

Supporting Information

Unexpected interactions between alkyl straps and pyridine ligands in sulfur-strapped porphyrin nanorings

Cécile Roche, Qianfu Luo, Guzmán Gil-Ramírez, Hua-Wei Jiang, Daniel R. Kohn, Yaoyao Xiong, Amber L. Thompson and Harry L. Anderson*

Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Oxford OX1 3TA, United Kingdom

TABLE OF CONTENTS

1. SUPPLEMENTARY FIGURES.....	S3
1.1. ^1H - ^1H COSY and ROESY NMR spectra of the porphyrin nanoring <i>c</i> -P6 _{S-C7} •T6 (<i>n</i> = 7).....	S3
1.2. NMR spectra of 1:1 complexes of strapped dibromoporphyrins 7a-c with pyridine	S6
2. MOLECULAR MODELS	S8
2.1. General.....	S8
2.2. Frequencies	S8
2.3. Total energies of optimized structures.....	S8
2.4. Cartesian coordinates	S8
3. UV-VISIBLE TITRATIONS OF PORPHYRIN MONOMERS WITH PYRIDINE	S56
4. CHARACTERIZATION SPECTRA FOR NEW COMPOUNDS	S58
4.1. S,S-Bis(2-formylphenyl)nonanebis(thioate) 3a	S58
4.2. S,S-Bis(2-formylphenyl)decanebis(thioate) 3b	S60
4.3. S,S-Bis(2-formylphenyl)dodecanebis(thioate) 3c	S61
4.4. S,S-Bis(2-formylphenyl)benzene-1,4-bis(carbothioate) 3d	S63
4.5. S,S-Bis(2-formylphenyl)-3,3'-(1,4-phenylene)dipropanethioate 3e	S65
4.6. C ₇ -Strapped free-base porphyrin 5a	S67
4.7. C ₈ -Strapped free-base porphyrin 5b	S69
4.8. C ₁₀ -Strapped free-base porphyrin 5c	S70
4.9. 1,4-Diethylbenzene-strapped free-base porphyrin 5e.....	S72
4.10. C ₇ -Strapped zinc(II) porphyrin 6a	S74
4.11. C ₈ -Strapped zinc(II) porphyrin 6b	S76
4.12. C ₁₀ -Strapped zinc(II) porphyrin 6c	S78
4.13. C ₇ -Strapped dibromoporphyrin 7a	S80
4.14. C ₈ -Strapped dibromoporphyrin 7b	S82
4.15. C ₁₀ -Strapped dibromoporphyrin 7c	S84
4.16. C ₇ -Strapped bis-TMS porphyrin 8a.....	S86
4.17. C ₈ -Strapped bis-TMS porphyrin 8b.....	S88
4.18. C ₁₀ -Strapped bis-TMS porphyrin 8c.....	S90
4.19. C ₇ -Strapped bis-deprotected porphyrin 9a	S92
4.20. C ₈ -Strapped bis-deprotected porphyrin 9b	S94
4.21. C ₁₀ -Strapped bis-deprotected porphyrin 9c	S96
4.22. Mono-deprotected t-Bu porphyrin 10.....	S98
4.23. C ₇ -Strapped bis-TMS porphyrin trimer 11a.....	S100
4.24. C ₈ -Strapped bis-TMS porphyrin trimer 11b	S102
4.25. C ₁₀ -Strapped bis-TMS porphyrin trimer 11c	S104

4.26. C ₇ -Strapped bis-deprotected porphyrin trimer 12a	S106
4.27. C ₈ -Strapped bis-deprotected porphyrin trimer 12b	S108
4.28. C ₁₀ -Strapped bis-deprotected porphyrin trimer 12c	S110
4.29. C ₇ -Strapped porphyrin nanoring <i>c</i> -P6 _{S-C7} •T6.....	S112
4.30. C ₈ -Strapped porphyrin nanoring <i>c</i> -P6 _{S-C8} •T6.....	S115
4.31. C ₁₀ -Strapped porphyrin nanoring <i>c</i> -P6 _{S-C10} •T6	S117
4.32. Template-free C ₁₀ -strapped porphyrin nanoring <i>c</i> -P6 _{S-C10}	S119
5. UV-VISIBLE ABSORPTION SPECTRA (MOLAR EXTINCTION COEFFICIENTS).....	S121
5.1. Strapped free-base porphyrins 5a-e	S121
5.2. Strapped zinc(II) porphyrins 6a-c	S121
5.3. Strapped dibromoporphyrins 7a-c	S122
5.4. Strapped bis-TMS porphyrins 8a-c.....	S122
5.5. Strapped bis-deprotected porphyrins 9a-c	S123
5.6. Mono-deprotected <i>t</i> -Bu porphyrin 10	S123
5.7. Strapped bis-TMS porphyrin trimers 11a-c.....	S124
5.8. Strapped bis-deprotected porphyrin trimers 12a-c	S124
5.9. Strapped porphyrin nanorings <i>c</i> -P6 _{S-C7-10} •T6	S125
5.10. Template-free strapped porphyrin nanoring <i>c</i> -P6 _{S-C10}	S126
6. SINGLE CRYSTAL X-RAY DIFFRACTION STUDIES.....	S127
6.1 Variable Temperature Study for Compound 6c-I.....	S128
6.2 Unit Cell Parameters for Compound 6c-I as a Function of Temperature	S130
6.3 Selected Reciprocal Lattice Section Reconstructions for 6c-I	S130
6.4 Overlay of molecules in the crystal structure of 6c-I at 150 K	S132
6.5 Displacement ellipsoid plots	S133
7. REFERENCES.....	S137

1. SUPPLEMENTARY FIGURES

1.1. ^1H - ^1H COSY and ROESY NMR spectra of the porphyrin nanoring *c*-P6_{S-C7} \bullet T6 (*n* = 7)

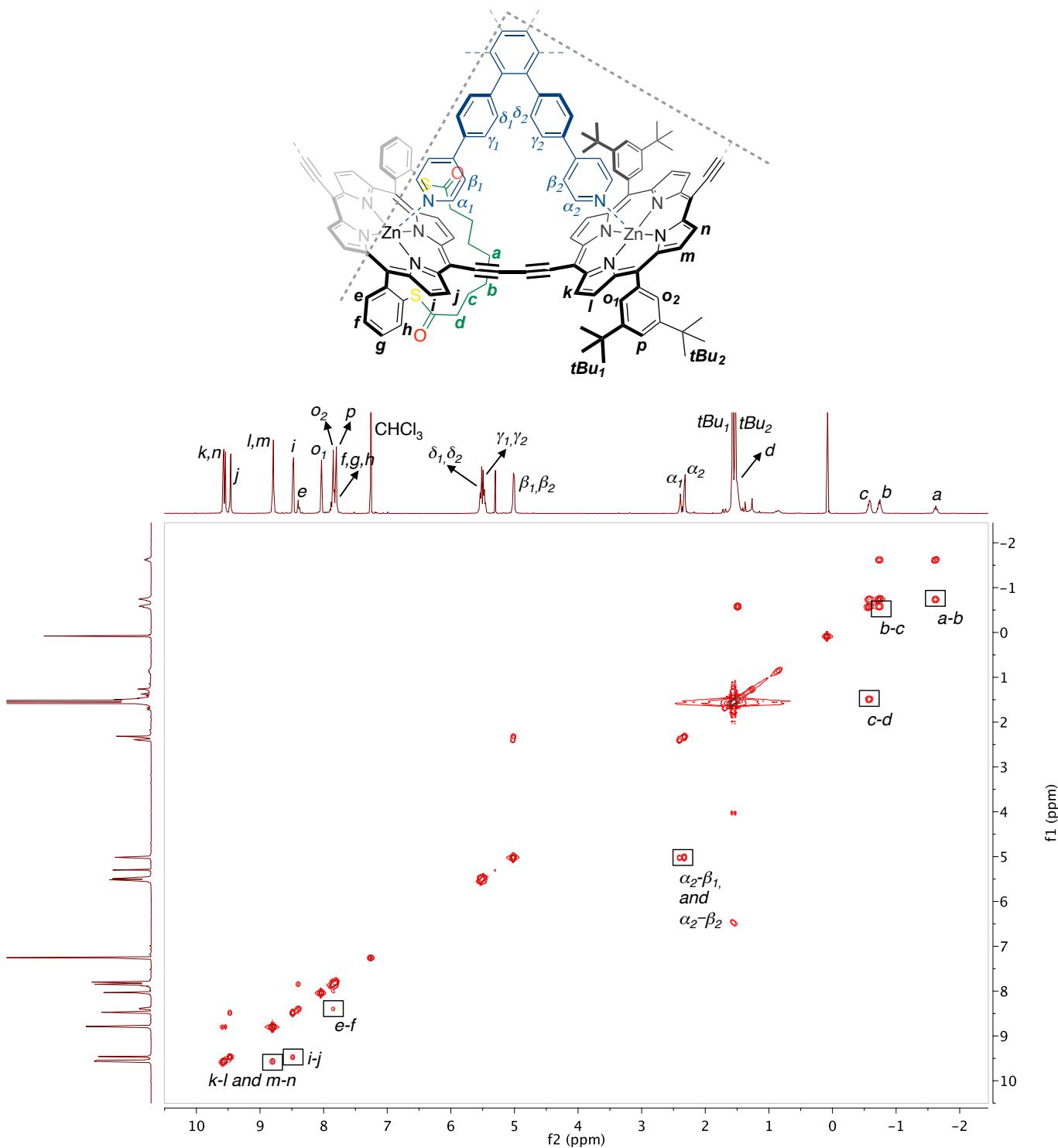


Figure S1: ^1H - ^1H COSY NMR spectrum of *c*-P6_{S-C7} \bullet T6 (500 MHz, CDCl_3 , 298 K).

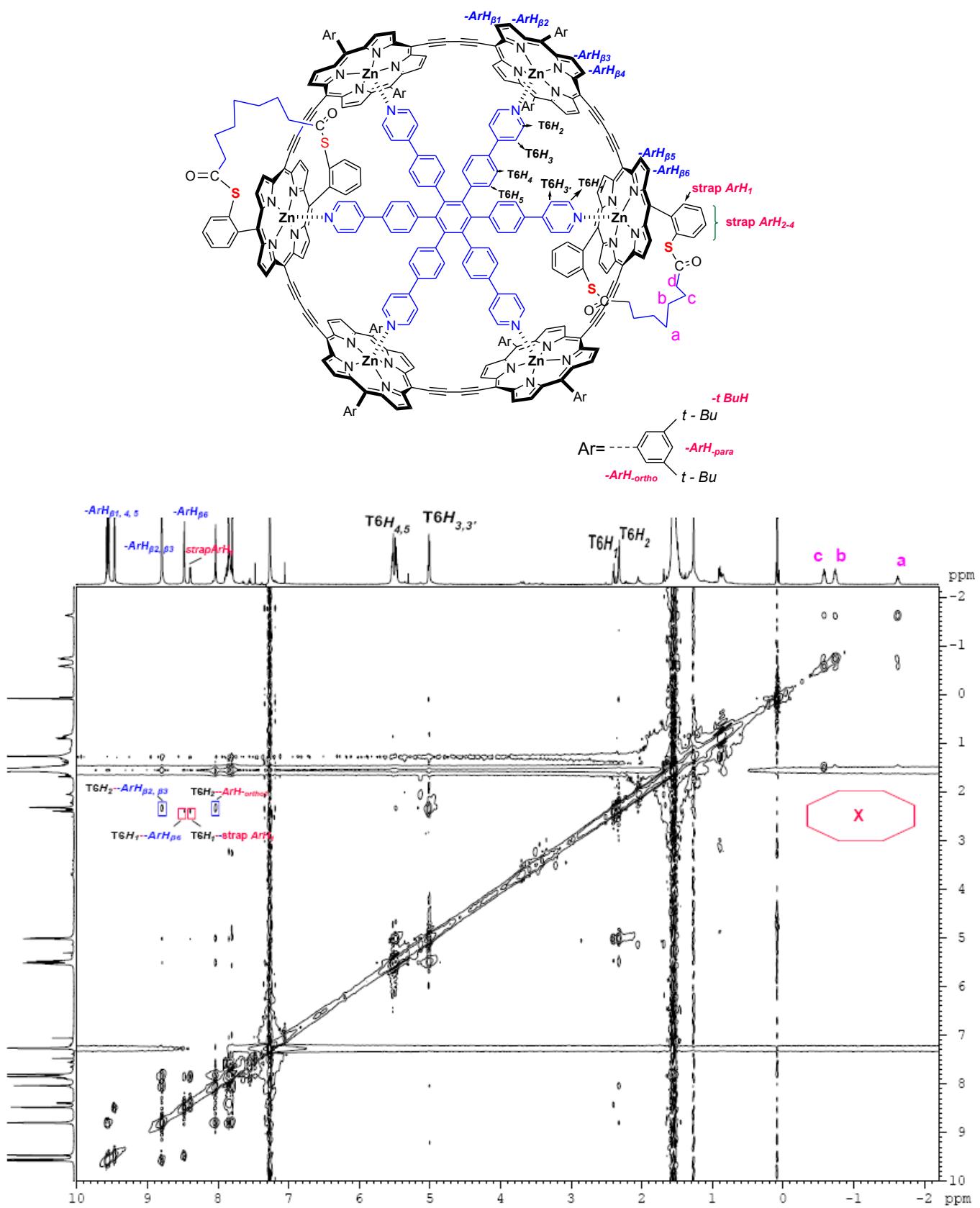


Figure S2. ¹H-¹H ROESY NMR spectrum of *c*-P6s-*c*7•T6 (500 MHz, CDCl₃, 298 K). The region labeled X shows no NOE between the strap-CH₂ and the T6-Ar-H, confirming that the strap is located outside the nanoring.

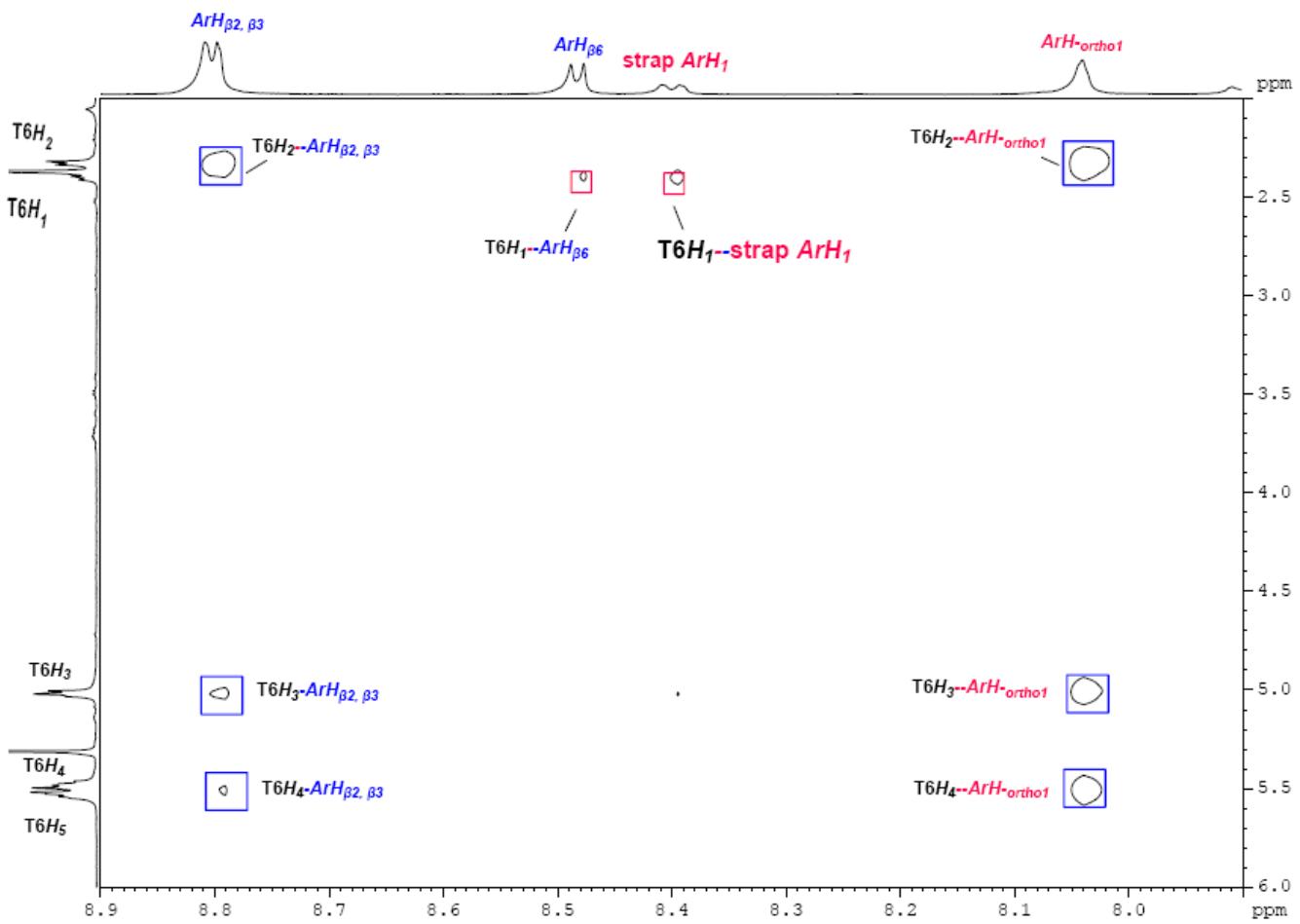


Figure S3. Part of the ^1H - ^1H ROESY spectrum of **c-P6S-C7•T6** showing NOEs between the strapped-ArH protons and the *b* protons of the strapped porphyrin, and between the strapped-ArH protons and the template **T6** (500 MHz, CDCl_3 , 298 K).

1.2. NMR spectra of 1:1 complexes of strapped dibromoporphyrins **7a-c** with pyridine

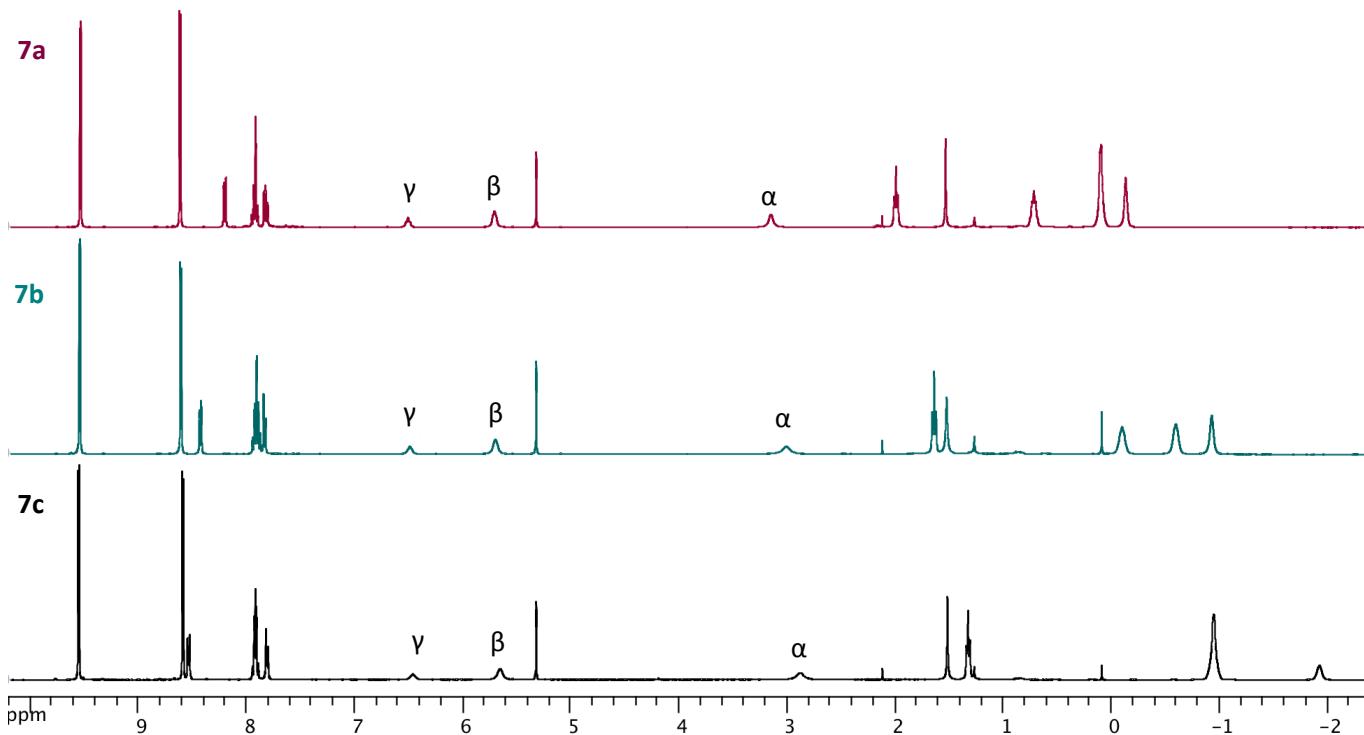


Figure S4. ¹H NMR spectra of 1:1 complexes of strapped dibromoporphyrins **7a-c** with pyridine at 298 K (CD_2Cl_2 , 400 MHz, pyridine protons indicated by α , β , and γ). At this temperature pyridine binding is dynamic and the *in* and *out* complexes cannot be distinguished by NMR.

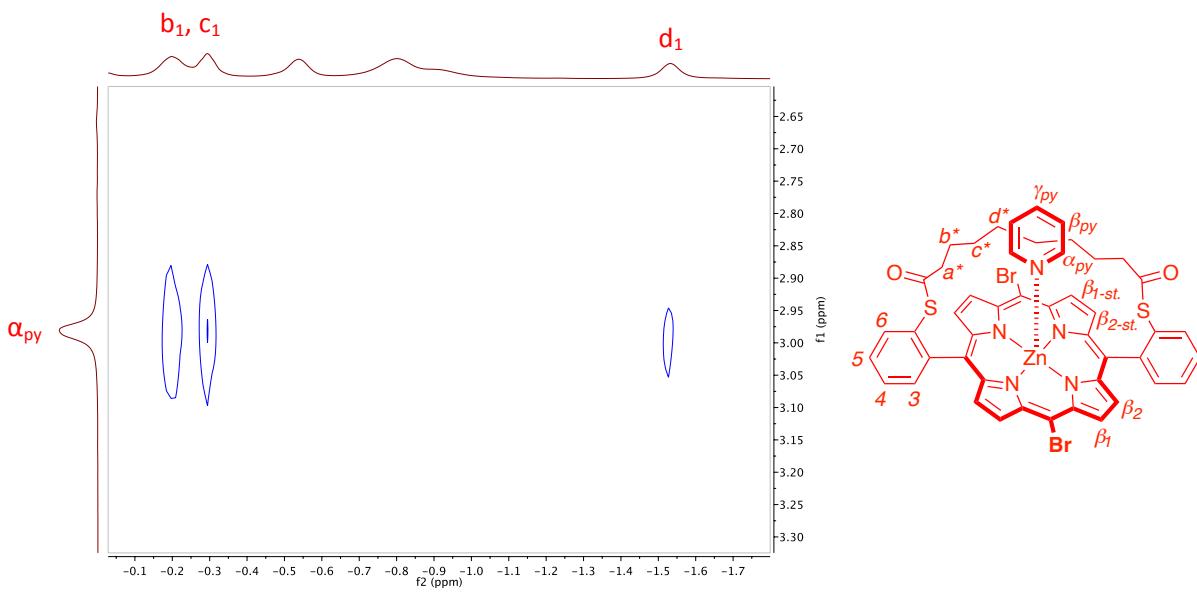


Figure S5. Part of the ROESY spectrum of the **7b**/pyridine complex showing NOEs between strap protons and the H_α pyridine proton in the *in* isomer (500 MHz, CD_2Cl_2 , 193 K).

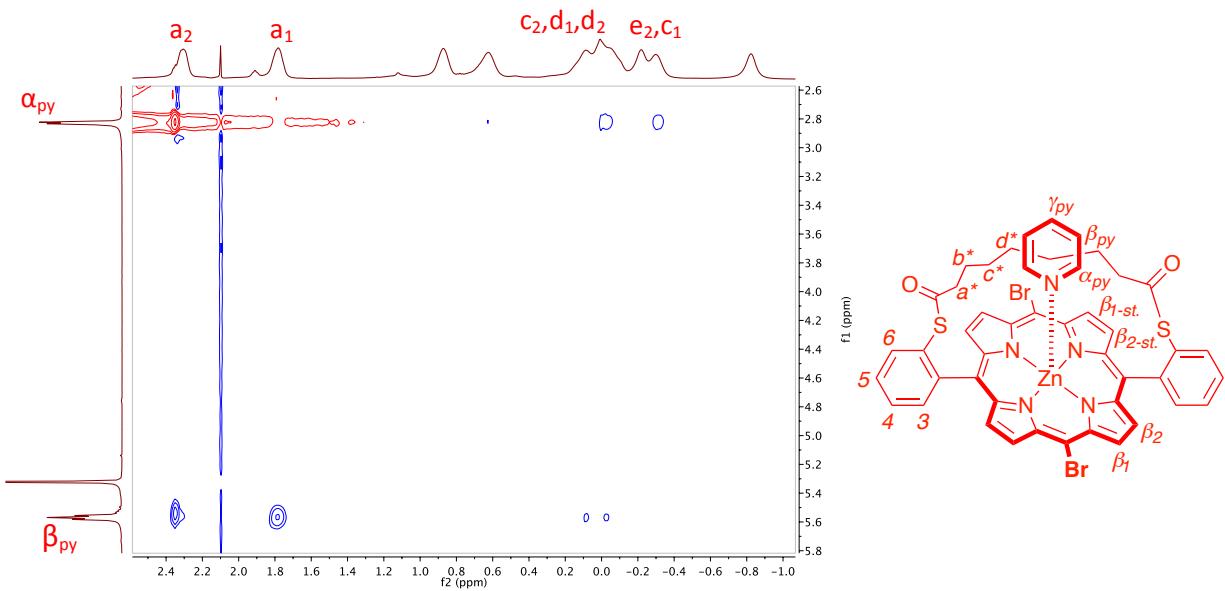


Figure S6. Part of the ROESY spectrum of the **7c**/pyridine complex showing NOEs between strap protons and the H_α and H_β pyridine protons in the *in* isomer (500 MHz, CD_2Cl_2 , 193 K).

2. MOLECULAR MODELS

2.1. General

Molecular models were built in HyperChem v. 7.0 using the MM+ forcefield with parameters modified for the description of porphyrins.^{S1,2,3,4} The Polak-Ribiere algorithm was used for geometry optimizations. The resulting geometries were subjected to further optimization in MOPAC2016 using the PM7 level of theory, and in the absence of symmetry.^{S5,6} The BFGS (Broyden-Fletcher-Goldfarb-Shanno) procedure was used for the geometry optimization.

To model the ring in a molecular junction (Fig. 1c in the main text) we optimized the geometry of the ring with free thiol groups **c-P6_{SH}•T6** (*out* isomer), based on the assumption that the strap is cleaved spontaneously on the gold surface.

The frequency calculations on **c-P6_{S-C7}•T6** and **c-P6_{SH}•T6** generated a very small imaginary mode (4.0 cm⁻¹ and 3.4 cm⁻¹, respectively), to which we attribute no significance.

2.2. Frequencies

- **c-P6_{S-C7}•T6** (*out* isomer)
1 imaginary frequency: -4.0 cm⁻¹
- **c-P6_{S-C10}•T6** (*in* isomer)
No imaginary frequency
- **c-P6_{SH}•T6** (*out* isomer)
1 imaginary frequency: -3.4 cm⁻¹

2.3. Total energies of optimized structures

- **c-P6_{S-C7}•T6** (*out* isomer)
FINAL HEAT OF FORMATION = 1501.11528 kcal/mol = 6280.66632 kJ/mol
TOTAL ENERGY = -57227.48065 eV
- **c-P6_{S-C10}•T6** (*in* isomer)
FINAL HEAT OF FORMATION = 1415.12429 kcal/mol = 5920.88004 kJ/mol
TOTAL ENERGY = -58127.21389 eV
- **c-P6_{SH}•T6** (*out* isomer)
FINAL HEAT OF FORMATION = 1718.49856 kcal/mol = 7190.19799 kJ/mol
TOTAL ENERGY = -53509.58169 eV

2.4. Cartesian coordinates

- **c-P6_{S-C7}•T6** (*out* isomer)

1	N	35.6746217	23.14620505	27.09486510
2	C	34.8680079	23.77108583	28.04716989

3	C	34.23944190	24.93537243	27.46290598
4	C	34.67063805	25.00860272	26.16048994
5	C	35.56418819	23.88731205	25.95963568
6	N	37.50207869	21.63682569	25.52720019
7	C	37.10583536	22.58682457	24.54094529
8	C	37.83389823	22.28937437	23.28395092
9	C	38.64259826	21.23617098	23.52857690
10	N	37.86272002	19.78977978	27.68325922
11	C	38.72306697	19.23642985	26.80530595
12	C	39.26849181	17.95539718	27.33784757
13	C	38.71765688	17.77058361	28.55593149
14	C	37.83807120	18.93488778	28.82275215
15	N	36.08826895	21.29485144	29.31035511
16	C	36.34388579	20.31727834	30.21302276
17	C	35.65533162	20.57303703	31.46664293
18	C	34.96641239	21.74603433	31.30005686
19	C	35.22818848	22.19781786	29.94681722
20	C	34.69972618	23.35155248	29.37409413
21	C	39.10557704	19.77725892	25.56427163
22	C	36.24967280	23.61741873	24.73148760
23	C	37.18165427	19.17779054	29.98072538
24	C	36.01676581	24.57398152	23.63161003
25	C	34.90083347	24.47672420	22.79809642
26	C	34.70702271	25.38578549	21.76189048
27	C	35.63516079	26.40641665	21.55994624
28	C	36.74895731	26.51296723	22.39113467
29	C	36.94167818	25.60027572	23.42518374
30	C	37.34659406	18.25457122	31.12007517
31	C	36.43788807	17.22538422	31.37180105
32	C	36.61406853	16.37292301	32.45832542
33	C	37.70732516	16.55334508	33.30444626
34	C	38.61774895	17.57948644	33.05993268
35	C	38.44024464	18.42992646	31.97157009
36	C	38.41996012	20.84213553	24.94769287
37	H	33.56491752	25.58790648	27.97643336
38	H	34.41571792	25.73147338	25.41843961
39	H	37.69307151	22.84851274	22.37982385
40	H	39.32709861	20.72757244	22.88170859
41	H	39.95930112	17.34307434	26.79450640
42	H	38.83988926	16.95903364	29.24782464
43	H	35.69874885	19.94357928	32.32717809
44	H	34.33970747	22.25816525	32.00000498
45	S	33.72871997	23.17952212	23.08592364
46	H	35.49040570	27.11624994	20.74775062
47	H	37.81271891	25.68133531	24.07371010
48	S	35.04577725	17.02021503	30.29458926

49	H	37.85119304	15.88733262	34.15282700
50	H	39.14941092	19.23378620	31.78184388
51	Zn	36.98748022	21.64172670	27.50941475
52	H	33.84306689	25.30454506	21.09890434
53	H	37.47375193	27.30976134	22.22967722
54	H	35.91131194	15.56003616	32.65297510
55	H	39.47234877	17.71627801	33.72073875
56	C	35.69289774	15.78192322	29.10853945
57	C	34.97419391	15.78259098	27.79791585
58	C	35.62733858	16.84212878	26.89756211
59	C	34.75950504	17.11385651	25.66626231
60	C	35.34892779	18.27784136	24.86156606
61	C	34.37121052	18.71700948	23.76598381
62	C	34.89517689	19.97822574	23.07278989
63	C	33.82681104	20.56261236	22.13614738
64	H	33.88804319	15.97848298	27.90778441
65	H	35.04668177	14.77994472	27.32361747
66	H	36.63930493	16.51248114	26.59225921
67	H	35.77815638	17.79440958	27.45334658
68	H	33.72636208	17.36018867	25.98017788
69	H	34.68179673	16.21024273	25.03658112
70	H	36.32151566	17.99112120	24.42187911
71	H	35.56782359	19.13334522	25.53717651
72	H	33.37760351	18.91621449	24.21313142
73	H	34.22085563	17.90437541	23.03335773
74	H	35.81837886	19.75098735	22.50624202
75	H	35.19597242	20.71923944	23.84652379
76	H	32.82201748	20.50423943	22.60450020
77	H	33.75532582	19.95122377	21.21062542
78	O	36.62552503	15.08729153	29.38425883
79	C	34.20521121	21.96769193	21.79238756
80	O	34.77980554	22.30900231	20.80240362
81	Zn	48.64485087	18.83733235	25.59276556
82	N	50.32569593	19.58701998	24.69065307
83	C	51.59068489	19.50145784	25.14859317
84	C	52.51410935	20.31196134	24.30276933
85	C	51.75738053	20.90979053	23.35960048
86	C	50.35182610	20.49408141	23.59454953
87	N	47.53963987	19.62292573	24.05798193
88	C	47.92659423	20.53722612	23.13694046
89	C	46.78891682	21.01631270	22.36990488
90	C	45.68819118	20.35873431	22.85383256
91	N	47.09225572	17.63464370	26.13260532
92	C	45.78642608	17.73430414	25.65027751
93	C	44.93450641	16.80746870	26.36300311
94	C	45.72760740	16.16248193	27.28089035

95	C	47.06122650	16.70271606	27.12291428
96	N	49.86915539	17.73943289	26.80801180
97	C	49.44472346	16.77296005	27.76373906
98	C	50.61937800	16.3614696	28.57033512
99	C	51.68126671	17.06151169	28.11686789
100	C	51.18620033	17.92423079	27.00883924
101	C	52.01401047	18.82067848	26.30529469
102	C	53.23151063	19.19425988	26.84703293
103	C	54.22915578	19.69302946	27.34896707
104	C	43.95947223	18.70159246	24.48060765
105	C	42.74574476	18.82860637	24.47841233
106	C	49.27421334	20.97668149	22.93254606
107	C	48.17954472	16.32394588	27.93229006
108	C	49.48545378	22.07112809	21.96769733
109	C	49.52602474	21.82773967	20.60154410
110	C	49.77483780	22.88126271	19.71220484
111	C	49.97692210	24.16036692	20.22274945
112	C	49.93299943	24.41430843	21.60075533
113	C	49.67841378	23.36143886	22.47177198
114	C	49.83371967	22.58045380	18.22658689
115	C	50.06786021	23.83651231	17.37078588
116	C	48.49970076	21.94573157	17.79386958
117	C	50.99480770	21.60001234	17.97669544
118	C	50.18733737	25.82495824	22.09605489
119	C	47.89970862	15.41652473	29.06071885
120	C	47.80075843	14.04523435	28.86618335
121	C	47.55853934	13.20145238	29.95762403
122	C	47.41486298	13.76231156	31.22370152
123	C	47.50636060	15.14635006	31.42600877
124	C	47.75027295	15.97250435	30.33461717
125	C	47.46488336	11.70711024	29.71472776
126	C	48.78699209	11.22658827	29.08810674
127	C	47.22464173	10.90556971	31.00483337
128	C	46.29264708	11.44006868	28.75326217
129	C	47.34917452	15.69453151	32.83146815
130	C	48.47275769	15.11549372	33.71085556
131	C	45.97378717	15.27261745	33.38008892
132	C	47.43698963	17.22978859	32.88413581
133	C	40.29848625	19.33912942	25.01322528
134	C	41.42957811	19.04201378	24.65755178
135	C	34.00678545	24.23319868	30.21160464
136	C	33.54502002	25.10476698	30.93049817
137	C	46.15316857	19.47860493	23.91041525
138	C	45.34859160	18.62321522	24.65695937
139	Zn	34.27506117	31.42745473	34.28718122
140	N	33.63598778	30.84523992	32.43232961

141	C	33.29132452	29.60185127	32.05411334
142	C	33.08651055	29.53548264	30.57843668
143	C	33.33911856	30.76885491	30.09210549
144	C	33.69720240	31.63054644	31.24463469
145	N	34.38901181	33.34555273	33.58570542
146	C	34.33086455	33.76958472	32.29880208
147	C	34.62423192	35.18763195	32.20612409
148	C	34.87963351	35.61733750	33.48393625
149	C	34.73917992	34.46490534	34.34894540
150	N	34.41923683	32.08545551	36.20780742
151	C	34.76925377	33.38426464	36.59190135
152	C	34.93338312	33.43524120	38.03118875
153	C	34.68107054	32.17347864	38.50521392
154	C	34.37225550	31.35327993	37.34839647
155	N	33.63212018	29.61450304	35.01546254
156	C	33.69517515	29.19034875	36.37349681
157	C	33.33704403	27.75262369	36.43516575
158	C	33.08454668	27.34840099	35.17196018
159	C	33.28596629	28.53335140	34.29192572
160	C	33.18810072	28.47005962	32.89026203
161	C	33.12045917	27.23477297	32.27270685
162	C	33.20976036	26.17610096	31.66762414
163	C	34.95984048	34.46483436	35.72671770
164	C	35.55582371	35.60190003	36.28742607
165	C	36.26411830	36.46474689	36.78109727
166	C	34.04282565	32.93580276	31.16940421
167	C	34.06164212	29.95672309	37.42609127
168	C	34.17527594	33.57132560	29.84598770
169	C	33.19462604	34.44204338	29.37958238
170	C	33.34844195	35.06639087	28.13883083
171	C	34.48772727	34.79495437	27.37898683
172	C	35.47197511	33.91672379	27.83617630
173	C	35.30833370	33.30331828	29.08007692
174	C	32.26665100	36.02147981	27.66989989
175	C	30.94579589	35.24046424	27.54352071
176	C	32.11908138	37.14799024	28.70968107
177	C	32.58084557	36.66340390	26.30843169
178	C	36.72056183	33.60302700	27.03320299
179	C	36.75401821	32.09022455	26.74500969
180	C	36.77506986	34.35041479	25.69065246
181	C	37.95349068	34.01109381	27.86227256
182	C	34.18185863	29.33682773	38.75832318
183	C	33.04657737	29.04952244	39.50572684
184	C	33.17290291	28.45909691	40.76921292
185	C	34.44581205	28.17012568	41.25248237
186	C	35.59566382	28.45514657	40.50307453

187	C	35.45665999	29.04416159	39.2509601
188	C	31.91406631	28.16341654	41.56201145
189	C	36.95336623	28.12582578	41.09367879
190	N	48.23756326	20.46322110	26.89546715
191	C	48.81454337	21.66756705	26.68459361
192	C	48.49098598	22.79940905	27.43795502
193	C	47.52948807	22.69214009	28.44730867
194	C	46.93978159	21.44573972	28.67424401
195	C	47.31913542	20.35789352	27.88125889
196	C	47.14686412	23.86688156	29.24088899
197	C	46.82027645	25.06583588	28.59967536
198	C	46.46560675	26.18569319	29.34577303
199	C	46.43129516	26.11471453	30.74015507
200	C	46.75195651	24.91706234	31.38359054
201	C	47.10872410	23.79812244	30.63636964
202	C	46.08138232	27.30496440	31.53466230
203	N	38.56176180	22.85102512	28.29054169
204	C	38.48493884	24.20084991	28.26767106
205	C	39.46669604	25.02224428	28.83181498
206	C	40.57542588	24.43584542	29.44785926
207	C	40.65813341	23.04087705	29.47242137
208	C	39.63728583	22.28628975	28.88475373
209	C	41.63106767	25.26695394	30.04622488
210	C	42.32966894	26.18483258	29.25679223
211	C	43.33870681	26.96538674	29.81454717
212	C	43.66090526	26.83609965	31.16808486
213	C	42.95491248	25.92829401	31.96121806
214	C	41.94635663	25.14665736	31.40235636
215	C	44.74196172	27.65179500	31.75110290
216	N	36.30327776	30.90983061	33.98157257
217	C	37.28108417	31.83970309	34.05985985
218	C	38.62598897	31.53557149	33.82393092
219	C	38.97528247	30.22246842	33.50286666
220	C	37.96843928	29.25805475	33.42482187
221	C	36.64548677	29.64080339	33.66537708
222	C	40.37648498	29.85513667	33.25061966
223	C	40.97954445	30.18633959	32.03547962
224	C	42.30305087	29.82743135	31.79382760
225	C	43.03138499	29.14536066	32.77085377
226	C	42.42877483	28.81645089	33.98756363
227	C	41.10295245	29.16721542	34.22517658
228	C	44.43672503	28.77761239	32.52592630
229	H	53.57034771	20.35549628	24.47029327
230	H	52.04474533	21.56479440	22.56091213
231	H	46.84605555	21.74127213	21.58840098
232	H	44.66820448	20.44183255	22.54226055

233	H	43.88971975	16.67479245	26.17871465
234	H	45.45365948	15.40868461	27.98551712
235	H	50.56206815	15.62953479	29.35154617
236	H	52.70311780	17.04830757	28.43277688
237	H	49.36875904	20.81583469	20.23042885
238	H	50.17776483	24.99052689	19.54828446
239	H	49.62773165	23.51608258	23.54657581
240	H	50.09206452	23.58396248	16.30456414
241	H	51.02319905	24.31571639	17.60902970
242	H	49.26901309	24.57265420	17.50966755
243	H	48.48865290	21.73911552	16.71910369
244	H	48.31180321	20.99743322	18.30920931
245	H	47.65756953	22.61086458	18.01479495
246	H	51.10768478	21.38282887	16.90997789
247	H	51.94377907	22.01362176	18.33539785
248	H	50.83811818	20.64505983	18.48996202
249	H	47.91300670	13.63441063	27.86373946
250	H	47.22821090	13.12338509	32.08466597
251	H	47.83019162	17.05118672	30.44679795
252	H	48.79205519	10.13988064	28.95834843
253	H	49.64150273	11.49142568	29.72058322
254	H	48.95708005	11.67306570	28.10240510
255	H	47.16856979	9.831720324	30.79330941
256	H	48.03623907	11.04955489	31.72588903
257	H	46.28206567	11.18792362	31.48570334
258	H	46.16015588	10.36802109	28.57768808
259	H	45.35308978	11.83087314	29.15959318
260	H	46.44930414	11.91410690	27.77802254
261	H	48.42273289	15.51091853	34.72993570
262	H	49.45864486	15.36619271	33.30260690
263	H	48.41479695	14.02447266	33.77943598
264	H	45.79639625	15.69458774	34.37390834
265	H	45.88523655	14.18493407	33.46708120
266	H	45.16768896	15.61519225	32.72129891
267	H	47.31386218	17.59359924	33.90956826
268	H	48.40933038	17.58935338	32.52893129
269	H	46.65418400	17.69708562	32.27688302
270	H	32.78996663	28.64210343	30.06919081
271	H	33.29970433	31.13161679	29.08398975
272	H	34.63183587	35.75061654	31.29906802
273	H	35.13137243	36.60105883	33.81952709
274	H	35.19517979	34.31399150	38.58211540
275	H	34.69438187	31.82274119	39.51369078
276	H	33.30324911	27.19968594	37.35279398
277	H	32.79308352	26.38867928	34.79983223
278	H	32.31525389	34.63493135	29.99296960

279	H	34.61145415	35.27796926	26.41261775
280	H	36.06328373	32.62040553	29.46437730
281	H	30.13786208	35.88366939	27.18136638
282	H	30.62576690	34.82355682	28.50470125
283	H	31.04787266	34.40542794	26.84180659
284	H	31.36791622	37.87984436	28.39703557
285	H	33.06624014	37.68044936	28.85053900
286	H	31.81119847	36.76339204	29.68821857
287	H	31.78157146	37.34969529	26.00642631
288	H	33.50890350	37.24395492	26.34121526
289	H	32.67331654	35.91079234	25.51848469
290	H	37.62835141	31.81984371	26.14598113
291	H	36.79270572	31.50029820	27.66665314
292	H	35.86079818	31.77645184	26.19291113
293	H	37.68718820	34.09912600	25.13860628
294	H	36.77348376	35.43643139	25.83421385
295	H	35.92717055	34.08775503	25.04873364
296	H	38.87886313	33.85385527	27.30106143
297	H	37.90527502	35.07047055	28.13933285
298	H	38.02886159	33.43433183	28.78996179
299	H	32.06336035	29.29348699	39.10607462
300	H	34.56519406	27.71563512	42.23399016
301	H	36.32152542	29.29242076	38.63945510
302	H	49.56177083	21.71863587	25.87654670
303	H	48.98557695	23.74739039	27.24121462
304	H	46.18415589	21.32134678	29.44571665
305	H	46.87067596	19.36104765	28.02995154
306	H	46.83635322	25.12217170	27.51106300
307	H	46.21757277	27.11890370	28.84313726
308	H	46.72790167	24.86258655	32.47085316
309	H	47.36916803	22.86914856	31.14277898
310	H	37.59669000	24.6353473	27.77871903
311	H	39.35972391	26.10396408	28.79756556
312	H	41.50873360	22.54534026	29.93412997
313	H	39.67416727	21.18512204	28.88312222
314	H	42.09022149	26.28404910	28.19840086
315	H	43.88111962	27.67631201	29.19353691
316	H	43.19348386	25.83427552	33.01959583
317	H	41.39692526	24.44309962	32.02720955
318	H	36.96324251	32.863801590	34.31990976
319	H	39.38500234	32.31148030	33.89294428
320	H	38.20525572	28.22626972	33.17552228
321	H	35.82060965	28.91127143	33.60064804
322	H	40.41235719	30.72177788	31.27481965
323	H	42.77127185	30.07693871	30.84317159
324	H	42.99939834	28.28915822	34.75030159

325	H	40.63230813	28.9089564	35.17303300
326	N	41.13133140	37.17722187	40.00250945
327	C	39.87673635	37.28340265	39.52224608
328	C	38.92689883	36.47871921	40.34530667
329	C	39.65534449	35.87762381	41.30853331
330	C	41.06841465	36.28522865	41.11018728
331	N	43.89169410	37.14462869	40.71095356
332	C	43.47574384	36.25899653	41.64734013
333	C	44.59211826	35.78578082	42.44856295
334	C	45.71206307	36.40892733	41.96282433
335	N	44.40367754	39.11635282	38.62934295
336	C	45.70268076	38.98130698	39.12008172
337	C	46.58201975	39.89510014	38.42378164
338	C	45.81042061	40.57099069	37.51028635
339	C	44.46339538	40.05976715	37.65096578
340	N	41.64923261	39.03117438	37.89238471
341	C	42.09376954	40.01580203	36.96433633
342	C	40.93393682	40.45177313	36.14967094
343	C	39.85896285	39.75651745	36.57850421
344	C	40.33037180	38.87152383	37.68018595
345	C	39.47839026	37.99120467	38.37319388
346	C	38.24188288	37.67570307	37.83841718
347	C	37.21660549	37.22522901	37.34713162
348	C	47.49477888	37.92082287	40.25858573
349	C	48.69531110	37.70833679	40.21489395
350	C	42.12102080	35.83045992	41.82879706
351	C	43.35970890	40.47696823	36.84004094
352	C	41.89083344	34.79157818	42.84809259
353	C	41.89849034	35.11146678	44.20223226
354	C	41.681111001	34.11354317	45.15649227
355	C	41.44402231	32.80552131	44.72994028
356	C	41.42790947	32.47814889	43.37310826
357	C	41.66335052	33.48129690	42.43086004
358	C	41.70325790	34.49825692	46.62411691
359	C	41.53031881	33.29319468	47.56325715
360	C	43.05500619	35.16365328	46.94291535
361	C	40.55103387	35.48628042	46.88353604
362	C	41.16027285	31.07083223	42.87456348
363	C	43.65630532	41.46967981	35.79087833
364	C	43.82729375	42.80610757	36.13137702
365	C	44.10483295	43.75142916	35.13705988
366	C	44.20622214	43.32654874	33.81521762
367	C	44.03579606	41.98034965	33.46415611
368	C	43.75977411	41.05090554	34.46188691
369	C	44.28455189	45.20147759	35.54424945
370	C	42.98358906	45.68872338	36.20853583

371	C	44.59278519	46.12329079	34.35281614
372	C	45.45541169	45.29042253	36.54023496
373	C	44.16168381	41.58547610	32.00499651
374	C	43.12616713	42.37562000	31.18376834
375	C	45.58627932	41.92228201	31.52702722
376	C	43.91517052	40.08509545	31.77098930
377	N	53.98227797	34.90570678	39.00265233
378	C	52.96448531	35.58081092	39.56514940
379	C	52.62623115	35.01522743	40.90168378
380	C	53.48744685	34.00019246	41.12502912
381	C	54.37676969	33.90859608	39.94073806
382	N	56.06431921	33.70233679	37.49266183
383	C	56.22098604	32.94914881	38.61588856
384	C	57.29159705	31.99187646	38.44647184
385	C	57.75602020	32.14738349	37.16131566
386	N	55.67323485	35.67554927	35.39841808
387	C	56.61719268	34.86809067	34.74689759
388	C	56.97863070	35.47325629	33.48055860
389	C	56.26967432	36.64262954	33.38342979
390	C	55.44738973	36.72954726	34.57858622
391	N	53.66876283	36.91315127	36.98691225
392	C	53.70428316	37.84915346	35.91552549
393	C	52.68337815	38.89740945	36.17196480
394	C	52.06955159	38.58424063	37.33133667
395	C	52.70216817	37.32812971	37.83128121
396	C	52.28382855	36.67983180	39.00553450
397	C	51.09581103	37.09689655	39.58257924
398	C	49.98860064	37.42354074	39.98292122
399	C	57.13762956	33.67946236	35.24943577
400	C	57.78659144	32.80722013	34.36751968
401	C	58.15083506	31.91404741	33.61796477
402	C	55.39540176	33.03251156	39.78413432
403	C	54.49259176	37.77280527	34.81851585
404	C	55.67796135	32.05285139	40.85086440
405	C	56.39659617	32.40576310	41.99527455
406	C	56.67781905	31.46017197	42.97744498
407	C	56.22827166	30.14995544	42.81983476
408	C	55.50474640	29.79143242	41.68392238
409	C	55.22898286	30.73854964	40.70074872
410	C	54.34720357	38.77820629	33.74903272
411	C	54.91567245	40.04966459	33.84616671
412	C	54.78332559	40.96852782	32.80825720
413	C	54.06904701	40.61649865	31.66435954
414	C	53.49457767	39.35074928	31.56130772
415	C	53.63060039	38.43326132	32.59971535
416	C	56.98767009	33.21572124	36.56712210

417	C	45.27775191	37.26526360	40.87511699
418	C	46.11006046	38.07559402	40.1101732
419	N	57.96271217	26.14697041	32.12712039
420	C	58.30378684	27.39848265	32.48375778
421	C	58.61972336	27.46575063	33.93899047
422	C	58.44957488	26.22194615	34.43435153
423	C	58.01932437	25.35505232	33.31021088
424	N	57.18637566	23.61789890	31.02793665
425	C	57.31620446	23.20675211	32.31304139
426	C	56.98539600	21.79896614	32.44270647
427	C	56.63846704	21.36223216	31.18955804
428	C	56.76449213	22.49836725	30.30004687
429	N	57.09141670	24.83727094	28.39670349
430	C	56.69704647	23.54242669	28.04353491
431	C	56.51259776	23.46796984	26.60839657
432	C	56.79938793	24.71136774	26.10533580
433	C	57.14644822	25.54534801	27.24119896
434	N	57.86188276	27.34699076	29.54460378
435	C	57.82053001	27.73144759	28.17379083
436	C	58.17493304	29.16857020	28.07912260
437	C	58.40644516	29.60837982	29.33469689
438	C	58.20506690	28.44552367	30.24287692
439	C	58.33628180	28.53121355	31.64209588
440	C	58.42915827	29.77037432	32.25047783
441	C	58.39418714	30.83049366	32.86065239
442	C	56.49830736	22.48018992	28.93108996
443	C	55.87168823	21.34599269	28.39765249
444	C	55.16393987	20.47770656	27.91263521
445	C	57.71137726	24.04121093	33.40961838
446	C	57.48856774	26.93288933	27.13352460
447	C	57.76772086	23.39629475	34.73402567
448	C	58.79328545	22.50089331	35.02642611
449	C	58.85155192	21.89091725	36.28188228
450	C	57.87360885	22.19640658	37.23039165
451	C	56.84327132	23.09462078	36.94659248
452	C	56.79290485	23.69210617	35.68494281
453	C	59.98049492	20.91624808	36.56008793
454	C	61.32082648	21.65560733	36.39179193
455	C	59.88469606	19.75584218	35.55235137
456	C	59.93002355	20.32818499	37.97972218
457	C	55.77204295	23.45041381	37.96063956
458	C	55.79677945	24.97312029	38.19353836
459	C	55.97495857	22.75522122	39.31706916
460	C	54.40350493	23.02296016	37.39789264
461	C	57.46045730	27.50153598	25.77323107
462	C	58.65316990	27.73757005	25.10013691

463	C	58.63256322	28.27465859	23.80755474
464	C	57.40436623	28.56222655	23.21926869
465	C	56.19687205	28.32216795	23.88980886
466	C	56.23135670	27.78899507	25.17422620
467	C	59.95266978	28.51081701	23.09894743
468	C	54.89396363	28.64693019	23.18409726
469	H	37.87502133	36.44003353	40.15060527
470	H	39.34309677	35.22557782	42.10004204
471	H	44.51101803	35.08609547	43.25096564
472	H	46.72523242	36.31849431	42.29431370
473	H	47.62845776	40.00033414	38.61673504
474	H	46.10734101	41.32788764	36.81850711
475	H	41.00861990	41.19517943	35.38090145
476	H	38.84152056	39.78547593	36.24959839
477	H	42.07638990	36.14217795	44.50719374
478	H	41.26784867	32.02659414	45.46822281
479	H	41.67252866	33.24889746	41.36833762
480	H	41.56705445	33.60775878	48.61249516
481	H	40.56653131	32.79626716	47.41123133
482	H	42.32528757	32.55367130	47.41963714
483	H	43.12838235	35.42455078	48.00329536
484	H	43.20255277	36.08602320	46.37063903
485	H	43.88873053	34.49377142	46.70493283
486	H	40.51946117	35.79158434	47.93400141
487	H	39.58311104	35.03621156	46.63740903
488	H	40.65200260	36.39555873	46.28083540
489	H	43.74625416	43.10837406	37.17499422
490	H	44.42224320	44.04553316	33.02739522
491	H	43.62338266	39.99694161	34.23250276
492	H	43.05572153	46.74221257	36.49613815
493	H	42.13145655	45.58559245	35.52778276
494	H	42.75006135	45.11818187	37.11406764
495	H	44.71525475	47.16105564	34.68328839
496	H	43.78333046	46.11391220	33.61542916
497	H	45.52090443	45.83391906	33.84881055
498	H	45.64580129	46.32635824	36.83744679
499	H	46.37714077	44.89385387	36.10039020
500	H	45.25767621	44.71986875	37.45440203
501	H	43.15806188	42.09223648	30.12718616
502	H	42.11017865	42.18858400	31.54986258
503	H	43.30008314	43.45507454	31.23675638
504	H	45.73596160	41.62472242	30.48480234
505	H	45.79556750	42.99478355	31.59467684
506	H	46.33643046	41.40372210	32.13489321
507	H	44.00516493	39.83537960	30.70861219
508	H	42.90912915	39.78940015	32.08908644

509	H	44.64176897	39.46897071	32.31146350
510	H	51.83819626	35.39913132	41.51579337
511	H	53.57024549	33.34884581	41.97146341
512	H	57.63146041	31.31191595	39.19601091
513	H	58.53977738	31.61043990	36.66987651
514	H	57.68331682	35.05940809	32.78968558
515	H	56.29133467	37.37185364	32.60352085
516	H	52.51711415	39.72598622	35.51353936
517	H	51.28415543	39.09104796	37.85352761
518	S	56.95533039	34.07554417	42.17594574
519	H	56.45059891	29.40644468	43.58252367
520	H	54.67470264	30.45741160	39.80677637
521	S	55.82391942	40.47753698	35.30570900
522	H	53.96813725	41.32919618	30.84820734
523	H	53.19383727	37.43905932	32.51578023
524	H	58.92760925	28.36568909	34.42983819
525	H	58.58578475	25.85629484	35.43313216
526	H	57.01582216	21.24759142	33.35654625
527	H	56.33593847	20.38311855	30.88345561
528	H	56.21735345	22.58726768	26.07816252
529	H	56.78541375	25.04000817	25.08945907
530	H	58.21929817	29.69703263	27.14748806
531	H	58.68793895	30.57923789	29.68462857
532	H	59.54333798	22.28126127	34.26704920
533	H	57.91543644	21.72434505	38.20918711
534	H	55.99444777	24.38707185	35.43336072
535	H	62.16631303	21.00304226	36.63029915
536	H	61.46380312	22.01241739	35.36606126
537	H	61.37492427	22.52761914	37.05284411
538	H	60.66217539	19.00748489	35.73428902
539	H	58.91378696	19.25315585	35.62180188
540	H	60.00049949	20.10181467	34.51924362
541	H	60.76165664	19.63376502	38.14490333
542	H	59.00465117	19.76871005	38.15230554
543	H	60.00745903	21.10993687	38.74282296
544	H	55.06950856	25.26969683	38.95510015
545	H	55.55964089	25.52915332	37.28085535
546	H	56.78672448	25.30209472	38.53059046
547	H	55.19126492	23.04271367	40.02632859
548	H	55.93771277	21.66473052	39.22109774
549	H	56.93523775	23.02774268	39.76868066
550	H	53.59825690	23.23803860	38.10609374
551	H	54.38545660	21.94778391	37.18657585
552	H	54.16828408	23.54236108	36.46307100
553	H	59.59925716	27.49373952	25.58160409
554	H	57.36698001	28.97944457	22.21480383

555	H	55.31879940	27.58148860	25.72878496
556	N	43.27223955	36.30469123	37.84023368
557	C	42.79289443	35.06882022	38.10566807
558	C	43.12566691	33.95126859	37.33482509
559	C	43.99500212	34.10655862	36.25056568
560	C	44.48526122	35.38522849	35.97049581
561	C	44.10108847	36.45642133	36.78363455
562	C	44.38770760	32.95084391	35.43381619
563	C	44.81571794	31.77109754	36.05114003
564	C	45.17873736	30.66887488	35.28314710
565	C	45.11660496	30.73624471	33.88937876
566	C	44.70072225	31.91659070	33.26907837
567	C	44.33817328	33.01863866	34.03850862
568	C	45.46344631	29.55696682	33.07811981
569	N	53.15363417	33.91204702	36.15709588
570	C	53.24519127	32.56344290	36.12673079
571	C	52.24154336	31.75060218	35.58687217
572	C	51.09099873	32.34310961	35.05803465
573	C	50.99794303	33.73795508	35.08374300
574	C	52.04401501	34.48332686	35.63594299
575	C	50.00033439	31.53467174	34.49258234
576	C	49.43180365	30.49474658	35.23400921
577	C	48.38451497	29.74394728	34.70561376
578	C	47.89613300	30.02152166	33.42635677
579	C	48.46505996	31.05674391	32.68085236
580	C	49.50994858	31.80898605	33.21197307
581	C	46.80195822	29.21283185	32.85732873
582	N	55.24907888	26.01855429	30.62594575
583	C	54.26468656	25.12757465	30.37472940
584	C	52.91499353	25.41978115	30.59704927
585	C	52.57131080	26.67852671	31.09301740
586	C	53.58532394	27.60313309	31.35160012
587	C	54.91169933	27.23574459	31.10814672
588	C	51.16651571	27.03151940	31.34351845
589	C	50.55466808	26.64917766	32.53882577
590	C	49.22912527	26.99661231	32.78408953
591	C	48.51144394	27.72282245	31.83156138
592	C	49.12187840	28.10048157	30.63331873
593	C	50.44858378	27.75667902	30.39050567
594	C	47.10656797	28.08671172	32.08235259
595	H	42.11955548	34.98187681	38.97378325
596	H	42.70880599	32.97673610	37.57643135
597	H	45.16844750	35.54812089	35.14072883
598	H	44.47126192	37.47807777	36.59396127
599	H	44.87222223	31.71643586	37.13846294
600	H	45.51159673	29.75205639	35.76763490

601	H	44.65269316	31.96986706	32.18265833
602	H	44.00389988	33.93320748	33.54953217
603	H	54.16443582	32.12717575	36.55243578
604	H	52.36232069	30.66999809	35.57538792
605	H	50.11746752	34.24136908	34.69101906
606	H	51.99627512	35.58344620	35.66827935
607	H	49.80359065	30.27558383	36.23463078
608	H	47.94602880	28.93648700	35.28940734
609	H	48.09107293	31.27359878	31.68143799
610	H	49.95187236	32.61165004	32.62209530
611	H	54.58101615	24.14564400	29.98298592
612	H	52.14916837	24.67714812	30.38556021
613	H	53.35033593	28.59228560	31.73742924
614	H	55.74406751	27.93393777	31.30399703
615	H	51.11585031	26.08085228	33.27980937
616	H	48.75136413	26.70443032	33.71751065
617	H	48.55796320	28.66169512	29.89023139
618	H	50.92664813	28.05206422	29.45736905
619	Zn	42.83331077	37.92170816	39.13815253
620	Zn	54.65681446	35.11593660	37.08115878
621	Zn	57.27242754	25.52983283	30.30272680
622	C	50.10597216	25.94373311	23.62814104
623	C	49.13579473	26.76647241	21.48177078
624	C	51.60001860	26.24866818	21.65542362
625	C	32.20300345	27.49023086	42.91404044
626	C	31.01976350	27.22009347	40.73628320
627	C	31.18183858	29.49127456	41.82841675
628	C	38.10755488	28.40794603	40.11639430
629	C	36.99685390	26.63101996	41.46129055
630	C	37.15153053	28.98666243	42.35448776
631	C	40.80905147	30.08935801	44.00448562
632	C	42.42349937	30.55772024	42.15810591
633	C	39.97680025	31.11437592	41.89034867
634	H	57.25808112	31.72829877	43.86339357
635	H	55.15851802	28.76617485	41.56029211
636	H	55.24338987	41.95709610	32.87283239
637	H	52.94380704	39.07498658	30.66304743
638	C	59.78155369	29.17161289	21.72123005
639	C	60.64774795	27.15086060	22.90404234
640	C	60.82667007	29.43385818	23.96847018
641	C	53.65782920	28.33381564	24.04442034
642	C	54.81282470	27.81046286	21.89398855
643	C	54.87547475	30.14852136	22.84330027
644	H	50.84891620	25.30533601	24.12009431
645	H	49.11277522	25.66799705	23.99887495
646	H	50.29941490	26.97213316	23.95108237

647	H	48.12110118	26.43918699	21.73538510
648	H	49.20457517	26.79749102	20.38956191
649	H	49.25785416	27.79085762	21.84595068
650	H	51.70415506	26.25275894	20.56602747
651	H	52.35826747	25.56434446	22.05478987
652	H	51.83899269	27.25615865	22.01223932
653	H	32.81871084	28.12674172	43.55834267
654	H	32.71626791	26.53155479	42.78542439
655	H	31.27252415	27.28789478	43.45657933
656	H	31.54932612	26.29436138	40.48626648
657	H	30.69924909	27.68067800	39.79573727
658	H	30.11516494	26.94757554	41.28905875
659	H	30.87392311	29.98031304	40.89758389
660	H	31.82590521	30.19432222	42.36859915
661	H	30.28073176	29.33443354	42.42904572
662	H	38.15712158	29.46937778	39.84738788
663	H	37.99955677	27.82809089	39.19304311
664	H	39.07182046	28.13537590	40.55813047
665	H	36.78050075	26.00640749	40.58741743
666	H	36.26485625	26.37730485	42.23457514
667	H	37.98269221	26.34474739	41.84083129
668	H	36.39025270	28.77669965	43.11271522
669	H	37.08543781	30.05471104	42.11421524
670	H	38.12883682	28.80490885	42.81286833
671	H	39.91341550	30.40876083	44.54870293
672	H	41.62953406	29.99131367	44.72361728
673	H	40.60943068	29.08811452	43.60739927
674	H	43.28822119	30.57054869	42.83124018
675	H	42.67720674	31.17617780	41.29062393
676	H	42.29011093	29.53094801	41.80586767
677	H	40.20439069	31.70637123	40.99812456
678	H	39.09140786	31.55721116	42.36149155
679	H	39.70644335	30.10820523	41.55302009
680	H	59.28594109	30.14473779	21.80088566
681	H	59.19779457	28.54284967	21.04091650
682	H	60.75413946	29.34203107	21.24570402
683	H	60.02024882	26.46778776	22.32056753
684	H	60.85911276	26.66160483	23.86144176
685	H	61.59946937	27.26356146	22.37612759
686	H	61.07709168	28.97350216	24.93015488
687	H	60.31290646	30.37829119	24.17831251
688	H	61.77053768	29.67229874	23.46798450
689	H	53.67109470	28.89429224	24.98554916
690	H	53.59486806	27.26566594	24.28297556
691	H	52.73551396	28.60598255	23.52065799
692	H	54.85036728	26.73806742	22.11945929

693	H	55.64124143	28.02954293	21.21283805
694	H	53.88422194	28.00804151	21.34969035
695	H	55.68694026	30.42230585	22.16163216
696	H	54.98888183	30.75702425	23.74757740
697	H	53.93522483	30.43551579	22.36278925
698	C	57.55612856	40.35481085	34.69756482
699	C	58.54151913	40.06832497	35.78304817
700	C	58.52449291	38.56394401	36.09520058
701	C	59.18018694	38.30211916	37.45383113
702	C	58.98317548	36.84052914	37.87186902
703	C	59.47244981	36.64310934	39.31115527
704	C	59.10188849	35.24552773	39.81458883
705	C	59.39044303	35.13523925	41.31936269
706	H	58.33248490	40.66023497	36.69917111
707	H	59.56009398	40.37711797	35.46036952
708	H	59.04421625	38.00006544	35.29701484
709	H	57.48645707	38.16606199	36.10506902
710	H	58.73647017	38.96820377	38.21979341
711	H	60.25588136	38.54954634	37.41880469
712	H	59.51614527	36.16145927	37.18234399
713	H	57.91034493	36.56270684	37.79277150
714	H	59.01607892	37.41164926	39.96591917
715	H	60.56437829	36.79945624	39.37096459
716	H	59.66194650	34.47044371	39.25696961
717	H	58.03022994	35.04589349	39.59589456
718	H	59.03428190	36.04193762	41.85194298
719	H	60.48836740	35.10259178	41.49377512
720	O	57.81192199	40.49061166	33.54014091
721	C	58.75553958	33.89109480	41.84824767
722	O	59.31237108	32.85506756	42.05026268

■ *c-P6_{S-C10}•T6 (in isomer)*

1	Zn	49.23658326	18.49365974	27.44332807
2	N	50.90126332	19.26973966	26.56406975
3	C	52.19746817	19.18068686	27.07287600
4	C	53.09553337	19.96410014	26.25491908
5	C	52.33185833	20.54369463	25.27012355
6	C	50.96774534	20.12037313	25.50497934
7	N	48.11984036	19.22924388	25.88955023
8	C	48.56594549	20.18338183	24.92942307
9	C	47.39209406	20.65537075	24.15718642
10	C	46.30982494	20.00396828	24.63430705
11	N	47.65047667	17.28526941	27.92103211
12	C	46.39028068	17.38523568	27.45172501

13	C	45.49271184	16.41547423	28.14331838
14	C	46.24922057	15.75414438	29.04392269
15	C	47.62853566	16.29193974	28.94064463
16	N	50.39363197	17.38973549	28.71196054
17	C	49.99772277	16.46247255	29.61442435
18	C	51.10425176	16.06416232	30.47044060
19	C	52.18974388	16.79964055	30.07244610
20	C	51.75371312	17.62421113	28.96150500
21	C	52.56134814	18.50069834	28.24593151
22	C	53.80249022	18.85815240	28.78954217
23	C	54.77276060	19.38763659	29.30816014
24	C	44.55916926	18.48791312	26.37637185
25	C	43.35856891	18.71995542	26.38849069
26	C	49.84008957	20.60748359	24.76757309
27	C	48.66844778	15.93784585	29.73062353
28	C	50.11776211	21.71643633	23.83645872
29	C	50.09945010	21.52944858	22.46107439
30	C	50.35692189	22.60956277	21.60645816
31	C	50.63673864	23.85560664	22.16008541
32	C	50.67361303	24.04751839	23.54849693
33	C	50.40352523	22.97125251	24.38468036
34	C	50.33518642	22.37143034	20.10849314
35	C	50.55263373	23.65805420	19.29480382
36	C	48.96808537	21.78172720	19.71510659
37	C	51.46063352	21.37978555	19.76123444
38	C	51.01591873	25.42029207	24.09429958
39	C	48.44556285	14.97472877	30.82381302
40	C	48.29685527	13.62011836	30.55424507
41	C	48.08771580	12.71736950	31.60427379
42	C	48.03413403	13.20218822	32.90809417
43	C	48.18356303	14.56767288	33.18793516
44	C	48.38871541	15.45338626	32.13594642
45	C	47.93141044	11.24469137	31.27628340
46	C	49.21823108	10.75647987	30.58632583
47	C	47.69263625	10.37695174	32.52304325
48	C	46.72634791	11.07436515	30.33259851
49	C	48.13034019	15.03045815	34.63143556
50	C	49.29538367	14.37603382	35.39648975
51	C	46.78421782	14.60310826	35.24485237
52	C	48.25820152	16.55727323	34.77091241
53	C	46.78939473	19.11555930	25.72975328
54	C	45.92629070	18.30118300	26.49067764
55	Zn	34.89398380	31.06868837	35.94206801
56	N	34.22675985	30.55627228	34.09006349
57	C	33.73568784	29.29997646	33.72537573
58	C	33.48593243	29.27317422	32.29813077

59	C	33.83574991	30.50676618	31.81024890
60	C	34.29817504	31.28221710	32.94577837
61	N	35.06748398	33.01113526	35.27522581
62	C	35.03770816	33.42701660	33.91300092
63	C	35.41770356	34.85881050	33.85080333
64	C	35.65732404	35.26614810	35.11529703
65	C	35.45497980	34.08185946	35.99658428
66	N	35.11451425	31.76414386	37.84840382
67	C	35.50401196	32.99730623	38.22188487
68	C	35.72779146	33.05653118	39.69604151
69	C	35.46799041	31.82508751	40.18139037
70	C	35.07011387	30.97395585	39.03248355
71	N	34.20028429	29.30803844	36.72124740
72	C	34.28379366	28.87408218	38.00402130
73	C	33.87434585	27.48606592	38.10876871
74	C	33.53966699	27.08072743	36.84144042
75	C	33.74599219	28.21834984	35.96950175
76	C	33.55536597	28.21424782	34.58821043
77	C	33.30164327	26.98216499	33.97143962
78	C	33.31454579	25.92507677	33.36134566
79	C	35.72620649	34.10238473	37.37529845
80	C	36.37752050	35.19733961	37.92050609
81	C	37.07128040	36.06915421	38.42424323
82	C	34.74499479	32.64021321	32.85123767
83	C	34.72502493	29.66788168	39.11227211
84	C	34.89905412	33.18241008	31.48949718
85	C	34.02408380	34.15166109	31.01174816
86	C	34.19124142	34.67066183	29.72321143
87	C	35.23879641	34.19715709	28.93579973
88	C	36.12756251	33.22539730	29.41015314
89	C	35.94433439	32.71178696	30.69194056
90	C	33.21748130	35.72567433	29.23332454
91	C	31.81139868	35.10152185	29.17913936
92	C	33.23446193	36.91184405	30.21600881
93	C	33.56632346	36.25922567	27.83402686
94	C	37.23373692	32.70028379	28.51440472
95	C	36.63599125	31.56235963	27.67197114
96	C	37.77230807	33.80241620	27.58374030
97	C	38.42362750	32.17080791	29.33706632
98	C	34.80640156	28.99075698	40.41924578
99	C	33.64553157	28.66862273	41.11274403
100	C	33.72699190	28.04436457	42.36295964
101	C	34.98336859	27.75962876	42.89111181
102	C	36.15829100	28.07179193	42.19445497
103	C	36.06297844	28.69057231	40.95208146
104	C	32.44085890	27.70491275	43.09228190

105	C	37.49654124	27.75639078	42.83568938
106	N	48.84490902	20.13627262	28.73391099
107	C	49.58980269	21.26285883	28.67306405
108	C	49.29329888	22.40266705	29.42608405
109	C	48.18601452	22.38256785	30.27763193
110	C	47.42066413	21.21618075	30.35246697
111	C	47.78060124	20.11682269	29.56682894
112	C	47.83368616	23.56548014	31.07272895
113	C	47.64525621	24.79897492	30.44296091
114	C	47.30468081	25.92087784	31.19268165
115	C	47.15350525	25.81430380	32.57677434
116	C	47.34737659	24.58470422	33.20958528
117	C	47.68473114	23.46281681	32.45832026
118	C	46.78811405	26.99789490	33.37121754
119	C	45.44198255	27.32378946	33.56666597
120	N	36.90477057	30.46640702	35.63644775
121	C	37.78739844	31.33750019	35.09808125
122	C	39.12477505	31.00774076	34.86800611
123	C	39.57641553	29.72804439	35.20344769
124	C	38.66782789	28.82556925	35.76170373
125	C	37.34362596	29.23025660	35.96179946
126	C	40.97813940	29.36274543	34.97153778
127	C	41.57937647	29.64649108	33.74115864
128	C	42.92103977	29.34481876	33.53242841
129	C	43.67088288	28.75694600	34.55417650
130	C	43.06941909	28.45849145	35.77869849
131	C	41.72554524	28.75719901	35.98494155
132	C	45.09190543	28.43963406	34.33676942
133	H	54.14978034	20.04603169	26.41317605
134	H	52.64480054	21.18250143	24.47413803
135	H	47.46400874	21.38082679	23.37143531
136	H	45.28365378	20.06099662	24.33685968
137	H	44.45272568	16.31608275	27.91060556
138	H	45.97656472	14.97972202	29.73317758
139	H	51.03962291	15.33200262	31.24515398
140	H	53.18550199	16.78945945	30.46299565
141	H	49.89312290	20.54054753	22.05462386
142	H	50.83800075	24.70689903	21.51292027
143	H	50.41600759	23.07658009	25.46725636
144	H	50.51853242	23.45090075	18.21911205
145	H	51.52874933	24.10841084	19.50351681
146	H	49.77773700	24.40271717	19.50530889
147	H	48.89346087	21.64454164	18.63166855
148	H	48.79586197	20.80415090	20.17780049
149	H	48.15096917	22.44227860	20.02466396
150	H	51.51228015	21.19933583	18.68321737

151	H	52.43572067	21.76222268	20.08341374
152	H	51.31309355	20.41023193	20.24987092
153	H	48.35351604	13.26687615	29.52580833
154	H	47.87696417	12.51641953	33.73831594
155	H	48.51644017	16.52006147	32.30812658
156	H	49.16764326	9.686617226	30.36220516
157	H	50.09399785	10.92324885	31.22361109
158	H	49.39811142	11.28045222	29.64117168
159	H	47.58377200	9.321191719	32.24974871
160	H	48.52991828	10.44069209	33.22611113
161	H	46.77784675	10.66987610	33.04892128
162	H	46.55028877	10.01881433	30.10235021
163	H	45.81221900	11.47368945	30.78518243
164	H	46.87711827	11.59388614	29.38038295
165	H	49.31538167	14.69963063	36.44154175
166	H	50.25844518	14.64208709	34.94497702
167	H	49.22311755	13.28379572	35.39213969
168	H	46.68013508	14.97216414	36.26965076
169	H	46.67815256	13.51418752	35.27880008
170	H	45.94482484	14.99646662	34.66053921
171	H	48.21849205	16.85911380	35.82257476
172	H	49.21075952	16.91951146	34.36707782
173	H	47.44589467	17.07682769	34.25149549
174	H	33.09382650	28.43326123	31.76415676
175	H	33.78207001	30.86803309	30.80627971
176	H	35.46449071	35.41076643	32.93304342
177	H	35.94001450	36.22847661	35.48834574
178	H	36.03425318	33.94730428	40.20481547
179	H	35.50840441	31.46121721	41.18923546
180	H	33.85224376	26.92410642	39.01633630
181	H	33.18936568	26.12319847	36.51757200
182	H	33.20494789	34.49376573	31.64241188
183	H	35.36944212	34.57969552	27.92571311
184	H	36.59680721	31.93478738	31.08511024
185	H	31.07396925	35.81650020	28.80166162
186	H	31.47353820	34.77266914	30.16801916
187	H	31.79488691	34.22513282	28.52112973
188	H	32.58577726	37.72251126	29.86887244
189	H	34.24578660	37.31797559	30.32495496
190	H	32.88480629	36.62229387	31.21249004
191	H	32.85909260	37.03715314	27.52468302
192	H	34.56653322	36.70431484	27.81043899
193	H	33.52339351	35.46812011	27.07777173
194	H	37.37579296	31.12719794	26.99465435
195	H	36.24811628	30.75058387	28.30186473
196	H	35.79666910	31.91452832	27.06148633

197	H	38.64604298	33.45396950	27.02360199
198	H	38.07264306	34.68839671	28.15270184
199	H	37.02765502	34.11397287	26.84387695
200	H	39.24285451	31.85619091	28.68326216
201	H	38.81187403	32.94605247	30.00671432
202	H	38.14206904	31.30719219	29.94990543
203	H	32.67610666	28.90695090	40.67606525
204	H	35.06816725	27.28592844	43.86722292
205	H	36.94987952	28.95104910	40.37914748
206	H	50.45867790	21.24527251	27.99307884
207	H	49.92145667	23.28732576	29.35177749
208	H	46.54913181	21.16479384	31.00006456
209	H	47.19808463	19.18193691	29.59641923
210	H	47.75634592	24.88023695	29.36153596
211	H	47.15585961	26.88126369	30.70234063
212	H	47.23343259	24.50577881	34.28919342
213	H	47.83919583	22.50415345	32.95237075
214	H	37.40203718	32.33857881	34.84521395
215	H	39.80404488	31.74441594	34.44590569
216	H	38.97513811	27.81631297	36.02559163
217	H	36.59948568	28.54265074	36.39813370
218	H	40.99560836	30.10262282	32.94203686
219	H	43.38871073	29.56293721	32.57370683
220	H	43.65515306	27.99790554	36.57245137
221	H	41.26068258	28.53108786	36.94412310
222	N	41.89771823	36.92958454	41.74504574
223	C	40.60418702	37.02384493	41.23239847
224	C	39.69583538	36.26356742	42.06073470
225	C	40.45082739	35.69575991	43.05883128
226	C	41.82038889	36.09960678	42.82020765
227	N	44.68240639	36.93120036	42.40640910
228	C	44.22440064	36.00322632	43.38572270
229	C	45.39712425	35.51083750	44.14753533
230	C	46.48983020	36.12267825	43.64272398
231	N	45.17067049	38.85920169	40.36093320
232	C	46.43507993	38.72459050	40.80818102
233	C	47.34388420	39.67965789	40.10945021
234	C	46.58659422	40.37324185	39.23419275
235	C	45.19764110	39.86444720	39.35295865
236	N	42.42111646	38.79858236	39.59156410
237	C	42.82319687	39.72457702	38.68987594
238	C	41.72391024	40.11589145	37.82234195
239	C	40.63694209	39.37782089	38.21204576
240	C	41.06446363	38.56006111	39.33102350
241	C	40.24937499	37.69201289	40.04965305
242	C	39.00609662	37.34318306	39.50580736

243	C	38.02752094	36.82872413	38.98800936
244	C	48.25593725	37.58945743	41.86208776
245	C	49.45597867	37.35492273	41.83600188
246	C	42.94165659	35.61228459	43.56815408
247	C	44.15382817	40.24760436	38.58203038
248	C	42.64239930	34.54818757	44.54368035
249	C	42.71057874	34.78819643	45.91219831
250	C	42.41600334	33.76288196	46.81619149
251	C	42.04434756	32.51001093	46.32593795
252	C	41.96882228	32.26207487	44.95387543
253	C	42.27955773	33.29014445	44.06285287
254	C	42.49657577	34.06130358	48.30190146
255	C	42.24796335	32.82179814	49.17728396
256	C	43.90093769	34.60222195	48.62965542
257	C	41.42898900	35.11826154	48.63891765
258	C	41.54938246	30.91916467	44.38641585
259	C	44.36945520	41.24977513	37.52294044
260	C	44.50194527	42.59362162	37.84964801
261	C	44.69703087	43.54300728	36.83902395
262	C	44.75235982	43.11487859	35.51582289
263	C	44.61620826	41.76115699	35.17813292
264	C	44.42774750	40.82779851	36.19169764
265	C	44.83337169	45.00219763	37.23022098
266	C	43.53368007	45.44523361	37.92591968
267	C	45.07535921	45.92439558	36.02378014
268	C	46.02679542	45.14593278	38.19289983
269	C	44.66960966	41.36397192	33.71518165
270	C	43.52984013	42.08172103	32.96868148
271	C	46.03238910	41.78605704	33.13607262
272	C	44.50332717	39.84934601	33.50342556
273	C	46.01833064	37.01126301	42.54360317
274	C	46.89050061	37.79824685	41.76494547
275	N	58.75705653	25.69285711	34.06611317
276	C	59.27604690	26.94727582	34.40112969
277	C	59.66445245	26.95400061	35.79773785
278	C	59.36364143	25.71379276	36.29865813
279	C	58.78661206	24.95536304	35.20342151
280	N	57.83395057	23.23460800	32.94180971
281	C	57.92519795	22.82581825	34.30342757
282	C	57.50593369	21.40721473	34.39640265
283	C	57.19858518	20.99646563	33.14741451
284	C	57.39453415	22.16680164	32.24735721
285	N	57.68326889	24.47171907	30.36863216
286	C	57.28806380	23.23480061	30.01530612
287	C	57.04130883	23.15914999	28.54585887
288	C	57.29625318	24.38420999	28.04163148

289	C	57.70755565	25.24923451	29.17498505
290	N	58.61434751	26.94760679	31.45227809
291	C	58.47675506	27.37224021	30.17223543
292	C	58.83050476	28.77507051	30.05102771
293	C	59.19141495	29.19756628	31.30549172
294	C	59.06433859	28.05428248	32.18415722
295	C	59.35116485	28.05202869	33.54770972
296	C	59.59472520	29.28015096	34.17839331
297	C	59.57368587	30.30673646	34.83889764
298	C	57.07756846	22.13931157	30.87790649
299	C	56.41654986	21.04010858	30.35470734
300	C	55.72131130	20.16157195	29.86523820
301	C	58.31185010	23.60881705	35.33721309
302	C	58.04271976	26.55621800	29.07655559
303	C	58.22744324	23.09867776	36.71626632
304	C	59.04290759	22.05741879	37.14950449
305	C	58.94726856	21.59660796	38.46595590
306	C	58.04066187	22.20558678	39.33480668
307	C	57.22888472	23.26017632	38.91236656
308	C	57.31902713	23.69617511	37.58964044
309	C	59.85227197	20.46024753	38.90394345
310	C	61.31049606	20.94810992	38.82439512
311	C	59.64203674	19.26011630	37.96163222
312	C	59.57380263	19.99154998	40.34166823
313	C	56.26755495	23.97509365	39.84251388
314	C	56.68769633	25.45361242	39.92399924
315	C	56.26336004	23.39754202	41.26718600
316	C	54.84146331	23.84993763	39.27267741
317	C	57.97463877	27.21945180	27.76180418
318	C	59.14949724	27.54334501	27.09224078
319	C	59.09409179	28.19302393	25.85401755
320	C	57.84882599	28.50091749	25.31311639
321	C	56.65985341	28.17003429	25.97701577
322	C	56.72902290	27.52517237	27.20803710
323	C	60.39548038	28.54148046	25.15706841
324	C	55.33805070	28.54141575	25.33222101
325	H	38.64155137	36.18796009	41.89971334
326	H	40.12768120	35.07707792	43.86659320
327	H	45.31742425	34.79885735	44.94473192
328	H	47.51895467	36.03866183	43.92313703
329	H	48.39079109	39.74841979	40.32135106
330	H	46.86450855	41.15184331	38.55179171
331	H	41.79265908	40.84543760	37.04541849
332	H	39.64531792	39.38269374	37.81109635
333	H	42.98400026	35.78001512	46.26951231
334	H	41.8042417	31.71278096	47.02535746

335	H	42.22945706	33.12399877	42.98855866
336	H	42.33751354	33.07029698	50.24088675
337	H	41.24228043	32.41531004	49.02736798
338	H	42.97418757	32.02931015	48.96804142
339	H	44.01279079	34.78833659	49.70259610
340	H	44.10681849	35.54644470	48.11462077
341	H	44.67640332	33.88783062	48.33281788
342	H	41.43813593	35.36621624	49.70462237
343	H	40.42508717	34.75797514	48.38792780
344	H	41.58926858	36.04897020	48.08322786
345	H	44.44356856	42.90188961	38.89255598
346	H	44.90028991	43.83710400	34.71525614
347	H	44.31352666	39.76830219	35.97373193
348	H	43.57357787	46.50237649	38.20583372
349	H	42.66816636	45.30558763	37.26845729
350	H	43.34452297	44.87123749	38.83972938
351	H	45.17562540	46.96795990	36.34355421
352	H	44.24367964	45.88457903	35.31236047
353	H	45.99570691	45.65973345	35.49252270
354	H	46.19023398	46.19287407	38.46767836
355	H	46.94937890	44.77343645	37.73489159
356	H	45.87131893	44.58705658	39.12211468
357	H	43.50469166	41.79504159	31.91295708
358	H	42.55646872	41.83165499	33.40684976
359	H	43.63714538	43.17025065	33.00959936
360	H	46.12986497	41.48223053	32.08932009
361	H	46.17412785	42.87082652	33.17566773
362	H	46.85524646	41.32746274	33.69579668
363	H	44.54297187	39.59671504	32.43860863
364	H	43.53875143	39.49459326	33.88408626
365	H	45.29800268	39.28368083	34.00123538
366	H	60.11024093	27.78519956	36.30245360
367	H	59.51504531	25.33844094	37.28723778
368	H	57.48130133	20.86496296	35.32082593
369	H	56.87168682	20.03999804	32.79697989
370	H	56.72684561	22.26309211	28.05162400
371	H	57.24219640	24.73605182	27.03010515
372	H	58.80221944	29.33433114	29.14166379
373	H	59.51631236	30.16821222	31.61558795
374	H	59.76163402	21.61684526	36.46055634
375	H	57.96889905	21.85815972	40.36287391
376	H	56.69582415	24.51463984	37.23254763
377	H	62.00747954	20.17266785	39.15611285
378	H	61.59041388	21.22653356	37.80242238
379	H	61.46519643	21.82993122	39.45646983
380	H	60.23955755	18.39921740	38.27812831

381	H	58.59163522	18.95005266	37.94888579
382	H	59.93104878	19.49297277	36.93148349
383	H	60.23361814	19.16120445	40.61714465
384	H	58.54354664	19.63847829	40.45717055
385	H	59.74636432	20.79222121	41.06891796
386	H	56.05817516	26.00422490	40.63431714
387	H	56.60859442	25.96064538	38.95709901
388	H	57.72580623	25.55078336	40.26080074
389	H	55.55142666	23.93990628	41.90207424
390	H	55.96995570	22.34344450	41.27710655
391	H	57.24668400	23.48805370	41.74112294
392	H	54.11845192	24.36107807	39.91734744
393	H	54.54053638	22.79941758	39.19999974
394	H	54.76229622	24.28240540	38.27064296
395	H	60.10948203	27.29272885	27.54280593
396	H	57.78413000	29.01252299	24.35467861
397	H	55.83105618	27.25730524	27.75957632
398	N	43.94872929	36.05483096	39.57159903
399	C	43.43751973	34.83370196	39.84470039
400	C	43.75157968	33.70173840	39.08789456
401	C	44.63130185	33.83010266	38.00950845
402	C	45.15235994	35.09368246	37.71813416
403	C	44.78631504	36.18015669	38.51869946
404	C	45.00310138	32.65791799	37.20842831
405	C	45.43897755	31.49101901	37.84339433
406	C	45.79278723	30.37607632	37.09048902
407	C	45.71723681	30.42240638	35.69660294
408	C	45.27896145	31.58520412	35.05939030
409	C	44.92316031	32.69933668	35.81383021
410	C	46.08976971	29.24315730	34.89914325
411	C	47.43601438	28.92204235	34.69487621
412	N	55.97008787	25.74167706	32.65520565
413	C	55.02122380	24.80268509	32.86913350
414	C	53.68561984	25.12671826	33.12145206
415	C	53.30714343	26.47173466	33.15266203
416	C	54.28609609	27.44470632	32.93967836
417	C	55.60234594	27.04134344	32.69121459
418	C	51.90392428	26.83859038	33.37884402
419	C	51.20801520	26.32715694	34.47766070
420	C	49.86477796	26.64152388	34.66236903
421	C	49.20842217	27.46579335	33.74570044
422	C	49.90412266	27.98694927	32.65246072
423	C	51.24936916	27.67860590	32.47369126
424	C	47.78641493	27.79758303	33.93811998
425	H	42.75024117	34.76929171	40.70508443
426	H	43.31103732	32.73892052	39.33425607

427	H	45.84336321	35.23190402	36.89069777
428	H	45.17511691	37.19205918	38.32072085
429	H	45.51026258	31.45726418	38.93063691
430	H	46.13045089	29.46787727	37.58636101
431	H	45.21230243	31.61633698	33.97305832
432	H	44.57290575	33.60269099	35.31527316
433	H	55.35005225	23.75160671	32.82837782
434	H	52.95187236	24.33920519	33.27549918
435	H	54.03390109	28.50271417	32.97306542
436	H	56.40177876	27.78089483	32.50934176
437	H	51.71773494	25.67991227	35.19086535
438	H	49.32238185	26.24311159	35.51767511
439	H	49.39174524	28.63299217	31.94185331
440	H	51.79008405	28.08338813	31.61909275
441	Zn	43.56743252	37.68685613	40.86127863
442	Zn	57.97628388	25.17541961	32.26353574
443	C	51.09685177	25.44780611	25.63088776
444	C	49.92893169	26.41338120	23.64545050
445	C	52.38643823	25.84399592	23.53711876
446	C	32.68506104	27.02403190	44.44936556
447	C	31.61633950	26.74717336	42.21278428
448	C	31.65615332	29.00643869	43.33918677
449	C	38.67824164	27.97760773	41.87541848
450	C	37.52162903	26.28353614	43.28389161
451	C	37.66454669	28.68191076	44.05425356
452	C	41.20080804	29.89022153	45.47405807
453	C	42.70908742	30.35608536	43.54269943
454	C	40.30694216	31.12729440	43.50102284
455	C	60.18045520	29.24779150	23.80820966
456	C	61.18054654	27.24172128	24.90238166
457	C	61.20482228	29.48017673	26.07082236
458	C	54.12400497	28.04722068	26.13740700
459	C	55.27218099	27.91727543	23.92655015
460	C	55.26184198	30.07625260	25.23146775
461	H	51.85442280	24.74750207	26.00330938
462	H	50.13563792	25.19176492	26.08880792
463	H	51.37255474	26.44475378	25.99069936
464	H	48.93673606	26.08337729	23.97369957
465	H	49.89495333	26.51172174	22.55563440
466	H	50.10479353	27.40997471	24.06069626
467	H	52.36990564	25.95625419	22.44896418
468	H	53.15436748	25.09919865	23.77895649
469	H	52.70522170	26.80220149	23.96130038
470	H	33.25595069	27.66772575	45.12674541
471	H	33.22586706	26.07871322	44.33467641
472	H	31.73626323	26.79380323	44.94734195

473	H	32.18025461	25.8354283	41.98686325
474	H	31.34029936	27.2062259	41.25705572
475	H	30.68832284	26.45081291	42.71169296
476	H	31.36069347	29.48823649	42.40074567
477	H	32.25734725	29.72799436	43.90324161
478	H	30.74183896	28.81584346	43.90979204
479	H	38.75219568	29.02396810	41.55776309
480	H	38.58237889	27.35544044	40.97843927
481	H	39.62749281	27.71689318	42.35485920
482	H	37.28052148	25.61583883	42.44914007
483	H	36.79931262	26.08467497	44.08197468
484	H	38.50807009	26.00049546	43.66423182
485	H	36.87871893	28.51566300	44.79863128
486	H	37.61334514	29.73640471	43.75832450
487	H	38.62696182	28.51895457	44.54956414
488	H	40.36185346	30.22874153	46.09242596
489	H	42.05393736	29.69436100	46.13252923
490	H	40.91166861	28.93169463	45.02940383
491	H	43.61939980	30.25925235	44.14454861
492	H	42.94561445	31.00484566	42.69303340
493	H	42.46531173	29.36693587	43.14488594
494	H	40.51426385	31.78555418	42.65057939
495	H	39.48951246	31.58243280	44.07249742
496	H	39.94425235	30.17577374	43.09807013
497	H	59.64406194	30.19470940	23.92993488
498	H	59.61723935	28.62033260	23.10965937
499	H	61.13954921	29.47985471	23.33131396
500	H	60.59442213	26.53955582	24.29949363
501	H	61.44102526	26.73282327	25.83690571
502	H	62.11496525	27.44105745	24.36855144
503	H	61.45879573	29.00288158	27.02378635
504	H	60.63922799	30.38973780	26.30109374
505	H	62.14412954	29.78177131	25.59699530
506	H	54.10652469	28.47861109	27.14409386
507	H	54.12370965	26.95505173	26.23271573
508	H	53.18657646	28.33331984	25.64877729
509	H	55.36168174	26.82584401	23.97754183
510	H	56.07545704	28.28115585	23.27804069
511	H	54.32618403	28.15576315	23.43009618
512	H	56.05056417	30.48044623	24.58859112
513	H	55.37525157	30.54038973	26.21767160
514	H	54.30283509	30.40059848	24.81680074
515	C	44.02200221	26.68854456	31.63246091
516	C	42.96634791	25.96388195	31.08805458
517	C	42.26672946	25.05056024	31.87967530
518	C	42.62643367	24.86210325	33.21636433

519	C	43.67610131	25.59172966	33.76406048
520	C	44.37074743	26.50922898	32.97274197
521	C	41.15680680	24.28106815	31.30811337
522	C	40.04549706	24.92564282	30.76133239
523	C	39.00678630	24.15072162	30.23702266
524	N	39.04040798	22.79945337	30.23705956
525	C	41.19709488	22.88528618	31.30627241
526	C	40.12181345	22.18009843	30.75975984
527	H	44.57491726	27.39633087	31.01760720
528	H	42.68918894	26.10301042	30.04265437
529	H	42.07550067	24.15268560	33.83345727
530	H	43.95202846	25.45734637	34.80829601
531	H	39.98580885	26.01035354	30.74654464
532	H	38.11100861	24.61766230	29.79481466
533	H	42.05685001	22.35174957	31.70394420
534	H	40.12258889	21.07600843	30.73529795
535	C	38.00213422	22.92571876	26.60291856
536	C	36.98808736	23.92680845	26.75952370
537	N	36.46357778	21.28739643	31.07939918
538	C	38.30259496	18.97067530	30.54833892
539	N	38.36994394	19.84915911	29.51278571
540	C	39.30681622	19.32722858	28.61896164
541	C	39.77908586	18.04966760	29.10439904
542	C	39.14753451	17.82120410	30.30364621
543	C	37.57152291	19.18744719	31.76117982
544	Zn	37.49201697	21.68140015	29.35798167
545	C	36.13304546	24.00376840	27.80555135
546	N	36.14496761	23.17084656	28.95969937
547	C	35.20179588	23.65241544	29.79312100
548	C	34.49790620	24.81538661	29.17701449
549	C	35.06360203	25.02143079	27.97008311
550	C	36.76199037	20.24403900	32.00138935
551	C	34.93540968	23.20722905	31.10093515
552	N	38.21759456	21.90141062	27.46101734
553	C	39.27372578	21.15238449	26.92445965
554	C	39.72453017	21.77193385	25.69297035
555	C	38.92905765	22.86953907	25.48521765
556	C	39.79083140	19.98341407	27.47671713
557	C	35.54463625	22.07230654	31.66977700
558	C	35.24967296	21.59475792	33.05016427
559	C	35.99837489	20.48943614	33.25011428
560	C	36.89126441	24.93038545	25.68427478
561	C	37.43720508	26.20766670	25.83491056
562	C	37.31084346	27.15351234	24.82033567
563	C	36.64214785	26.81787500	23.64436250
564	C	36.10726640	25.54081685	23.48298153

565	C	36.23304064	24.59679859	24.49871249
566	C	37.74745169	18.17032839	32.81456364
567	C	38.78398588	18.26051362	33.74576506
568	C	38.91738725	17.30362499	34.74948756
569	C	38.01700759	16.24177602	34.81247594
570	C	36.99027914	16.13726556	33.87498249
571	C	36.85345324	17.09897264	32.87797262
572	H	40.48483254	17.42693374	28.59657860
573	H	39.24081827	16.97961424	30.95142094
574	H	33.69707068	25.33777935	29.65924525
575	H	34.83552668	25.75734812	27.22396260
576	H	40.52483527	21.40224653	25.08625509
577	H	38.95622800	23.56835438	24.67965170
578	H	34.56361224	22.08775094	33.70722144
579	H	36.08305125	19.86755252	34.12046264
580	S	38.32272597	26.60079216	27.31847719
581	H	36.53645261	27.55694685	22.85245212
582	H	35.81744680	23.59577514	24.37665555
583	H	38.11673151	15.49343183	35.59609459
584	H	36.05125011	17.02195109	32.14316631
585	H	37.71855046	28.15891279	24.93583477
586	H	35.58675196	25.28010886	22.56169771
587	S	39.97905515	19.56108686	33.61038092
588	H	39.71646997	17.37266965	35.48916888
589	H	36.29124001	15.30238238	33.92324514
590	C	37.33451519	27.95323375	28.04951190
591	C	39.37155011	20.85598017	34.74886982
592	O	36.38957285	28.40787693	27.47512288
593	O	38.35791796	20.72607277	35.36605653
594	C	40.96745234	19.46086584	26.92353301
595	C	42.07883294	19.07759384	26.59371305
596	C	34.14742705	24.01694328	31.90051126
597	C	33.59696399	24.84676241	32.61056527
598	C	40.30041537	22.03000904	34.82025973
599	C	39.52799188	23.31386564	35.14780968
600	C	38.59460783	23.70812461	33.99868118
601	C	37.76058841	27.82415389	32.51391489
602	C	36.65046620	26.94417213	33.10512859
603	C	38.10629104	25.15135615	34.16645755
604	C	37.03317981	25.46235654	33.11935623
605	C	37.84697299	28.41682112	29.37482464
606	C	36.67574367	28.59094839	30.35301961
607	C	37.17606552	29.01275594	31.73968874
608	H	40.87481326	22.17194117	33.87945552
609	H	41.06214226	21.83512415	35.60801264
610	H	38.93742576	23.17645202	36.07694116

611	H	40.24156789	24.13267088	35.35985220
612	H	37.72939230	23.01412184	33.96239295
613	H	39.10579183	23.59729372	33.02403908
614	H	38.42117277	28.18802520	33.32174064
615	H	38.41571628	27.22513839	31.85561382
616	H	35.71364525	27.06583030	32.52229218
617	H	36.39455727	27.28675982	34.12493821
618	H	38.95347223	25.85406712	34.06981690
619	H	37.69374055	25.30255382	35.18131327
620	H	36.13110477	24.84981386	33.32605934
621	H	37.37183711	25.14895407	32.11359538
622	H	38.37071076	29.39033644	29.23185675
623	H	38.60534963	27.73918605	29.81700185
624	H	36.33460447	29.45677744	32.31567489
625	H	37.92696596	29.81708419	31.65313852
626	H	36.09767697	27.64755689	30.42968545
627	H	35.95792740	29.34129276	29.96325498
628	C	49.12099764	30.73520114	34.49397295
629	C	50.15661413	31.49422689	35.03053105
630	C	50.56800173	31.28484838	36.34929245
631	C	49.92703376	30.31939526	37.13273107
632	C	48.90131821	29.55132295	36.59441500
633	C	48.50014627	29.75694302	35.27277209
634	C	51.68427964	32.04983807	36.91172596
635	C	51.82347381	33.42078578	36.68706980
636	C	52.91827734	34.09034669	37.24268921
637	N	53.85019342	33.46067313	37.99173575
638	C	52.64487974	31.39920782	37.69093341
639	C	53.70746292	32.13572101	38.21617906
640	H	48.79821254	30.89656210	33.46690212
641	H	50.65160394	32.24676431	34.41696897
642	H	50.22565577	30.17363209	38.17135451
643	H	48.41287720	28.78876263	37.19795167
644	H	51.09191977	33.96977908	36.09989693
645	H	53.05669993	35.17439530	37.08960566
646	H	52.57581070	30.32988081	37.87565773
647	H	54.48116374	31.65732106	38.84007683
648	C	54.64651573	37.18955946	37.75368478
649	C	55.53368013	37.04670321	36.63852573
650	N	56.65326526	32.87059357	39.32719235
651	C	54.79886020	33.18672474	41.67639253
652	N	54.61884400	34.21810122	40.81510563
653	C	53.59638358	35.00715770	41.35540328
654	C	53.15741343	34.43231143	42.61198044
655	C	53.91146370	33.30603263	42.81953627
656	C	55.71121202	32.09903522	41.48154740

657	Zn	55.41886693	34.47451578	38.95217297
658	C	56.44324177	36.05584482	36.49268483
659	N	56.60511995	34.93370894	37.35422027
660	C	57.56436028	34.16587998	36.80561647
661	C	58.09665132	34.78707118	35.56043940
662	C	57.41098235	35.93370635	35.37283607
663	C	56.54619764	31.96980716	40.42416064
664	C	58.00484924	32.91430504	37.27592880
665	N	54.55522231	36.31522526	38.79019985
666	C	53.52944597	36.78741408	39.61160659
667	C	52.99850288	38.01613180	39.06302731
668	C	53.69618762	38.27109083	37.90705424
669	C	53.05258717	36.14723491	40.76388571
670	C	57.59124008	32.36471013	38.50219105
671	C	58.13251581	31.08292960	39.04198969
672	C	57.49440403	30.84834544	40.20744853
673	C	55.40993196	38.05235706	35.56721489
674	C	54.68072943	37.77677789	34.40709831
675	C	54.60533622	38.71608093	33.38156377
676	C	55.24688347	39.94513286	33.52437029
677	C	55.95716616	40.23388463	34.68903783
678	C	56.03994897	39.29016534	35.70949054
679	C	55.72861029	31.06210736	42.53093778
680	C	54.86674883	29.96199574	42.49406738
681	C	54.92256542	28.99131019	43.49077214
682	C	55.84421790	29.11882827	44.52887117
683	C	56.69801857	30.21903820	44.57731018
684	C	56.63933539	31.19065108	43.58161011
685	H	52.39050009	34.84653270	43.23313733
686	H	53.88017409	32.62752478	43.64225207
687	H	58.87982753	34.35108137	34.97502746
688	H	57.49611301	36.65895504	34.58610417
689	H	52.21200156	38.59143560	39.50488367
690	H	53.58534954	39.08953498	37.23233356
691	H	58.89188098	30.51385256	38.54638605
692	H	57.60226590	30.03360476	40.89557857
693	S	53.78515949	36.25196671	34.26463198
694	H	55.19380242	40.67939487	32.72279469
695	H	56.59588015	39.51017299	36.62169013
696	H	55.89350219	28.35573329	45.30359398
697	H	57.30288524	32.05546671	43.61669672
698	H	54.05376550	38.50426779	32.46440173
699	H	56.45183247	41.19867353	34.80079860
700	S	53.68715362	29.88009638	41.17684099
701	H	54.26137378	28.12150699	43.47163431
702	H	57.41338331	30.32015835	45.39292037

703	C	54.91175989	35.14039564	33.34918476
704	C	53.68471261	28.13889868	40.63920729
705	O	55.96114311	35.52435219	32.92702979
706	O	54.24506711	27.28537613	41.26233584
707	C	51.85871690	36.64941781	41.29907403
708	C	50.73842854	37.00971115	41.62465031
709	C	58.76382564	32.12170805	36.43130877
710	C	59.29138157	31.33557177	35.65760111
711	C	52.90436218	27.89465354	39.38214590
712	C	53.84108339	27.37247874	38.28181910
713	C	54.93622632	28.38240275	37.92569704
714	C	54.79131015	30.53348726	35.32343664
715	C	56.12658858	29.85438356	35.00989687
716	C	55.70770046	27.94389993	36.67357848
717	C	56.66233628	29.05031707	36.20209749
718	C	54.37798223	33.75065057	33.18666568
719	C	54.91761567	32.85032927	34.30755361
720	C	54.31729164	31.44416995	34.18342450
721	H	52.35166451	28.78555365	39.02422246
722	H	52.12037244	27.13332262	39.59356546
723	H	54.30518105	26.41793502	38.60717298
724	H	53.24294769	27.12875239	37.38253754
725	H	55.64297349	28.49738536	38.77108797
726	H	54.49796175	29.38405759	37.76140553
727	H	54.01996004	29.76562417	35.52491834
728	H	54.88952696	31.11725881	36.25941943
729	H	56.87656963	30.62166718	34.72510785
730	H	56.02487375	29.19719600	34.12911549
731	H	55.01148130	27.66835054	35.86138014
732	H	56.28322701	27.02283263	36.88993274
733	H	57.63382158	28.59391633	35.91466048
734	H	56.90432554	29.73778221	37.03569981
735	H	54.70416867	33.35194854	32.19908281
736	H	53.27058305	33.71643197	33.16569735
737	H	54.57986986	31.00183390	33.20508774
738	H	53.21215777	31.50628383	34.20064385
739	H	54.68188559	33.27877777	35.30277301
740	H	56.02453454	32.79880211	34.26247028

▪ **c-P6_{SH}•T6 (*out* isomer)**

1	N	35.68354225	23.14975874	27.10883067
2	C	34.86326694	23.76474230	28.05628112
3	C	34.21393729	24.91305541	27.46369704
4	C	34.64751446	24.98752281	26.16213935

5	C	35.56465798	23.88365549	25.97042436
6	N	37.57506932	21.68807433	25.55625202
7	C	37.16596306	22.63098267	24.57057133
8	C	37.91364602	22.35640781	23.31848208
9	C	38.73368255	21.31235264	23.56267286
10	N	37.91977188	19.82636640	27.69503171
11	C	38.78360393	19.27821435	26.81777559
12	C	39.32815493	17.99350924	27.34613757
13	C	38.76866486	17.80062259	28.55864049
14	C	37.88076073	18.96078929	28.82386992
15	N	36.10420725	21.30209680	29.31810481
16	C	36.36023892	20.31950002	30.21342014
17	C	35.66535488	20.56330304	31.46684616
18	C	34.97292375	21.73507024	31.30674683
19	C	35.23740787	22.19822398	29.95747688
20	C	34.70292676	23.34851783	29.38565100
21	C	39.17775187	19.82854708	25.58499160
22	C	36.26998810	23.62855521	24.75025871
23	C	37.20452696	19.18644149	29.97373677
24	C	36.01215849	24.56368559	23.63957738
25	C	34.92033151	24.39664387	22.78243743
26	C	34.69918734	25.30734974	21.75046874
27	C	35.57350141	26.37748053	21.57028796
28	C	36.66743169	26.54284592	22.41822243
29	C	36.88520014	25.63768081	23.45288504
30	C	37.35462260	18.24015301	31.09392351
31	C	36.45293648	17.19006101	31.29040273
32	C	36.61747468	16.32286315	32.36946280
33	C	37.68403864	16.50362437	33.24813902
34	C	38.58736275	17.54719468	33.05318011
35	C	38.42188557	18.41512267	31.97772643
36	C	38.49893962	20.90245671	24.97589888
37	H	33.52550447	25.55499724	27.97144298
38	H	34.37856674	25.69752461	25.41307215
39	H	37.77175125	22.92003588	22.41888923
40	H	39.42956748	20.81575922	22.91916651
41	H	40.02035117	17.38569161	26.80093902
42	H	38.88907517	16.98953121	29.24826693
43	H	35.70619376	19.92436654	32.32014189
44	H	34.34124310	22.23934345	32.00756306
45	S	33.87543728	22.99846076	23.05769988
46	H	35.40087855	27.08666259	20.76253716
47	H	37.73538695	25.76312012	24.12310292
48	S	35.13532411	17.02047985	30.12558533
49	H	37.81130482	15.82609369	34.09056231
50	H	39.11925071	19.23798293	31.82354775

51	Zn	37.00563860	21.65579018	27.52055260
52	H	33.85242217	25.20012476	21.07446971
53	H	37.34987893	27.37749411	22.27243380
54	H	35.92525228	15.50064302	32.54373942
55	H	39.41922689	17.68463533	33.74069099
56	Zn	48.65671914	18.83510806	25.59996936
57	N	50.34054499	19.59062497	24.70634464
58	C	51.60335569	19.50531977	25.16944893
59	C	52.52859720	20.32402674	24.33301736
60	C	51.77447868	20.92691637	23.39082600
61	C	50.36993563	20.5027024	23.61411999
62	N	47.56477874	19.59882359	24.04512165
63	C	47.95109866	20.51700425	23.12715326
64	C	46.81759657	20.97717065	22.34325713
65	C	45.71977417	20.30499381	22.81414409
66	N	47.11224669	17.61626203	26.12790841
67	C	45.81423747	17.69321297	25.62128096
68	C	44.96425364	16.75485545	26.32088729
69	C	45.75036690	16.12585076	27.25571023
70	C	47.07720480	16.68838376	27.12197257
71	N	49.87469391	17.75288909	26.83696742
72	C	49.44693544	16.79743472	27.80234153
73	C	50.61624144	16.40327591	28.62518689
74	C	51.68071662	17.09444647	28.16446299
75	C	51.19131619	17.93903463	27.03950345
76	C	52.02311754	18.82388417	26.32689103
77	C	53.24391117	19.19113311	26.86505372
78	C	54.24354853	19.68769629	27.36486500
79	C	43.99168068	18.65626558	24.44287380
80	C	42.78017882	18.80326053	24.45021440
81	C	49.29516457	20.97505302	22.94039019
82	C	48.18560813	16.33293336	27.95531967
83	C	49.50190203	22.07040408	21.97586564
84	C	49.52215290	21.82668212	20.60918965
85	C	49.75620549	22.87971395	19.71564247
86	C	49.96242000	24.15971889	20.22230450
87	C	49.93817461	24.41437960	21.60061236
88	C	49.70214337	23.36085584	22.47641544
89	C	49.79045023	22.57754482	18.22964045
90	C	50.02477607	23.83063573	17.36964559
91	C	48.44345149	21.95593828	17.81840145
92	C	50.93727212	21.58519385	17.96213742
93	C	50.18754505	25.82805130	22.08978630
94	C	47.89941618	15.42405294	29.08070815
95	C	47.79850839	14.05393599	28.87694686
96	C	47.54585168	13.20369405	29.96057849

97	C	47.39356328	13.7568402	31.22900433
98	C	47.48724232	15.13926402	31.44082023
99	C	47.74255901	15.97216274	30.35691379
100	C	47.44830827	11.71159638	29.70598324
101	C	48.77033583	11.23060935	29.07961328
102	C	47.20137824	10.90097311	30.98912007
103	C	46.27830144	11.45665724	28.73833603
104	C	47.31792391	15.67791989	32.84858718
105	C	48.42968934	15.08797551	33.73572518
106	C	45.93504235	15.25733382	33.37956682
107	C	47.41100356	17.21226276	32.91367664
108	C	40.35540212	19.37066645	25.02096963
109	C	41.47221134	19.04454258	24.64558443
110	C	34.01138450	24.23214926	30.22428829
111	C	33.55286814	25.10641205	30.94133652
112	C	46.18332053	19.43557179	23.87927308
113	C	45.37911296	18.57650446	24.62236282
114	Zn	34.27382838	31.42974887	34.29091139
115	N	33.62340836	30.84948024	32.43900184
116	C	33.27473425	29.60665281	32.06160673
117	C	33.05863379	29.54245908	30.58752254
118	C	33.31072818	30.77579432	30.10086050
119	C	33.68074275	31.63494880	31.25172639
120	N	34.39428425	33.34720366	33.58911627
121	C	34.33861338	33.76925929	32.30152790
122	C	34.64470010	35.18451819	32.20586645
123	C	34.90322416	35.61475854	33.48278901
124	C	34.75193212	34.46547851	34.35056279
125	N	34.42559408	32.08866373	36.21114851
126	C	34.77526709	33.38784600	36.59484236
127	C	34.93849257	33.43937941	38.03414060
128	C	34.68775400	32.17724319	38.50842300
129	C	34.37830133	31.35688232	37.35198828
130	N	33.62903025	29.61917959	35.02080302
131	C	33.68713976	29.19739913	36.37963817
132	C	33.31088578	27.76423077	36.44428987
133	C	33.05289235	27.36061069	35.18212193
134	C	33.27173244	28.54024404	34.29908400
135	C	33.17680710	28.47492074	32.89747430
136	C	33.11810644	27.23782041	32.28052302
137	C	33.21614330	26.17936853	31.67704468
138	C	34.96737869	34.46782807	35.72919682
139	C	35.55920368	35.60733689	36.28990287
140	C	36.26320658	36.47397706	36.78305109
141	C	34.03791777	32.93710345	31.17442728
142	C	34.06163157	29.96179156	37.43096101

143	C	34.16993121	33.56903298	29.84930042
144	C	33.19064423	34.44000241	29.38072033
145	C	33.34217611	35.05498801	28.13495975
146	C	34.47835535	34.77522842	27.37347342
147	C	35.46255025	33.89915373	27.83433615
148	C	35.30071495	33.29404459	29.08243535
149	C	32.26096481	36.00840866	27.66155092
150	C	30.93942683	35.22760031	27.54069038
151	C	32.11546329	37.14117448	28.69478000
152	C	32.57481299	36.64221812	26.29607877
153	C	36.70873330	33.57854071	27.03059179
154	C	36.74064380	32.06350155	26.75423558
155	C	36.75952899	34.31481099	25.68203674
156	C	37.94378797	33.99310317	27.85314724
157	C	34.18020811	29.34128790	38.76317788
158	C	33.04382790	29.05738799	39.51047707
159	C	33.16754986	28.46197912	40.77181149
160	C	34.43911667	28.16445823	41.25352336
161	C	35.59010401	28.44660368	40.50485373
162	C	35.45365342	29.04169644	39.25517520
163	C	31.90740075	28.16770870	41.56306856
164	C	36.94658226	28.10686220	41.09308324
165	N	48.22602088	20.46895019	26.88735057
166	C	48.82690810	21.66519708	26.69787828
167	C	48.50342014	22.79837229	27.44955113
168	C	47.51684481	22.70110833	28.43527056
169	C	46.90068119	21.46343560	28.63917315
170	C	47.28076163	20.37389965	27.84866145
171	C	47.13735389	23.87595476	29.23069295
172	C	46.82423718	25.08071667	28.59394049
173	C	46.47260709	26.19934713	29.34386157
174	C	46.43031485	26.12197174	30.73772917
175	C	46.73771756	24.91836383	31.37653466
176	C	47.08941754	23.80033986	30.62555500
177	C	46.08426625	27.30983737	31.53761490
178	N	38.56423561	22.87048373	28.31656248
179	C	38.47790711	24.21936556	28.30269721
180	C	39.46111049	25.04248230	28.86128559
181	C	40.57924008	24.45588896	29.45895420
182	C	40.67280710	23.06177208	29.47305980
183	C	39.64889611	22.30625029	28.89353477
184	C	41.63608802	25.28485664	30.05453272
185	C	42.30570046	26.23106423	29.27393279
186	C	43.31775050	27.00725214	29.83129551
187	C	43.66613861	26.84409501	31.17432230
188	C	42.98970008	25.90788932	31.95923356

189	C	41.97965014	25.12953879	31.40007174
190	C	44.74610771	27.65812218	31.75806189
191	N	36.29841057	30.91025956	33.97519823
192	C	37.28346680	31.82726687	34.10046776
193	C	38.62788516	31.52028395	33.86556059
194	C	38.96871663	30.21791968	33.49531624
195	C	37.95398831	29.26780535	33.36607684
196	C	36.63207657	29.65233257	33.60919804
197	C	40.37032621	29.84904027	33.24634140
198	C	40.97159437	30.16479655	32.02629202
199	C	42.29700277	29.80960906	31.79021430
200	C	43.02881182	29.14450479	32.77667499
201	C	42.42706504	28.82917585	33.99730112
202	C	41.09954847	29.17775072	34.23008956
203	C	44.43591643	28.78056190	32.53563033
204	H	53.58392827	20.36966629	24.50570274
205	H	52.06351416	21.58954496	22.59911724
206	H	46.87451919	21.70107355	21.56050271
207	H	44.70313767	20.37236823	22.48788696
208	H	43.92512740	16.60477401	26.11784585
209	H	45.47546590	15.36953019	27.95691946
210	H	50.55421933	15.68620954	29.41940033
211	H	52.70104307	17.08625149	28.48648466
212	H	49.35912228	20.81455792	20.24106950
213	H	50.15011800	24.98994576	19.54427978
214	H	49.66928235	23.51604205	23.55182009
215	H	50.03587449	23.57650174	16.30359728
216	H	50.98613914	24.30290842	17.59734913
217	H	49.23312341	24.57300325	17.51591299
218	H	48.41119301	21.75680707	16.74288240
219	H	48.25798808	21.00613459	18.33198838
220	H	47.61078379	22.62616575	18.05892699
221	H	51.03008261	21.36501545	16.89425780
222	H	51.89615696	21.99005781	18.30414653
223	H	50.78009008	20.63264733	18.47998807
224	H	47.91687298	13.64964666	27.87247612
225	H	47.19771206	13.11294902	32.08410773
226	H	47.82460097	17.04987810	30.47696398
227	H	48.76754770	10.14624984	28.93085132
228	H	49.62289227	11.47794083	29.72175036
229	H	48.95053836	11.69202625	28.10261694
230	H	47.14218716	9.829017027	30.76918820
231	H	48.01127099	11.03695797	31.71358141
232	H	46.25867104	11.18302959	31.46964598
233	H	46.14346569	10.38673114	28.55224964
234	H	45.33856395	11.84638050	29.14509621

235	H	46.43951789	11.93968742	27.76817059
236	H	48.37071024	15.47664260	34.75693754
237	H	49.42085613	15.33714476	33.33937760
238	H	48.36635018	13.99682394	33.79629920
239	H	45.74657843	15.67710045	34.37231383
240	H	45.84343726	14.16966133	33.46251392
241	H	45.13769523	15.60340028	32.71211330
242	H	47.28045774	17.56885283	33.94074801
243	H	48.38769561	17.57082580	32.56950701
244	H	46.63528237	17.68720617	32.30326486
245	H	32.75615986	28.65015495	30.07977313
246	H	33.26454191	31.14000843	29.09365590
247	H	34.65826595	35.74505027	31.29741914
248	H	35.16392680	36.59683278	33.81634727
249	H	35.19854298	34.31853155	38.58507867
250	H	34.70191121	31.82674276	39.51687121
251	H	33.26934697	27.21392455	37.36310380
252	H	32.74594204	26.40496555	34.81225731
253	H	32.31404531	34.63988102	29.99570028
254	H	34.59976999	35.25063959	26.40300896
255	H	36.05508726	32.61176933	29.46910891
256	H	30.13185777	35.86892615	27.17458728
257	H	30.61960429	34.81721210	28.50478409
258	H	31.04064092	34.38776488	26.84463115
259	H	31.37276066	37.87789302	28.37366618
260	H	33.06626571	37.66595121	28.83981195
261	H	31.79756458	36.76369157	29.67286687
262	H	31.77659434	37.32829407	25.99117300
263	H	33.50401732	37.22118159	26.32482431
264	H	32.66496637	35.88501304	25.51034918
265	H	37.60740436	31.78928995	26.14607458
266	H	36.79203398	31.48120463	27.68012266
267	H	35.84059116	31.74415485	26.21645125
268	H	37.66970651	34.05932146	25.12914403
269	H	36.75909153	35.40183219	25.81710868
270	H	35.90932024	34.04825339	25.04508556
271	H	38.86786389	33.82934343	27.29174412
272	H	37.89720586	35.05516058	28.12010331
273	H	38.02027490	33.42541619	28.78638353
274	H	32.06171244	29.30733751	39.11183433
275	H	34.55651507	27.70510387	42.23293130
276	H	36.31967446	29.28843037	38.64466287
277	H	49.59462501	21.70884337	25.90884398
278	H	49.01732030	23.73942527	27.26971450
279	H	46.12470745	21.34748522	29.39168940
280	H	46.81109467	19.38414286	27.97936610

281	H	46.84839604	25.14281054	27.50588155
282	H	46.23219758	27.13637388	28.84471798
283	H	46.70688409	24.85823598	32.46327191
284	H	47.33820528	22.86634294	31.12847630
285	H	37.58111682	24.65073723	27.82648153
286	H	39.34837809	26.12357649	28.83700669
287	H	41.53260349	22.56891696	29.91979374
288	H	39.69150330	21.20550187	28.88511776
289	H	42.04138593	26.35482083	28.22423341
290	H	43.84102237	27.74066456	29.22029189
291	H	41.45132891	24.40152513	32.01492150
292	H	36.97173756	32.84285208	34.39857063
293	H	39.39319904	32.28537083	33.97357746
294	H	38.18422668	28.24482548	33.07649632
295	H	35.80084710	28.93397776	33.50681673
296	H	40.40197056	30.68647606	31.25785664
297	H	42.76396560	30.04705320	30.83582048
298	H	42.99955152	28.31434851	34.76717052
299	H	40.62999674	28.93037068	35.18142539
300	N	41.12585841	37.19277053	40.00642457
301	C	39.87104764	37.30004428	39.52678991
302	C	38.92110706	36.49559215	40.34988229
303	C	39.64984382	35.89248112	41.31160286
304	C	41.06317119	36.29987884	41.11327934
305	N	43.88749179	37.15391468	40.71103369
306	C	43.47167851	36.26653905	41.64584760
307	C	44.59022699	35.78225589	42.43735860
308	C	45.71090518	36.40037117	41.94700762
309	N	44.39844593	39.13091851	38.63445513
310	C	45.69909801	38.98883487	39.11855980
311	C	46.57952343	39.89946220	38.42002517
312	C	45.80694700	40.58032475	37.51072881
313	C	44.45826598	40.07521775	37.65708416
314	N	41.64375225	39.04707219	37.89739658
315	C	42.08882688	40.03122010	36.96913883
316	C	40.93049379	40.46354294	36.15037948
317	C	39.85555265	39.76753671	36.57819816
318	C	40.32552953	38.88615911	37.68310463
319	C	39.47269317	38.00706306	38.37717180
320	C	38.23662792	37.69043544	37.84172440
321	C	37.21270730	37.23814625	37.34935990
322	C	47.49191201	37.91830972	40.24718948
323	C	48.69245727	37.70474112	40.20434145
324	C	42.11576872	35.84328952	41.83094517
325	C	43.35419740	40.49428667	36.84754558
326	C	41.88299120	34.80239452	42.84776228

327	C	41.89809917	35.11372423	44.20376153
328	C	41.67274654	34.11208482	45.15261024
329	C	41.42165523	32.80909678	44.71854067
330	C	41.39968242	32.49006064	43.35965166
331	C	41.64233107	33.49661637	42.42400860
332	C	41.70068562	34.48735178	46.62260136
333	C	41.52003388	33.27747087	47.55425268
334	C	43.05775168	35.14043985	46.94423830
335	C	40.55651609	35.48253112	46.89005277
336	C	41.12263566	31.08755029	42.85289882
337	C	43.65320617	41.48519307	35.79734656
338	C	43.82857913	42.82223686	36.13290871
339	C	44.11288080	43.76228523	35.13533468
340	C	44.21565408	43.33175110	33.81544888
341	C	44.04122518	41.98476809	33.46959374
342	C	43.75789716	41.06090128	34.47019863
343	C	44.29952346	45.21301406	35.53710177
344	C	43.00283867	45.70858123	36.20345348
345	C	44.60856398	46.12956793	34.34175672
346	C	45.47363486	45.29996287	36.52946071
347	C	44.16936265	41.5822635	32.01278042
348	C	43.12977082	42.36350739	31.18819710
349	C	45.59240433	41.92235839	31.53253032
350	C	43.92986647	40.07945952	31.78725560
351	N	53.96950380	34.88943007	38.99420486
352	C	52.96360589	35.57348949	39.56643790
353	C	52.64085924	35.01720635	40.91066365
354	C	53.50247807	34.00130679	41.12957699
355	C	54.37189678	33.89539054	39.93157343
356	N	56.02549295	33.65794752	37.45958497
357	C	56.17582705	32.89605527	38.57608933
358	C	57.21394632	31.90533406	38.38653946
359	C	57.67194249	32.06003967	37.09983008
360	N	55.61890651	35.62489489	35.36032036
361	C	56.54261155	34.8043362	34.69769084
362	C	56.87009267	35.38658608	33.41027296
363	C	56.16448266	36.55760471	33.31446029
364	C	55.38412726	36.67217097	34.53628817
365	N	53.65577945	36.89618862	36.98093606
366	C	53.70262225	37.83785946	35.91534992
367	C	52.71480528	38.91202137	36.19322164
368	C	52.10339751	38.60334007	37.35527619
369	C	52.70835670	37.32719757	37.83816946
370	C	52.28474513	36.67561919	39.00964199
371	C	51.09609692	37.09342602	39.58287471
372	C	49.98608175	37.42004540	39.97638422

373	C	57.08286353	33.62989865	35.20970967
374	C	57.76433427	32.77734728	34.33244602
375	C	58.17236659	31.90291952	33.58519323
376	C	55.37744384	33.00635525	39.76031452
377	C	54.46953407	37.74323795	34.80449873
378	C	55.67334278	32.03626566	40.83087284
379	C	56.44005288	32.39197186	41.94504059
380	C	56.70257195	31.45117759	42.93972491
381	C	56.20723179	30.15469004	42.81673611
382	C	55.44970788	29.79368451	41.70368017
383	C	55.18202713	30.73409897	40.71310303
384	C	54.34902306	38.76828103	33.75214555
385	C	55.00054121	40.00156062	33.85106637
386	C	54.86486519	40.94495662	32.83375681
387	C	54.08194349	40.65525567	31.71818221
388	C	53.43572886	39.42465402	31.61269272
389	C	53.56976362	38.48286935	32.62829974
390	C	56.92768325	33.15545285	36.52160427
391	C	45.27516536	37.26547017	40.86698346
392	C	46.10759956	38.07709558	40.10291413
393	N	57.99957420	26.14258566	32.12235521
394	C	58.35673109	27.39191752	32.47189996
395	C	58.68813012	27.46060624	33.92385654
396	C	58.51273858	26.21954907	34.42412803
397	C	58.06073342	25.35427074	33.30713208
398	N	57.18993780	23.62638450	31.03691073
399	C	57.32029984	23.21571633	32.32201184
400	C	56.97306642	21.81208383	32.45584966
401	C	56.61872312	21.37676940	31.20450135
402	C	56.75711406	22.50928272	30.31182285
403	N	57.09818757	24.84062383	28.39777562
404	C	56.70417571	23.54468515	28.04951414
405	C	56.52687647	23.46252885	26.61387989
406	C	56.81773027	24.70282148	26.10547360
407	C	57.15992321	25.54236892	27.23836378
408	N	57.88862820	27.34082379	29.53382702
409	C	57.84454160	27.72556267	28.16364109
410	C	58.20861999	29.16040328	28.06673388
411	C	58.45108277	29.59820440	29.32080799
412	C	58.24670915	28.43609031	30.22950637
413	C	58.39101234	28.51991280	31.62628811
414	C	58.48904142	29.76147575	32.22919419
415	C	58.44688822	30.82470846	32.83135951
416	C	56.49926017	22.48745160	28.94179264
417	C	55.87691685	21.35041187	28.41023697
418	C	55.17546046	20.47634301	27.92688445

419	C	57.73548341	24.04534602	33.41437682
420	C	57.50538613	26.92828201	27.12502722
421	C	57.79005531	23.40388430	34.74046176
422	C	58.80969518	22.50359197	35.03806481
423	C	58.86073068	21.89590492	36.29514221
424	C	57.88175059	22.20878208	37.24005159
425	C	56.85652449	23.11096456	36.95054700
426	C	56.81436326	23.70719252	35.68809337
427	C	59.98133639	20.91307500	36.57888181
428	C	61.32805824	21.64207558	36.41688511
429	C	59.88128712	19.75322740	35.57080055
430	C	59.91982114	20.32482098	37.99816177
431	C	55.77944895	23.46900743	37.95745311
432	C	55.80211527	24.99185407	38.18923541
433	C	55.97273966	22.77453214	39.31563797
434	C	54.41483075	23.04086584	37.38544581
435	C	57.47231157	27.49824334	25.76557548
436	C	58.66177538	27.74325536	25.08969315
437	C	58.63458806	28.28777449	23.80034409
438	C	57.40322760	28.57442321	23.21826755
439	C	56.19904178	28.32526762	23.89137566
440	C	56.24004956	27.78361983	25.17199790
441	C	59.95091361	28.53225252	23.08751854
442	C	54.89246535	28.64915180	23.19212652
443	H	37.86906347	36.45780611	40.15592401
444	H	39.33794957	35.23867234	42.10187072
445	H	44.50970573	35.07903688	43.23665931
446	H	46.72579822	36.30092175	42.27031334
447	H	47.62742492	39.99910059	38.60802270
448	H	46.10463896	41.33580300	36.81784766
449	H	41.00636367	41.20413384	35.37915780
450	H	38.83892041	39.79383570	36.24657352
451	H	42.08833361	36.14032325	44.51469787
452	H	41.23991440	32.02733105	45.45231304
453	H	41.64653375	33.27083455	41.35933612
454	H	41.56486748	33.58396317	48.60553840
455	H	40.55061856	32.79149821	47.40216851
456	H	42.30692925	32.53128459	47.40141387
457	H	43.13653719	35.38853431	48.00728252
458	H	43.20894555	36.06857993	46.38223323
459	H	43.88635475	34.46816634	46.69546136
460	H	40.52350680	35.77463651	47.94420706
461	H	39.58546442	35.04477307	46.63419694
462	H	40.66871014	36.39836845	46.29932456
463	H	43.74628330	43.12919728	37.17499766
464	H	44.43701048	44.04645617	33.02521858

465	H	43.61763576	40.00643478	34.24491751
466	H	43.07762118	46.76492756	36.47953016
467	H	42.14683198	45.59921488	35.52858199
468	H	42.77396016	45.14794368	37.11638489
469	H	44.73862788	47.16748693	34.66868388
470	H	43.79599506	46.12272428	33.60777049
471	H	45.53292758	45.83325801	33.83476128
472	H	45.66943158	46.33596287	36.82261691
473	H	46.39227772	44.89752886	36.08840830
474	H	45.27583792	44.73330344	37.44611552
475	H	43.15728957	42.06979491	30.13436591
476	H	42.11552386	42.17901764	31.56052825
477	H	43.30302973	43.44348689	31.23042676
478	H	45.74470732	41.61491124	30.49357948
479	H	45.79562836	42.99659594	31.58925582
480	H	46.34475398	41.4143620	32.14656331
481	H	44.02432111	39.82317567	30.72673248
482	H	42.92393288	39.78139331	32.10361373
483	H	44.65720126	39.46966333	32.33404442
484	H	51.86246308	35.40755415	41.53238107
485	H	53.59855347	33.35743683	41.97991978
486	H	57.54073397	31.21181330	39.12808082
487	H	58.43663568	31.50699192	36.59683798
488	H	57.55218980	34.95686943	32.70701887
489	H	56.16568283	37.27386902	32.52384162
490	H	52.56803449	39.75162455	35.54462875
491	H	51.33633439	39.12451656	37.89019895
492	S	57.05599232	34.04719941	42.02091973
493	H	56.41607258	29.42007972	43.59253658
494	H	54.59389827	30.45904615	39.83780433
495	S	55.98919137	40.29116523	35.28749397
496	H	53.97784092	41.39269181	30.92410824
497	H	53.07538565	37.51435549	32.54929400
498	H	59.00786942	28.35978007	34.40835775
499	H	58.65779970	25.85449076	35.42169604
500	H	56.99935303	21.26299705	33.37108635
501	H	56.30380073	20.40080813	30.90109583
502	H	56.23331783	22.57930658	26.08699805
503	H	56.81008681	25.02610038	25.08788571
504	H	58.25103759	29.68825697	27.13477441
505	H	58.74107320	30.56685186	29.66995468
506	H	59.56029434	22.27772884	34.28131430
507	H	57.91797699	21.73903141	38.22006353
508	H	56.02075874	24.40630026	35.43263237
509	H	62.16760209	20.98194220	36.65556310
510	H	61.47651979	22.00114747	35.39263181

511	H	61.38736548	22.51144349	37.0809329
512	H	60.65130706	18.99831334	35.75698882
513	H	58.90570619	19.25889966	35.63516874
514	H	60.00551029	20.09810943	34.53827352
515	H	60.74312903	19.62107501	38.16542079
516	H	58.98780632	19.77541096	38.16725577
517	H	60.00320550	21.10501626	38.76210641
518	H	55.06849236	25.28896864	38.94448065
519	H	55.57224339	25.54707348	37.27405080
520	H	56.78910485	25.32145287	38.53377518
521	H	55.18269483	23.06063716	40.01835054
522	H	55.93799393	21.68386947	39.21941281
523	H	56.92892690	23.04841130	39.77472090
524	H	53.60551213	23.24853748	38.09110829
525	H	54.40162173	21.96693856	37.16672969
526	H	54.18239618	23.56584694	36.45302962
527	H	59.61043984	27.50109098	25.56687166
528	H	57.36058944	28.99823202	22.21685814
529	H	55.33023500	27.56872033	25.72832717
530	N	43.27559491	36.31496444	37.84712792
531	C	42.78926577	35.08094895	38.10870631
532	C	43.12771652	33.96086720	37.34379060
533	C	44.00799563	34.11221032	36.26805842
534	C	44.50790733	35.38817177	35.99339290
535	C	44.11903604	36.46171761	36.80139416
536	C	44.39819486	32.95502124	35.45158247
537	C	44.86191533	31.78774130	36.06598509
538	C	45.22062819	30.68458993	35.29672161
539	C	45.11708653	30.73748573	33.90468556
540	C	44.66285156	31.90564899	33.28759249
541	C	44.30603181	33.00908798	34.05778777
542	C	45.46142527	29.55868533	33.09083102
543	N	53.13474653	33.90059909	36.16418489
544	C	53.24315163	32.55467594	36.10392217
545	C	52.24136911	31.74221324	35.56177488
546	C	51.07913038	32.33612936	35.06271006
547	C	50.96775229	33.72819989	35.11806588
548	C	52.01280902	34.47258332	35.67229709
549	C	49.99050320	31.52818342	34.49699022
550	C	49.42380270	30.49052562	35.24212426
551	C	48.37700923	29.73992136	34.71415844
552	C	47.89180453	30.01942184	33.43456706
553	C	48.45950036	31.05223071	32.68525216
554	C	49.50421169	31.80390196	33.21568321
555	C	46.79865761	29.21203200	32.86605611
556	N	55.26214262	26.03498441	30.63550653

557	C	54.27331981	25.15567622	30.36063588
558	C	52.92432763	25.44927647	30.58590417
559	C	52.58414958	26.69697306	31.11170119
560	C	53.60289462	27.60887455	31.39614393
561	C	54.92864363	27.24142686	31.14615160
562	C	51.17817784	27.04877018	31.36205105
563	C	50.56385707	26.66866089	32.55689450
564	C	49.23550868	27.01034549	32.79678525
565	C	48.51565484	27.72941784	31.84023918
566	C	49.12907513	28.10564680	30.64295130
567	C	50.45826912	27.76719917	30.40519057
568	C	47.10878981	28.08947032	32.08798130
569	H	42.10501819	34.99759948	38.96853953
570	H	42.70656126	32.98753099	37.58262296
571	H	45.20109022	35.54689179	35.17123140
572	H	44.49681638	37.48131849	36.61570186
573	H	44.95035693	31.74336779	37.15161756
574	H	45.58191637	29.77803888	35.77956074
575	H	44.57999518	31.94812136	32.20261975
576	H	43.94213655	33.91374910	33.57145662
577	H	54.17325963	32.11982854	36.50718343
578	H	52.37186506	30.66358366	35.52538236
579	H	50.07611005	34.22810315	34.74731173
580	H	51.95422705	35.57113461	35.73064356
581	H	49.79661921	30.27388945	36.24276706
582	H	47.93737935	28.93243363	35.29690750
583	H	48.08505511	31.26659700	31.68561495
584	H	49.94852724	32.60588343	32.62689838
585	H	54.58550012	24.18198070	29.94609281
586	H	52.15595241	24.71534158	30.35403598
587	H	53.37202548	28.58933130	31.80636108
588	H	55.76394039	27.93089500	31.35955577
589	H	51.12498725	26.10596847	33.30206550
590	H	48.75698178	26.71901142	33.73015539
591	H	48.56536025	28.66199378	29.89601884
592	H	50.93713346	28.06187249	29.47220771
593	Zn	42.82817896	37.93575360	39.14147881
594	Zn	54.64419891	35.10030852	37.07366992
595	Zn	57.28566693	25.53479610	30.30339767
596	C	50.12939003	25.94888874	23.62271764
597	C	49.11666910	26.75768442	21.49060723
598	C	51.58839595	26.26560266	21.62582332
599	C	32.19381486	27.49358818	42.91521921
600	C	31.01355414	27.22563805	40.73533908
601	C	31.17563623	29.49575586	41.82967437
602	C	38.10120726	28.38289327	40.11471562

603	C	36.98081468	26.61112953	41.45795449
604	C	37.15197860	28.96393324	42.35525726
605	C	40.74746843	30.10634849	43.97531199
606	C	42.39071746	30.56568813	42.15141031
607	C	39.95246375	31.14356030	41.85375630
608	H	57.29423995	31.70732308	43.81755388
609	H	55.07056380	28.77852325	41.60753477
610	H	55.36438468	41.91146350	32.88965973
611	H	52.83041237	39.19922526	30.73722082
612	C	59.77122971	29.18654497	21.70763782
613	C	60.65547067	27.17683247	22.89471787
614	C	60.82033890	29.46449575	23.95173333
615	C	53.66070760	28.33406228	24.05796788
616	C	54.80703870	27.81303350	21.90207385
617	C	54.86979630	30.15087660	22.85190318
618	H	50.88442392	25.31681476	24.10417861
619	H	49.14385126	25.66696935	24.00940309
620	H	50.32039541	26.97933558	23.94086963
621	H	48.10931955	26.41613507	21.75436112
622	H	49.17306636	26.79324712	20.39785551
623	H	49.22907181	27.78239812	21.85745650
624	H	51.67503903	26.26969909	20.53488875
625	H	52.35958256	25.58938944	22.01392700
626	H	51.82278290	27.27580066	21.97780377
627	H	32.80920910	28.12937167	43.56054786
628	H	32.70645196	26.53452044	42.78694665
629	H	31.26242805	27.29180025	43.45630496
630	H	31.54270955	26.29959645	40.48567734
631	H	30.69526325	27.68720625	39.79449914
632	H	30.10781634	26.95364108	41.28638453
633	H	30.86776982	29.98508896	40.89894741
634	H	31.82002874	30.19843144	42.36993164
635	H	30.27451978	29.33908613	42.43035096
636	H	38.15824471	29.44474731	39.84829534
637	H	37.98714780	27.80614598	39.18997681
638	H	39.06389674	28.10160229	40.55413719
639	H	36.75747052	25.98968364	40.58352434
640	H	36.24880320	26.36136283	42.23223239
641	H	37.96518858	26.31684530	41.83462925
642	H	36.39703940	28.74928708	43.11844919
643	H	37.08129093	30.03262076	42.11910108
644	H	38.13328840	28.78345786	42.80538052
645	H	39.85335396	30.43802540	44.51482483
646	H	41.56111452	29.99055010	44.69950099
647	H	40.53398675	29.11066578	43.57134247
648	H	43.24604511	30.56658085	42.83655774

649	H	42.66248138	31.18660771	41.29115053
650	H	42.25233255	29.54242676	41.79125374
651	H	40.19737265	31.73321957	40.96469129
652	H	39.06527516	31.59478269	42.31321744
653	H	39.67642840	30.14034354	41.51185998
654	H	59.27037606	30.15725252	21.78462416
655	H	59.18851719	28.55132193	21.03230207
656	H	60.74118703	29.36019836	21.22799818
657	H	60.02802527	26.48508368	22.32160780
658	H	60.87976841	26.69511103	23.85298014
659	H	61.60131732	27.29370045	22.35720072
660	H	61.07085778	29.01153850	24.91700022
661	H	60.30315158	30.40856301	24.15454949
662	H	61.76417058	29.70248819	23.45107177
663	H	53.67474319	28.89916038	24.99634555
664	H	53.60357870	27.26678072	24.30170923
665	H	52.73530662	28.59873398	23.53584301
666	H	54.84234642	26.74054939	22.12747519
667	H	55.63501807	28.03002217	21.21971466
668	H	53.87805180	28.01299535	21.35938062
669	H	55.67263419	30.42483962	22.16022986
670	H	54.99421531	30.75911957	23.75489424
671	H	53.92375316	30.43789755	22.38311500
672	H	32.93594300	23.21777653	22.12760382
673	H	34.48656587	15.97296837	30.65295848
674	H	43.25269875	25.78902525	33.00924400
675	H	57.66374236	34.01840354	43.21499246
676	H	56.40134503	41.54246492	35.04126372

3. UV-VISIBLE TITRATIONS OF PORPHYRIN MONOMERS WITH PYRIDINE

Titrations with zinc porphyrins *cis*-2SAC-P, **6a**, or **6c**, with pyridine were performed in order to compare their binding constants.

All titrations were performed in toluene at 298 K. The porphyrin concentration was kept constant throughout the titration by adding porphyrin to the ligand solution before titrations were started. In order to minimize relative errors between samples, the same stock solution of pyridine was used for the first series of titrations (Run 1), and a second stock solution was used for the second series of titrations (Run 2). The binding curves were fitted using a 1:1 binding isotherm using the equation:

$$\frac{A - A_{initial}}{A_{\infty} - A_{initial}} = \left(\frac{(K_a([L] + [P]_0) + 1) - \sqrt{(K_a([L] + [P]_0) + 1)^2 - 4K_a^2[P]_0[L]}}{2K_a[P]_0} \right)$$

where A is the observed absorption at a specific wavelength or the difference of absorbance between two wavelengths; $A_{initial}$ is the starting absorbance at this wavelength or difference of absorbance at these wavelengths; A_{∞} is the asymptotic final absorbance at this wavelength or difference of absorbance at these wavelengths; K_a is the association constant between ligand and porphyrin host; $[L]$ is the concentration of ligand; $[P]_0$ is the concentration of porphyrin host. The free variables which were adjusted to optimize the fit to the experimental data during the fitting procedure are $A_{initial}$, A_{∞} , and K_a . Fitting analysis was carried out using the Origin software.

The titration results are summarized in Table S1 and the binding curves are shown in Figure S7.

Table S1. Binding constants for *cis*-2SAC-P, **6a**, and **6c** with pyridine in toluene at 298 K (in M⁻¹).

Porphyrin	Run 1	Run 2	Average
<i>cis</i> -2SAC-P	1.16 ± 0.10 × 10 ⁴	1.14 ± 0.10 × 10 ⁴	1.15 ± 0.10 × 10 ⁴
6a	7.66 ± 0.70 × 10 ³	7.53 ± 0.70 × 10 ³	7.60 ± 0.70 × 10 ³
6c	2.04 ± 0.20 × 10 ⁴	2.05 ± 0.20 × 10 ⁴	2.05 ± 0.20 × 10 ⁴

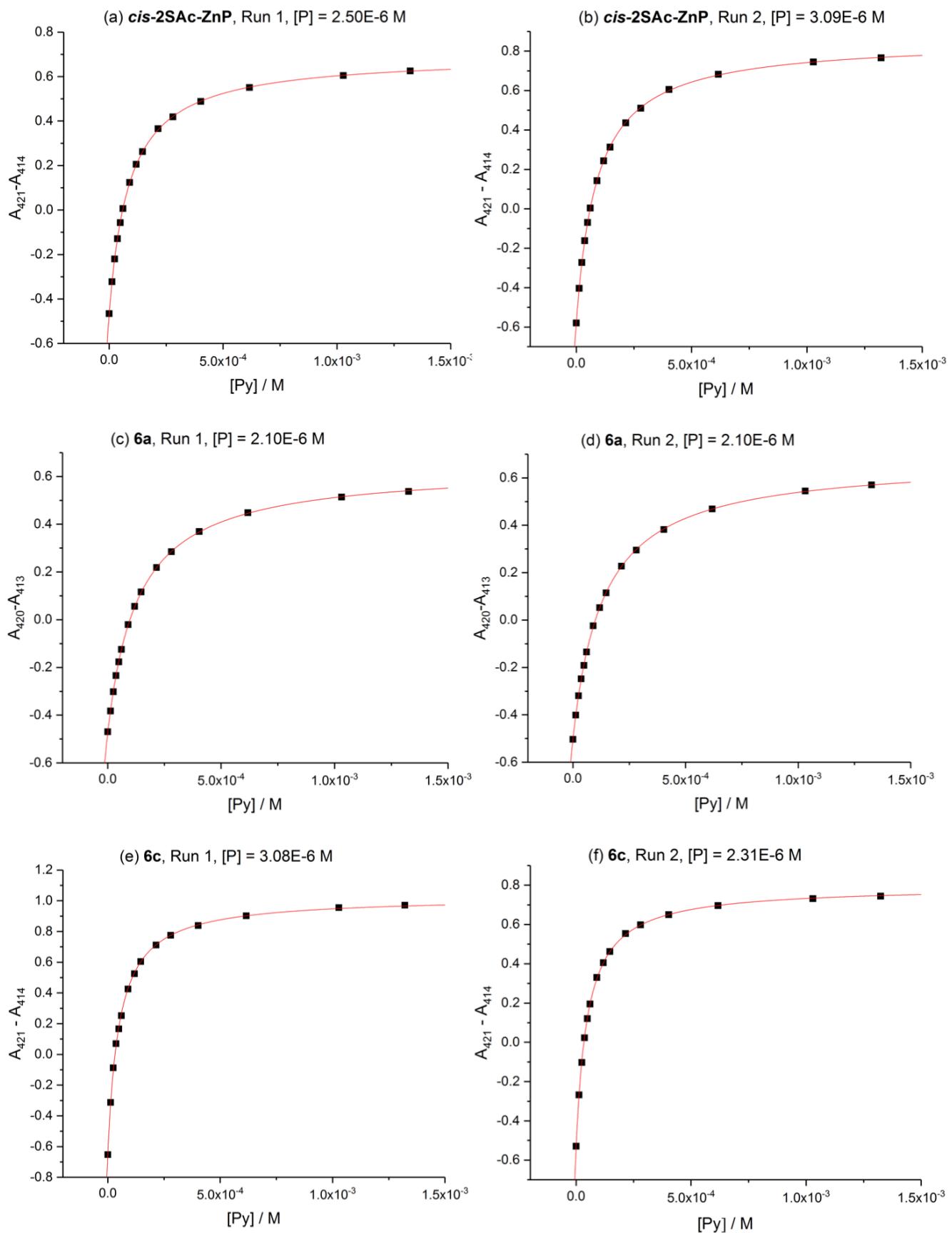
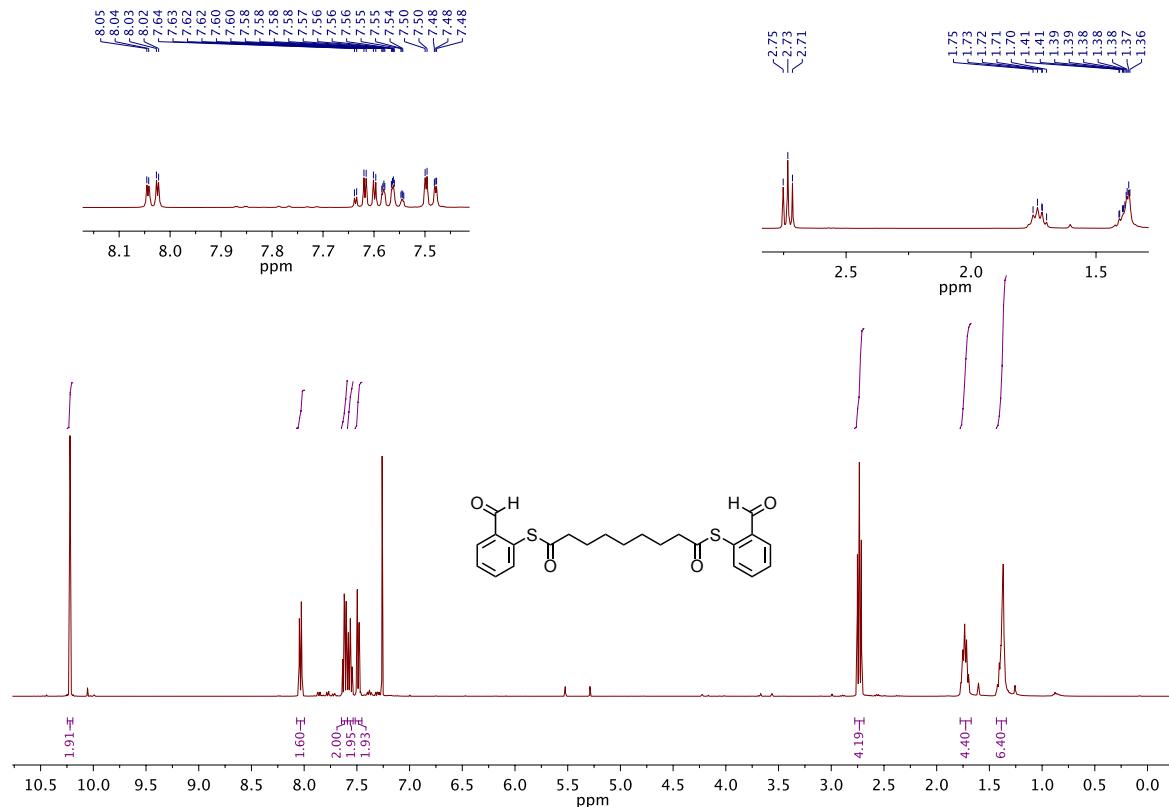


Figure S7. Binding curves and fitting results for the titrations of ***cis*-2SAC-P**, **6a**, and **6c**, with pyridine in toluene at 298 K.

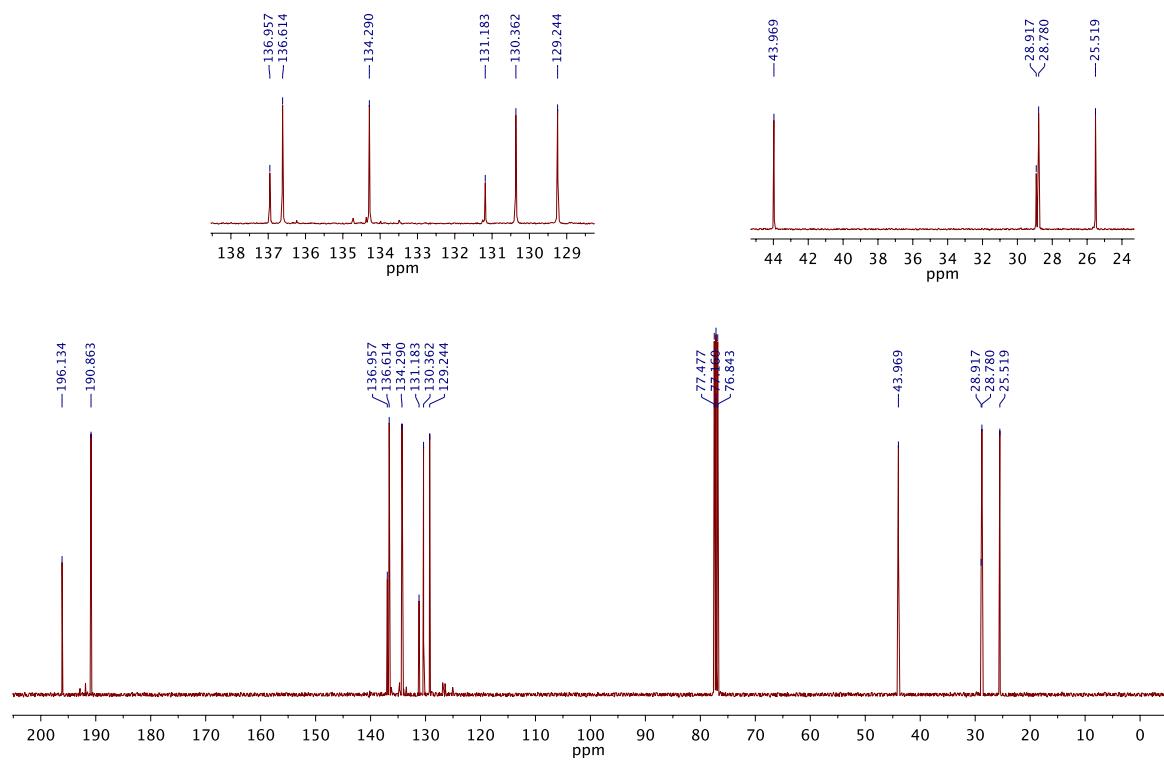
4. CHARACTERIZATION SPECTRA FOR NEW COMPOUNDS

4.1. S,S-Bis(2-formylphenyl)nonanebis(thioate) 3a

¹H NMR (CDCl₃, 400 MHz, 298K):



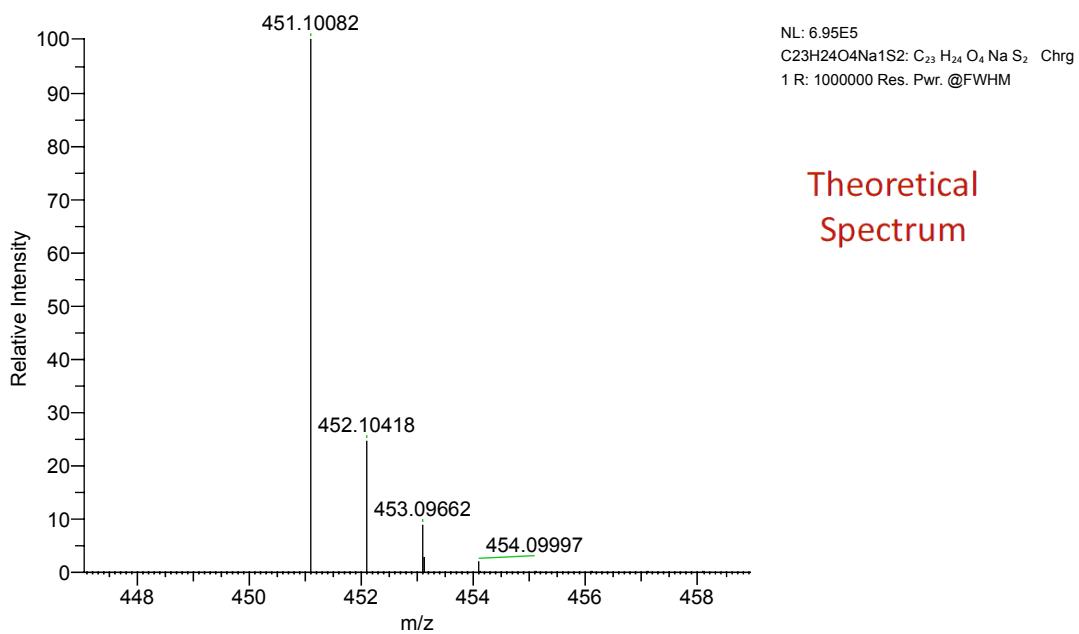
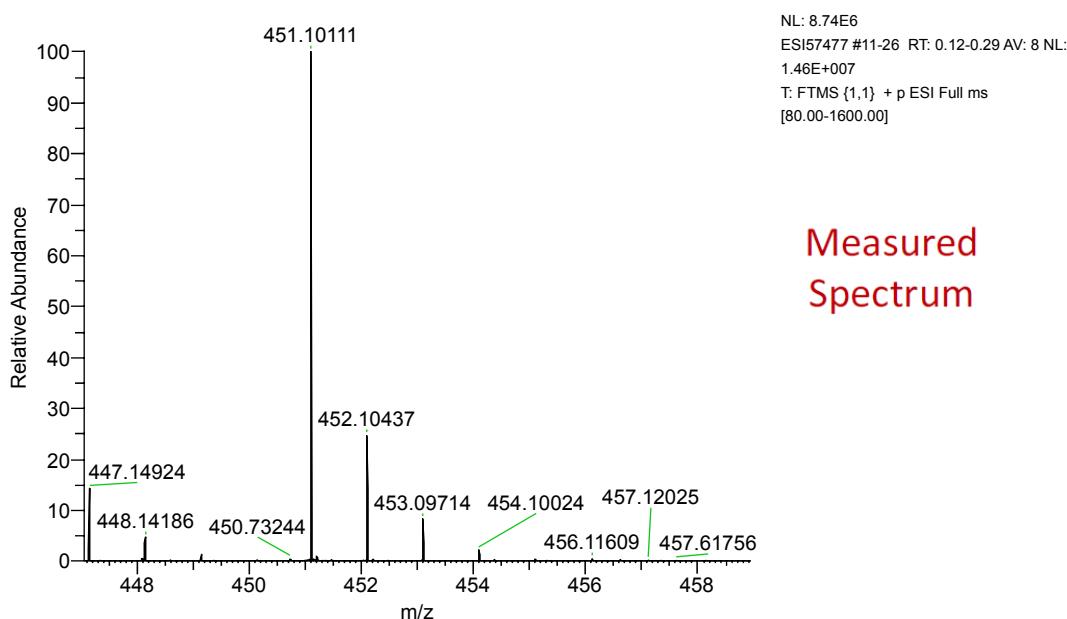
¹³C NMR (CDCl₃, 100 MHz, 298K):



ESI-HRMS:

W:\data\June 16\ESI57477.raw

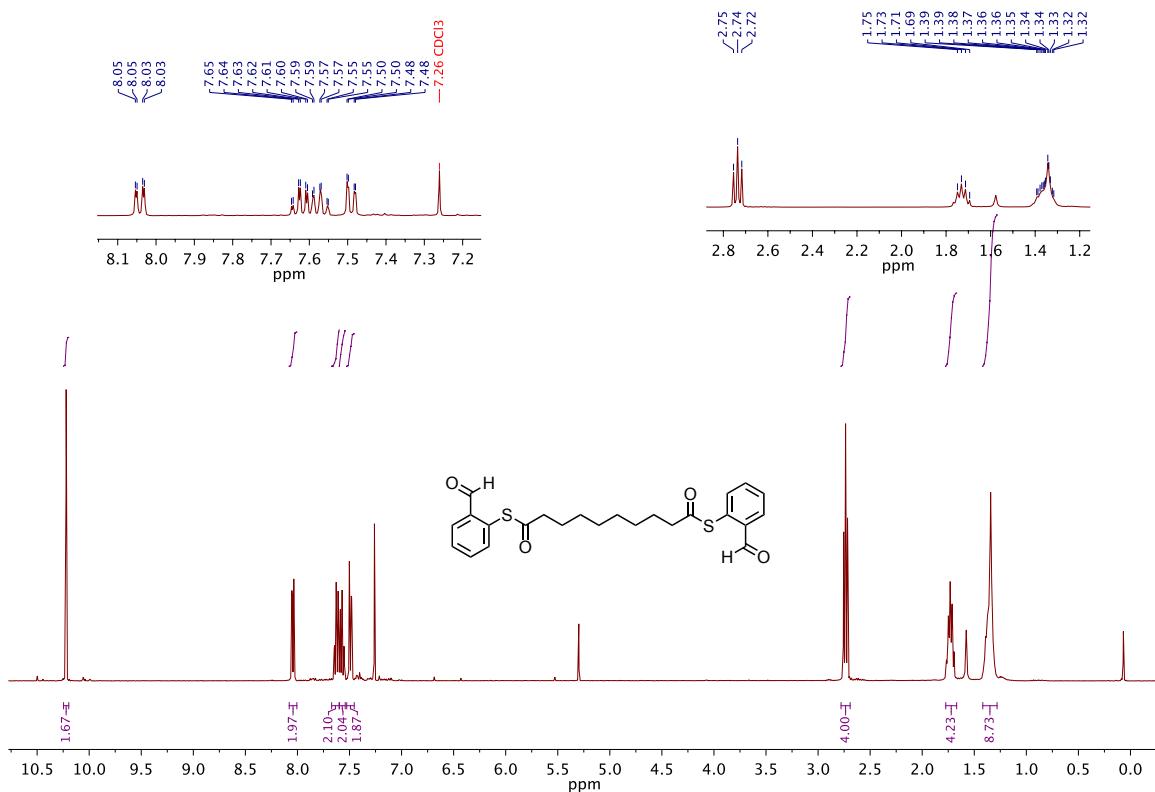
01/06/2016 8:15 am



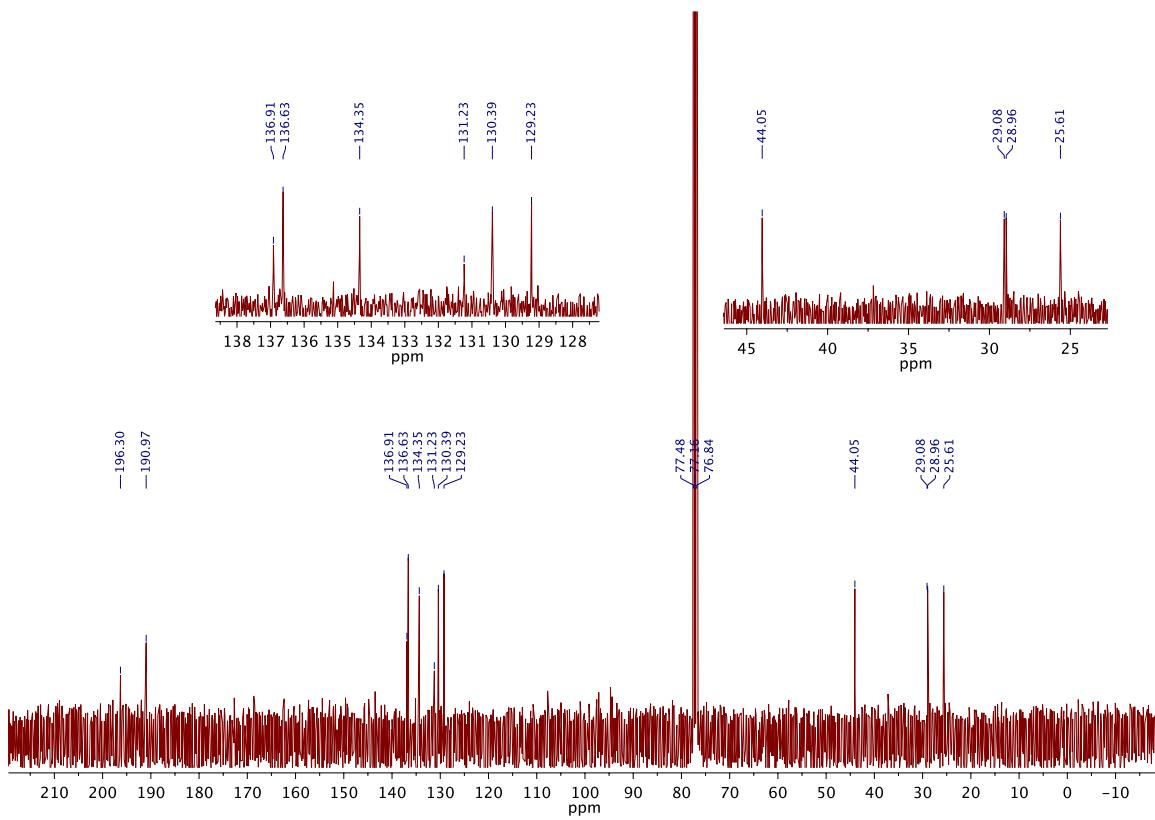
m/z	Formula	RDB	Delta ppm	Theo. Mass
451.10110	C ₂₃ H ₂₄ O ₄ ²³ Na ³² S ₂	11.5	0.63	451.10082

4.2. S,S-Bis(2-formylphenyl)decanebis(thioate) 3b

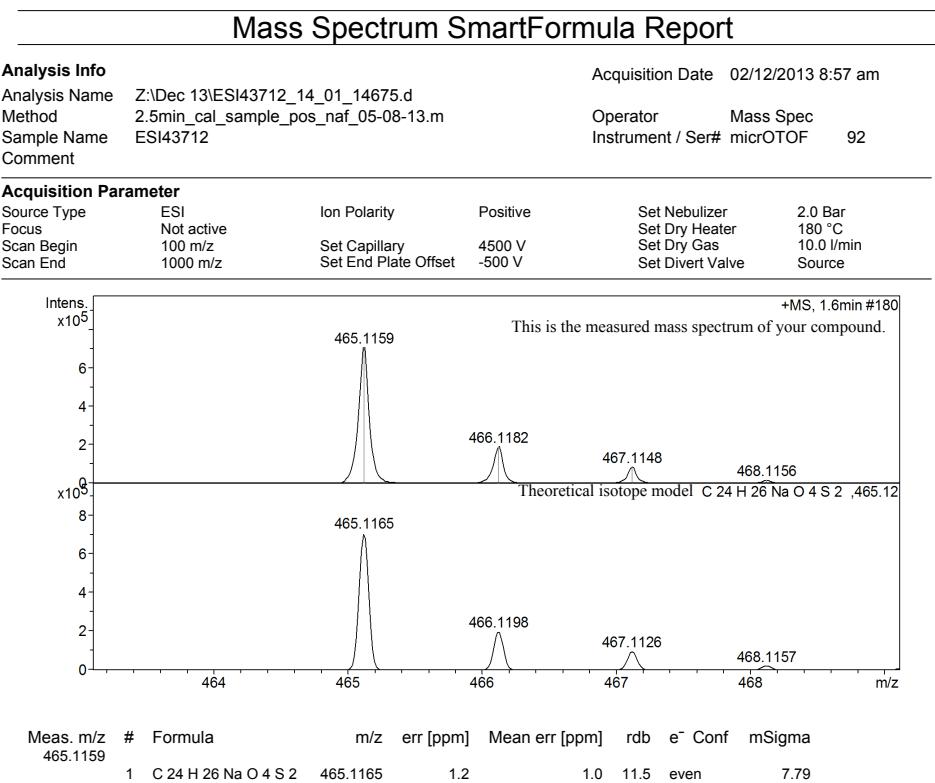
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

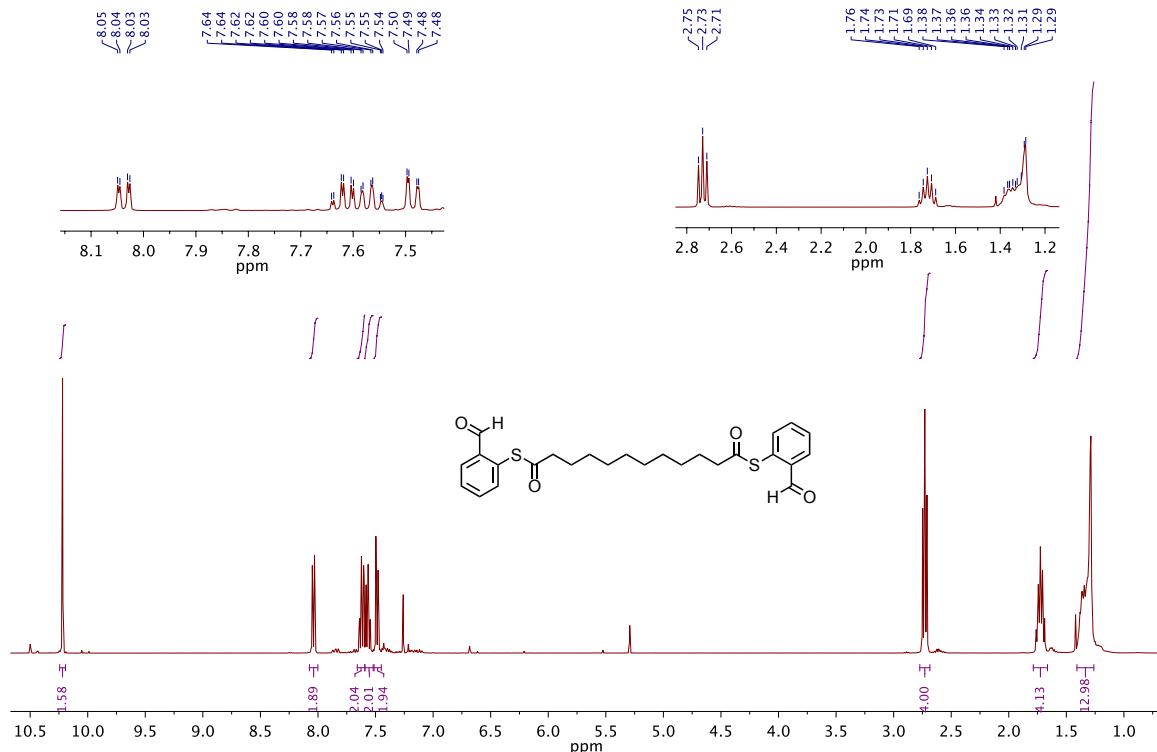


ESI-HRMS:

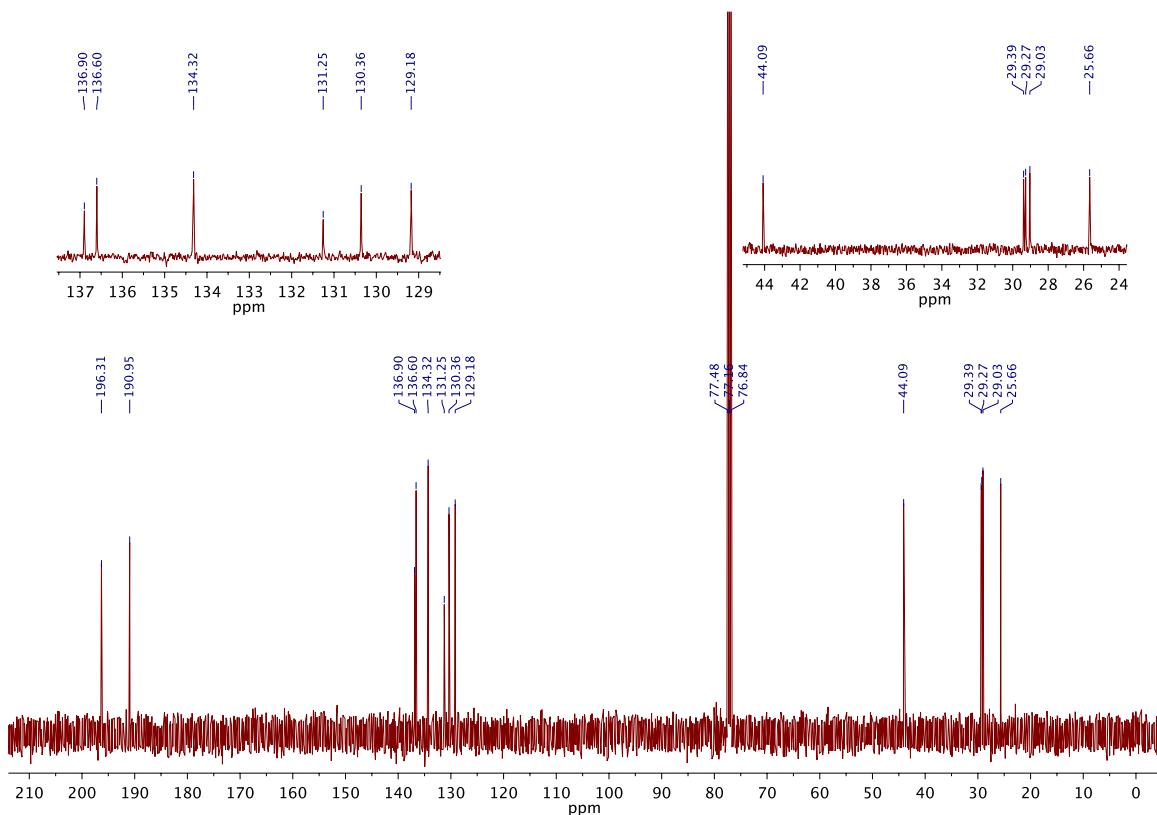


4.3. S,S-Bis(2-formylphenyl)dodecanabis(thioate) 3c

¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):



ESI-HRMS:

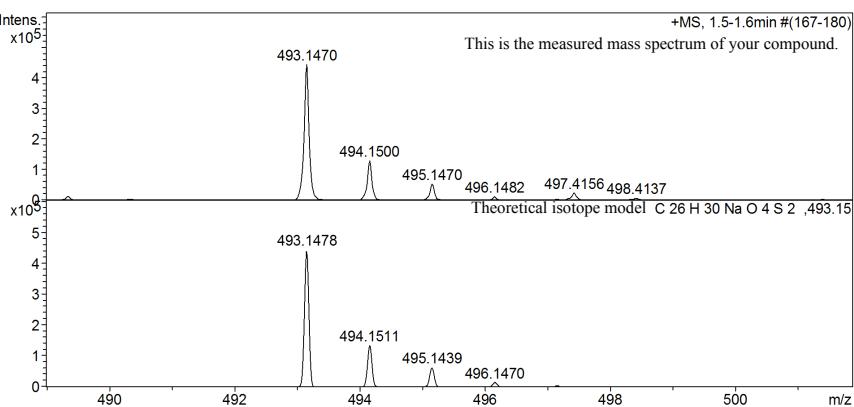
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	Z:\Dec 13\ESI43713_15_01_14676.d	Acquisition Date	02/12/2013 9:00 am
Method	2.5min_cal_sample_pos_naf_05-08-13.m	Operator	Mass Spec
Sample Name	ESI43713	Instrument / Ser#	micrOTOF 92
Comment			

Acquisition Parameter

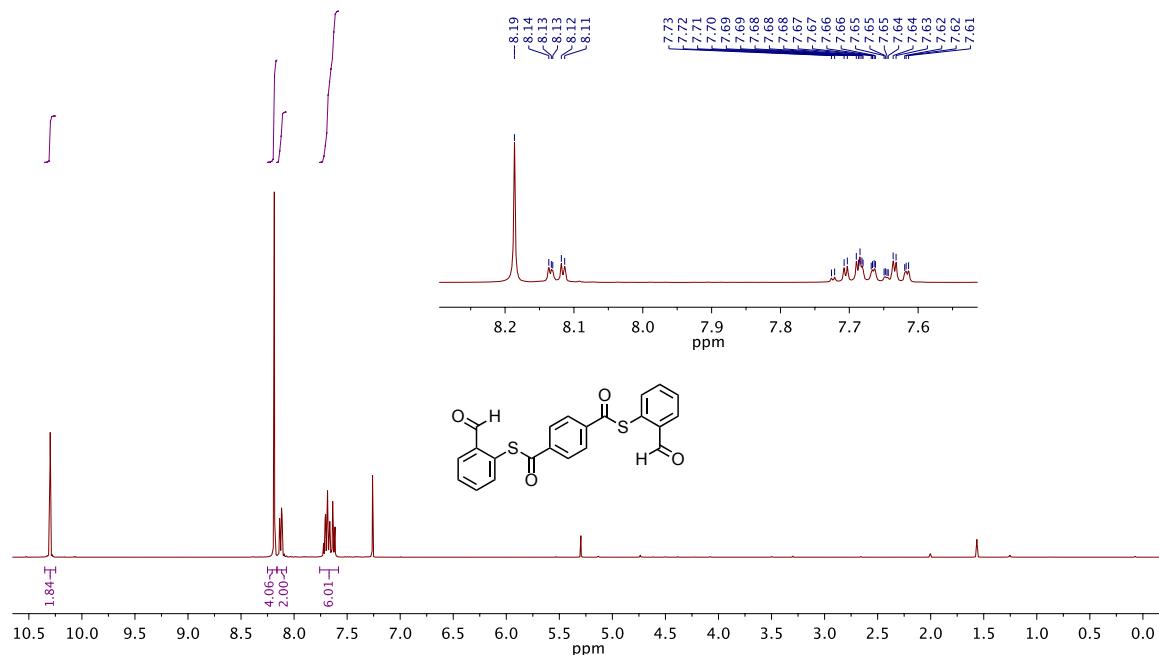
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



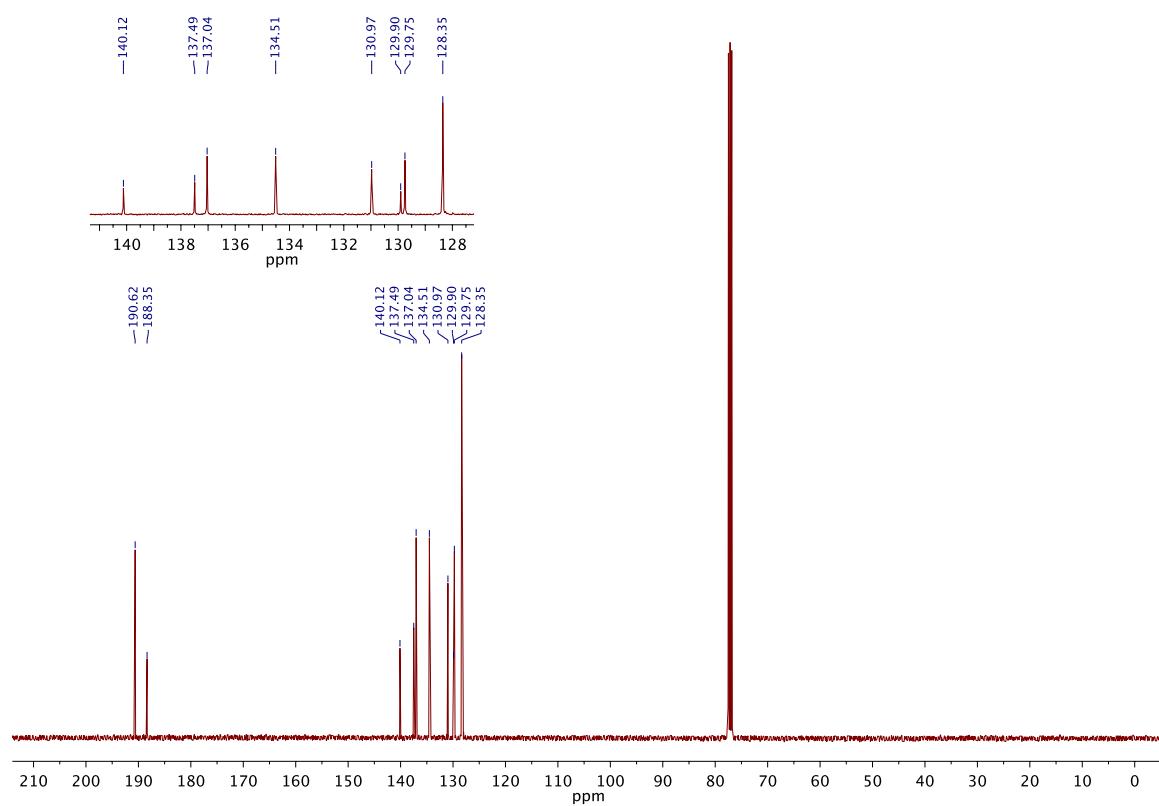
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	e-	Conf	mSigma
493.1470	1	C 26 H 30 Na O 4 S 2	493.1478	1.6	1.0	11.5	even		11.10

4.4. S,S-Bis(2-formylphenyl)benzene-1,4-bis(carbothioate) 3d

^1H NMR (CDCl_3 , 400 MHz, 298K):



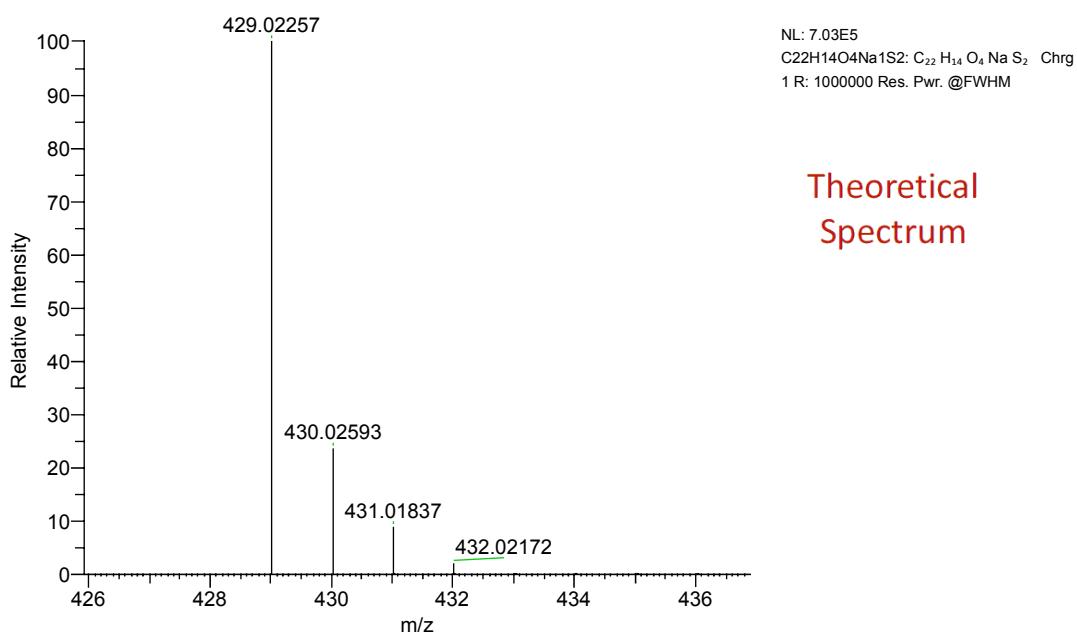
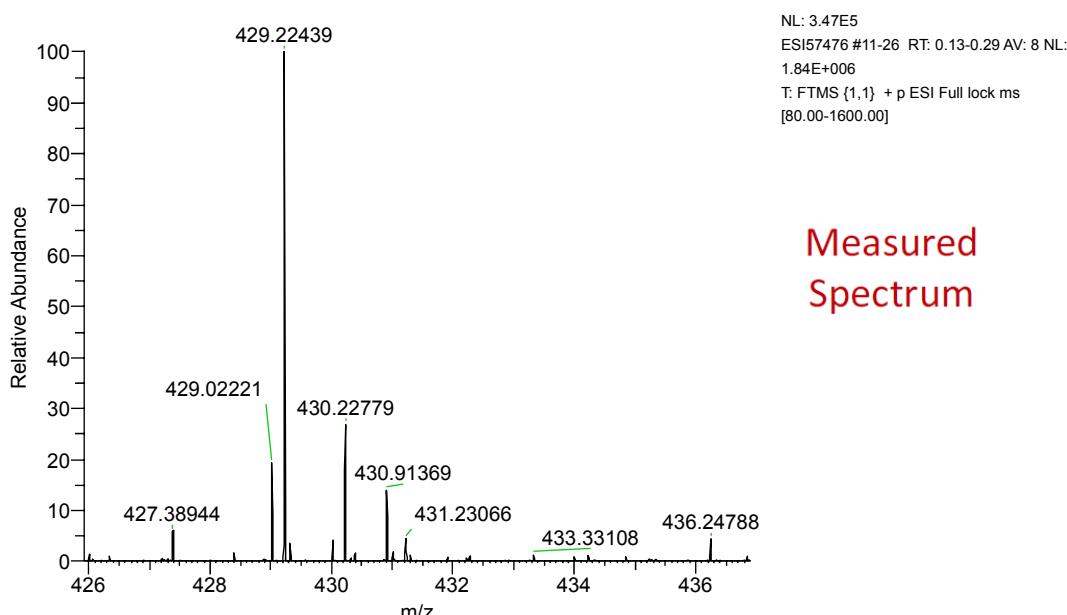
^{13}C NMR (CDCl_3 , 100 MHz, 298K):



ESI-HRMS:

W:\data\June 16\ESI57476.raw

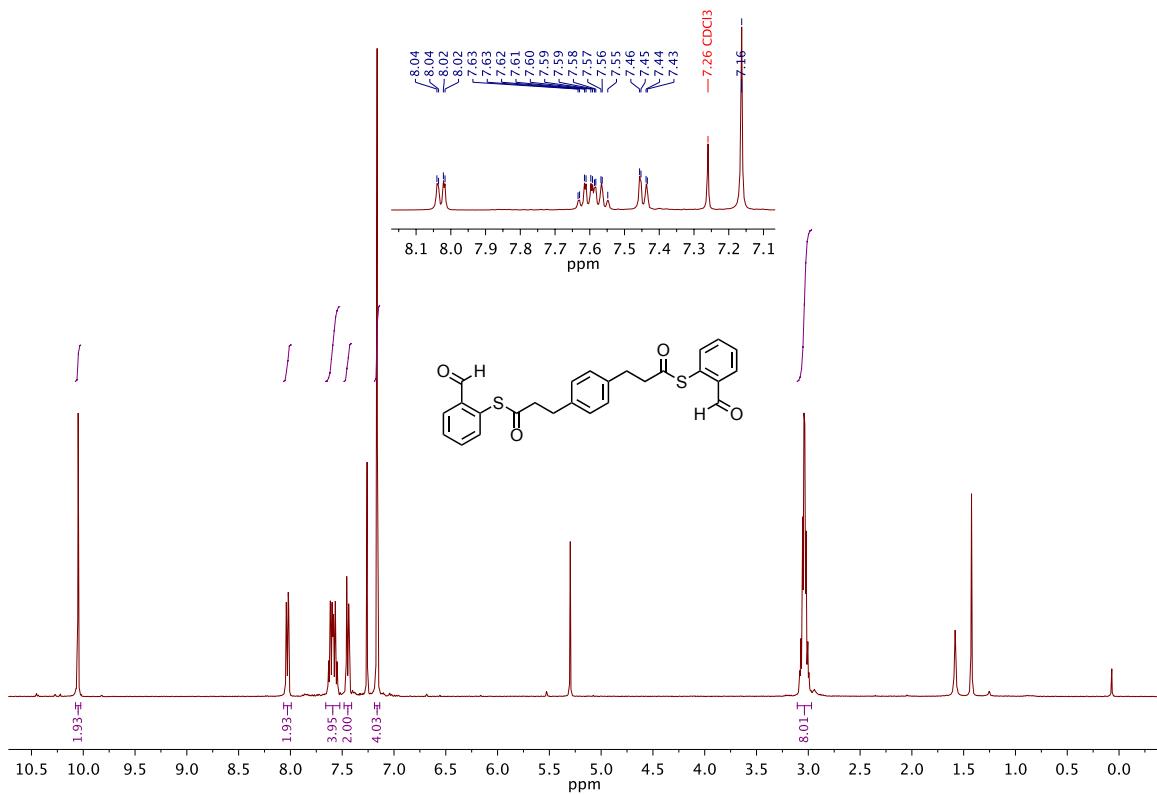
01/06/2016 8:13 am



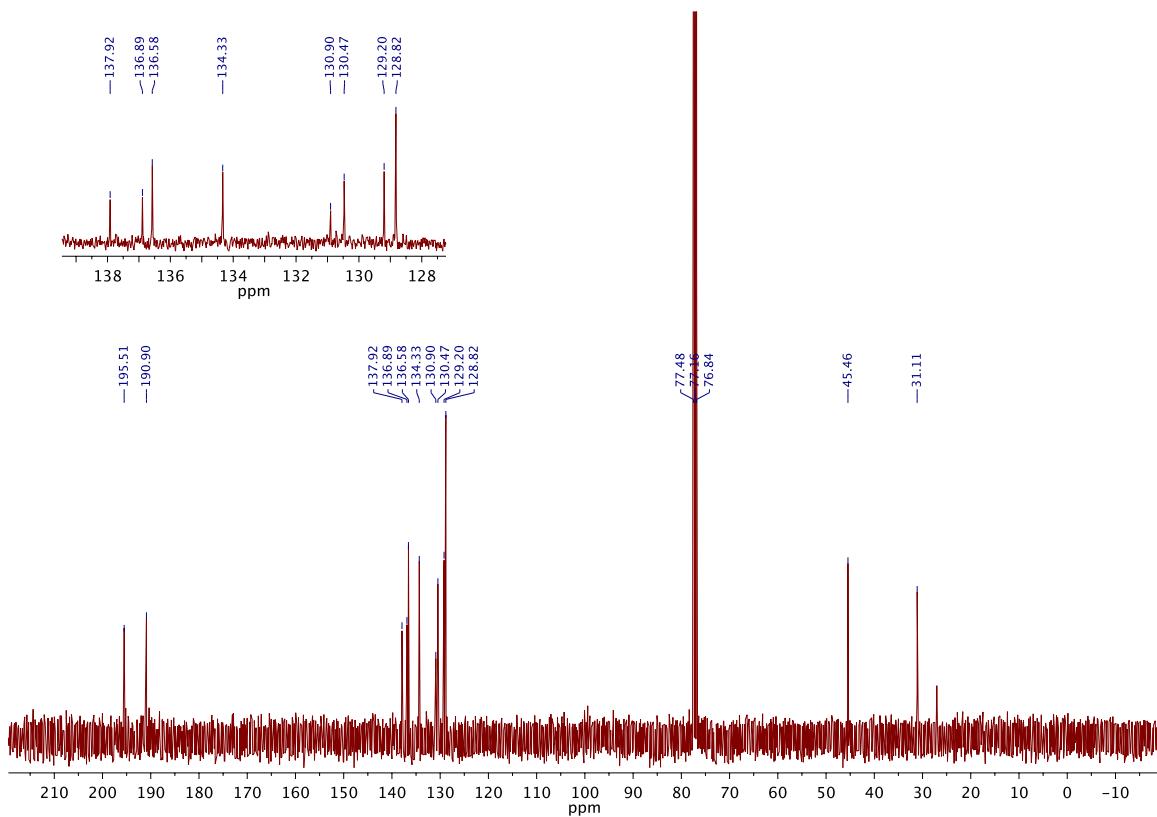
m/z	Formula	RDB	Delta ppm	Theo. Mass
429.02222	C ₂₂ H ₁₄ O ₄ ²³ Na ³² S ₂	15.5	-0.83	429.02257

4.5. S,S-Bis(2-formylphenyl)-3,3'-(1,4-phenylene)dipropanethioate 3e

¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):



ESI-HRMS:

Mass Spectrum SmartFormula Report

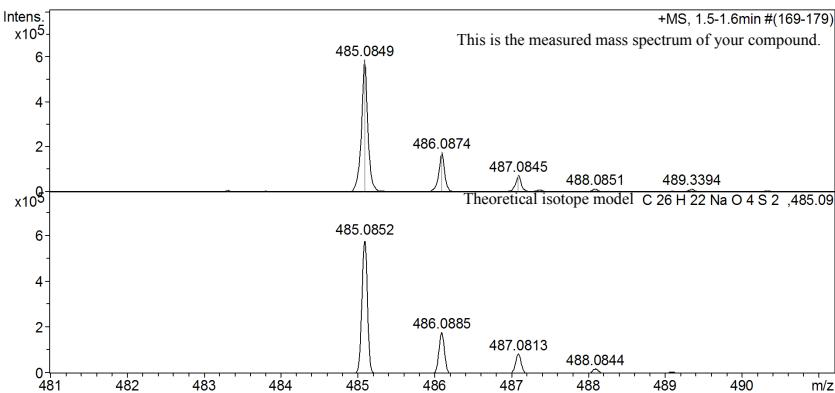
Analysis Info

Analysis Name Z:\Dec 13\ESI43715_17_01_14678.d
Method 2.5min_cal_sample_pos_naf_05-08-13.m
Sample Name ESI43715
Comment

Acquisition Date 02/12/2013 9:08 am
Operator Mass Spec
Instrument / Ser# micrOTOF 92

Acquisition Parameter

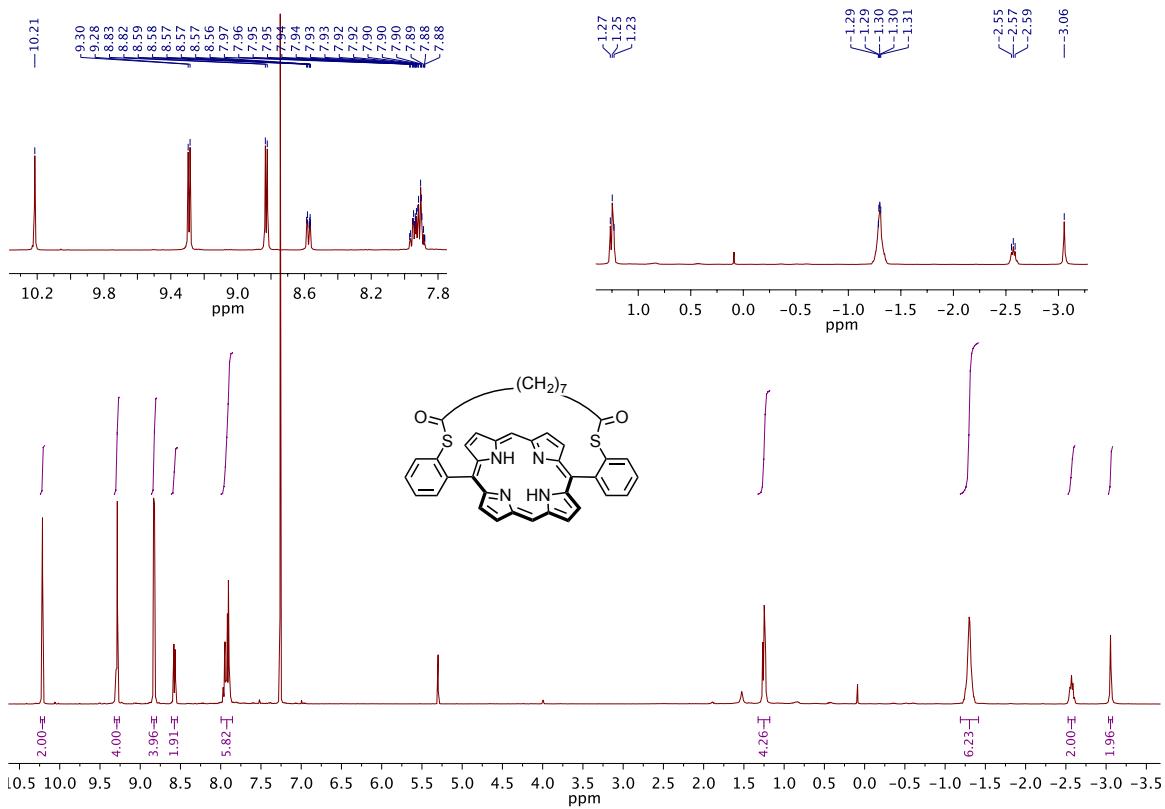
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



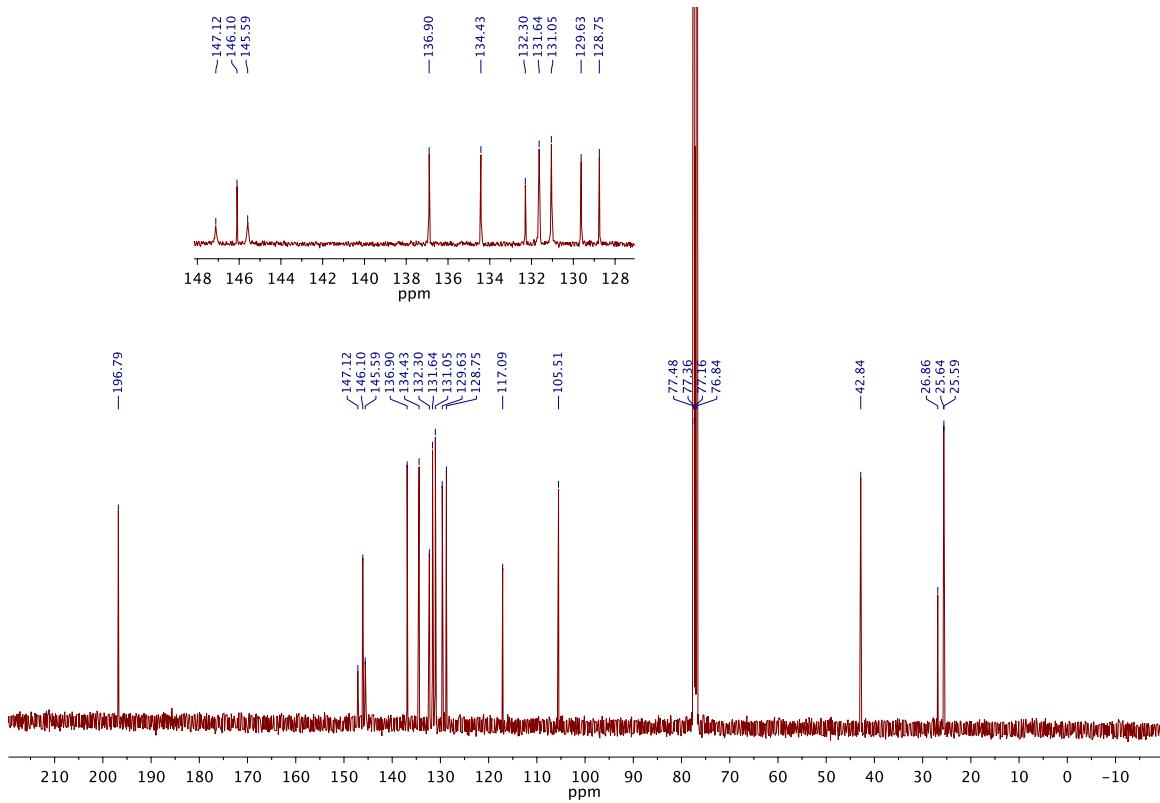
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	e ⁻	Conf	mSigma
485.0849	1	C ₂₆ H ₂₂ NaO ₄ S ₂	485.0852	0.6	0.3	15.5	even		9.40

4.6. C₇-Strapped free-base porphyrin 5a

¹H NMR (CDCl₃, 400 MHz, 298K):



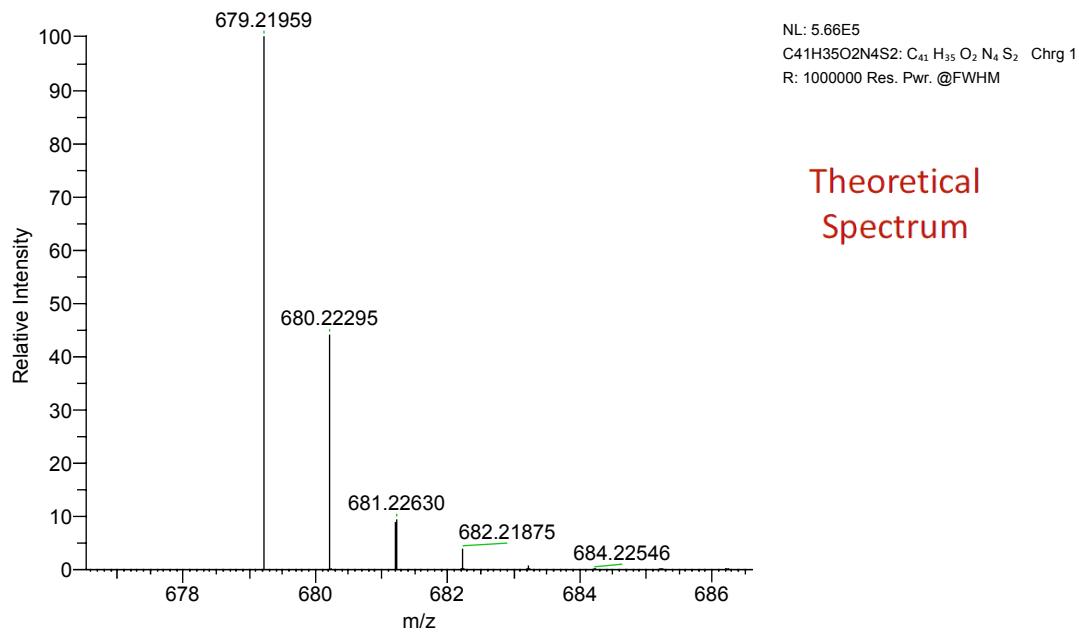
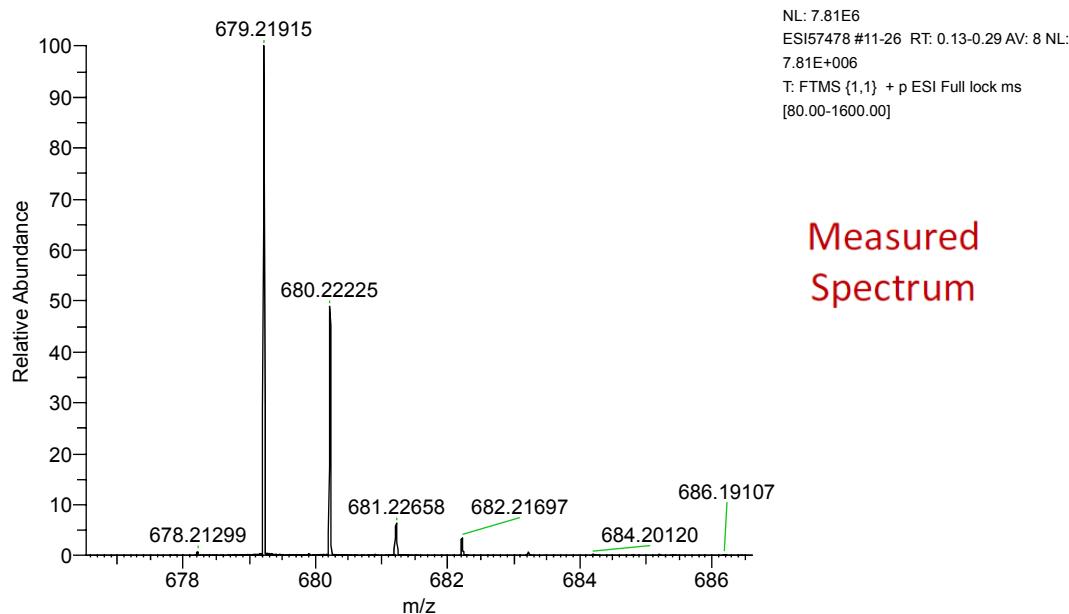
¹³C NMR (CDCl₃, 100 MHz, 298K):



ESI-HRMS:

W:\data\June 16\ESI57478.raw

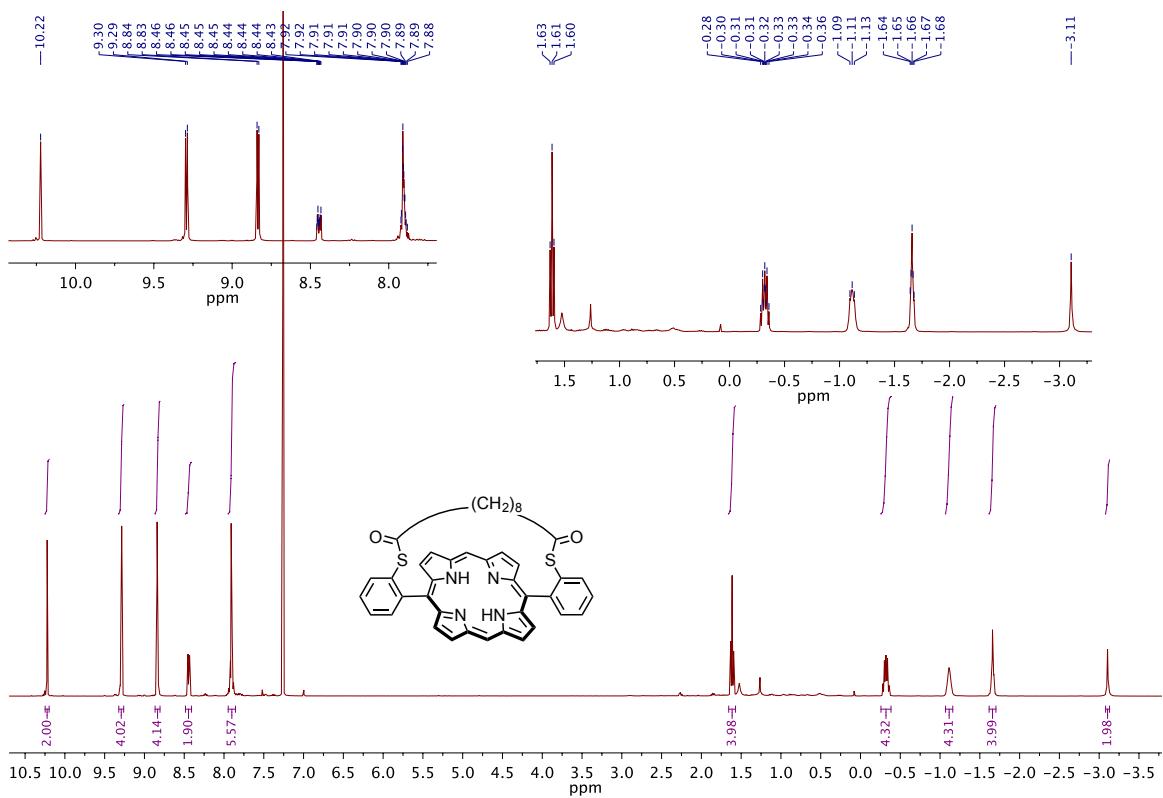
01/06/2016 8:17 am



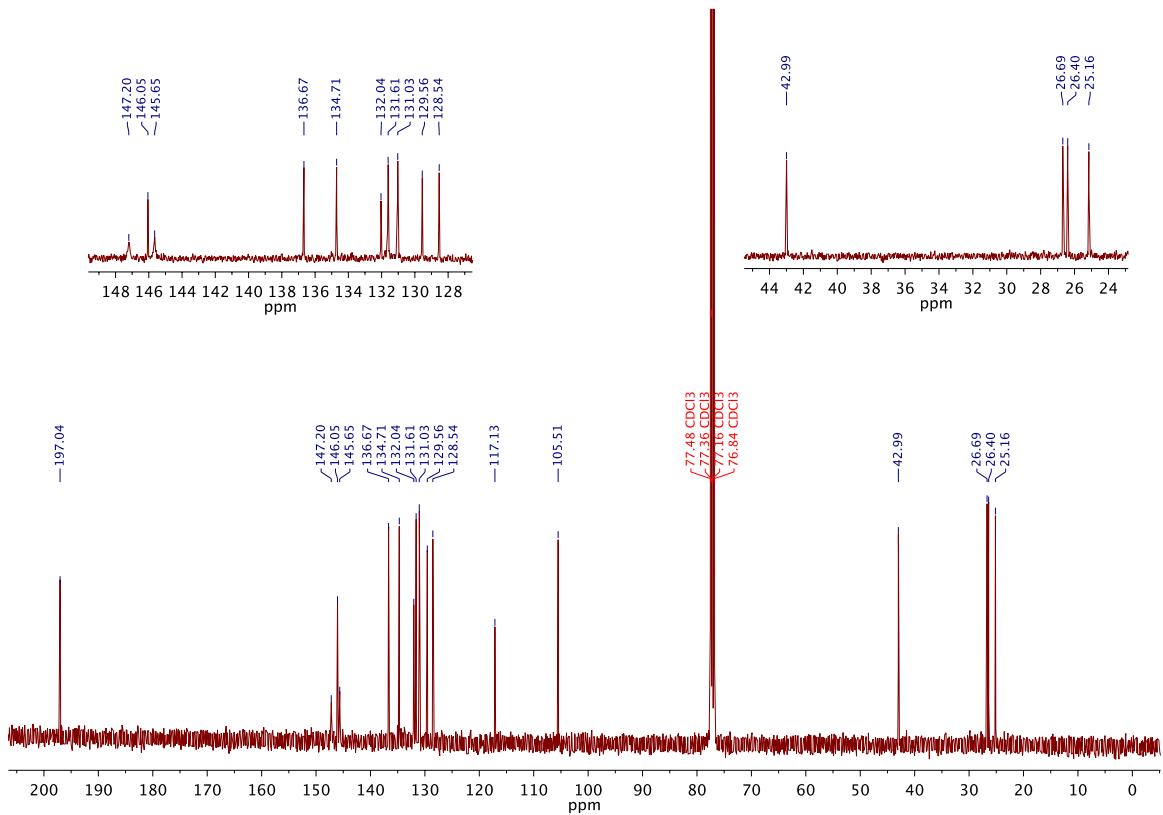
m/z	Formula	RDB	Delta ppm	Theo. Mass
679.21918	C ₄₁ H ₃₅ O ₂ N ₄ ³² S ₂	26.5	-0.61	679.21959

4.7. C₈-Strapped free-base porphyrin 5b

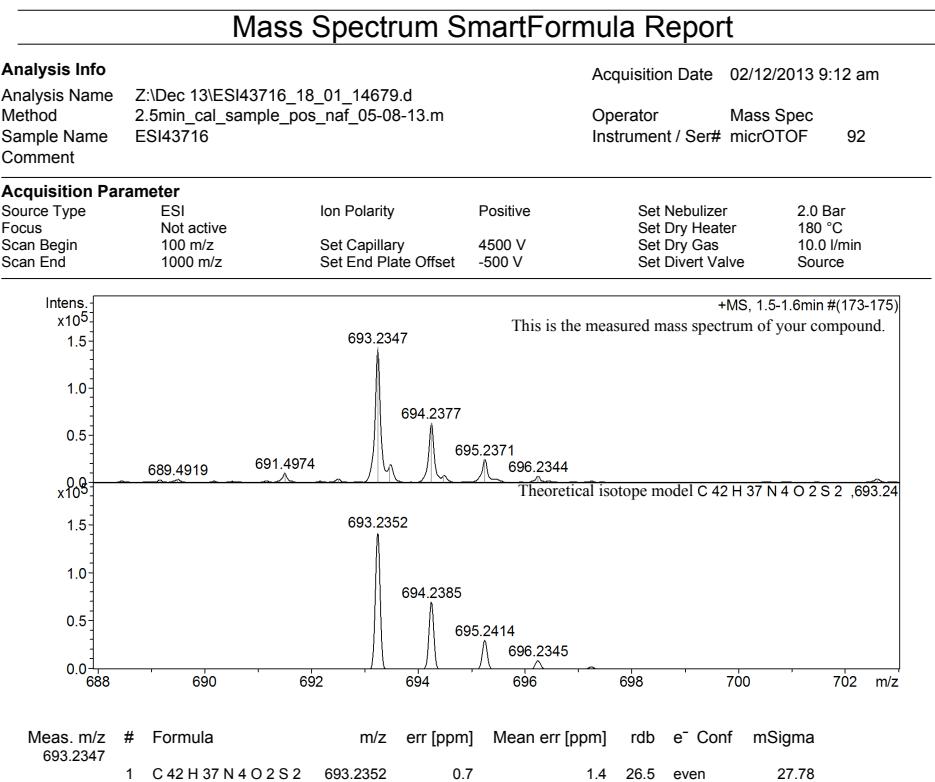
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

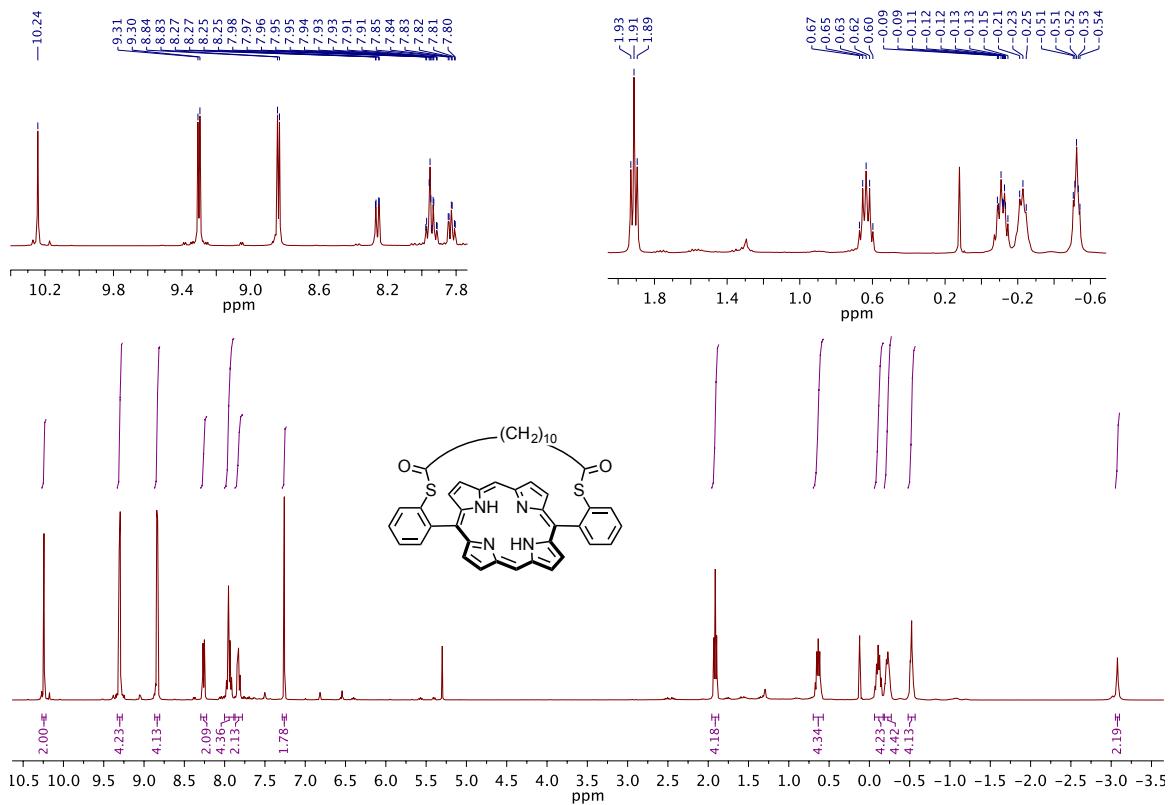


ESI-HRMS:

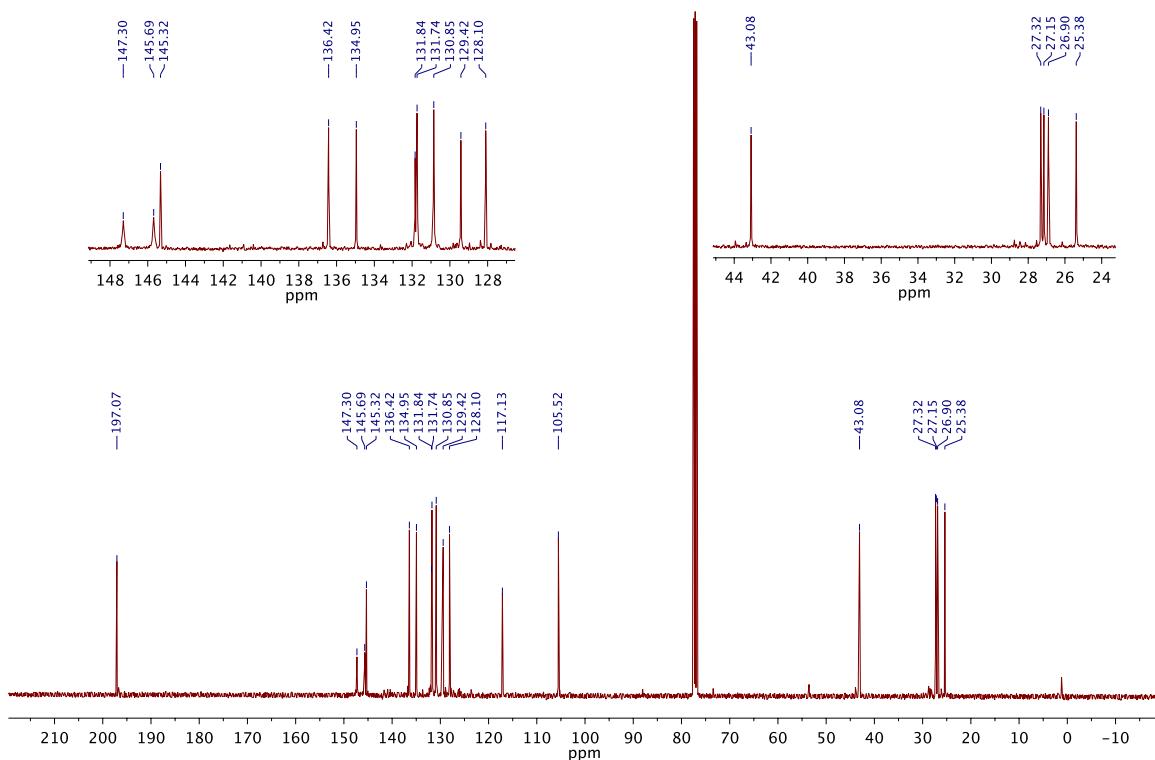


4.8. C₁₀-Strapped free-base porphyrin 5c

¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):



ESI-HRMS:

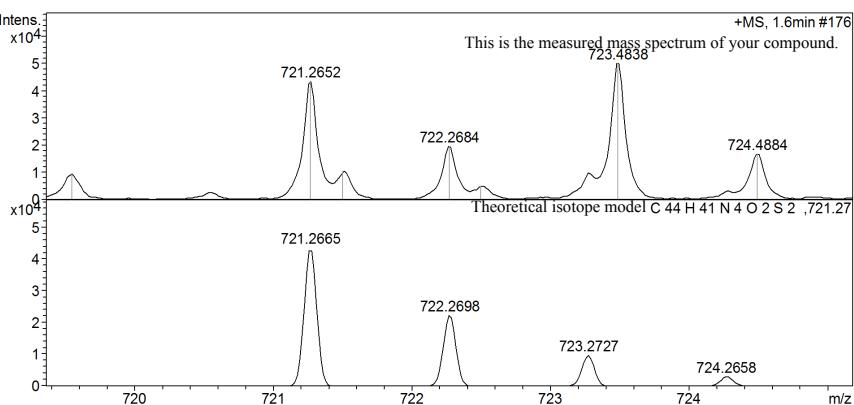
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	Z:\Dec 13\ESI43717_19_01_14680.d	Acquisition Date	02/12/2013 9:16 am
Method	2.5min_cal_sample_pos_naf_05-08-13.m	Operator	Mass Spec
Sample Name	ESI43717	Instrument / Ser#	micrOTOF 92
Comment			

Acquisition Parameter

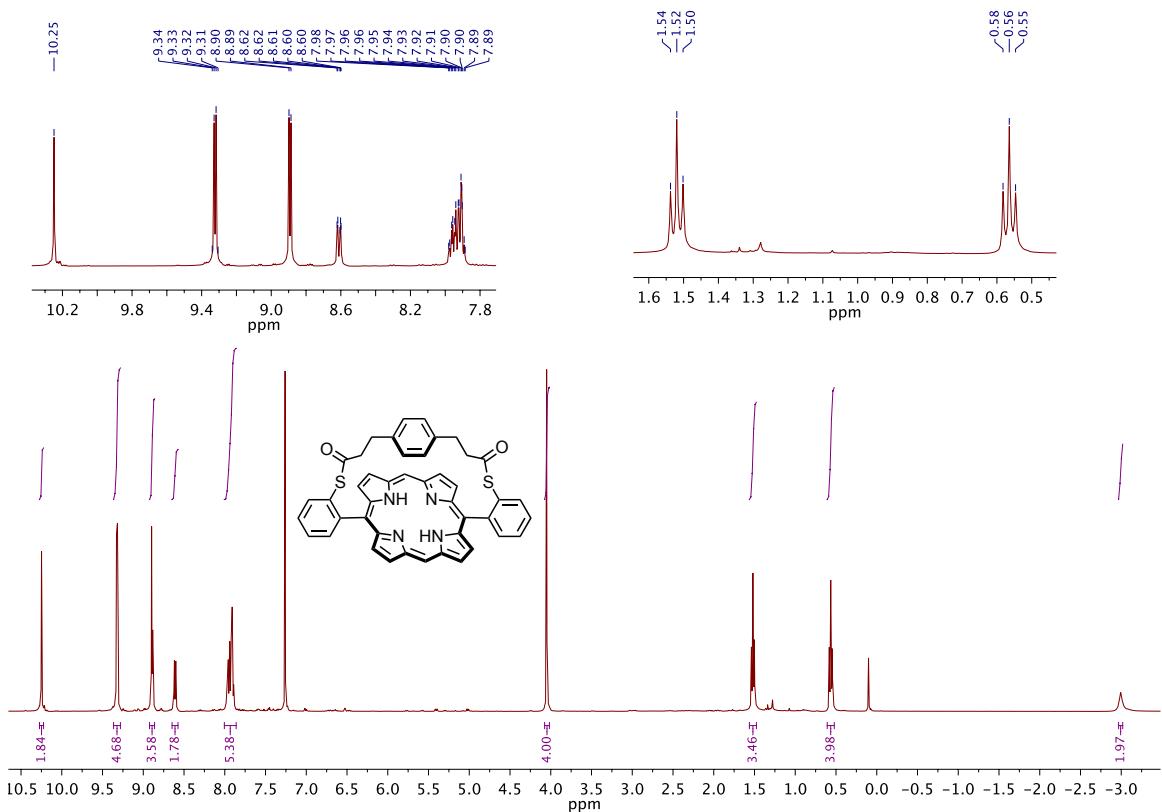
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



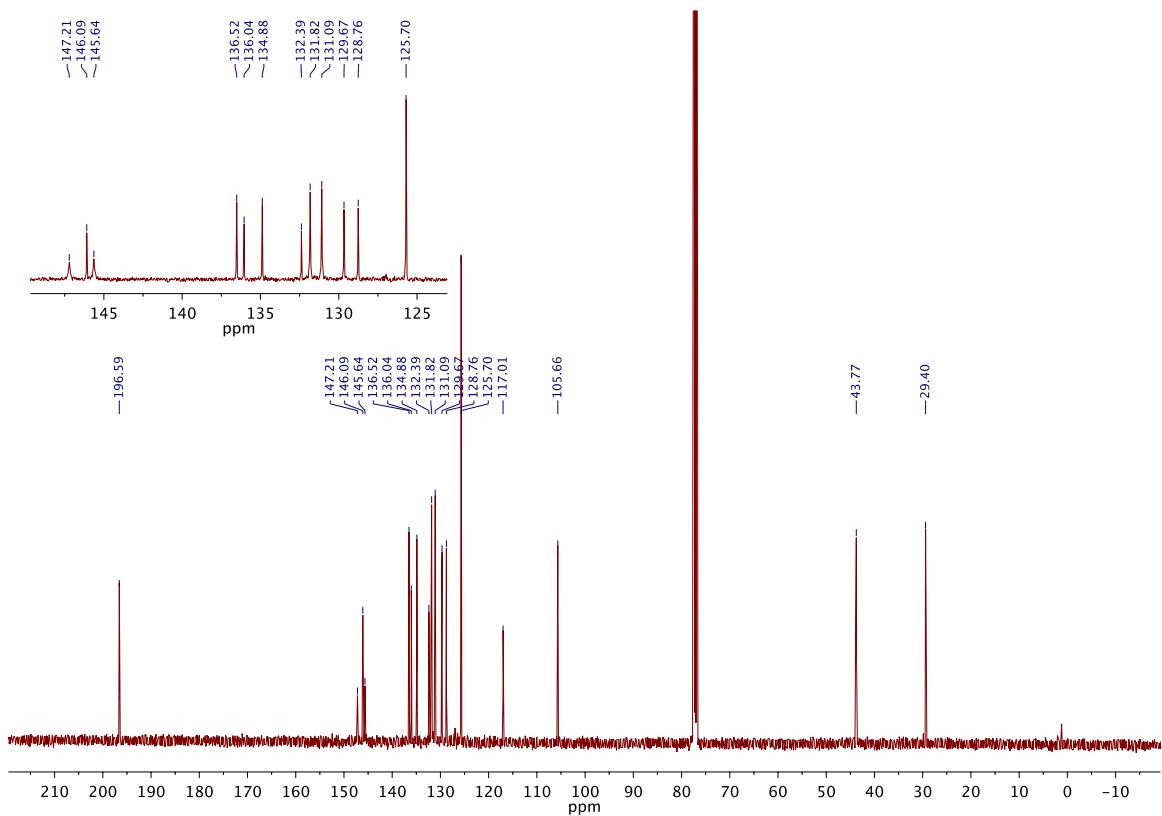
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	e ⁻	Conf	mSigma
721.2652	1	C ₄₄ H ₄₁ N ₄ O ₂ S ₂	721.2665	1.9	1.9	26.5	even		107.79

4.9. 1,4-Diethylbenzene-strapped free-base porphyrin 5e

^1H NMR (CDCl_3 , 400 MHz, 298K):



^{13}C NMR (CDCl_3 , 100 MHz, 298K):



ESI-HRMS:

Mass Spectrum SmartFormula Report

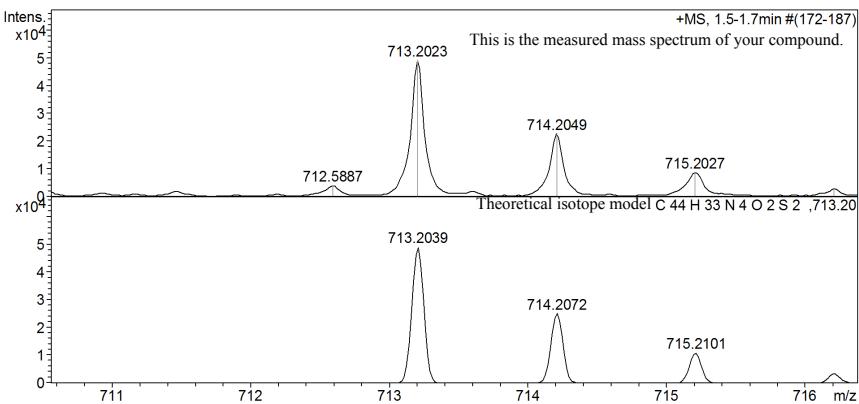
Analysis Info

Analysis Name Z:\Dec 13\ESI43718_20_01_14681.d
Method 2.5min_cal_sample_pos_naf_05-08-13.m
Sample Name ESI43718
Comment

Acquisition Date 02/12/2013 9:19 am
Operator Mass Spec
Instrument / Ser# micrOTOF 92

Acquisition Parameter

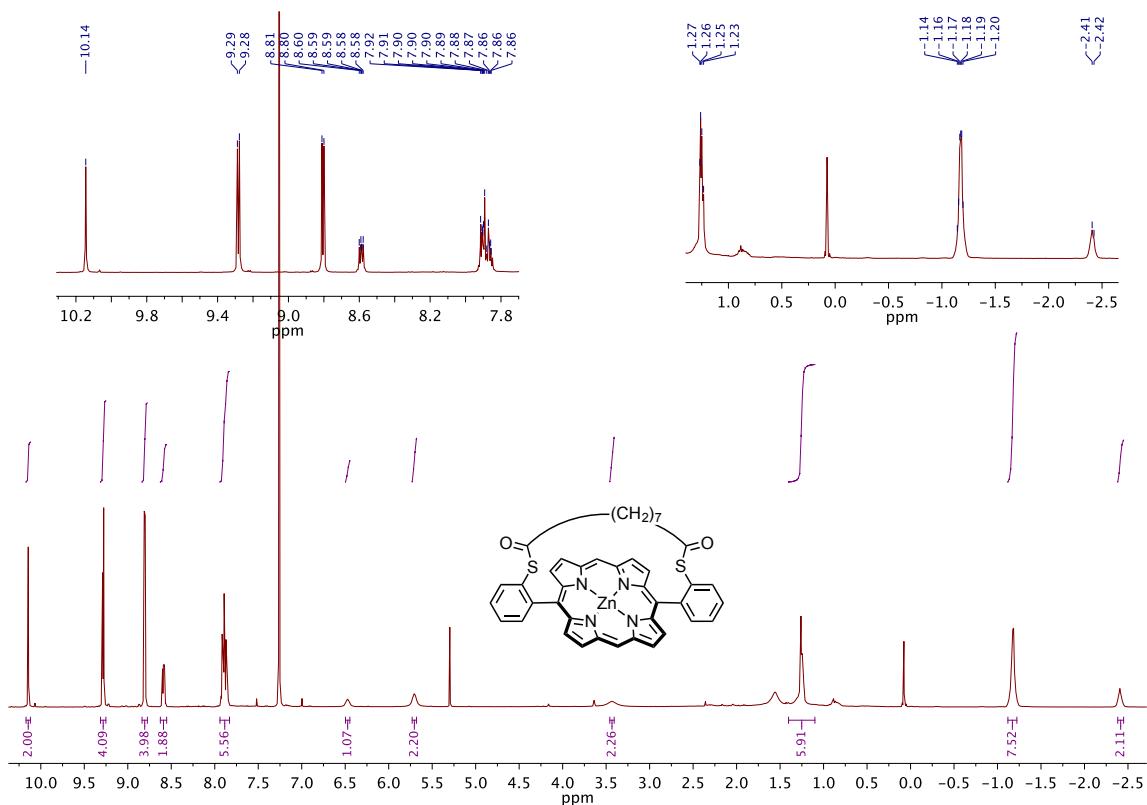
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



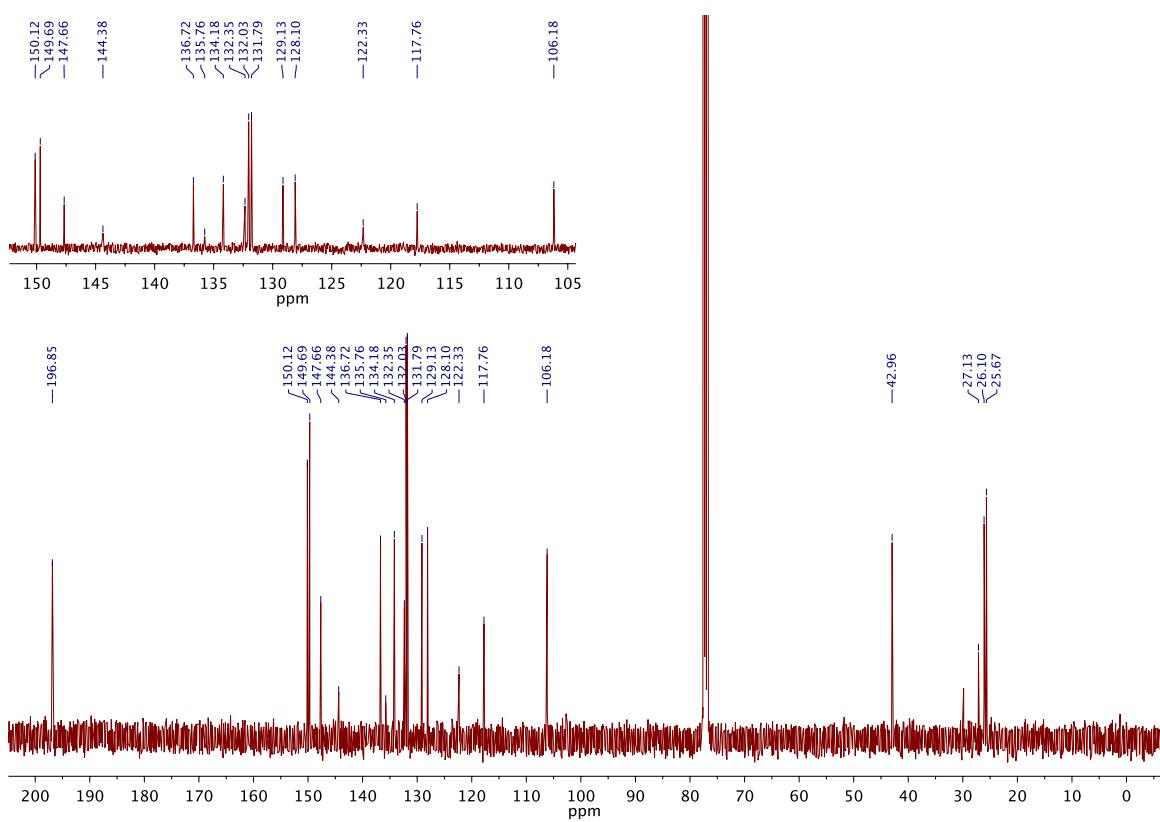
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	e ⁻	Conf	mSigma
713.2023	1	C44H33N4O2S2	713.2039	2.3	3.4	30.5	even		28.77

4.10. C₇-Strapped zinc(II) porphyrin 6a

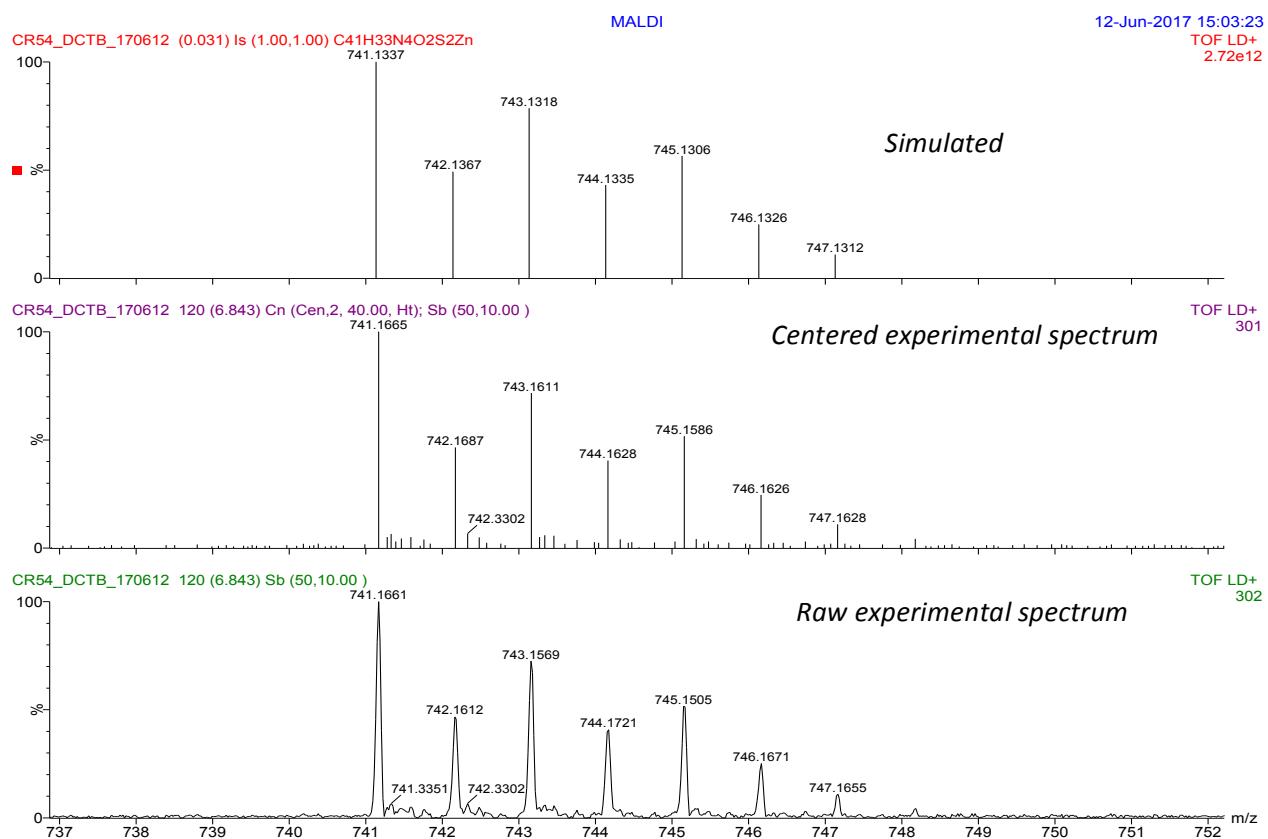
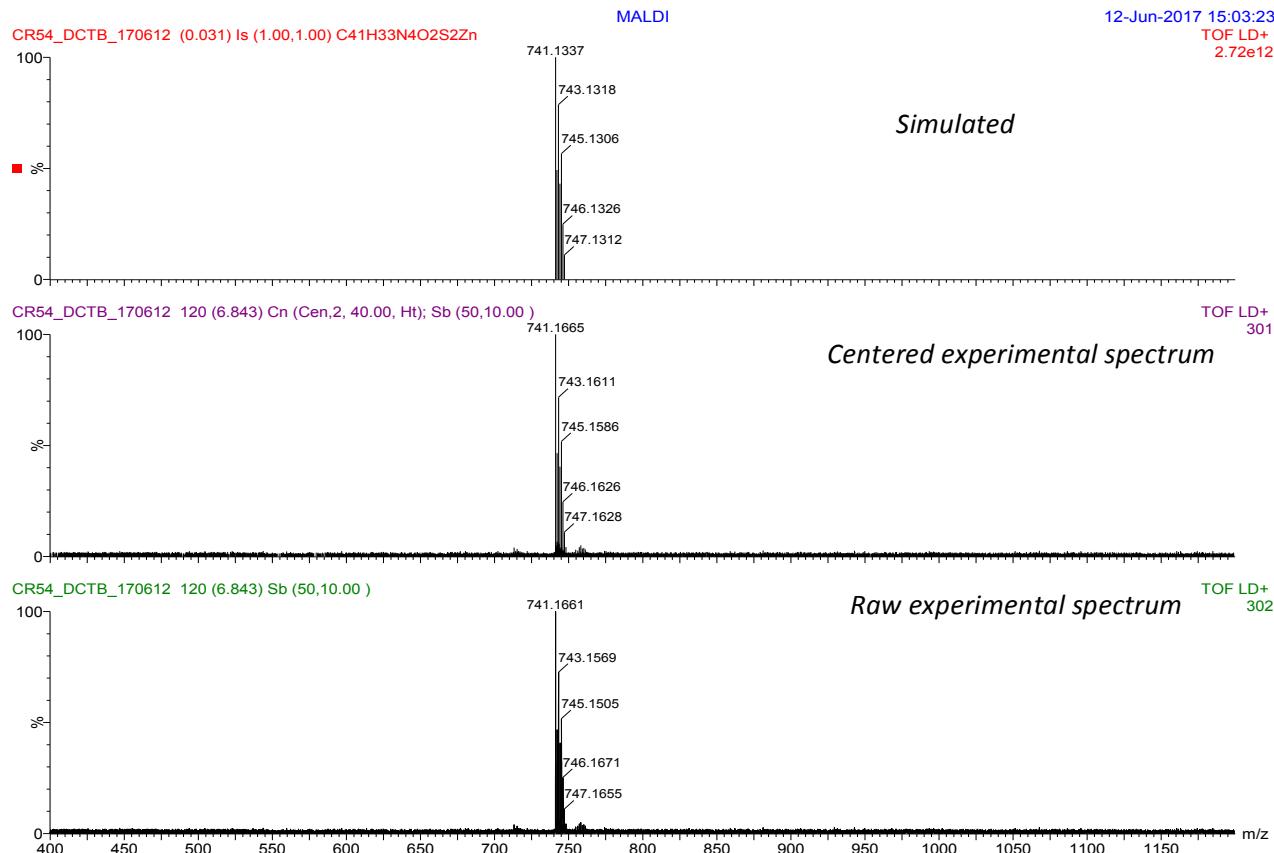
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

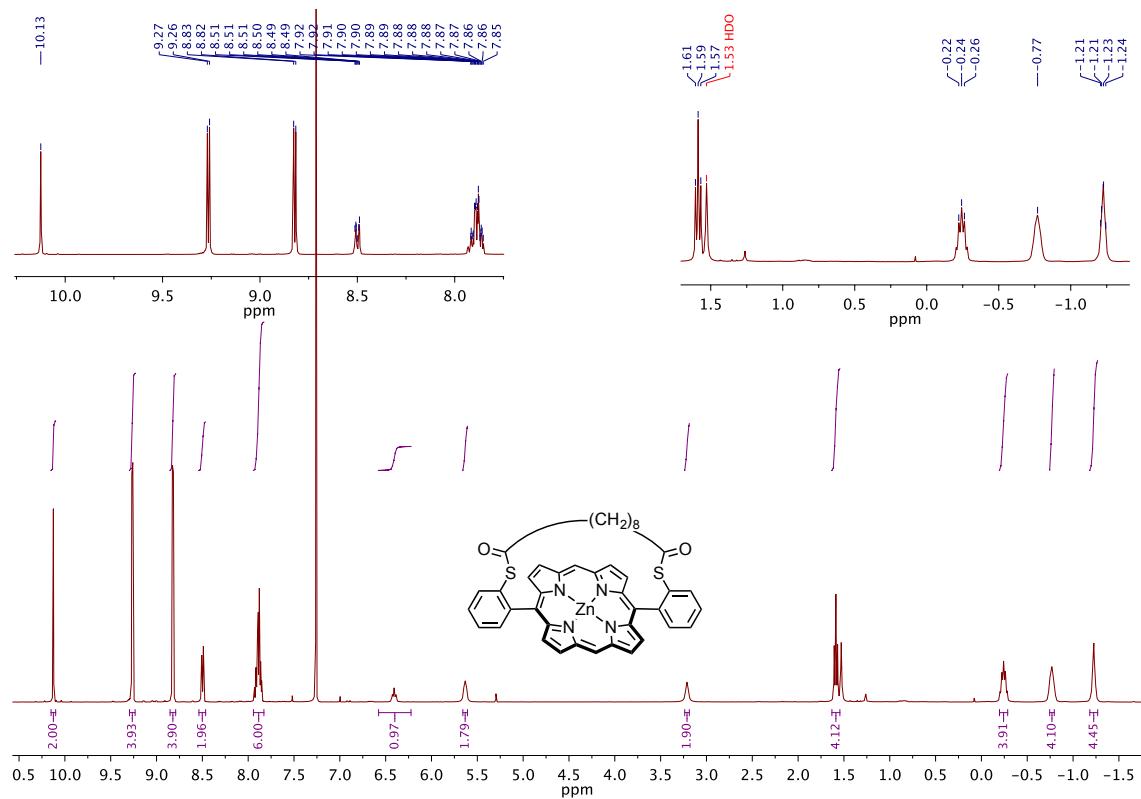


MALDI-TOF:

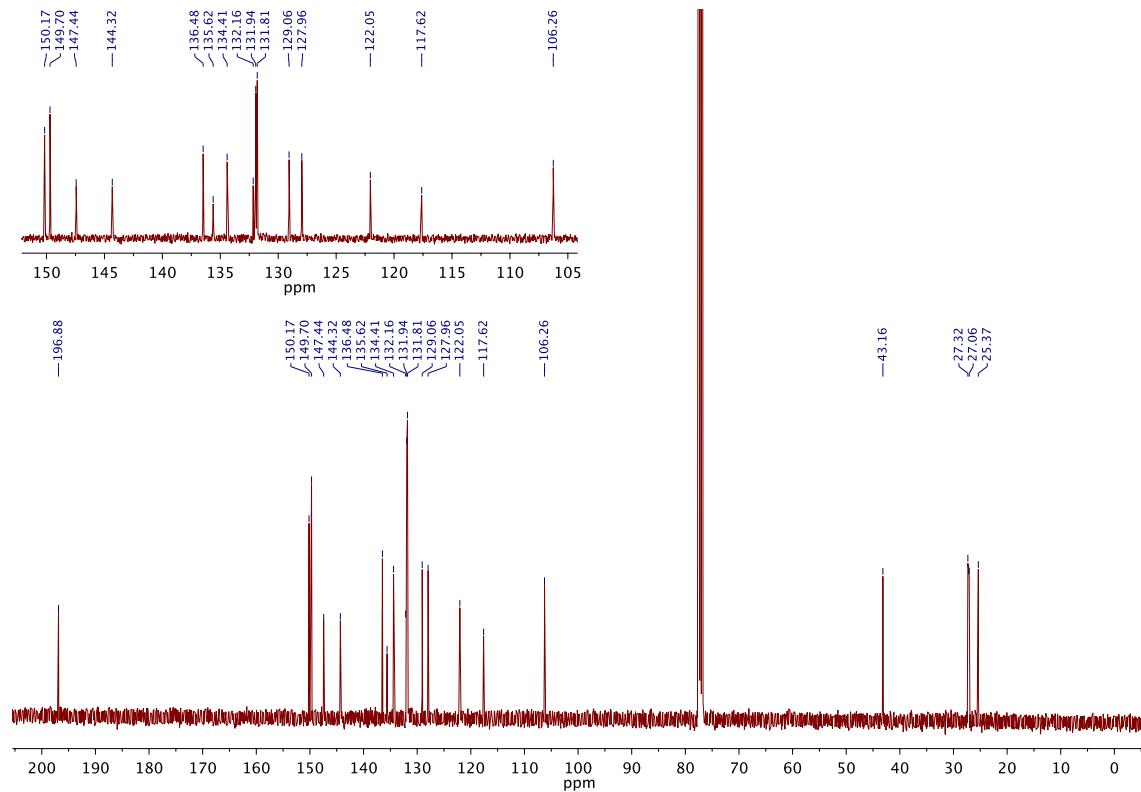


4.11. C₈-Strapped zinc(II) porphyrin 6b

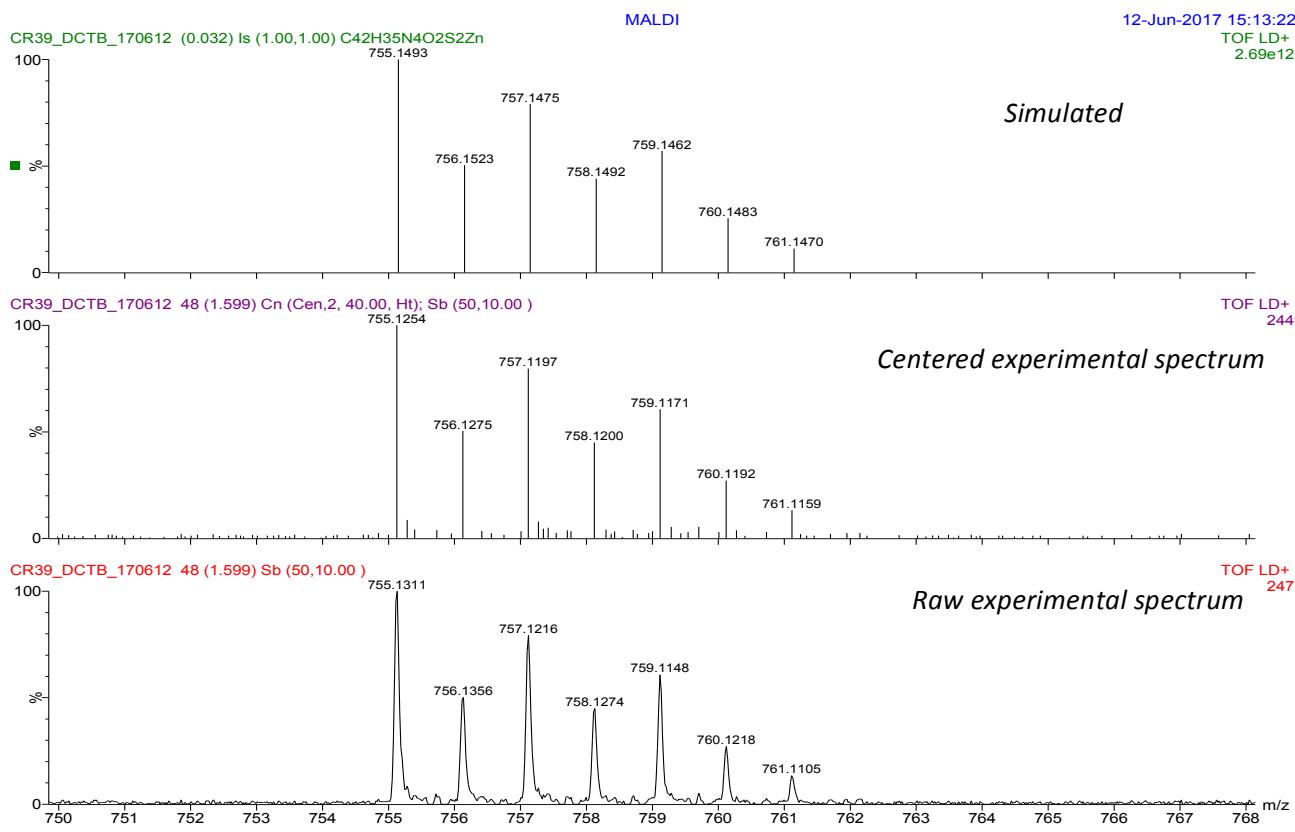
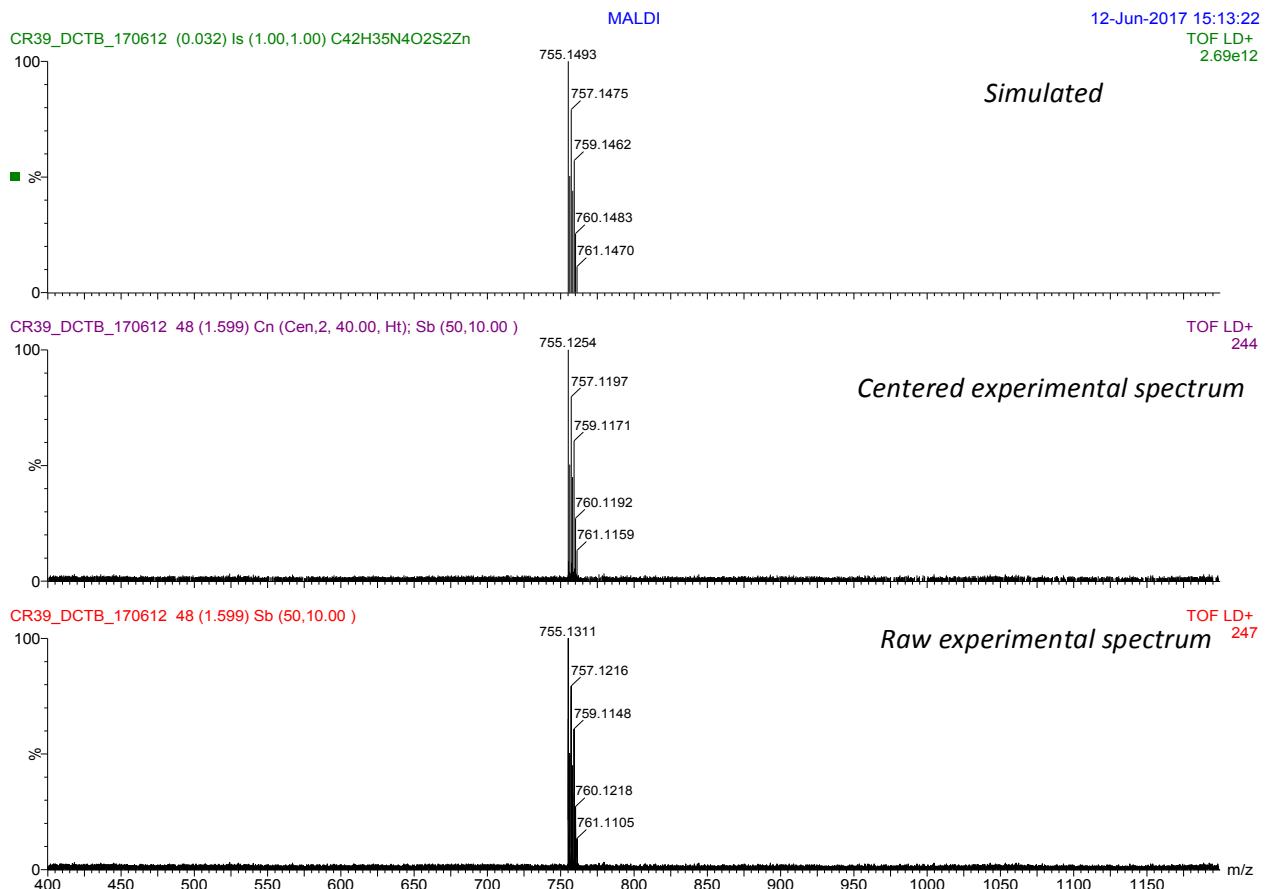
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

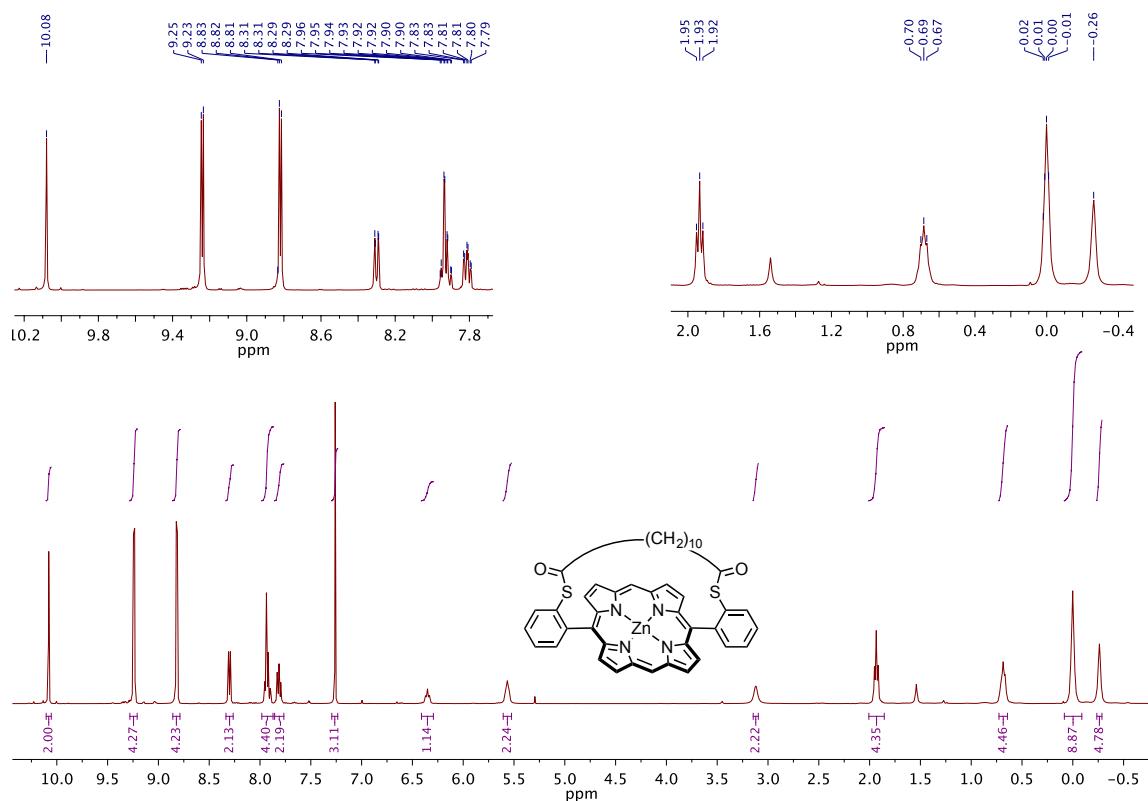


MALDI-TOF:

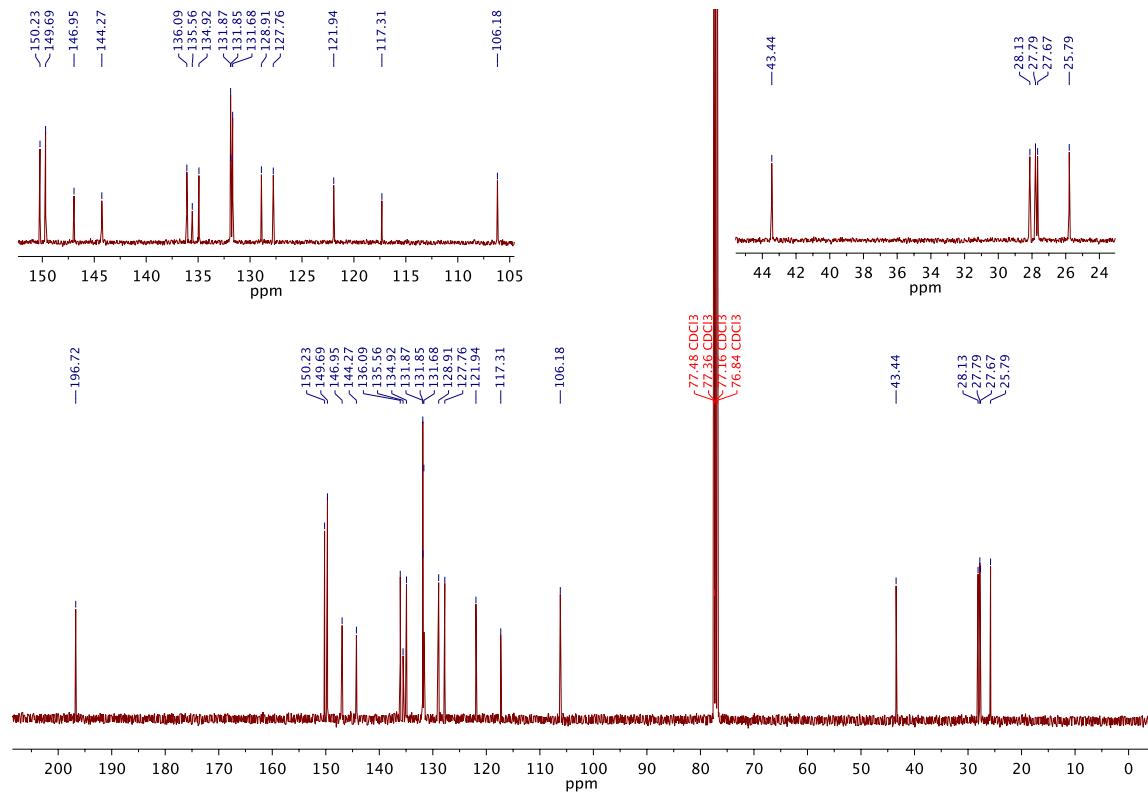


4.12. C₁₀-Strapped zinc(II) porphyrin 6c

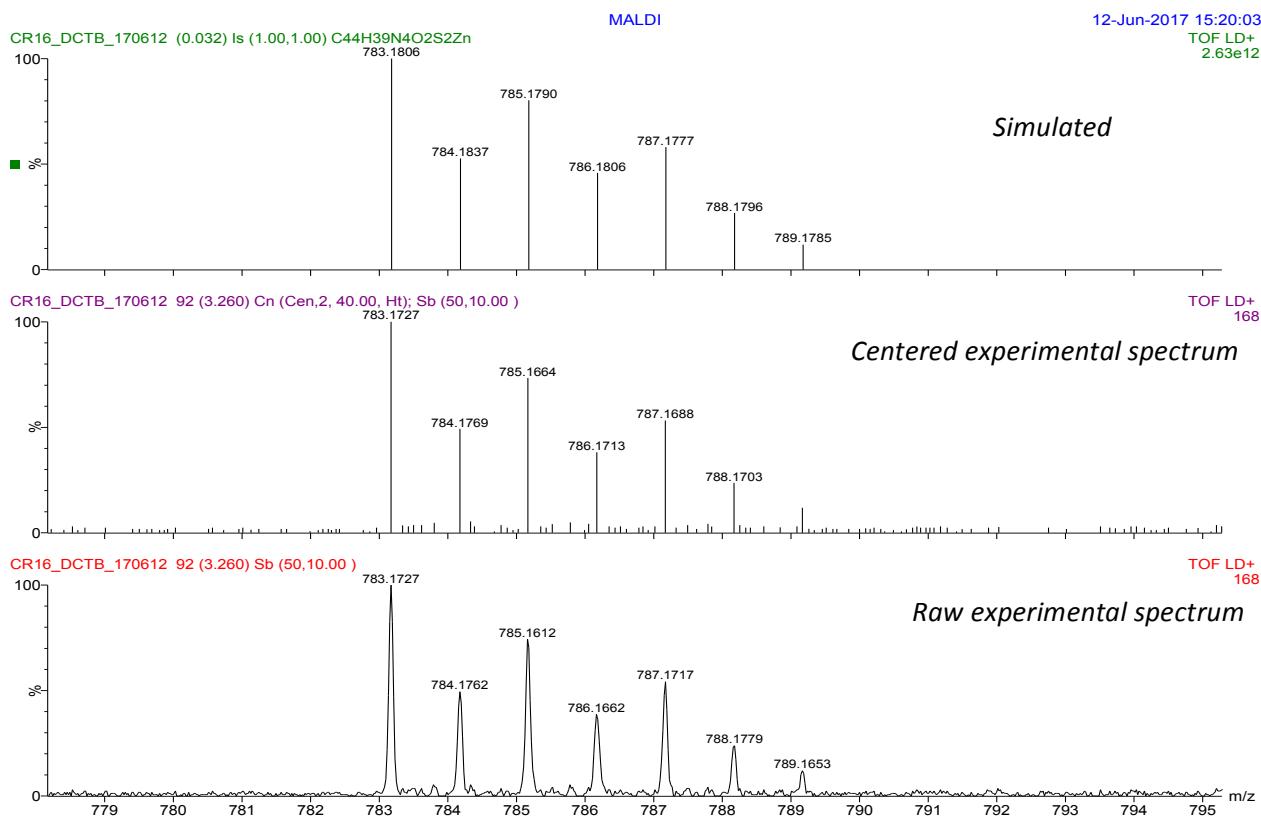
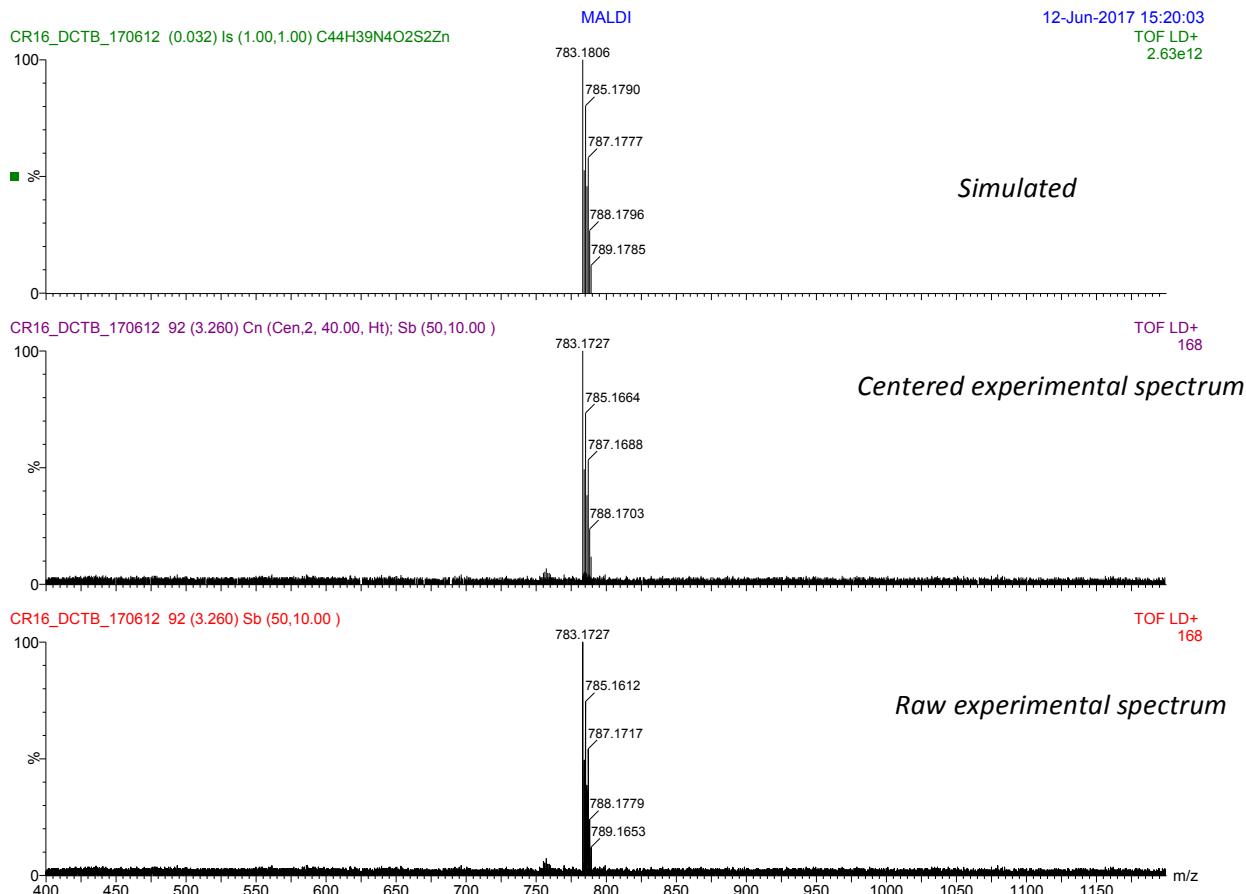
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

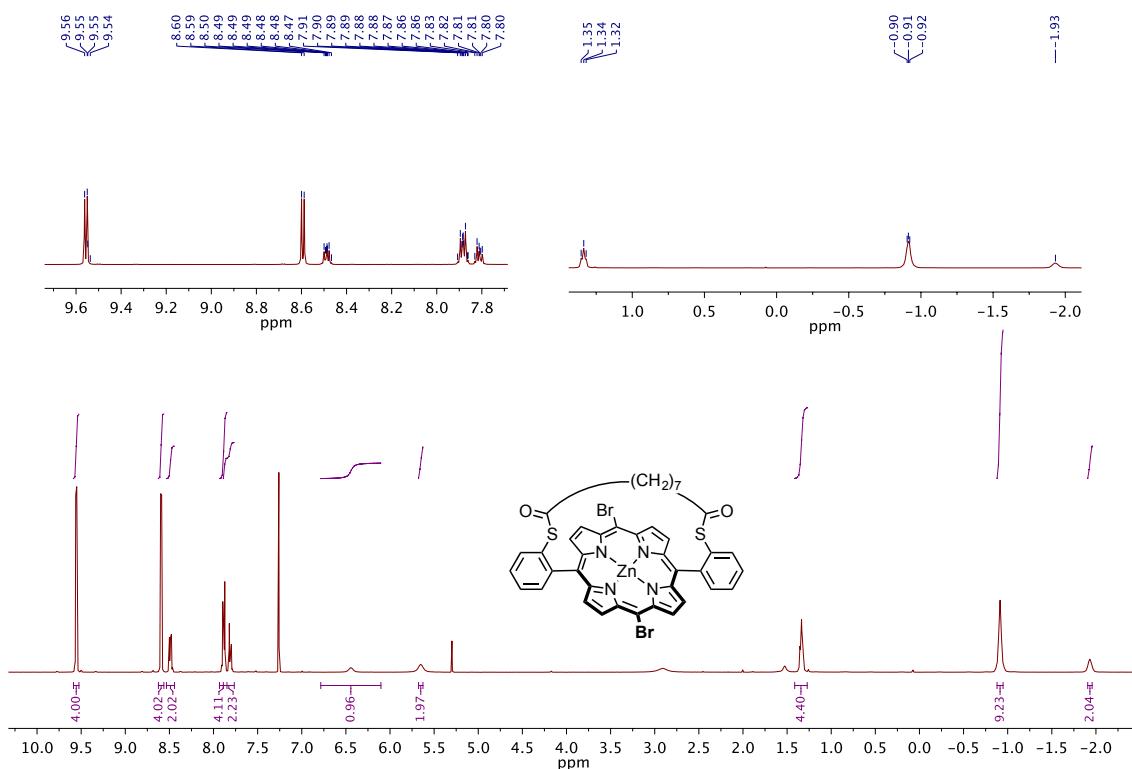


MALDI-TOF:

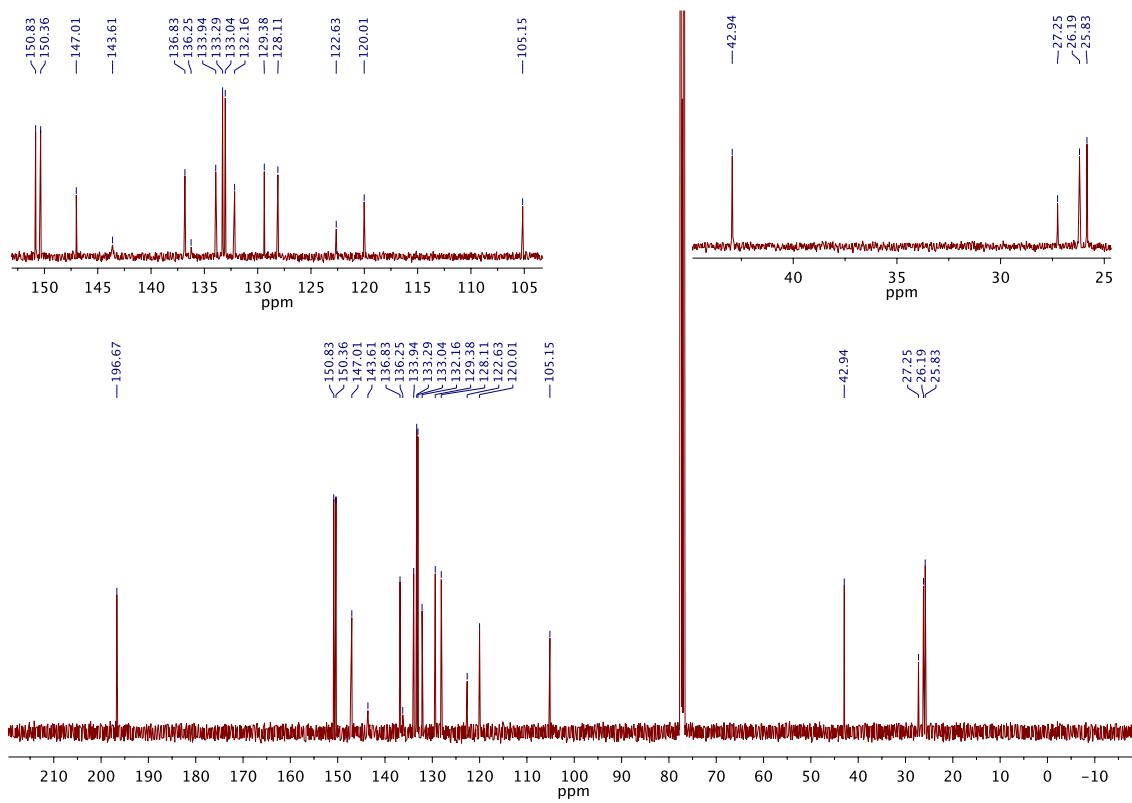


4.13. C₇-Strapped dibromoporphyrin 7a

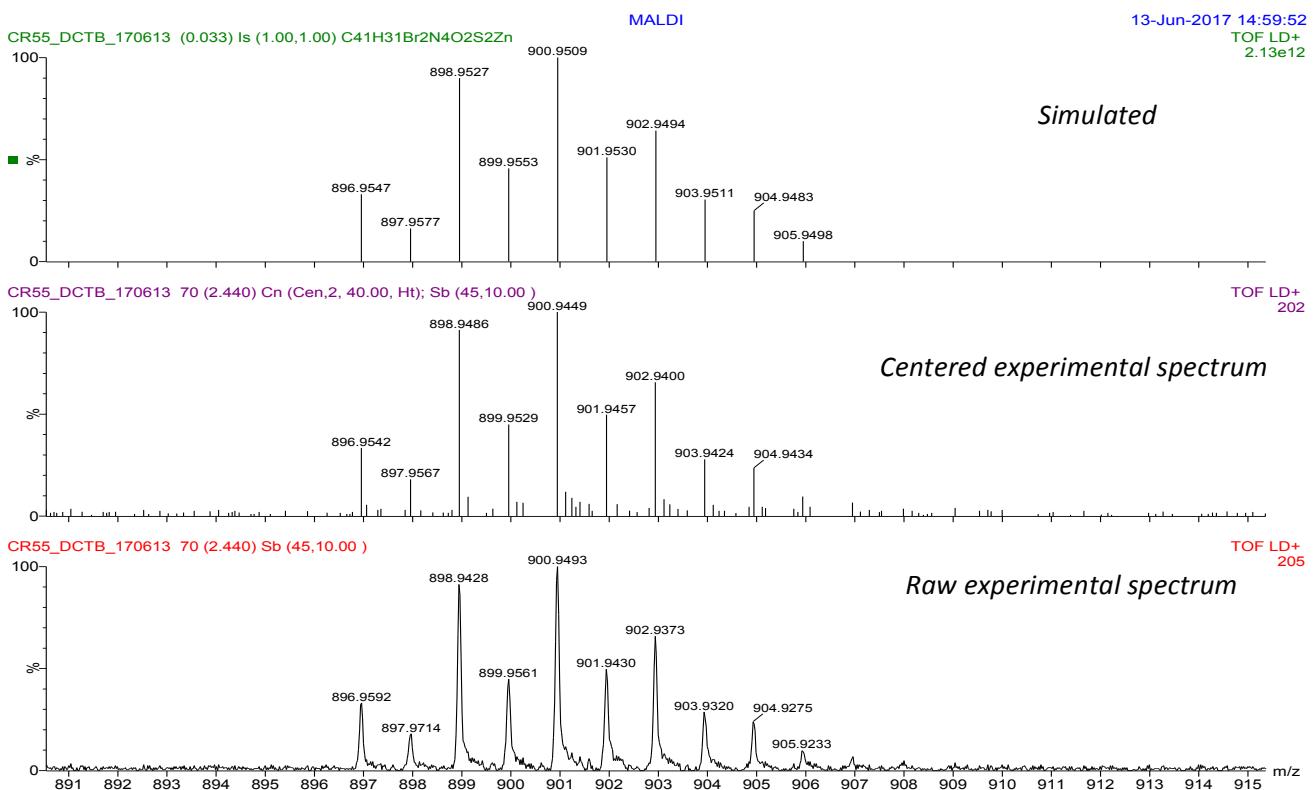
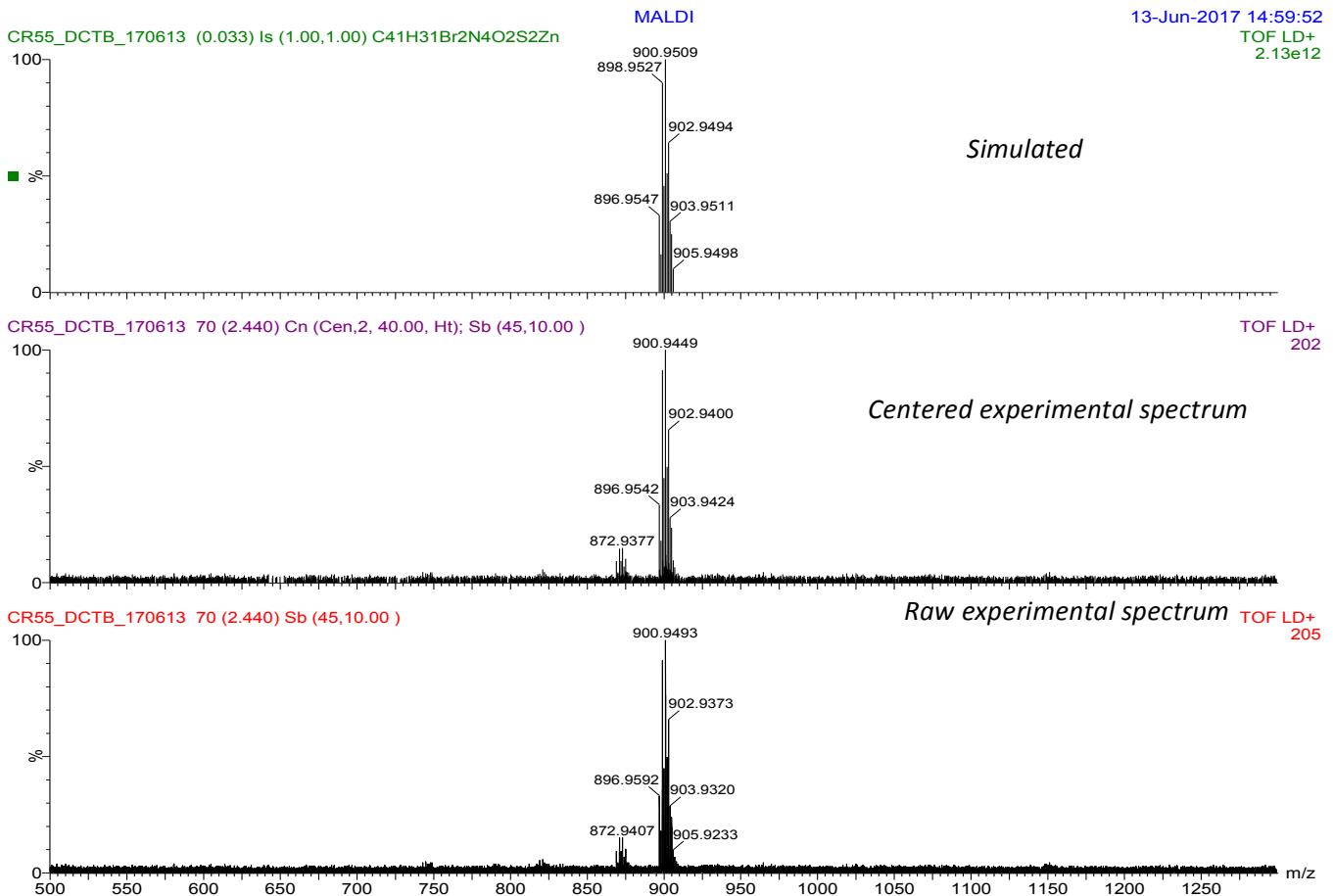
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

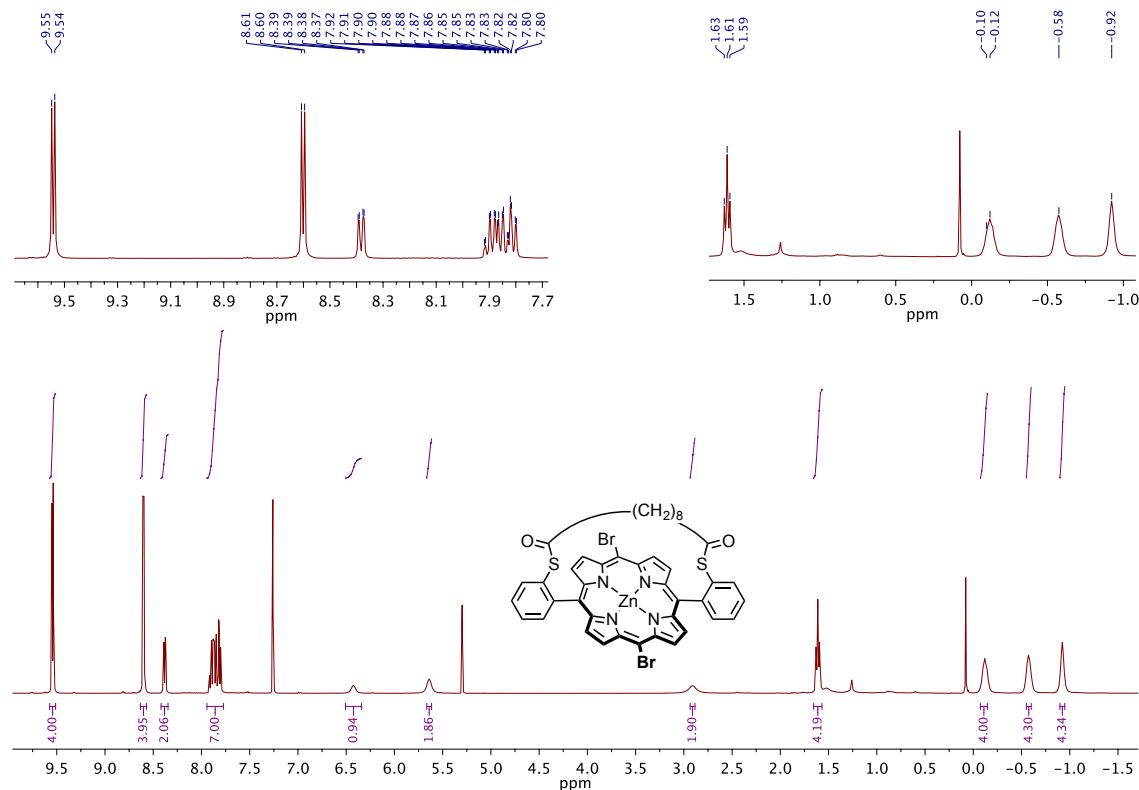


MALDI-TOF:

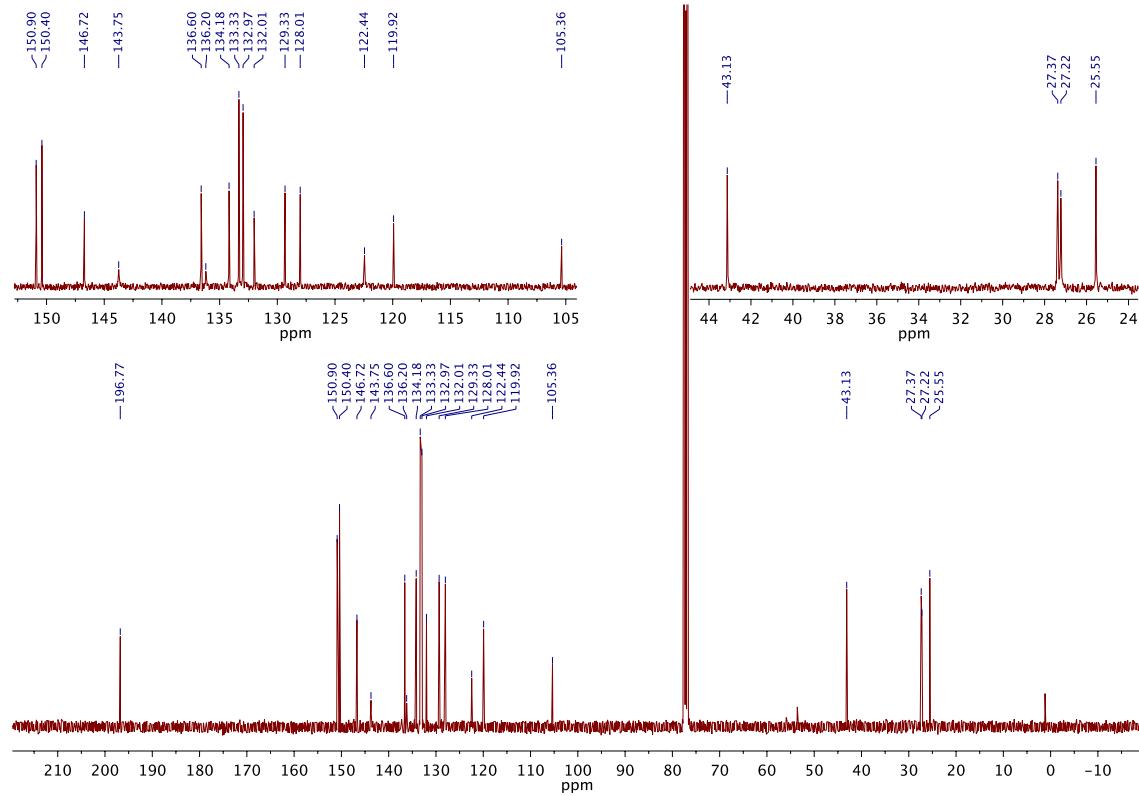


4.14. C₈-Strapped dibromoporphyrin 7b

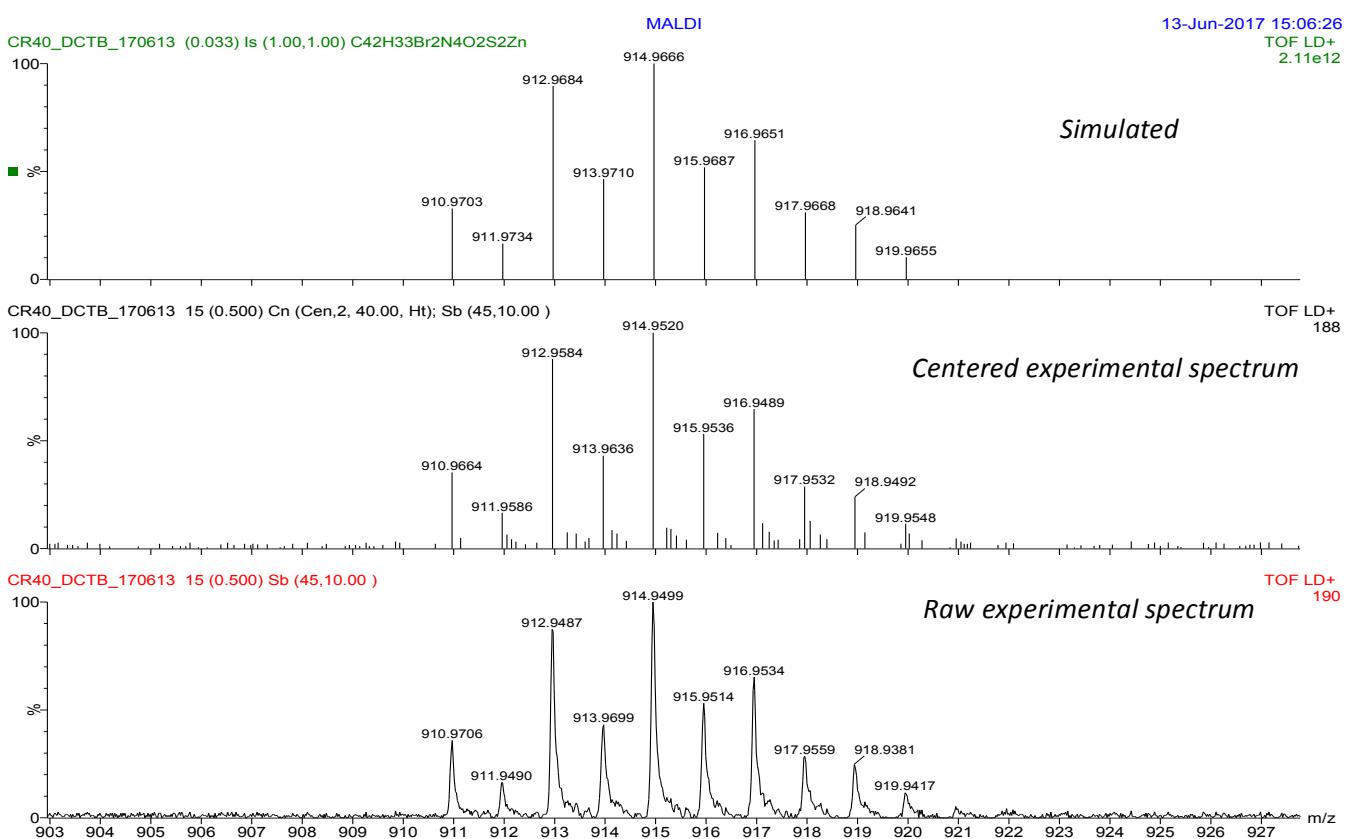
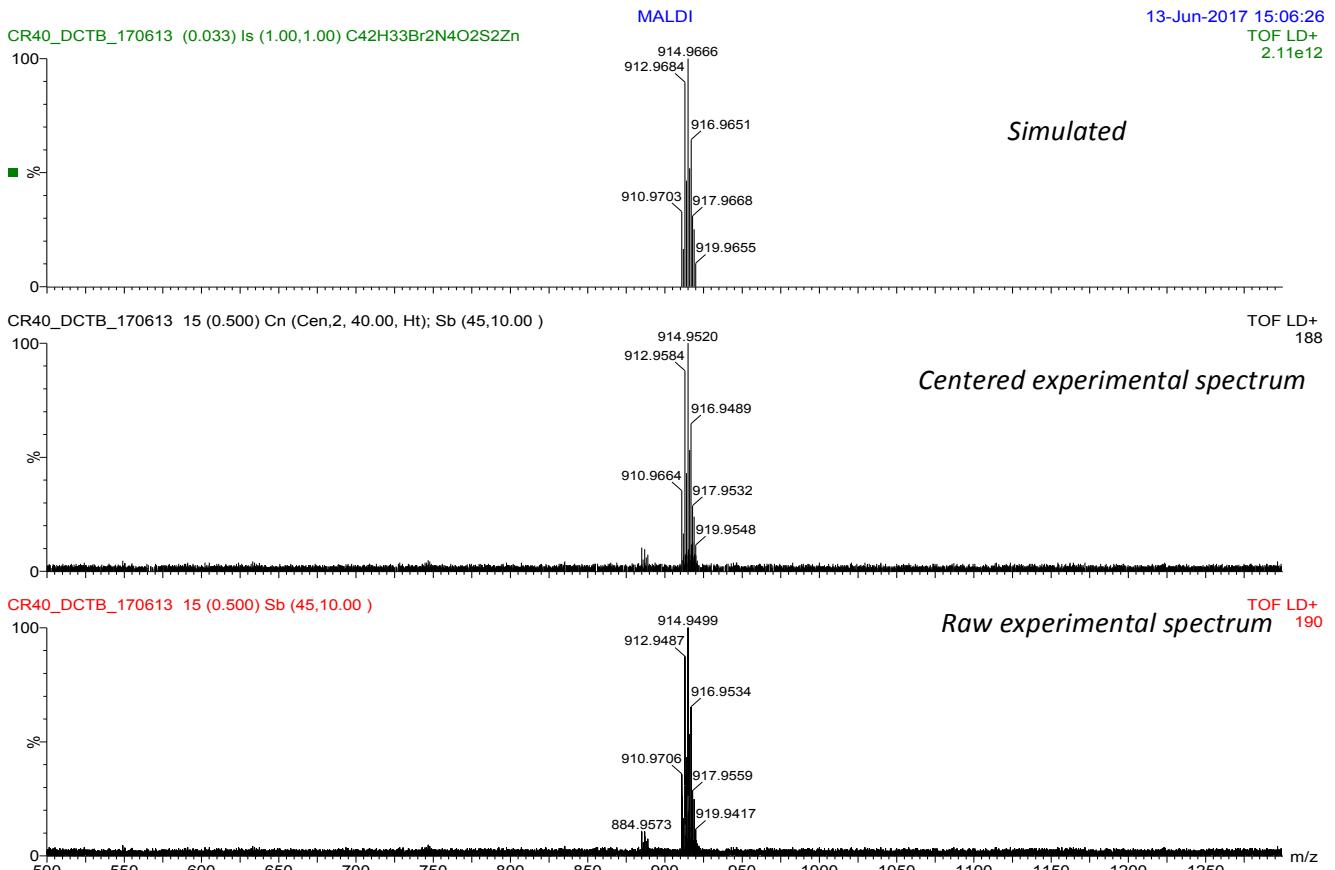
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

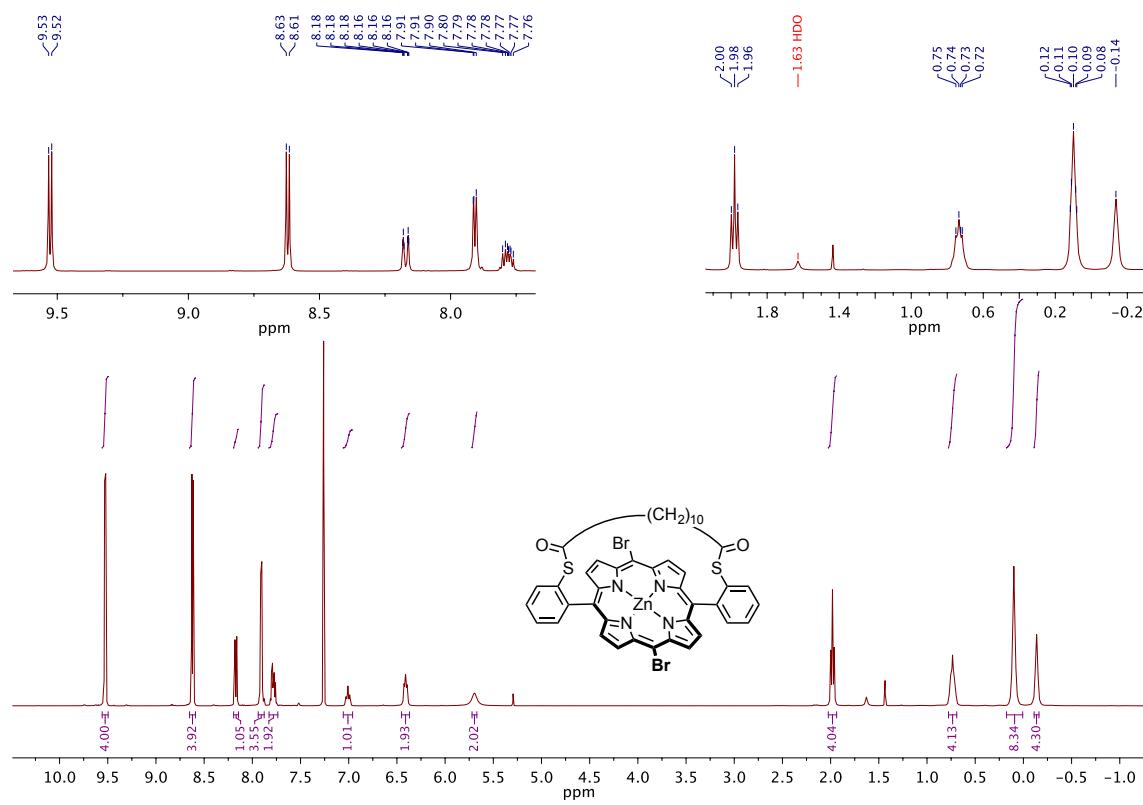


MALDI-TOF:

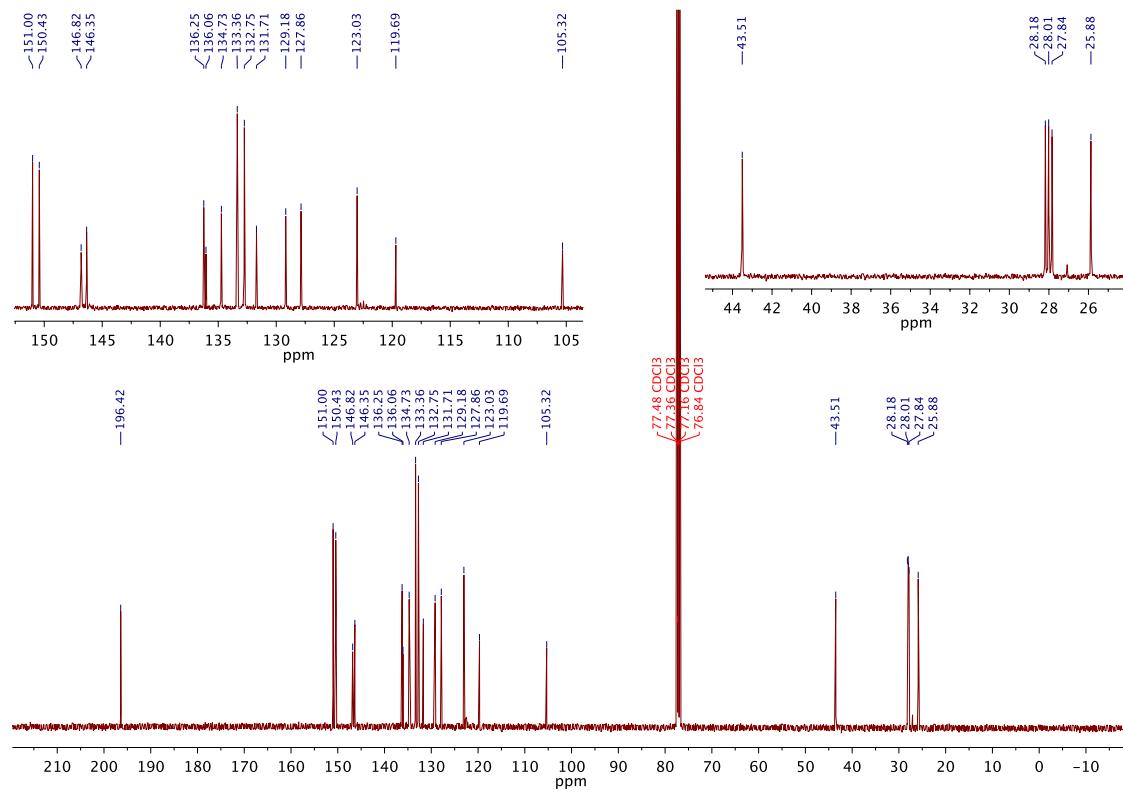


4.15. C₁₀-Strapped dibromoporphyrin 7c

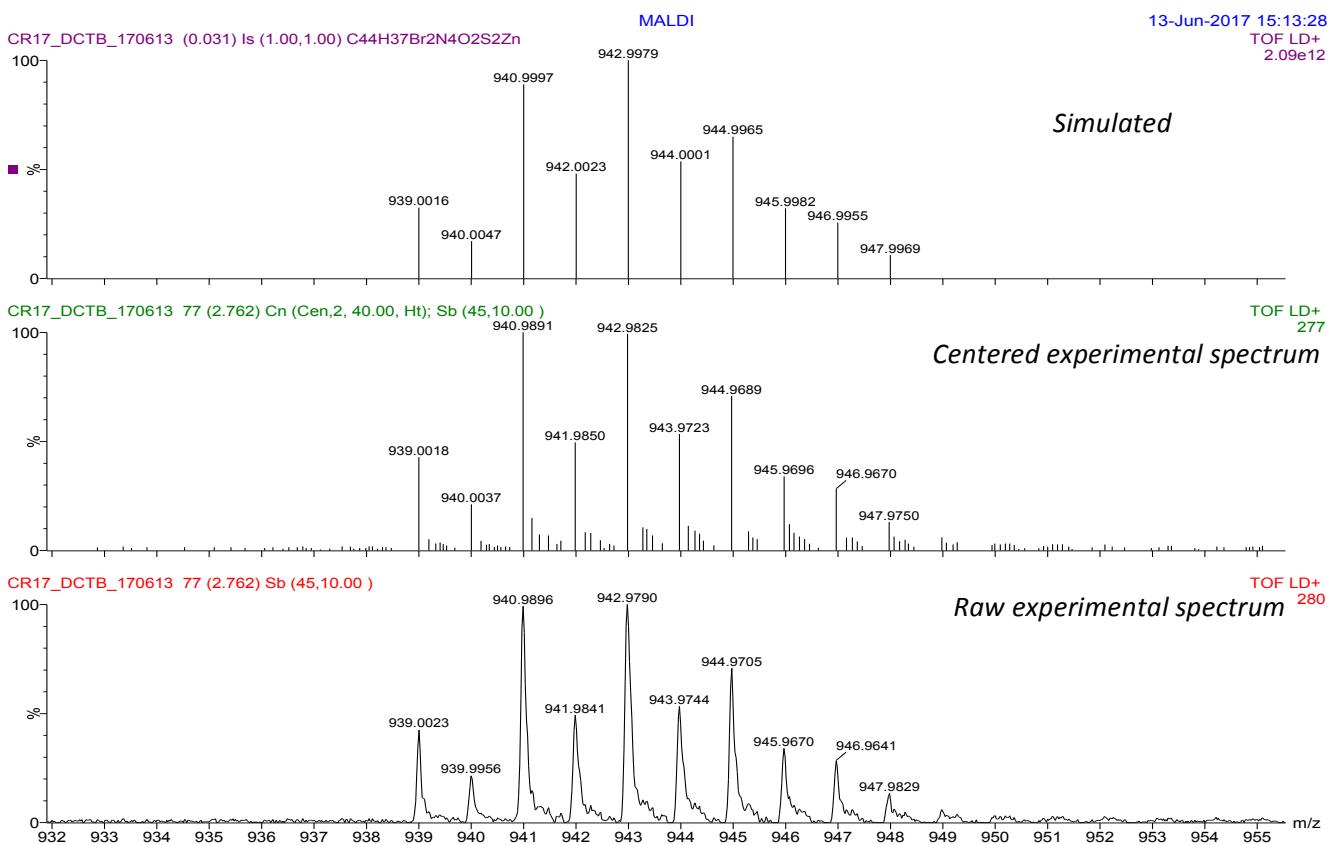
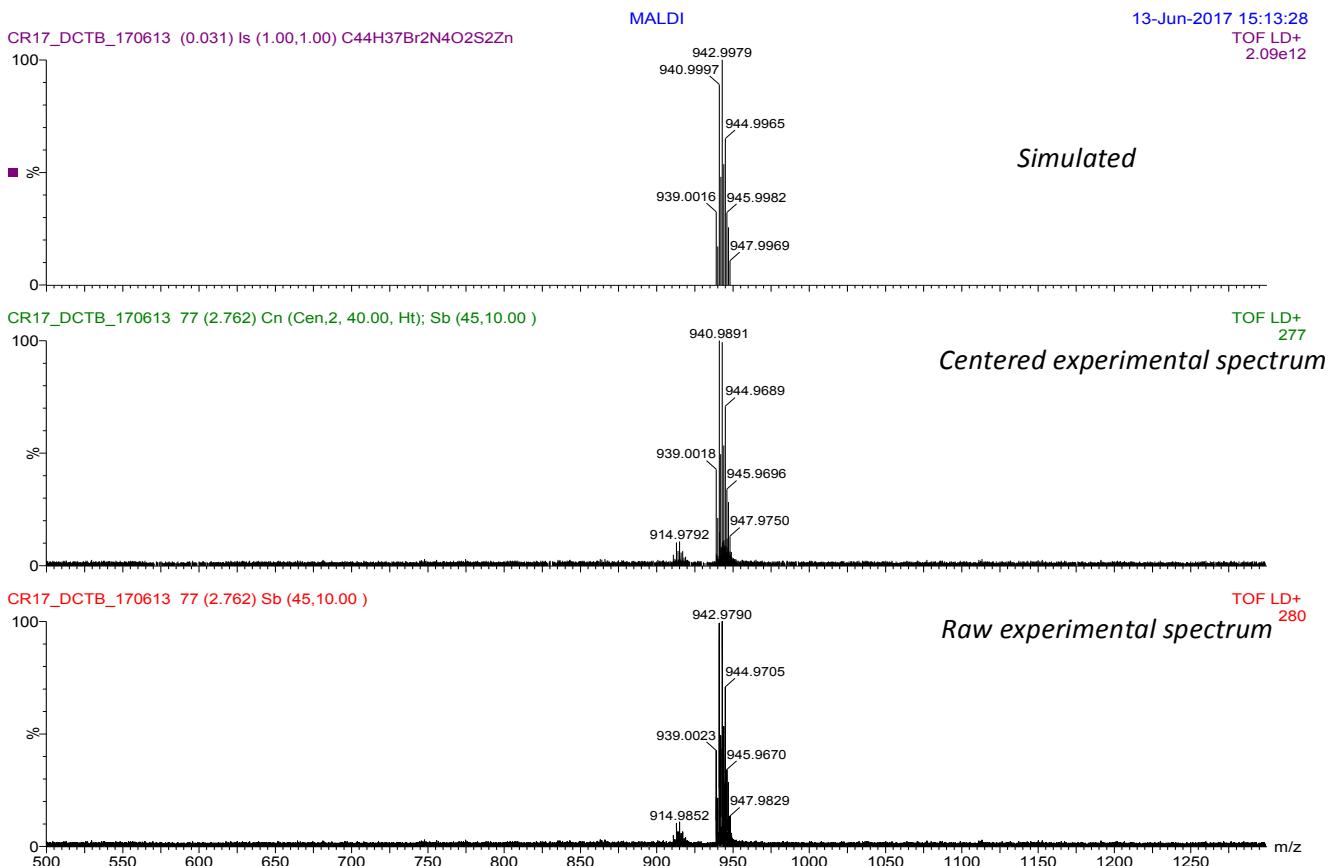
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

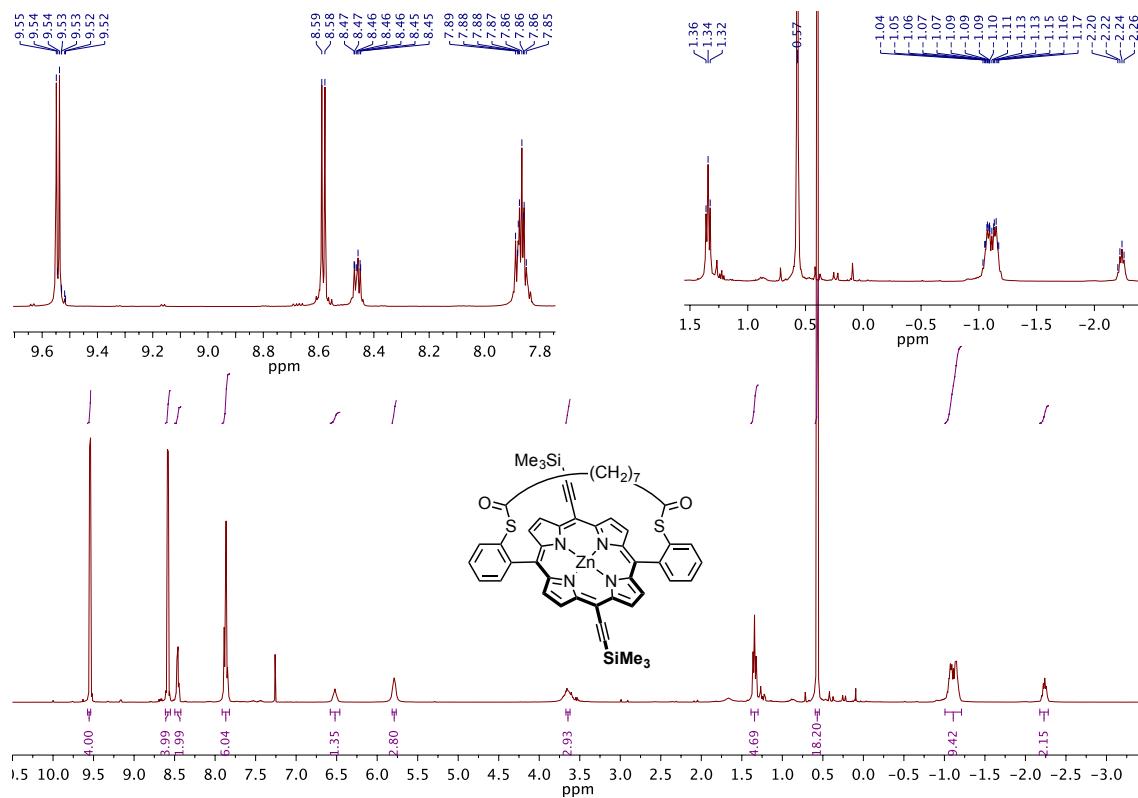


MALDI-TOF:

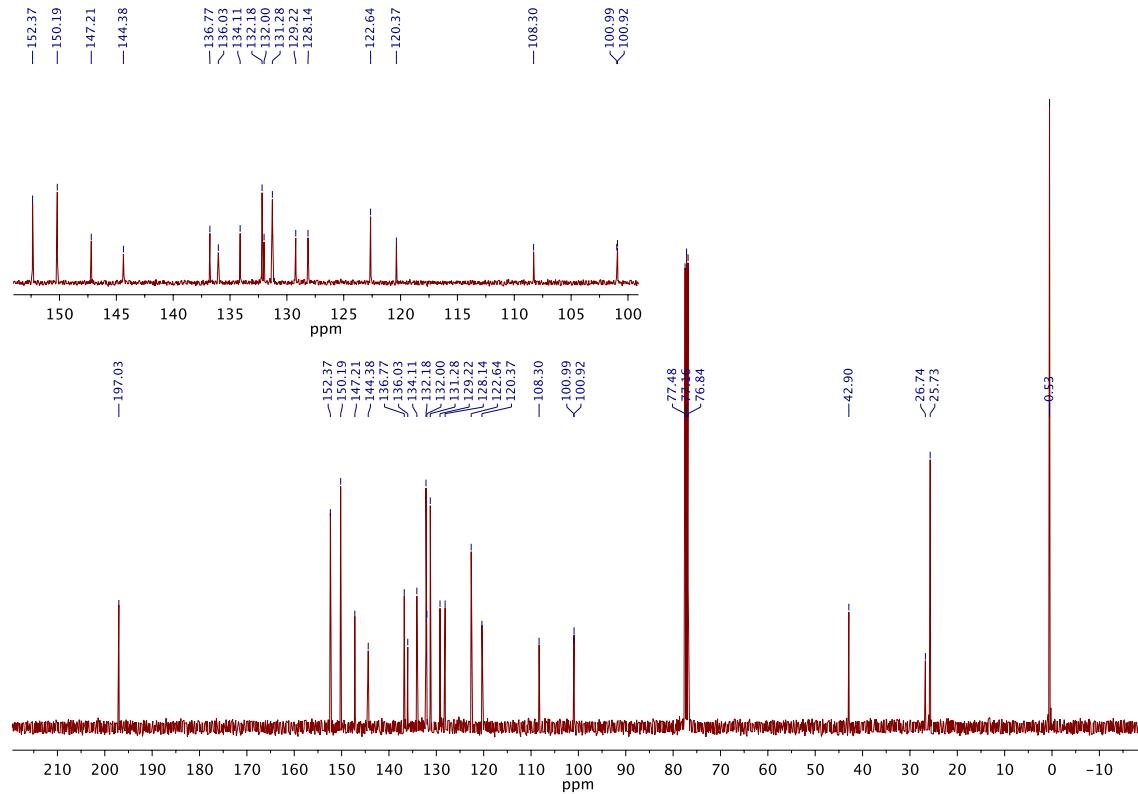


4.16. C₇-Strapped bis-TMS porphyrin 8a

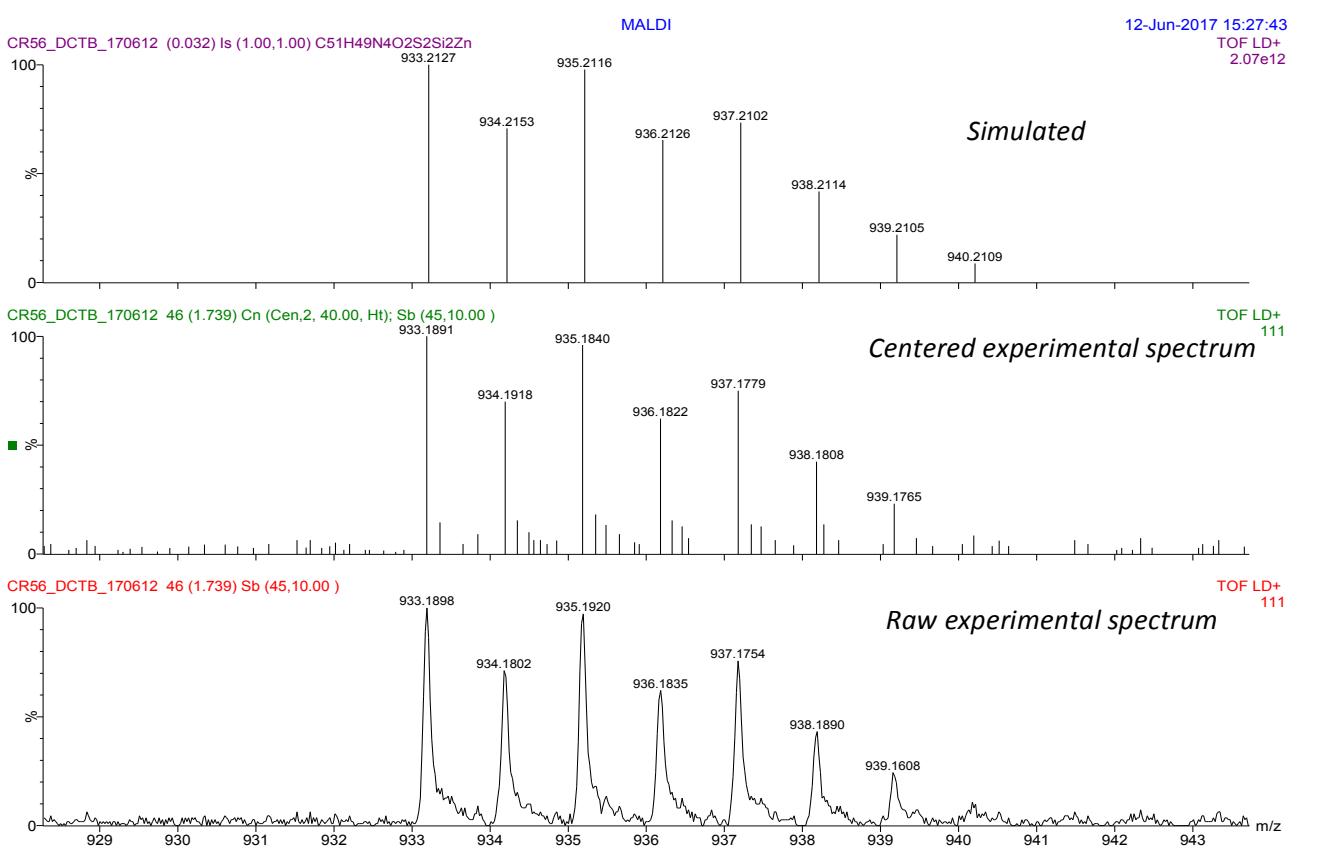
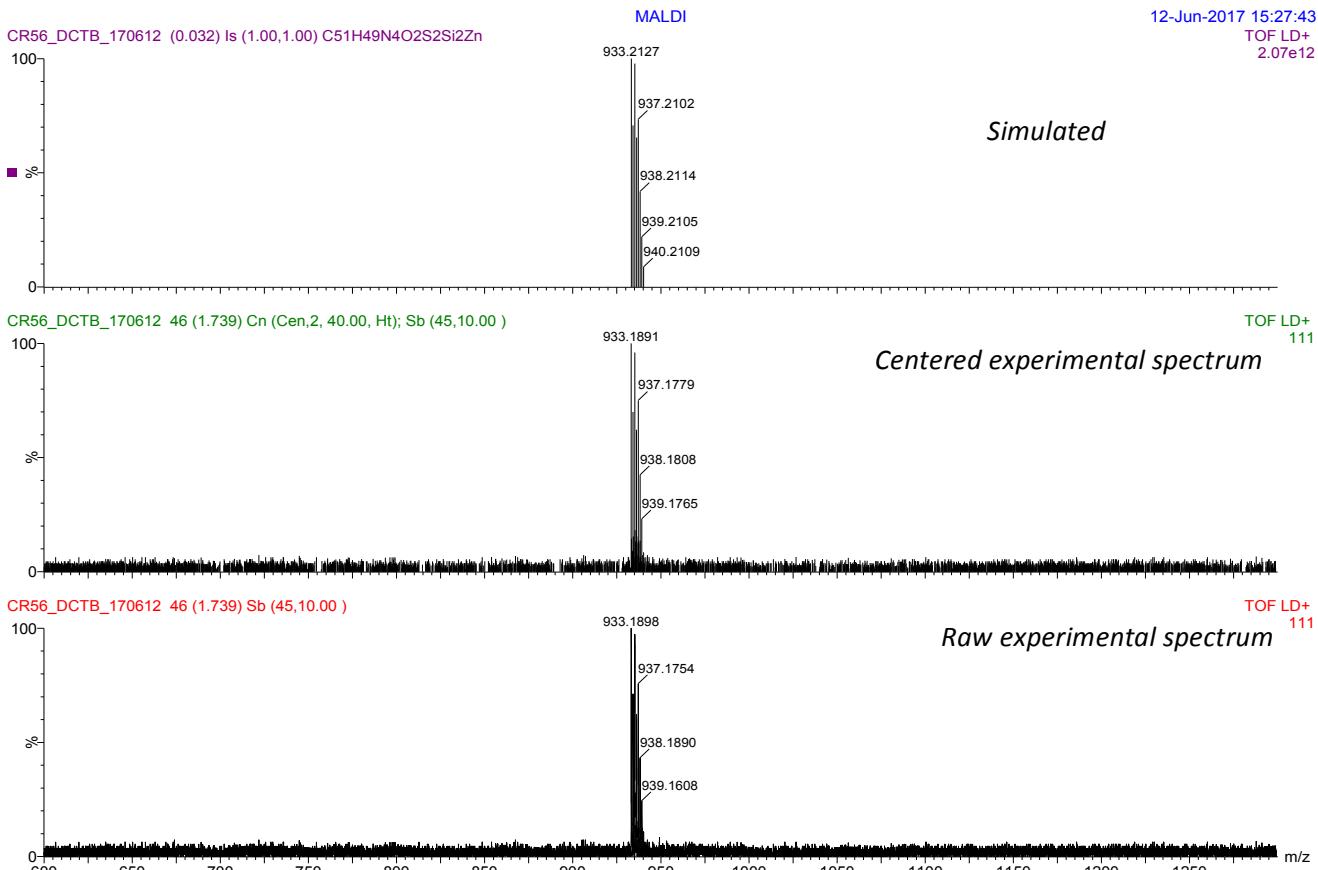
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

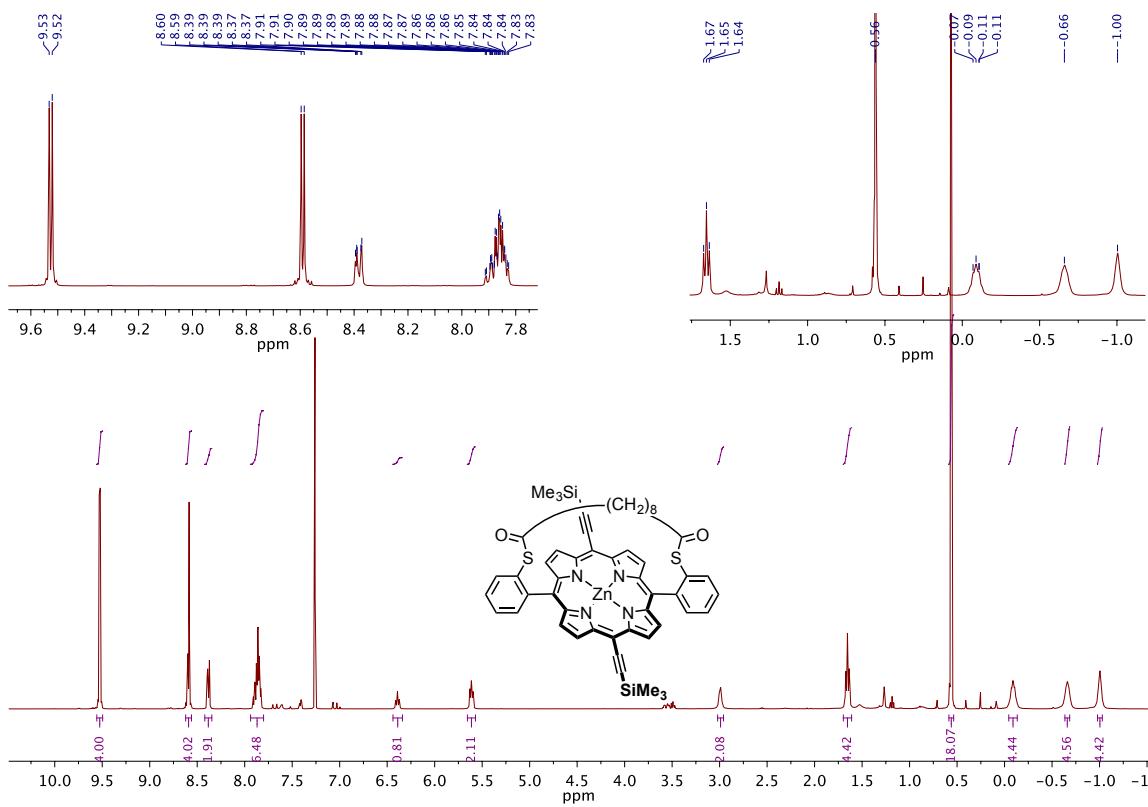


MALDI-TOF:

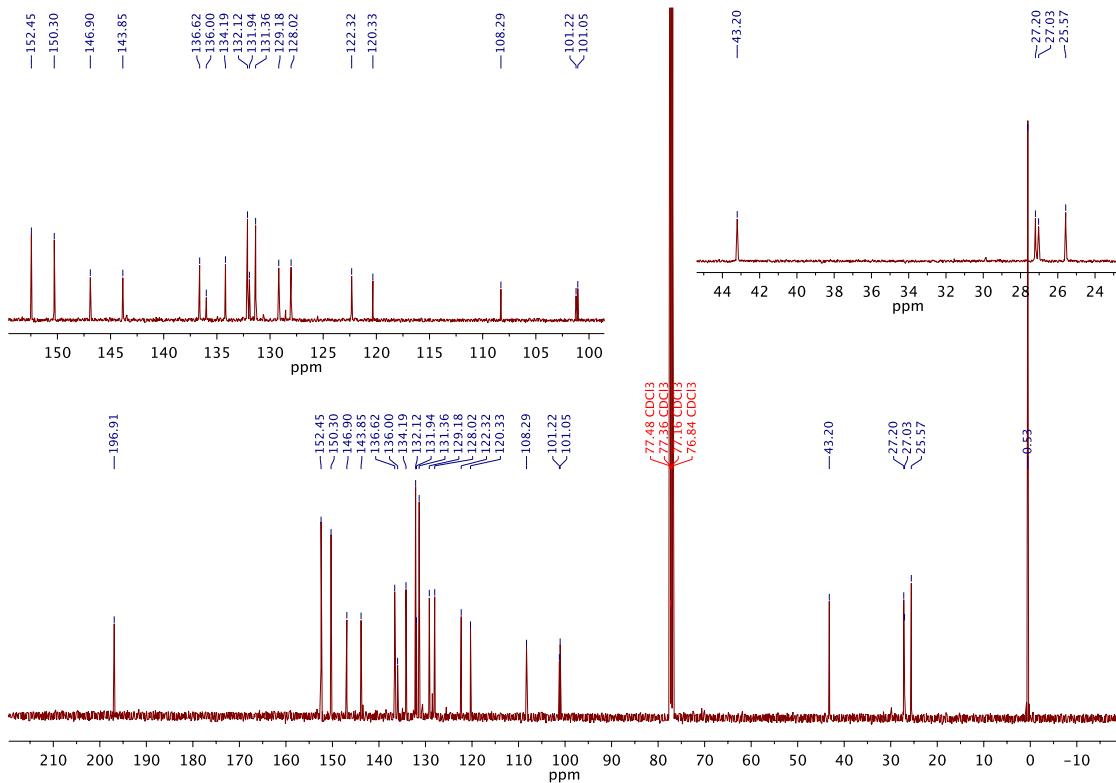


4.17. C₈-Strapped bis-TMS porphyrin 8b

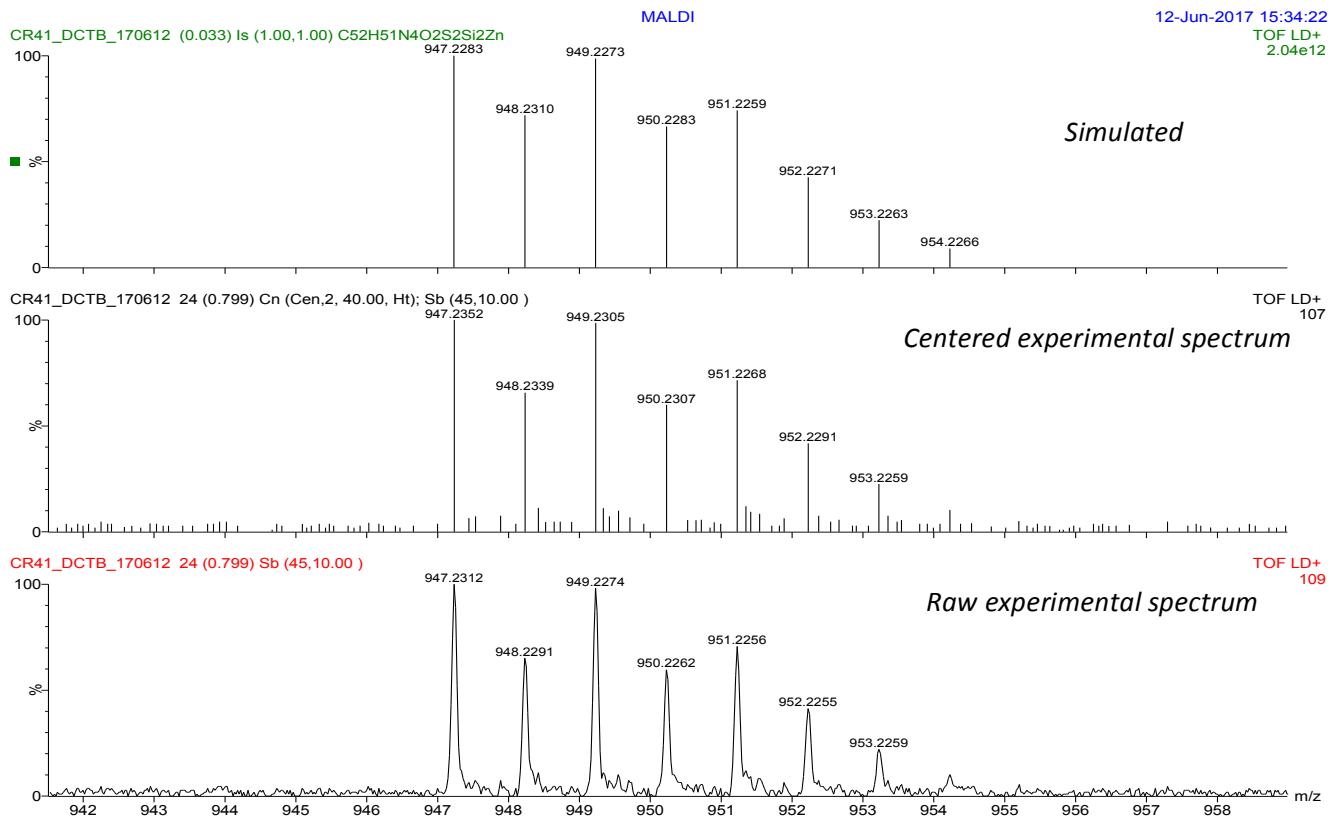
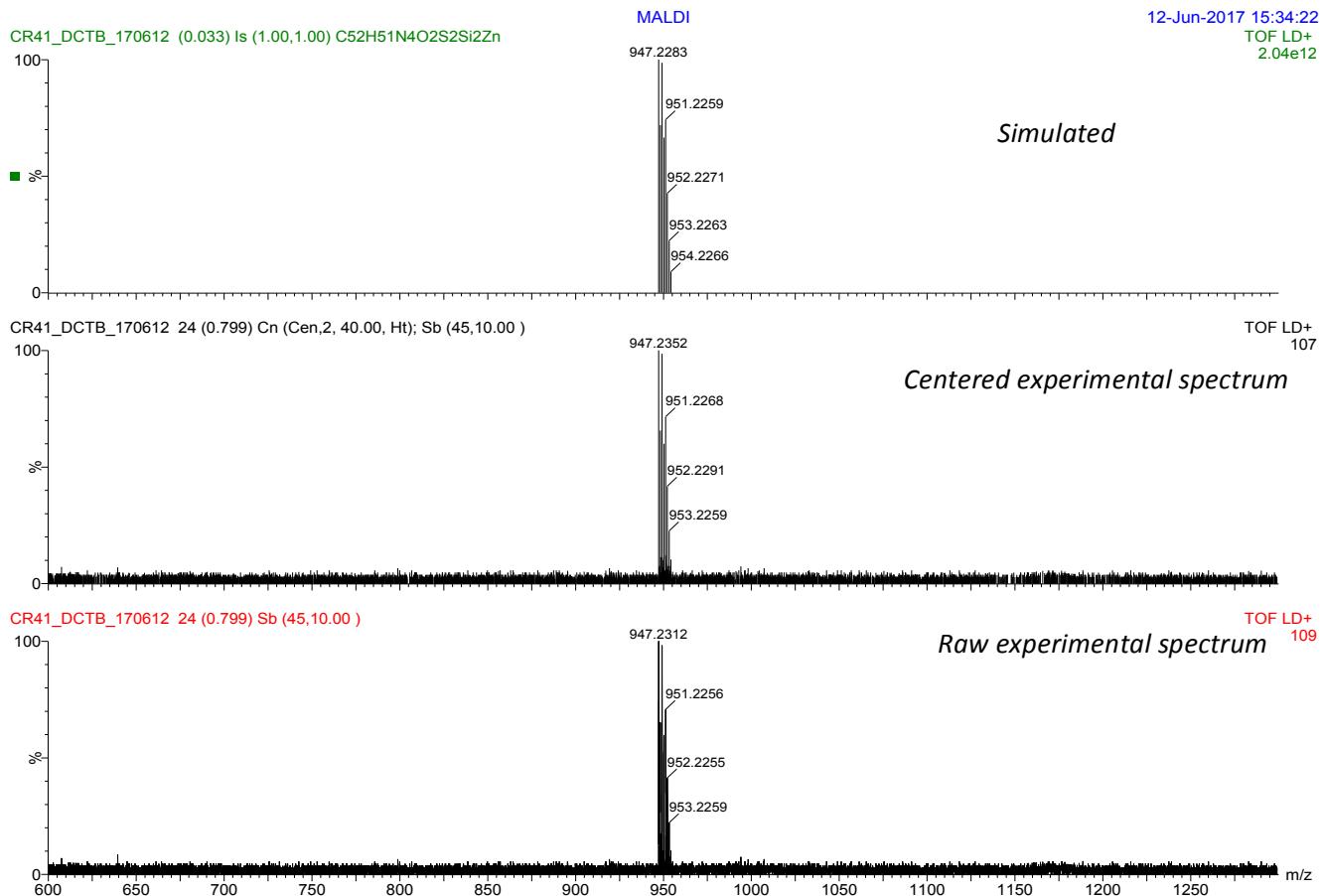
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

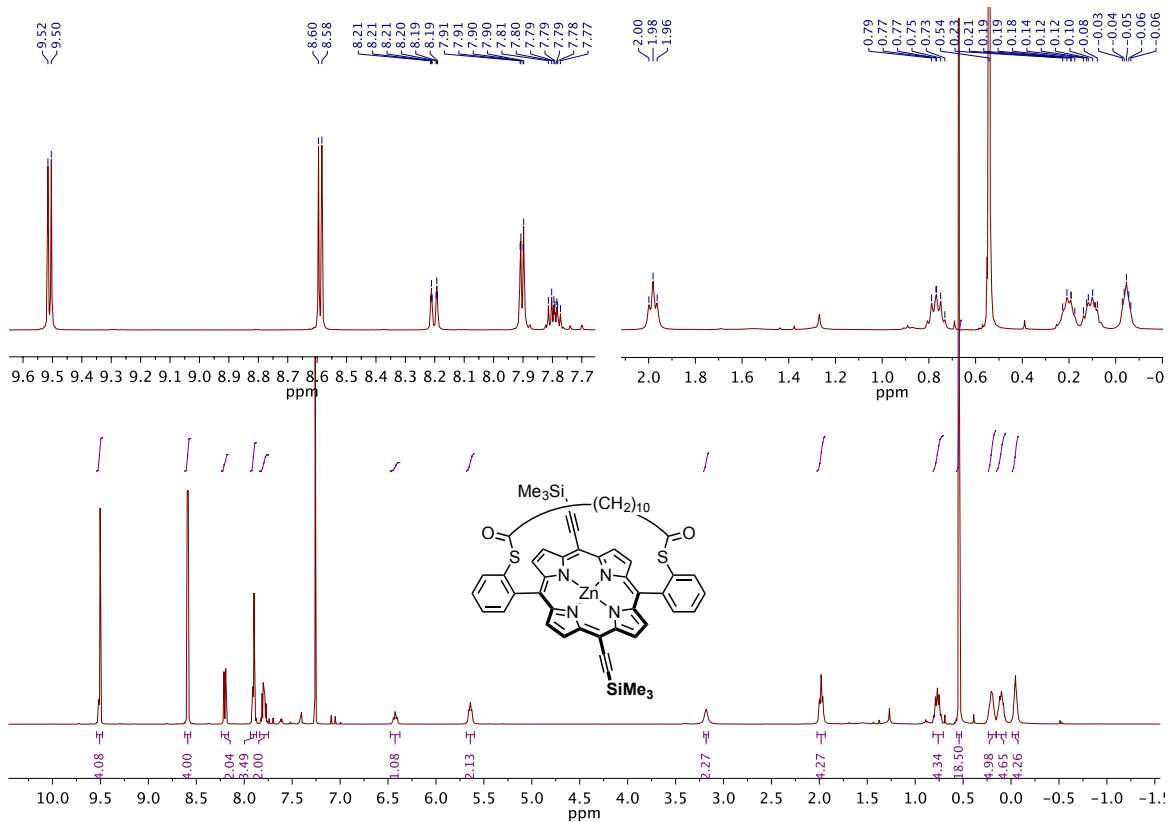


MALDI-TOF:

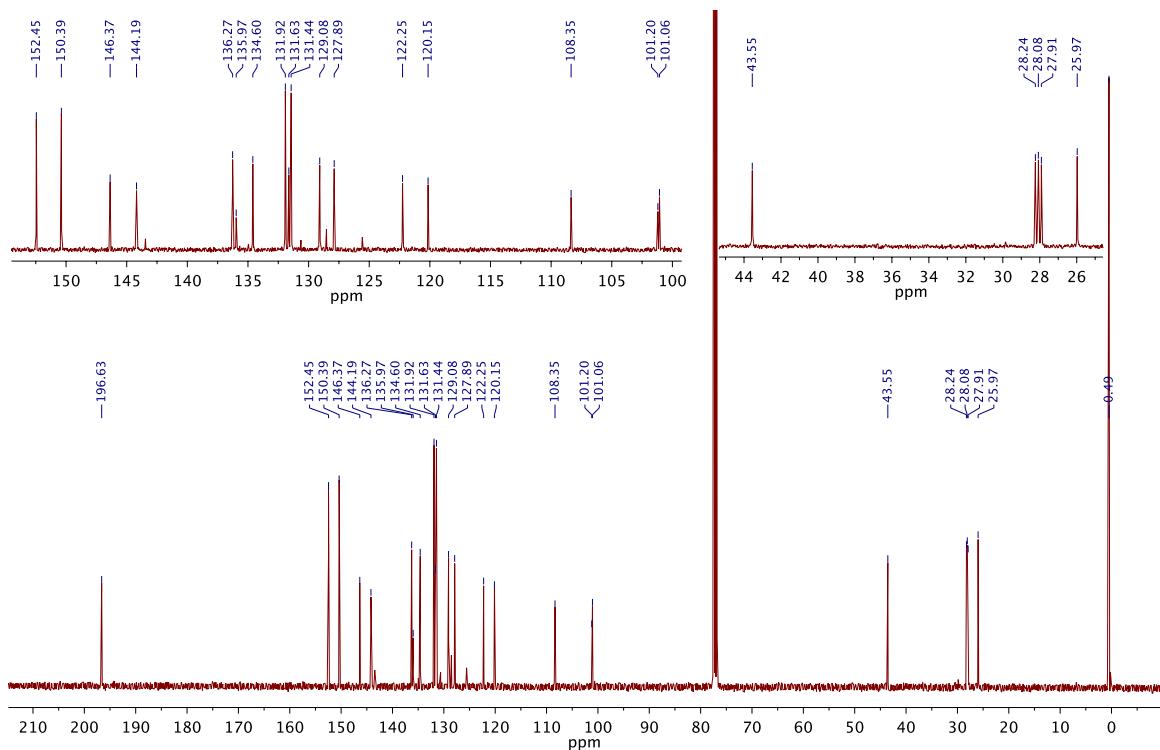


4.18. C₁₀-Strapped bis-TMS porphyrin 8c

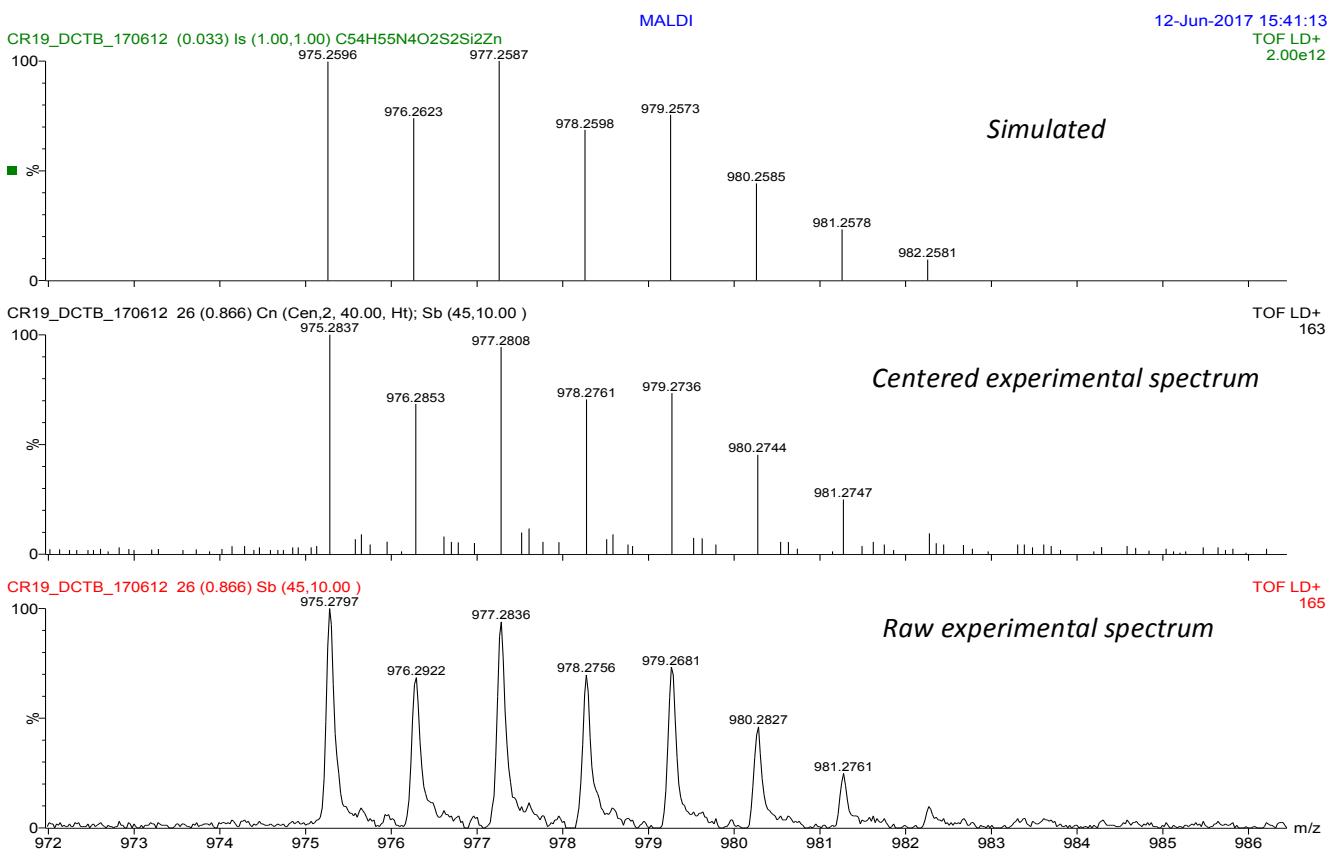
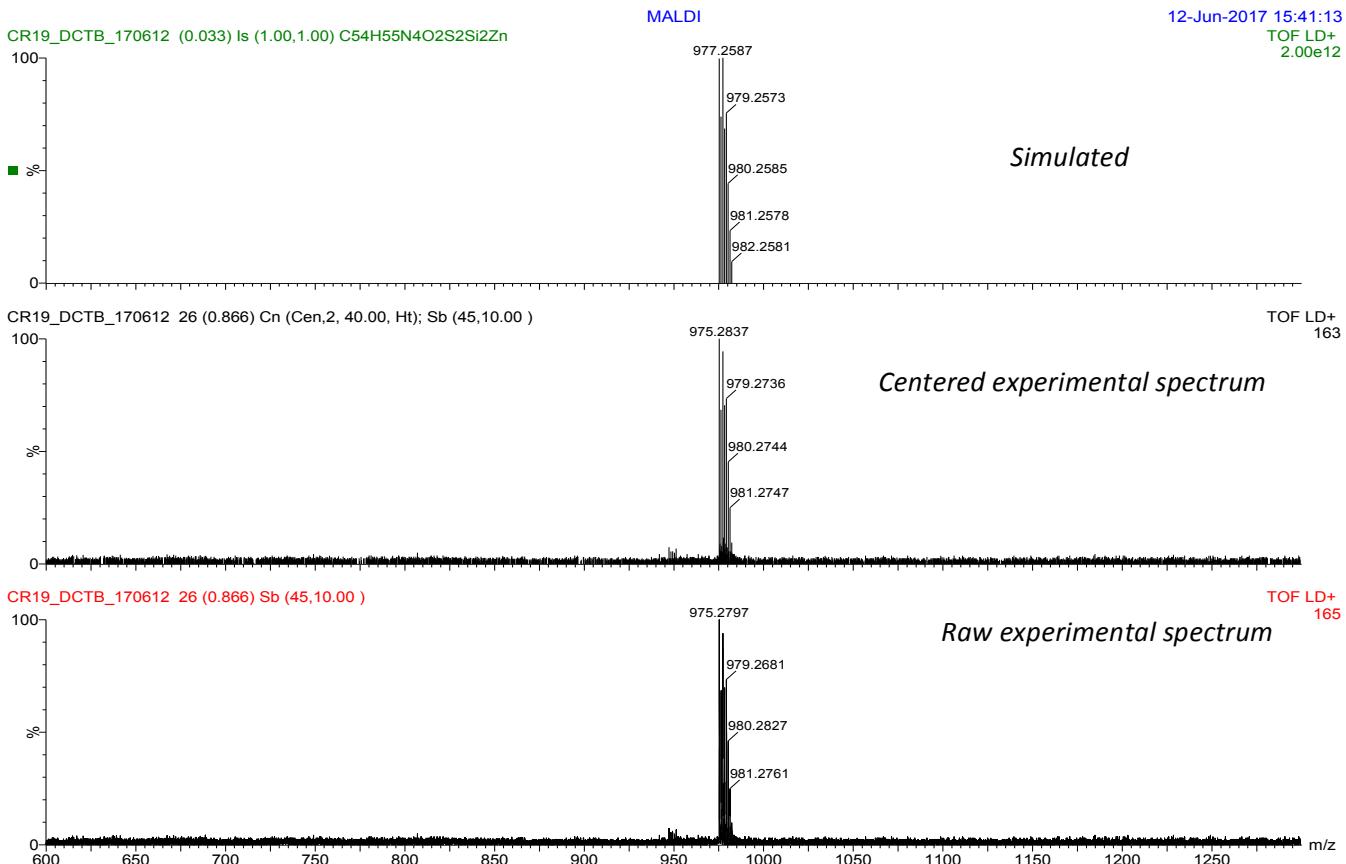
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

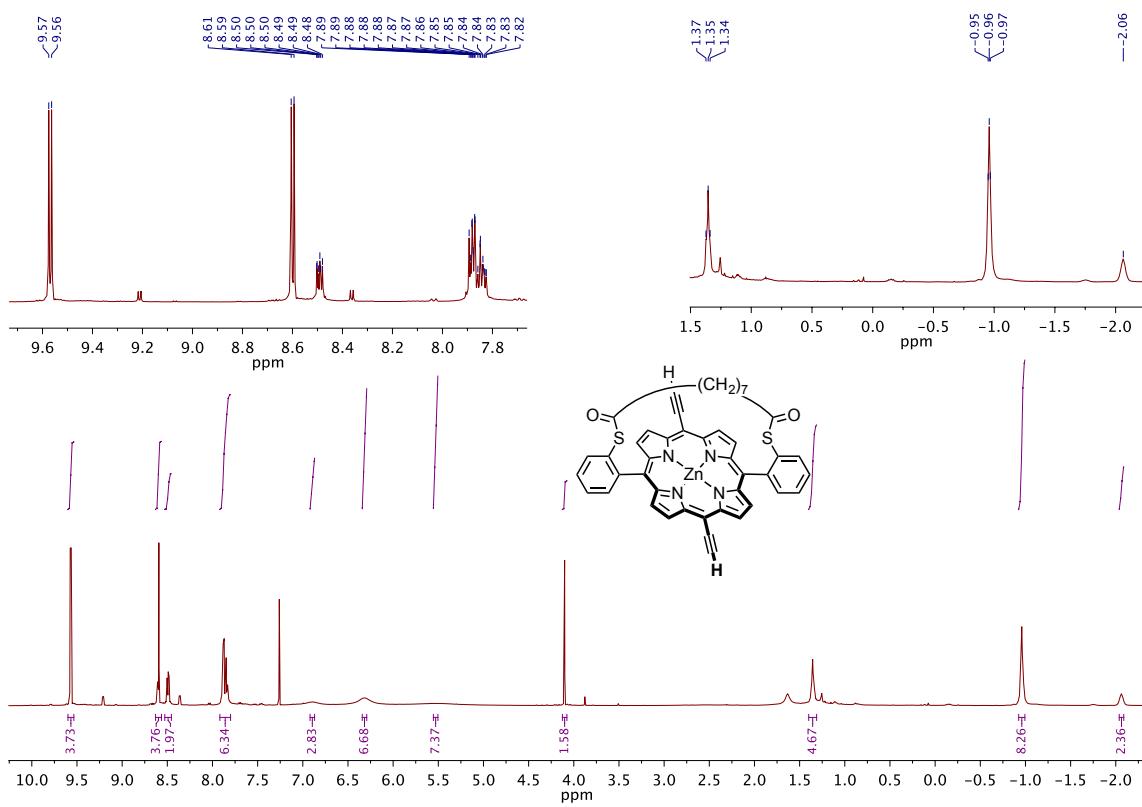


MALDI-TOF:

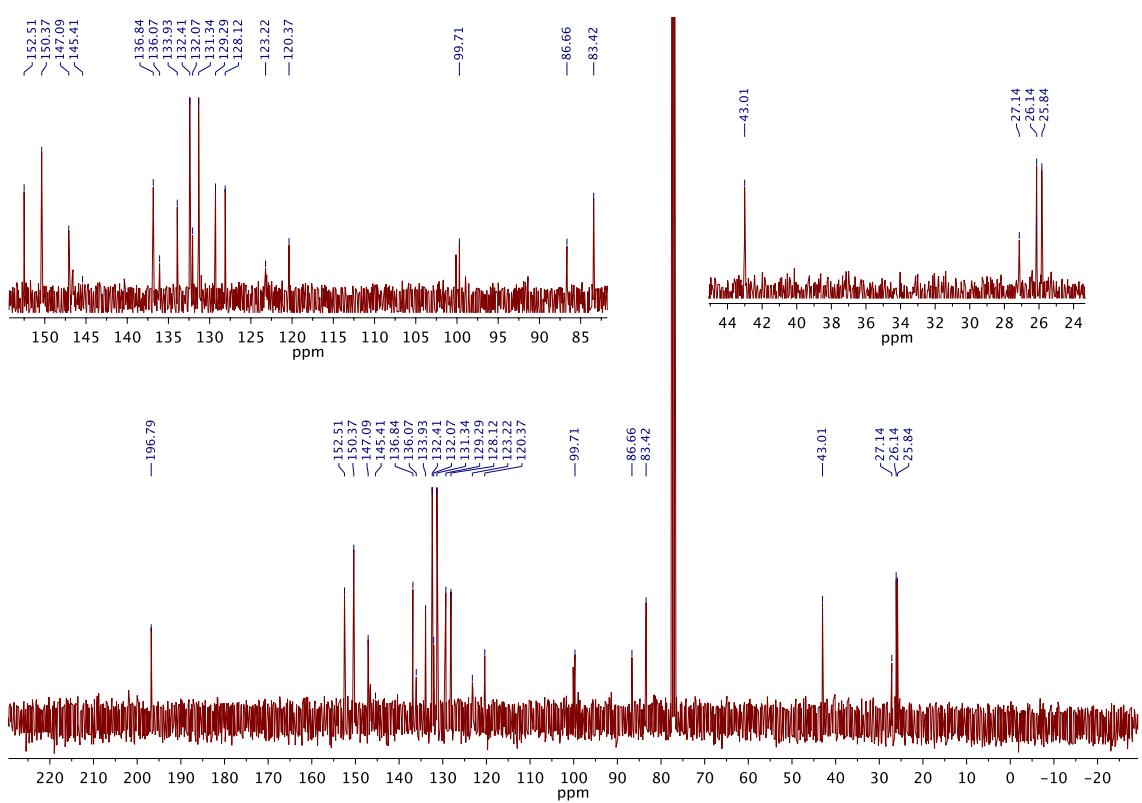


4.19. C₇-Strapped bis-deprotected porphyrin 9a

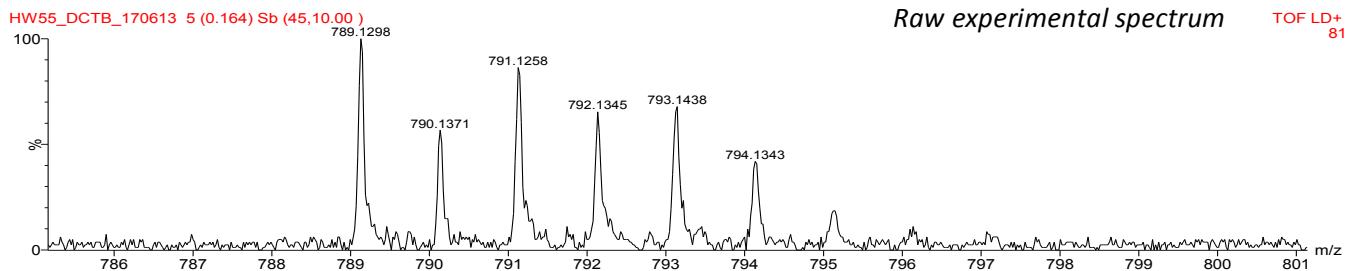
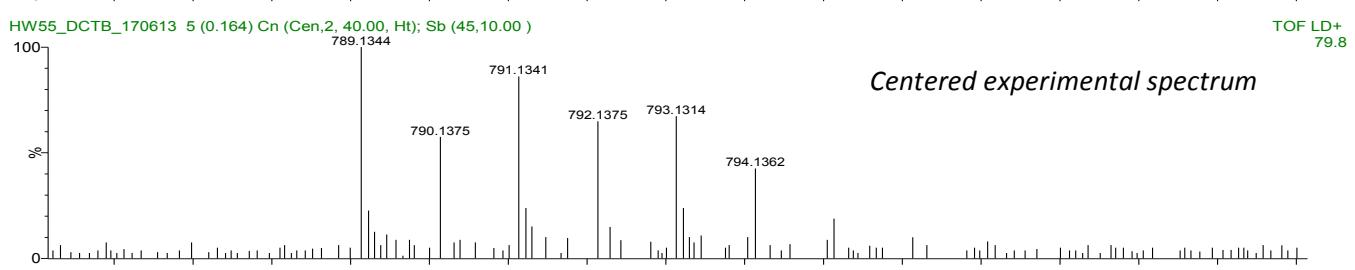
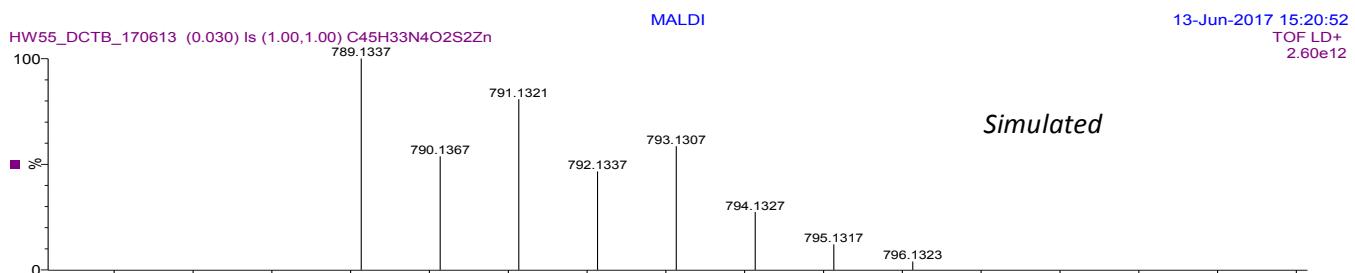
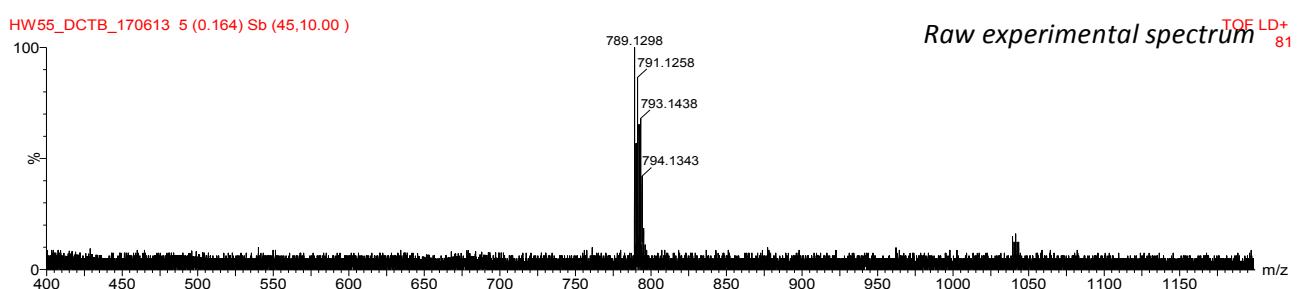
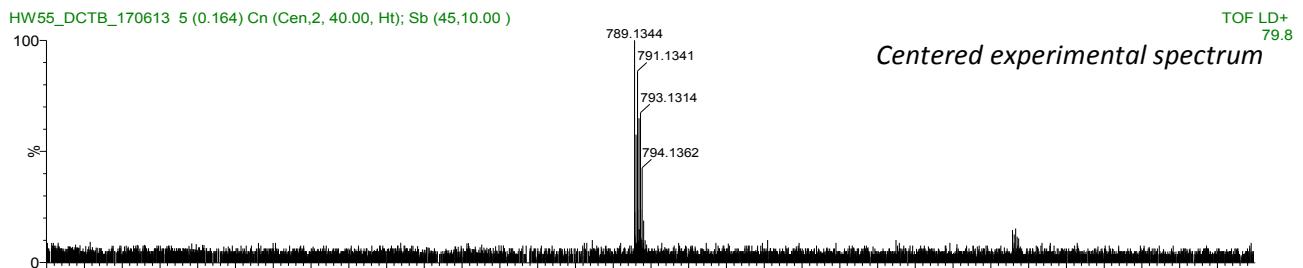
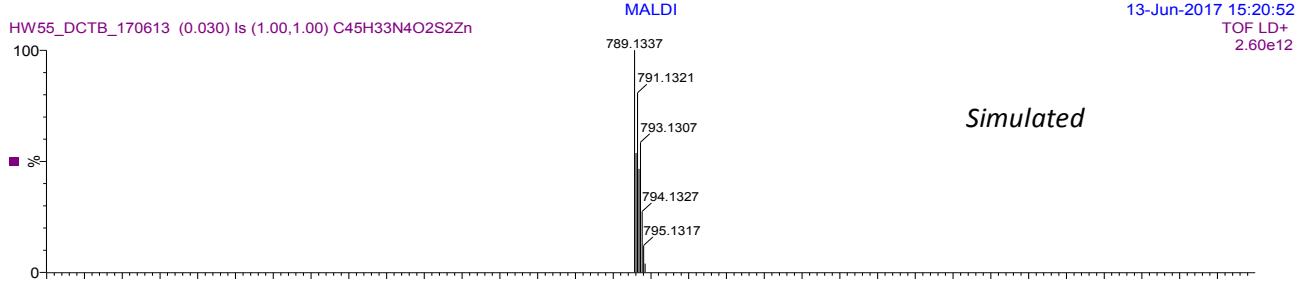
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

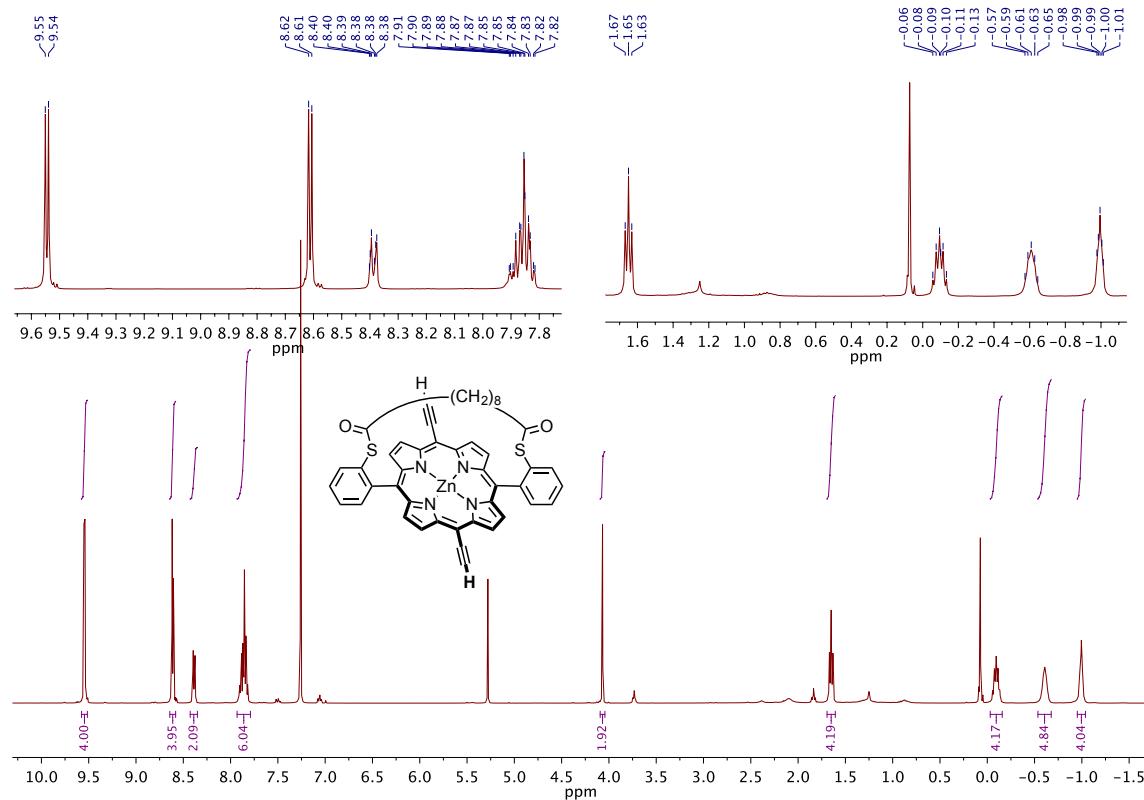


MALDI-TOF:

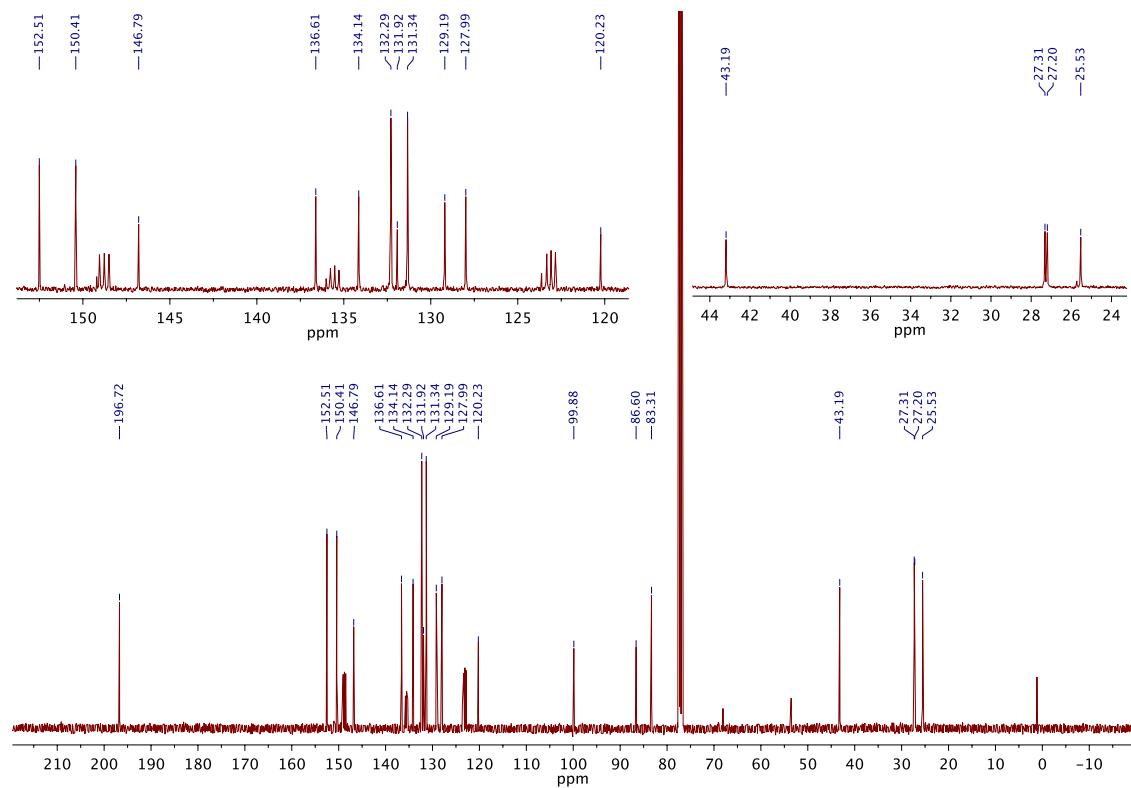


4.20. C₈-Strapped bis-deprotected porphyrin 9b

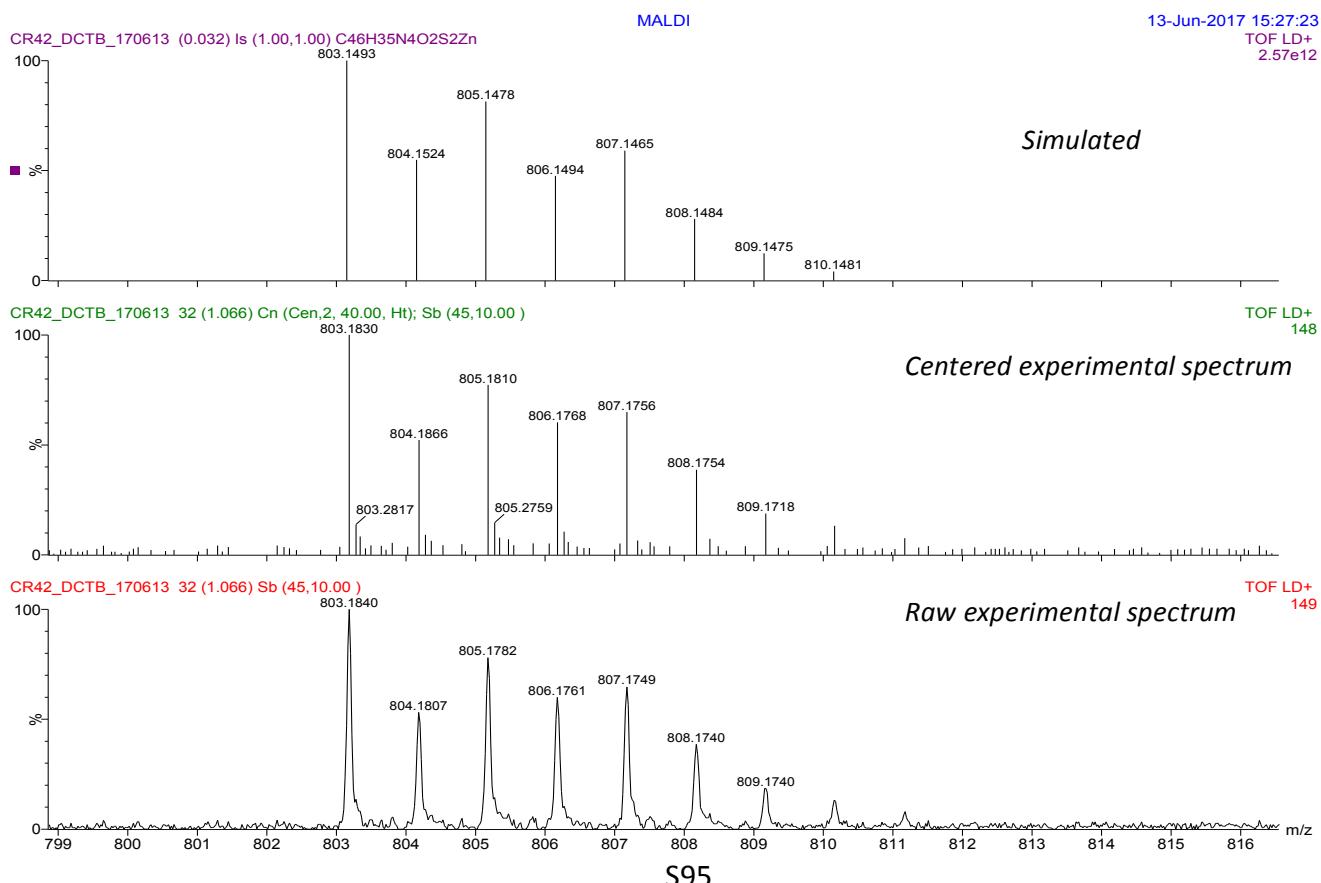
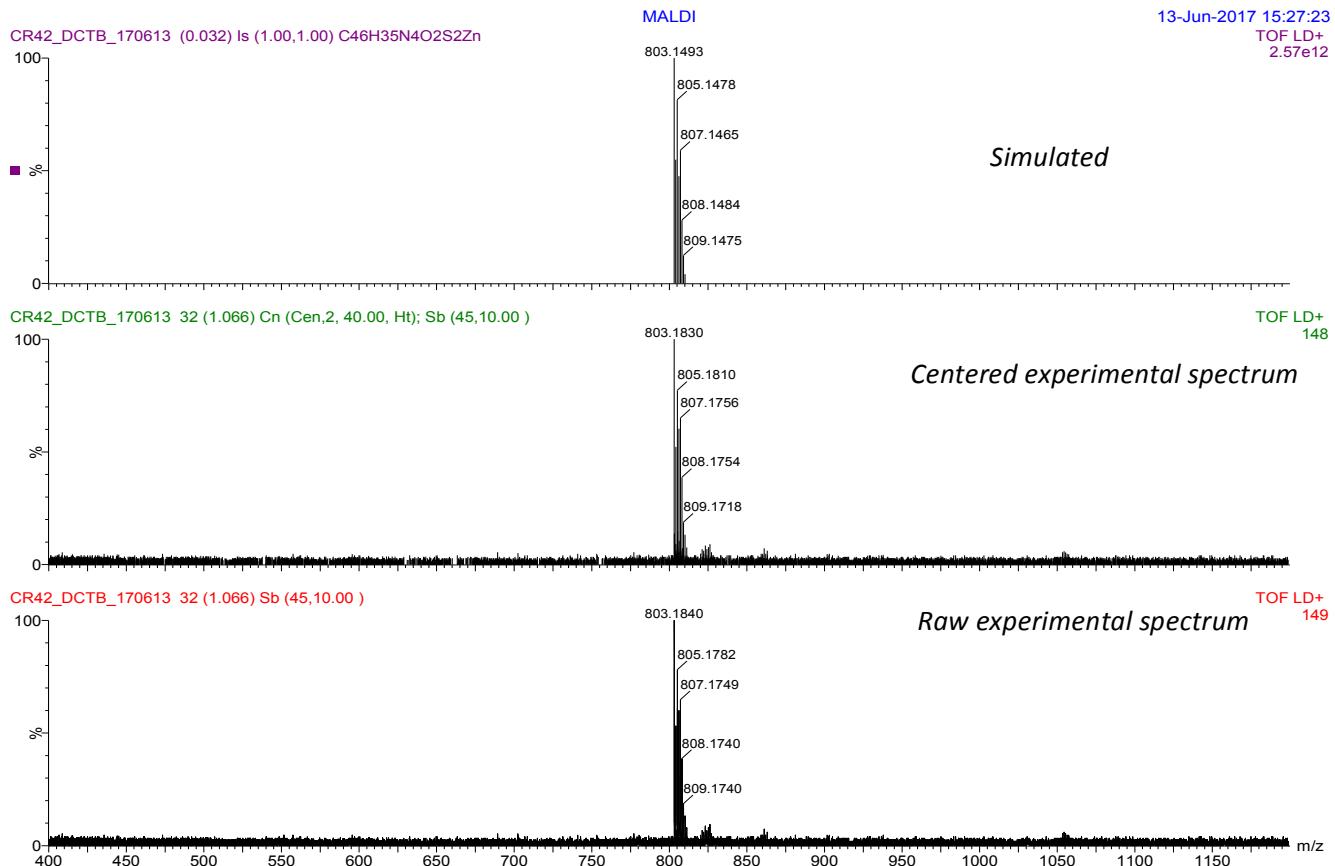
¹H NMR (CDCl₃/1% pyridine-d₅, 400 MHz, 298K):



¹³C NMR (CDCl₃/1% pyridine-d₅, 100 MHz, 298K):

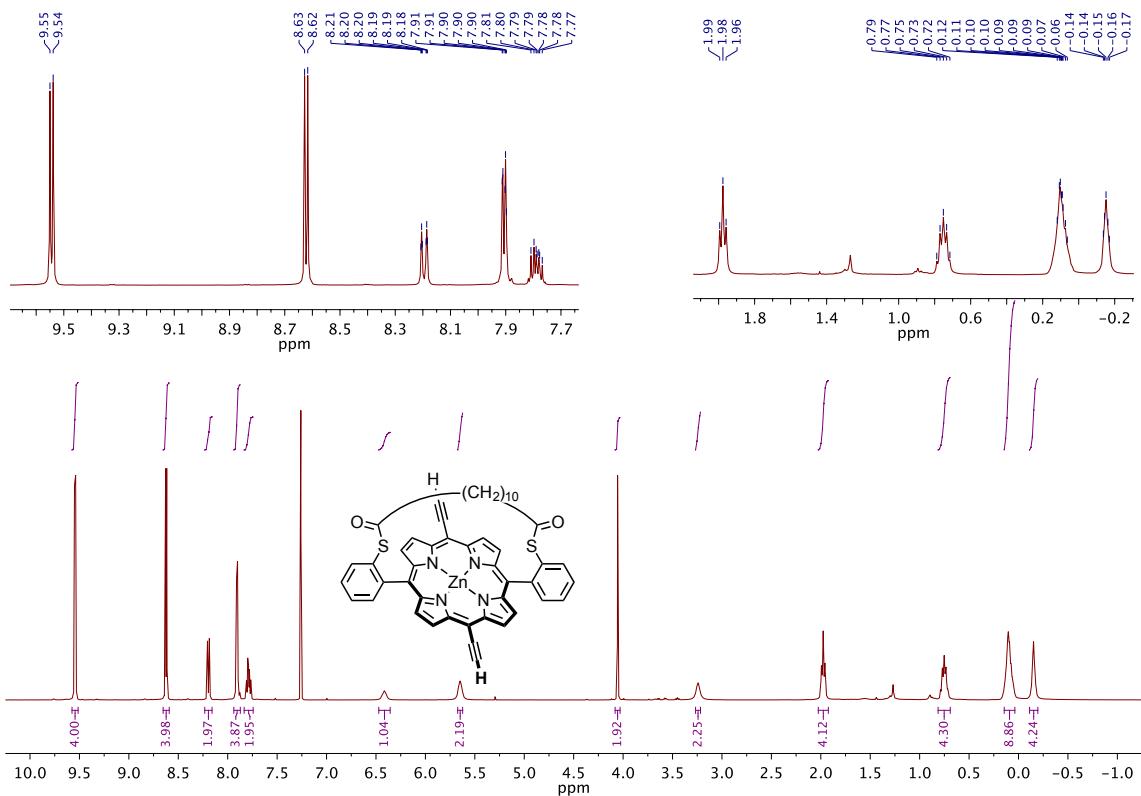


MALDI-TOF:

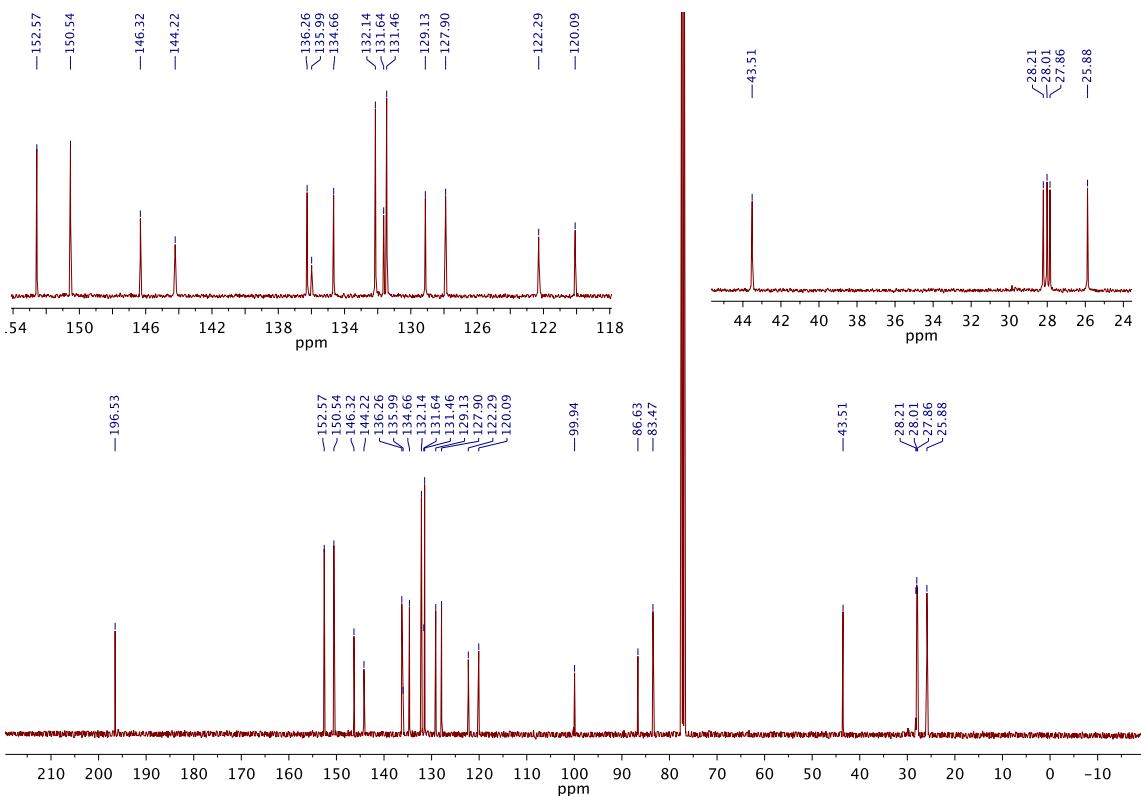


4.21. C₁₀-Strapped bis-deprotected porphyrin 9c

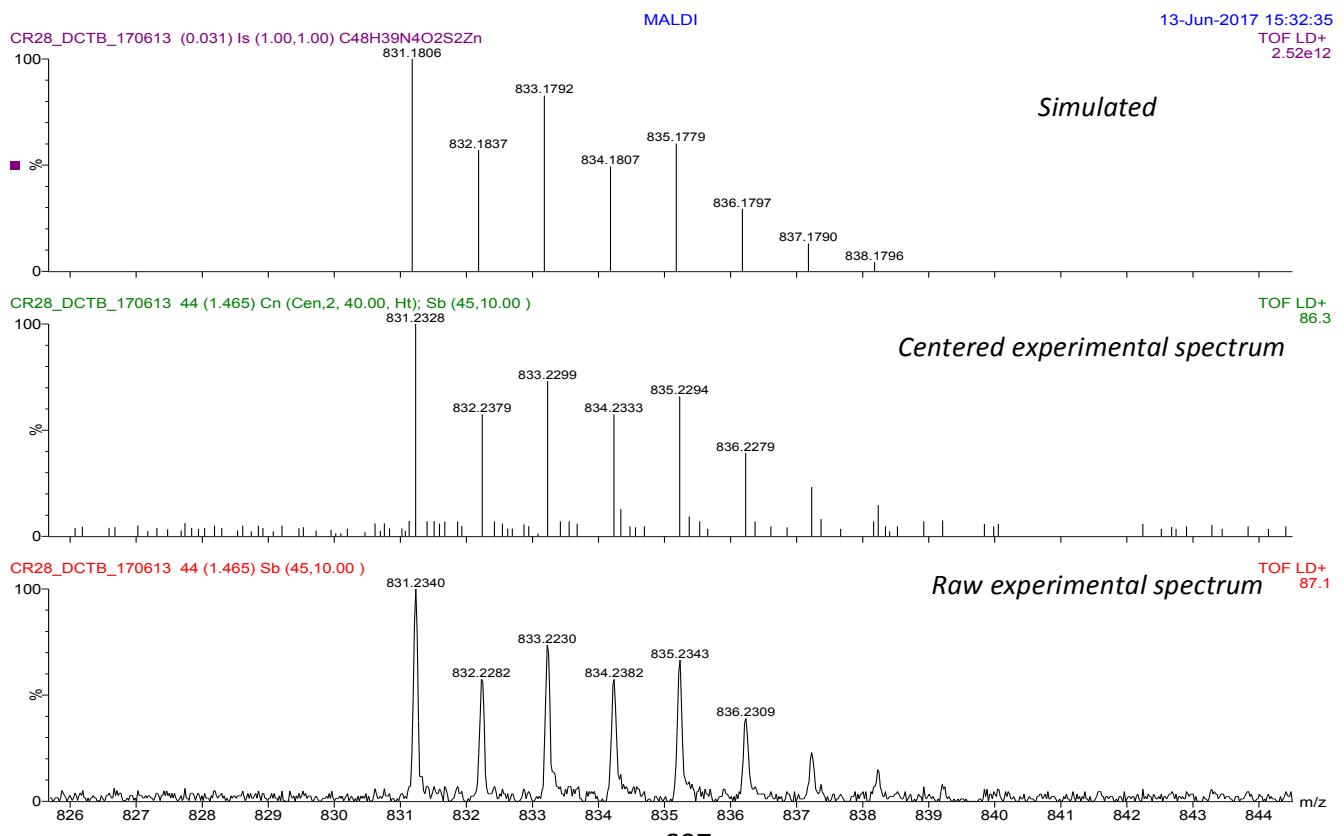
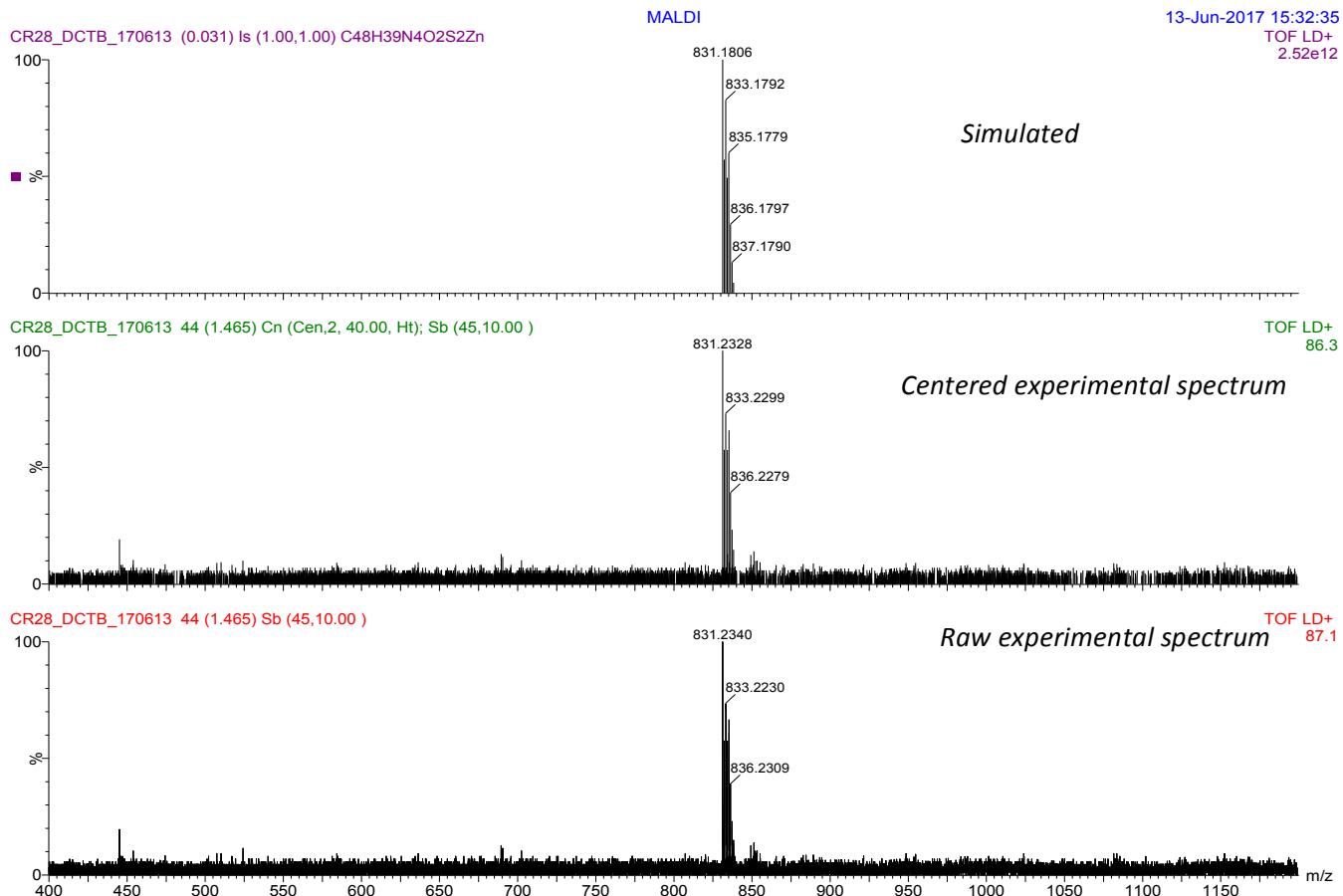
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

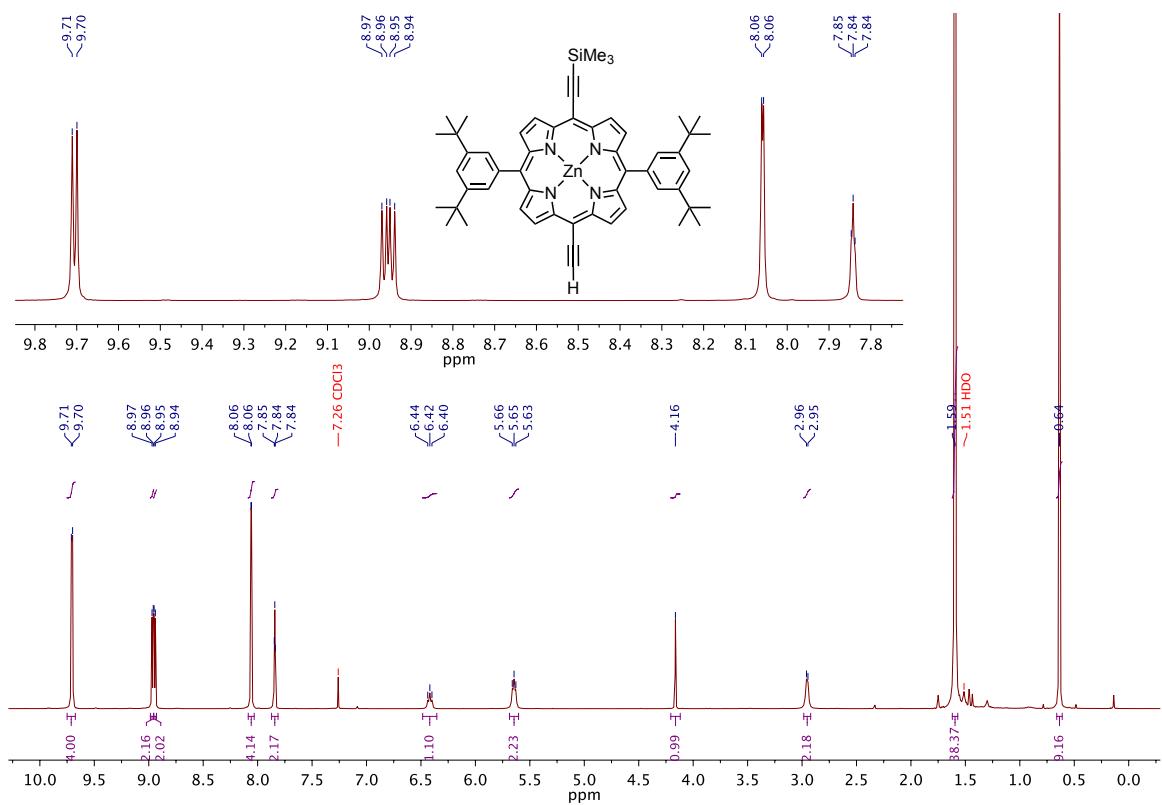


MALDI-TOF:

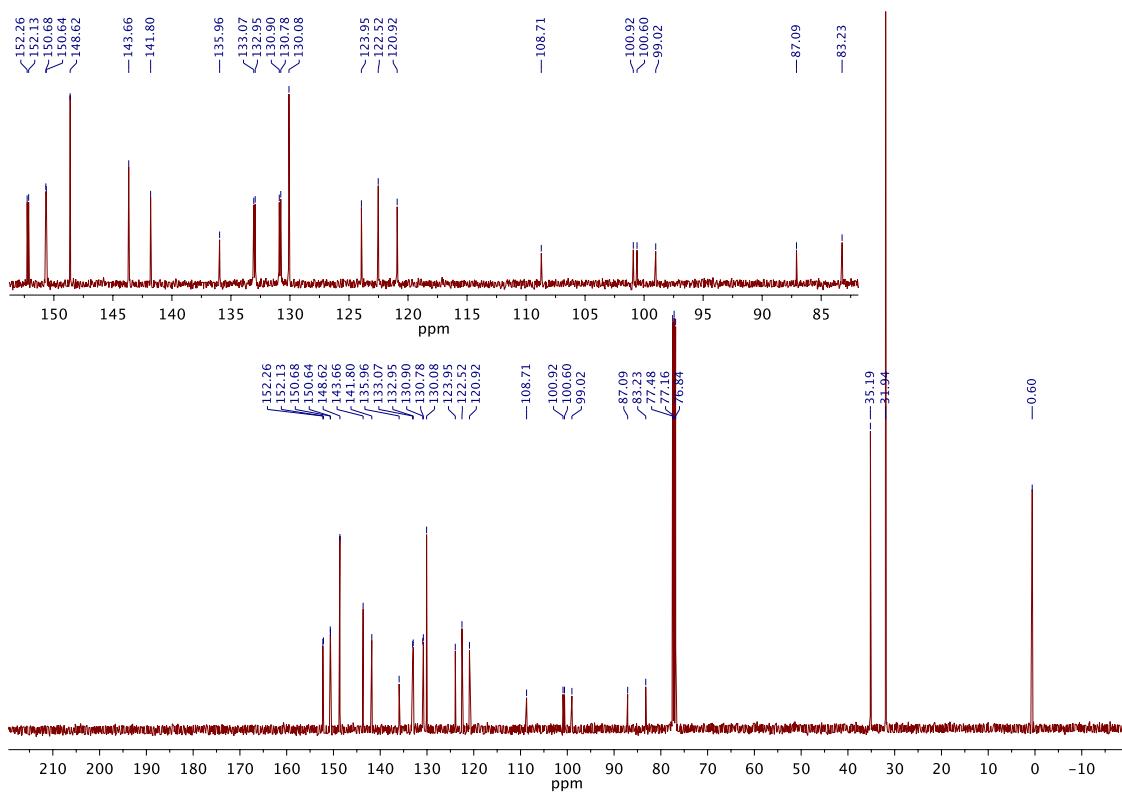


4.22. Mono-deprotected t-Bu porphyrin 10

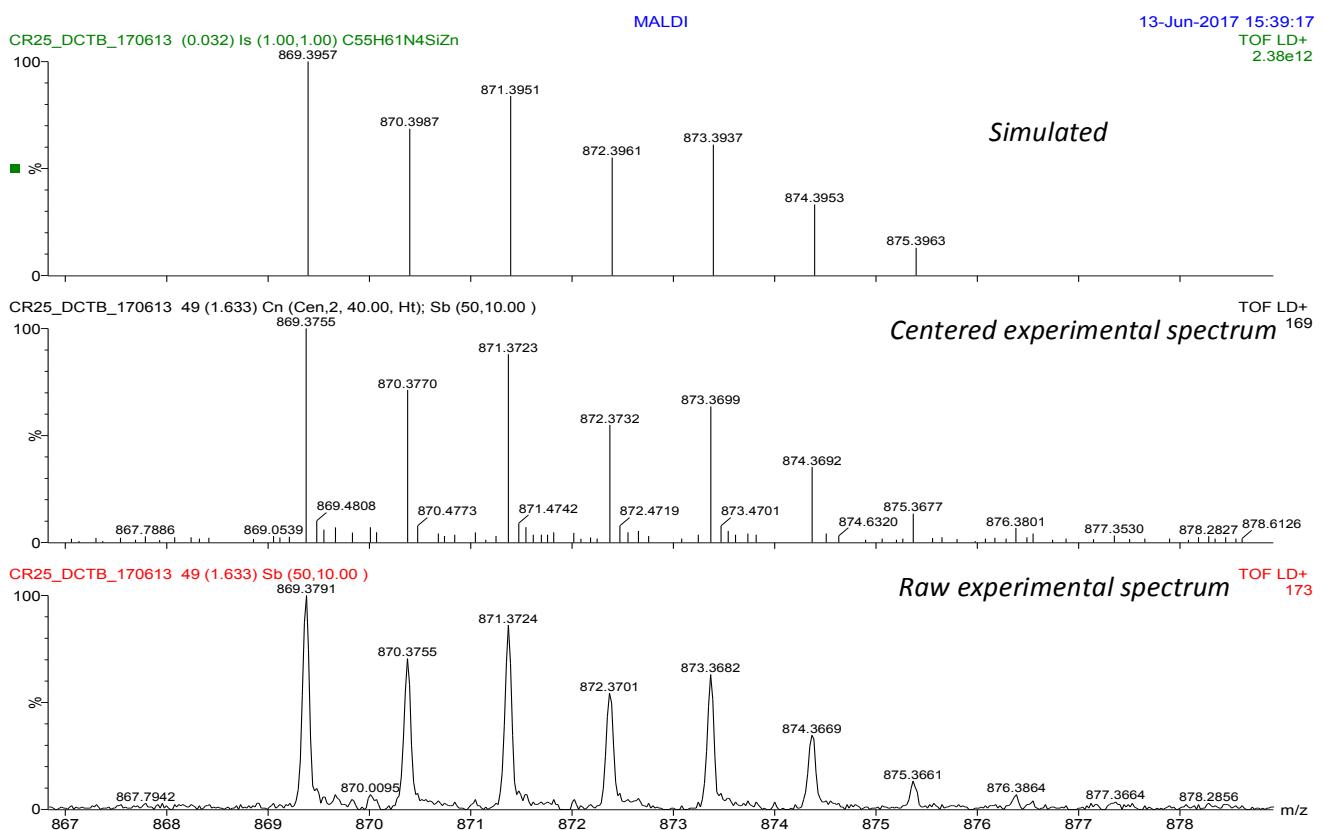
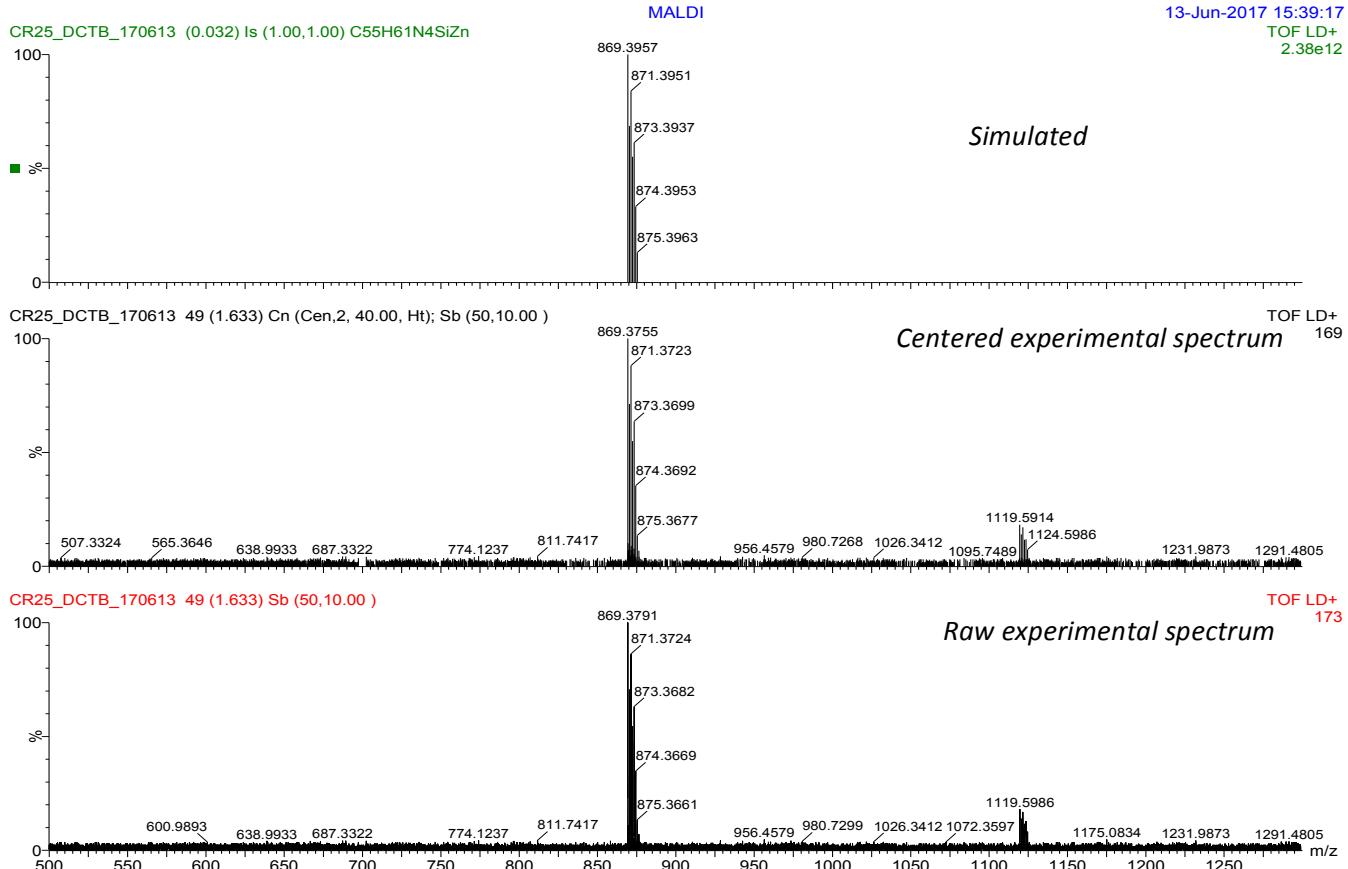
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

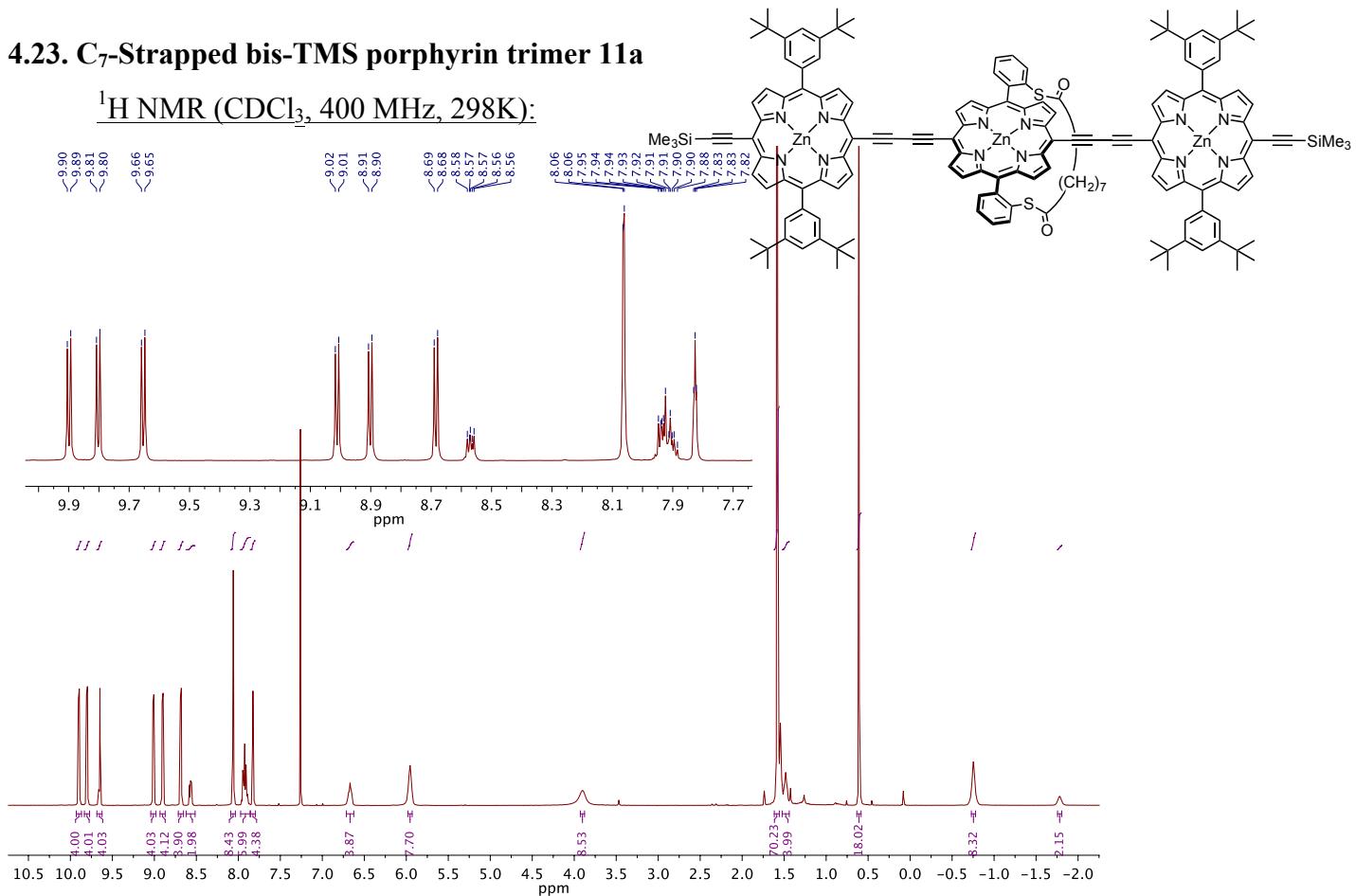


MALDI-TOF:

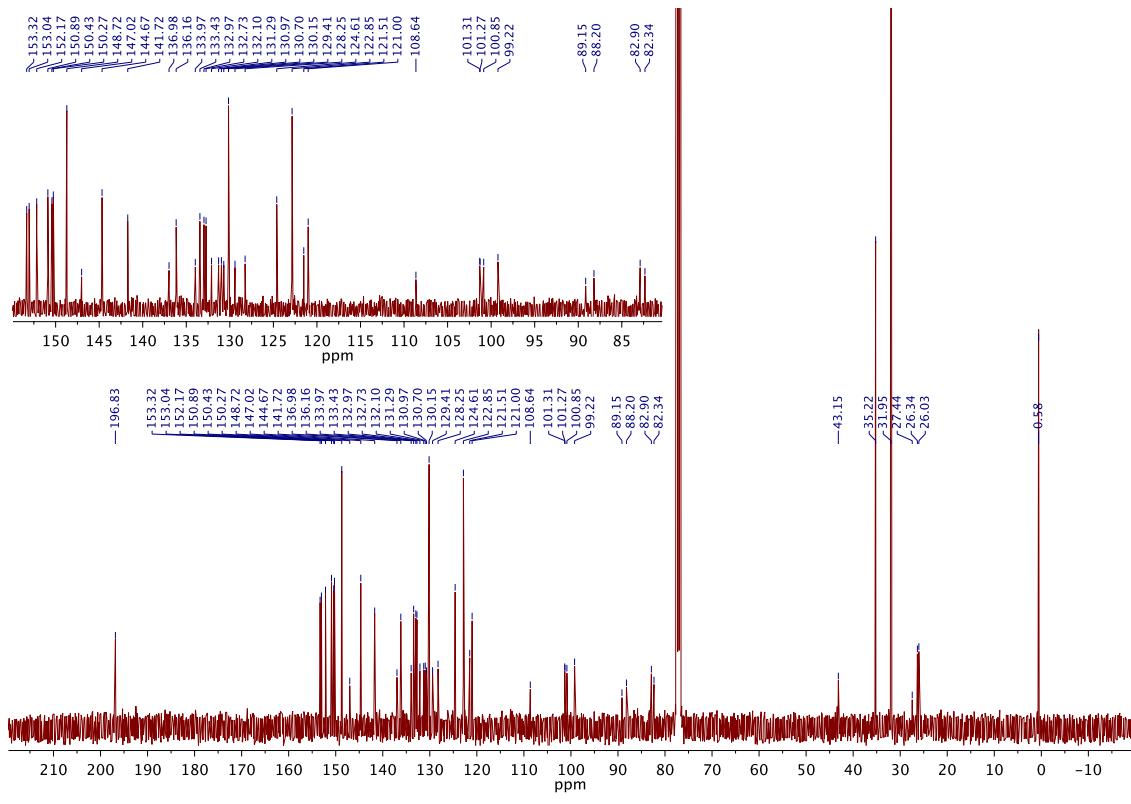


4.23. C₇-Strapped bis-TMS porphyrin trimer 11a

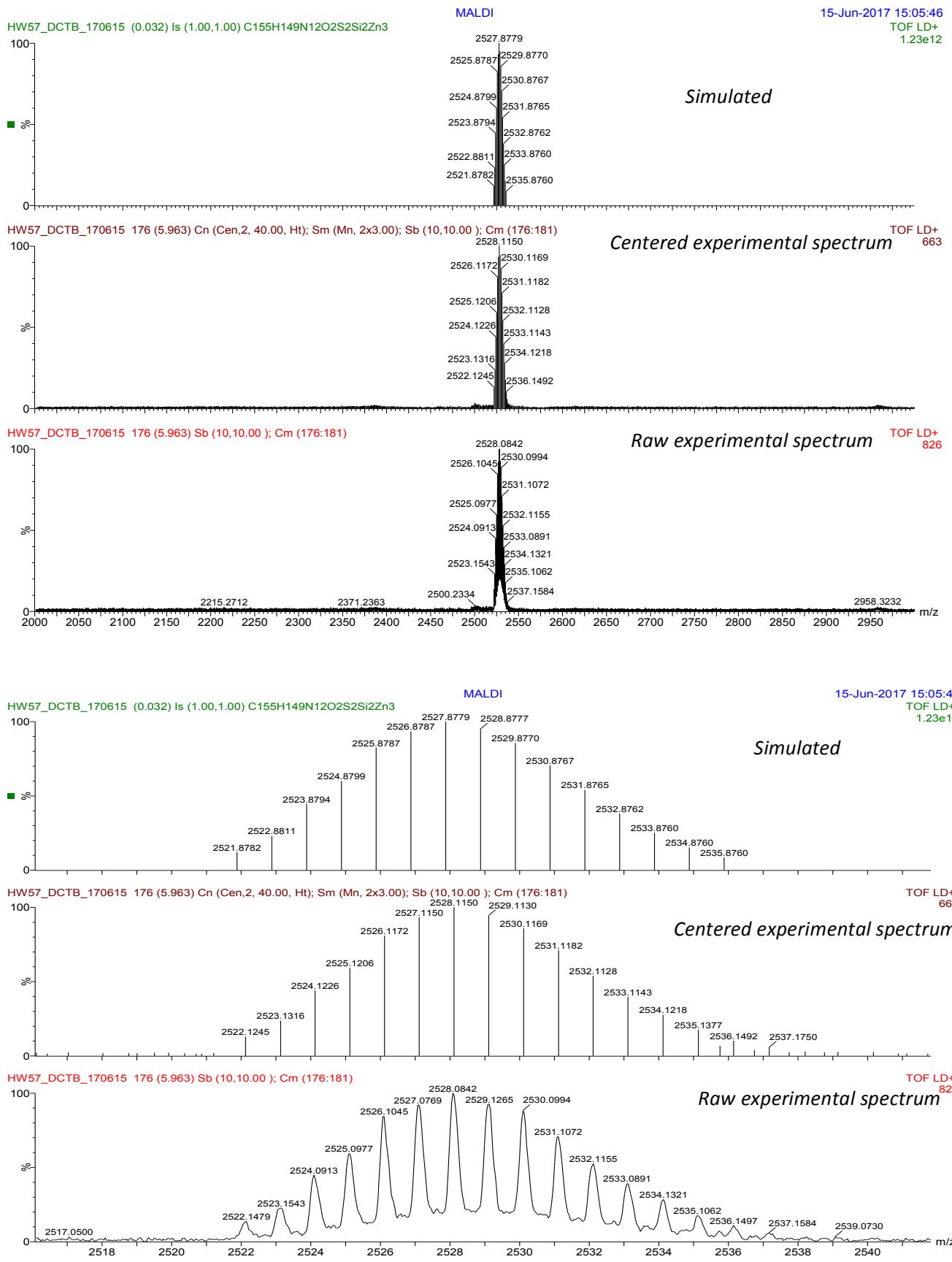
¹H NMR (CDCl_3 , 400 MHz, 298K):



¹³C NMR (CDCl_3 , 100 MHz, 298K):

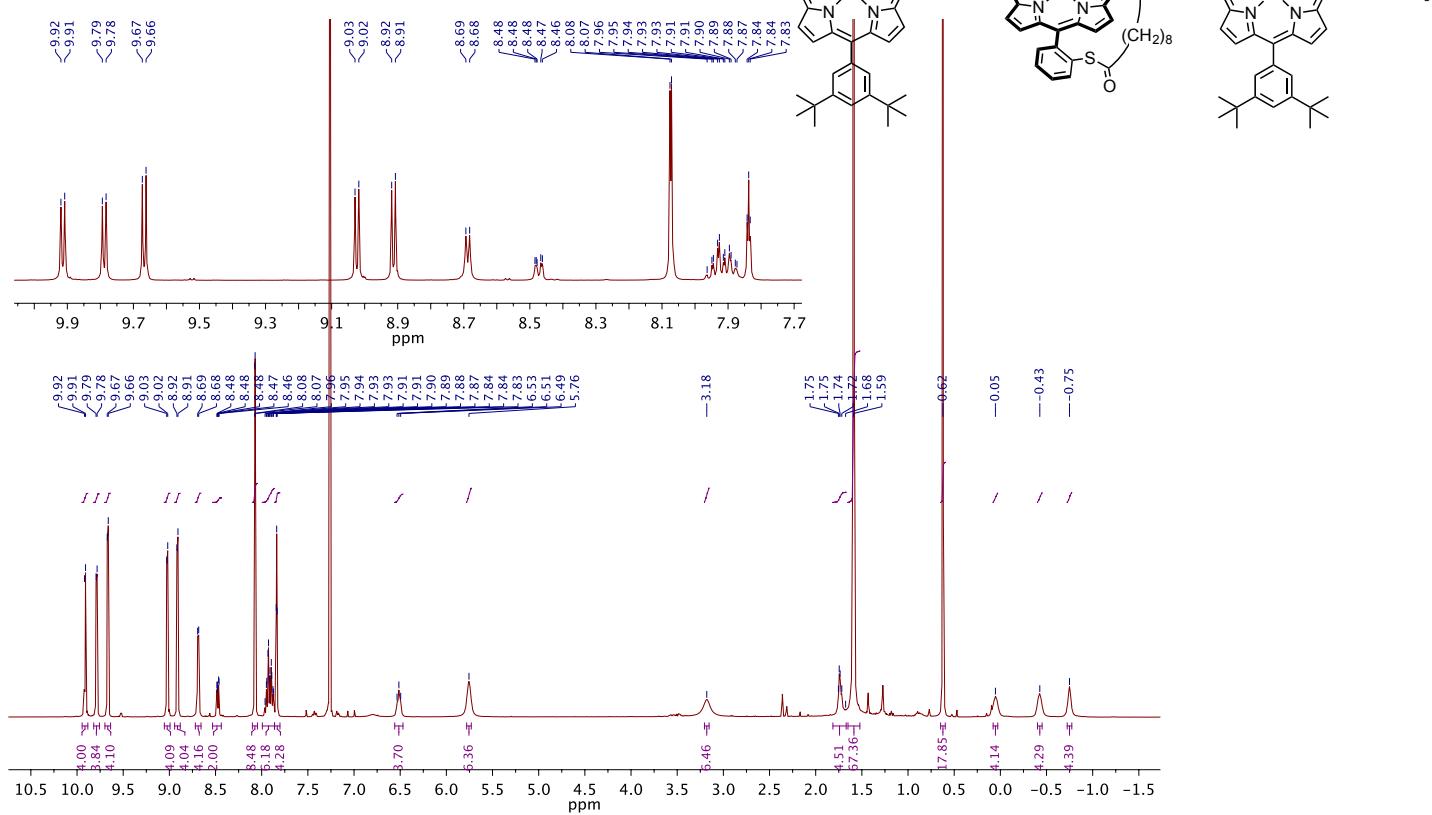


MALDI-TOF:

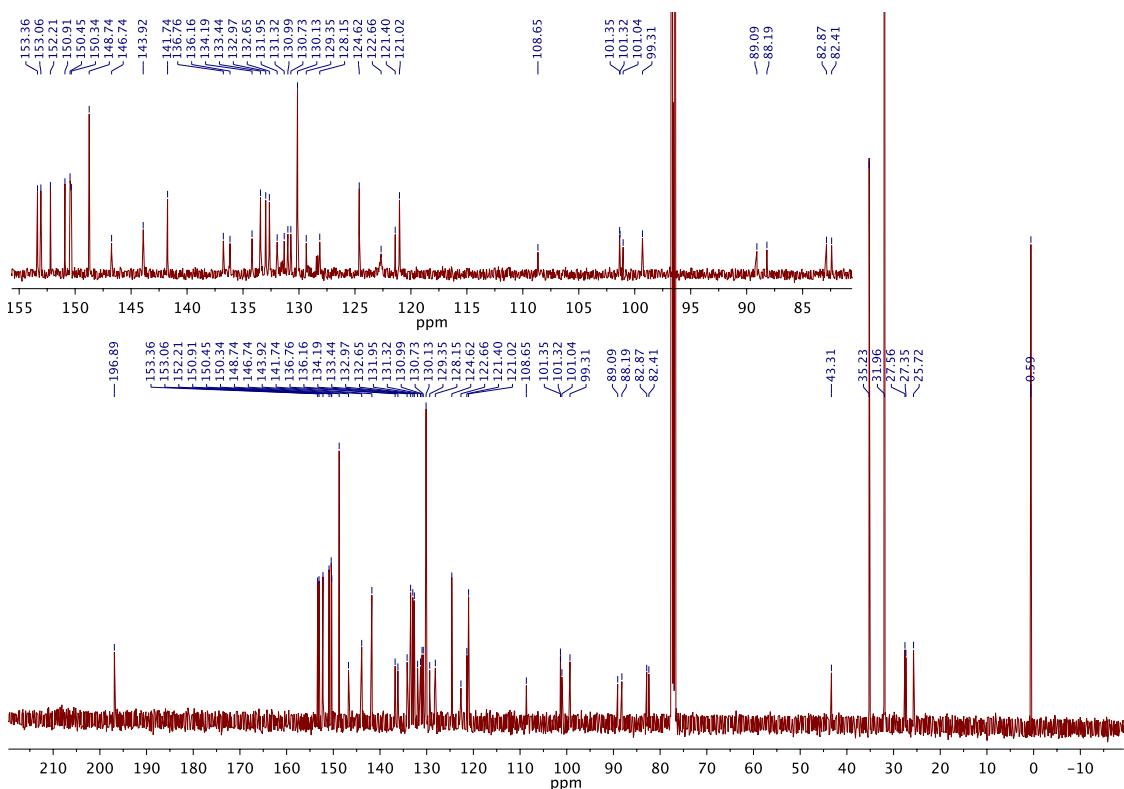


4.24. C₈-Strapped bis-TMS porphyrin trimer 11b

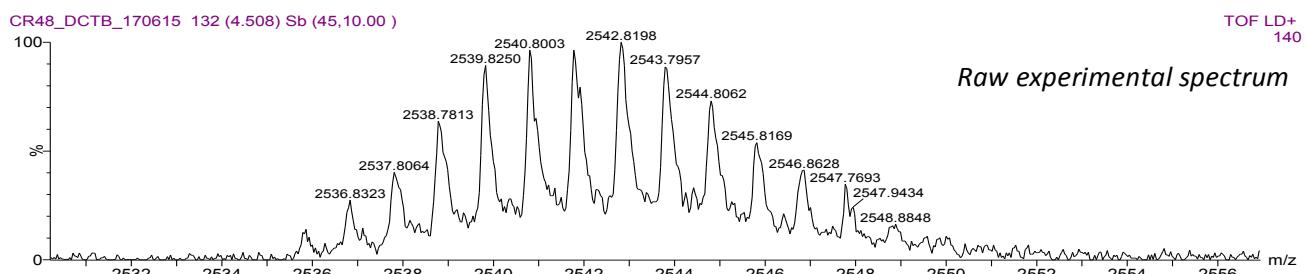
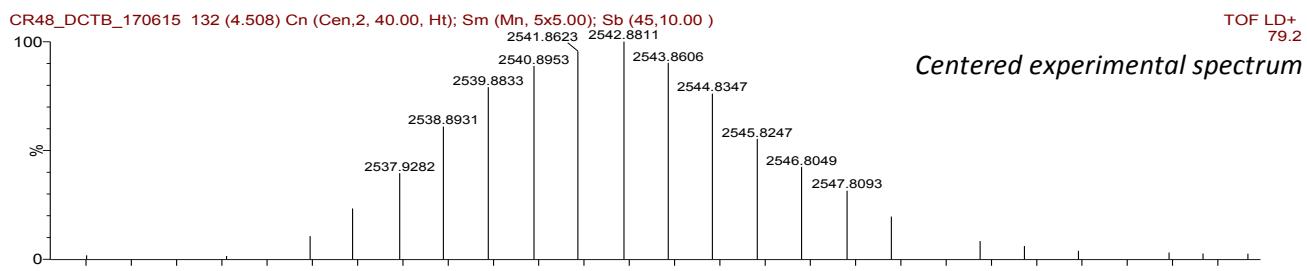
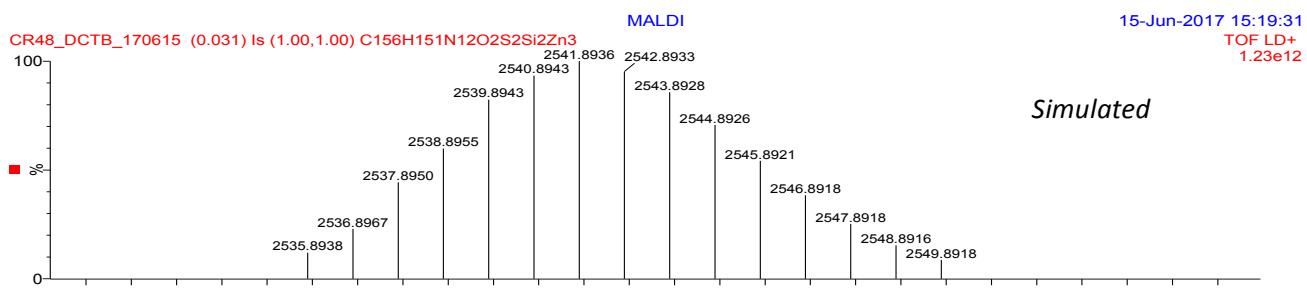
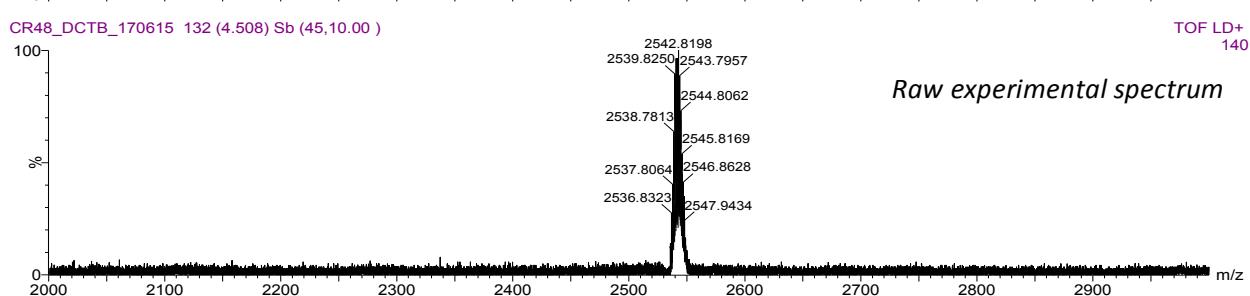
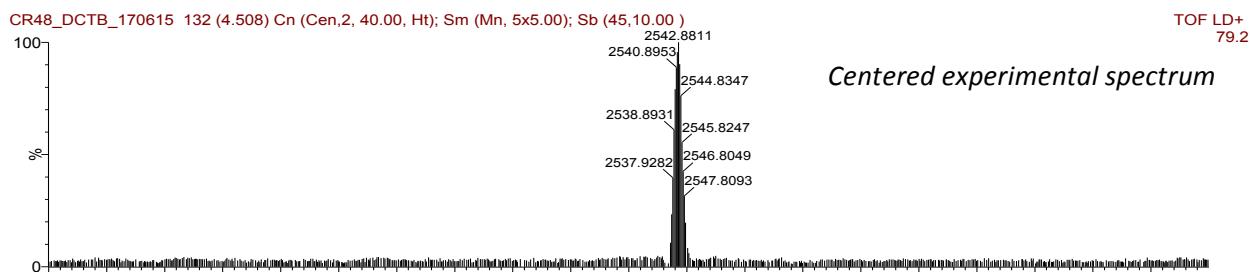
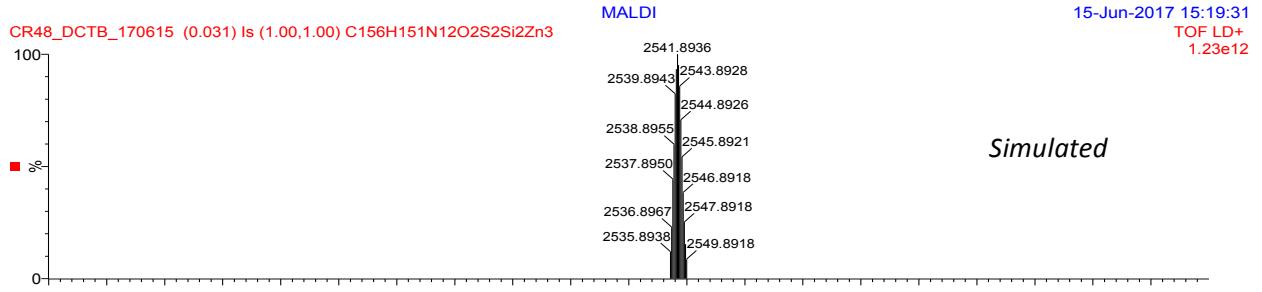
¹H NMR (CDCl₃, 400 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):

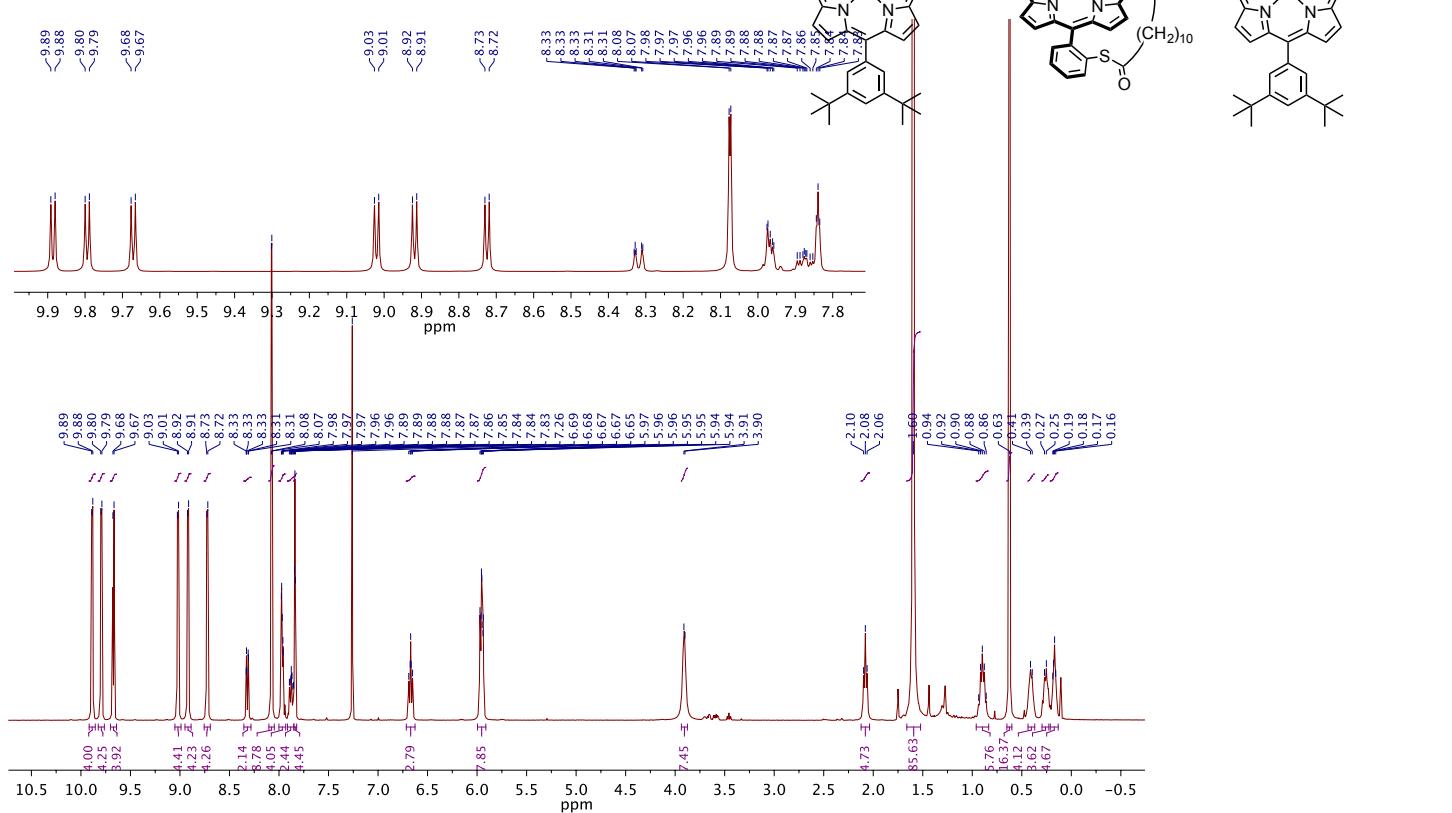


MALDI-TOF:

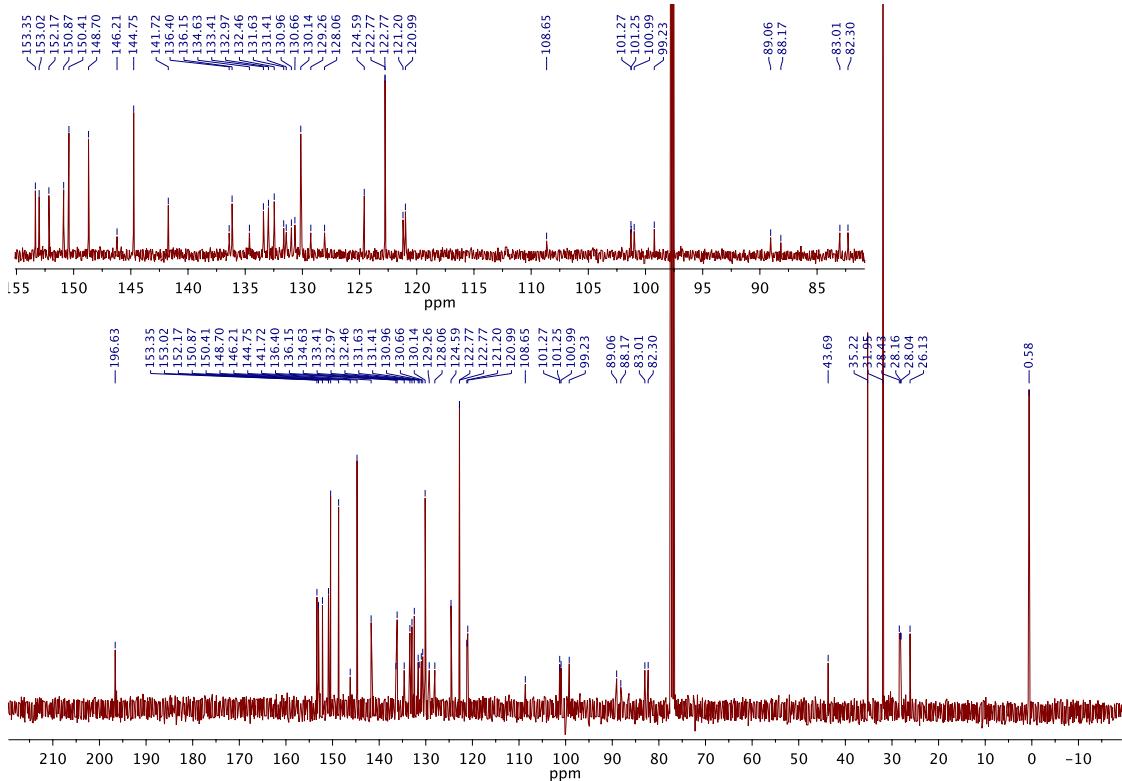


4.25. C₁₀-Strapped bis-TMS porphyrin trimer 11c

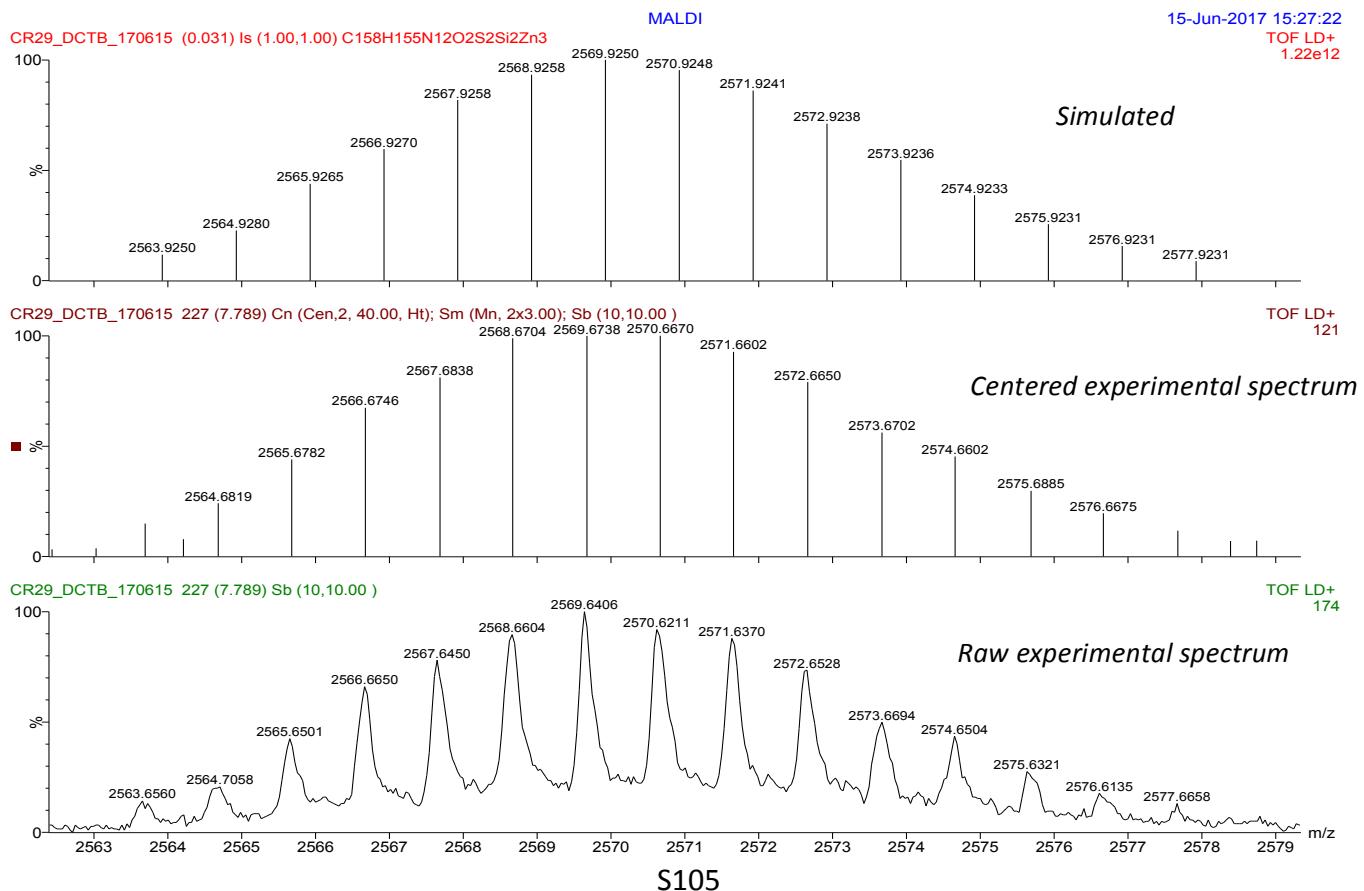
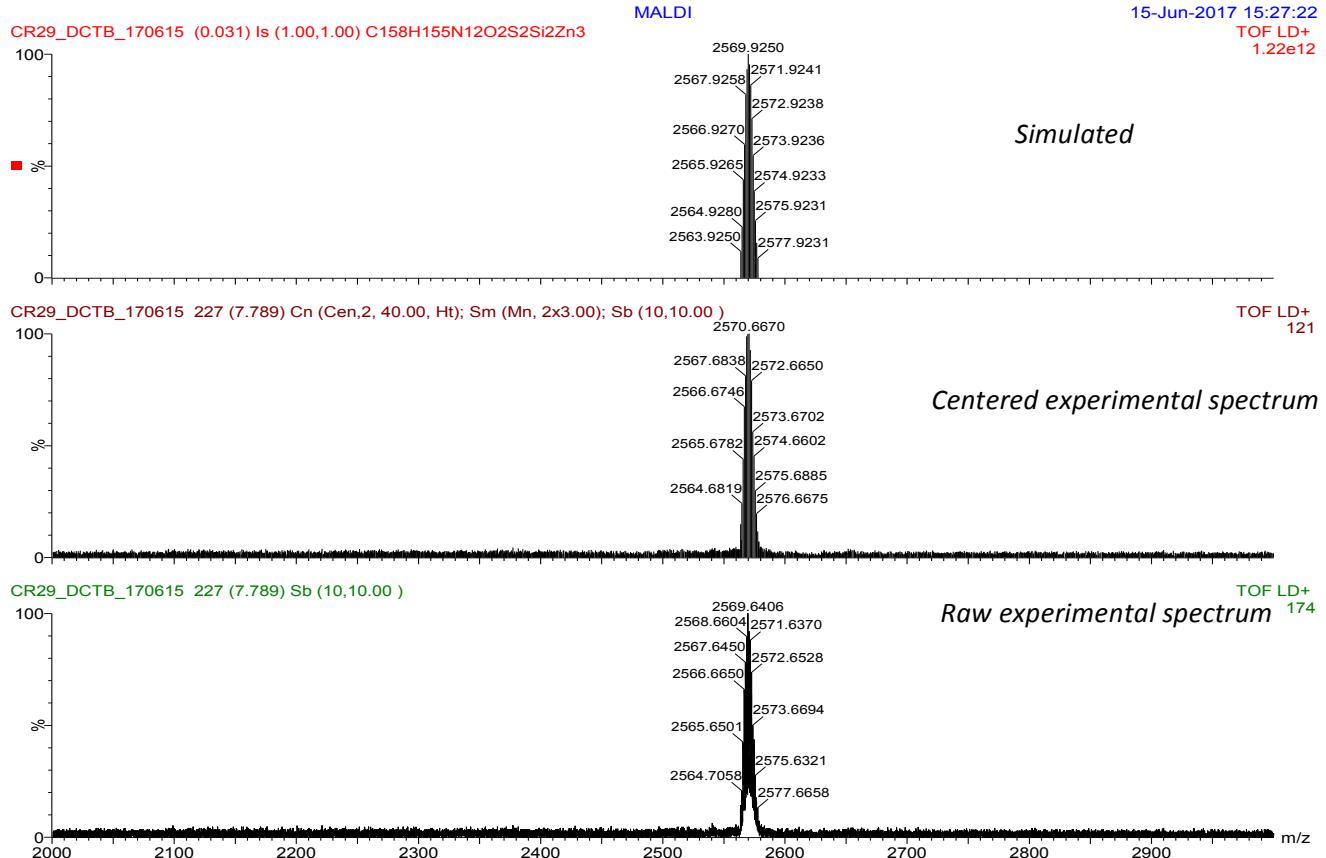
¹H NMR (CDCl₃, 400 MHz, 298K):



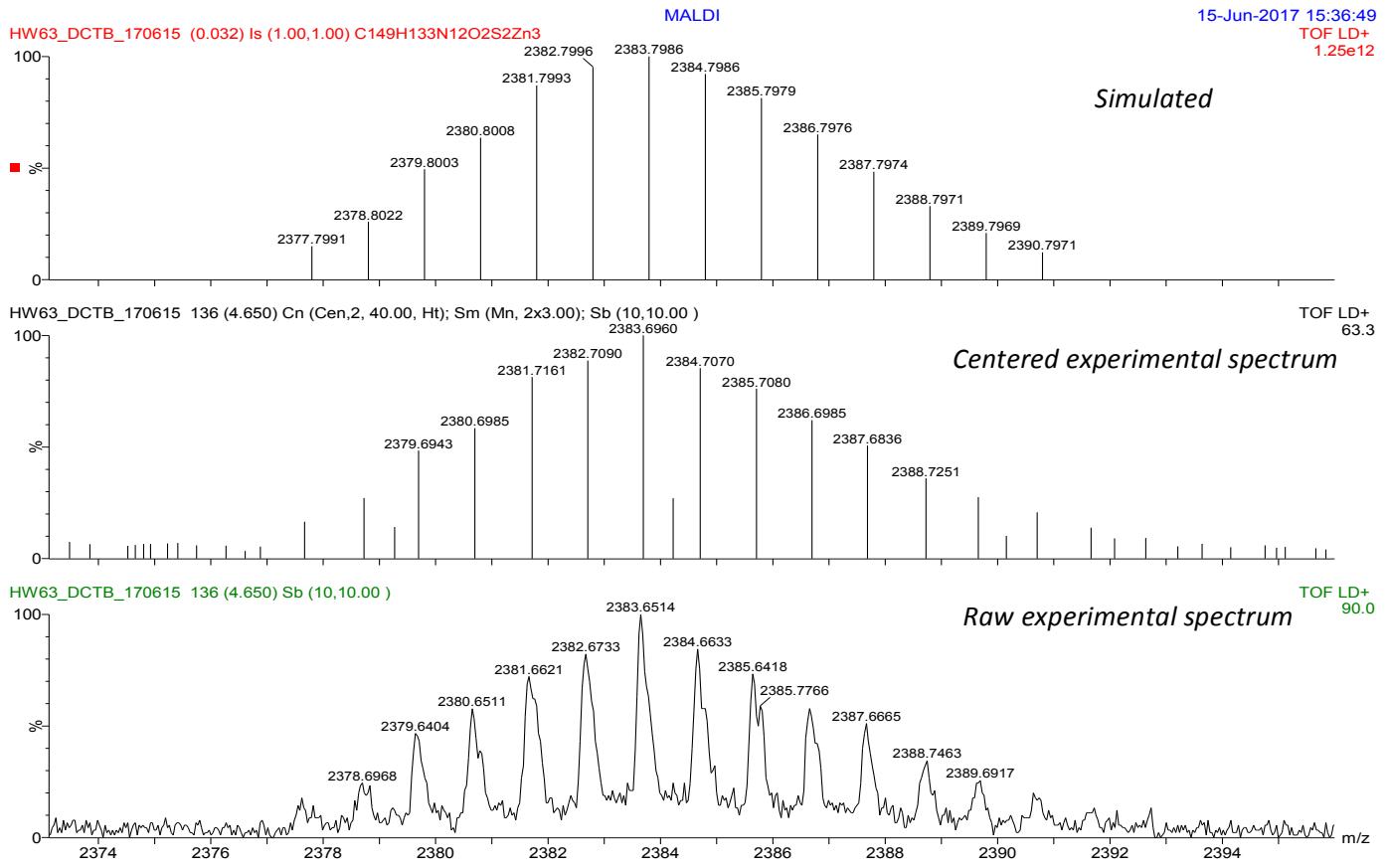
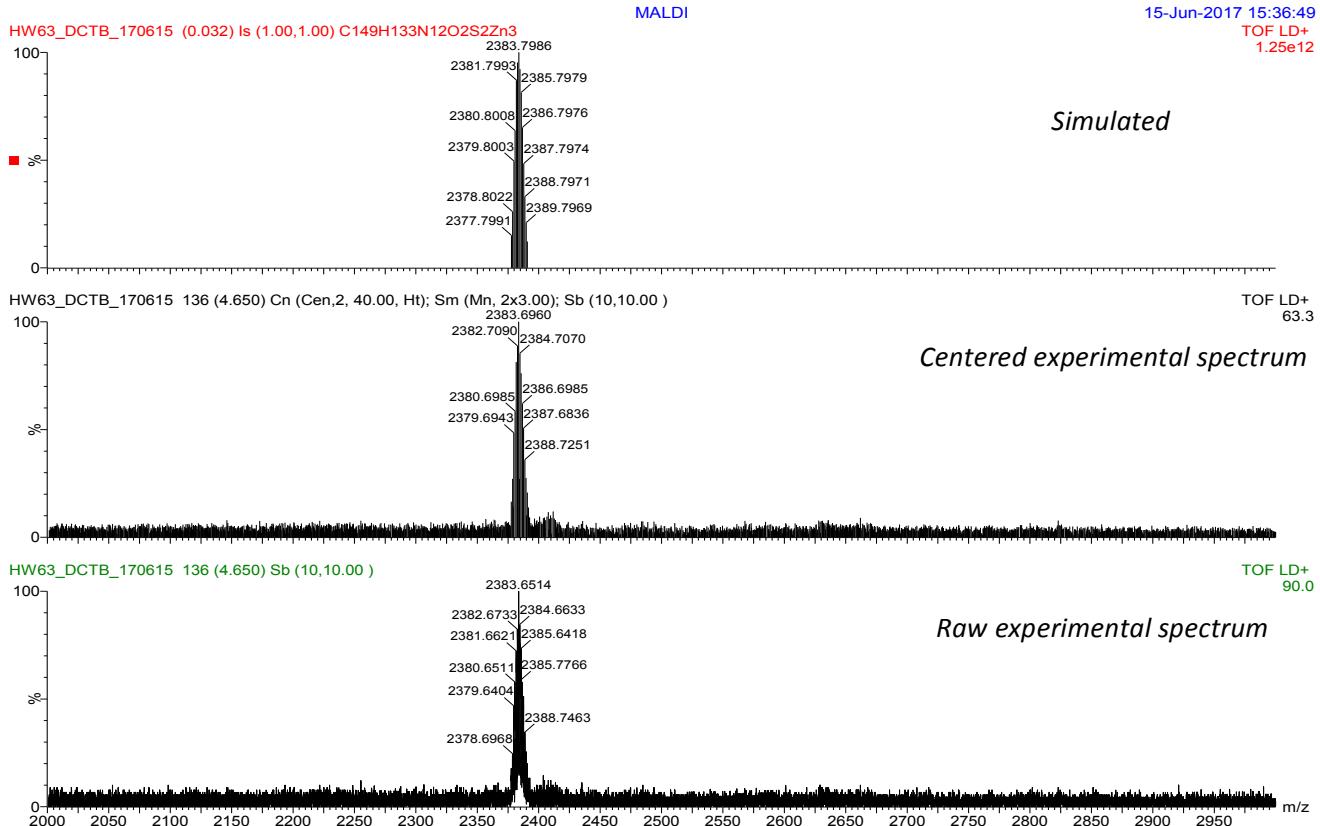
¹³C NMR (CDCl₃, 100 MHz, 298K):



MALDI-TOF:

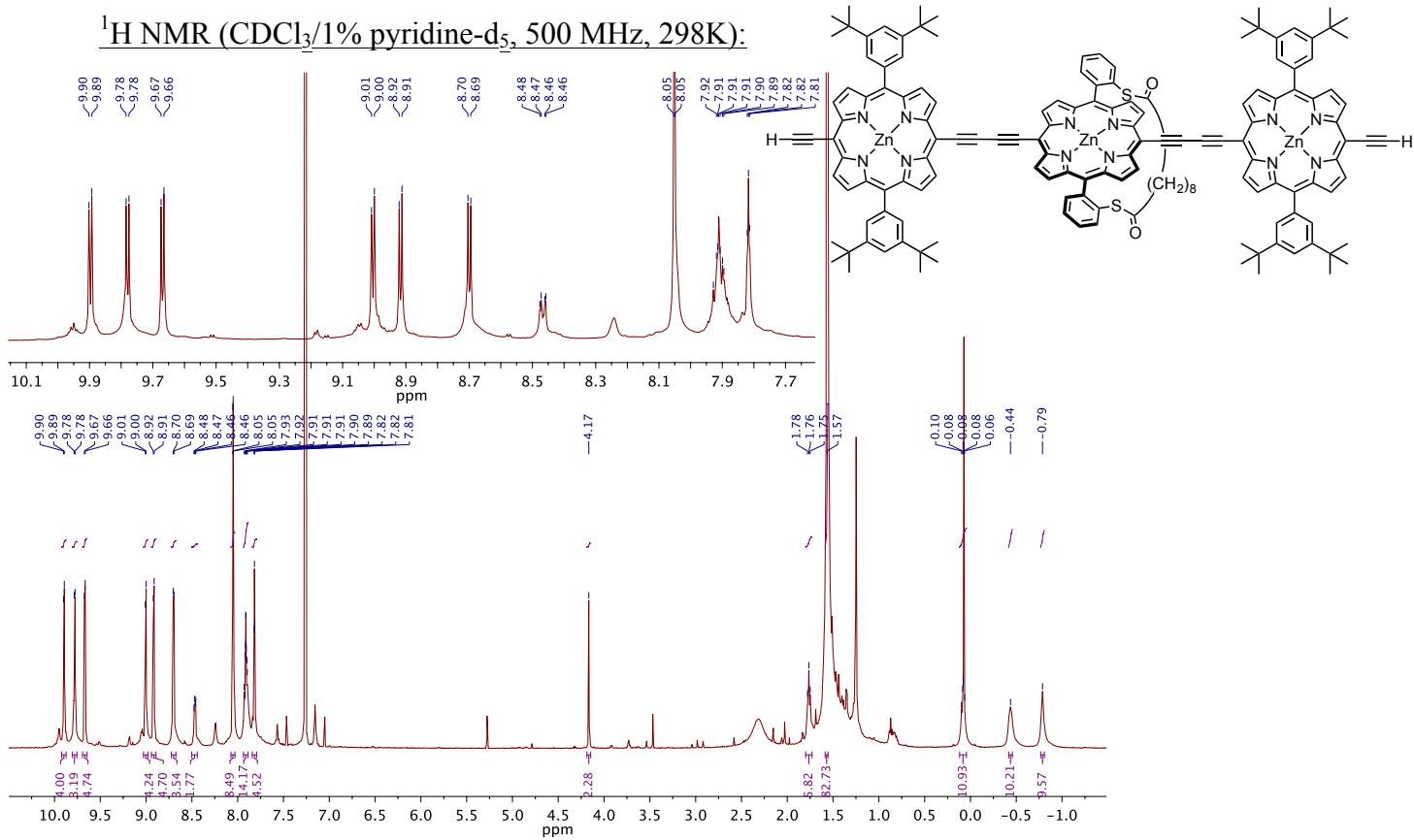


MALDI-TOF:

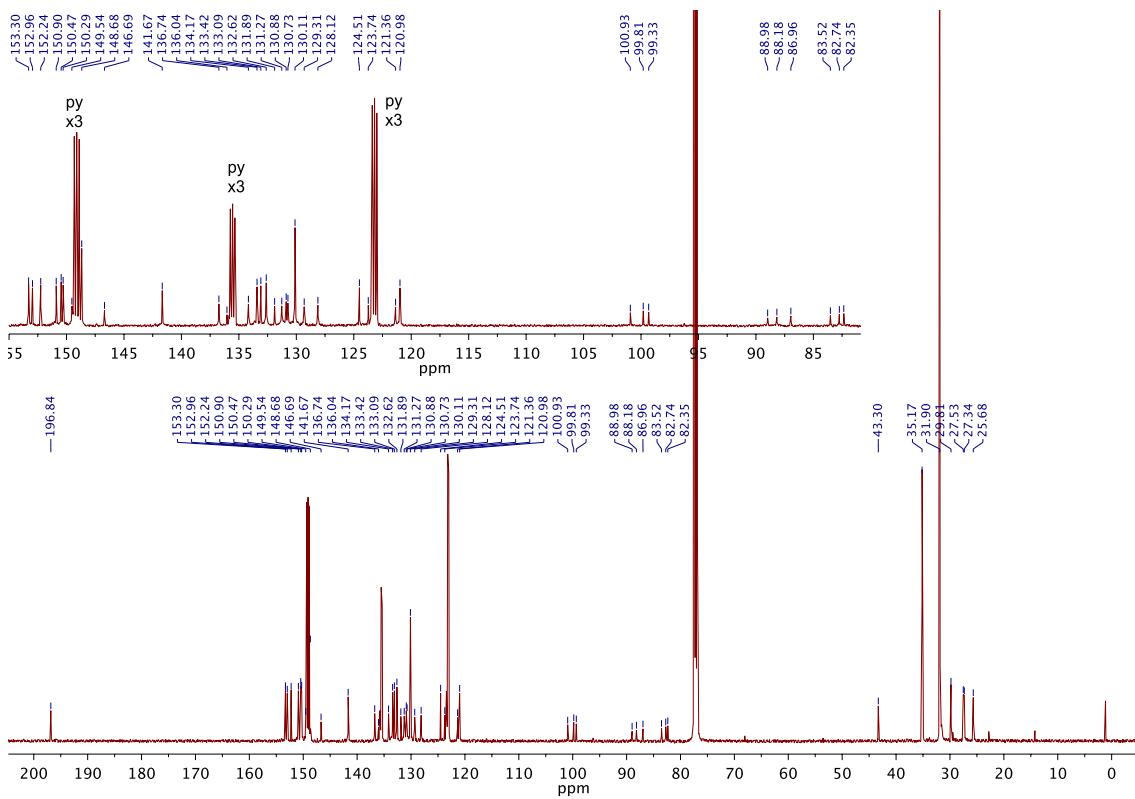


4.27. C₈-Strapped bis-deprotected porphyrin trimer 12b

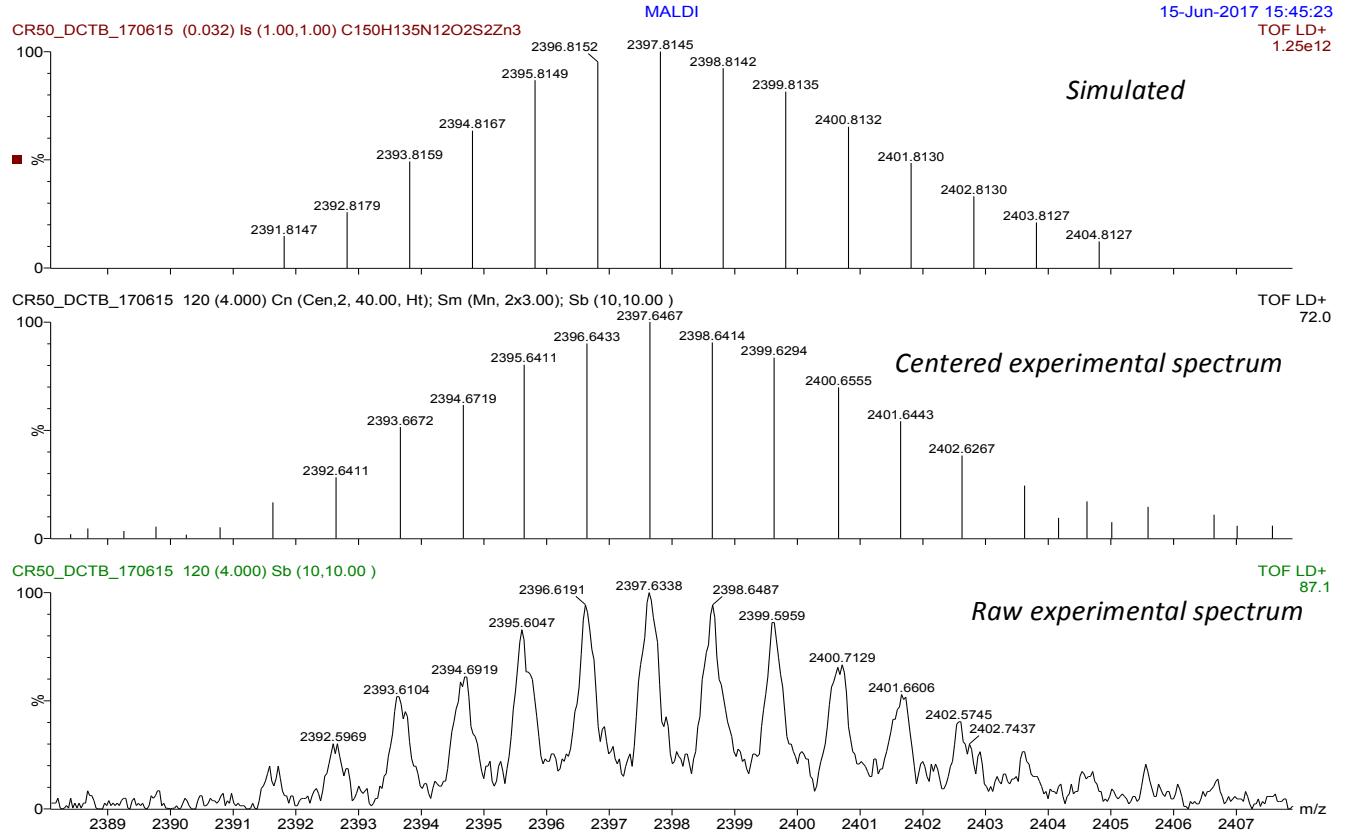
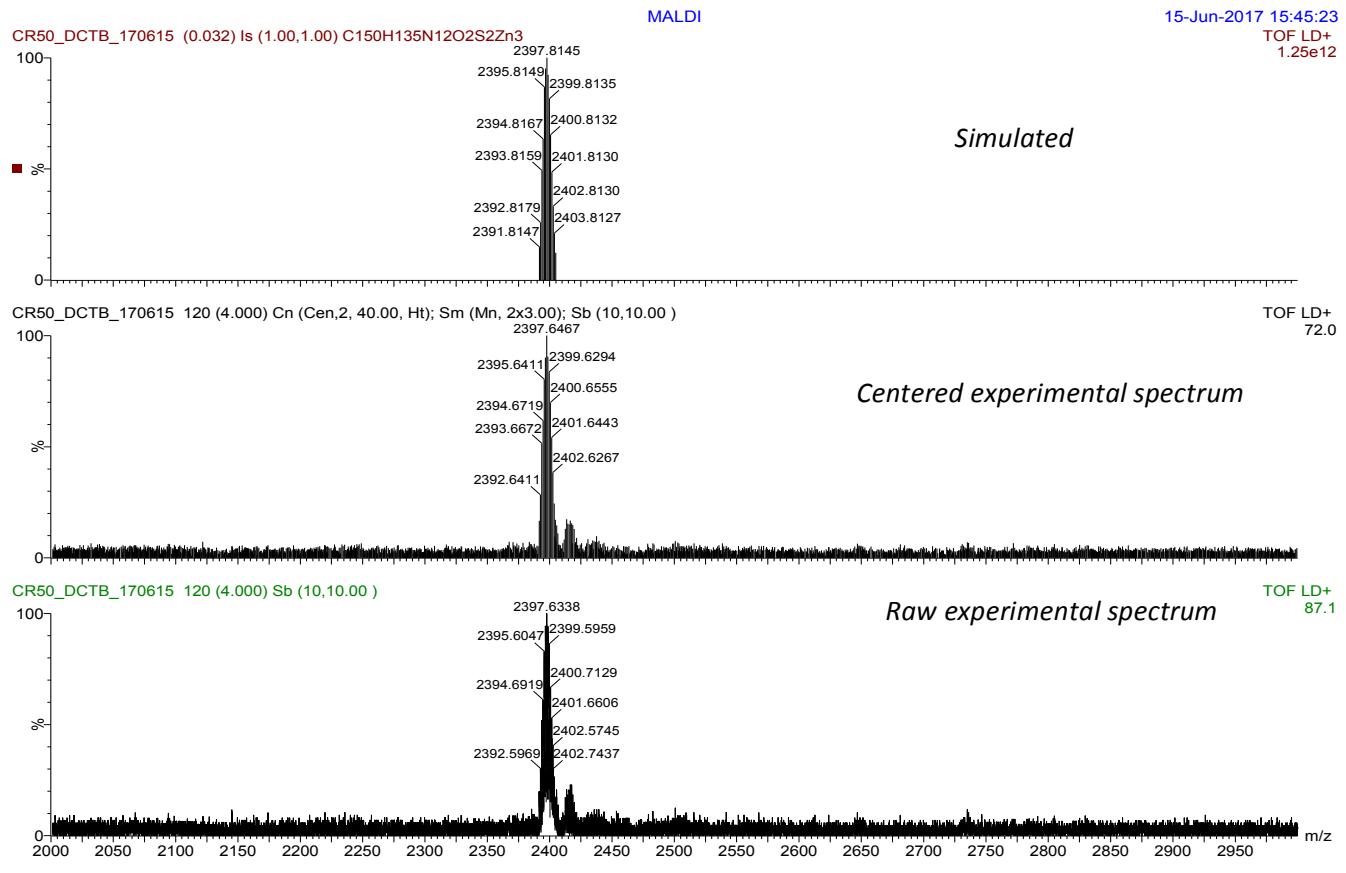
¹H NMR (CDCl₃/1% pyridine-d₅, 500 MHz, 298K):



¹³C NMR (CDCl₃/1% pyridine-d₅, 125 MHz, 298K):

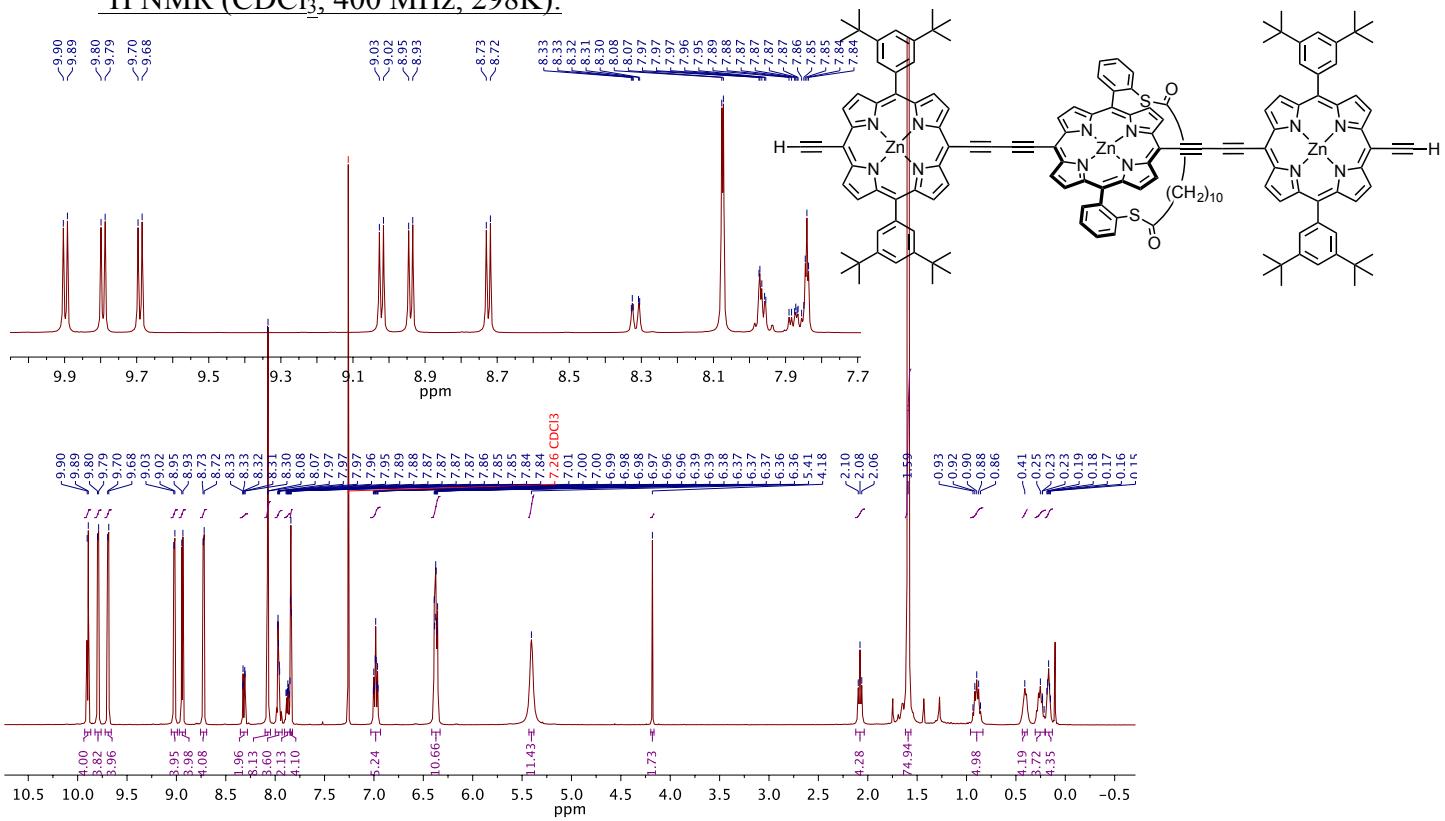


MALDI-TOF:

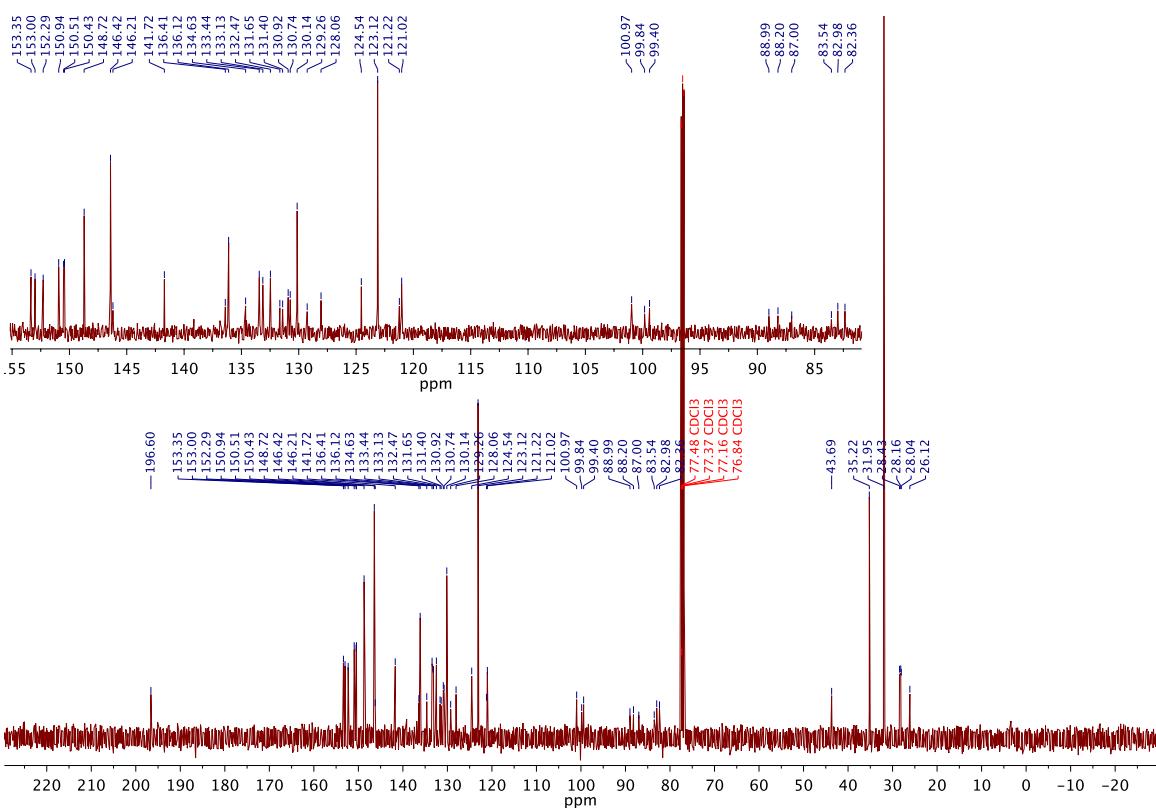


4.28. C₁₀-Strapped bis-deprotected porphyrin trimer 12c

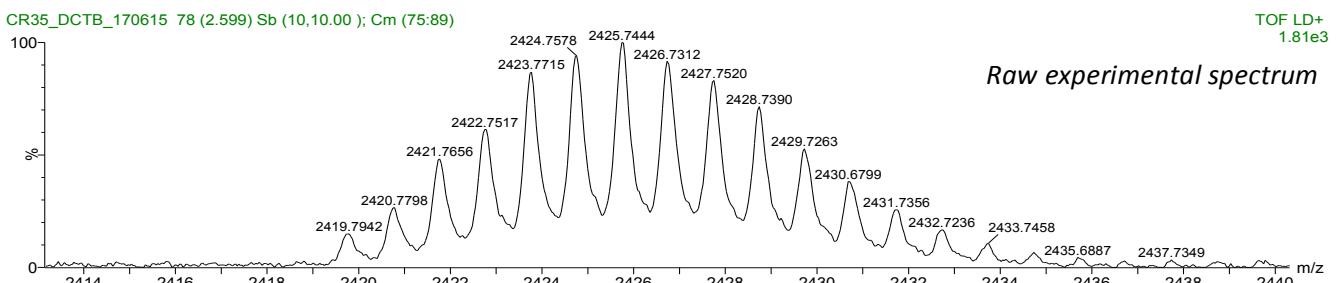
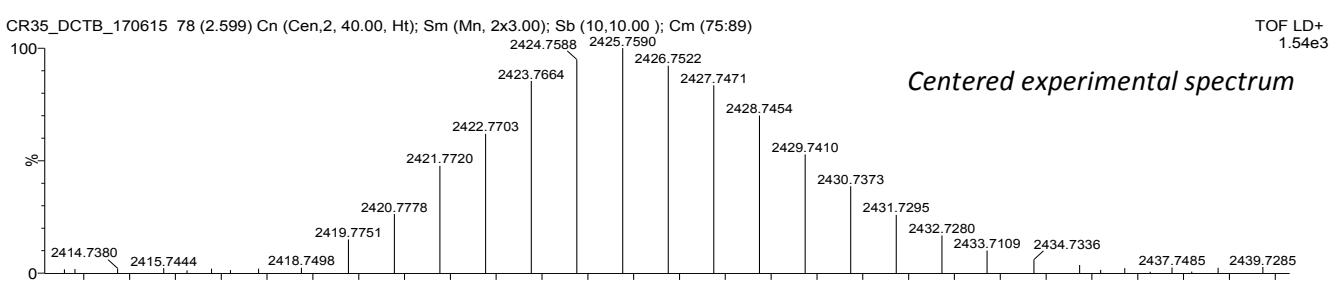
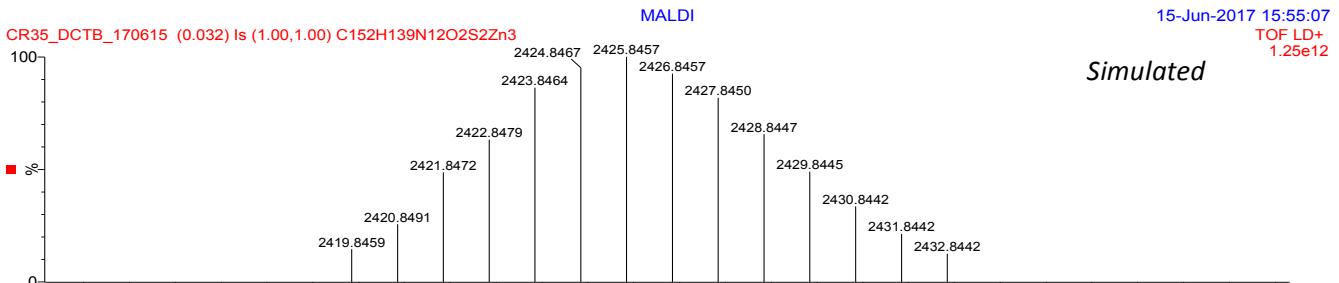
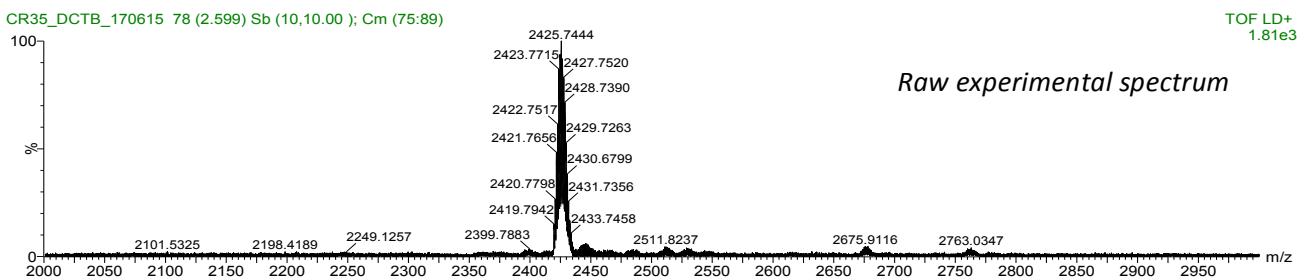
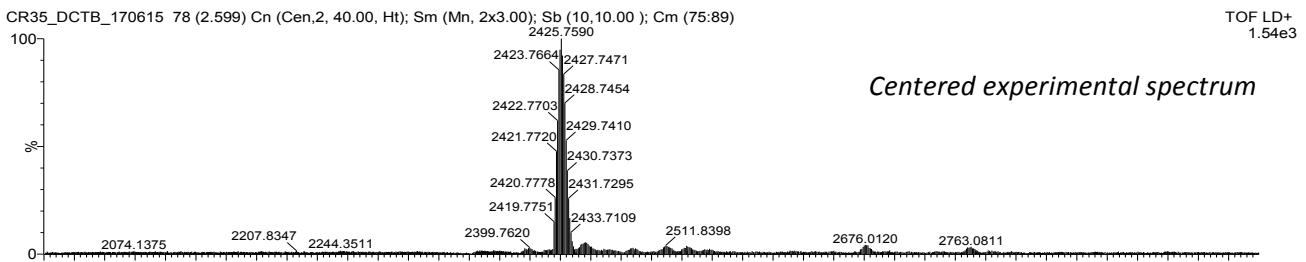
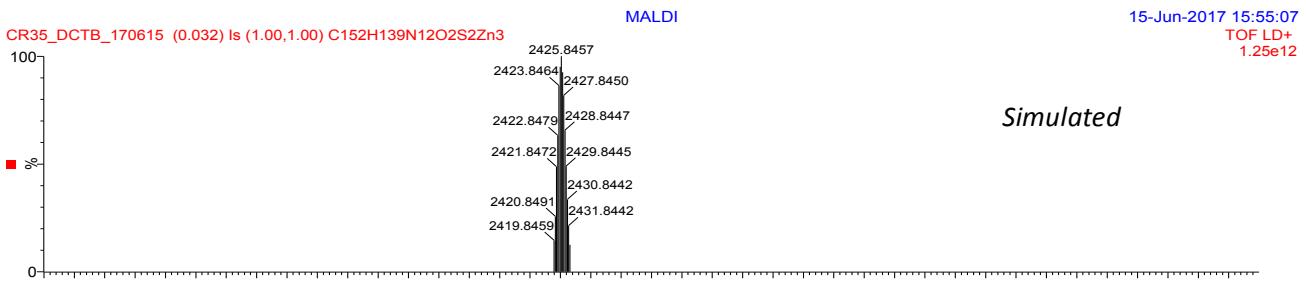
¹H NMR (CDCl₃, 400 MHz, 298K):



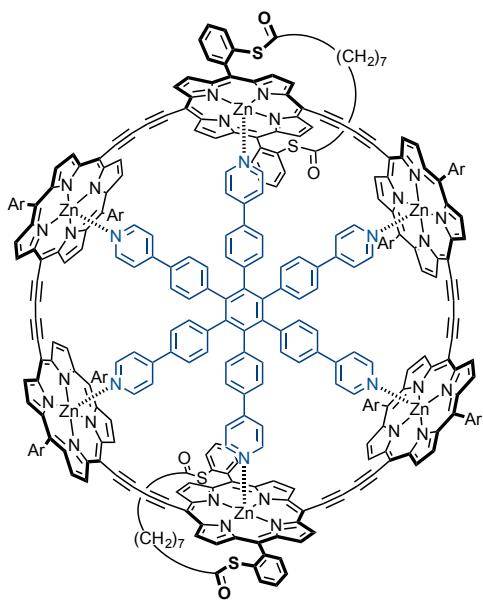
¹³C NMR (CDCl₃, 100 MHz, 298K):



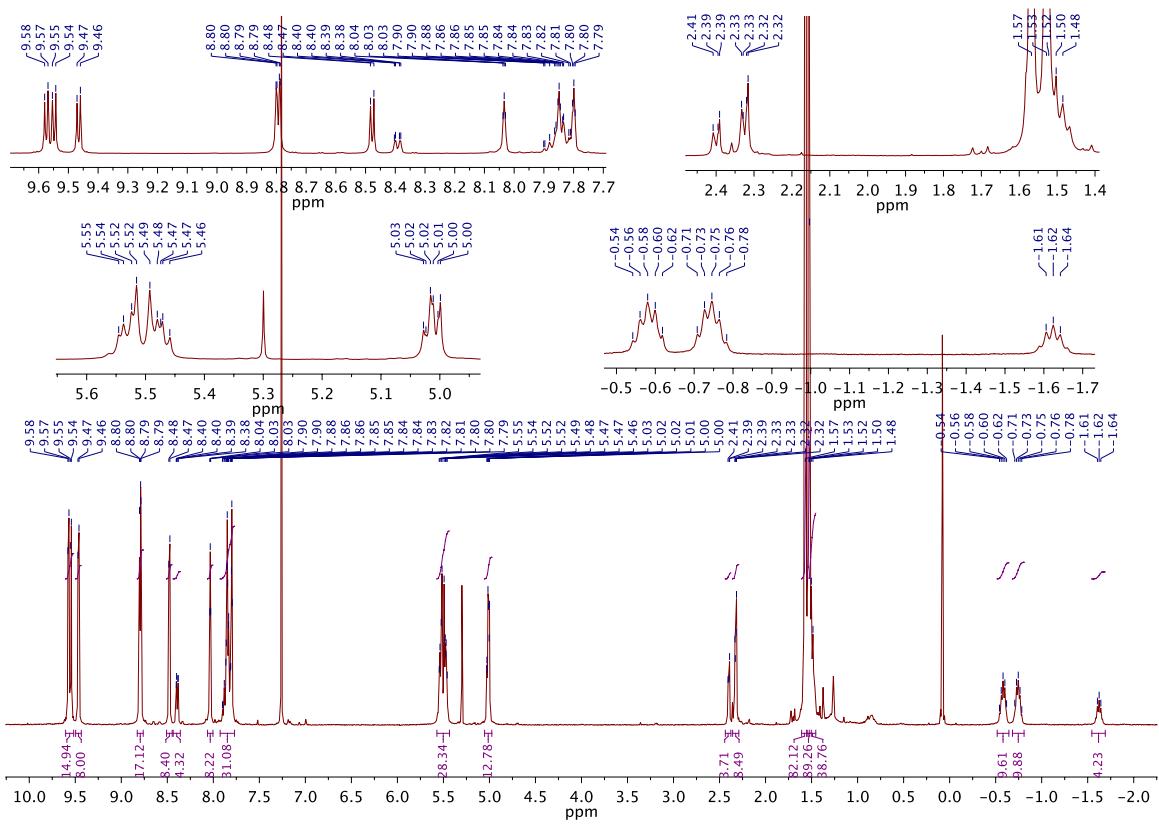
MALDI-TOF:



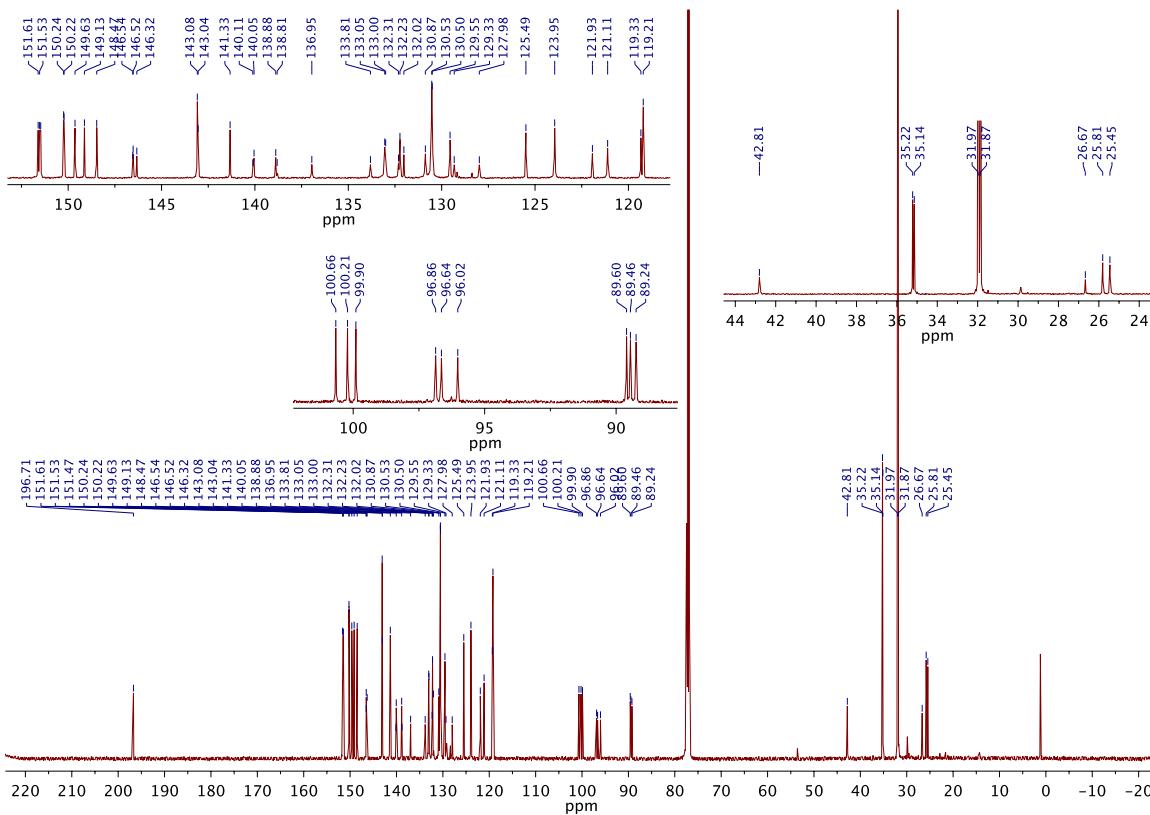
4.29. C₇-Strapped porphyrin nanoring *c*-P6_{S-C7}•T6



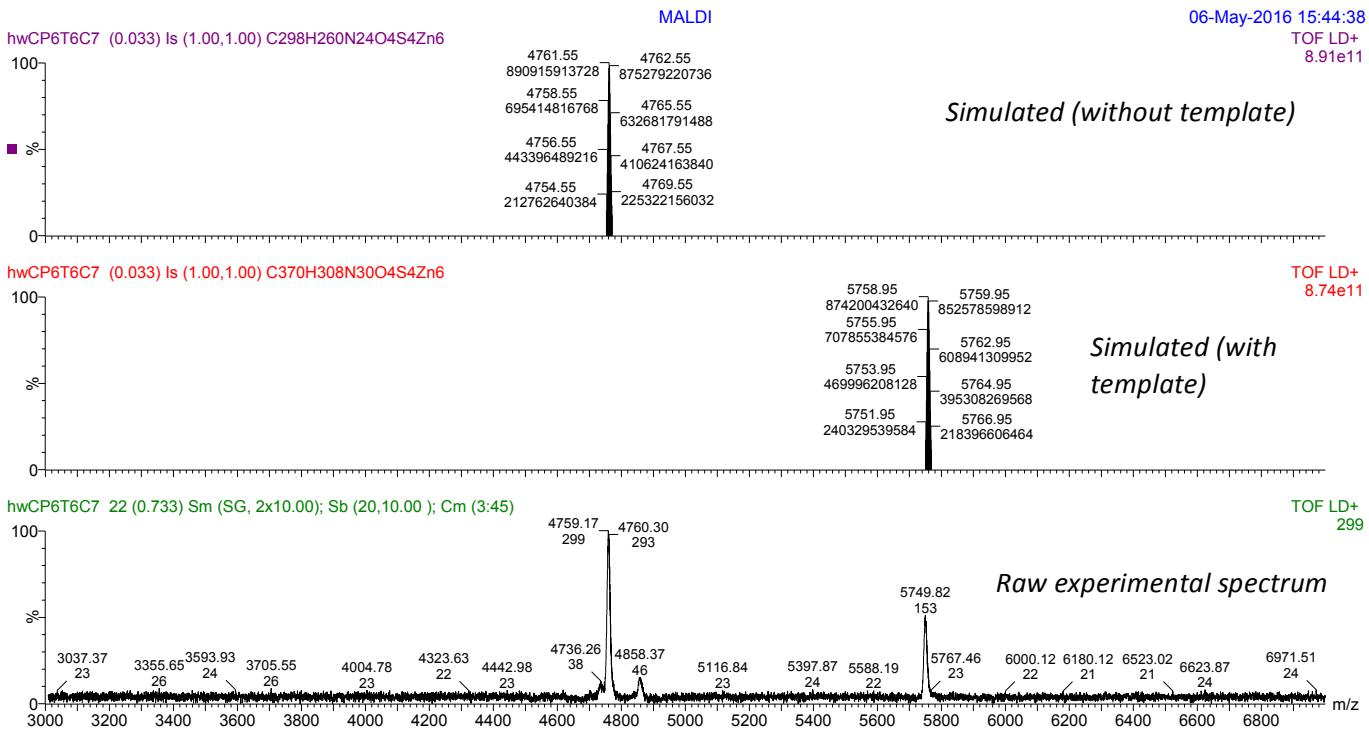
¹H NMR (CDCl_3 , 500 MHz, 298K):



¹³C NMR (CDCl₃, 100 MHz, 298K):



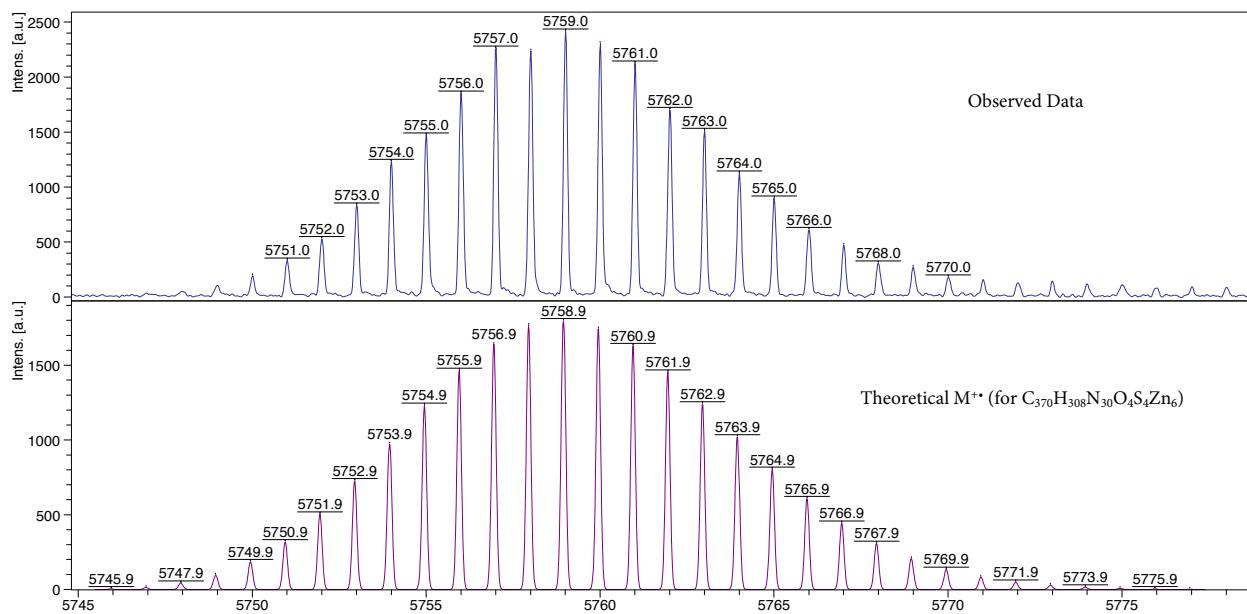
MALDI-TOF:



EPSRC UK National Mass Spectrometry Facility (NMSF), Swansea

D:\Data\NMSF\2016\June\OXFAND-QAQZN-UM-B\0_G5\1SRef

Comment 1 Prof. Anderson HW66 MW=5745?? PosRef Tol./%Pyr. [1:24] (DCTB;Tol./%Pyr.)



ultralleXtreme MALDI

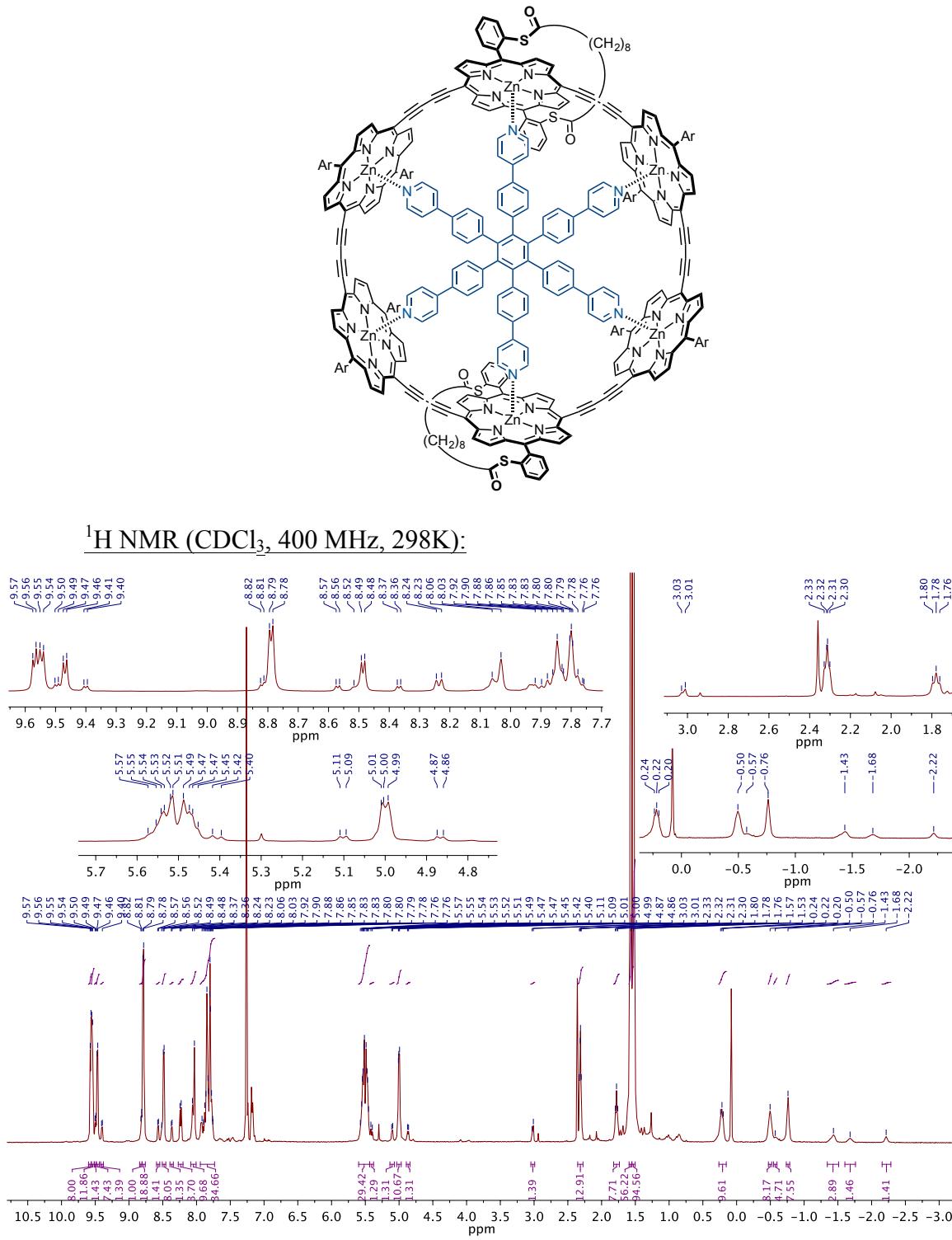
Date of Acquisition

2016-06-21T09:20:15.513+01:00

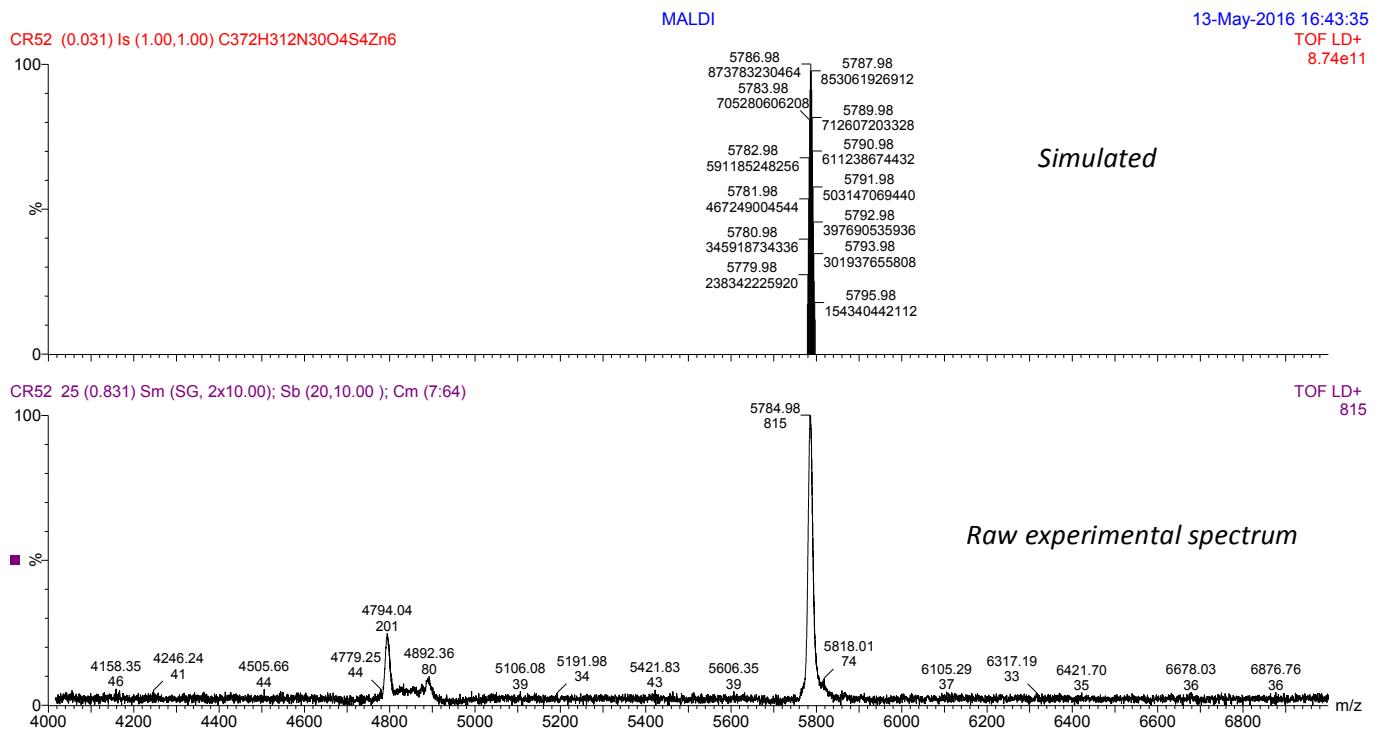
Printed

21/06/2016 14:31:03

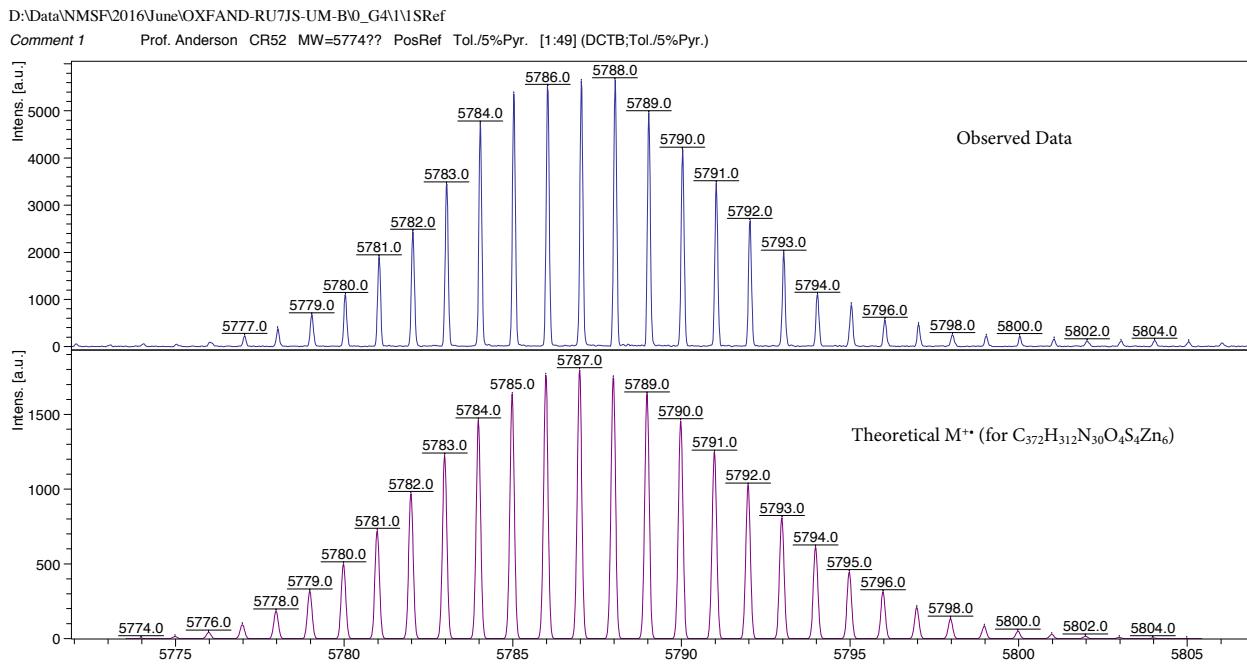
4.30. C₈-Strapped porphyrin nanoring c-P6_{S-C8}•T6



MALDI-TOF:



EPSRC UK National Mass Spectrometry Facility (NMSF), Swansea



ultraflexXtreme MALDI

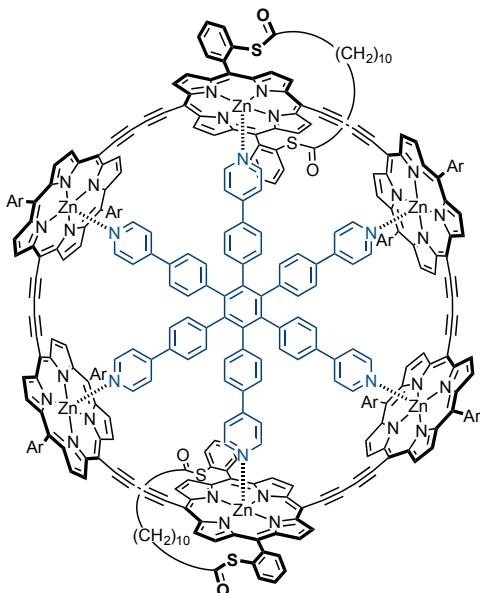
Date of Acquisition

2016-06-21T09:17:25.363+01:00

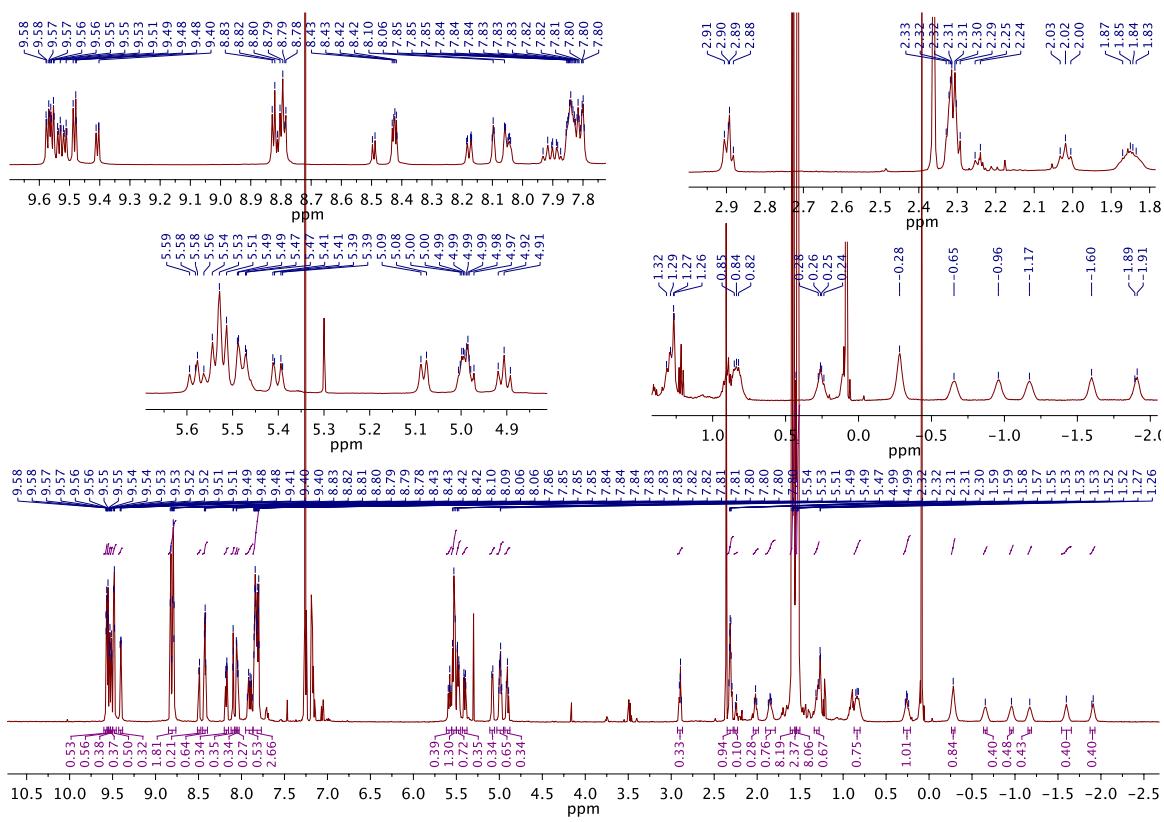
Printed

21/06/2016 14:24:19

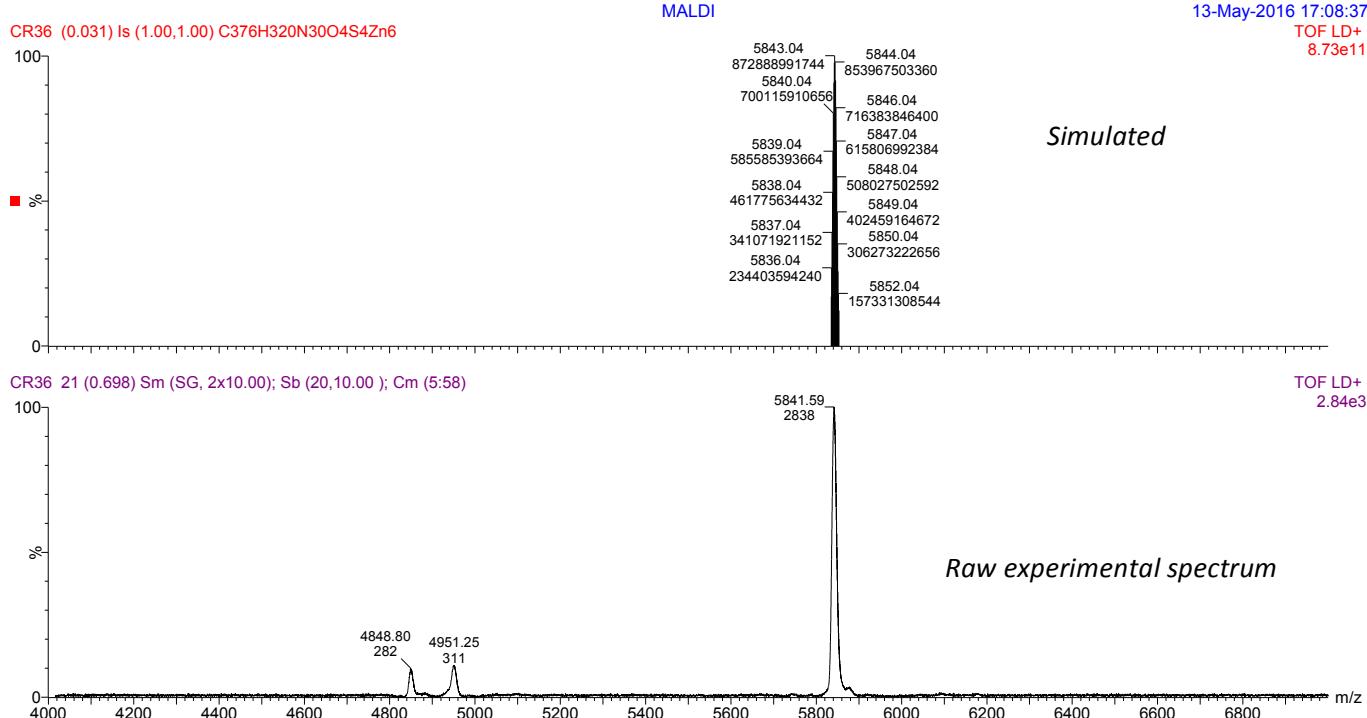
4.31. C₁₀-Strapped porphyrin nanoring c-P6S-C10•T6



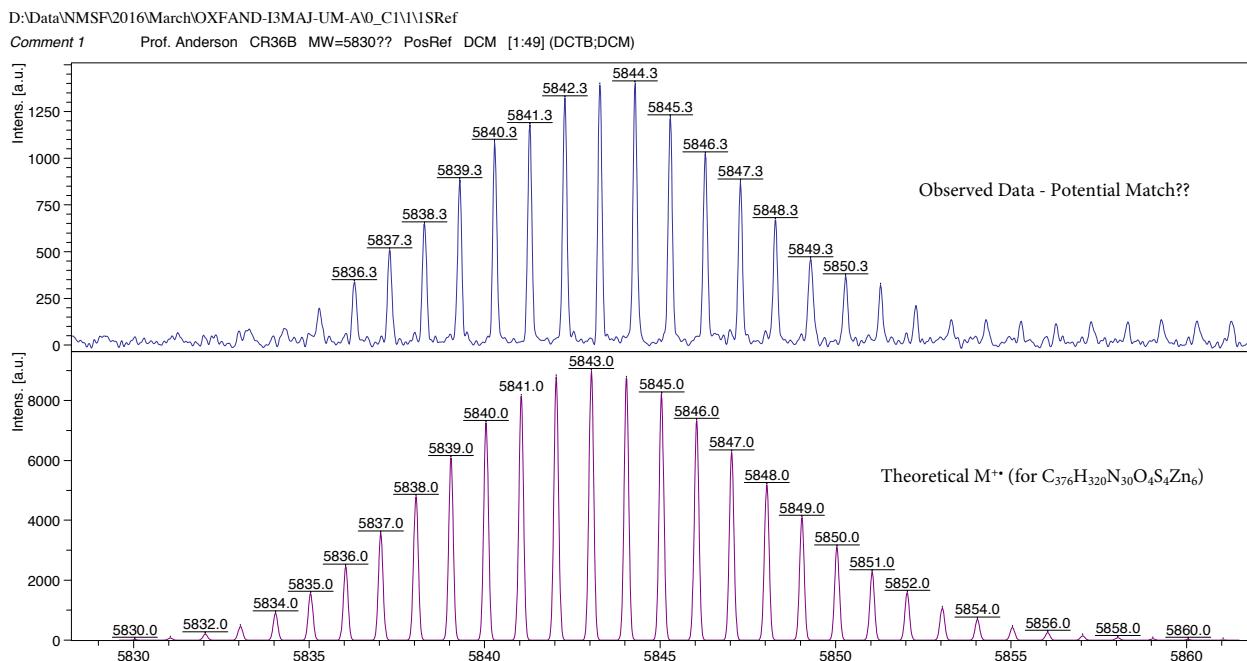
¹H NMR (CDCl₃, 500 MHz, 298K):



MALDI-TOF:



EPSRC UK National Mass Spectrometry Facility (NMSF), Swansea



ultraflleXtreme MALDI

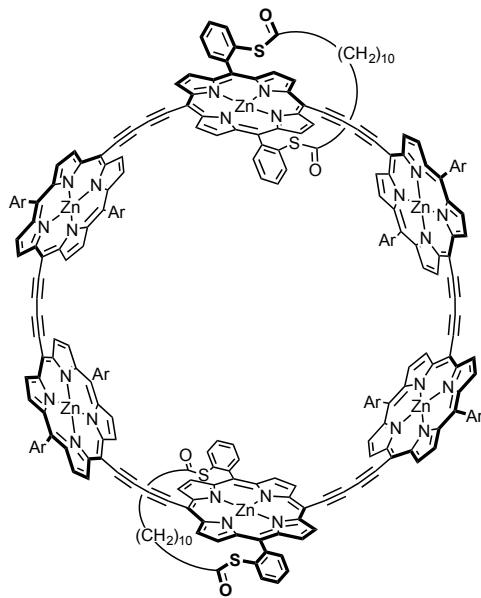
Date of Acquisition

2016-03-09T13:18:27.546+00:00

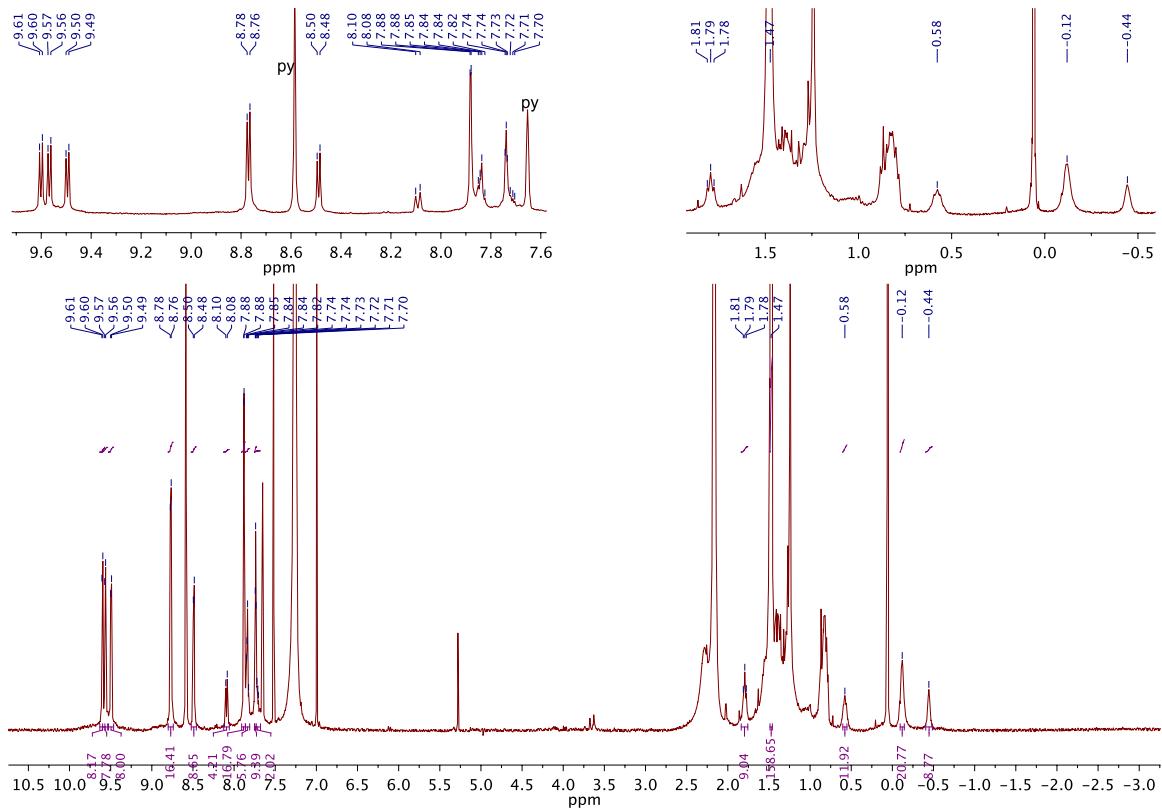
Printed

09/03/2016 13:52:06

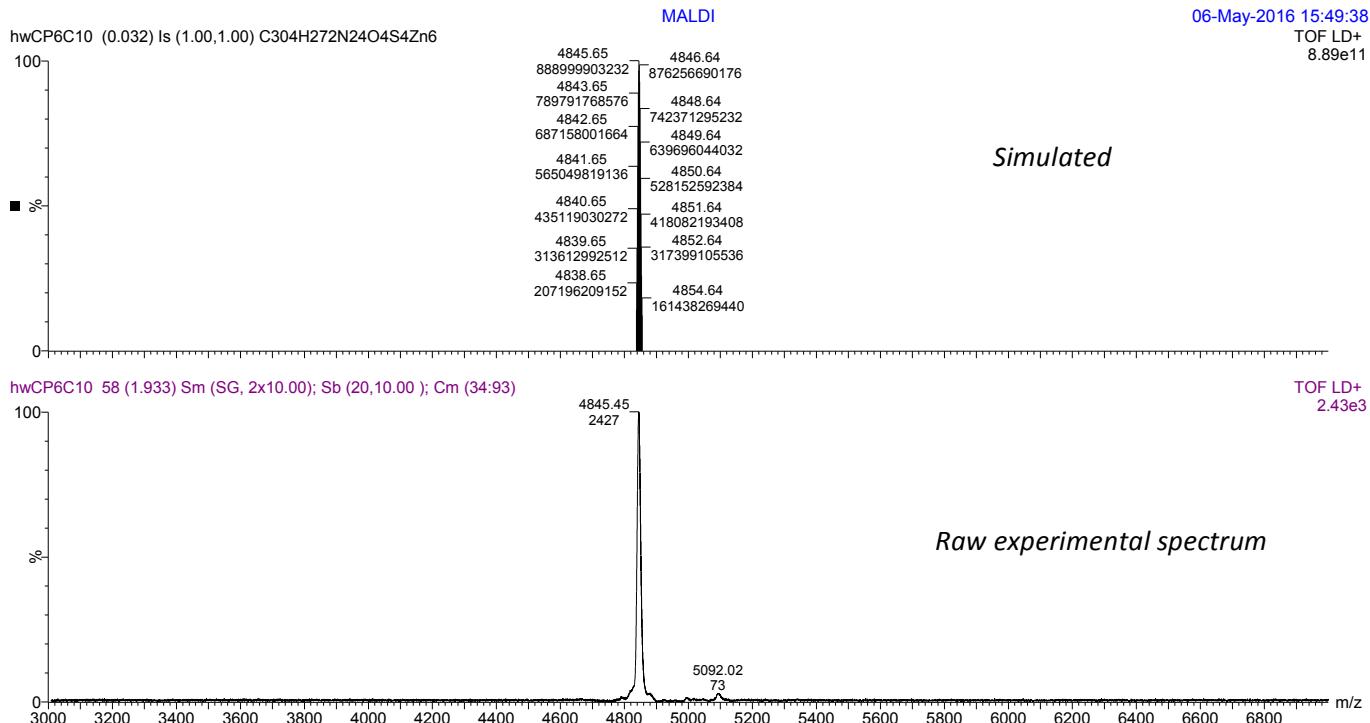
4.32. Template-free C₁₀-strapped porphyrin nanoring c-P6S-C₁₀



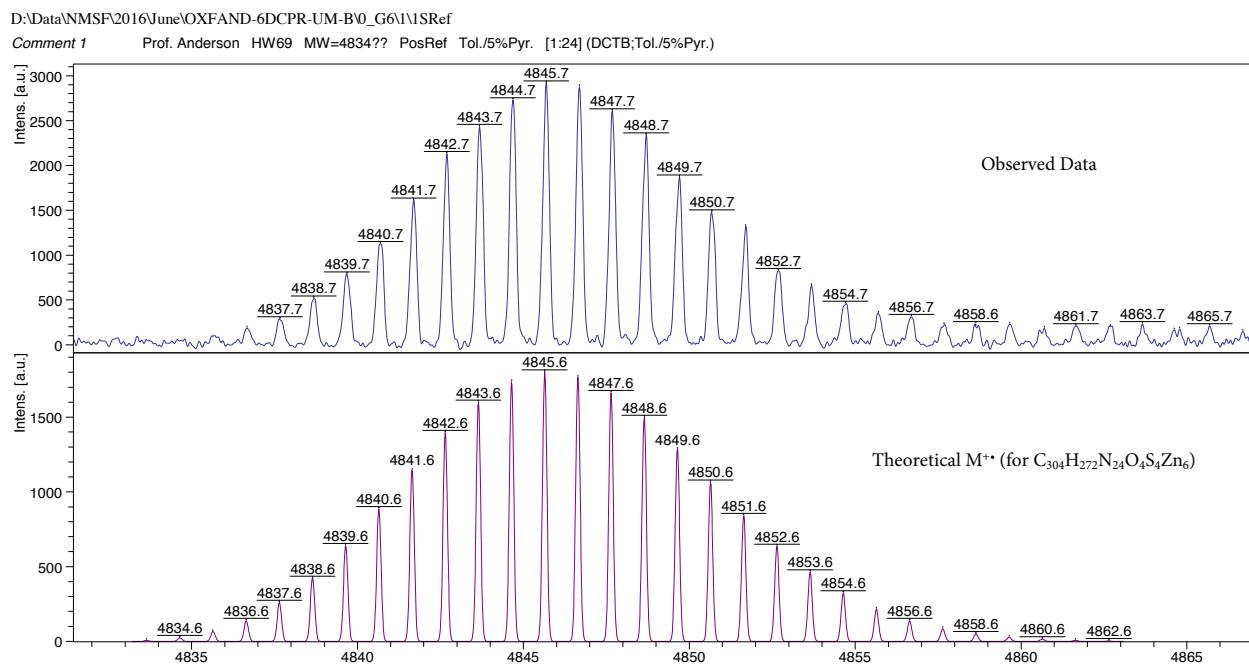
¹H NMR (CDCl₃/1% pyridine-d₅, 400 MHz, 298K):



MALDI-TOF:



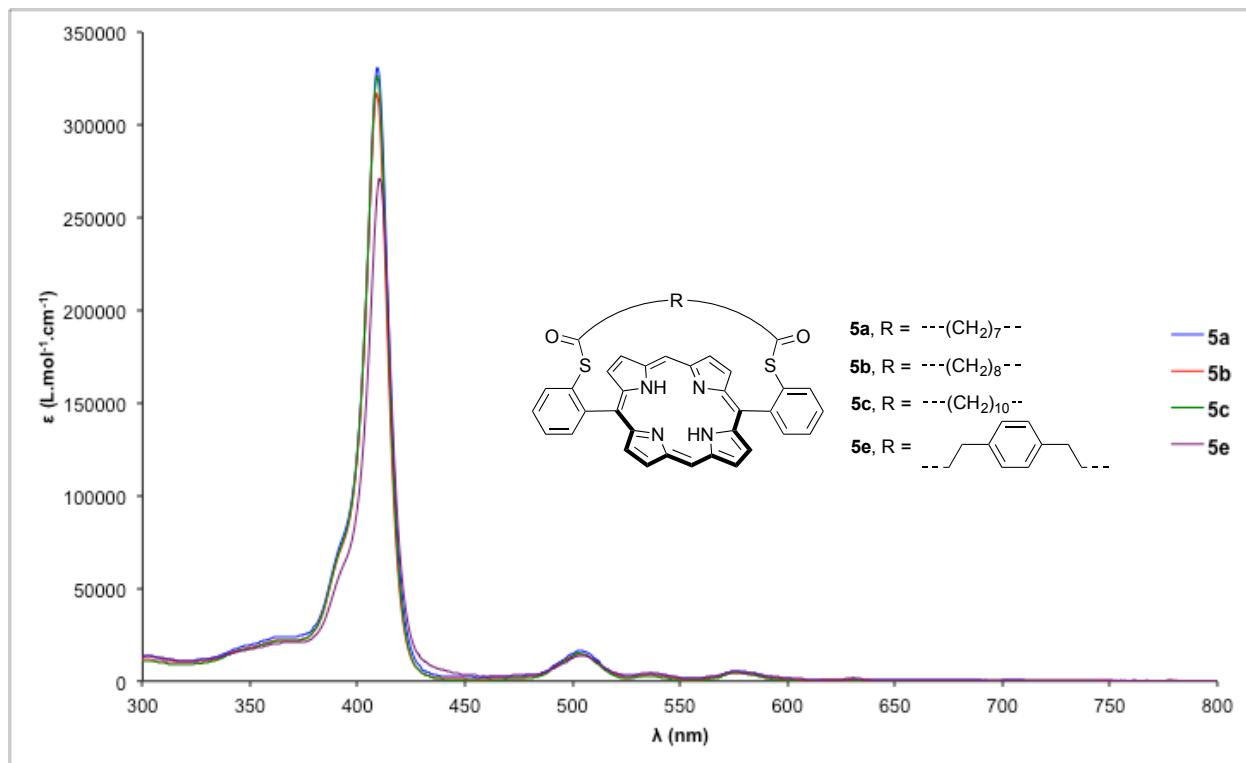
EPSRC UK National Mass Spectrometry Facility (NMSF), Swansea



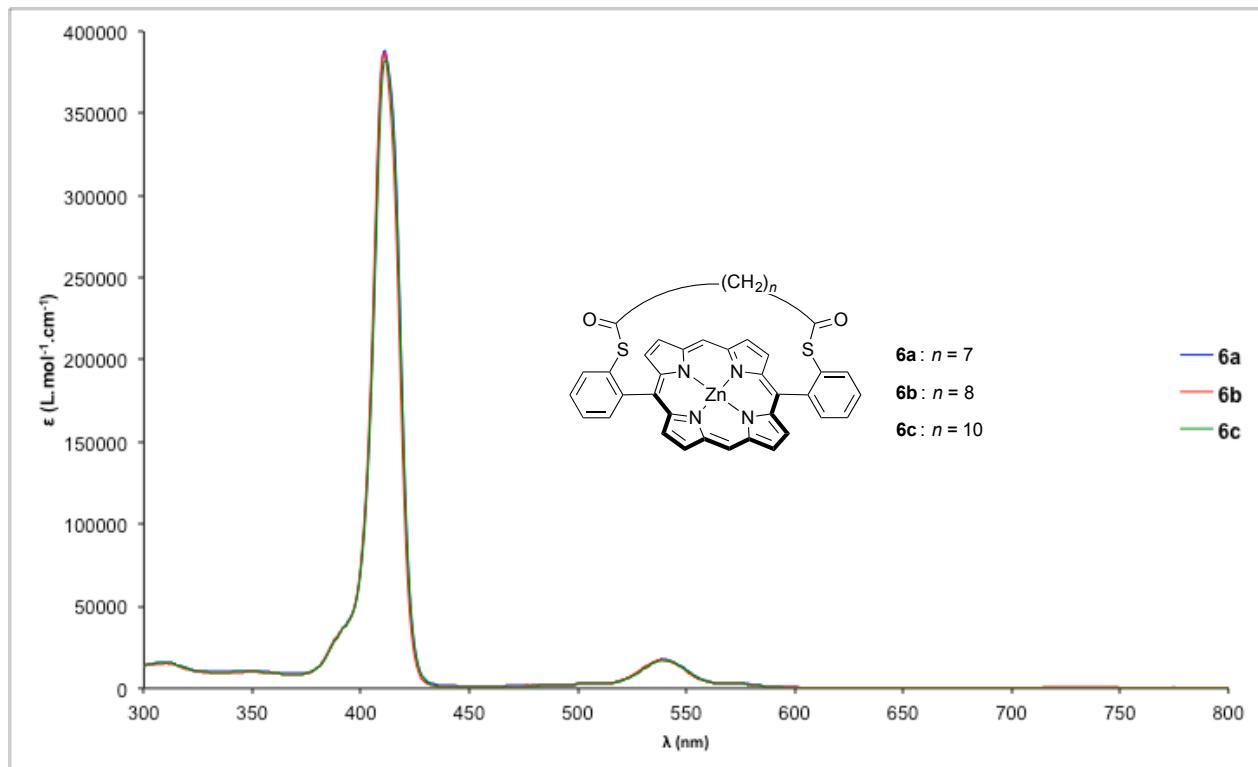
5. UV-VISIBLE ABSORPTION SPECTRA

(molar absorption coefficient spectra recorded in chloroform)

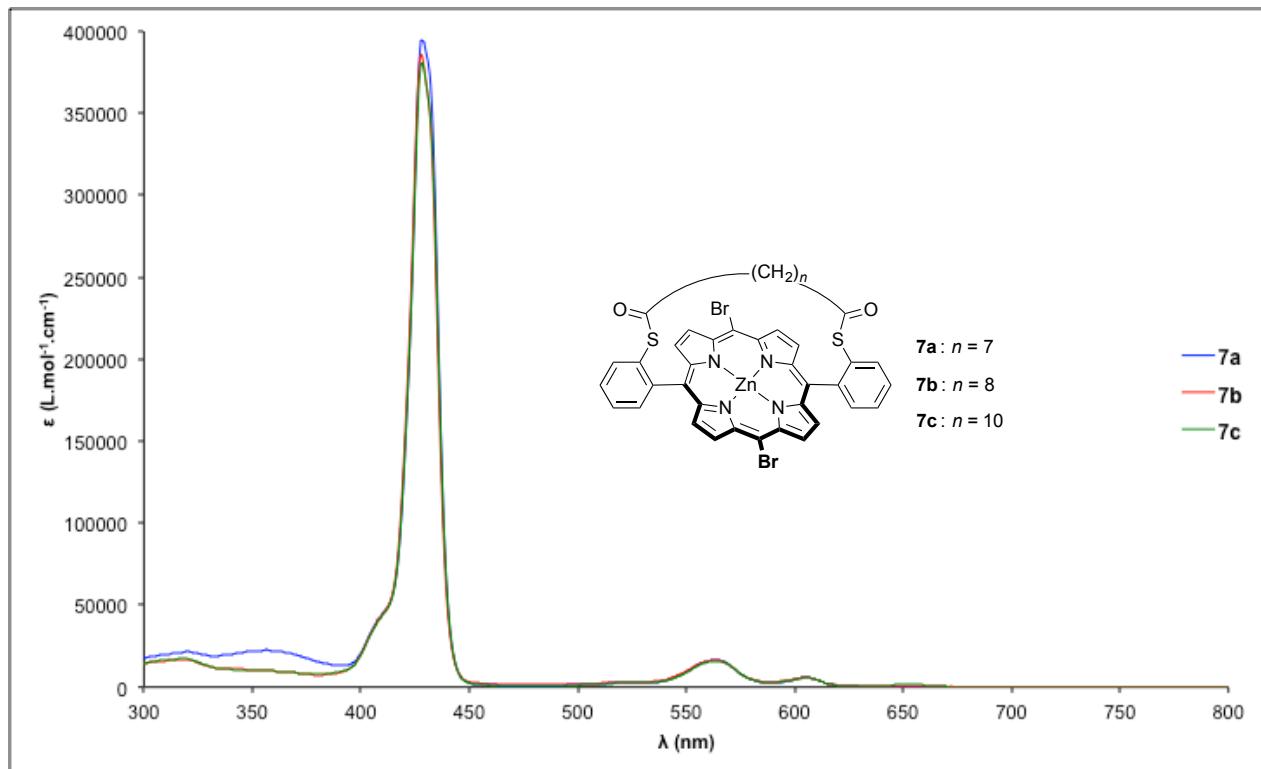
5.1. Strapped free-base porphyrins 5a-e



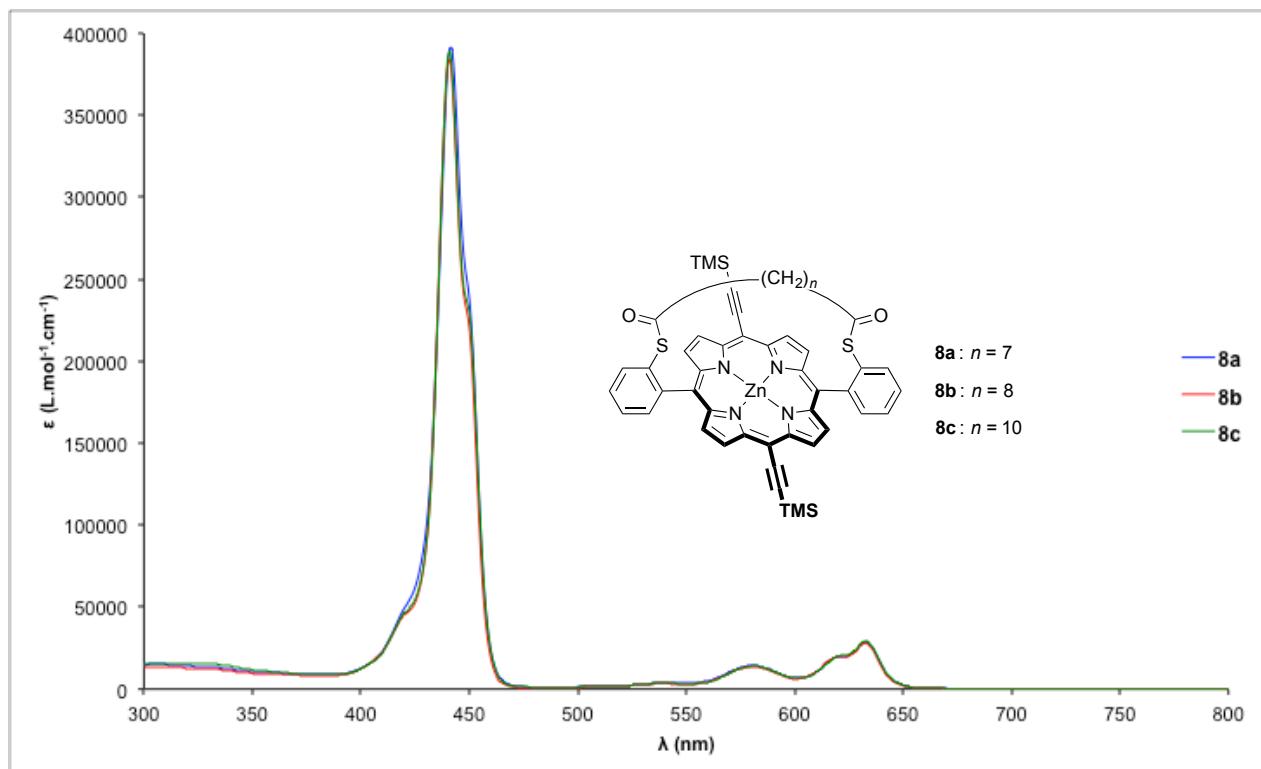
5.2. Strapped zinc(II) porphyrins 6a-c



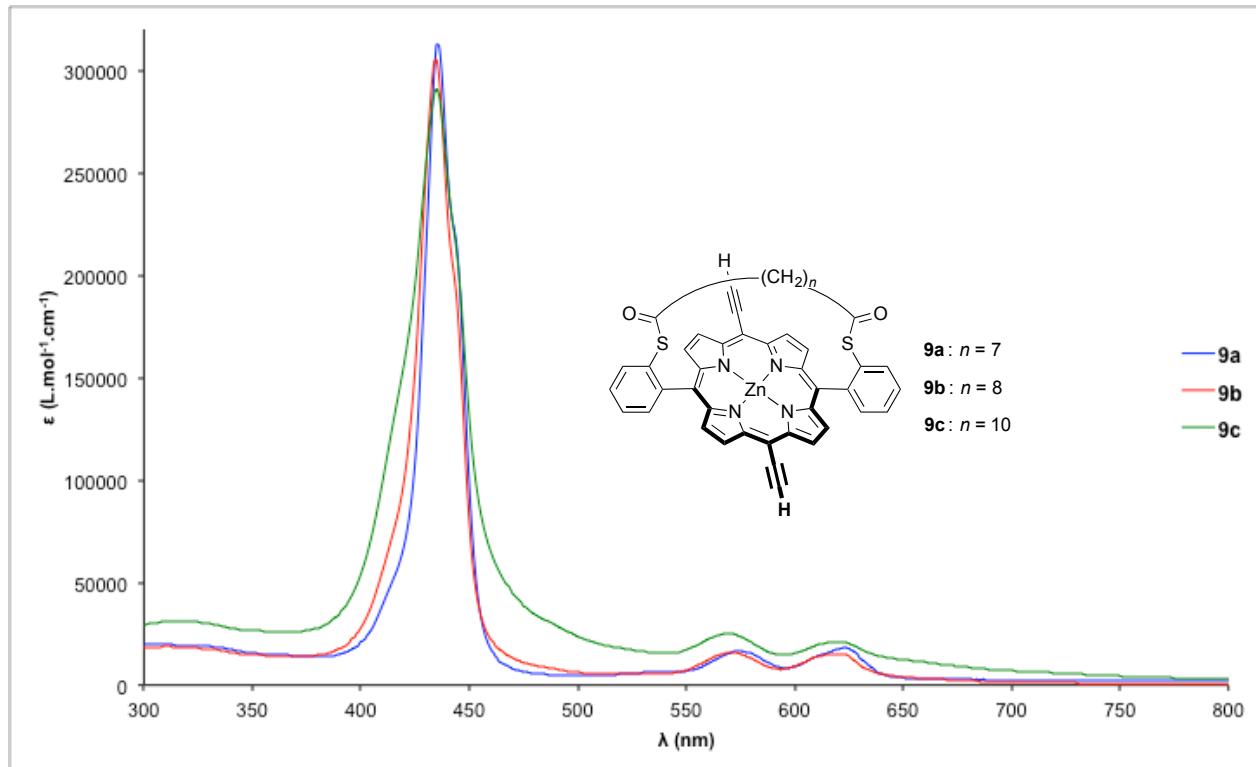
5.3. Strapped dibromoporphyrins 7a-c



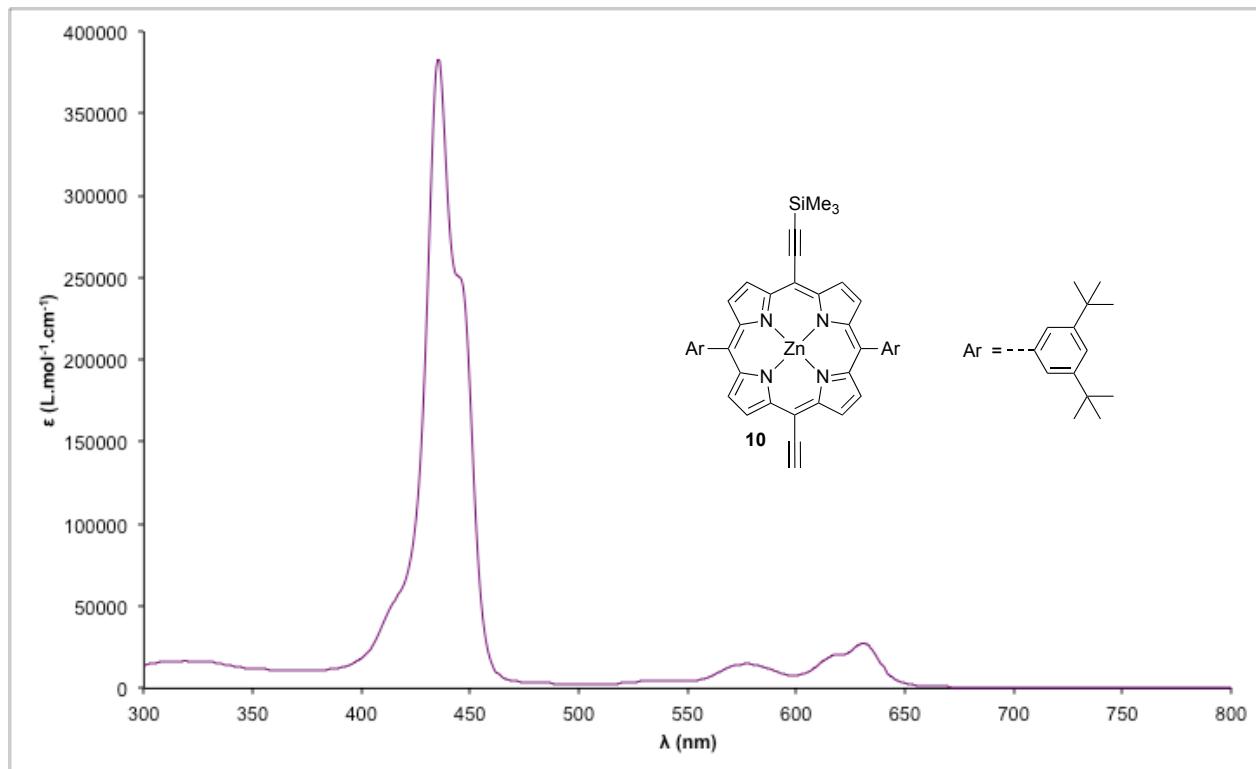
5.4. Strapped bis-TMS porphyrins 8a-c



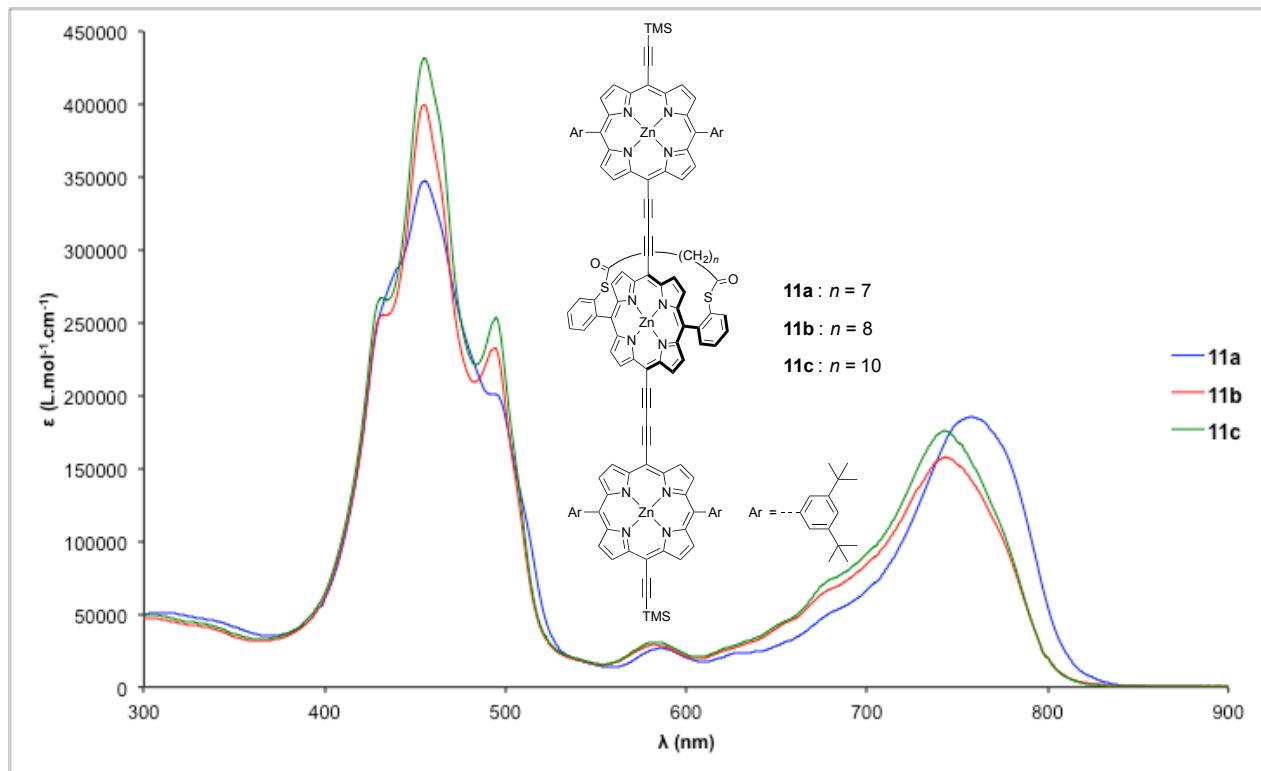
5.5. Strapped bis-deprotected porphyrins 9a-c



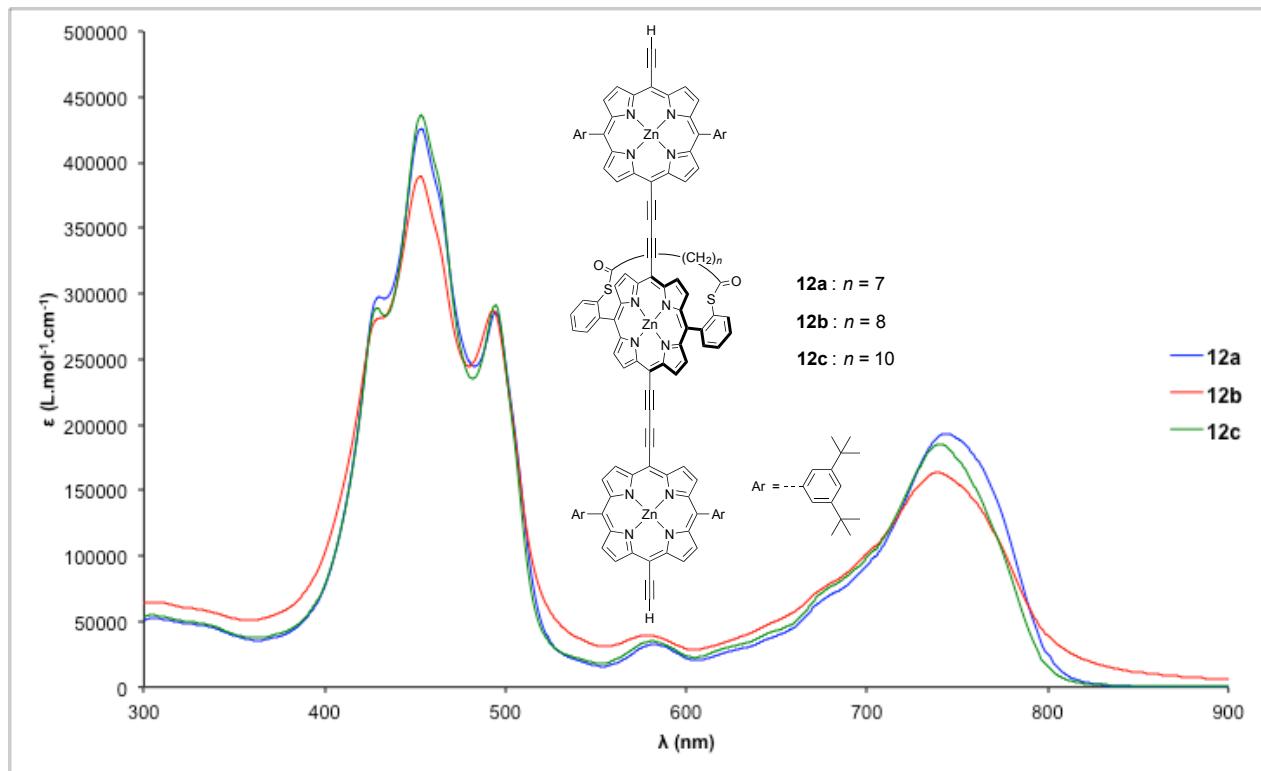
5.6. Mono-deprotected *t*-Bu porphyrin 10



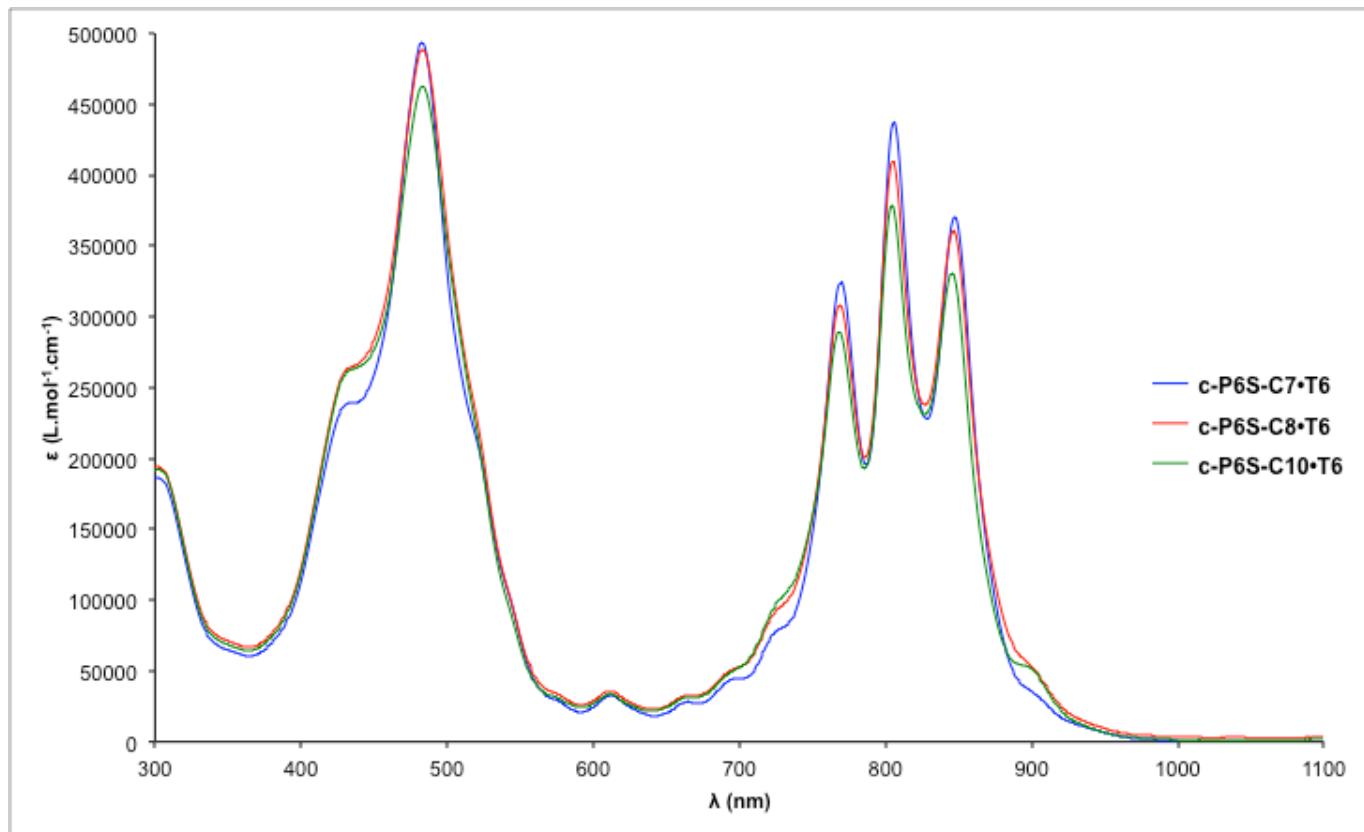
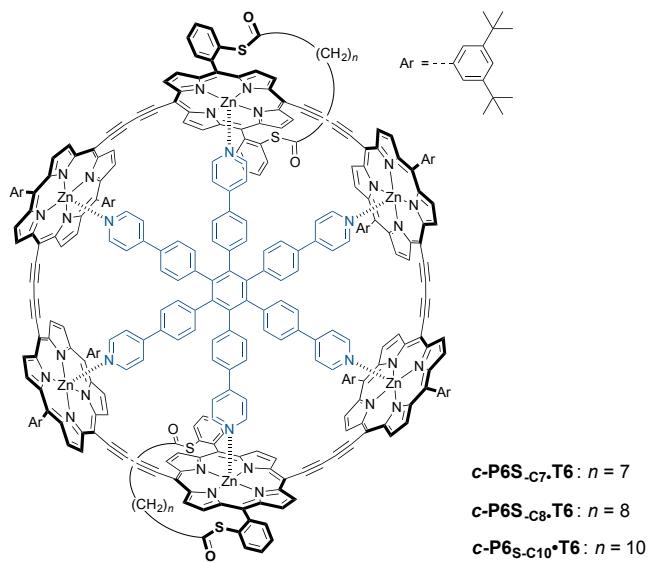
5.7. Strapped bis-TMS porphyrin trimers 11a-c



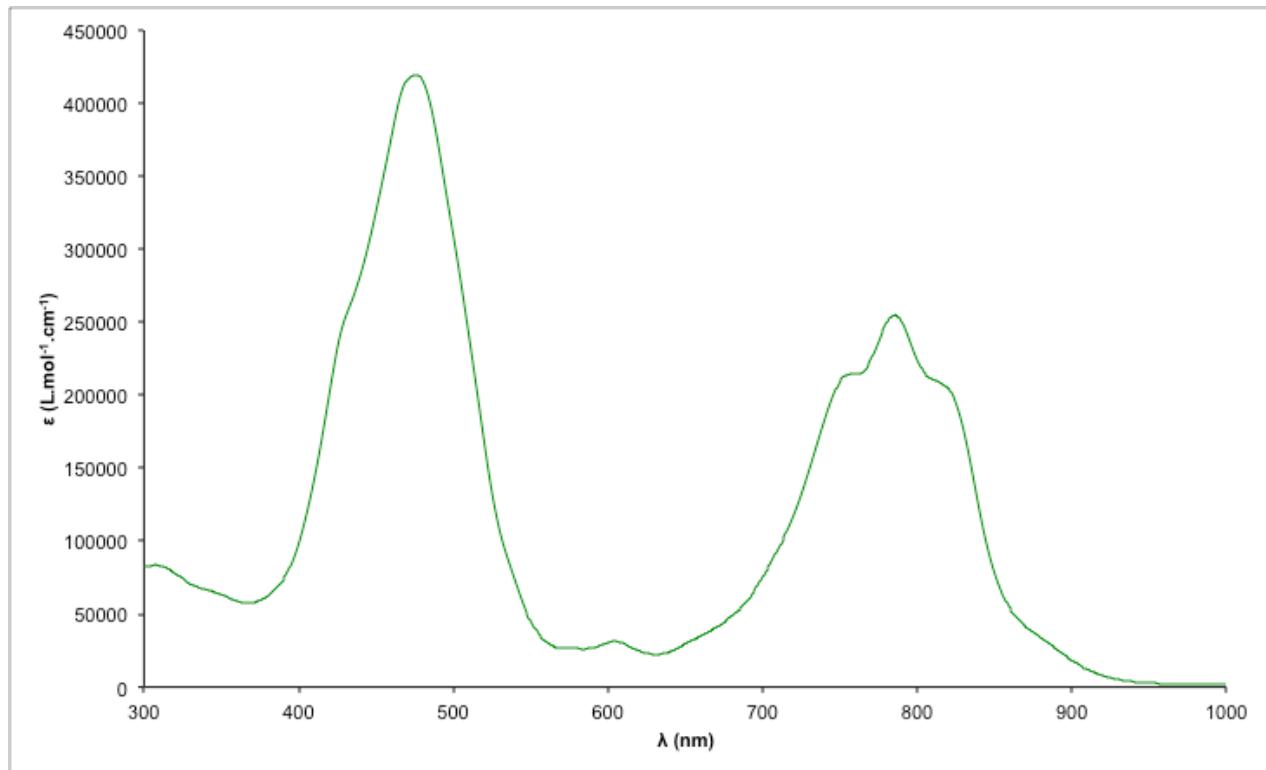
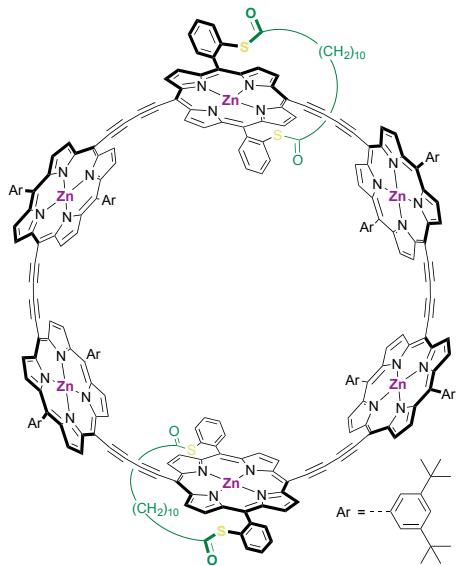
5.8. Strapped bis-deprotected porphyrin trimers 12a-c



5.9. Strapped porphyrin nanorings $c\text{-P6S-C}_7\text{--10}\bullet\text{T6}$



5.10. Template-free strapped porphyrin nanoring *c*-P6_{S-C10}



6. SINGLE CRYSTAL X-RAY DIFFRACTION STUDIES

Crystals of **6a**, **6b**, **6c**, **7b** and **7c** were grown by diffusion of MeOH vapor into a solution of the compound in CHCl₃/1% pyridine at 20 °C. Crystals of **6c** and **7a** were grown by diffusion of CH₃CN vapor into a solution of the compound in CHCl₃/1% pyridine at 20 °C. Crystals of **6c** resulting from diffusion of MeOH and MeCN were both studied as detailed below.

In general, crystals were mounted using the oil-drop technique, placing the sample directly into the cold N₂ flow of an Oxford CryoSystems^{S7} at 150 K. Diffraction images were collected using either a Nonius Kappa-CCD Diffractometer (Compounds **6a** & **7c**; $\lambda = 0.71073 \text{ \AA}$) or a (Rigaku) Oxford Diffraction Supernova A (**6b**, **6c-I**, **6c-II**, **7a** & **7b**; $\lambda = 1.54180 \text{ \AA}$). These raw frame data were collected and reduced using DENZO-SMN/HKL-COLLECT^{S8} or CrysAlisPro as appropriate. Structure solution was carried out using charge flipping^{S9} within SuperFlip^{S10} and the structures were refined using CRYSTALS.^{S11}

In general, all non-hydrogen atoms were refined with anisotropic displacement parameters, however, for **6b** & **7c** the ellipsoids for the alkyl strap were decidedly prolate suggesting disorder which was modeled using a two components with application of restraints as required.^{S12} The structure of **7b** turned out to be a chloroform solvate; disorder in the solvent sphere was modeled in a similar fashion. In the absence of disorder, hydrogen atoms on nitrogen atoms were generally visible in the difference map so were located at geometric positions and refined using restraints prior to inclusion in the final refinement using a riding model.^{S13}

Initial single crystal diffraction studies for Compound **6c** at 150 K, suggested that it crystallized with a triclinic cell of 8.99660(10) Å, 18.40620(29) Å, 26.24820(40) Å, 69.7540(6)°, 89.9432(6)°, 87.9057(7)° ($V = 4074.9(1) \text{ \AA}^3$) with two molecules in the asymmetric unit. On close inspection however, there was a clear symmetry relationship between the molecules. On re-examination, the raw data were inconclusive, so data were re-collected (see Section 6.1-4 for more details). In the meantime, crystals of a second polymorph (**6c-II**) was found to have grown from CHCl₃/ pyridine /MeOH (compared with original polymorph, **6c-I**, grown from CHCl₃/pyridine/MeCN). The structure of **6c-II** was a methanol solvate with a large amount of diffuse electron density found within voids in the structure. This was thought to be disordered methanol and despite best efforts could not be satisfactorily modeled. For this reason, PLATON/SQUEEZE^{S14} was used leaving a void from which the electron density was removed. The discrete Fourier transform of this void region were treated as contributions to the A and B parts of the calculated structure factors with in CRYSTALS.

Full crystallographic data for all structures have been deposited with the Cambridge Crystallographic Data Centre, CCDC 1534244-1534250. Copies of these data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

6.1 Variable Temperature Study for Compound 6c-I

Attempts to quench-cool the crystal using the oil-drop mounting method confirmed earlier suspicions that the crystals were sensitive to thermal change: the data would not index and visual examination of the diffraction suggested damage to the crystal. This crystal was removed from the cold stream which was warmed to 300 K where the crystal was returned to the flow before cooling to 250 K at 300 K/hr. Although the data were weak and of poor quality, the structure solved well in P₂₁ with a new cell, 9.1178(7) Å, 49.1865(19) Å, 9.3222(4) Å, 89.920(4)°, 92.344(4)°, 90.203(6)°, $V = 4177.2(4)$ Å³ (related to that seen previously). The two molecules in the asymmetric unit were related by approximate glide-symmetry suggesting that a more in-depth study would be appropriate with a new crystal. For this experiment a small red crystal was selected and mounted with a minimum quantity of oil to reduce strain on cooling should the sample undergo a phase change. A hemisphere of data (to a resolution of 0.8 Å) was collected at 300 K, before cooling to 275 K at 120 K/hr where another hemisphere was collected (maximum resolution of 1.2 Å). Similar hemispheres were collected at 25 K intervals to 100 K, with additional data collected at 150 K to give a resolution similar to that collected at 300 K.

The data at 300 K were initially indexed with an orthorhombic centered cell (13.36 Å, 12.81 Å, 49.31 Å), but it quickly became clear that the actual symmetry was much lower, in keeping with the monoclinic cell seen at 250 K. These data were then indexed using the monoclinic cell of 9.1886(3) Å, 49.108(2) Å, 9.3396(5) Å, 89.986(4)°, 92.348(4)°, 90.003(3)°, $V = 4210.8(3)$ Å³ (at 300 K). The associated orientation matrix was used to index the 1.2 Å data at each temperature, and the unit cells recorded to determine whether there were any discontinuities that could indicate the temperature of any transition (Section 6.2). Reciprocal lattice section reconstructions were also made for the $hk0$, $hk1$, $h0l$, $h1l$, $0kl$, $1kl$ layers at each temperature and examined. The most apparent features were the change in the α and γ angles with twinning and splitting thought to be the result of strain introduced by the transition taking place in the crystal coated in vitrified perfluoro polyether oil. These studies suggested the presence of a phase transition from monoclinic to triclinic, occurring between 250 K and 225 K on cooling. It is possible there are also super-lattice reflections at low temperature caused by either doubling of the b -axis, or modulation in another direction, but these additional reflections could not be resolved from the other features (Section 6.3).

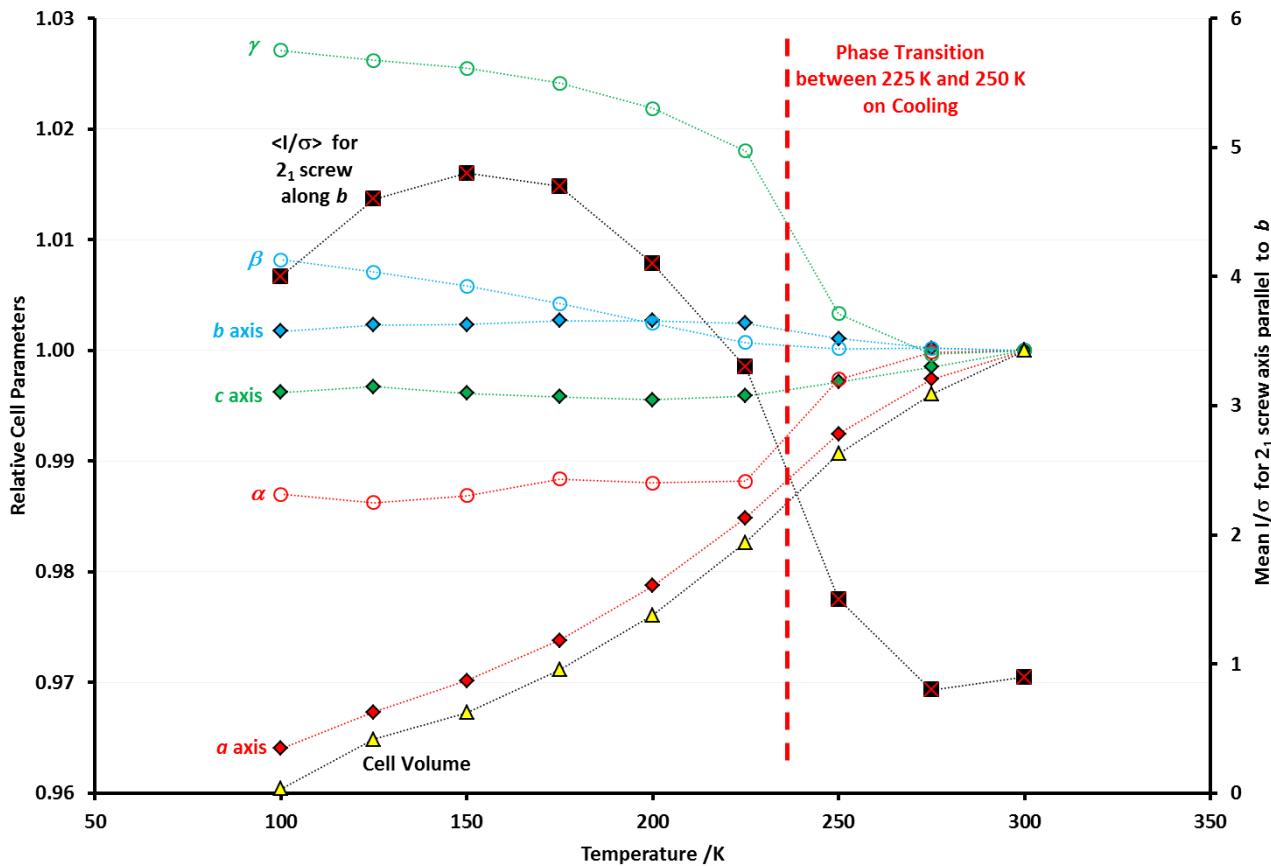
Again, the structure solved well from the full 300 K dataset (maximum resolution of 0.8 Å), however there was some ambiguity about the space group. The data were generally weak, but the systematic absences clearly indicated the presence of a 2₁ screw axis ($0k0$: $k \neq 2n$; $\langle I/\sigma \rangle = 0.3$) and the structure solved with direct methods giving an asymmetric unit with two crystallographically independent molecules. The initial solution clearly showed the porphyrin rings with the phenyl substituents and beginning of the strap. The missing atoms could be seen in the difference Fourier map, though the resolution of the central alkyl chain was poor and there were strong indications of disorder. There was clear additional symmetry between the well resolved parts of the structure suggesting the presence of an a -glide plane. Examination of the systematic absences ($h0l$: $h \neq 2n$) showed that although there was a clear systematic weakness for this operator ($\langle I/\sigma \rangle = 1.6$ compared with 5.7 and 6.1 for the c and n glides respectively), over 10% of the reflections were observed. It is possible that at 300 K the a -glide symmetry is broken by the alkyl chains, however, the resolution of the data was so poor that the structure was resolved (using charge-flipping) and refined in the space group P₂₁/a.

The raw frame data from the short, restricted resolution data collections were reduced and the systematic absences were examined with respect to temperature. The mean I/σ for the $0k0$ ($k \neq 2n$) absences at 250 K was 1.5 (i.e. unobserved), but increased to 3.3 at 225 K (i.e. observed, though weak; Section 6.2). Similarly, the R_{int} for the monoclinic setting went from 9% at 250 K to 27% at 225 K, while the R_{int} for the triclinic setting remained below 5% throughout the temperature range studied. The behavior of the intensity for the a -glide ($h0l$: $h \neq 2n$) absence was less clear cut. At 300 K, the mean I/σ for the restricted resolution data collection was 6.9, i.e. much larger than that for the full data collection to 0.8 Å. This was thought to be result from the fact that the weaker high angle data were not included in the statistics effectively diluting them. On cooling, the $\langle I/\sigma \rangle$ for $h0l$ ($h \neq 2n$) increased significantly, to over 15, still significantly weaker than the intensity of the systematic absence violations for the c - and n -glides (both 26), but unambiguously present.

Although the structure solved from the full dataset collected at 150 K in $P\bar{1}$, the refinement was poor. Initially this was thought to be the result of twinning associated with the phase transition. Although including a 30% twin component^{S15} improved the refinement the end result was still very poor ($R_1 > 18\%$), possibly due to additional structural changes not clear in the raw data or further damage or strain introduced by the transition. Comparing the two molecules in the asymmetric unit (Section 6.4), however, suggested a possible origin of the transition: it is clear that the porphyrins match well, but the symmetry is broken by the alkyl chain of the strap. It is likely that the strap is dynamic at room temperature, but as the motion decreases on cooling, packing becomes more efficient with an associated gradual loss of symmetry.

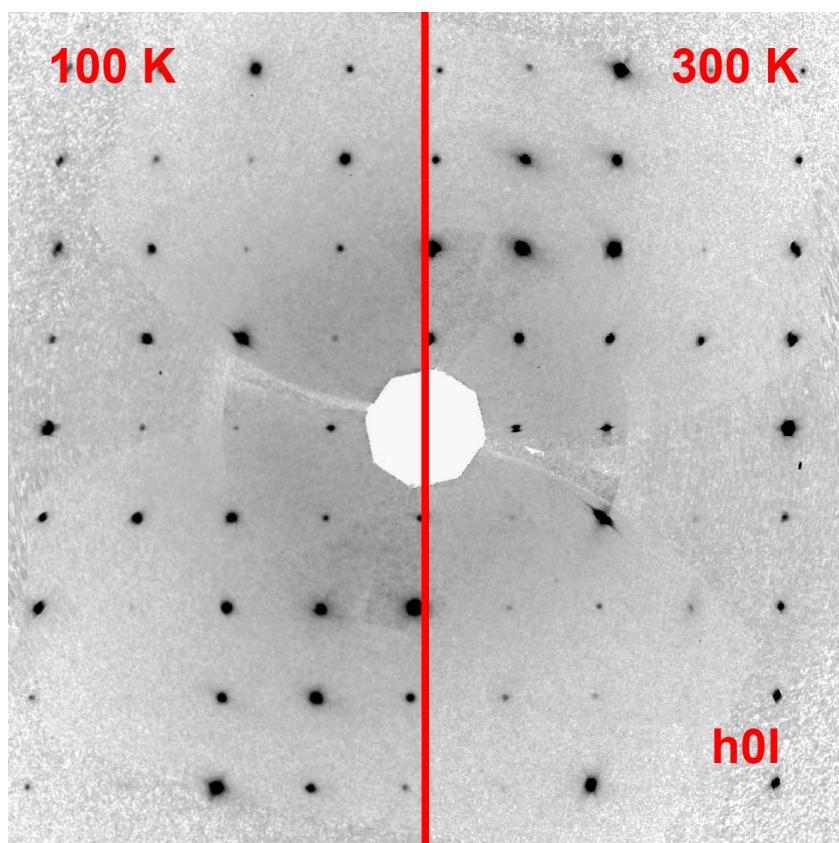
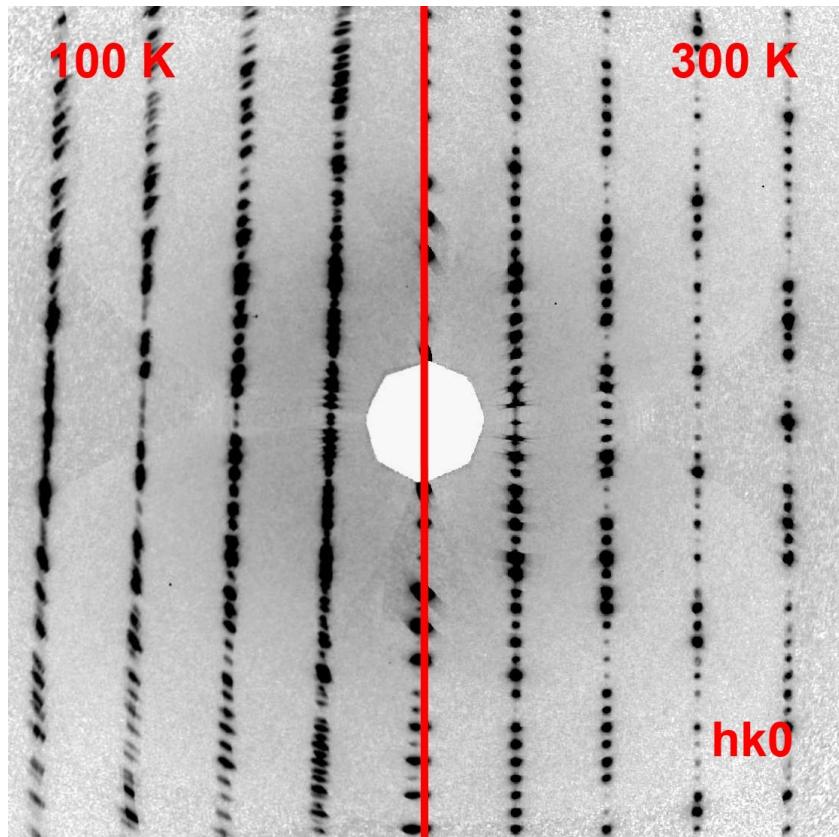
6.2 Unit Cell Parameters for Compound 6c-I as a Function of Temperature

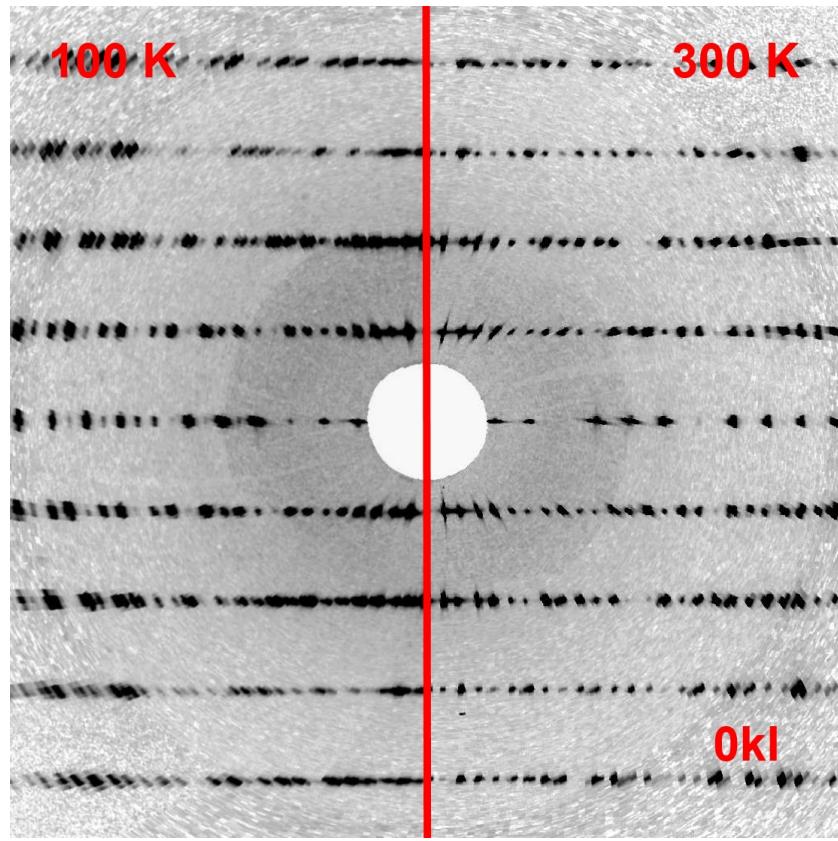
The variation of unit cell parameters with temperature is shown below for Compound **6c-I**. Each parameter is plotted as the relative value with respect to 300 K; the lines are drawn to guide the eye. Some parameters show little change, but it is clear that α and γ display a significant discontinuity between 250 K and 225 K. The $\langle I/\sigma \rangle$ for the systematic absence violations for the 2_1 screw axis parallel to b ($0k0$; $k \neq 2n$) are also shown and support the conclusion that there is a phase transition between 250 K and 225 K.



6.3 Selected Reciprocal Lattice Section Reconstructions for **6c-I**

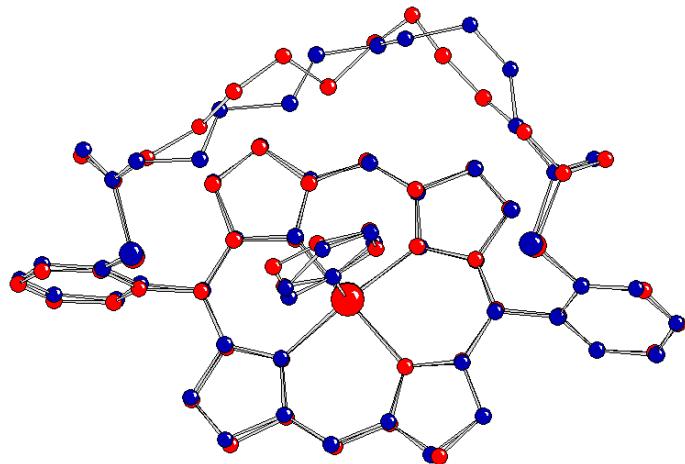
Reciprocal lattice sections were constructed up for **6c-I** at all temperatures. These were compared throughout the temperature range. The most apparent features were the change in the α and γ angles with twinning and splitting thought to be the result of strain introduced by the transition taking place in the crystal coated in vitrified perfluoro polyether oil. It is possible there are also super-lattice reflections at 100 K caused either doubling of the b -axis or modulation in another direction, but these additional reflections could not be resolved from the other features. The zero order layers are shown below for the 100 K and 300 K data plotted to 2 Å.



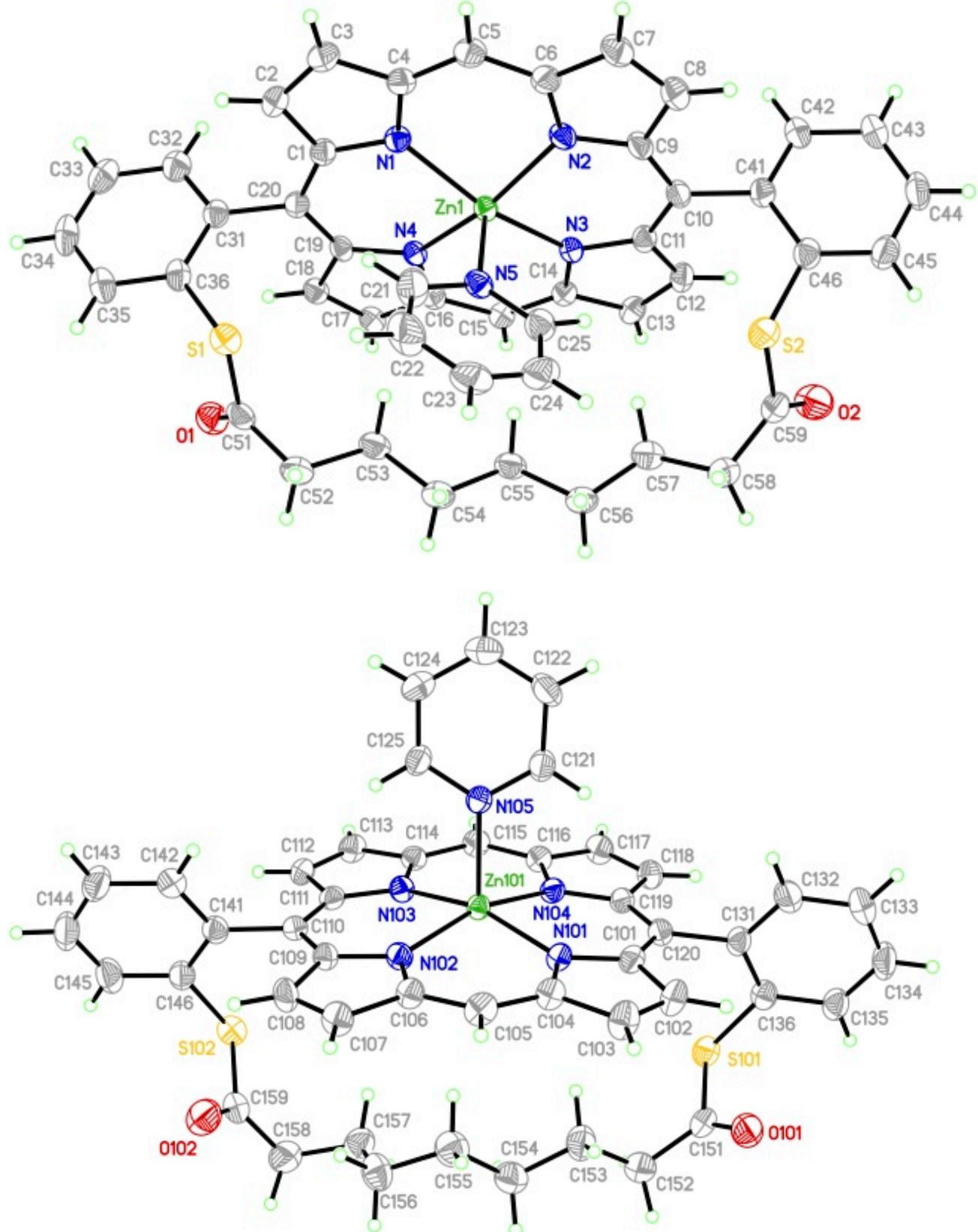


6.4 Overlay of molecules in the crystal structure of 6c-I at 150 K

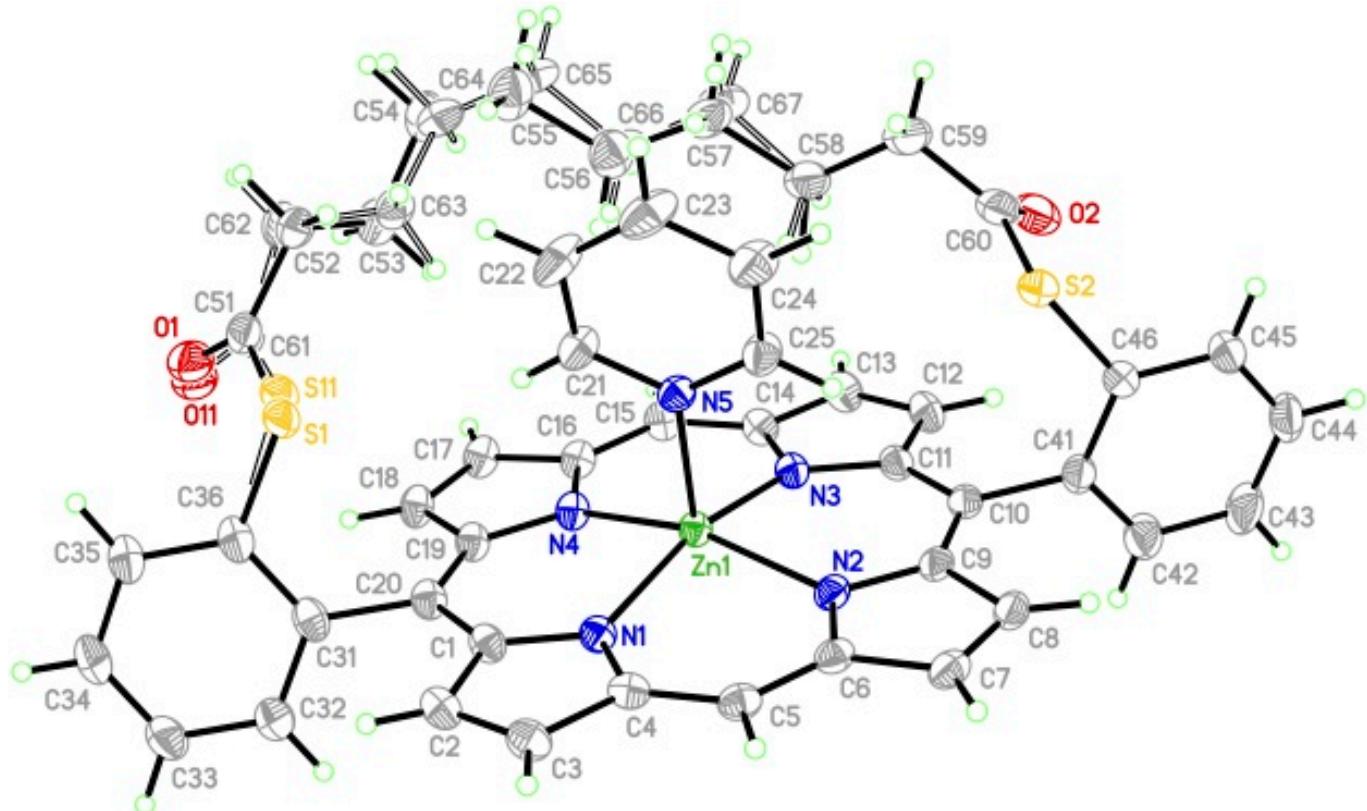
A least-squares fit was performed for all non-hydrogen atoms in the two crystallographically independent molecules seen at 100 K. The resultant overlay below shows a good agreement between the atoms in the porphyrin and significant deviation in the strap. It is possible that the strap is dynamic at room temperature, but as the motion decreases on cooling, packing becomes more efficient with an associated gradual loss of symmetry.



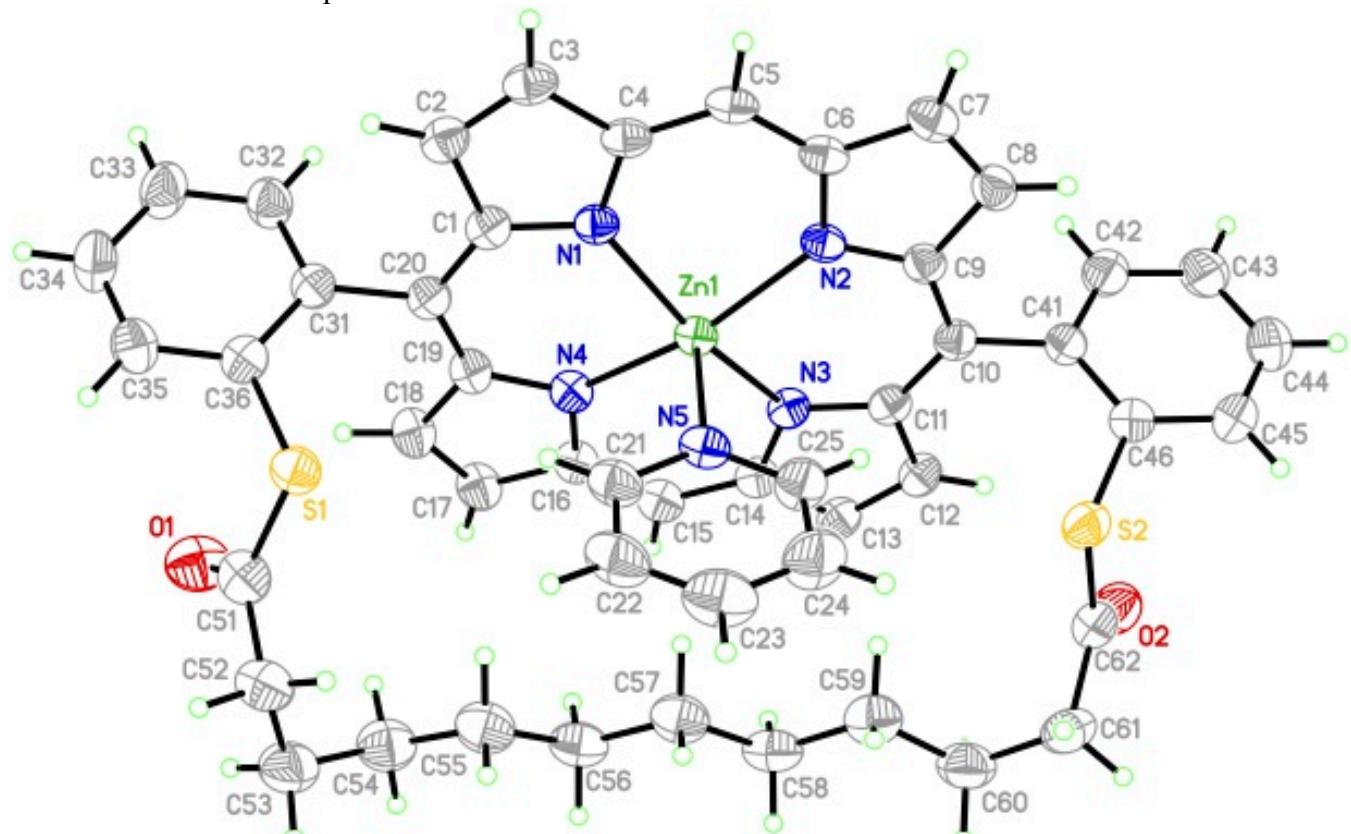
6.5 Displacement ellipsoid plots



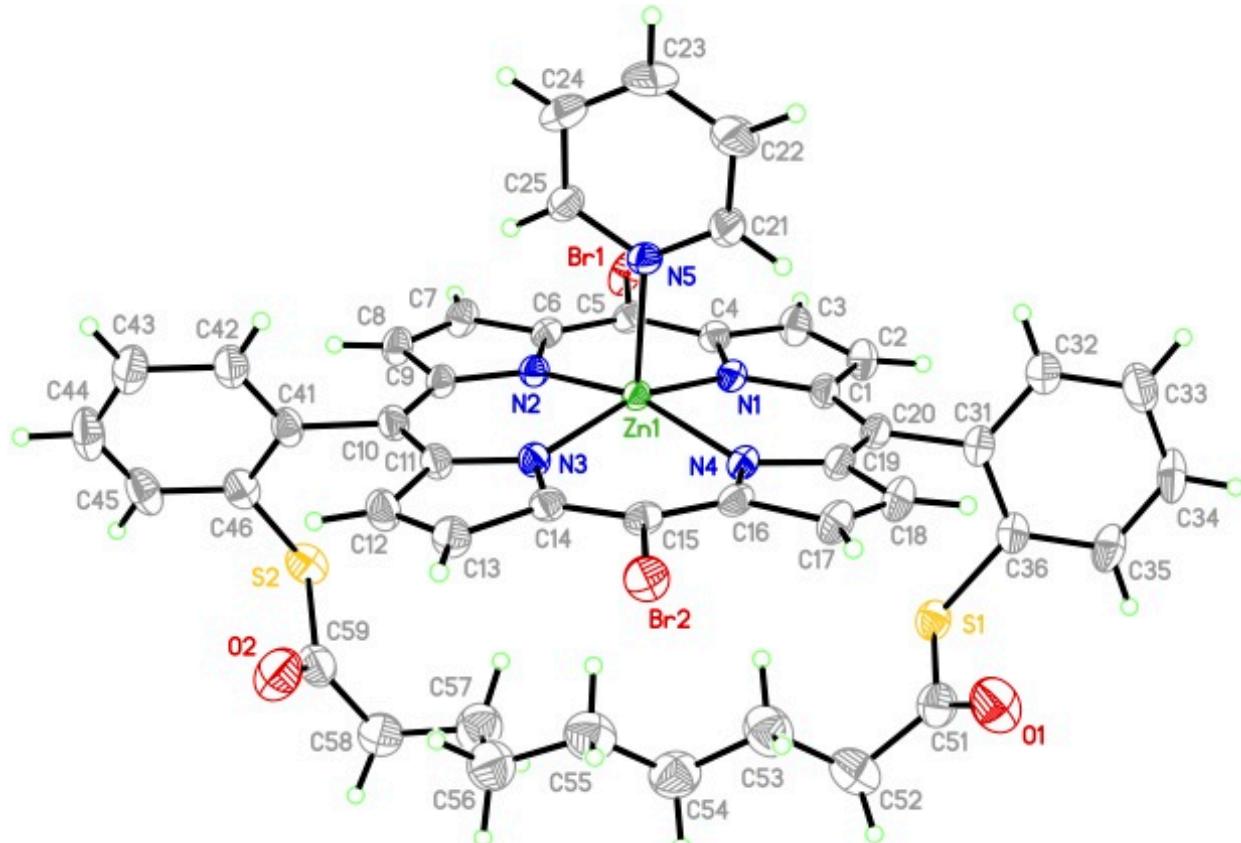
Displacement ellipsoid plot of the two porphyrins in asymmetric unit of porphyrin **6a** displayed at the 50% probability level.



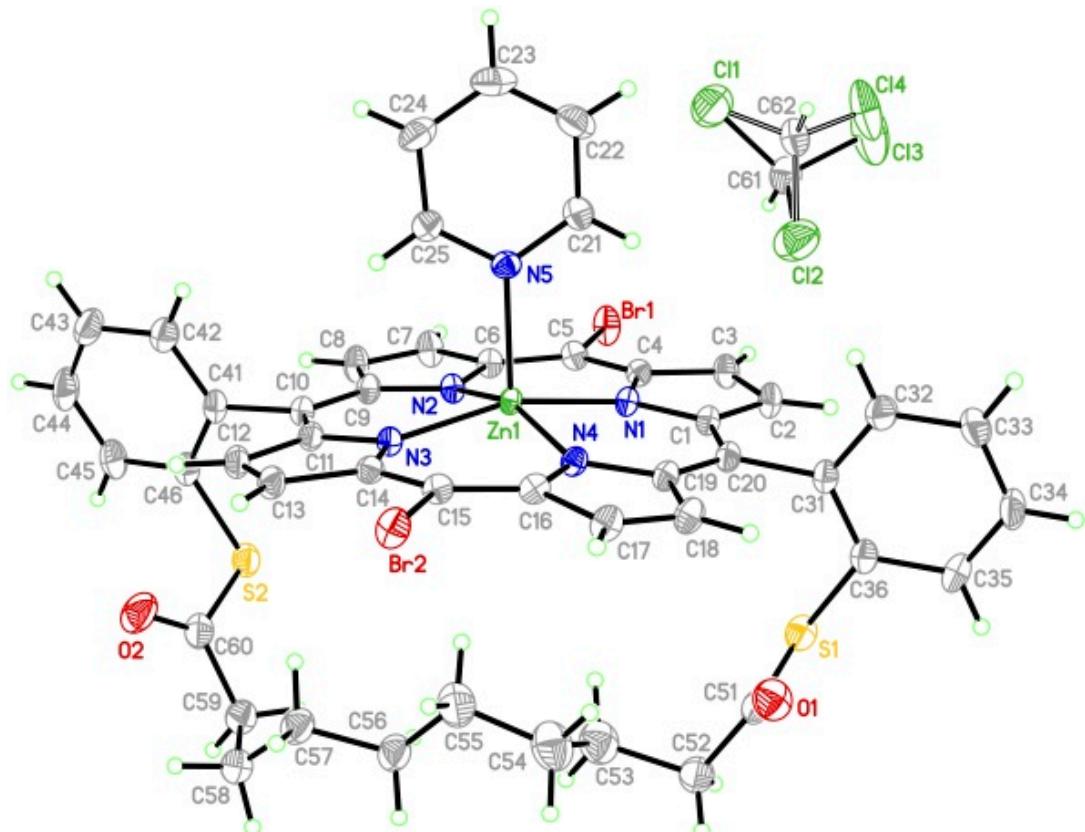
Displacement ellipsoid plot of porphyrin **6b** displayed at the 50% probability level; a minor component of disorder is shown with open bonds.



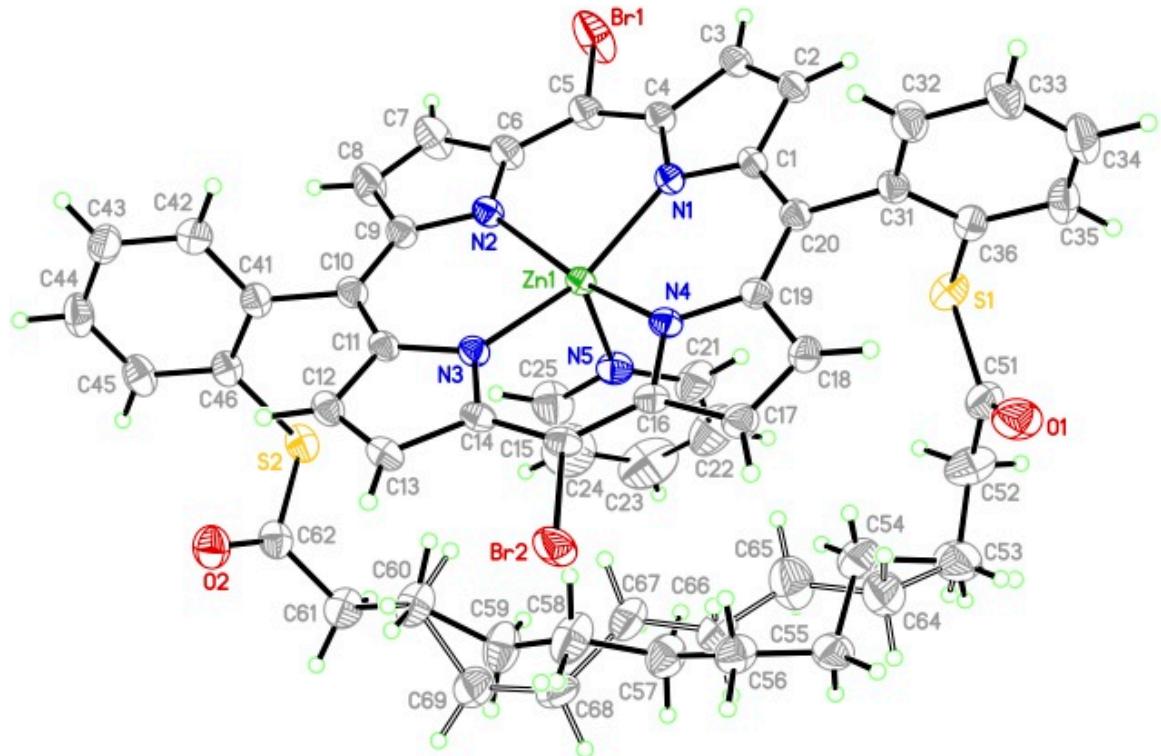
Displacement ellipsoid plot of porphyrin **6c** displayed at the 50% probability level



Displacement ellipsoid plot of porphyrin 7a displayed at the 50% probability level.



Displacement ellipsoid plot of porphyrin 7b displayed at the 50% probability level; modeled disordered solvent displayed.



Displacement ellipsoid plot of porphyrin **7c** displayed at the 50% probability level; a minor component of disorder is shown with open bonds.

7. REFERENCES

- S1. Goldstein, E.; Ma, B. Y.; Lii, J. H.; Allinger, N. L. *J. Phys. Org. Chem.* **1996**, *9*, 191.
- S2. Marques, H. M.; Cukrowski, I. *Phys. Chem. Chem. Phys.* **2002**, *4*, 5878.
- S3. Marques, H. M.; Cukrowski, I. *Phys. Chem. Chem. Phys.* **2003**, *5*, 5499.
- S4. Jarowski, P. D.; Diederich, F.; Houk, K. N. *J. Org. Chem.* **2005**, *70*, 1671.
- S5. Stewart, J. J. P. *J. Mol. Model.* **2007**, *13*, 1173.
- S6. Stewart, J. J. P. MOPAC2016, Stewart Computational Chemistry, Colorado Springs, CO, USA, <http://OpenMOPAC.net>.
- S7. Cosier, J.; Glazer, A. M. *J. Appl. Cryst.* **1986**, *19*, 105.
- S8. Otwinowski, Z.; Minor, W. Processing of X-ray Diffraction Data Collected in Oscillation Mode, *Methods Enzymol.* **1997**, *276*, Eds C. W. Carter, R. M. Sweet, Academic Press.
- S9. Oszlányi, G.; Süto, A. *Acta Cryst.* **2004**, *A60*, 134.
- S10. Palatinus, L. Chapuis, G. *J. Appl. Cryst.* **2007**, *40*, 786.
- S11. Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. *J. Appl. Cryst.* **2003**, *36*, 1487.
- S12. Parois, P.; Cooper, R. I.; Thompson, A. L. *Chemistry Central Journal* **2015**, *9:30*.
- S13. Cooper, R. I.; Thompson, A. L.; Watkin, D. J. *J. Appl. Cryst.* **2010**, *43*, 1100.
- S14. PLATON, A Multipurpose Crystallographic Tool, A. L. Spek. Utrecht, the Netherlands, 1998; Spek, A. *J. Appl. Cryst.* **2003**, *36*, 7; van der Sluis, P.; Spek, A. L. *Acta Cryst.* **1990**, *A46*, 194.
- S15. Cooper, R. I.; Gould, R. O.; Parsons, S. D.; Watkin, J. *J. Appl. Cryst.* **2002**, *35*, 168.