Supporting Information

for

Dye-sensitized solar cells based on triazine-linked porphyrin dyads containing one or two carboxylic acid anchoring groups

Galateia E. Zervaki[†], Panagiotis A. Angaridis[†], Emmanouel N. Koukaras[‡], Ganesh D. Sharma[§], and Athanassios G. Coutsolelos[†]**

[†]Laboratory of Bioinorganic Chemistry, Department of Chemistry, University of Crete, Voutes Campus, P.O. Box 2208, 71003 Heraklion, Crete, Greece

[‡]Institute of Chemical Engineering Sciences, Foundation for Research & Technology Hellas (FORTH/ICE-HT), Stadiou Str. Platani, Patras, 26504 Greece

[§]R&D Center for Engineering and Science, JEC Group of Colleges, Jaipur Engineering College, Kukas, Jaipur (Raj.) 303101, India

Corresponding authors: coutsole@chemistry.uoc.gr, gdsharma273@gmail.com

Table of contents

Table S1: Cartesian coordinates of structures **5a** and **5b**.....**S3**

Figure S1: Total and partial density of states of structures **5a** and **5b**.....**S8**

Figure S2: ^{1}H NMR spectrum of **3a** **S9**

Figure S3: Focus on ^{1}H NMR spectrum of **3a**.....**S10**

Figure S4: ^{1}H NMR spectrum of **4a** **S11**

Figure S5: Focus on ^{1}H NMR spectrum of **4a**.....**S12**

Figure S6: ^{1}H NMR spectrum of **5a** **S13**

Figure S7: Focus on ^{1}H NMR spectrum of **5a** **S14**

Figure S8: ^{1}H NMR spectrum of **3b** **S15**

Figure S9: Focus on ^{1}H NMR spectrum of **3b** **S16**

Figure S10: ^{1}H NMR spectrum of **4b** **S17**

Figure S11: Focus on ^{1}H NMR spectrum of **4b** **S18**

Figure S12: ^{13}C NMR spectrum of **4b** **S19**

Figure S13: Focus on ^{13}C NMR spectrum of **4b**.....**S20**

Figure S14: ^{1}H NMR spectrum of **5b** **S21**

Figure S15: Focus on ^{1}H NMR spectrum of **5b** **S22**

Figure S16: ^{13}C NMR spectrum of **5b** **S23**

Figure S17: Focus on ^{13}C NMR spectrum of **5b**.....**S24**

Figure S18: Square wave voltammograms of **5a** and **5b**.....**S25**

Figure S19: FTIR spectra of **5a** and **5a/TiO_2** **S25**

Table S1. Cartesian coordinates of structures **5a** and **5b** optimized at the DFT/B3LYP/TZVP level of theory (units in Ångströms).

5a				5b			
atom	**x**	**Y**	**z**	**atom**	**x**	**y**	**z**
c	11.246	6.453	-4.980	c	11.309	6.329	-4.991
c	9.339	5.777	-3.526	c	9.389	5.663	-3.548
c	8.368	4.814	-9.517	c	8.373	4.896	-9.561
c	6.490	4.073	-8.056	c	6.473	4.182	-8.114
n	10.705	6.116	-6.197	n	10.756	6.040	-6.214
n	8.497	5.296	-4.498	n	8.529	5.240	-4.531
n	7.006	4.459	-6.843	n	7.005	4.516	-6.894
n	9.232	5.240	-8.538	n	9.251	5.271	-8.574
c	12.563	7.009	-5.182	c	12.640	6.853	-5.182
c	8.702	5.644	-2.237	c	8.755	5.505	-2.261
c	8.964	5.046	-10.812	c	8.974	5.142	-10.850
c	5.221	3.420	-7.847	c	5.180	3.572	-7.919
c	10.353	5.720	-9.168	c	10.386	5.732	-9.194
c	10.184	5.601	-10.597	c	10.211	5.654	-10.625
c	11.633	6.440	-7.155	c	11.690	6.362	-7.167
c	12.804	6.994	-6.517	c	12.878	6.865	-6.518
c	4.983	3.424	-6.510	c	4.945	3.550	-6.582
c	6.101	4.085	-5.880	c	6.090	4.150	-5.938
c	7.356	4.863	-3.870	c	7.378	4.821	-3.911
c	7.480	5.093	-2.449	c	7.516	4.997	-2.485
zn	8.860	5.278	-6.519	zn	8.885	5.267	-6.553
c	6.330	3.816	-10.517	c	6.304	3.986	-10.581
c	6.714	2.681	-11.237	c	6.655	2.857	-11.328
c	5.212	4.535	-10.951	c	5.206	4.746	-10.996
c	5.999	2.275	-12.360	c	5.927	2.496	-12.457
h	7.576	2.112	-10.910	h	7.501	2.257	-11.015
c	4.498	4.133	-12.075	c	4.480	4.389	-12.128
h	4.905	5.419	-10.403	h	4.925	5.625	-10.428
c	4.889	3.000	-12.783	c	4.838	3.262	-12.862
h	6.307	1.388	-12.902	h	6.210	1.614	-13.020
h	3.638	4.706	-12.400	h	3.636	4.994	-12.438
h	4.333	2.685	-13.658	h	4.272	2.983	-13.743
c	11.388	6.749	-2.522	c	11.466	6.554	-2.526
c	11.093	7.963	-1.893	c	11.199	7.753	-1.859
c	12.412	5.956	-1.997	c	12.477	5.725	-2.030
c	11.804	8.372	-0.770	c	11.923	8.115	-0.727
h	10.303	8.589	-2.292	h	10.420	8.407	-2.234
c	13.124	6.365	-0.874	c	13.201	6.085	-0.898
h	12.649	5.011	-2.473	h	12.693	4.791	-2.536
c	12.822	7.574	-0.256	c	12.926	7.281	-0.243
h	11.564	9.318	-0.297	h	11.704	9.050	-0.225

h	13.913	5.735	-0.479	h	13.979	5.428	-0.527
h	13.376	7.893	0.619	h	13.490	7.562	0.639
c	12.616	6.706	-9.419	c	12.676	6.655	-9.425
c	13.476	5.767	-9.994	c	13.506	5.705	-10.028
c	12.833	8.062	-9.681	c	12.936	8.010	-9.652
c	14.528	6.172	-10.811	c	14.568	6.099	-10.837
h	13.321	4.713	-9.796	h	13.317	4.651	-9.858
c	13.884	8.468	-10.499	c	13.996	8.405	-10.462
h	12.171	8.800	-9.244	h	12.298	8.756	-9.194
c	14.735	7.524	-11.066	c	14.816	7.451	-11.057
h	15.188	5.430	-11.245	h	15.203	5.349	-11.293
h	14.035	9.523	-10.694	h	14.180	9.460	-10.630
h	15.553	7.841	-11.702	h	15.642	7.758	-11.687
c	5.106	3.848	-3.619	c	5.097	3.874	-3.681
c	3.864	4.489	-3.668	c	3.888	4.577	-3.676
c	5.250	2.787	-2.721	c	5.200	2.760	-2.845
c	2.819	4.089	-2.850	c	2.837	4.189	-2.860
h	3.718	5.320	-4.348	h	3.775	5.449	-4.310
c	4.210	2.370	-1.898	c	4.152	2.352	-2.028
h	6.197	2.264	-2.668	h	6.119	2.187	-2.839
c	2.976	3.024	-1.952	c	2.953	3.072	-2.021
h	1.870	4.613	-2.898	h	1.917	4.764	-2.860
h	4.347	1.548	-1.214	h	4.252	1.483	-1.399
c	7.098	4.255	-9.308	c	7.086	4.373	-9.364
c	6.237	4.285	-4.495	c	6.238	4.302	-4.549
c	10.622	6.306	-3.732	c	10.685	6.164	-3.745
c	11.483	6.267	-8.540	c	11.532	6.228	-8.555
c	0.283	1.030	1.437	c	0.286	1.114	1.400
c	1.712	1.864	-0.091	n	1.272	0.469	2.042
n	0.441	1.799	0.366	c	2.492	0.622	1.510
c	-2.223	1.340	1.672	c	1.696	1.942	-0.138
c	-3.268	1.029	2.555	n	0.426	1.870	0.314
c	-2.518	2.077	0.520	n	2.752	1.347	0.397
c	-4.566	1.435	2.292	c	-2.227	1.394	1.634
h	-3.055	0.467	3.458	c	-3.268	1.069	2.517
c	-3.826	2.480	0.275	c	-2.533	2.127	0.483
h	-1.727	2.321	-0.169	c	-4.571	1.460	2.257
c	-4.874	2.170	1.143	h	-3.048	0.508	3.419
h	-5.354	1.181	2.991	c	-3.845	2.517	0.240
h	-4.035	3.045	-0.627	h	-1.745	2.380	-0.207
c	-6.277	2.604	0.851	c	-4.889	2.195	1.110
c	-6.574	3.971	0.983	h	-5.354	1.197	2.957
c	-7.194	1.613	0.462	h	-4.062	3.080	-0.660
n	-7.788	4.561	0.731	c	-6.296	2.618	0.825
c	-5.639	4.978	1.428	c	-6.604	3.982	0.957
n	-8.519	1.812	0.164	c	-7.208	1.619	0.444

c	-6.875	0.214	0.297	n	-7.824	4.562	0.713
c	-7.650	5.902	0.993	c	-5.674	4.997	1.395
c	-6.300	6.165	1.430	n	-8.538	1.807	0.156
c	-9.047	0.591	-0.175	c	-6.879	0.222	0.277
c	-8.015	-0.414	-0.087	c	-7.695	5.904	0.974
c	-8.649	6.879	0.862	c	-6.345	6.178	1.401
c	-10.373	0.338	-0.560	c	-9.058	0.580	-0.177
c	-9.969	6.629	0.458	c	-8.018	-0.416	-0.097
c	-8.277	8.301	1.176	c	-8.704	6.872	0.851
c	-11.372	1.314	-0.687	c	-10.385	0.317	-0.550
c	-10.751	-1.086	-0.862	c	-10.024	6.612	0.457
n	-10.505	5.403	0.149	c	-8.341	8.298	1.162
c	-10.980	7.645	0.296	c	-11.393	1.284	-0.671
c	-8.449	8.805	2.479	c	-10.754	-1.111	-0.847
c	-7.753	9.131	0.169	n	-10.553	5.381	0.152
n	-11.221	2.663	-0.475	c	-11.045	7.620	0.302
c	-12.737	1.042	-1.068	c	-8.505	8.800	2.466
c	-10.639	-1.583	-2.172	c	-7.832	9.132	0.150
c	-11.214	-1.924	0.169	n	-11.251	2.635	-0.463
c	-11.816	5.610	-0.199	c	-12.759	1.001	-1.042
c	-12.114	7.021	-0.113	c	-10.651	-1.609	-2.158
c	-8.096	10.128	2.747	c	-11.201	-1.951	0.189
c	-7.414	10.448	0.482	c	-11.868	5.578	-0.186
c	-12.438	3.249	-0.713	c	-12.177	6.986	-0.098
c	-13.394	2.230	-1.081	c	-8.160	10.125	2.732
c	-10.995	-2.908	-2.428	c	-7.500	10.452	0.460
c	-11.560	-3.242	-0.132	c	-12.475	3.211	-0.694
c	-12.728	4.619	-0.598	c	-13.425	2.184	-1.053
c	-7.580	10.968	1.763	c	-10.999	-2.937	-2.408
h	-8.227	10.509	3.755	c	-11.540	-3.272	-0.107
h	-7.007	11.083	-0.299	c	-12.774	4.579	-0.578
c	-11.461	-3.754	-1.424	c	-7.659	10.970	1.744
h	-10.903	-3.288	-3.440	h	-8.285	10.506	3.741
h	-11.915	-3.885	0.667	h	-7.105	11.090	-0.324
c	-14.121	5.058	-0.926	c	-11.449	-3.785	-1.398
c	-15.008	5.446	0.084	h	-10.913	-3.318	-3.421
c	-14.566	5.091	-2.253	h	-11.883	-3.917	0.697
c	-16.300	5.854	-0.217	c	-14.173	5.007	-0.899
h	-14.679	5.421	1.116	c	-15.057	5.389	0.116
c	-15.854	5.501	-2.561	c	-14.626	5.034	-2.223
h	-13.889	4.798	-3.047	c	-16.354	5.787	-0.178
c	-16.733	5.885	-1.545	h	-14.722	5.368	1.146
h	-16.977	6.145	0.575	c	-15.919	5.435	-2.525
h	-16.196	5.533	-3.588	h	-13.952	4.745	-3.020
zn	-9.508	3.609	0.143	c	-16.794	5.814	-1.504
n	1.855	2.671	-1.183	h	-17.028	6.075	0.617

h	0.990	3.125	-1.434	h	-16.267	5.463	-3.549
n	-0.947	0.866	2.010	zn	-9.541	3.596	0.140
h	-0.901	0.277	2.829	n	1.831	2.726	-1.252
c	-18.102	6.316	-1.924	h	0.965	3.179	-1.503
o	-18.528	6.360	-3.055	n	-0.946	0.938	1.973
o	-18.864	6.668	-0.856	h	-0.890	0.362	2.800
h	-19.730	6.929	-1.206	c	-18.169	6.234	-1.875
c	-7.551	8.627	-1.240	o	-18.602	6.276	-3.003
h	-6.871	7.773	-1.268	o	-18.928	6.582	-0.803
h	-8.493	8.296	-1.686	h	-19.797	6.837	-1.149
h	-7.135	9.411	-1.874	c	-7.639	8.630	-1.261
c	-9.002	7.943	3.589	h	-6.955	7.779	-1.294
h	-10.004	7.578	3.352	h	-8.583	8.295	-1.699
h	-8.377	7.065	3.764	h	-7.232	9.416	-1.897
h	-9.060	8.507	4.520	c	-9.041	7.934	3.581
c	-7.237	12.405	2.070	h	-10.042	7.560	3.353
h	-8.106	13.055	1.925	h	-8.407	7.060	3.751
h	-6.911	12.524	3.105	h	-9.096	8.497	4.513
h	-6.442	12.772	1.418	c	-7.325	12.409	2.048
c	-10.140	-0.717	-3.304	h	-8.196	13.055	1.894
h	-10.113	-1.281	-4.237	h	-7.007	12.534	3.084
h	-10.780	0.155	-3.454	h	-6.527	12.778	1.401
h	-9.133	-0.341	-3.107	c	-10.168	-0.741	-3.295
c	-11.341	-1.429	1.589	h	-10.147	-1.305	-4.228
h	-10.378	-1.100	1.988	h	-10.816	0.127	-3.440
h	-12.020	-0.575	1.658	h	-9.162	-0.359	-3.109
h	-11.723	-2.217	2.239	c	-11.319	-1.454	1.610
c	-11.875	-5.171	-1.732	h	-10.355	-1.118	1.999
h	-12.932	-5.220	-2.012	h	-12.004	-0.606	1.684
h	-11.299	-5.583	-2.563	h	-11.689	-2.245	2.264
h	-11.737	-5.823	-0.867	c	-11.854	-5.206	-1.700
h	8.501	4.824	-11.759	h	-12.913	-5.263	-1.974
h	10.903	5.915	-11.337	h	-11.280	-5.616	-2.534
h	13.692	7.327	-7.029	h	-11.707	-5.855	-0.835
h	13.214	7.364	-4.400	n	3.540	0.019	2.126
h	9.135	5.938	-1.296	c	4.908	0.105	1.617
h	6.728	4.865	-1.713	c	3.362	-0.865	3.279
h	4.604	2.997	-8.622	c	5.878	0.520	2.728
h	4.137	3.002	-5.994	h	4.923	0.817	0.799
h	-13.065	7.473	-0.342	c	4.296	-0.465	4.424
h	-10.833	8.700	0.467	h	3.583	-1.895	2.965
h	-5.916	7.133	1.707	c	5.753	-0.391	3.954
h	-4.615	4.795	1.708	h	6.898	0.499	2.333
h	-5.901	-0.223	0.447	h	4.188	-1.186	5.239
h	-8.150	-1.462	-0.304	h	6.102	-1.399	3.696
h	-13.136	0.066	-1.289	h	2.320	-0.824	3.580

h	-14.432	2.403	-1.312	h	3.982	0.510	4.812
n	1.263	0.352	2.069	h	6.398	-0.034	4.761
c	2.470	0.496	1.519	h	5.665	1.555	3.014
n	2.759	1.236	0.429	h	5.199	-0.877	1.218
c	4.738	-1.528	3.636	h	8.503	4.958	-11.801
o	5.766	-1.304	3.050	h	10.937	5.964	-11.358
o	4.658	-2.314	4.729	h	13.774	7.187	-7.023
h	5.552	-2.638	4.925	h	13.303	7.169	-4.394
n	3.508	-0.151	2.091	h	9.201	5.755	-1.313
h	4.425	-0.033	1.688	h	6.761	4.765	-1.752
c	3.381	-0.979	3.261	h	4.546	3.193	-8.703
h	2.981	-0.423	4.115	h	4.084	3.149	-6.074
h	2.697	-1.817	3.097	h	-13.133	7.430	-0.321
–	–	–	–	h	-10.905	8.675	0.471
–	–	–	–	h	-5.967	7.150	1.675
–	–	–	–	h	-4.647	4.822	1.668
–	–	–	–	h	-5.901	-0.206	0.420
–	–	–	–	h	-8.146	-1.465	-0.311
–	–	–	–	h	-13.152	0.021	-1.258
–	–	–	–	h	-14.466	2.348	-1.277

Figure S1. Total and partial density of states of structures of (a) **5a** and (b) **5b,** performed at the DFT/B3LYP/TZVP level of theory.

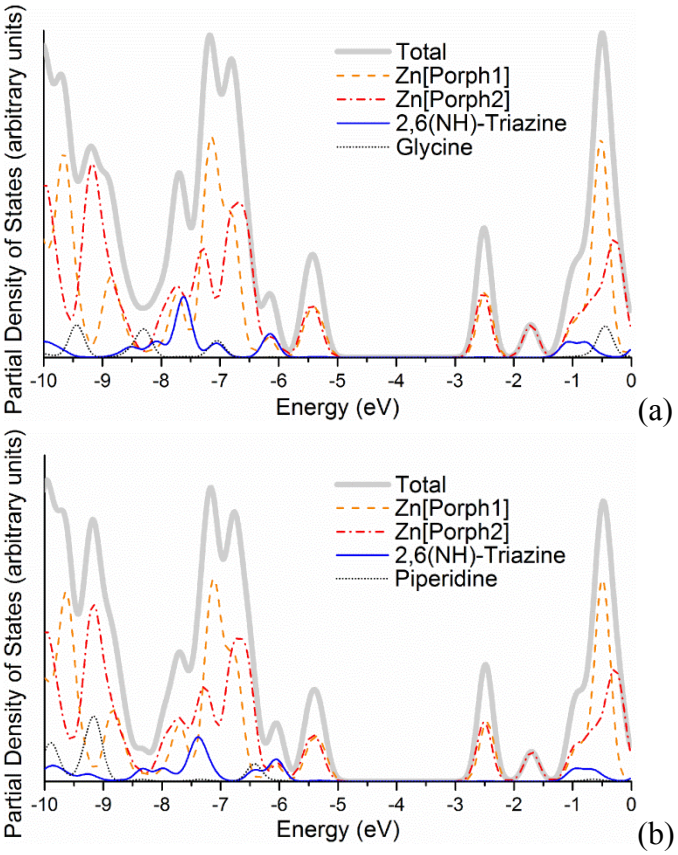

Figure S2. ^{1}H NMR spectrum of **3a** (300 MHz, $CDCl_3$).

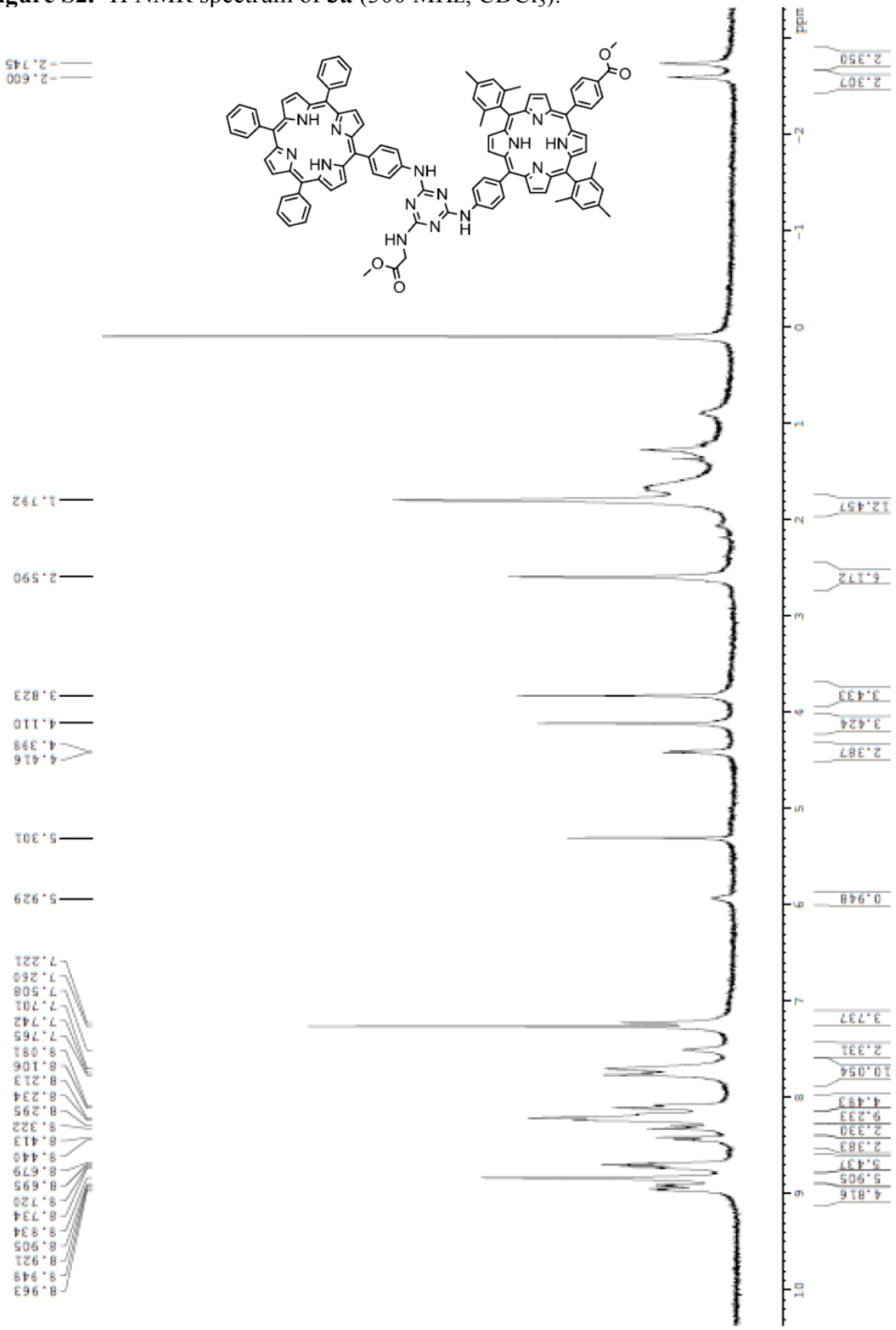

Figure S3. Focus on ^{1}H NMR spectrum of **3a** (300 MHz, $CDCl_3$).

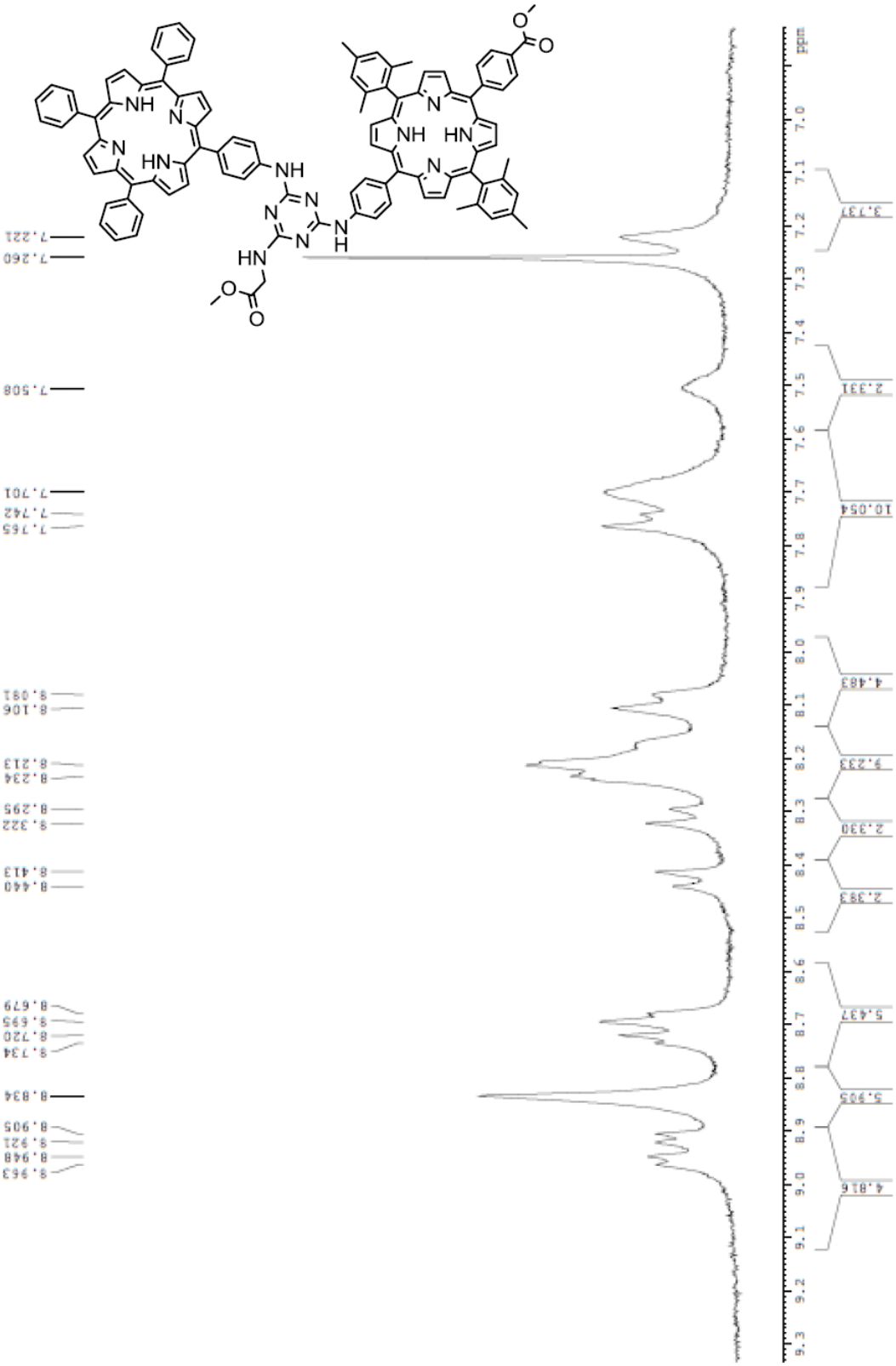

Figure S4. ^{1}H NMR spectrum of **4a** (300 MHz, $CDCl_3$).

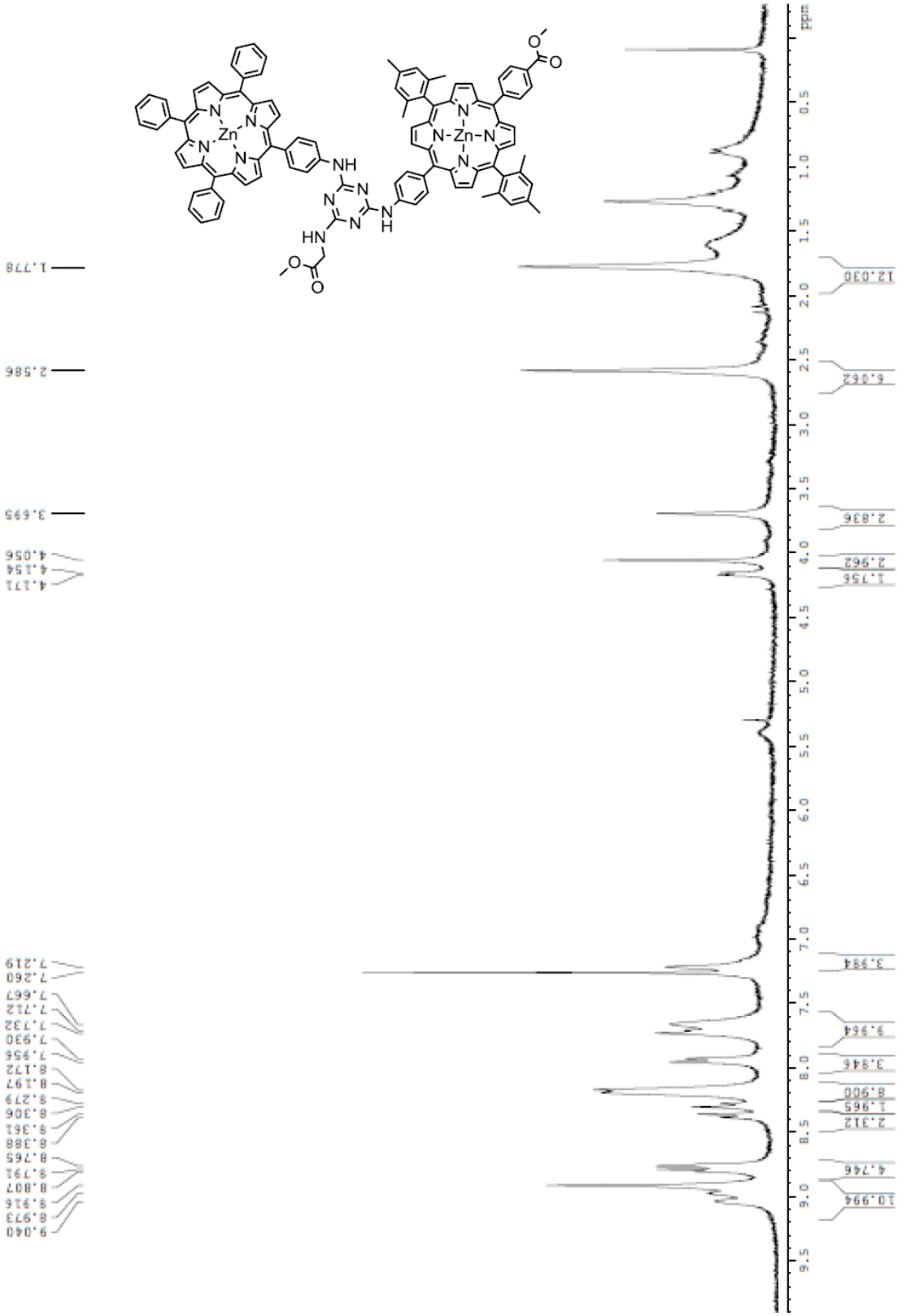

Figure S5. Focus on ^{1}H NMR spectrum of **4a** (300 MHz, $CDCl_3$).

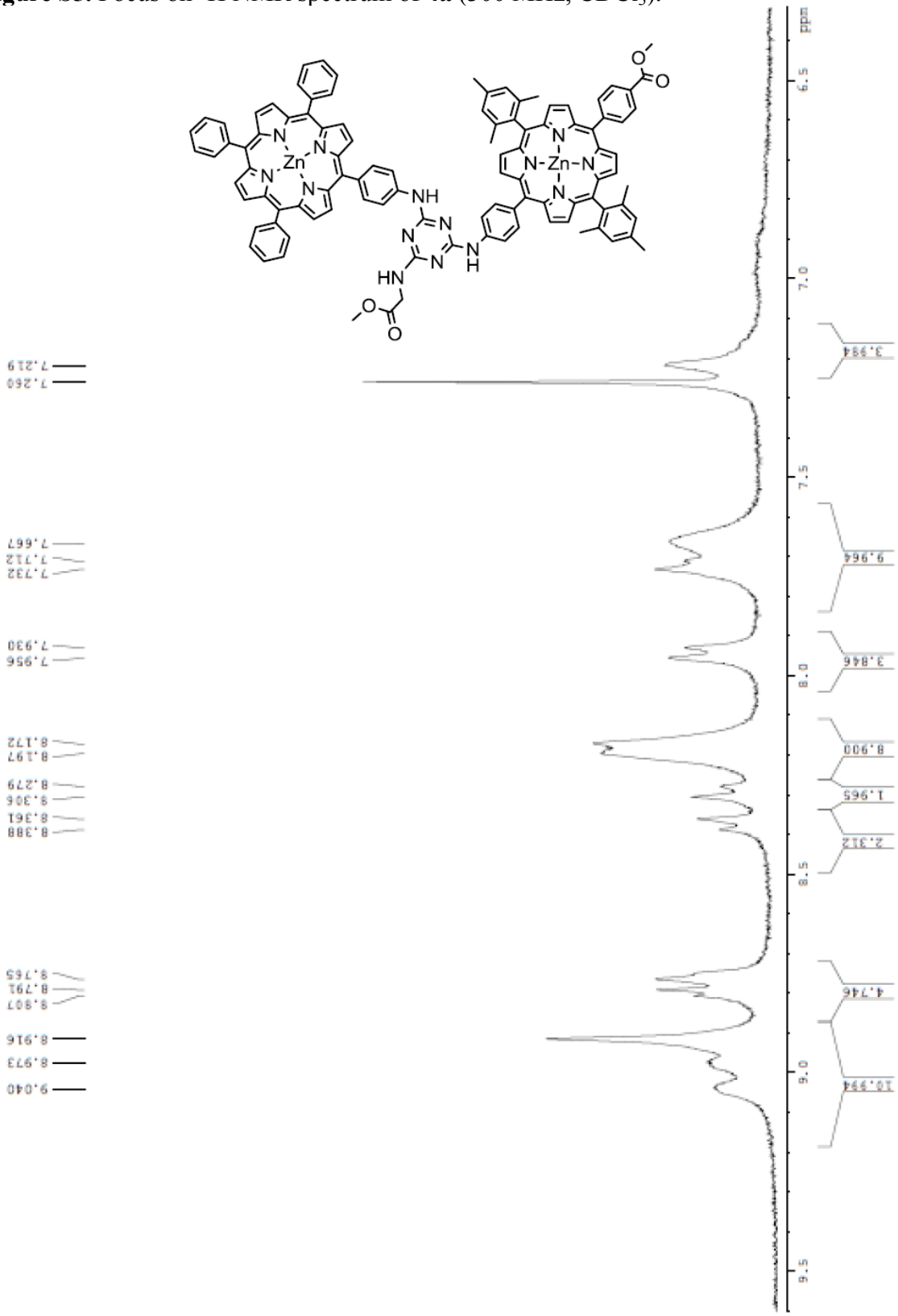

Figure S6. ^{1}H NMR spectrum of **5a** (300 MHz, $CDCl_3$).

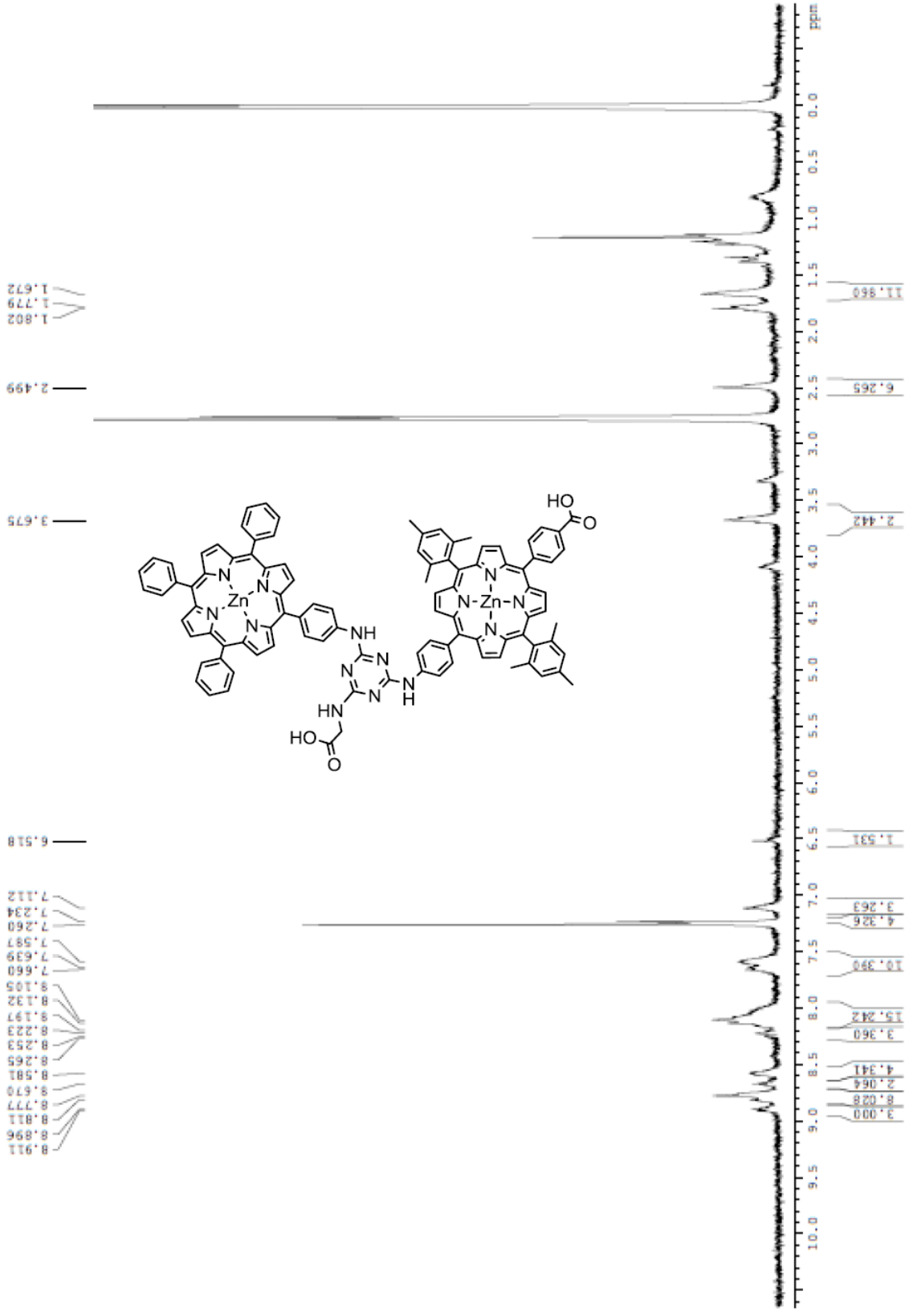

Figure S7. Focus on ^{1}H NMR spectrum of **5a** (300 MHz, $CDCl_3$).

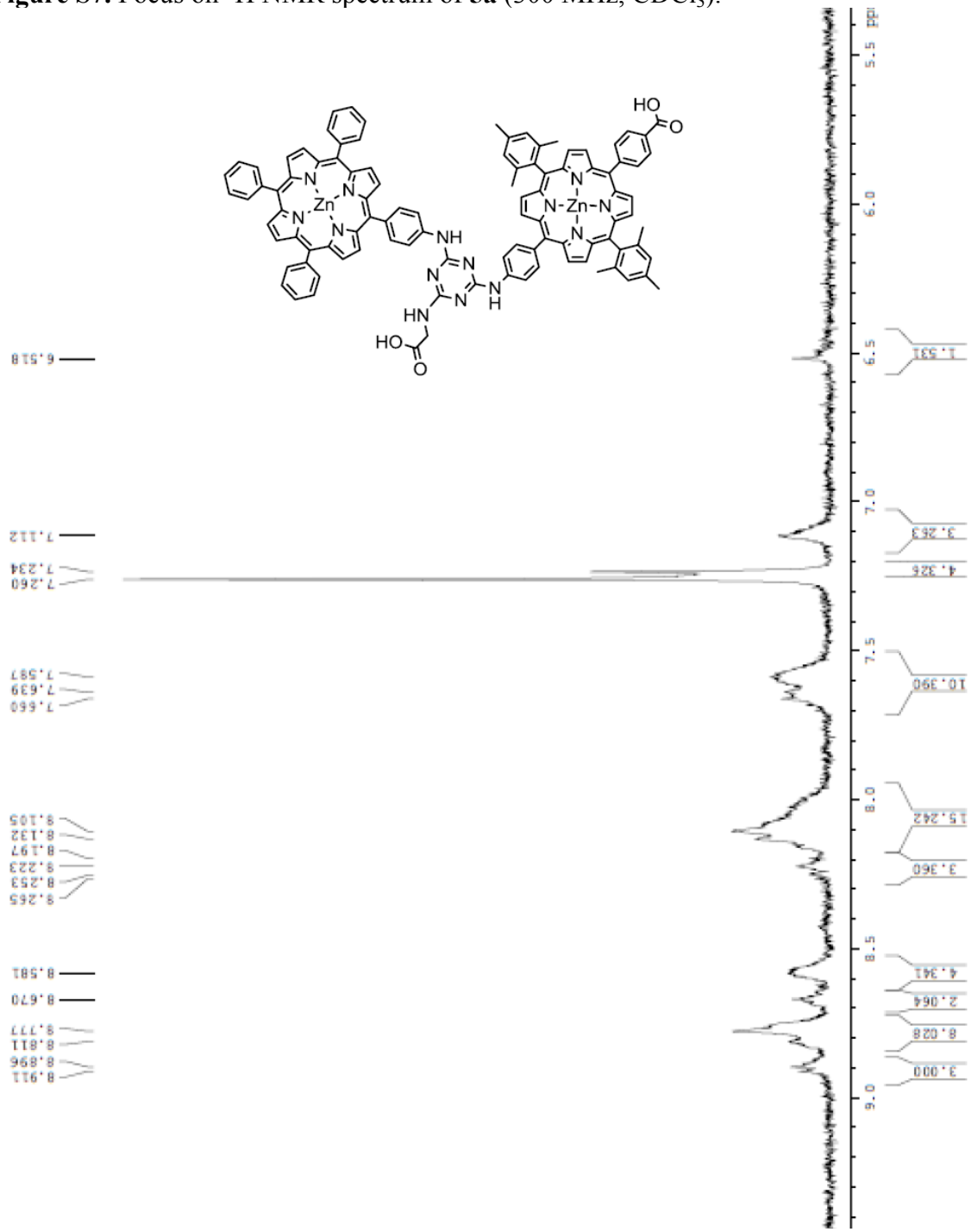

Figure S8. ^{1}H NMR spectrum of **3b** (300 MHz, $CDCl_3$).

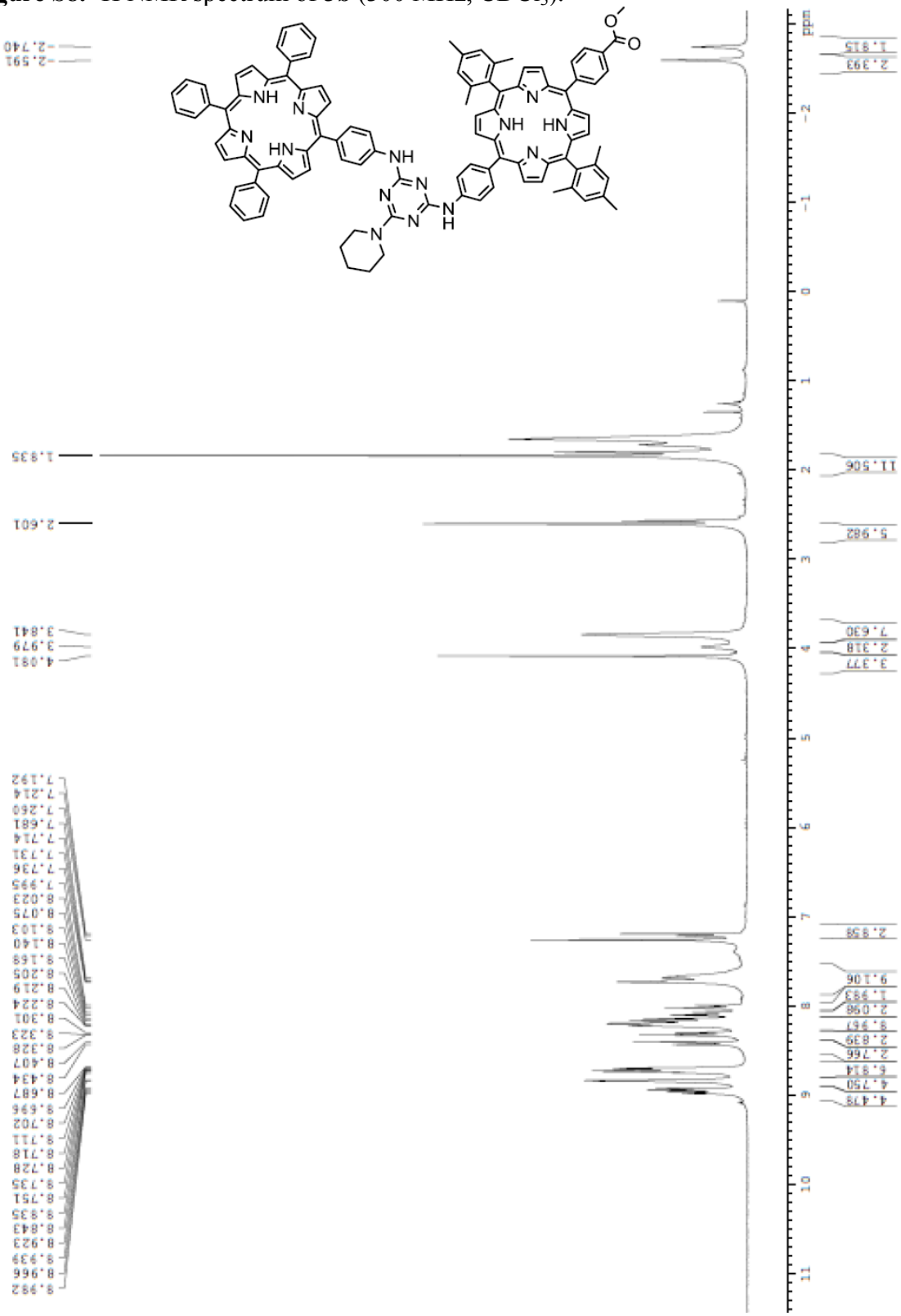

Figure S9. Focus on ^{1}H NMR spectrum of **3b** (300 MHz, $CDCl_3$).

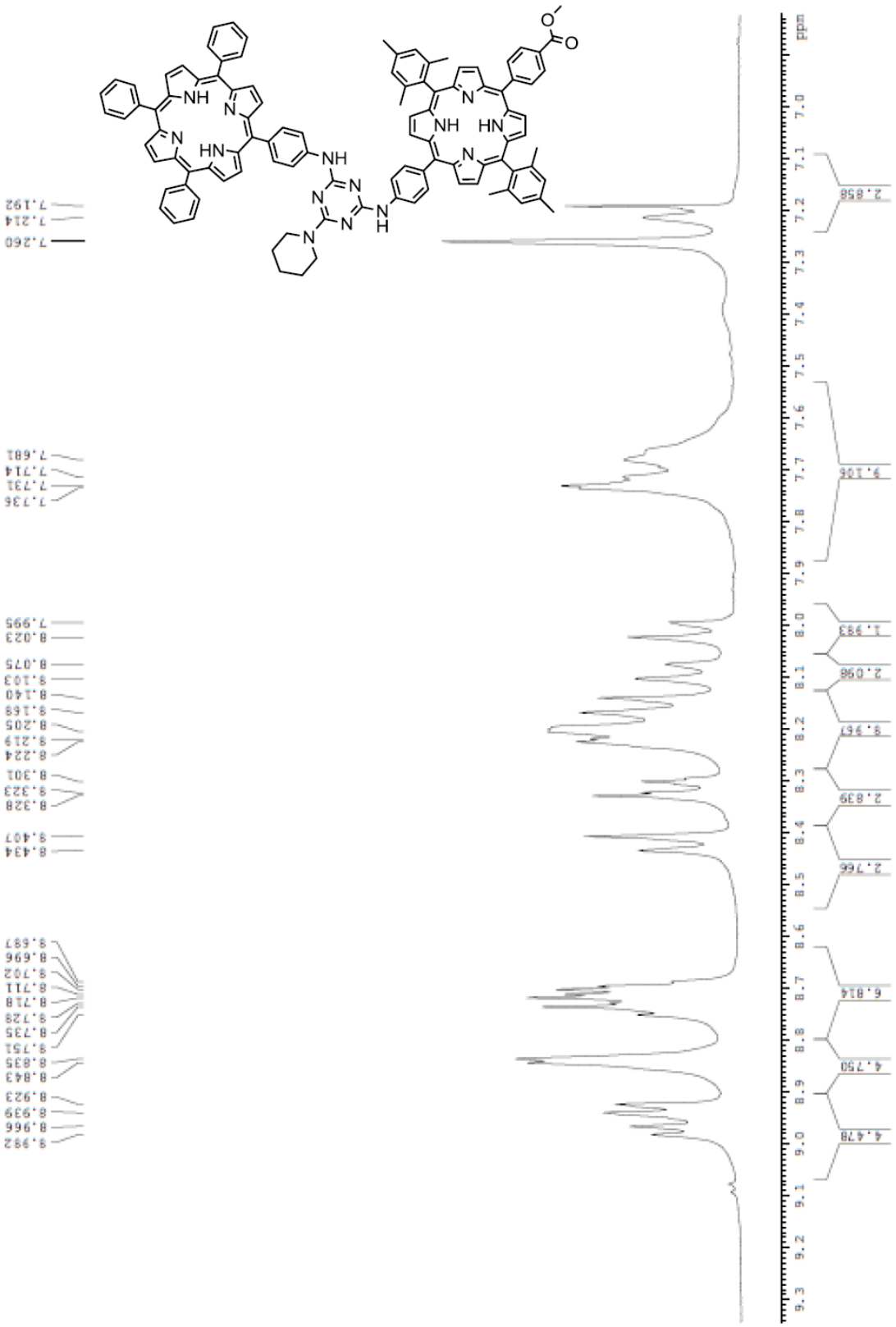

Figure S10. ^{1}H NMR spectrum of **4b** (300 MHz, $CDCl_3$).

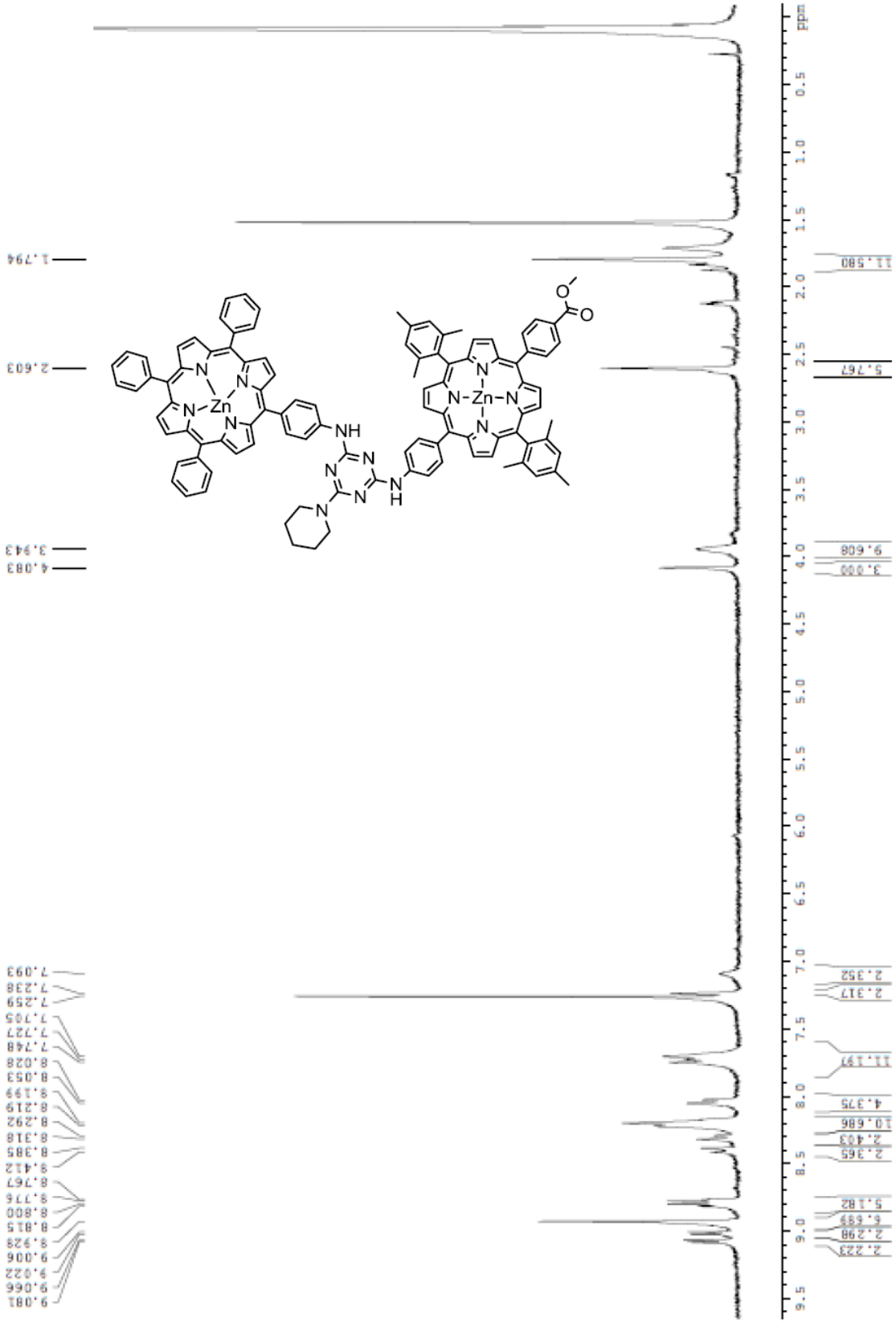

Figure S11. Focus on ^{1}H NMR spectrum of **4b** (300 MHz, $CDCl_3$).

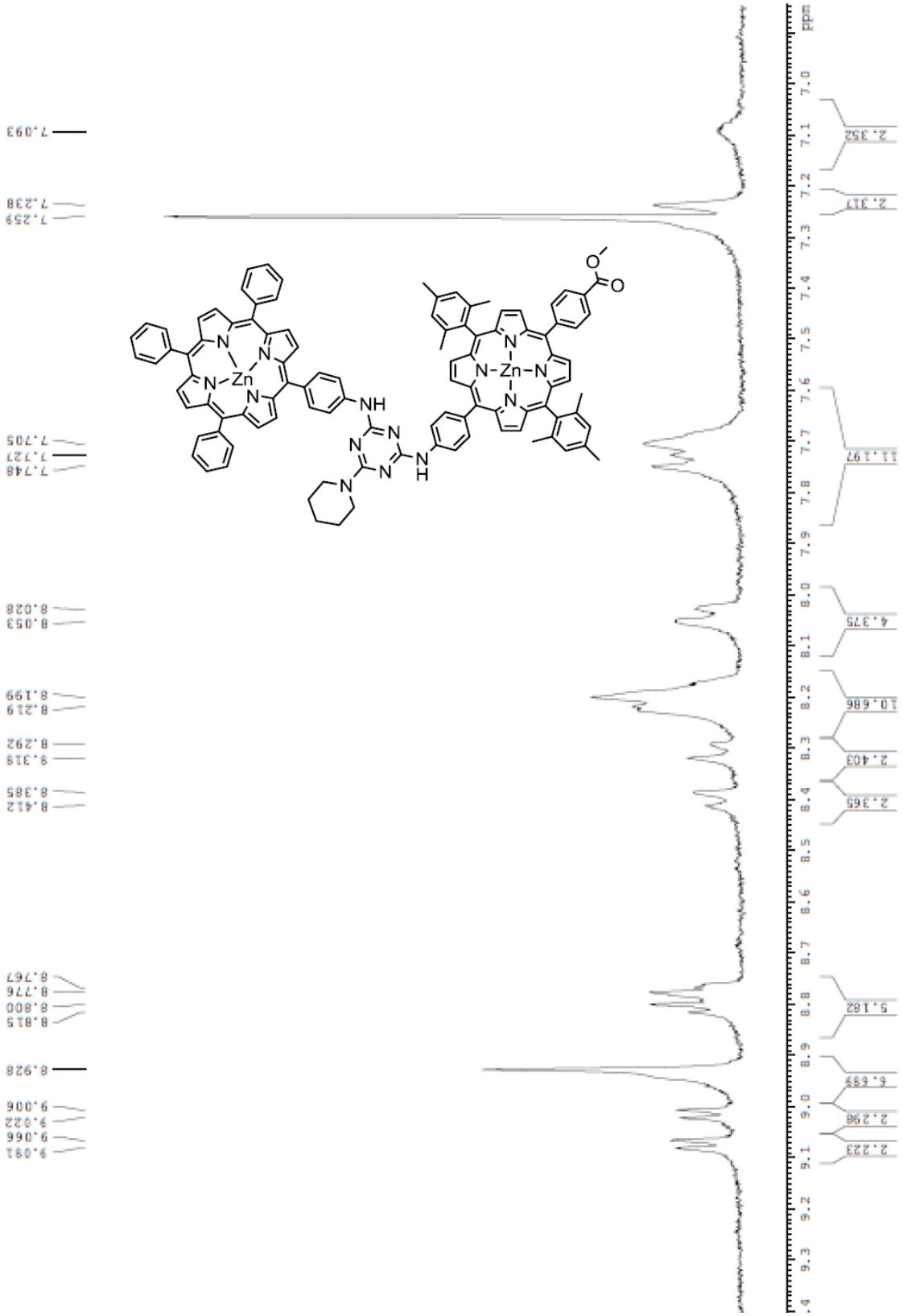

Figure S12. ^{13}C NMR spectrum of **4b** (75 MHz, $CDCl_3$).

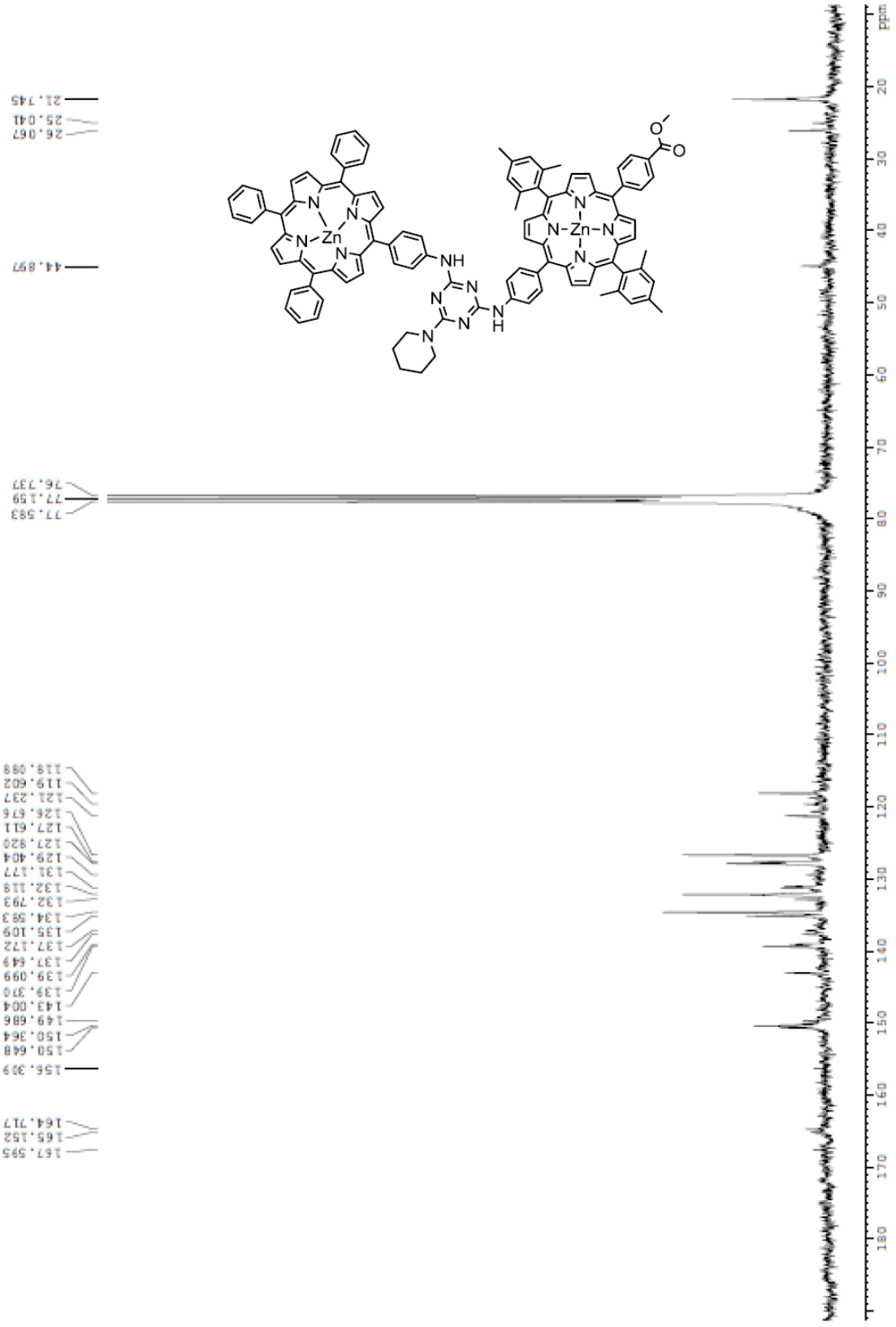

Figure S13. Focus on ^{13}C NMR spectrum of **4b** (75 MHz, $CDCl_3$).

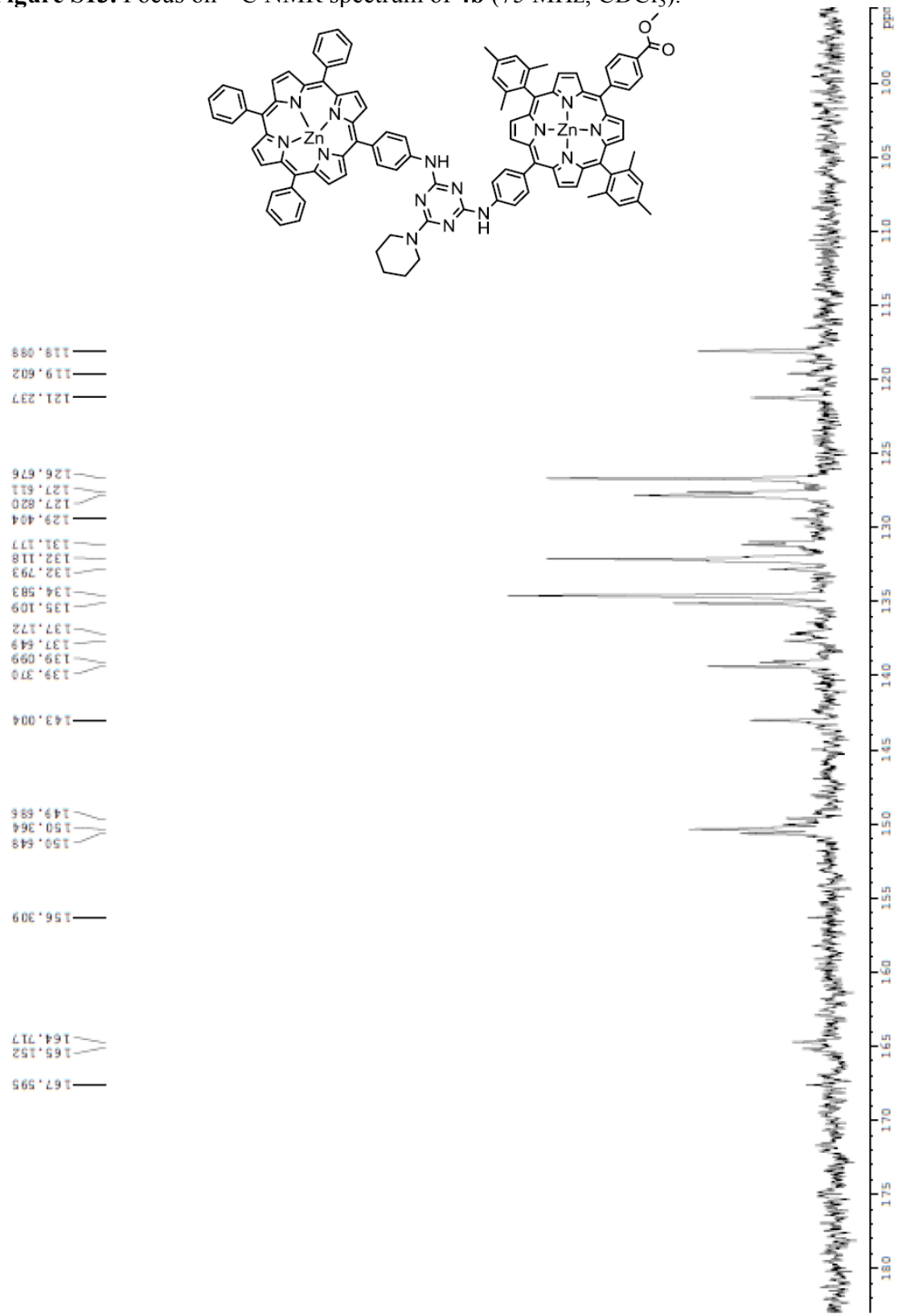

Figure S14. ^{1}H NMR spectrum of **5b** (300 MHz, $CDCl_3$).

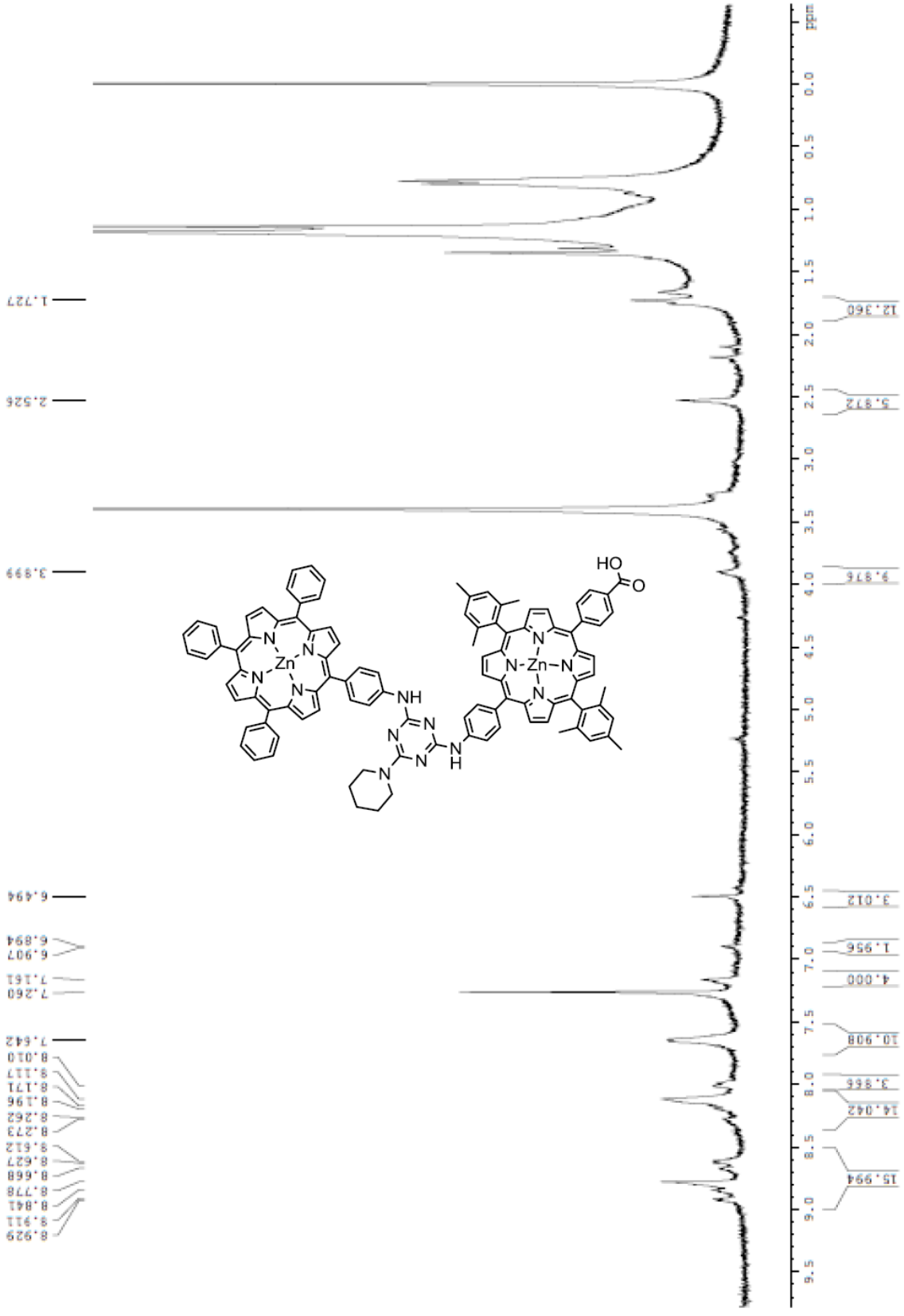

Figure S15. Focus on ^{1}H NMR spectrum of **5b** (300 MHz, $CDCl_3$).

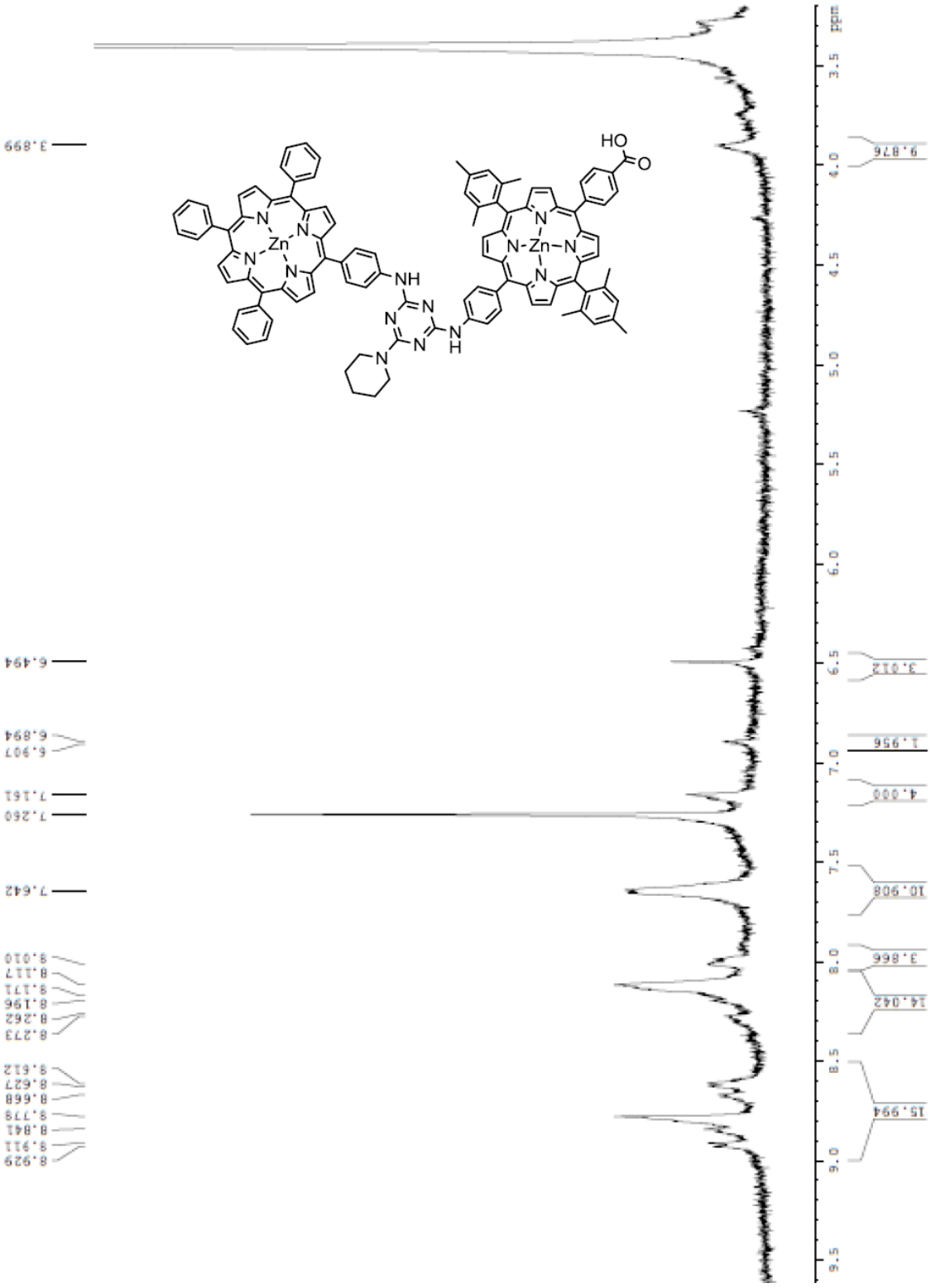

Figure S16. ^{13}C NMR spectrum of **5b** (75 MHz, $CDCl_3$).

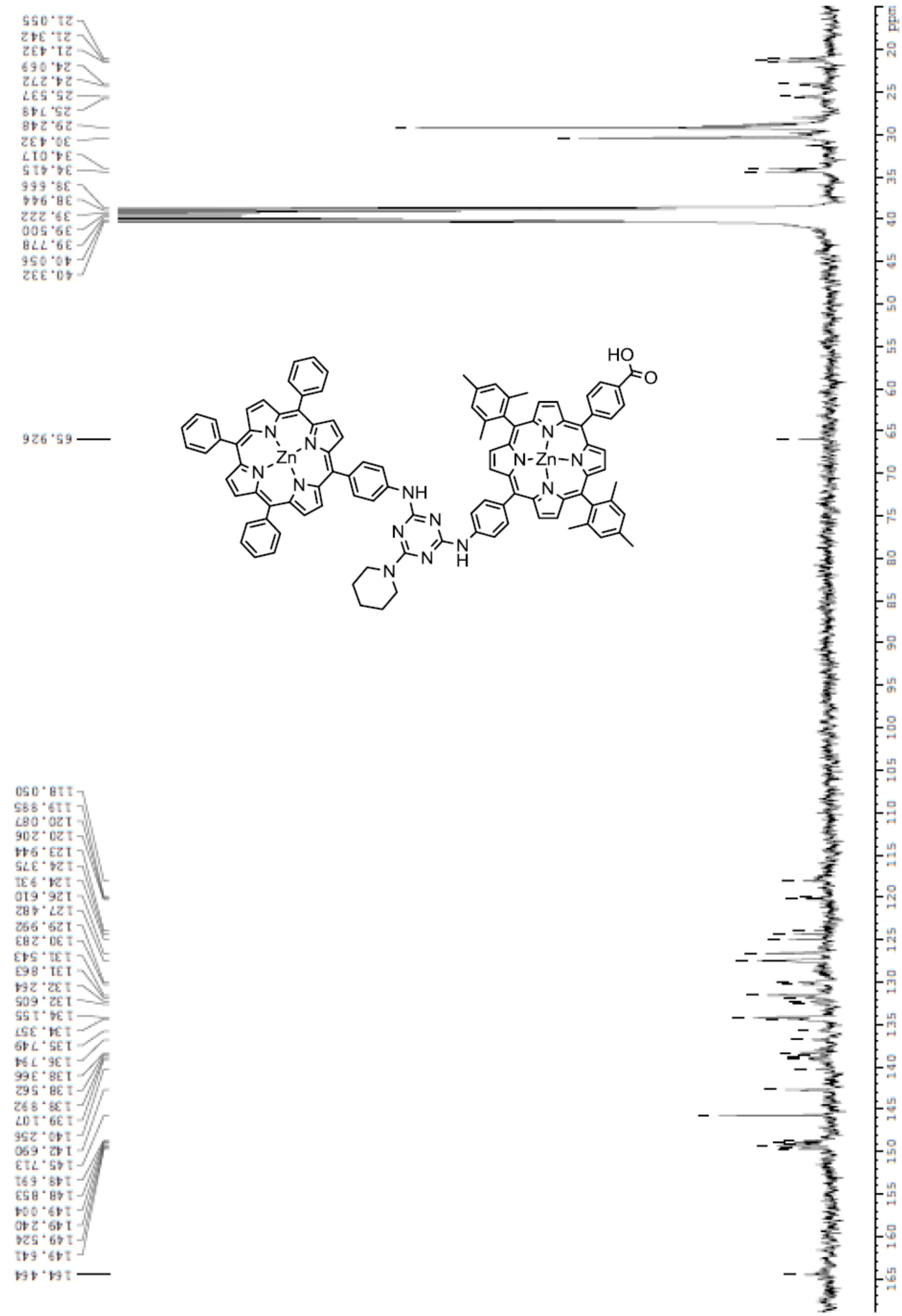

Figure S17. Focus on ^{13}C NMR spectrum of **5b** (75 MHz, $CDCl_3$).

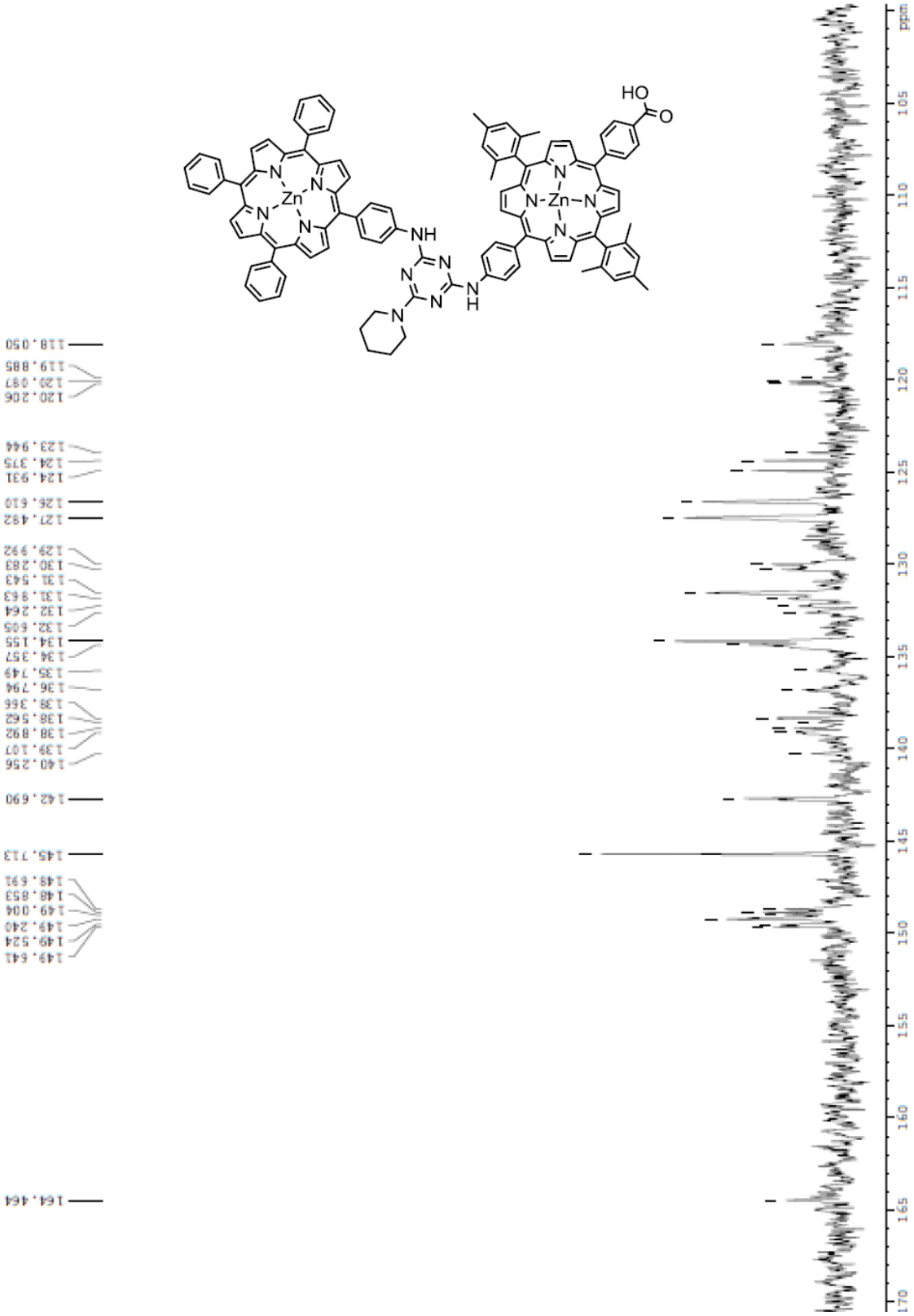

Figure S18. Square wave voltammograms of **5a** and **5b**. The ferrocene/ferrocenium (Fc/Fc^+) redox couple wave is also shown. Voltage is reported *vs* NHE.

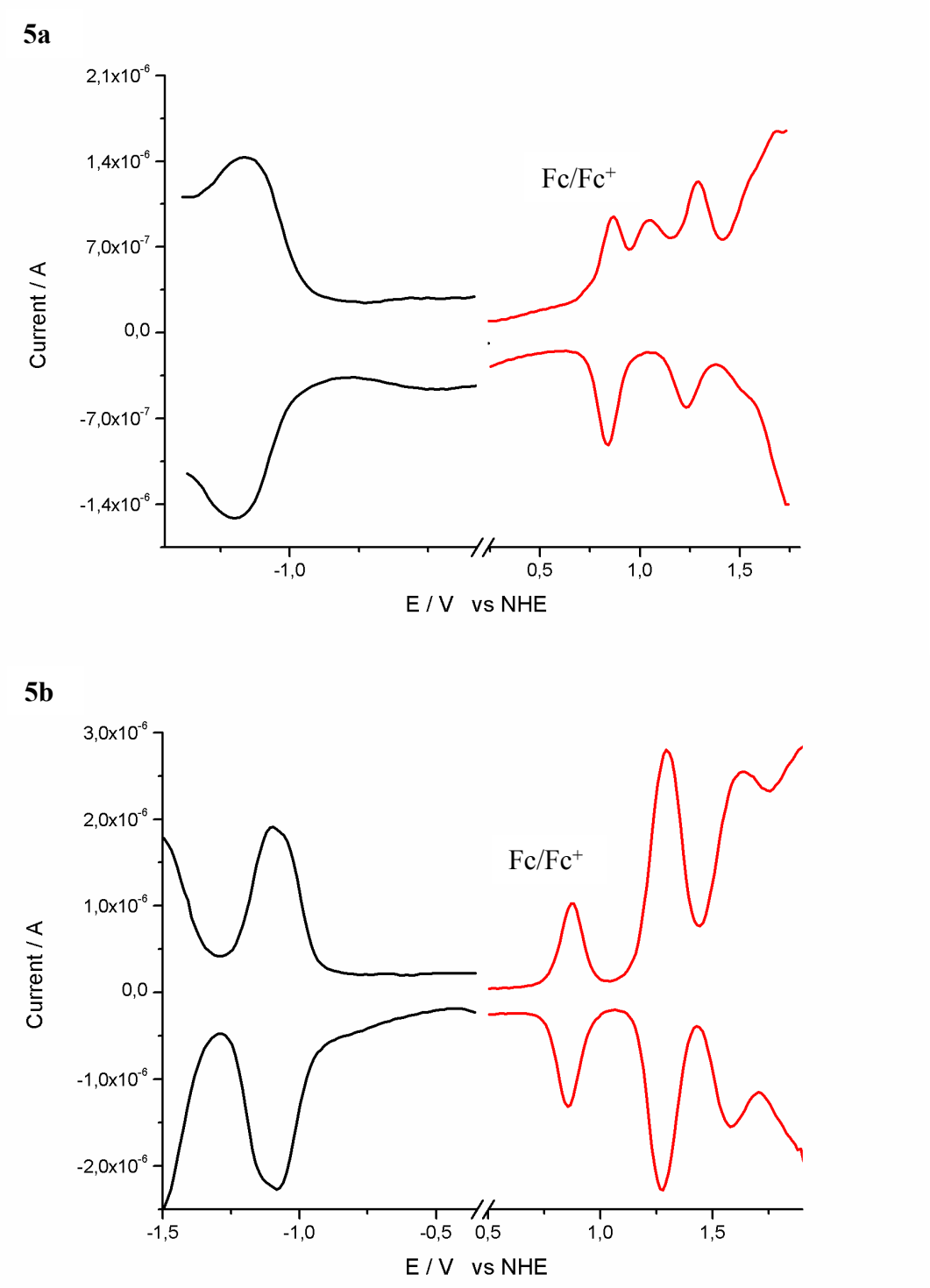

Figure S19. FTIR spectra of **5a** and **5a/TiO$_2$**