38	1149.0077	142496	1403.1	4.3	0.0081
39	1221.9908	118904	5185.8	16.3	0.0103
40	1521.9707	97333	1955.8	6.5	0.0156

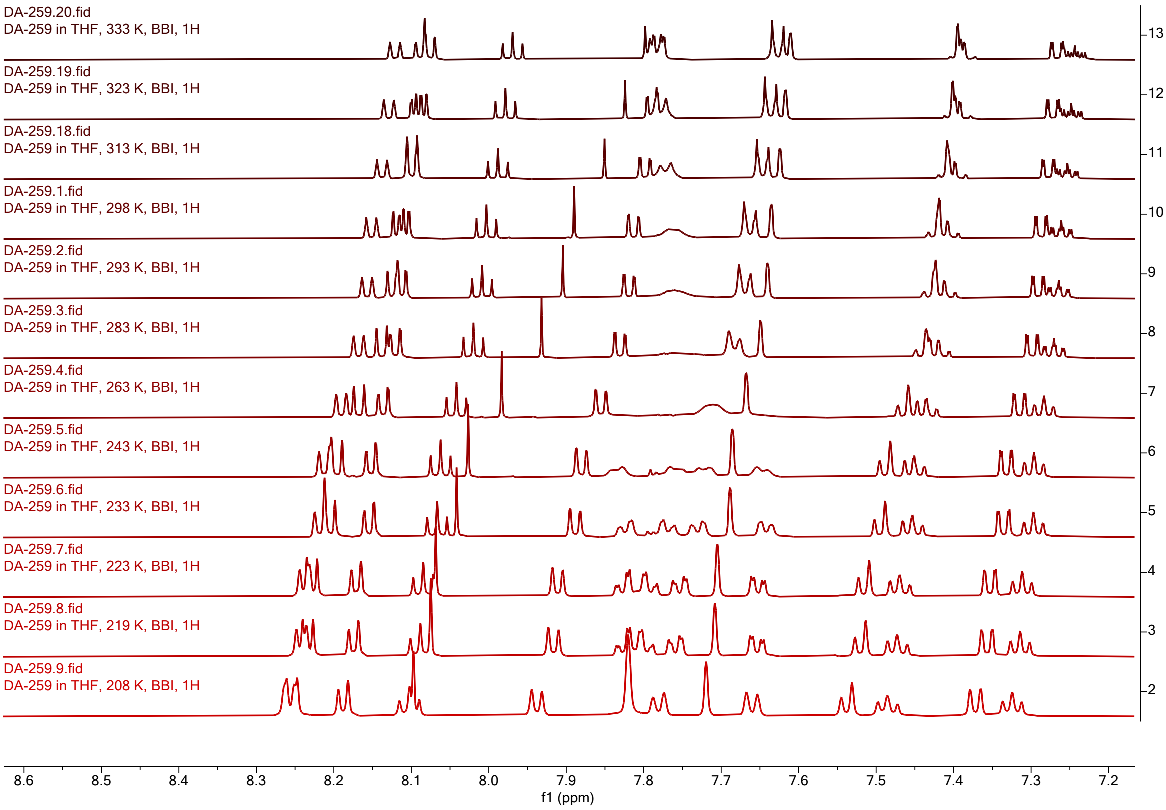
#	m/z	Res.	S/N	I %	FWHM
1	820.2105	240736		100.0	0.0034
2	821.2075	241028		1.5	0.0034
3	821.2139	241030		61.0	0.0034
4	822.2109	241323		0.9	0.0034
5	822.2171	241325		19.1	0.0034
6	823.2142	241617		0.3	0.0034
7	823.2203	241619		4.1	0.0034
8	824.2234	241914		0.7	0.0034

Full assignment at 218 K:



Nr	^{1}H [ppm]	^{13}C [ppm]	Nr	^{1}H [ppm]	^{13}C [ppm]
1		75.29	15		136.82
2	-	85.66	16	7.79	128.82
3	-	119.45	17	7.83	130.14
4	7.71	117.48	18	-	132.55
5	-	141.40	19	7.65	129.23
6	-	125.05	20	7.76	128.13
7	8.23	121.57	21	-	167.12
8	7.36	122.52	22	-	130.80
9	-	123.80	23	-	132.74
10	-	142.26	24	-	167.30
11	7.52	110.82	25	-	135.83
12	7.47	128.05	26	7.92	136.70
13	7.31	121.53	27	8.09	135.63
14	8.24	121.92	28	8.17	124.53

VT-1H NMR (600 MHz, THF-d8):

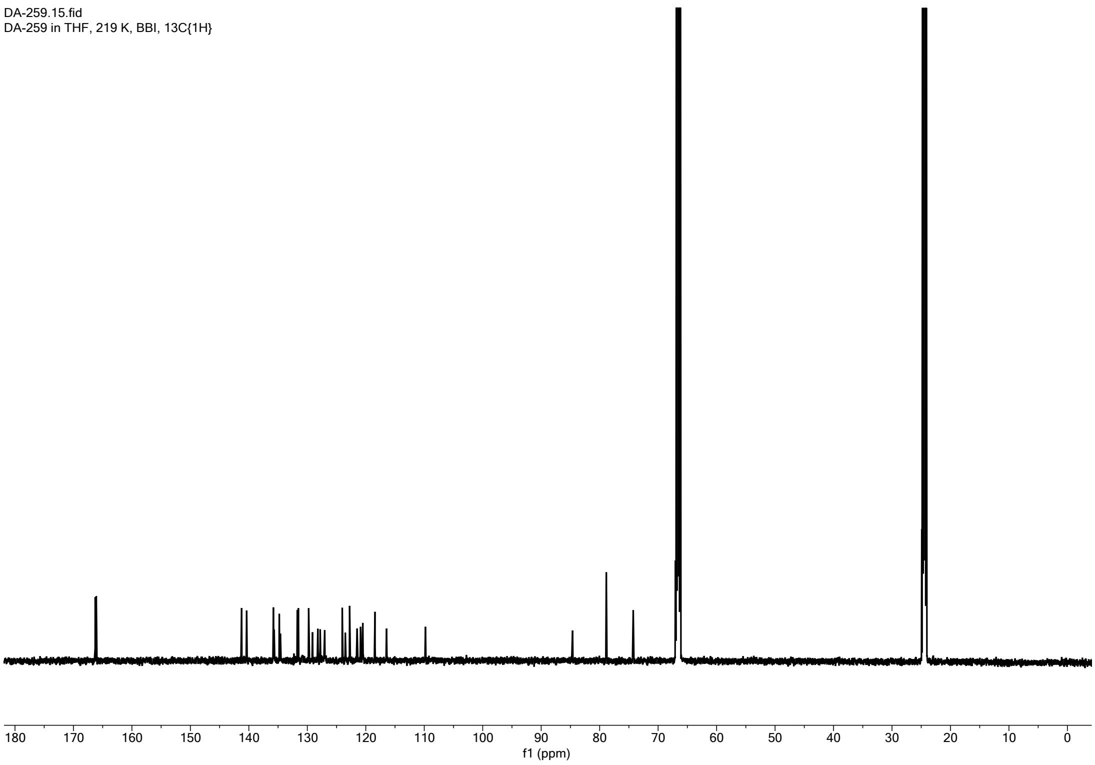


VT-NMR shows coalescence at 265 K for the exchanging protons H-17 and H-19, and at 253 K for protons H-16 and H-20 coalesce. The shift difference $|\nu_A \;\; \nu_B|$ between the exchanging was determined as 109.6 and 22.9 Hz, respectively. The Eyring equation can be rewritten followingly to determine the rotational barrier.[1]

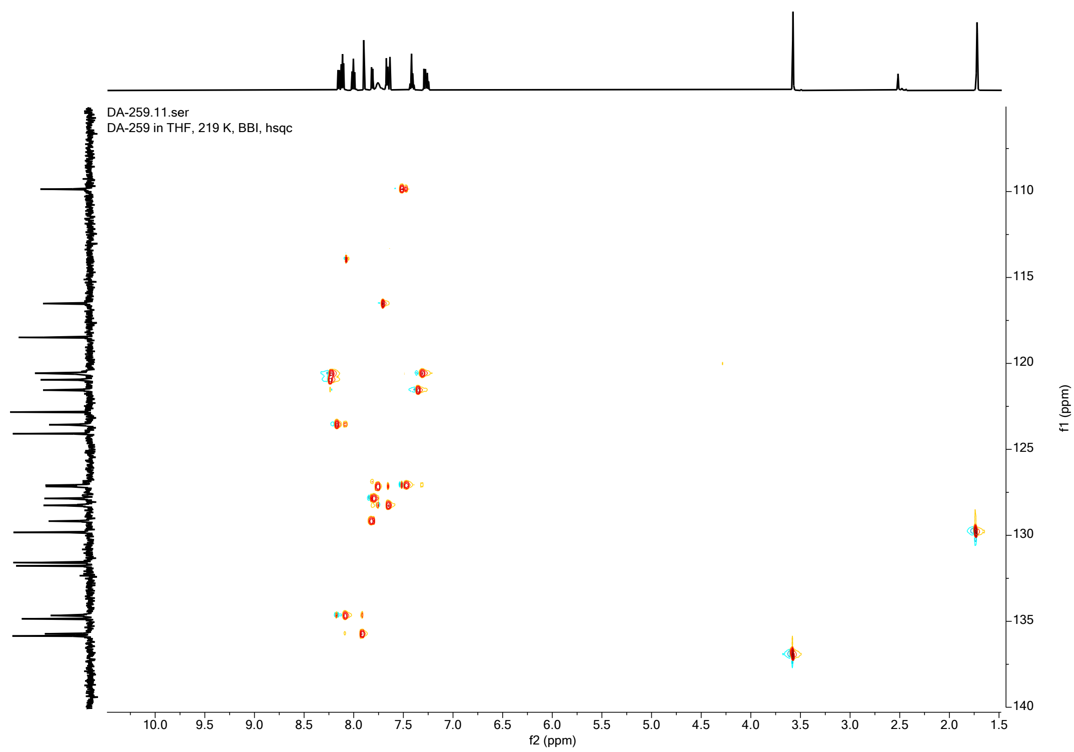
$$\Delta G = RT_c \cdot ln \frac{RT_c\sqrt{2}}{\pi N_A h |\nu_A - \nu_B|}$$

With the above mentioned T_C and shift differences we obtain activation barriers of 52.4 kJ/mol for H-17/19 and 53.2 kJ/mol, or an an averaged rotational barrier of 52.8 kJ/mol. The uncertainty of the activation barrier is estimated to be ±1 kJ/mol.

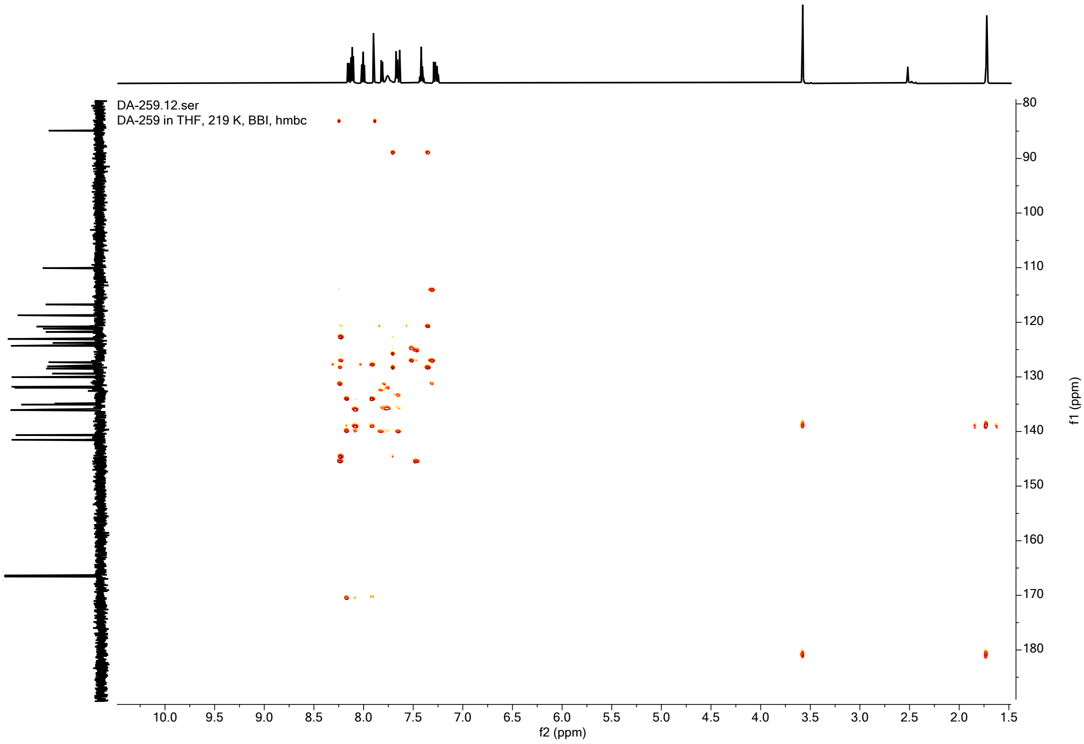
^{13}C NMR (150 MHz, THF-d8): at 219 K



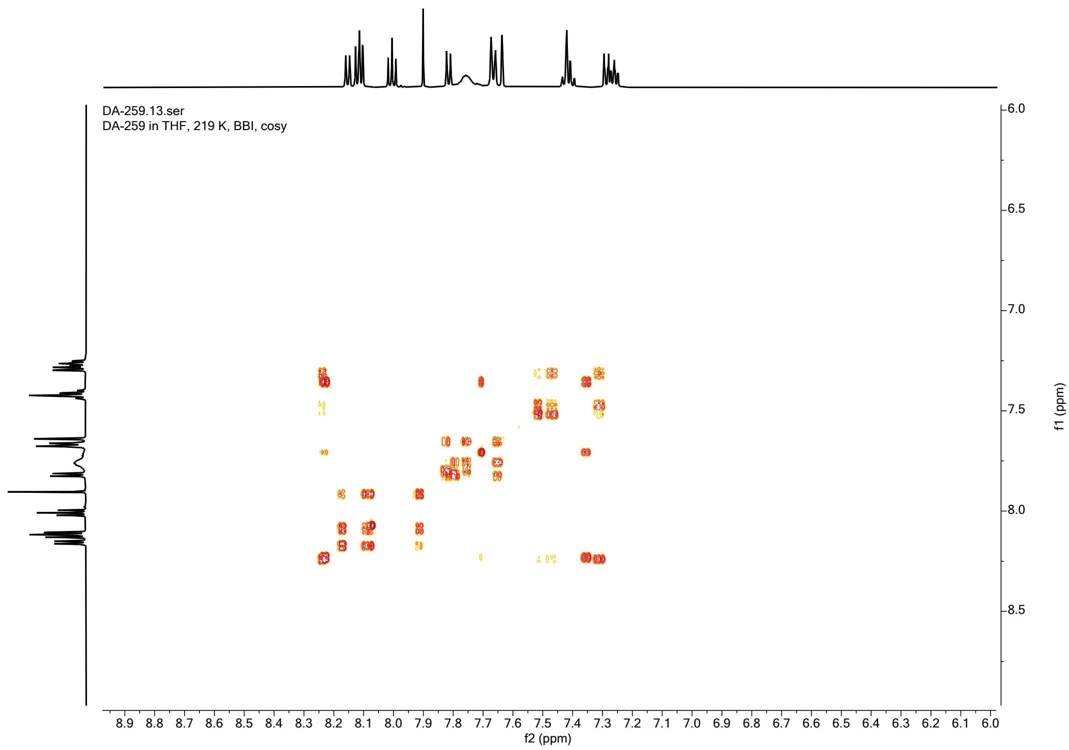
HSQC: at 219 K



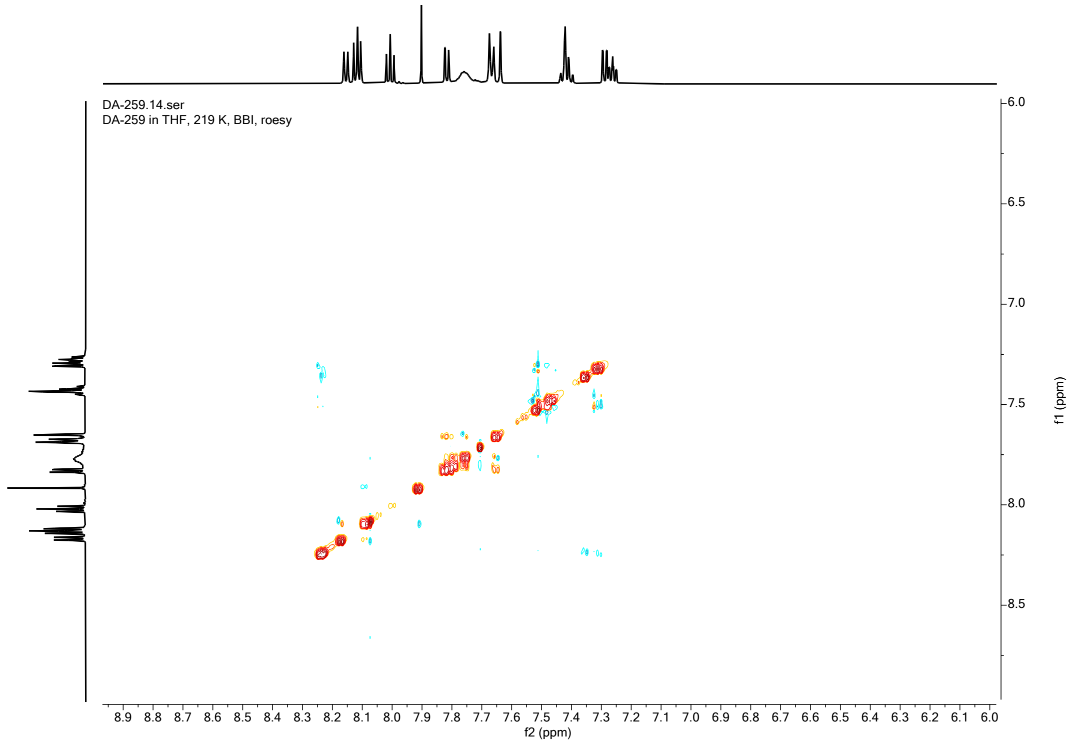
HMBC: at 219 K



COSY: at 219 K

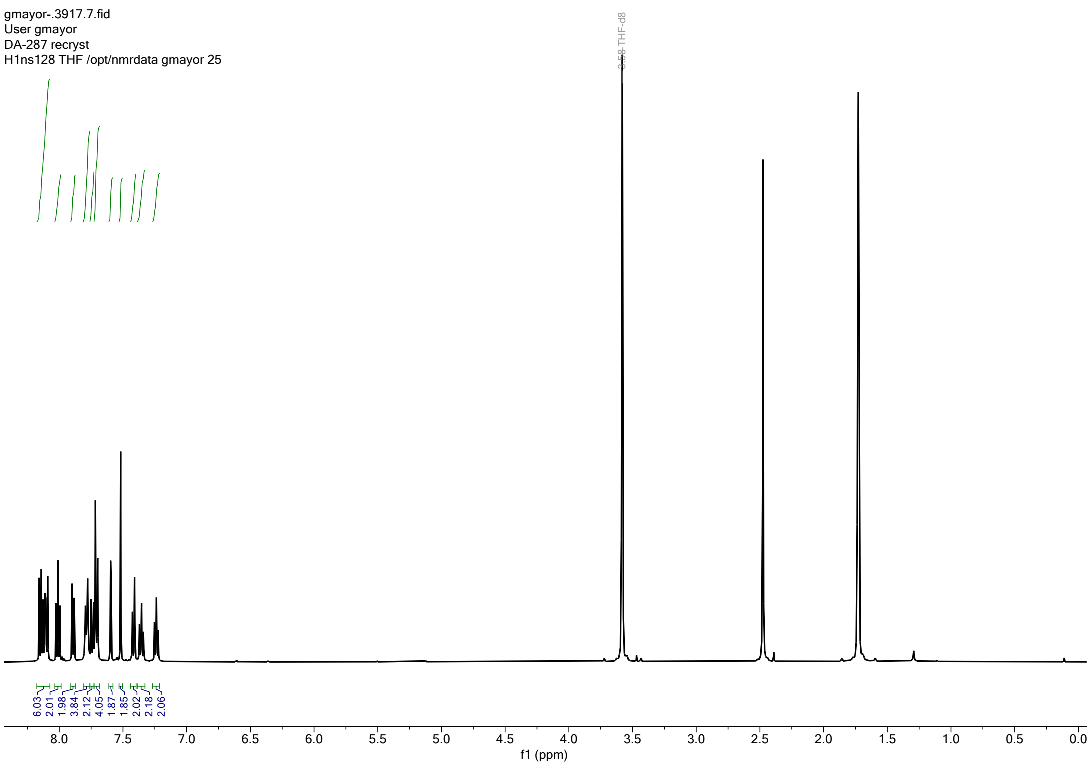


ROESY: at 219 K

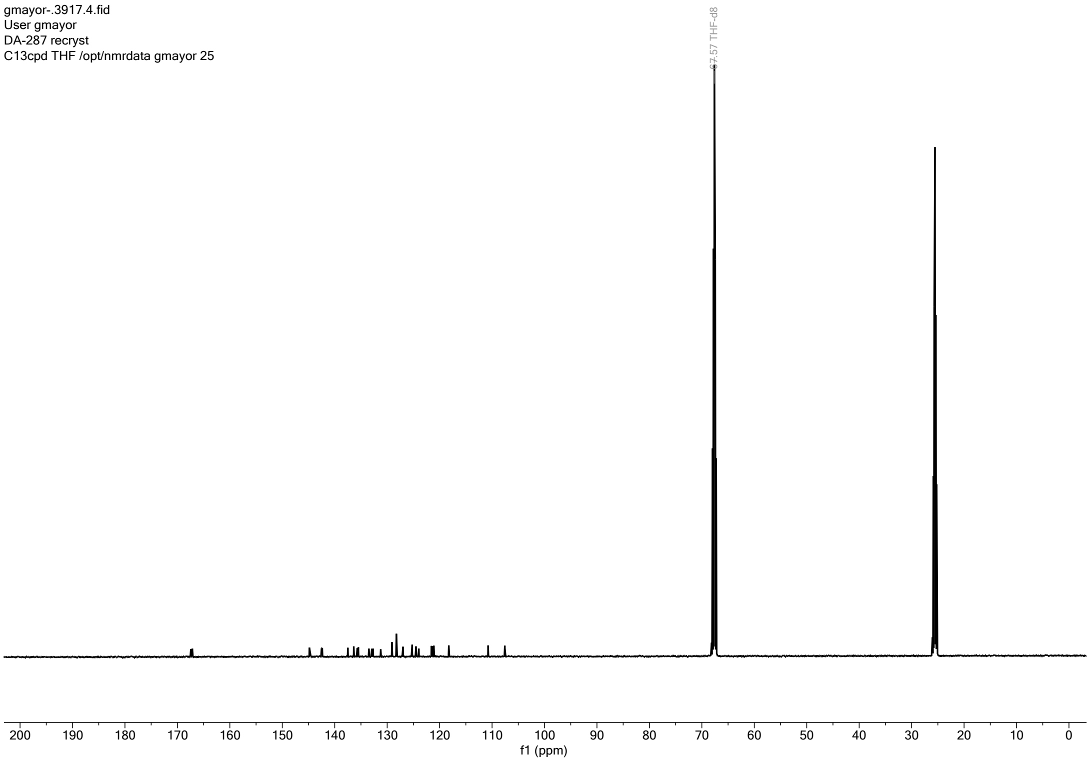


Thiophene macrocycle 1:

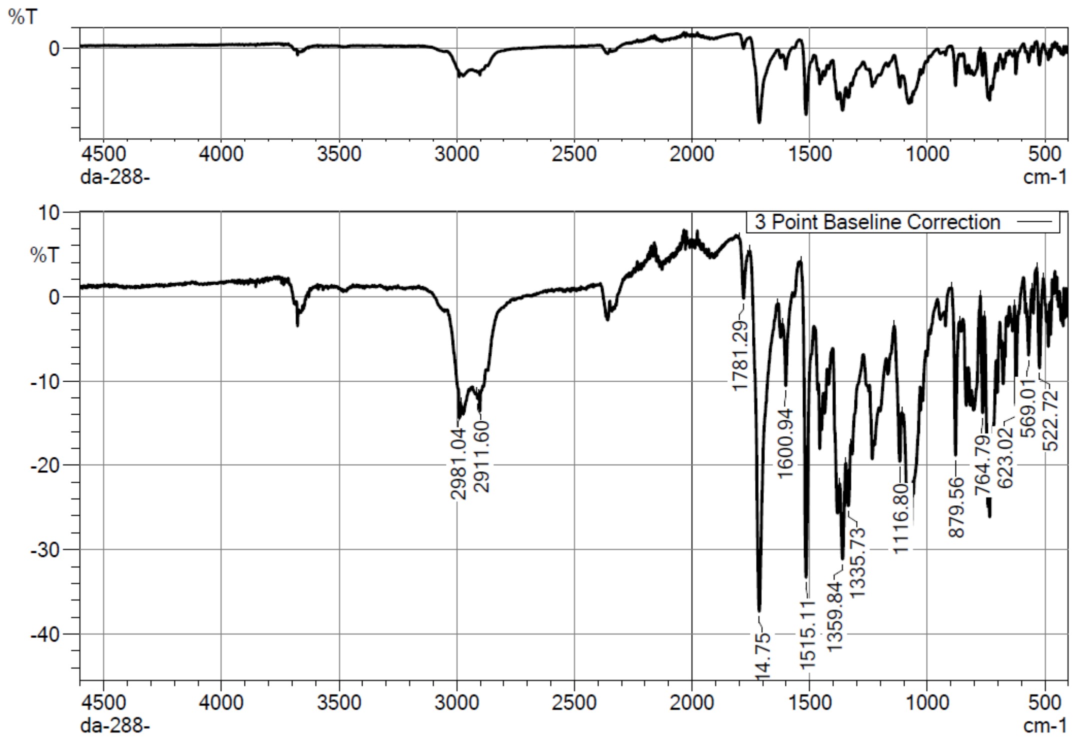
^1H NMR (500 MHz, $CDCl_3$):



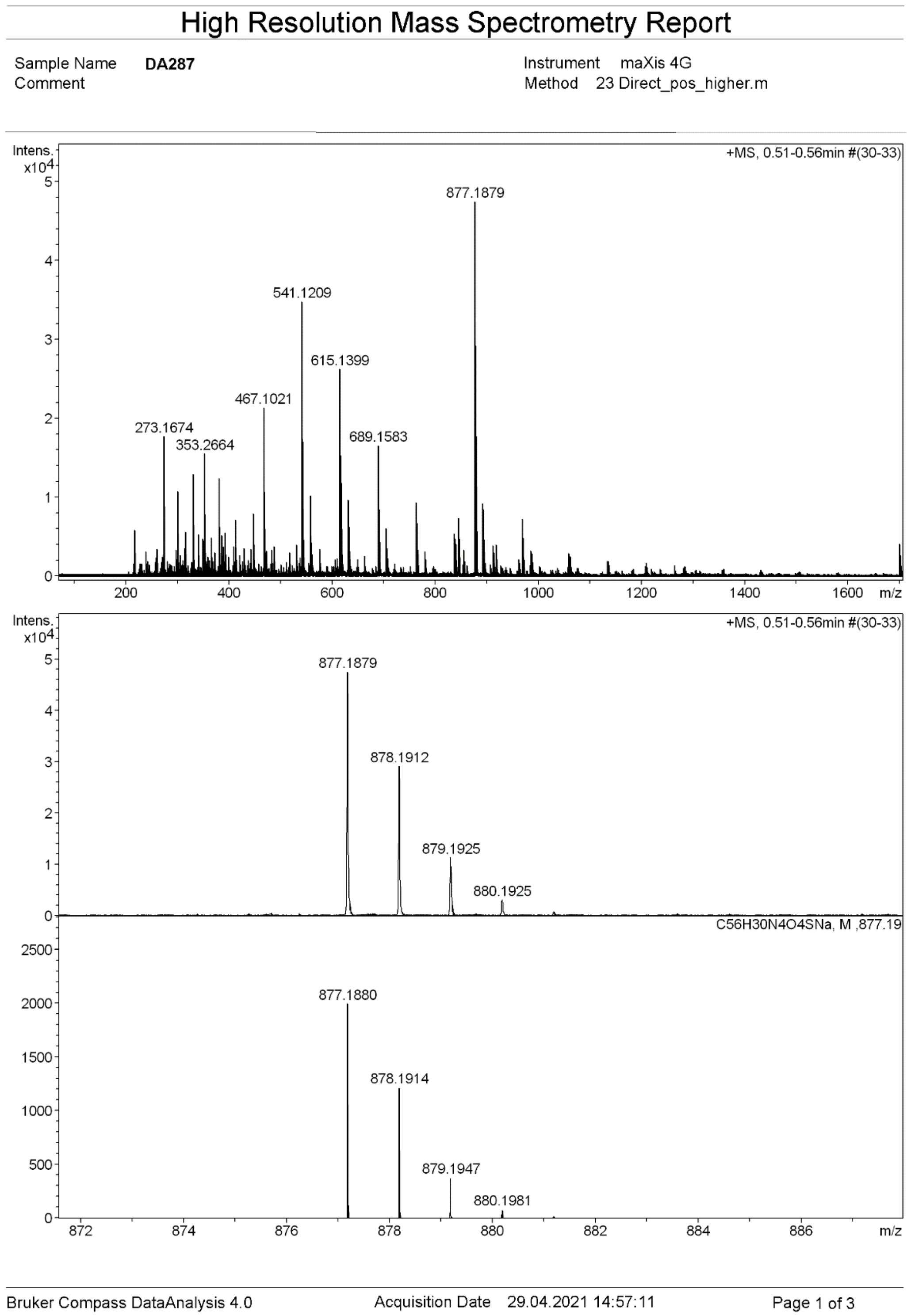
^{13}C NMR (126 MHz, $CDCl_3$):



FT-IR (neat)



HRMS (ESI-ToF):



High Resolution Mass Spectrometry Report
Sample Name DA287
Comment
Instrument maXis 4G
Method 23 Direct_pos_higher.m
Intens. x10^4
+MS, 0.51-0.56min #(30-33)
877.1879
541.1209
615.1399
467.1021
273.1674
353.2664
689.1583
m/z
878.1912
879.1925
880.1925
C56H30N4O4SNa, M ,877.19
877.1880
878.1914
879.1947
880.1981
Bruker Compass DataAnalysis 4.0
Acquisition Date 29.04.2021 14:57:11
Page 1 of 3

High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	z
877.1879	1	C 56 H 30 N 4 Na O 4 S	100.00	877.1880	0.1	0.1	10.3	43.5	even	1+
893.1617	1	C 56 H 30 K N 4 O 4 S	100.00	893.1619	0.2	0.2	57.0	43.5	even	

Mass list

#	m/z	I %	I
1	217.1043	12.3	5867
2	239.0898	6.6	3148
3	261.1309	7.4	3527
4	273.1674	37.4	17771
5	297.2403	7.2	3404
6	301.1411	22.7	10776
7	301.1621	7.9	3767
8	305.1574	5.6	2667
9	313.2349	7.6	3590
10	315.1778	11.9	5641
11	331.2093	27.3	12976
12	341.2664	11.2	5338
13	348.9903	10.1	4819
14	349.1836	5.9	2788
15	350.9872	9.7	4590
16	353.2664	32.8	15596
17	354.2696	6.4	3040
18	365.1059	10.3	4910
19	373.2197	6.5	3075
20	381.2973	26.2	12432
21	382.3008	6.3	3010
22	385.2921	10.9	5198
23	389.2512	8.1	3843
24	393.2975	11.6	5507
25	409.1310	8.1	3830
26	413.2659	15.2	7217
27	421.2321	5.6	2674
28	429.3181	7.4	3536
29	443.3344	7.3	3477
30	447.3443	16.7	7952
31	467.1021	45.1	21429
32	468.1025	17.8	8439
33	469.1003	12.8	6062
34	469.3286	8.8	4158
35	473.3445	6.9	3263
36	483.0756	7.1	3393
37	487.3606	8.1	3829
38	517.3709	6.5	3082
39	531.3869	8.4	3993
40	541.1209	73.3	34835
41	542.1214	36.1	17144
42	543.1196	25.7	12221
43	544.1197	10.0	4728
44	557.0951	21.6	10261
45	558.0952	11.0	5205
46	559.0937	9.1	4337
47	561.3964	5.9	2792
48	575.4128	7.4	3522
49	615.1399	55.3	26273
50	616.1405	32.4	15403
51	617.1382	25.0	11890
52	618.1380	9.6	4551
53	619.4389	6.0	2866
54	631.1136	20.5	9744
55	632.1142	13.3	6336
56	633.1121	11.1	5259
57	663.4658	5.5	2620
58	689.1583	35.0	16631
59	690.1591	23.2	11034
60	691.1572	17.8	8452
61	692.1571	8.7	4125

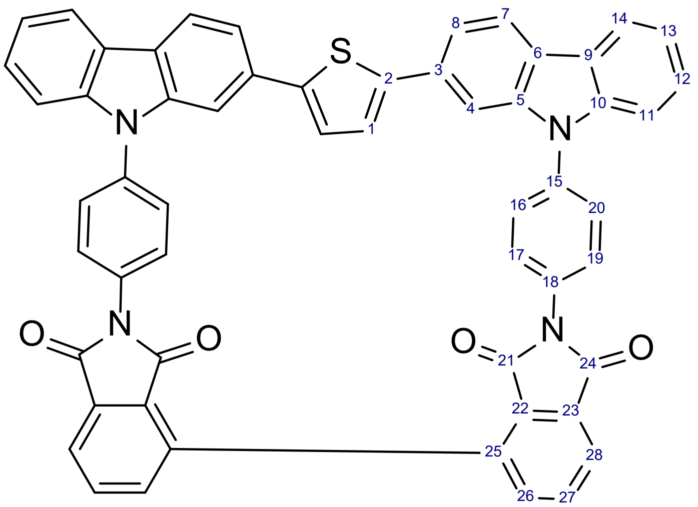
High Resolution Mass Spectrometry Report

#	m/z	I %	I
62	705.1324	12.8	6059
63	706.1327	7.6	3613
64	707.1306	7.5	3551
65	763.1769	19.8	9423
66	764.1783	14.3	6777
67	765.1756	11.4	5403
68	766.1761	6.0	2841
69	779.1505	6.6	3159
70	780.1503	6.2	2962
71	837.1958	11.5	5461
72	838.1967	10.1	4781
73	839.1940	8.7	4147
74	845.2156	15.7	7445
75	846.2195	10.1	4786
76	854.1967	7.1	3351
77	855.2028	7.0	3341
78	877.1879	100.0	47510
79	878.1912	61.5	29195
80	879.1925	24.0	11419
81	880.1925	6.8	3219
82	891.2032	19.6	9295
83	892.2068	11.6	5516
84	893.1617	18.0	8543
85	893.2055	5.6	2651
86	894.1656	11.6	5532
87	895.1963	6.7	3189
88	911.2143	8.2	3895
89	912.2154	7.4	3518
90	913.2127	6.4	3026
91	918.2144	8.4	3992
92	969.2354	15.4	7316
93	970.2383	10.2	4866
94	985.2337	6.8	3242
95	986.2345	5.7	2718
96	987.2323	6.1	2902
97	1059.2540	6.2	2952
98	1699.4165	6.5	3107
99	1700.4181	8.7	4149
100	1701.4197	5.8	2749

Acquisition Parameter

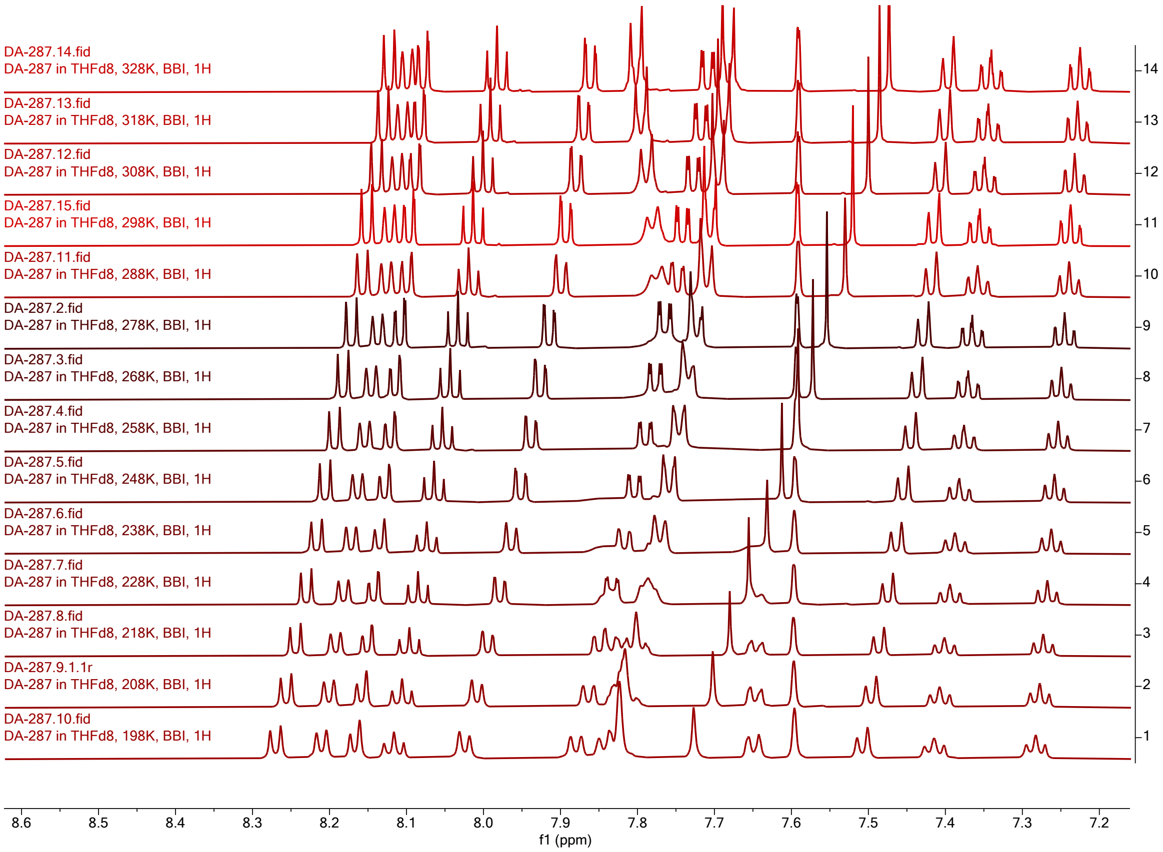
General	Fore Vacuum	2.39e+000 mBar	High Vacuum	1.05e-007 mBar	Source Type	ESI
	Scan Begin	75 m/z	Scan End	1700 m/z	Ion Polarity	Positive
Source	Set Nebulizer	0.4 Bar	Set Capillary	3600 V	Set Dry Gas	4.0 l/min
	Set Dry Heater	180 °C	Set End Plate Offset	-500 V		
Quadrupole	Set Ion Energy (MS only)	4.0 eV				
Coll. Cell	Collision Energy	8.0 eV	Set Collision Cell RF	500.0 Vpp	100.0 Vpp	
Ion Cooler	Set Ion Cooler Transfer Time	100.0 µs	Set Ion Cooler Pre Pulse Storage Time	18.0 µs		

Complete Assignment at 218 K:



Nr	^1H [ppm]	^{13}C [ppm]	Nr	^1H [ppm]	^{13}C [ppm]
1	7.69	125.3	15		137.2
2	-	144.3	16	7.81	128.17
3	-	133.1	17	7.85	130.3
4	7.61	107.0	18	-	132.1
5	-	141.8	19	7.65	129.5
6	-	123.6	20	7.82	128.20
7	8.25	121.8	21	-	167.4
8	7.85	118.1	22	-	131.1
9	-	124.1	23	-	132.7
10	-	142.0	24	-	167.2
11	7.50	110.8	25	-	135.3
12	7.40	127.1	26	8.01	136.2
13	7.29	121.4	27	8.11	135.7
14	8.20	121.3	28	8.16	124.2

VT-^{1}H NMR (600 MHz, THF-d8):



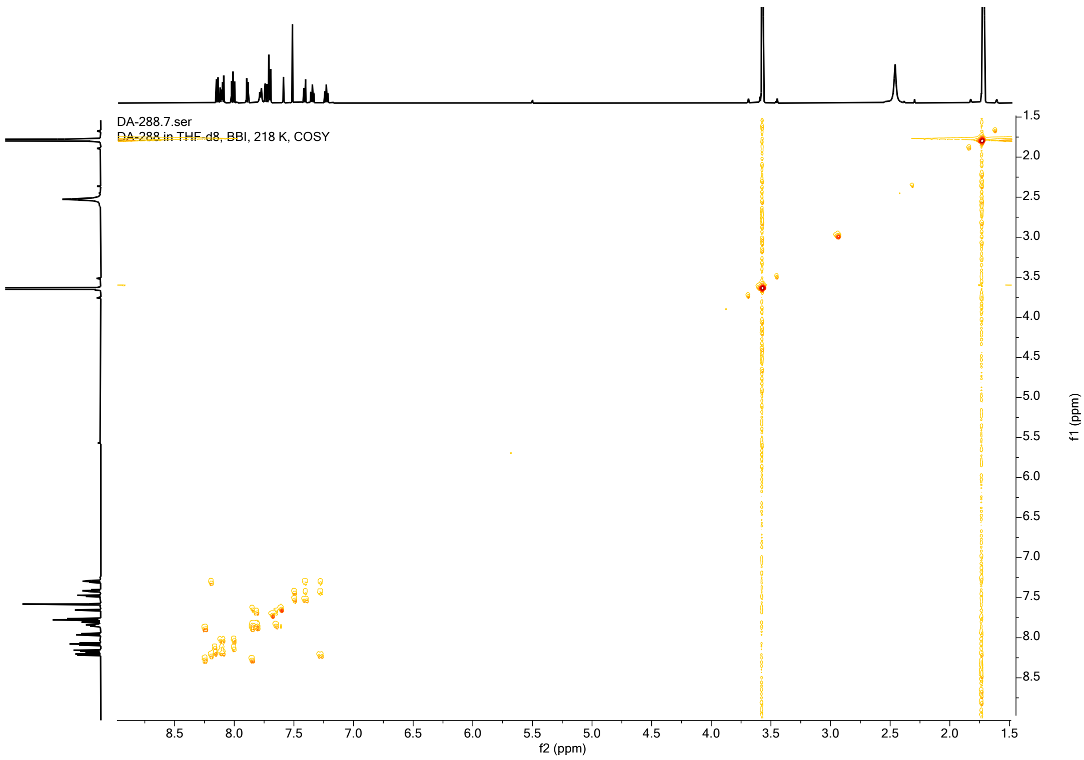
VT-NMR shows coalescence of protons H-17 and H-19 at 263 K. Unfortunately the protons H-16 and H-20 experience different temperature shifts, resulting in accidental isochrony, thus, preventing further analysis. The chemical shift difference for H-17 and H-19 was determined as 120.8 Hz.

The Eyring equation can be rewritten followingly to determine the rotational barrier[1]

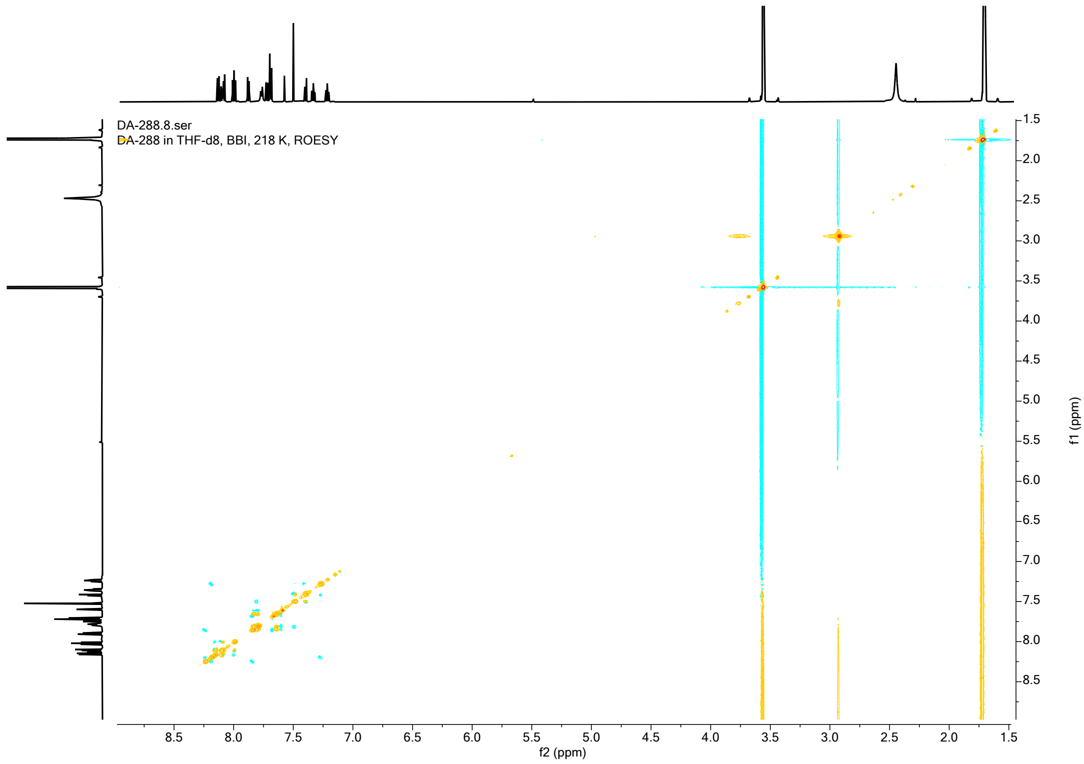
$$\Delta G = RT_c \cdot ln\frac{RT_c\sqrt{2}}{\pi N_A h|\nu_A - \nu_B|}$$

With T_C = 263 K ΔG the rotational barrier is determined as 51.8 kJ/mol. The uncertainty of the activation barrier is estimated to be ±1 kJ/mol.

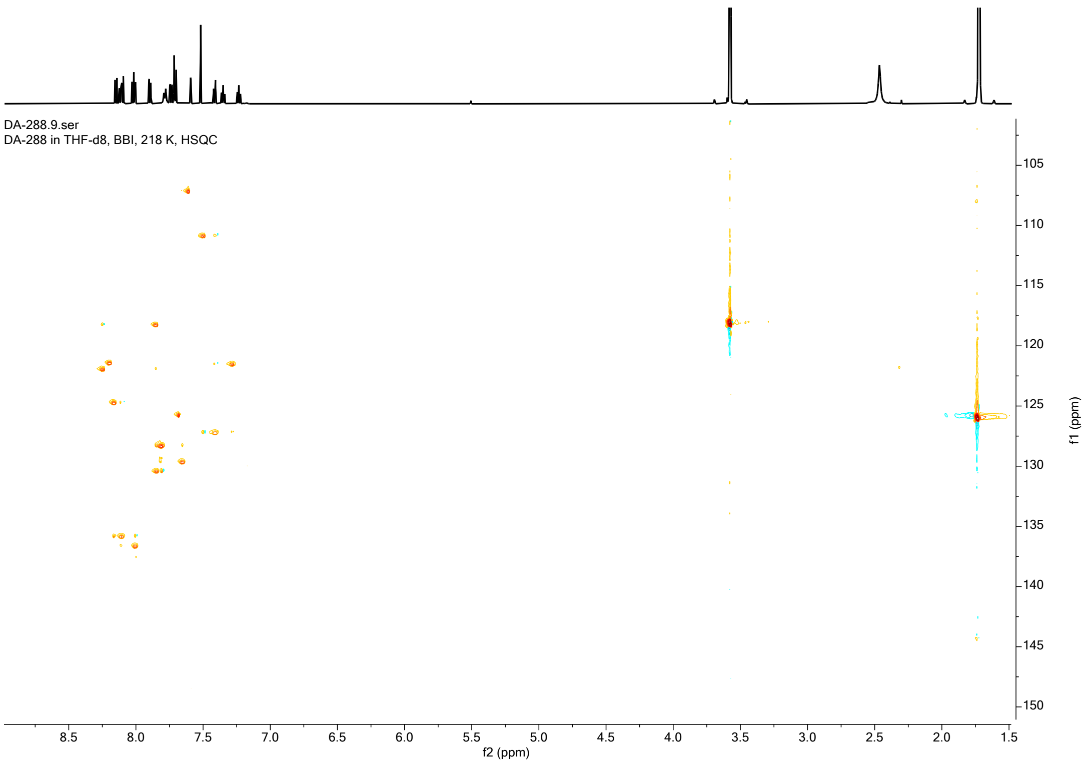
COSY: at 218 K



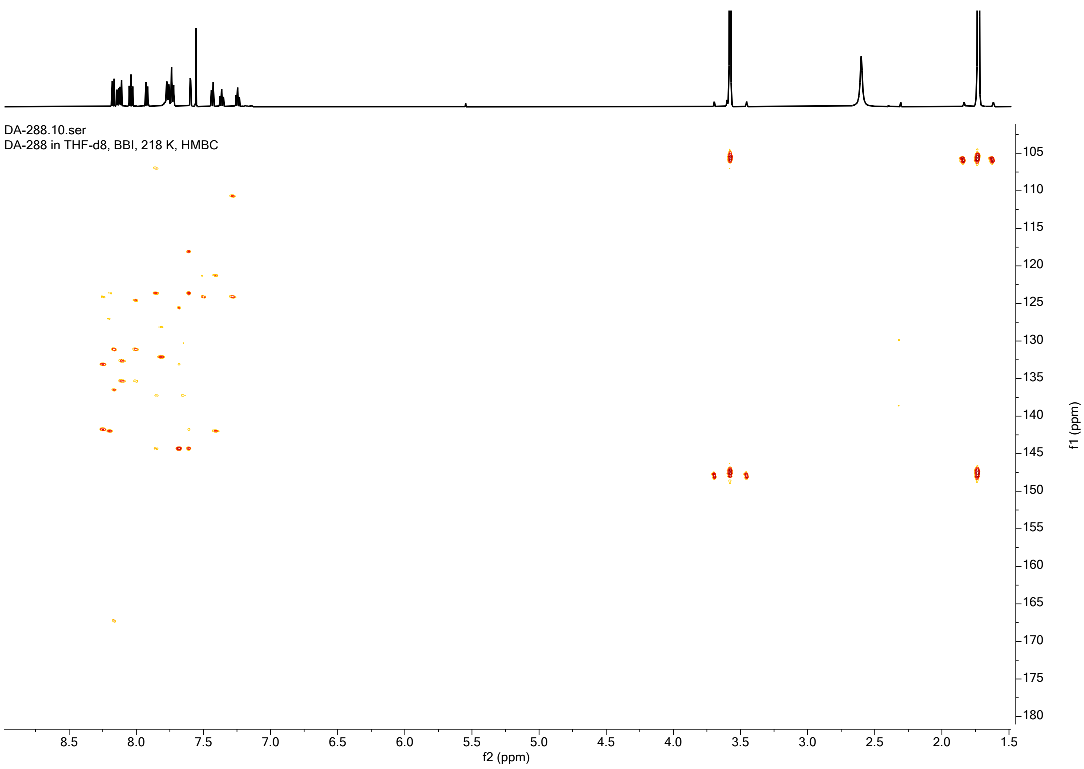
ROESY: at 218 K



HSQC: at 218 K



HMBC: at 218 K



Calculations and Structure Analysis

Geometry Optimization and Conformer Analysis

Optimization, frequency analysis and TD-DFT calculations were preformed using Gaussian 09 (E.01)[2], automated conformational analysis was carried out using CREST[3] and the obtained structures submitted again to DFT optimization. For geometry optimization coordinates of (*P)*-**2** was extracted from the crystalstructure of (*rac)*-**2**. The initial guess for (*P)*-**1** was modeled from the optimized structure of *(P)*-**2**.

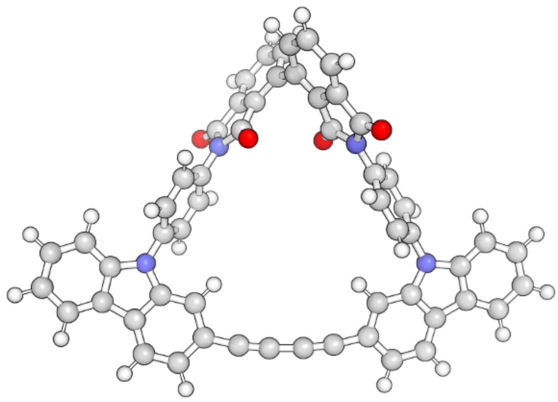


Figure S6. Optimized Geometry of (*P*)-**2** calculated with B3LYP/6311G* level of theory.

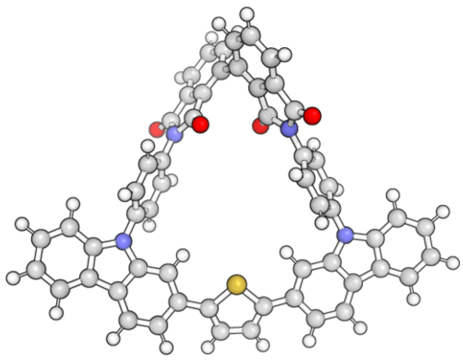


Figure S7. Optimized geometry of (*P*)-**1** calculated with B3LYP/6311G* level of theory.

For both macrocycles automated conformation analysis was carried out within a 6 kcal/mol energy-window using CREST and yielded five conformers. Optimization on the same level as the initial guess reduced the ensemble to three conformers for (*P*)-**2** and four for (*P*)-**1**.

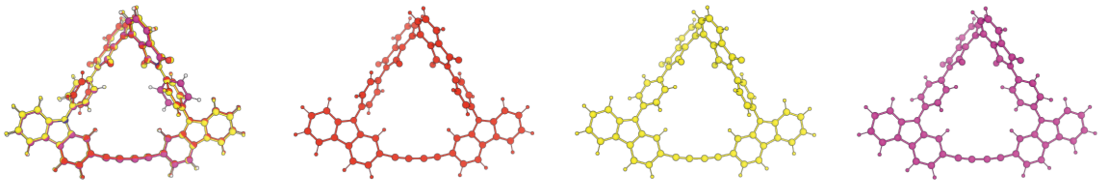


Figure S8. Optimized conformers of *(P)*-**2** at the level of B3LYP/6311G(d,p), left all conformers overlapped, red conformer 1, yellow conformer 2, magenta conformer 3. Conformer 4 and 2 as well as conformer 5 and 1 from CREST converged to the same structure respectively.

Table S1. Boltzmann distribution of (*P*)-**2**

Conformer	*SP E [Hartree]*	*ZPC [Hartree]*	*corr E [Hartree]*	*Thermal corrections [Hartree]*	*G [Hartree]*	$p_i = e^{\frac{G_i - G_1}{kT}}$	$\frac{p_i}{p_{tot}}$	$\frac{p_i}{p_{tot}} * 100$
1	-2670.770101	0.683216	-2670.086885	0.601458	-2670.168643	1	0.967327278	96.73
2	-2670.767768	0.683657	-2670.084111	0.602331	-2670.165437	0.033523056	0.032427767	3.24
3	-2670.764627	0.684234	-2670.080393	0.603803	-2670.160824	0.000253229	0.000244955	0.02

The conformers of (*P*)-**2** vary in the orientation of the benzene bridge with a large population (96.73%) of the first conformer.

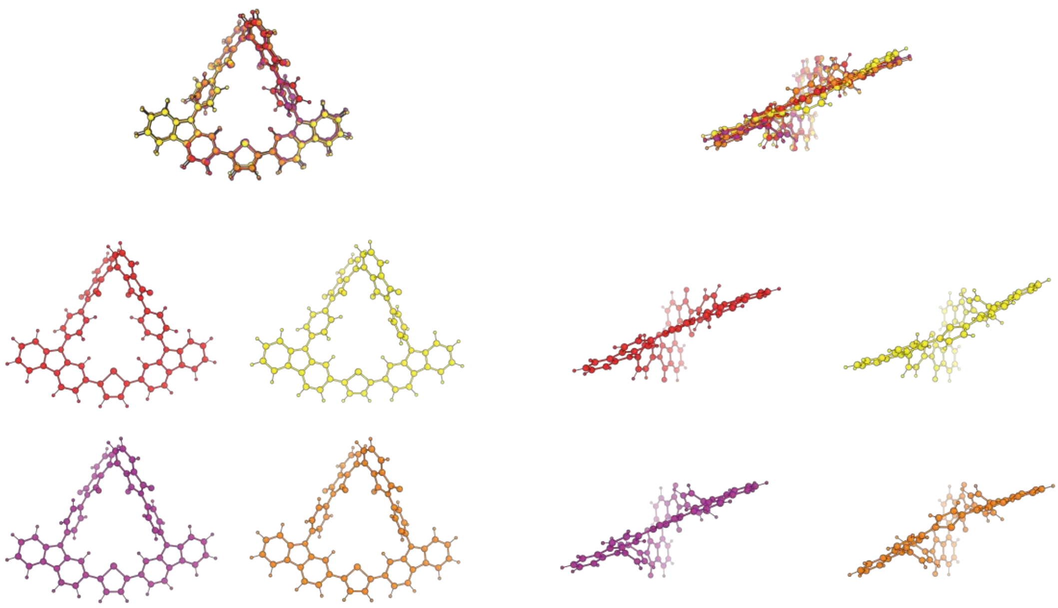


Figure S9. Optimized conformers of *(P)*-**1** at the level of B3LYP/6311G(d,p), left topview, right frontview, top overlayd geometries, red conformer 1, magenta conformer 2, yellow conformer 3, and orange conformer 5. Conformer 4 from CREST converged to the same geometry than conformer 2.

Table S2. Boltzmann distribution of *(P)*-**1**

Conformer	*SP E [Hartree]*	*ZPC [Hartree]*	*Corr E [Hartree]*	*Thermal corrections [Hartree]*	*G [Hartree]*	$p_i = e^{\frac{G_i - G_1}{kT}}$	$\frac{p_i}{p_{tot}}$	$\frac{p_i}{p_{tot}} * 100$
1	-3070.262991	0.710579	-3069.552412	0.62904	-3069.633951	0.000987	0.000479259	0.047926
2	-3070.266079	0.710131	-3069.555948	0.628256	-3069.637823	0.059581	0.028944461	2.894446
3	-3070.267977	0.709726	-3069.558251	0.627493	-3069.640484	0.997884	0.484774165	48.47742
5	-3070.267978	0.709726	-3069.558252	0.627492	-3069.640486	1	0.485802116	48.58021

The conformers of (*P)*-**1** vary in the orientation of the benzene bridge and in the orientation of the thiophene with a large population of 48.58% and 48.48% of the conformer 5 and 2, respectively. Rotation around the backbone (C_2 symmetry operation) shows that conformers 5 and 3 are very similar with only minute differences.

TD-DFT:

Vertical singlet transitions where calculated, for all the conformers of *(P)*-**1** found, at the TD-B3LYP/ 6311G(d,p) level of theory, the Polarizable Continuum Model was used to take the effects of acetonitrile into account. SpecDis 1.71 was used to extract the transitions and fit the calculated data.[4,5] Only conformers with significant population (above 5% were taken into account). The minute difference between conformers 3 and 5 did not yield in different computed transitions.

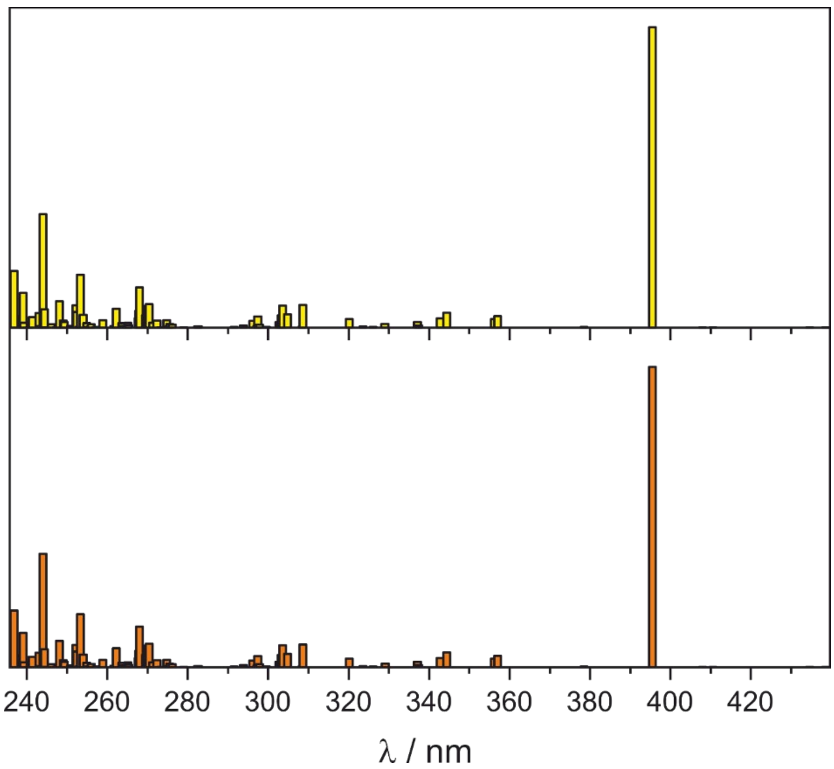


Figure S9. Computed transitions as bar plot at TD-B3LYP/6-311G(d,p) level of theory. In yellow conformer 3 is depicted and in orangege conformer 5 of (*P*)-**1**.

X-Ray Structure and Optimized Geometries

Crystals of (*rac)*-**2** were obtained by slow vapor diffusion of n-hexane into a solution of $CHCl_3$.

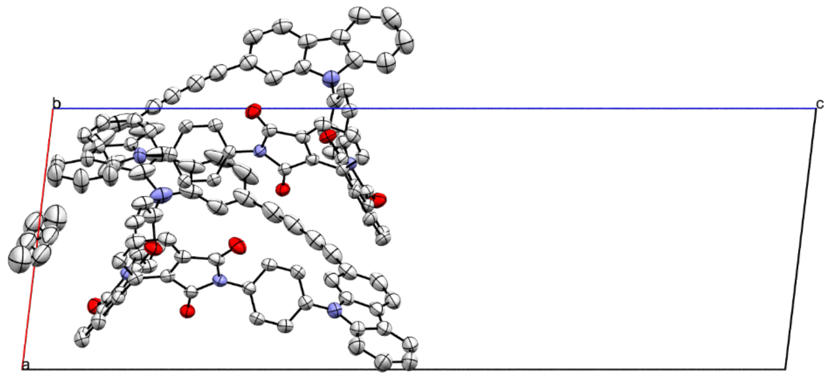


Figure S10. Unit cell of the crystal of rac-**2** obtained from slow diffusion of hexane to a solution of *rac*-**2** in chloroform. Visualized in the ORTEP representation with 50% probability. Hydrogens are omitted for clarity.

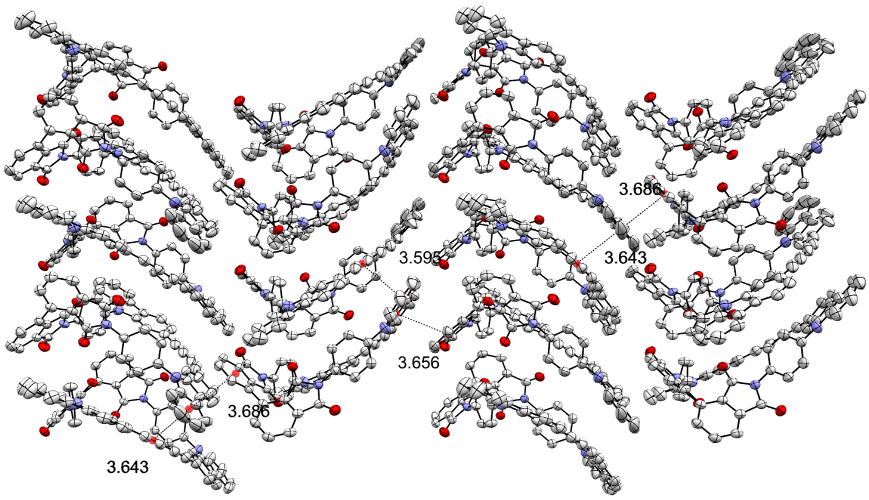


Figure S11. Herringbone-type packing of the crystal of rac-**2** obtained from slow diffusion of hexane to a solution of *rac*-**2** in chloroform. Close contacts which indicate weak π-π interaction are illustrated.

Mercury 2021.3.0 was used to measure the angles in the modeled structures of (*P*)-**1** and (*P*)-**2** as well as (*P*)-**2** extracted from the solid state structure above. Four centroids (dummy atoms) were calculated as pivots for measuring the angle between the rung and axis (α), the rung and bannister (β), and as anchors for measuring the dihedral angle ϕ_a. The pivot to measure α was calculated as center point of benzene ring in the phthalimide subunit. For β the pivot was determined as the middle point of the axis from C2 to C7 in a carbazole subunit. For ϕ_a the centroids of the 7 membered scaffold of the individual phthalimides found in the axis were calculated. The dihedral angle was measured from these centroids over the CC bond connecting the phtahlimides units.Two different dihedral angles ϕ_i are found between rung and axis, the angles are measured from either C1 or C3 over N2 in the phthalimide subunit to the directly bond carbon and the closest C-*ortho*. As each dihedral angle exist twice we report the outer ϕ_1 and inner ϕ_2 as average in the main text. The same is found between rung and banister, with the dihedral angles span by either C8a or C9a over N9 to the bonded quaternary C of the rung and the closest C-*ortho*. As each dihedral angle exist twice we report the outer ϕ_3 and inner ϕ_4 as average in the main text.

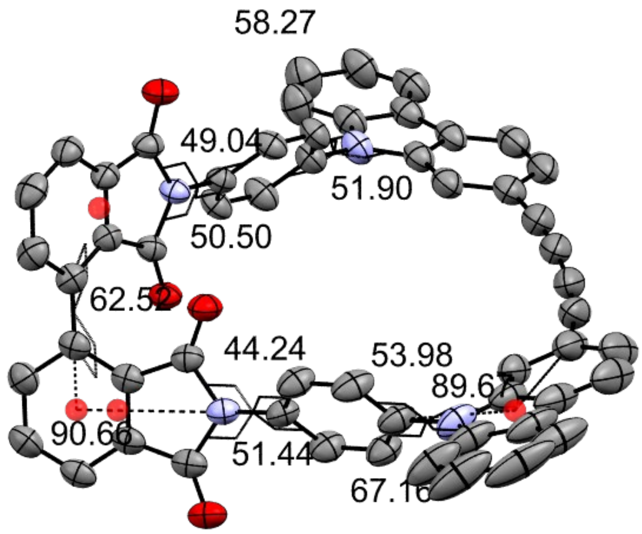


Figure S12. ORTEP representation of (*P*)-**2** with the discussed angles, (*M*)-**2** and solvents are omitted for clarity. Centroids are visualized as red spheres.

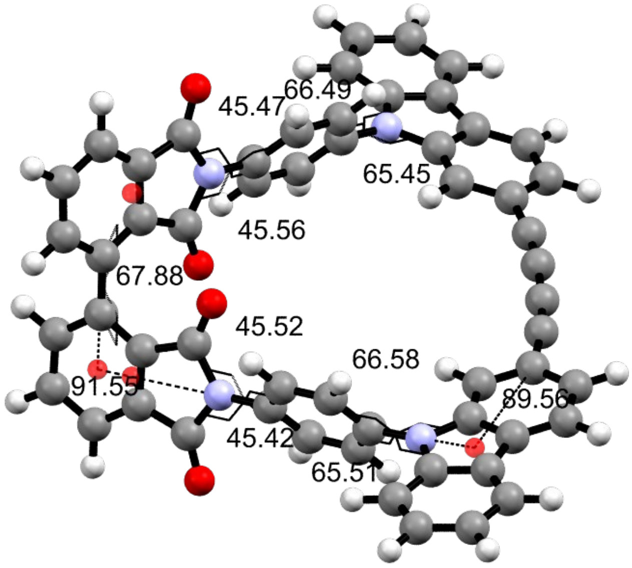


Figure S13. Optimized geomertry of (*P*)-**2** visualized in Mercury with the discussed angles. Centroids are visualized as red spheres.

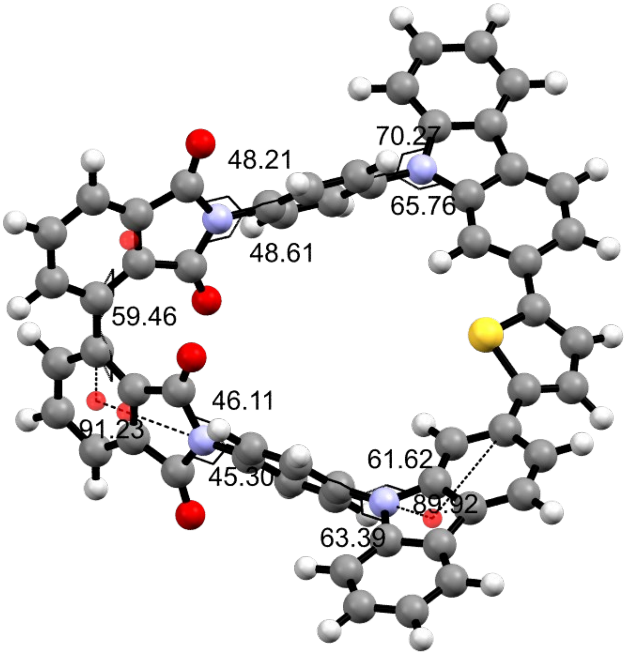


Figure S14. Optimized geomertry of (*P*)-**1** visualized in Mercury with the discussed angles. Centroids are visualized as red spheres.

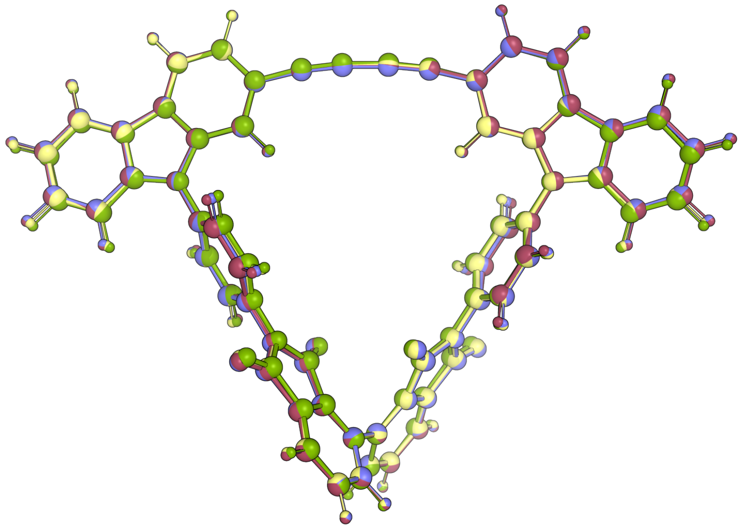


Figure S15. Optimized geomertry of (*P*)-**2** calculated with different functionals and basis-sets all staggered over each other. Red: B3LYP/cc-pVDZ. Green: M06-2X/6311G**. Blue: B3LYP/631G**. Yellow: wB97xd/6311G**.

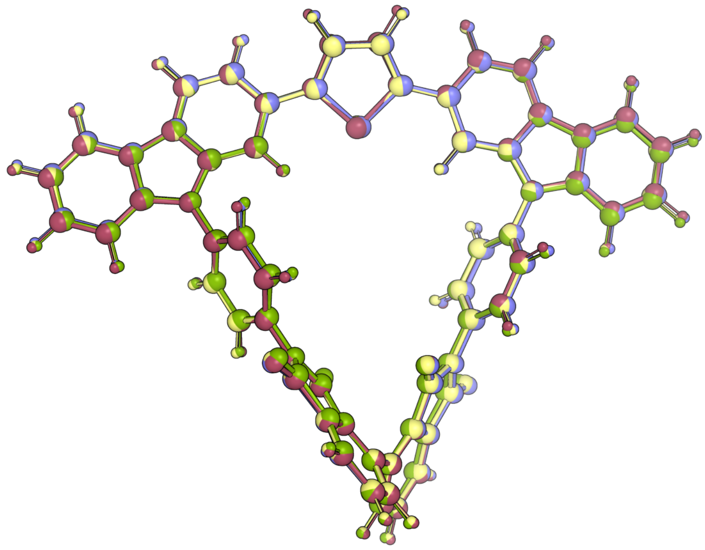


Figure S16. Optimized geomertry of (*P*)-**1** calculated with different functionals and basis-sets all staggered over each other. Red: B3LYP/cc-pVDZ. Green: M06-2X/6311G**. Blue: B3LYP/631G**. Yellow: wB97xd/6311G**

Cartesians

Energies are reported in kcal/mol.

Macrocycle **2**

92

da-276-P-6311.out Energy: -1676279.7370661

O	1.48606	3.01066	-0.80796
O	3.56890	3.19658	3.29514
O	-1.48678	3.01085	0.80811
O	-3.56889	3.19625	-3.29536
N	2.72146	2.78220	1.15662
N	5.56358	-1.92368	-0.10581
N	-5.56346	-1.92404	0.10546
N	-2.72174	2.78212	-1.15670
C	1.77795	3.39751	0.29543
C	1.27407	4.59511	1.03399
C	0.35825	5.57582	0.65264
C	0.14801	6.62165	1.56701
H	-0.56031	7.40282	1.31136
C	0.80230	6.67114	2.79939
H	0.59723	7.49426	3.47540
C	1.70810	5.67581	3.16876
H	2.22662	5.69483	4.12045
C	1.92617	4.65364	2.26096
C	2.84941	3.49157	2.37474
C	3.45230	1.60036	0.83804
C	4.05412	1.46291	-0.41497
H	3.95302	2.24702	-1.15340
C	4.75286	0.30165	-0.72559
H	5.19609	0.17889	-1.70732
C	4.87530	-0.71987	0.21794
C	4.28895	-0.56933	1.47618
H	4.39216	-1.35908	2.21152
C	3.57036	0.57954	1.78370
H	3.11683	0.68967	2.75949
C	6.92702	-2.06089	-0.37091
C	7.93077	-1.09229	-0.36510
H	7.71095	-0.05579	-0.13583
C	9.22665	-1.50334	-0.65753
H	10.02601	-0.76934	-0.65962
C	9.52194	-2.84521	-0.94585
H	10.54401	-3.13112	-1.17061
C	8.52031	-3.80729	-0.94211
H	8.75504	-4.84453	-1.15970
C	7.20681	-3.42342	-0.65204
C	4.96458	-3.17873	-0.21989
C	5.95371	-4.13731	-0.55512
C	5.57132	-5.47255	-0.73206
H	6.30897	-6.22685	-0.98659
C	4.24002	-5.83010	-0.58948
H	3.93286	-6.85999	-0.72875
C	3.25693	-4.86073	-0.27276
C	3.62659	-3.51815	-0.08281
H	2.87279	-2.77749	0.15223
C	1.88156	-5.18757	-0.15965
C	0.67548	-5.30798	-0.05564
C	-0.67510	-5.30805	0.05536
C	-1.88120	-5.18770	0.15929
C	-4.96436	-3.17907	0.21948
C	-3.62639	-3.51845	0.08222
H	-2.87263	-2.77781	-0.15299
C	-3.25660	-4.86097	0.27237
C	-4.23958	-5.83035	0.58938
H	-3.93234	-6.86020	0.72886
C	-5.57087	-5.47284	0.73216
H	-6.30843	-6.22713	0.98700
C	-5.95336	-4.13765	0.55509
C	-6.92681	-2.06129	0.37110
C	-7.20645	-3.42381	0.65240
C	-8.51983	-3.80774	0.94287
H	-8.75446	-4.84500	1.16051
C	-9.52152	-2.84572	0.94688
H	-10.54350	-3.13170	1.17195
C	-9.22640	-1.50386	0.65839
H	-10.02579	-0.76989	0.66072
C	-7.93063	-1.09275	0.36553
H	-7.71098	-0.05627	0.13604
C	-4.87529	-0.72019	-0.21822
C	-4.75409	0.30189	0.72489
H	-5.19816	0.17948	1.70630
C	-4.05544	1.46321	0.41432
H	-3.95532	2.24776	1.15242
C	-3.45249	1.60021	-0.83819
C	-3.56931	0.57887	-1.78343
H	-3.11489	0.68867	-2.75884
C	-4.28782	-0.57008	-1.47599
H	-4.39016	-1.36019	-2.21108
C	-1.77859	3.39765	-0.29531
C	-1.27455	4.59515	-1.03394
C	-0.35870	5.57585	-0.65261
C	-0.14841	6.62164	-1.56699
H	0.55991	7.40281	-1.31133
C	-0.80265	6.67111	-2.79941
H	-0.59755	7.49423	-3.47541
C	-1.70840	5.67575	-3.16880
H	-2.22683	5.69467	-4.12055
C	-1.92653	4.65362	-2.26097
C	-2.84950	3.49134	-2.37491

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da276-P-prop1.out Energy: -1676310.9479878

O	-1.48709	3.01139	0.80895
O	-3.56719	3.19465	-3.29580
O	1.48710	3.01139	-0.80896
O	3.56719	3.19465	3.29580
N	-2.72155	2.78129	-1.15623
N	-5.56406	-1.92283	0.10774
N	5.56406	-1.92284	-0.10774
N	2.72155	2.78129	1.15623
C	-1.77852	3.39715	-0.29504
C	-1.27374	4.59397	-1.03411
C	-0.35800	5.57471	-0.65295
C	-0.14620	6.61952	-1.56801
H	0.56124	7.40008	-1.31202
C	-0.79968	6.66811	-2.80071
H	-0.59381	7.48988	-3.47658
C	-1.70565	5.67310	-3.17023
H	-2.22328	5.69103	-4.12134
C	-1.92483	4.65208	-2.26154
C	-2.84826	3.48994	-2.37503
C	-3.45306	1.59983	-0.83718
C	-4.04364	1.45821	0.42065
H	-3.93200	2.23786	1.16092
C	-4.74229	0.29716	0.73163
H	-5.17747	0.17025	1.71540
C	-4.87591	-0.71852	-0.21640
C	-4.30137	-0.56349	-1.47934
H	-4.41330	-1.34911	-2.21649
C	-3.58228	0.58472	-1.78744
H	-3.13841	0.70053	-2.76601
C	-6.92751	-2.06073	0.37156
C	-7.93142	-1.09243	0.36547
H	-7.71101	-0.05686	0.13769
C	-9.22711	-1.50453	0.65704

H	-10.02624	-0.77191	0.65927
C	-9.52187	-2.84660	0.94452
H	-10.54299	-3.13243	1.16812
C	-8.52001	-3.80842	0.94114
H	-8.75328	-4.84494	1.15798
C	-7.20676	-3.42349	0.65209
C	-4.96434	-3.17734	0.22176
C	-5.95313	-4.13666	0.55592
C	-5.57069	-5.47180	0.73233
H	-6.30812	-6.22511	0.98567
C	-4.23924	-5.82863	0.58991
H	-3.93089	-6.85714	0.72832
C	-3.25684	-4.85839	0.27401
C	-3.62610	-3.51568	0.08492
H	-2.87337	-2.77535	-0.15006
C	-1.88129	-5.18506	0.16042
C	-0.67527	-5.30572	0.05585
C	0.67527	-5.30572	-0.05586
C	1.88128	-5.18505	-0.16043
C	4.96434	-3.17734	-0.22176
C	3.62609	-3.51568	-0.08492
H	2.87337	-2.77535	0.15005
C	3.25683	-4.85839	-0.27401
C	4.23923	-5.82863	-0.58991
H	3.93088	-6.85714	-0.72832
C	5.57069	-5.47181	-0.73233
H	6.30811	-6.22511	-0.98566
C	5.95313	-4.13666	-0.55592
C	6.92751	-2.06073	-0.37156
C	7.20676	-3.42350	-0.65209
C	8.52001	-3.80843	-0.94113
H	8.75328	-4.84495	-1.15798
C	9.52187	-2.84661	-0.94452
H	10.54299	-3.13244	-1.16812
C	9.22711	-1.50454	-0.65704
H	10.02624	-0.77192	-0.65927
C	7.93143	-1.09244	-0.36547
H	7.71101	-0.05686	-0.13770
C	4.87591	-0.71852	0.21640
C	4.74229	0.29716	-0.73163
H	5.17747	0.17025	-1.71540
C	4.04364	1.45821	-0.42065
H	3.93200	2.23786	-1.16092
C	3.45307	1.59983	0.83718
C	3.58228	0.58472	1.78744
H	3.13841	0.70054	2.76601
C	4.30137	-0.56349	1.47934
H	4.41331	-1.34911	2.21649
C	1.77852	3.39715	0.29504
C	1.27374	4.59397	1.03411
C	0.35800	5.57471	0.65295
C	0.14620	6.61952	1.56801
H	-0.56124	7.40008	1.31202
C	0.79968	6.66810	2.80071
H	0.59381	7.48987	3.47658
C	1.70565	5.67310	3.17023
H	2.22328	5.69103	4.12134
C	1.92483	4.65208	2.26154
C	2.84827	3.48994	2.37503

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da276-P-prop2.out Energy: -1676310.0324138

O	1.49658	2.97146	-0.79848
O	3.62900	3.19368	3.27639
O	-1.49284	3.17458	0.86795
O	-3.43906	3.17141	-3.31734
N	2.75374	2.76018	1.15318
N	5.50603	-2.00558	-0.08360
N	-5.58492	-1.84749	0.18815
N	-2.68508	2.83180	-1.11961
C	1.81652	3.38047	0.28950
C	1.35466	4.60852	1.00396
C	0.46264	5.60489	0.60679
C	0.28401	6.67395	1.49969
H	-0.40399	7.46755	1.23127
C	0.94690	6.73056	2.72728
H	0.76682	7.57125	3.38703
C	1.82958	5.72059	3.11283
H	2.35342	5.74609	4.06034
C	2.01654	4.67467	2.22527
C	2.91023	3.49053	2.35621
C	3.45818	1.55965	0.84350
C	4.04161	1.39741	-0.41522
H	3.94483	2.17478	-1.16005
C	4.71677	0.22117	-0.71966
H	5.14994	0.07977	-1.70234
C	4.83225	-0.79067	0.23476
C	4.26255	-0.61724	1.49729
H	4.36057	-1.40077	2.23870
C	3.56845	0.54848	1.80014
H	3.13040	0.68089	2.77942
C	6.87582	-2.16271	-0.29879
C	7.89538	-1.21350	-0.22957
H	7.68421	-0.17997	0.01568
C	9.19394	-1.64239	-0.48145
H	10.00547	-0.92506	-0.43421
C	9.47584	-2.98224	-0.79148
H	10.49973	-3.28148	-0.98247
C	8.45773	-3.92490	-0.85195
H	8.68087	-4.95979	-1.08649
C	7.14118	-3.52262	-0.60426
C	4.88791	-3.24457	-0.25423
C	5.87199	-4.21349	-0.57578
C	5.47380	-5.53641	-0.80123
H	6.20723	-6.29616	-1.04676
C	4.13229	-5.87264	-0.71657
H	3.81167	-6.89163	-0.89233
C	3.15556	-4.89367	-0.40996
C	3.53992	-3.56236	-0.17389
H	2.79216	-2.81476	0.05438
C	1.77355	-5.20588	-0.34572
C	0.56539	-5.32733	-0.27115
C	-0.78617	-5.32793	-0.17175
C	-1.99127	-5.20591	-0.05769
C	-5.01095	-3.12325	0.22390
C	-3.69591	-3.49993	-0.00965
H	-2.93231	-2.78039	-0.26769
C	-3.35688	-4.85879	0.10731
C	-4.35130	-5.81601	0.42117
H	-4.06741	-6.85735	0.50506
C	-5.66576	-5.42876	0.62626
H	-6.41850	-6.17265	0.86150
C	-6.01265	-4.07567	0.53589
C	-6.94787	-1.97452	0.47811
C	-7.24779	-3.34363	0.69576
C	-8.55414	-3.72106	1.02197
H	-8.79743	-4.76402	1.19149
C	-9.53341	-2.74298	1.13236
H	-10.55002	-3.02218	1.38312
C	-9.21697	-1.39105	0.92943
H	-9.99321	-0.64119	1.03183
C	-7.92665	-0.98756	0.60361
H	-7.69240	0.05961	0.46277
C	-4.88744	-0.64734	-0.11089
C	-5.36031	0.23446	-1.08491
H	-6.27509	0.00766	-1.61788
C	-4.65761	1.39269	-1.39549
H	-5.03428	2.05199	-2.16121
C	-3.43775	1.66915	-0.76505
C	-2.96084	0.78600	0.21100
H	-2.03673	0.99309	0.72609
C	-3.69357	-0.34414	0.54801
H	-3.32805	-1.00044	1.32729
C	-1.75155	3.48498	-0.26839
C	-1.19264	4.62231	-1.05447
C	-0.25173	5.58878	-0.70015

C	0.00766	6.58400	-1.65678
H	0.73564	7.35306	-1.42453
C	-0.62129	6.59319	-2.90363
H	-0.37886	7.37653	-3.61222
C	-1.54518	5.60543	-3.24778
H	-2.03849	5.58970	-4.21168
C	-1.81413	4.63765	-2.29509
C	-2.75277	3.48735	-2.37786

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da276-P-prop3.out Energy: -1676308.9854645

O	1.51895	3.14774	-0.85737
O	3.45571	3.16602	3.33341
O	-1.51896	3.14774	0.85736
O	-3.45572	3.16602	-3.33341
N	2.70259	2.80681	1.13704
N	5.52800	-1.92998	-0.14791
N	-5.52799	-1.92999	0.14792
N	-2.70261	2.80681	-1.13704
C	1.78993	3.47265	0.27246
C	1.26437	4.64124	1.03395
C	0.35070	5.62554	0.65709
C	0.11468	6.64518	1.59281
H	-0.59154	7.42898	1.34354
C	0.73967	6.66010	2.84193
H	0.51588	7.46263	3.53498
C	1.63478	5.65415	3.20929
H	2.12255	5.64348	4.17605
C	1.88130	4.66132	2.27624
C	2.78453	3.48479	2.38405
C	3.42979	1.62163	0.79949
C	4.61914	1.30093	1.46735
H	4.98827	1.93842	2.25463
C	5.30145	0.12912	1.16183
H	6.19212	-0.12807	1.72118
C	4.84165	-0.72505	0.15725
C	3.67636	-0.38260	-0.53227
H	3.32017	-1.01568	-1.33472
C	2.96228	0.76168	-0.20253
H	2.06393	0.99999	-0.74805
C	6.89767	-2.06853	-0.40101
C	7.89430	-1.09350	-0.46454
H	7.67152	-0.04780	-0.29742
C	9.18800	-1.50629	-0.76423
H	9.97774	-0.76556	-0.81852
C	9.49095	-2.85563	-1.00170
H	10.51065	-3.14242	-1.23036
C	8.49439	-3.82112	-0.95396
H	8.72723	-4.86165	-1.15083
C	7.18424	-3.43379	-0.65577
C	4.93630	-3.19456	-0.24780
C	5.93413	-4.15105	-0.56062
C	5.57254	-5.49491	-0.70952
H	6.32264	-6.24090	-0.94650
C	4.24725	-5.86975	-0.56023
H	3.95208	-6.90335	-0.68887
C	3.25618	-4.90957	-0.24490
C	3.60904	-3.56012	-0.07061
H	2.84684	-2.83909	0.18761
C	1.88339	-5.24813	-0.12942
C	0.67622	-5.37307	-0.04413
C	-0.67620	-5.37307	0.04409
C	-1.88337	-5.24813	0.12939
C	-4.93628	-3.19457	0.24780
C	-3.60903	-3.56012	0.07060
H	-2.84684	-2.83909	-0.18762
C	-3.25616	-4.90957	0.24488
C	-4.24723	-5.86976	0.56021
H	-3.95205	-6.90336	0.68884
C	-5.57252	-5.49493	0.70951
H	-6.32261	-6.24092	0.94649
C	-5.93411	-4.15106	0.56062
C	-6.89767	-2.06855	0.40102
C	-7.18422	-3.43380	0.65578
C	-8.49437	-3.82115	0.95398
H	-8.72721	-4.86168	1.15084
C	-9.49094	-2.85566	1.00172
H	-10.51063	-3.14245	1.23039
C	-9.18799	-1.50631	0.76427
H	-9.97773	-0.76559	0.81856
C	-7.89429	-1.09352	0.46457
H	-7.67152	-0.04782	0.29746
C	-4.84165	-0.72506	-0.15724
C	-3.67635	-0.38261	0.53227
H	-3.32016	-1.01568	1.33472
C	-2.96228	0.76168	0.20252
H	-2.06393	0.99999	0.74804
C	-3.42980	1.62162	-0.79949
C	-4.61915	1.30092	-1.46734
H	-4.98829	1.93842	-2.25462
C	-5.30146	0.12911	-1.16182
H	-6.19214	-0.12808	-1.72116
C	-1.78994	3.47265	-0.27246
C	-1.26438	4.64124	-1.03395
C	-0.35071	5.62554	-0.65710
C	-0.11470	6.64518	-1.59282
H	0.59153	7.42898	-1.34355
C	-0.73969	6.66010	-2.84194
H	-0.51590	7.46263	-3.53498
C	-1.63480	5.65415	-3.20930
H	-2.12257	5.64348	-4.17606
C	-1.88132	4.66131	-2.27624
C	-2.78455	3.48479	-2.38405

Macrocycle **1**

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da-288-P-6311.out Energy: -1926982.2877855

O	-1.49666	3.37146	0.81743
O	-3.70327	3.36718	-3.22194
O	1.27061	3.41775	-0.90084
O	3.41963	3.59654	3.16490
N	-2.75518	3.03099	-1.11267
N	-5.03403	-1.94591	0.24291
N	5.14852	-1.66600	-0.13659
N	2.51275	3.17436	1.05365
C	-1.84019	3.72391	-0.28298
C	-1.44423	4.94716	-1.04535
C	-0.57254	5.98325	-0.70758
C	-0.46785	7.03535	-1.63287
C	-1.17900	7.03822	-2.83434
C	-2.03339	5.98485	-3.16328
C	-2.14742	4.95497	-2.24489
C	-2.98088	3.72325	-2.32571
C	-3.34945	1.78028	-0.77381
C	-3.88633	1.58135	0.49984
C	-4.43582	0.34968	0.83648
C	-4.47694	-0.68365	-0.10144
C	-3.95739	-0.47272	-1.38072
C	-3.38473	0.74850	-1.71409
C	-6.36360	-2.18829	0.59908
C	-7.42944	-1.29454	0.70344
C	-8.67004	-1.80677	1.06852
C	-8.85111	-3.17554	1.31989
C	-7.78860	-4.06294	1.20383
C	-6.52960	-3.57577	0.83896
C	-4.34468	-3.16063	0.25660
C	-5.24258	-4.19491	0.61625
C	-4.76350	-5.50638	0.69473
C	-3.42783	-5.76404	0.42962
C	-2.53175	-4.72602	0.08113
C	-3.00052	-3.40850	-0.00377
C	4.54166	-2.91688	-0.26117
C	3.18801	-3.23698	-0.24675
C	2.80918	-4.57673	-0.40991

C	3.81279	-5.56156	-0.58100
C	5.15672	-5.23008	-0.62008
C	5.54446	-3.89522	-0.46577
C	6.53070	-1.83021	-0.25837
C	6.81348	-3.20408	-0.46634
C	8.14216	-3.61542	-0.61280
C	9.15595	-2.66787	-0.54587
C	8.85678	-1.31387	-0.32936
C	7.54474	-0.87598	-0.18118
C	4.47994	-0.44412	0.15848
C	4.43666	0.58169	-0.78697
C	3.79654	1.78027	-0.49163
C	3.17795	1.95103	0.74815
C	3.20890	0.92342	1.69265
C	3.86666	-0.26509	1.40021
C	1.58103	3.80800	0.19652
C	1.12197	5.02907	0.92728
C	0.20865	6.01748	0.55813
C	0.05158	7.08696	1.45567
C	0.75087	7.15016	2.66247
C	1.64437	6.14140	3.02530
C	1.81100	5.09563	2.13329
C	2.69402	3.90232	2.25305
C	-1.12558	-5.03741	-0.19285
C	-0.59006	-6.15210	-0.79171
C	0.81994	-6.10929	-0.92519
C	1.39622	-4.96436	-0.42439
S	0.15341	-3.92447	0.24556
H	0.20562	7.85761	-1.41442
H	-1.05503	7.86874	-3.52100
H	-2.58834	5.96447	-4.09419
H	-3.84810	2.37504	1.23374
H	-4.82627	0.18258	1.83386
H	-4.00188	-1.26974	-2.11404
H	-2.98198	0.90507	-2.70582
H	-7.30033	-0.23741	0.50161
H	-9.51505	-1.13157	1.15719
H	-9.83200	-3.54202	1.60374
H	-7.93529	-5.12201	1.39175
H	-5.42600	-6.31910	0.97571
H	-3.04843	-6.77532	0.52307
H	-2.33164	-2.60525	-0.28874
H	2.44137	-2.45866	-0.13920
H	3.52324	-6.60221	-0.66786
H	5.90104	-6.00738	-0.76221
H	8.37939	-4.66246	-0.77375
H	10.19028	-2.97533	-0.65865
H	9.66461	-0.59129	-0.27354
H	7.32121	0.17033	-0.00662
H	4.90222	0.43515	-1.75501
H	3.75960	2.57172	-1.22856
H	2.73632	1.05989	2.65647
H	3.90821	-1.06044	2.13560
H	-0.65495	7.87343	1.21139
H	0.58581	7.99160	3.32681
H	2.18978	6.16621	3.96173
H	-1.20134	-6.96196	-1.17151
H	1.38936	-6.88744	-1.41818

95
da288-P-prop1-freq.out Energy: -1927013.9410385

O	-1.44341	3.49232	0.82905
O	-3.28260	3.42862	-3.40088
O	1.44347	3.49231	-0.82904
O	3.28267	3.42856	3.40088
N	-2.53190	3.08667	-1.20283
N	-5.05818	-1.81559	0.07271
N	5.05815	-1.81565	-0.07274
N	2.53195	3.08664	1.20283
C	-1.69285	3.80487	-0.30938
C	-1.21776	5.00719	-1.05159
C	-0.35290	6.02820	-0.65518
C	-0.16289	7.07175	-1.57508
C	-0.78250	7.07437	-2.82707
C	-1.62074	6.02850	-3.21657
C	-1.82264	5.01022	-2.29993
C	-2.64570	3.77803	-2.43879
C	-3.16980	1.84521	-0.89093
C	-4.33987	1.45608	-1.55462
C	-4.94372	0.24033	-1.25438
C	-4.42392	-0.59045	-0.25889
C	-3.26598	-0.19031	0.41189
C	-2.63002	0.99960	0.08659
C	-6.41351	-1.97893	0.39116
C	-7.43864	-1.03336	0.43759
C	-8.70602	-1.46638	0.81357
C	-8.95434	-2.80714	1.14229
C	-7.92766	-3.74192	1.11383
C	-6.64355	-3.33262	0.74204
C	-4.41898	-3.05116	0.23475
C	-5.37276	-4.01163	0.64687
C	-4.95377	-5.32537	0.87842
C	-3.62099	-5.65916	0.70938
C	-2.66885	-4.70416	0.27835
C	-3.08569	-3.38982	0.02419
C	4.41893	-3.05121	-0.23476
C	3.08565	-3.38986	-0.02415
C	2.66878	-4.70420	-0.27829
C	3.62089	-5.65921	-0.70935
C	4.95367	-5.32543	-0.87843
C	5.37268	-4.01170	-0.64689
C	6.41348	-1.97901	-0.39122
C	6.64349	-3.33271	-0.74210
C	7.92758	-3.74203	-1.11392
C	8.95427	-2.80726	-1.14240
C	8.70598	-1.46650	-0.81369
C	7.43861	-1.03346	-0.43768
C	4.42391	-0.59051	0.25887
C	4.94375	0.24027	1.25434
C	4.33992	1.45603	1.55460
C	3.16984	1.84517	0.89093
C	2.63003	0.99957	-0.08658
C	3.26597	-0.19035	-0.41189
C	1.69292	3.80485	0.30939
C	1.21784	5.00717	1.05162
C	0.35298	6.02819	0.65521
C	0.16298	7.07174	1.57513
C	0.78260	7.07434	2.82712
C	1.62083	6.02846	3.21661
C	1.82272	5.01018	2.29996
C	2.64578	3.77799	2.43880
C	-1.26373	-5.08822	0.12142
C	-0.70483	-6.34437	0.06639
C	0.70478	-6.34438	-0.06607
C	1.26366	-5.08824	-0.12132
S	-0.00004	-3.87915	-0.00006
H	0.50725	7.88289	-1.31381
H	-0.59478	7.89690	-3.50727
H	-2.09680	6.00526	-4.18894
H	-4.75633	2.07981	-2.32970
H	-5.82452	-0.06630	-1.80414
H	-2.86086	-0.80920	1.20202
H	-1.74109	1.28668	0.62394
H	-7.25835	0.00680	0.20054
H	-9.51693	-0.74805	0.85539
H	-9.95454	-3.11155	1.42759
H	-8.11738	-4.77501	1.38317
H	-5.66277	-6.07818	1.20442
H	-3.29753	-6.66803	0.93120
H	-2.38130	-2.65217	-0.33650
H	2.38127	-2.65220	0.33656
H	3.29741	-6.66807	-0.93117
H	5.66265	-6.07826	-1.20445
H	8.11728	-4.77512	-1.38326
H	9.95446	-3.11170	-1.42773
H	9.51690	-0.74819	-0.85553

H	7.25835	0.00671	-0.20063
H	5.82456	-0.06637	1.80409
H	4.75640	2.07976	2.32967
H	1.74109	1.28666	-0.62392
H	2.86083	-0.80924	-1.20201
H	-0.50716	7.88288	1.31386
H	0.59488	7.89686	3.50733
H	2.09689	6.00521	4.18898
H	-1.29105	-7.25237	0.10866
H	1.29101	-7.25238	-0.10815

95
da288-P-prop2-freq.out Energy: -1927015.2765481

O	1.36823	3.32420	-0.86909
O	3.61017	3.50408	3.14538
O	-1.39879	3.56074	0.87802
O	-3.46600	3.45050	-3.24284
N	2.64541	3.07653	1.06100
N	5.04203	-1.89426	-0.10047
N	-5.11604	-1.72684	0.31347
N	-2.60587	3.14407	-1.08141
C	1.73019	3.73514	0.20525
C	1.35584	5.00168	0.90521
C	0.49528	6.03069	0.51933
C	0.40745	7.12878	1.39065
C	1.12342	7.18199	2.58810
C	1.96623	6.13610	2.96675
C	2.06469	5.06071	2.10016
C	2.88580	3.82514	2.23801
C	3.24833	1.81813	0.76667
C	3.81234	1.59292	-0.49059
C	4.39218	0.36279	-0.77835
C	4.42828	-0.64126	0.19013
C	3.86968	-0.40896	1.44824
C	3.27294	0.81329	1.73562
C	6.41684	-2.11940	-0.19983
C	7.47115	-1.21548	-0.07359
C	8.76436	-1.70947	-0.21001
C	9.00534	-3.06877	-0.46263
C	7.95107	-3.96593	-0.57971
C	6.64007	-3.49761	-0.44681
C	4.37960	-3.10955	-0.27950
C	5.34046	-4.12725	-0.49591
C	4.89588	-5.43673	-0.70309
C	3.53786	-5.70690	-0.69910
C	2.57764	-4.68312	-0.51058
C	3.01274	-3.36714	-0.29895
C	-4.48105	-2.97420	0.28270
C	-3.16578	-3.28638	-0.04831
C	-2.76050	-4.62667	-0.01056
C	-3.69445	-5.63019	0.33607
C	-5.00896	-5.31399	0.64027
C	-5.41979	-3.97755	0.62268
C	-6.45234	-1.92428	0.68214
C	-6.67530	-3.31000	0.87992
C	-7.94014	-3.75638	1.27395
C	-8.95463	-2.82842	1.47078
C	-8.71345	-1.45880	1.28679
C	-7.46491	-0.98769	0.89430
C	-4.50816	-0.48748	-0.01429
C	-3.29040	-0.12419	0.56550
C	-2.65631	1.05702	0.20582
C	-3.25730	1.92776	-0.71061
C	-4.49545	1.58557	-1.26662
C	-5.10030	0.37870	-0.93641
C	-1.69104	3.84971	-0.25594
C	-1.20819	5.00829	-1.06192
C	-0.28662	6.00708	-0.74650
C	-0.10990	7.01500	-1.70889
C	-0.79702	7.00537	-2.92461
C	-1.69436	5.98202	-3.23338
C	-1.88166	5.00006	-2.27529
C	-2.76088	3.80090	-2.32990
C	1.14938	-5.00919	-0.54762
C	0.52796	-6.11660	-1.07854
C	-0.88291	-6.10730	-0.94475
C	-1.37297	-4.98838	-0.31611
S	-0.05081	-3.93783	0.14722
H	-0.25525	7.94706	1.13276
H	1.01230	8.04626	3.23243
H	2.52409	6.15506	3.89481
H	3.77929	2.36745	-1.24403
H	4.81897	0.17501	-1.75602
H	3.90663	-1.18828	2.19959
H	2.84659	0.99446	2.71258
H	7.29088	-0.16662	0.12750
H	9.60261	-1.02830	-0.11648
H	10.02567	-3.41979	-0.56410
H	8.14254	-5.01632	-0.76929
H	5.60685	-6.24085	-0.85747
H	3.20173	-6.72790	-0.82725
H	2.30056	-2.56054	-0.17601
H	-2.46908	-2.51819	-0.35523
H	-3.36249	-6.65968	0.39115
H	-5.70834	-6.09972	0.90349
H	-8.12491	-4.81352	1.42929
H	-9.93993	-3.16168	1.77511
H	-9.51479	-0.74874	1.45719
H	-7.28776	0.07263	0.76920
H	-2.83191	-0.77170	1.30176
H	-1.71181	1.31236	0.65871
H	-4.96292	2.23536	-1.98974
H	-6.03357	0.10242	-1.41048
H	0.60235	7.80772	-1.50959
H	-0.61732	7.79996	-3.63935
H	-2.22629	5.94853	-4.17607
H	1.06734	-6.90427	-1.58737
H	-1.52583	-6.88317	-1.33956

95
da288-P-prop3-freq.out Energy: -1927015.7697768

O	-1.41771	3.37571	0.80025
O	-3.41284	3.44407	-3.34696
O	1.41186	3.37706	-0.80214
O	3.40579	3.44955	3.34558
N	-2.58022	3.07342	-1.19541
N	-5.09932	-1.81495	0.04685
N	5.10189	-1.80791	-0.04430
N	2.57418	3.07704	1.19396
C	-1.69659	3.74197	-0.31400
C	-1.23915	4.96316	-1.04384
C	-0.36656	5.97902	-0.65168
C	-0.19777	7.03907	-1.55800
C	-0.84828	7.06725	-2.79306
C	-1.70231	6.03242	-3.17713
C	-1.88037	4.99552	-2.27706
C	-2.73047	3.77948	-2.41230
C	-3.22919	1.84152	-0.88934
C	-3.83658	1.66515	0.35573
C	-4.44605	0.45545	0.66299
C	-4.47580	-0.57735	-0.27621
C	-3.88396	-0.38983	-1.52662
C	-3.25142	0.81044	-1.83019
C	-6.44917	-1.98889	0.36296
C	-7.48935	-1.05992	0.34082
C	-8.76026	-1.50437	0.68992
C	-8.99511	-2.84076	1.04821
C	-7.95700	-3.76378	1.06042
C	-6.66816	-3.34425	0.71603
C	-4.44651	-3.04021	0.20492
C	-5.39065	-4.01150	0.61708
C	-4.94998	-5.31650	0.85795
C	-3.61086	-5.62739	0.69602
C	-2.66703	-4.65537	0.28216
C	-3.10021	-3.34530	0.03347
C	4.45158	-3.03422	-0.20453

C	3.10519	-3.34135	-0.03768
C	2.67456	-4.65199	-0.28793
C	3.62146	-5.62244	-0.69864
C	4.96055	-5.30946	-0.85641
C	5.39856	-4.00385	-0.61399
C	6.45300	-1.97961	-0.35617
C	6.67527	-3.33454	-0.70886
C	7.96586	-3.75186	-1.04941
C	9.00240	-2.82713	-1.03382
C	8.76426	-1.49120	-0.67597
C	7.49155	-1.04892	-0.33067
C	4.47558	-0.57138	0.27755
C	4.44531	0.46110	-0.66197
C	3.83367	1.66997	-0.35573
C	3.22477	1.84579	0.88867
C	3.24731	0.81493	1.82976
C	3.88191	-0.38451	1.52719
C	1.69022	3.74429	0.31191
C	1.23106	4.96519	1.04117
C	0.35725	5.97979	0.64844
C	0.18699	7.04003	1.55427
C	0.83722	7.06955	2.78944
C	1.69241	6.03592	3.17413
C	1.87196	4.99887	2.27453
C	2.72356	3.78396	2.41046
C	-1.25874	-5.02815	0.12683
C	-0.70054	-6.28386	0.05581
C	0.70700	-6.28304	-0.08777
C	1.26611	-5.02663	-0.13806
S	0.00396	-3.81745	0.00484
H	0.47745	7.84594	-1.29652
H	-0.67628	7.90218	-3.46226
H	-2.20941	6.03104	-4.13406
H	-3.80667	2.45872	1.08885
H	-4.89657	0.30434	1.63626
H	-3.91940	-1.18669	-2.25932
H	-2.79369	0.95324	-2.79903
H	-7.31654	-0.02927	0.05700
H	-9.58620	-0.80215	0.68075
H	-9.99799	-3.15358	1.31453
H	-8.14413	-4.79682	1.33196
H	-5.64654	-6.08033	1.18532
H	-3.27447	-6.63285	0.91354
H	-2.40212	-2.58328	-0.28958
H	2.40504	-2.57986	0.28218
H	3.28806	-6.62881	-0.91638
H	5.65931	-6.07232	-1.18136
H	8.15553	-4.78453	-1.32058
H	10.00660	-3.13825	-1.29715
H	9.58901	-0.78762	-0.66416
H	7.31613	-0.01860	-0.04723
H	4.89728	0.31042	-1.63464
H	3.80346	2.46336	-1.08904
H	2.78827	0.95733	2.79805
H	3.91767	-1.18120	2.26006
H	-0.48919	7.84594	1.29230
H	0.66407	7.90456	3.45824
H	2.19930	6.03554	4.13117
H	-1.28651	-7.19215	0.09223
H	1.29188	-7.19118	-0.14074

95
da288-P-prop5-freq.out Energy: -1927015.9953100

O	-1.27174	3.41891	0.90033
O	-3.41537	3.59265	-3.16853
O	1.49517	3.37347	-0.81846
O	3.69705	3.36616	3.22358
N	-2.51121	3.17255	-1.05561
N	-5.14544	-1.66726	0.13598
N	5.03209	-1.94437	-0.24136
N	2.75153	3.03110	1.11287
C	-1.58125	3.80774	-0.19789
C	-1.12217	5.02859	-0.92887
C	-0.21016	6.01798	-0.55930
C	-0.05267	7.08703	-1.45717
C	-0.75079	7.14887	-2.66457
C	-1.64293	6.13933	-3.02826
C	-1.80969	5.09414	-2.13571
C	-2.69134	3.89967	-2.25582
C	-3.17613	1.94901	-0.74987
C	-3.78235	1.77377	0.49533
C	-4.42171	0.57504	0.79085
C	-4.47681	-0.44509	-0.15985
C	-3.87626	-0.26144	-1.40694
C	-3.21858	0.92685	-1.69976
C	-6.52733	-1.83062	0.26011
C	-7.54080	-0.87591	0.18302
C	-8.85259	-1.31326	0.33452
C	-9.15186	-2.66669	0.55392
C	-8.13861	-3.61478	0.62079
C	-6.81025	-3.20397	0.47123
C	-4.53864	-2.91784	0.26179
C	-5.54145	-3.89550	0.47003
C	-5.15464	-5.23026	0.62653
C	-3.81112	-5.56260	0.58490
C	-2.80770	-4.57845	0.40921
C	-3.18519	-3.23853	0.24501
C	4.34354	-3.15929	-0.25698
C	2.99931	-3.40829	0.00179
C	2.53247	-4.72631	-0.08543
C	3.42963	-5.76344	-0.43405
C	4.76545	-5.50453	-0.69638
C	5.24281	-4.19267	-0.61598
C	6.36233	-2.18531	-0.59541
C	6.52977	-3.57249	-0.83599
C	7.78945	-4.05866	-1.19939
C	8.85110	-3.17004	-1.31342
C	8.66854	-1.80160	-1.06175
C	7.42723	-1.29035	-0.69795
C	4.47364	-0.68208	0.10263
C	3.96520	-0.46773	1.38560
C	3.39184	0.75308	1.71872
C	3.34604	1.78034	0.77403
C	3.87215	1.57812	-0.50353
C	4.42156	0.34647	-0.83970
C	1.83779	3.72485	0.28269
C	1.44101	4.94762	1.04530
C	0.56990	5.98402	0.70722
C	0.46407	7.03561	1.63286
C	1.17412	7.03766	2.83484
C	2.02798	5.98420	3.16452
C	2.14282	4.95502	2.24557
C	2.97582	3.72281	2.32662
C	-1.39496	-4.96736	0.41867
C	-0.82018	-6.12125	0.90042
C	0.58951	-6.16359	0.76608
C	1.12614	-5.03968	0.18535
S	-0.15115	-3.91718	-0.23256
H	0.65180	7.87375	-1.21194
H	-0.58582	7.98945	-3.32844
H	-2.18704	6.16267	-3.96438
H	-3.73451	2.56089	1.23486
H	-4.87816	0.42414	1.76150
H	-3.92695	-1.05276	-2.14476
H	-2.75674	1.06899	-2.66690
H	-7.31630	0.16885	0.00707
H	-9.65965	-0.59144	0.27917
H	-10.18515	-2.97281	0.66886
H	-8.37493	-4.66046	0.78399
H	-5.89913	-6.00520	0.77187
H	-3.52105	-6.60159	0.67570
H	-2.43860	-2.46232	0.13150
H	2.32963	-2.60663	0.28585
H	3.05105	-6.77384	-0.52748
H	5.42922	-6.31491	-0.97669
H	7.93628	-5.11647	-1.38755

H	9.83182	-3.53476	-1.59574
H	9.51239	-1.12658	-1.14924
H	7.29584	-0.23447	-0.49685
H	4.01794	-1.26158	2.12047
H	2.99843	0.91450	2.71243
H	3.82393	2.36847	-1.23910
H	4.80469	0.17587	-1.83830
H	-0.20797	7.85756	1.41353
H	1.04961	7.86722	3.52104
H	2.58169	5.96282	4.09502
H	-1.39117	-6.90680	1.37689
H	1.19954	-6.98036	1.1292

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