Supporting Information

Martin Tlustý,[†] Hana Dvořáková,[ʃ] Jan Čejka,[§] Michal Kohout[†] and Pavel Lhoták[†*]

[†]Department of Organic Chemistry, University of Chemistry and Technology, Prague (UCTP), Technicka 5, 166 28 Prague 6, Czech Republic
[ʃ]Laboratory of NMR Spectroscopy, UCTP, Technická 5, 166 28 Prague 6, Czech Republic.
[§]Solid State Department, UCTP, Technicka 5, 166 28 Prague 6, Czech Republic

Table of Contents

1. Spectral characterization of compounds

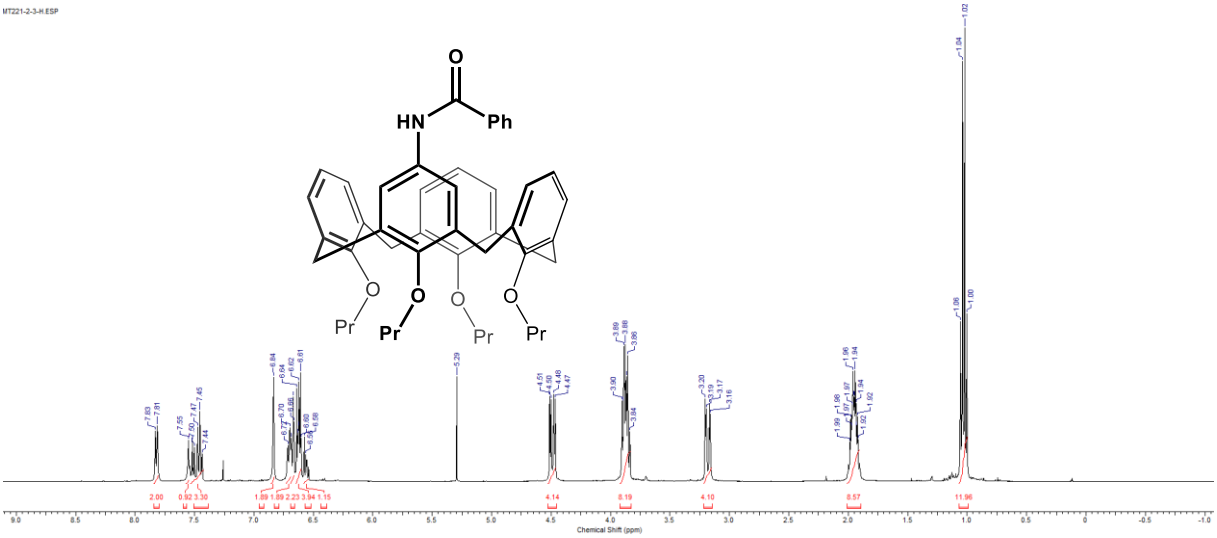


Figure 1: ^{1}H NMR of compound **5a** ($CDCl_3$, 400 MHz).

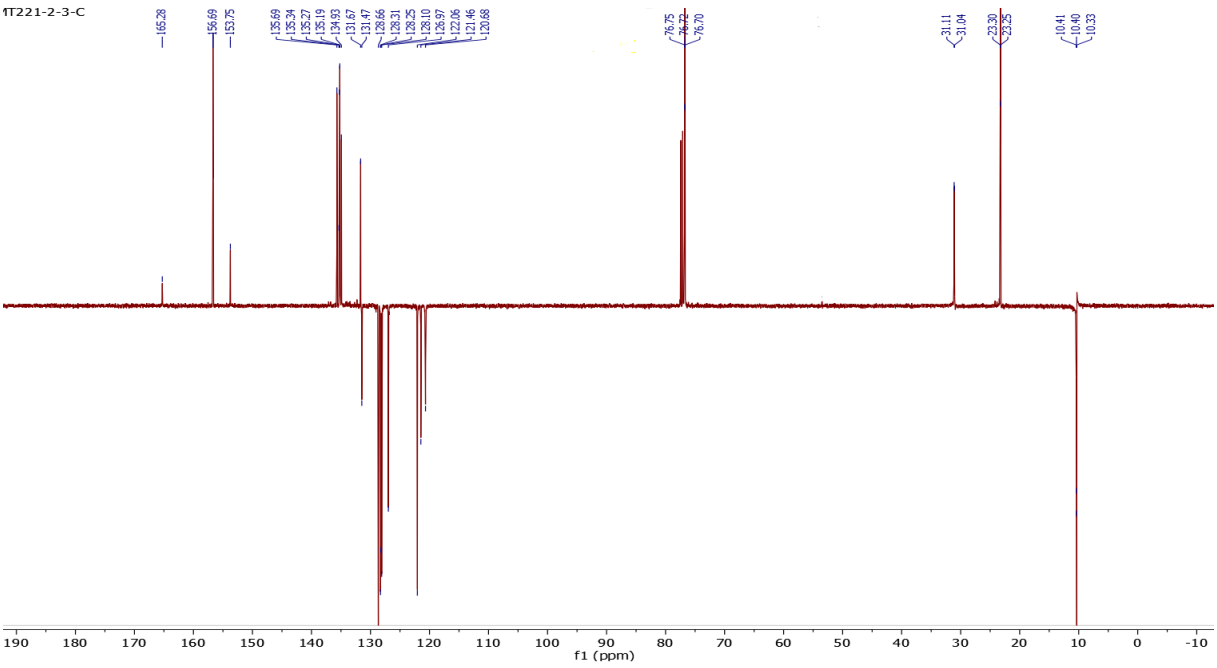


Figure 2: ^{13}C(APT) NMR of compound **5a** ($CDCl_3$, 100 MHz).

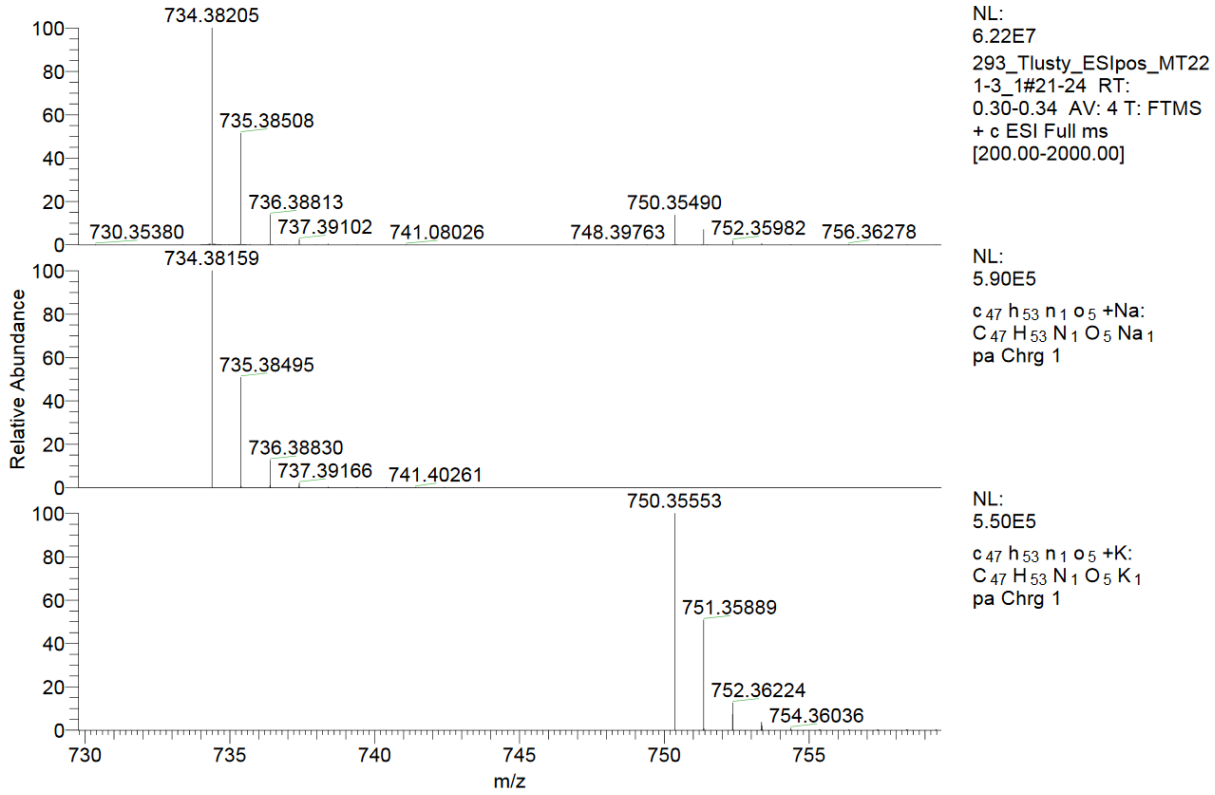


Figure 3: HRMS of compound **5a** (ESI^+).

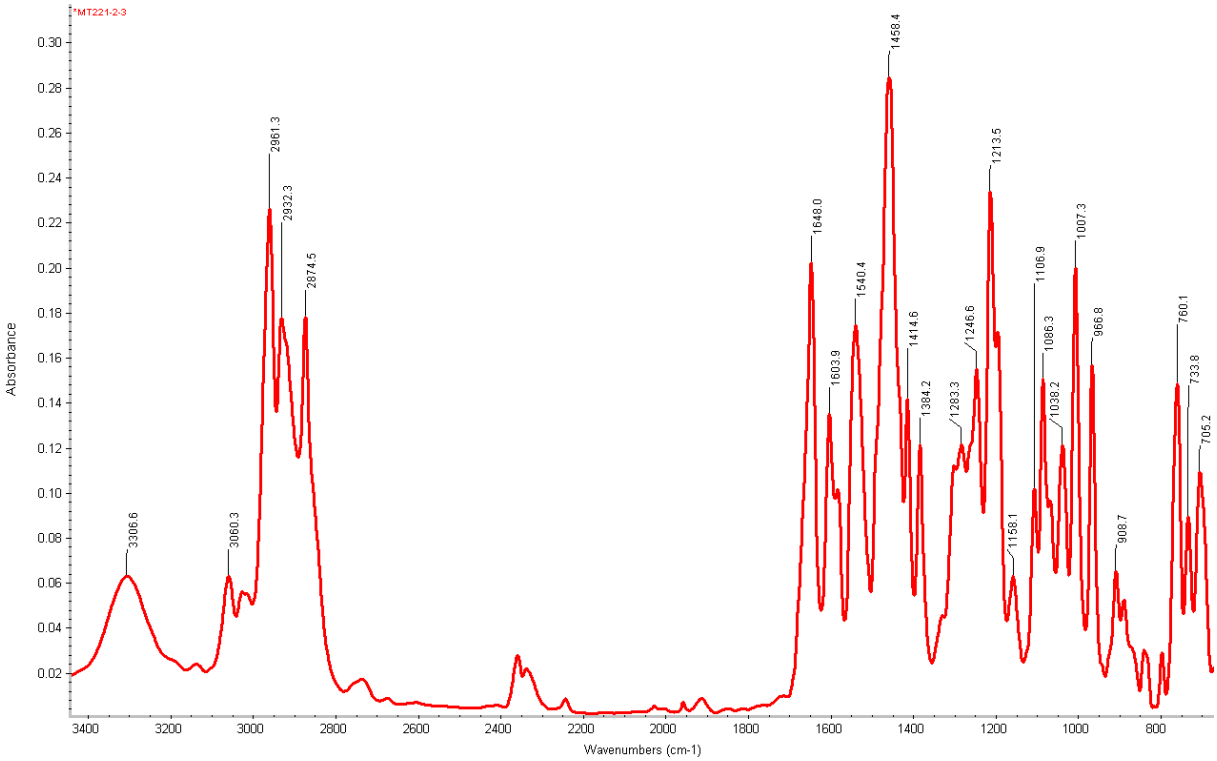


Figure 4: IR of compound **5a** (KBr).

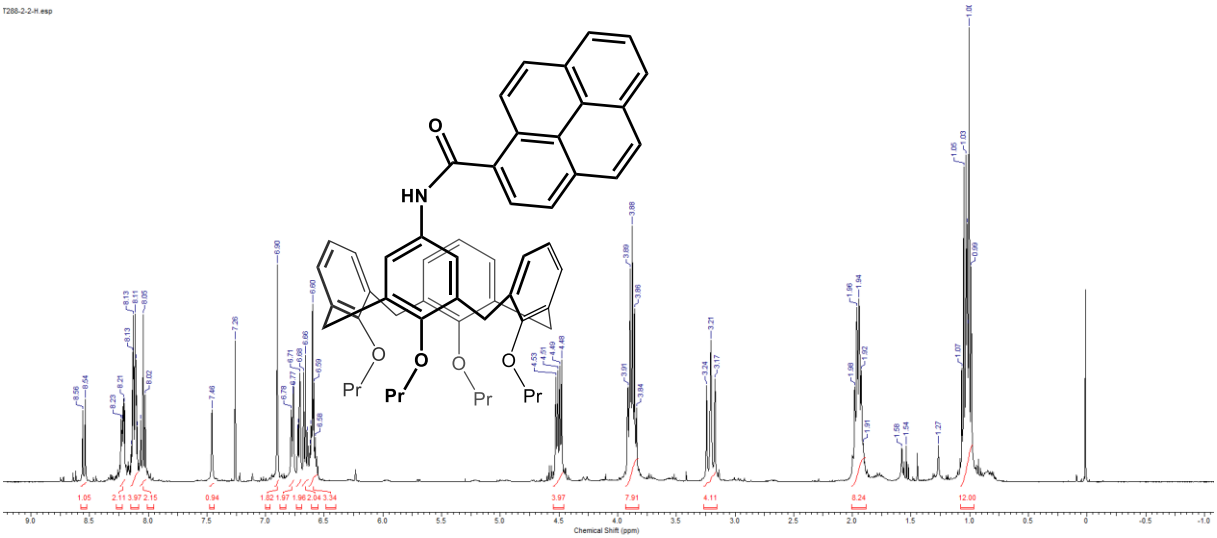


Figure 5: ^{1}H NMR of compound **5b** ($CDCl_3$, 400 MHz).

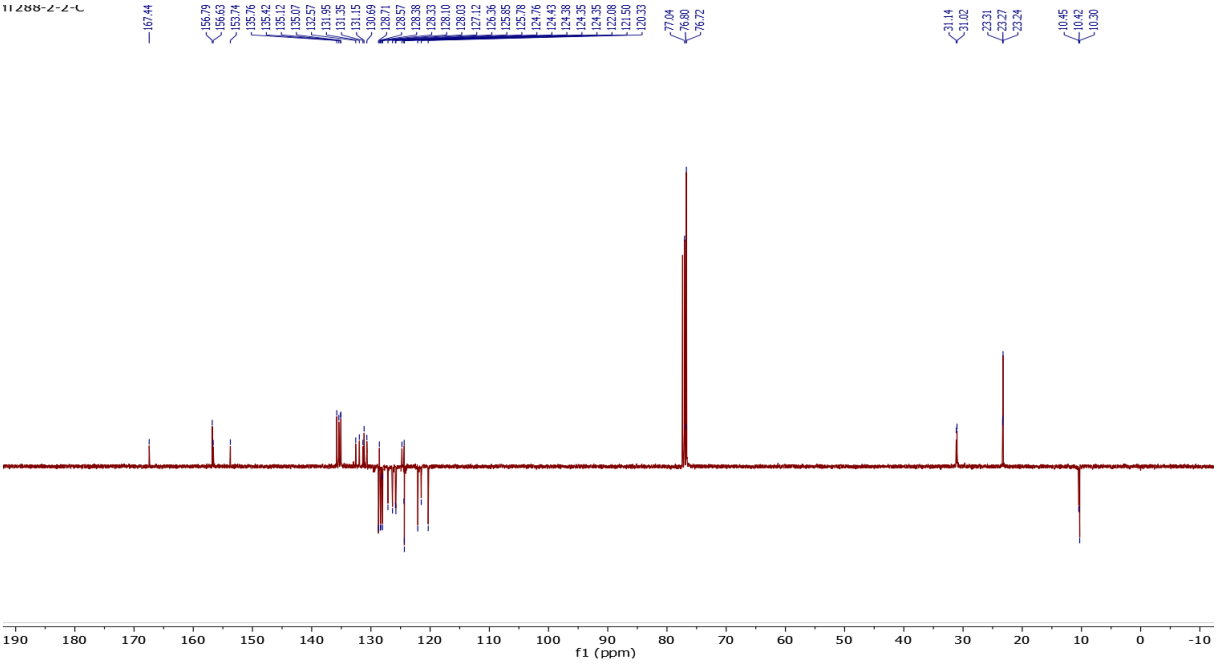


Figure 6: ^{13}C(APT) NMR of compound **5b** ($CDCl_3$, 100 MHz).

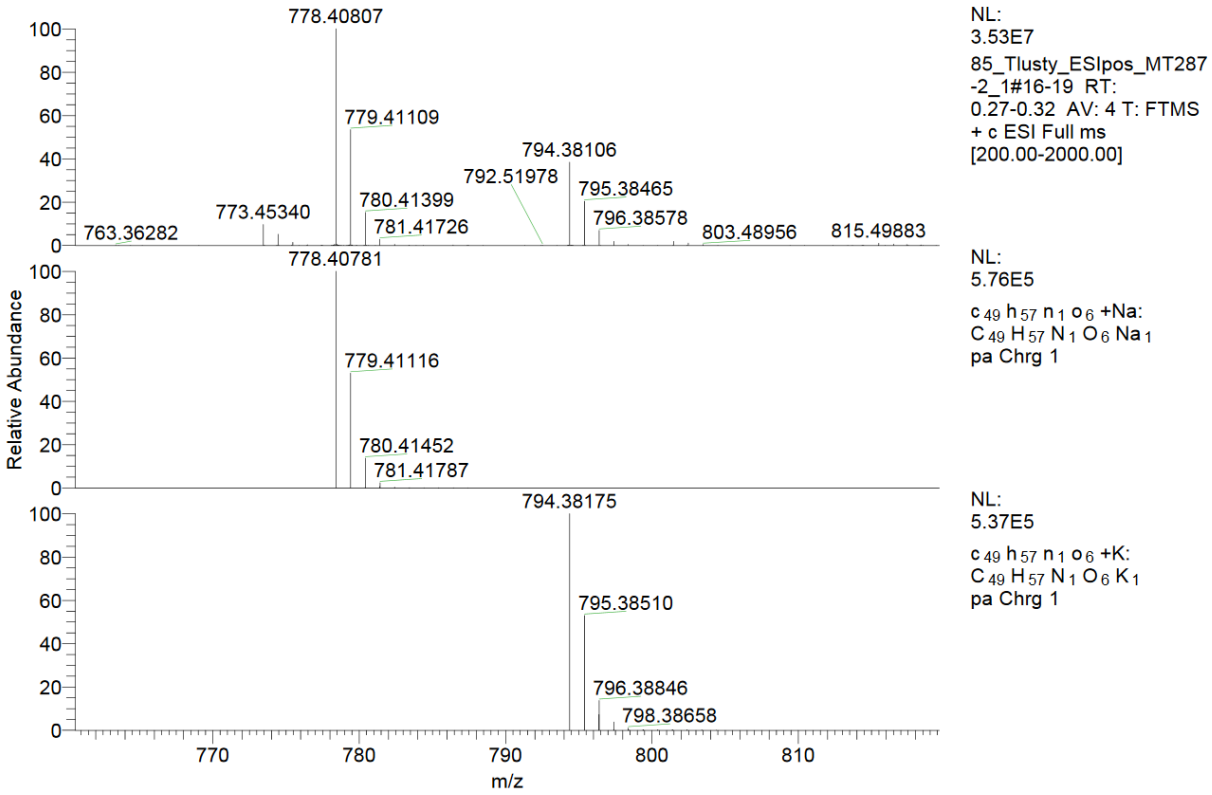


Figure 7: HRMS of compound **5b** (ESI^+).

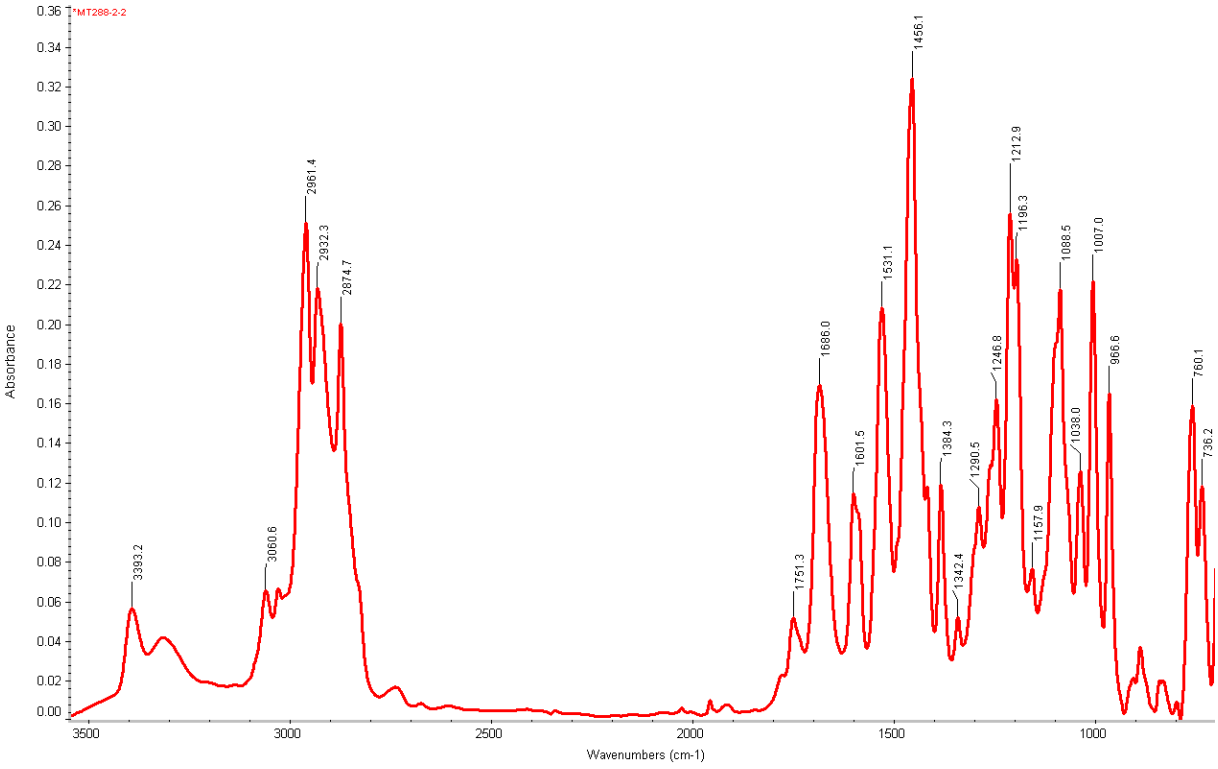


Figure 8: IR of compound **5b** (KBr).

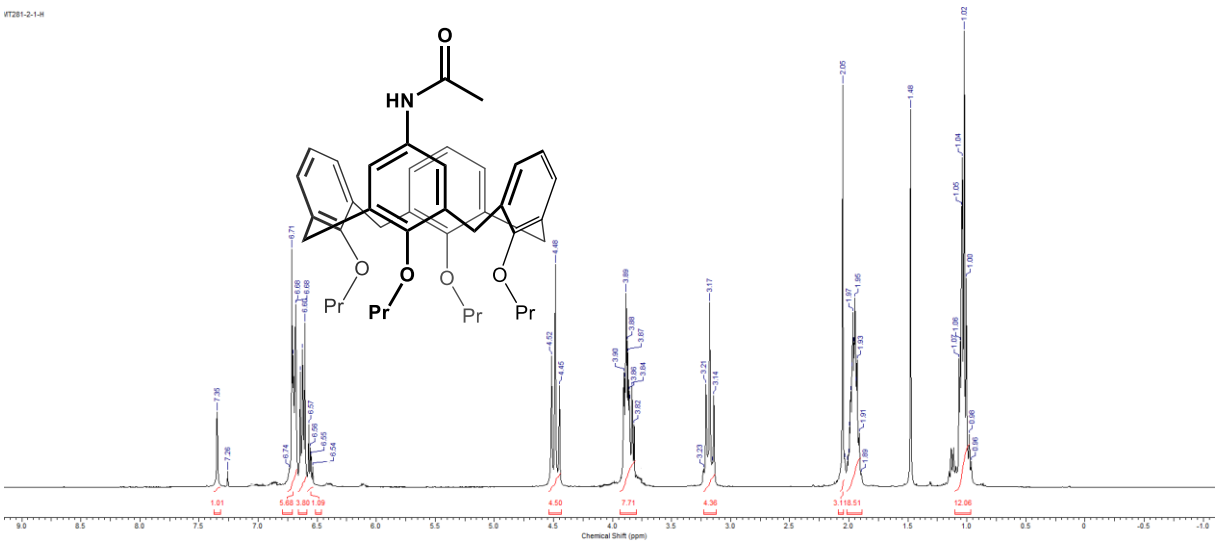


Figure 9: ^{1}H NMR of compound **5c** ($CDCl_3$, 400 MHz).

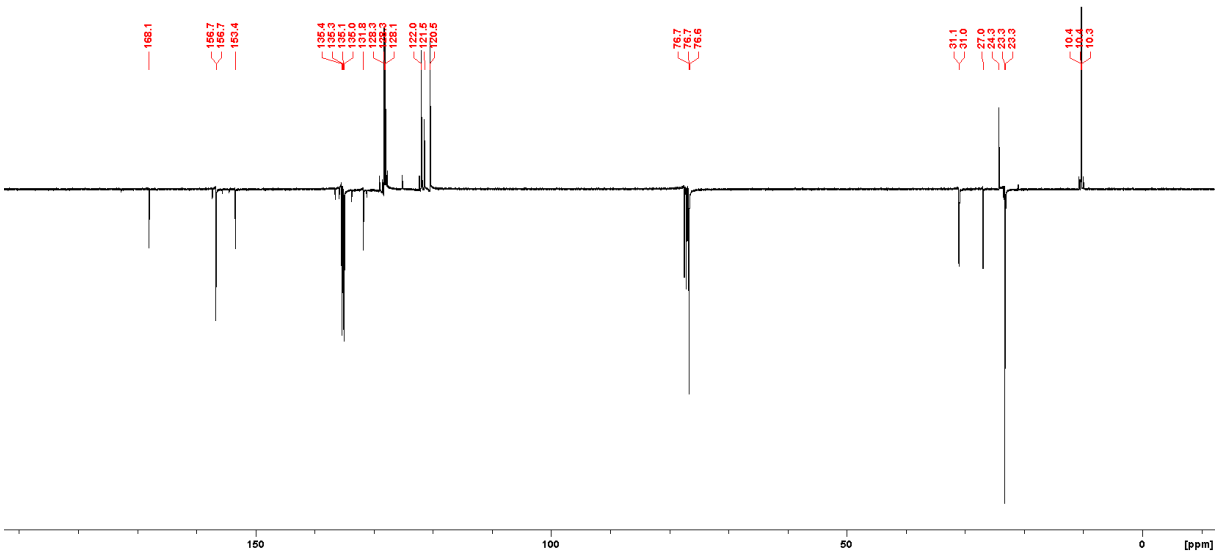


Figure 10: ^{13}C(APT) NMR of compound **5c** ($CDCl_3$, 100 MHz).

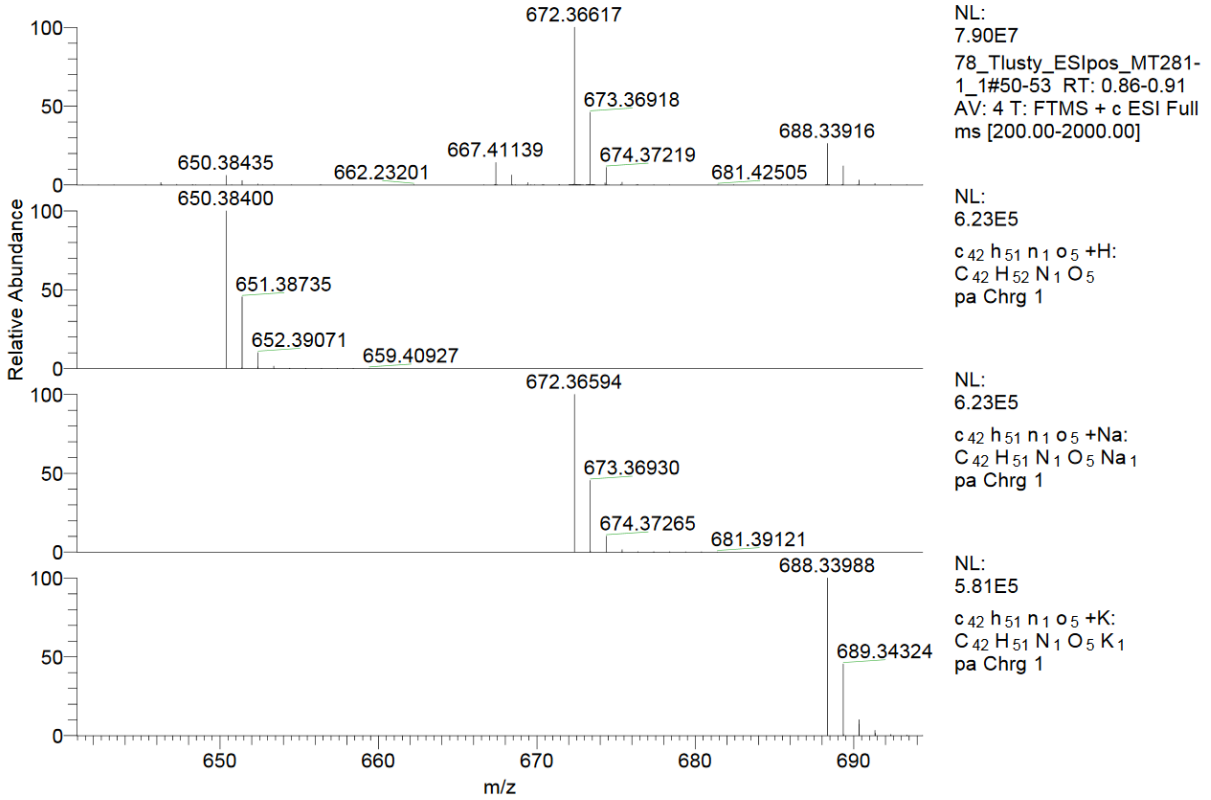


Figure 11: HRMS of compound **5c** (ESI^+).

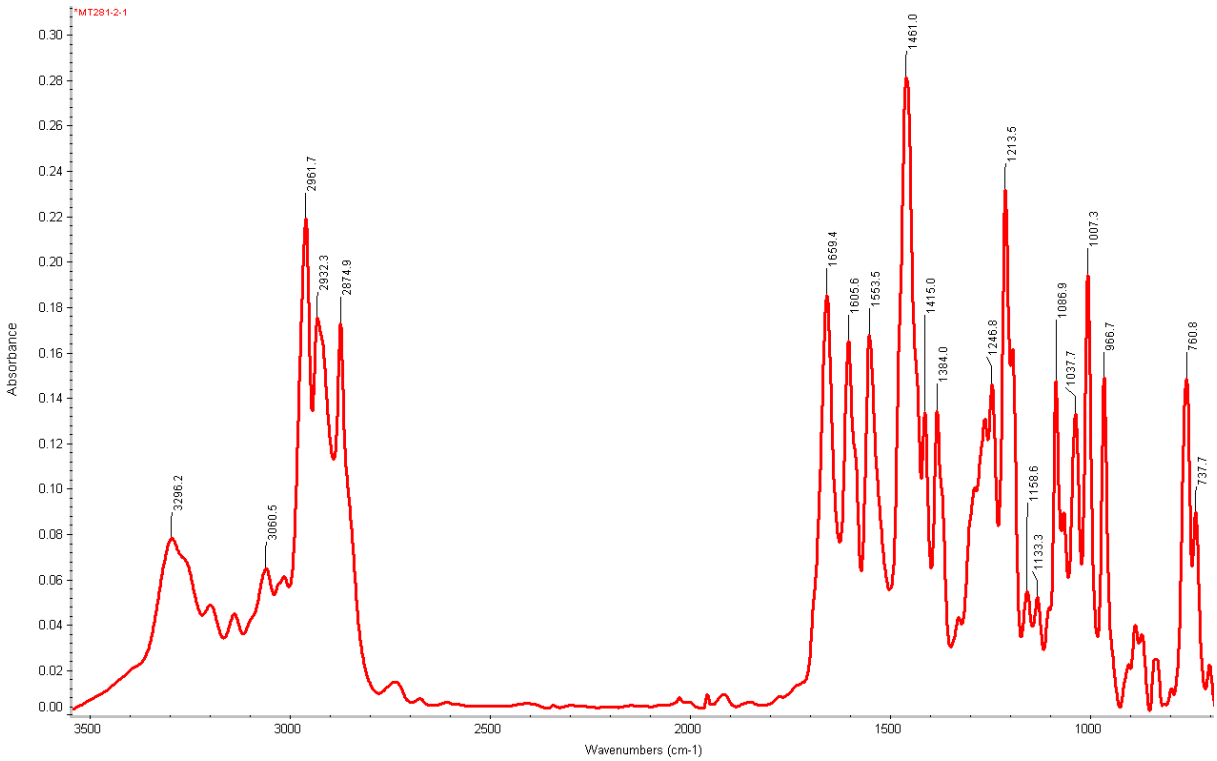


Figure 12: IR of compound **5c** (KBr).

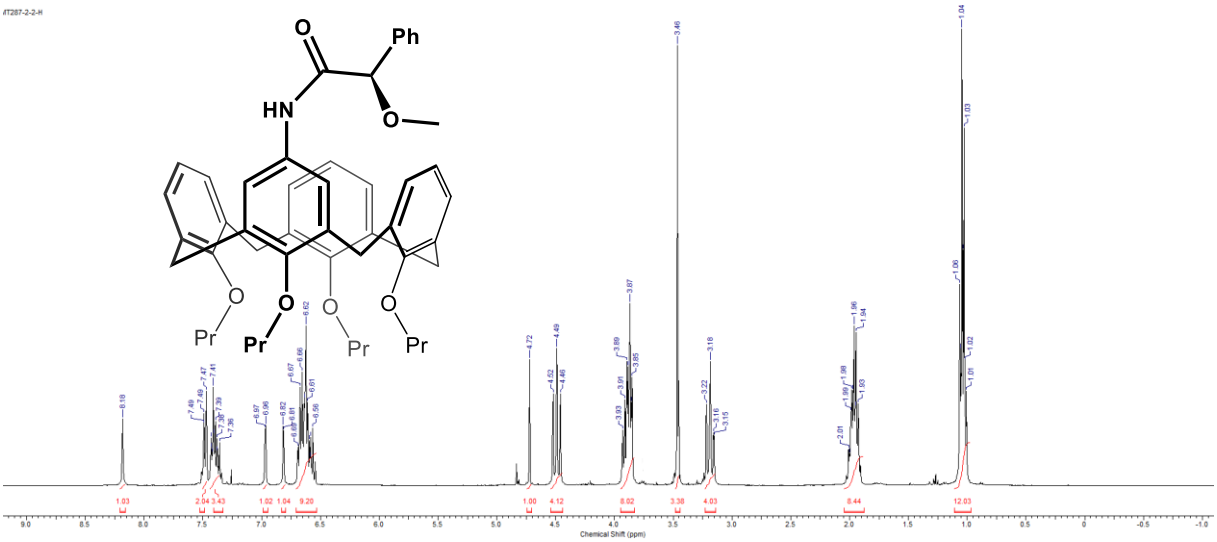


Figure 13: ^{1}H NMR of compound **5d** ($CDCl_3$, 400 MHz).

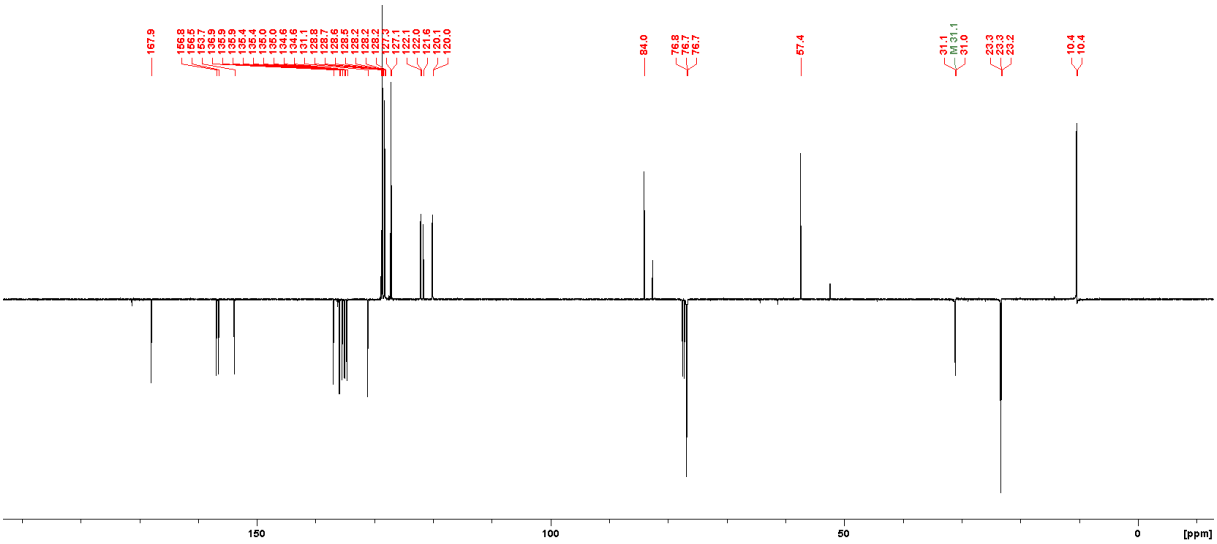


Figure 14: ^{13}C(APT) NMR of compound **5d** ($CDCl_3$, 100 MHz).

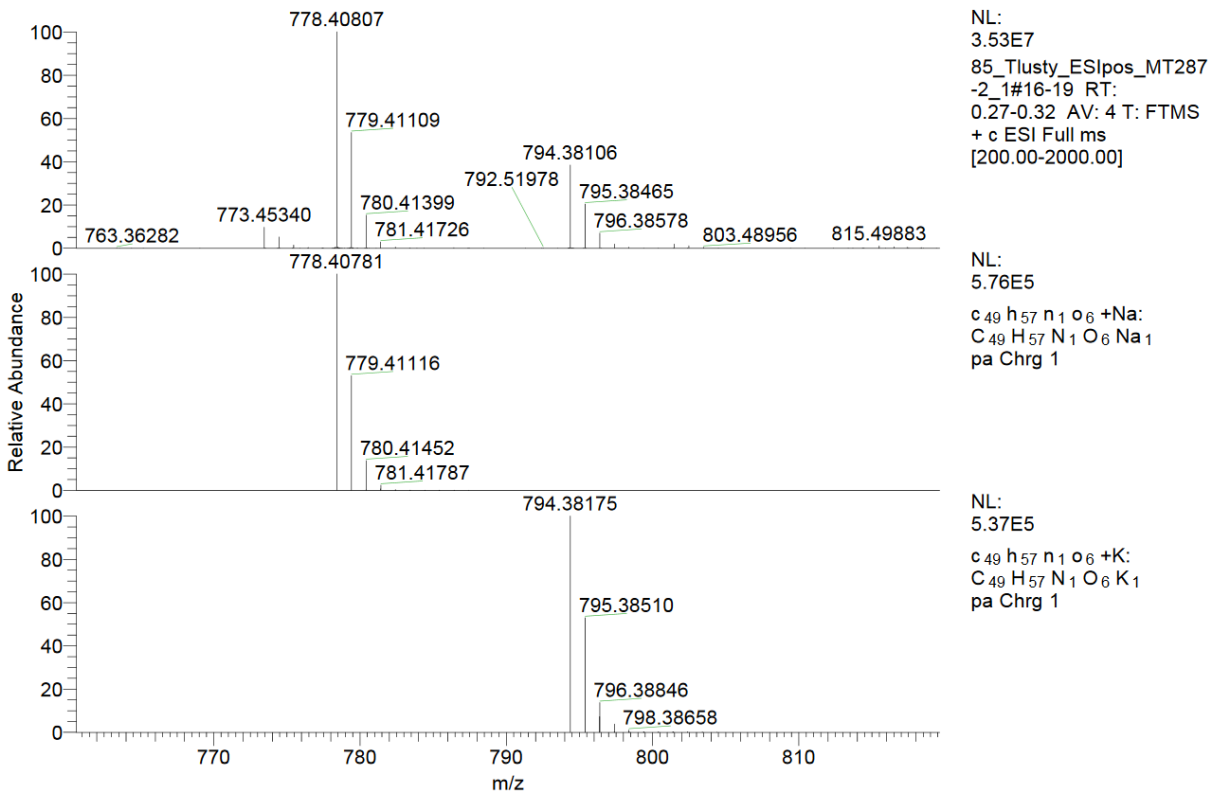


Figure 15: HRMS of compound **5d** (ESI^+).

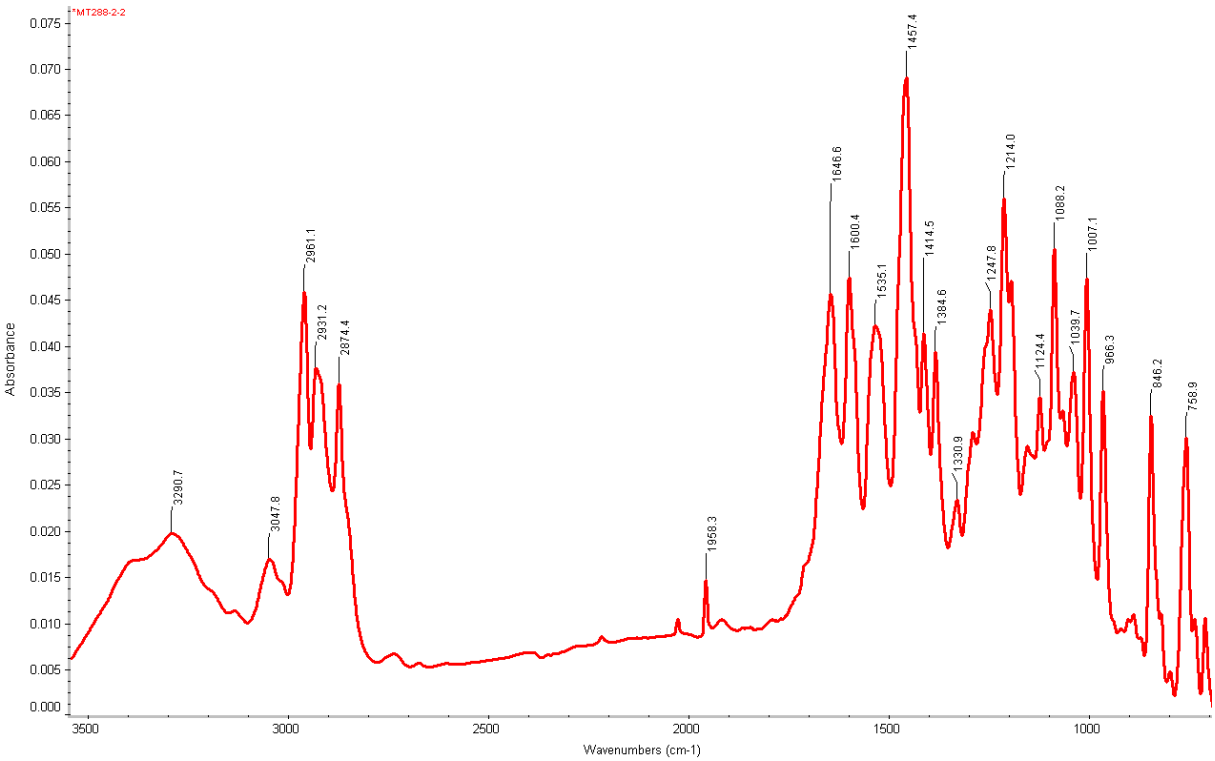


Figure 16: IR of compound **5d** (KBr).

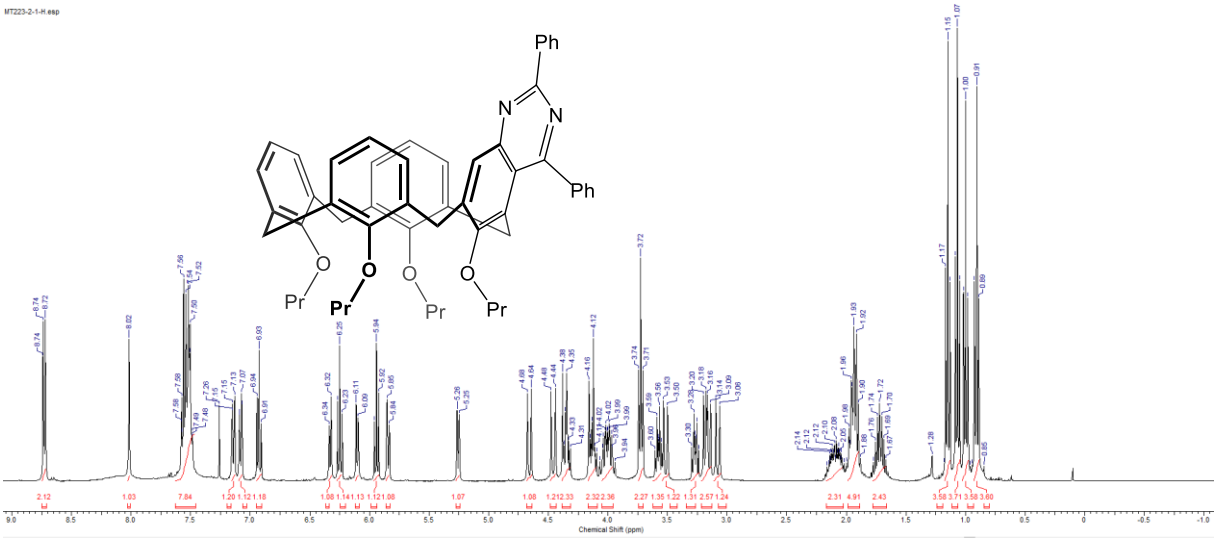


Figure 17: ^{1}H NMR of compound **8aa** ($CDCl_3$, 400 MHz).

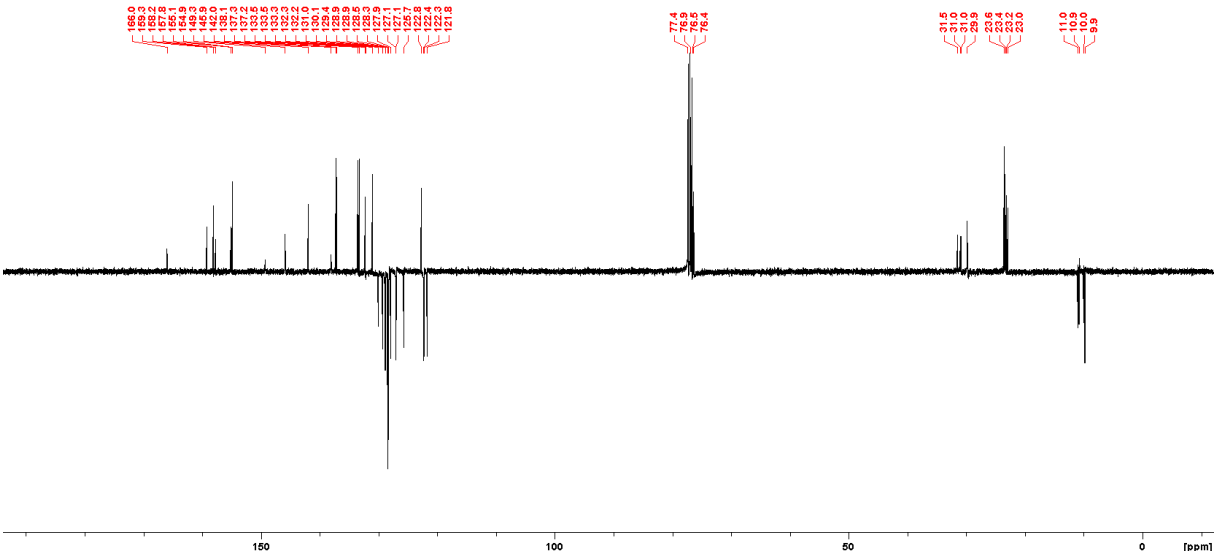


Figure 18: ^{13}C(APT) NMR of compound **8aa** ($CDCl_3$, 100 MHz).

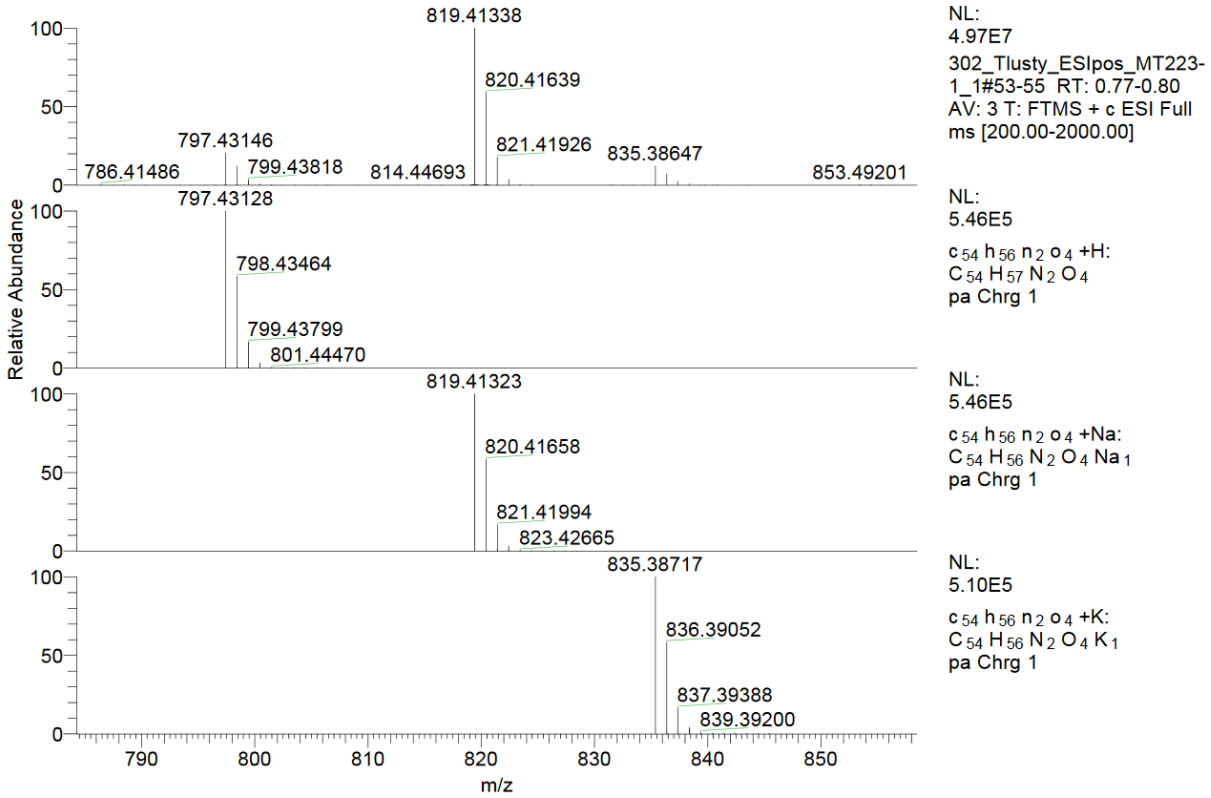


Figure 19: HRMS of compound **8aa** (ESI^+).

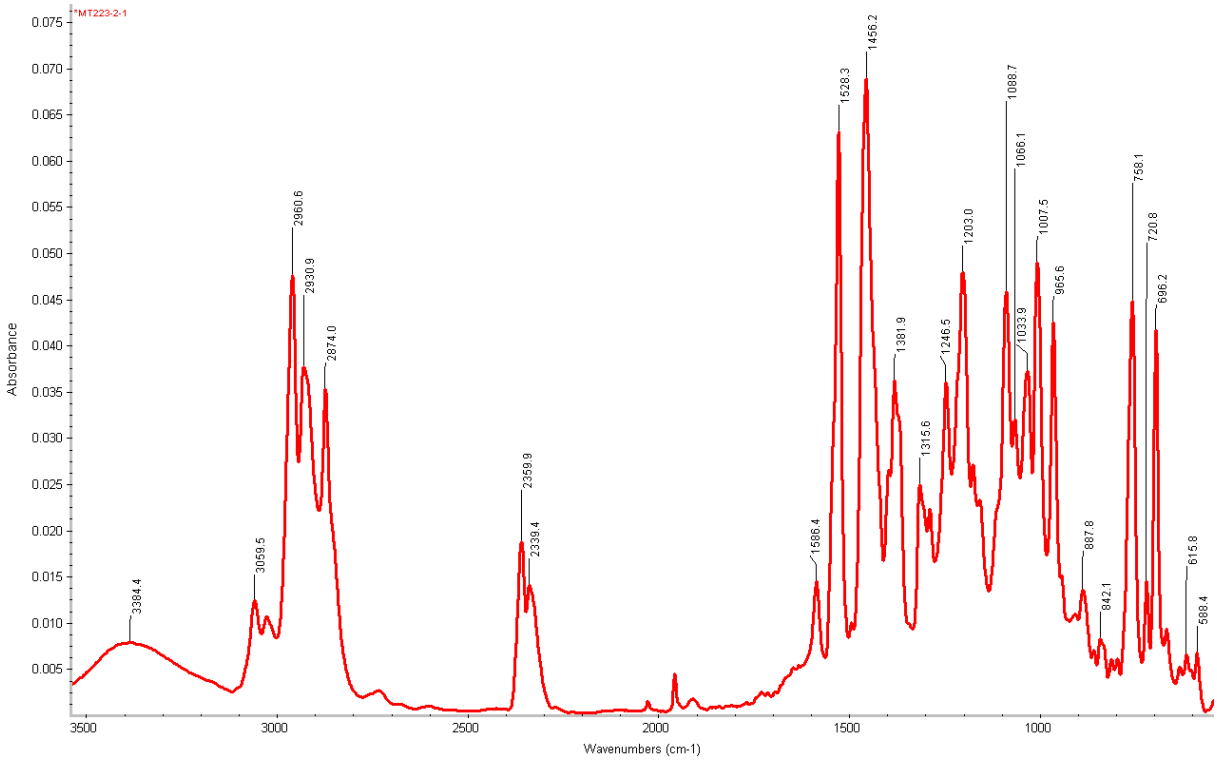


Figure 20: IR of compound **8aa** (KBr).

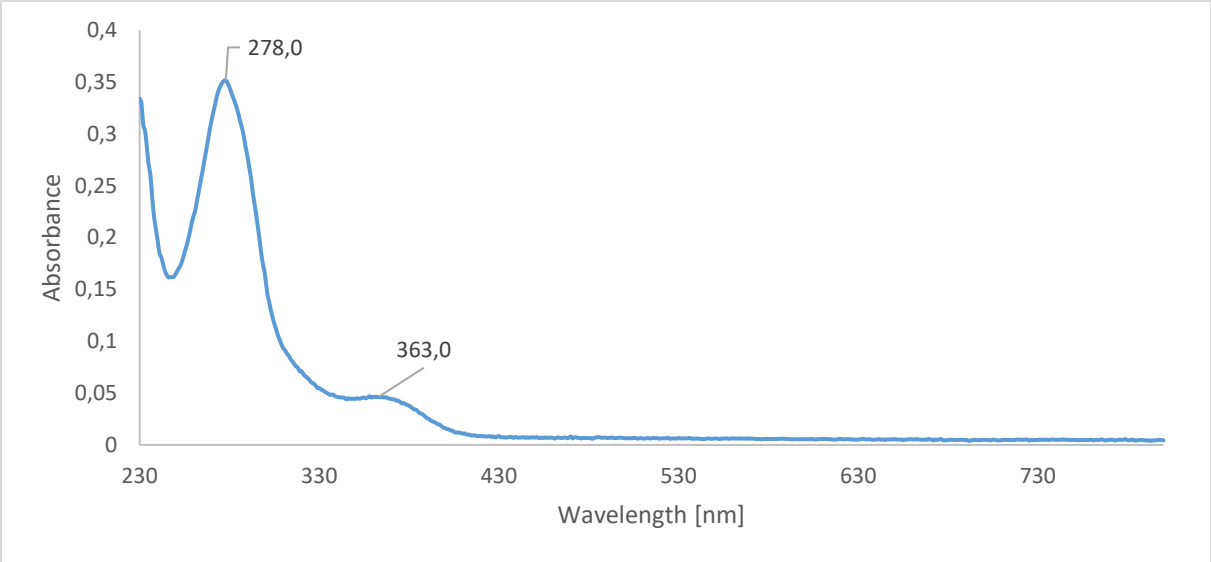


Figure 21: UV of compound **8aa** (CH_2Cl_2).

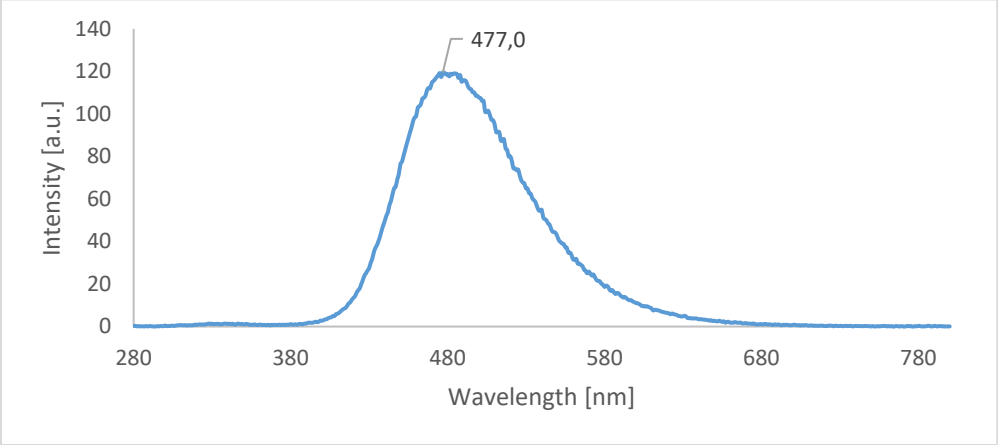


Figure 22: Fluorescence of compound **8aa** (CH_2Cl_2, excitation wavelength 278 nm).

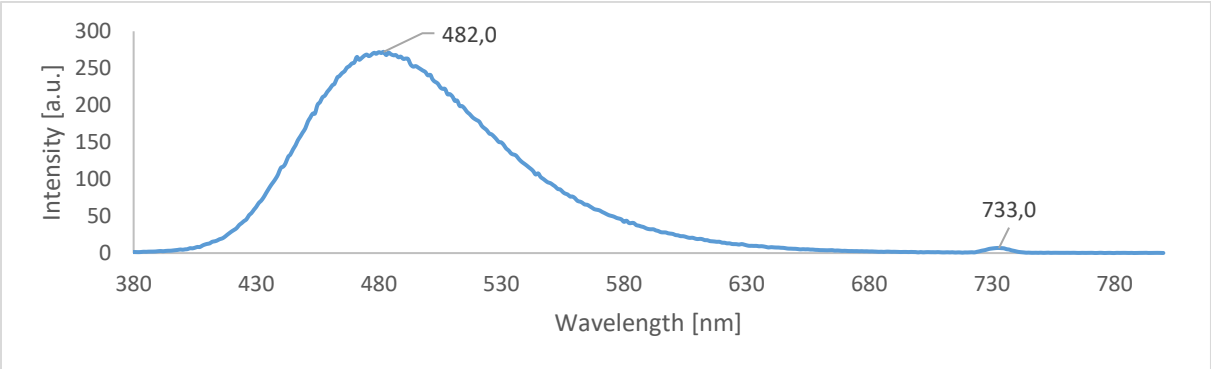


Figure 23: Fluorescence of compound **8aa** (CH_2Cl_2, excitation wavelength 367 nm).

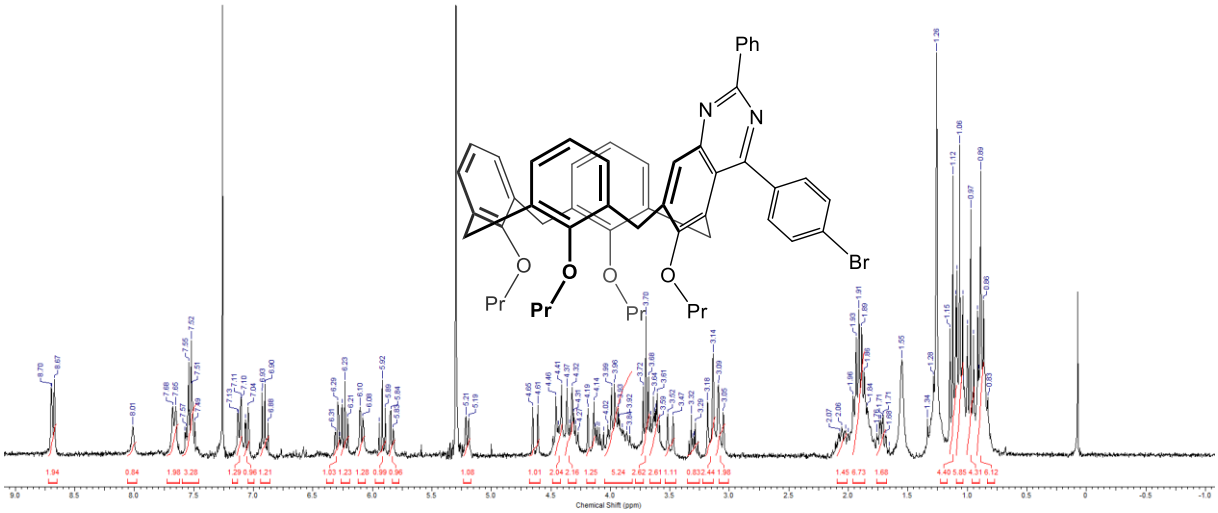


Figure 24: ^{1}H NMR of compound **8ab** ($CDCl_3$, 400 MHz).

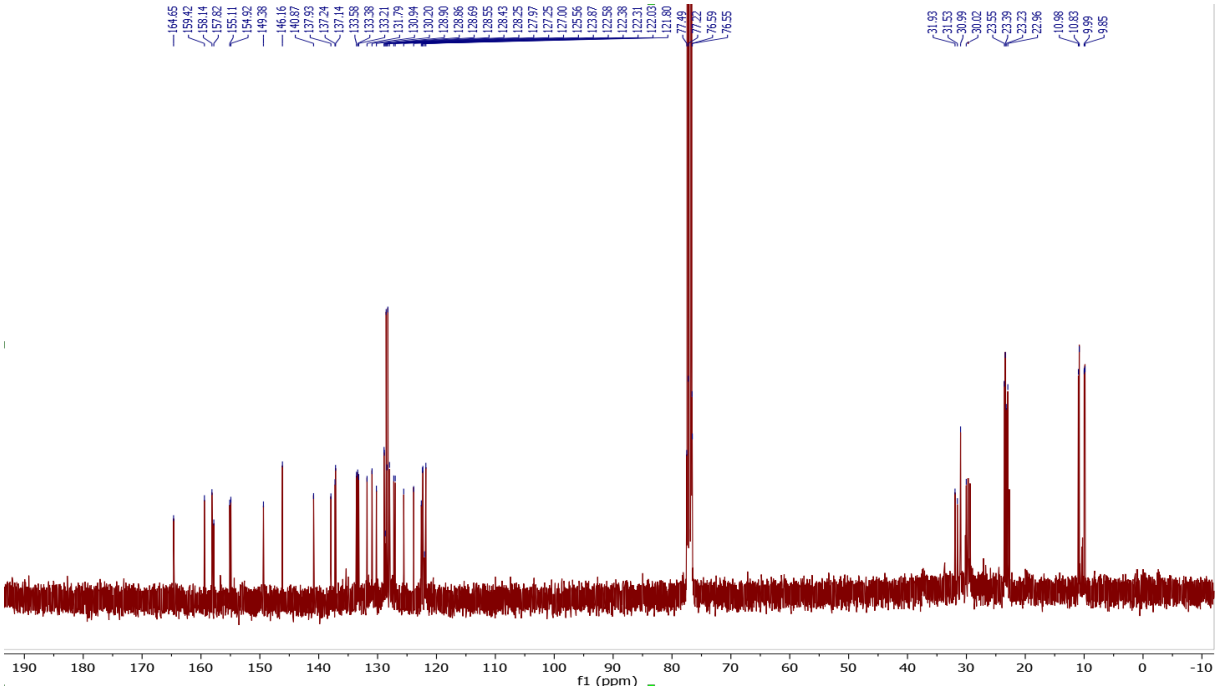


Figure 25: ^{13}C NMR of compound **8ab** ($CDCl_3$, 100 MHz).

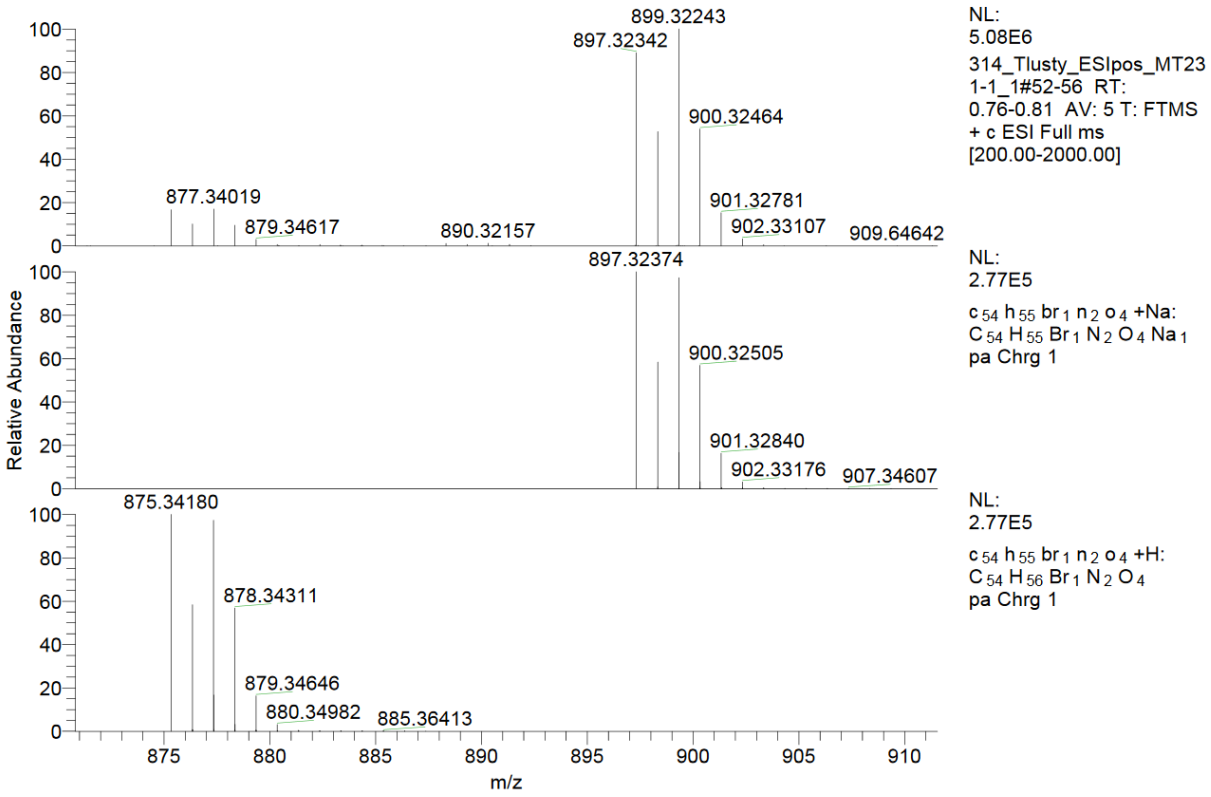


Figure 26: HRMS of compound **8ab** (ESI^+).

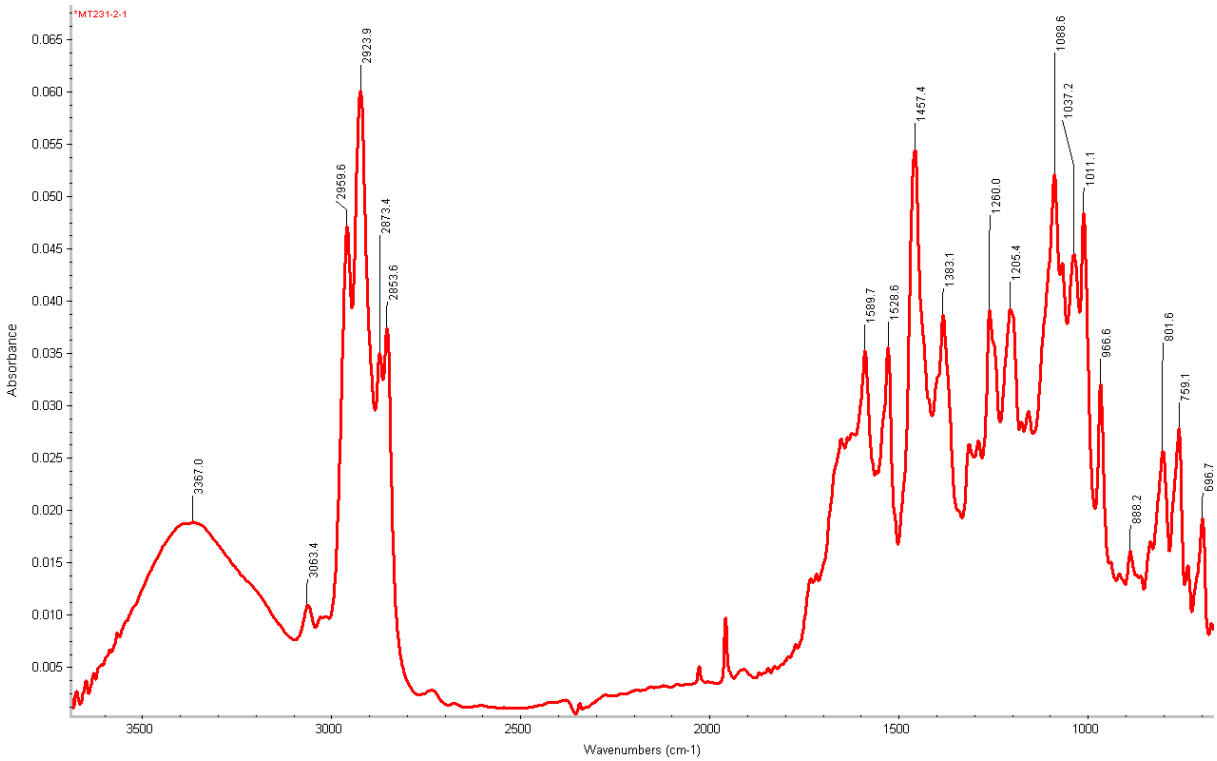


Figure 27: IR of compound **8ab** (KBr).

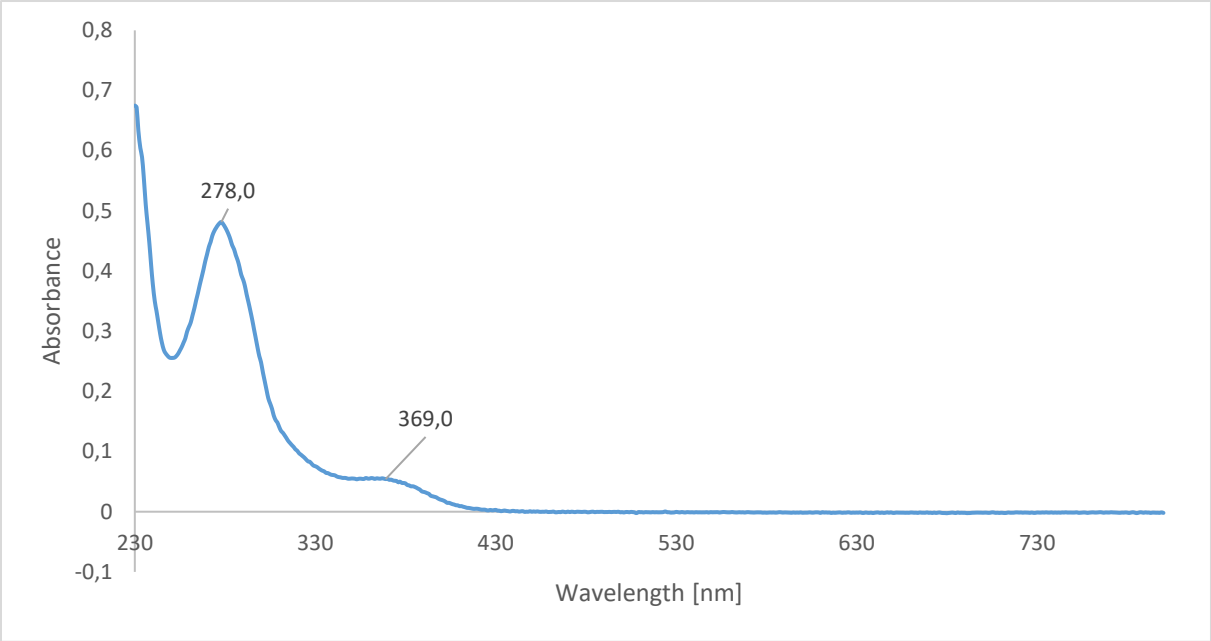


Figure 28: UV of compound **8ab** (CH_2Cl_2).

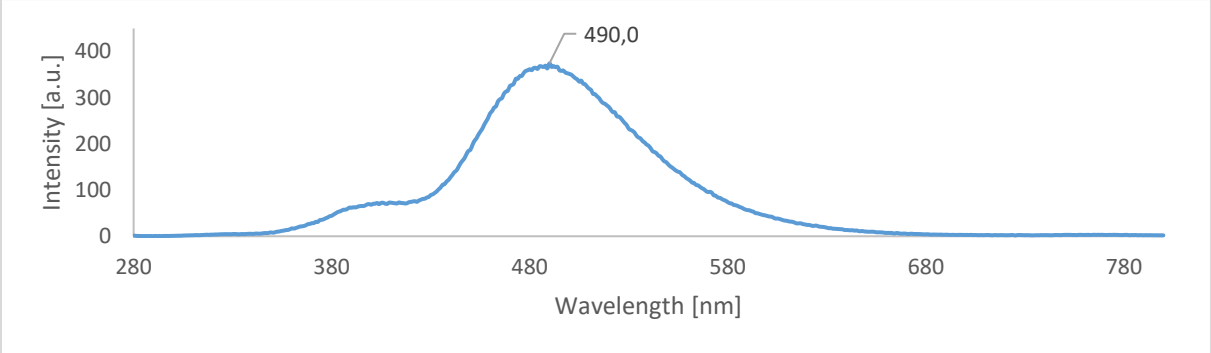


Figure 29: Fluorescence of compound **8ab** (CH_2Cl_2, excitation wavelength 278 nm).

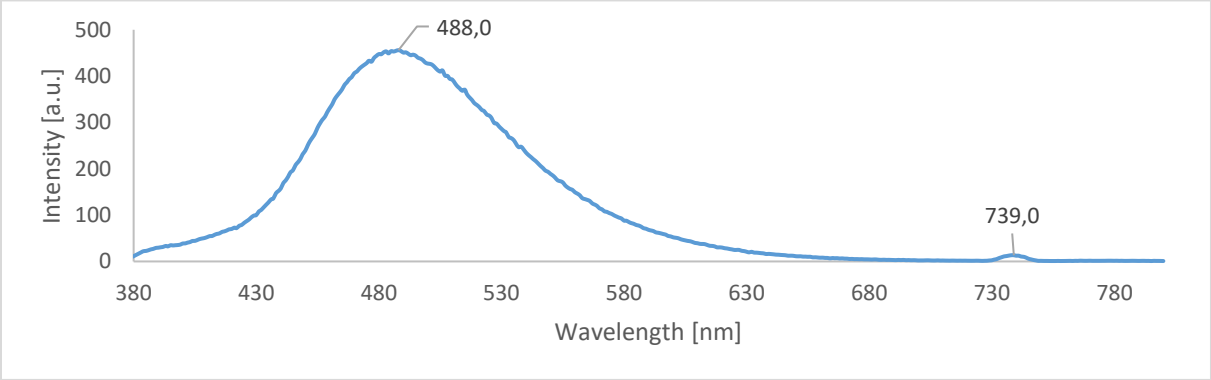


Figure 30: Fluorescence of compound **8ab** (CH_2Cl_2, excitation wavelength 370 nm).

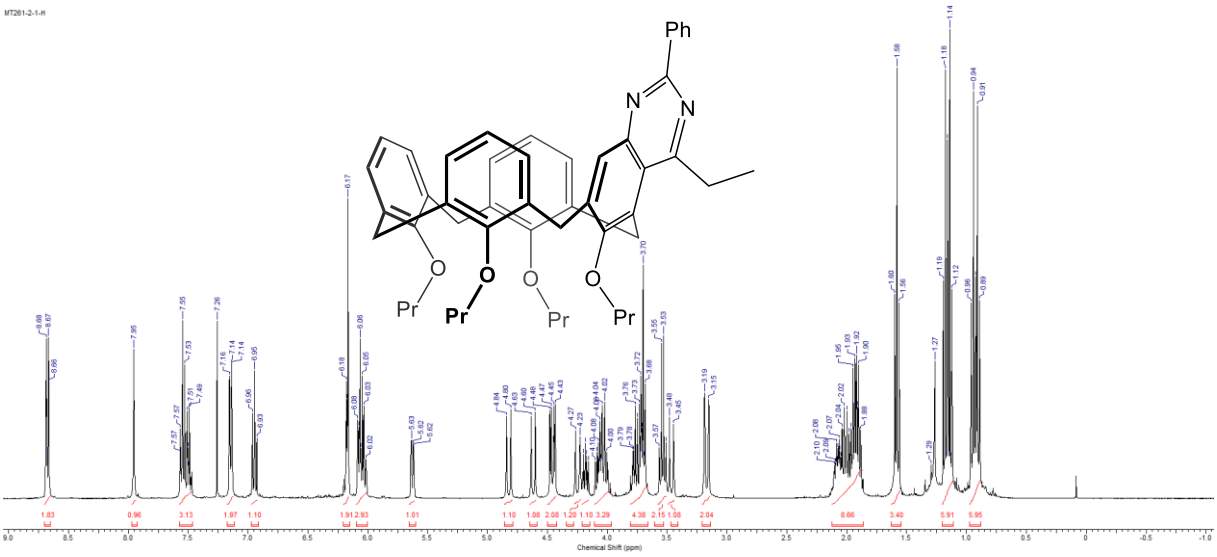


Figure 31: ^{1}H NMR of compound **8ac** ($CDCl_3$, 400 MHz).

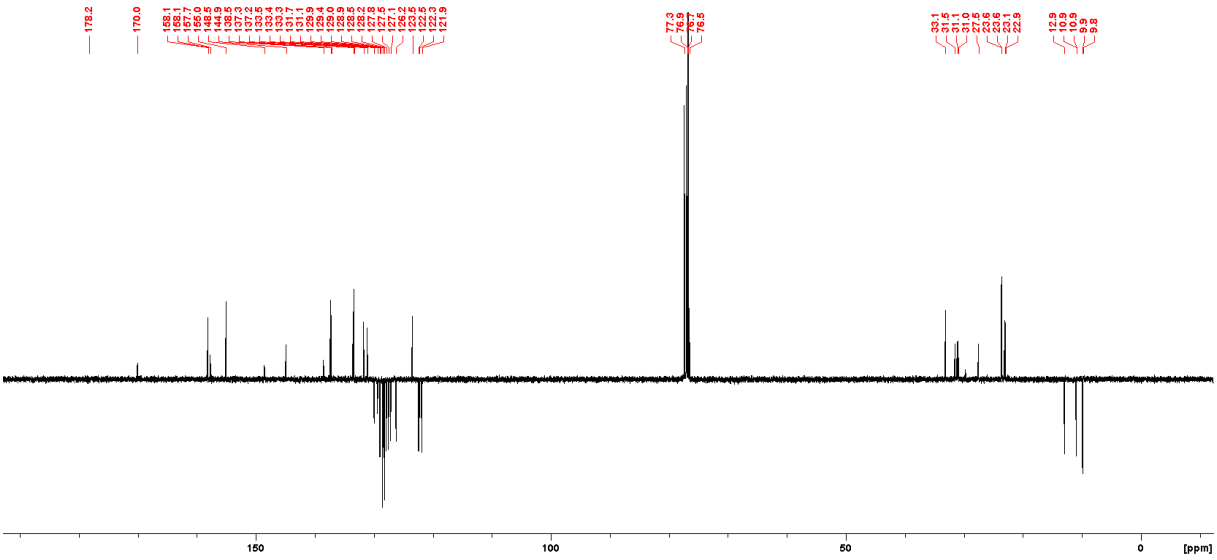


Figure 32: ^{13}C(APT) NMR of compound **8ac** ($CDCl_3$, 100 MHz).

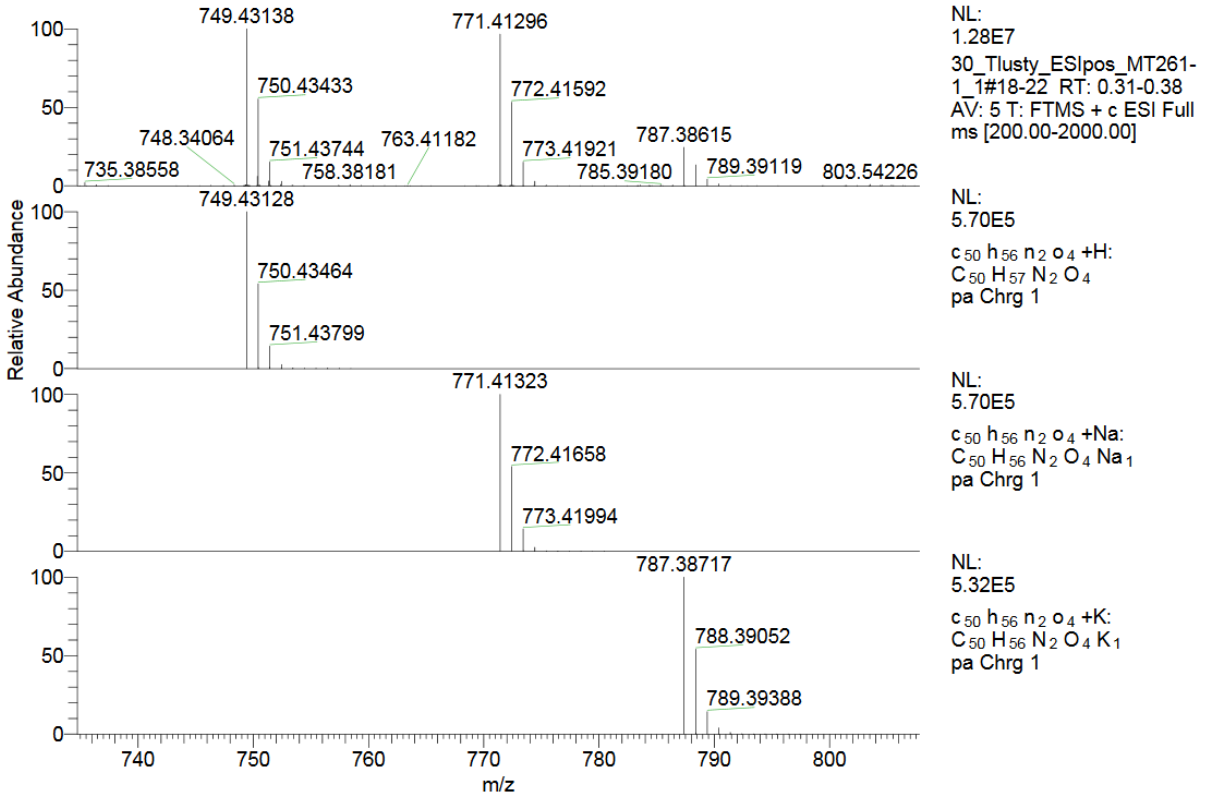


Figure 33: HRMS of compound **8ac** (ESI^+).

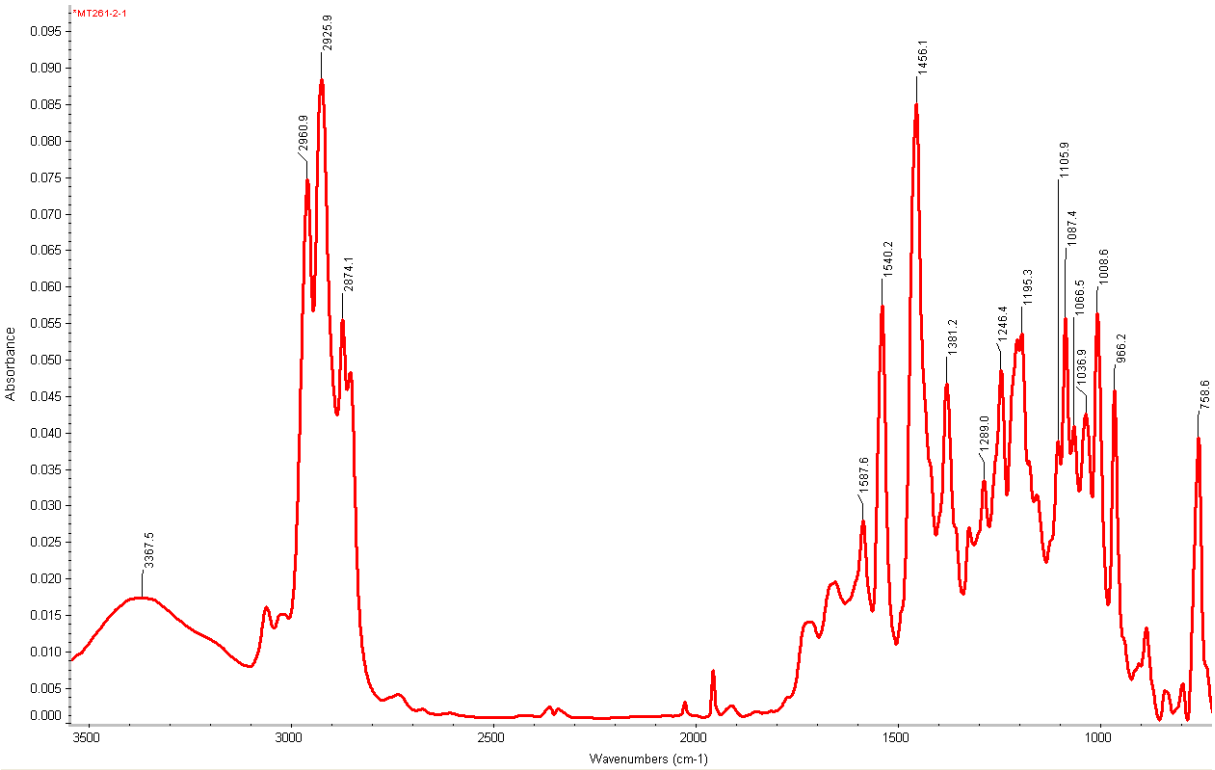


Figure 34: IR of compound **8ac** (KBr).

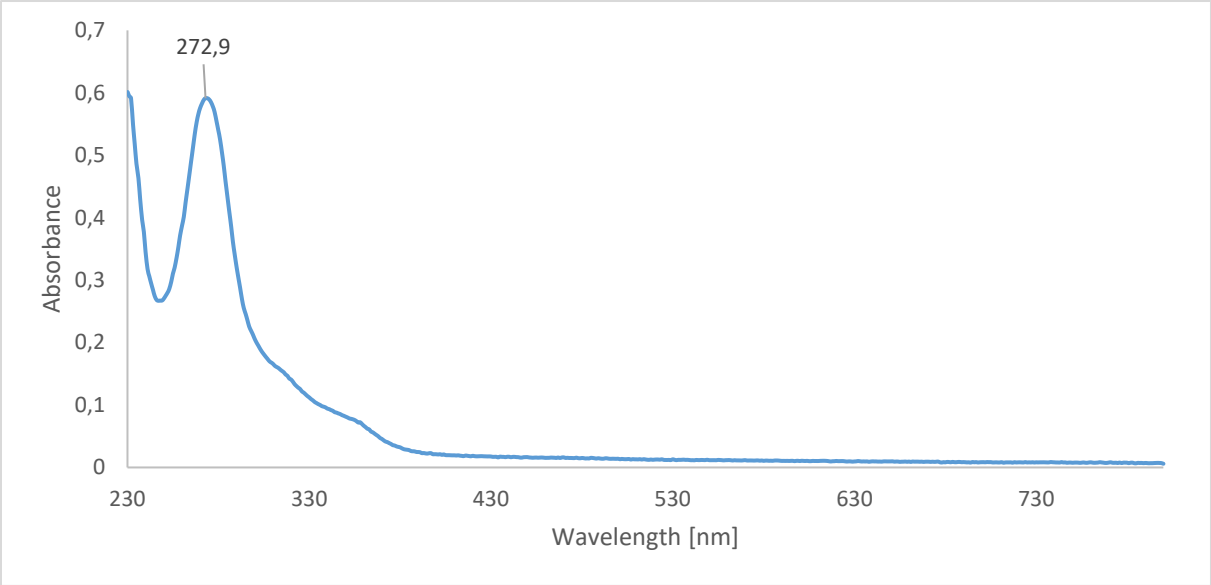


Figure 35: UV of compound **8ac** (CH_2Cl_2).

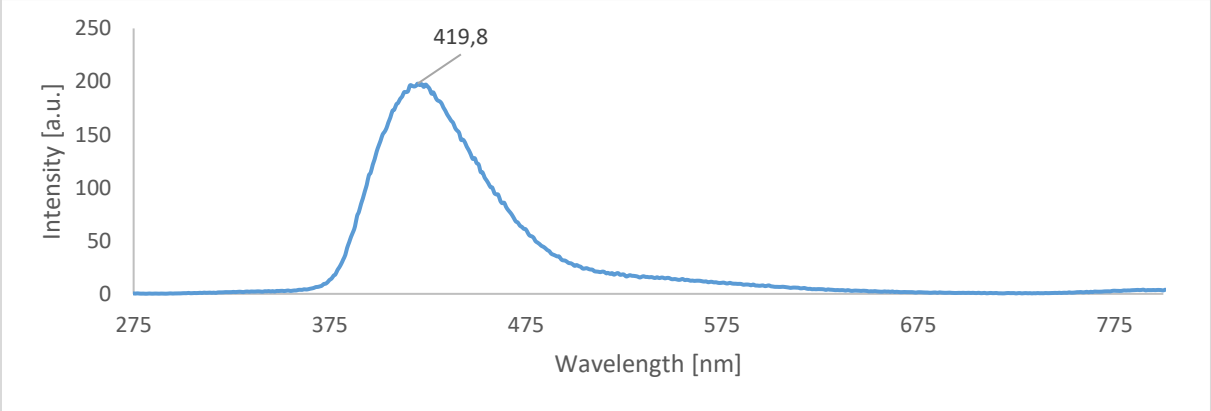


Figure 36: Fluorescence of compound **8ac** (CH_2Cl_2, excitation wavelength 273 nm).

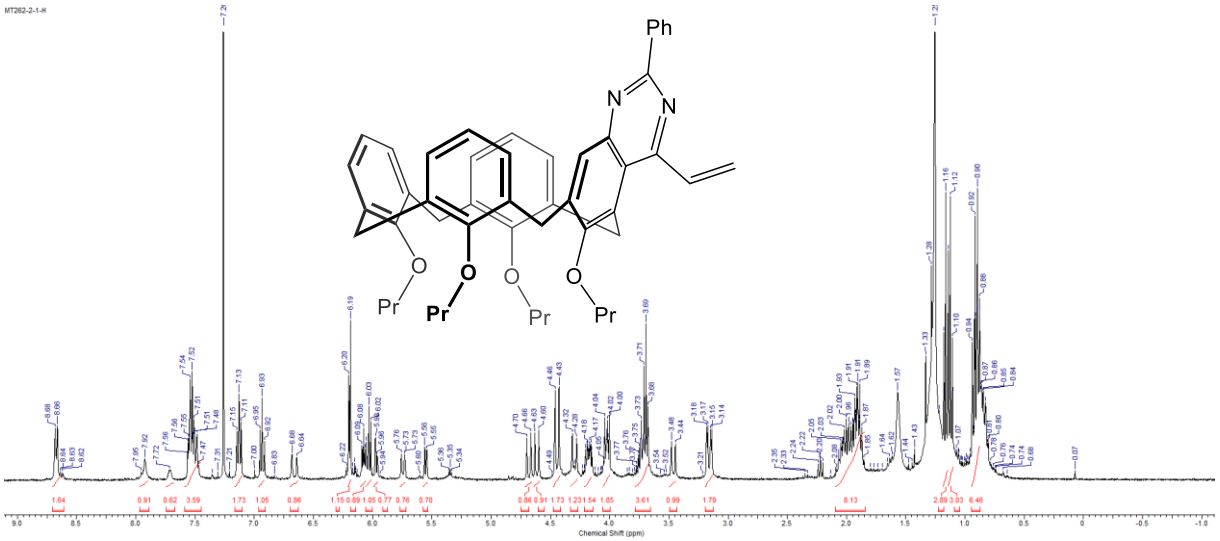


Figure 37: ^{1}H NMR of compound **8ad** ($CDCl_3$, 400 MHz).

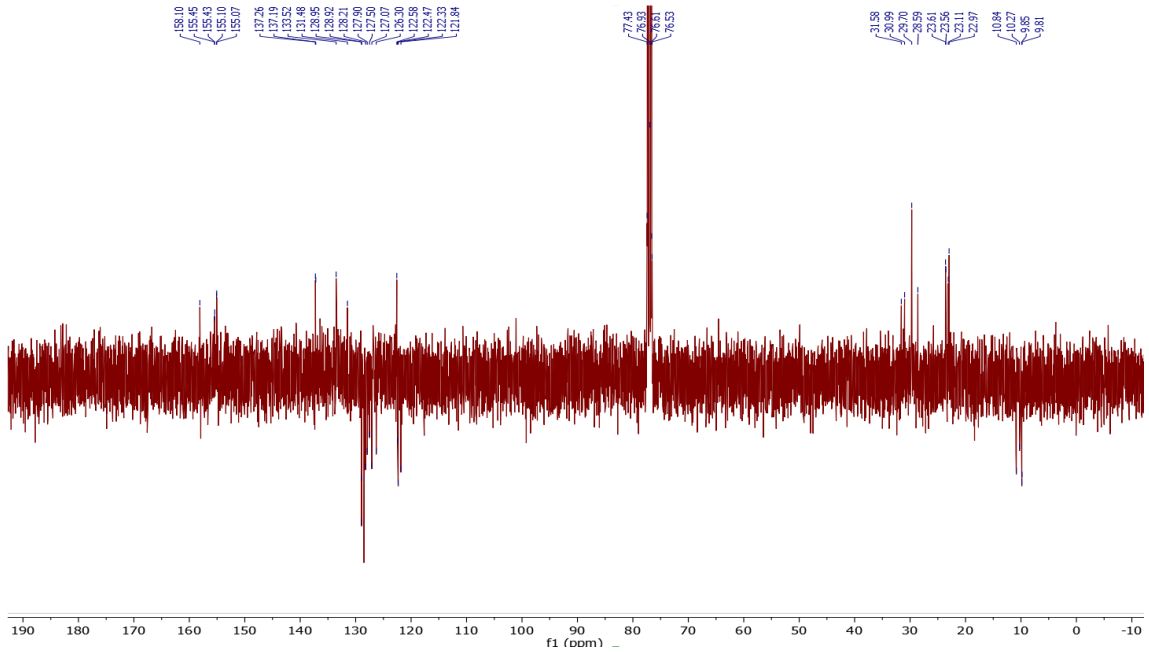


Figure 38: ^{13}C(APT) NMR of compound **8ad** ($CDCl_3$, 100 MHz).

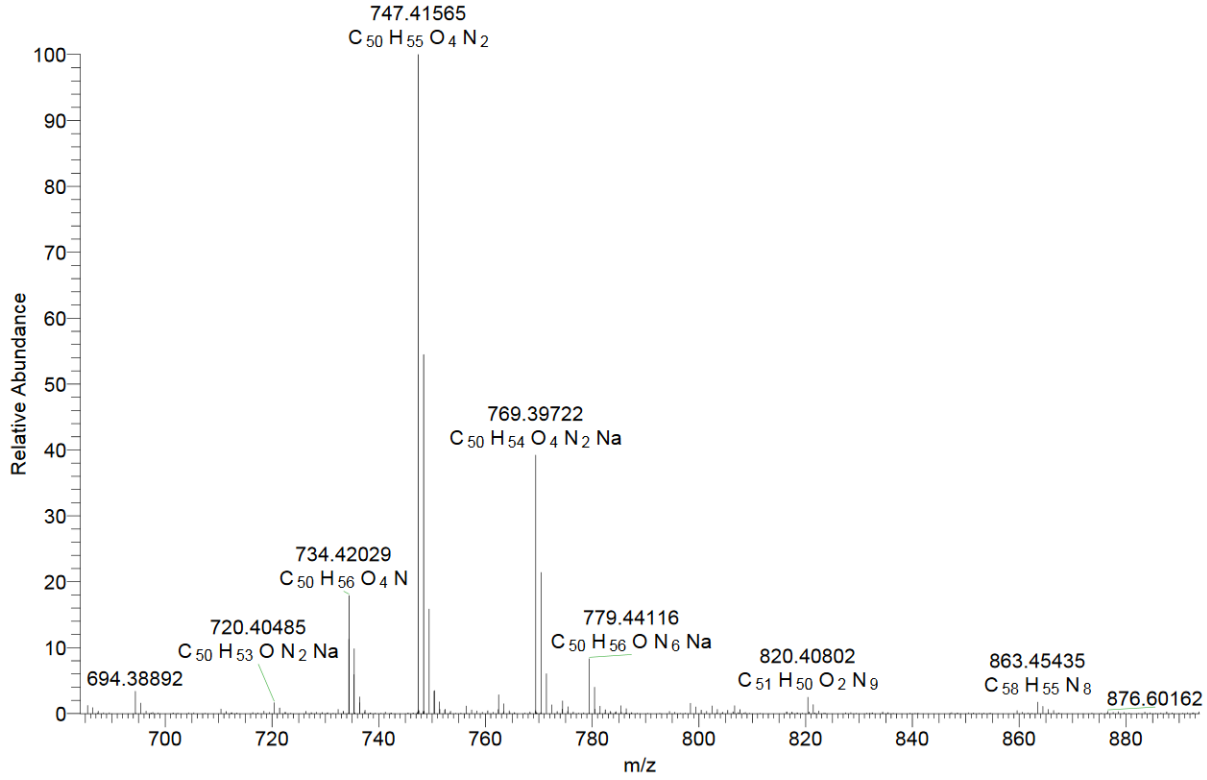


Figure 39: HRMS of compound **8ad** (ESI^+).

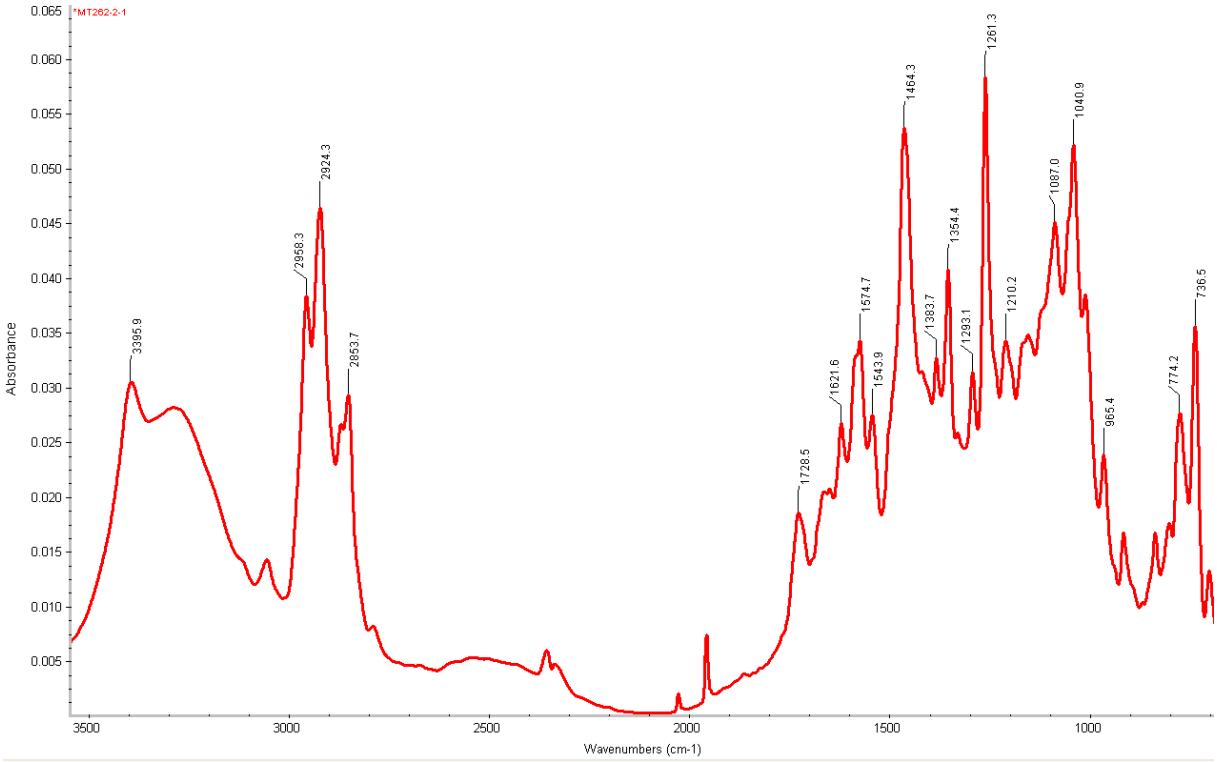


Figure 40: IR of compound **8ad** (KBr).

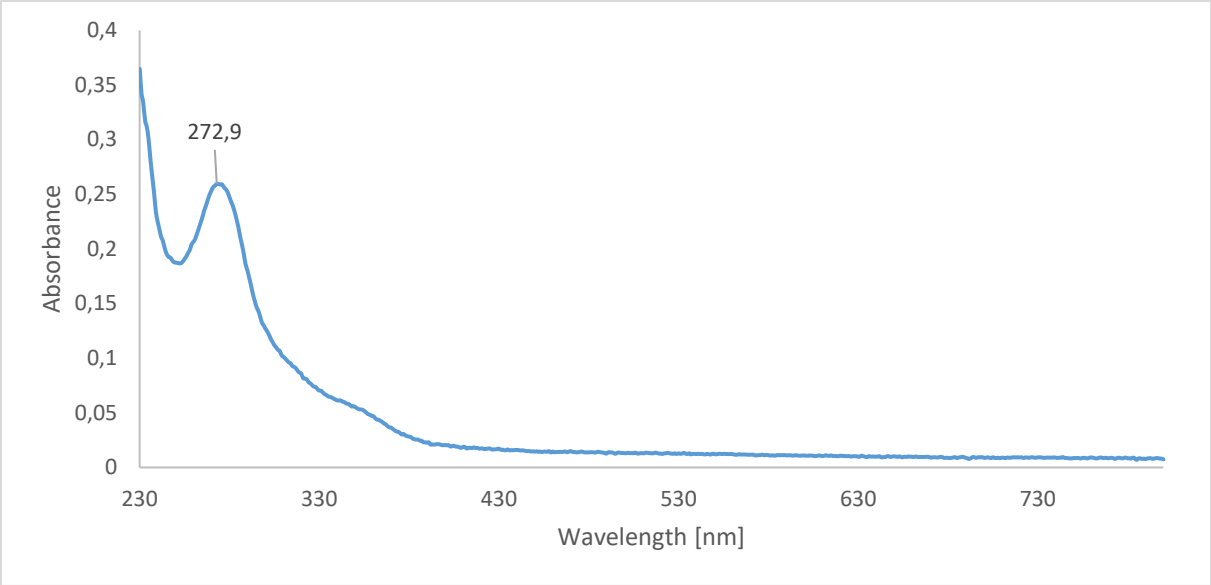


Figure 41: UV of compound **8ad** (CH_2Cl_2).

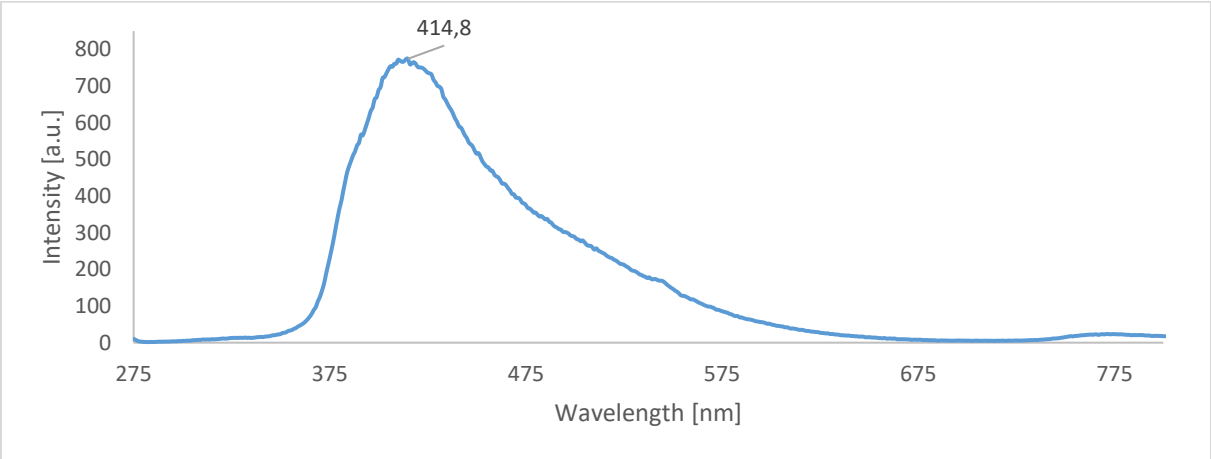


Figure 42: Fluorescence of compound **8ad** (CH_2Cl_2, excitation wavelength 273 nm).

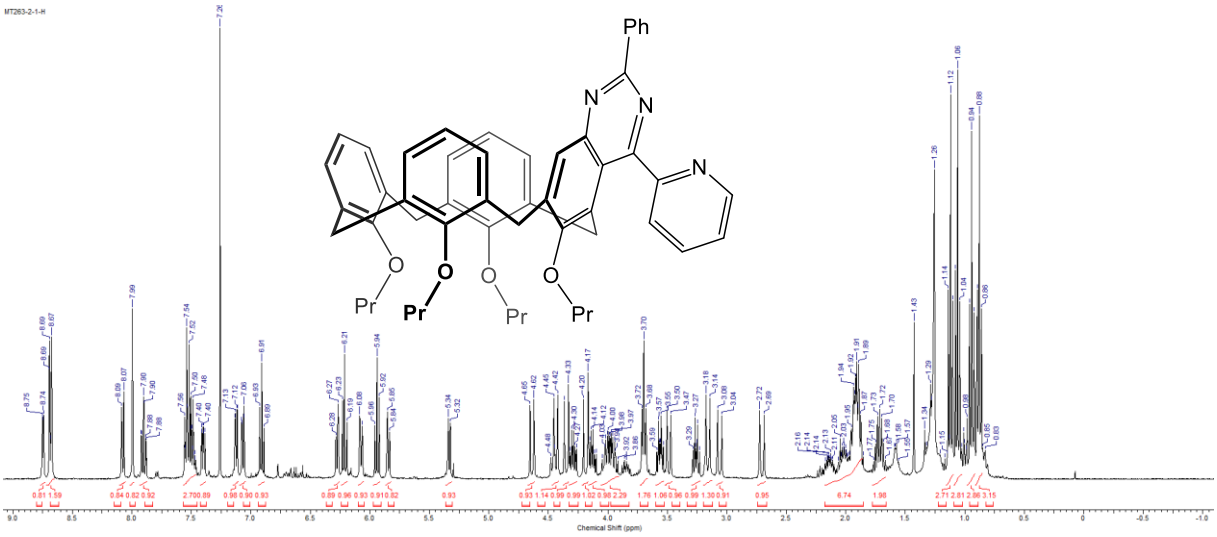


Figure 43: ^{1}H NMR of compound **8ae** ($CDCl_3$, 400 MHz).

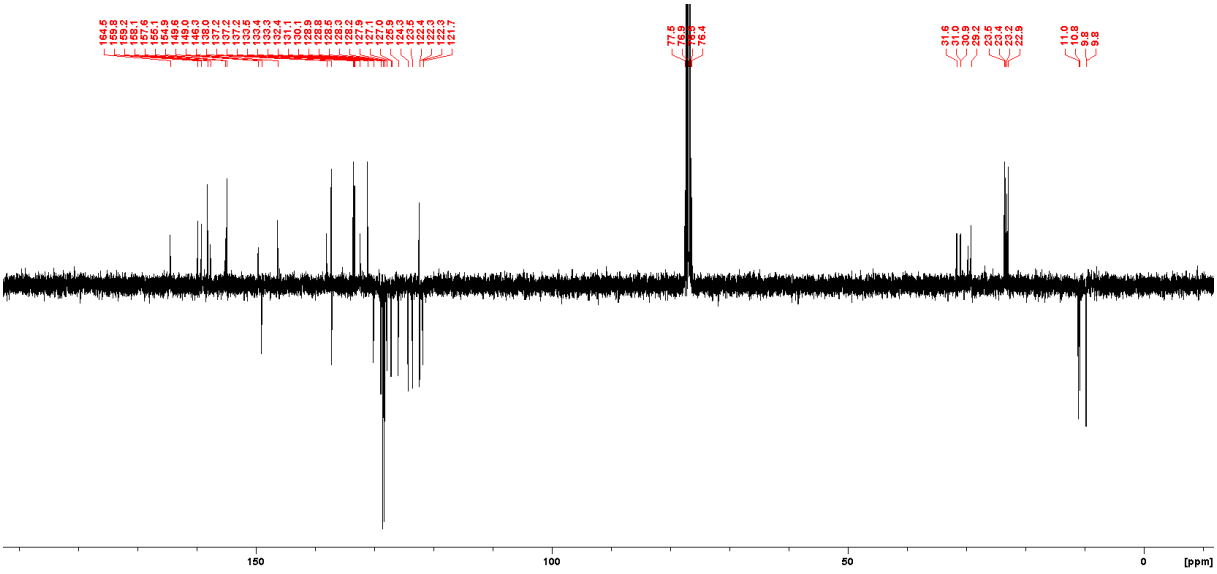


Figure 44: ^{13}C(APT) NMR of compound **8ae** ($CDCl_3$, 100 MHz).

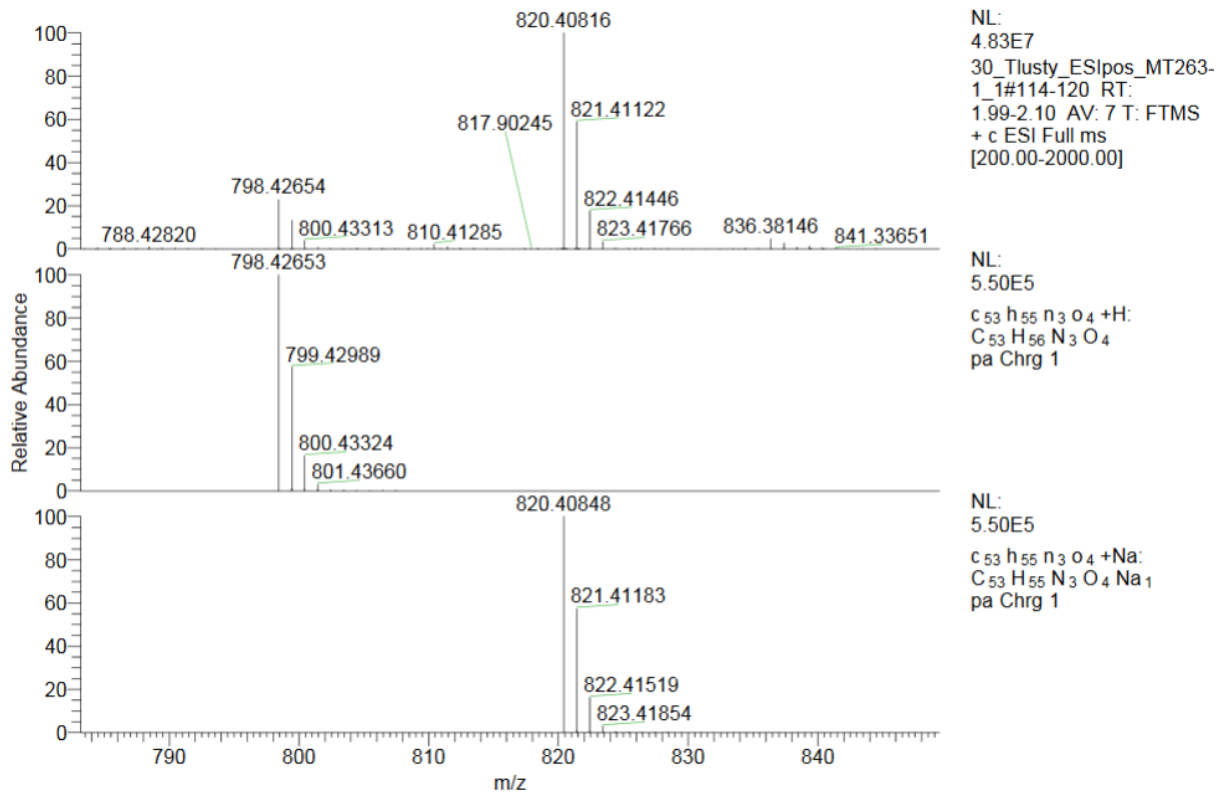


Figure 45: HRMS of compound **8ae** (ESI^+).

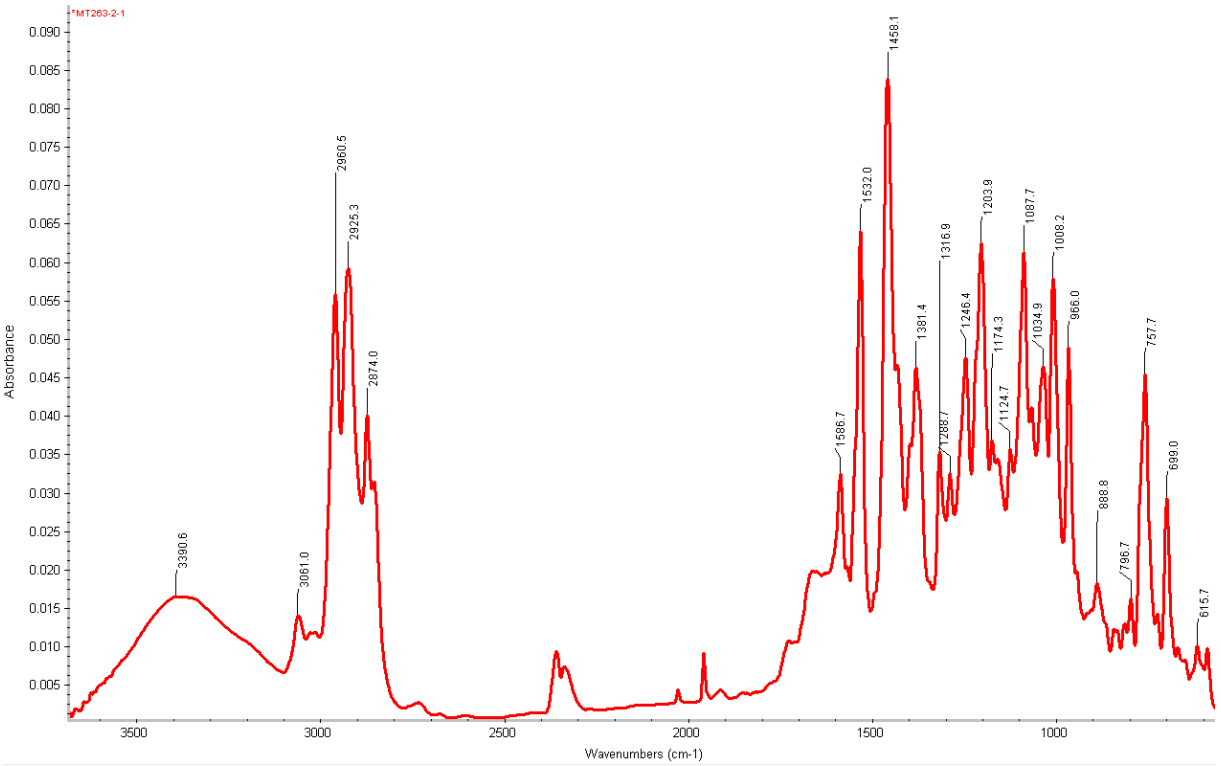


Figure 46: IR of compound **8ae** (KBr).

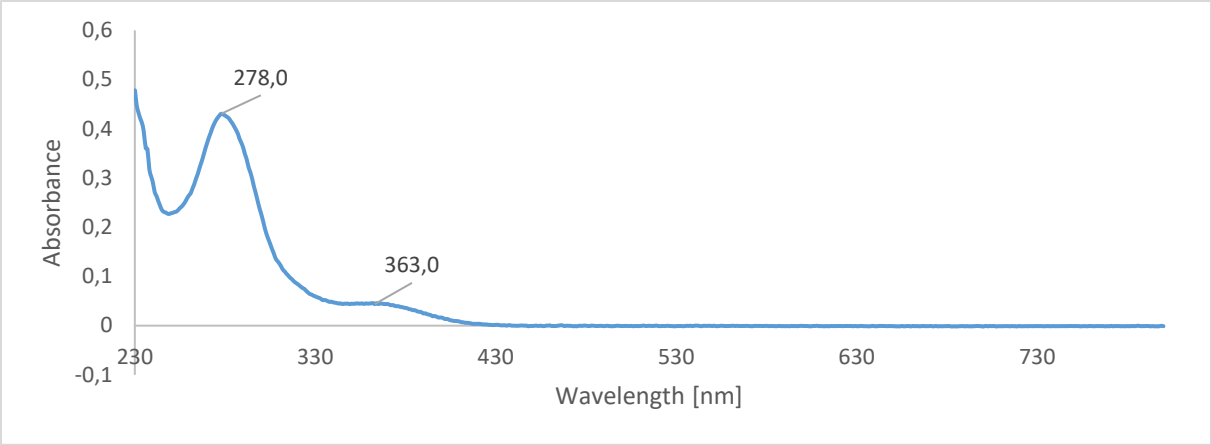


Figure 47: UV of compound **8ae** (CH_2Cl_2).

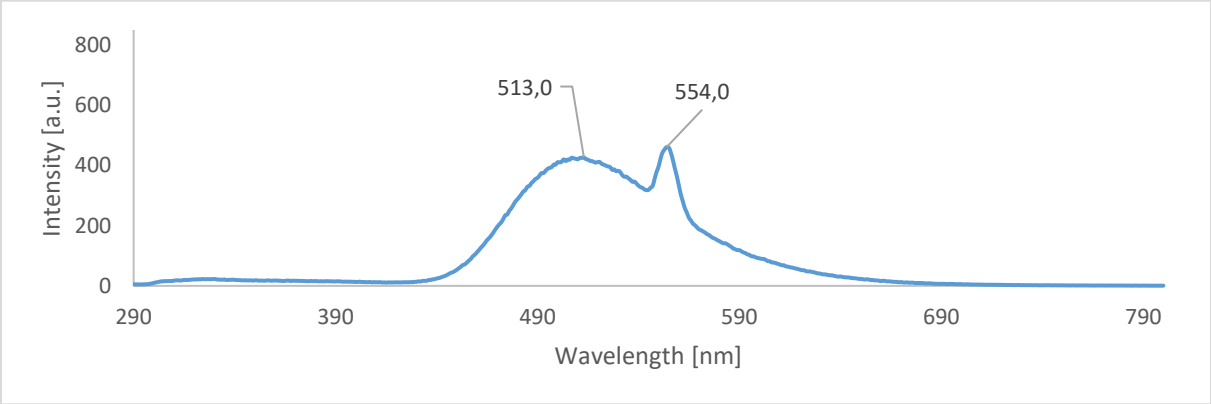


Figure 48: Fluorescence of compound **8ae** (CH_2Cl_2, excitation wavelength 278 nm).

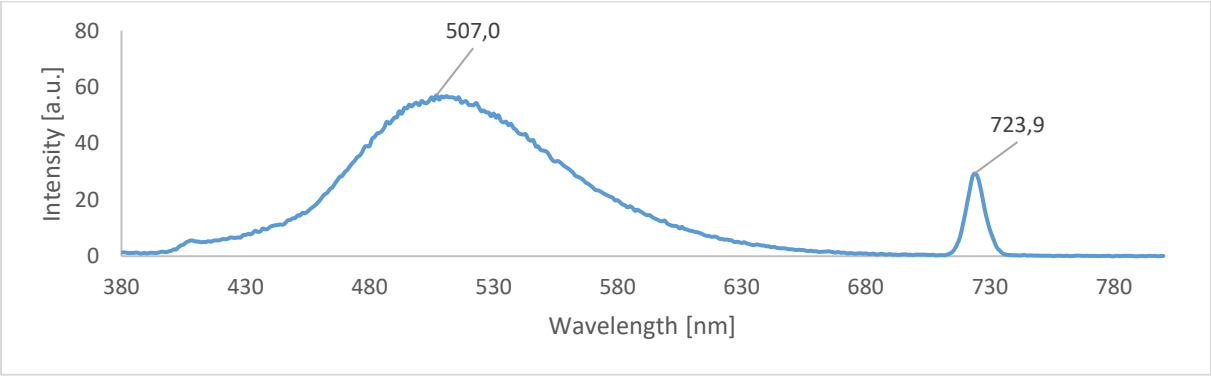


Figure 49: Fluorescence of compound **8ae** (CH_2Cl_2, excitation wavelength 363 nm).

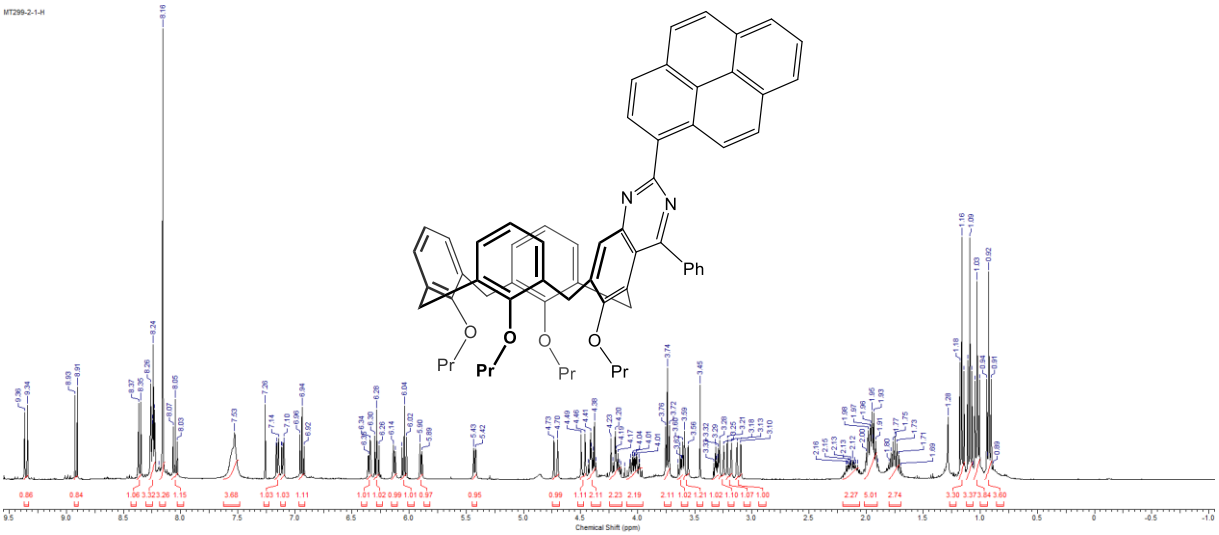


Figure 50: ^{1}H NMR of compound **8ba** ($CDCl_3$, 400 MHz).

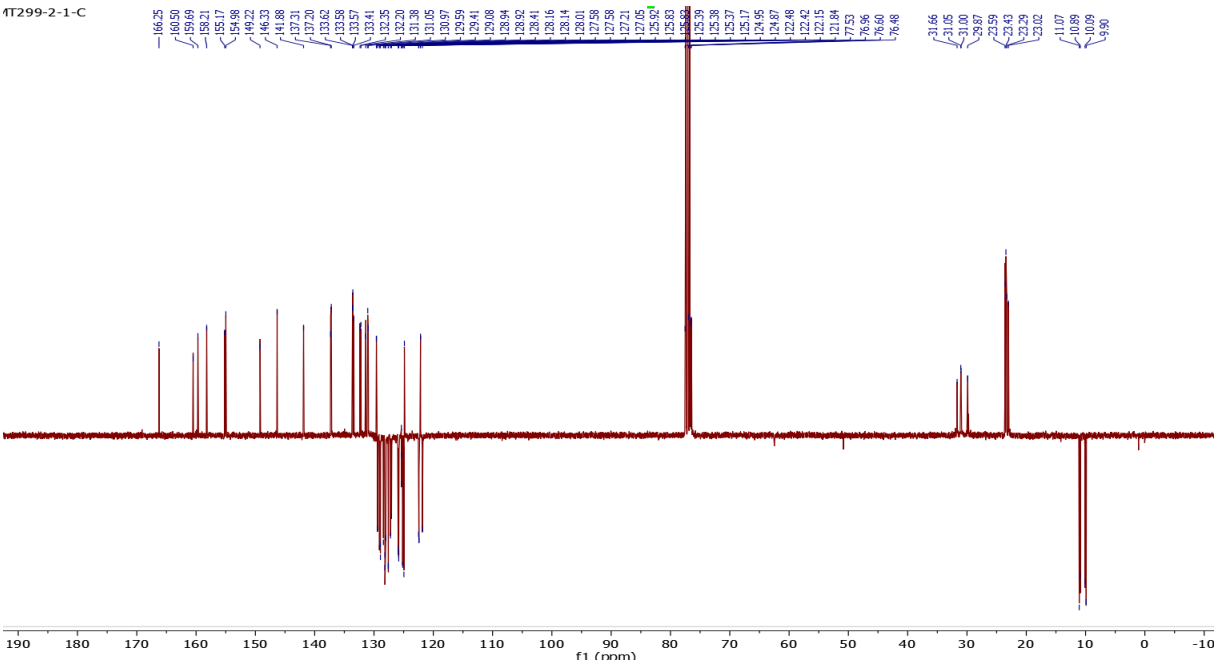


Figure 51: ^{13}C(APT) NMR of compound **8ba** ($CDCl_3$, 100 MHz).

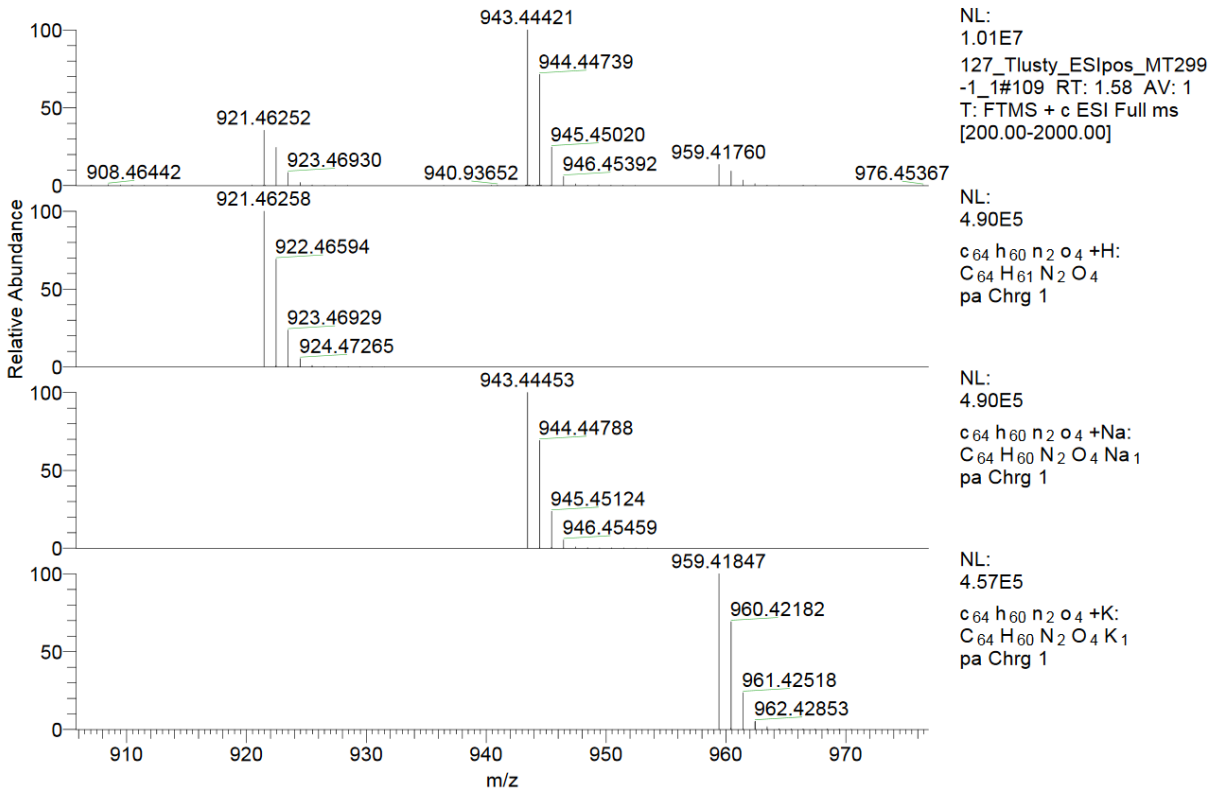


Figure 52: HRMS of compound **8ba** (ESI^+).

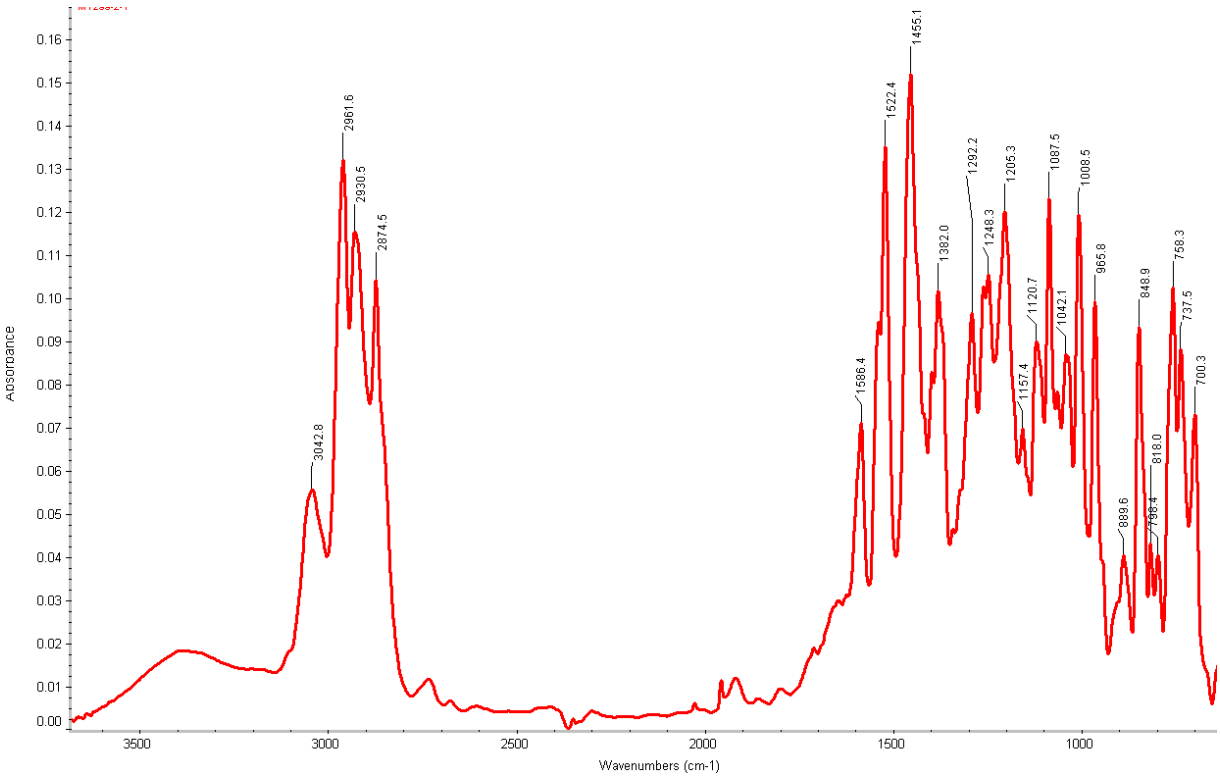


Figure 53: IR of compound **8ba** (KBr).

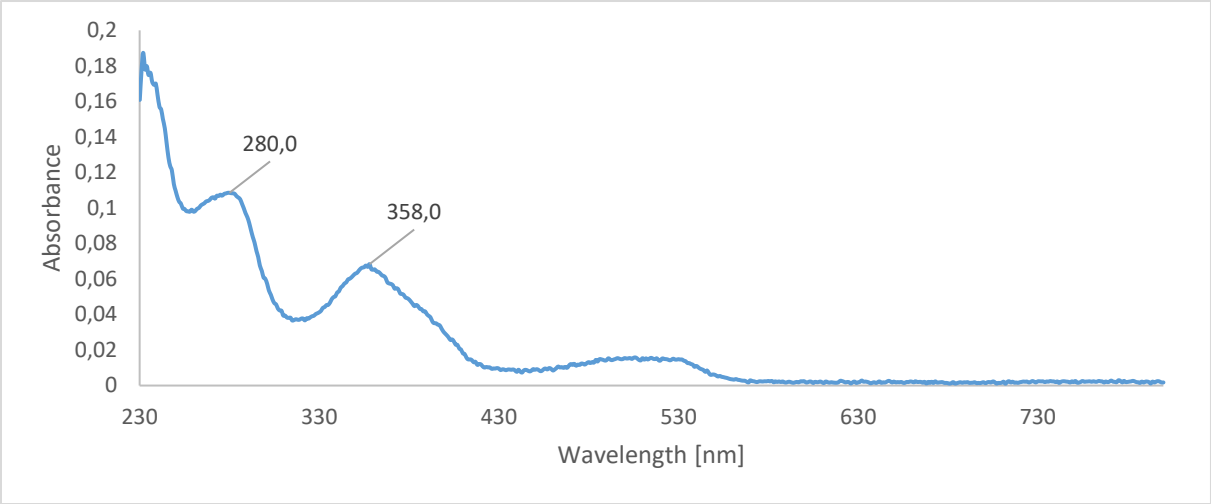


Figure 54: UV of compound **8ba** (CH_2Cl_2).

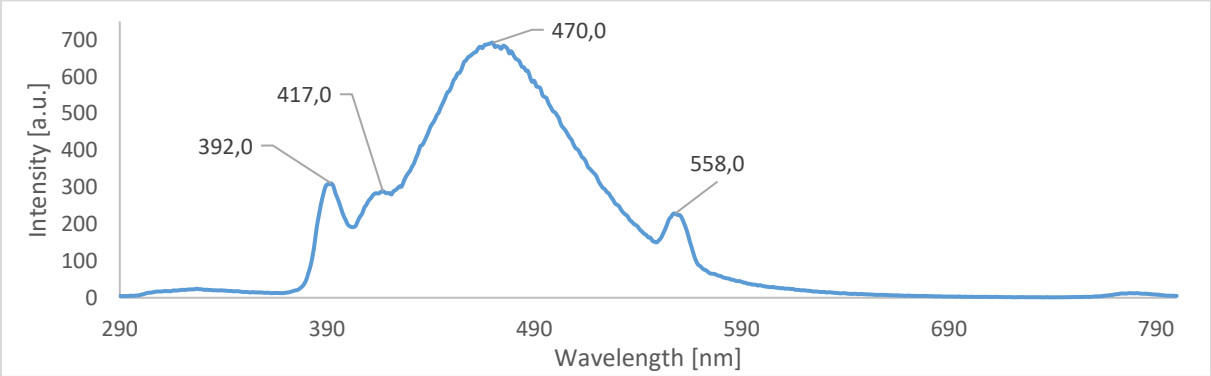


Figure 55: Fluorescence of compound **8ba** (CH_2Cl_2, excitation wavelength 280 nm).

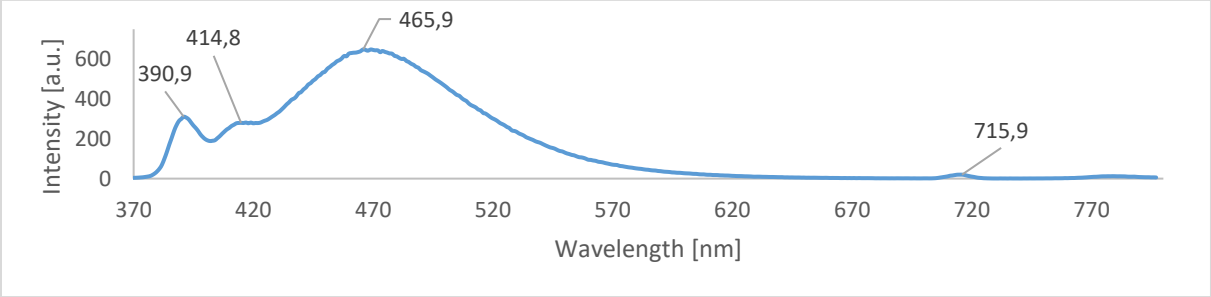


Figure 56: Fluorescence of compound **8ba** (CH_2Cl_2, excitation wavelength 358 nm).

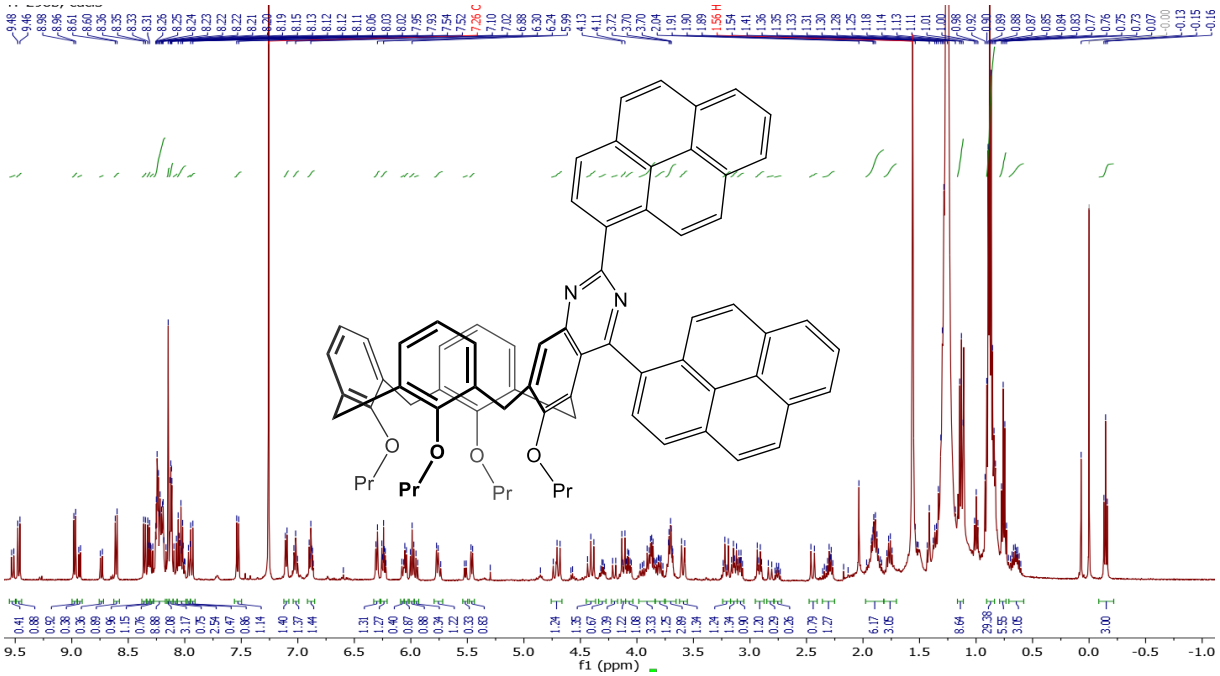


Figure 57: ^{1}H NMR of compound **8bb** ($CDCl_3$, 400 MHz).

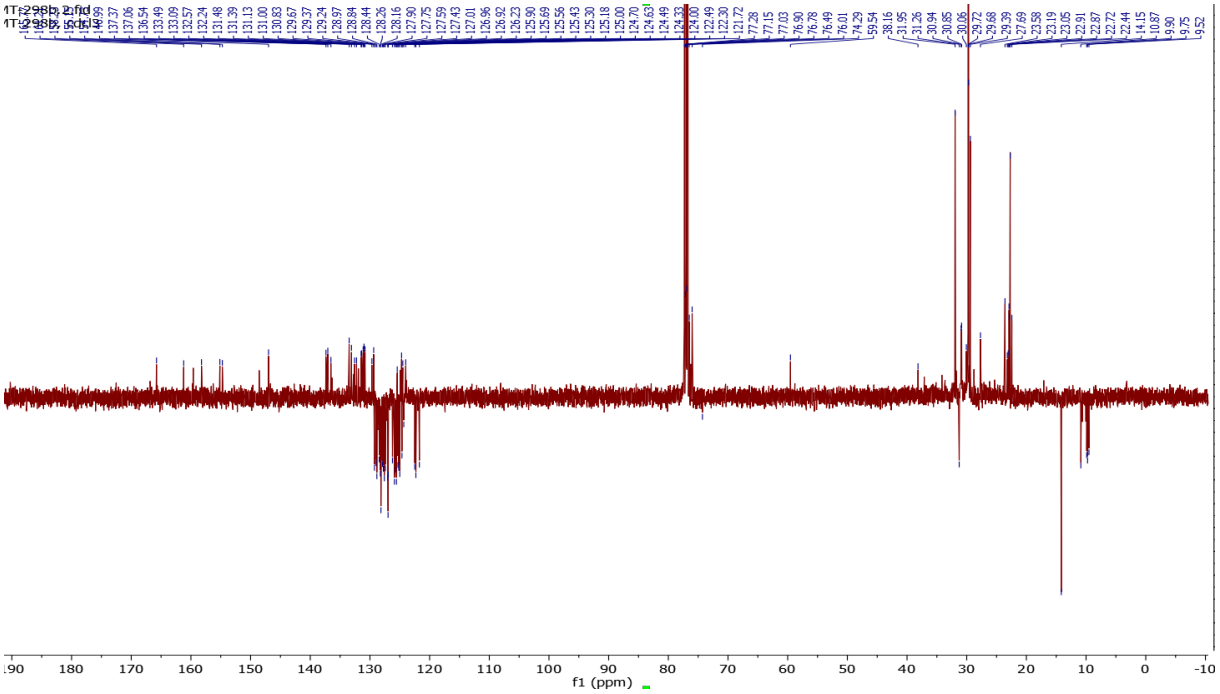


Figure 58: ^{13}C(APT) NMR of compound **8bb** ($CDCl_3$, 100 MHz).

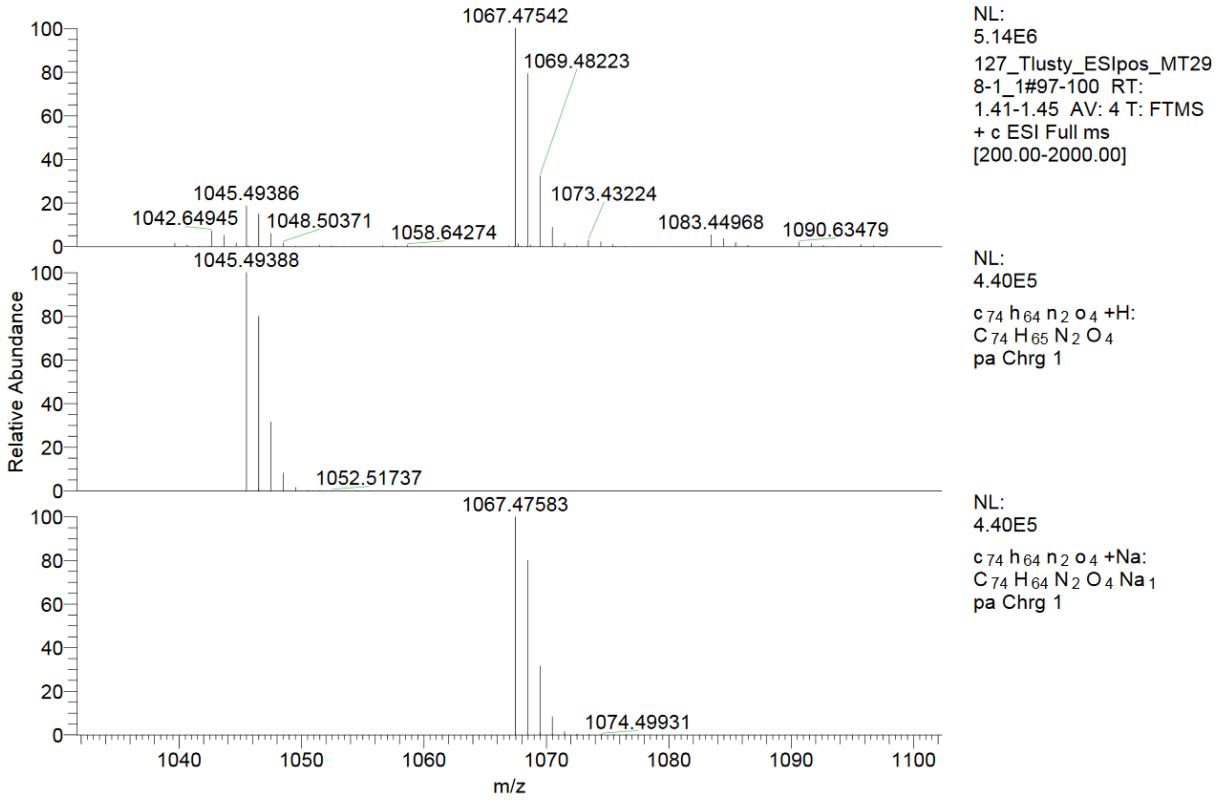


Figure 59: HRMS of compound **8bb** (ESI^+).

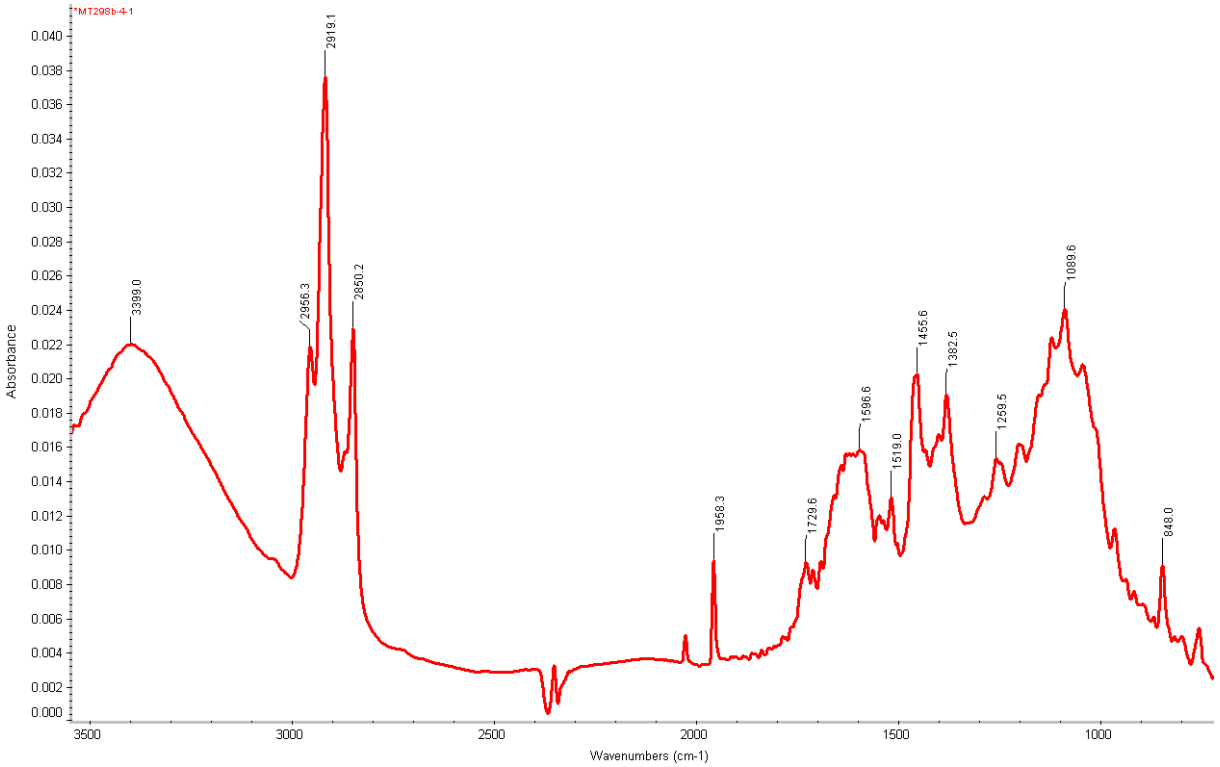


Figure 60: IR of compound **8bb** (KBr).

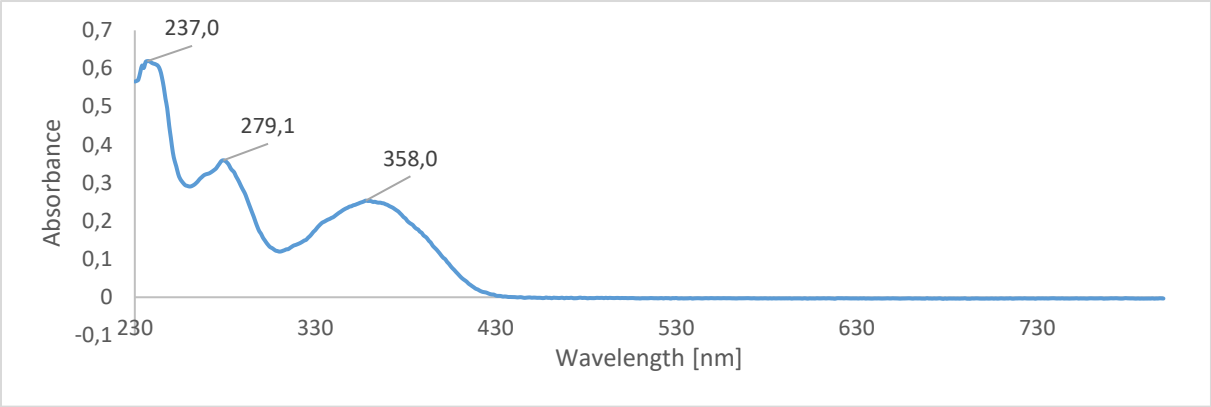


Figure 61: UV of compound **8bb** (CH_2Cl_2).

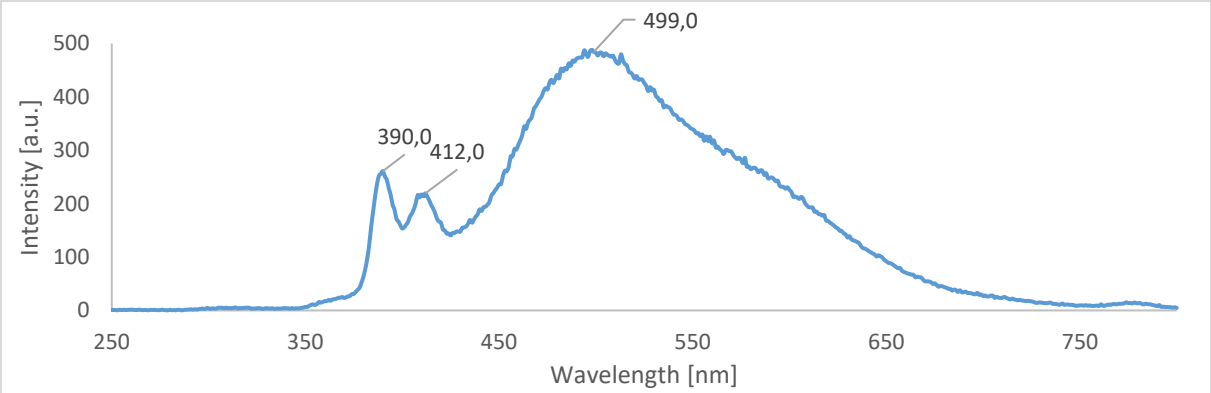


Figure 62: Fluorescence of compound **8bb** (CH_2Cl_2, excitation wavelength 237 nm).

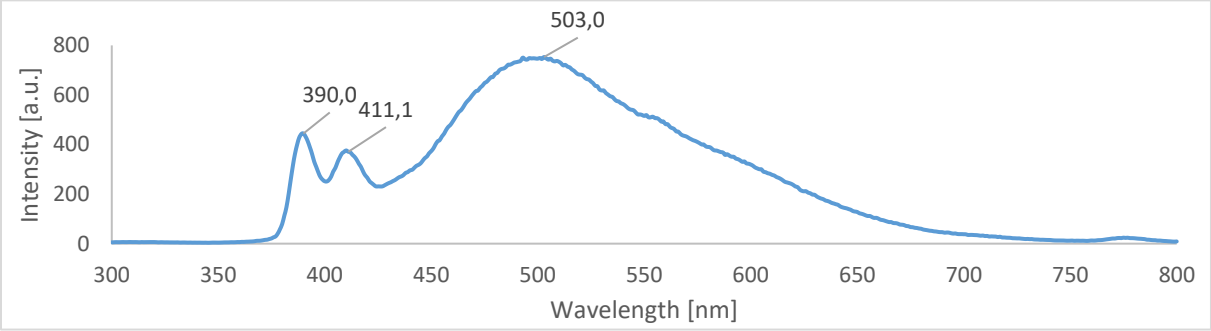


Figure 63: Fluorescence of compound **8bb** (CH_2Cl_2, excitation wavelength 279 nm).

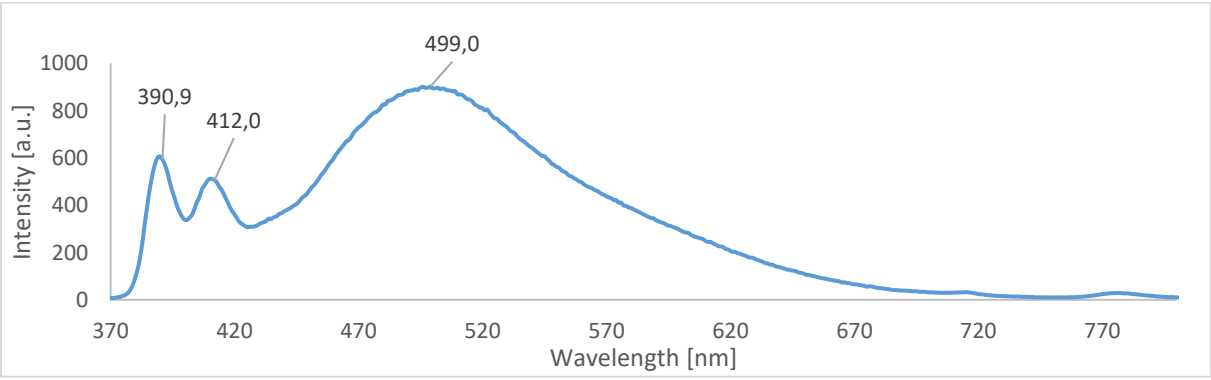


Figure 64: Fluorescence of compound **8bb** (CH_2Cl_2, excitation wavelength 358 nm).

2. Dynamic NMR measurements

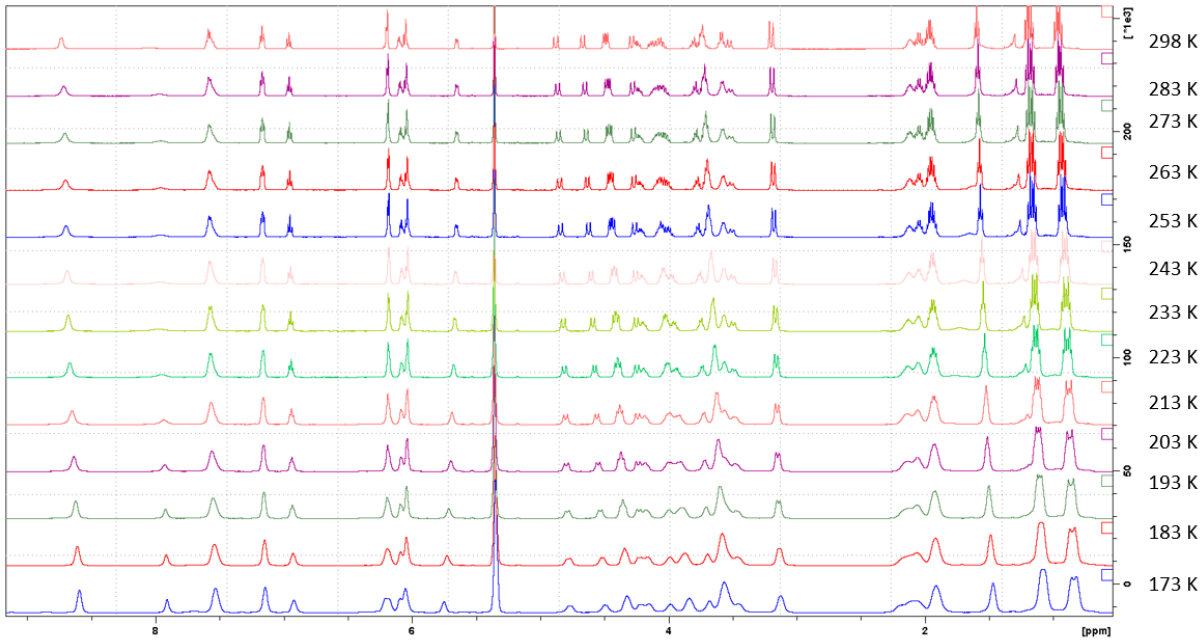


Figure 65: Dynamic ^{1}H NMR measurements of **8ac** (298 – 173 K, CD_2Cl_2, 500 MHz)

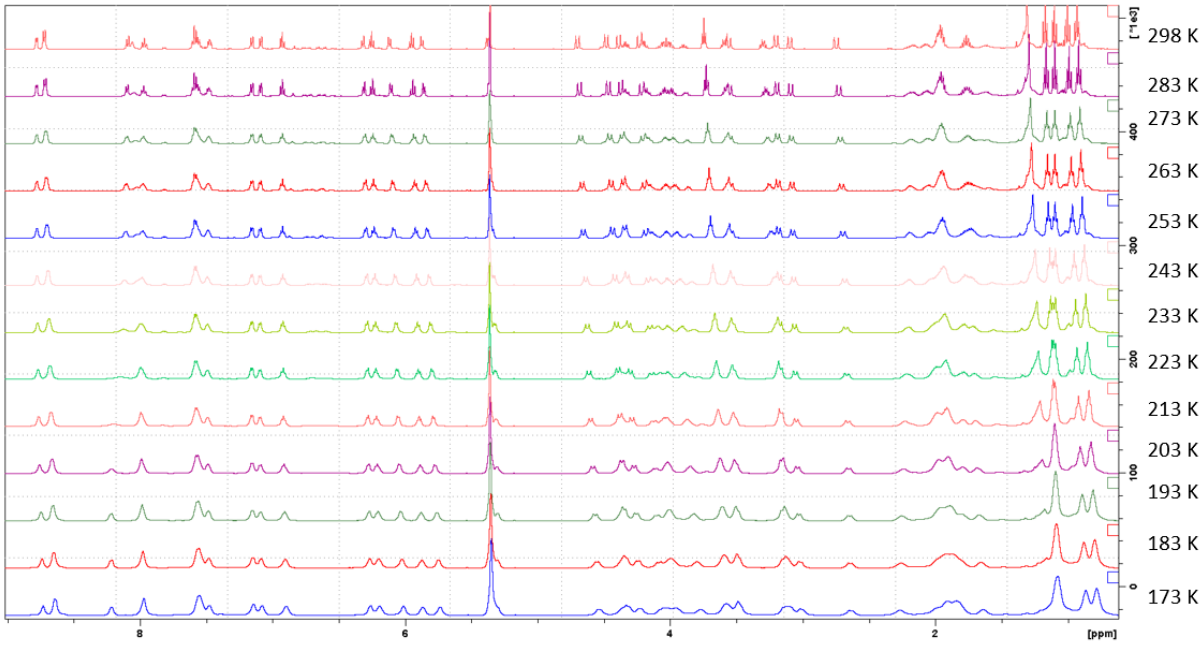


Figure 66: Dynamic ^{1}H NMR measurements of **8ae** (298 – 173 K, CD_2Cl_2, 500 MHz)

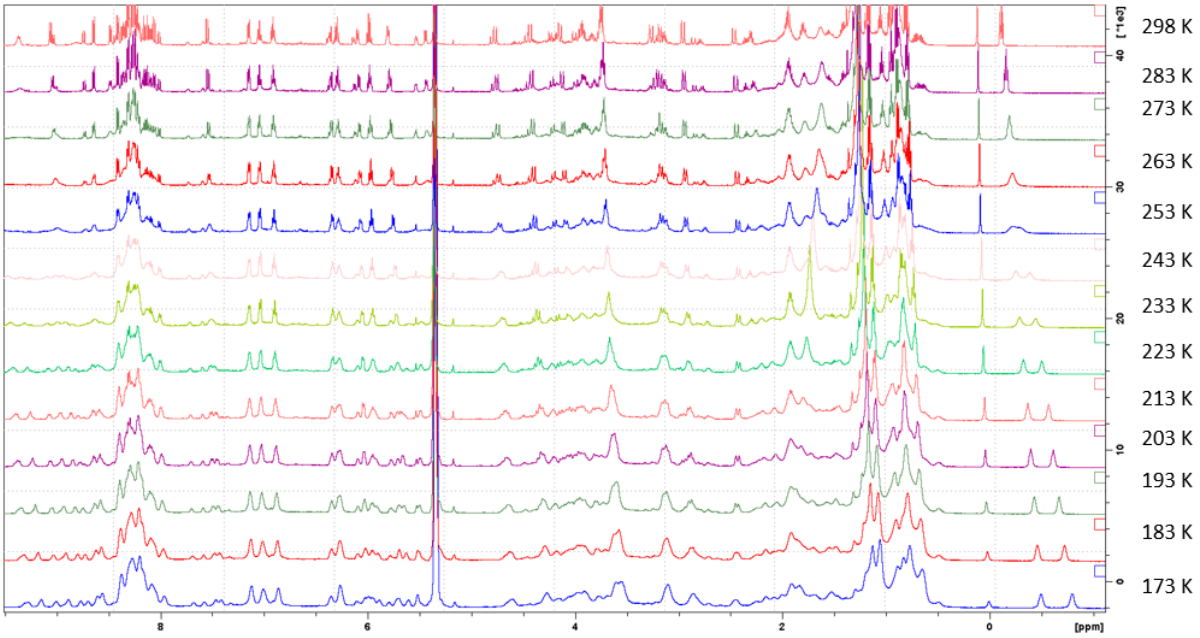


Figure 67: Dynamic ^{1}H NMR measurements of **8ae** (298 – 173 K, CD_2Cl_2, 500 MHz)

3. Chiral separation and ECD spectra

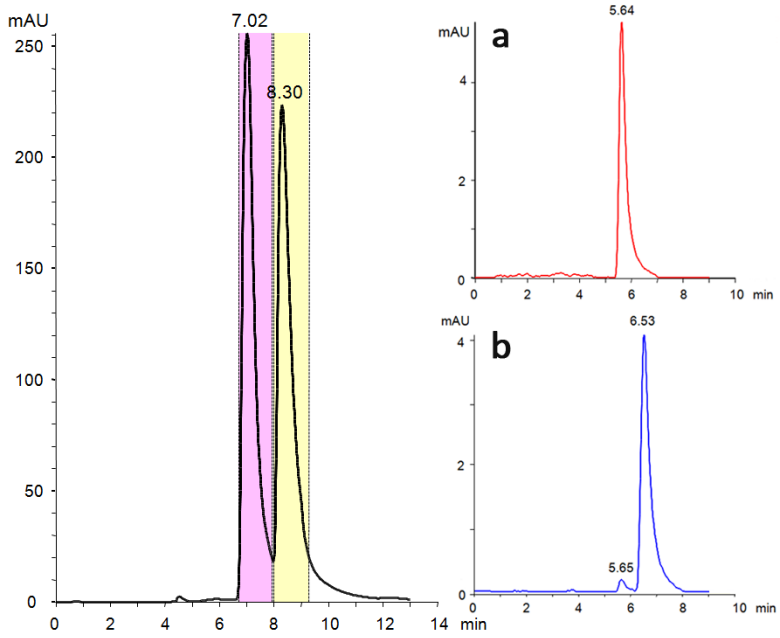


Figure 68: Preparative separation of **8aa** on Chiralpak IA (250×20 mm ID, 5 µm); the collected intervals of peaks are marked in colour. The analytical fraction purity control on ChiralArt Amylose-SA (250×4.6 mm ID, 5 µm) is depicted in the inset on the right: a) the first eluting enantiomer (**8aa-1**), b) the second eluting enantiomer (**8aa-2**).

The enantiomeric character of the separated substances **8aa-1** and **8aa-2** was verified by ECD spectroscopy using Jasco J-810 (Jasco).

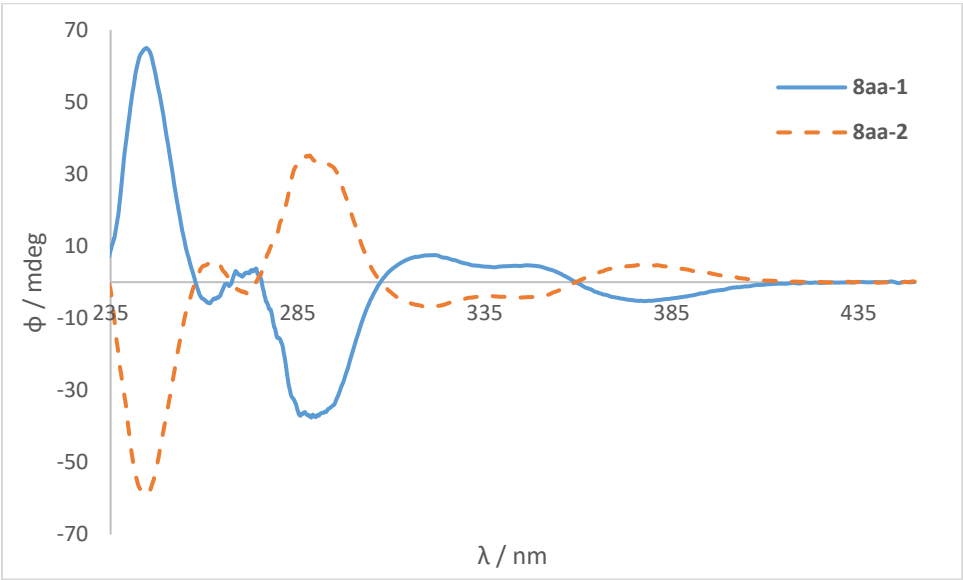


Figure 69: ECD spectra of both separated enantiomers of **8aa** in MeOH, the first eluting enantiomer **8aa-1** full (blue) line, the second eluting enantiomer **8aa-2** dashed (orange) line.

4. Crystallographic data

Crystallographic data for ***8aa***

Data were collected at 180 (2) K on a D8 Venture Photon CMOS diffractometer with Incoatec microfocus sealed tube Cu-Kα radiation. M = 813.07 $g \cdot mol^{-1}$, monoclinic system, space group P21/c , a = 9.5527(2) Å, b = 17.1196(4) Å, c = 28.2418(6) Å, β = 91.7686(8)°, Z = 4, V = 4616.42(17) $Å^3$, D_c = 1.170 $g \cdot cm^{-3}$, μ(Cu-Kα) = 0.576 mm^{-1} , crystal dimensions of 0.169 × 0.185 × 0.449 mm. The structure was solved by direct methods[17] and anisotropically refined by full matrix least squares on F squared using the CRYSTALS suite of programs[18] to final value R = 0.059 and wR = 0.155 using 9364 independent reflections (Θmax = 74.4°), 560 parameters and 0 restrains. The hydrogen atoms were placed in calculated positions and refined with riding constrains. The structure was deposited into Cambridge Structural Database under number CCDC 1985895.

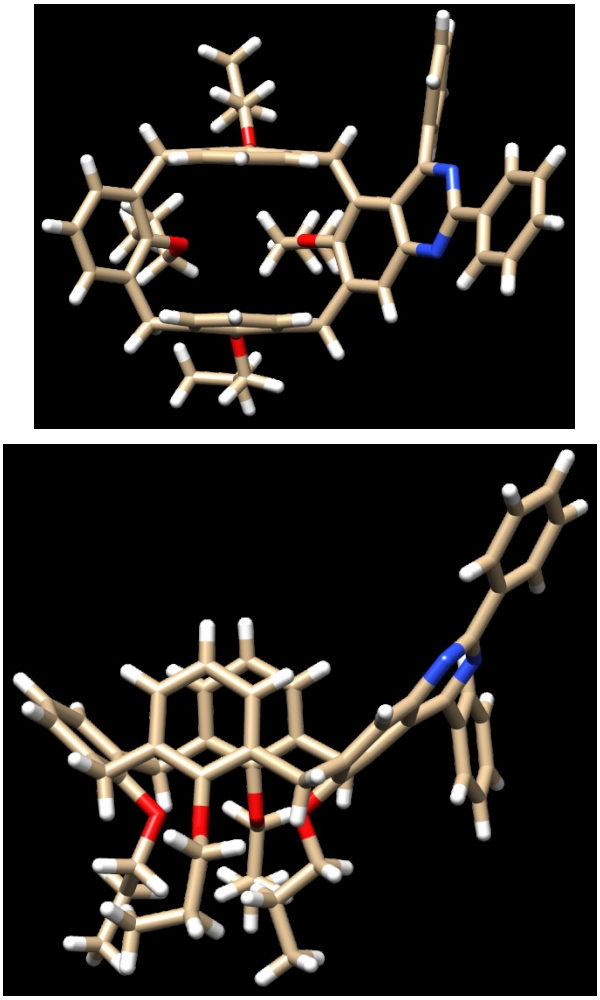


Figure 70: X-ray structure of compound **8aa**

17. A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. C. Burla, G. Polidori and M. Camalli, *J. Appl. Crystallogr.*, 1994, **27**, 435-436.
18. P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout and D. J. Watkin, *J. Appl. Crystallogr.*, 2003, **36**, 1487.

5. Titration experiments

Calixarene **8aa** was dissolved in specified amount of CH_2Cl_2 (solution 1). 0.9 ml of calixarene solution 1 was put in a volumetric flask and diluted to total volume of 5 ml (solution 2). 2.5 ml of solution 2 was put to a fluorescence cuvette. Specified amount of *N*-methylquinolinium iodide (NMQI) was put to another volumetric flask, 0.9 ml of solution 1 was added and the solution was diluted to total volume of 5 ml (solution 3). The aliquots of NMQI were gradually added to fluorescence tube to achieve different calixarene/guest rations (1:0.000-29.258), ensuring constant host concentration during the experiment. The complexation constants were determined by analyzing fluorescence intensity using nonlinear curve-fitting procedure (program BindFit).

	V (total) [m	V(addition, total) [n	V(addition) [ml]	c(NMQI) [mol/l]	c(**8aa**) [mol/l]	c(NMQI)/c(**8a**	fluorescer	fluorescer	fluorescer
1	2.500000	0.000000	0.000000	0.000000	0.000131	0.000000	259.4109	214.634	172.8671
2	2.503000	0.003000	0.003000	0.000017	0.000131	0.131502	260.0261	216.1471	173.4606
3	2.510000	0.010000	0.007000	0.000057	0.000131	0.437119	255.4534	213.2857	168.7682
4	2.520000	0.020000	0.010000	0.000114	0.000131	0.870768	248.1394	210.6184	166.4995
5	2.535000	0.035000	0.015000	0.000198	0.000131	1.514828	220.8578	195.1219	153.7419
6	2.563000	0.063000	0.028000	0.000353	0.000131	2.696902	175.3186	163.8034	134.8889
7	2.613000	0.113000	0.050000	0.000621	0.000131	4.744738	130.4499	135.6293	112.7
8	2.681000	0.181000	0.068000	0.000970	0.000131	7.407216	82.97461	99.07418	84.9652
9	2.749000	0.249000	0.068000	0.001302	0.000131	9.937974	54.70518	74.07558	67.35785
10	2.500000	0.300000	0.300000	0.001725	0.000131	13.166019	31.80076	49.06158	46.55412
11	2.600000	0.400000	0.100000	0.002211	0.000131	16.879512	18.80015	35.57058	35.26059
12	2.700000	0.500000	0.100000	0.002661	0.000131	20.317931	13.07971	27.01264	26.90764
13	2.800000	0.600000	0.100000	0.003080	0.000131	23.510748	7.7923	19.87785	20.12643
14	2.900000	0.700000	0.100000	0.003469	0.000131	26.483372	5.599566	15.2689	16.598
15	3.000000	0.800000	0.100000	0.003832	0.000131	29.257820	3.624555	11.72142	13.00782

K	899.1 M^{-1}
Error	53.0621847 M^{-1}

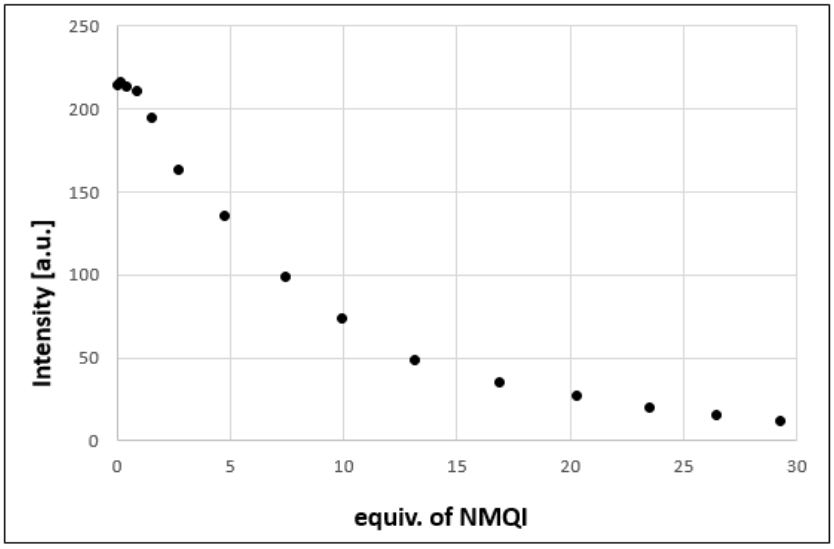


Figure 71: ^{1}H NMR titration of compound **8aa** with NMQI (CH_2Cl_2).

Calixarene **8aa** was dissolved in specified amount of CH_2Cl_2 (solution 1). 0.9 ml of calixarene solution 1 was put in a volumetric flask and diluted to total volume of 5 ml (solution 2). 2.5 ml of solution 2 was put to a fluorescence cuvette. Specified amount of *N*-methylisoquinolinium iodide (NMII) was put to another volumetric flask, 0.9 ml of solution 1 was added and the solution was diluted to total volume of 5 ml (solution 3). The aliquots of NMII were gradually added to fluorescence tube to achieve different calixarene/guest rations (1:0.000-29.829), ensuring constant host concentration during the experiment. The complexation constants were determined by analyzing fluorescence intensity using nonlinear curve-fitting procedure (program BindFit).

	V (total) [m	V(addition, total) [n	V(addition) [ml]	c(NMII) [mol/l]	c(**8aa**) [mol/l]	c(NMII)/c(**8a**	fluorescer	fluorescer
1	2.500000	0.000000	0.000000	0.000000	0.000131	0.000000	199.50	243.23
2	2.503000	0.003000	0.003000	0.000018	0.000131	0.134068	197.76	242.87
3	2.510000	0.010000	0.007000	0.000058	0.000131	0.445646	195.15	234.48
4	2.520000	0.020000	0.010000	0.000116	0.000131	0.887755	186.37	227.34
5	2.535000	0.035000	0.015000	0.000202	0.000131	1.544378	171.23	206.87
6	2.563000	0.063000	0.028000	0.000360	0.000131	2.749511	160.41	193.46
7	2.613000	0.113000	0.050000	0.000634	0.000131	4.837295	123.14	145.56
8	2.681000	0.181000	0.068000	0.000989	0.000131	7.551710	90.53	106.22
9	2.749000	0.249000	0.068000	0.001327	0.000131	10.131836	69.44	80.25
10	2.500000	0.300000	0.300000	0.001758	0.000131	13.422851	41.66	46.33
11	2.600000	0.400000	0.100000	0.002254	0.000131	17.208783	28.83	31.09
12	2.700000	0.500000	0.100000	0.002713	0.000131	20.714276	20.07	20.68
13	2.800000	0.600000	0.100000	0.003140	0.000131	23.969377	14.18	14.46
14	2.900000	0.700000	0.100000	0.003537	0.000131	26.999988	9.61	8.60
15	3.000000	0.800000	0.100000	0.003907	0.000131	29.828558	5.83	6.29

K	697.45 M^{-1}
Error	31.2806325 M^{-1}

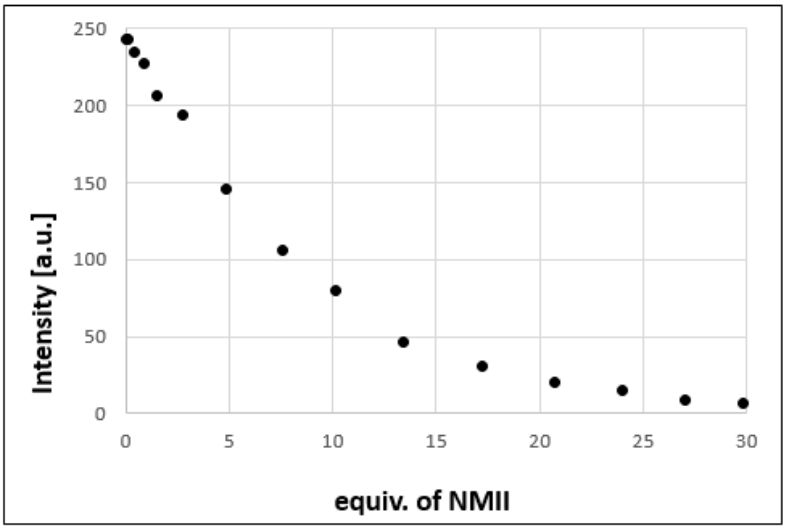


Figure 72: ^{1}H NMR titration of compound **8aa** with NMII (CH_2Cl_2).

Calixarene **8aa-1** was dissolved in specified amount of CH_2Cl_2 (solution 1). 0.55 ml of calixarene solution 1 was put in a volumetric flask and diluted to total volume of 5 ml (solution 2). 2.5 ml of solution 2 was put to a fluorescence cuvette. Specified amount of (*S*)-1-Methyl-3-(1-methylpyrrolidin-2-yl)pyridinium iodide (NMNI) was put to another volumetric flask, 0.55 ml of solution 1 was added and the solution was diluted to total volume of 5 ml (solution 3). The aliquots of NMNI were gradually added to fluorescence tube to achieve different calixarene/guest rations (1:0.000-28.323), ensuring constant host concentration during the experiment. The complexation constants were determined by analyzing fluorescence intensity using nonlinear curve-fitting procedure (program BindFit).

	V (total) [m	V(addition, total) [n	V(addition) [ml]	c(NMNI) [mol/l]	c(**8aa-1**) [mol/l	c(NMNI)/c(**8a**	fluorescer	fluorescer	fluorescer
1	2.500000	0.000000	0.000000	0.000000	0.000115	0.000000	214.554	168.6094	11.92773
2	2.503000	0.003000	0.003000	0.000015	0.000115	0.127300	220.0388	172.3604	12.35316
3	2.510000	0.010000	0.007000	0.000049	0.000115	0.423149	216.0294	170.5441	12.06353
4	2.520000	0.020000	0.010000	0.000097	0.000115	0.842939	199.5746	160.2873	10.7974
5	2.535000	0.035000	0.015000	0.000169	0.000115	1.466415	194.2098	154.7734	10.0219
6	2.563000	0.063000	0.028000	0.000300	0.000115	2.610710	157.0061	124.2024	7.802997
7	2.613000	0.113000	0.050000	0.000528	0.000115	4.593098	122.8441	97.17803	5.562119
8	2.681000	0.181000	0.068000	0.000824	0.000115	7.170484	86.11126	69.17575	3.225509
9	2.749000	0.249000	0.068000	0.001106	0.000115	9.620359	62.52728	49.62094	1.671861
10	2.500000	0.300000	0.300000	0.001465	0.000115	12.745237	36.09595	29.07918	0.903414
11	2.600000	0.400000	0.100000	0.001878	0.000115	16.340048	25.90681	20.86432	0.522382
12	2.700000	0.500000	0.100000	0.002261	0.000115	19.668576	18.55095	15.5127	0.429352
13	2.800000	0.600000	0.100000	0.002616	0.000115	22.759352	14.23187	11.17925	0.187106
14	2.900000	0.700000	0.100000	0.002947	0.000115	25.636972	11.35532	9.01088	0.215326
15	3.000000	0.800000	0.100000	0.003256	0.000115	28.322750	9.48248	7.566717	0.05596

K	1023.09 M^{-1}
Error	58.1831283 M^{-1}

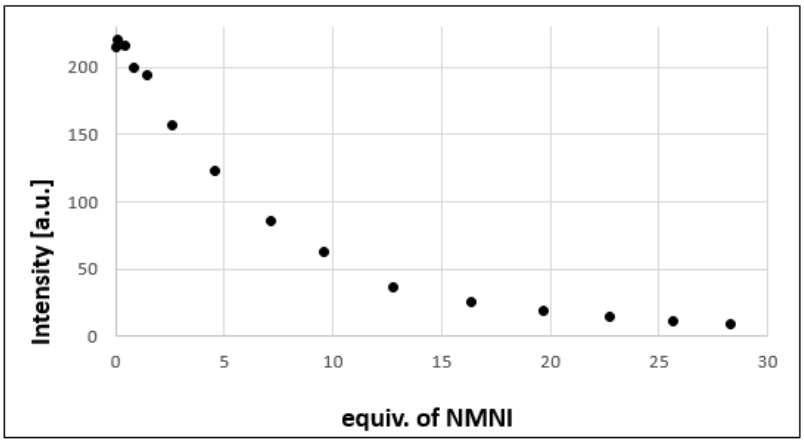


Figure 73: ^{1}H NMR titration of compound **8aa-1** with NMNI (CH_2Cl_2).

Calixarene **8aa-2** was dissolved in specified amount of CH_2Cl_2 (solution 1). 0.8 ml of calixarene solution 1 was put in a volumetric flask and diluted to total volume of 5 ml (solution 2). 2.5 ml of solution 2 was put to a fluorescence cuvette. Specified amount of (*S*)-1-Methyl-3-(1-methylpyrrolidin-2-yl)pyridinium iodide (NMNI) was put to another volumetric flask, 0.8 ml of solution 1 was added and the solution was diluted to total volume of 5 ml (solution 3). The aliquots of NMNI were gradually added to fluorescence tube to achieve different calixarene/guest rations (1:0.000-32.032), ensuring constant host concentration during the experiment. The complexation constants were determined by analyzing fluorescence intensity using nonlinear curve-fitting procedure (program BindFit).

	V (total) [m	V(addition, total) [n	V(addition) [ml]	c(NMNI) [mol/l]	c(**8aa-2**) [mol/l	c(NMNI)/c(**8a**	fluorescer	fluorescer	fluorescen
1	2.500000	0.000000	0.000000	0.000000	0.000115	0.000000	262.0602	202.5699	7.959859
2	2.503000	0.003000	0.003000	0.000017	0.000115	0.143970	262.1531	205.9744	7.704388
3	2.510000	0.010000	0.007000	0.000055	0.000115	0.478563	254.4821	199.7941	7.562208
4	2.520000	0.020000	0.010000	0.000110	0.000115	0.953328	246.8108	195.6015	6.998728
5	2.535000	0.035000	0.015000	0.000191	0.000115	1.658451	226.1117	177.2112	6.483453
6	2.563000	0.063000	0.028000	0.000340	0.000115	2.952600	180.8214	142.5319	4.997797
7	2.613000	0.113000	0.050000	0.000599	0.000115	5.194595	131.2368	105.4533	3.291471
8	2.681000	0.181000	0.068000	0.000934	0.000115	8.109507	93.04965	72.8703	2.186102
9	2.749000	0.249000	0.068000	0.001254	0.000115	10.880210	67.74667	54.28183	0.969769
10	2.500000	0.300000	0.300000	0.001661	0.000115	14.414313	41.72074	33.80562	0.665596
11	2.600000	0.400000	0.100000	0.002129	0.000115	18.479888	29.27642	24.25861	0.448374
12	2.700000	0.500000	0.100000	0.002563	0.000115	22.244309	23.11673	18.18512	0.182004
13	2.800000	0.600000	0.100000	0.002966	0.000115	25.739844	17.3428	14.39961	0.156406
14	2.900000	0.700000	0.100000	0.003341	0.000115	28.994307	13.2909	10.82477	0.218079
15	3.000000	0.800000	0.100000	0.003691	0.000115	32.031806	12.00225	9.671965	0.041457

K	1145.54 M^{-1}
Error	63.41938548 M^{-1}

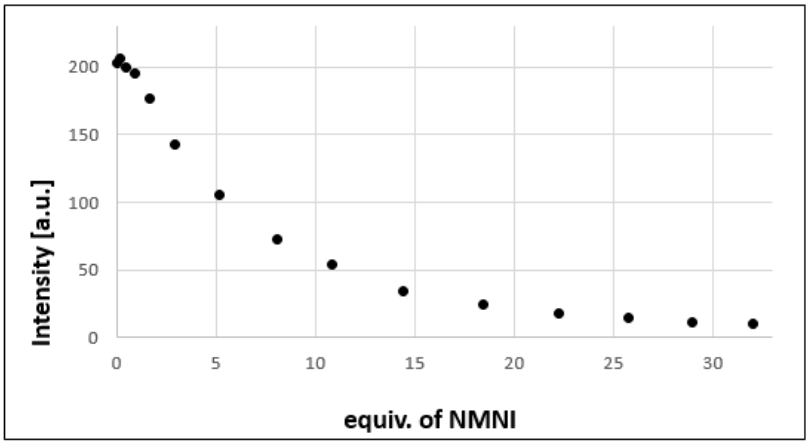


Figure 74: ^{1}H NMR titration of compound **8aa-2** with NMNI (CH_2Cl_2).

Calixarene **8bb** was dissolved in specified amount of CH_2Cl_2 (solution 1). 0.25 ml of calixarene solution 1 was put in a volumetric flask and diluted to total volume of 5 ml (solution 2). 2.5 ml of solution 2 was put to a fluorescence cuvette. Specified amount of *N*-methylisoquinolinium iodide (NMII) was put to another volumetric flask, 0.25 ml of solution 1 was added and the solution was diluted to total volume of 5 ml (solution 3). The aliquots of NMII were gradually added to fluorescence tube to achieve different calixarene/guest rations (1:0.000-47.816), ensuring constant host concentration during the experiment. The complexation constants were determined by analyzing fluorescence intensity using nonlinear curve-fitting procedure (program BindFit).

M(NMII)	271.10147 g/mol	M(**8bb**)	1045.336 g/mol		
m(NMII)	0.0236 g	m(**8bb**)	0.00051 g	0.00203	
c(NMII)	0.017410455 mol/l	c(**8bb**)	0.000097 mol/l		
V(CH2Cl2_NMII)	5 ml	V(CH2Cl2_**8bb**)	5 ml		

	V (total) [m	V(addition, total) [n	V(addition) [ml]	c(NMII) [mol/l]	c(**8bb**) [mol/l]	c(NMII)/c(**8bl**	fluorescer	fluorescer	fluorescer	fluorescer
1	2.500000	0.000000	0.000000	0.000000	0.000097	0.000000	912.8894	554.7544	707.7678	231.7736
2	2.503000	0.003000	0.003000	0.000021	0.000097	0.214912	918.936	550.1825	706.7305	219.8474
3	2.510000	0.010000	0.007000	0.000069	0.000097	0.714375	854.0452	503.3274	675.0663	193.0115
4	2.520000	0.020000	0.010000	0.000138	0.000097	1.423080	756.7221	435.3731	600.1621	158.2693
5	2.535000	0.035000	0.015000	0.000240	0.000097	2.475655	636.897	352.2045	493.3597	113.8643
6	2.563000	0.063000	0.028000	0.000428	0.000097	4.407496	416.2254	212.9528	318.4914	64.62449
7	2.613000	0.113000	0.050000	0.000753	0.000097	7.754236	267.4121	131.3659	194.7122	36.99195
8	2.681000	0.181000	0.068000	0.001175	0.000097	12.105473	167.2709	77.98933	116.62	18.89854
9	2.749000	0.249000	0.068000	0.001577	0.000097	16.241442	101.6831	48.08674	66.85209	9.97151
10	2.500000	0.300000	0.300000	0.002089	0.000097	21.516976	51.65318	25.47579	30.22287	6.16394
11	2.600000	0.400000	0.100000	0.002679	0.000097	27.585867	43.51534	20.50124	23.91788	4.603973
12	2.700000	0.500000	0.100000	0.003224	0.000097	33.205210	29.09026	14.19861	12.89789	3.268435
13	2.800000	0.600000	0.100000	0.003731	0.000097	38.423172	19.23077	9.838295	8.578782	2.40634
14	2.900000	0.700000	0.100000	0.004203	0.000097	43.281274	13.95126	7.491844	5.394998	1.796158
15	3.000000	0.800000	0.100000	0.004643	0.000097	47.815502	12.45473	6.806807	4.390254	1.555014

K	2345.01 M^{-1}
Error	160.1946681 M^{-1}

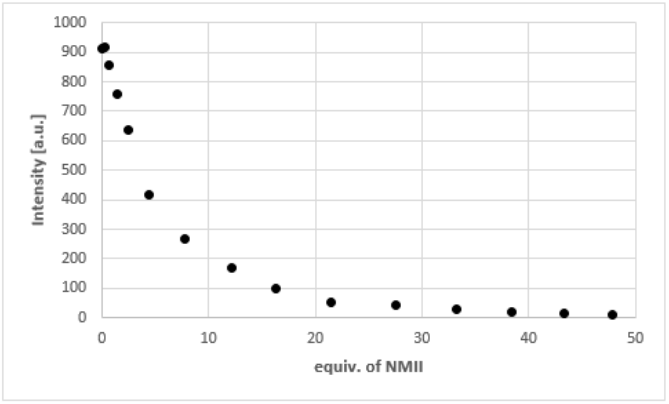


Figure 75: ^{1}H NMR titration of compound **8bb** with NMII (CH_2Cl_2).

Calixarene **8bb** was dissolved in specified amount of CH_2Cl_2 (solution 1). 0.20 ml of calixarene solution 1 was put in a volumetric flask and diluted to total volume of 5 ml (solution 2). 2.5 ml of solution 2 was put to a fluorescence cuvette. Specified amount of *N*-methylquinolinium iodide (NMII) was put to another volumetric flask, 0.20 ml of solution 1 was added and the solution was diluted to total volume of 5 ml (solution 3). The aliquots of NMQI were gradually added to fluorescence tube to achieve different calixarene/guest rations (1:0.000-48.930), ensuring constant host concentration during the experiment. The complexation constants were determined by analyzing fluorescence intensity using nonlinear curve-fitting procedure (program BindFit).

M(NMQI)	271.10147 g/mol	M(**8bb**)	1045.336 g/mol		
m(NMQI)	0.01932 g	m(**8bb**)	0.00041 g	0.00203	
c(NMQI)	0.014252966 mol/l	c(**8bb**)	0.000078 mol/l		
V(CH2Cl2_NMQI)	5 ml	V(CH2Cl2_**8bb**)	5 ml		

	V (total) [m	V(addition, total) [n	V(addition) [ml]	c(NMQI) [mol/l]	c(**8bb**) [mol/l]	c(NMQI)/c(**8b**	fluorescer	fluorescer	fluorescenc
1	2.500000	0.000000	0.000000	0.000000	0.000078	0.000000	365.1827	485.1543	607.8722
2	2.503000	0.003000	0.003000	0.000017	0.000078	0.219920	342.6986	469.8418	609.3022
3	2.510000	0.010000	0.007000	0.000057	0.000078	0.731024	302.6639	445.1225	568.4015
4	2.520000	0.020000	0.010000	0.000113	0.000078	1.456245	274.4518	431.9343	558.2444
5	2.535000	0.035000	0.015000	0.000197	0.000078	2.533350	214.0205	368.4146	479.0066
6	2.563000	0.063000	0.028000	0.000350	0.000078	4.510213	155.8725	304.4912	396.8813
7	2.613000	0.113000	0.050000	0.000616	0.000078	7.934949	102.4513	235.2298	297.187
8	2.681000	0.181000	0.068000	0.000962	0.000078	12.387592	66.37468	160.5352	195.5901
9	2.749000	0.249000	0.068000	0.001291	0.000078	16.619951	40.62778	96.61857	103.943
10	2.500000	0.300000	0.300000	0.001710	0.000078	22.018431	23.0515	55.73735	57.59327
11	2.600000	0.400000	0.100000	0.002193	0.000078	28.228758	12.44105	29.93987	24.47273
12	2.700000	0.500000	0.100000	0.002639	0.000078	33.979060	8.291224	19.32528	14.38439
13	2.800000	0.600000	0.100000	0.003054	0.000078	39.318627	6.288636	13.7365	9.15774
14	2.900000	0.700000	0.100000	0.003440	0.000078	44.289947	4.905201	9.962555	5.378346
15	3.000000	0.800000	0.100000	0.003801	0.000078	48.929847	3.255194	7.288543	3.323562

K	1567.44 M^{-1}
Error	118.4827896 M^{-1}

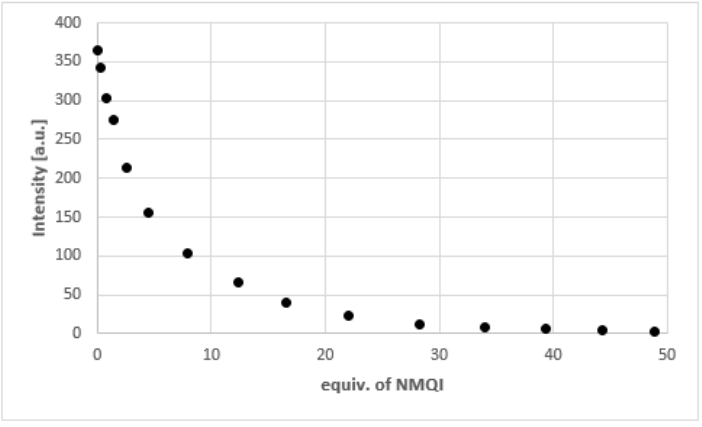
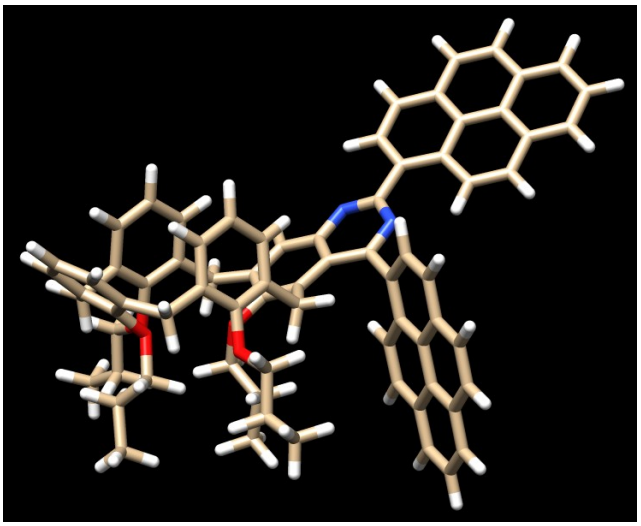


Figure 76: ^{1}H NMR titration of compound **8bb** with NMQI (CH_2Cl_2).

6. Theoretical calculations

Internal coordinates

8bb conformer **A**



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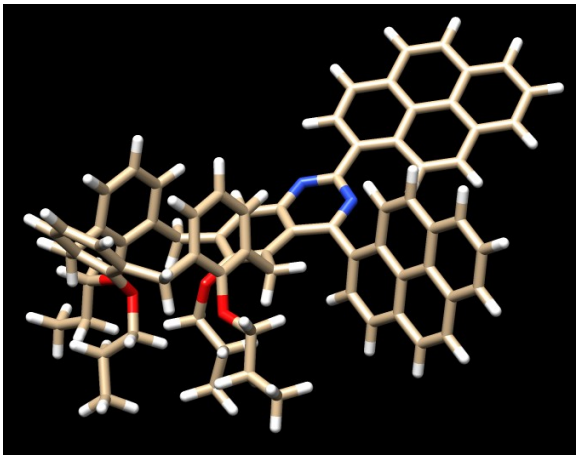
8bb conformer **B**



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H	0.808358	-8.17686	0.469154
H	2.22024	-3.61077	0.989895
H	2.466845	-2.0533	1.807717
H	-0.18814	-3.57398	1.758154
H	0.104854	-2.04877	2.592562
H	1.810758	-3.17878	4.091486
H	1.510265	-4.71754	3.266622
H	0.227294	-3.95831	4.222941
H	-3.57456	-2.83497	-0.04753
H	-3.70089	-4.18031	-1.20324
H	-2.75619	-5.7381	0.52138
H	-2.63521	-4.40597	1.666547
H	6.118	-2.79499	-0.50972
H	6.025132	-4.29303	-1.46366
H	7.417136	-5.44945	1.889715
H	7.776299	-5.40828	0.156595
H	7.853349	-3.91937	1.114267
H	2.746064	-5.81922	-0.06924
H	2.410958	-7.134	-1.19585
H	-5.15797	-4.12412	1.615688
H	-5.28101	-5.46376	0.462094
H	-4.70827	-5.76301	2.109892
H	5.274935	-5.54022	0.57474

H	5.350632	-4.05677	1.521245
H	3.745561	-5.36454	-2.2888
H	4.52013	-5.22072	-3.85995
H	-0.3904	-6.06464	-11.7953
H	0.055783	-5.92609	-9.36757
H	4.408432	-7.96811	-8.76086
H	6.014717	-9.04219	-10.2656
H	1.955282	-7.78503	-15.5736
H	0.306745	-6.73524	-14.0611
H	6.703368	-9.72294	-12.5552
H	6.234546	-9.85425	-14.9904
H	4.122629	-8.92612	-15.9064
H	3.682445	-8.13851	-3.98823
H	5.716322	-9.08643	-2.95846
H	7.491954	-4.57183	-8.31552
H	5.275278	-5.23091	-7.5095
H	8.186763	-9.25515	-2.83906
H	10.41528	-8.60762	-3.67983
H	11.81447	-7.30496	-5.26269
H	12.00798	-5.70675	-7.15002
H	9.970913	-4.75388	-8.1989