Supporting Information

A Different Approach: Highly Encapsulating Macrocycles Being Used as Organic Tectons in the Building of CPs

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1. NMR, Mass and IR spectra

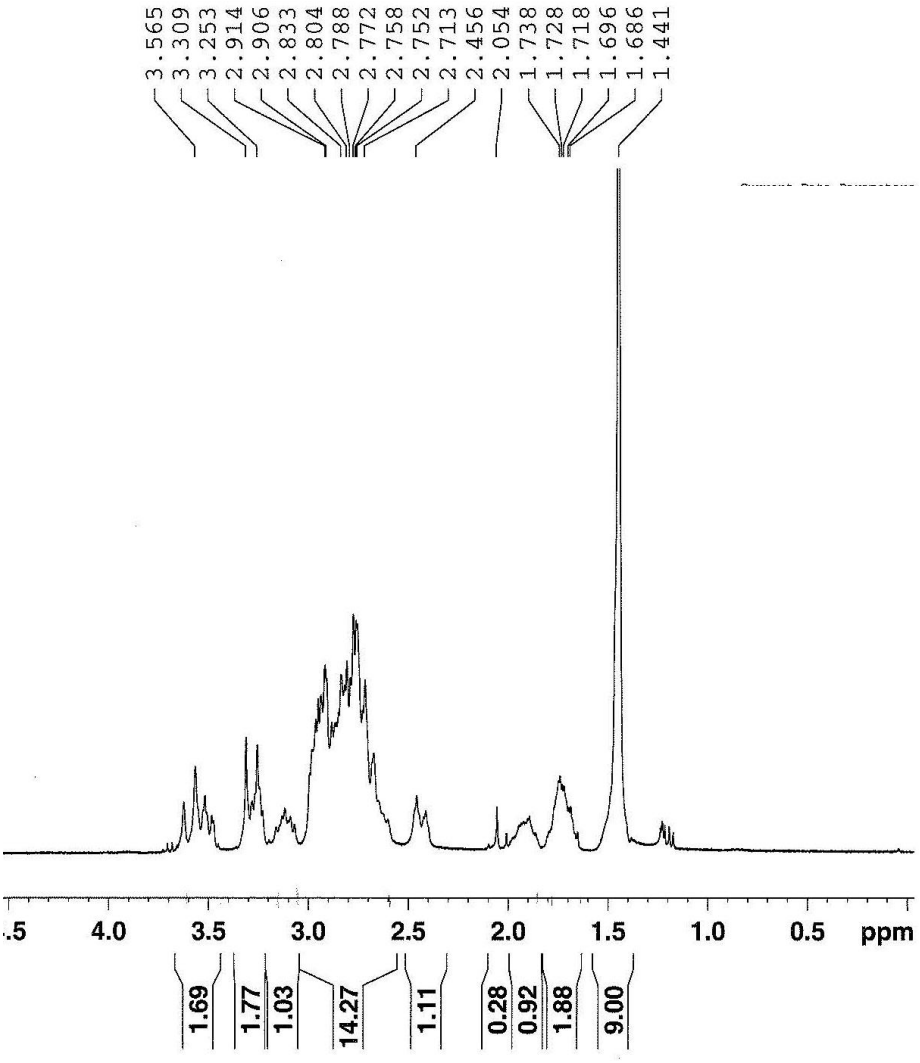


Figure S1. ^{1}H NMR spectrum of (**1**) in $CDCl_3$ (300 MHz, 298 K).

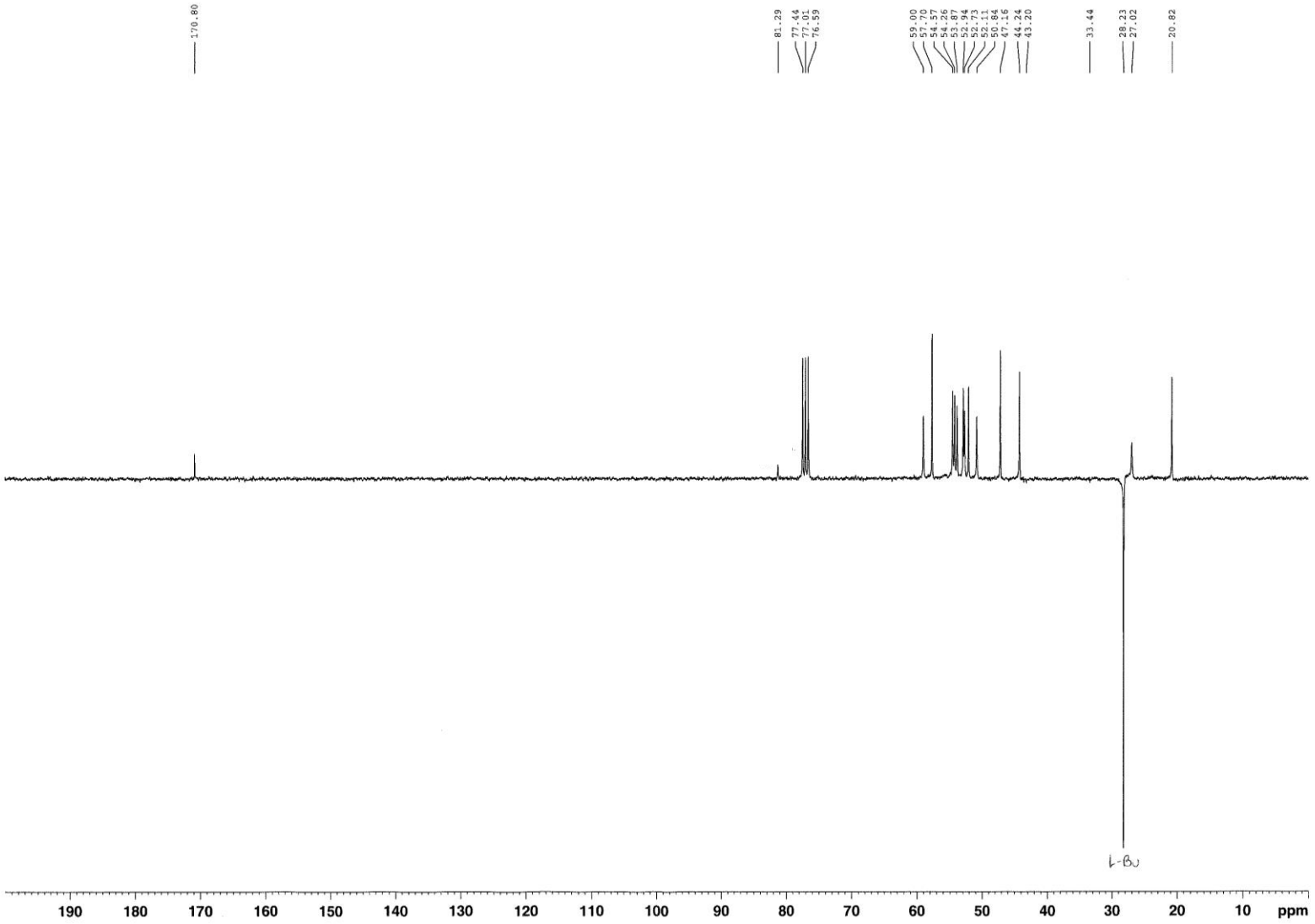


Figure S2. J-mod ^{13}C NMR spectrum of (**1**) in $CDCl_3$ (300 MHz, 298 K).

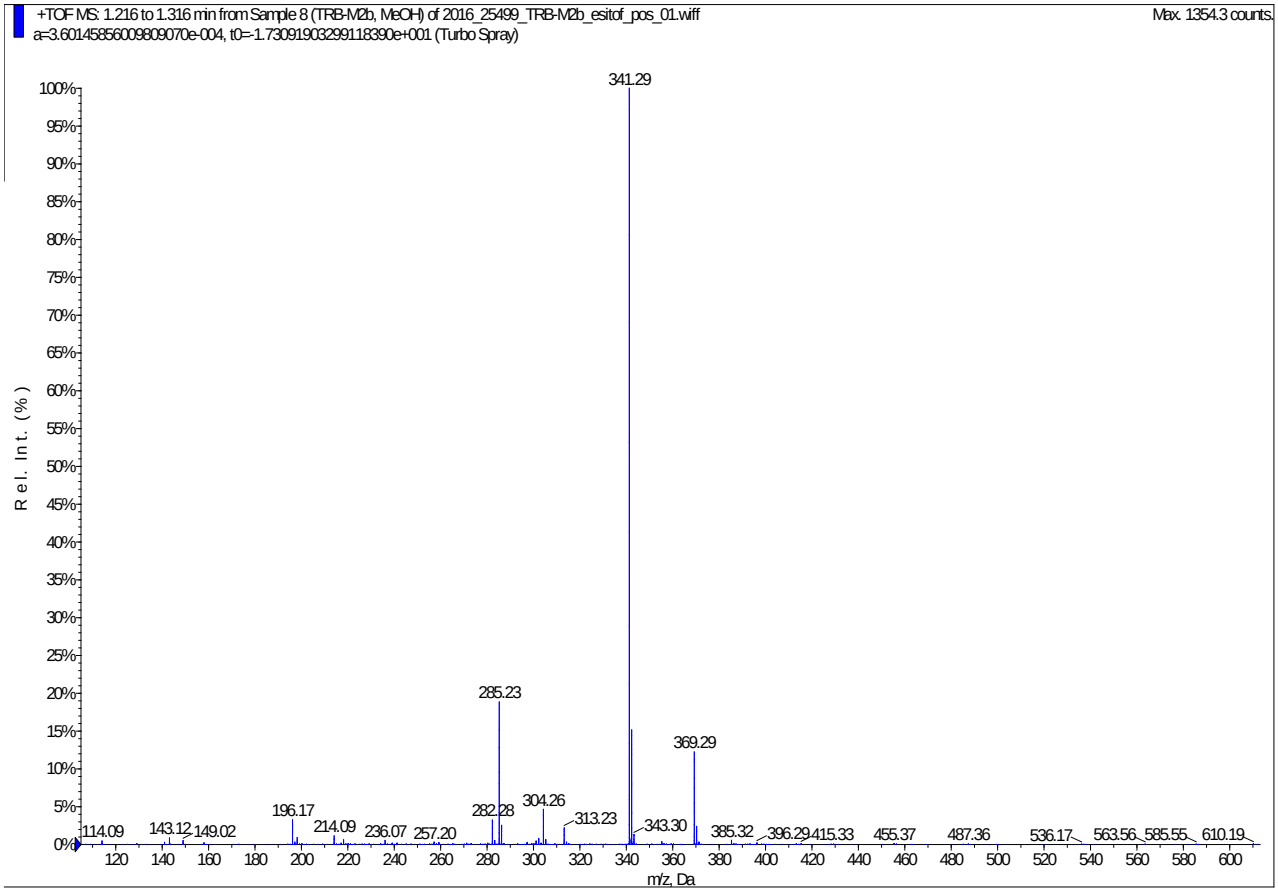


Figure S3. Mass spectrum (ESI-TOF^{+}) of (**1**).

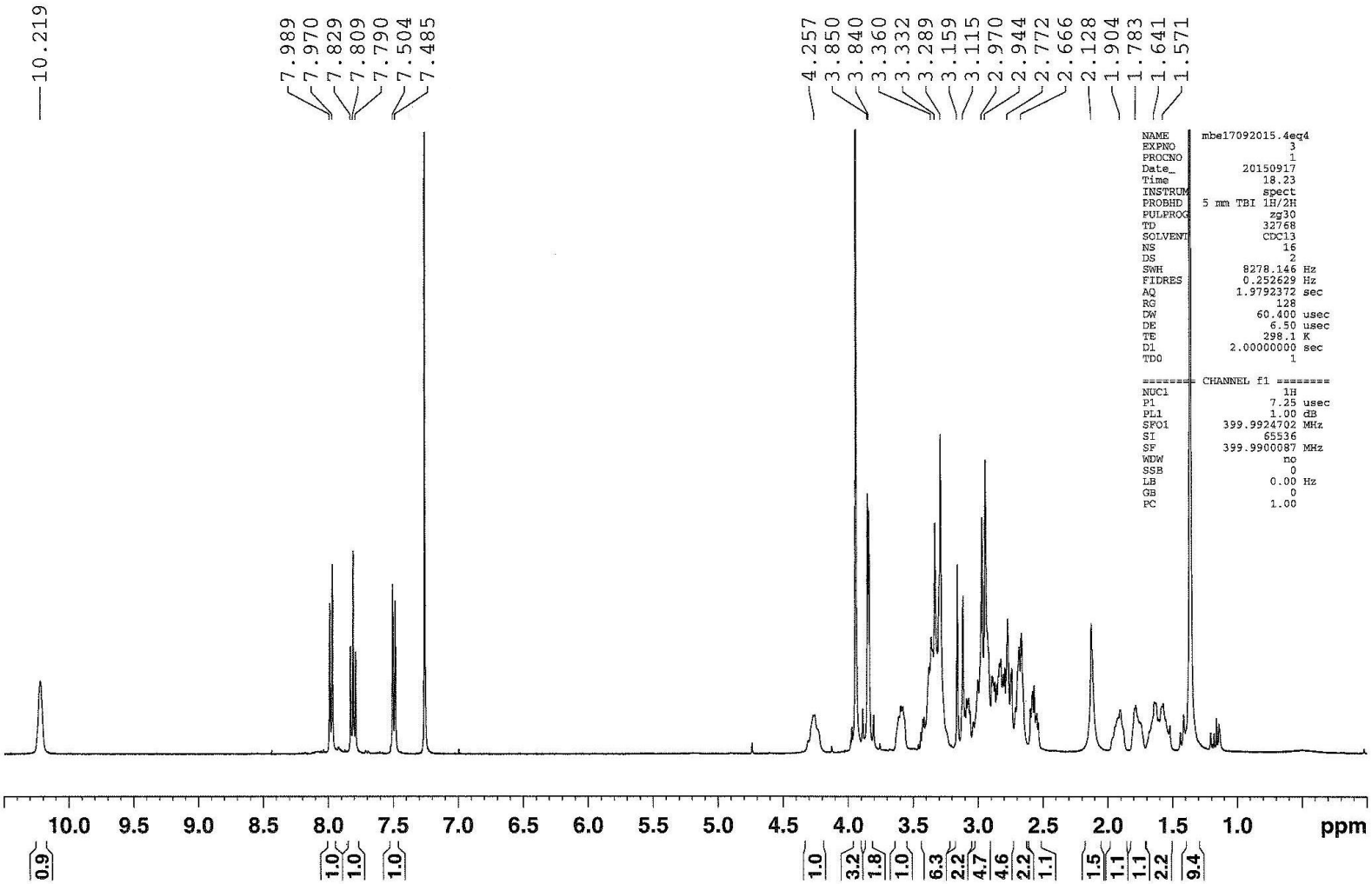


Figure S4. ^{1}H NMR spectrum of (**2**) in $CDCl_3$ (400 MHz, 298 K).

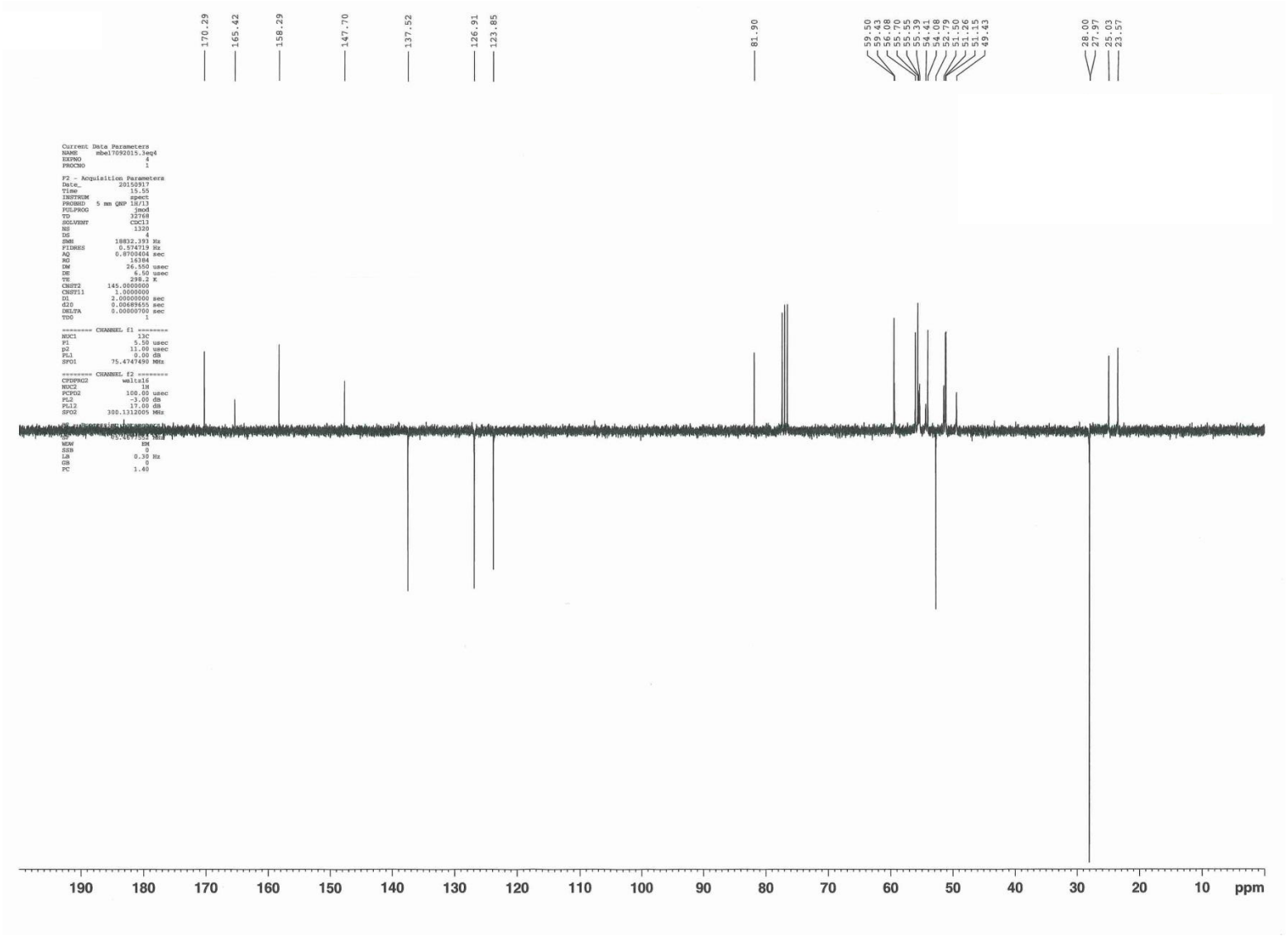
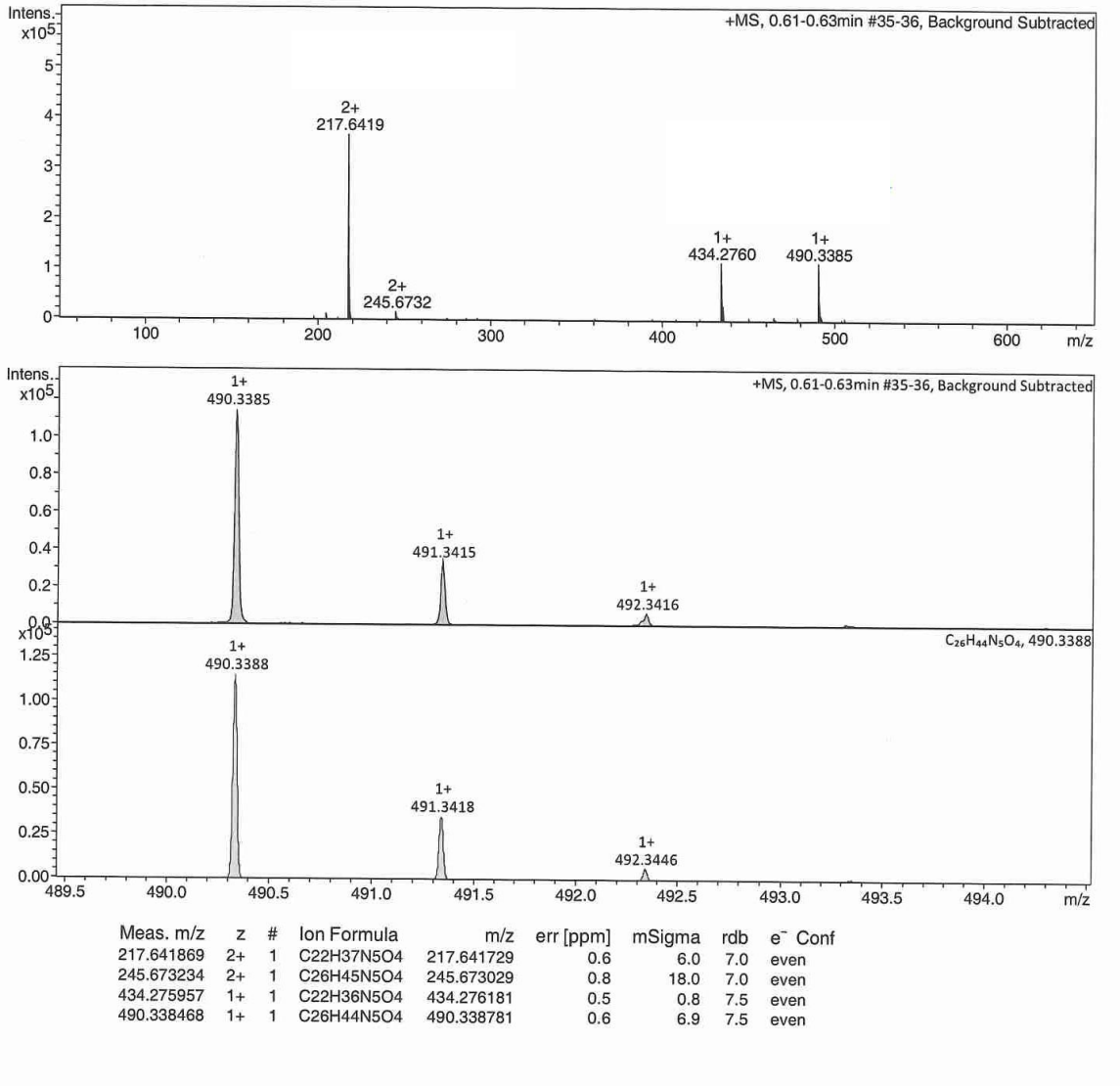
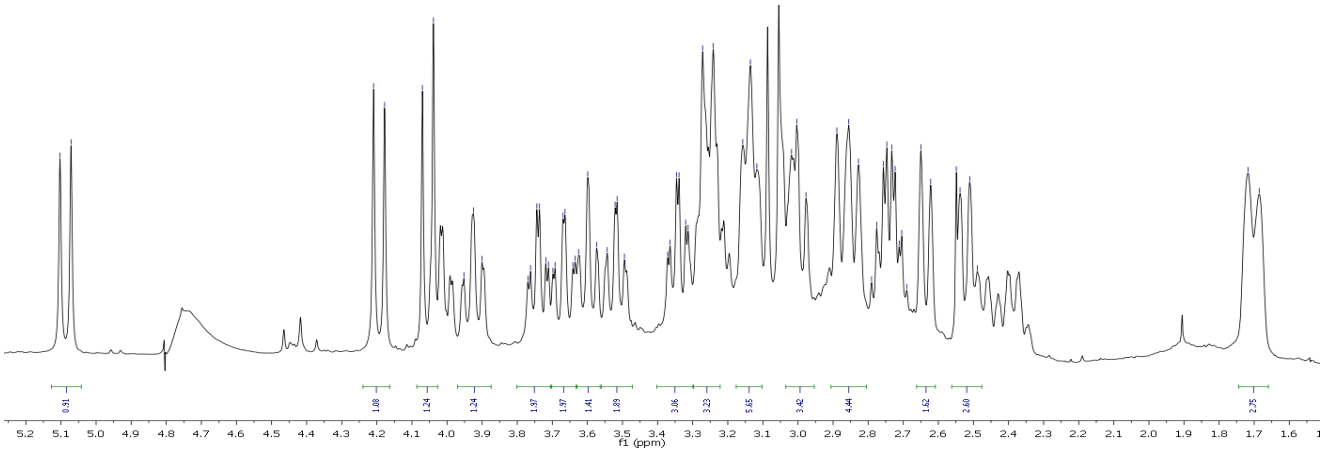


Figure S5. J-mod ^{13}C NMR spectrum of (**2**) in $CDCl_3$ (400 MHz, 298 K).

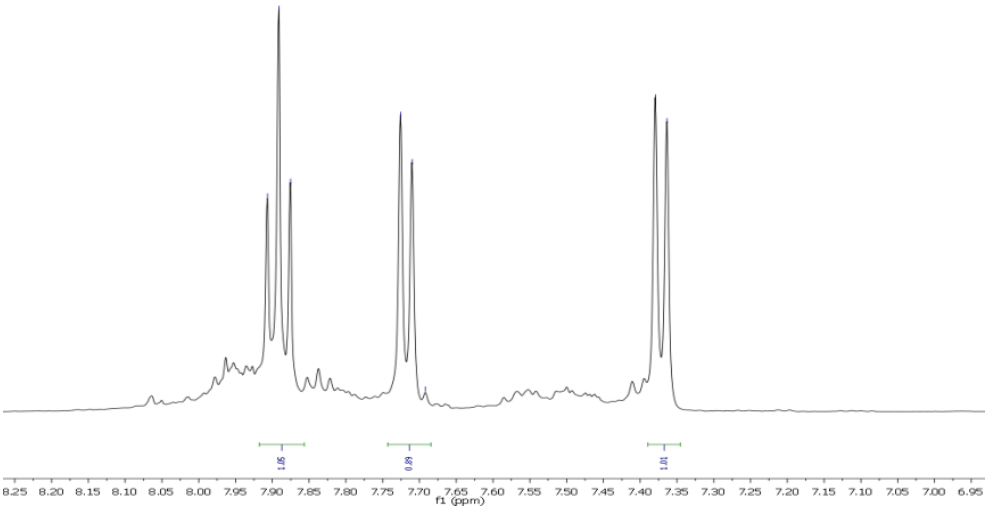


Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf
217.641869	2+	1	C22H37N5O4	217.641729	0.6	6.0	7.0	even
245.673234	2+	1	C26H45N5O4	245.673029	0.8	18.0	7.0	even
434.275957	1+	1	C22H36N5O4	434.276181	0.5	0.8	7.5	even
490.338468	1+	1	C26H44N5O4	490.338781	0.6	6.9	7.5	even

Figure S6. High Resolution Mass spectrometry (ESI^+) of (**2**). *m/z* calcd for $[C_{26}H_{43}N_5O_4 + H]^+$: 490.3388, found: 490.3385, $[M+H]^+$.



(a)



(b)

Figure S7. ^{1}H NMR spectrum of ligand **H_2cb-teapa** (**3**) in D_2O (500 MHz, 298 K, pD=7.55): **a)** Aliphatic region. **b)** Aromatic region.

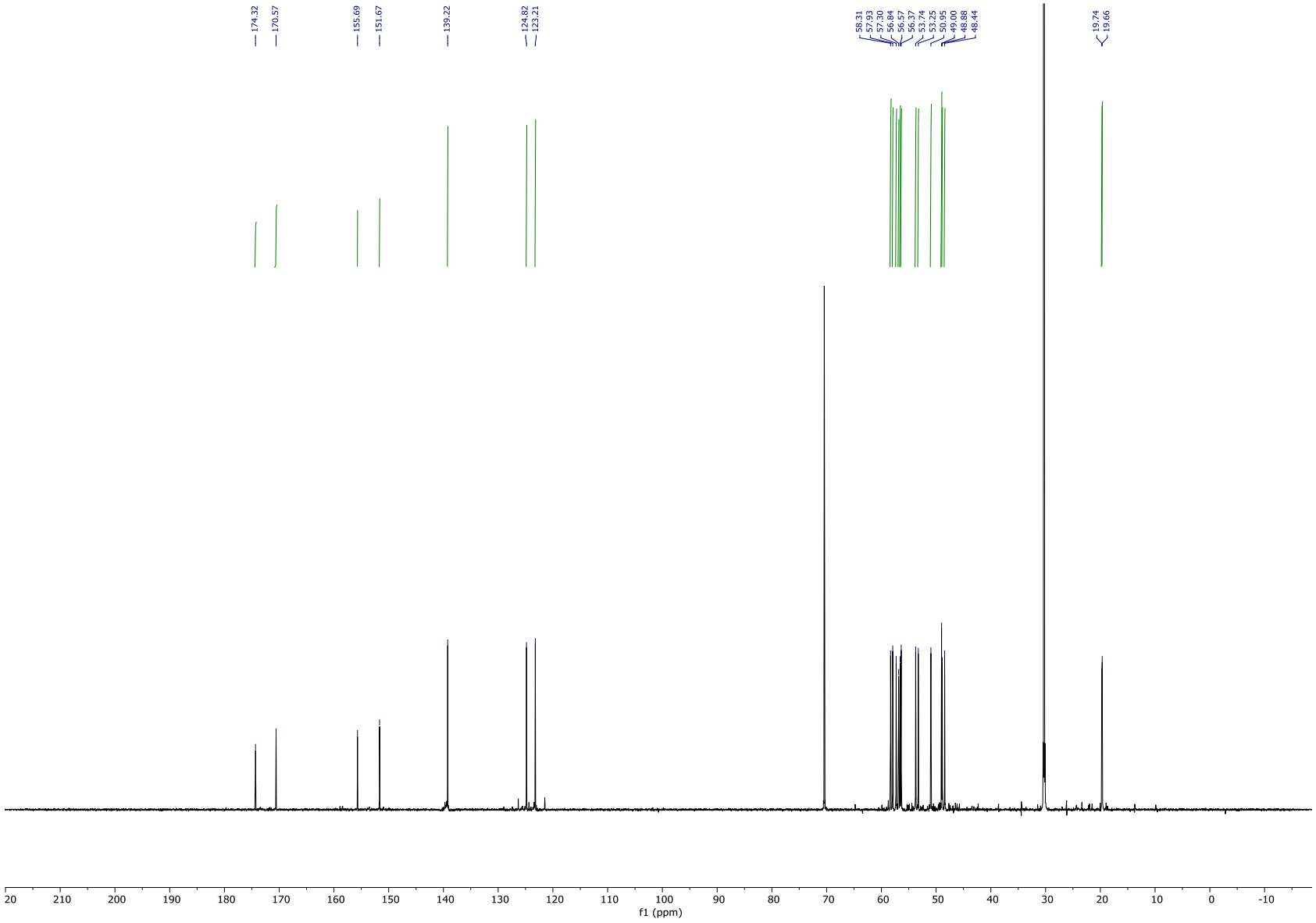


Figure S8. ^{13}C NMR spectrum of ligand **H_2cb-teapa** (**3**) in D_2O (298 K, pD=7.55, ^{t}BuOH as internal standard).

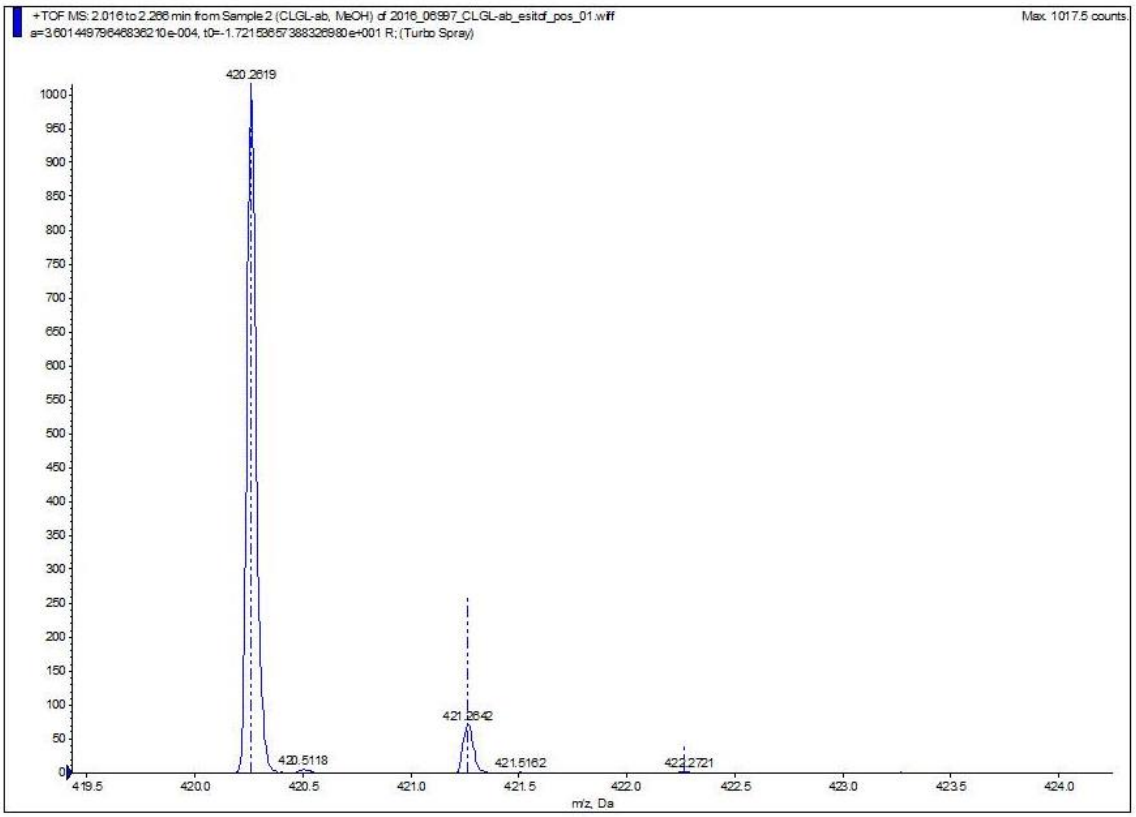


Figure S9. High Resolution Mass spectrometry (ESI-TOF^{+}) of the ligand **H_2cb-teapa** (**3**). *m/z* calcd. for $[C_{21}H_{33}N_5O_4+H]^+$: 420.2605; found: 420.2619, $[M+H]^+$**.**

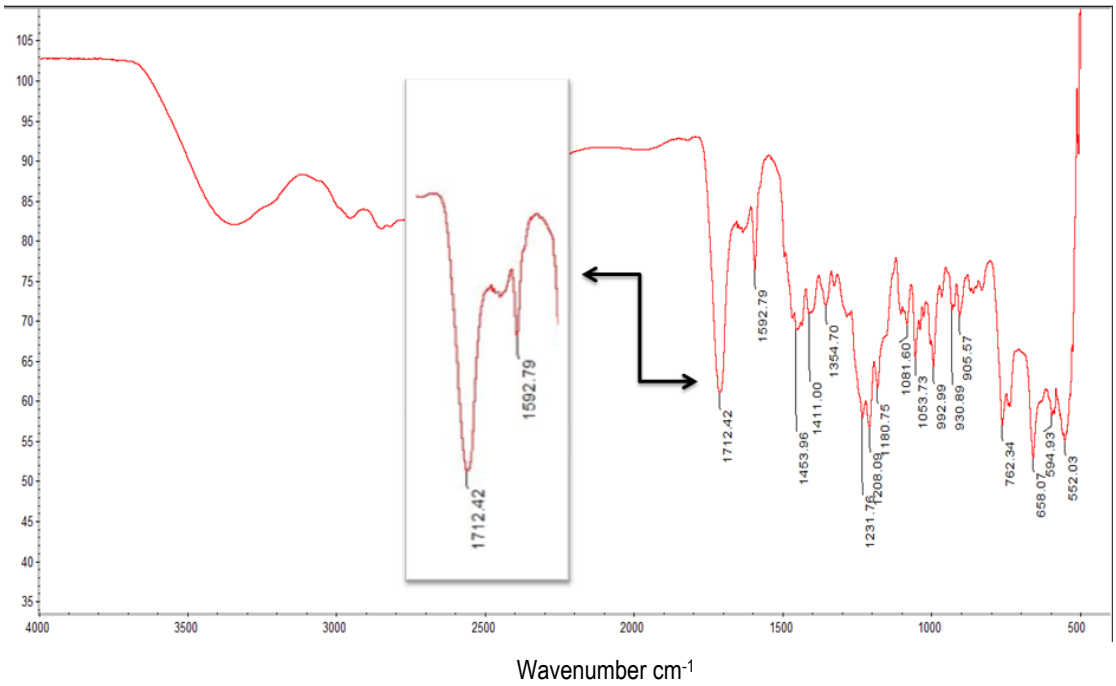


Figure S10. IR spectrum of the ligand **H_2cb-teapa** (**3**).

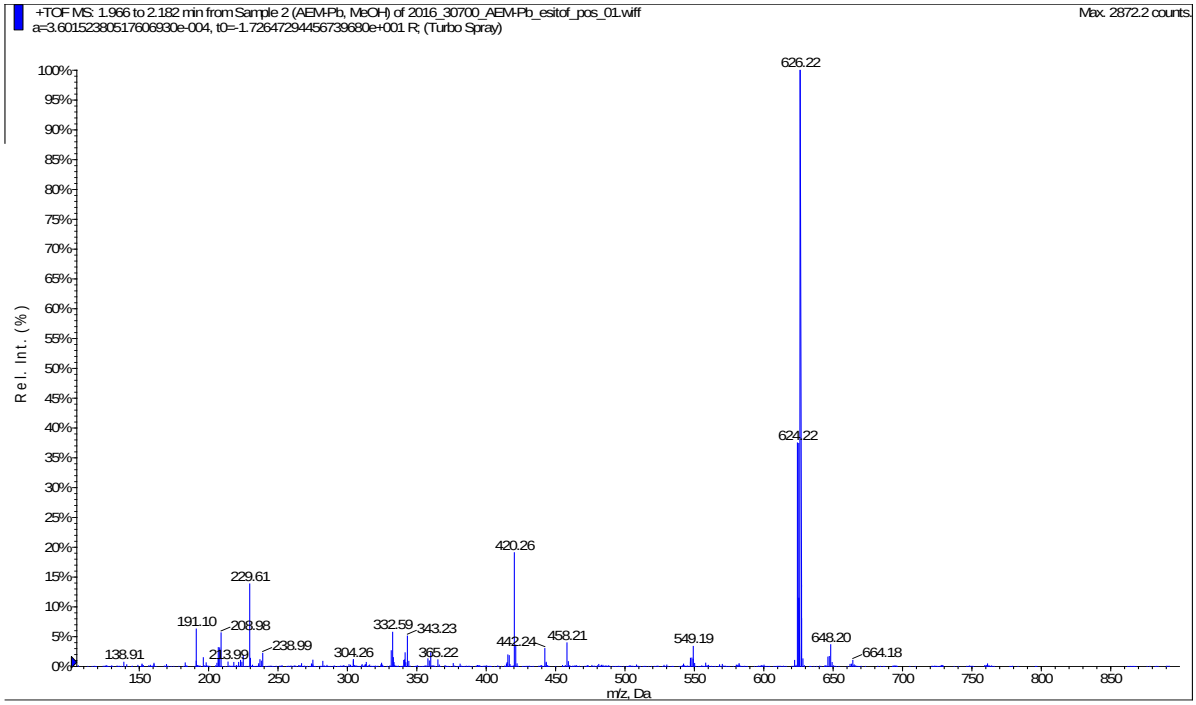


Figure S11. Mass spectrum (ESI-TOF^{+}) of (**4**).

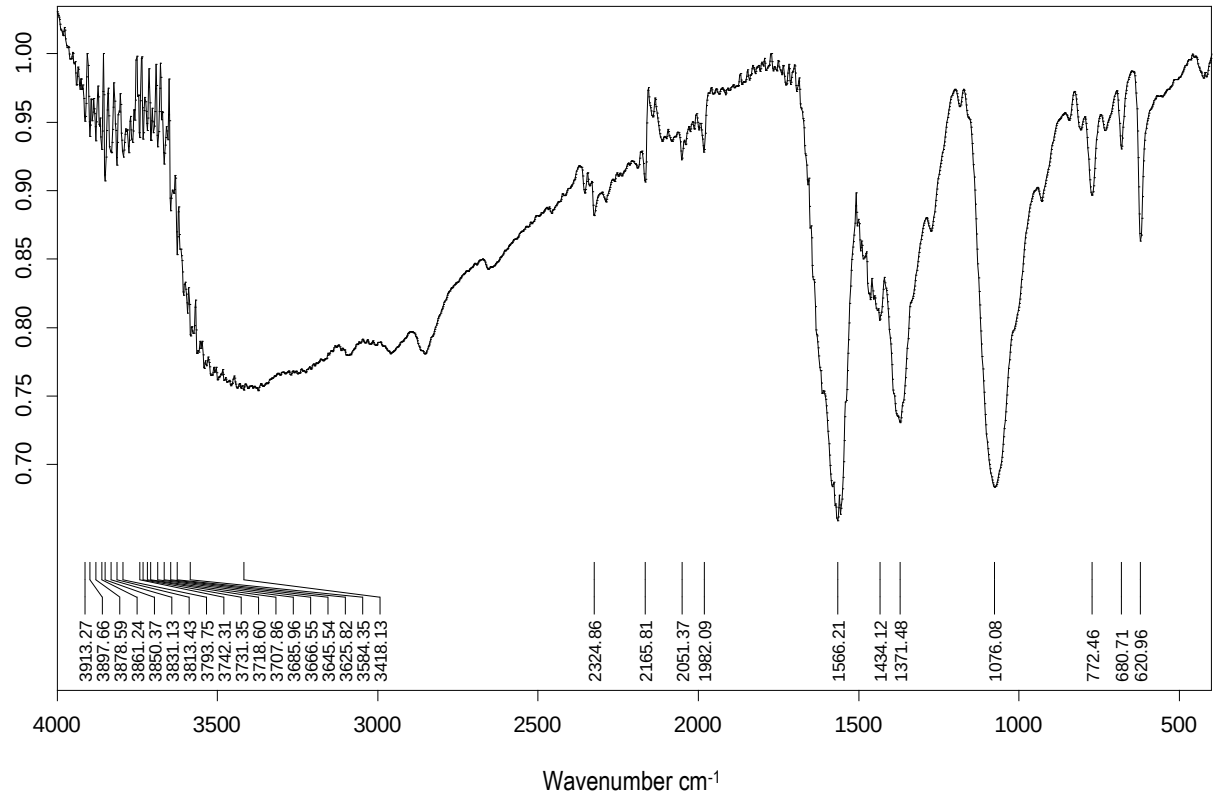


Figure S12. IR spectrum of (**4**).

2. ^{1}H NMR titration of H_2cb-teapa.

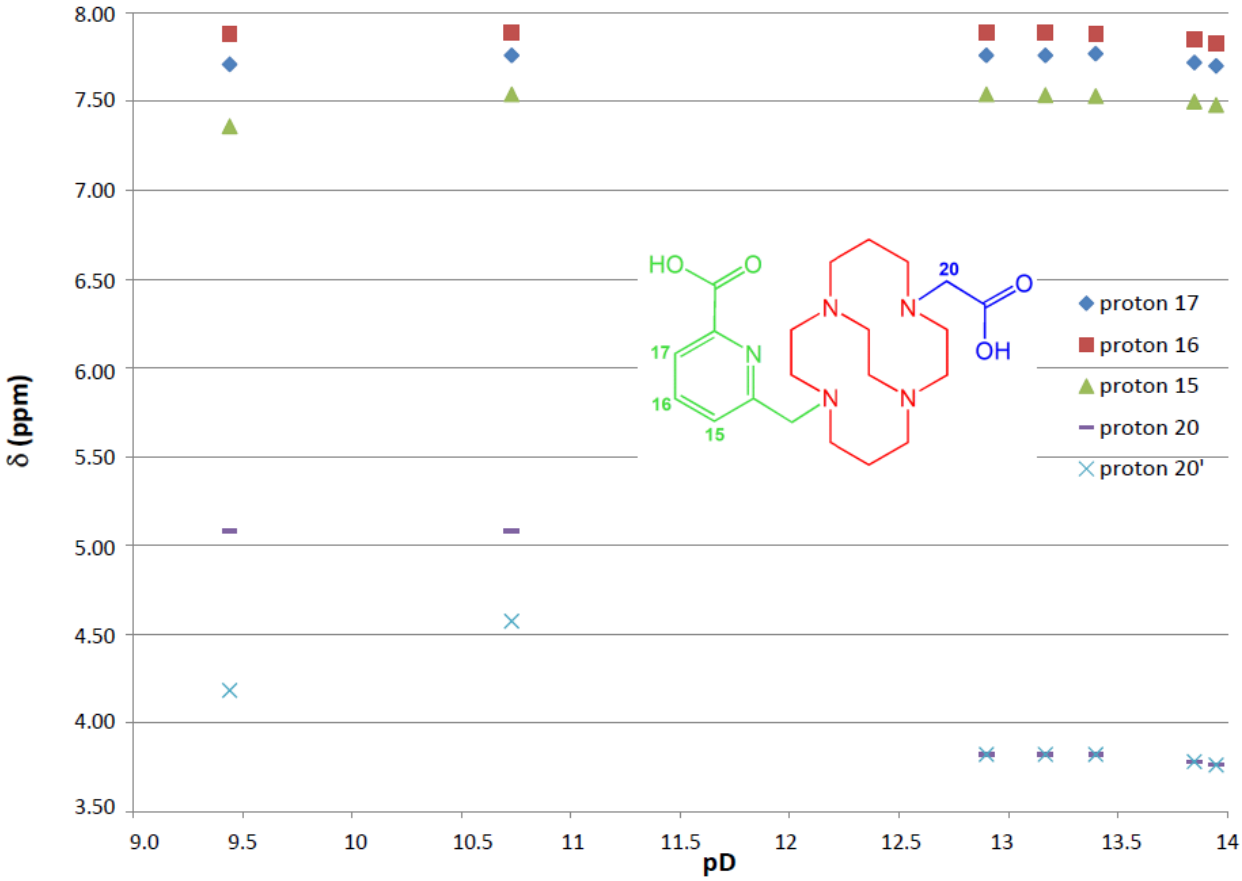


Figure S13. ^{1}H NMR titration of **H_2cb-teapa** in D_2O solution at basic pD.

2. Thermal Decomposition of (4).

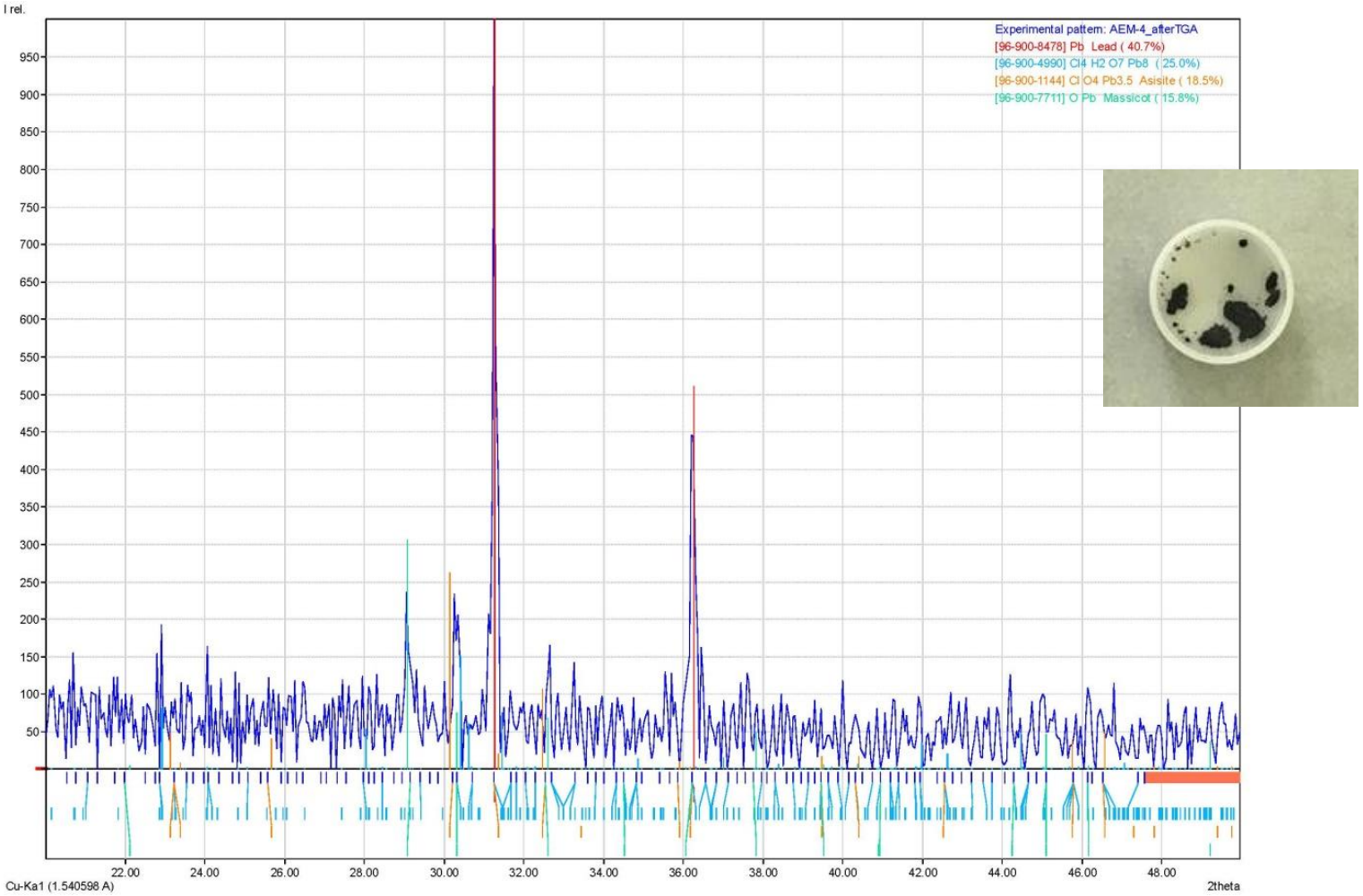


Figure S14. PXRD pattern of the black residue resulting from the thermal decomposition of (**4**).

3. Tables with optimized Cartesian coordinates.

Table S1. Calculated Cartesian coordinates for compound at DFT level using the functional RTPSSh and 6-31G(d) basis set for all atoms except Pb for which the ECP ECP60MDF with the associated basis set was used. (0 imaginary frequencies)

Center Number	Symbol	Coordinates (Angstroms) X	Y	Z
1	Pb	-0.4802360	1.7526315	0.1580967
2	C	1.0587768	-0.2567935	1.5166155
3	C	1.9420266	-1.3125331	2.1395225
4	C	1.6356129	-1.7839399	3.4208502
5	H	0.7836835	-1.3742810	3.9502318
6	C	2.4376038	-2.7821786	3.9750228
7	H	2.2191377	-3.1867472	4.9582481
8	C	3.5247178	-3.2530432	3.2411604
9	H	4.1724246	-4.0296325	3.6357800
10	C	3.7731916	-2.6953894	1.9791851
11	C	5.0224103	-3.0988468	1.2265871
12	H	5.8240342	-2.4167509	1.5321985
13	H	5.2992400	-4.1335997	1.4413651
14	C	6.1777271	-3.3204872	-0.9708922
15	H	5.9316760	-3.4528734	-2.0244053
16	H	6.5051490	-4.2874472	-0.5812899
17	C	7.2955442	-2.2975353	-0.7955684
18	H	7.5489280	-2.1934530	0.2621149
19	H	8.1737717	-2.7327450	-1.3042199
20	C	8.1696344	-0.0743849	-0.9763755
21	H	9.0412769	-0.3330703	-1.5990366
22	H	8.4276157	-0.2843769	0.0656646
23	C	7.8715726	1.4260333	-1.1069330
24	H	8.7938427	1.9670285	-0.8663887
25	H	7.6323495	1.7036964	-2.1392894
26	C	6.8022636	1.9282091	-0.1355013
27	H	7.1412047	1.7929093	0.8919710
28	H	6.5560373	2.9804298	-0.3019511
29	C	4.7698495	1.4587839	-1.5080780
30	H	5.5125291	1.5655249	-2.3005289
31	H	4.2806691	2.4255158	-1.3667860
32	C	3.7173961	0.4177626	-1.8748527
33	H	2.9387533	0.3804239	-1.1095824
34	H	3.2465269	0.7790305	-2.8057324
35	C	3.0235497	-1.8296709	-2.3149119
36	H	2.5947221	-1.6088008	-3.3055156
37	H	2.2775798	-1.5629482	-1.5599528
38	C	3.3183429	-3.3330562	-2.2134363
39	H	2.3904442	-3.8667440	-2.4479898
40	H	4.0393979	-3.6589692	-2.9703863
41	C	3.7369615	-3.7931798	-0.8156685
42	H	4.0538103	-4.8391734	-0.8037918
43	H	2.9098918	-3.6630872	-0.1189242
44	C	6.7045566	-0.9049371	-2.7540243
45	H	7.3042320	-1.6541261	-3.2949589
46	H	7.0380922	0.0655839	-3.1243920
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48	H	4.9665163	-0.3870363	-3.9580285
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51	H	3.7044911	0.8997126	0.8136874
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53	C	5.3487519	0.4363280	2.1507786
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55	N	4.8873701	-2.9697815	-0.2645787
56	N	7.0070863	-0.9471367	-1.3076786
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58	N	4.2139171	-0.9641462	-2.0543257
59	O	1.1862821	-0.0010033	0.2677493
60	O	0.2157852	0.3313449	2.2512067
61	O	6.2505764	-0.3785933	1.7759785
62	O	4.8861919	0.6365678	3.2939343
63	Cl	-0.6310332	1.1078700	-2.5132950
64	H	4.6755235	-1.9737177	-0.5433087
65	H	5.8360468	0.1380970	-0.2998117
66	O	-2.2150466	0.0607545	0.4048956
67	O	-2.6904729	1.7791396	1.7745812
68	O	-6.8295065	0.7830803	1.9091525
69	O	-7.6281274	2.8976632	1.7879389
70	C	-6.9277370	1.9331131	1.3845464
71	C	-6.0964003	2.2079095	0.1196683
72	C	-5.9758999	3.5273939	-0.3413353
73	N	-5.5092135	1.1736628	-0.5173969
74	H	-6.4789931	4.3121834	0.2111585
75	C	-5.2313741	3.7881376	-1.4896714
76	H	-5.1219461	4.8014167	-1.8657112
77	C	-4.6448587	2.7161358	-2.1663776
78	H	-4.0761375	2.8679898	-3.0787201
79	C	-4.8137136	1.4320232	-1.6380546
80	C	-4.1498719	0.2530310	-2.3168860
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82	H	-4.0188958	0.4341516	-3.3862005
83	N	-4.9439199	-1.0164734	-2.1748896
84	C	-4.2130283	-2.1967138	-2.7696143
85	H	-4.9379327	-3.0056312	-2.8585941
86	H	-3.9070534	-1.9114936	-3.7788749
87	C	-2.9888208	-2.6436955	-1.9764403
88	H	-2.2511736	-1.8377007	-1.9322525
89	H	-2.5391894	-3.4642266	-2.5615163
90	N	-3.2583565	-3.0780691	-0.5921826
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93	H	-1.2679376	-2.5871247	-0.1881999
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124	H	-4.8918456	0.0880012	1.8705481
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