Electronic Supplementary Information

Intramolecular axial α/β-coordination of the 13^2-terminal pyridyl group to the central zinc atom in chlorophyll-*a* derivatives

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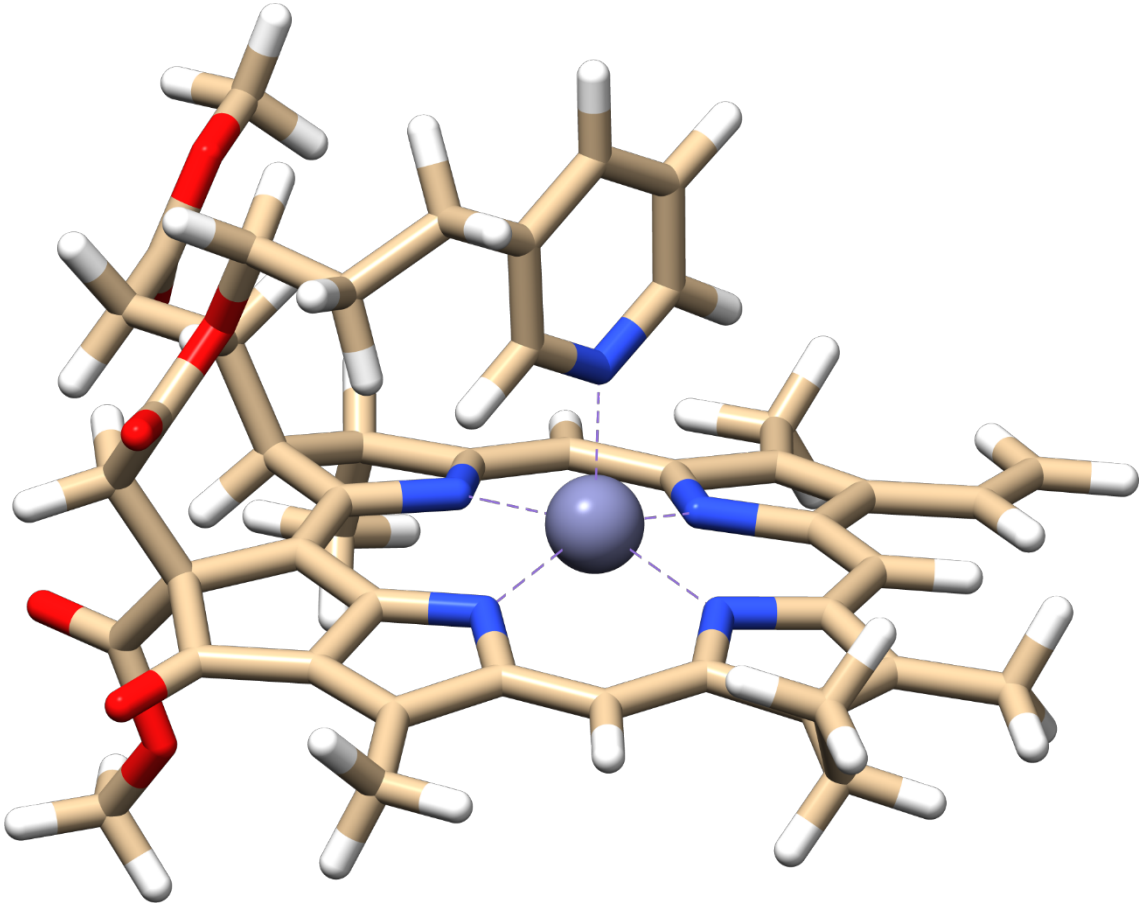
Table S1. Optimized molecular configuration image and its Cartesian coordinates of **Zn-4($C_{1,3}$)** (MM+/PM3).[a]



106116 0 0 0 0 0 0 0 0999 V2000

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71.0524	15.2480	-18.2655	O	0	0	0	0	0	0	0	0	0	0
70.7229	13.0649	-18.5331	O	0	0	0	0	0	0	0	0	0	0
68.6810	15.3417	-19.3581	H	0	0	0	0	0	0	0	0	0	0
68.2009	13.6795	-18.9842	H	0	0	0	0	0	0	0	0	0	0
72.4354	15.0208	-18.1077	C	0	0	0	0	0	0	0	0	0	0
72.8776	14.5598	-18.9974	H	0	0	0	0	0	0	0	0	0	0
72.6474	14.4036	-17.2280	H	0	0	0	0	0	0	0	0	0	0
69.1304	13.9544	-11.7186	C	0	0	0	0	0	0	0	0	0	0
68.0057	14.5281	-11.2012	N	0	0	0	0	0	0	0	0	0	0
68.1759	14.6267	-9.7785	C	0	0	0	0	0	0	0	0	0	0
69.5235	14.1043	-9.4545	C	0	0	0	0	0	0	0	0	0	0
67.2574	15.0523	-8.8766	C	0	0	0	0	0	0	0	0	0	0
65.9076	15.4149	-9.1725	C	0	0	0	0	0	0	0	0	0	0
65.3461	15.4529	-10.4221	N	0	0	0	0	0	0	0	0	0	0
63.9608	15.6901	-10.2734	C	0	0	0	0	0	0	0	0	0	0

63.6925	15.8692	-8.8625	C	0	0	0	0	0	0	0	0	0	0	0	0
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63.0068	15.6377	-11.2914	C	0	0	0	0	0	0	0	0	0	0	0	0
63.2733	15.3596	-12.6186	C	0	0	0	0	0	0	0	0	0	0	0	0
64.5914	15.1349	-13.1422	N	0	0	0	0	0	0	0	0	0	0	0	0
64.4473	14.8992	-14.4564	C	0	0	0	0	0	0	0	0	0	0	0	0
63.0506	14.9298	-14.8397	C	0	0	0	0	0	0	0	0	0	0	0	0
62.3128	15.2144	-13.7091	C	0	0	0	0	0	0	0	0	0	0	0	0
65.3292	14.5951	-15.5523	C	0	0	0	0	0	0	0	0	0	0	0	0
66.6570	14.3718	-15.3596	C	0	0	0	0	0	0	0	0	0	0	0	0
67.2571	14.4405	-14.0610	N	0	0	0	0	0	0	0	0	0	0	0	0
68.4843	13.8299	-14.1086	C	0	0	0	0	0	0	0	0	0	0	0	0
68.8215	13.3349	-15.5043	C	0	0	0	0	0	0	0	0	0	0	0	0
67.6752	13.8988	-16.3804	C	0	0	0	0	0	0	0	0	0	0	0	0
69.3689	13.6394	-13.0614	C	0	0	0	0	0	0	0	0	0	0	0	0
69.9945	14.0869	-8.0897	C	0	0	0	0	0	0	0	0	0	0	0	0
67.5596	15.0666	-7.8135	H	0	0	0	0	0	0	0	0	0	0	0	0
62.3834	16.1501	-8.2315	C	0	0	0	0	0	0	0	0	0	0	0	0
61.9522	15.8060	-11.0131	H	0	0	0	0	0	0	0	0	0	0	0	0
62.9506	14.6152	-16.2601	C	0	0	0	0	0	0	0	0	0	0	0	0
60.8568	15.3481	-13.5792	C	0	0	0	0	0	0	0	0	0	0	0	0
64.4402	14.4660	-16.7885	C	0	0	0	0	0	0	0	0	0	0	0	0
69.8095	13.7521	-15.8173	H	0	0	0	0	0	0	0	0	0	0	0	0
67.2268	13.0914	-17.0108	H	0	0	0	0	0	0	0	0	0	0	0	0
70.3387	13.1570	-13.2723	H	0	0	0	0	0	0	0	0	0	0	0	0
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61.9061	17.5623	-8.4991	C	0	0	0	0	0	0	0	0	0	0	0	0
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62.4899	15.9858	-7.1340	H	0	0	0	0	0	0	0	0	0	0	0	0
61.6333	15.4156	-8.5852	H	0	0	0	0	0	0	0	0	0	0	0	0
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60.4708	16.1181	-14.2612	H	0	0	0	0	0	0	0	0	0	0	0	0
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61.7581	17.7442	-9.5721	H	0	0	0	0	0	0	0	0	0	0	0	0
62.6262	18.3078	-8.1383	H	0	0	0	0	0	0	0	0	0	0	0	0
60.9498	17.7566	-7.9968	H	0	0	0	0	0	0	0	0	0	0	0	0
71.4013	13.0582	-10.8717	C	0	0	0	0	0	0	0	0	0	0	0	0
71.5127	12.1258	-10.3008	H	0	0	0	0	0	0	0	0	0	0	0	0
71.5171	12.8153	-11.9423	H	0	0	0	0	0	0	0	0	0	0	0	0
68.1563	15.0369	-17.2819	C	0	0	0	0	0	0	0	0	0	0	0	0
68.8648	15.6944	-16.7397	H	0	0	0	0	0	0	0	0	0	0	0	0
67.2892	15.6875	-17.5311	H	0	0	0	0	0	0	0	0	0	0	0	0
67.9368	11.3502	-15.3030	H	0	0	0	0	0	0	0	0	0	0	0	0
69.6536	11.4327	-14.8782	H	0	0	0	0	0	0	0	0	0	0	0	0
69.1577	11.4854	-16.5807	H	0	0	0	0	0	0	0	0	0	0	0	0
69.2464	14.4529	-7.3634	H	0	0	0	0	0	0	0	0	0	0	0	0
71.1961	13.6835	-7.6813	C	0	0	0	0	0	0	0	0	0	0	0	0
66.4397	15.3116	-12.2416	Zn	0	0	0	0	0	0	0	0	0	0	0	0
72.2256	13.7272	-10.5877	H	0	0	0	0	0	0	0	0	0	0	0	0
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71.4815	13.6978	-6.6337	H	0	0	0	0	0	0	0	0	0	0	0	0
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   65.7020    16.6053    -6.4381 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.0961    15.8619    -6.2286 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.5522    14.8404    -6.3452 H  0  0  0  0  0  0  0  0  0  0  0  0
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   63.6756    10.6078   -18.0718 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.7330    10.1652   -16.3296 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.2574    10.4198   -17.2492 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.1658    18.0827   -13.4176 C  0  0  0  0  0  0  0  0  0  0  0  0
   68.0921    17.8638   -12.0940 C  0  0  0  0  0  0  0  0  0  0  0  0
   66.4953    19.4034   -13.7490 C  0  0  0  0  0  0  0  0  0  0  0  0
   68.4693    19.1747   -12.3906 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.6707    19.9490   -13.2256 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.9583    20.9787   -13.4684 H  0  0  0  0  0  0  0  0  0  0  0  0
   69.3914    19.5844   -11.9648 H  0  0  0  0  0  0  0  0  0  0  0  0
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   65.2464    17.6189   -13.8281 H  0  0  0  0  0  0  0  0  0  0  0  0
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   64.7211    19.4418   -15.5680 C  0  0  0  0  0  0  0  0  0  0  0  0
   65.4524    19.0484   -16.8550 C  0  0  0  0  0  0  0  0  0  0  0  0
   66.1964    20.9823   -15.1622 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.9476    20.8209   -13.9220 H  0  0  0  0  0  0  0  0  0  0  0  0
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   64.4179    16.9566   -17.4794 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.7068    15.5212   -17.8704 C  0  0  0  0  0  0  0  0  0  0  0  0
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   63.8323    20.0498   -15.8286 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.3156    18.5409   -15.0526 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.5282    19.2994   -16.8250 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.0073    19.5485   -17.7352 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.3599    17.5458   -17.5470 O  0  0  0  0  0  0  0  0  0  0  0  0
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 1  5  1  0  0  0  0
 1  6  1  0  0  0  0
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 7 72  1  0  0  0  0
10 11  1  0  0  0  0
10 32  1  0  0  0  0
10 43  2  0  0  0  0
11 12  1  0  0  0  0
11 67  1  0  0  0  0
12 13  2  0  0  0  0
12 14  1  0  0  0  0
13 33  1  0  0  0  0
13 43  1  0  0  0  0
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14	34	1	0	0	0	0
15	16	1	0	0	0	0
15	19	1	0	0	0	0
16	17	2	0	0	0	0
16	67	1	0	0	0	0
17	18	1	0	0	0	0
17	20	1	0	0	0	0
18	19	2	0	0	0	0
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21	25	1	0	0	0	0
22	23	1	0	0	0	0
22	67	1	0	0	0	0
23	24	1	0	0	0	0
23	26	2	0	0	0	0
24	25	2	0	0	0	0
24	37	1	0	0	0	0
25	38	1	0	0	0	0
26	27	1	0	0	0	0
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27	31	1	0	0	0	0
28	29	1	0	0	0	0
28	67	1	0	0	0	0
29	30	1	0	0	0	0
29	32	2	0	0	0	0
30	31	1	0	0	0	0
30	40	1	0	0	0	0
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35	46	1	0	0	0	0
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37	39	1	0	0	0	0
37	48	2	0	0	0	0
38	49	1	0	0	0	0
38	50	1	0	0	0	0
38	51	1	0	0	0	0
39	52	1	0	0	0	0
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43	56	1	0	0	0	0
44	53	1	0	0	0	0
44	54	1	0	0	0	0
44	55	1	0	0	0	0
45	62	1	0	0	0	0
45	63	1	0	0	0	0

```
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 52 77    1    0    0    0    0
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 56 57    1    0    0    0    0
 56 58    1    0    0    0    0
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 59 60    1    0    0    0    0
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 71 74    1    0    0    0    0
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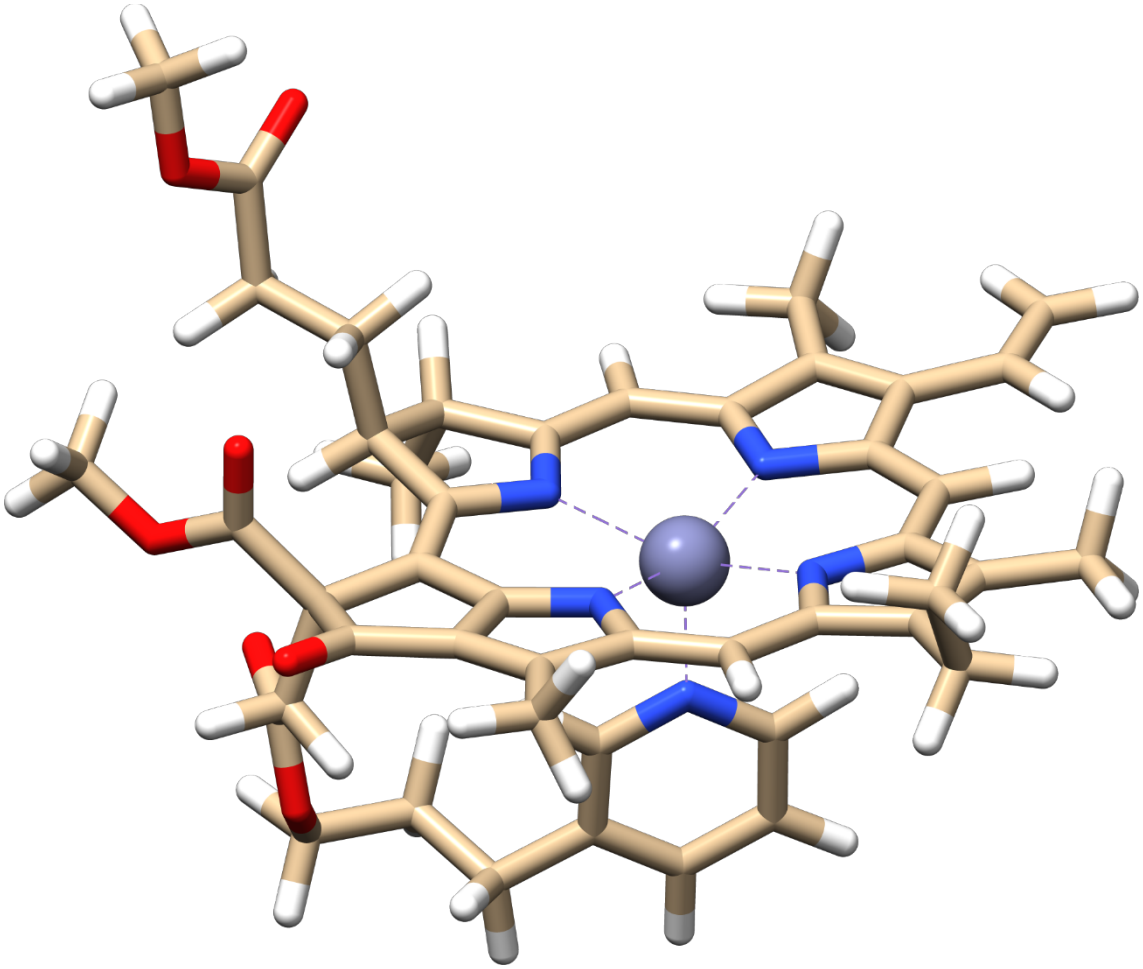
 99101    1    0    0    0    0
M    END
```

[a] The MM+/PM3 calculations were performed until the RMS gradient reached a value below 0.01 kcal $Å^{-1}$ mol^{-1} by using Polak-Ribiere algorithm.

Table S2. Optimized molecular configuration image and its Cartesian coordinates of **Zn-4'($C_{1,3}$)** (MM+/PM3).[a]



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69.8654	15.5572	-16.5716	C	0	0	0	0	0	0	0	0	0	0	0
71.1757	16.0229	-15.9785	C	0	0	0	0	0	0	0	0	0	0	0
71.7060	17.1043	-16.6251	O	0	0	0	0	0	0	0	0	0	0	0
71.7810	15.5438	-15.0395	O	0	0	0	0	0	0	0	0	0	0	0
69.7527	15.9247	-17.6187	H	0	0	0	0	0	0	0	0	0	0	0
69.8766	14.4502	-16.6338	H	0	0	0	0	0	0	0	0	0	0	0
72.8905	17.6837	-16.1244	C	0	0	0	0	0	0	0	0	0	0	0
73.7359	16.9896	-16.1788	H	0	0	0	0	0	0	0	0	0	0	0
72.7691	18.0373	-15.0949	H	0	0	0	0	0	0	0	0	0	0	0
65.5122	13.6005	-12.0358	C	0	0	0	0	0	0	0	0	0	0	0
64.6817	14.6460	-11.7888	N	0	0	0	0	0	0	0	0	0	0	0
64.1558	14.4919	-10.4607	C	0	0	0	0	0	0	0	0	0	0	0
64.7168	13.2393	-9.9069	C	0	0	0	0	0	0	0	0	0	0	0
63.3311	15.3505	-9.8110	C	0	0	0	0	0	0	0	0	0	0	0
62.8620	16.6005	-10.3163	C	0	0	0	0	0	0	0	0	0	0	0

63.1236	17.1145	-11.5641	N	0	0	0	0	0	0	0	0	0	0	0	0
62.5704	18.4082	-11.6302	C	0	0	0	0	0	0	0	0	0	0	0	0
61.9153	18.6759	-10.3699	C	0	0	0	0	0	0	0	0	0	0	0	0
62.0921	17.5623	-9.5632	C	0	0	0	0	0	0	0	0	0	0	0	0
62.6929	19.3064	-12.6991	C	0	0	0	0	0	0	0	0	0	0	0	0
63.4021	19.0720	-13.8569	C	0	0	0	0	0	0	0	0	0	0	0	0
64.0797	17.8352	-14.1416	N	0	0	0	0	0	0	0	0	0	0	0	0
64.6981	17.9934	-15.3215	C	0	0	0	0	0	0	0	0	0	0	0	0
64.4538	19.3209	-15.8578	C	0	0	0	0	0	0	0	0	0	0	0	0
63.6563	19.9973	-14.9614	C	0	0	0	0	0	0	0	0	0	0	0	0
65.6051	17.2185	-16.1256	C	0	0	0	0	0	0	0	0	0	0	0	0
66.1851	16.0896	-15.6164	C	0	0	0	0	0	0	0	0	0	0	0	0
65.6856	15.4496	-14.4484	N	0	0	0	0	0	0	0	0	0	0	0	0
66.3507	14.2464	-14.2766	C	0	0	0	0	0	0	0	0	0	0	0	0
67.2902	13.9609	-15.4350	C	0	0	0	0	0	0	0	0	0	0	0	0
67.3949	15.3364	-16.1399	C	0	0	0	0	0	0	0	0	0	0	0	0
66.2586	13.3829	-13.2110	C	0	0	0	0	0	0	0	0	0	0	0	0
64.3654	12.8048	-8.5758	C	0	0	0	0	0	0	0	0	0	0	0	0
63.0226	15.0754	-8.7855	H	0	0	0	0	0	0	0	0	0	0	0	0
61.1784	19.9005	-9.9853	C	0	0	0	0	0	0	0	0	0	0	0	0
62.2042	20.2874	-12.5881	H	0	0	0	0	0	0	0	0	0	0	0	0
65.1675	19.4437	-17.1210	C	0	0	0	0	0	0	0	0	0	0	0	0
63.1475	21.3720	-15.0503	C	0	0	0	0	0	0	0	0	0	0	0	0
65.7594	17.9892	-17.4364	C	0	0	0	0	0	0	0	0	0	0	0	0
68.2834	13.6306	-15.0441	H	0	0	0	0	0	0	0	0	0	0	0	0
67.3586	15.2356	-17.2503	H	0	0	0	0	0	0	0	0	0	0	0	0
66.8462	12.4490	-13.2298	H	0	0	0	0	0	0	0	0	0	0	0	0
65.5429	12.7034	-10.8597	C	0	0	0	0	0	0	0	0	0	0	0	0
62.1062	21.0552	-9.6678	C	0	0	0	0	0	0	0	0	0	0	0	0
66.7504	12.8792	-16.3503	C	0	0	0	0	0	0	0	0	0	0	0	0
60.5584	19.6574	-9.0913	H	0	0	0	0	0	0	0	0	0	0	0	0
60.4718	20.1824	-10.7902	H	0	0	0	0	0	0	0	0	0	0	0	0
65.2892	20.4033	-17.8472	O	0	0	0	0	0	0	0	0	0	0	0	0
62.0487	21.3798	-15.0666	H	0	0	0	0	0	0	0	0	0	0	0	0
63.5033	21.8801	-15.9557	H	0	0	0	0	0	0	0	0	0	0	0	0
63.4692	21.9636	-14.1818	H	0	0	0	0	0	0	0	0	0	0	0	0
64.8044	17.4707	-18.5316	C	0	0	0	0	0	0	0	0	0	0	0	0
67.2017	18.1720	-17.8930	C	0	0	0	0	0	0	0	0	0	0	0	0
62.7112	21.3427	-10.5384	H	0	0	0	0	0	0	0	0	0	0	0	0
62.8020	20.8027	-8.8573	H	0	0	0	0	0	0	0	0	0	0	0	0
61.5394	21.9408	-9.3533	H	0	0	0	0	0	0	0	0	0	0	0	0
66.3574	11.4796	-10.8293	C	0	0	0	0	0	0	0	0	0	0	0	0
65.7342	10.5865	-10.6817	H	0	0	0	0	0	0	0	0	0	0	0	0
66.9038	11.3573	-11.7806	H	0	0	0	0	0	0	0	0	0	0	0	0
68.6950	16.0349	-15.7219	C	0	0	0	0	0	0	0	0	0	0	0	0
68.9016	15.8499	-14.6474	H	0	0	0	0	0	0	0	0	0	0	0	0
68.5869	17.1340	-15.8097	H	0	0	0	0	0	0	0	0	0	0	0	0
65.7873	13.1587	-16.8010	H	0	0	0	0	0	0	0	0	0	0	0	0
66.6008	11.9394	-15.8025	H	0	0	0	0	0	0	0	0	0	0	0	0
67.4500	12.6817	-17.1733	H	0	0	0	0	0	0	0	0	0	0	0	0
63.6857	13.5012	-8.0525	H	0	0	0	0	0	0	0	0	0	0	0	0
64.7827	11.6883	-7.9817	C	0	0	0	0	0	0	0	0	0	0	0	0
64.0524	16.0416	-13.1404	Zn	0	0	0	0	0	0	0	0	0	0	0	0
67.0974	11.5114	-10.0175	H	0	0	0	0	0	0	0	0	0	0	0	0

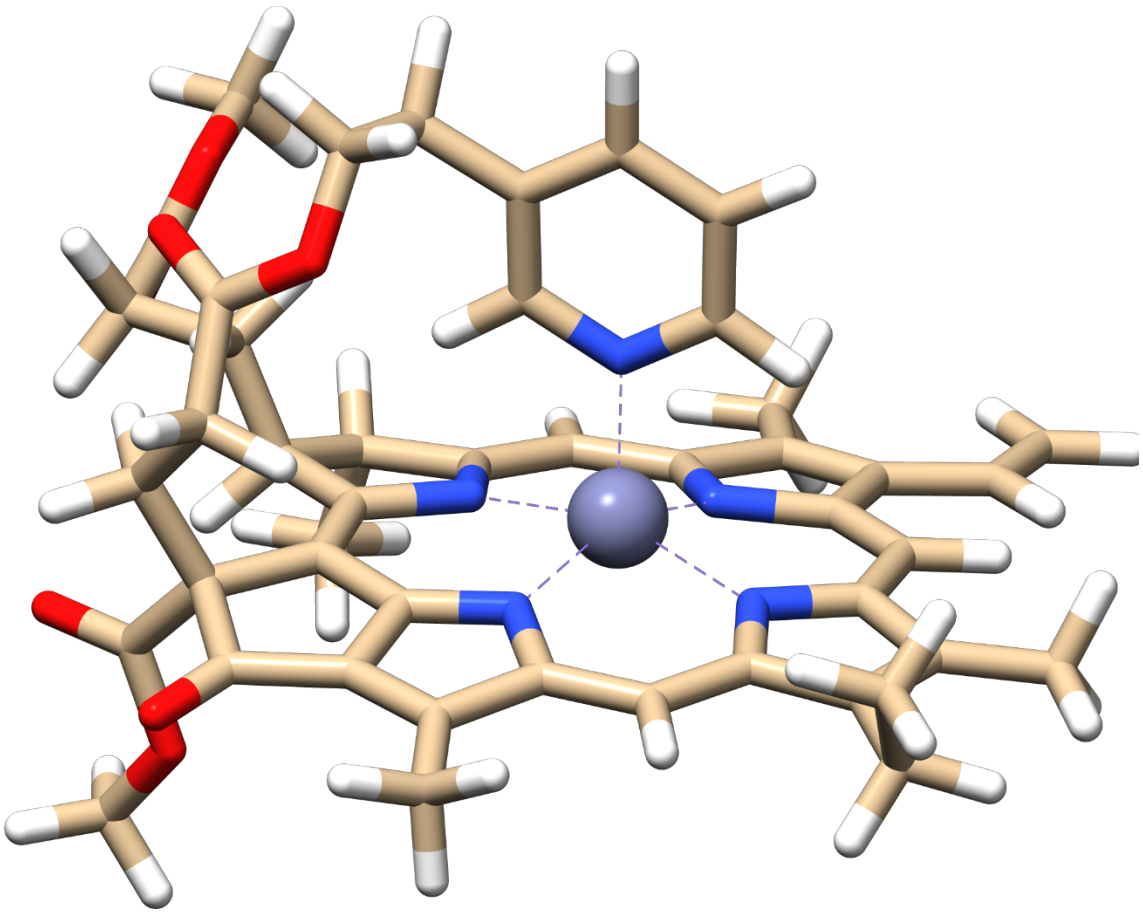
```
   65.4492    10.9666    -8.4462 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.4745    11.4236    -6.9746 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.5802    17.3972    -8.1936 C  0  0  0  0  0  0  0  0  0  0  0  0
   73.0447    18.5275   -16.8017 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.0302    16.4540    -8.0787 H  0  0  0  0  0  0  0  0  0  0  0  0
   62.3963    17.4005    -7.4591 H  0  0  0  0  0  0  0  0  0  0  0  0
   60.8960    18.2274    -7.9480 H  0  0  0  0  0  0  0  0  0  0  0  0
   68.0583    18.8404   -17.3490 O  0  0  0  0  0  0  0  0  0  0  0  0
   67.5186    17.5507   -19.0693 O  0  0  0  0  0  0  0  0  0  0  0  0
   68.8460    17.6245   -19.5413 C  0  0  0  0  0  0  0  0  0  0  0  0
   69.5324    17.0928   -18.8646 H  0  0  0  0  0  0  0  0  0  0  0  0
   68.7806    17.1068   -20.5015 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.0165    18.0050   -19.4825 H  0  0  0  0  0  0  0  0  0  0  0  0
   69.1855    18.6560   -19.6833 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.7743    17.7772   -18.2396 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.7682    15.9962   -18.8594 C  0  0  0  0  0  0  0  0  0  0  0  0
   63.5175    15.6364   -19.3038 O  0  0  0  0  0  0  0  0  0  0  0  0
   63.1869    14.2699   -19.4997 C  0  0  0  0  0  0  0  0  0  0  0  0
   62.7652    13.5888   -18.1984 C  0  0  0  0  0  0  0  0  0  0  0  0
   61.4837    14.1858   -17.6206 C  0  0  0  0  0  0  0  0  0  0  0  0
   60.6035    13.6282   -17.9990 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.3434    15.2293   -17.9722 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.4835    14.2044   -16.1279 C  0  0  0  0  0  0  0  0  0  0  0  0
   60.5264    13.5045   -15.3910 C  0  0  0  0  0  0  0  0  0  0  0  0
   60.5486    13.5777   -14.0008 C  0  0  0  0  0  0  0  0  0  0  0  0
   61.5311    14.3376   -13.3650 C  0  0  0  0  0  0  0  0  0  0  0  0
   62.4432    14.9604   -15.4398 C  0  0  0  0  0  0  0  0  0  0  0  0
   62.4690    15.0169   -14.0818 N  0  0  0  0  0  0  0  0  0  0  0  0
   63.2166    15.5398   -15.9744 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.5906    14.4206   -12.2686 H  0  0  0  0  0  0  0  0  0  0  0  0
   59.8025    13.0425   -13.4030 H  0  0  0  0  0  0  0  0  0  0  0  0
   59.7613    12.9067   -15.9012 H  0  0  0  0  0  0  0  0  0  0  0  0
   62.6224    12.5087   -18.3957 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.5963    13.6457   -17.4638 H  0  0  0  0  0  0  0  0  0  0  0  0
   62.3469    14.3579   -20.2118 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.0047    13.7115   -19.9928 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.6395    15.1530   -18.8455 O  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  5  1  0  0  0  0
 1  6  1  0  0  0  0
 1 60  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  2  0  0  0  0
 3  7  1  0  0  0  0
 7  8  1  0  0  0  0
 7  9  1  0  0  0  0
 7 73  1  0  0  0  0
10 11  1  0  0  0  0
10 32  1  0  0  0  0
10 43  2  0  0  0  0
11 12  1  0  0  0  0
11 68  1  0  0  0  0
12 13  2  0  0  0  0
12 14  1  0  0  0  0
```

13	33	1	0	0	0	0
13	43	1	0	0	0	0
14	15	2	0	0	0	0
14	34	1	0	0	0	0
15	16	1	0	0	0	0
15	19	1	0	0	0	0
16	17	2	0	0	0	0
16	68	1	0	0	0	0
17	18	1	0	0	0	0
17	20	1	0	0	0	0
18	19	2	0	0	0	0
18	35	1	0	0	0	0
19	72	1	0	0	0	0
20	21	2	0	0	0	0
20	36	1	0	0	0	0
21	22	1	0	0	0	0
21	25	1	0	0	0	0
22	23	1	0	0	0	0
22	68	1	0	0	0	0
23	24	1	0	0	0	0
23	26	2	0	0	0	0
24	25	2	0	0	0	0
24	37	1	0	0	0	0
25	38	1	0	0	0	0
26	27	1	0	0	0	0
26	39	1	0	0	0	0
27	28	2	0	0	0	0
27	31	1	0	0	0	0
28	29	1	0	0	0	0
28	68	1	0	0	0	0
29	30	1	0	0	0	0
29	32	2	0	0	0	0
30	31	1	0	0	0	0
30	40	1	0	0	0	0
30	45	1	0	0	0	0
31	41	1	0	0	0	0
31	60	1	0	0	0	0
32	42	1	0	0	0	0
33	66	1	0	0	0	0
33	67	2	0	0	0	0
35	44	1	0	0	0	0
35	46	1	0	0	0	0
35	47	1	0	0	0	0
37	39	1	0	0	0	0
37	48	2	0	0	0	0
38	49	1	0	0	0	0
38	50	1	0	0	0	0
38	51	1	0	0	0	0
39	52	1	0	0	0	0
39	53	1	0	0	0	0
43	57	1	0	0	0	0
44	54	1	0	0	0	0
44	55	1	0	0	0	0
44	56	1	0	0	0	0

```
 45 63    1    0    0    0    0
 45 64    1    0    0    0    0
 45 65    1    0    0    0    0
 52 82    1    0    0    0    0
 52 84    1    0    0    0    0
 52 85    1    0    0    0    0
 53 77    2    0    0    0    0
 53 78    1    0    0    0    0
 57 58    1    0    0    0    0
 57 59    1    0    0    0    0
 57 69    1    0    0    0    0
 60 61    1    0    0    0    0
 60 62    1    0    0    0    0
 67 70    1    0    0    0    0
 67 71    1    0    0    0    0
 68 97    1    0    0    0    0
 72 74    1    0    0    0    0
 72 75    1    0    0    0    0
 72 76    1    0    0    0    0
 78 79    1    0    0    0    0
 79 80    1    0    0    0    0
 79 81    1    0    0    0    0
 79 83    1    0    0    0    0
 85 86    1    0    0    0    0
 85106    2    0    0    0    0
 86 87    1    0    0    0    0
 87 88    1    0    0    0    0
 87104    1    0    0    0    0
 87105    1    0    0    0    0
 88 89    1    0    0    0    0
 88102    1    0    0    0    0
 88103    1    0    0    0    0
 89 90    1    0    0    0    0
 89 91    1    0    0    0    0
 89 92    1    0    0    0    0
 92 93    1    0    0    0    0
 92 96    2    0    0    0    0
 93 94    2    0    0    0    0
 93101    1    0    0    0    0
 94 95    1    0    0    0    0
 94100    1    0    0    0    0
 95 97    2    0    0    0    0
 95 99    1    0    0    0    0
 96 97    1    0    0    0    0
 96 98    1    0    0    0    0
M    END
```

[a] The MM+/PM3 calculations were performed until the RMS gradient reached a value below 0.01 kcal $Å^{-1}$ mol^{-1} by using Polak-Ribiere algorithm.

Table S3. Optimized molecular configuration image and its Cartesian coordinates of **Zn-4($C_{2,2}$)** (MM+/PM3).[a]



106116 0 0 0 0 0 0 0 0999 V2000

68.6322	14.7863	-18.5311	C	0	0	0	0	0	0	0	0	0	0
70.1026	14.4618	-18.3972	C	0	0	0	0	0	0	0	0	0	0
70.8778	15.5499	-18.0926	O	0	0	0	0	0	0	0	0	0	0
70.6476	13.3870	-18.5535	O	0	0	0	0	0	0	0	0	0	0
68.5242	15.6164	-19.2590	H	0	0	0	0	0	0	0	0	0	0
68.1060	13.9186	-18.9809	H	0	0	0	0	0	0	0	0	0	0
72.2659	15.3660	-17.9234	C	0	0	0	0	0	0	0	0	0	0
72.7444	15.0000	-18.8382	H	0	0	0	0	0	0	0	0	0	0
72.4863	14.6857	-17.0937	H	0	0	0	0	0	0	0	0	0	0
69.0846	14.1006	-11.7226	C	0	0	0	0	0	0	0	0	0	0
67.9426	14.6185	-11.1910	N	0	0	0	0	0	0	0	0	0	0
68.1292	14.7329	-9.7710	C	0	0	0	0	0	0	0	0	0	0
69.5115	14.2962	-9.4685	C	0	0	0	0	0	0	0	0	0	0
67.1987	15.0964	-8.8545	C	0	0	0	0	0	0	0	0	0	0
65.8228	15.3660	-9.1264	C	0	0	0	0	0	0	0	0	0	0
65.2340	15.3485	-10.3672	N	0	0	0	0	0	0	0	0	0	0
63.8440	15.5099	-10.1947	C	0	0	0	0	0	0	0	0	0	0

63.5894	15.6822	-8.7823	C	0	0	0	0	0	0	0	0	0	0	0
64.8065	15.5892	-8.1249	C	0	0	0	0	0	0	0	0	0	0	0
62.8732	15.4143	-11.1996	C	0	0	0	0	0	0	0	0	0	0	0
63.1305	15.1700	-12.5321	C	0	0	0	0	0	0	0	0	0	0	0
64.4555	15.0438	-13.0781	N	0	0	0	0	0	0	0	0	0	0	0
64.3103	14.7934	-14.3873	C	0	0	0	0	0	0	0	0	0	0	0
62.9077	14.7363	-14.7542	C	0	0	0	0	0	0	0	0	0	0	0
62.1671	14.9650	-13.6146	C	0	0	0	0	0	0	0	0	0	0	0
65.1934	14.5454	-15.4961	C	0	0	0	0	0	0	0	0	0	0	0
66.5315	14.3731	-15.3168	C	0	0	0	0	0	0	0	0	0	0	0
67.1369	14.4389	-14.0230	N	0	0	0	0	0	0	0	0	0	0	0
68.4036	13.9074	-14.0973	C	0	0	0	0	0	0	0	0	0	0	0
68.7445	13.4517	-15.5050	C	0	0	0	0	0	0	0	0	0	0	0
67.5651	13.9835	-16.3573	C	0	0	0	0	0	0	0	0	0	0	0
69.3142	13.7760	-13.0685	C	0	0	0	0	0	0	0	0	0	0	0
70.0084	14.3197	-8.1131	C	0	0	0	0	0	0	0	0	0	0	0
67.5175	15.1324	-7.7967	H	0	0	0	0	0	0	0	0	0	0	0
62.2774	15.8874	-8.1285	C	0	0	0	0	0	0	0	0	0	0	0
61.8219	15.5201	-10.8876	H	0	0	0	0	0	0	0	0	0	0	0
62.8147	14.4379	-16.1802	C	0	0	0	0	0	0	0	0	0	0	0
60.7053	14.9836	-13.4769	C	0	0	0	0	0	0	0	0	0	0	0
64.3003	14.4108	-16.7299	C	0	0	0	0	0	0	0	0	0	0	0
69.7102	13.9153	-15.8226	H	0	0	0	0	0	0	0	0	0	0	0
67.1570	13.1776	-17.0157	H	0	0	0	0	0	0	0	0	0	0	0
70.3059	13.3466	-13.2915	H	0	0	0	0	0	0	0	0	0	0	0
70.0827	13.8975	-10.6471	C	0	0	0	0	0	0	0	0	0	0	0
61.7145	17.2696	-8.3867	C	0	0	0	0	0	0	0	0	0	0	0
68.8781	11.9432	-15.5965	C	0	0	0	0	0	0	0	0	0	0	0
62.4127	15.7305	-7.0331	H	0	0	0	0	0	0	0	0	0	0	0
61.5645	15.1106	-8.4686	H	0	0	0	0	0	0	0	0	0	0	0
61.8293	14.2589	-16.8589	O	0	0	0	0	0	0	0	0	0	0	0
60.3748	15.7121	-12.7242	H	0	0	0	0	0	0	0	0	0	0	0
60.3421	13.9939	-13.1643	H	0	0	0	0	0	0	0	0	0	0	0
60.2144	15.2299	-14.4276	H	0	0	0	0	0	0	0	0	0	0	0
64.5621	13.0769	-17.4363	C	0	0	0	0	0	0	0	0	0	0	0
61.5384	17.4431	-9.4569	H	0	0	0	0	0	0	0	0	0	0	0
62.3960	18.0556	-8.0370	H	0	0	0	0	0	0	0	0	0	0	0
60.7571	17.4081	-7.8684	H	0	0	0	0	0	0	0	0	0	0	0
71.4204	13.3480	-10.9127	C	0	0	0	0	0	0	0	0	0	0	0
71.6015	12.4349	-10.3288	H	0	0	0	0	0	0	0	0	0	0	0
71.5274	13.0933	-11.9815	H	0	0	0	0	0	0	0	0	0	0	0
67.9779	15.1820	-17.2143	C	0	0	0	0	0	0	0	0	0	0	0
68.6335	15.8676	-16.6400	H	0	0	0	0	0	0	0	0	0	0	0
67.0711	15.7817	-17.4524	H	0	0	0	0	0	0	0	0	0	0	0
67.9449	11.4287	-15.3317	H	0	0	0	0	0	0	0	0	0	0	0
69.6605	11.5766	-14.9184	H	0	0	0	0	0	0	0	0	0	0	0
69.1483	11.6366	-16.6160	H	0	0	0	0	0	0	0	0	0	0	0
69.2508	14.6372	-7.3741	H	0	0	0	0	0	0	0	0	0	0	0
71.2432	14.0043	-7.7266	C	0	0	0	0	0	0	0	0	0	0	0
66.3084	15.2891	-12.2054	Zn	0	0	0	0	0	0	0	0	0	0	0
72.2081	14.0713	-10.6594	H	0	0	0	0	0	0	0	0	0	0	0
72.0291	13.6867	-8.4064	H	0	0	0	0	0	0	0	0	0	0	0
71.5473	14.0453	-6.6850	H	0	0	0	0	0	0	0	0	0	0	0
65.0129	15.6720	-6.6703	C	0	0	0	0	0	0	0	0	0	0	0

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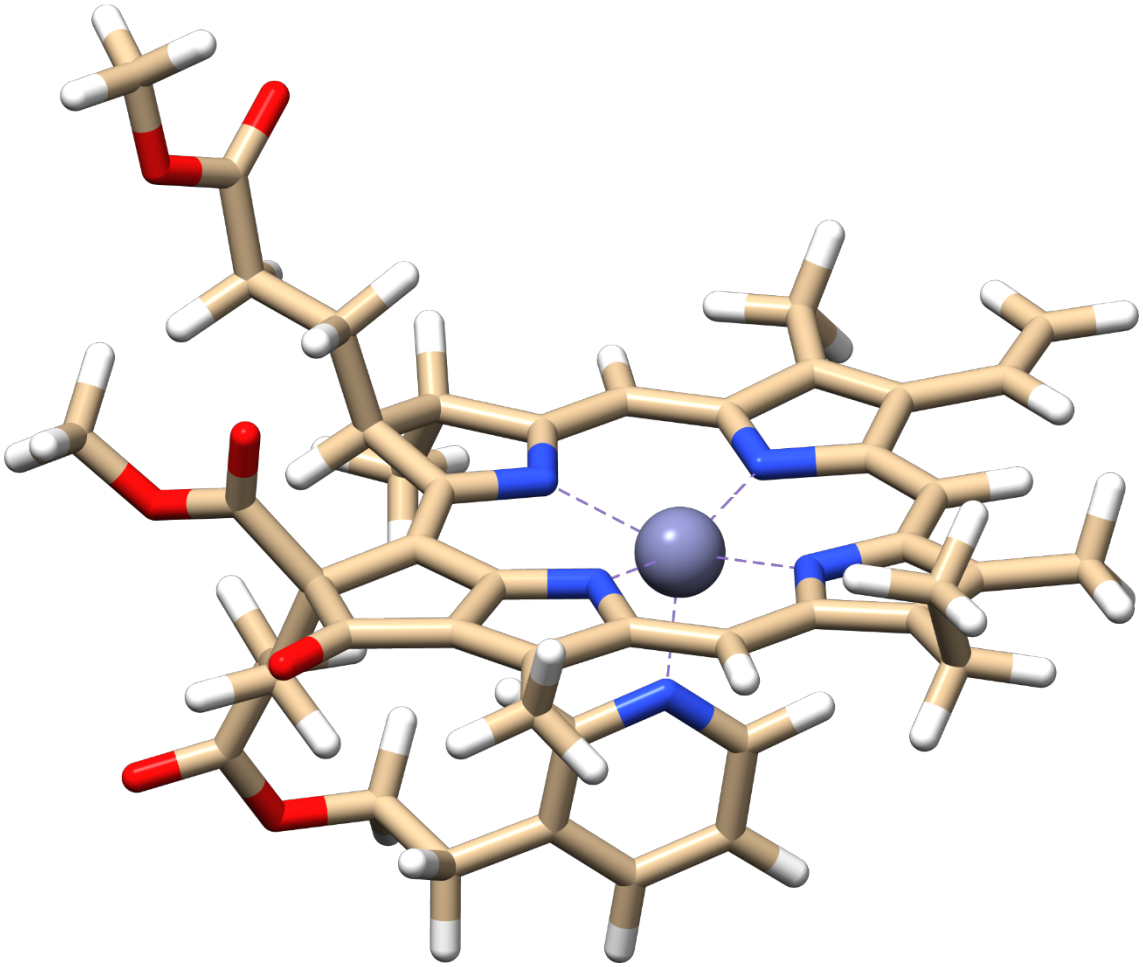
   72.6115    16.3763   -17.6907 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.5834    16.5695    -6.3975 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.0377    15.7169    -6.1557 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.5600    14.7993    -6.2903 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.6981    17.3309   -12.5777 N  0  0  0  0  0  0  0  0  0  0  0  0
   64.1603    11.9871   -16.7219 O  0  0  0  0  0  0  0  0  0  0  0  0
   64.3369    10.7040   -17.2845 C  0  0  0  0  0  0  0  0  0  0  0  0
   65.0772    12.9045   -18.5249 O  0  0  0  0  0  0  0  0  0  0  0  0
   63.7938    10.5914   -18.2289 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.9092    10.0547   -16.5164 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.3970    10.4732   -17.4356 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.8717    17.7600   -13.8571 C  0  0  0  0  0  0  0  0  0  0  0  0
   66.7458    18.2314   -11.5580 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.0918    19.1108   -14.1570 C  0  0  0  0  0  0  0  0  0  0  0  0
   66.9627    19.5886   -11.8025 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.1346    20.0334   -13.1095 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.3011    21.0969   -13.3175 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.9920    20.2940   -10.9649 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.6010    17.8342   -10.5406 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.8233    16.9937   -14.6510 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.2772    19.5411   -15.5742 C  0  0  0  0  0  0  0  0  0  0  0  0
   65.9668    19.9791   -16.2348 C  0  0  0  0  0  0  0  0  0  0  0  0
   65.0087    18.9386   -16.3251 O  0  0  0  0  0  0  0  0  0  0  0  0
   67.7481    18.7242   -16.1596 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.9877    20.3909   -15.6138 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.1072    17.9912   -17.3120 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.0438    16.9264   -17.1776 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.4678    15.5679   -17.7296 C  0  0  0  0  0  0  0  0  0  0  0  0
   63.1442    17.2933   -17.7129 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.7369    16.8352   -16.1123 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.8653    15.3402   -18.6332 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.5216    15.5892   -18.0849 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.1667    20.4340   -17.2235 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.4204    20.7122   -15.6148 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.9757    18.1096   -18.1537 O  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  5  1  0  0  0  0
 1  6  1  0  0  0  0
 1 59  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  2  0  0  0  0
 3  7  1  0  0  0  0
 7  8  1  0  0  0  0
 7  9  1  0  0  0  0
 7 72  1  0  0  0  0
10 11  1  0  0  0  0
10 32  1  0  0  0  0
10 43  2  0  0  0  0
11 12  1  0  0  0  0
11 67  1  0  0  0  0
12 13  2  0  0  0  0
12 14  1  0  0  0  0
13 33  1  0  0  0  0
13 43  1  0  0  0  0
```

14	15	2	0	0	0	0
14	34	1	0	0	0	0
15	16	1	0	0	0	0
15	19	1	0	0	0	0
16	17	2	0	0	0	0
16	67	1	0	0	0	0
17	18	1	0	0	0	0
17	20	1	0	0	0	0
18	19	2	0	0	0	0
18	35	1	0	0	0	0
19	71	1	0	0	0	0
20	21	2	0	0	0	0
20	36	1	0	0	0	0
21	22	1	0	0	0	0
21	25	1	0	0	0	0
22	23	1	0	0	0	0
22	67	1	0	0	0	0
23	24	1	0	0	0	0
23	26	2	0	0	0	0
24	25	2	0	0	0	0
24	37	1	0	0	0	0
25	38	1	0	0	0	0
26	27	1	0	0	0	0
26	39	1	0	0	0	0
27	28	2	0	0	0	0
27	31	1	0	0	0	0
28	29	1	0	0	0	0
28	67	1	0	0	0	0
29	30	1	0	0	0	0
29	32	2	0	0	0	0
30	31	1	0	0	0	0
30	40	1	0	0	0	0
30	45	1	0	0	0	0
31	41	1	0	0	0	0
31	59	1	0	0	0	0
32	42	1	0	0	0	0
33	65	1	0	0	0	0
33	66	2	0	0	0	0
35	44	1	0	0	0	0
35	46	1	0	0	0	0
35	47	1	0	0	0	0
37	39	1	0	0	0	0
37	48	2	0	0	0	0
38	49	1	0	0	0	0
38	50	1	0	0	0	0
38	51	1	0	0	0	0
39	52	1	0	0	0	0
39	99	1	0	0	0	0
43	56	1	0	0	0	0
44	53	1	0	0	0	0
44	54	1	0	0	0	0
44	55	1	0	0	0	0
45	62	1	0	0	0	0
45	63	1	0	0	0	0

```
 45 64    1    0    0    0    0
 52 77    1    0    0    0    0
 52 79    2    0    0    0    0
 56 57    1    0    0    0    0
 56 58    1    0    0    0    0
 56 68    1    0    0    0    0
 59 60    1    0    0    0    0
 59 61    1    0    0    0    0
 66 69    1    0    0    0    0
 66 70    1    0    0    0    0
 67 76    1    0    0    0    0
 71 73    1    0    0    0    0
 71 74    1    0    0    0    0
 71 75    1    0    0    0    0
 76 83    2    0    0    0    0
 76 84    1    0    0    0    0
 77 78    1    0    0    0    0
 78 80    1    0    0    0    0
 78 81    1    0    0    0    0
 78 82    1    0    0    0    0
 83 85    1    0    0    0    0
 83 91    1    0    0    0    0
 84 86    2    0    0    0    0
 84 90    1    0    0    0    0
 85 87    2    0    0    0    0
 85 92    1    0    0    0    0
 86 87    1    0    0    0    0
 86 89    1    0    0    0    0
 87 88    1    0    0    0    0
 92 93    1    0    0    0    0
 92 95    1    0    0    0    0
 92 96    1    0    0    0    0
 93 94    1    0    0    0    0
 93104    1    0    0    0    0
 93105    1    0    0    0    0
 94 97    1    0    0    0    0
 97 98    1    0    0    0    0
 97106    2    0    0    0    0
 98 99    1    0    0    0    0
 98100    1    0    0    0    0
 98101    1    0    0    0    0
 99102    1    0    0    0    0
 99103    1    0    0    0    0
M    END
```

[a] The MM+/PM3 calculations were performed until the RMS gradient reached a value below 0.01 kcal $Å^{-1}$ mol^{-1} by using Polak-Ribiere algorithm.

Table S4. Optimized molecular configuration image and its Cartesian coordinates of **Zn-4'($C_{2,2}$)** (MM+/PM3).[a]



106116 0 0 0 0 0 0 0 0999 V2000

69.8107	15.2914	-16.6035	C	0	0	0	0	0	0	0	0	0	0	0	0
71.1613	15.7866	-16.1369	C	0	0	0	0	0	0	0	0	0	0	0	0
71.6420	16.8259	-16.8835	O	0	0	0	0	0	0	0	0	0	0	0	0
71.8308	15.3609	-15.2166	O	0	0	0	0	0	0	0	0	0	0	0	0
69.6644	15.5047	-17.6832	H	0	0	0	0	0	0	0	0	0	0	0	0
69.7831	14.1868	-16.5038	H	0	0	0	0	0	0	0	0	0	0	0	0
72.8636	17.4252	-16.5101	C	0	0	0	0	0	0	0	0	0	0	0	0
73.6999	16.7226	-16.5897	H	0	0	0	0	0	0	0	0	0	0	0	0
72.8230	17.8386	-15.4968	H	0	0	0	0	0	0	0	0	0	0	0	0
65.4284	13.5693	-11.9553	C	0	0	0	0	0	0	0	0	0	0	0	0
64.5995	14.6179	-11.7227	N	0	0	0	0	0	0	0	0	0	0	0	0
64.0417	14.4613	-10.4080	C	0	0	0	0	0	0	0	0	0	0	0	0
64.5795	13.2020	-9.8494	C	0	0	0	0	0	0	0	0	0	0	0	0
63.2109	15.3244	-9.7700	C	0	0	0	0	0	0	0	0	0	0	0	0
62.7594	16.5795	-10.2746	C	0	0	0	0	0	0	0	0	0	0	0	0

63.0538	17.1034	-11.5130	N	0	0	0	0	0	0	0	0	0	0	0
62.4950	18.3921	-11.5889	C	0	0	0	0	0	0	0	0	0	0	0
61.8066	18.6517	-10.3455	C	0	0	0	0	0	0	0	0	0	0	0
61.9681	17.5356	-9.5379	C	0	0	0	0	0	0	0	0	0	0	0
62.6201	19.2889	-12.6625	C	0	0	0	0	0	0	0	0	0	0	0
63.3700	19.0672	-13.7953	C	0	0	0	0	0	0	0	0	0	0	0
64.1361	17.8689	-14.0146	N	0	0	0	0	0	0	0	0	0	0	0
64.7285	17.9993	-15.2113	C	0	0	0	0	0	0	0	0	0	0	0
64.3793	19.2677	-15.8254	C	0	0	0	0	0	0	0	0	0	0	0
63.5551	19.9447	-14.9546	C	0	0	0	0	0	0	0	0	0	0	0
65.6401	17.2174	-15.9990	C	0	0	0	0	0	0	0	0	0	0	0
66.1974	16.0719	-15.5009	C	0	0	0	0	0	0	0	0	0	0	0
65.7051	15.4491	-14.3255	N	0	0	0	0	0	0	0	0	0	0	0
66.3276	14.2181	-14.1719	C	0	0	0	0	0	0	0	0	0	0	0
67.2476	13.9113	-15.3401	C	0	0	0	0	0	0	0	0	0	0	0
67.3496	15.2691	-16.0802	C	0	0	0	0	0	0	0	0	0	0	0
66.2002	13.3491	-13.1182	C	0	0	0	0	0	0	0	0	0	0	0
64.1942	12.7617	-8.5296	C	0	0	0	0	0	0	0	0	0	0	0
62.8785	15.0432	-8.7533	H	0	0	0	0	0	0	0	0	0	0	0
61.0544	19.8715	-9.9753	C	0	0	0	0	0	0	0	0	0	0	0
62.0828	20.2466	-12.5769	H	0	0	0	0	0	0	0	0	0	0	0
65.0234	19.3358	-17.1315	C	0	0	0	0	0	0	0	0	0	0	0
62.9651	21.2796	-15.1153	C	0	0	0	0	0	0	0	0	0	0	0
65.7670	17.9387	-17.3395	C	0	0	0	0	0	0	0	0	0	0	0
68.2444	13.5857	-14.9536	H	0	0	0	0	0	0	0	0	0	0	0
67.2249	15.1510	-17.1899	H	0	0	0	0	0	0	0	0	0	0	0
66.7665	12.4019	-13.1325	H	0	0	0	0	0	0	0	0	0	0	0
65.4239	12.6650	-10.7867	C	0	0	0	0	0	0	0	0	0	0	0
61.9680	21.0344	-9.6471	C	0	0	0	0	0	0	0	0	0	0	0
66.6936	12.8135	-16.2279	C	0	0	0	0	0	0	0	0	0	0	0
60.4222	19.6259	-9.0905	H	0	0	0	0	0	0	0	0	0	0	0
60.3579	20.1456	-10.7917	H	0	0	0	0	0	0	0	0	0	0	0
65.0035	20.2271	-17.9486	O	0	0	0	0	0	0	0	0	0	0	0
61.9178	21.2999	-14.7842	H	0	0	0	0	0	0	0	0	0	0	0
62.9988	21.6143	-16.1602	H	0	0	0	0	0	0	0	0	0	0	0
63.5183	22.0136	-14.5122	H	0	0	0	0	0	0	0	0	0	0	0
64.9593	17.2225	-18.4416	C	0	0	0	0	0	0	0	0	0	0	0
67.2086	18.2680	-17.7173	C	0	0	0	0	0	0	0	0	0	0	0
62.5843	21.3235	-10.5092	H	0	0	0	0	0	0	0	0	0	0	0
62.6530	20.7900	-8.8250	H	0	0	0	0	0	0	0	0	0	0	0
61.3895	21.9165	-9.3446	H	0	0	0	0	0	0	0	0	0	0	0
66.2269	11.4339	-10.7440	C	0	0	0	0	0	0	0	0	0	0	0
65.5939	10.5463	-10.6052	H	0	0	0	0	0	0	0	0	0	0	0
66.7866	11.3060	-11.6867	H	0	0	0	0	0	0	0	0	0	0	0
68.6969	15.9330	-15.7853	C	0	0	0	0	0	0	0	0	0	0	0
68.9271	15.8652	-14.7022	H	0	0	0	0	0	0	0	0	0	0	0
68.6445	17.0172	-16.0070	H	0	0	0	0	0	0	0	0	0	0	0
65.7314	13.0931	-16.6814	H	0	0	0	0	0	0	0	0	0	0	0
66.5329	11.8892	-15.6573	H	0	0	0	0	0	0	0	0	0	0	0
67.3885	12.5857	-17.0472	H	0	0	0	0	0	0	0	0	0	0	0
63.5027	13.4565	-8.0197	H	0	0	0	0	0	0	0	0	0	0	0
64.5959	11.6425	-7.9300	C	0	0	0	0	0	0	0	0	0	0	0
64.0431	16.0531	-13.0582	Zn	0	0	0	0	0	0	0	0	0	0	0
66.9551	11.4597	-9.9214	H	0	0	0	0	0	0	0	0	0	0	0

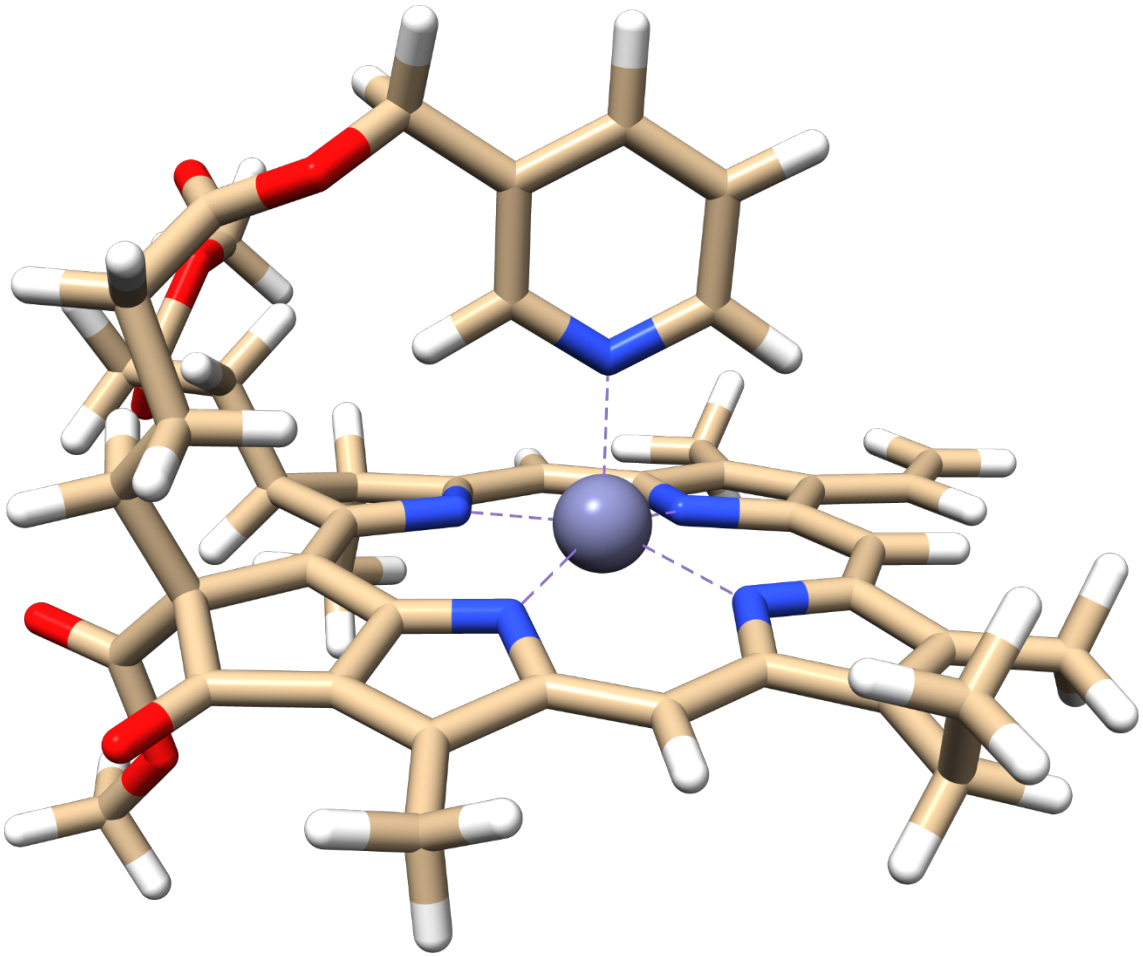
```
   65.2735    10.9222    -8.3806 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.2625    11.3737    -6.9319 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.4228    17.3638    -8.1821 C  0  0  0  0  0  0  0  0  0  0  0  0
   72.9658    18.2268   -17.2460 H  0  0  0  0  0  0  0  0  0  0  0  0
   60.8697    16.4205    -8.0853 H  0  0  0  0  0  0  0  0  0  0  0  0
   62.2209    17.3629    -7.4280 H  0  0  0  0  0  0  0  0  0  0  0  0
   60.7333    18.1932    -7.9487 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.9394    19.0683   -17.1684 O  0  0  0  0  0  0  0  0  0  0  0  0
   67.6907    17.6023   -18.8119 O  0  0  0  0  0  0  0  0  0  0  0  0
   68.9676    17.9464   -19.3068 C  0  0  0  0  0  0  0  0  0  0  0  0
   69.7561    17.7376   -18.5738 H  0  0  0  0  0  0  0  0  0  0  0  0
   69.0643    17.2868   -20.1730 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.1655    17.7112   -19.4164 H  0  0  0  0  0  0  0  0  0  0  0  0
   69.0155    18.9957   -19.6162 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.8790    17.3907   -18.2410 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.1859    15.7243   -18.5569 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.4278    15.1547   -19.7336 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.8740    15.2117   -17.6152 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.2699    15.4901   -18.6639 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.3718    14.2845   -19.6275 O  0  0  0  0  0  0  0  0  0  0  0  0
   62.9093    13.8805   -18.3530 C  0  0  0  0  0  0  0  0  0  0  0  0
   61.7719    14.7787   -17.8470 C  0  0  0  0  0  0  0  0  0  0  0  0
   60.8248    14.5289   -18.3647 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.9761    15.8416   -18.0969 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.6171    14.6437   -16.3684 C  0  0  0  0  0  0  0  0  0  0  0  0
   60.5583    13.9381   -15.7944 C  0  0  0  0  0  0  0  0  0  0  0  0
   60.4749    13.8499   -14.4071 C  0  0  0  0  0  0  0  0  0  0  0  0
   61.4487    14.4584   -13.6124 C  0  0  0  0  0  0  0  0  0  0  0  0
   62.5597    15.2459   -15.5250 C  0  0  0  0  0  0  0  0  0  0  0  0
   62.4808    15.1483   -14.1705 N  0  0  0  0  0  0  0  0  0  0  0  0
   63.4048    15.8318   -15.9349 H  0  0  0  0  0  0  0  0  0  0  0  0
   61.4217    14.4100   -12.5135 H  0  0  0  0  0  0  0  0  0  0  0  0
   59.6497    13.3059   -13.9336 H  0  0  0  0  0  0  0  0  0  0  0  0
   59.7998    13.4627   -16.4283 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.6402    15.3396   -20.9119 O  0  0  0  0  0  0  0  0  0  0  0  0
   62.5618    12.8504   -18.5416 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.7418    13.8384   -17.6154 H  0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  5  1  0  0  0  0
  1  6  1  0  0  0  0
  1 60  1  0  0  0  0
  2  3  1  0  0  0  0
  2  4  2  0  0  0  0
  3  7  1  0  0  0  0
  7  8  1  0  0  0  0
  7  9  1  0  0  0  0
  7 73  1  0  0  0  0
 10 11  1  0  0  0  0
 10 32  1  0  0  0  0
 10 43  2  0  0  0  0
 11 12  1  0  0  0  0
 11 68  1  0  0  0  0
 12 13  2  0  0  0  0
 12 14  1  0  0  0  0
```

13	33	1	0	0	0	0
13	43	1	0	0	0	0
14	15	2	0	0	0	0
14	34	1	0	0	0	0
15	16	1	0	0	0	0
15	19	1	0	0	0	0
16	17	2	0	0	0	0
16	68	1	0	0	0	0
17	18	1	0	0	0	0
17	20	1	0	0	0	0
18	19	2	0	0	0	0
18	35	1	0	0	0	0
19	72	1	0	0	0	0
20	21	2	0	0	0	0
20	36	1	0	0	0	0
21	22	1	0	0	0	0
21	25	1	0	0	0	0
22	23	1	0	0	0	0
22	68	1	0	0	0	0
23	24	1	0	0	0	0
23	26	2	0	0	0	0
24	25	2	0	0	0	0
24	37	1	0	0	0	0
25	38	1	0	0	0	0
26	27	1	0	0	0	0
26	39	1	0	0	0	0
27	28	2	0	0	0	0
27	31	1	0	0	0	0
28	29	1	0	0	0	0
28	68	1	0	0	0	0
29	30	1	0	0	0	0
29	32	2	0	0	0	0
30	31	1	0	0	0	0
30	40	1	0	0	0	0
30	45	1	0	0	0	0
31	41	1	0	0	0	0
31	60	1	0	0	0	0
32	42	1	0	0	0	0
33	66	1	0	0	0	0
33	67	2	0	0	0	0
35	44	1	0	0	0	0
35	46	1	0	0	0	0
35	47	1	0	0	0	0
37	39	1	0	0	0	0
37	48	2	0	0	0	0
38	49	1	0	0	0	0
38	50	1	0	0	0	0
38	51	1	0	0	0	0
39	52	1	0	0	0	0
39	53	1	0	0	0	0
43	57	1	0	0	0	0
44	54	1	0	0	0	0
44	55	1	0	0	0	0
44	56	1	0	0	0	0

```
 45 63    1    0    0    0    0
 45 64    1    0    0    0    0
 45 65    1    0    0    0    0
 52 82    1    0    0    0    0
 52 84    1    0    0    0    0
 52 85    1    0    0    0    0
 53 77    2    0    0    0    0
 53 78    1    0    0    0    0
 57 58    1    0    0    0    0
 57 59    1    0    0    0    0
 57 69    1    0    0    0    0
 60 61    1    0    0    0    0
 60 62    1    0    0    0    0
 67 70    1    0    0    0    0
 67 71    1    0    0    0    0
 68 99    1    0    0    0    0
 72 74    1    0    0    0    0
 72 75    1    0    0    0    0
 72 76    1    0    0    0    0
 78 79    1    0    0    0    0
 79 80    1    0    0    0    0
 79 81    1    0    0    0    0
 79 83    1    0    0    0    0
 85 86    1    0    0    0    0
 85 87    1    0    0    0    0
 85 88    1    0    0    0    0
 86 89    1    0    0    0    0
 86104    2    0    0    0    0
 89 90    1    0    0    0    0
 90 91    1    0    0    0    0
 90105    1    0    0    0    0
 90106    1    0    0    0    0
 91 92    1    0    0    0    0
 91 93    1    0    0    0    0
 91 94    1    0    0    0    0
 94 95    1    0    0    0    0
 94 98    2    0    0    0    0
 95 96    2    0    0    0    0
 95103    1    0    0    0    0
 96 97    1    0    0    0    0
 96102    1    0    0    0    0
 97 99    2    0    0    0    0
 97101    1    0    0    0    0
 98 99    1    0    0    0    0
 98100    1    0    0    0    0
M    END
```

[a] The MM+/PM3 calculations were performed until the RMS gradient reached a value below 0.01 kcal $Å^{-1}$ mol^{-1} by using Polak-Ribiere algorithm.

Table S5. Optimized molecular configuration image and its Cartesian coordinates of **Zn-4($C_{3,1}$)** (MM+/PM3).[a]



106116 0 0 0 0 0 0 0 0999 V2000

68.2939	14.4568	-18.6704	C	0	0	0	0	0	0	0	0	0	0	0
69.6354	13.7600	-18.6545	C	0	0	0	0	0	0	0	0	0	0	0
70.6900	14.6073	-18.4367	O	0	0	0	0	0	0	0	0	0	0	0
69.8669	12.5805	-18.8326	O	0	0	0	0	0	0	0	0	0	0	0
68.3496	15.3076	-19.3797	H	0	0	0	0	0	0	0	0	0	0	0
67.5280	13.7666	-19.0827	H	0	0	0	0	0	0	0	0	0	0	0
71.9904	14.0659	-18.3698	C	0	0	0	0	0	0	0	0	0	0	0
72.2819	13.5825	-19.3084	H	0	0	0	0	0	0	0	0	0	0	0
72.0907	13.3555	-17.5419	H	0	0	0	0	0	0	0	0	0	0	0
69.0170	13.8356	-11.8099	C	0	0	0	0	0	0	0	0	0	0	0
67.9609	14.4830	-11.2409	N	0	0	0	0	0	0	0	0	0	0	0
68.2117	14.5791	-9.8298	C	0	0	0	0	0	0	0	0	0	0	0
69.5460	13.9896	-9.5743	C	0	0	0	0	0	0	0	0	0	0	0
67.3611	15.0452	-8.8824	C	0	0	0	0	0	0	0	0	0	0	0
66.0134	15.4609	-9.1062	C	0	0	0	0	0	0	0	0	0	0	0

65.3824	15.5095	-10.3253 N	0	0	0	0	0	0	0	0	0	0	0
64.0234	15.8127	-10.1026 C	0	0	0	0	0	0	0	0	0	0	0
63.8387	16.0055	-8.6819 C	0	0	0	0	0	0	0	0	0	0	0
65.0624	15.7852	-8.0688 C	0	0	0	0	0	0	0	0	0	0	0
63.0124	15.8219	-11.0714 C	0	0	0	0	0	0	0	0	0	0	0
63.1968	15.5616	-12.4130 C	0	0	0	0	0	0	0	0	0	0	0
64.4826	15.3050	-13.0039 N	0	0	0	0	0	0	0	0	0	0	0
64.2707	15.0923	-14.3107 C	0	0	0	0	0	0	0	0	0	0	0
62.8589	15.1860	-14.6312 C	0	0	0	0	0	0	0	0	0	0	0
62.1830	15.4718	-13.4649 C	0	0	0	0	0	0	0	0	0	0	0
65.0864	14.7661	-15.4505 C	0	0	0	0	0	0	0	0	0	0	0
66.3957	14.4205	-15.3182 C	0	0	0	0	0	0	0	0	0	0	0
67.0528	14.4205	-14.0474 N	0	0	0	0	0	0	0	0	0	0	0
68.2305	13.7211	-14.1564 C	0	0	0	0	0	0	0	0	0	0	0
68.4526	13.1997	-15.5650 C	0	0	0	0	0	0	0	0	0	0	0
67.3231	13.8712	-16.3865 C	0	0	0	0	0	0	0	0	0	0	0
69.1561	13.4813	-13.1588 C	0	0	0	0	0	0	0	0	0	0	0
70.0919	13.9610	-8.2379 C	0	0	0	0	0	0	0	0	0	0	0
67.7197	15.0466	-7.8369 H	0	0	0	0	0	0	0	0	0	0	0
62.5791	16.3420	-7.9813 C	0	0	0	0	0	0	0	0	0	0	0
61.9892	16.0330	-10.7220 H	0	0	0	0	0	0	0	0	0	0	0
62.6920	14.9325	-16.0600 C	0	0	0	0	0	0	0	0	0	0	0
60.7361	15.6386	-13.2777 C	0	0	0	0	0	0	0	0	0	0	0
64.1499	14.7857	-16.6594 C	0	0	0	0	0	0	0	0	0	0	0
69.4593	13.5214	-15.9278 H	0	0	0	0	0	0	0	0	0	0	0
66.7770	13.1117	-16.9993 H	0	0	0	0	0	0	0	0	0	0	0
70.0772	12.9301	-13.4140 H	0	0	0	0	0	0	0	0	0	0	0
70.0240	13.5231	-10.7692 C	0	0	0	0	0	0	0	0	0	0	0
62.1524	17.7757	-8.2193 C	0	0	0	0	0	0	0	0	0	0	0
68.3774	11.6853	-15.6247 C	0	0	0	0	0	0	0	0	0	0	0
62.7366	16.1682	-6.8914 H	0	0	0	0	0	0	0	0	0	0	0
61.7785	15.6437	-8.2955 H	0	0	0	0	0	0	0	0	0	0	0
61.6718	14.8581	-16.7063 O	0	0	0	0	0	0	0	0	0	0	0
60.5073	16.3878	-12.5076 H	0	0	0	0	0	0	0	0	0	0	0
60.2834	14.6877	-12.9619 H	0	0	0	0	0	0	0	0	0	0	0
60.2425	15.9458	-14.2090 H	0	0	0	0	0	0	0	0	0	0	0
64.2527	13.4848	-17.4586 C	0	0	0	0	0	0	0	0	0	0	0
61.9570	17.9702	-9.2825 H	0	0	0	0	0	0	0	0	0	0	0
62.9232	18.4862	-7.8943 H	0	0	0	0	0	0	0	0	0	0	0
61.2333	18.0100	-7.6670 H	0	0	0	0	0	0	0	0	0	0	0
71.2787	12.8219	-11.0789 C	0	0	0	0	0	0	0	0	0	0	0
71.3793	11.9008	-10.4882 H	0	0	0	0	0	0	0	0	0	0	0
71.3116	12.5448	-12.1470 H	0	0	0	0	0	0	0	0	0	0	0
67.8671	14.9698	-17.3019 C	0	0	0	0	0	0	0	0	0	0	0
68.7023	15.5112	-16.8132 H	0	0	0	0	0	0	0	0	0	0	0
67.0778	15.7382	-17.4577 H	0	0	0	0	0	0	0	0	0	0	0
67.3952	11.3075	-15.3113 H	0	0	0	0	0	0	0	0	0	0	0
69.1305	11.2287	-14.9686 H	0	0	0	0	0	0	0	0	0	0	0
68.5605	11.3254	-16.6463 H	0	0	0	0	0	0	0	0	0	0	0
69.3996	14.3572	-7.4732 H	0	0	0	0	0	0	0	0	0	0	0
71.2999	13.5172	-7.8956 C	0	0	0	0	0	0	0	0	0	0	0
66.3811	15.3359	-12.2041 Zn	0	0	0	0	0	0	0	0	0	0	0
72.1530	13.4537	-10.8688 H	0	0	0	0	0	0	0	0	0	0	0
72.0222	13.1183	-8.6025 H	0	0	0	0	0	0	0	0	0	0	0

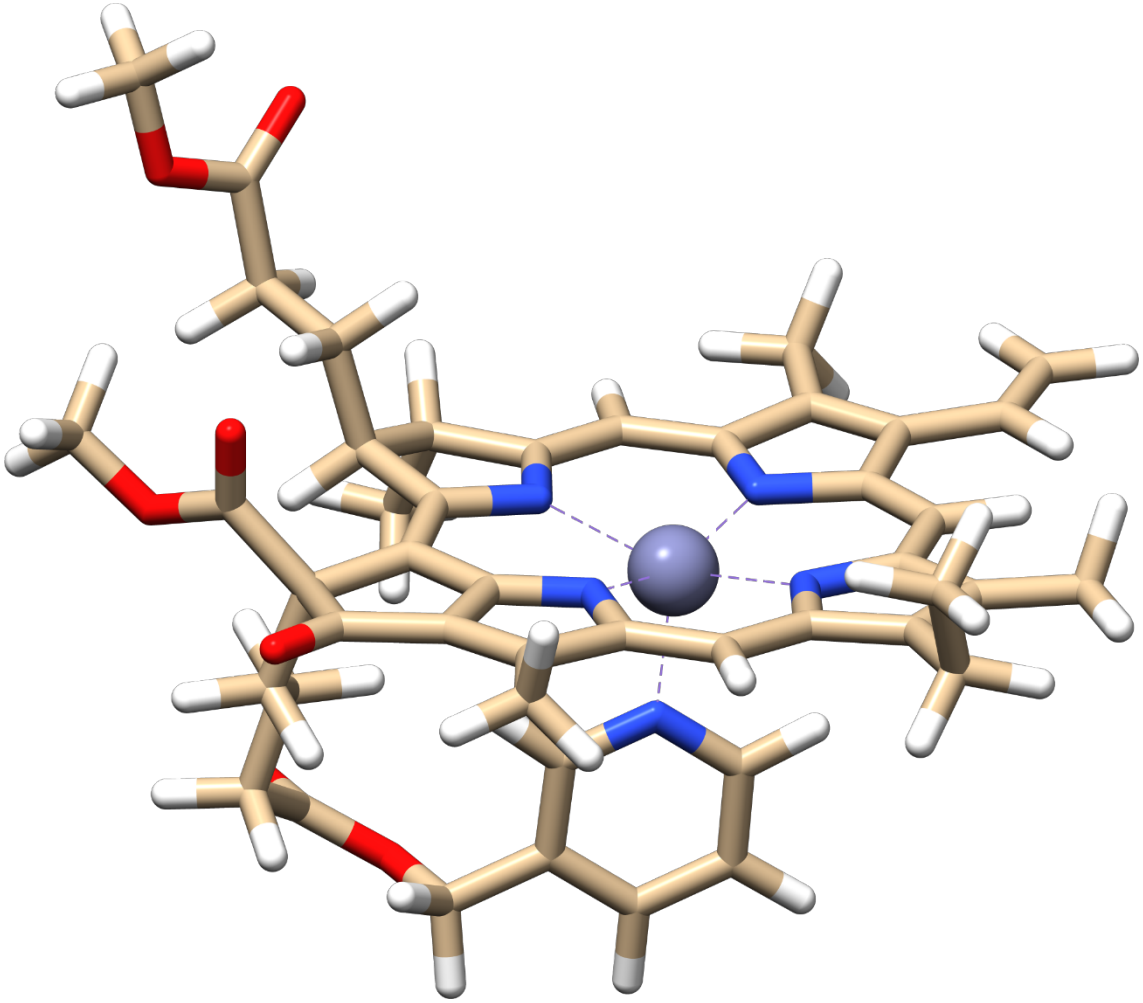
```
   71.6448    13.5259    -6.8660 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.3281    15.8408    -6.6226 C  0  0  0  0  0  0  0  0  0  0  0  0
   72.6060    14.9508   -18.1897 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.9981    16.6732    -6.3705 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.3819    15.9846    -6.0732 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.7950    14.9146    -6.2624 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.9925    17.3280   -12.5590 N  0  0  0  0  0  0  0  0  0  0  0  0
   63.8078    12.3866   -16.7833 O  0  0  0  0  0  0  0  0  0  0  0  0
   63.8471    11.1315   -17.4293 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.6786    13.3429   -18.5894 O  0  0  0  0  0  0  0  0  0  0  0  0
   63.2399    11.1192   -18.3408 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.4172    10.4693   -16.6735 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.8748    10.8323   -17.6627 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.9402    17.8900   -13.7981 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.4600    18.0563   -11.5085 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.3577    19.2081   -14.0195 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.8844    19.3754   -11.6759 C  0  0  0  0  0  0  0  0  0  0  0  0
   67.8308    19.9563   -12.9380 C  0  0  0  0  0  0  0  0  0  0  0  0
   68.1548    20.9942   -13.0818 H  0  0  0  0  0  0  0  0  0  0  0  0
   68.2507    19.9437   -10.8141 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.4790    17.5520   -10.5279 H  0  0  0  0  0  0  0  0  0  0  0  0
   66.5473    17.2558   -14.6119 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.3414    19.8326   -15.3867 C  0  0  0  0  0  0  0  0  0  0  0  0
   66.1203    19.5627   -16.0575 O  0  0  0  0  0  0  0  0  0  0  0  0
   66.1050    18.7924   -17.1919 C  0  0  0  0  0  0  0  0  0  0  0  0
   68.2441    19.5148   -15.9470 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.3492    20.9366   -15.3200 H  0  0  0  0  0  0  0  0  0  0  0  0
   67.1562    18.4433   -17.6890 O  0  0  0  0  0  0  0  0  0  0  0  0
   64.7010    18.5032   -17.6766 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.0979    17.3263   -16.9202 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.4192    15.9902   -17.5768 C  0  0  0  0  0  0  0  0  0  0  0  0
   64.0695    19.4044   -17.5438 H  0  0  0  0  0  0  0  0  0  0  0  0
   62.9978    17.4559   -16.8670 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.4434    17.3271   -15.8649 H  0  0  0  0  0  0  0  0  0  0  0  0
   63.8219    15.8835   -18.5059 H  0  0  0  0  0  0  0  0  0  0  0  0
   65.4816    15.9709   -17.9039 H  0  0  0  0  0  0  0  0  0  0  0  0
   64.7223    18.3032   -18.7668 H  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  5  1  0  0  0  0
 1  6  1  0  0  0  0
 1 59  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  2  0  0  0  0
 3  7  1  0  0  0  0
 7  8  1  0  0  0  0
 7  9  1  0  0  0  0
 7 72  1  0  0  0  0
10 11  1  0  0  0  0
10 32  1  0  0  0  0
10 43  2  0  0  0  0
11 12  1  0  0  0  0
11 67  1  0  0  0  0
12 13  2  0  0  0  0
12 14  1  0  0  0  0
```

13 33 1 0 0 0 0
13 43 1 0 0 0 0
14 15 2 0 0 0 0
14 34 1 0 0 0 0
15 16 1 0 0 0 0
15 19 1 0 0 0 0
16 17 2 0 0 0 0
16 67 1 0 0 0 0
17 18 1 0 0 0 0
17 20 1 0 0 0 0
18 19 2 0 0 0 0
18 35 1 0 0 0 0
19 71 1 0 0 0 0
20 21 2 0 0 0 0
20 36 1 0 0 0 0
21 22 1 0 0 0 0
21 25 1 0 0 0 0
22 23 1 0 0 0 0
22 67 1 0 0 0 0
23 24 1 0 0 0 0
23 26 2 0 0 0 0
24 25 2 0 0 0 0
24 37 1 0 0 0 0
25 38 1 0 0 0 0
26 27 1 0 0 0 0
26 39 1 0 0 0 0
27 28 2 0 0 0 0
27 31 1 0 0 0 0
28 29 1 0 0 0 0
28 67 1 0 0 0 0
29 30 1 0 0 0 0
29 32 2 0 0 0 0
30 31 1 0 0 0 0
30 40 1 0 0 0 0
30 45 1 0 0 0 0
31 41 1 0 0 0 0
31 59 1 0 0 0 0
32 42 1 0 0 0 0
33 65 1 0 0 0 0
33 66 2 0 0 0 0
35 44 1 0 0 0 0
35 46 1 0 0 0 0
35 47 1 0 0 0 0
37 39 1 0 0 0 0
37 48 2 0 0 0 0
38 49 1 0 0 0 0
38 50 1 0 0 0 0
38 51 1 0 0 0 0
39 52 1 0 0 0 0
39100 1 0 0 0 0
43 56 1 0 0 0 0
44 53 1 0 0 0 0
44 54 1 0 0 0 0
44 55 1 0 0 0 0

```
 45 62    1    0    0    0    0
 45 63    1    0    0    0    0
 45 64    1    0    0    0    0
 52 77    1    0    0    0    0
 52 79    2    0    0    0    0
 56 57    1    0    0    0    0
 56 58    1    0    0    0    0
 56 68    1    0    0    0    0
 59 60    1    0    0    0    0
 59 61    1    0    0    0    0
 66 69    1    0    0    0    0
 66 70    1    0    0    0    0
 67 76    1    0    0    0    0
 71 73    1    0    0    0    0
 71 74    1    0    0    0    0
 71 75    1    0    0    0    0
 76 83    2    0    0    0    0
 76 84    1    0    0    0    0
 77 78    1    0    0    0    0
 78 80    1    0    0    0    0
 78 81    1    0    0    0    0
 78 82    1    0    0    0    0
 83 85    1    0    0    0    0
 83 91    1    0    0    0    0
 84 86    2    0    0    0    0
 84 90    1    0    0    0    0
 85 87    2    0    0    0    0
 85 92    1    0    0    0    0
 86 87    1    0    0    0    0
 86 89    1    0    0    0    0
 87 88    1    0    0    0    0
 92 93    1    0    0    0    0
 92 95    1    0    0    0    0
 92 96    1    0    0    0    0
 93 94    1    0    0    0    0
 94 97    2    0    0    0    0
 94 98    1    0    0    0    0
 98 99    1    0    0    0    0
 98101    1    0    0    0    0
 98106    1    0    0    0    0
 99100    1    0    0    0    0
 99102    1    0    0    0    0
 99103    1    0    0    0    0
100104    1    0    0    0    0
100105    1    0    0    0    0
M    END
```

[a] The MM+/PM3 calculations were performed until the RMS gradient reached a value below 0.01 kcal $Å^{-1}$ mol^{-1} by using Polak-Ribiere algorithm.

Table S6. Optimized molecular configuration image and its Cartesian coordinates of **Zn-4'($C_{3,1}$)** (MM+/PM3).[a]



106116 0 0 0 0 0 0 0 0999 V2000

69.8812	15.3447	-16.4758	C	0	0	0	0	0	0	0	0	0	0
71.2074	15.9465	-16.0727	C	0	0	0	0	0	0	0	0	0	0
71.6478	16.9099	-16.9381	O	0	0	0	0	0	0	0	0	0	0
71.8911	15.6611	-15.1100	O	0	0	0	0	0	0	0	0	0	0
69.7950	15.2939	-17.5801	H	0	0	0	0	0	0	0	0	0	0
69.8245	14.2951	-16.1060	H	0	0	0	0	0	0	0	0	0	0
72.8377	17.6044	-16.6340	C	0	0	0	0	0	0	0	0	0	0
73.7055	16.9364	-16.6258	H	0	0	0	0	0	0	0	0	0	0
72.7691	18.1332	-15.6774	H	0	0	0	0	0	0	0	0	0	0
65.6391	13.6639	-12.0071	C	0	0	0	0	0	0	0	0	0	0
64.7608	14.6686	-11.7623	N	0	0	0	0	0	0	0	0	0	0
64.2206	14.4760	-10.4453	C	0	0	0	0	0	0	0	0	0	0
64.8311	13.2467	-9.8945	C	0	0	0	0	0	0	0	0	0	0
63.3414	15.2857	-9.8026	C	0	0	0	0	0	0	0	0	0	0

62.8135	16.5123	-10.3030	C	0	0	0	0	0	0	0	0	0	0	0
63.0724	17.0582	-11.5406	N	0	0	0	0	0	0	0	0	0	0	0
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M    END
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[a] The MM+/PM3 calculations were performed until the RMS gradient reached a value below 0.01 kcal $Å^{-1}$ mol^{-1} by using Polak-Ribiere algorithm.

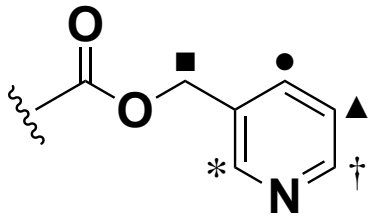

Table S7. Specific ^{1}H NMR (600 MHz) spectral signals in the 13^2-pyridine terminal of **Zn-4(C$_{3,1}$)** in $CDCl_3$ with/without pyridine-d_5.

Proton	δ / ppm		$\lvert\Delta\delta\rvert$ / ppm [a]
	Without pyridine-d_5	With pyridine-d_5	
*	4.20	6.94	2.74
■	4.26 / 4.17	4.67 / 4.63	0.41 / 0.46
●	6.52	7.17	0.65
▲	5.92	6.71	0.79
†	3.74	6.79	3.05

[a] $|\Delta\delta| = |\delta$[without pyridine-d_5] $- \delta$[with pyridine-d_5]$|$

Table S8. Specific ^{1}H NMR (600 MHz) spectral signals in the 13^2-pyridine terminal of **Zn-4'(C$_{3,1}$)** in $CDCl_3$ with/without pyridine-d_5.

Proton	δ / ppm		$\lvert\Delta\delta\rvert$ / ppm [a]
	Without pyridine-d_5	With pyridine-d_5	
*	4.01	7.07	3.06
■	4.31 / 4.13	4.74 / 4.69	0.43 / 0.56
●	6.44	7.20	0.76
▲	5.76	6.73	0.97
†	3.81–3.70	7.07	3.26–3.37

[a] $|\Delta\delta| = |\delta$[without pyridine-d_5] $- \delta$[with pyridine-d_5]$|$

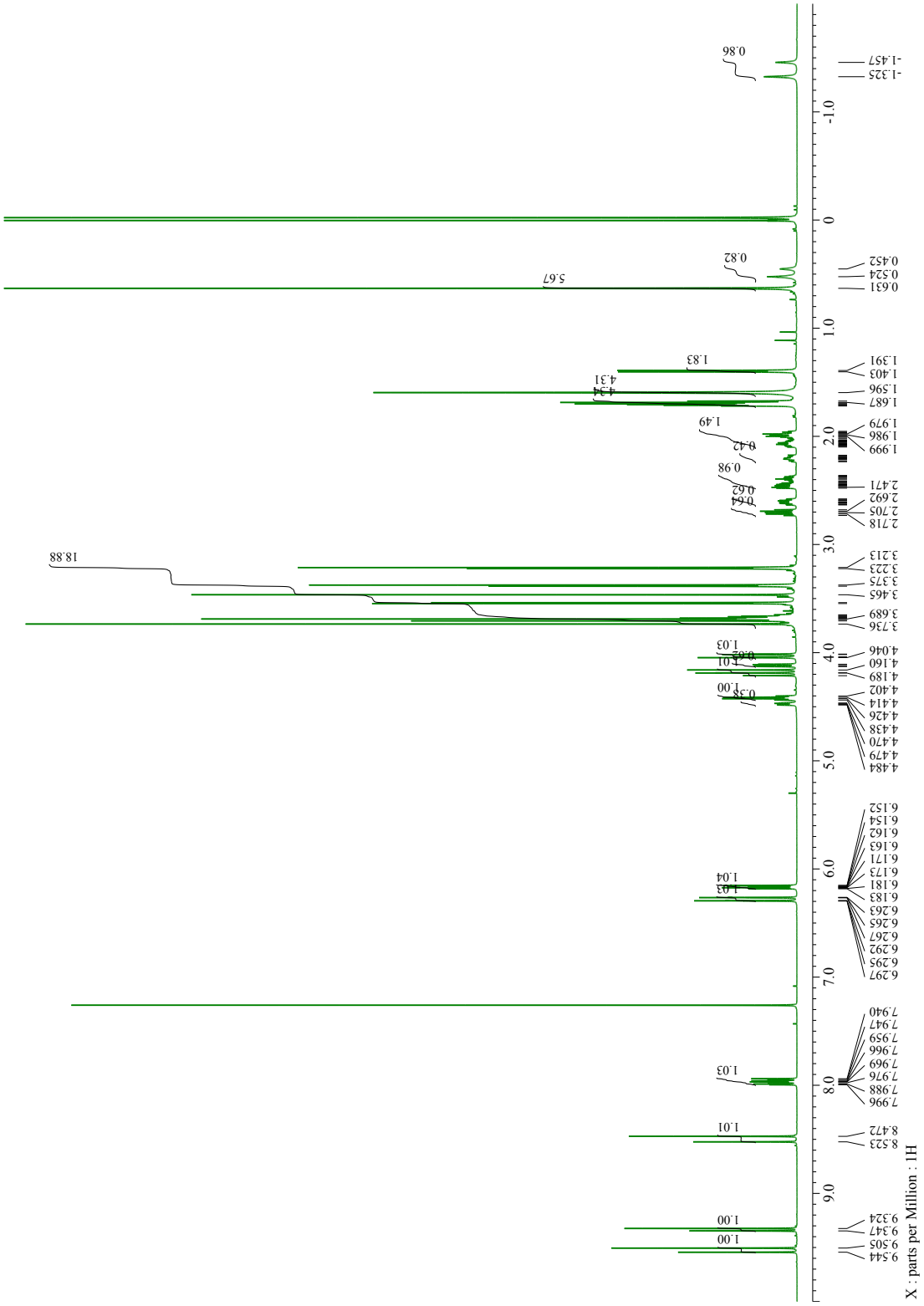

Figure S1. ^{1}H NMR (600 MHz) spectrum of methyl 13^{2}-(*tert*-butoxycarbonylmethyl)-pheophorbides-*a*/*a*' [**H$_2$-2/2'(C$_1$)**] in $CDCl_3$.

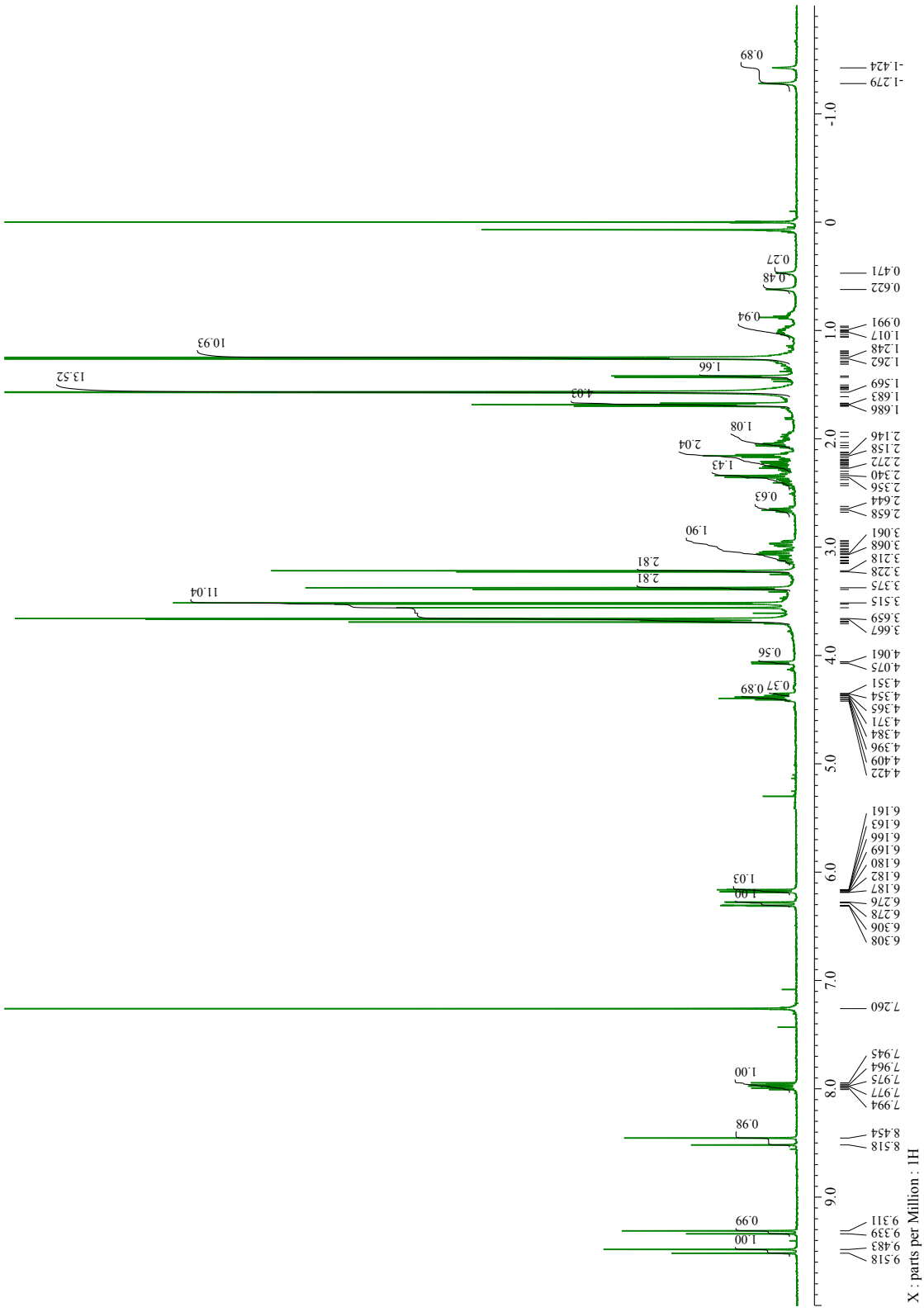

Figure S2. ^{1}H NMR (600 MHz) spectrum of methyl 13^{2}-[3-(*tert*-butoxycarbonyl)-propyl]pheophorbides-*a*/*a*' [**H$_2$-2/2'(C$_3$)**] in $CDCl_3$.

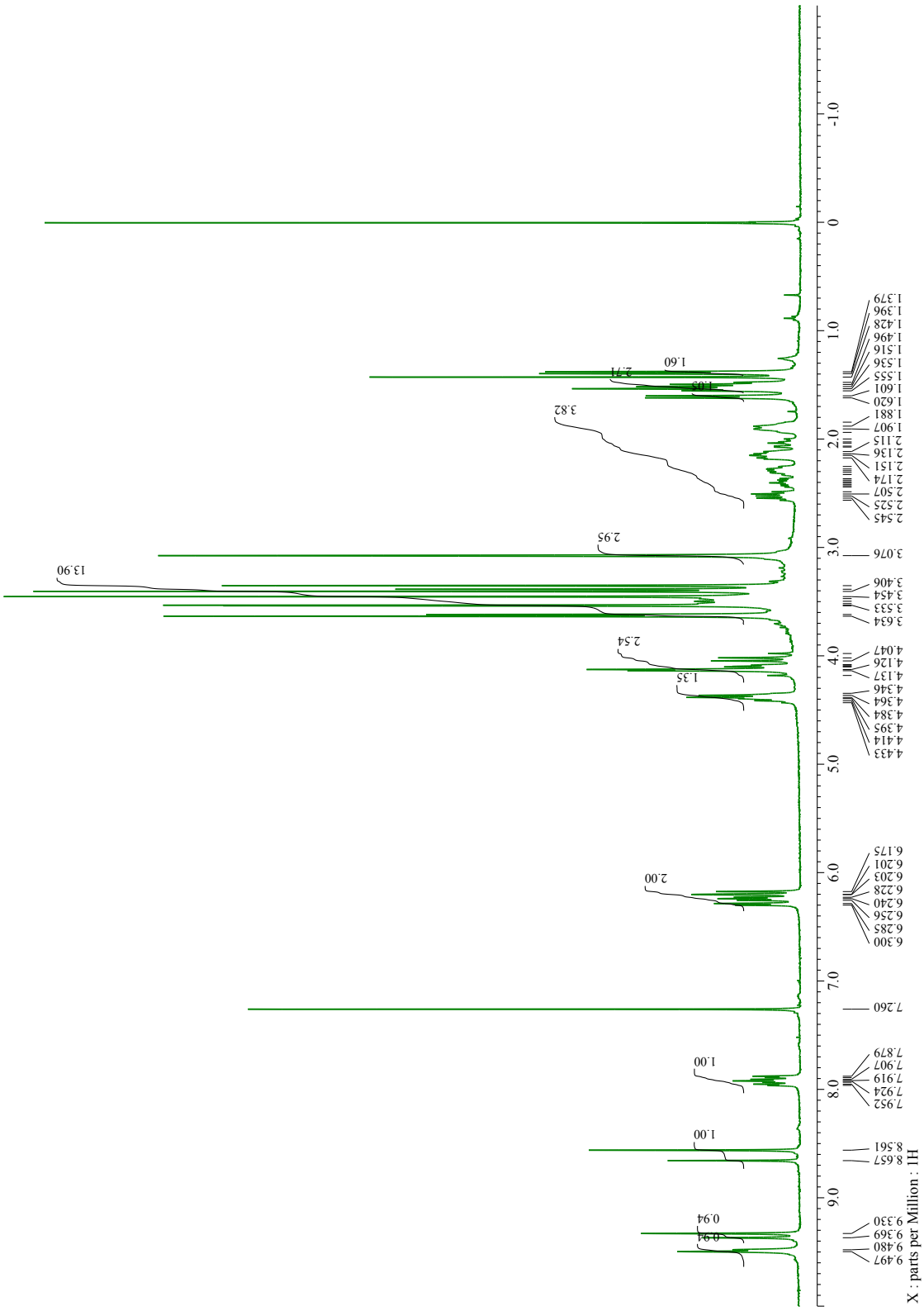

Figure S3. ^{1}H NMR (600 MHz) spectrum of methyl 13^{2}-(carboxymethyl)pheophorbides-*a*/*a*' [**H$_2$-3/3'(C$_1$)**] in $CDCl_3$.

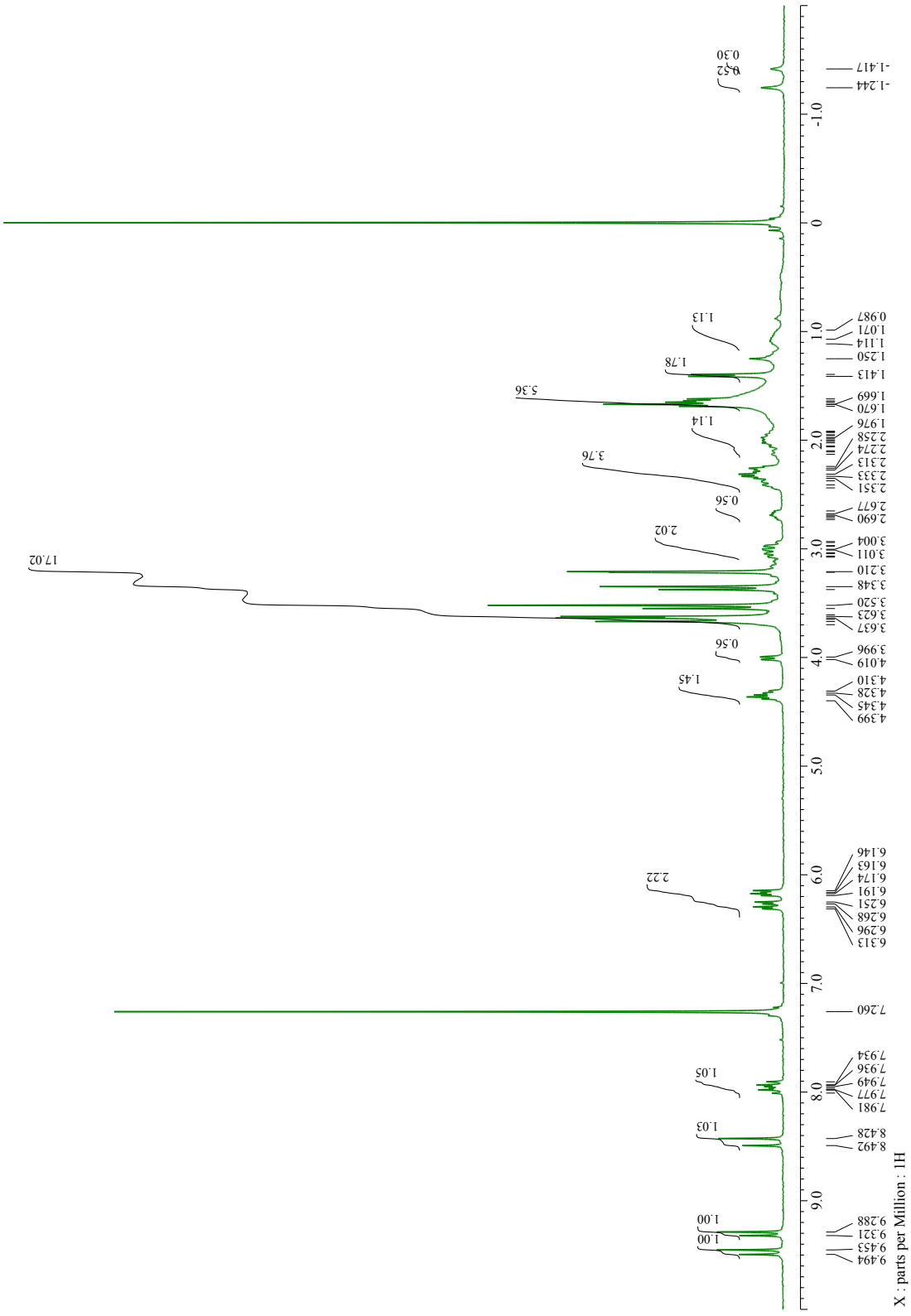

Figure S4. ^{1}H NMR (600 MHz) spectrum of methyl 13^{2}-(3-carboxypropyl)pheophorbides-*a*/*a*' [**H$_2$-3/3'(C$_3$)**] in $CDCl_3$.

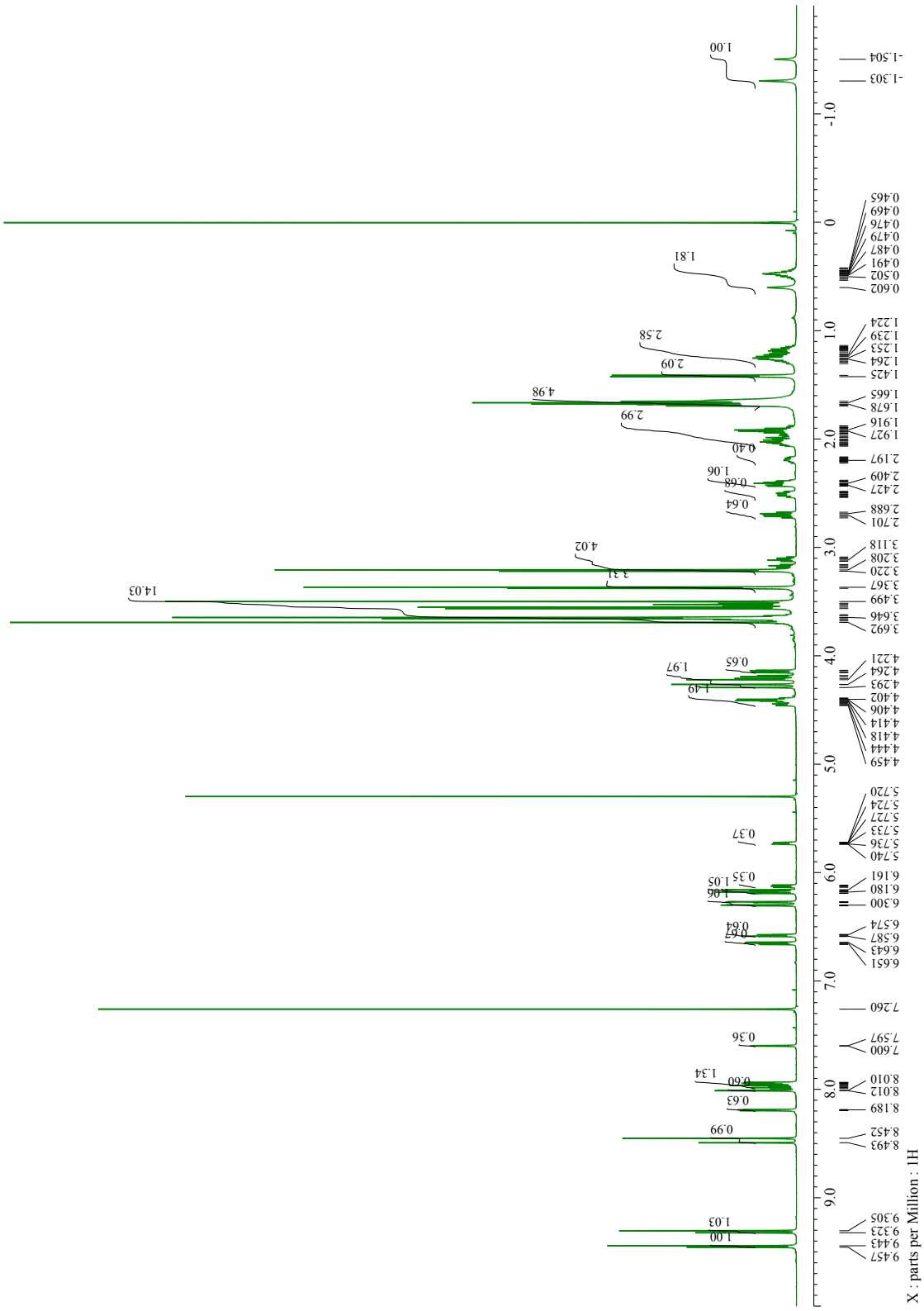

Figure S5. ^{1}H NMR (600 MHz) spectrum of methyl 13^{2}-[{3-(3-pyridyl)propyl}oxy-carbonylmethyl]pheophorbides-*a*/*a*' [**H$_2$-4/4'(C$_{1,3}$)**] in $CDCl_3$.

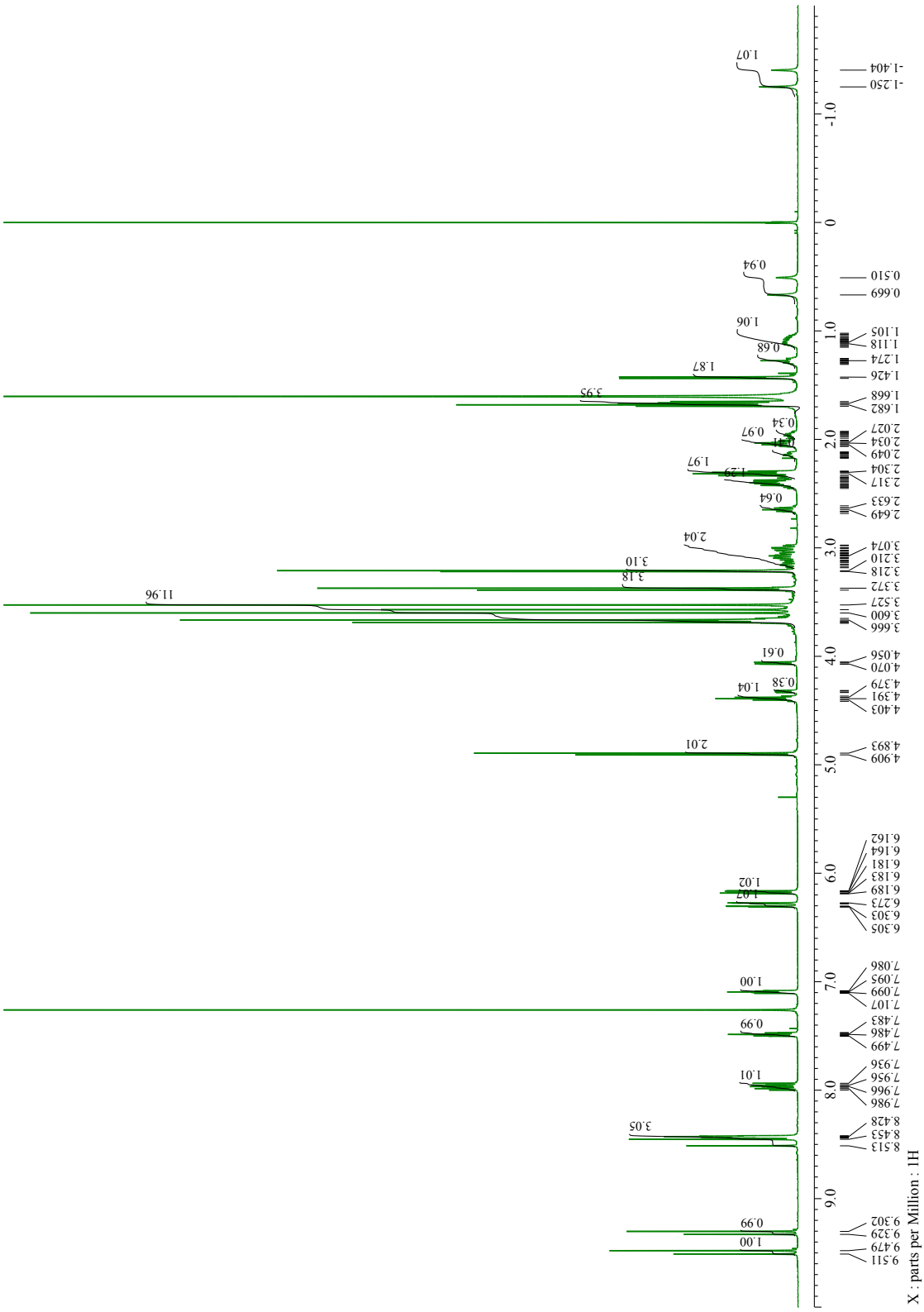

Figure S6. ^{1}H NMR (600 MHz) spectrum of methyl 13^{2}-[3-{(3-pyridyl)methyloxy-carbonyl}propyl]pheophorbides-*a*/*a*' [**H_2-4/4'($C_{3,1}$)**] in $CDCl_3$.

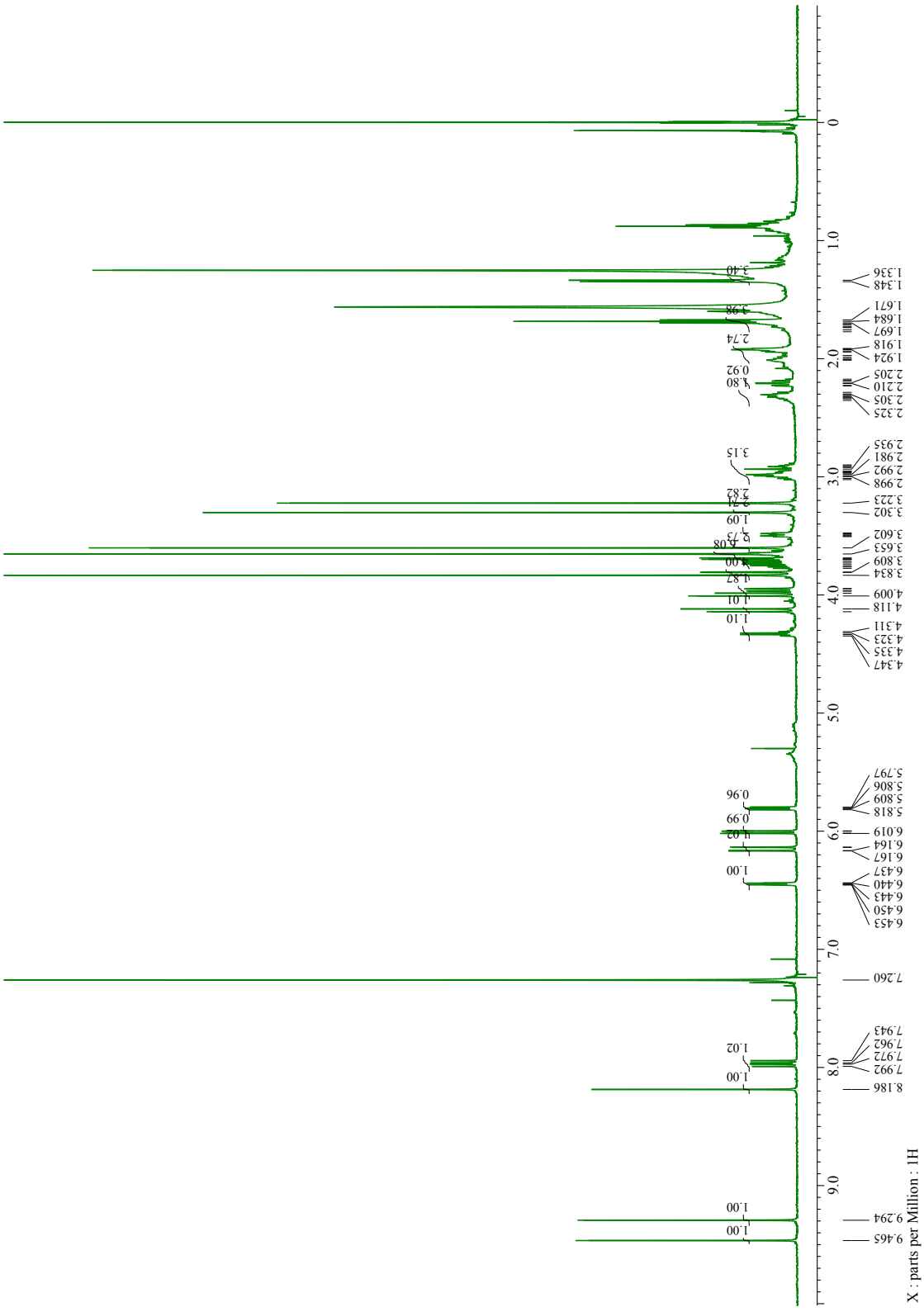

Figure S7. ^{1}H NMR (600 MHz) spectrum of zinc methyl 13^{2}-[{3-(3-pyridyl)propyl}oxy-carbonylmethyl]pheophorbide-*a* [**Zn-4(C$_{1,3}$)**] in $CDCl_3$.

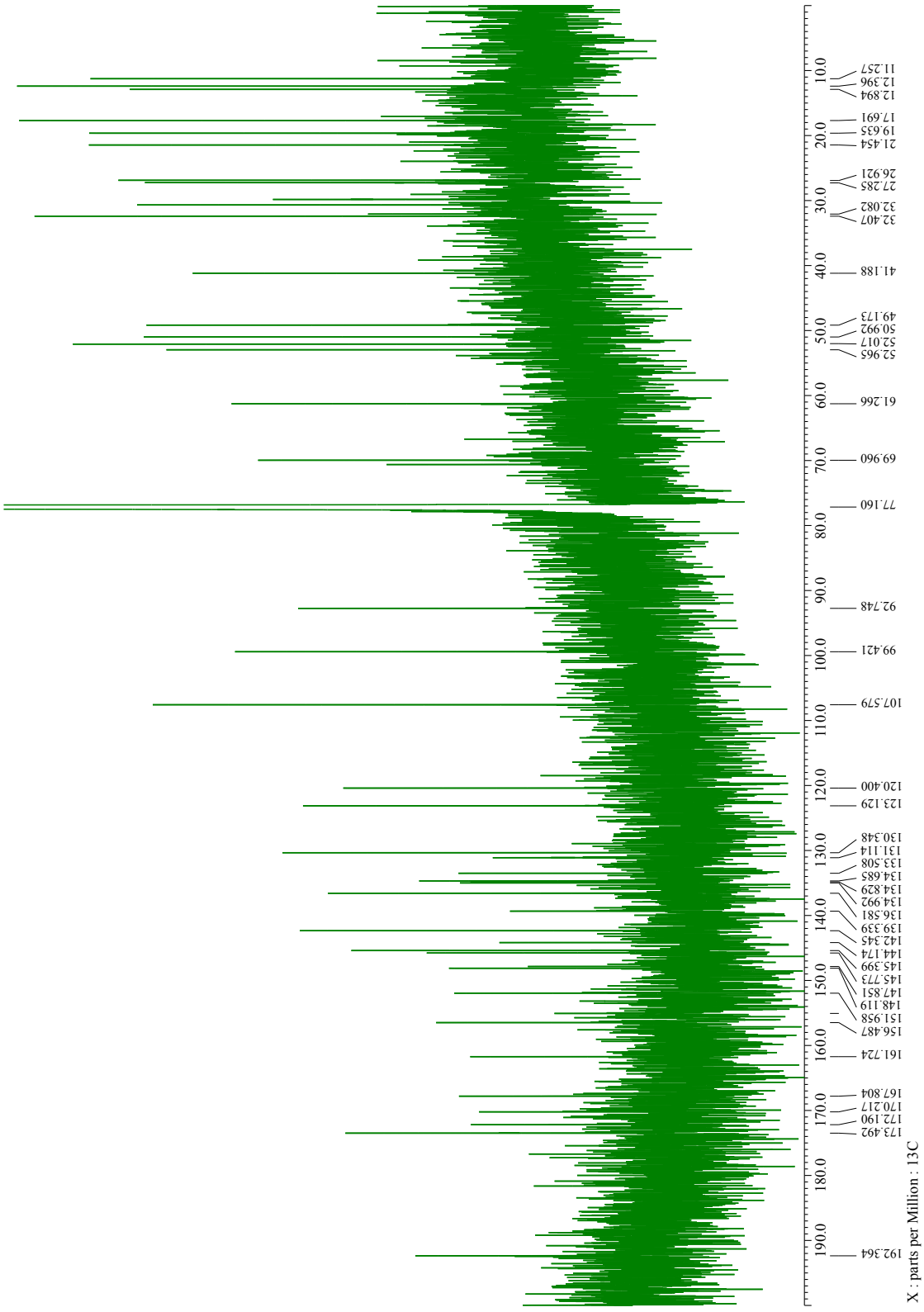

Figure S8. ^{13}C NMR (151 MHz) spectrum of zinc methyl 13^2-[{3-(3-pyridyl)propyl}oxy-carbonylmethyl]pheophorbide-*a* [**Zn-4(C$_{1,3}$)**] in $CDCl_3$.

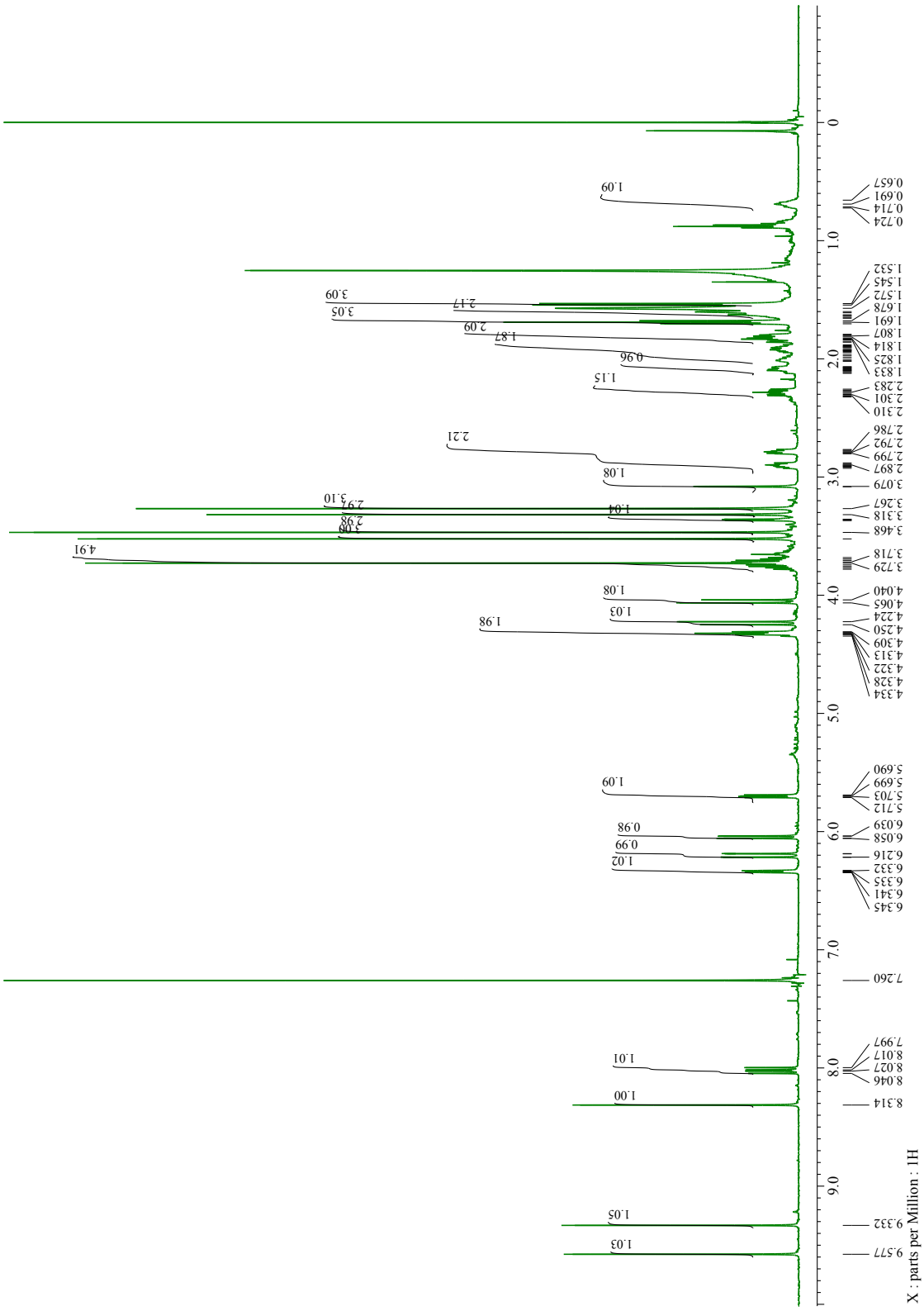

Figure S9. ^{1}H NMR (600 MHz) spectrum of zinc methyl 13^{2}-[{3-(3-pyridyl)propyl}oxy-carbonylmethyl]pheophorbide-*a*' [**Zn-4'($C_{1,3}$)**] in $CDCl_3$.

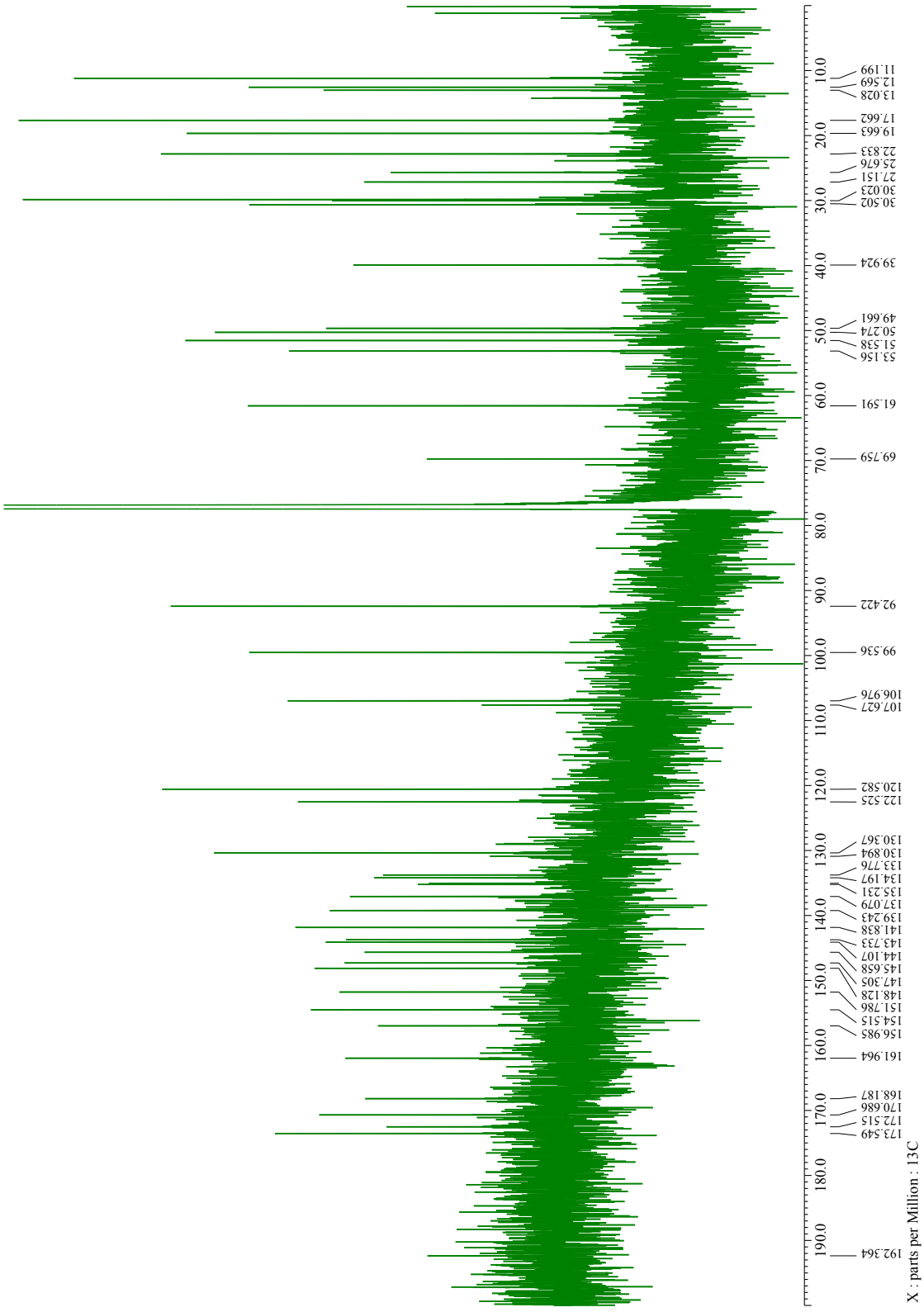

Figure S10. ^{13}C NMR (151 MHz) spectrum of zinc methyl 13^2-[{3-(3-pyridyl)propyl}-oxycarbonylmethyl]pheophorbide-*a*' [**Zn-4'($C_{1,3}$)**] in $CDCl_3$.

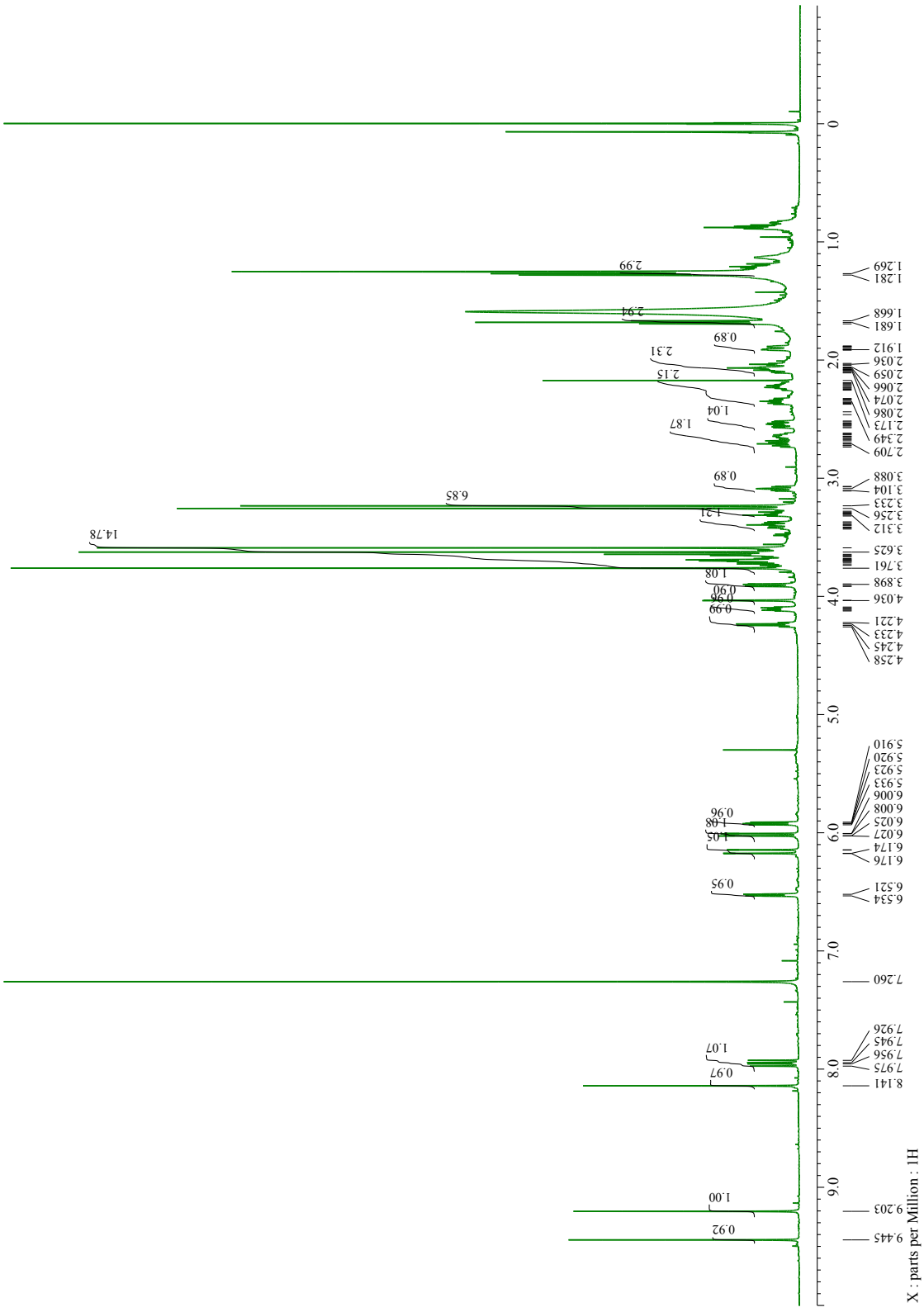

Figure S11. ^{1}H NMR (600 MHz) spectrum of zinc methyl 13^{2}-(2-[{2-(3-pyridyl)ethyl}-oxycarbonyl]ethyl)pheophorbide-*a* [**Zn-4(C$_{2,2}$)**] in $CDCl_3$.

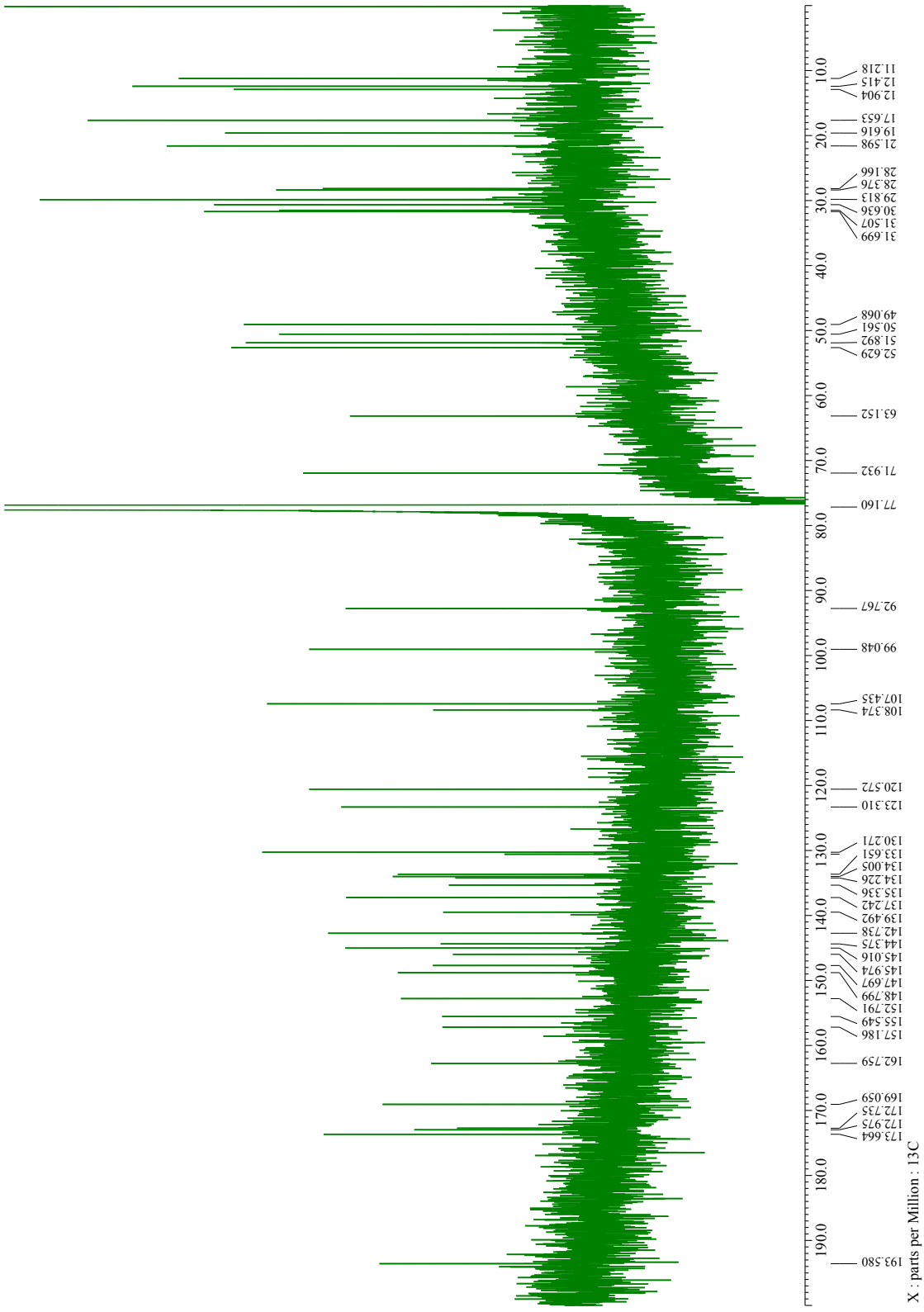

Figure S12. ^{13}C NMR (151 MHz) spectrum of zinc methyl 13^2-(2-[{2-(3-pyridyl)ethyl}-oxycarbonyl]ethyl)pheophorbide-*a* [**Zn-4(C$_{2,2}$)**] in $CDCl_3$.

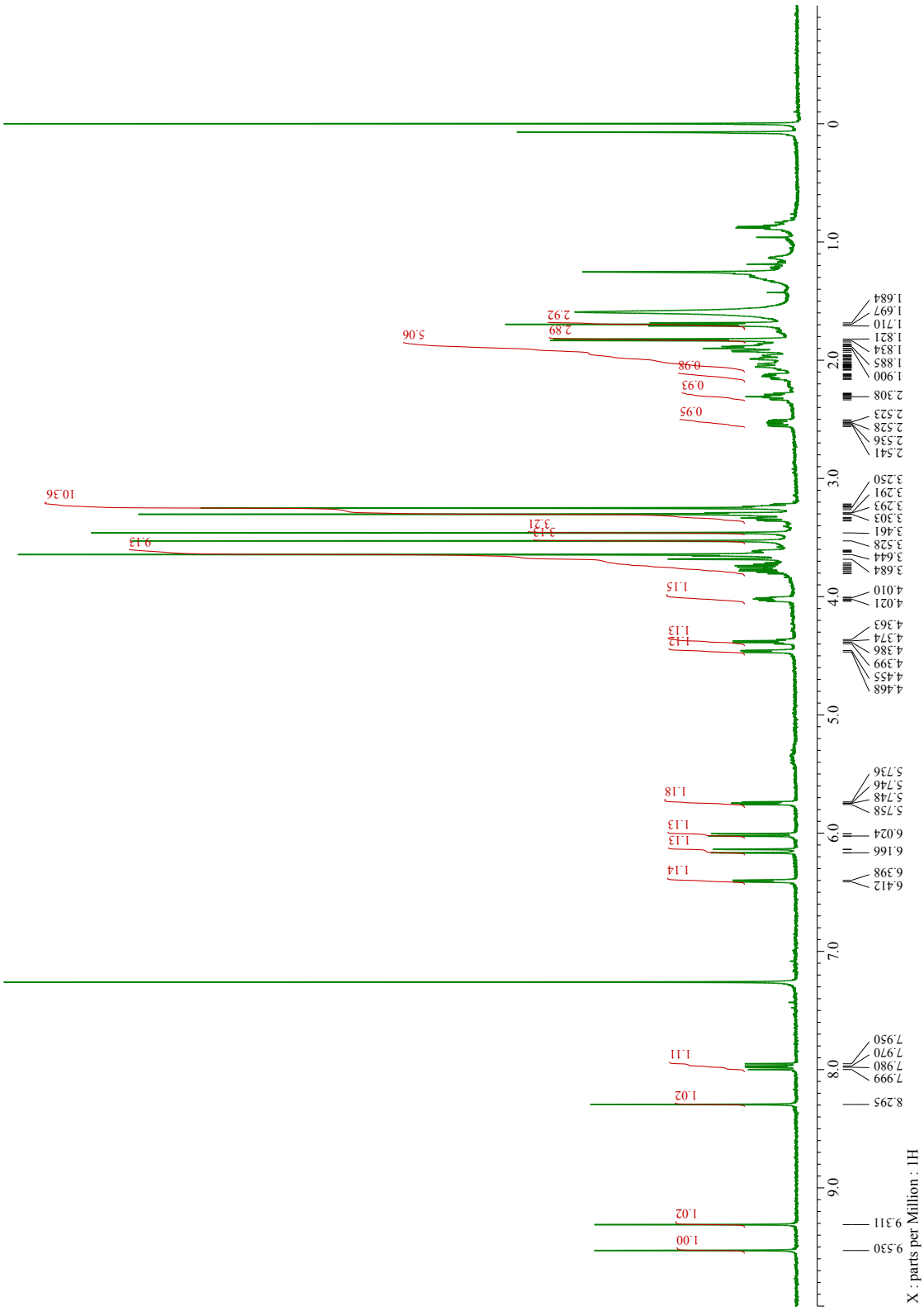

Figure S13. ^{1}H NMR (600 MHz) spectrum of zinc methyl 13^{2}-(2-[{2-(3-pyridyl)ethyl}-oxycarbonyl]ethyl)pheophorbide-*a*' [**Zn-4'($C_{2,2}$)**] in $CDCl_3$.

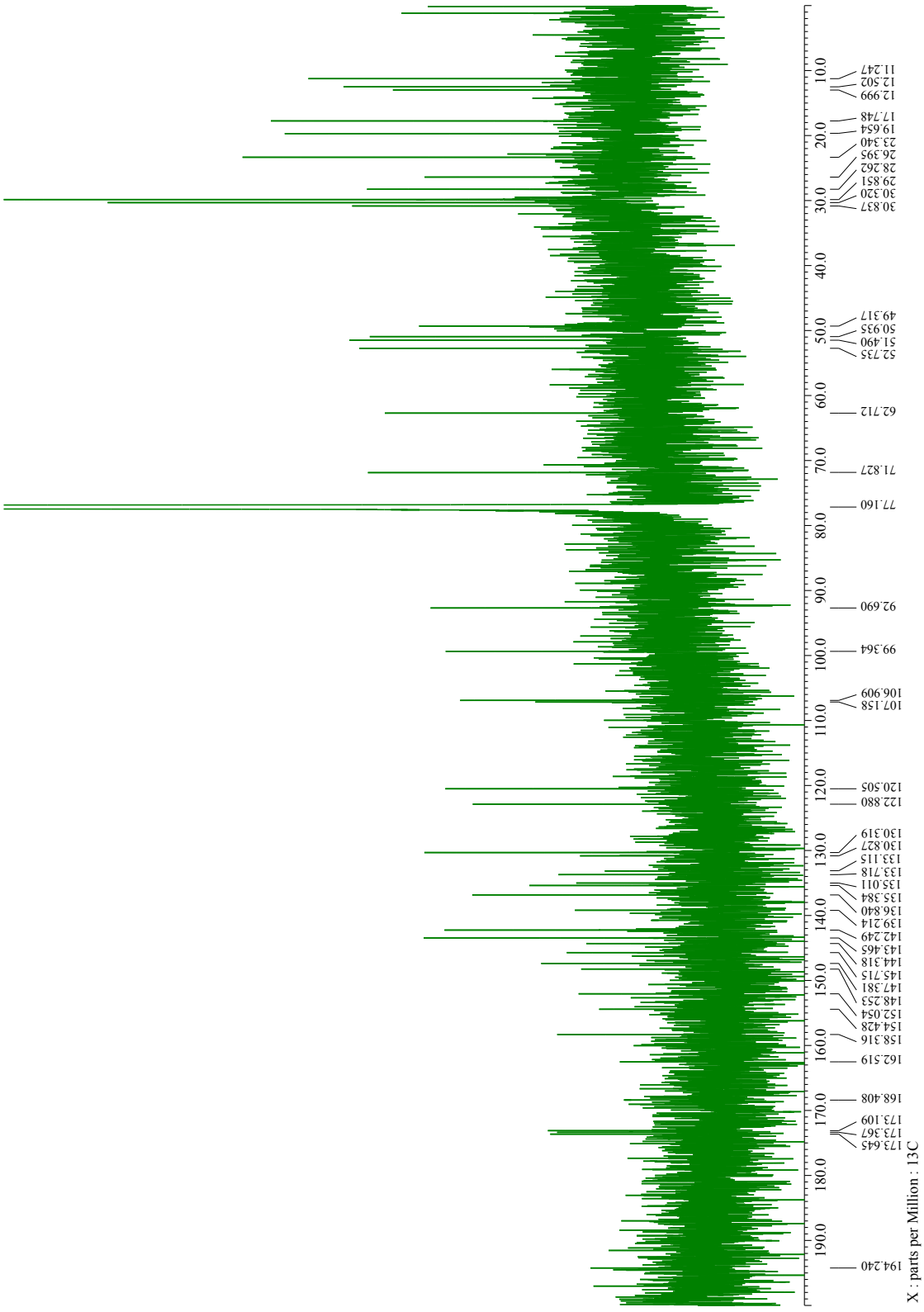

Figure S14. ^{13}C NMR (151 MHz) spectrum of zinc methyl 13^2-(2-[{2-(3-pyridyl)ethyl}-oxycarbonyl]ethyl)pheophorbide-*a*' [**Zn-4'($C_{2,2}$)**] in $CDCl_3$.

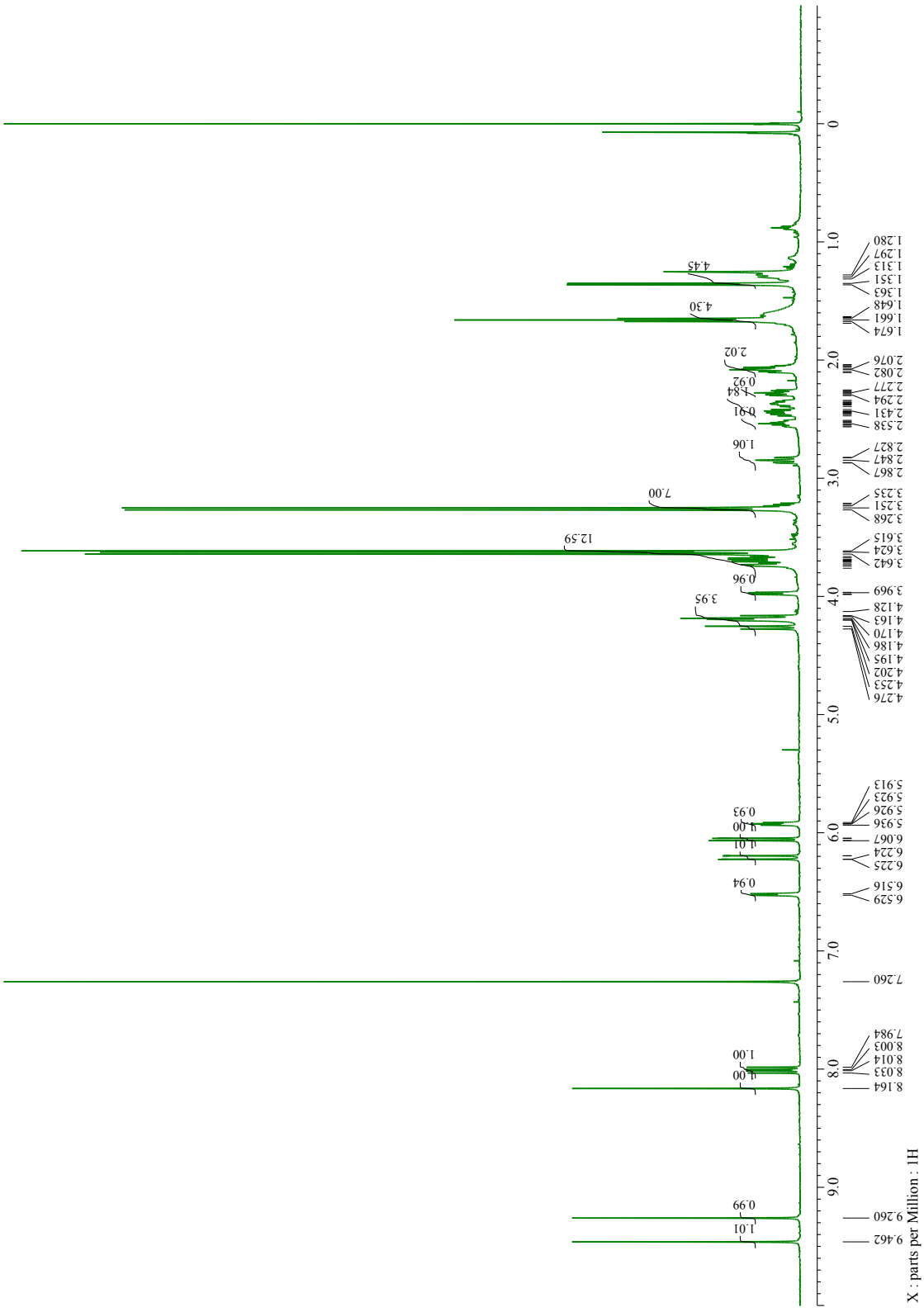

Figure S15. ^{1}H NMR (600 MHz) spectrum of zinc methyl 13^{2}-[3-{(3-pyridyl)methyloxy-carbonyl}propyl]pheophorbide-*a* [**Zn-4(C$_{3,1}$)**] in $CDCl_3$.

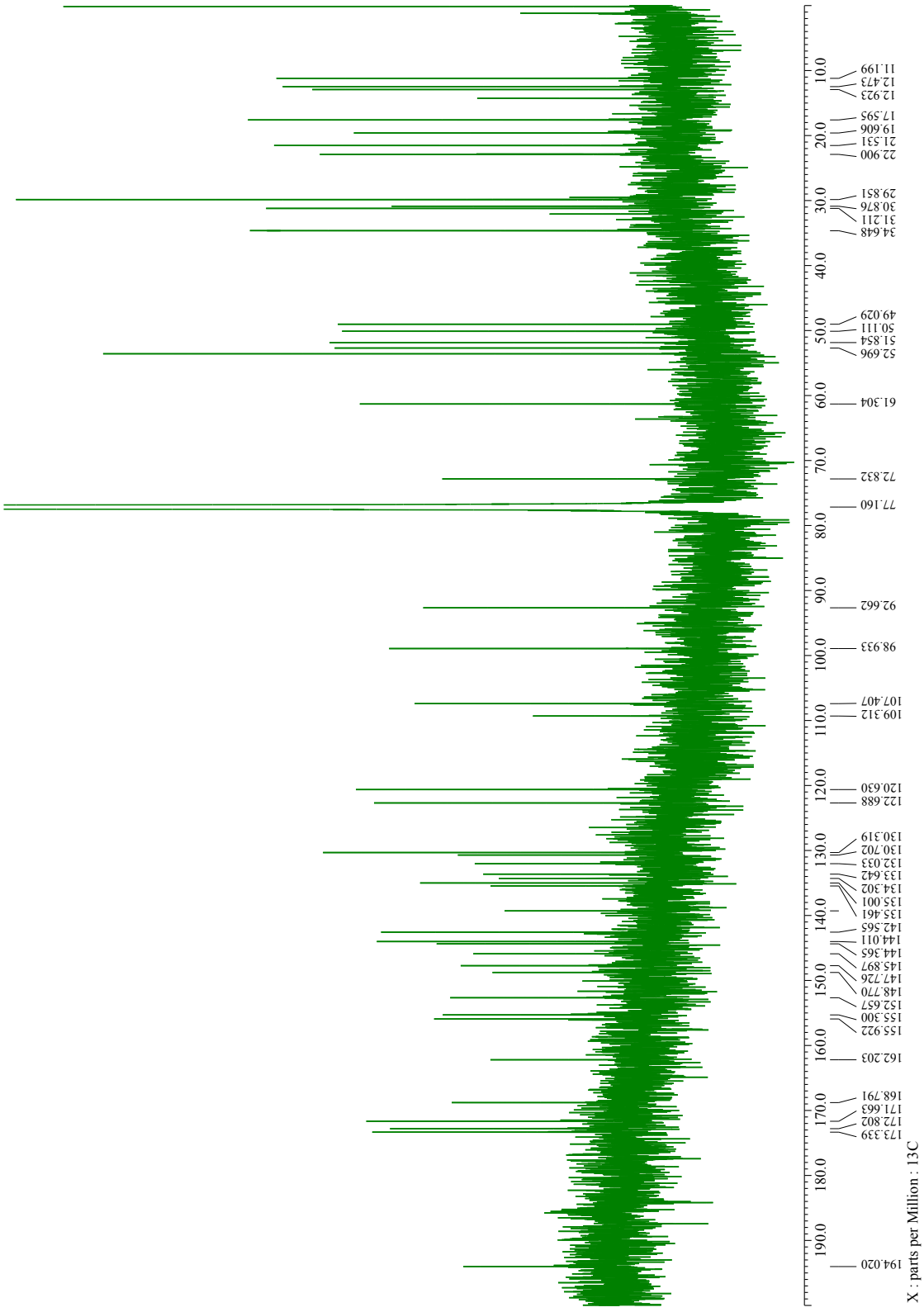

Figure S16. ^{13}C NMR (151 MHz) spectrum of zinc methyl 13^2-[3-{(3-pyridyl)methyl-oxycarbonyl}propyl]pheophorbide-*a* [**Zn-4(C$_{3,1}$)**] in $CDCl_3$.

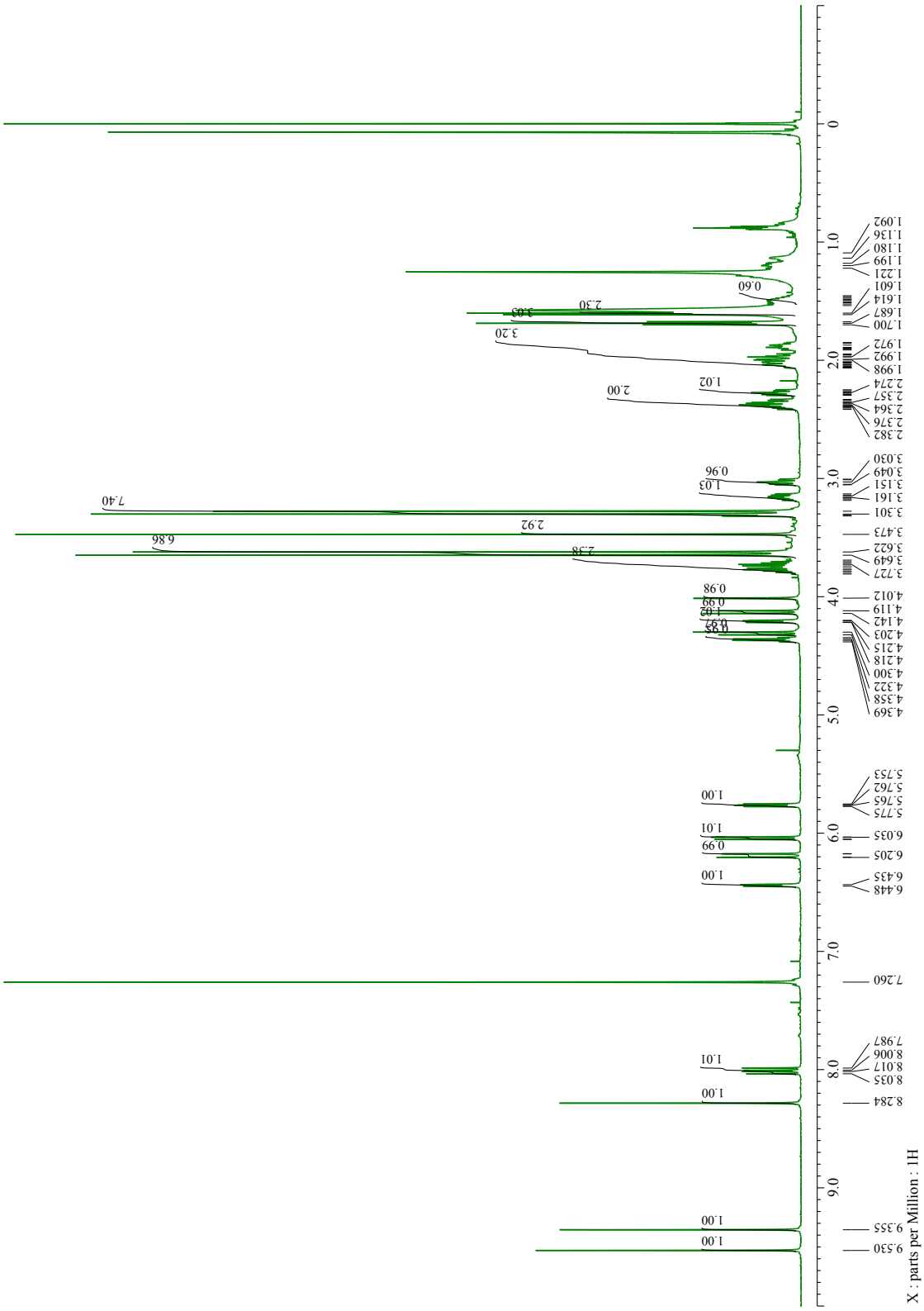

Figure S17. ^{1}H NMR (600 MHz) spectrum of zinc methyl 13^{2}-[3-{(3-pyridyl)methyl-oxycarbonyl}propyl]pheophorbide-*a*' [**Zn-4'($C_{3,1}$)**] in $CDCl_3$.

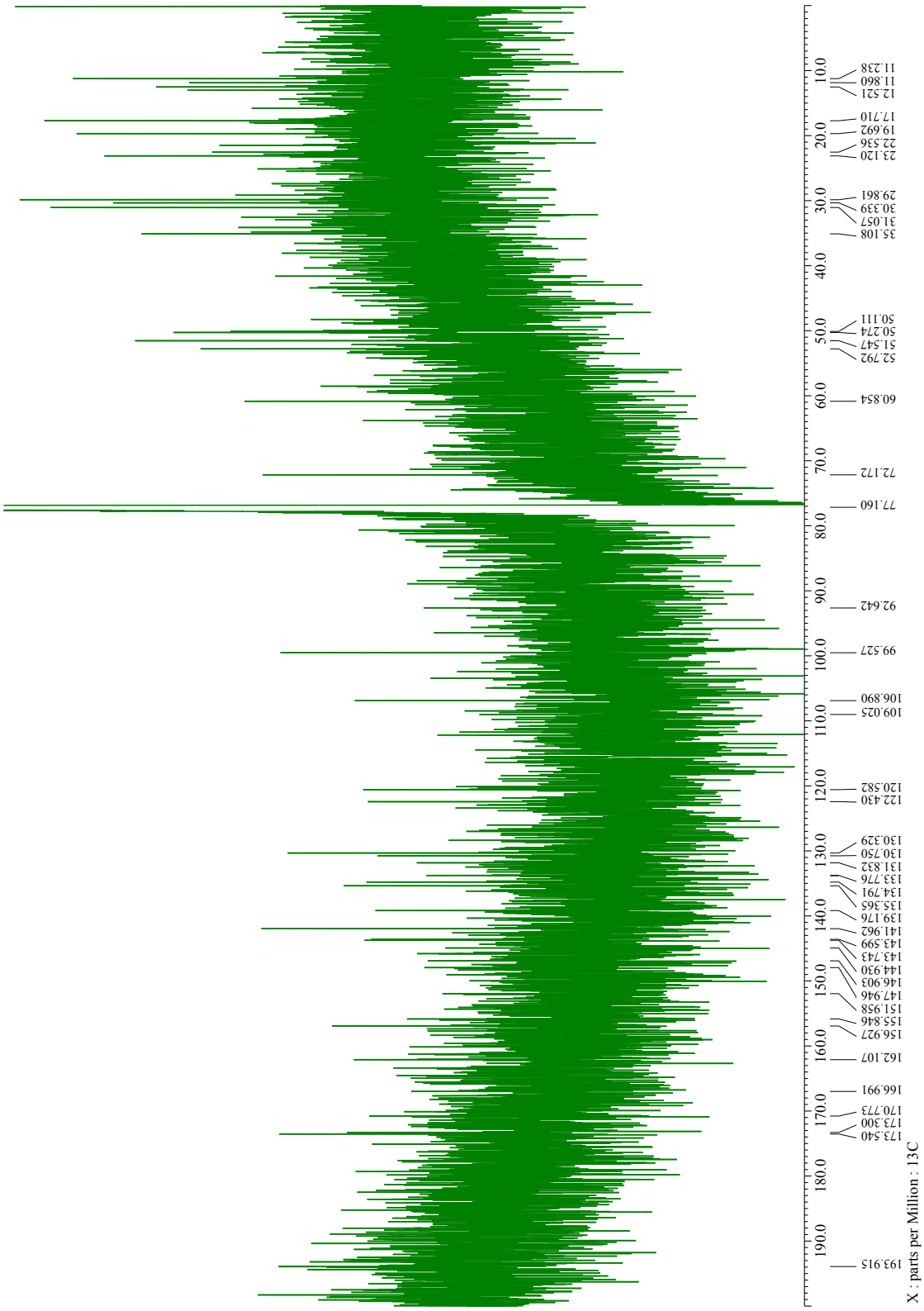

Figure S18. ^{13}C NMR (151 MHz) spectrum of zinc methyl 13^2-[3-{(3-pyridyl)methyl-oxycarbonyl}propyl]pheophorbide-*a*' [**Zn-4'($C_{3,1}$)**] in $CDCl_3$.

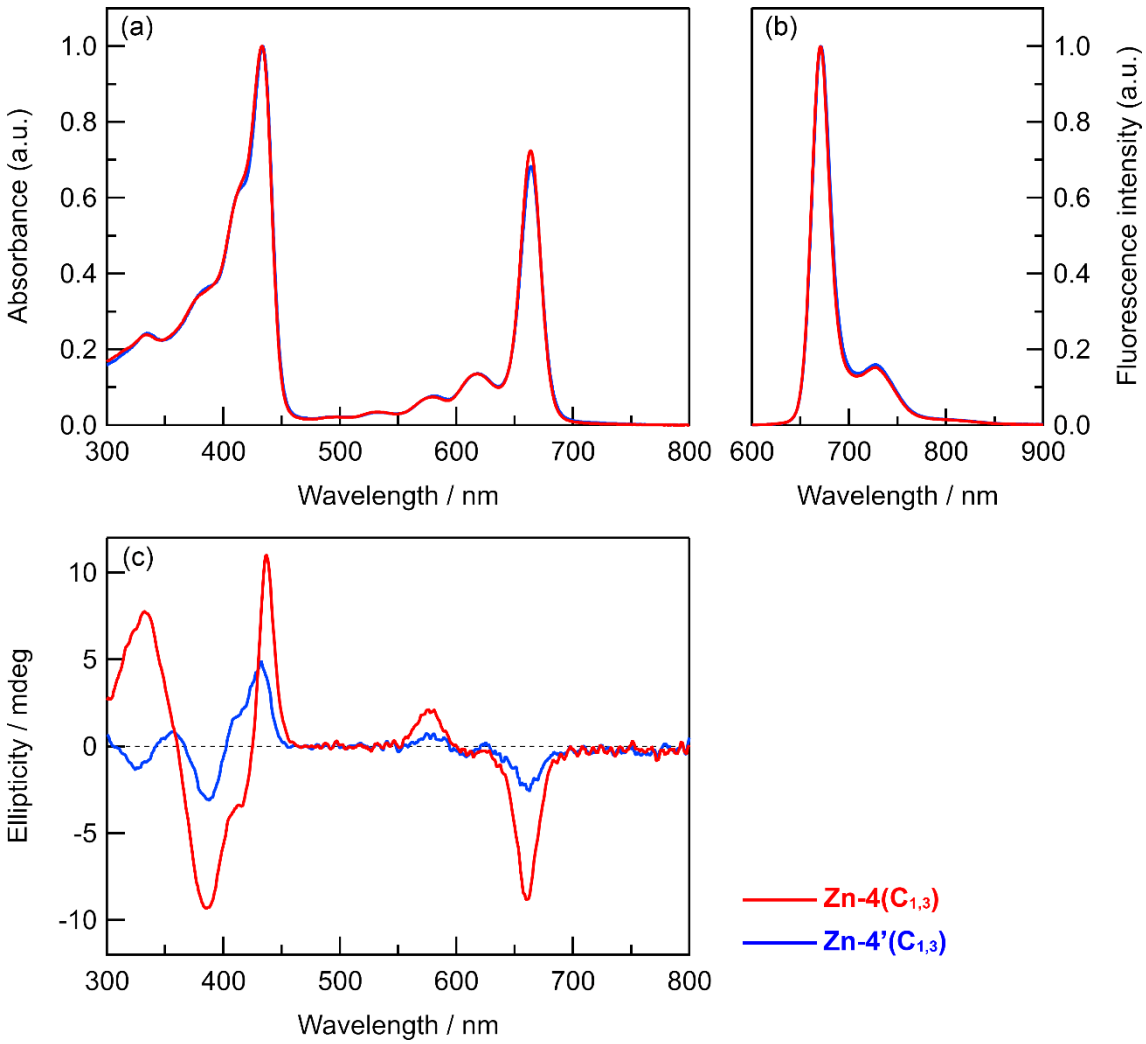

Fig. S19 (a) UV-visible absorption, (b) fluorescence emission (excited at Soret maxima), and (c) CD spectra of **Zn-4($C_{1,3}$)** (red line) and **Zn-4'($C_{1,3}$)** (blue line) in aerated $CHCl_3$ at rt; visible spectra were normalized at Soret maxima and fluorescence spectra were normalized at intense maxima.

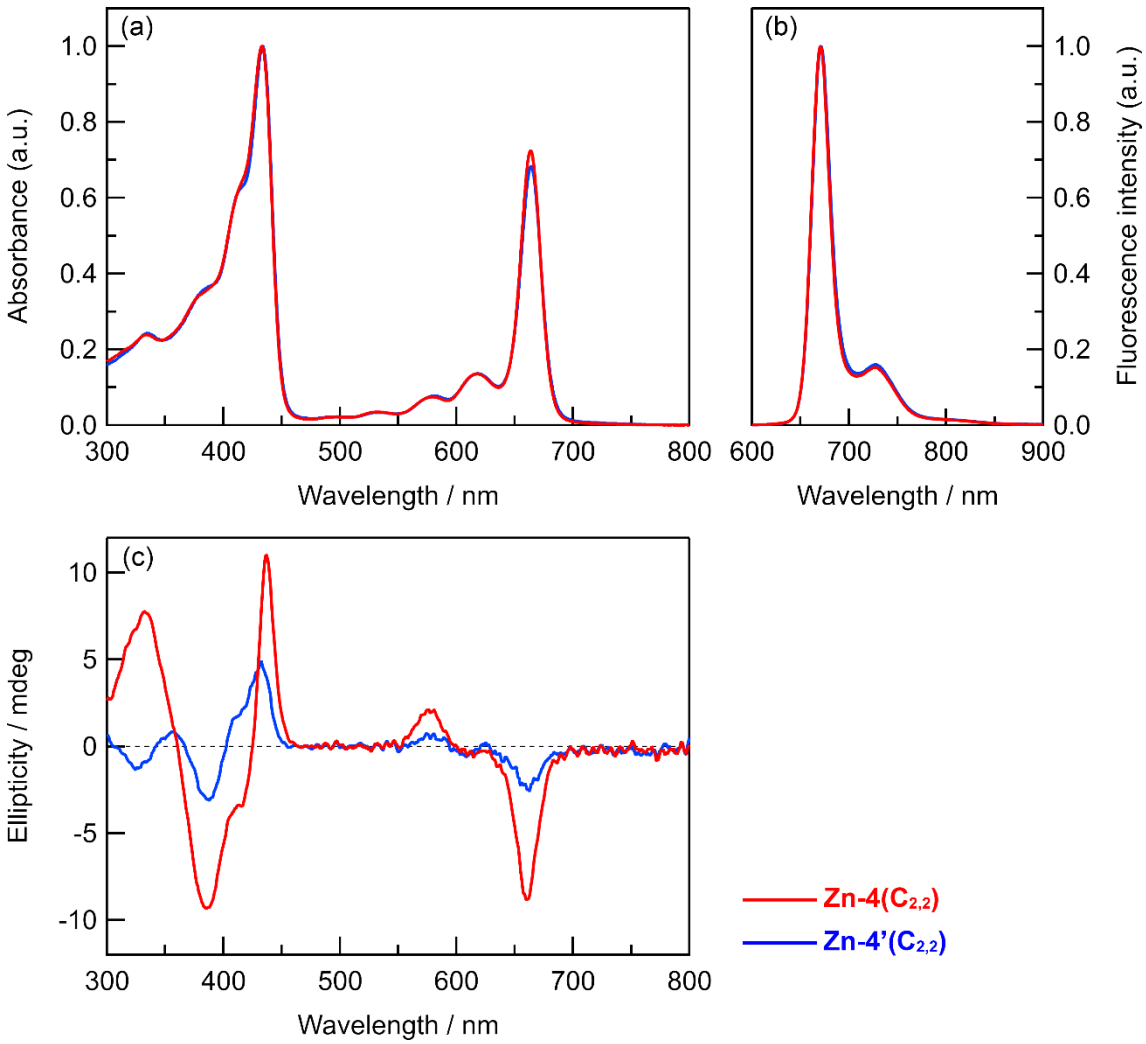

Fig. S20 (a) UV-visible absorption, (b) fluorescence emission (excited at Soret maxima), and (c) CD spectra of **Zn-4($C_{2,2}$)** (red line) and **Zn-4'($C_{2,2}$)** (blue line) in aerated $CHCl_3$ at rt; visible spectra were normalized at Soret maxima and fluorescence spectra were normalized at intense maxima.