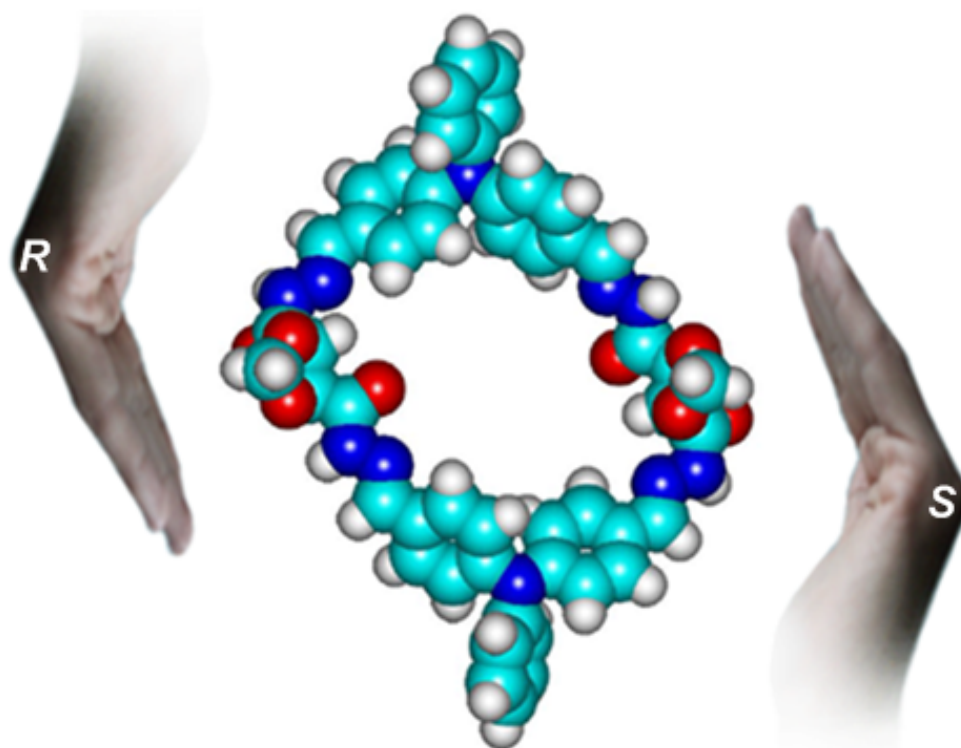


**Supplementary Information:**

**Synthesis of novel enantiomerically pure tetra-carbohydrazide cyclophane macrocycles**

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*School of Engineering and Science, Jacobs University Bremen, P.O. Box 750 561, 28725 Bremen, Germany.*



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**\*Corresponding Author:**

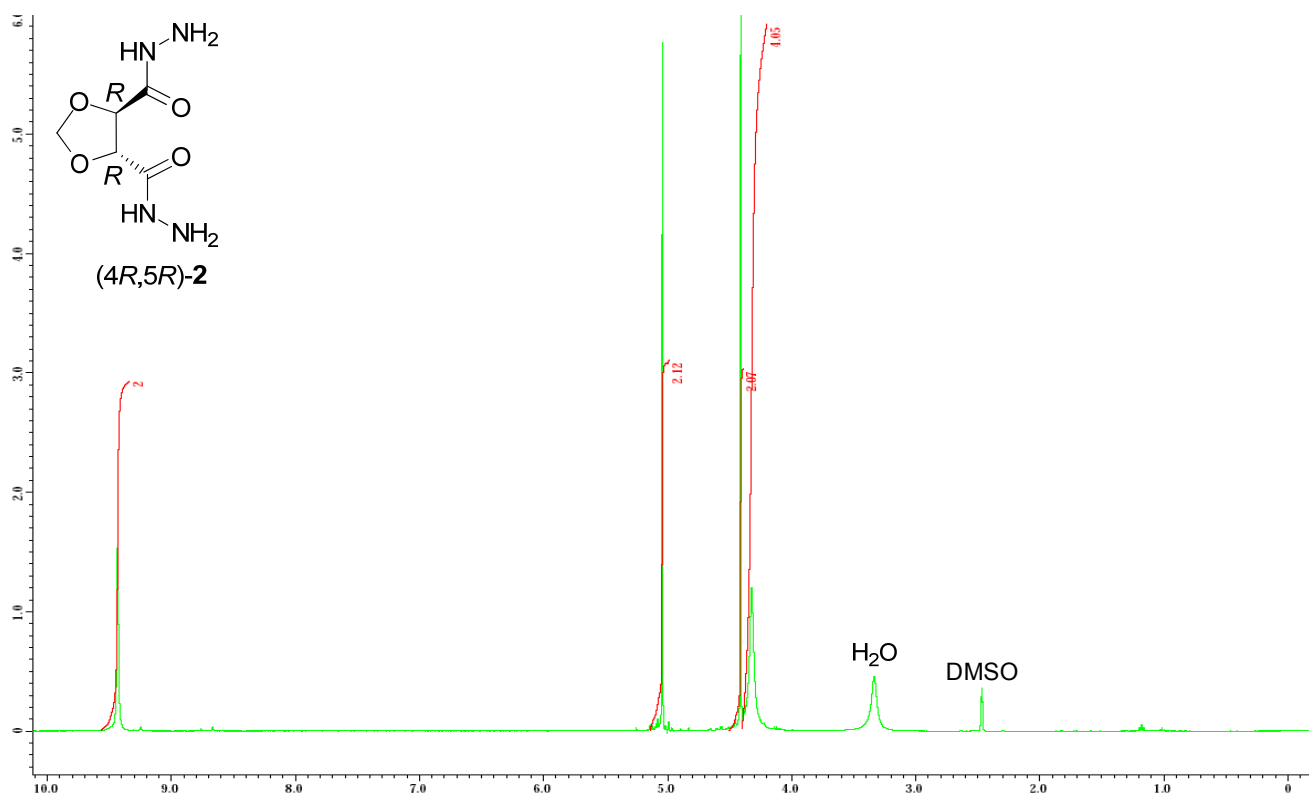
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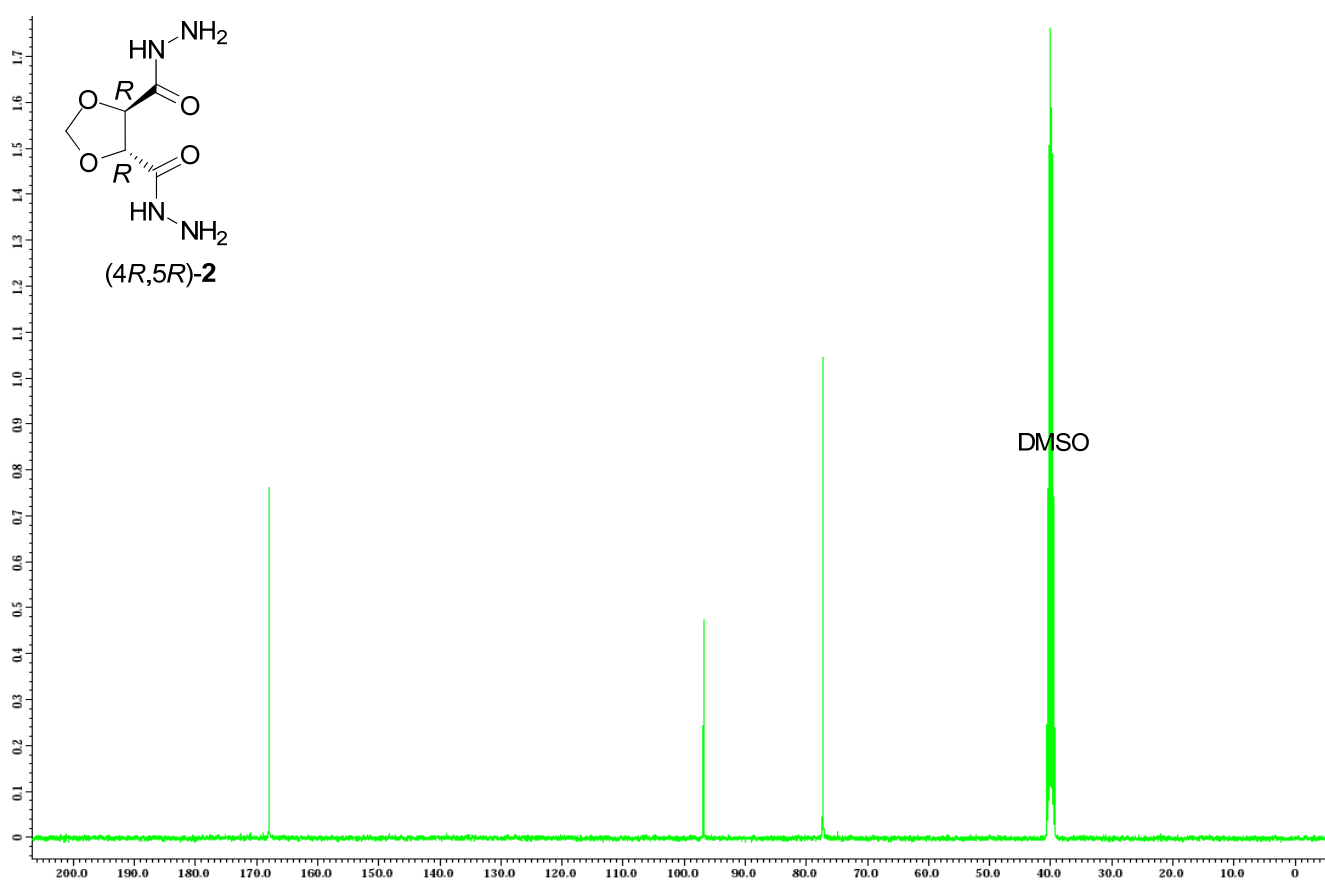
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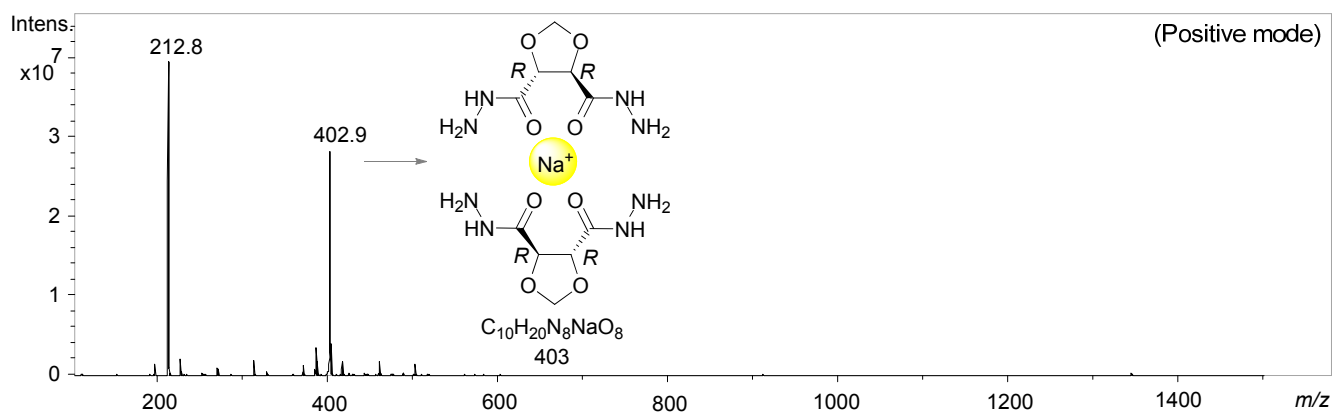
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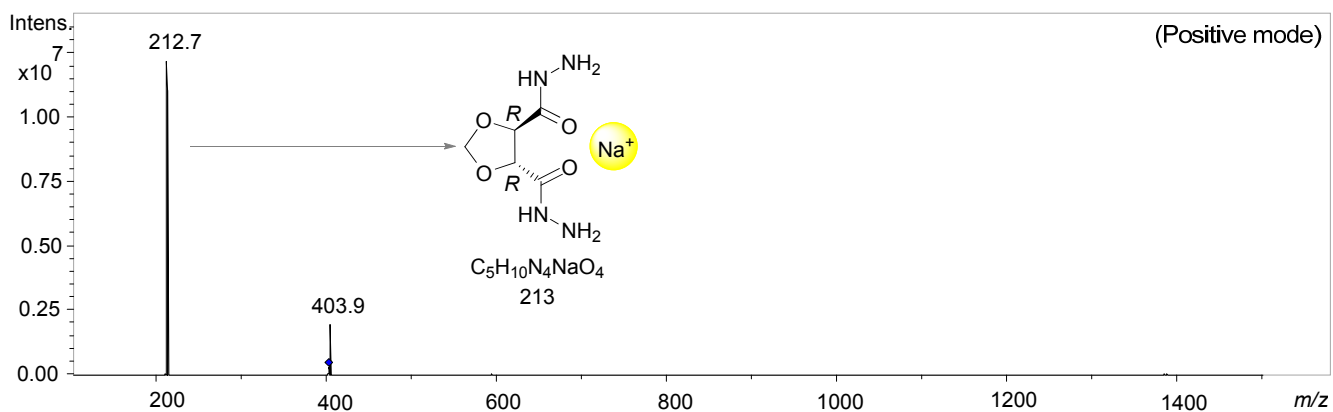
**Figure 1.**  $^1\text{H-NMR}$  spectrum for (4*R*,5*R*)-1,3-dioxolane-4,5-dicarbohydrazide (**2**),  $\text{DMSO-d}_6$ , 400 MHz.



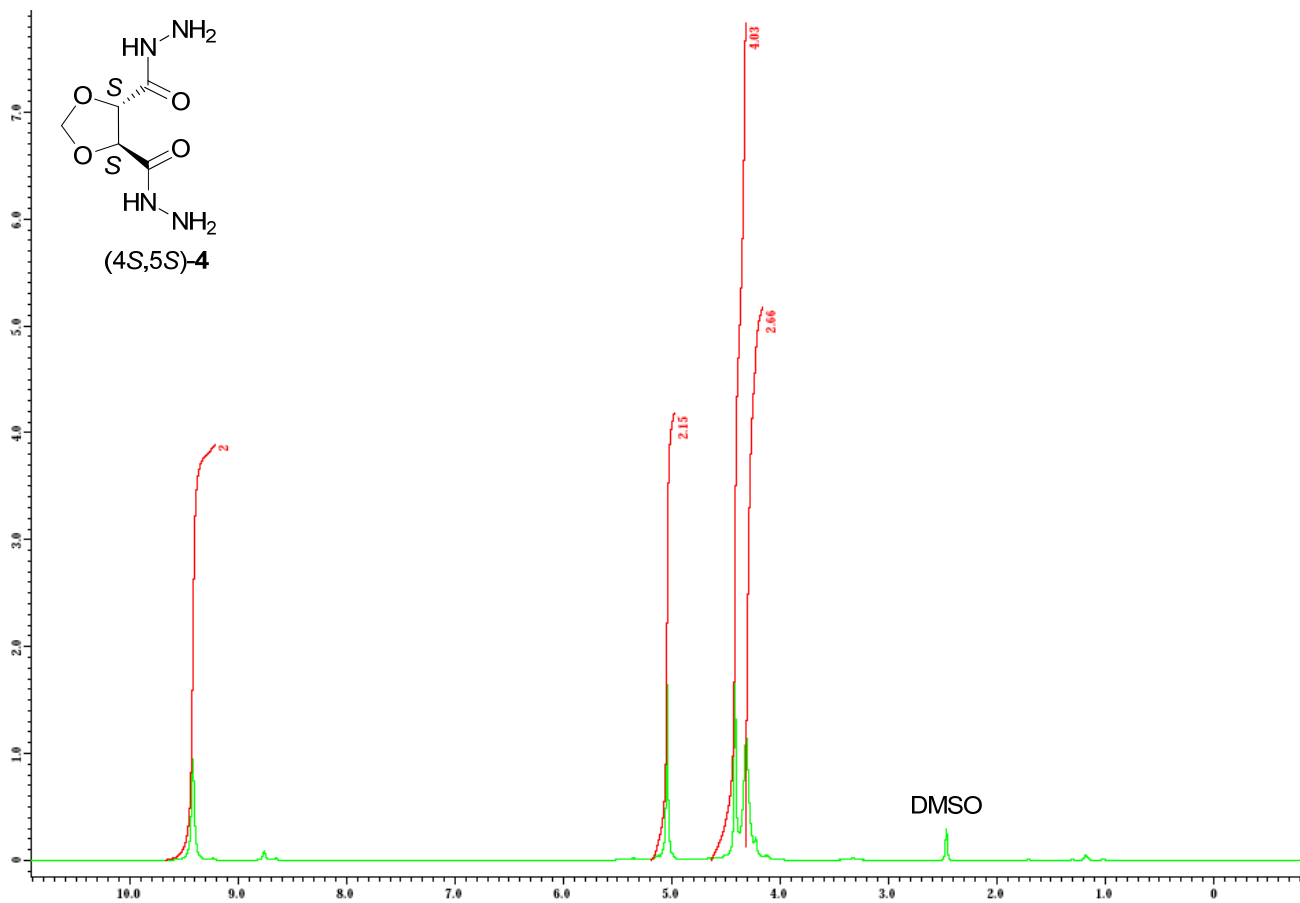
**Figure 2.**  $^{13}\text{C-NMR}$  spectrum for (4*R*,5*R*)-1,3-dioxolane-4,5-dicarbohydrazide (**2**),  $\text{DMSO-d}_6$ , 100 MHz.



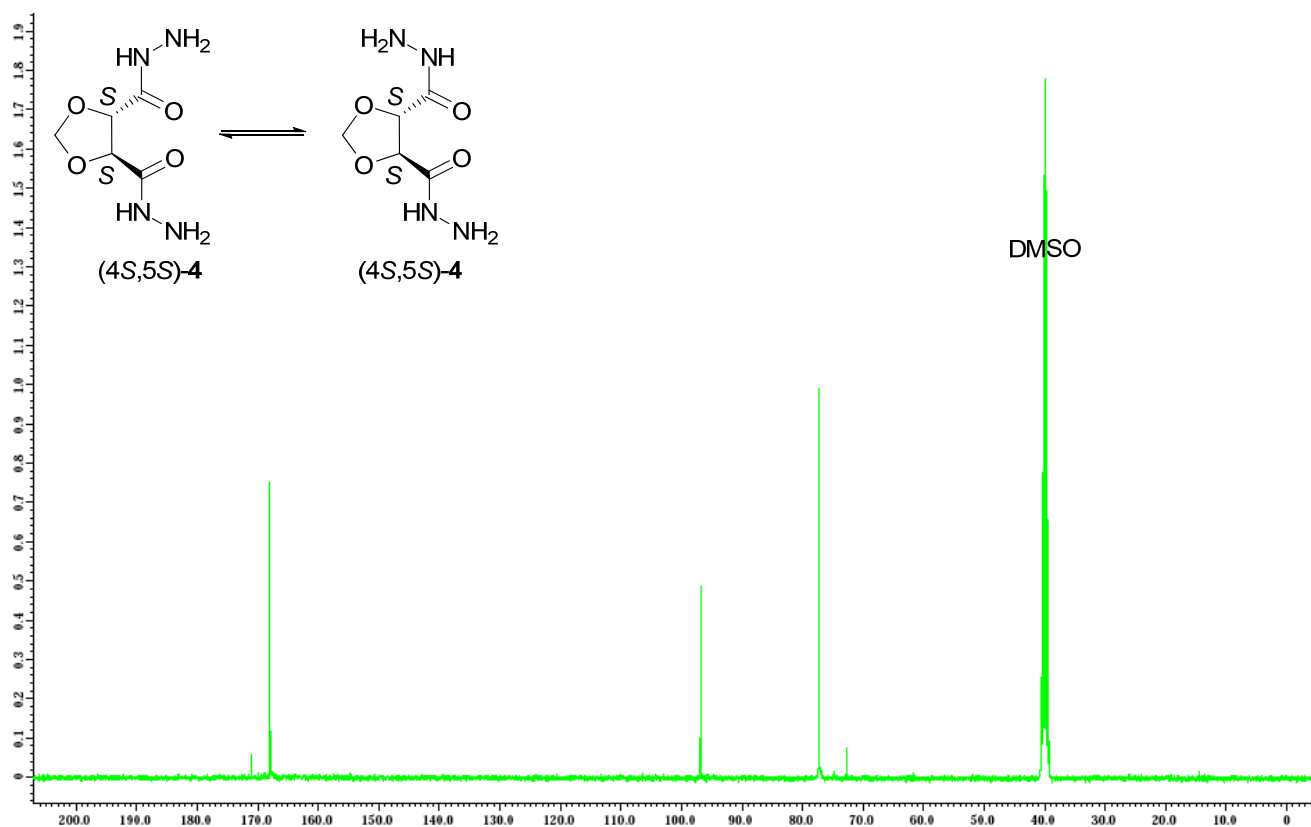
**Figure 3.** ESI-MS spectrum for (4*R*,5*R*)-1,3-dioxolane-4,5-dicarbohydrazide (**2**) from H<sub>2</sub>O.



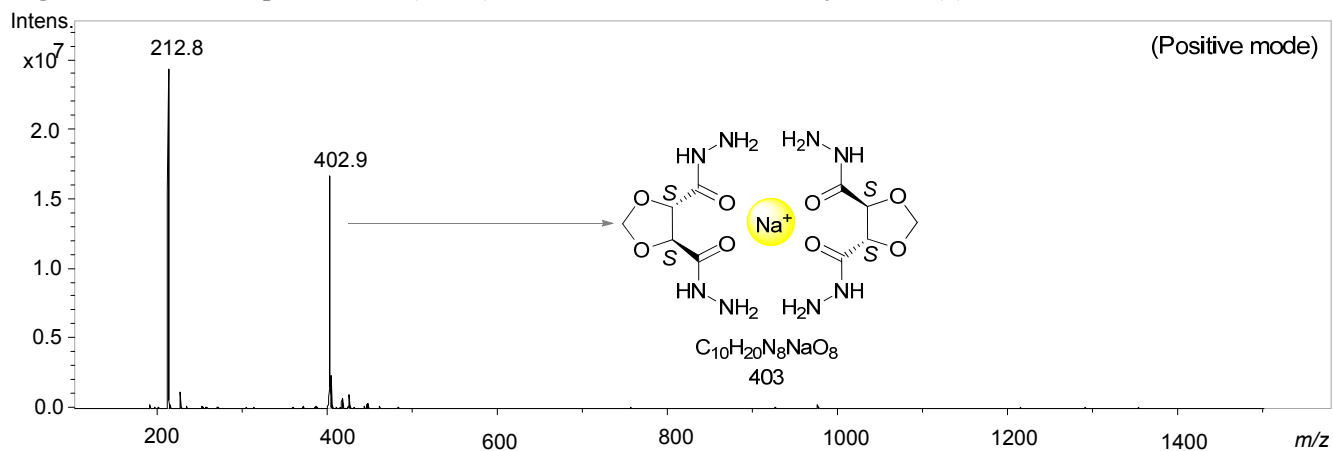
**Figure 4.** Tandem ESI-MS<sup>2</sup> spectrum for (4*R*,5*R*)-1,3-dioxolane-4,5-dicarbohydrazide (**2**) from H<sub>2</sub>O.



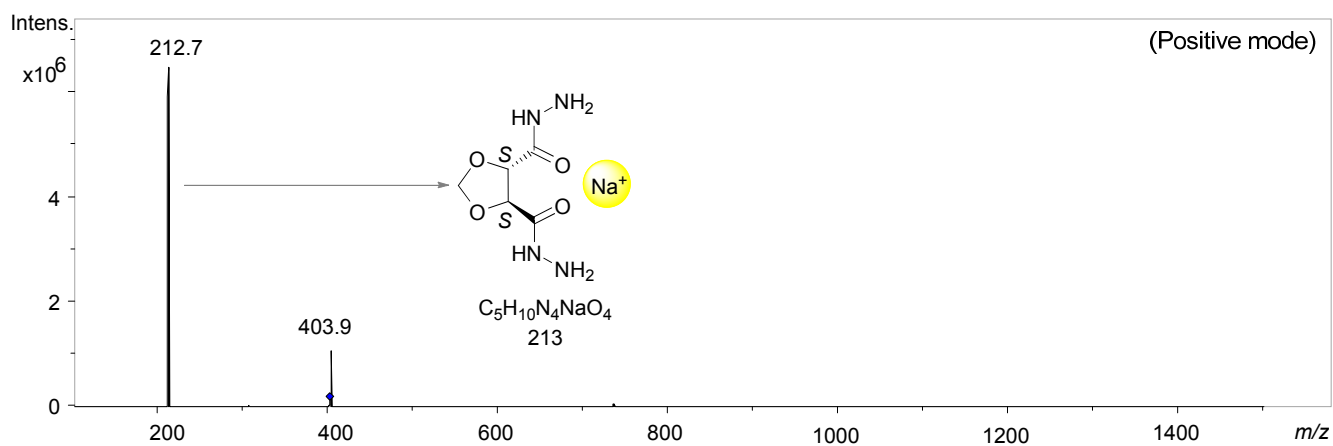
**Figure 5.** <sup>1</sup>H-NMR spectrum for (4*S*,5*S*)-1,3-dioxolane-4,5-dicarbohydrazide (**4**), DMSO-*d*<sub>6</sub>, 400 MHz.



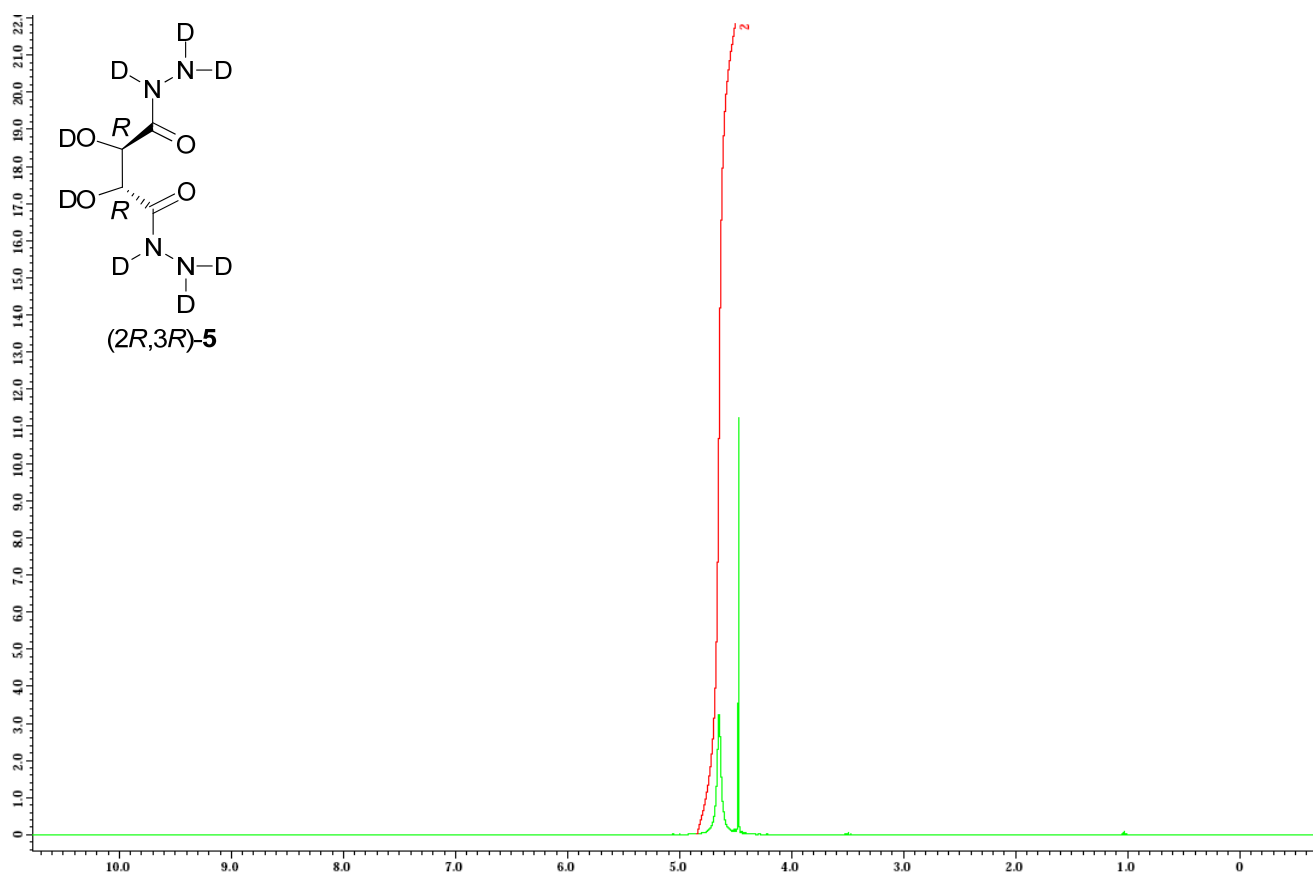
**Figure 6.**  $^{13}\text{C}$ -NMR spectrum for (4*S*,5*S*)-1,3-dioxolane-4,5-dicarbohydrazide (**4**), DMSO- $d_6$ , 100 MHz.



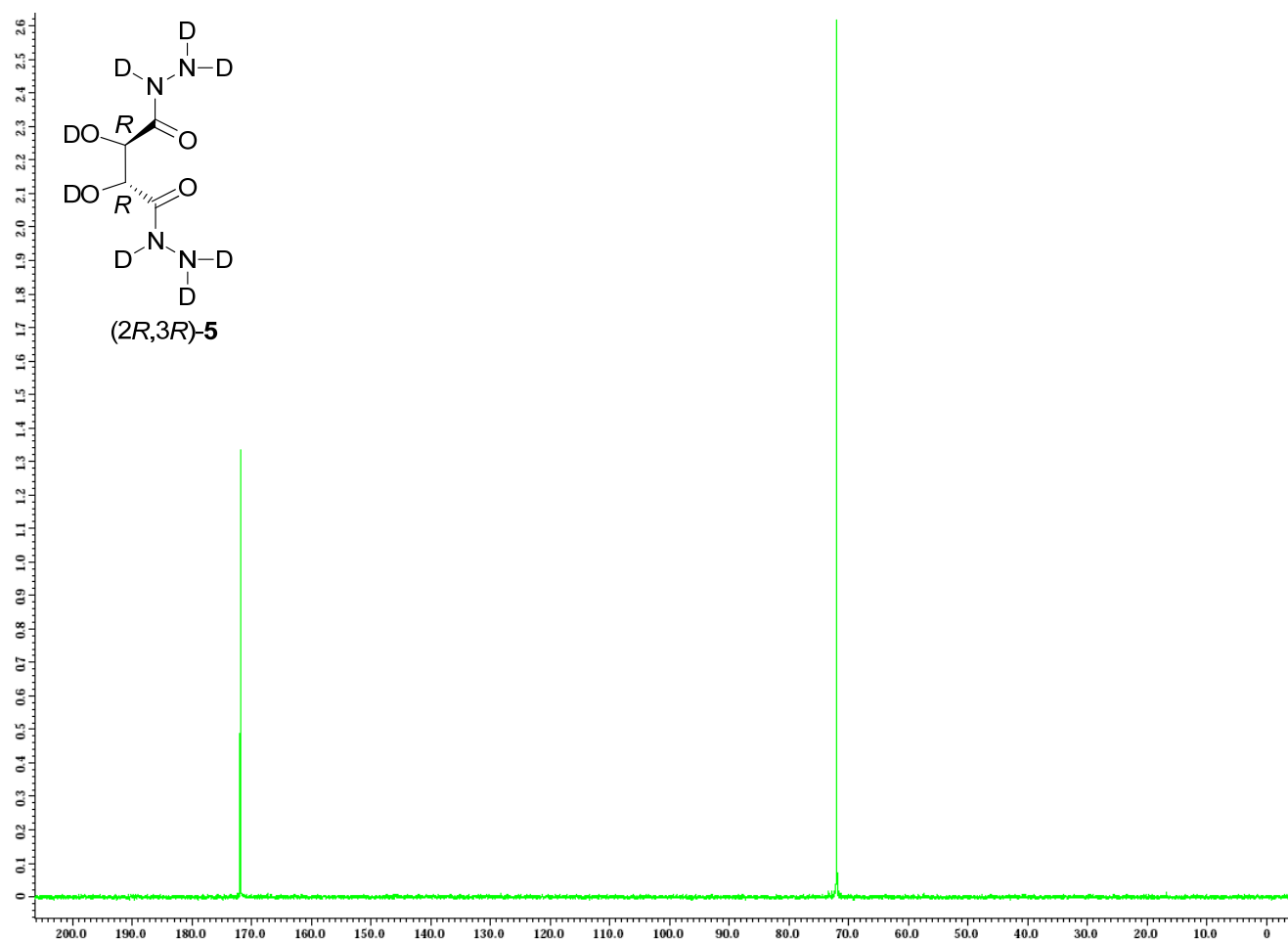
**Figure 7.** ESI-MS spectrum for (4*S*,5*S*)-1,3-dioxolane-4,5-dicarbohydrazide (**4**) from  $\text{H}_2\text{O}$ .



**Figure 8.** Tandem ESI- $\text{MS}^2$  spectrum for (4*S*,5*S*)-1,3-dioxolane-4,5-dicarbohydrazide (**4**) from  $\text{H}_2\text{O}$ .

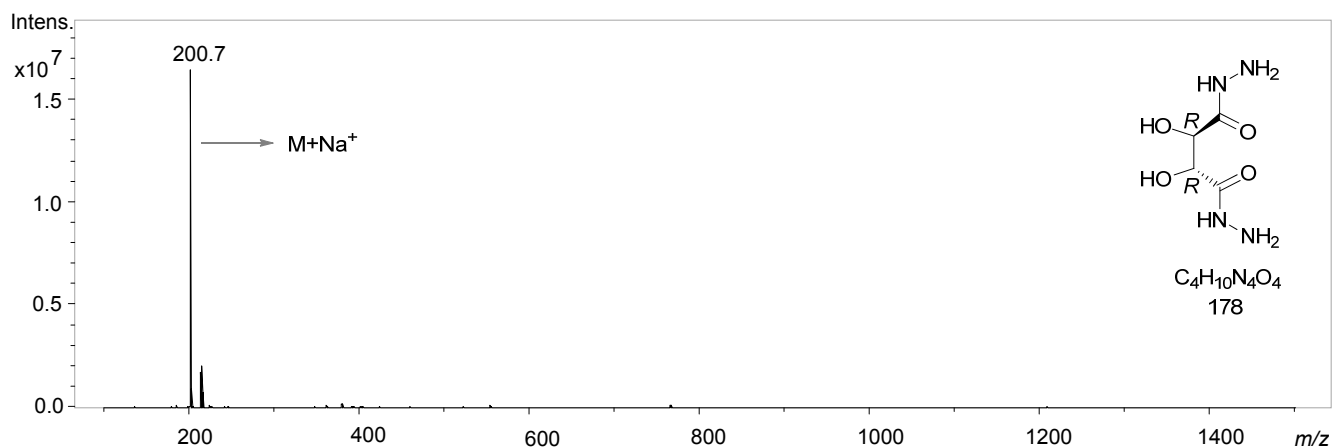


**Figure 9.**  $^1\text{H}$ -NMR spectrum for (2R,3R)-2,3-dihydroxy dicarbohydrazide (**5**),  $\text{D}_2\text{O}$ , 400 MHz.

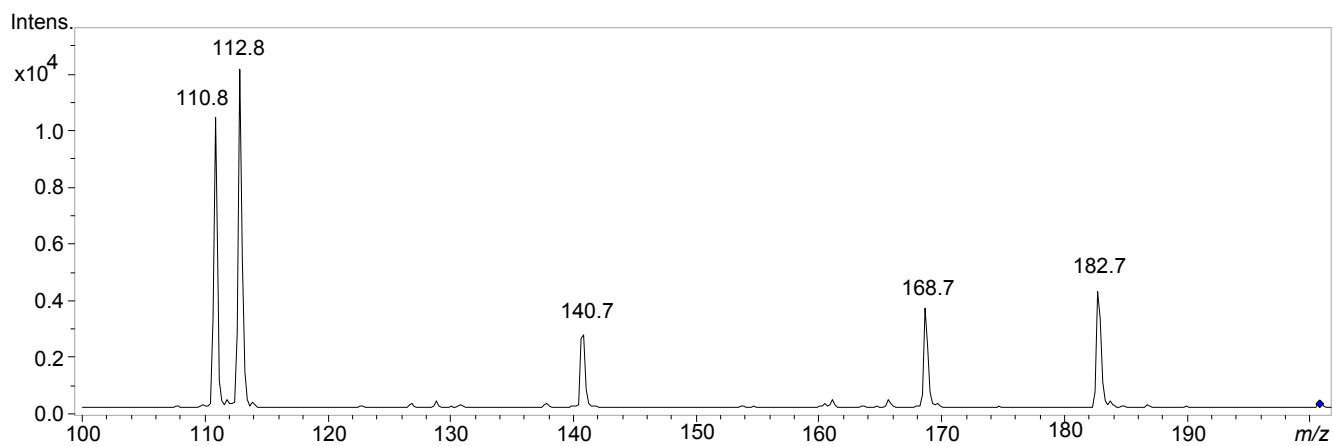


**Figure 10.**  $^{13}\text{C}$ -NMR spectrum for (2R,3R)-2,3-dihydroxy dicarbohydrazide (**5**),  $\text{D}_2\text{O}$ , 100 MHz.

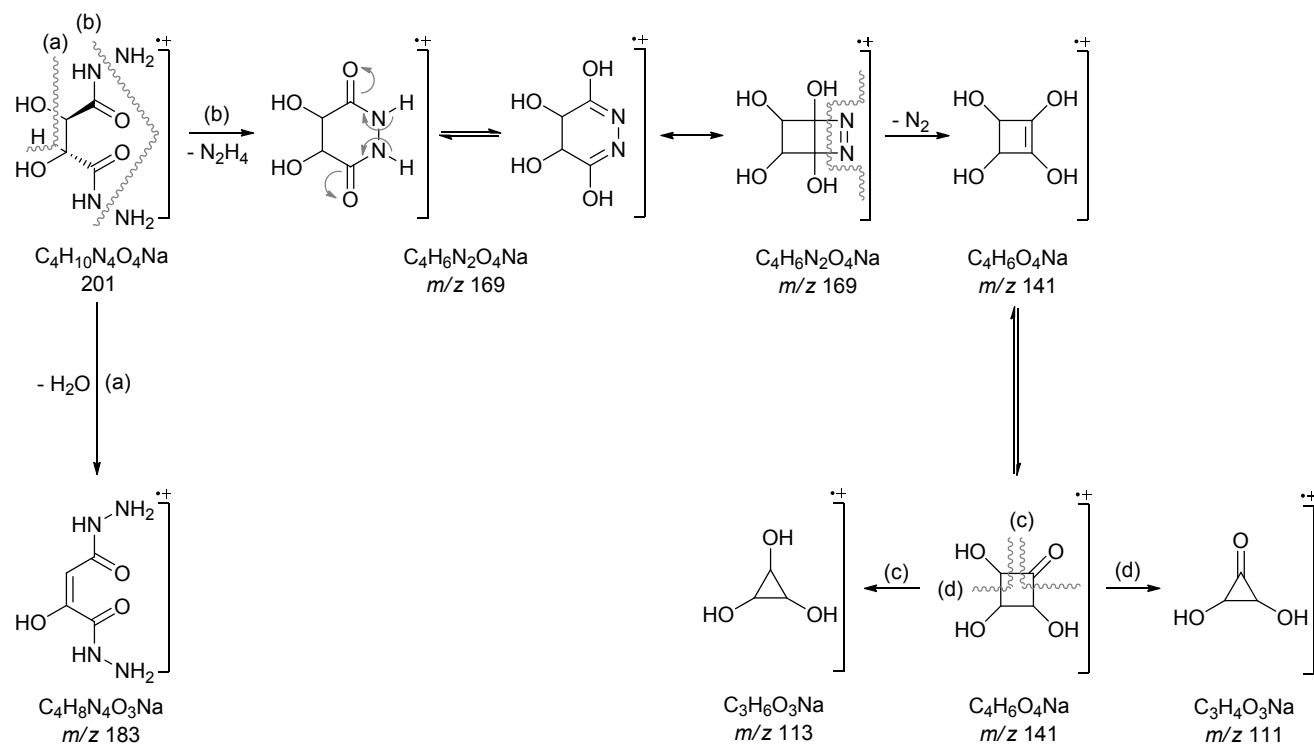




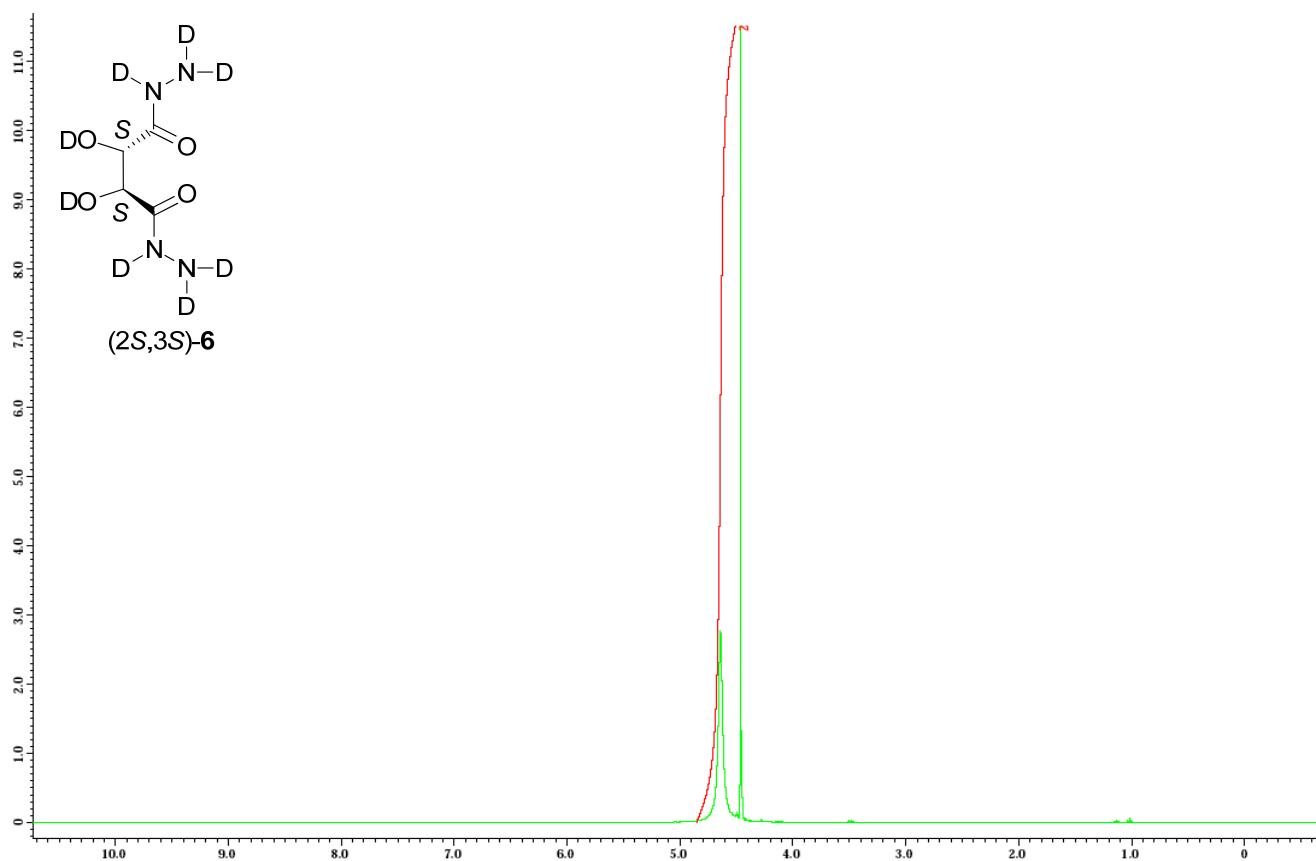
**Figure 11.** ESI-MS spectrum for (2*R*,3*R*)-2,3-dihydroxy dicarbohydrazide (**5**) from H<sub>2</sub>O (Positive mode).



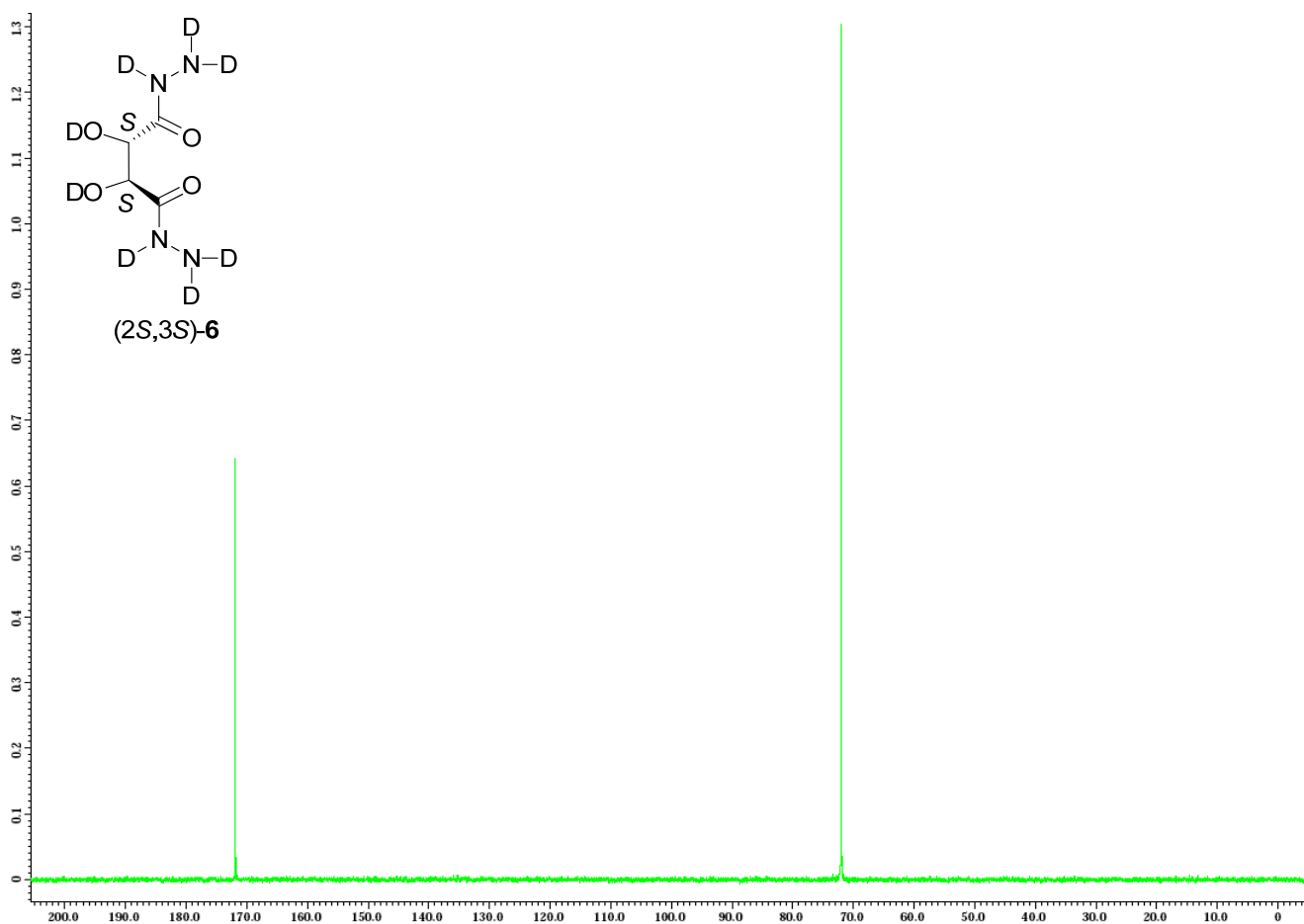
**Figure 12.** Tandem ESI-MS<sup>2</sup> spectrum for (2*R*,3*R*)-2,3-dihydroxy dicarbohydrazide (**5**) from H<sub>2</sub>O (Positive mode).



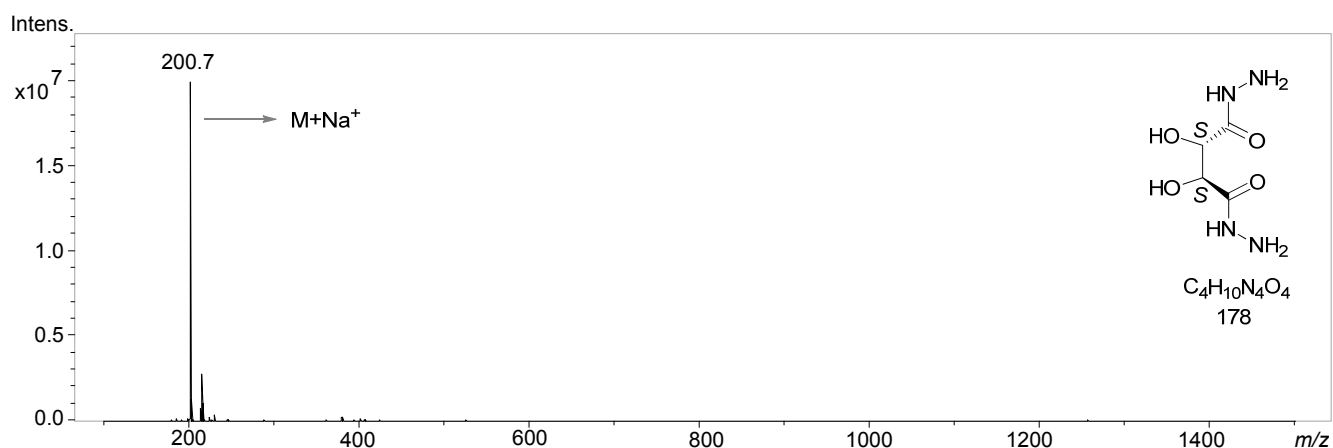
**Scheme 1.** Proposed fragmentation mechanism for (2*R*,3*R*)-2,3-dihydroxy dicarbohydrazide (**5**).



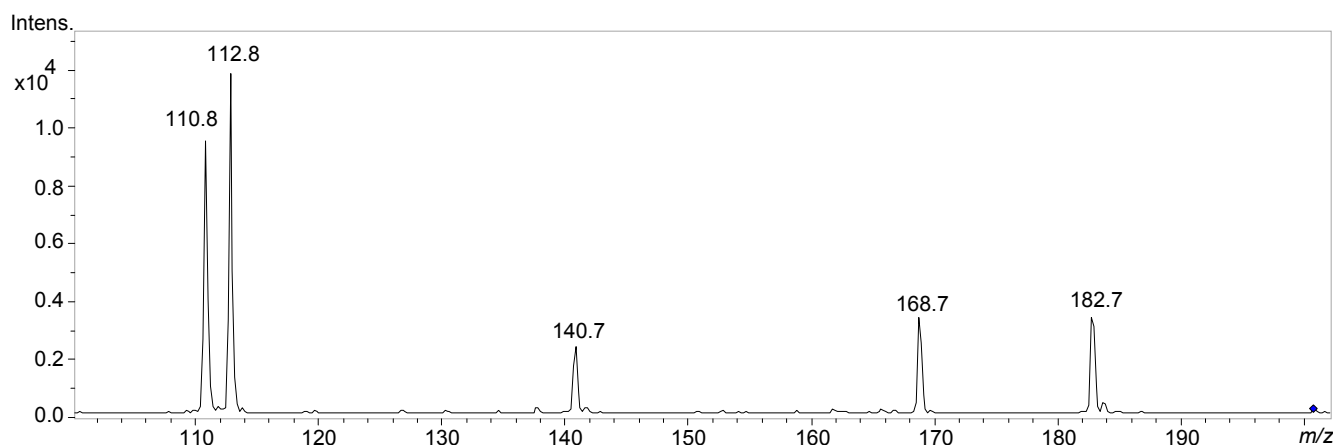
**Figure 13.**  $^1\text{H}$ -NMR spectrum for (2*S*,3*S*)- 2,3-dihydroxy dicarbohydrazide (**6**),  $\text{D}_2\text{O}$ , 400 MHz.



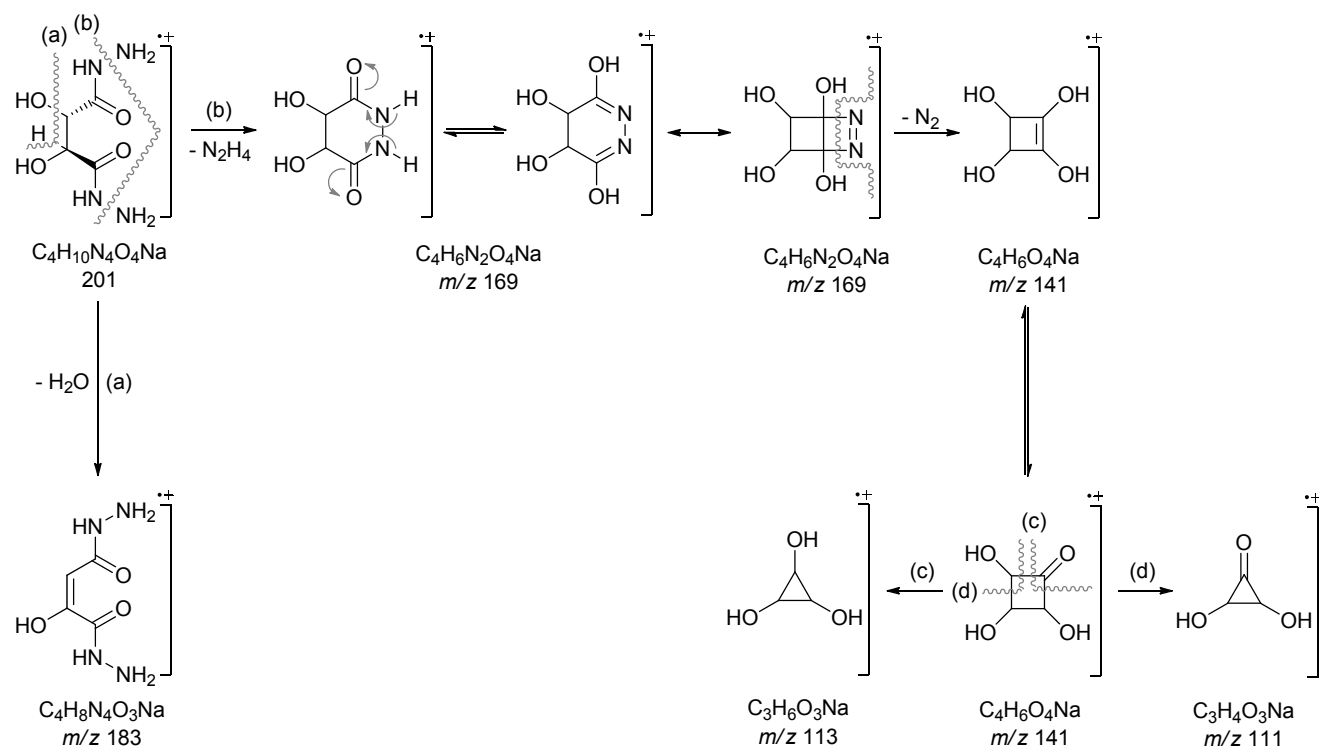
**Figure 14.**  $^{13}\text{C}$ -NMR spectrum for (2*S*,3*S*)- 2,3-dihydroxy dicarbohydrazide (**6**),  $\text{D}_2\text{O}$ , 100 MHz.



**Figure 15.** ESI-MS spectrum for (2*S*,3*S*)-2,3-dihydroxy dicarbohydrazide (**6**) from H<sub>2</sub>O (Positive mode).

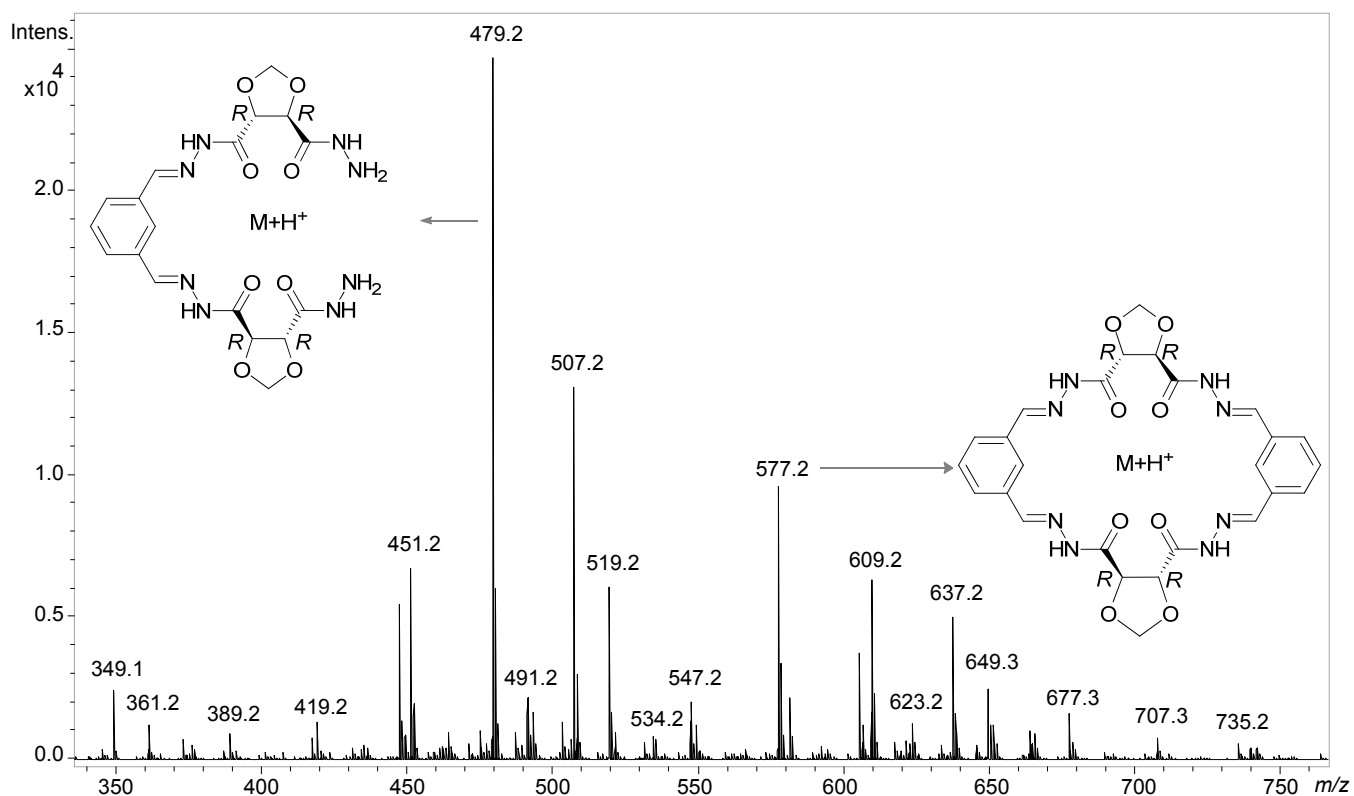


**Figure 16.** Tandem ESI-MS<sup>2</sup> spectrum for (2*S*,3*S*)-2,3-dihydroxy dicarbohydrazide (**6**) from H<sub>2</sub>O (Positive mode).

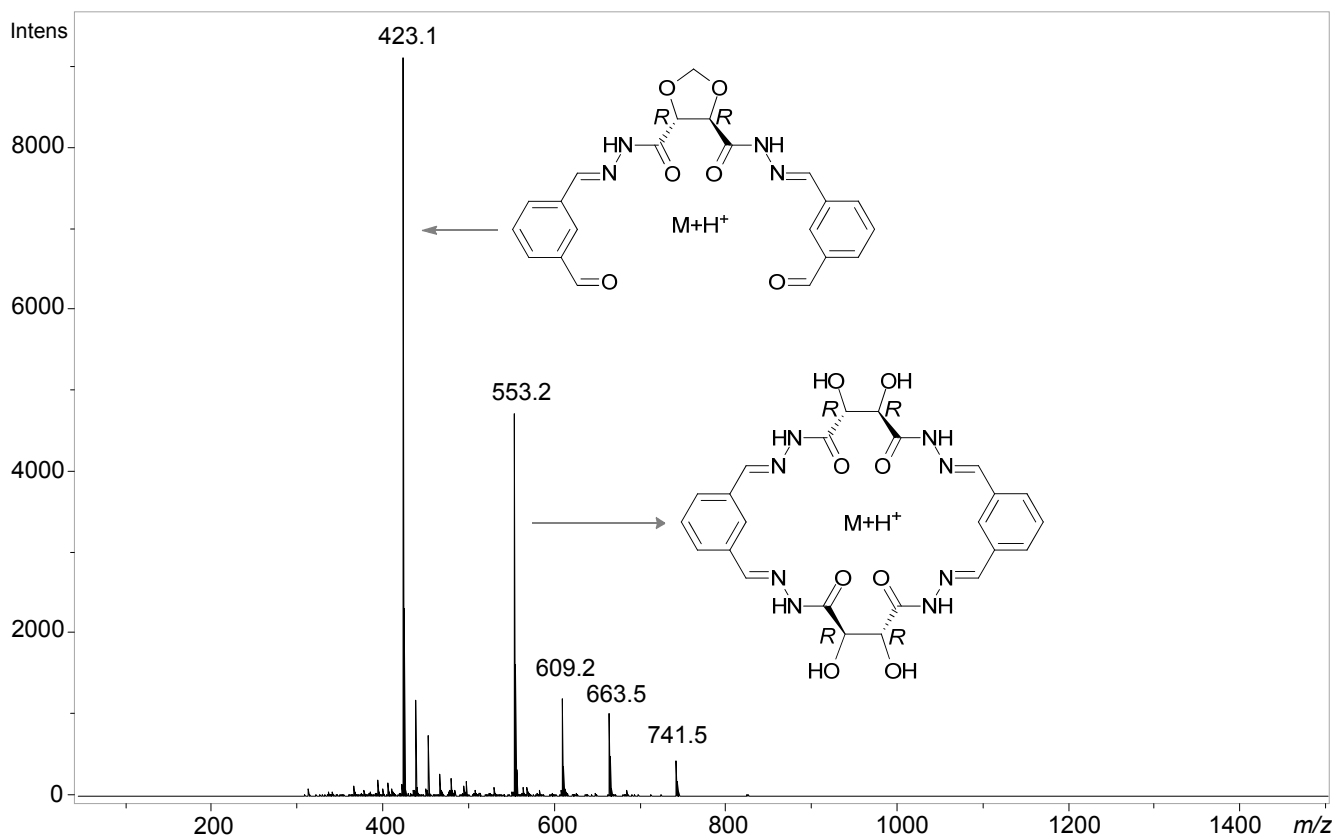


**Scheme 2.** Proposed fragmentation mechanism for (2*S*,3*S*)-2,3-dihydroxy dicarbohydrazide (**6**).

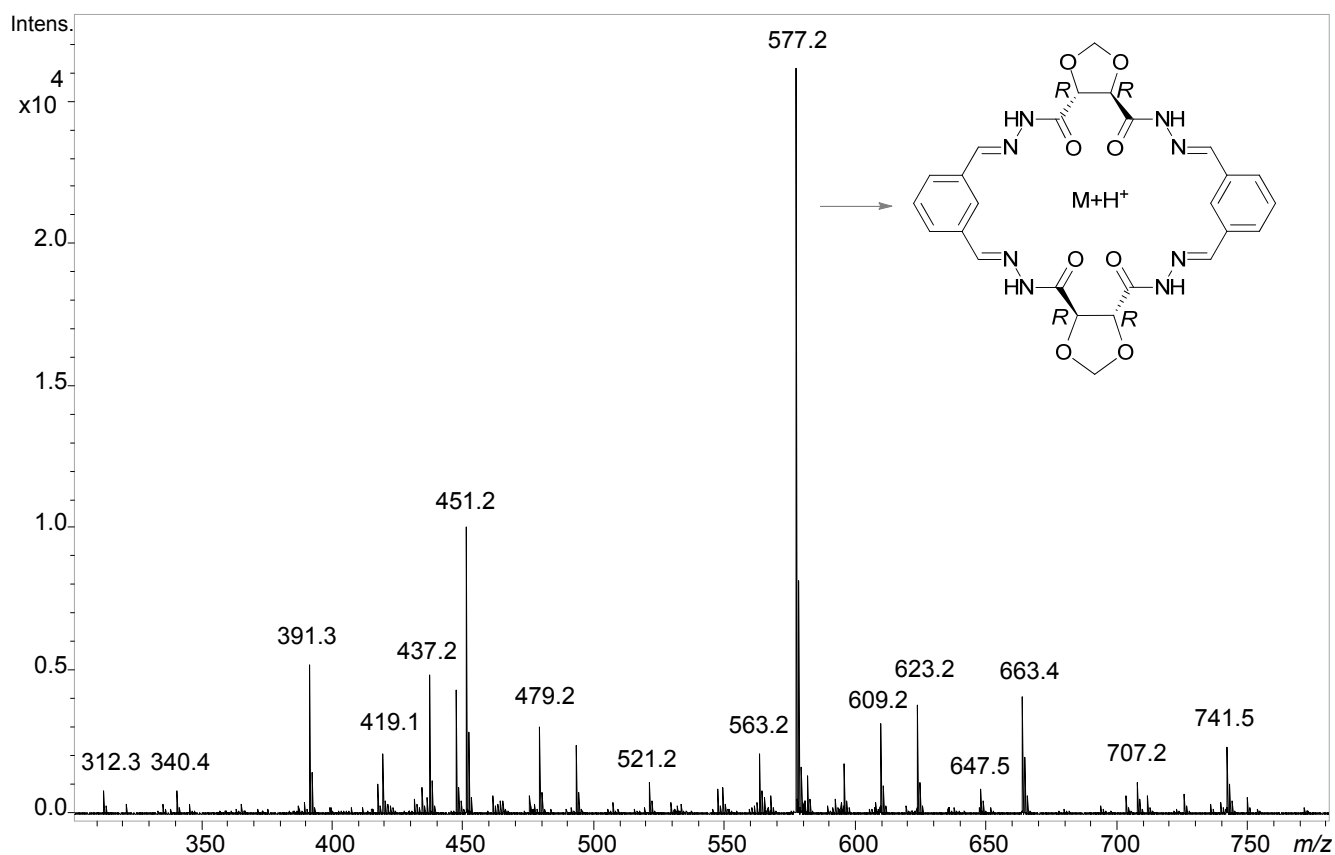
### Optimisation of the [2+2]-cyclocondensation reaction



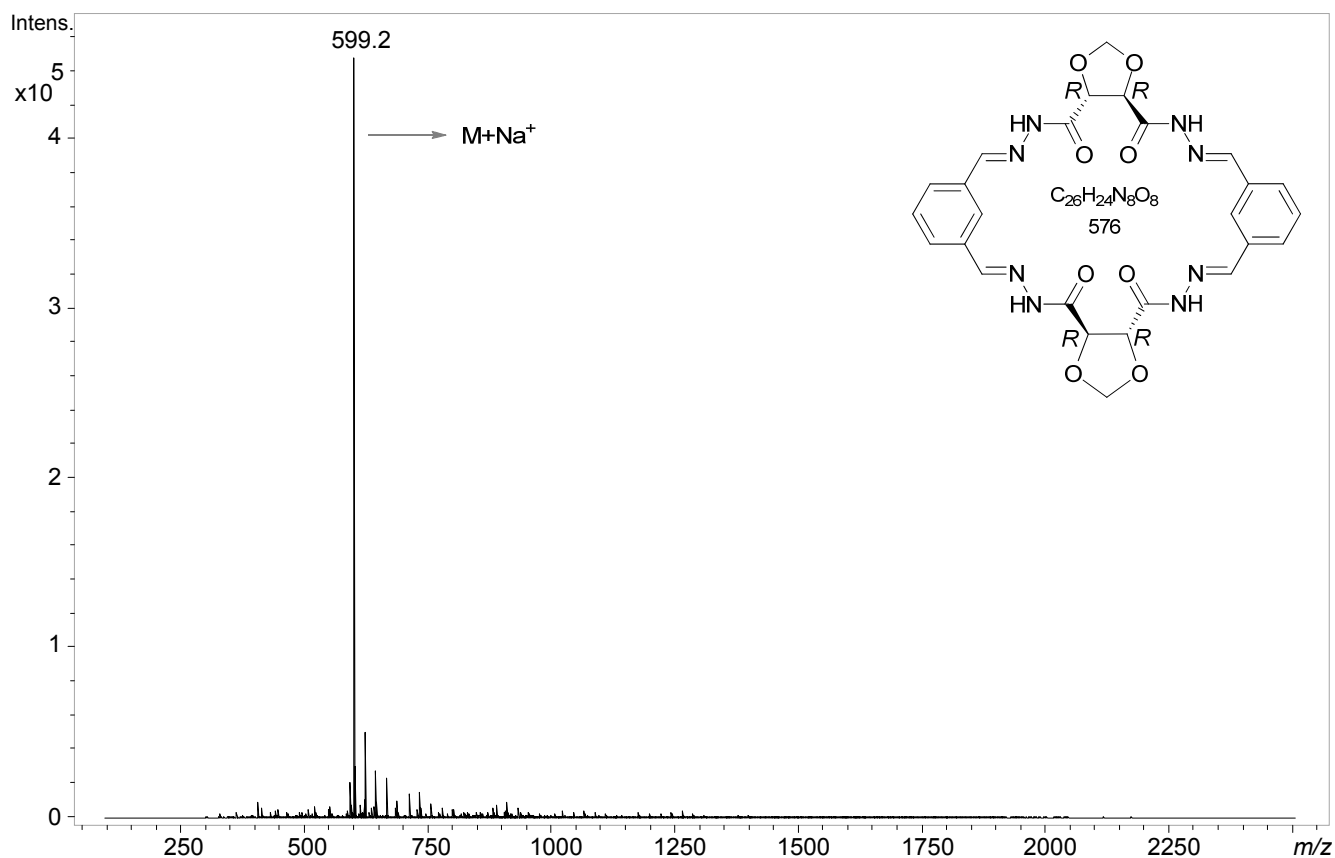
**Figure 17.** APCI-TOF MS from DMSO (macrocycle 7, reaction was conducted in DMF in the presence of few drops of AcOH, ratio of hydrazide to dialdehyde is 2:1, positive mode).



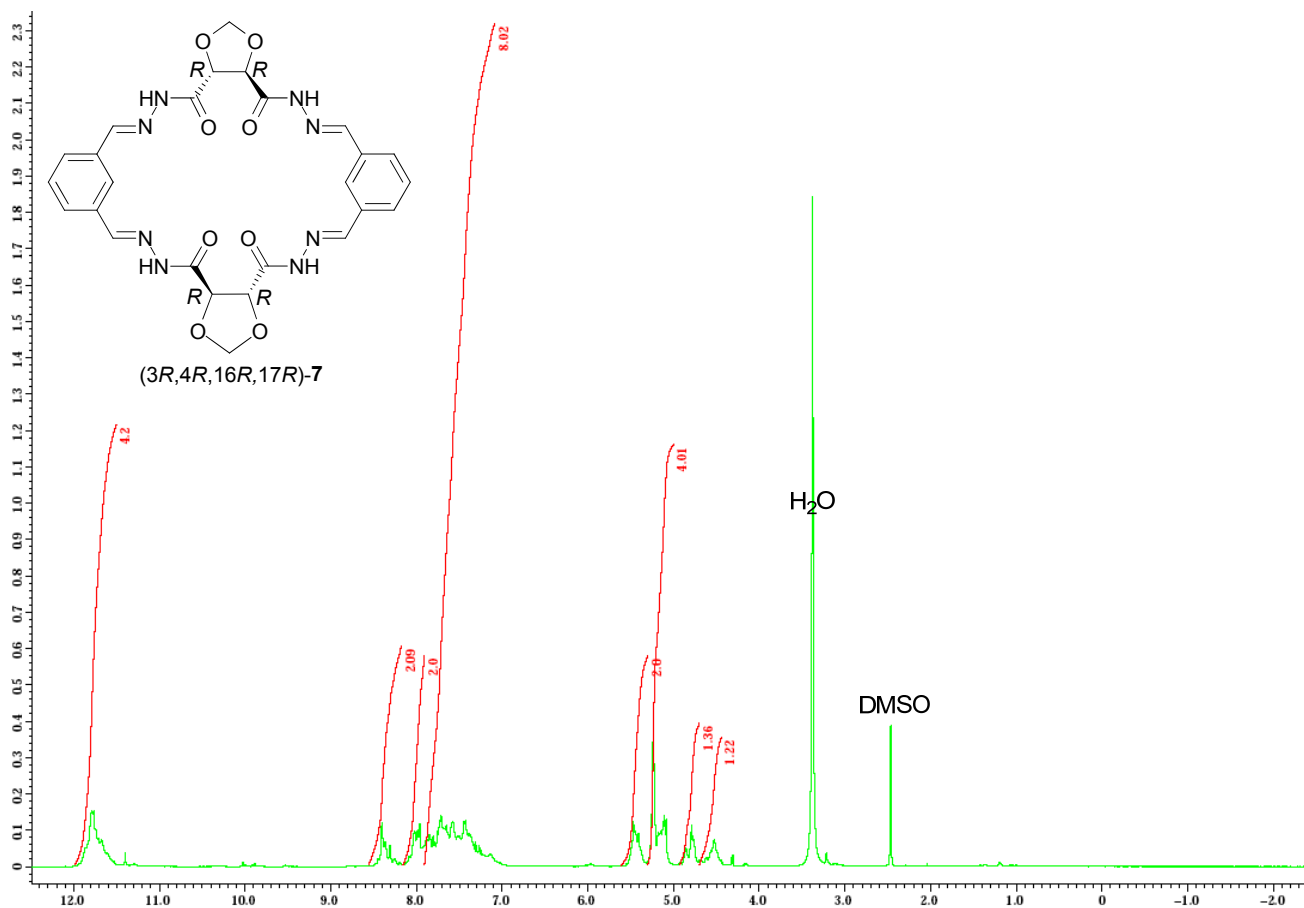
**Figure 18.** APCI-TOF MS from DMSO (macrocycle 7, reaction was conducted in DMF in the presence of few drops of AcOH, ratio of hydrazide to dialdehyde is 1:2, positive mode).



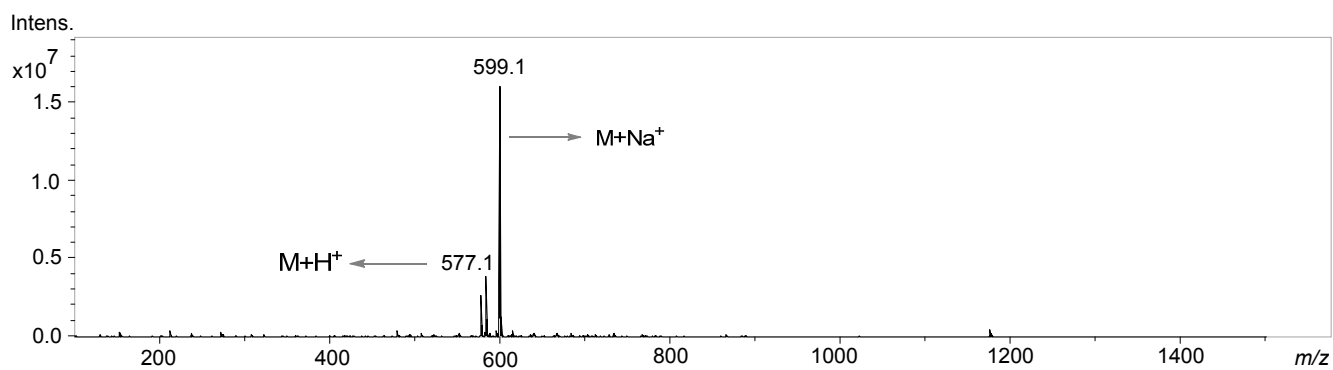
**Figure 19.** APCI-TOF MS from DMSO (macrocycle 7, reaction was conducted in MeOH in the presence of few drops of AcOH, ratio of hydrazide to dialdehyde is 1:1, positive mode).



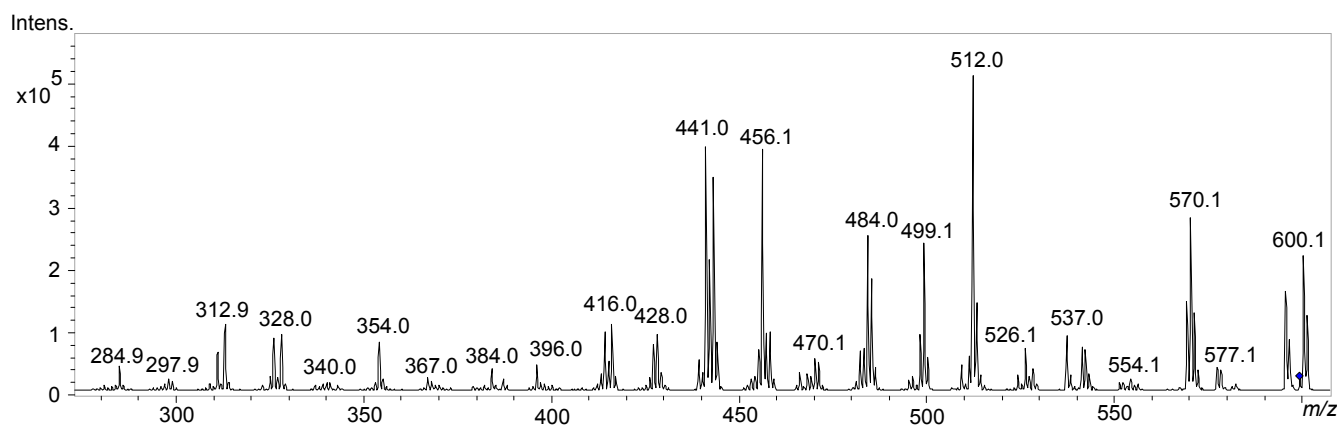
**Figure 20.** APCI-TOF MS from DMSO (macrocycle 7, reaction was conducted in MeOH in the presence of few drops of AcOH, ratio of hydrazide to dialdehyde is 1.2:1, positive mode).



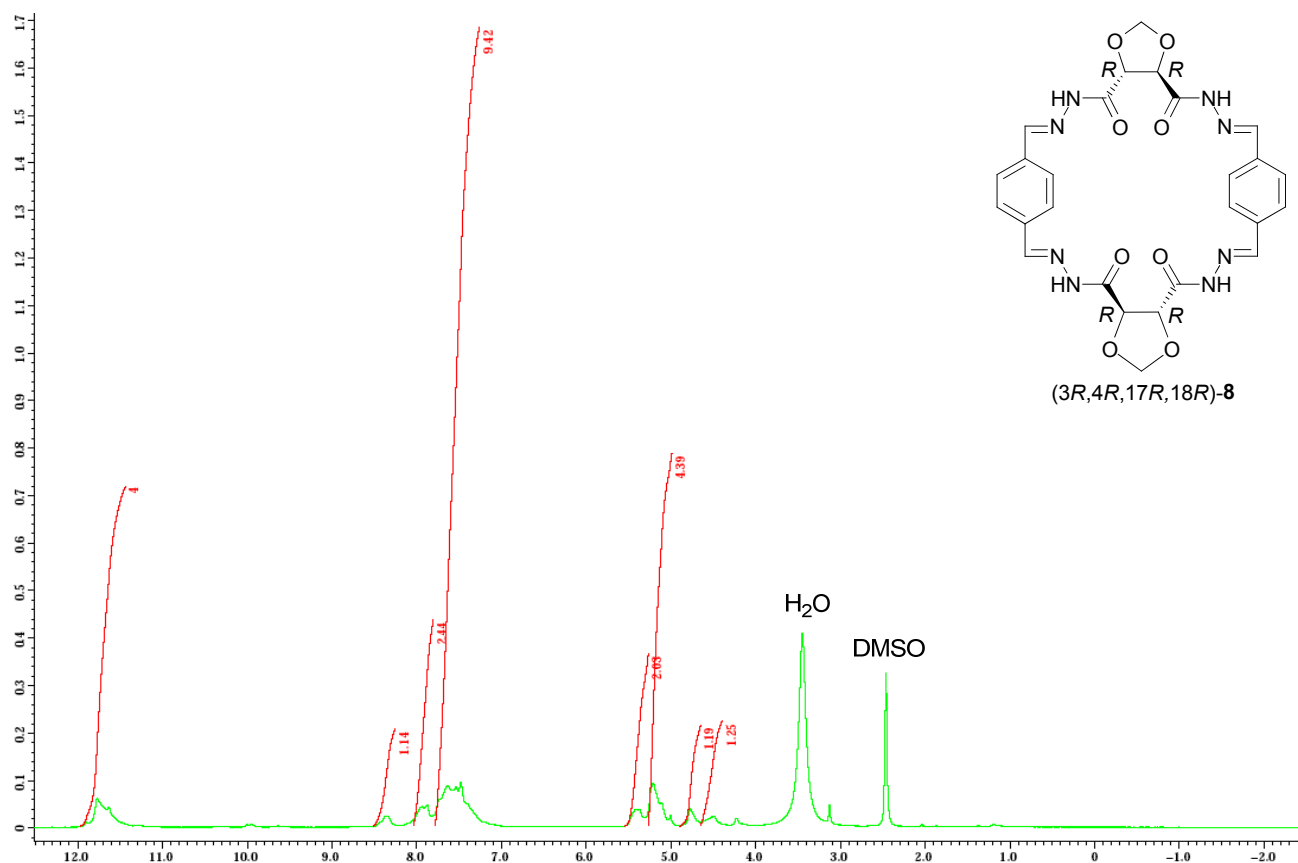
**Figure 21.**  $^1\text{H-NMR}$  spectrum for macrocycle (7),  $\text{DMSO-d}_6$ , 400 MHz.



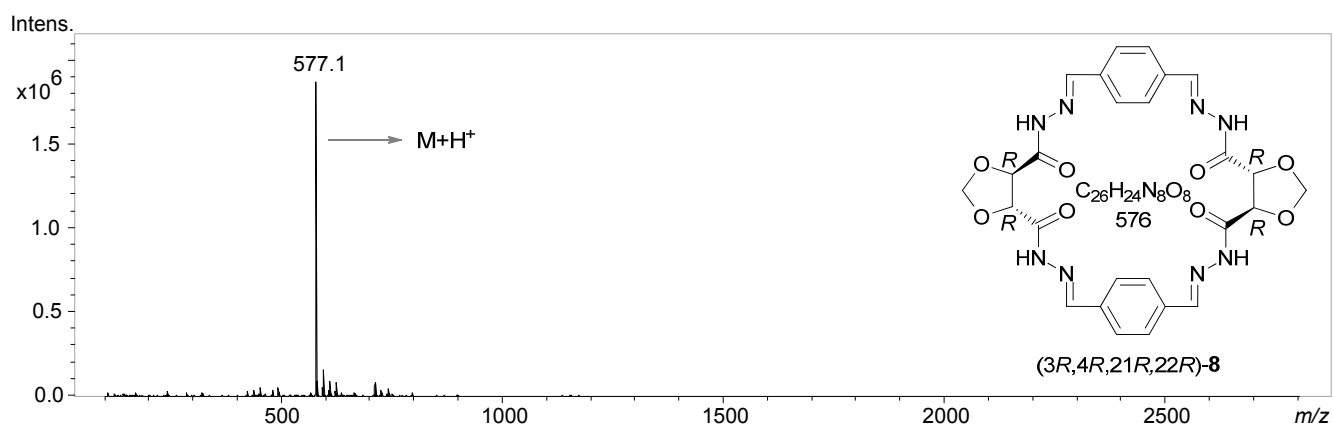
**Figure 22.** ESI-MS spectrum for macrocycle (7) from DMF and ACN (Positive mode).



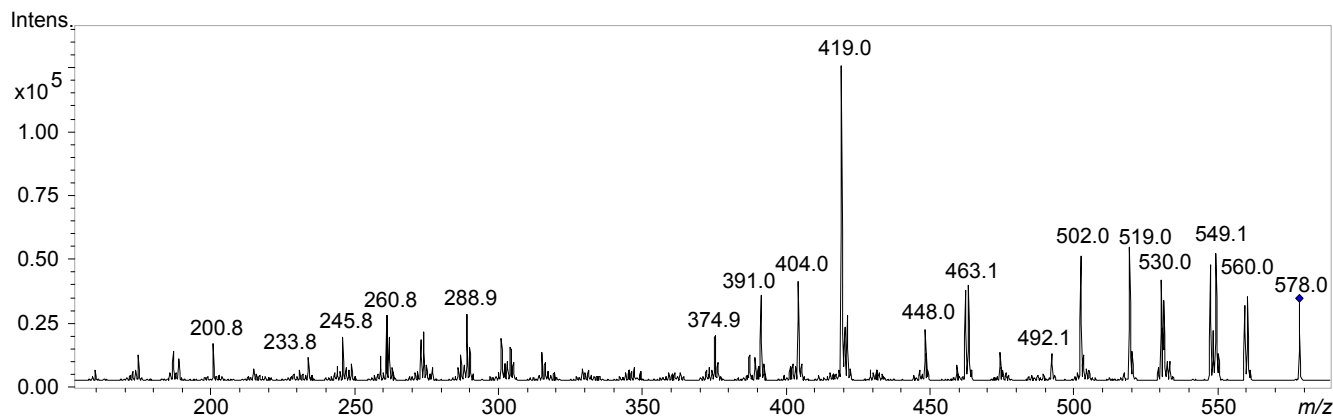
**Figure 23.** Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (7) from DMF and ACN (Positive mode).



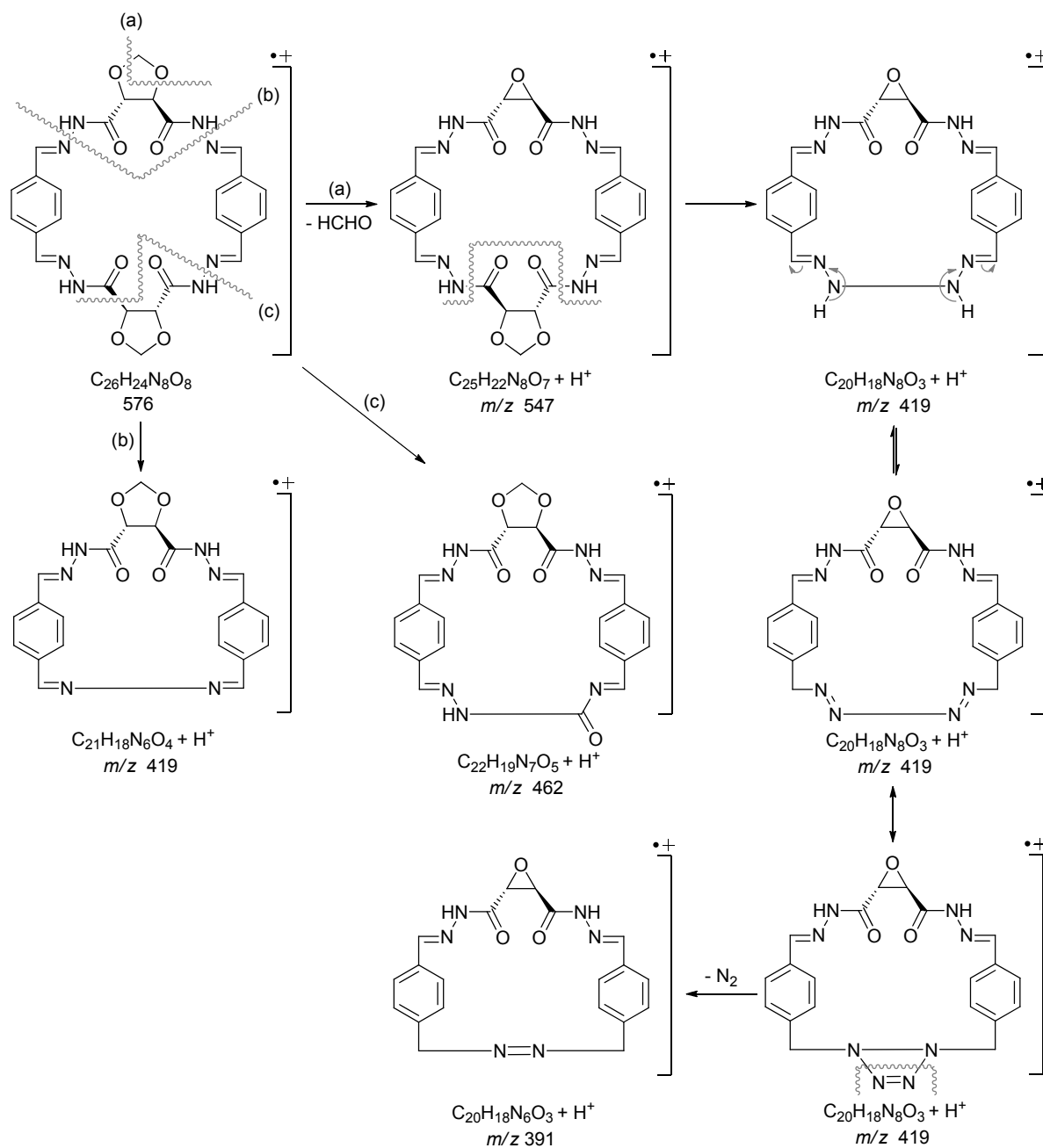
**Figure 24.**  $^1\text{H-NMR}$  spectrum for macrocycle (**8**),  $\text{DMSO-d}_6$ , 400 MHz.



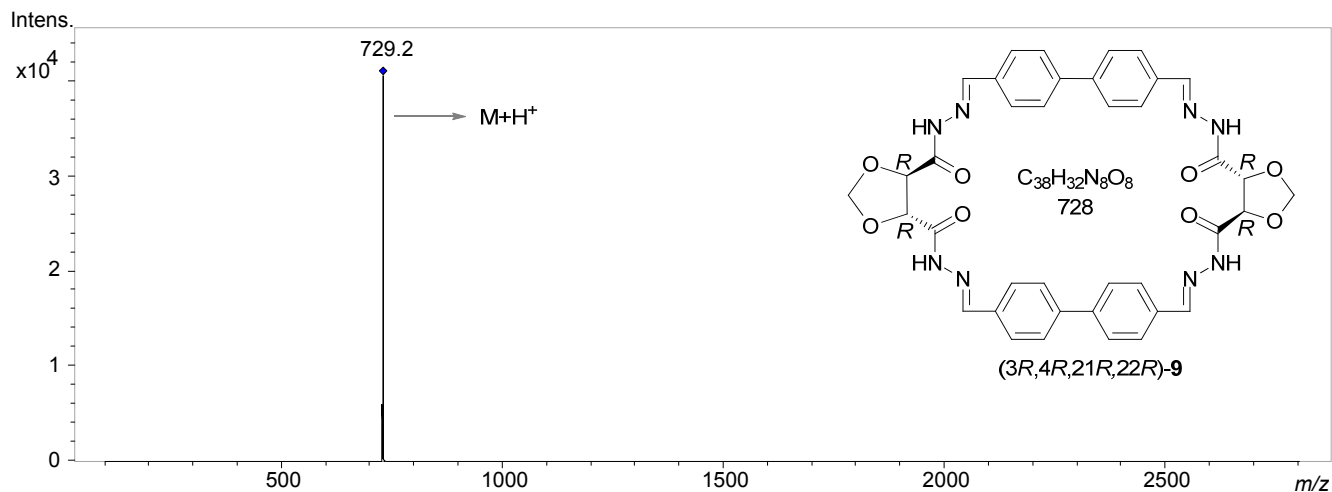
**Figure 25.** ESI-MS spectrum for macrocycle (**8**) from DMF and ACN (Positive mode).



**Figure 26.** Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (**8**) from DMF and ACN (Positive mode).



**Scheme 3.** Proposed fragmentation mechanism for macrocycle (**8**).



**Figure 27.** APCI-MS<sup>2</sup> spectrum for macrocycle (**9**), DMSO (Positive mode).



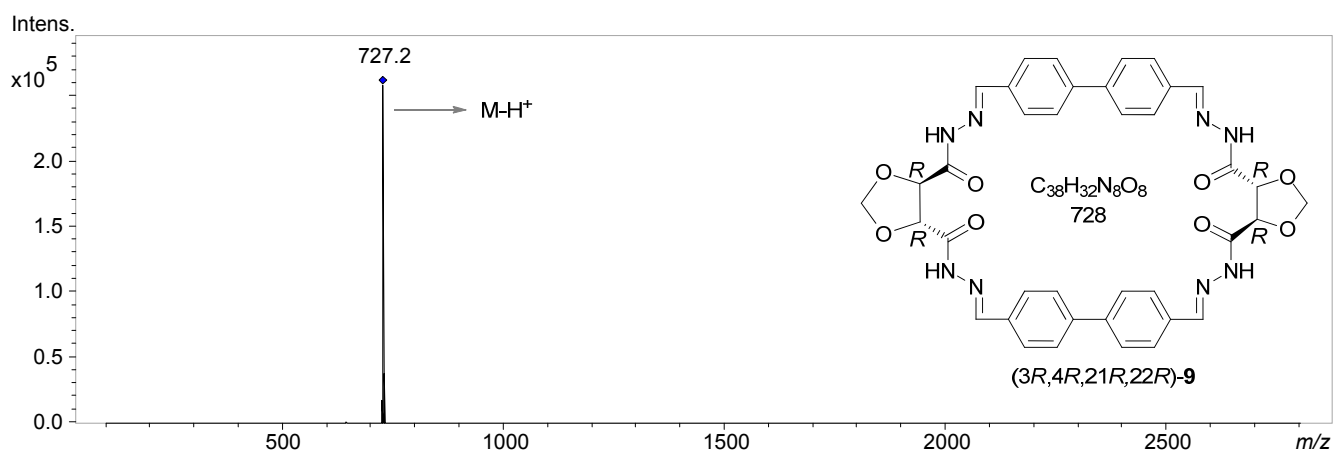


Figure 28. APCI-MS<sup>2</sup> spectrum for macrocycle (9), DMSO (negative mode).

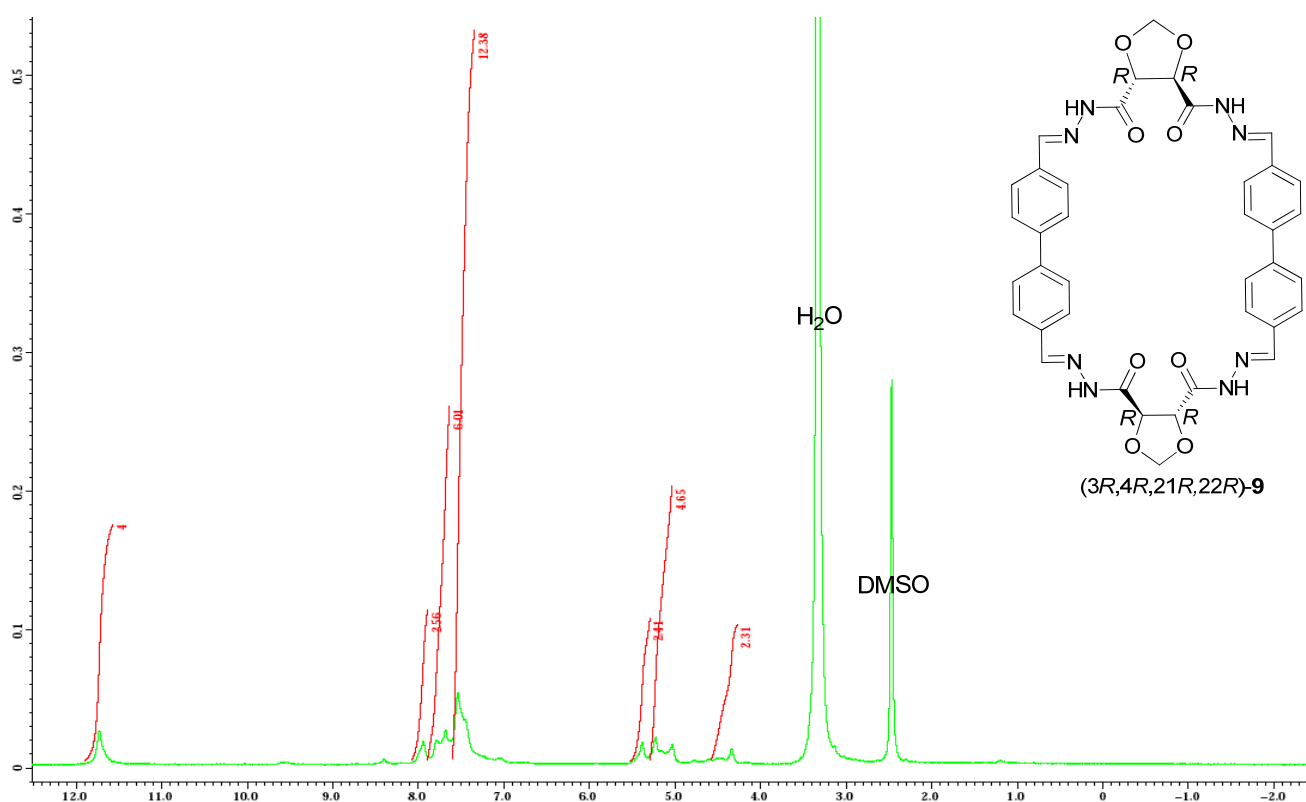


Figure 29. <sup>1</sup>H-NMR spectrum for macrocycle (9), DMSO-d<sub>6</sub>, 400 MHz.

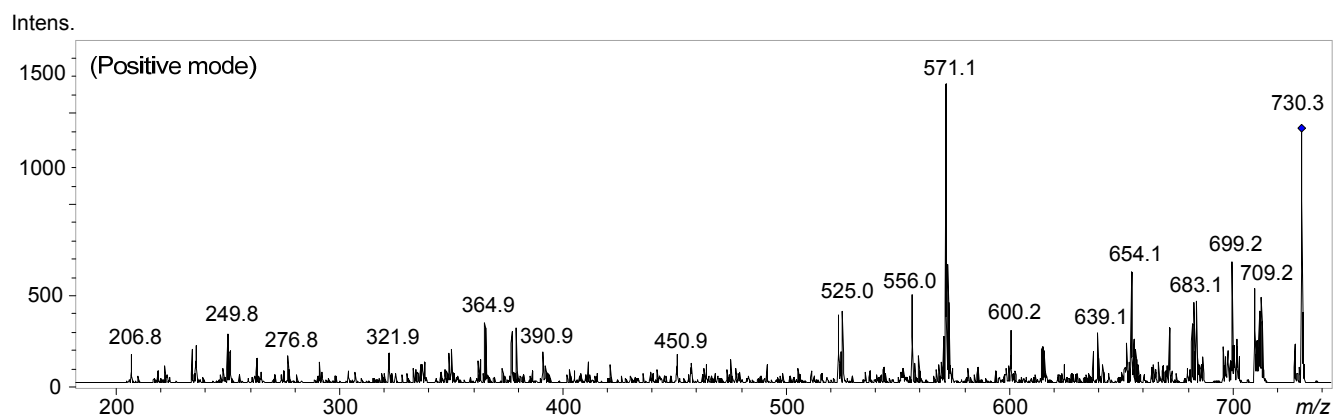
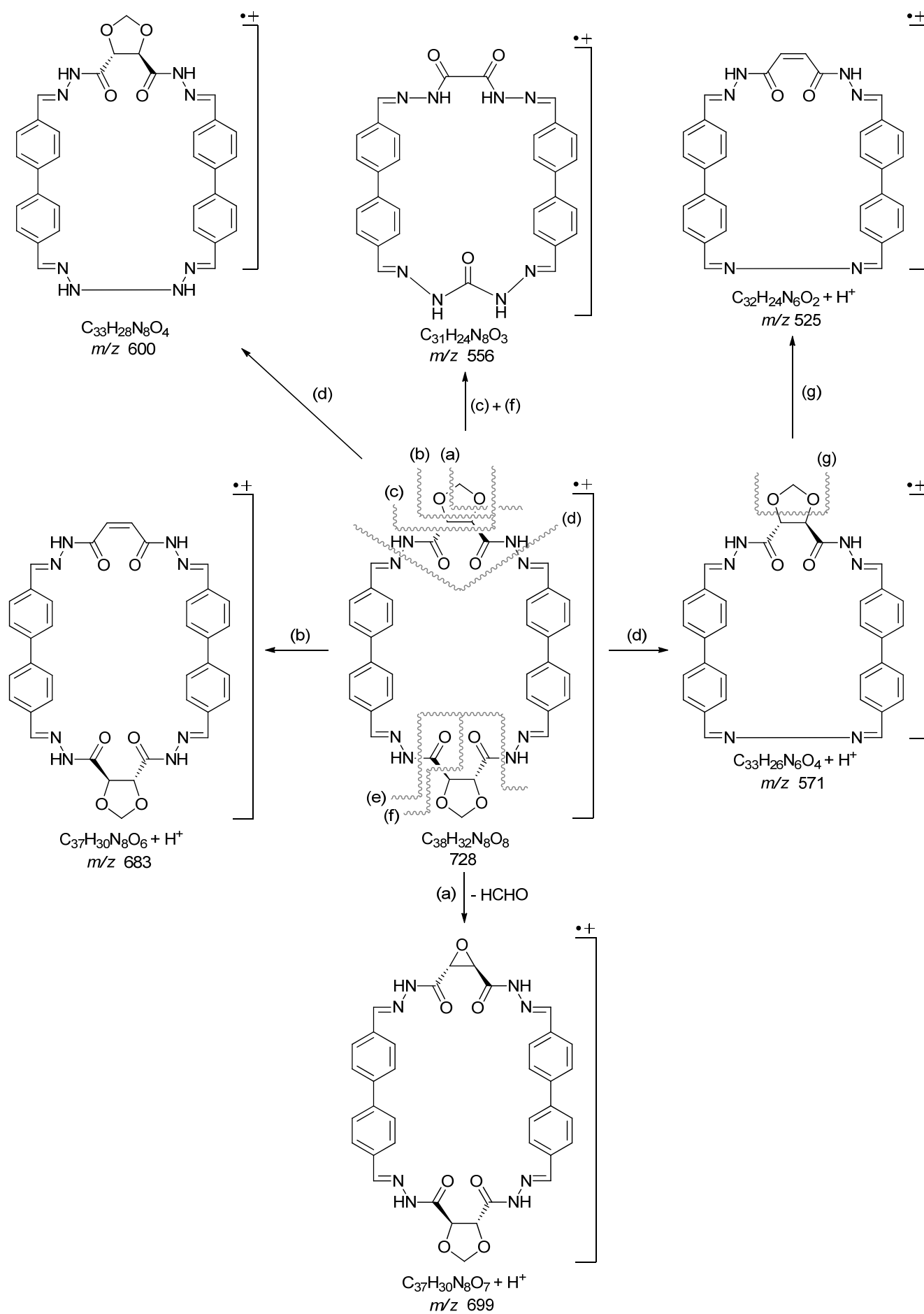
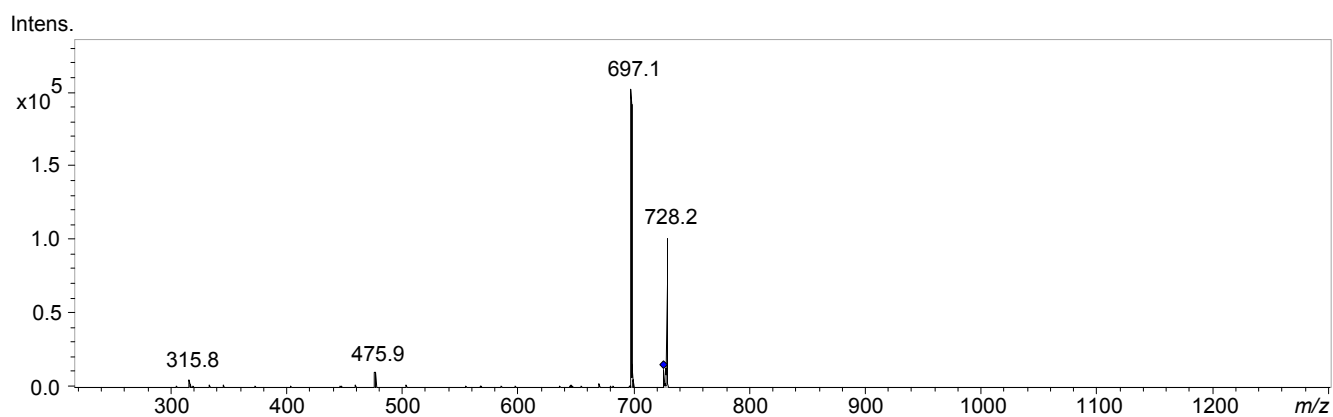


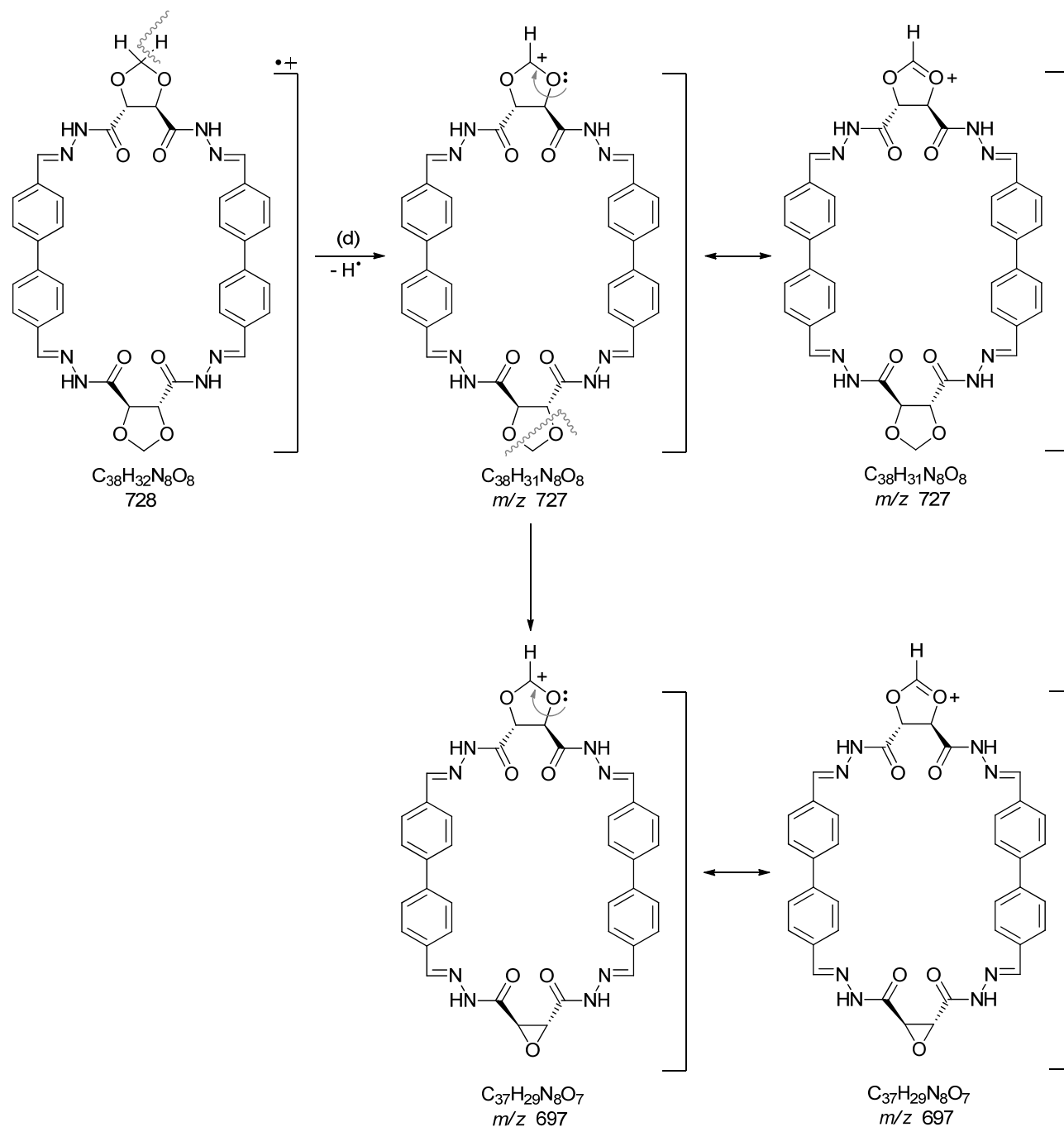
Figure 30. Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (9), DMSO.



Scheme 4. Proposed fragmentation mechanism for macrocycle (9).



**Figure 31.** Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (**9**) from DMSO (negative mode).



**Scheme 5.** Proposed fragmentation mechanism for macrocycle (**9**).

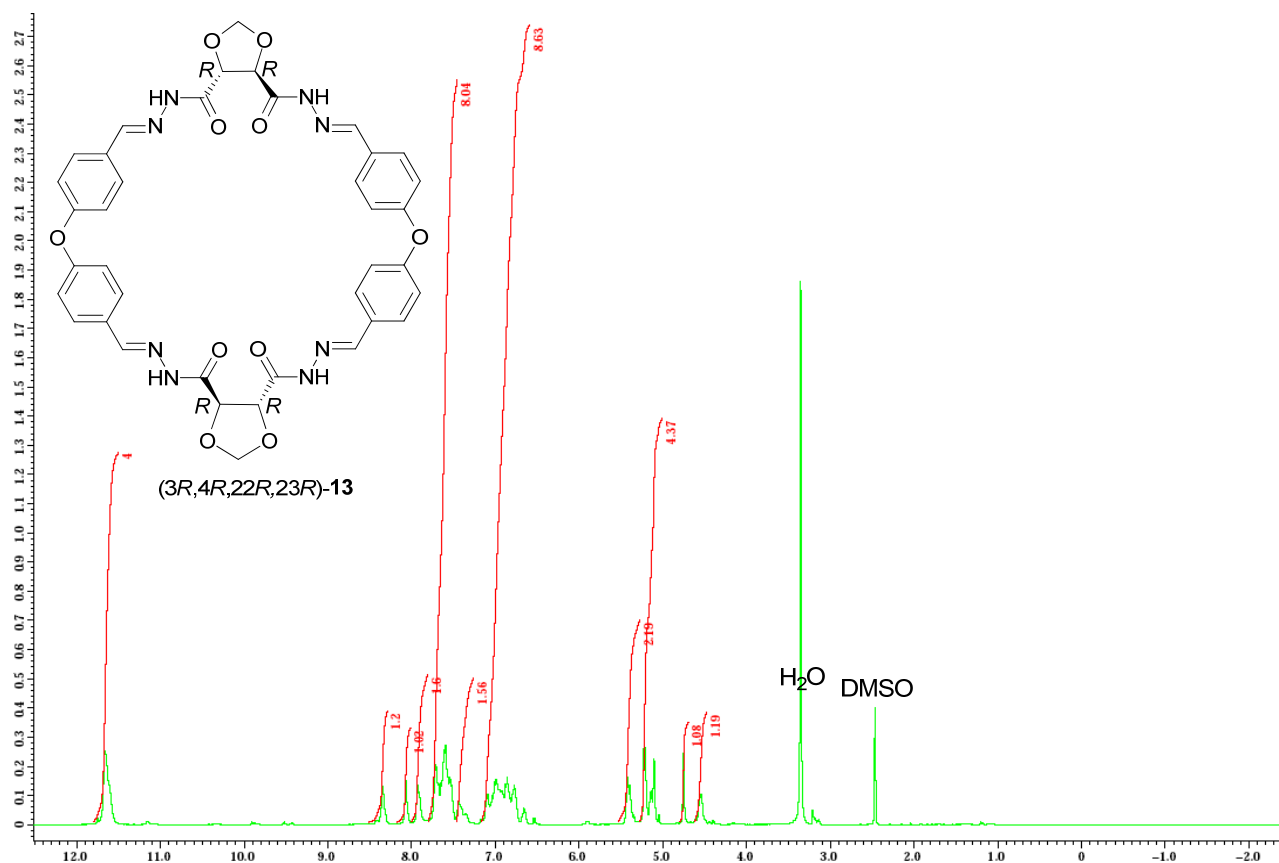


Figure 32. <sup>1</sup>H-NMR spectrum for macrocycle (13), DMSO-d<sub>6</sub>, 400 MHz.

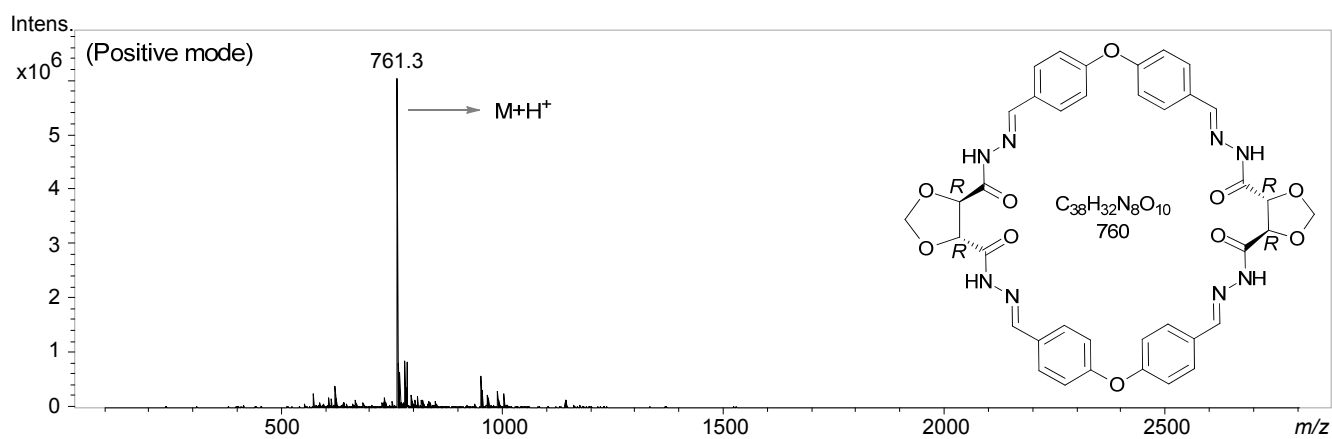


Figure 33. ESI-MS spectrum for macrocycle (13) from DMF and ACN.

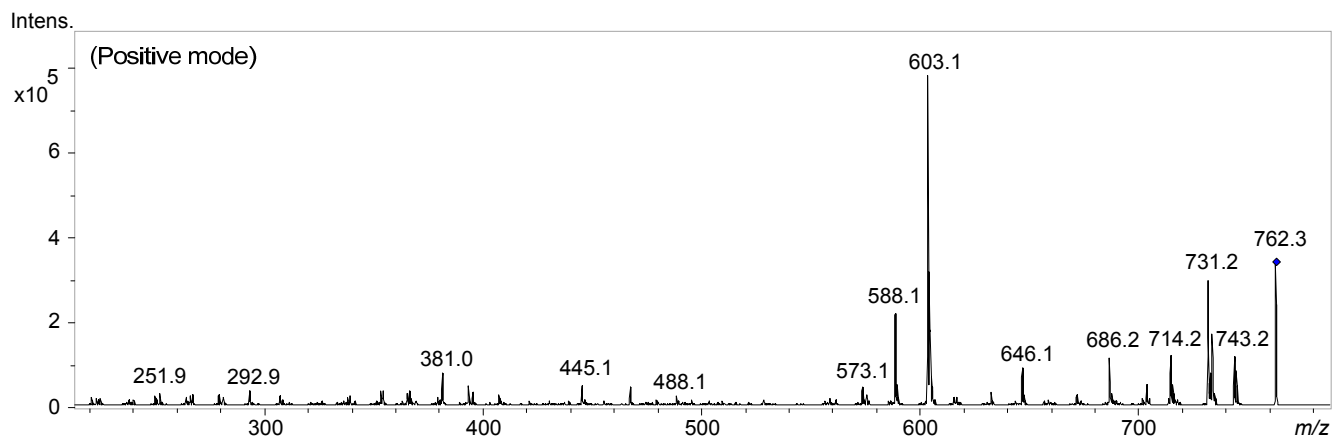
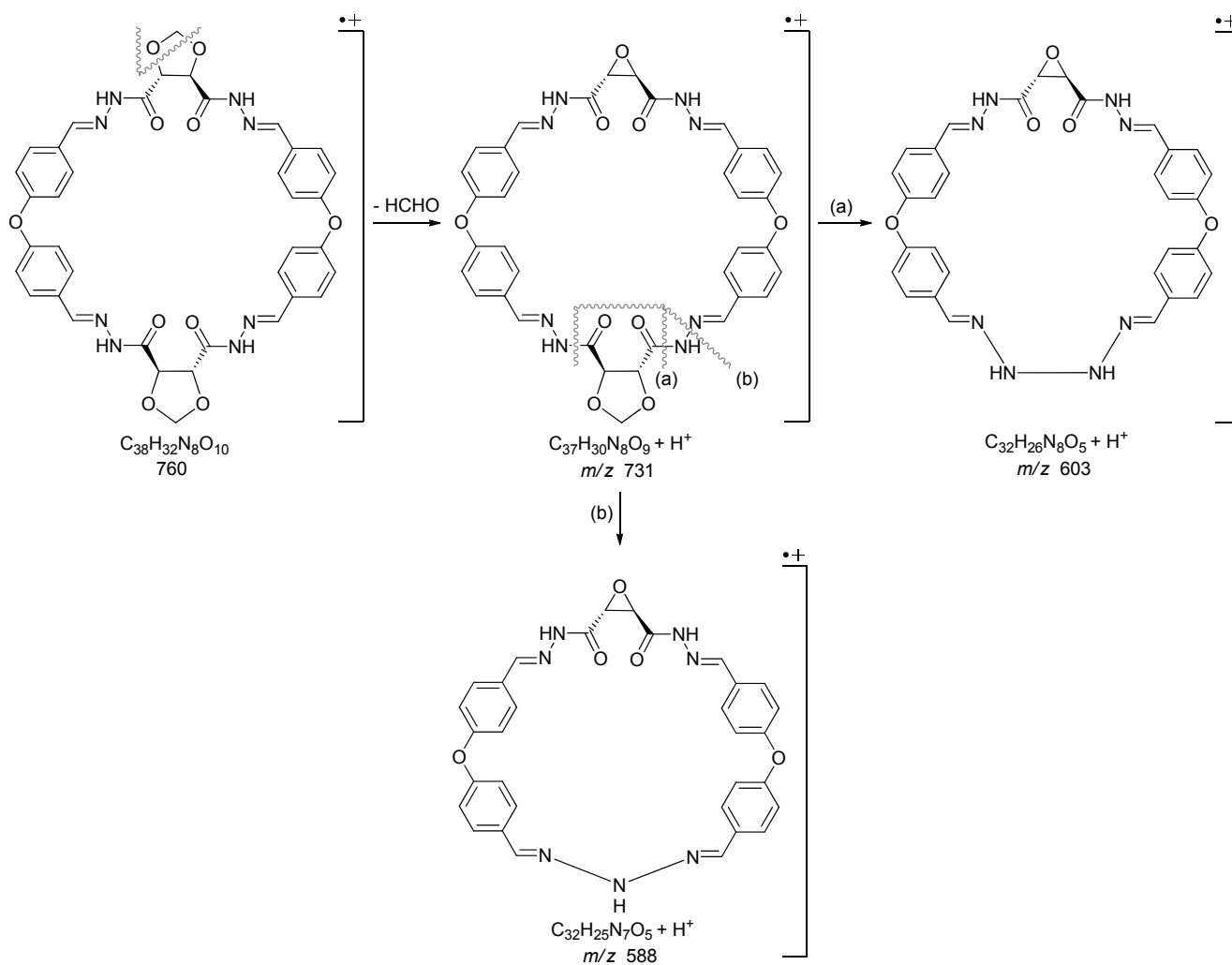
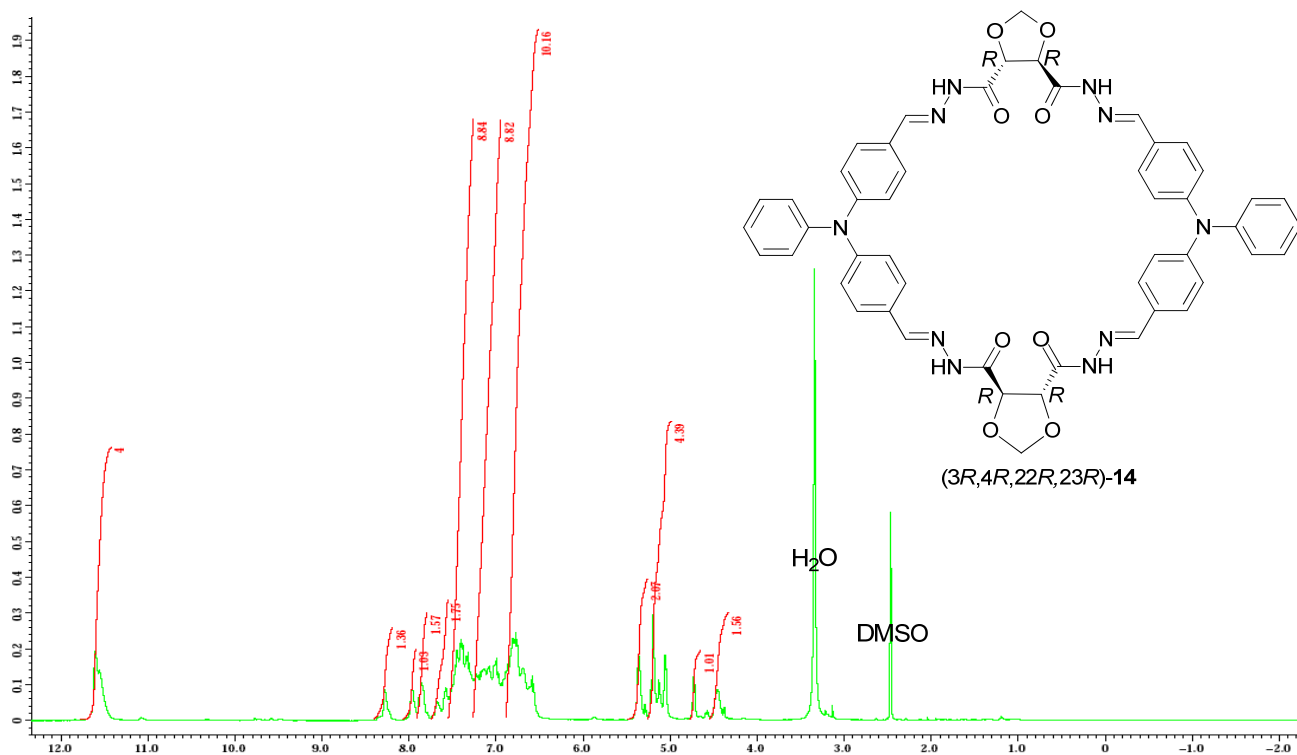


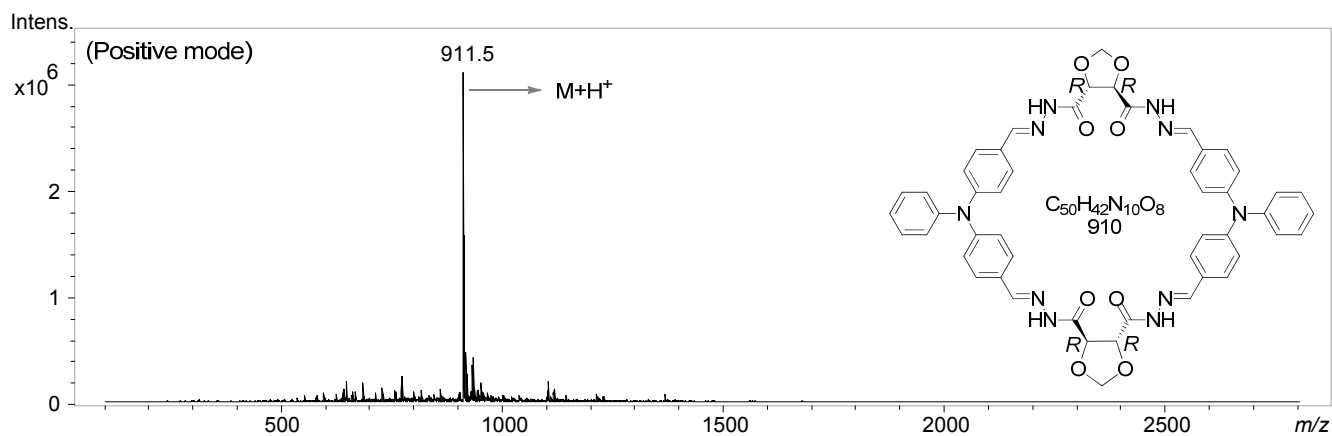
Figure 34. Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (13) from DMF and ACN.



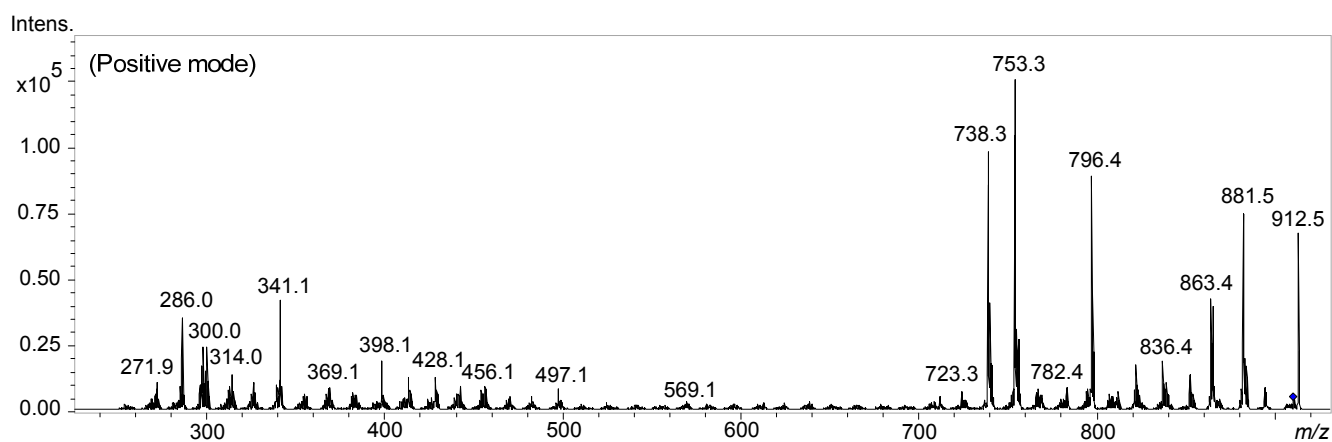
**Scheme 6.** Proposed fragmentation mechanism for macrocycle (13).



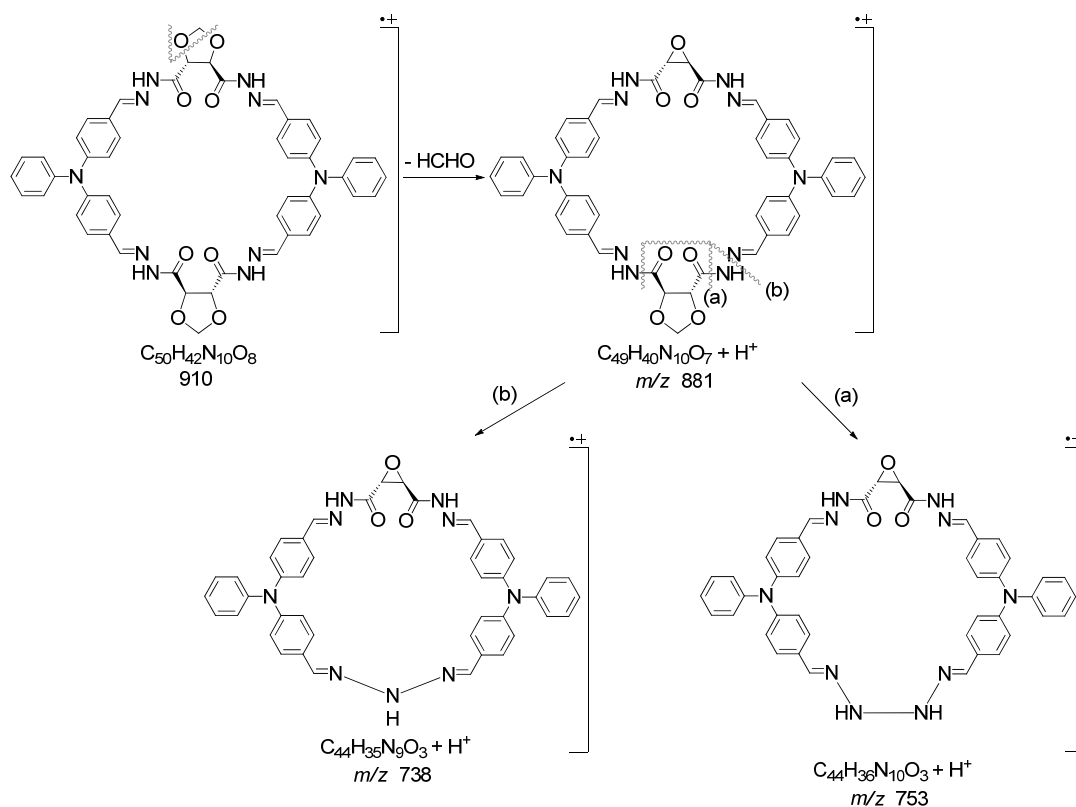
**Figure 35.**  $^1H$ -NMR spectrum for macrocycle (14),  $DMSO-d_6$ , 400 MHz.



**Figure 36.** ESI-MS spectrum for macrocycle (14) from DMF and ACN.



**Figure 37.** Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (14) from DMF and ACN.



**Scheme 7.** Proposed fragmentation mechanism for macrocycle (14).

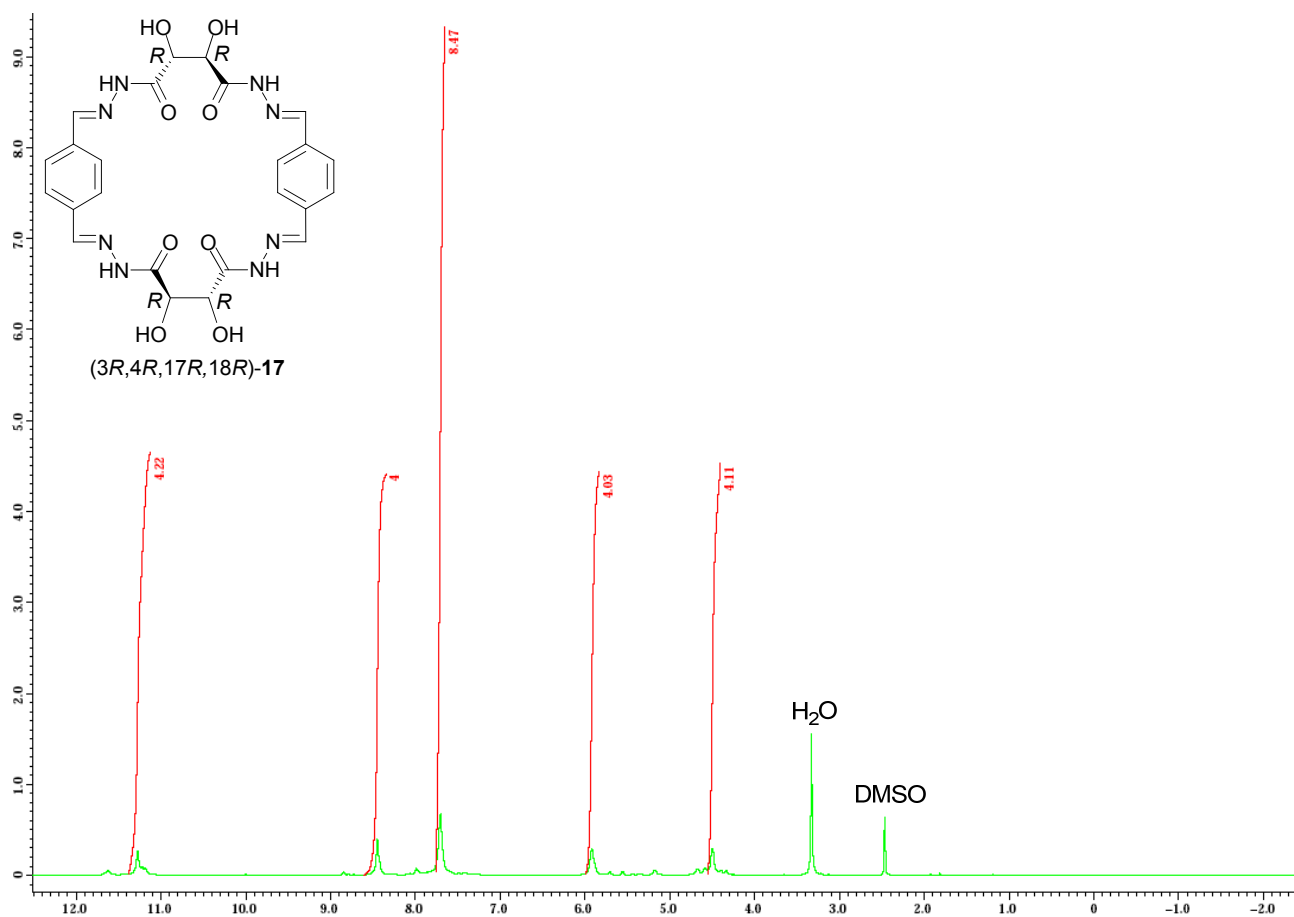


Figure 38. <sup>1</sup>H-NMR spectrum for macrocycle (17), DMSO-d<sub>6</sub>, 400 MHz.

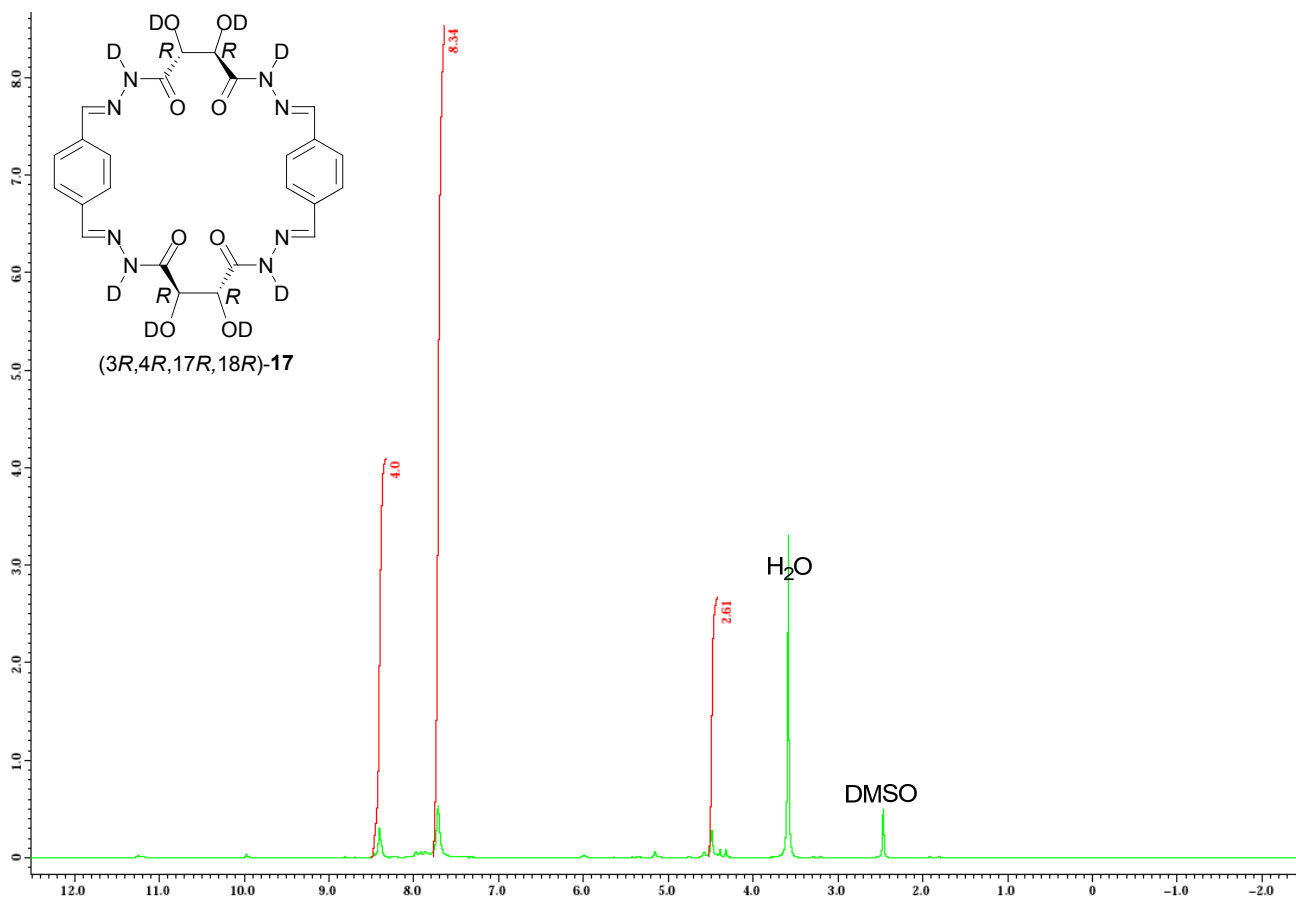
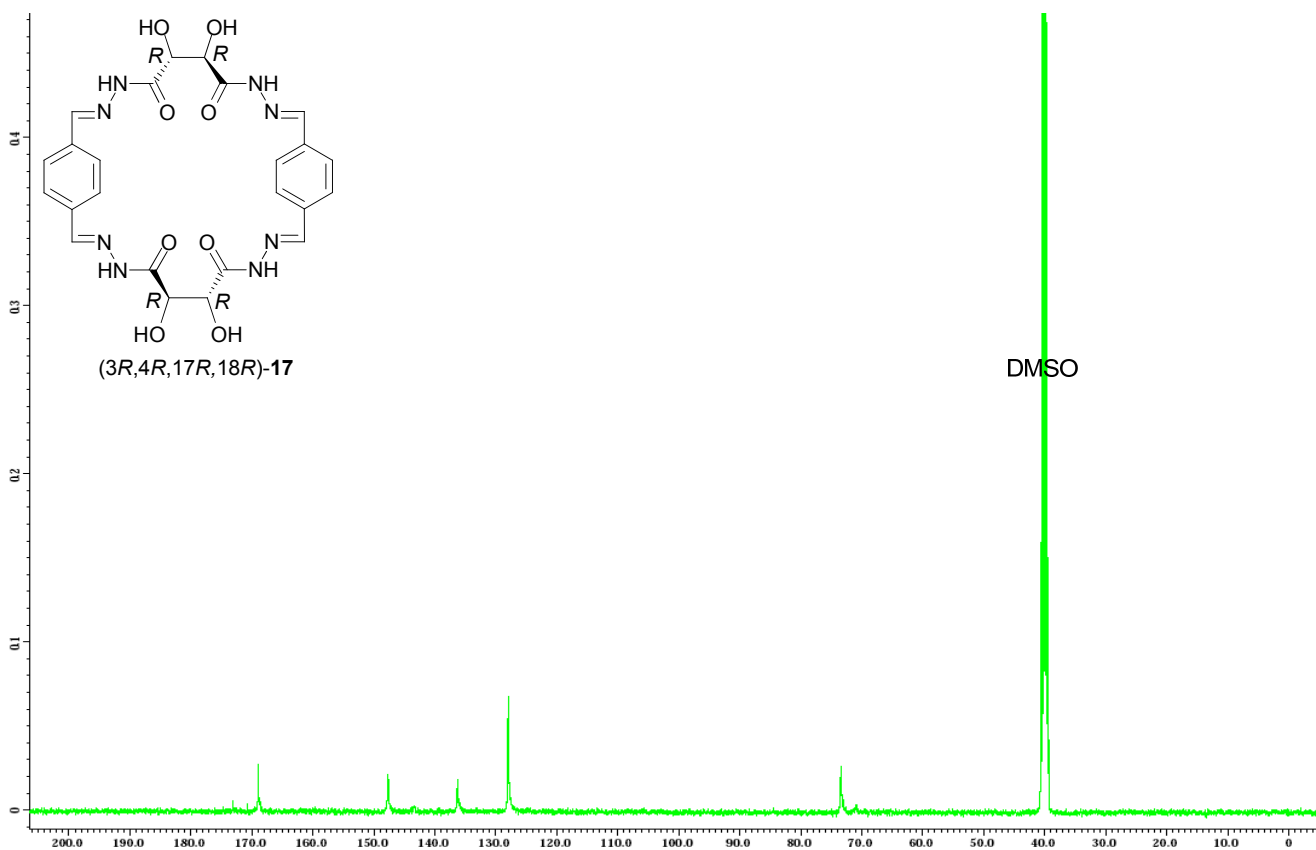
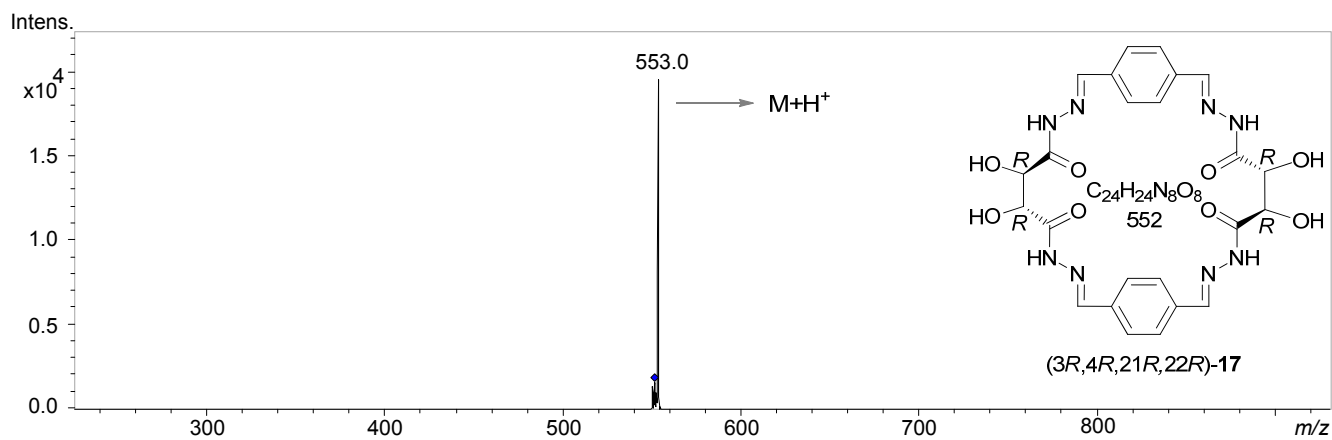


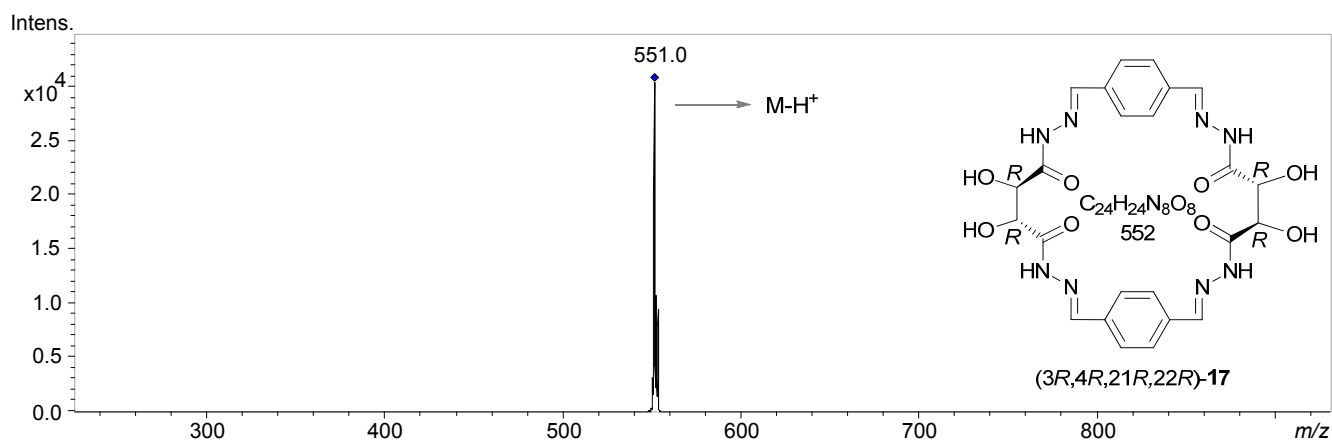
Figure 39. <sup>1</sup>H-NMR spectrum for macrocycle (17), DMSO-d<sub>6</sub> and D<sub>2</sub>O, 400 MHz.



**Figure 40.**  $^{13}\text{C}$ -NMR spectrum for macrocycle (**17**), DMSO- $d_6$ , 100 MHz.

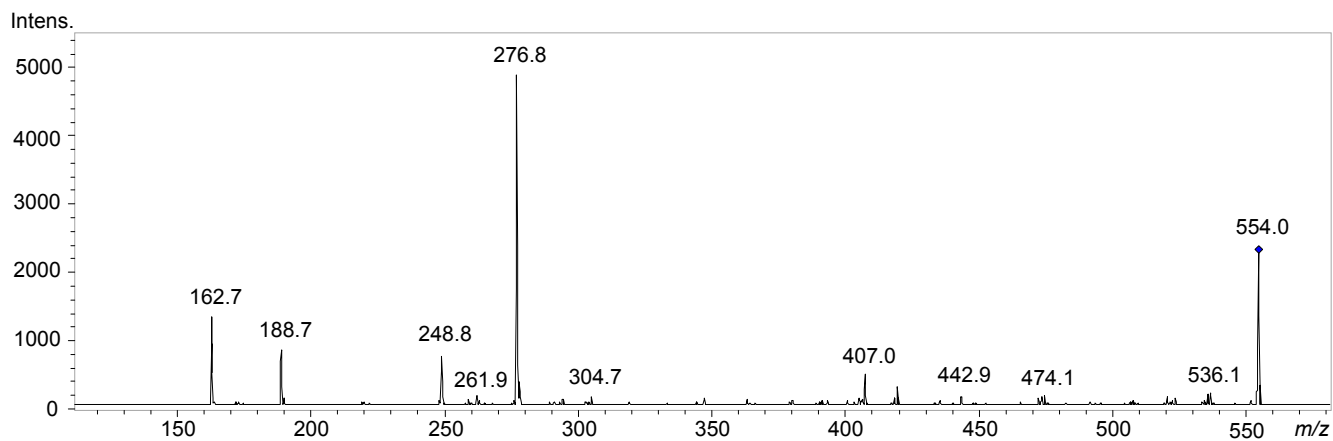


**Figure 41.** APCI- $\text{MS}^2$  spectrum for macrocycle (**17**), DMSO (positive mode).

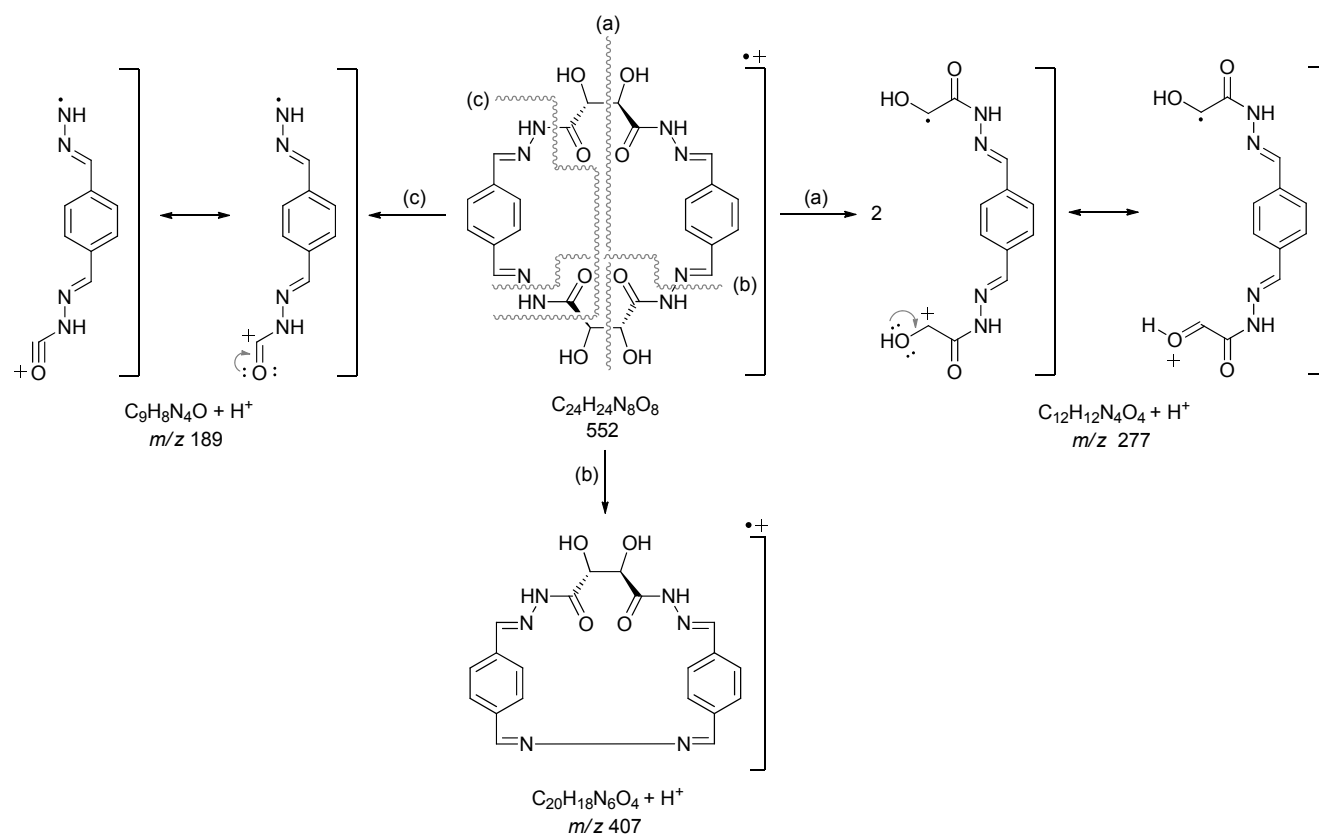


**Figure 42.** APCI- $\text{MS}^2$  spectrum for macrocycle (**17**), DMSO (negative mode).

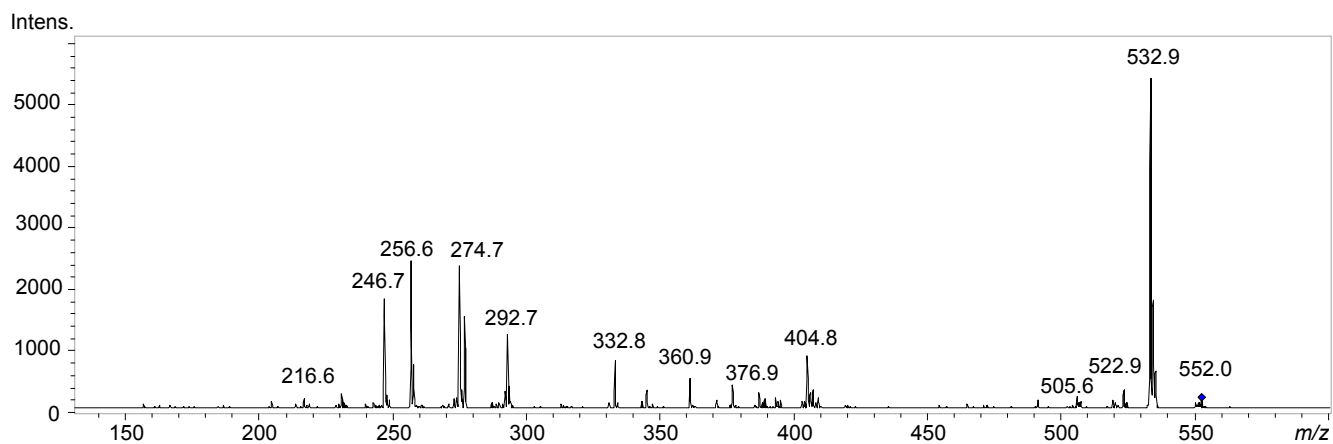




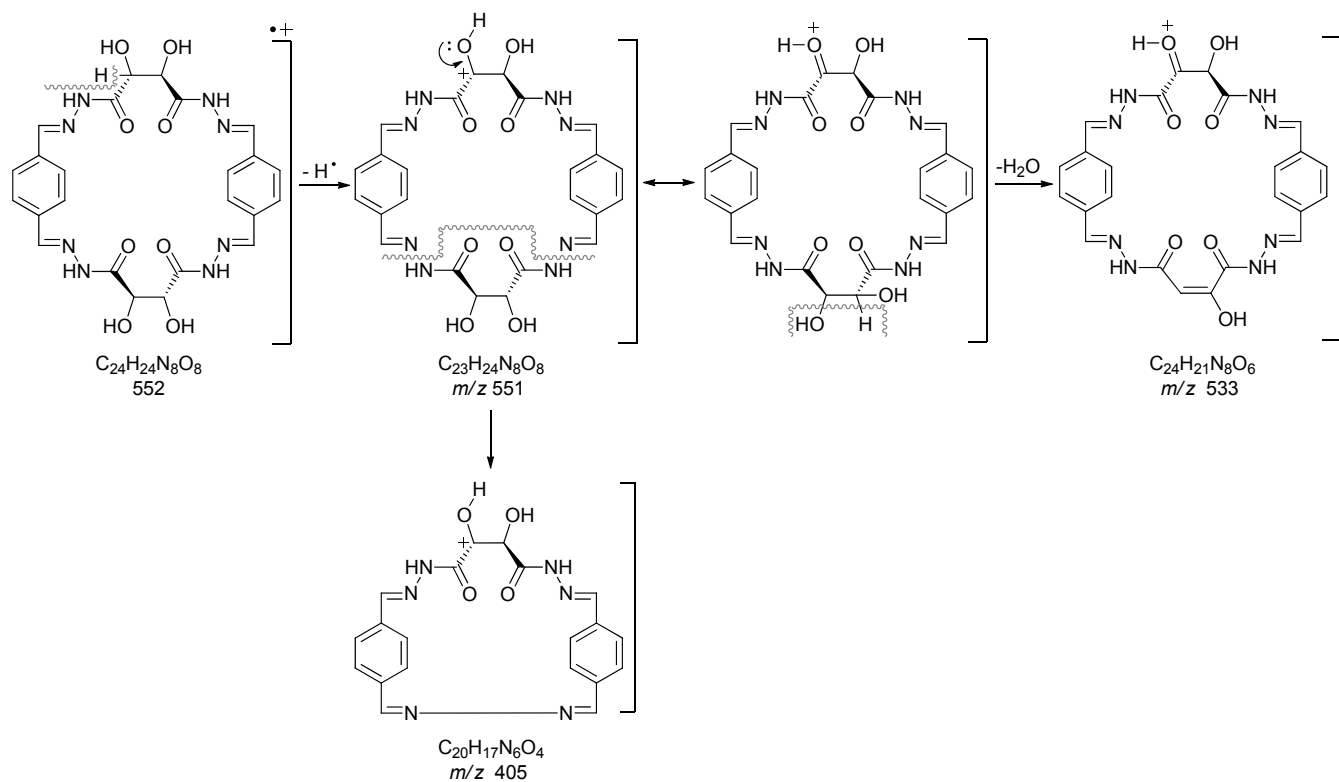
**Figure 43.** Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (17), DMSO (positive mode).



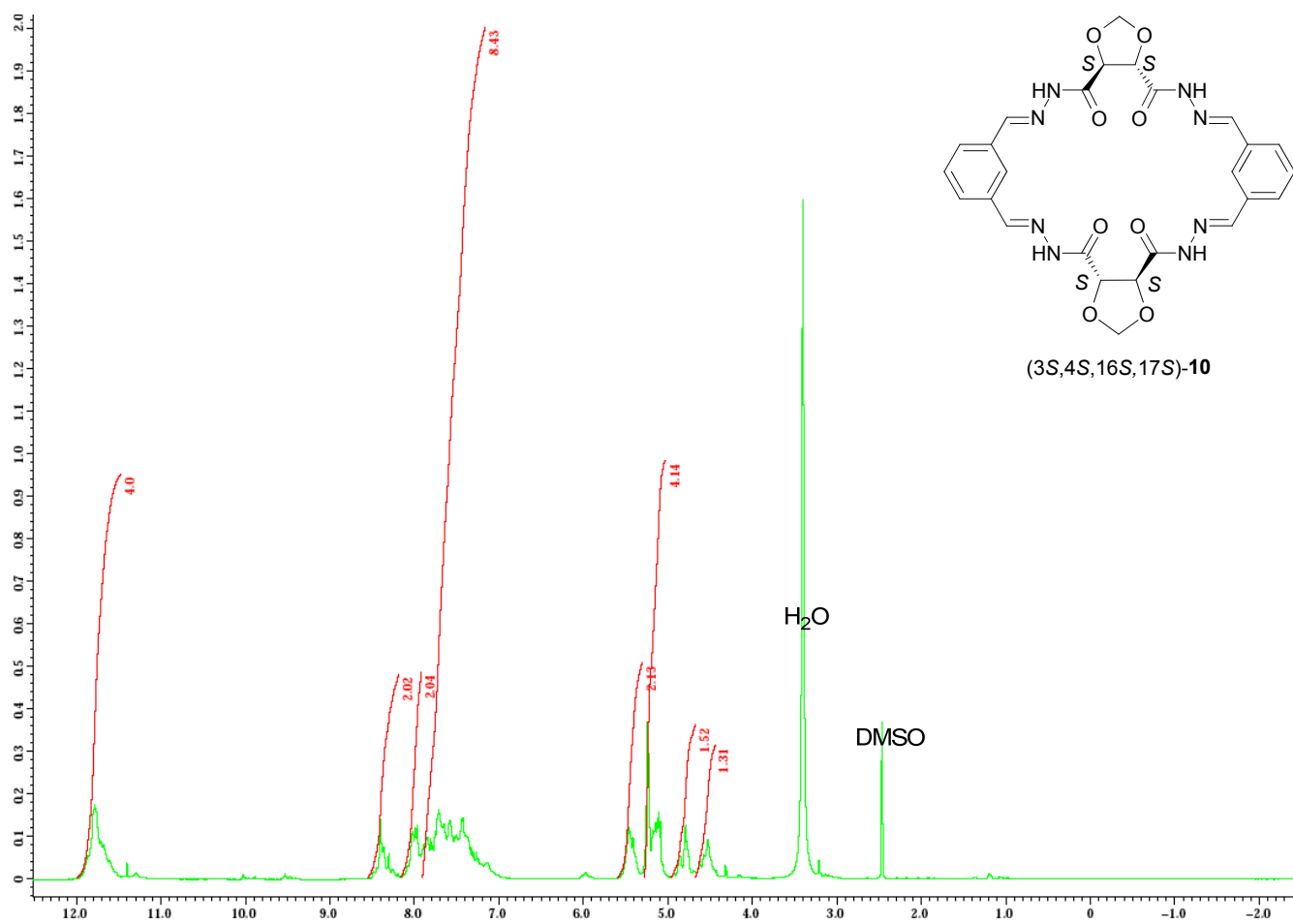
**Scheme 8.** Proposed fragmentation mechanism for macrocycle (17).



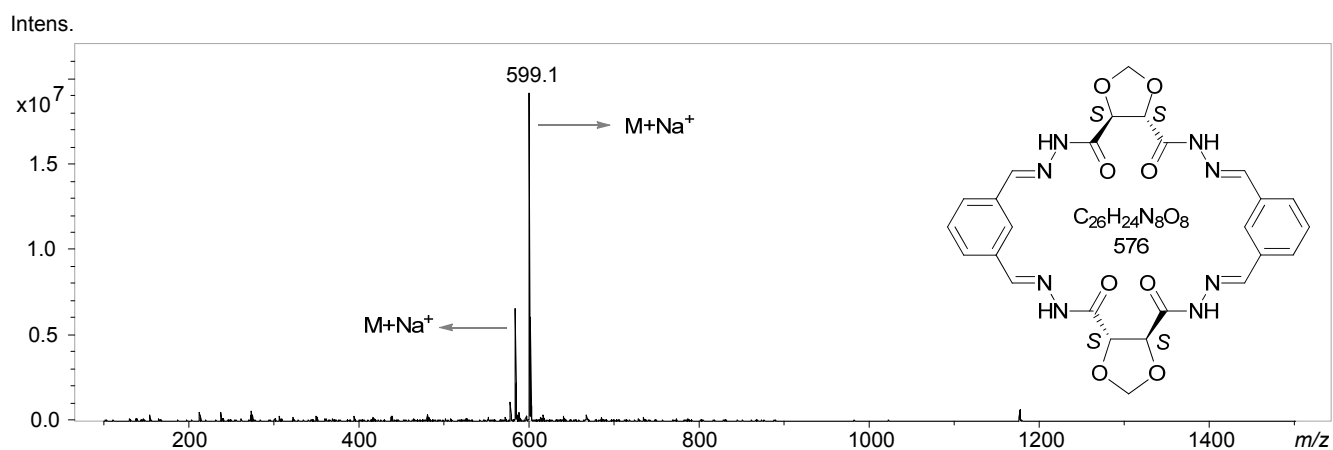
**Figure 44.** Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (17), DMSO (negative mode).



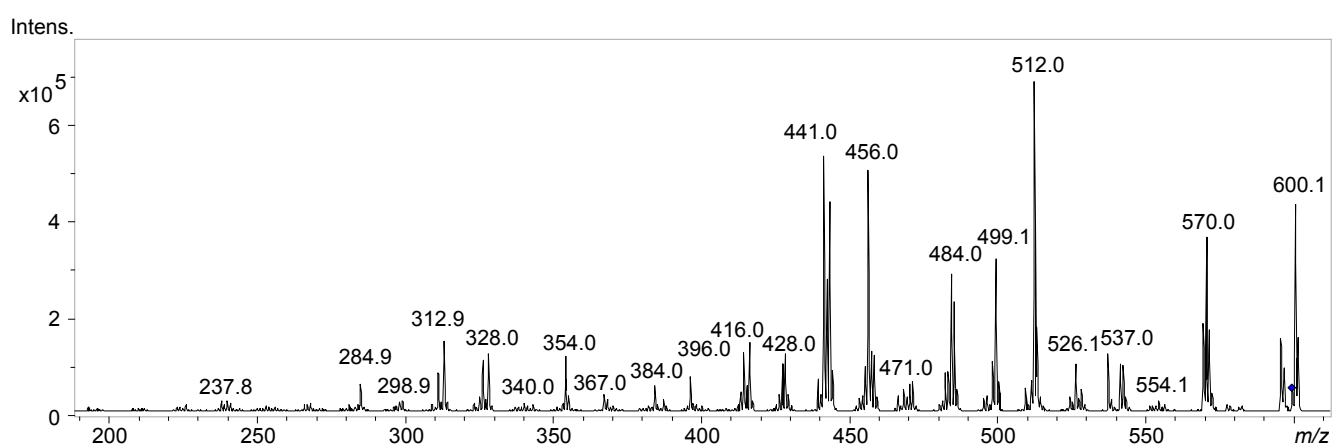
**Scheme 9.** Proposed fragmentation mechanism for macrocycle (17).



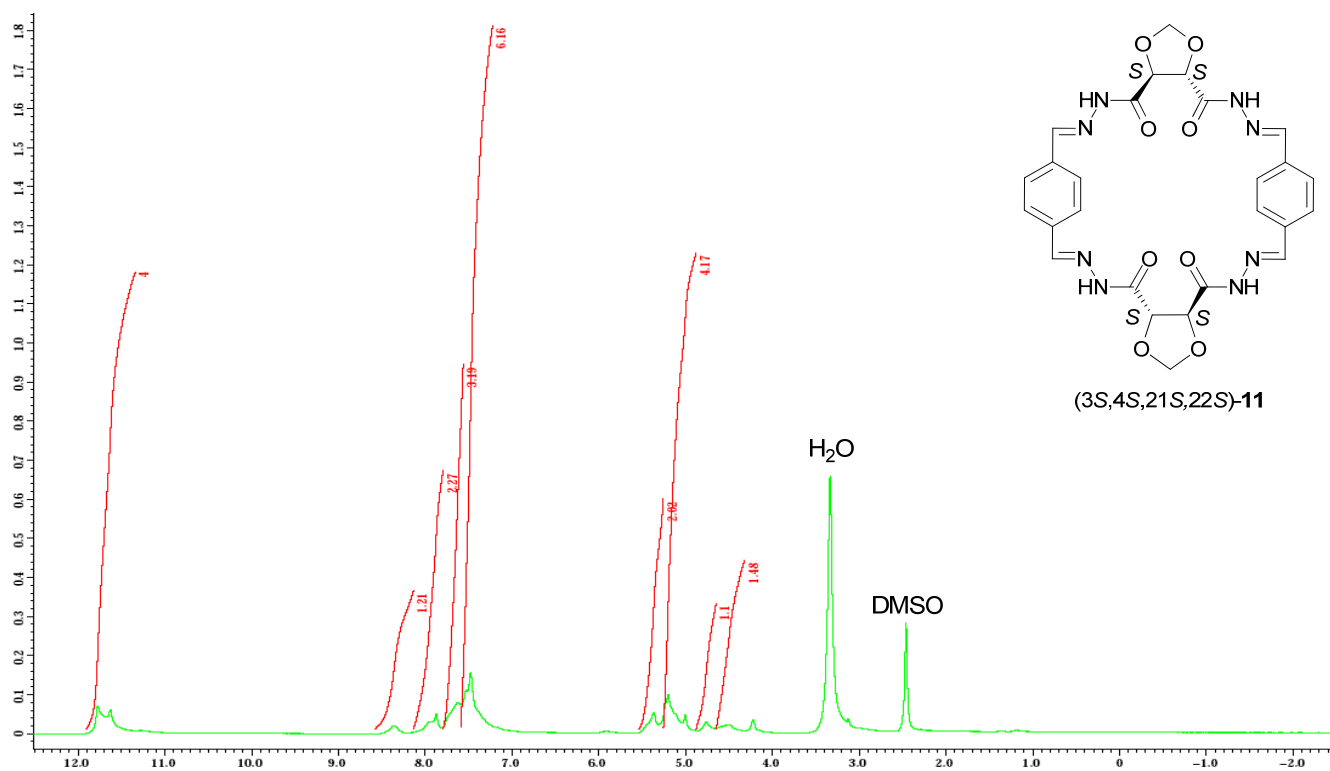
**Figure 45.**  $^1H$ -NMR spectrum for macrocycle (10), DMSO- $d_6$ , 400 MHz.



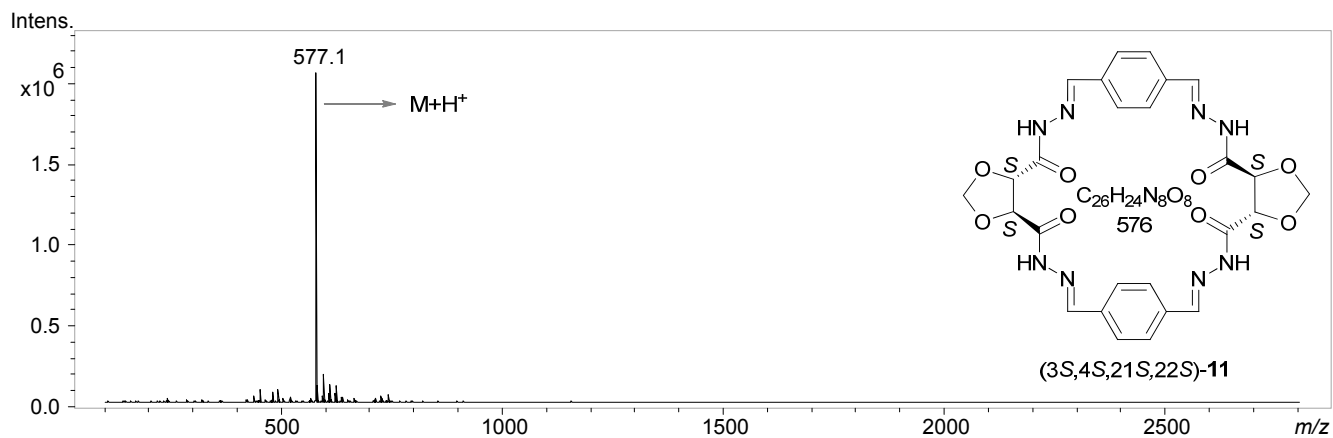
**Figure 46.** ESI-MS spectrum for macrocycle (10) from DMF and ACN (positive mode).



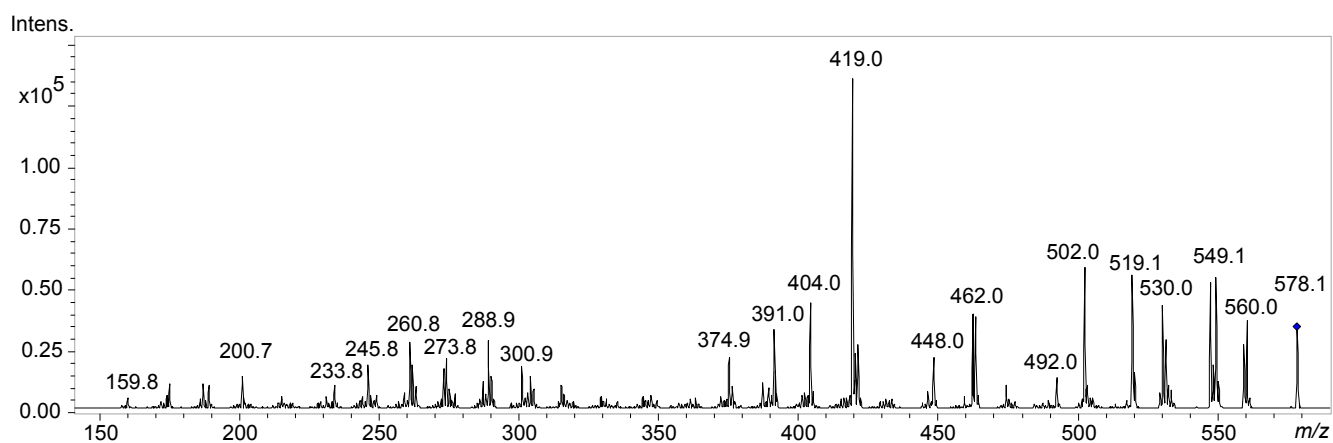
**Figure 47.** Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (10) from DMF and ACN (positive mode).



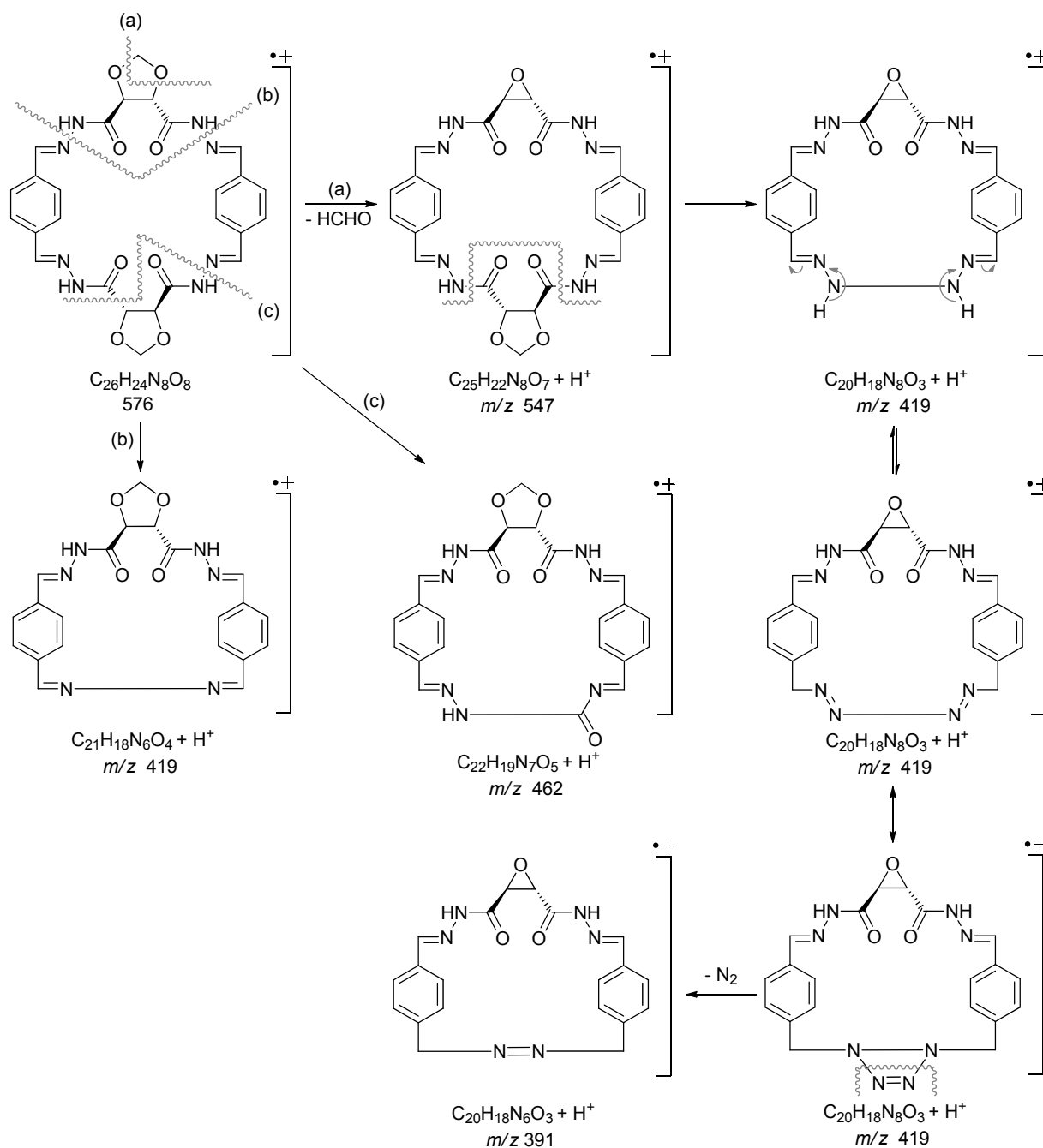
**Figure 48.** <sup>1</sup>H-NMR spectrum for macrocycle (11), DMSO-d<sub>6</sub>, 400 MHz.



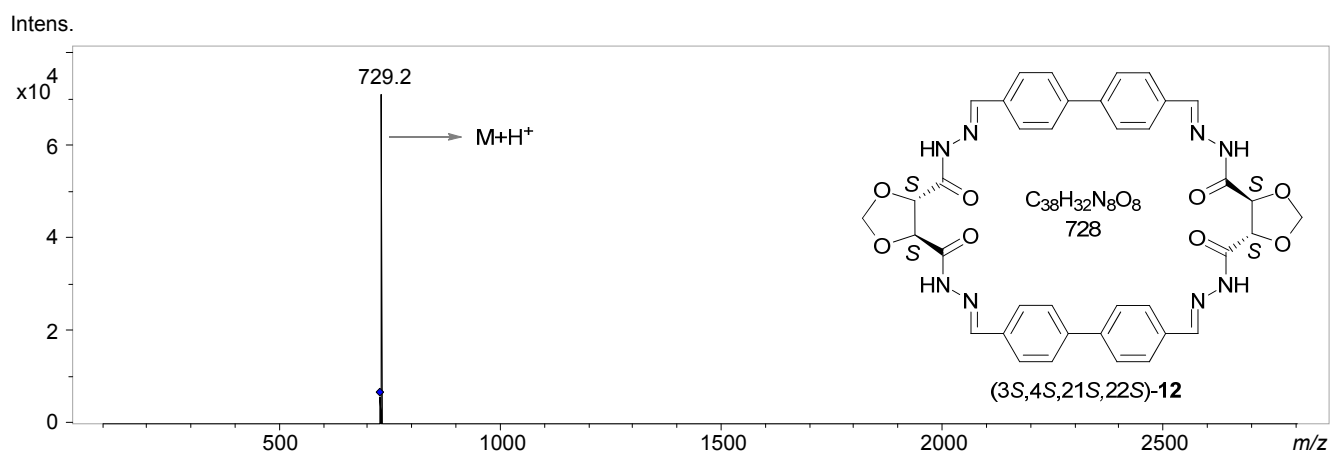
**Figure 49.** APCI-MS spectrum for macrocycle (11) from DMF and ACN (positive mode).



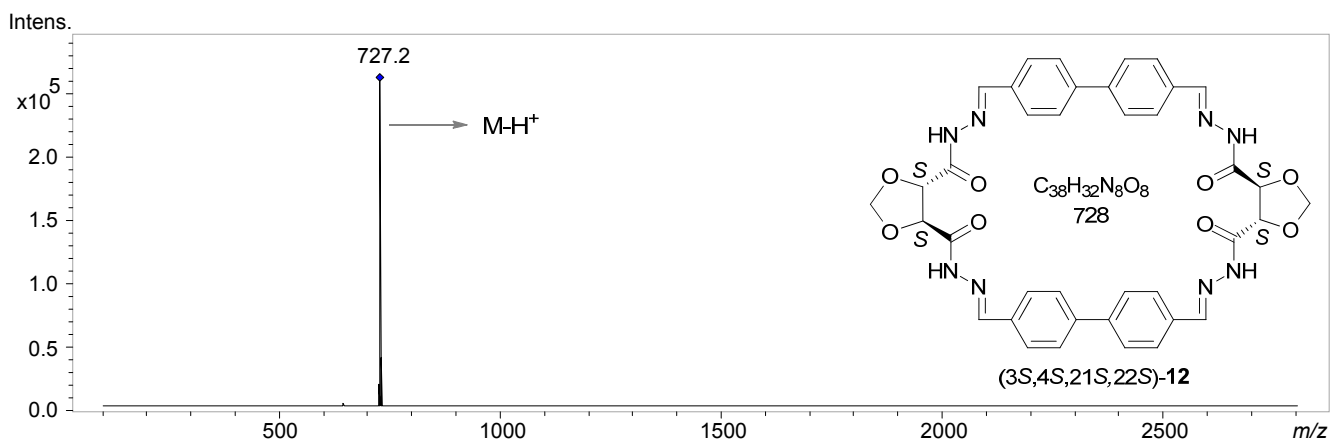
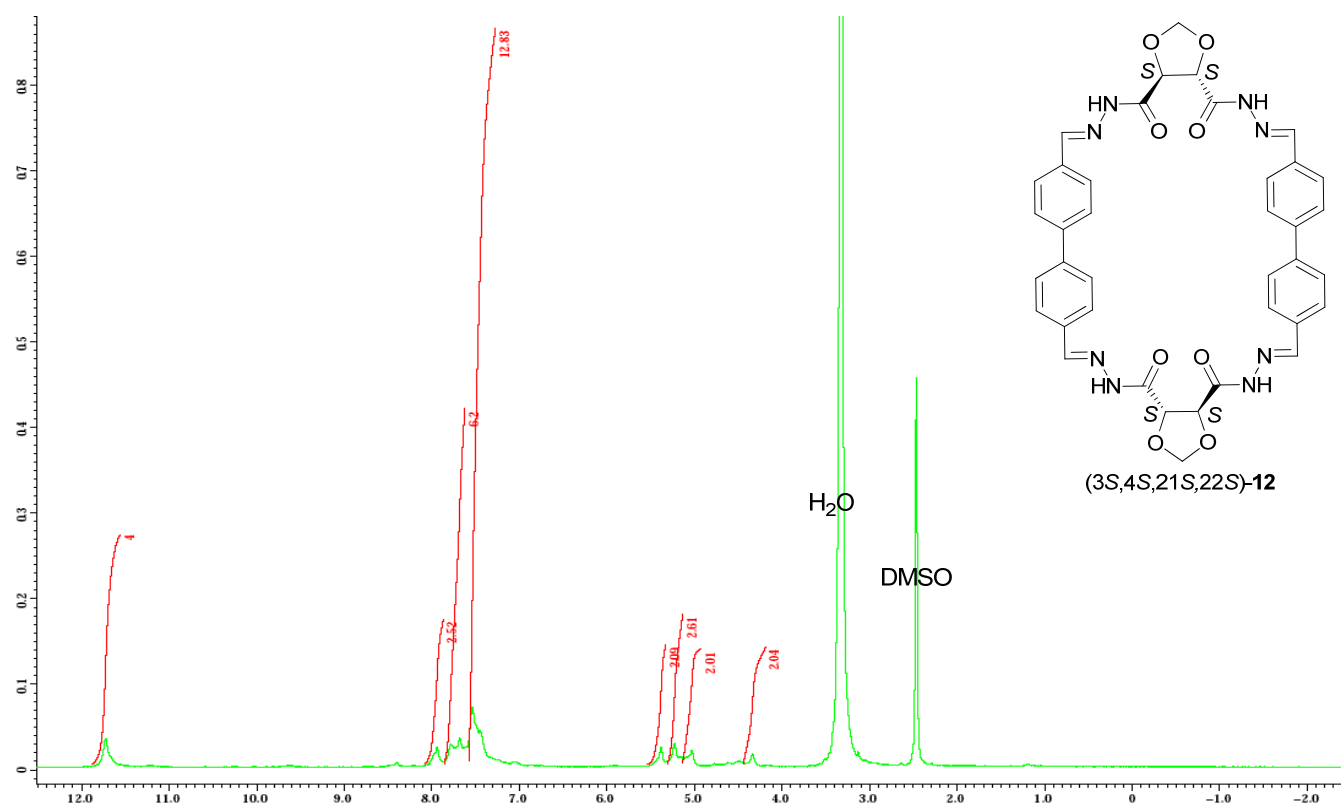
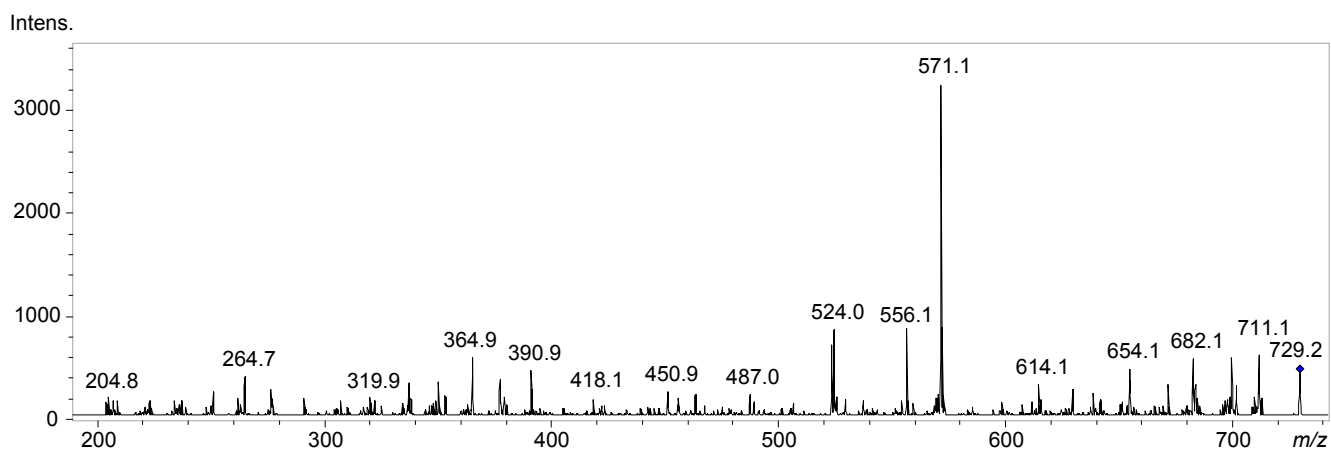
**Figure 50.** Tandem ESI-MS<sup>2</sup> spectrum for macrocycle (11) from DMF and ACN (positive mode).

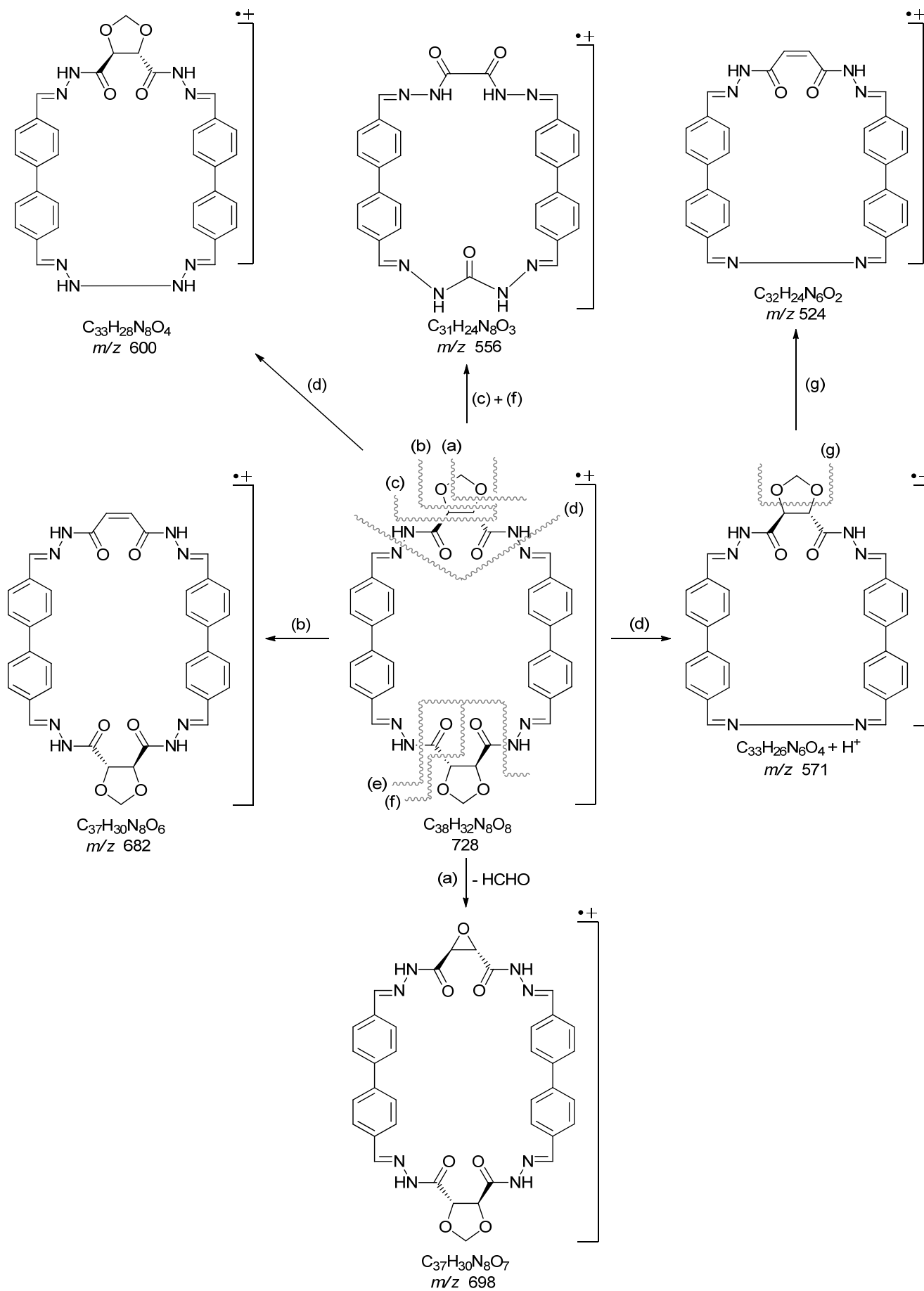


**Scheme 10.** Proposed fragmentation mechanism for macrocycle (11).

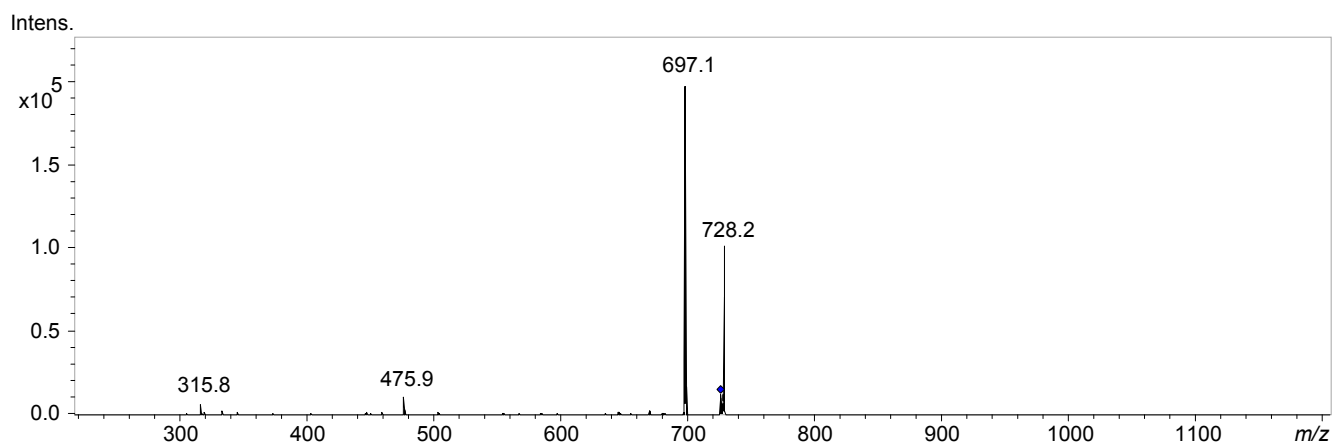


**Figure 51.** APCI-MS<sup>2</sup> spectrum for macrocycle (12) from DMSO (positive mode).

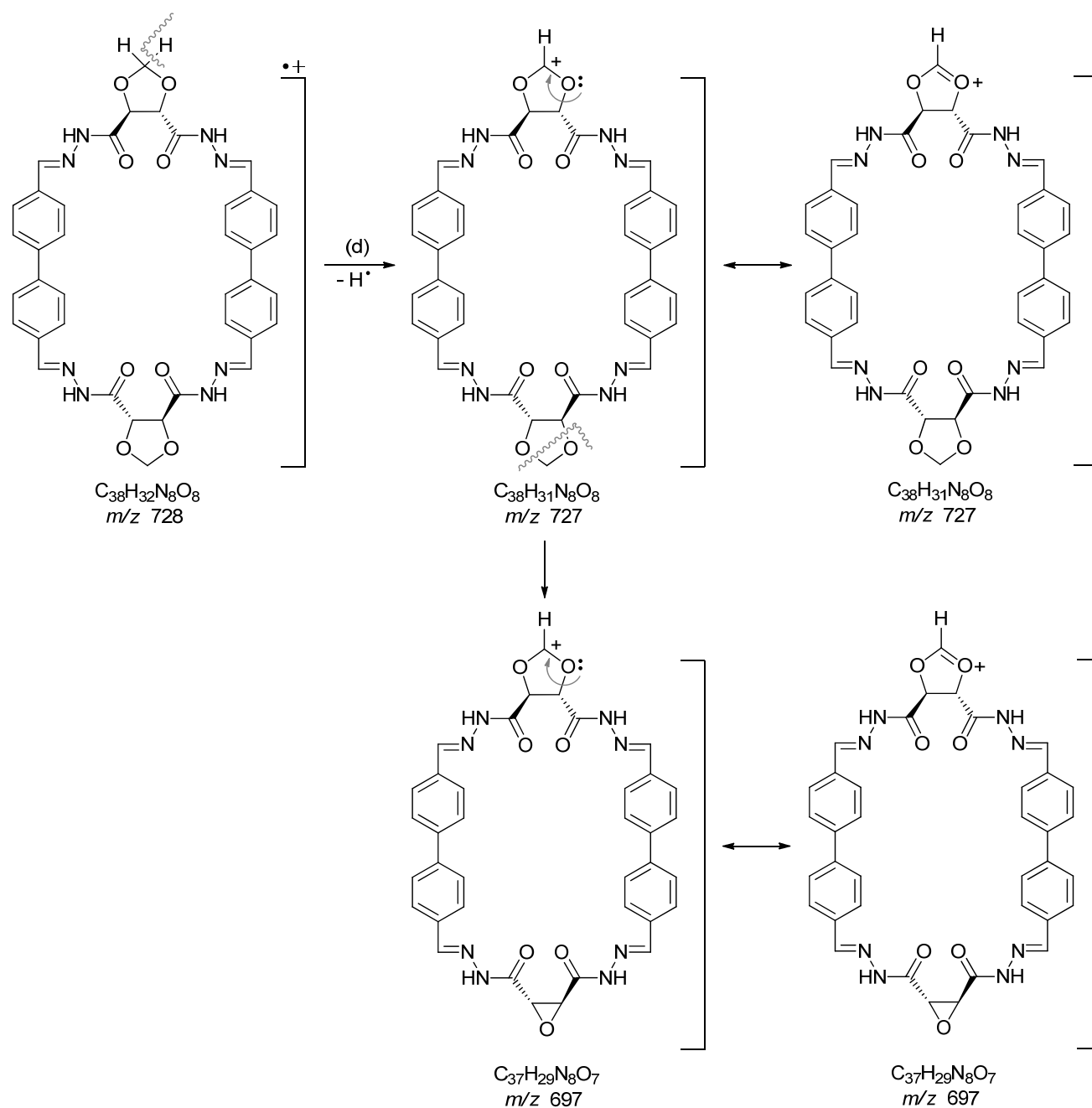




**Scheme 11.** Proposed fragmentation mechanism for macrocycle (12), positive mode.

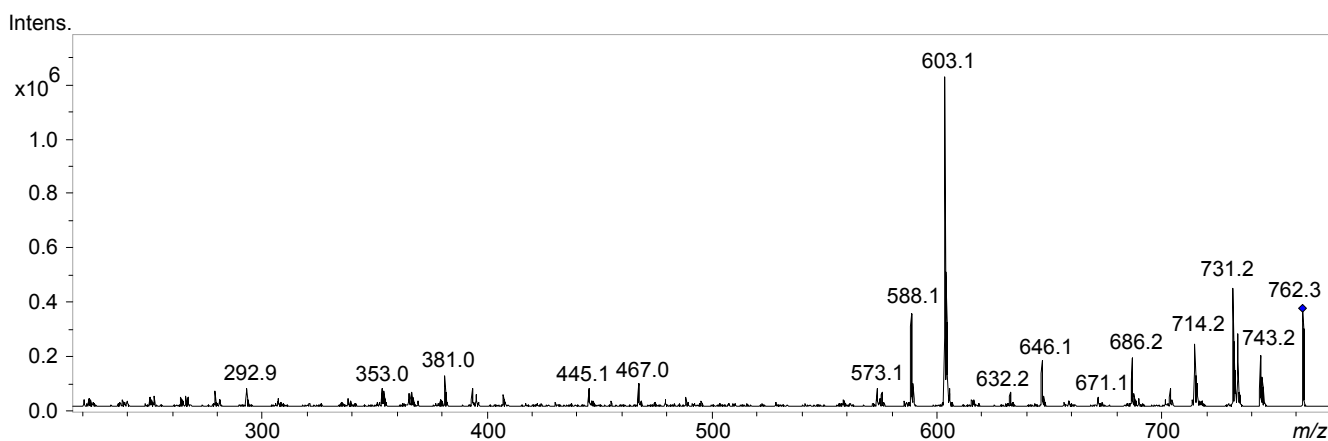
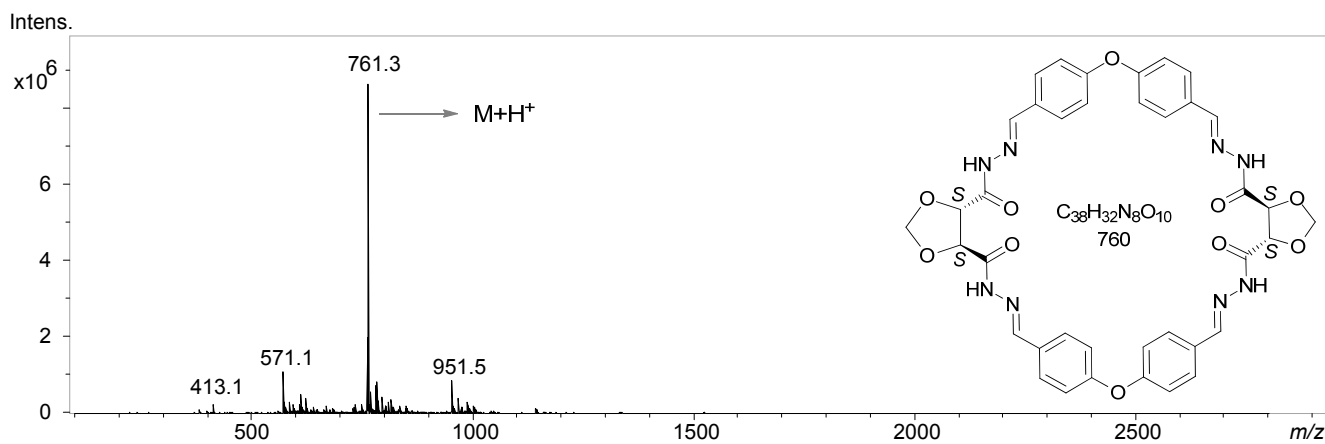
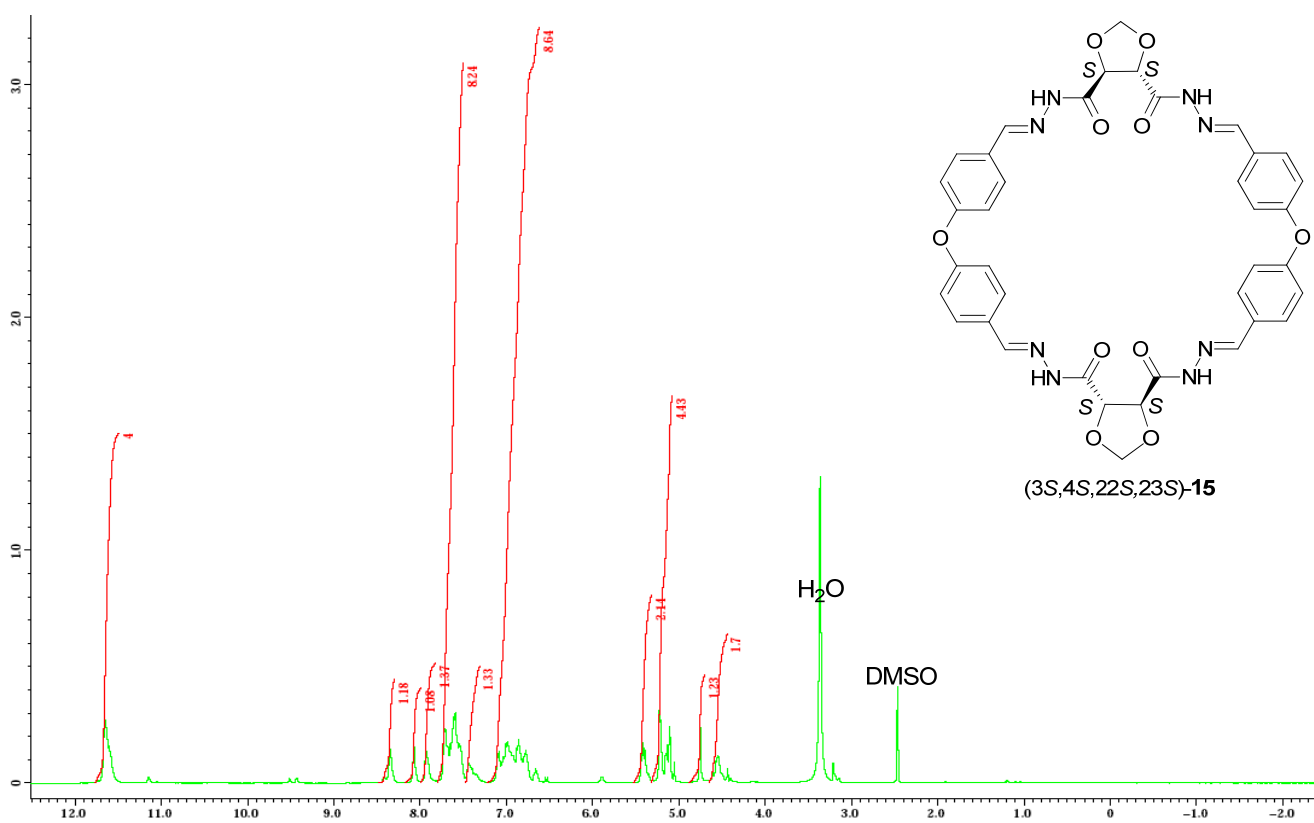


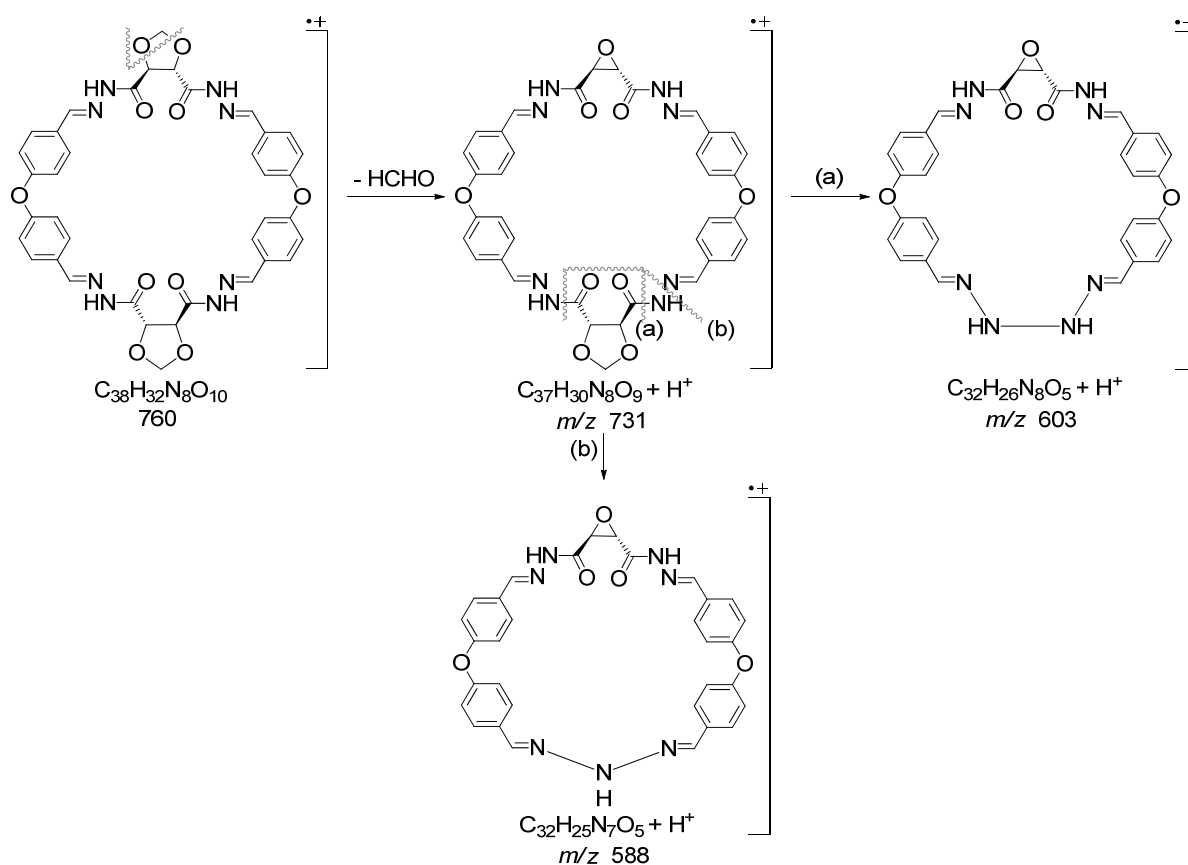
**Figure 55.** Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (**12**) from DMSO (negative mode).



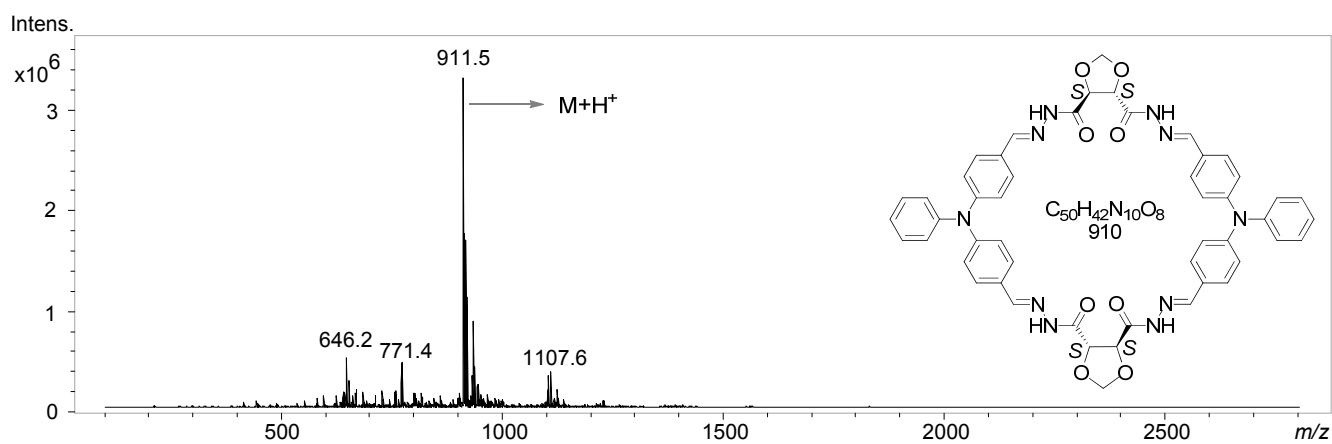
**Scheme 12.** Proposed fragmentation mechanism for macrocycle (**12**), negative mode.



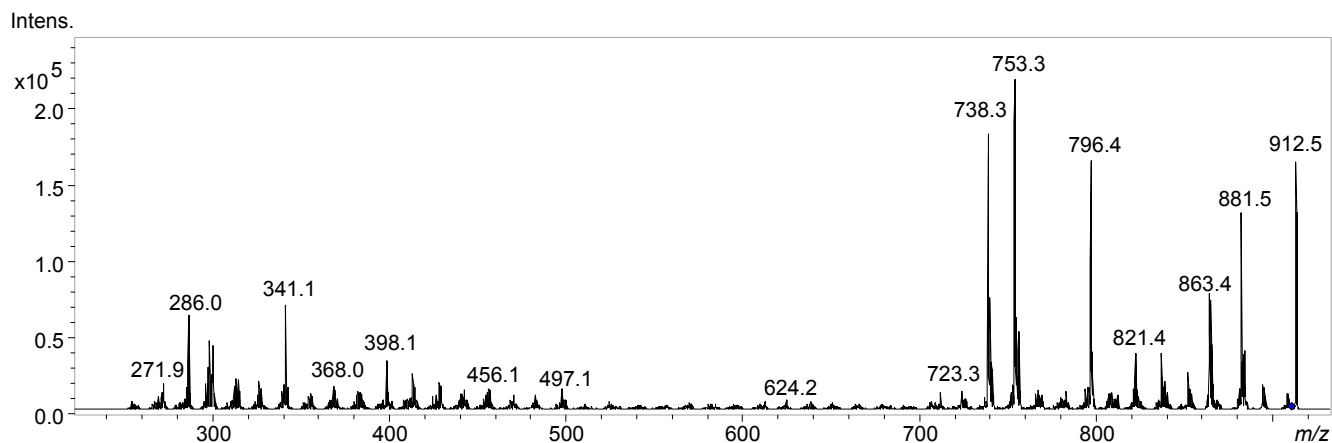




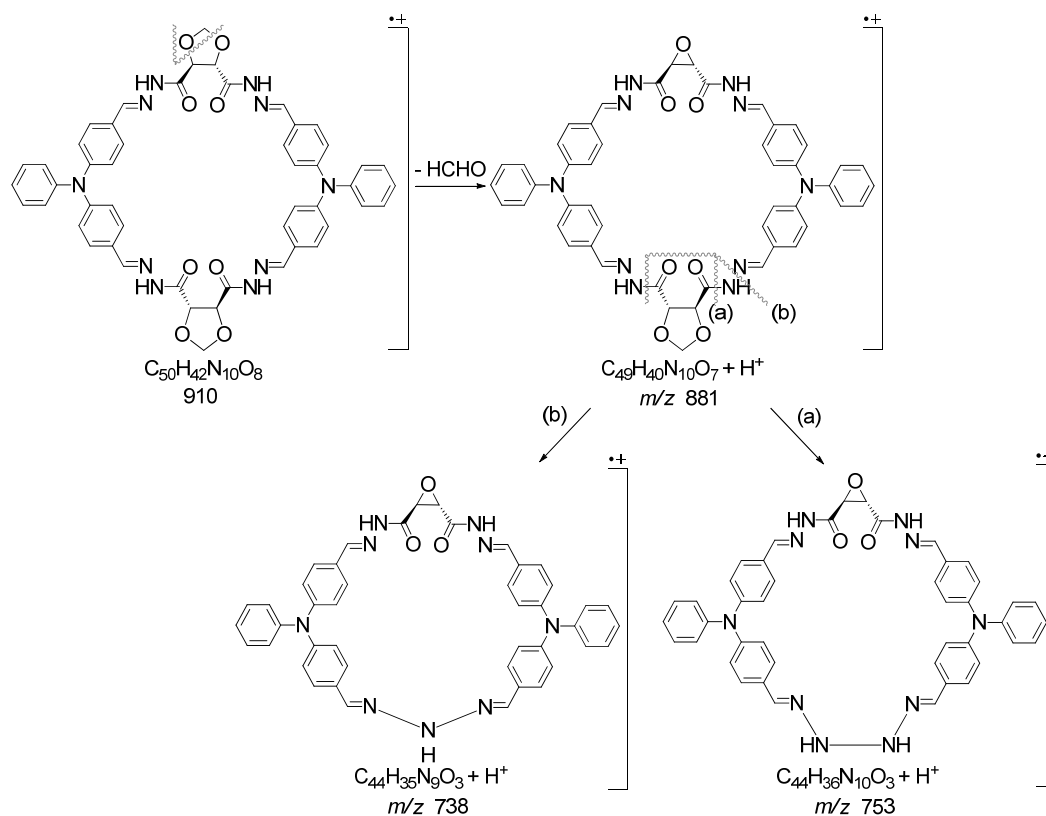
**Scheme 13.** Proposed fragmentation mechanism for macrocycle (15), positive mode.



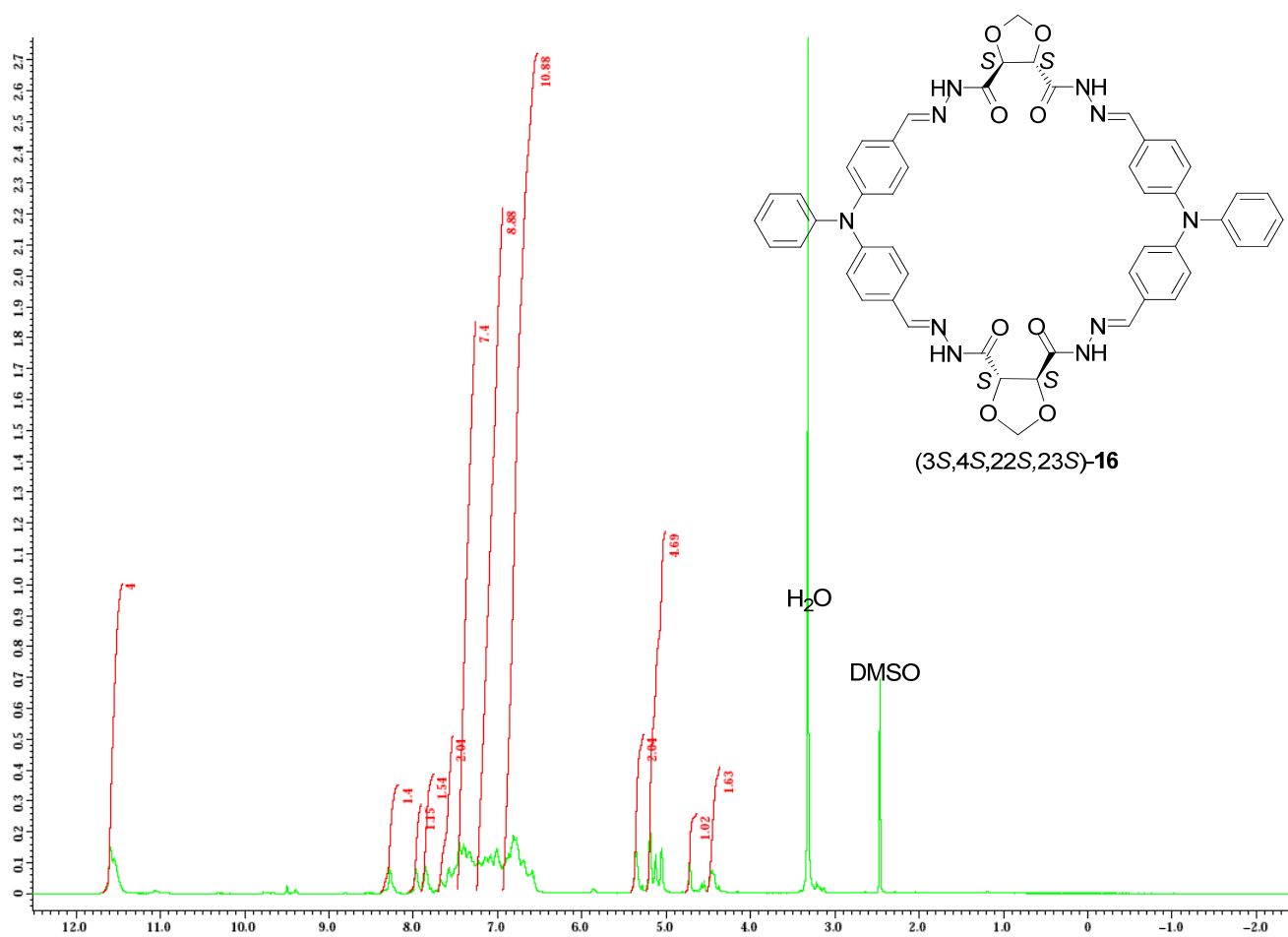
**Figure 59.** APCI-MS spectrum for macrocycle (16) from DMSO (positive mode).



**Figure 60.** Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (16) from DMSO (positive mode).



**Scheme 14.** Proposed fragmentation mechanism for macrocycle (16), positive mode.



**Figure 61.**  $^1H$ -NMR spectrum for macrocycle (16), DMSO- $d_6$ , 400 MHz.

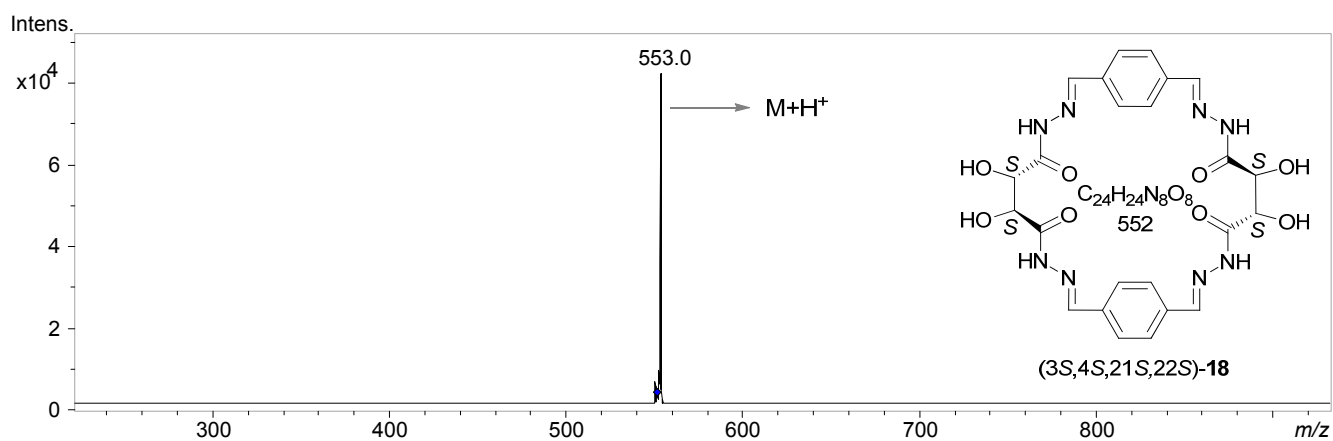


Figure 62. APCI-MS<sup>2</sup> spectrum for macrocycle (18) from DMSO (positive mode).

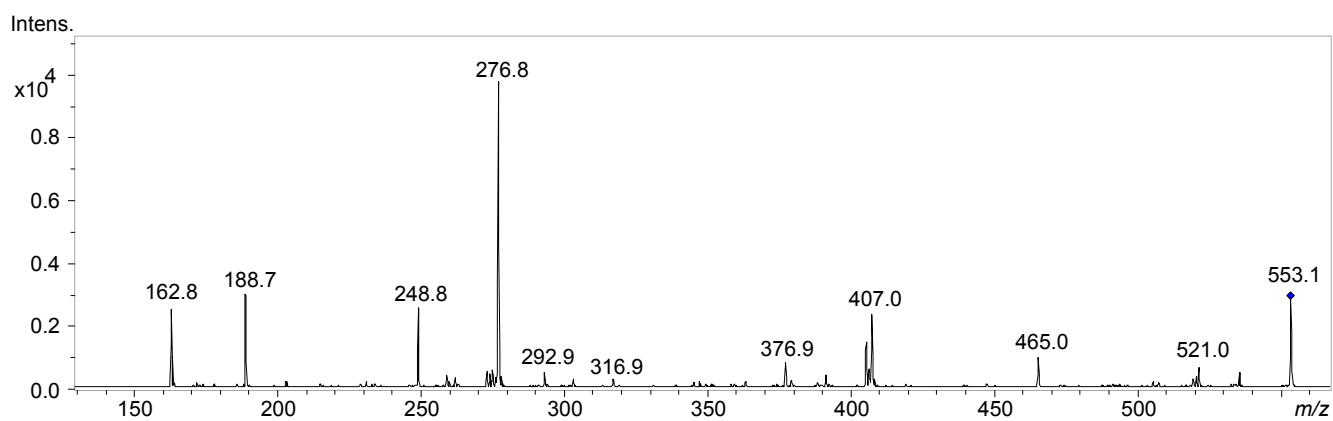
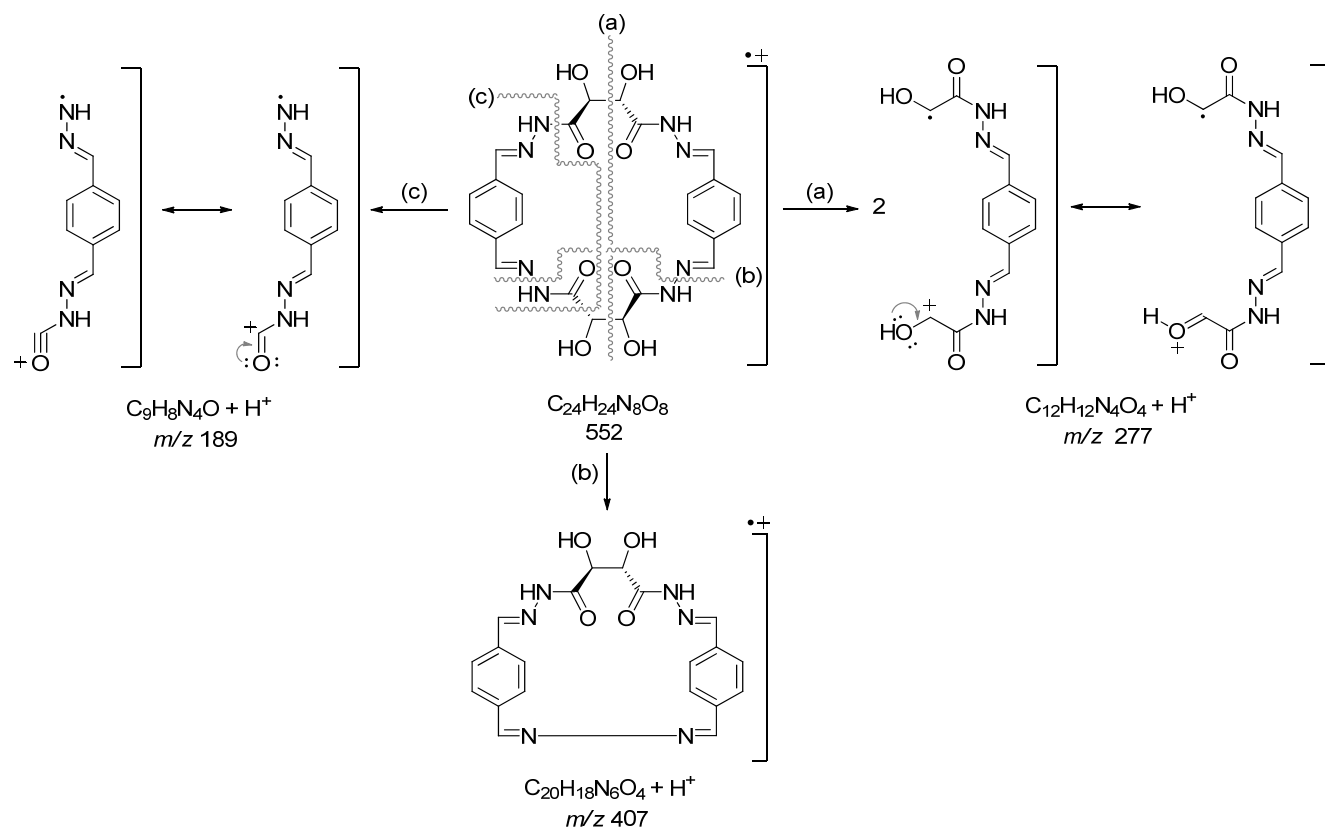
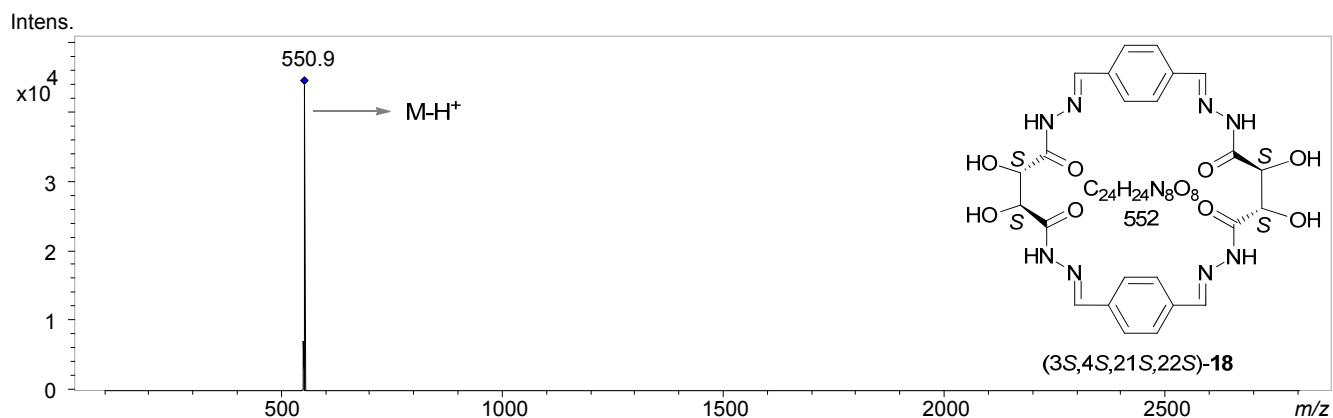


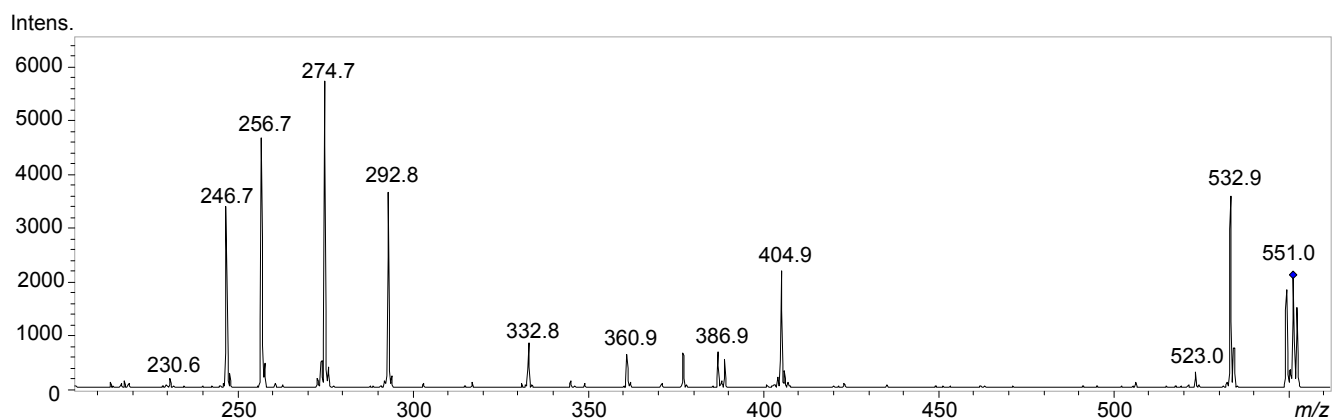
Figure 63. Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (18) from DMSO (positive mode).



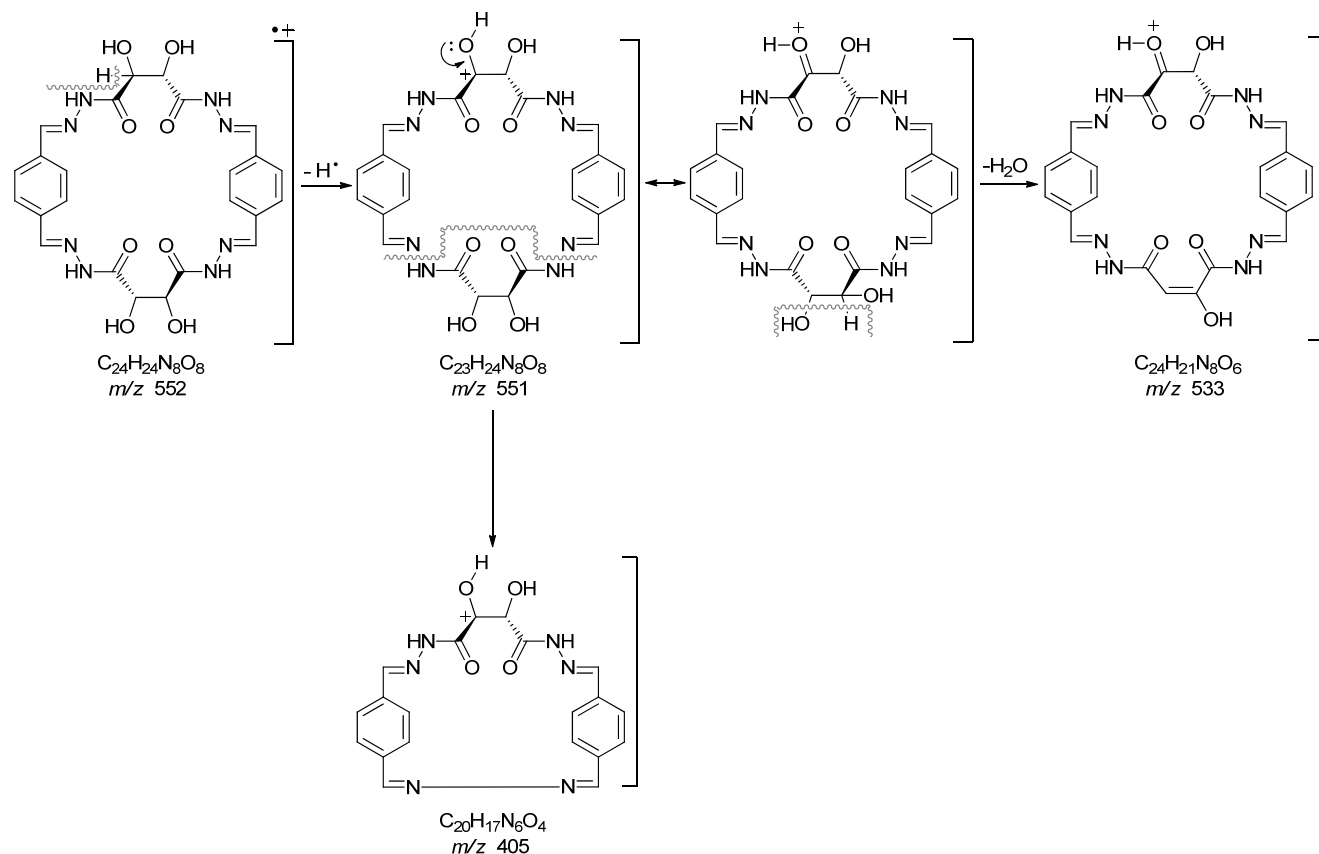
Scheme 15. Proposed fragmentation mechanism for macrocycle (17), positive mode.



**Figure 64.** APCI-MS<sup>2</sup> spectrum for macrocycle (**18**) from DMSO (negative mode).



**Figure 65.** Tandem APCI-MS<sup>2</sup> spectrum for macrocycle (**18**) from DMSO (negative mode).



**Scheme 16.** Proposed fragmentation mechanism for macrocycle (**18**), negative mode.

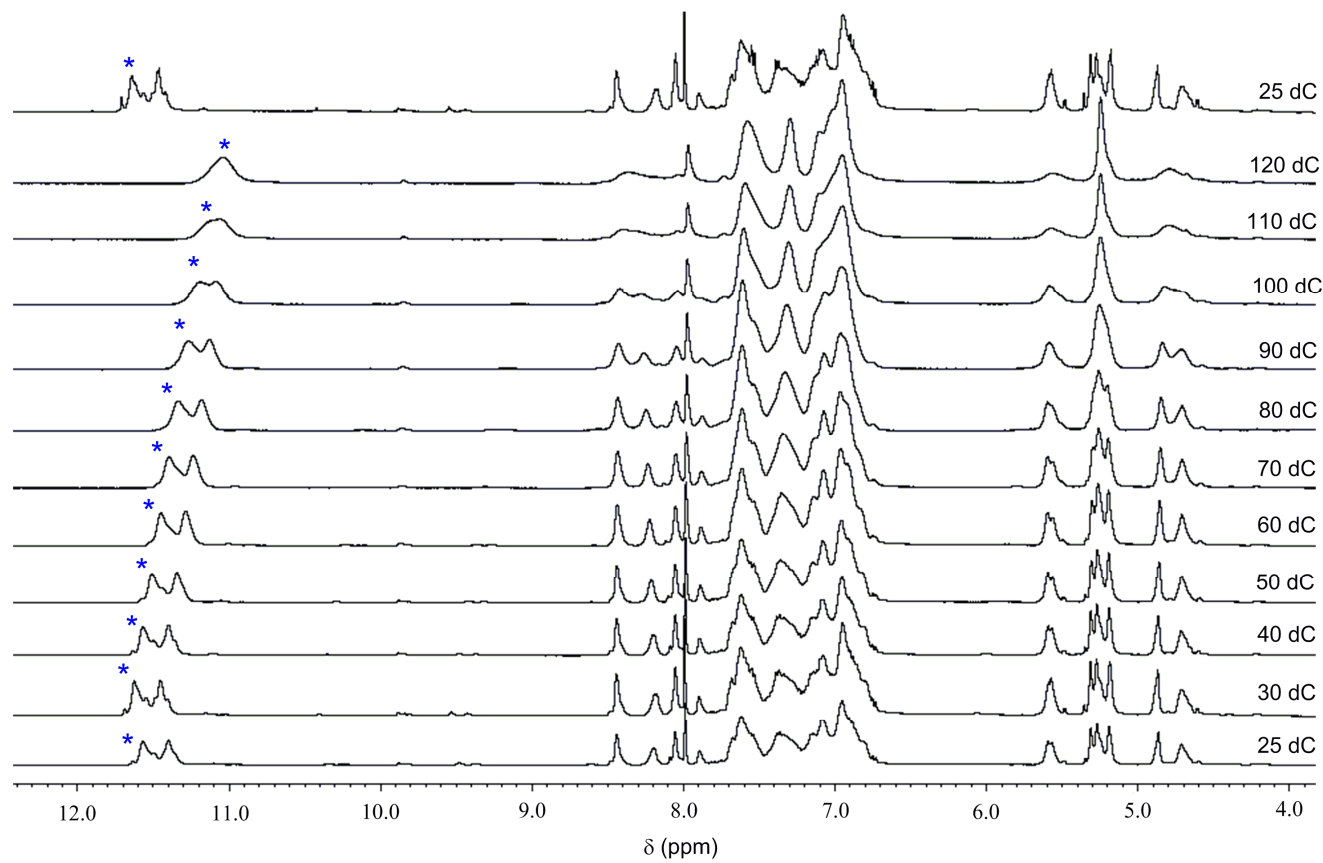
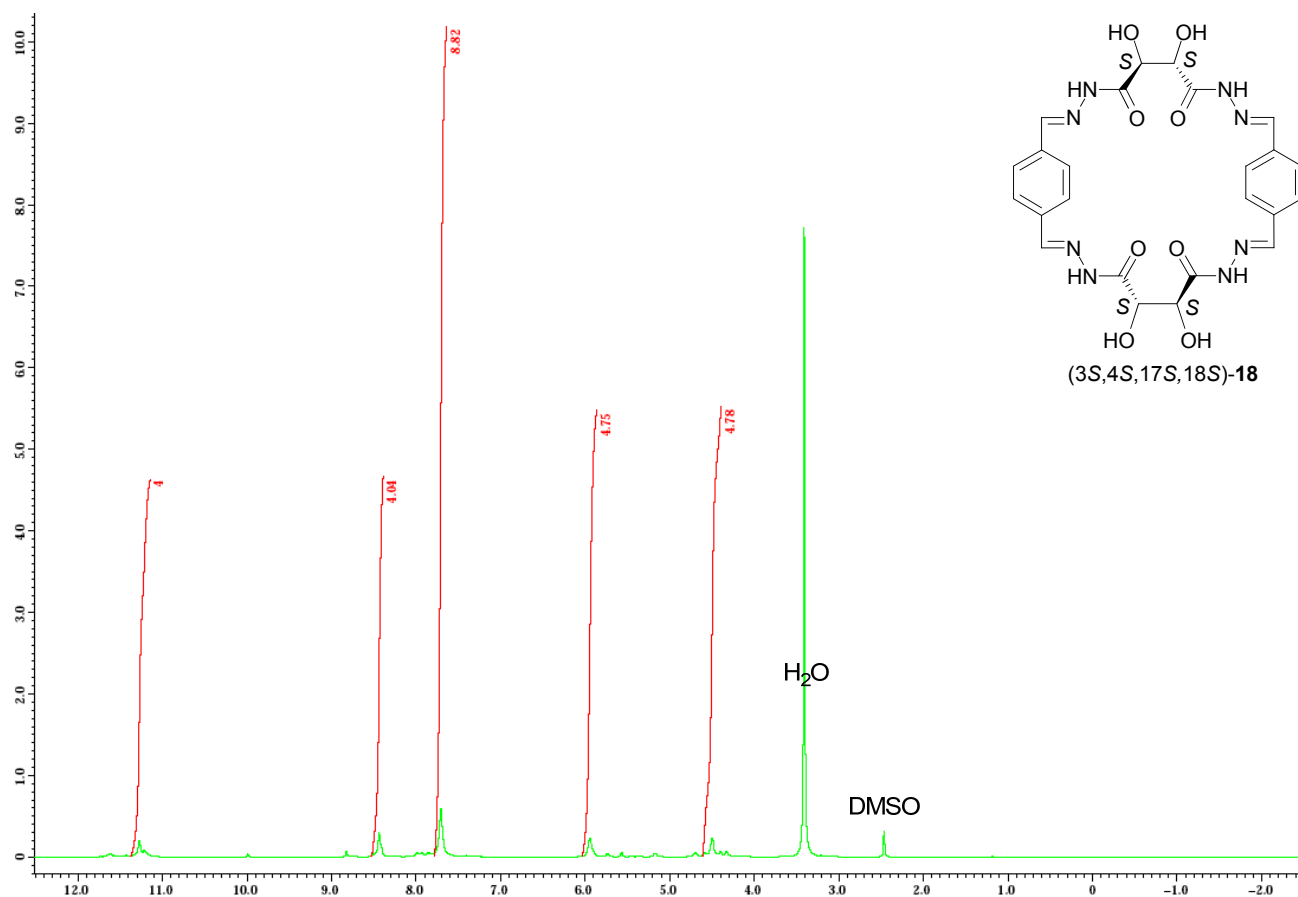
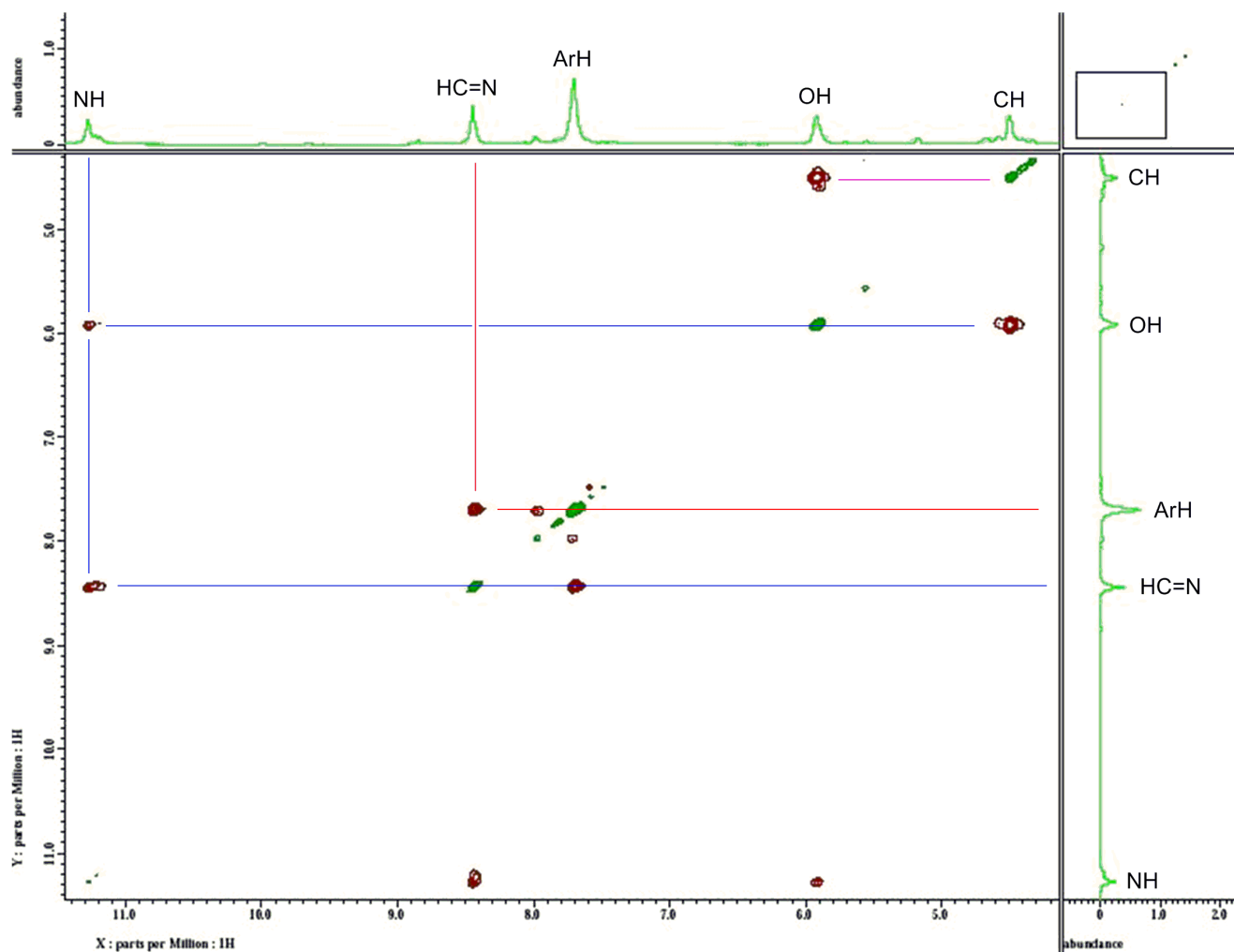
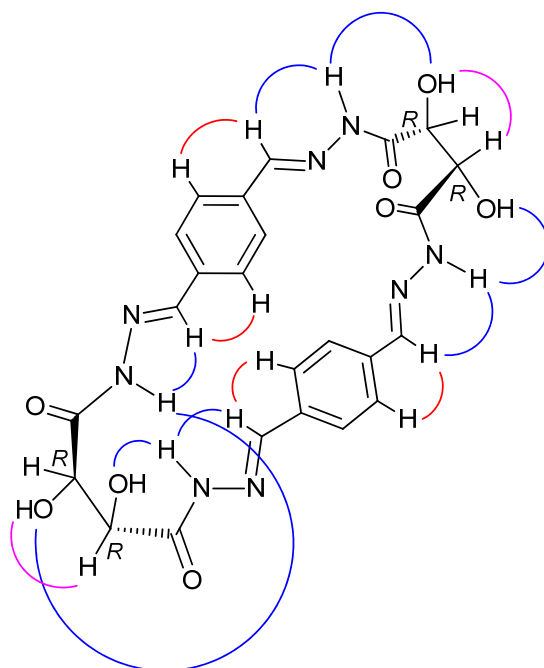


Figure 67. Stacked <sup>1</sup>H NMR spectra for macrocycle (14), 400 MHz, DMF-d<sub>7</sub>.



**Figure 68.** 2D-ROESY spectrum for macrocycle (17), 400 MHz, DMSO-d<sub>6</sub>.



**Figure 69.** Through space interactions of different protons for macrocycle (17) as suggested by 2D-ROESY NMR spectrum.

## Molecular modelling data for the computed structure (14a)

Geometry optimization, SemiEmpirical, PM3

Polak-Ribiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.0100 kcal/(Å mol) Maximum cycles = 3000

RHF Calculation:

Singlet state calculation

Number of electrons = 340

Number of Double Occupied Levels = 170

Charge on the System = 0

Total Orbitals = 314

### ENERGIES AND GRADIENT

Total Energy = -242937.5595208 (kcal/mol)

Total Energy = -387.145596287 (a.u.)

Binding Energy = -12294.3055588 (kcal/mol)

Isolated Atomic Energy = -230643.2539620 (kcal/mol)

Electronic Energy = -2903965.4422912 (kcal/mol)

Core-Core Interaction = 2661027.8827704 (kcal/mol)

Heat of Formation = 44.9504412 (kcal/mol)

Gradient = 0.0079269 (kcal/mol/Å)

NET CHARGES AND COORDINATES						
Atom	Z	Charge	Coordinates (Angstrom)			Mass
			x	y	z	
2	8	-0.298640	0.59400	-6.02677	-3.61096	15.99900
1	6	0.024839	0.47095	-5.92143	-2.18590	12.01100
3	6	0.052485	1.72562	-5.12759	-1.74703	12.01100
4	8	-0.260549	2.33389	-4.73332	-2.97806	15.99900
5	6	0.215626	1.87150	-5.57389	-4.01112	12.01100
6	6	-0.102575	4.87162	-1.86220	0.44087	12.01100
7	6	-0.031176	3.68854	-1.17549	0.72063	12.01100
8	6	-0.151295	3.70271	0.20052	0.91352	12.01100
9	6	-0.043679	4.90149	0.91597	0.80966	12.01100
10	6	-0.133505	6.09239	0.22390	0.53064	12.01100
11	6	-0.061921	6.07420	-1.14970	0.35691	12.01100
12	7	0.160628	4.96098	2.35699	0.91092	14.00700
13	6	-0.073621	-4.08705	-4.78449	-3.35478	12.01100
14	6	-0.082216	-5.30050	-3.98873	-3.15807	12.01100
15	6	-0.039822	-5.62500	-3.40510	-1.93014	12.01100
16	6	-0.126476	-6.80114	-2.68114	-1.78647	12.01100
17	6	-0.056961	-7.66987	-2.52158	-2.87506	12.01100
18	6	-0.141218	-7.33716	-3.09312	-4.11068	12.01100
19	6	-0.068811	-6.16672	-3.82425	-4.24467	12.01100
20	7	0.157986	-8.93311	-1.84342	-2.66609	14.00700
21	6	-0.049274	-8.91603	-0.51618	-2.08457	12.01100
22	6	-0.143474	-7.76510	0.27887	-2.05071	12.01100
23	6	-0.032999	-7.78744	1.51727	-1.42040	12.01100



24	6	-0.097494	-8.95882	1.98143	-0.81688	12.01100
25	6	-0.067215	-10.11331	1.18849	-0.86193	12.01100
26	6	-0.123366	-10.09717	-0.04695	-1.48733	12.01100
27	6	-0.038331	-9.03940	3.26728	-0.12390	12.01100
28	6	0.025424	-4.41545	6.46319	0.16120	12.01100
29	6	0.051495	-5.78572	5.95237	-0.34157	12.01100
30	8	-0.261344	-6.10026	6.81675	-1.32211	15.99900
31	6	0.214811	-5.33977	8.00074	-1.43323	12.01100
32	8	-0.282365	-4.19115	7.67875	-0.56275	15.99900
54	6	0.242632	2.70660	-5.94367	-0.89579	12.01100
55	8	-0.356959	2.60320	-7.13609	-0.65894	15.99900
56	7	0.012766	3.90040	-5.32423	-0.39632	14.00700
57	6	-0.028702	4.91433	-3.31032	0.22862	12.01100
58	7	-0.127430	3.84348	-3.94868	-0.14029	14.00700
60	6	-0.086106	-9.96484	-2.07243	-3.67378	12.01100
61	6	-0.089549	-10.65509	-3.29012	-3.64345	12.01100
62	6	-0.098311	-11.66505	-3.53083	-4.56769	12.01100
63	6	-0.102764	-11.99370	-2.56851	-5.51673	12.01100
64	6	-0.094219	-11.30903	-1.35823	-5.54500	12.01100
65	6	-0.113122	-10.29411	-1.10508	-4.62981	12.01100
66	6	-0.088820	6.05060	2.88915	1.72812	12.01100
67	6	-0.085202	6.80701	3.94414	1.20515	12.01100
68	6	-0.099284	7.86473	4.46316	1.94338	12.01100
69	6	-0.100240	8.17415	3.93770	3.19334	12.01100
70	6	-0.096149	7.42247	2.88845	3.71198	12.01100
71	6	-0.111384	6.35999	2.36204	2.98708	12.01100
82	7	-0.081515	-3.12291	-4.73487	-2.48355	14.00700
83	6	0.239310	-3.23974	5.50016	-0.10080	12.01100
84	8	-0.300086	-3.36561	4.37455	-0.53636	15.99900
85	6	-0.059920	3.72630	3.11728	0.94230	12.01100
86	6	-0.137665	3.46244	4.03992	1.96391	12.01100
87	6	-0.071391	2.32731	4.83416	1.90692	12.01100
88	6	-0.076432	1.42549	4.70830	0.84554	12.01100
89	6	-0.043133	1.67503	3.77255	-0.16095	12.01100
90	6	-0.122163	2.82138	2.98887	-0.12044	12.01100
95	6	-0.084994	0.25837	5.59378	0.81838	12.01100
96	7	-0.070363	-0.85295	5.19551	0.27355	14.00700
97	7	0.021293	-1.94073	6.05296	0.17982	14.00700
100	6	0.238972	-6.88498	6.04509	0.72728	12.01100
101	8	-0.360252	-6.86621	6.80915	1.67916	15.99900
102	7	-0.125697	-8.00133	4.04901	-0.05415	14.00700
104	7	0.019640	-8.09202	5.28448	0.58778	14.00700
106	6	0.239361	-0.84952	-5.22751	-1.80751	12.01100
107	8	-0.308300	-0.96450	-4.55369	-0.80277	15.99900
108	7	0.016911	-1.99375	-5.53662	-2.62794	14.00700
47	1	0.120136	-11.01058	-0.65382	-1.51660	1.00800
48	1	0.039075	-5.90673	8.80645	-0.82387	1.00800
49	1	0.059418	-5.02671	8.29630	-2.33380	1.00800
72	1	0.118675	-10.40062	-4.05471	-2.89973	1.00800
73	1	0.105379	-12.20528	-4.48315	-4.54514	1.00800
74	1	0.105013	-12.79143	-2.76339	-6.24085	1.00800
75	1	0.105520	-11.56770	-0.60017	-6.29175	1.00800

76	1	0.117651	-9.76336	-0.14542	-4.65413	1.00800
77	1	0.118725	6.56780	4.36537	0.22137	1.00800
78	1	0.105873	8.45737	5.28886	1.53553	1.00800
79	1	0.105262	9.00953	4.34937	3.76907	1.00800
80	1	0.105718	7.66622	2.47459	4.69612	1.00800
81	1	0.116612	5.77619	1.53019	3.39940	1.00800
50	1	0.132041	1.48463	-4.16763	-1.23157	1.00800
51	1	0.115563	0.44211	-6.96350	-1.78674	1.00800
52	1	0.096582	-4.42673	6.73161	1.24439	1.00800
53	1	0.138439	-5.74543	4.93341	-0.79483	1.00800
33	1	0.058626	1.76264	-4.96475	-4.91960	1.00800
34	1	0.038135	2.54546	-6.43211	-4.17967	1.00800
35	1	0.120654	2.73725	-1.71745	0.78901	1.00800
36	1	0.126959	2.76110	0.72006	1.13663	1.00800
37	1	0.120538	7.04264	0.76724	0.45414	1.00800
91	1	0.120232	4.15624	4.14918	2.80761	1.00800
92	1	0.102587	2.13755	5.56255	2.70374	1.00800
93	1	0.124598	0.96760	3.65521	-0.99113	1.00800
94	1	0.122420	3.01055	2.26842	-0.92630	1.00800
59	1	0.099231	5.88945	-3.80330	0.38848	1.00800
38	1	0.103141	7.01014	-1.67852	0.14126	1.00800
39	1	0.097623	-4.04882	-5.40185	-4.27023	1.00800
98	1	0.062899	-1.94223	6.82475	0.81663	1.00800
99	1	0.099374	0.38982	6.58539	1.28714	1.00800
40	1	0.128841	-4.95240	-3.51809	-1.07025	1.00800
41	1	0.121186	-7.04292	-2.23267	-0.81469	1.00800
42	1	0.120355	-8.00295	-2.97557	-4.97533	1.00800
103	1	0.098734	-10.01281	3.51740	0.33555	1.00800
43	1	0.102163	-5.92177	-4.27309	-5.21453	1.00800
105	1	0.075427	-8.70985	5.30592	1.37602	1.00800
44	1	0.126267	-6.83257	-0.07464	-2.51046	1.00800
45	1	0.125747	-6.87484	2.12696	-1.40288	1.00800
46	1	0.102854	-11.04067	1.54305	-0.39621	1.00800
109	1	0.072266	-1.77870	-5.78173	-3.57367	1.00800
110	1	0.077758	4.40578	-5.84871	0.29020	1.00800

### Molecular modelling data for the computed structure (14b)

Single Point, MolecularMechanics, AMBER

Total Energy = 119.979437 kcal/mol Gradient = 27.619543.

Bond = 50.4237 Angle = 16.5468 Dihedral = 61.4234 Vdw = 4.53074 Electrostatic = -12.9453.

Polak-Ribiere optimizer

Energy=72.483180 kcal/mol Gradient=9.192527 Converged=NO (1 cycles 3 points).

Energy=65.589485 kcal/mol Gradient=3.426232 Converged=NO (2 cycles 6 points).

Energy=63.729839 kcal/mol Gradient=3.124597 Converged=NO (3 cycles 9 points).

Energy=61.682132 kcal/mol Gradient=3.197076 Converged=NO (4 cycles 11 points).

Energy=60.070983 kcal/mol Gradient=2.758009 Converged=NO (5 cycles 13 points).

Energy=58.587777 kcal/mol Gradient=2.135706 Converged=NO (6 cycles 16 points).

Energy=57.695786 kcal/mol Gradient=2.069894 Converged=NO (7 cycles 18 points).

Energy=56.728267 kcal/mol Gradient=2.171227 Converged=NO (8 cycles 20 points).  
Energy=55.980020 kcal/mol Gradient=2.200601 Converged=NO (9 cycles 22 points).  
Energy=55.152884 kcal/mol Gradient=2.003619 Converged=NO (10 cycles 24 points).  
Energy=54.362531 kcal/mol Gradient=2.008199 Converged=NO (11 cycles 26 points).  
Energy=53.696196 kcal/mol Gradient=1.946764 Converged=NO (12 cycles 28 points).  
Energy=52.931895 kcal/mol Gradient=1.620541 Converged=NO (13 cycles 30 points).  
Energy=52.486583 kcal/mol Gradient=1.273557 Converged=NO (14 cycles 32 points).  
Energy=52.128932 kcal/mol Gradient=1.297944 Converged=NO (15 cycles 34 points).  
Energy=51.910754 kcal/mol Gradient=0.908417 Converged=NO (16 cycles 36 points).  
Energy=51.748593 kcal/mol Gradient=0.916035 Converged=NO (17 cycles 39 points).  
Energy=51.618929 kcal/mol Gradient=0.872896 Converged=NO (18 cycles 41 points).  
Energy=51.476052 kcal/mol Gradient=0.947766 Converged=NO (19 cycles 43 points).  
Energy=51.316908 kcal/mol Gradient=0.724334 Converged=NO (20 cycles 45 points).  
Energy=51.193164 kcal/mol Gradient=0.807903 Converged=NO (21 cycles 47 points).  
Energy=51.079763 kcal/mol Gradient=0.688217 Converged=NO (22 cycles 49 points).  
Energy=51.011856 kcal/mol Gradient=0.523589 Converged=NO (23 cycles 51 points).  
Energy=50.948147 kcal/mol Gradient=0.545196 Converged=NO (24 cycles 53 points).  
Energy=50.881540 kcal/mol Gradient=0.577503 Converged=NO (25 cycles 55 points).  
Energy=50.831692 kcal/mol Gradient=0.574606 Converged=NO (26 cycles 57 points).  
Energy=50.780271 kcal/mol Gradient=0.443207 Converged=NO (27 cycles 59 points).  
Energy=50.737025 kcal/mol Gradient=0.519577 Converged=NO (28 cycles 61 points).  
Energy=50.663051 kcal/mol Gradient=0.545873 Converged=NO (29 cycles 64 points).  
Energy=50.616010 kcal/mol Gradient=0.491719 Converged=NO (30 cycles 66 points).  
Energy=50.560750 kcal/mol Gradient=0.581060 Converged=NO (31 cycles 69 points).  
Energy=50.490381 kcal/mol Gradient=0.477397 Converged=NO (32 cycles 71 points).  
Energy=50.447952 kcal/mol Gradient=0.595633 Converged=NO (33 cycles 73 points).  
Energy=50.381656 kcal/mol Gradient=0.559295 Converged=NO (34 cycles 76 points).  
Energy=50.322631 kcal/mol Gradient=0.550970 Converged=NO (35 cycles 78 points).  
Energy=50.264279 kcal/mol Gradient=0.626870 Converged=NO (36 cycles 80 points).  
Energy=50.171871 kcal/mol Gradient=0.656903 Converged=NO (37 cycles 82 points).  
Energy=50.092197 kcal/mol Gradient=0.519057 Converged=NO (38 cycles 84 points).  
Energy=50.017426 kcal/mol Gradient=0.661550 Converged=NO (39 cycles 86 points).  
Energy=49.933510 kcal/mol Gradient=0.646010 Converged=NO (40 cycles 88 points).  
Energy=49.873257 kcal/mol Gradient=0.581789 Converged=NO (41 cycles 90 points).  
Energy=49.811747 kcal/mol Gradient=0.555271 Converged=NO (42 cycles 92 points).  
Energy=49.755816 kcal/mol Gradient=0.570819 Converged=NO (43 cycles 94 points).  
Energy=49.693757 kcal/mol Gradient=0.531042 Converged=NO (44 cycles 96 points).  
Energy=49.639278 kcal/mol Gradient=0.504507 Converged=NO (45 cycles 98 points).  
Energy=49.565625 kcal/mol Gradient=0.560988 Converged=NO (46 cycles 101 points).  
Energy=49.507592 kcal/mol Gradient=0.607898 Converged=NO (47 cycles 103 points).  
Energy=49.440090 kcal/mol Gradient=0.528917 Converged=NO (48 cycles 105 points).  
Energy=49.378172 kcal/mol Gradient=0.637095 Converged=NO (49 cycles 107 points).  
Energy=49.305934 kcal/mol Gradient=0.673730 Converged=NO (50 cycles 109 points).  
Energy=49.238847 kcal/mol Gradient=0.512702 Converged=NO (51 cycles 111 points).  
Energy=49.171306 kcal/mol Gradient=0.582046 Converged=NO (52 cycles 114 points).  
Energy=49.102227 kcal/mol Gradient=0.530076 Converged=NO (53 cycles 116 points).  
Energy=49.045109 kcal/mol Gradient=0.602022 Converged=NO (54 cycles 118 points).  
Energy=48.973274 kcal/mol Gradient=0.587912 Converged=NO (55 cycles 120 points).  
Energy=48.897515 kcal/mol Gradient=0.573411 Converged=NO (56 cycles 123 points).  
Energy=48.839830 kcal/mol Gradient=0.636583 Converged=NO (57 cycles 125 points).  
Energy=48.771511 kcal/mol Gradient=0.603980 Converged=NO (58 cycles 127 points).  
Energy=48.704080 kcal/mol Gradient=0.573557 Converged=NO (59 cycles 129 points).

Energy=48.614622 kcal/mol Gradient=0.703926 Converged=NO (60 cycles 132 points).  
Energy=48.519255 kcal/mol Gradient=0.662557 Converged=NO (61 cycles 134 points).  
Energy=48.443945 kcal/mol Gradient=0.624545 Converged=NO (62 cycles 136 points).  
Energy=48.353115 kcal/mol Gradient=0.624668 Converged=NO (63 cycles 138 points).  
Energy=48.277005 kcal/mol Gradient=0.775922 Converged=NO (64 cycles 140 points).  
Energy=48.151411 kcal/mol Gradient=0.818264 Converged=NO (65 cycles 142 points).  
Energy=48.052629 kcal/mol Gradient=0.711810 Converged=NO (66 cycles 144 points).  
Energy=47.891557 kcal/mol Gradient=0.880861 Converged=NO (67 cycles 149 points).  
Energy=47.784912 kcal/mol Gradient=0.827880 Converged=NO (68 cycles 151 points).  
Energy=47.549127 kcal/mol Gradient=1.036123 Converged=NO (69 cycles 154 points).  
Energy=47.277708 kcal/mol Gradient=1.015578 Converged=NO (70 cycles 156 points).  
Energy=47.125693 kcal/mol Gradient=1.015708 Converged=NO (71 cycles 158 points).  
Energy=46.921232 kcal/mol Gradient=1.122425 Converged=NO (72 cycles 160 points).  
Energy=46.689249 kcal/mol Gradient=1.022672 Converged=NO (73 cycles 162 points).  
Energy=46.491095 kcal/mol Gradient=1.063289 Converged=NO (74 cycles 164 points).  
Energy=46.297535 kcal/mol Gradient=0.934287 Converged=NO (75 cycles 166 points).  
Energy=46.066248 kcal/mol Gradient=0.941210 Converged=NO (76 cycles 169 points).  
Energy=45.928662 kcal/mol Gradient=0.833463 Converged=NO (77 cycles 171 points).  
Energy=45.794800 kcal/mol Gradient=0.954137 Converged=NO (78 cycles 173 points).  
Energy=45.629778 kcal/mol Gradient=0.886093 Converged=NO (79 cycles 175 points).  
Energy=45.473758 kcal/mol Gradient=1.006306 Converged=NO (80 cycles 177 points).  
Energy=45.288465 kcal/mol Gradient=0.971970 Converged=NO (81 cycles 179 points).  
Energy=45.121295 kcal/mol Gradient=0.859500 Converged=NO (82 cycles 181 points).  
Energy=44.941067 kcal/mol Gradient=0.814929 Converged=NO (83 cycles 183 points).  
Energy=44.809286 kcal/mol Gradient=0.879387 Converged=NO (84 cycles 185 points).  
Energy=44.674727 kcal/mol Gradient=0.974458 Converged=NO (85 cycles 187 points).  
Energy=44.483138 kcal/mol Gradient=0.854913 Converged=NO (86 cycles 189 points).  
Energy=44.380416 kcal/mol Gradient=0.742683 Converged=NO (87 cycles 191 points).  
Energy=44.267169 kcal/mol Gradient=0.740657 Converged=NO (88 cycles 193 points).  
Energy=44.179477 kcal/mol Gradient=0.625588 Converged=NO (89 cycles 195 points).  
Energy=44.086054 kcal/mol Gradient=0.695116 Converged=NO (90 cycles 197 points).  
Energy=43.976913 kcal/mol Gradient=0.682582 Converged=NO (91 cycles 199 points).  
Energy=43.922241 kcal/mol Gradient=0.545635 Converged=NO (92 cycles 201 points).  
Energy=43.852085 kcal/mol Gradient=0.609158 Converged=NO (93 cycles 204 points).  
Energy=43.795459 kcal/mol Gradient=0.519126 Converged=NO (94 cycles 206 points).  
Energy=43.749029 kcal/mol Gradient=0.509862 Converged=NO (95 cycles 208 points).  
Energy=43.687450 kcal/mol Gradient=0.535587 Converged=NO (96 cycles 211 points).  
Energy=43.624760 kcal/mol Gradient=0.531738 Converged=NO (97 cycles 213 points).  
Energy=43.577569 kcal/mol Gradient=0.515685 Converged=NO (98 cycles 215 points).  
Energy=43.532259 kcal/mol Gradient=0.474843 Converged=NO (99 cycles 217 points).  
Energy=43.493229 kcal/mol Gradient=0.473043 Converged=NO (100 cycles 219 points).  
Energy=43.451127 kcal/mol Gradient=0.494816 Converged=NO (101 cycles 221 points).  
Energy=43.409975 kcal/mol Gradient=0.419673 Converged=NO (102 cycles 223 points).  
Energy=43.369803 kcal/mol Gradient=0.428056 Converged=NO (103 cycles 225 points).  
Energy=43.326913 kcal/mol Gradient=0.433474 Converged=NO (104 cycles 228 points).  
Energy=43.292458 kcal/mol Gradient=0.519821 Converged=NO (105 cycles 230 points).  
Energy=43.244125 kcal/mol Gradient=0.459861 Converged=NO (106 cycles 232 points).  
Energy=43.200238 kcal/mol Gradient=0.517178 Converged=NO (107 cycles 235 points).  
Energy=43.151560 kcal/mol Gradient=0.506485 Converged=NO (108 cycles 237 points).  
Energy=43.108152 kcal/mol Gradient=0.438077 Converged=NO (109 cycles 239 points).  
Energy=43.055459 kcal/mol Gradient=0.537976 Converged=NO (110 cycles 242 points).  
Energy=43.004612 kcal/mol Gradient=0.504143 Converged=NO (111 cycles 244 points).

Energy=42.955401 kcal/mol Gradient=0.557325 Converged=NO (112 cycles 246 points).  
Energy=42.898220 kcal/mol Gradient=0.532211 Converged=NO (113 cycles 248 points).  
Energy=42.850007 kcal/mol Gradient=0.521750 Converged=NO (114 cycles 250 points).  
Energy=42.803107 kcal/mol Gradient=0.500736 Converged=NO (115 cycles 252 points).  
Energy=42.750127 kcal/mol Gradient=0.510325 Converged=NO (116 cycles 254 points).  
Energy=42.689097 kcal/mol Gradient=0.481844 Converged=NO (117 cycles 256 points).  
Energy=42.646729 kcal/mol Gradient=0.479583 Converged=NO (118 cycles 258 points).  
Energy=42.609960 kcal/mol Gradient=0.472606 Converged=NO (119 cycles 260 points).  
Energy=42.561138 kcal/mol Gradient=0.477227 Converged=NO (120 cycles 263 points).  
Energy=42.523559 kcal/mol Gradient=0.520006 Converged=NO (121 cycles 265 points).  
Energy=42.463991 kcal/mol Gradient=0.514057 Converged=NO (122 cycles 268 points).  
Energy=42.419941 kcal/mol Gradient=0.437088 Converged=NO (123 cycles 270 points).  
Energy=42.372296 kcal/mol Gradient=0.464107 Converged=NO (124 cycles 272 points).  
Energy=42.334008 kcal/mol Gradient=0.426288 Converged=NO (125 cycles 274 points).  
Energy=42.304363 kcal/mol Gradient=0.449534 Converged=NO (126 cycles 276 points).  
Energy=42.260189 kcal/mol Gradient=0.439401 Converged=NO (127 cycles 279 points).  
Energy=42.230010 kcal/mol Gradient=0.428794 Converged=NO (128 cycles 281 points).  
Energy=42.199237 kcal/mol Gradient=0.367078 Converged=NO (129 cycles 283 points).  
Energy=42.167257 kcal/mol Gradient=0.382358 Converged=NO (130 cycles 286 points).  
Energy=42.131269 kcal/mol Gradient=0.485396 Converged=NO (131 cycles 288 points).  
Energy=42.087426 kcal/mol Gradient=0.457566 Converged=NO (132 cycles 290 points).  
Energy=42.053778 kcal/mol Gradient=0.410873 Converged=NO (133 cycles 292 points).  
Energy=42.018914 kcal/mol Gradient=0.463376 Converged=NO (134 cycles 295 points).  
Energy=41.983978 kcal/mol Gradient=0.438382 Converged=NO (135 cycles 297 points).  
Energy=41.950045 kcal/mol Gradient=0.394703 Converged=NO (136 cycles 299 points).  
Energy=41.907043 kcal/mol Gradient=0.459607 Converged=NO (137 cycles 301 points).  
Energy=41.860945 kcal/mol Gradient=0.498809 Converged=NO (138 cycles 303 points).  
Energy=41.822380 kcal/mol Gradient=0.425940 Converged=NO (139 cycles 305 points).  
Energy=41.789725 kcal/mol Gradient=0.465072 Converged=NO (140 cycles 307 points).  
Energy=41.735830 kcal/mol Gradient=0.532918 Converged=NO (141 cycles 309 points).  
Energy=41.699110 kcal/mol Gradient=0.418095 Converged=NO (142 cycles 311 points).  
Energy=41.660998 kcal/mol Gradient=0.439267 Converged=NO (143 cycles 314 points).  
Energy=41.620060 kcal/mol Gradient=0.424628 Converged=NO (144 cycles 316 points).  
Energy=41.581677 kcal/mol Gradient=0.494514 Converged=NO (145 cycles 318 points).  
Energy=41.534699 kcal/mol Gradient=0.471134 Converged=NO (146 cycles 320 points).  
Energy=41.497870 kcal/mol Gradient=0.453452 Converged=NO (147 cycles 322 points).  
Energy=41.457174 kcal/mol Gradient=0.497351 Converged=NO (148 cycles 324 points).  
Energy=41.417019 kcal/mol Gradient=0.458808 Converged=NO (149 cycles 326 points).  
Energy=41.371792 kcal/mol Gradient=0.446822 Converged=NO (150 cycles 328 points).  
Energy=41.317159 kcal/mol Gradient=0.504546 Converged=NO (151 cycles 330 points).  
Energy=41.282364 kcal/mol Gradient=0.440359 Converged=NO (152 cycles 332 points).  
Energy=41.239346 kcal/mol Gradient=0.433054 Converged=NO (153 cycles 334 points).  
Energy=41.204160 kcal/mol Gradient=0.474702 Converged=NO (154 cycles 336 points).  
Energy=41.164820 kcal/mol Gradient=0.482625 Converged=NO (155 cycles 338 points).  
Energy=41.125102 kcal/mol Gradient=0.431513 Converged=NO (156 cycles 340 points).  
Energy=41.077304 kcal/mol Gradient=0.445411 Converged=NO (157 cycles 342 points).  
Energy=41.040313 kcal/mol Gradient=0.455715 Converged=NO (158 cycles 344 points).  
Energy=40.994413 kcal/mol Gradient=0.524272 Converged=NO (159 cycles 346 points).  
Energy=40.949024 kcal/mol Gradient=0.476317 Converged=NO (160 cycles 348 points).  
Energy=40.905733 kcal/mol Gradient=0.492773 Converged=NO (161 cycles 350 points).  
Energy=40.861671 kcal/mol Gradient=0.512896 Converged=NO (162 cycles 352 points).  
Energy=40.820861 kcal/mol Gradient=0.403882 Converged=NO (163 cycles 354 points).

Energy=40.782191 kcal/mol Gradient=0.442000 Converged=NO (164 cycles 356 points).  
Energy=40.737410 kcal/mol Gradient=0.468137 Converged=NO (165 cycles 358 points).  
Energy=40.708581 kcal/mol Gradient=0.373087 Converged=NO (166 cycles 360 points).  
Energy=40.674349 kcal/mol Gradient=0.440092 Converged=NO (167 cycles 363 points).  
Energy=40.647211 kcal/mol Gradient=0.368094 Converged=NO (168 cycles 365 points).  
Energy=40.624711 kcal/mol Gradient=0.338422 Converged=NO (169 cycles 367 points).  
Energy=40.597994 kcal/mol Gradient=0.348645 Converged=NO (170 cycles 369 points).  
Energy=40.573233 kcal/mol Gradient=0.322412 Converged=NO (171 cycles 371 points).  
Energy=40.551076 kcal/mol Gradient=0.371847 Converged=NO (172 cycles 373 points).  
Energy=40.530742 kcal/mol Gradient=0.334005 Converged=NO (173 cycles 375 points).  
Energy=40.505416 kcal/mol Gradient=0.364266 Converged=NO (174 cycles 378 points).  
Energy=40.481751 kcal/mol Gradient=0.370886 Converged=NO (175 cycles 380 points).  
Energy=40.460324 kcal/mol Gradient=0.293501 Converged=NO (176 cycles 382 points).  
Energy=40.439593 kcal/mol Gradient=0.352394 Converged=NO (177 cycles 385 points).  
Energy=40.410024 kcal/mol Gradient=0.348004 Converged=NO (178 cycles 387 points).  
Energy=40.390316 kcal/mol Gradient=0.361429 Converged=NO (179 cycles 389 points).  
Energy=40.367978 kcal/mol Gradient=0.315699 Converged=NO (180 cycles 391 points).  
Energy=40.350305 kcal/mol Gradient=0.332534 Converged=NO (181 cycles 393 points).  
Energy=40.324412 kcal/mol Gradient=0.368413 Converged=NO (182 cycles 395 points).  
Energy=40.303543 kcal/mol Gradient=0.310117 Converged=NO (183 cycles 397 points).  
Energy=40.279624 kcal/mol Gradient=0.355058 Converged=NO (184 cycles 399 points).  
Energy=40.255318 kcal/mol Gradient=0.314893 Converged=NO (185 cycles 401 points).  
Energy=40.241809 kcal/mol Gradient=0.293922 Converged=NO (186 cycles 403 points).  
Energy=40.223352 kcal/mol Gradient=0.301992 Converged=NO (187 cycles 406 points).  
Energy=40.206188 kcal/mol Gradient=0.318625 Converged=NO (188 cycles 408 points).  
Energy=40.186562 kcal/mol Gradient=0.344702 Converged=NO (189 cycles 410 points).  
Energy=40.159388 kcal/mol Gradient=0.317806 Converged=NO (190 cycles 412 points).  
Energy=40.137460 kcal/mol Gradient=0.345417 Converged=NO (191 cycles 414 points).  
Energy=40.114624 kcal/mol Gradient=0.374188 Converged=NO (192 cycles 416 points).  
Energy=40.095516 kcal/mol Gradient=0.297571 Converged=NO (193 cycles 418 points).  
Energy=40.077018 kcal/mol Gradient=0.308672 Converged=NO (194 cycles 420 points).  
Energy=40.054609 kcal/mol Gradient=0.343822 Converged=NO (195 cycles 422 points).  
Energy=40.033386 kcal/mol Gradient=0.350088 Converged=NO (196 cycles 424 points).  
Energy=40.008219 kcal/mol Gradient=0.351848 Converged=NO (197 cycles 426 points).  
Energy=39.984480 kcal/mol Gradient=0.335756 Converged=NO (198 cycles 428 points).  
Energy=39.963519 kcal/mol Gradient=0.389964 Converged=NO (199 cycles 430 points).  
Energy=39.939376 kcal/mol Gradient=0.319355 Converged=NO (200 cycles 432 points).  
Energy=39.912782 kcal/mol Gradient=0.364651 Converged=NO (201 cycles 434 points).  
Energy=39.891012 kcal/mol Gradient=0.348576 Converged=NO (202 cycles 436 points).  
Energy=39.864566 kcal/mol Gradient=0.340727 Converged=NO (203 cycles 438 points).  
Energy=39.844524 kcal/mol Gradient=0.312568 Converged=NO (204 cycles 440 points).  
Energy=39.826702 kcal/mol Gradient=0.341640 Converged=NO (205 cycles 442 points).  
Energy=39.805660 kcal/mol Gradient=0.338646 Converged=NO (206 cycles 444 points).  
Energy=39.786362 kcal/mol Gradient=0.284834 Converged=NO (207 cycles 446 points).  
Energy=39.765407 kcal/mol Gradient=0.354752 Converged=NO (208 cycles 448 points).  
Energy=39.742418 kcal/mol Gradient=0.338597 Converged=NO (209 cycles 450 points).  
Energy=39.723131 kcal/mol Gradient=0.328132 Converged=NO (210 cycles 452 points).  
Energy=39.691466 kcal/mol Gradient=0.381437 Converged=NO (211 cycles 455 points).  
Energy=39.673255 kcal/mol Gradient=0.319310 Converged=NO (212 cycles 457 points).  
Energy=39.653318 kcal/mol Gradient=0.340581 Converged=NO (213 cycles 459 points).  
Energy=39.629937 kcal/mol Gradient=0.306332 Converged=NO (214 cycles 461 points).  
Energy=39.609936 kcal/mol Gradient=0.304993 Converged=NO (215 cycles 463 points).

Energy=39.593718 kcal/mol Gradient=0.323208 Converged=NO (216 cycles 465 points).  
Energy=39.570951 kcal/mol Gradient=0.325336 Converged=NO (217 cycles 467 points).  
Energy=39.553806 kcal/mol Gradient=0.313844 Converged=NO (218 cycles 469 points).  
Energy=39.535886 kcal/mol Gradient=0.317131 Converged=NO (219 cycles 471 points).  
Energy=39.518555 kcal/mol Gradient=0.297966 Converged=NO (220 cycles 473 points).  
Energy=39.497842 kcal/mol Gradient=0.284636 Converged=NO (221 cycles 475 points).  
Energy=39.483791 kcal/mol Gradient=0.279443 Converged=NO (222 cycles 477 points).  
Energy=39.471318 kcal/mol Gradient=0.252537 Converged=NO (223 cycles 479 points).  
Energy=39.457377 kcal/mol Gradient=0.243561 Converged=NO (224 cycles 481 points).  
Energy=39.447415 kcal/mol Gradient=0.280970 Converged=NO (225 cycles 483 points).  
Energy=39.430466 kcal/mol Gradient=0.284975 Converged=NO (226 cycles 486 points).  
Energy=39.413222 kcal/mol Gradient=0.288833 Converged=NO (227 cycles 488 points).  
Energy=39.397544 kcal/mol Gradient=0.251977 Converged=NO (228 cycles 490 points).  
Energy=39.385108 kcal/mol Gradient=0.302420 Converged=NO (229 cycles 492 points).  
Energy=39.366624 kcal/mol Gradient=0.296587 Converged=NO (230 cycles 494 points).  
Energy=39.351215 kcal/mol Gradient=0.281117 Converged=NO (231 cycles 496 points).  
Energy=39.337304 kcal/mol Gradient=0.306370 Converged=NO (232 cycles 498 points).  
Energy=39.318941 kcal/mol Gradient=0.279893 Converged=NO (233 cycles 500 points).  
Energy=39.302765 kcal/mol Gradient=0.272519 Converged=NO (234 cycles 502 points).  
Energy=39.284336 kcal/mol Gradient=0.339537 Converged=NO (235 cycles 504 points).  
Energy=39.265267 kcal/mol Gradient=0.311915 Converged=NO (236 cycles 506 points).  
Energy=39.249779 kcal/mol Gradient=0.293865 Converged=NO (237 cycles 508 points).  
Energy=39.232673 kcal/mol Gradient=0.279215 Converged=NO (238 cycles 510 points).  
Energy=39.218719 kcal/mol Gradient=0.292993 Converged=NO (239 cycles 512 points).  
Energy=39.200295 kcal/mol Gradient=0.298720 Converged=NO (240 cycles 514 points).  
Energy=39.182509 kcal/mol Gradient=0.298689 Converged=NO (241 cycles 516 points).  
Energy=39.164477 kcal/mol Gradient=0.323574 Converged=NO (242 cycles 518 points).  
Energy=39.149492 kcal/mol Gradient=0.285316 Converged=NO (243 cycles 520 points).  
Energy=39.131219 kcal/mol Gradient=0.304038 Converged=NO (244 cycles 522 points).  
Energy=39.113442 kcal/mol Gradient=0.312964 Converged=NO (245 cycles 524 points).  
Energy=39.097801 kcal/mol Gradient=0.288063 Converged=NO (246 cycles 526 points).  
Energy=39.077251 kcal/mol Gradient=0.275692 Converged=NO (247 cycles 528 points).  
Energy=39.062993 kcal/mol Gradient=0.298550 Converged=NO (248 cycles 530 points).  
Energy=39.048948 kcal/mol Gradient=0.286440 Converged=NO (249 cycles 532 points).  
Energy=39.033383 kcal/mol Gradient=0.266753 Converged=NO (250 cycles 534 points).  
Energy=39.018089 kcal/mol Gradient=0.285940 Converged=NO (251 cycles 536 points).  
Energy=39.002188 kcal/mol Gradient=0.290115 Converged=NO (252 cycles 538 points).  
Energy=38.987240 kcal/mol Gradient=0.282639 Converged=NO (253 cycles 540 points).  
Energy=38.969252 kcal/mol Gradient=0.307331 Converged=NO (254 cycles 542 points).  
Energy=38.954705 kcal/mol Gradient=0.275254 Converged=NO (255 cycles 544 points).  
Energy=38.940803 kcal/mol Gradient=0.299793 Converged=NO (256 cycles 546 points).  
Energy=38.923731 kcal/mol Gradient=0.246950 Converged=NO (257 cycles 548 points).  
Energy=38.910760 kcal/mol Gradient=0.270843 Converged=NO (258 cycles 550 points).  
Energy=38.898376 kcal/mol Gradient=0.244007 Converged=NO (259 cycles 552 points).  
Energy=38.888061 kcal/mol Gradient=0.223475 Converged=NO (260 cycles 554 points).  
Energy=38.875693 kcal/mol Gradient=0.268546 Converged=NO (261 cycles 556 points).  
Energy=38.865878 kcal/mol Gradient=0.240875 Converged=NO (262 cycles 558 points).  
Energy=38.852577 kcal/mol Gradient=0.236594 Converged=NO (263 cycles 560 points).  
Energy=38.842137 kcal/mol Gradient=0.215330 Converged=NO (264 cycles 562 points).  
Energy=38.834287 kcal/mol Gradient=0.213090 Converged=NO (265 cycles 564 points).  
Energy=38.823365 kcal/mol Gradient=0.263369 Converged=NO (266 cycles 566 points).  
Energy=38.811873 kcal/mol Gradient=0.204120 Converged=NO (267 cycles 568 points).

Energy=38.803360 kcal/mol Gradient=0.260169 Converged=NO (268 cycles 570 points).  
Energy=38.791922 kcal/mol Gradient=0.210547 Converged=NO (269 cycles 572 points).  
Energy=38.784065 kcal/mol Gradient=0.199771 Converged=NO (270 cycles 574 points).  
Energy=38.772109 kcal/mol Gradient=0.245031 Converged=NO (271 cycles 576 points).  
Energy=38.762753 kcal/mol Gradient=0.225504 Converged=NO (272 cycles 578 points).  
Energy=38.753666 kcal/mol Gradient=0.212110 Converged=NO (273 cycles 580 points).  
Energy=38.746135 kcal/mol Gradient=0.193271 Converged=NO (274 cycles 582 points).  
Energy=38.739693 kcal/mol Gradient=0.201005 Converged=NO (275 cycles 584 points).  
Energy=38.730839 kcal/mol Gradient=0.217283 Converged=NO (276 cycles 586 points).  
Energy=38.721195 kcal/mol Gradient=0.208924 Converged=NO (277 cycles 588 points).  
Energy=38.712364 kcal/mol Gradient=0.209666 Converged=NO (278 cycles 590 points).  
Energy=38.705274 kcal/mol Gradient=0.199921 Converged=NO (279 cycles 592 points).  
Energy=38.698192 kcal/mol Gradient=0.188486 Converged=NO (280 cycles 594 points).  
Energy=38.691173 kcal/mol Gradient=0.200906 Converged=NO (281 cycles 596 points).  
Energy=38.684182 kcal/mol Gradient=0.213304 Converged=NO (282 cycles 598 points).  
Energy=38.674040 kcal/mol Gradient=0.183477 Converged=NO (283 cycles 600 points).  
Energy=38.666668 kcal/mol Gradient=0.184337 Converged=NO (284 cycles 602 points).  
Energy=38.660801 kcal/mol Gradient=0.196950 Converged=NO (285 cycles 604 points).  
Energy=38.653625 kcal/mol Gradient=0.198006 Converged=NO (286 cycles 606 points).  
Energy=38.646069 kcal/mol Gradient=0.208630 Converged=NO (287 cycles 608 points).  
Energy=38.636839 kcal/mol Gradient=0.216533 Converged=NO (288 cycles 610 points).  
Energy=38.629195 kcal/mol Gradient=0.199056 Converged=NO (289 cycles 612 points).  
Energy=38.620740 kcal/mol Gradient=0.193276 Converged=NO (290 cycles 614 points).  
Energy=38.612684 kcal/mol Gradient=0.215878 Converged=NO (291 cycles 616 points).  
Energy=38.604346 kcal/mol Gradient=0.227991 Converged=NO (292 cycles 618 points).  
Energy=38.595863 kcal/mol Gradient=0.199421 Converged=NO (293 cycles 620 points).  
Energy=38.587869 kcal/mol Gradient=0.206160 Converged=NO (294 cycles 622 points).  
Energy=38.579168 kcal/mol Gradient=0.226035 Converged=NO (295 cycles 624 points).  
Energy=38.569845 kcal/mol Gradient=0.207352 Converged=NO (296 cycles 626 points).  
Energy=38.560212 kcal/mol Gradient=0.221483 Converged=NO (297 cycles 628 points).  
Energy=38.551321 kcal/mol Gradient=0.217214 Converged=NO (298 cycles 630 points).  
Energy=38.544771 kcal/mol Gradient=0.192736 Converged=NO (299 cycles 632 points).  
Energy=38.535674 kcal/mol Gradient=0.202259 Converged=NO (300 cycles 634 points).  
Energy=38.529556 kcal/mol Gradient=0.177848 Converged=NO (301 cycles 636 points).  
Energy=38.521309 kcal/mol Gradient=0.222657 Converged=NO (302 cycles 638 points).  
Energy=38.513594 kcal/mol Gradient=0.182818 Converged=NO (303 cycles 640 points).  
Energy=38.505465 kcal/mol Gradient=0.192991 Converged=NO (304 cycles 642 points).  
Energy=38.499483 kcal/mol Gradient=0.213404 Converged=NO (305 cycles 644 points).  
Energy=38.491094 kcal/mol Gradient=0.190168 Converged=NO (306 cycles 646 points).  
Energy=38.481642 kcal/mol Gradient=0.210754 Converged=NO (307 cycles 648 points).  
Energy=38.473817 kcal/mol Gradient=0.187647 Converged=NO (308 cycles 650 points).  
Energy=38.467358 kcal/mol Gradient=0.212062 Converged=NO (309 cycles 652 points).  
Energy=38.457252 kcal/mol Gradient=0.202913 Converged=NO (310 cycles 654 points).  
Energy=38.451270 kcal/mol Gradient=0.185599 Converged=NO (311 cycles 656 points).  
Energy=38.444725 kcal/mol Gradient=0.208454 Converged=NO (312 cycles 658 points).  
Energy=38.434802 kcal/mol Gradient=0.199653 Converged=NO (313 cycles 660 points).  
Energy=38.427311 kcal/mol Gradient=0.189629 Converged=NO (314 cycles 662 points).  
Energy=38.420935 kcal/mol Gradient=0.186440 Converged=NO (315 cycles 664 points).  
Energy=38.414505 kcal/mol Gradient=0.181873 Converged=NO (316 cycles 666 points).  
Energy=38.408885 kcal/mol Gradient=0.164501 Converged=NO (317 cycles 668 points).  
Energy=38.403733 kcal/mol Gradient=0.195164 Converged=NO (318 cycles 670 points).  
Energy=38.396178 kcal/mol Gradient=0.190161 Converged=NO (319 cycles 672 points).



Energy=38.389031 kcal/mol Gradient=0.167941 Converged=NO (320 cycles 674 points).  
Energy=38.381824 kcal/mol Gradient=0.202784 Converged=NO (321 cycles 676 points).  
Energy=38.375989 kcal/mol Gradient=0.173412 Converged=NO (322 cycles 678 points).  
Energy=38.369605 kcal/mol Gradient=0.185017 Converged=NO (323 cycles 680 points).  
Energy=38.363660 kcal/mol Gradient=0.178712 Converged=NO (324 cycles 682 points).  
Energy=38.358444 kcal/mol Gradient=0.165686 Converged=NO (325 cycles 684 points).  
Energy=38.353117 kcal/mol Gradient=0.172299 Converged=NO (326 cycles 686 points).  
Energy=38.346508 kcal/mol Gradient=0.152378 Converged=NO (327 cycles 688 points).  
Energy=38.340419 kcal/mol Gradient=0.211690 Converged=NO (328 cycles 690 points).  
Energy=38.333376 kcal/mol Gradient=0.177425 Converged=NO (329 cycles 692 points).  
Energy=38.328241 kcal/mol Gradient=0.165693 Converged=NO (330 cycles 694 points).  
Energy=38.322460 kcal/mol Gradient=0.181880 Converged=NO (331 cycles 696 points).  
Energy=38.316986 kcal/mol Gradient=0.163642 Converged=NO (332 cycles 698 points).  
Energy=38.311394 kcal/mol Gradient=0.169474 Converged=NO (333 cycles 700 points).  
Energy=38.305163 kcal/mol Gradient=0.166643 Converged=NO (334 cycles 702 points).  
Energy=38.300560 kcal/mol Gradient=0.159571 Converged=NO (335 cycles 704 points).  
Energy=38.296319 kcal/mol Gradient=0.160499 Converged=NO (336 cycles 706 points).  
Energy=38.290674 kcal/mol Gradient=0.171486 Converged=NO (337 cycles 708 points).  
Energy=38.285105 kcal/mol Gradient=0.187839 Converged=NO (338 cycles 710 points).  
Energy=38.278510 kcal/mol Gradient=0.173294 Converged=NO (339 cycles 712 points).  
Energy=38.272290 kcal/mol Gradient=0.167397 Converged=NO (340 cycles 714 points).  
Energy=38.266007 kcal/mol Gradient=0.180129 Converged=NO (341 cycles 716 points).  
Energy=38.261105 kcal/mol Gradient=0.184980 Converged=NO (342 cycles 718 points).  
Energy=38.252829 kcal/mol Gradient=0.197245 Converged=NO (343 cycles 720 points).  
Energy=38.246198 kcal/mol Gradient=0.187765 Converged=NO (344 cycles 722 points).  
Energy=38.240467 kcal/mol Gradient=0.171095 Converged=NO (345 cycles 724 points).  
Energy=38.233555 kcal/mol Gradient=0.190845 Converged=NO (346 cycles 726 points).  
Energy=38.226433 kcal/mol Gradient=0.182057 Converged=NO (347 cycles 728 points).  
Energy=38.219331 kcal/mol Gradient=0.212349 Converged=NO (348 cycles 730 points).  
Energy=38.212159 kcal/mol Gradient=0.200212 Converged=NO (349 cycles 732 points).  
Energy=38.205037 kcal/mol Gradient=0.181862 Converged=NO (350 cycles 734 points).  
Energy=38.197981 kcal/mol Gradient=0.187882 Converged=NO (351 cycles 736 points).  
Energy=38.192711 kcal/mol Gradient=0.155594 Converged=NO (352 cycles 738 points).  
Energy=38.187476 kcal/mol Gradient=0.164216 Converged=NO (353 cycles 740 points).  
Energy=38.181918 kcal/mol Gradient=0.168397 Converged=NO (354 cycles 742 points).  
Energy=38.177326 kcal/mol Gradient=0.177416 Converged=NO (355 cycles 744 points).  
Energy=38.171759 kcal/mol Gradient=0.142212 Converged=NO (356 cycles 746 points).  
Energy=38.167270 kcal/mol Gradient=0.172584 Converged=NO (357 cycles 748 points).  
Energy=38.161856 kcal/mol Gradient=0.151848 Converged=NO (358 cycles 750 points).  
Energy=38.158063 kcal/mol Gradient=0.141128 Converged=NO (359 cycles 752 points).  
Energy=38.153013 kcal/mol Gradient=0.155372 Converged=NO (360 cycles 754 points).  
Energy=38.149366 kcal/mol Gradient=0.145662 Converged=NO (361 cycles 756 points).  
Energy=38.145681 kcal/mol Gradient=0.147244 Converged=NO (362 cycles 758 points).  
Energy=38.141557 kcal/mol Gradient=0.131459 Converged=NO (363 cycles 760 points).  
Energy=38.136920 kcal/mol Gradient=0.162704 Converged=NO (364 cycles 762 points).  
Energy=38.131787 kcal/mol Gradient=0.171448 Converged=NO (365 cycles 764 points).  
Energy=38.127230 kcal/mol Gradient=0.138233 Converged=NO (366 cycles 766 points).  
Energy=38.122973 kcal/mol Gradient=0.169368 Converged=NO (367 cycles 768 points).  
Energy=38.118051 kcal/mol Gradient=0.157674 Converged=NO (368 cycles 770 points).  
Energy=38.114000 kcal/mol Gradient=0.146523 Converged=NO (369 cycles 772 points).  
Energy=38.109229 kcal/mol Gradient=0.144029 Converged=NO (370 cycles 774 points).  
Energy=38.104925 kcal/mol Gradient=0.145413 Converged=NO (371 cycles 776 points).

Energy=38.101382 kcal/mol Gradient=0.149413 Converged=NO (372 cycles 778 points).  
Energy=38.096652 kcal/mol Gradient=0.154329 Converged=NO (373 cycles 780 points).  
Energy=38.092285 kcal/mol Gradient=0.167735 Converged=NO (374 cycles 782 points).  
Energy=38.087150 kcal/mol Gradient=0.164742 Converged=NO (375 cycles 784 points).  
Energy=38.082106 kcal/mol Gradient=0.154067 Converged=NO (376 cycles 786 points).  
Energy=38.075850 kcal/mol Gradient=0.160336 Converged=NO (377 cycles 789 points).  
Energy=38.071883 kcal/mol Gradient=0.161543 Converged=NO (378 cycles 791 points).  
Energy=38.066825 kcal/mol Gradient=0.152266 Converged=NO (379 cycles 793 points).  
Energy=38.062390 kcal/mol Gradient=0.158420 Converged=NO (380 cycles 795 points).  
Energy=38.058217 kcal/mol Gradient=0.159078 Converged=NO (381 cycles 797 points).  
Energy=38.053528 kcal/mol Gradient=0.132159 Converged=NO (382 cycles 799 points).  
Energy=38.049762 kcal/mol Gradient=0.148497 Converged=NO (383 cycles 801 points).  
Energy=38.044025 kcal/mol Gradient=0.173093 Converged=NO (384 cycles 804 points).  
Energy=38.039934 kcal/mol Gradient=0.139088 Converged=NO (385 cycles 806 points).  
Energy=38.036471 kcal/mol Gradient=0.149757 Converged=NO (386 cycles 808 points).  
Energy=38.031155 kcal/mol Gradient=0.152493 Converged=NO (387 cycles 810 points).  
Energy=38.027999 kcal/mol Gradient=0.135593 Converged=NO (388 cycles 812 points).  
Energy=38.023102 kcal/mol Gradient=0.148355 Converged=NO (389 cycles 814 points).  
Energy=38.019120 kcal/mol Gradient=0.135075 Converged=NO (390 cycles 816 points).  
Energy=38.015643 kcal/mol Gradient=0.143060 Converged=NO (391 cycles 818 points).  
Energy=38.012461 kcal/mol Gradient=0.127304 Converged=NO (392 cycles 820 points).  
Energy=38.009232 kcal/mol Gradient=0.136209 Converged=NO (393 cycles 822 points).  
Energy=38.005575 kcal/mol Gradient=0.143750 Converged=NO (394 cycles 824 points).  
Energy=38.002074 kcal/mol Gradient=0.123434 Converged=NO (395 cycles 826 points).  
Energy=37.999069 kcal/mol Gradient=0.116846 Converged=NO (396 cycles 828 points).  
Energy=37.996232 kcal/mol Gradient=0.120296 Converged=NO (397 cycles 830 points).  
Energy=37.993710 kcal/mol Gradient=0.129889 Converged=NO (398 cycles 832 points).  
Energy=37.990646 kcal/mol Gradient=0.126105 Converged=NO (399 cycles 834 points).  
Energy=37.987393 kcal/mol Gradient=0.126830 Converged=NO (400 cycles 836 points).  
Energy=37.984221 kcal/mol Gradient=0.146135 Converged=NO (401 cycles 838 points).  
Energy=37.980488 kcal/mol Gradient=0.116486 Converged=NO (402 cycles 840 points).  
Energy=37.977074 kcal/mol Gradient=0.131375 Converged=NO (403 cycles 842 points).  
Energy=37.973836 kcal/mol Gradient=0.146368 Converged=NO (404 cycles 844 points).  
Energy=37.970307 kcal/mol Gradient=0.135980 Converged=NO (405 cycles 846 points).  
Energy=37.967136 kcal/mol Gradient=0.118998 Converged=NO (406 cycles 848 points).  
Energy=37.963936 kcal/mol Gradient=0.139292 Converged=NO (407 cycles 850 points).  
Energy=37.959461 kcal/mol Gradient=0.155699 Converged=NO (408 cycles 852 points).  
Energy=37.955646 kcal/mol Gradient=0.131953 Converged=NO (409 cycles 854 points).  
Energy=37.952017 kcal/mol Gradient=0.137152 Converged=NO (410 cycles 856 points).  
Energy=37.949072 kcal/mol Gradient=0.141170 Converged=NO (411 cycles 858 points).  
Energy=37.944979 kcal/mol Gradient=0.133577 Converged=NO (412 cycles 860 points).  
Energy=37.941598 kcal/mol Gradient=0.132378 Converged=NO (413 cycles 862 points).  
Energy=37.938053 kcal/mol Gradient=0.137563 Converged=NO (414 cycles 864 points).  
Energy=37.934615 kcal/mol Gradient=0.139985 Converged=NO (415 cycles 866 points).  
Energy=37.930786 kcal/mol Gradient=0.124839 Converged=NO (416 cycles 868 points).  
Energy=37.927735 kcal/mol Gradient=0.153629 Converged=NO (417 cycles 870 points).  
Energy=37.923437 kcal/mol Gradient=0.140630 Converged=NO (418 cycles 872 points).  
Energy=37.920205 kcal/mol Gradient=0.121275 Converged=NO (419 cycles 874 points).  
Energy=37.916633 kcal/mol Gradient=0.130506 Converged=NO (420 cycles 876 points).  
Energy=37.913643 kcal/mol Gradient=0.121165 Converged=NO (421 cycles 878 points).  
Energy=37.911216 kcal/mol Gradient=0.122147 Converged=NO (422 cycles 880 points).  
Energy=37.907698 kcal/mol Gradient=0.124517 Converged=NO (423 cycles 882 points).

Energy=37.905553 kcal/mol Gradient=0.113866 Converged=NO (424 cycles 884 points).  
Energy=37.903041 kcal/mol Gradient=0.114972 Converged=NO (425 cycles 886 points).  
Energy=37.899861 kcal/mol Gradient=0.116432 Converged=NO (426 cycles 888 points).  
Energy=37.897053 kcal/mol Gradient=0.134806 Converged=NO (427 cycles 890 points).  
Energy=37.893451 kcal/mol Gradient=0.136208 Converged=NO (428 cycles 892 points).  
Energy=37.890214 kcal/mol Gradient=0.129487 Converged=NO (429 cycles 894 points).  
Energy=37.887098 kcal/mol Gradient=0.135273 Converged=NO (430 cycles 896 points).  
Energy=37.884045 kcal/mol Gradient=0.126006 Converged=NO (431 cycles 898 points).  
Energy=37.881003 kcal/mol Gradient=0.123888 Converged=NO (432 cycles 900 points).  
Energy=37.877592 kcal/mol Gradient=0.121719 Converged=NO (433 cycles 902 points).  
Energy=37.874956 kcal/mol Gradient=0.126871 Converged=NO (434 cycles 904 points).  
Energy=37.871915 kcal/mol Gradient=0.127299 Converged=NO (435 cycles 906 points).  
Energy=37.868566 kcal/mol Gradient=0.135331 Converged=NO (436 cycles 908 points).  
Energy=37.865198 kcal/mol Gradient=0.141803 Converged=NO (437 cycles 910 points).  
Energy=37.862362 kcal/mol Gradient=0.109798 Converged=NO (438 cycles 912 points).  
Energy=37.859365 kcal/mol Gradient=0.109131 Converged=NO (439 cycles 914 points).  
Energy=37.856929 kcal/mol Gradient=0.113564 Converged=NO (440 cycles 916 points).  
Energy=37.854652 kcal/mol Gradient=0.114843 Converged=NO (441 cycles 918 points).  
Energy=37.852325 kcal/mol Gradient=0.116324 Converged=NO (442 cycles 920 points).  
Energy=37.849883 kcal/mol Gradient=0.104664 Converged=NO (443 cycles 922 points).  
Energy=37.847739 kcal/mol Gradient=0.116306 Converged=NO (444 cycles 924 points).  
Energy=37.845483 kcal/mol Gradient=0.095208 Converged=NO (445 cycles 926 points).  
Energy=37.843347 kcal/mol Gradient=0.106904 Converged=NO (446 cycles 928 points).  
Energy=37.841035 kcal/mol Gradient=0.106704 Converged=NO (447 cycles 930 points).  
Energy=37.839361 kcal/mol Gradient=0.104091 Converged=NO (448 cycles 932 points).  
Energy=37.836814 kcal/mol Gradient=0.105797 Converged=NO (449 cycles 934 points).  
Energy=37.835190 kcal/mol Gradient=0.094106 Converged=NO (450 cycles 936 points).  
Energy=37.833282 kcal/mol Gradient=0.106902 Converged=NO (451 cycles 938 points).  
Energy=37.830995 kcal/mol Gradient=0.096939 Converged=NO (452 cycles 940 points).  
Energy=37.828713 kcal/mol Gradient=0.110241 Converged=NO (453 cycles 942 points).  
Energy=37.826846 kcal/mol Gradient=0.102108 Converged=NO (454 cycles 944 points).  
Energy=37.825175 kcal/mol Gradient=0.095609 Converged=NO (455 cycles 946 points).  
Energy=37.823147 kcal/mol Gradient=0.101413 Converged=NO (456 cycles 948 points).  
Energy=37.821352 kcal/mol Gradient=0.085930 Converged=NO (457 cycles 950 points).  
Energy=37.819966 kcal/mol Gradient=0.099911 Converged=NO (458 cycles 952 points).  
Energy=37.817634 kcal/mol Gradient=0.097139 Converged=NO (459 cycles 954 points).  
Energy=37.815772 kcal/mol Gradient=0.103711 Converged=NO (460 cycles 956 points).  
Energy=37.814161 kcal/mol Gradient=0.098483 Converged=NO (461 cycles 958 points).  
Energy=37.812165 kcal/mol Gradient=0.098586 Converged=NO (462 cycles 960 points).  
Energy=37.810054 kcal/mol Gradient=0.111848 Converged=NO (463 cycles 962 points).  
Energy=37.807255 kcal/mol Gradient=0.110068 Converged=NO (464 cycles 964 points).  
Energy=37.805500 kcal/mol Gradient=0.097558 Converged=NO (465 cycles 966 points).  
Energy=37.803318 kcal/mol Gradient=0.105128 Converged=NO (466 cycles 968 points).  
Energy=37.801389 kcal/mol Gradient=0.107369 Converged=NO (467 cycles 970 points).  
Energy=37.799595 kcal/mol Gradient=0.100206 Converged=NO (468 cycles 972 points).  
Energy=37.796914 kcal/mol Gradient=0.113239 Converged=NO (469 cycles 975 points).  
Energy=37.794439 kcal/mol Gradient=0.110805 Converged=NO (470 cycles 977 points).  
Energy=37.792504 kcal/mol Gradient=0.101609 Converged=NO (471 cycles 979 points).  
Energy=37.790339 kcal/mol Gradient=0.097723 Converged=NO (472 cycles 981 points).  
Energy=37.788489 kcal/mol Gradient=0.113385 Converged=NO (473 cycles 983 points).  
Energy=37.786291 kcal/mol Gradient=0.109195 Converged=NO (474 cycles 985 points).  
Energy=37.784129 kcal/mol Gradient=0.097432 Converged=NO (475 cycles 987 points).

Energy=37.781823 kcal/mol Gradient=0.105070 Converged=NO (476 cycles 989 points).  
Energy=37.780032 kcal/mol Gradient=0.097898 Converged=NO (477 cycles 991 points).  
Energy=37.778056 kcal/mol Gradient=0.107241 Converged=NO (478 cycles 993 points).  
Energy=37.775964 kcal/mol Gradient=0.108967 Converged=NO (479 cycles 995 points).  
Energy=37.773476 kcal/mol Gradient=0.115806 Converged=NO (480 cycles 997 points).  
Energy=37.771631 kcal/mol Gradient=0.092043 Converged=NO (481 cycles 999 points).  
Energy=37.769970 kcal/mol Gradient=0.090068 Converged=NO (482 cycles 1001 points).  
Energy=37.767790 kcal/mol Gradient=0.105278 Converged=NO (483 cycles 1004 points).  
Energy=37.766157 kcal/mol Gradient=0.091644 Converged=NO (484 cycles 1006 points).  
Energy=37.764424 kcal/mol Gradient=0.101353 Converged=NO (485 cycles 1008 points).  
Energy=37.762214 kcal/mol Gradient=0.109352 Converged=NO (486 cycles 1010 points).  
Energy=37.760634 kcal/mol Gradient=0.090378 Converged=NO (487 cycles 1012 points).  
Energy=37.758541 kcal/mol Gradient=0.106155 Converged=NO (488 cycles 1014 points).  
Energy=37.756377 kcal/mol Gradient=0.087091 Converged=NO (489 cycles 1016 points).  
Energy=37.754793 kcal/mol Gradient=0.103750 Converged=NO (490 cycles 1018 points).  
Energy=37.753015 kcal/mol Gradient=0.089738 Converged=NO (491 cycles 1020 points).  
Energy=37.751666 kcal/mol Gradient=0.082803 Converged=NO (492 cycles 1022 points).  
Energy=37.750303 kcal/mol Gradient=0.092508 Converged=NO (493 cycles 1024 points).  
Energy=37.748880 kcal/mol Gradient=0.084397 Converged=NO (494 cycles 1026 points).  
Energy=37.747412 kcal/mol Gradient=0.077786 Converged=NO (495 cycles 1028 points).  
Energy=37.746089 kcal/mol Gradient=0.082332 Converged=NO (496 cycles 1030 points).  
Energy=37.744609 kcal/mol Gradient=0.099057 Converged=NO (497 cycles 1032 points).  
Energy=37.743219 kcal/mol Gradient=0.078003 Converged=NO (498 cycles 1034 points).  
Energy=37.741952 kcal/mol Gradient=0.083685 Converged=NO (499 cycles 1036 points).  
Energy=37.740770 kcal/mol Gradient=0.080190 Converged=NO (500 cycles 1038 points).  
Energy=37.739563 kcal/mol Gradient=0.069102 Converged=NO (501 cycles 1040 points).  
Energy=37.738663 kcal/mol Gradient=0.072402 Converged=NO (502 cycles 1042 points).  
Energy=37.737392 kcal/mol Gradient=0.078037 Converged=NO (503 cycles 1044 points).  
Energy=37.736417 kcal/mol Gradient=0.082849 Converged=NO (504 cycles 1046 points).  
Energy=37.735101 kcal/mol Gradient=0.075357 Converged=NO (505 cycles 1048 points).  
Energy=37.733950 kcal/mol Gradient=0.083896 Converged=NO (506 cycles 1050 points).  
Energy=37.732645 kcal/mol Gradient=0.082658 Converged=NO (507 cycles 1052 points).  
Energy=37.731446 kcal/mol Gradient=0.066385 Converged=NO (508 cycles 1054 points).  
Energy=37.730274 kcal/mol Gradient=0.088485 Converged=NO (509 cycles 1056 points).  
Energy=37.728793 kcal/mol Gradient=0.091224 Converged=NO (510 cycles 1058 points).  
Energy=37.727548 kcal/mol Gradient=0.079474 Converged=NO (511 cycles 1060 points).  
Energy=37.726334 kcal/mol Gradient=0.076176 Converged=NO (512 cycles 1062 points).  
Energy=37.725197 kcal/mol Gradient=0.079367 Converged=NO (513 cycles 1064 points).  
Energy=37.723941 kcal/mol Gradient=0.087618 Converged=NO (514 cycles 1066 points).  
Energy=37.722448 kcal/mol Gradient=0.076006 Converged=NO (515 cycles 1068 points).  
Energy=37.721182 kcal/mol Gradient=0.084353 Converged=NO (516 cycles 1070 points).  
Energy=37.720072 kcal/mol Gradient=0.081111 Converged=NO (517 cycles 1072 points).  
Energy=37.718969 kcal/mol Gradient=0.074834 Converged=NO (518 cycles 1074 points).  
Energy=37.717677 kcal/mol Gradient=0.079872 Converged=NO (519 cycles 1076 points).  
Energy=37.716523 kcal/mol Gradient=0.076204 Converged=NO (520 cycles 1078 points).  
Energy=37.715393 kcal/mol Gradient=0.081515 Converged=NO (521 cycles 1080 points).  
Energy=37.713914 kcal/mol Gradient=0.080024 Converged=NO (522 cycles 1082 points).  
Energy=37.712908 kcal/mol Gradient=0.081757 Converged=NO (523 cycles 1084 points).  
Energy=37.711491 kcal/mol Gradient=0.093903 Converged=NO (524 cycles 1086 points).  
Energy=37.709774 kcal/mol Gradient=0.089407 Converged=NO (525 cycles 1088 points).  
Energy=37.708318 kcal/mol Gradient=0.076260 Converged=NO (526 cycles 1090 points).  
Energy=37.707321 kcal/mol Gradient=0.081144 Converged=NO (527 cycles 1092 points).

Energy=37.706003 kcal/mol Gradient=0.071174 Converged=NO (528 cycles 1094 points).  
Energy=37.704904 kcal/mol Gradient=0.080115 Converged=NO (529 cycles 1096 points).  
Energy=37.703844 kcal/mol Gradient=0.080538 Converged=NO (530 cycles 1098 points).  
Energy=37.702786 kcal/mol Gradient=0.071124 Converged=NO (531 cycles 1100 points).  
Energy=37.701646 kcal/mol Gradient=0.070410 Converged=NO (532 cycles 1102 points).  
Energy=37.700660 kcal/mol Gradient=0.075749 Converged=NO (533 cycles 1104 points).  
Energy=37.699653 kcal/mol Gradient=0.069078 Converged=NO (534 cycles 1106 points).  
Energy=37.698747 kcal/mol Gradient=0.072383 Converged=NO (535 cycles 1108 points).  
Energy=37.697612 kcal/mol Gradient=0.078591 Converged=NO (536 cycles 1110 points).  
Energy=37.696828 kcal/mol Gradient=0.062438 Converged=NO (537 cycles 1112 points).  
Energy=37.695870 kcal/mol Gradient=0.070806 Converged=NO (538 cycles 1114 points).  
Energy=37.694909 kcal/mol Gradient=0.064091 Converged=NO (539 cycles 1116 points).  
Energy=37.693982 kcal/mol Gradient=0.077982 Converged=NO (540 cycles 1118 points).  
Energy=37.692978 kcal/mol Gradient=0.067091 Converged=NO (541 cycles 1120 points).  
Energy=37.692174 kcal/mol Gradient=0.062482 Converged=NO (542 cycles 1122 points).  
Energy=37.691538 kcal/mol Gradient=0.066491 Converged=NO (543 cycles 1124 points).  
Energy=37.690637 kcal/mol Gradient=0.060139 Converged=NO (544 cycles 1126 points).  
Energy=37.689790 kcal/mol Gradient=0.072947 Converged=NO (545 cycles 1128 points).  
Energy=37.688579 kcal/mol Gradient=0.073092 Converged=NO (546 cycles 1130 points).  
Energy=37.687796 kcal/mol Gradient=0.064495 Converged=NO (547 cycles 1132 points).  
Energy=37.686964 kcal/mol Gradient=0.072136 Converged=NO (548 cycles 1134 points).  
Energy=37.685846 kcal/mol Gradient=0.072865 Converged=NO (549 cycles 1136 points).  
Energy=37.685075 kcal/mol Gradient=0.071774 Converged=NO (550 cycles 1138 points).  
Energy=37.683722 kcal/mol Gradient=0.077080 Converged=NO (551 cycles 1141 points).  
Energy=37.682608 kcal/mol Gradient=0.066197 Converged=NO (552 cycles 1143 points).  
Energy=37.681642 kcal/mol Gradient=0.073811 Converged=NO (553 cycles 1145 points).  
Energy=37.680799 kcal/mol Gradient=0.073920 Converged=NO (554 cycles 1147 points).  
Energy=37.679557 kcal/mol Gradient=0.080751 Converged=NO (555 cycles 1149 points).  
Energy=37.678402 kcal/mol Gradient=0.077824 Converged=NO (556 cycles 1151 points).  
Energy=37.677387 kcal/mol Gradient=0.071767 Converged=NO (557 cycles 1153 points).  
Energy=37.676226 kcal/mol Gradient=0.075191 Converged=NO (558 cycles 1155 points).  
Energy=37.675024 kcal/mol Gradient=0.081746 Converged=NO (559 cycles 1157 points).  
Energy=37.673817 kcal/mol Gradient=0.082094 Converged=NO (560 cycles 1159 points).  
Energy=37.672705 kcal/mol Gradient=0.077133 Converged=NO (561 cycles 1161 points).  
Energy=37.671518 kcal/mol Gradient=0.080892 Converged=NO (562 cycles 1163 points).  
Energy=37.670340 kcal/mol Gradient=0.077063 Converged=NO (563 cycles 1165 points).  
Energy=37.669415 kcal/mol Gradient=0.069770 Converged=NO (564 cycles 1167 points).  
Energy=37.667875 kcal/mol Gradient=0.076889 Converged=NO (565 cycles 1170 points).  
Energy=37.666820 kcal/mol Gradient=0.080749 Converged=NO (566 cycles 1172 points).  
Energy=37.665827 kcal/mol Gradient=0.072462 Converged=NO (567 cycles 1174 points).  
Energy=37.664778 kcal/mol Gradient=0.071428 Converged=NO (568 cycles 1176 points).  
Energy=37.663868 kcal/mol Gradient=0.073399 Converged=NO (569 cycles 1178 points).  
Energy=37.662777 kcal/mol Gradient=0.073569 Converged=NO (570 cycles 1180 points).  
Energy=37.661815 kcal/mol Gradient=0.070984 Converged=NO (571 cycles 1182 points).  
Energy=37.660491 kcal/mol Gradient=0.077126 Converged=NO (572 cycles 1185 points).  
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Energy=37.657353 kcal/mol Gradient=0.071015 Converged=NO (575 cycles 1191 points).  
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Energy=37.655301 kcal/mol Gradient=0.076013 Converged=NO (577 cycles 1195 points).  
Energy=37.654242 kcal/mol Gradient=0.063044 Converged=NO (578 cycles 1197 points).  
Energy=37.653308 kcal/mol Gradient=0.077362 Converged=NO (579 cycles 1199 points).

Energy=37.652486 kcal/mol Gradient=0.060880 Converged=NO (580 cycles 1201 points).  
Energy=37.651788 kcal/mol Gradient=0.066203 Converged=NO (581 cycles 1203 points).  
Energy=37.650801 kcal/mol Gradient=0.066086 Converged=NO (582 cycles 1205 points).  
Energy=37.650126 kcal/mol Gradient=0.061218 Converged=NO (583 cycles 1207 points).  
Energy=37.649292 kcal/mol Gradient=0.063168 Converged=NO (584 cycles 1209 points).  
Energy=37.648521 kcal/mol Gradient=0.060516 Converged=NO (585 cycles 1211 points).  
Energy=37.647752 kcal/mol Gradient=0.073226 Converged=NO (586 cycles 1213 points).  
Energy=37.647001 kcal/mol Gradient=0.058975 Converged=NO (587 cycles 1215 points).  
Energy=37.646154 kcal/mol Gradient=0.057764 Converged=NO (588 cycles 1217 points).  
Energy=37.645490 kcal/mol Gradient=0.066034 Converged=NO (589 cycles 1219 points).  
Energy=37.644648 kcal/mol Gradient=0.062594 Converged=NO (590 cycles 1221 points).  
Energy=37.643905 kcal/mol Gradient=0.065188 Converged=NO (591 cycles 1223 points).  
Energy=37.643033 kcal/mol Gradient=0.066723 Converged=NO (592 cycles 1225 points).  
Energy=37.642368 kcal/mol Gradient=0.062174 Converged=NO (593 cycles 1227 points).  
Energy=37.641664 kcal/mol Gradient=0.056317 Converged=NO (594 cycles 1229 points).  
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Energy=37.638040 kcal/mol Gradient=0.063627 Converged=NO (599 cycles 1239 points).  
Energy=37.637469 kcal/mol Gradient=0.055050 Converged=NO (600 cycles 1241 points).  
Energy=37.636657 kcal/mol Gradient=0.061697 Converged=NO (601 cycles 1244 points).  
Energy=37.635889 kcal/mol Gradient=0.059075 Converged=NO (602 cycles 1246 points).  
Energy=37.635342 kcal/mol Gradient=0.057427 Converged=NO (603 cycles 1248 points).  
Energy=37.634654 kcal/mol Gradient=0.054086 Converged=NO (604 cycles 1250 points).  
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Energy=37.631726 kcal/mol Gradient=0.054724 Converged=NO (609 cycles 1260 points).  
Energy=37.631241 kcal/mol Gradient=0.057362 Converged=NO (610 cycles 1262 points).  
Energy=37.630505 kcal/mol Gradient=0.057050 Converged=NO (611 cycles 1264 points).  
Energy=37.629980 kcal/mol Gradient=0.058009 Converged=NO (612 cycles 1266 points).  
Energy=37.629339 kcal/mol Gradient=0.057663 Converged=NO (613 cycles 1268 points).  
Energy=37.628662 kcal/mol Gradient=0.055912 Converged=NO (614 cycles 1270 points).  
Energy=37.628025 kcal/mol Gradient=0.056382 Converged=NO (615 cycles 1272 points).  
Energy=37.627427 kcal/mol Gradient=0.059789 Converged=NO (616 cycles 1274 points).  
Energy=37.626799 kcal/mol Gradient=0.056283 Converged=NO (617 cycles 1276 points).  
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Energy=37.625626 kcal/mol Gradient=0.052379 Converged=NO (619 cycles 1280 points).  
Energy=37.625109 kcal/mol Gradient=0.053495 Converged=NO (620 cycles 1282 points).  
Energy=37.624431 kcal/mol Gradient=0.054990 Converged=NO (621 cycles 1284 points).  
Energy=37.623788 kcal/mol Gradient=0.056526 Converged=NO (622 cycles 1286 points).  
Energy=37.623268 kcal/mol Gradient=0.056963 Converged=NO (623 cycles 1288 points).  
Energy=37.622729 kcal/mol Gradient=0.049588 Converged=NO (624 cycles 1290 points).  
Energy=37.622189 kcal/mol Gradient=0.054202 Converged=NO (625 cycles 1292 points).  
Energy=37.621751 kcal/mol Gradient=0.050385 Converged=NO (626 cycles 1294 points).  
Energy=37.621092 kcal/mol Gradient=0.054435 Converged=NO (627 cycles 1297 points).  
Energy=37.620524 kcal/mol Gradient=0.050375 Converged=NO (628 cycles 1299 points).  
Energy=37.620059 kcal/mol Gradient=0.053605 Converged=NO (629 cycles 1301 points).  
Energy=37.619606 kcal/mol Gradient=0.046997 Converged=NO (630 cycles 1303 points).  
Energy=37.619223 kcal/mol Gradient=0.045486 Converged=NO (631 cycles 1305 points).

Energy=37.618750 kcal/mol Gradient=0.049141 Converged=NO (632 cycles 1307 points).  
Energy=37.618387 kcal/mol Gradient=0.041849 Converged=NO (633 cycles 1309 points).  
Energy=37.617955 kcal/mol Gradient=0.049273 Converged=NO (634 cycles 1311 points).  
Energy=37.617400 kcal/mol Gradient=0.053781 Converged=NO (635 cycles 1313 points).  
Energy=37.617018 kcal/mol Gradient=0.045394 Converged=NO (636 cycles 1315 points).  
Energy=37.616588 kcal/mol Gradient=0.048707 Converged=NO (637 cycles 1317 points).  
Energy=37.616126 kcal/mol Gradient=0.045275 Converged=NO (638 cycles 1319 points).  
Energy=37.615766 kcal/mol Gradient=0.047401 Converged=NO (639 cycles 1321 points).  
Energy=37.615295 kcal/mol Gradient=0.044545 Converged=NO (640 cycles 1323 points).  
Energy=37.614956 kcal/mol Gradient=0.041420 Converged=NO (641 cycles 1325 points).  
Energy=37.614563 kcal/mol Gradient=0.050484 Converged=NO (642 cycles 1327 points).  
Energy=37.614158 kcal/mol Gradient=0.048988 Converged=NO (643 cycles 1329 points).  
Energy=37.613677 kcal/mol Gradient=0.046609 Converged=NO (644 cycles 1331 points).  
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Energy=37.606336 kcal/mol Gradient=0.032422 Converged=NO (665 cycles 1373 points).  
Energy=37.606096 kcal/mol Gradient=0.042509 Converged=NO (666 cycles 1375 points).  
Energy=37.605800 kcal/mol Gradient=0.034414 Converged=NO (667 cycles 1377 points).  
Energy=37.605577 kcal/mol Gradient=0.037653 Converged=NO (668 cycles 1379 points).  
Energy=37.605311 kcal/mol Gradient=0.036227 Converged=NO (669 cycles 1381 points).  
Energy=37.605075 kcal/mol Gradient=0.034444 Converged=NO (670 cycles 1383 points).  
Energy=37.604752 kcal/mol Gradient=0.037447 Converged=NO (671 cycles 1385 points).  
Energy=37.604542 kcal/mol Gradient=0.036936 Converged=NO (672 cycles 1387 points).  
Energy=37.604245 kcal/mol Gradient=0.039079 Converged=NO (673 cycles 1389 points).  
Energy=37.604020 kcal/mol Gradient=0.030981 Converged=NO (674 cycles 1391 points).  
Energy=37.603829 kcal/mol Gradient=0.036958 Converged=NO (675 cycles 1393 points).  
Energy=37.603550 kcal/mol Gradient=0.035466 Converged=NO (676 cycles 1395 points).  
Energy=37.603294 kcal/mol Gradient=0.032158 Converged=NO (677 cycles 1397 points).  
Energy=37.603081 kcal/mol Gradient=0.037149 Converged=NO (678 cycles 1399 points).  
Energy=37.602840 kcal/mol Gradient=0.035590 Converged=NO (679 cycles 1401 points).  
Energy=37.602645 kcal/mol Gradient=0.032718 Converged=NO (680 cycles 1403 points).  
Energy=37.602361 kcal/mol Gradient=0.037967 Converged=NO (681 cycles 1405 points).  
Energy=37.602136 kcal/mol Gradient=0.035694 Converged=NO (682 cycles 1407 points).  
Energy=37.601864 kcal/mol Gradient=0.035378 Converged=NO (683 cycles 1409 points).

Energy=37.601601 kcal/mol Gradient=0.035708 Converged=NO (684 cycles 1411 points).  
Energy=37.601363 kcal/mol Gradient=0.040686 Converged=NO (685 cycles 1413 points).  
Energy=37.601070 kcal/mol Gradient=0.038777 Converged=NO (686 cycles 1415 points).  
Energy=37.600773 kcal/mol Gradient=0.039308 Converged=NO (687 cycles 1417 points).  
Energy=37.600517 kcal/mol Gradient=0.030734 Converged=NO (688 cycles 1419 points).  
Energy=37.600354 kcal/mol Gradient=0.032284 Converged=NO (689 cycles 1421 points).  
Energy=37.600102 kcal/mol Gradient=0.034933 Converged=NO (690 cycles 1423 points).  
Energy=37.599867 kcal/mol Gradient=0.032997 Converged=NO (691 cycles 1425 points).  
Energy=37.599712 kcal/mol Gradient=0.032427 Converged=NO (692 cycles 1427 points).  
Energy=37.599500 kcal/mol Gradient=0.027890 Converged=NO (693 cycles 1429 points).  
Energy=37.599326 kcal/mol Gradient=0.032107 Converged=NO (694 cycles 1431 points).  
Energy=37.599153 kcal/mol Gradient=0.029961 Converged=NO (695 cycles 1433 points).  
Energy=37.598974 kcal/mol Gradient=0.030438 Converged=NO (696 cycles 1435 points).  
Energy=37.598758 kcal/mol Gradient=0.033078 Converged=NO (697 cycles 1437 points).  
Energy=37.598594 kcal/mol Gradient=0.028641 Converged=NO (698 cycles 1439 points).  
Energy=37.598477 kcal/mol Gradient=0.026283 Converged=NO (699 cycles 1441 points).  
Energy=37.598262 kcal/mol Gradient=0.030953 Converged=NO (700 cycles 1444 points).  
Energy=37.598107 kcal/mol Gradient=0.027519 Converged=NO (701 cycles 1446 points).  
Energy=37.597950 kcal/mol Gradient=0.029394 Converged=NO (702 cycles 1448 points).  
Energy=37.597801 kcal/mol Gradient=0.028726 Converged=NO (703 cycles 1450 points).  
Energy=37.597637 kcal/mol Gradient=0.028733 Converged=NO (704 cycles 1452 points).  
Energy=37.597496 kcal/mol Gradient=0.031023 Converged=NO (705 cycles 1454 points).  
Energy=37.597311 kcal/mol Gradient=0.027989 Converged=NO (706 cycles 1456 points).  
Energy=37.597144 kcal/mol Gradient=0.027965 Converged=NO (707 cycles 1458 points).  
Energy=37.596997 kcal/mol Gradient=0.029011 Converged=NO (708 cycles 1460 points).  
Energy=37.596846 kcal/mol Gradient=0.027791 Converged=NO (709 cycles 1462 points).  
Energy=37.596702 kcal/mol Gradient=0.026128 Converged=NO (710 cycles 1464 points).  
Energy=37.596579 kcal/mol Gradient=0.029031 Converged=NO (711 cycles 1466 points).  
Energy=37.596428 kcal/mol Gradient=0.027245 Converged=NO (712 cycles 1468 points).  
Energy=37.596286 kcal/mol Gradient=0.025573 Converged=NO (713 cycles 1470 points).  
Energy=37.596119 kcal/mol Gradient=0.028067 Converged=NO (714 cycles 1472 points).  
Energy=37.595998 kcal/mol Gradient=0.026197 Converged=NO (715 cycles 1474 points).  
Energy=37.595868 kcal/mol Gradient=0.026778 Converged=NO (716 cycles 1476 points).  
Energy=37.595719 kcal/mol Gradient=0.026724 Converged=NO (717 cycles 1478 points).  
Energy=37.595615 kcal/mol Gradient=0.025180 Converged=NO (718 cycles 1480 points).  
Energy=37.595488 kcal/mol Gradient=0.024901 Converged=NO (719 cycles 1483 points).  
Energy=37.595334 kcal/mol Gradient=0.026408 Converged=NO (720 cycles 1485 points).  
Energy=37.595187 kcal/mol Gradient=0.028849 Converged=NO (721 cycles 1487 points).  
Energy=37.595053 kcal/mol Gradient=0.026347 Converged=NO (722 cycles 1489 points).  
Energy=37.594938 kcal/mol Gradient=0.024681 Converged=NO (723 cycles 1491 points).  
Energy=37.594820 kcal/mol Gradient=0.026066 Converged=NO (724 cycles 1493 points).  
Energy=37.594700 kcal/mol Gradient=0.022515 Converged=NO (725 cycles 1495 points).  
Energy=37.594608 kcal/mol Gradient=0.023733 Converged=NO (726 cycles 1497 points).  
Energy=37.594460 kcal/mol Gradient=0.023647 Converged=NO (727 cycles 1499 points).  
Energy=37.594373 kcal/mol Gradient=0.024200 Converged=NO (728 cycles 1501 points).  
Energy=37.594265 kcal/mol Gradient=0.022715 Converged=NO (729 cycles 1503 points).  
Energy=37.594167 kcal/mol Gradient=0.024114 Converged=NO (730 cycles 1505 points).  
Energy=37.594047 kcal/mol Gradient=0.026882 Converged=NO (731 cycles 1507 points).  
Energy=37.593919 kcal/mol Gradient=0.024621 Converged=NO (732 cycles 1509 points).  
Energy=37.593770 kcal/mol Gradient=0.025527 Converged=NO (733 cycles 1511 points).  
Energy=37.593662 kcal/mol Gradient=0.022729 Converged=NO (734 cycles 1513 points).  
Energy=37.593577 kcal/mol Gradient=0.023398 Converged=NO (735 cycles 1515 points).



Energy=37.593477 kcal/mol Gradient=0.022414 Converged=NO (736 cycles 1517 points).  
Energy=37.593369 kcal/mol Gradient=0.024662 Converged=NO (737 cycles 1519 points).  
Energy=37.593249 kcal/mol Gradient=0.025066 Converged=NO (738 cycles 1521 points).  
Energy=37.593142 kcal/mol Gradient=0.022626 Converged=NO (739 cycles 1523 points).  
Energy=37.593035 kcal/mol Gradient=0.021944 Converged=NO (740 cycles 1525 points).  
Energy=37.592942 kcal/mol Gradient=0.023835 Converged=NO (741 cycles 1527 points).  
Energy=37.592856 kcal/mol Gradient=0.022951 Converged=NO (742 cycles 1529 points).  
Energy=37.592735 kcal/mol Gradient=0.021017 Converged=NO (743 cycles 1531 points).  
Energy=37.592657 kcal/mol Gradient=0.021935 Converged=NO (744 cycles 1533 points).  
Energy=37.592566 kcal/mol Gradient=0.020914 Converged=NO (745 cycles 1535 points).  
Energy=37.592474 kcal/mol Gradient=0.020707 Converged=NO (746 cycles 1537 points).  
Energy=37.592391 kcal/mol Gradient=0.023695 Converged=NO (747 cycles 1539 points).  
Energy=37.592288 kcal/mol Gradient=0.023211 Converged=NO (748 cycles 1541 points).  
Energy=37.592203 kcal/mol Gradient=0.020849 Converged=NO (749 cycles 1543 points).  
Energy=37.592096 kcal/mol Gradient=0.022217 Converged=NO (750 cycles 1545 points).  
Energy=37.592017 kcal/mol Gradient=0.021651 Converged=NO (751 cycles 1547 points).  
Energy=37.591913 kcal/mol Gradient=0.024437 Converged=NO (752 cycles 1549 points).  
Energy=37.591786 kcal/mol Gradient=0.022183 Converged=NO (753 cycles 1551 points).  
Energy=37.591706 kcal/mol Gradient=0.023372 Converged=NO (754 cycles 1553 points).  
Energy=37.591609 kcal/mol Gradient=0.023283 Converged=NO (755 cycles 1555 points).  
Energy=37.591503 kcal/mol Gradient=0.019907 Converged=NO (756 cycles 1557 points).  
Energy=37.591403 kcal/mol Gradient=0.024968 Converged=NO (757 cycles 1559 points).  
Energy=37.591284 kcal/mol Gradient=0.024490 Converged=NO (758 cycles 1561 points).  
Energy=37.591187 kcal/mol Gradient=0.022889 Converged=NO (759 cycles 1563 points).  
Energy=37.591072 kcal/mol Gradient=0.024405 Converged=NO (760 cycles 1565 points).  
Energy=37.590988 kcal/mol Gradient=0.021036 Converged=NO (761 cycles 1567 points).  
Energy=37.590895 kcal/mol Gradient=0.023640 Converged=NO (762 cycles 1569 points).  
Energy=37.590785 kcal/mol Gradient=0.020233 Converged=NO (763 cycles 1571 points).  
Energy=37.590695 kcal/mol Gradient=0.022954 Converged=NO (764 cycles 1573 points).  
Energy=37.590603 kcal/mol Gradient=0.022500 Converged=NO (765 cycles 1575 points).  
Energy=37.590511 kcal/mol Gradient=0.020297 Converged=NO (766 cycles 1577 points).  
Energy=37.590437 kcal/mol Gradient=0.022669 Converged=NO (767 cycles 1579 points).  
Energy=37.590344 kcal/mol Gradient=0.021604 Converged=NO (768 cycles 1581 points).  
Energy=37.590252 kcal/mol Gradient=0.018965 Converged=NO (769 cycles 1583 points).  
Energy=37.590182 kcal/mol Gradient=0.019009 Converged=NO (770 cycles 1585 points).  
Energy=37.590106 kcal/mol Gradient=0.021250 Converged=NO (771 cycles 1587 points).  
Energy=37.590028 kcal/mol Gradient=0.021992 Converged=NO (772 cycles 1589 points).  
Energy=37.589934 kcal/mol Gradient=0.020478 Converged=NO (773 cycles 1591 points).  
Energy=37.589855 kcal/mol Gradient=0.023209 Converged=NO (774 cycles 1593 points).  
Energy=37.589756 kcal/mol Gradient=0.020918 Converged=NO (775 cycles 1595 points).  
Energy=37.589665 kcal/mol Gradient=0.020487 Converged=NO (776 cycles 1597 points).  
Energy=37.589572 kcal/mol Gradient=0.021803 Converged=NO (777 cycles 1599 points).  
Energy=37.589496 kcal/mol Gradient=0.021480 Converged=NO (778 cycles 1601 points).  
Energy=37.589410 kcal/mol Gradient=0.021865 Converged=NO (779 cycles 1603 points).  
Energy=37.589314 kcal/mol Gradient=0.022537 Converged=NO (780 cycles 1605 points).  
Energy=37.589219 kcal/mol Gradient=0.023163 Converged=NO (781 cycles 1607 points).  
Energy=37.589116 kcal/mol Gradient=0.022575 Converged=NO (782 cycles 1609 points).  
Energy=37.588998 kcal/mol Gradient=0.023826 Converged=NO (783 cycles 1611 points).  
Energy=37.588896 kcal/mol Gradient=0.024874 Converged=NO (784 cycles 1613 points).  
Energy=37.588783 kcal/mol Gradient=0.025356 Converged=NO (785 cycles 1615 points).  
Energy=37.588673 kcal/mol Gradient=0.023729 Converged=NO (786 cycles 1617 points).  
Energy=37.588555 kcal/mol Gradient=0.023130 Converged=NO (787 cycles 1619 points).

Energy=37.588478 kcal/mol Gradient=0.022252 Converged=NO (788 cycles 1621 points).  
Energy=37.588306 kcal/mol Gradient=0.024513 Converged=NO (789 cycles 1624 points).  
Energy=37.588207 kcal/mol Gradient=0.023197 Converged=NO (790 cycles 1626 points).  
Energy=37.588120 kcal/mol Gradient=0.023801 Converged=NO (791 cycles 1628 points).  
Energy=37.588003 kcal/mol Gradient=0.023864 Converged=NO (792 cycles 1630 points).  
Energy=37.587893 kcal/mol Gradient=0.024447 Converged=NO (793 cycles 1632 points).  
Energy=37.587771 kcal/mol Gradient=0.025389 Converged=NO (794 cycles 1634 points).  
Energy=37.587669 kcal/mol Gradient=0.021216 Converged=NO (795 cycles 1636 points).  
Energy=37.587576 kcal/mol Gradient=0.020926 Converged=NO (796 cycles 1638 points).  
Energy=37.587506 kcal/mol Gradient=0.018250 Converged=NO (797 cycles 1640 points).  
Energy=37.587452 kcal/mol Gradient=0.019569 Converged=NO (798 cycles 1642 points).  
Energy=37.587367 kcal/mol Gradient=0.019347 Converged=NO (799 cycles 1644 points).  
Energy=37.587303 kcal/mol Gradient=0.016856 Converged=NO (800 cycles 1646 points).  
Energy=37.587249 kcal/mol Gradient=0.018426 Converged=NO (801 cycles 1648 points).  
Energy=37.587180 kcal/mol Gradient=0.017242 Converged=NO (802 cycles 1650 points).  
Energy=37.587115 kcal/mol Gradient=0.019174 Converged=NO (803 cycles 1652 points).  
Energy=37.587059 kcal/mol Gradient=0.018120 Converged=NO (804 cycles 1654 points).  
Energy=37.587004 kcal/mol Gradient=0.015577 Converged=NO (805 cycles 1656 points).  
Energy=37.586955 kcal/mol Gradient=0.014276 Converged=NO (806 cycles 1658 points).  
Energy=37.586917 kcal/mol Gradient=0.015896 Converged=NO (807 cycles 1660 points).  
Energy=37.586858 kcal/mol Gradient=0.017094 Converged=NO (808 cycles 1662 points).  
Energy=37.586812 kcal/mol Gradient=0.014559 Converged=NO (809 cycles 1664 points).  
Energy=37.586765 kcal/mol Gradient=0.016210 Converged=NO (810 cycles 1666 points).  
Energy=37.586732 kcal/mol Gradient=0.012990 Converged=NO (811 cycles 1668 points).  
Energy=37.586693 kcal/mol Gradient=0.013605 Converged=NO (812 cycles 1671 points).  
Energy=37.586641 kcal/mol Gradient=0.016677 Converged=NO (813 cycles 1673 points).  
Energy=37.586598 kcal/mol Gradient=0.014101 Converged=NO (814 cycles 1675 points).  
Energy=37.586561 kcal/mol Gradient=0.015281 Converged=NO (815 cycles 1677 points).  
Energy=37.586510 kcal/mol Gradient=0.014902 Converged=NO (816 cycles 1679 points).  
Energy=37.586480 kcal/mol Gradient=0.013229 Converged=NO (817 cycles 1681 points).  
Energy=37.586441 kcal/mol Gradient=0.014598 Converged=NO (818 cycles 1684 points).  
Energy=37.586398 kcal/mol Gradient=0.013970 Converged=NO (819 cycles 1686 points).  
Energy=37.586360 kcal/mol Gradient=0.013353 Converged=NO (820 cycles 1688 points).  
Energy=37.586329 kcal/mol Gradient=0.013550 Converged=NO (821 cycles 1690 points).  
Energy=37.586292 kcal/mol Gradient=0.014514 Converged=NO (822 cycles 1692 points).  
Energy=37.586254 kcal/mol Gradient=0.013649 Converged=NO (823 cycles 1694 points).  
Energy=37.586223 kcal/mol Gradient=0.014085 Converged=NO (824 cycles 1696 points).  
Energy=37.586180 kcal/mol Gradient=0.013490 Converged=NO (825 cycles 1698 points).  
Energy=37.586137 kcal/mol Gradient=0.014542 Converged=NO (826 cycles 1700 points).  
Energy=37.586102 kcal/mol Gradient=0.013922 Converged=NO (827 cycles 1702 points).  
Energy=37.586066 kcal/mol Gradient=0.013574 Converged=NO (828 cycles 1704 points).  
Energy=37.586033 kcal/mol Gradient=0.013957 Converged=NO (829 cycles 1706 points).  
Energy=37.585996 kcal/mol Gradient=0.013737 Converged=NO (830 cycles 1708 points).  
Energy=37.585967 kcal/mol Gradient=0.012666 Converged=NO (831 cycles 1710 points).  
Energy=37.585930 kcal/mol Gradient=0.011680 Converged=NO (832 cycles 1712 points).  
Energy=37.585900 kcal/mol Gradient=0.012733 Converged=NO (833 cycles 1714 points).  
Energy=37.585871 kcal/mol Gradient=0.013620 Converged=NO (834 cycles 1716 points).  
Energy=37.585838 kcal/mol Gradient=0.012788 Converged=NO (835 cycles 1718 points).  
Energy=37.585809 kcal/mol Gradient=0.012252 Converged=NO (836 cycles 1720 points).  
Energy=37.585780 kcal/mol Gradient=0.013249 Converged=NO (837 cycles 1722 points).  
Energy=37.585749 kcal/mol Gradient=0.011013 Converged=NO (838 cycles 1724 points).  
Energy=37.585721 kcal/mol Gradient=0.011875 Converged=NO (839 cycles 1726 points).

Energy=37.585696 kcal/mol Gradient=0.012302 Converged=NO (840 cycles 1728 points).  
Energy=37.585669 kcal/mol Gradient=0.012244 Converged=NO (841 cycles 1730 points).  
Energy=37.585642 kcal/mol Gradient=0.011490 Converged=NO (842 cycles 1732 points).  
Energy=37.585618 kcal/mol Gradient=0.011864 Converged=NO (843 cycles 1734 points).  
Energy=37.585588 kcal/mol Gradient=0.013631 Converged=NO (844 cycles 1736 points).  
Energy=37.585553 kcal/mol Gradient=0.010939 Converged=NO (845 cycles 1738 points).  
Energy=37.585528 kcal/mol Gradient=0.011707 Converged=NO (846 cycles 1740 points).  
Energy=37.585500 kcal/mol Gradient=0.013299 Converged=NO (847 cycles 1742 points).  
Energy=37.585476 kcal/mol Gradient=0.010323 Converged=NO (848 cycles 1744 points).  
Energy=37.585446 kcal/mol Gradient=0.013161 Converged=NO (849 cycles 1747 points).  
Energy=37.585420 kcal/mol Gradient=0.011398 Converged=NO (850 cycles 1749 points).  
Energy=37.585392 kcal/mol Gradient=0.012262 Converged=NO (851 cycles 1751 points).  
Energy=37.585361 kcal/mol Gradient=0.011635 Converged=NO (852 cycles 1753 points).  
Energy=37.585336 kcal/mol Gradient=0.011983 Converged=NO (853 cycles 1755 points).  
Energy=37.585312 kcal/mol Gradient=0.012177 Converged=NO (854 cycles 1757 points).  
Energy=37.585285 kcal/mol Gradient=0.010624 Converged=NO (855 cycles 1759 points).  
Energy=37.585263 kcal/mol Gradient=0.011122 Converged=NO (856 cycles 1761 points).  
Energy=37.585238 kcal/mol Gradient=0.011271 Converged=NO (857 cycles 1763 points).  
Energy=37.585216 kcal/mol Gradient=0.010115 Converged=NO (858 cycles 1765 points).  
Energy=37.585194 kcal/mol Gradient=0.010475 Converged=NO (859 cycles 1767 points).  
Energy=37.585176 kcal/mol Gradient=0.010831 Converged=NO (860 cycles 1769 points).  
Energy=37.585155 kcal/mol Gradient=0.010409 Converged=NO (861 cycles 1771 points).  
Energy=37.585133 kcal/mol Gradient=0.010144 Converged=NO (862 cycles 1773 points).  
Energy=37.585111 kcal/mol Gradient=0.011705 Converged=NO (863 cycles 1775 points).  
Energy=37.585088 kcal/mol Gradient=0.009352 Converged=NO (864 cycles 1777 points).  
Energy=37.585088 kcal/mol Gradient=0.009352 Converged=YES (864 cycles 1777 points).

Bond = 1.98755 Angle = 8.78296 Dihedral = 41.8076 Vdw = 4.14276 Electrostatic = -19.1358.