

Novel Short PEG Chains Substituted Porphyrins: Synthesis, Photochemistry and In Vitro Photodynamic Activity Against Cancer Cells

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1. NMR data

1.1. NMR experiments of compound 1.

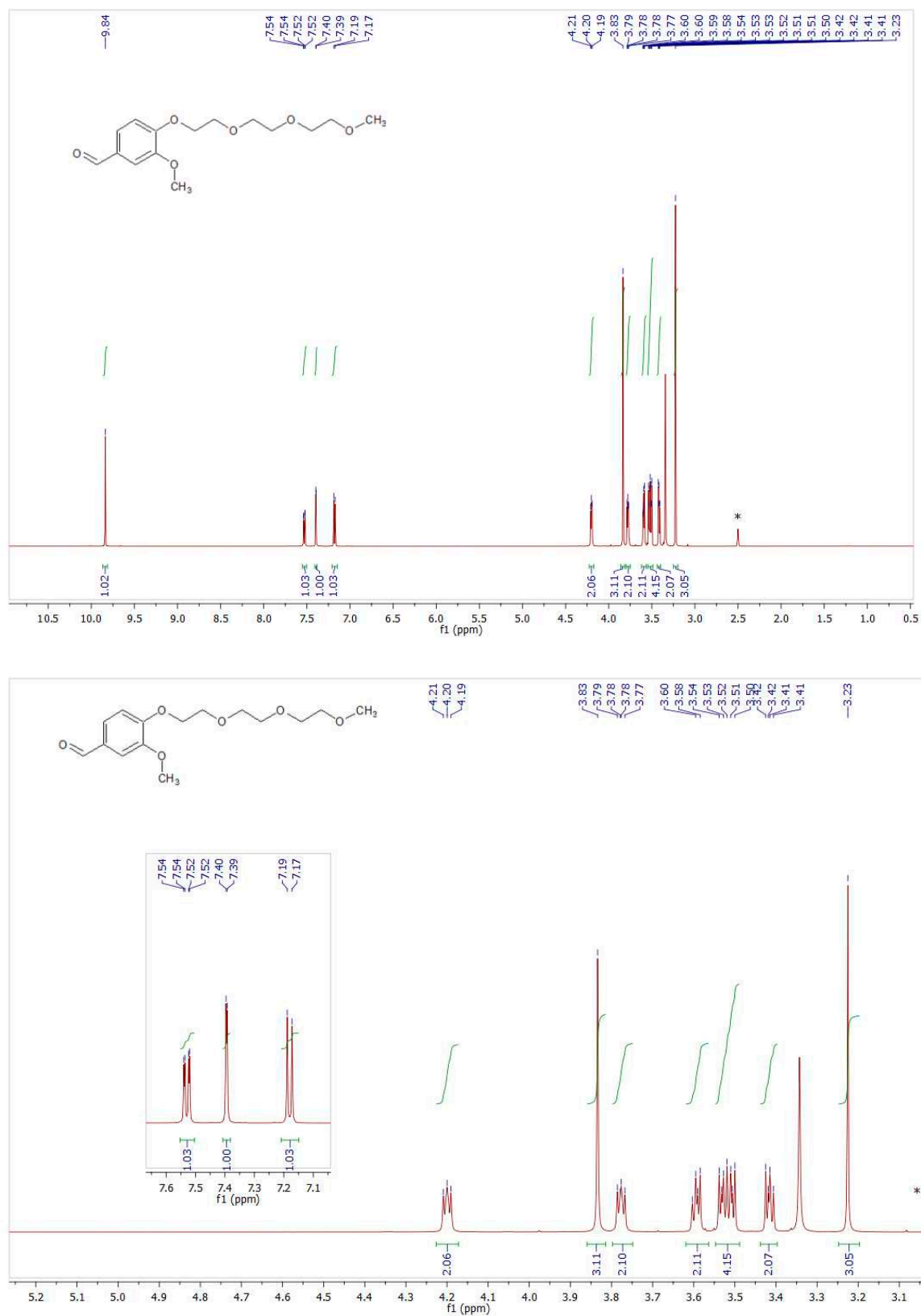


Figure S1. ^1H spectra NMR of aldehyde 1.

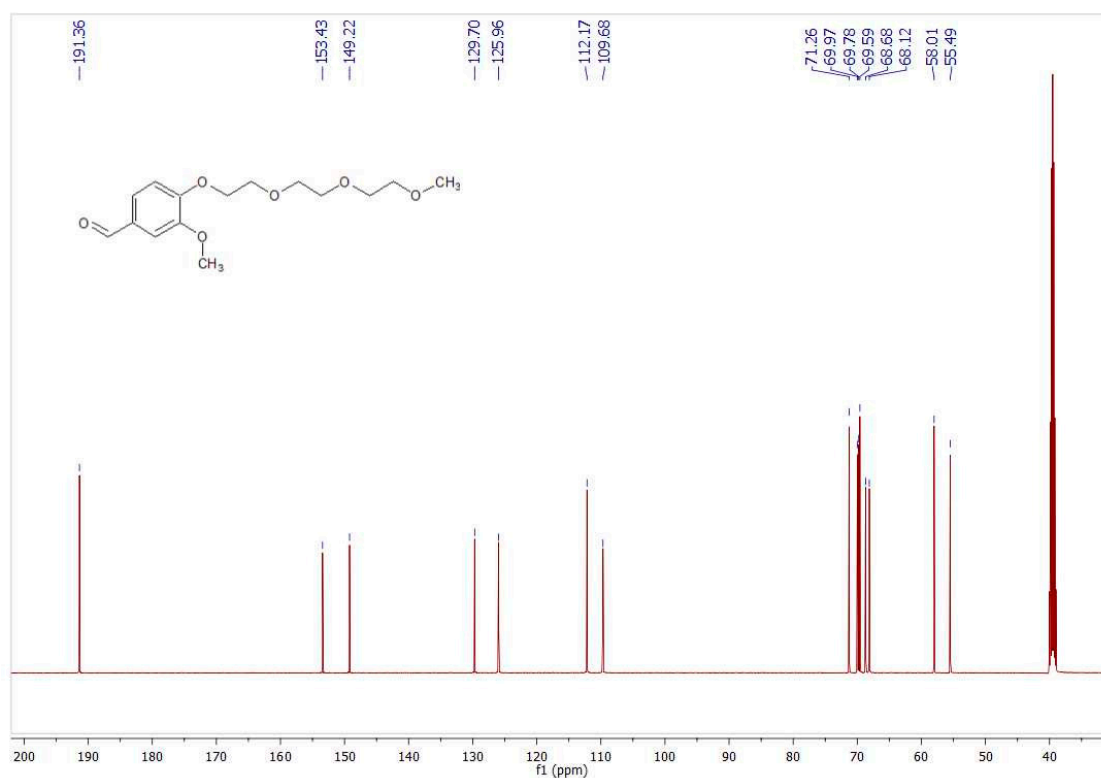


Figure S2. ¹³C NMR spectrum of aldehyde 1.

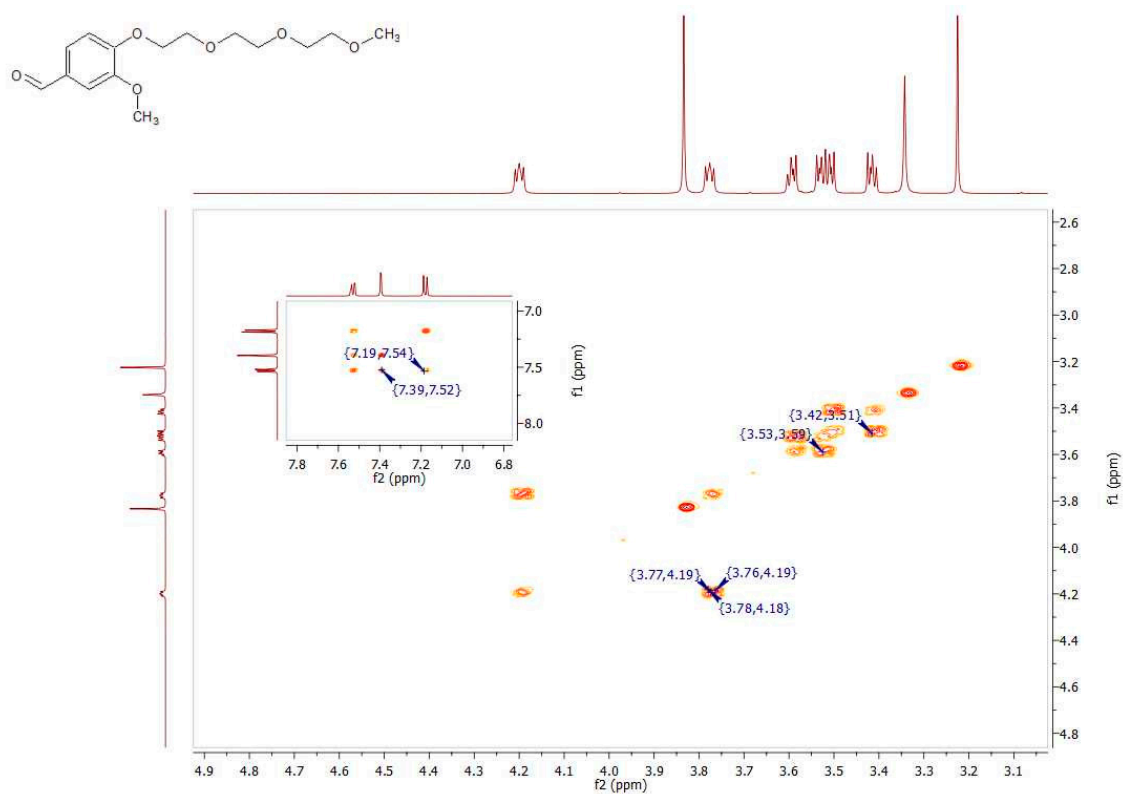


Figure S3. ¹H-¹H COSY spectrum of aldehyde 1.

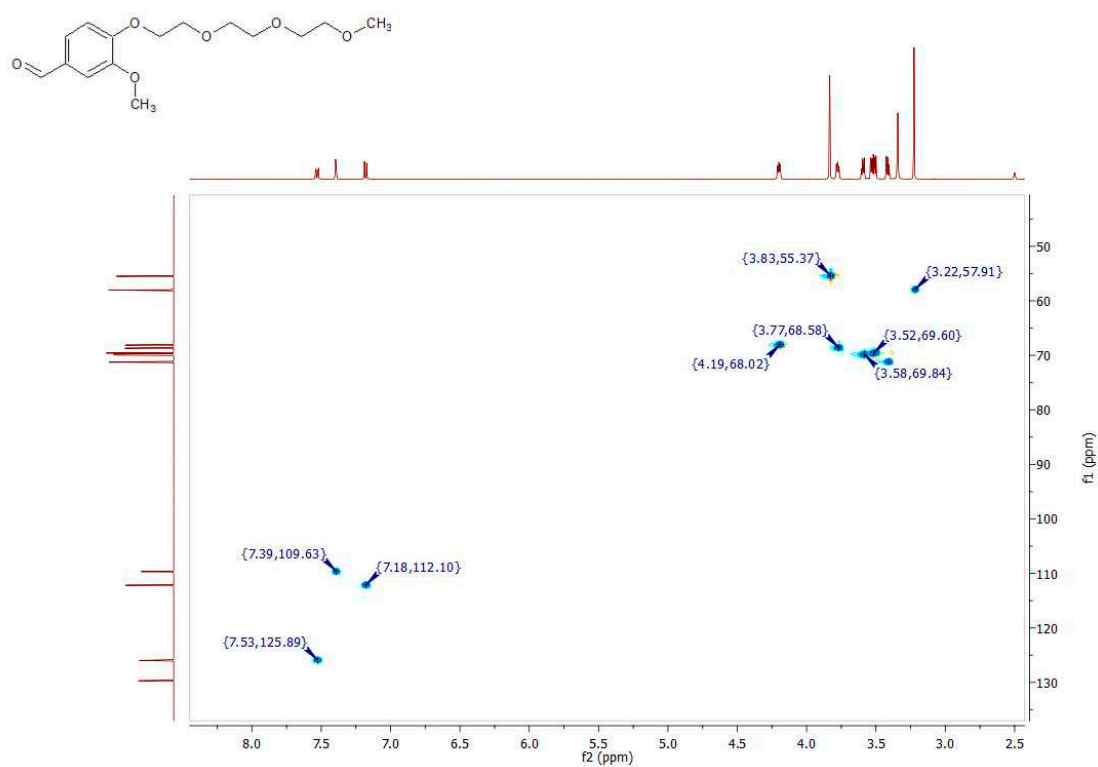


Figure S4. ¹H-¹³C HSQC spectrum of aldehyde 1.

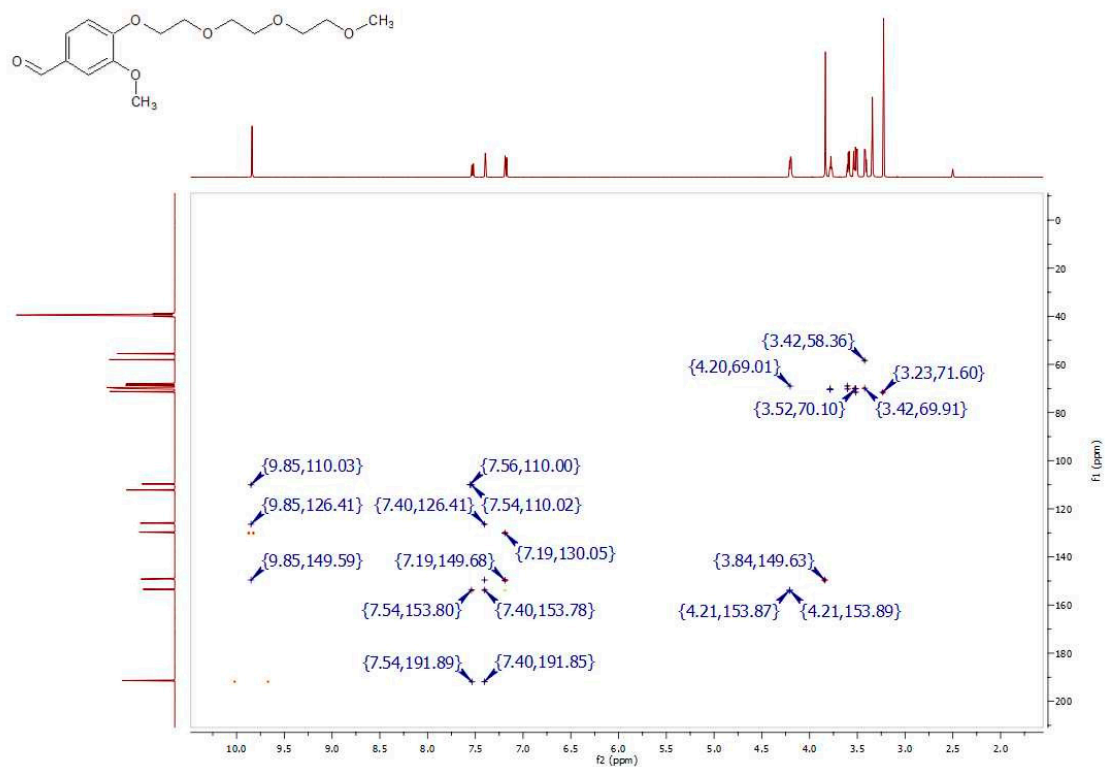


Figure S5. ¹H-¹³C HMBC spectrum of aldehyde 1.

1.2. NMR experiments of compound 2.

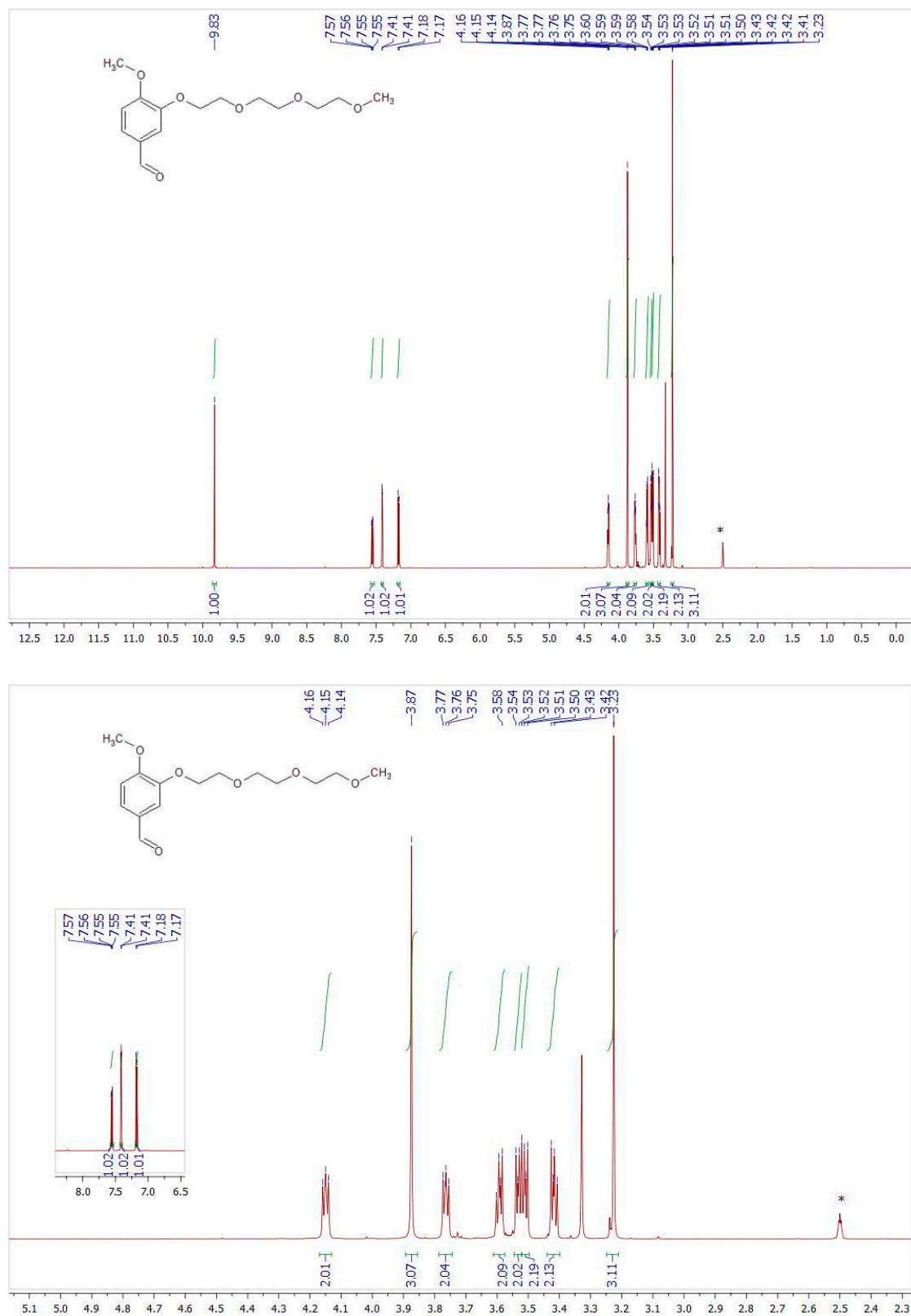


Figure S6. ^1H NMR spectra of aldehyde 2.

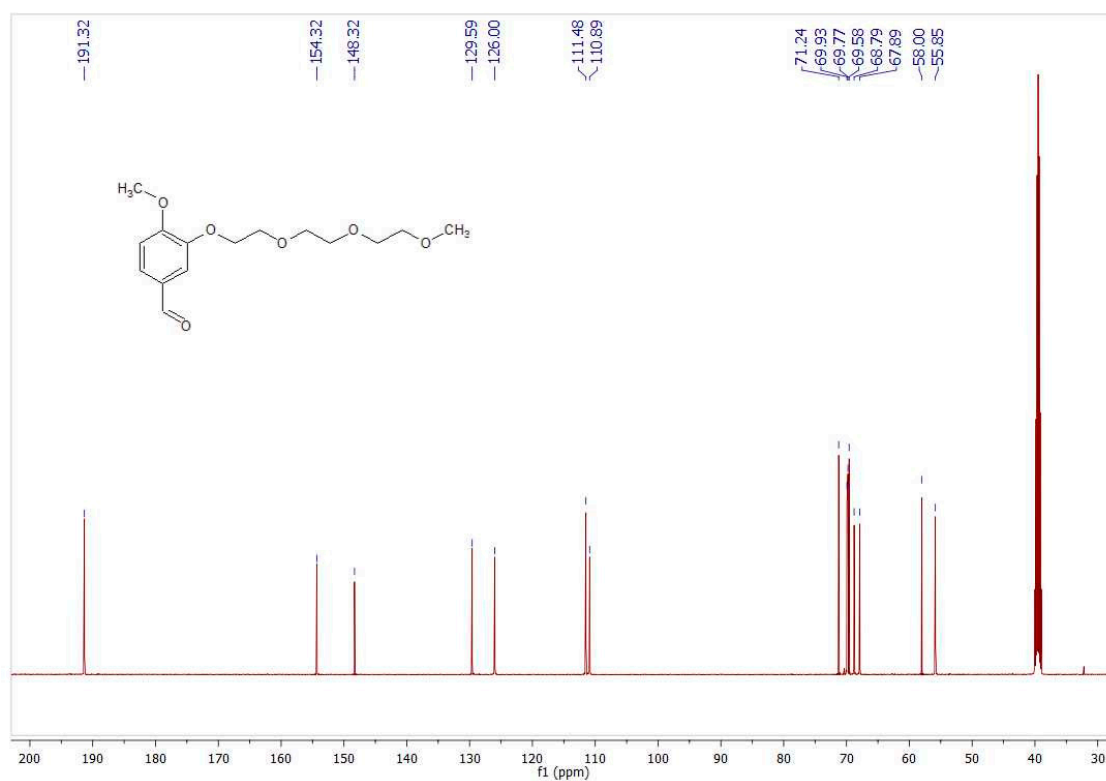


Figure S7. ^{13}C spectrum NMR of aldehyde 2.

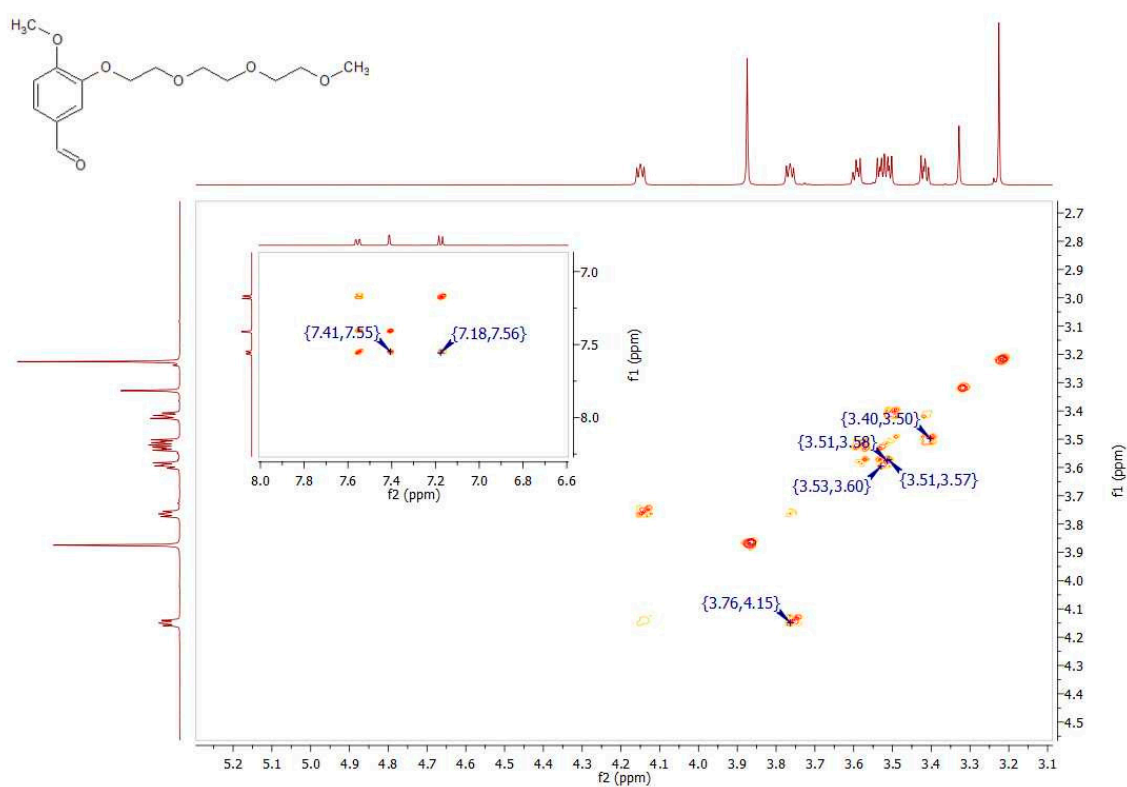


Figure S8. ^1H - ^1H COSY spectrum of aldehyde 2.

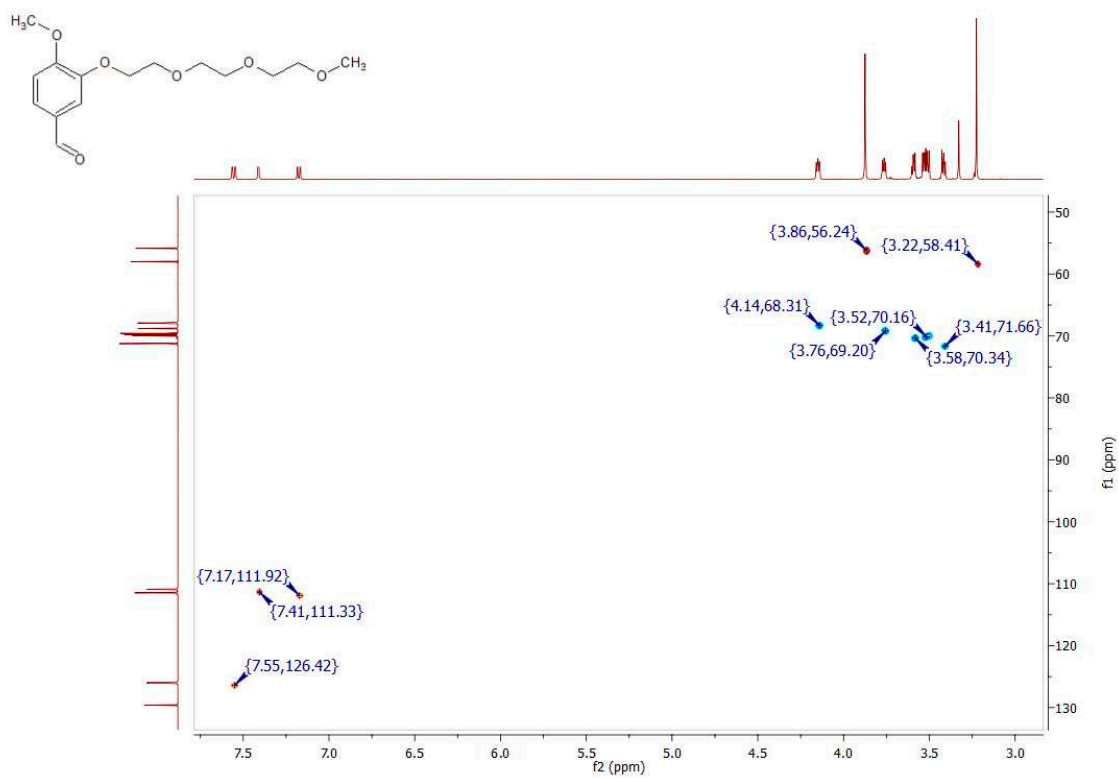


Figure S9. ¹H-¹³C HSQC spectrum of aldehyde 2.

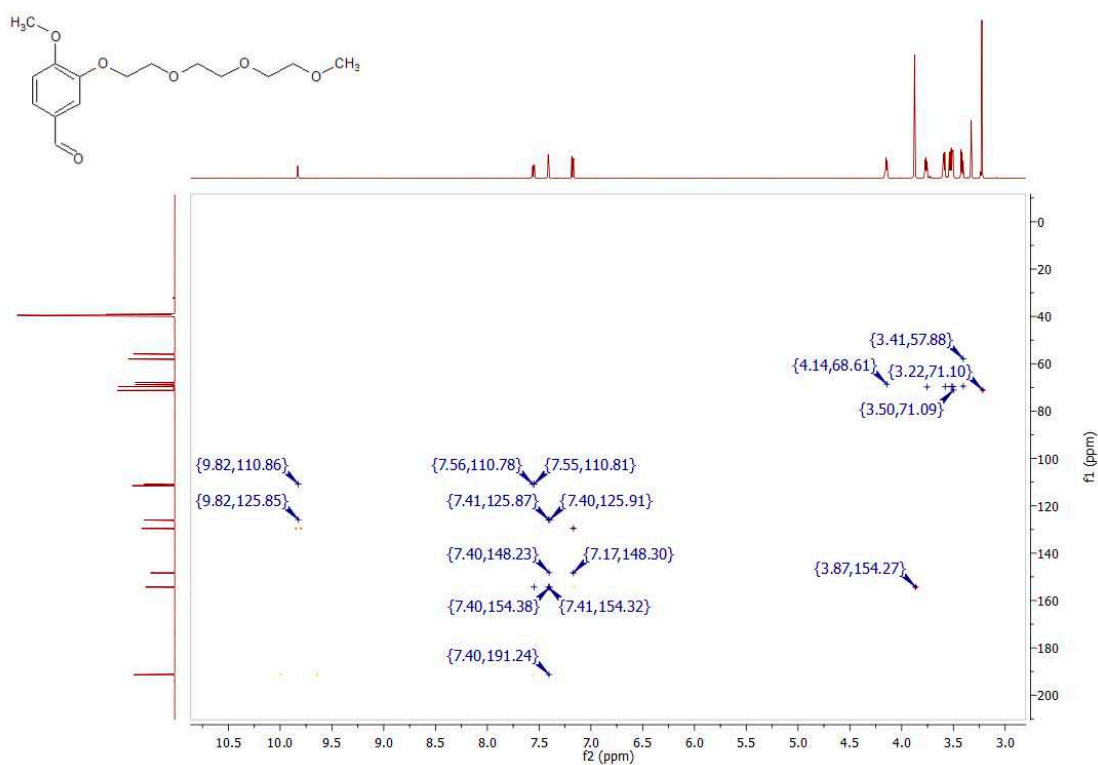


Figure S10. ¹H-¹³C HMBC spectrum of aldehyde 2.

1.3. NMR experiments of compound 3.

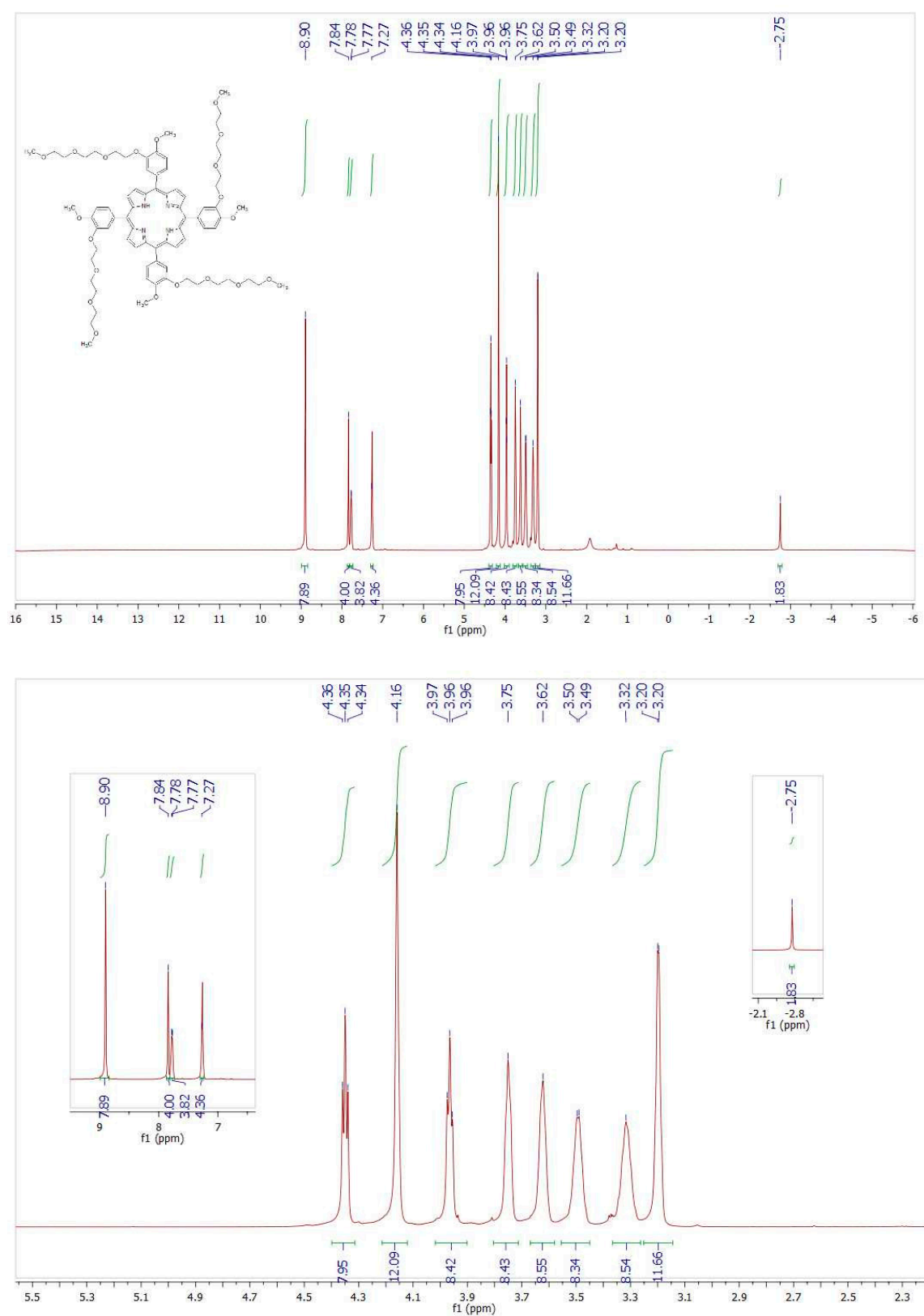


Figure S11. ^1H spectra NMR of porphyrin 3.

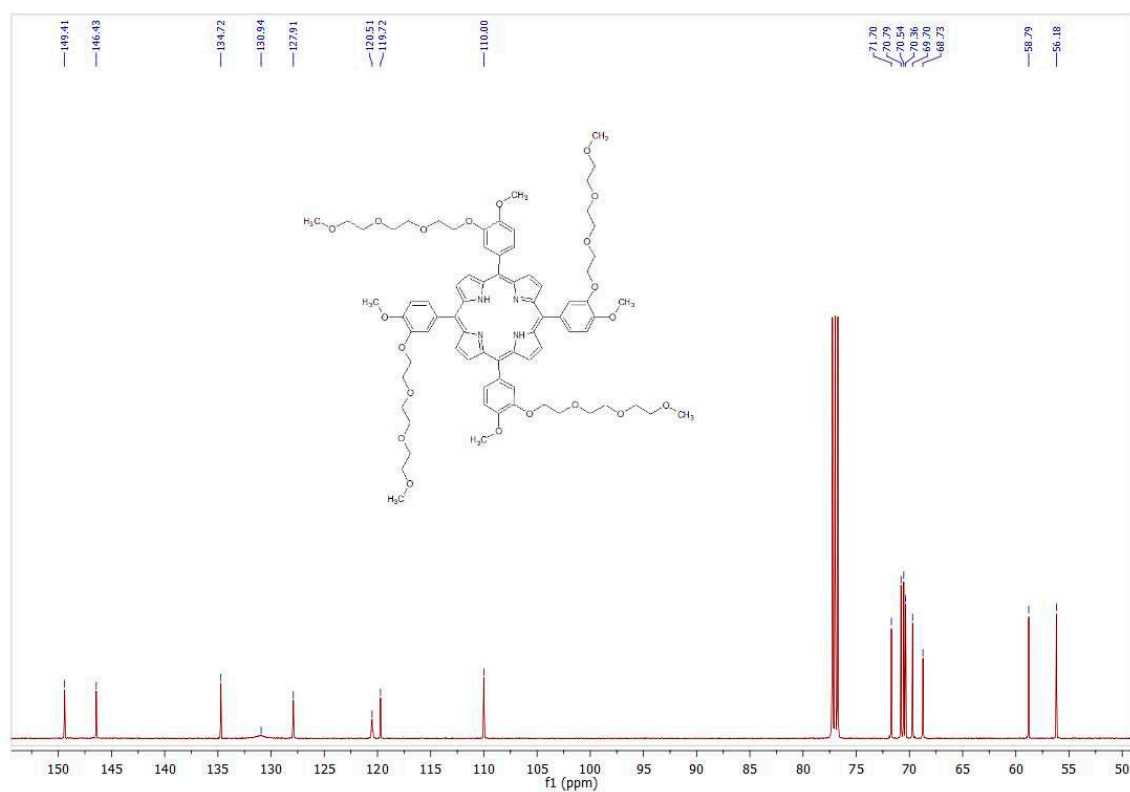


Figure S12. ^{13}C spectrum NMR of porphyrin 3.

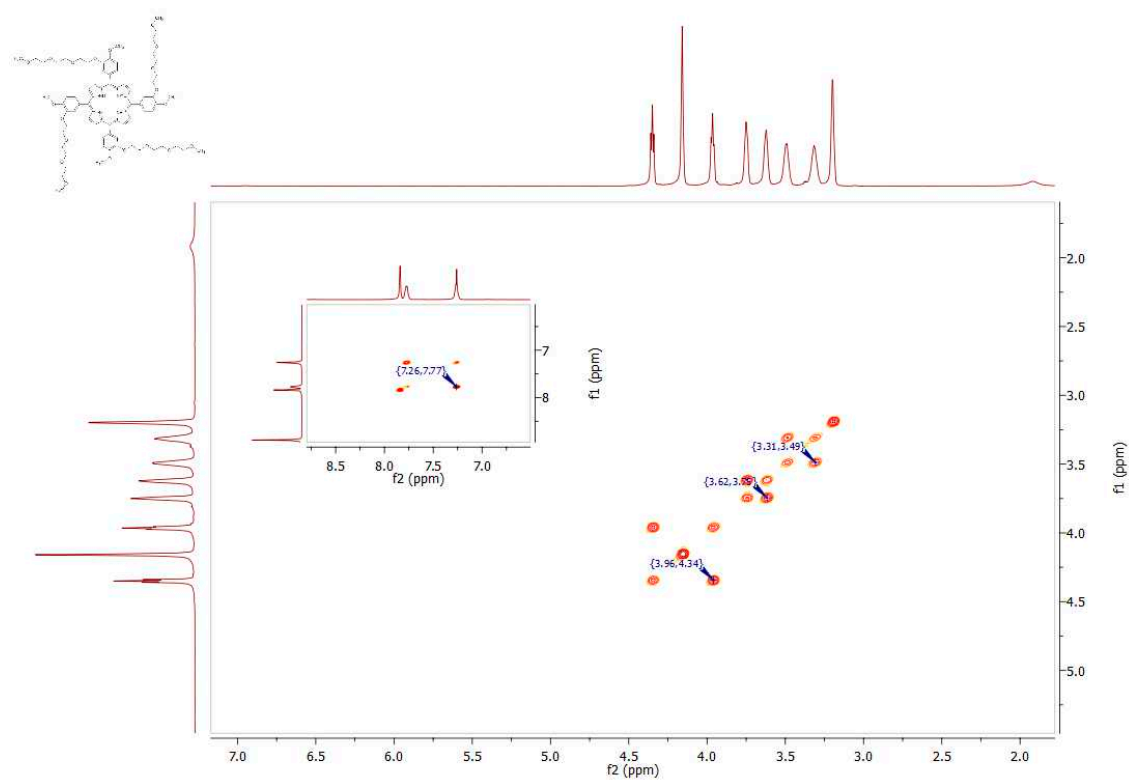


Figure S13. ^1H - ^1H COSY spectrum of porphyrin 3.

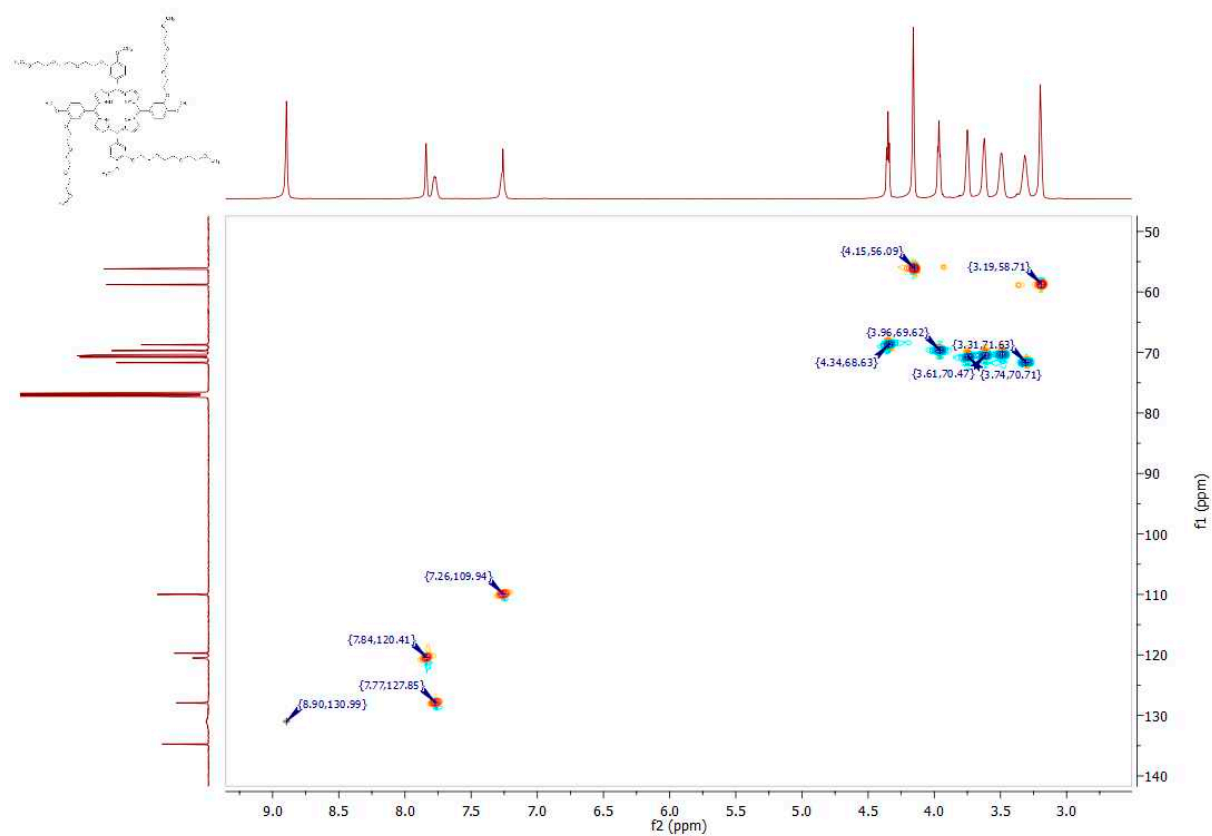


Figure S14. ^1H - ^{13}C HSQC spectrum of porphyrin 3.

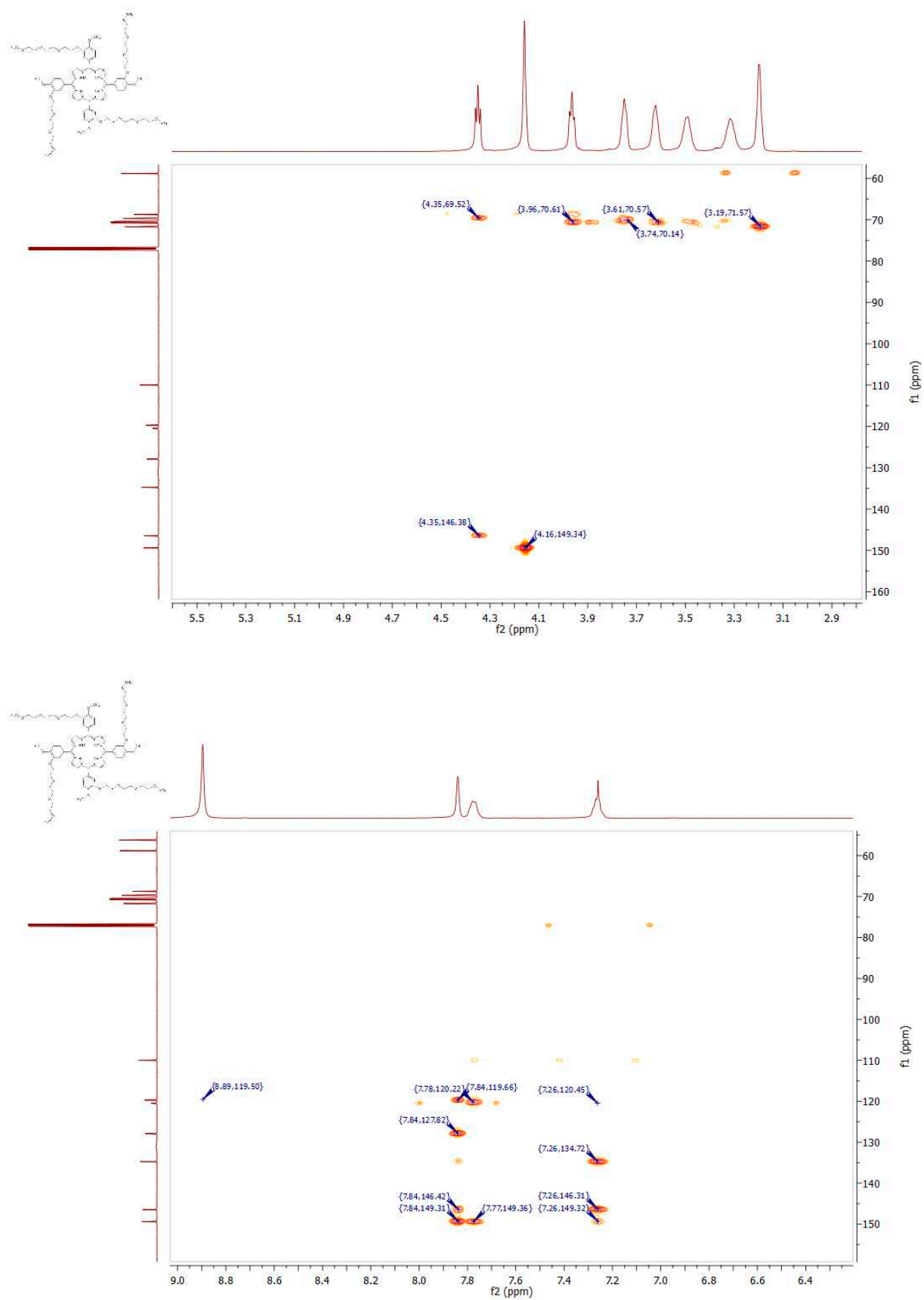


Figure S15. ^1H - ^{13}C HMBC spectra of porphyrin 3.

1.4. NMR experiments of compound 4.

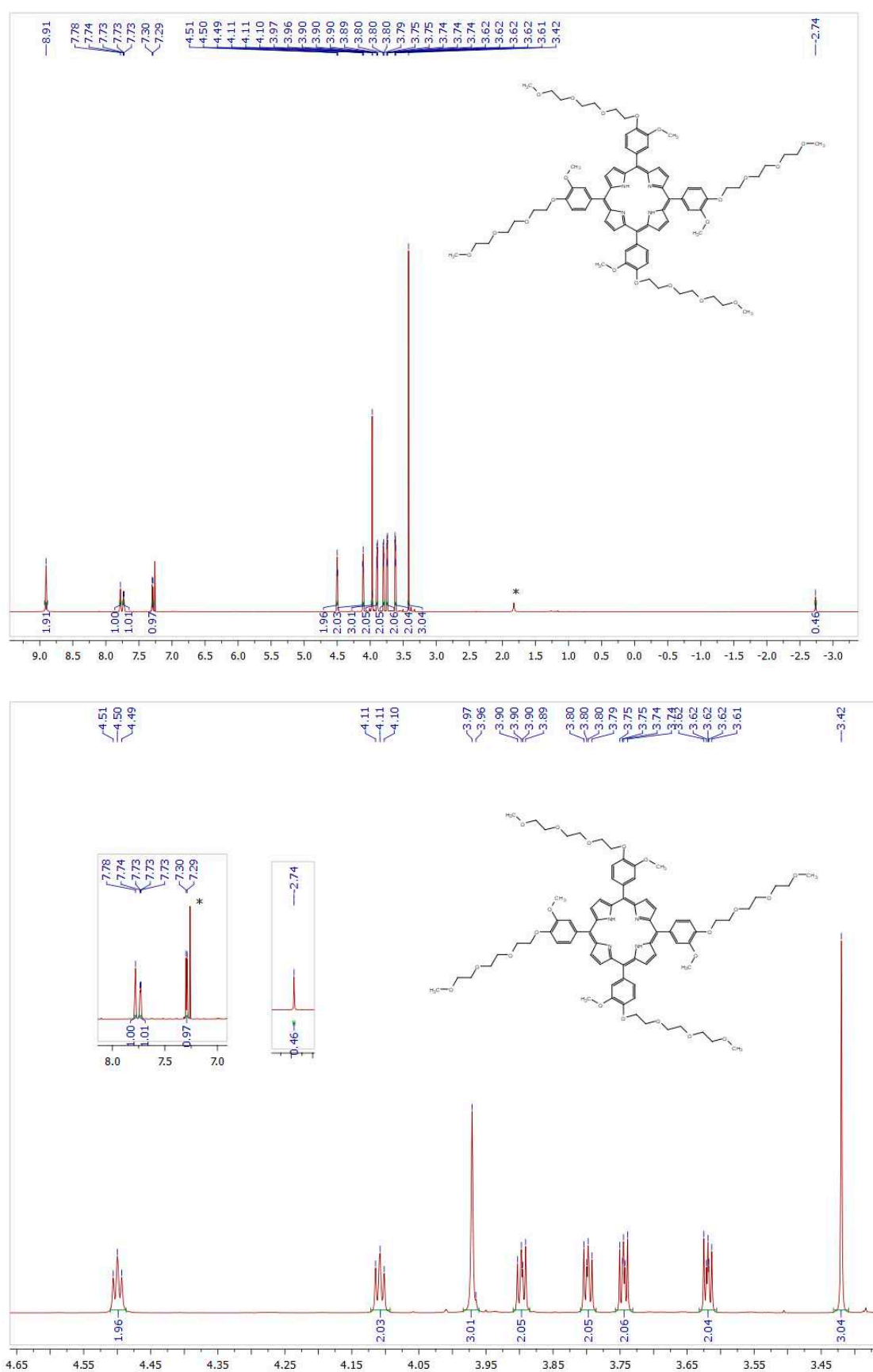


Figure S16. ^1H NMR spectra of porphyrin 4.

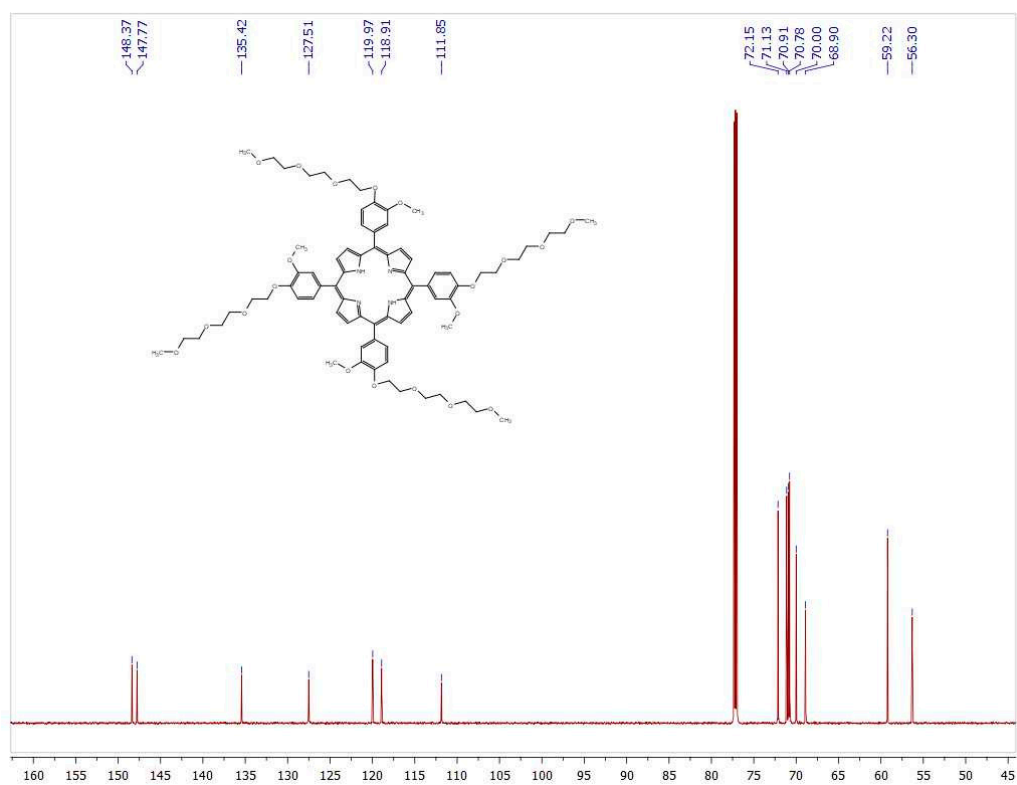


Figure S17. ¹³C NMR spectrum of porphyrin 4.

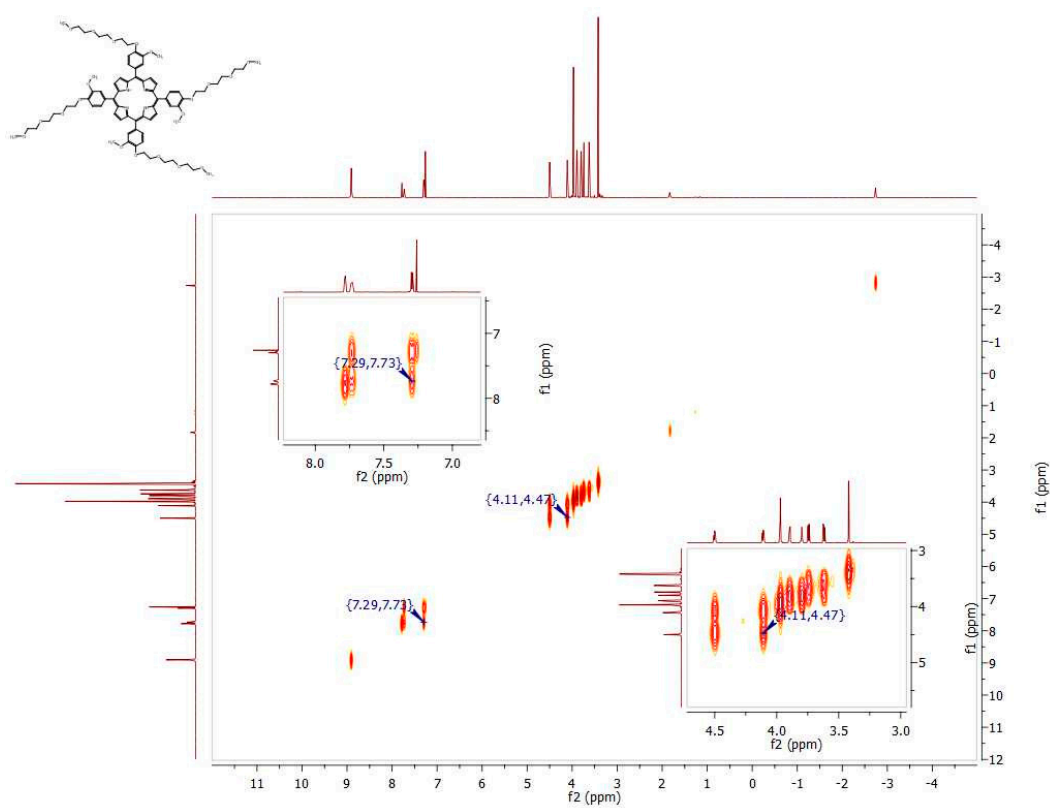


Figure S18. ¹H-¹H COSY spectrum of porphyrin 4.

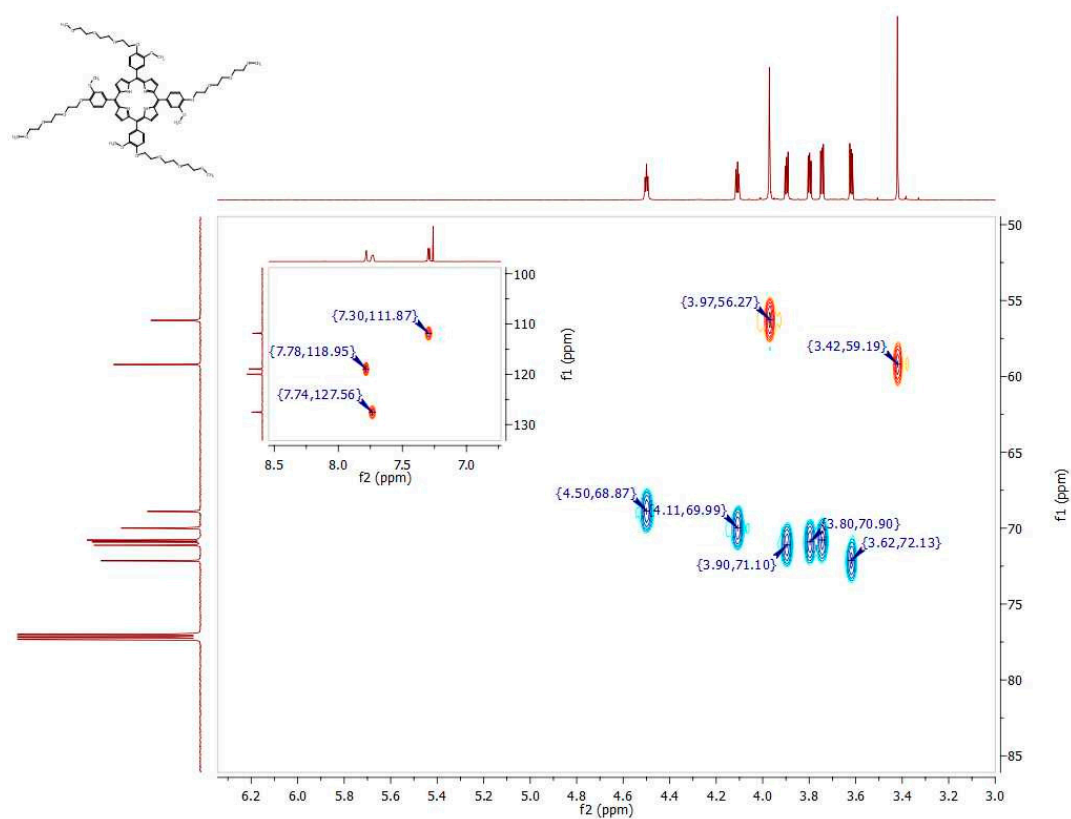


Figure S19. ^1H - ^{13}C HSQC spectrum of porphyrin 4.

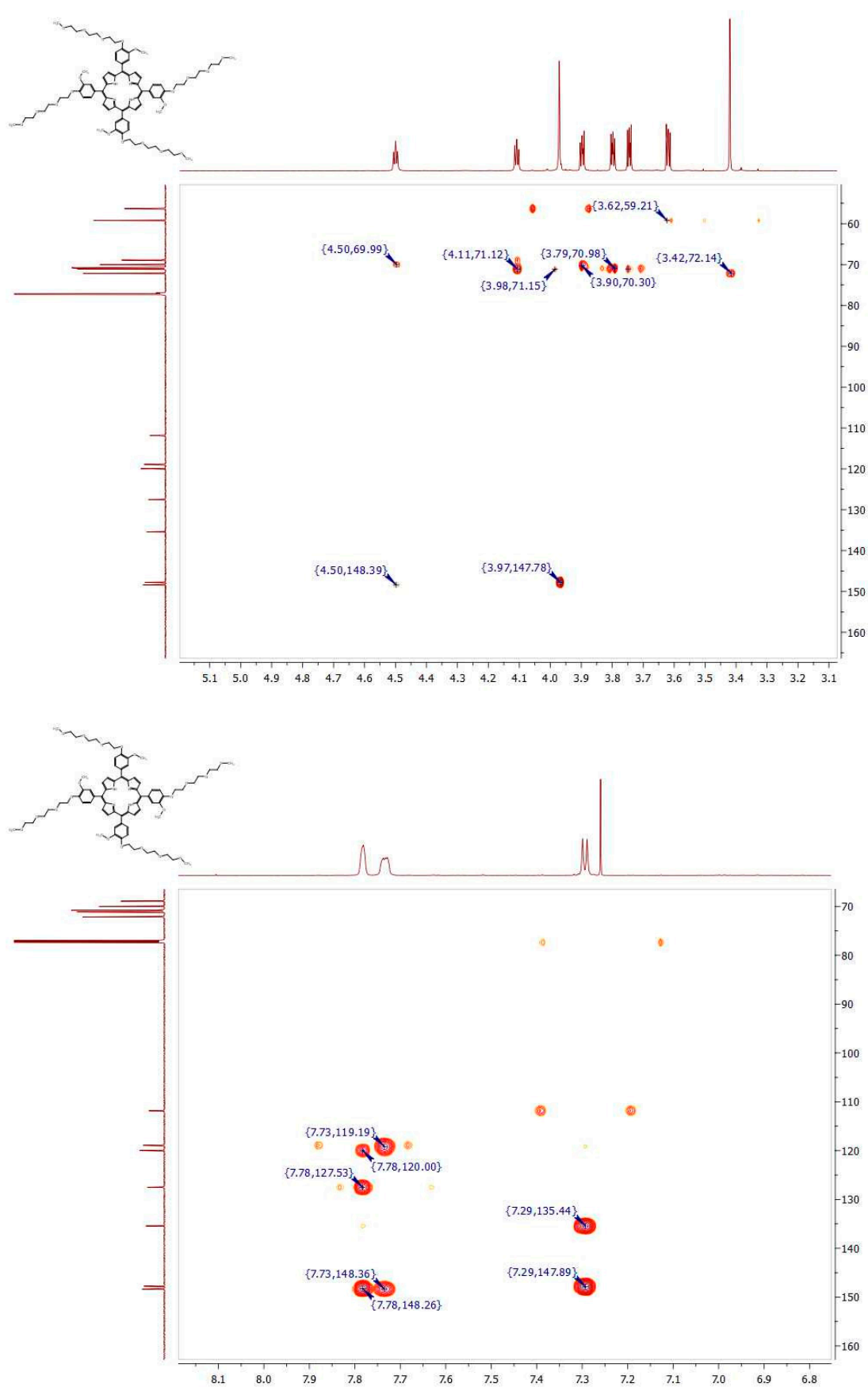


Figure S20. ^1H - ^{13}C HMBC spectra of porphyrin **4**.

1.5. NMR experiments of compound 5.

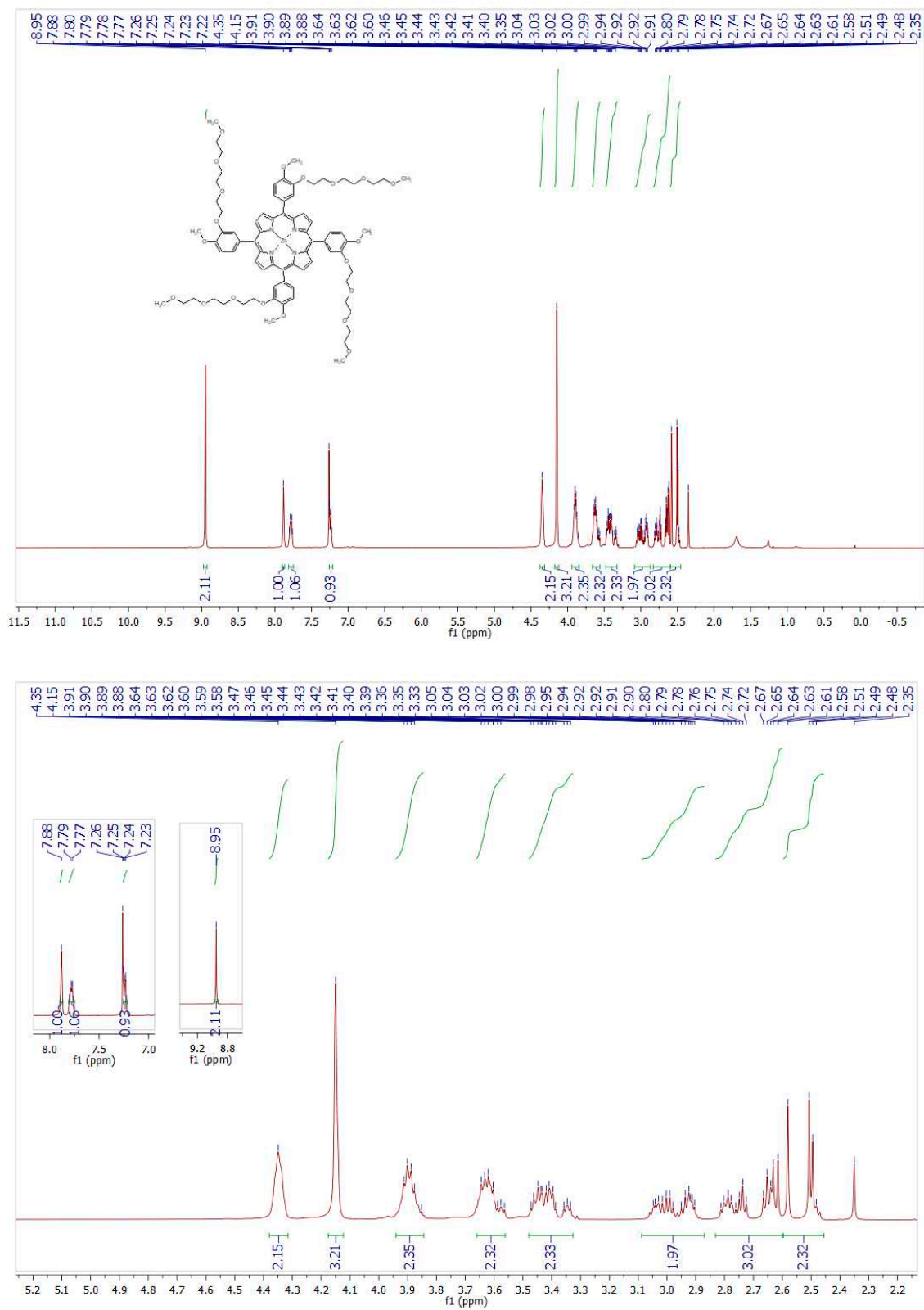


Figure S21. ^1H NMR spectra of porphyrin 5.

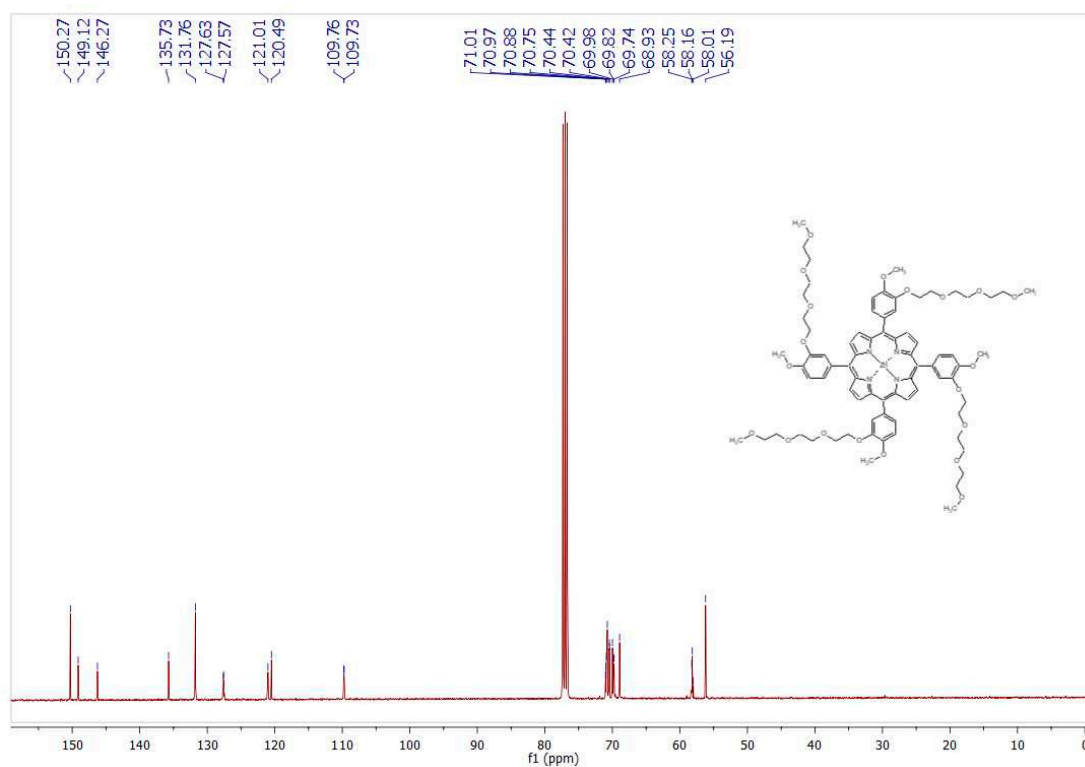


Figure S22. ¹³C NMR spectrum of porphyrin 5.

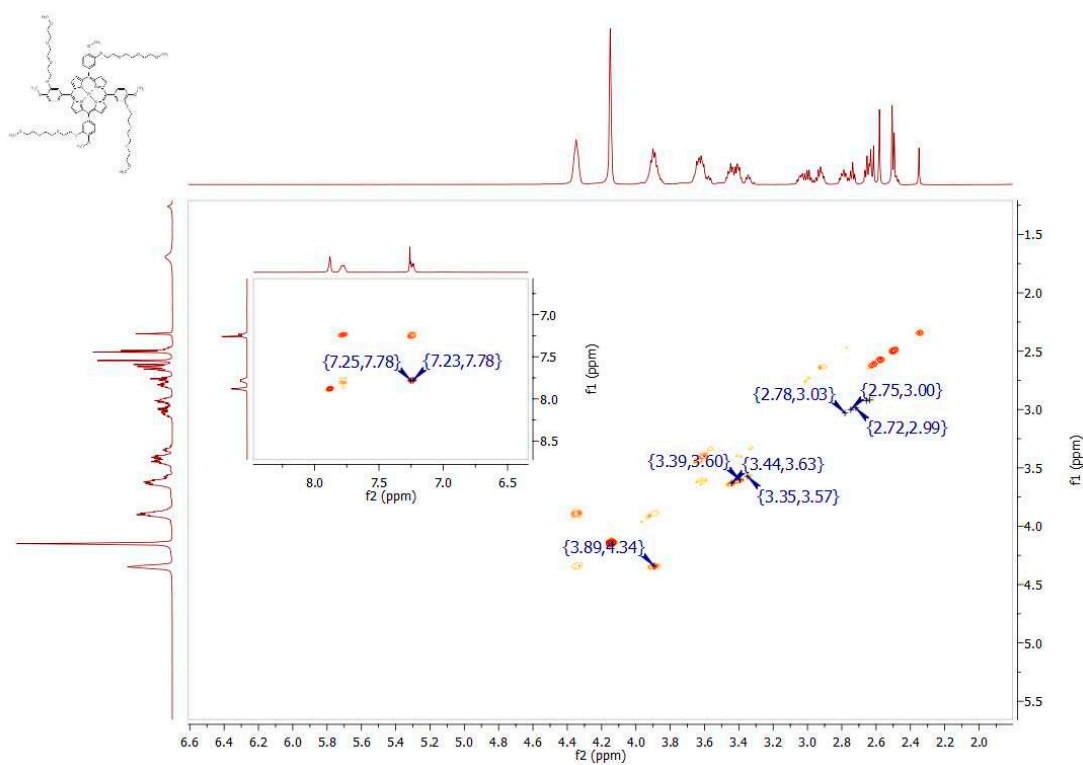


Figure S23. ¹H-¹H COSY spectrum of porphyrin 5.

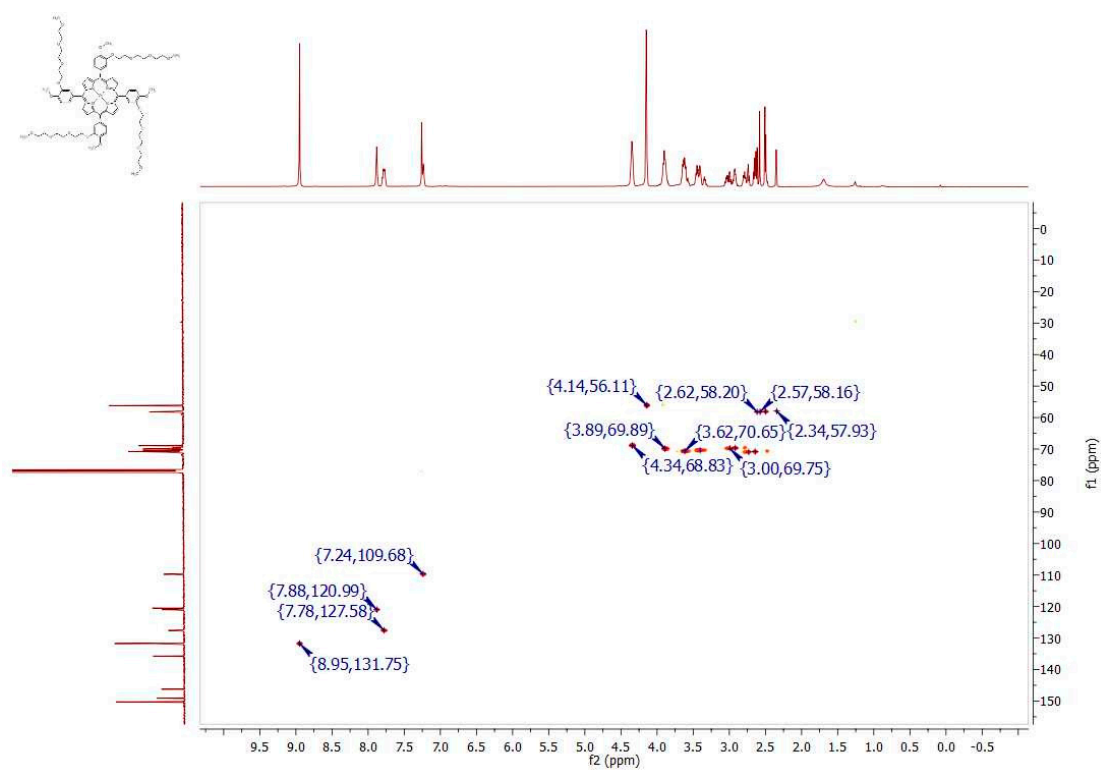


Figure S24. ^1H - ^{13}C HSQC spectrum of porphyrin 5.

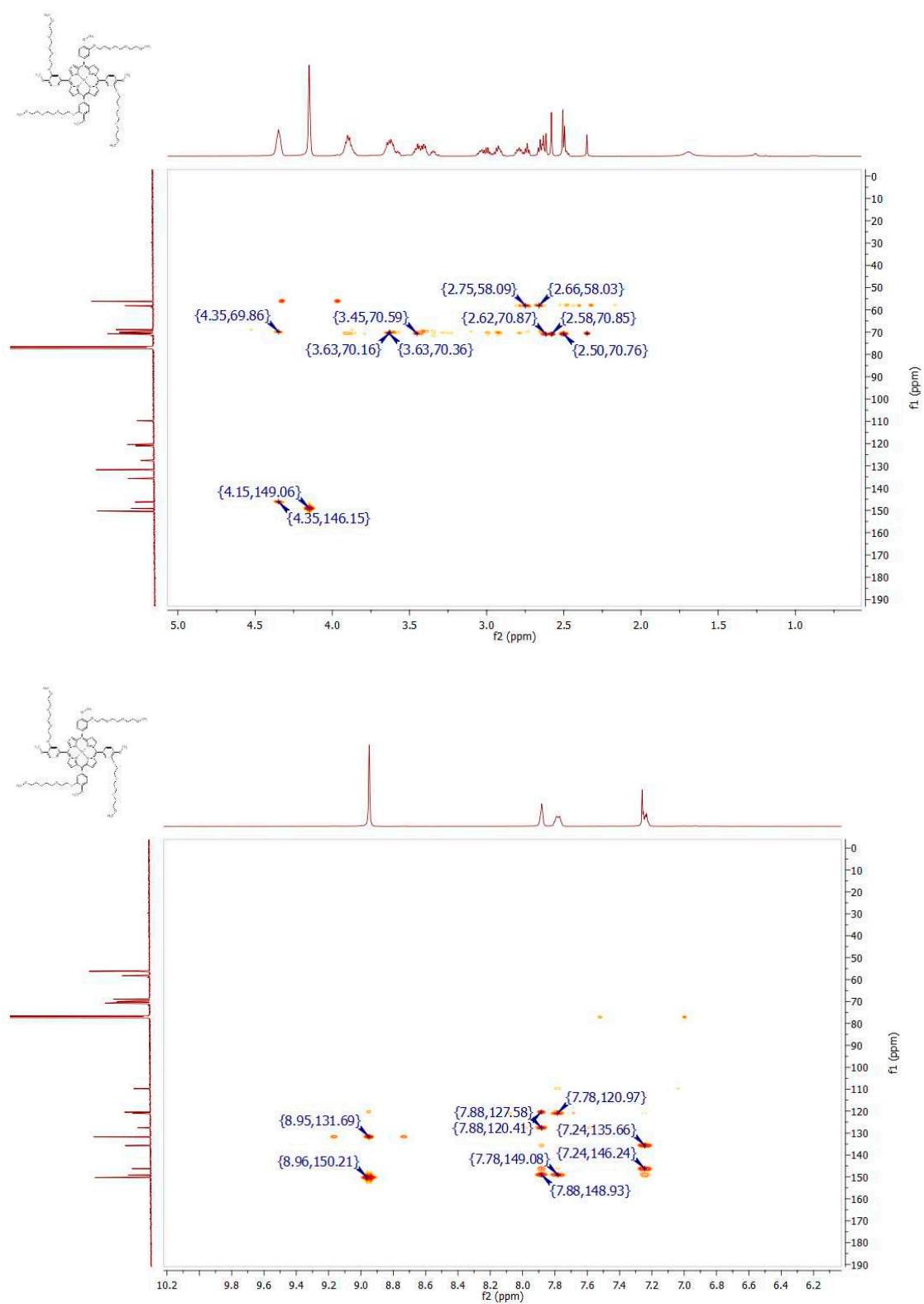


Figure S25. ^1H - ^{13}C HMBC spectra of porphyrin **5**.

1.6. NMR experiments of compound 6.

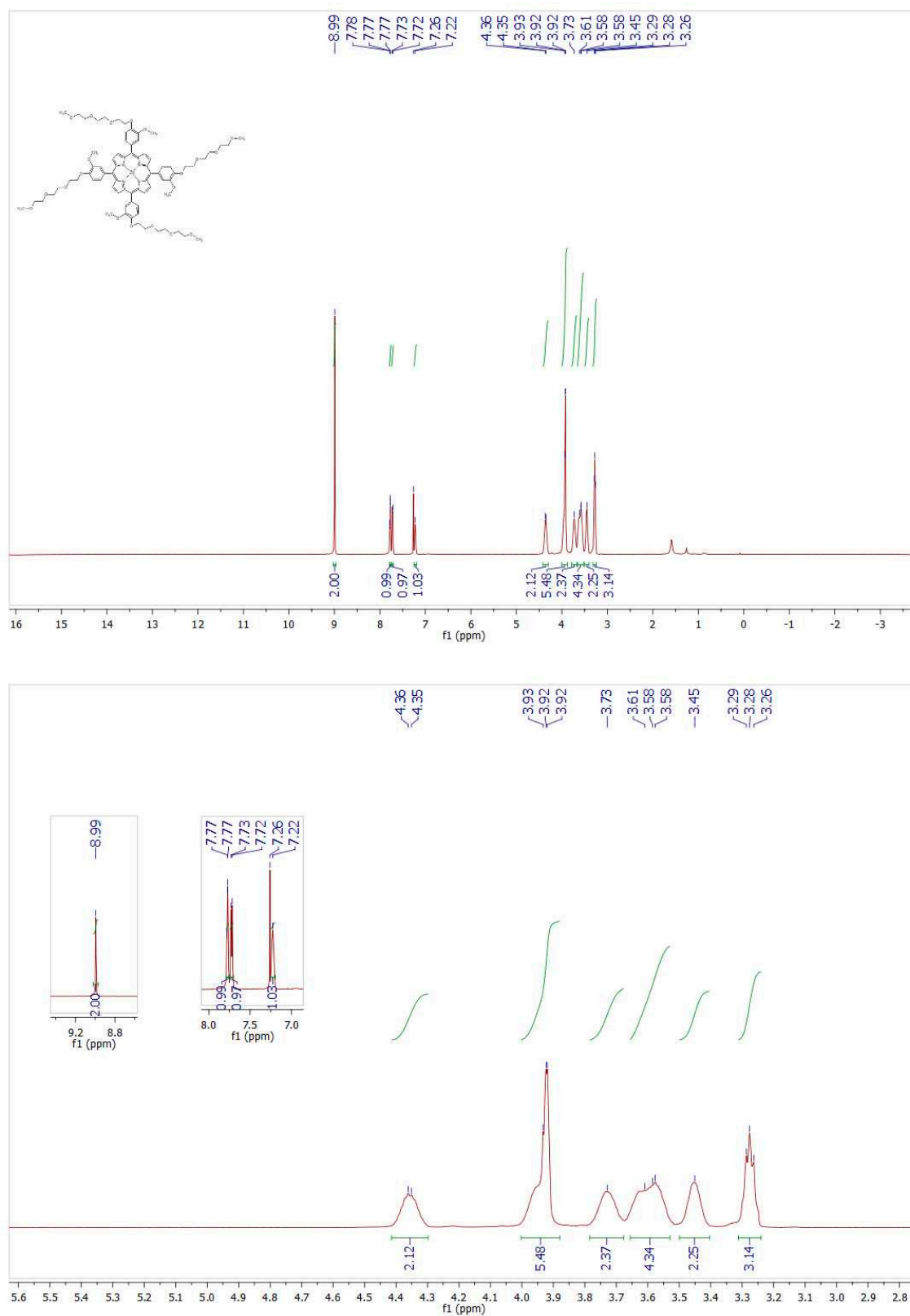


Figure S26. ^1H NMR spectra of porphyrin 6.

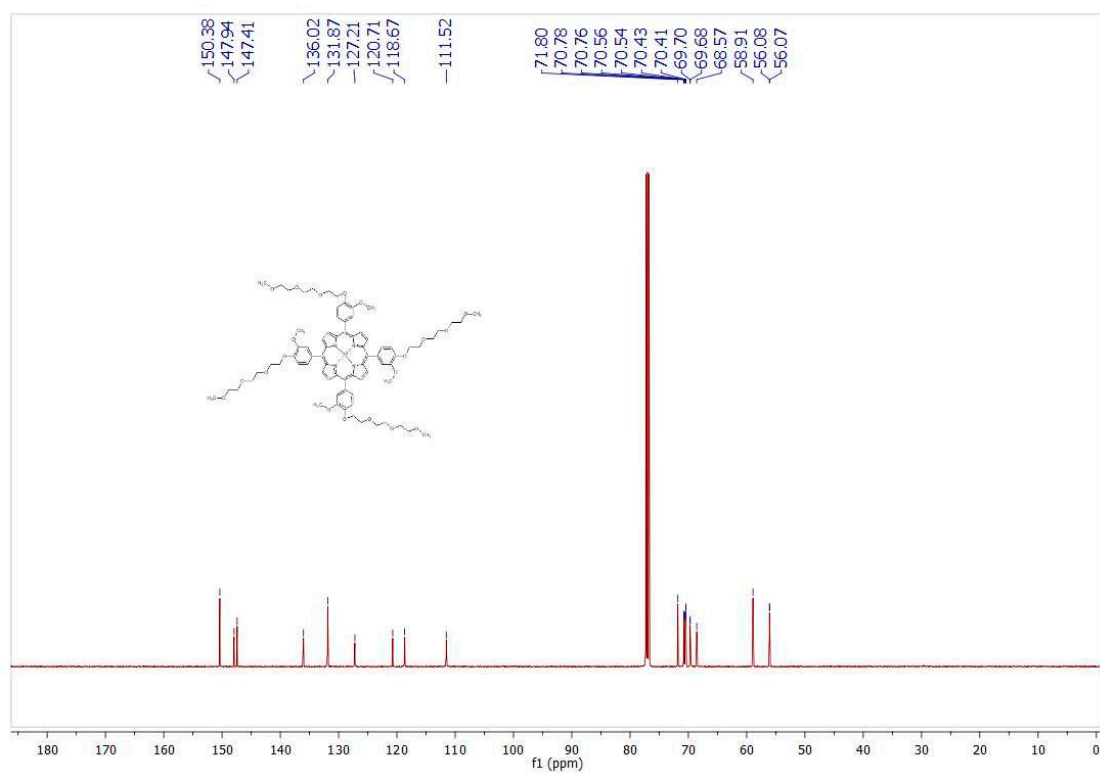


Figure S27. ¹³C NMR spectrum of porphyrin 6.

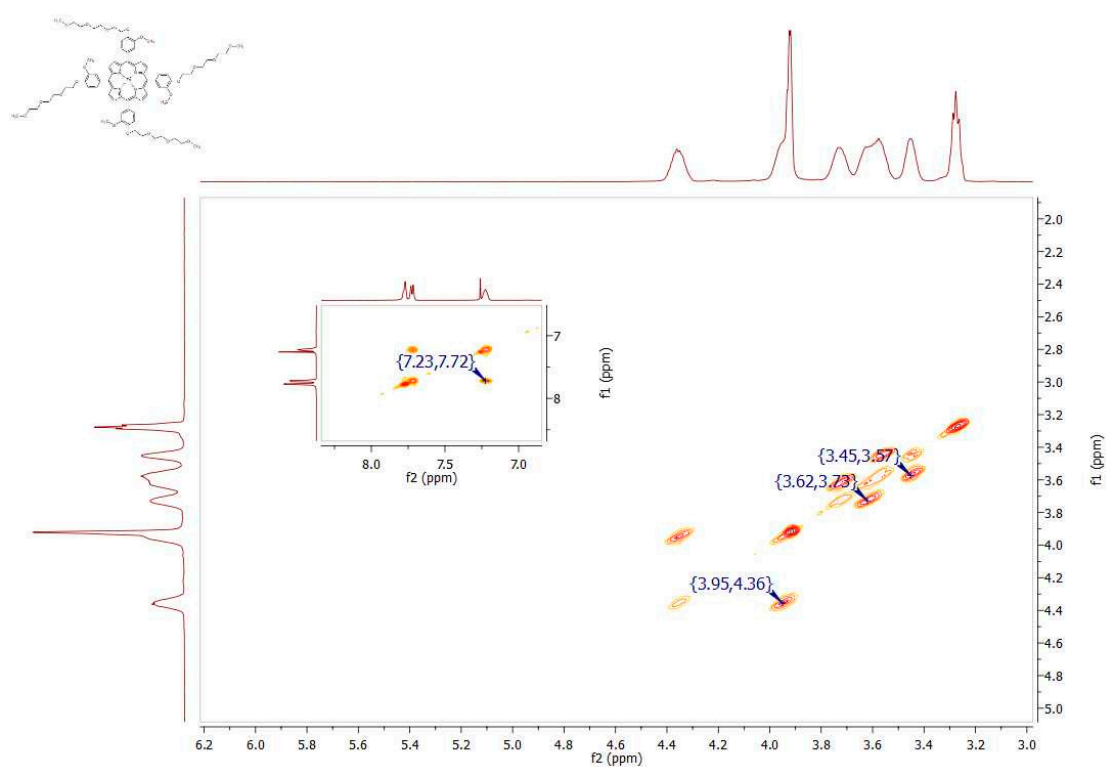


Figure S28. ¹H-¹H COSY spectrum of porphyrin 5.

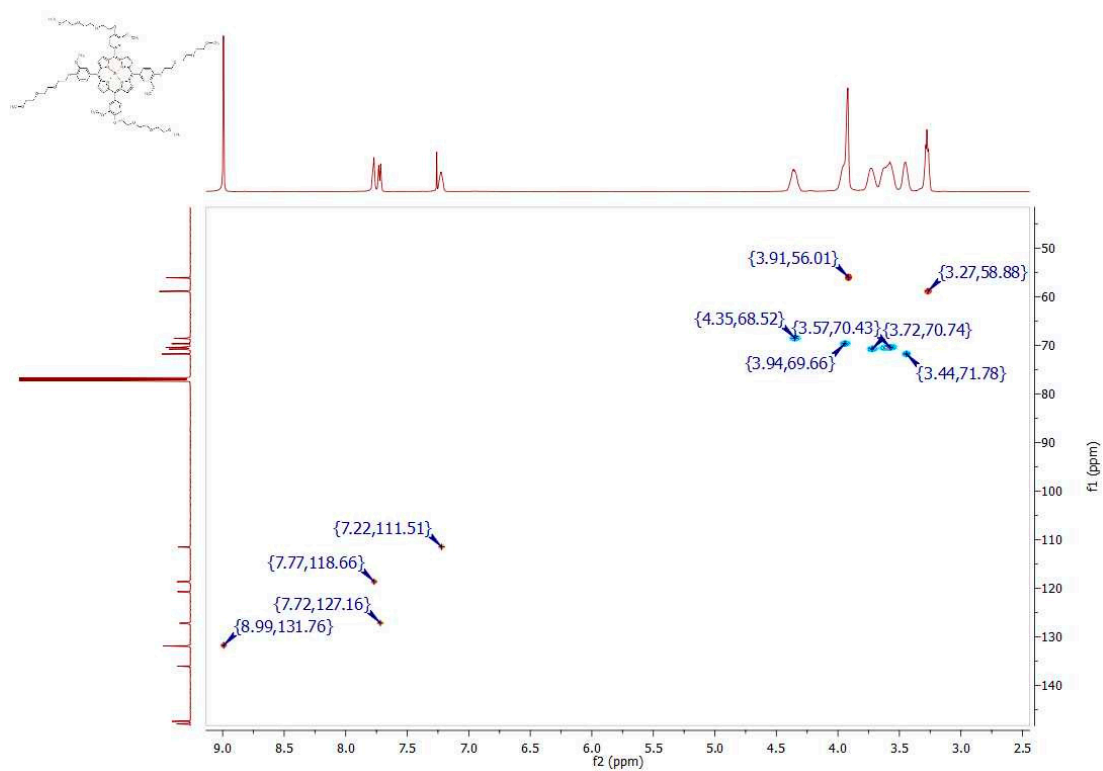


Figure S29. ^1H - ^{13}C HSQC spectrum of porphyrin 6.

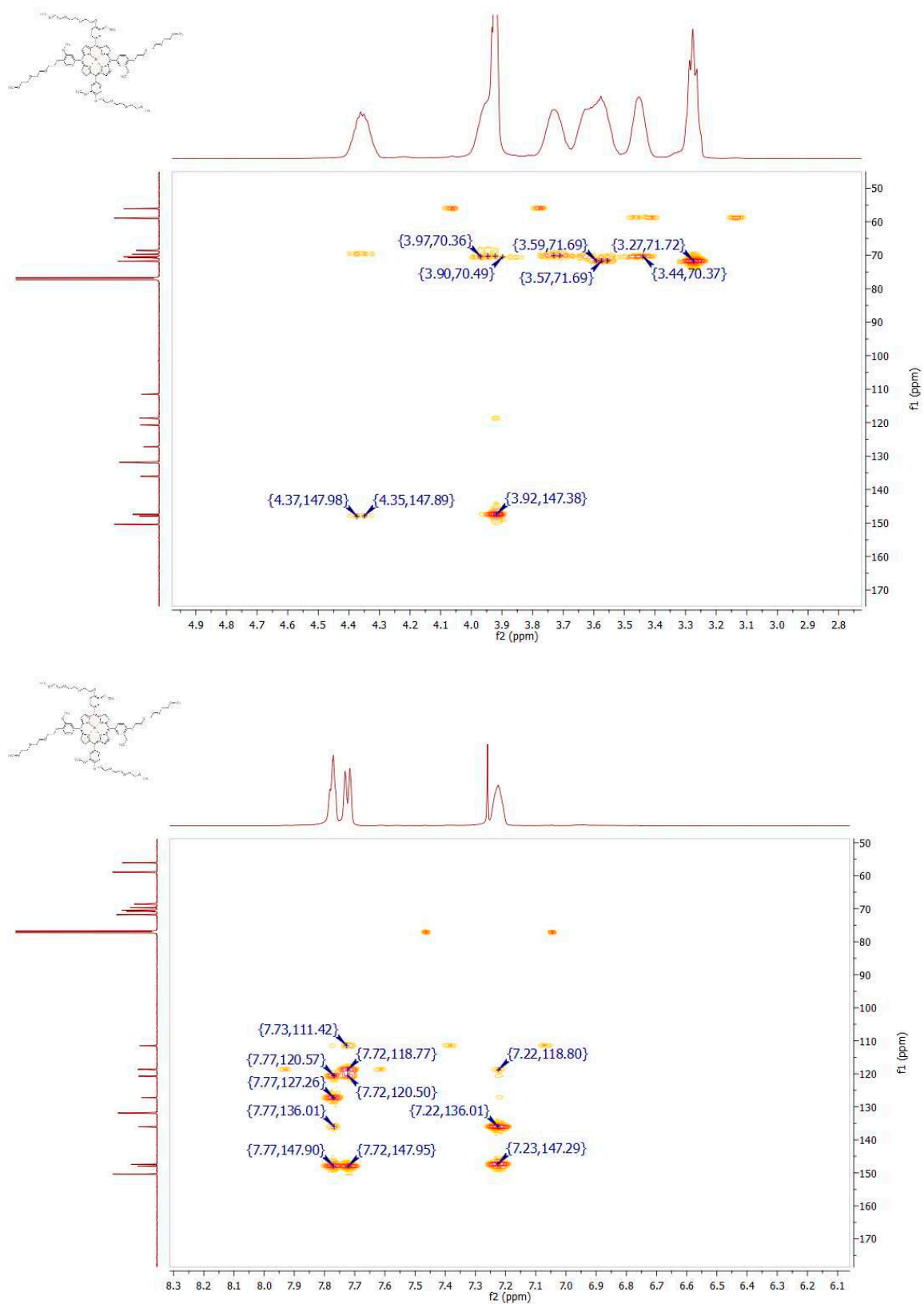


Figure S30. ^1H - ^{13}C HMBC spectra of porphyrin 6.

2. Mass spectrometry data

1.7. ESI experiments

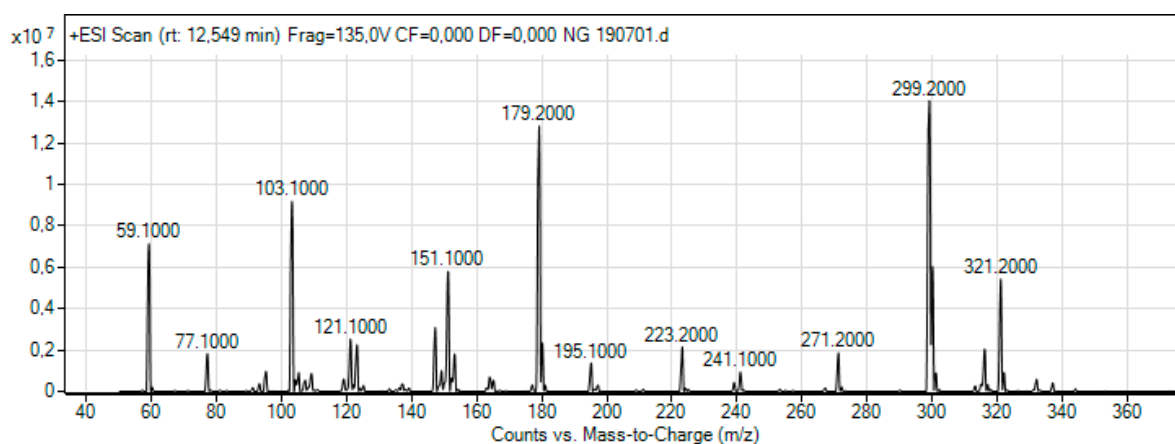


Figure S32. Mass spectra of aldehyde 1.

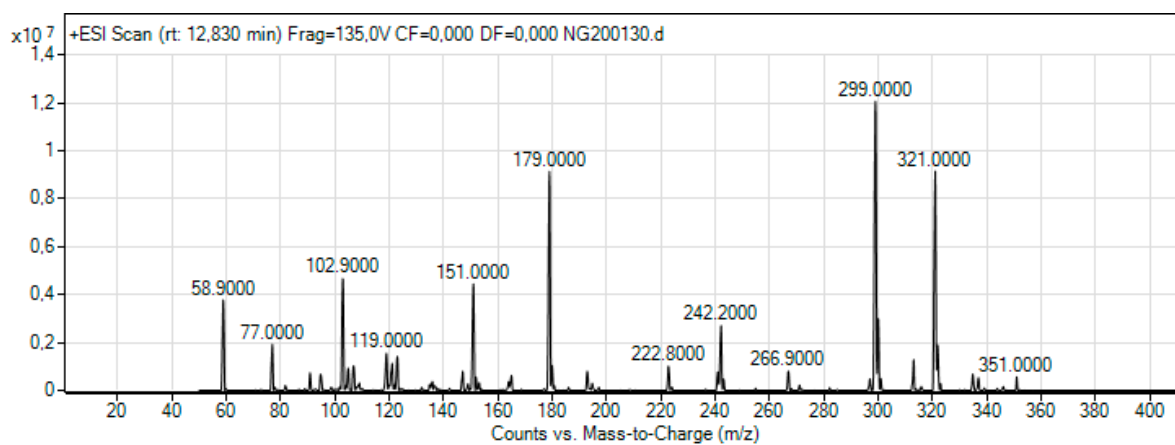


Figure S33. Mass spectra of aldehyde 2.

1.8. Data from MALDI-TOF experiments

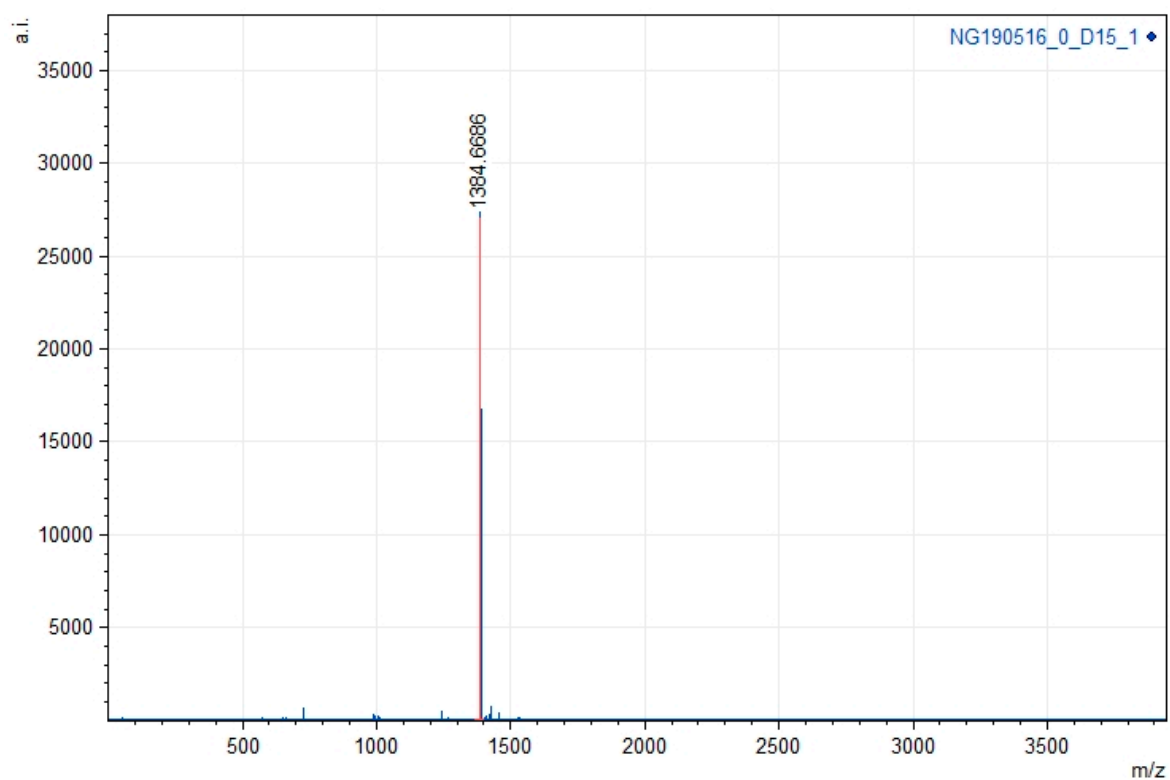


Figure S34. Mass spectra of porphyrin 3.

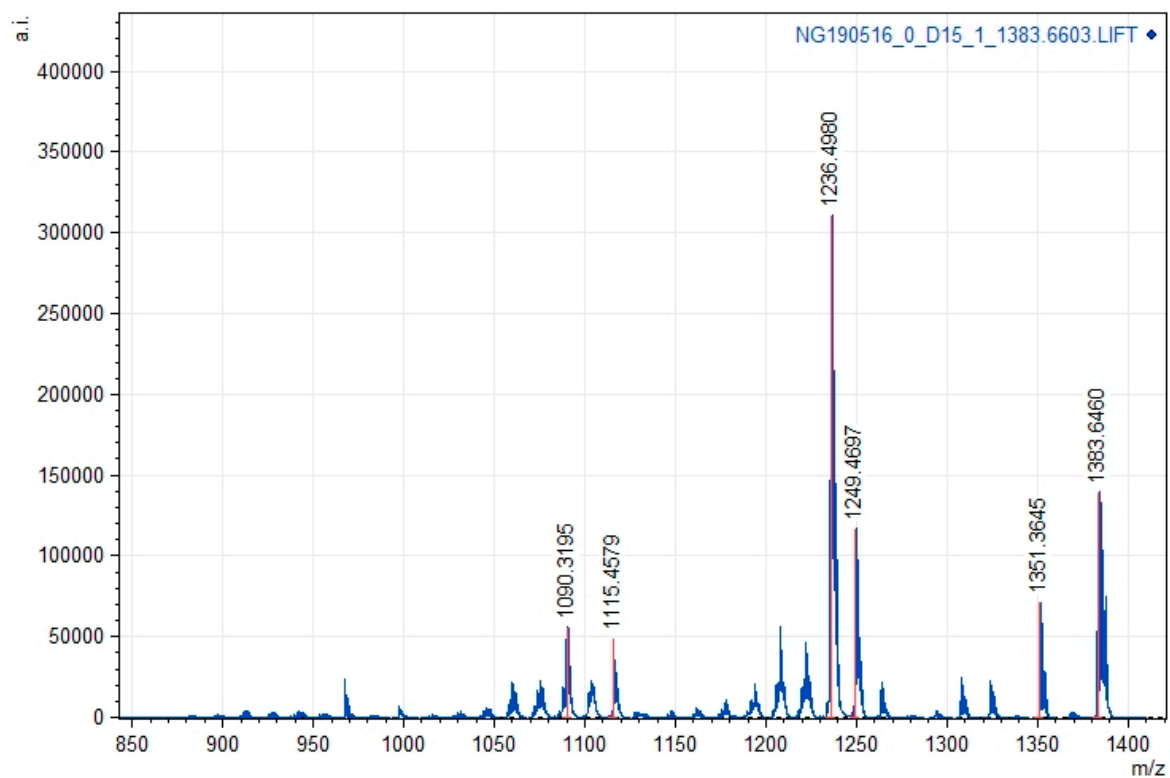


Figure S34. Fragmentation mass spectra of porphyrin 3.

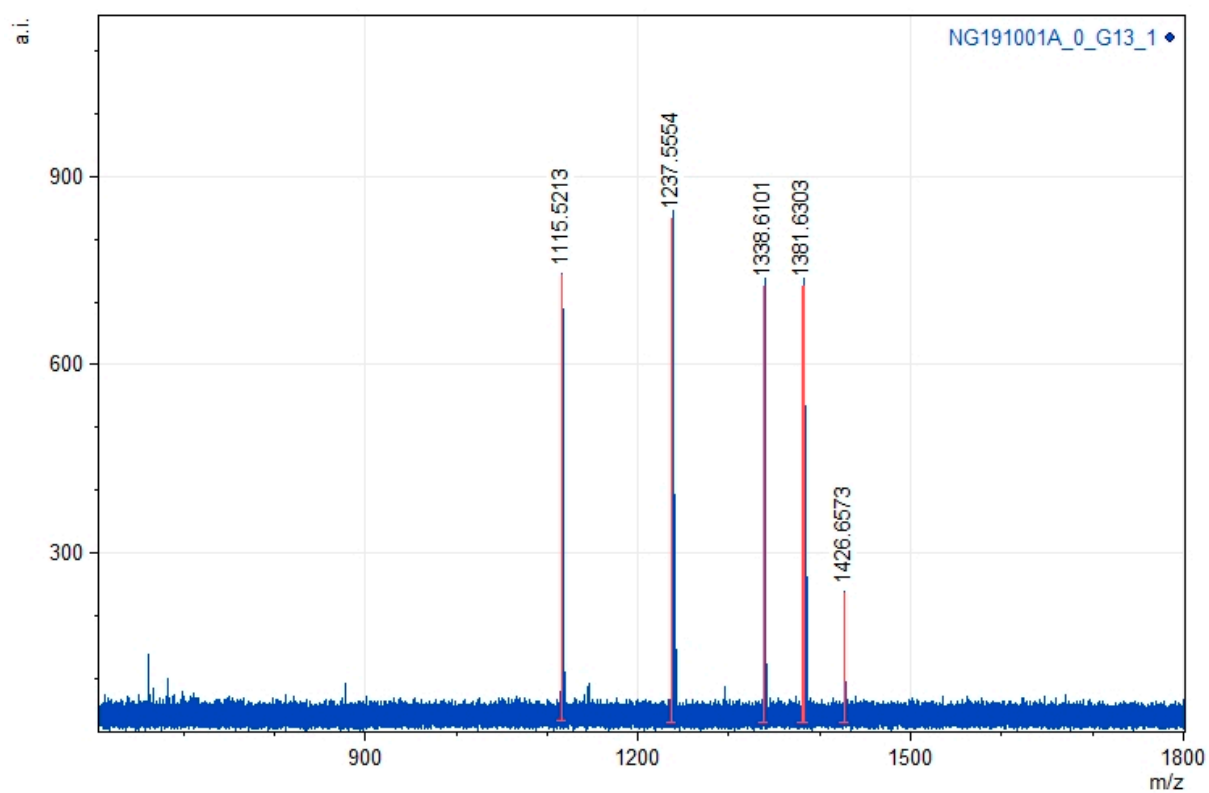


Figure S35. Mass spectra of porphyrin 4.

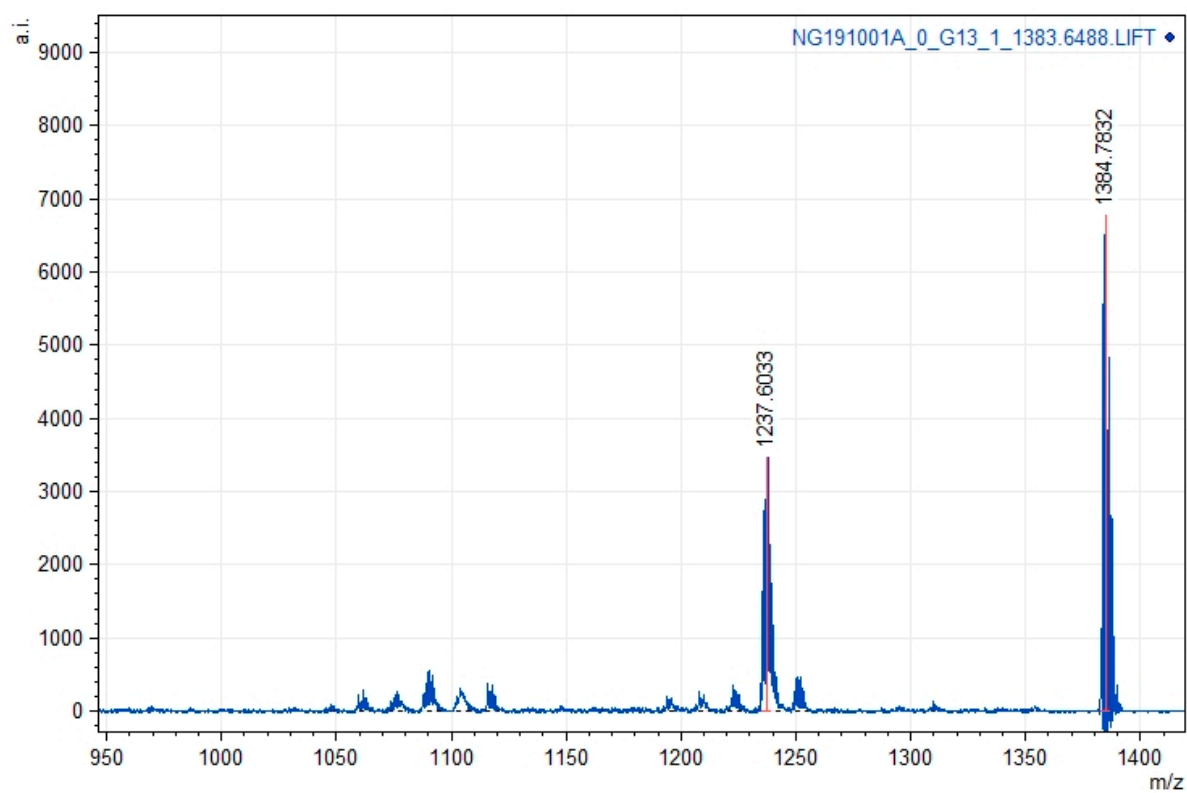


Figure S36. Fragmentation mass spectra of porphyrin 4.

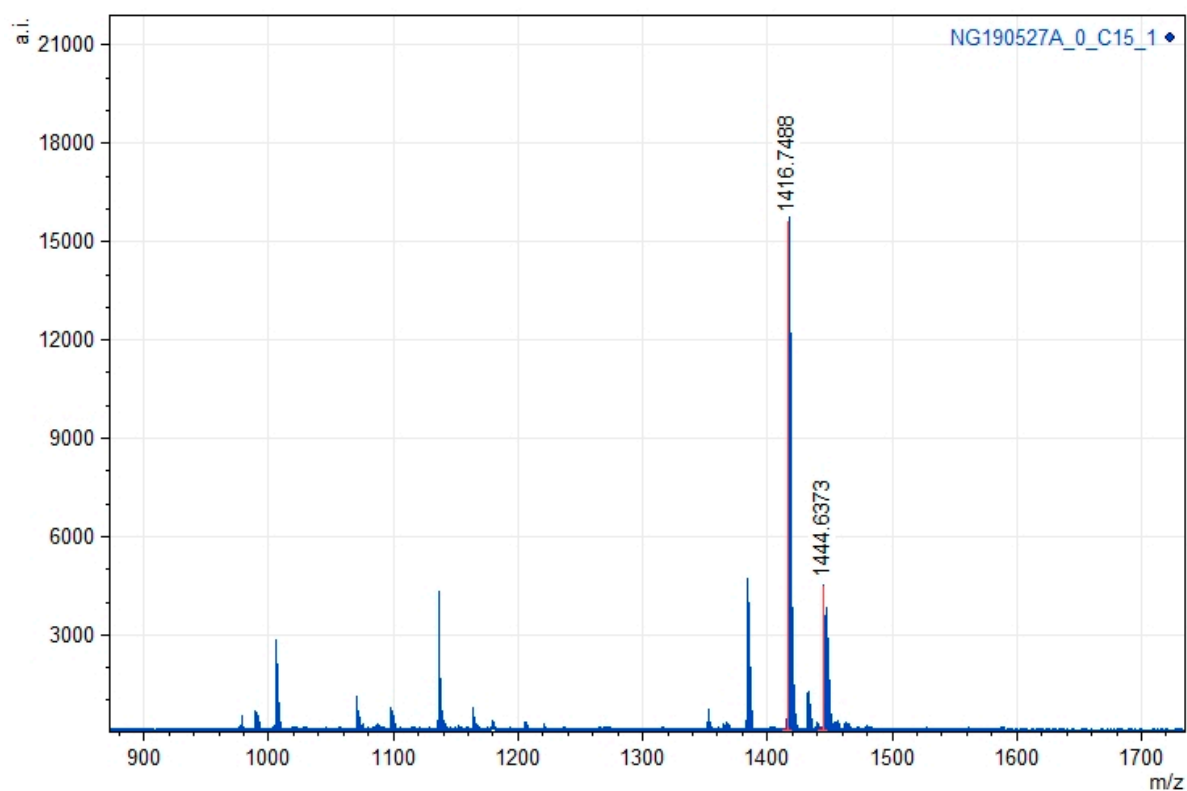


Figure S37. Mass spectra of porphyrin 5.

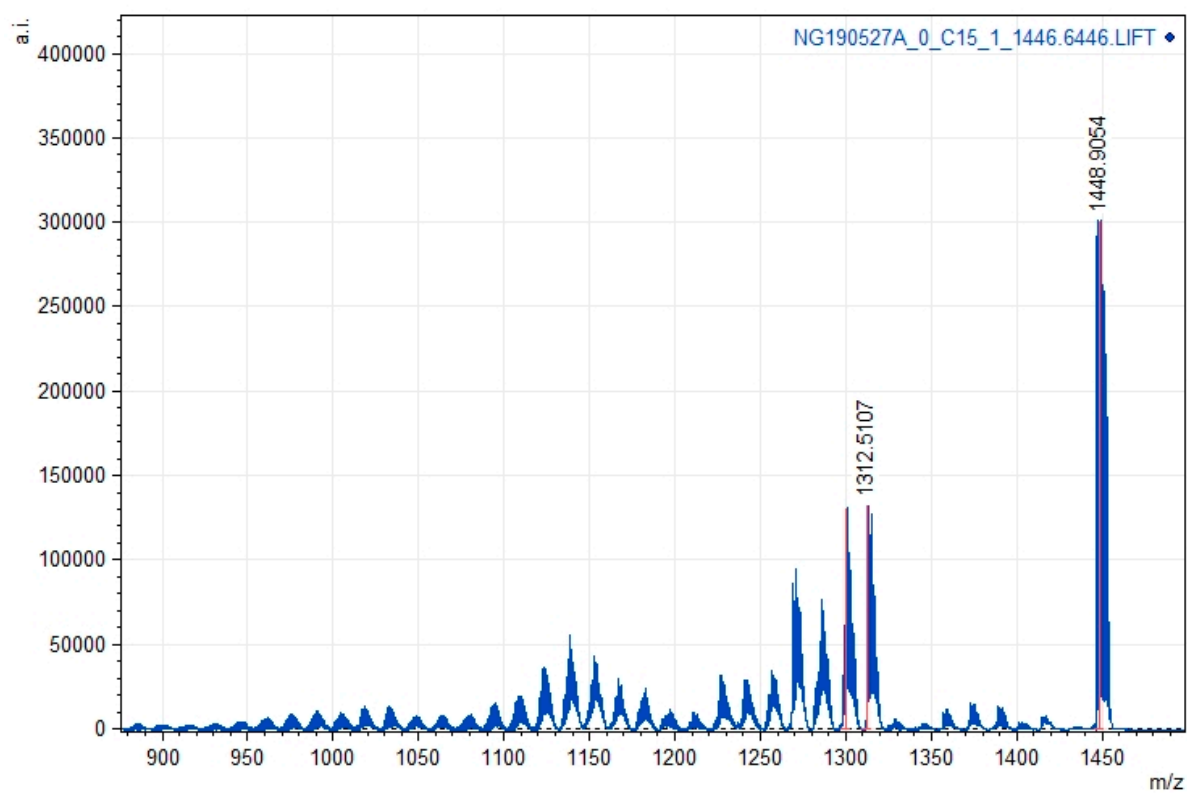


Figure S38. Fragmentation mass spectra of porphyrin 5.

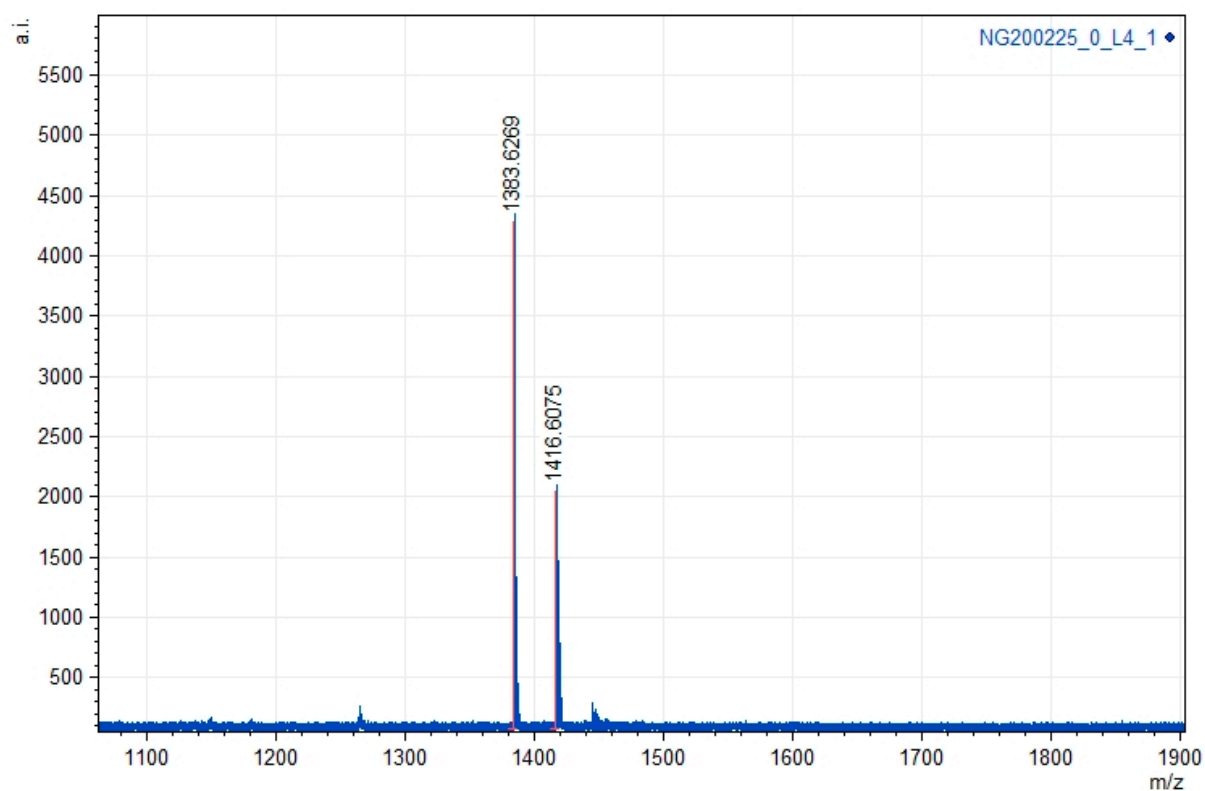


Figure S39. Fragmentation mass spectra of porphyrin 6.

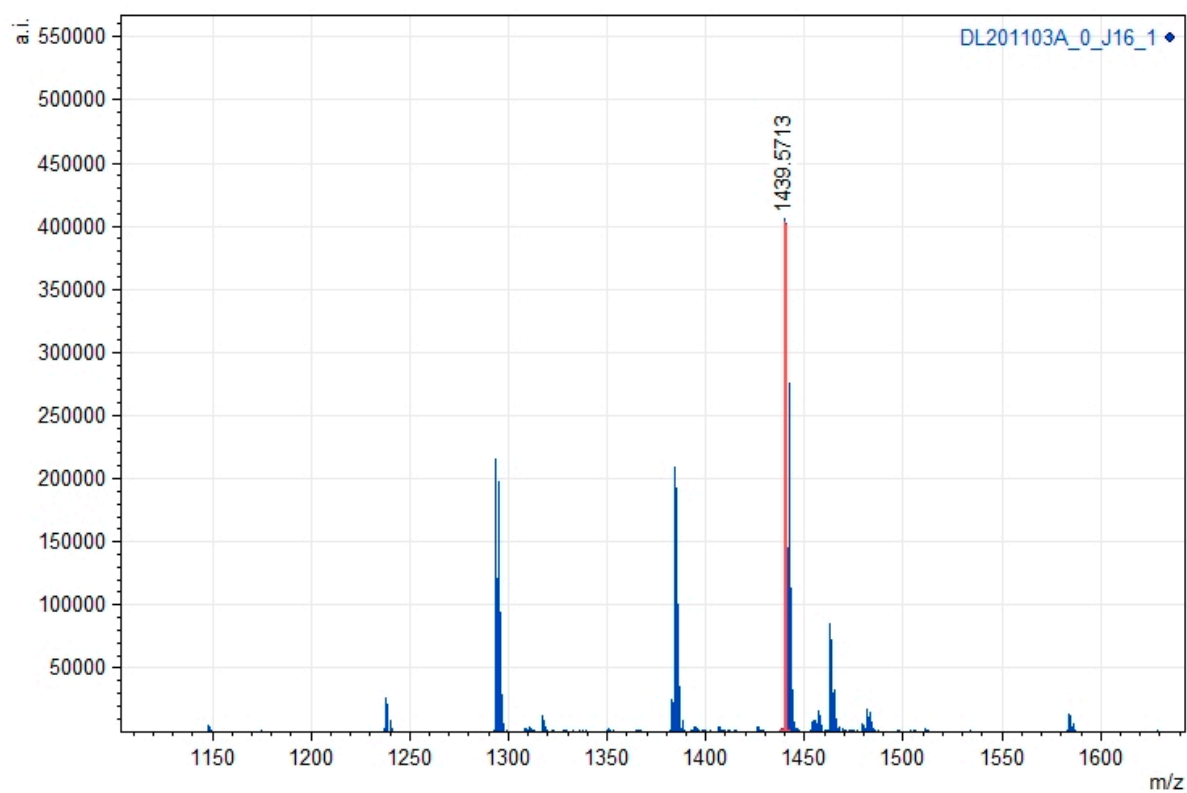


Figure S40. Mass spectra of porphyrin 7.

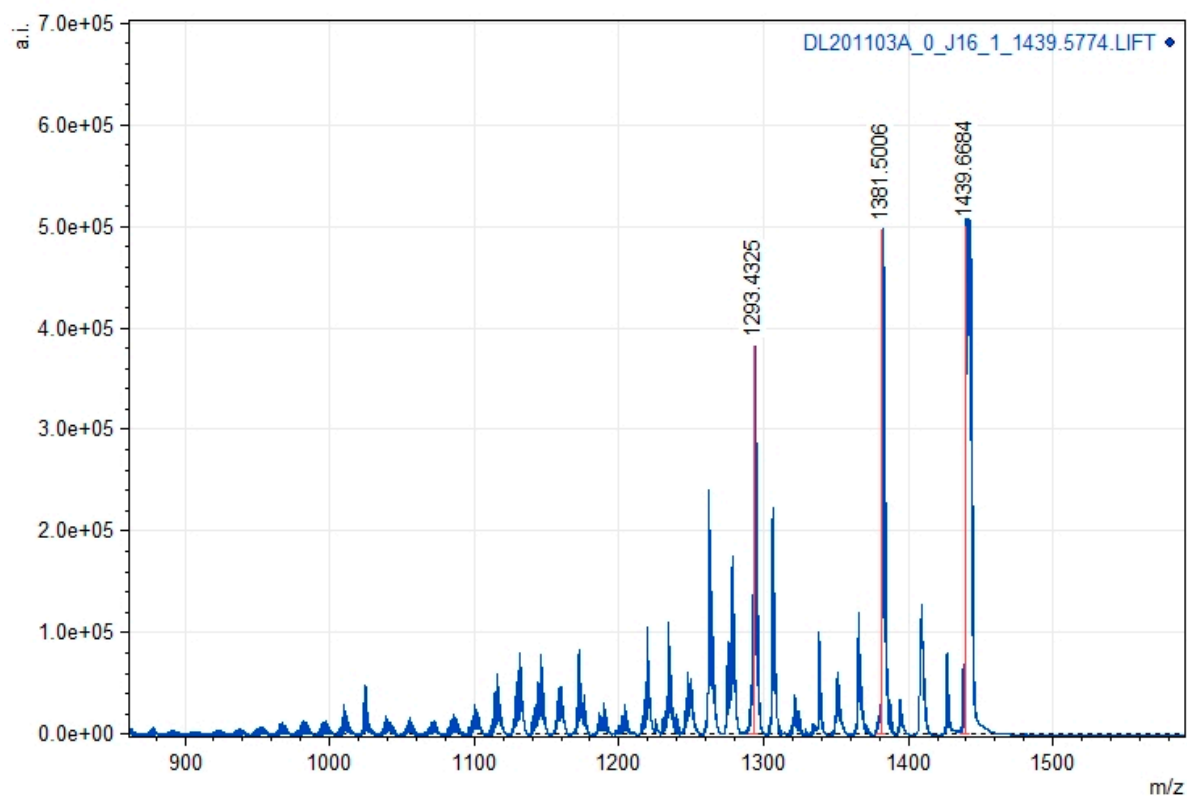


Figure S41. Fragmentation mass spectra of porphyrin 7.

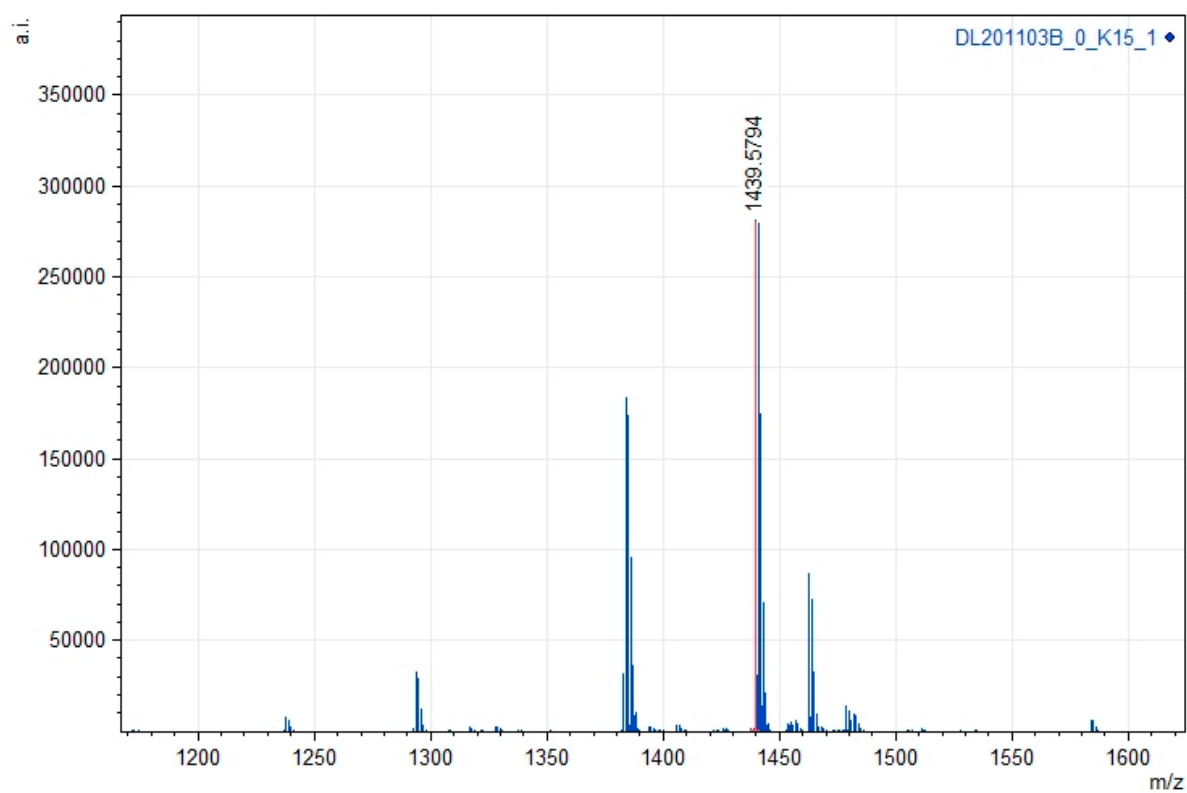


Figure S42. Mass spectra of porphyrin 8.

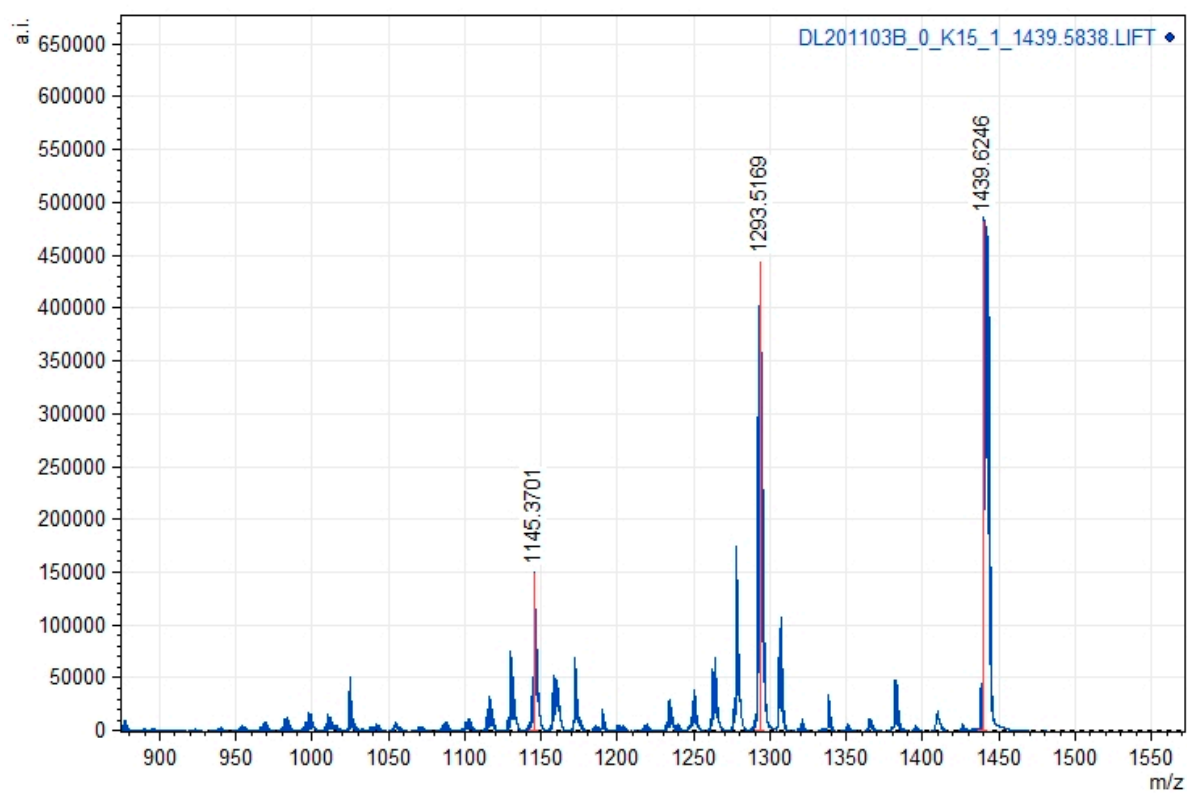


Figure S43. Fragmentation mass spectra of porphyrin 8.

3. IR data

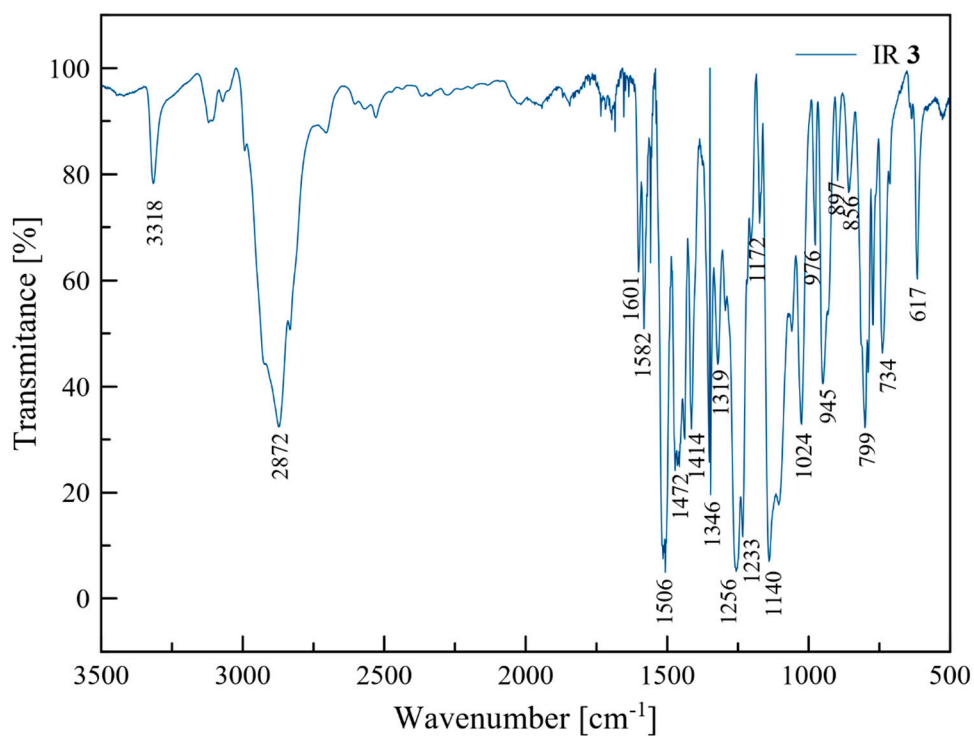


Figure S44. IR spectrum of porphyrin 3.

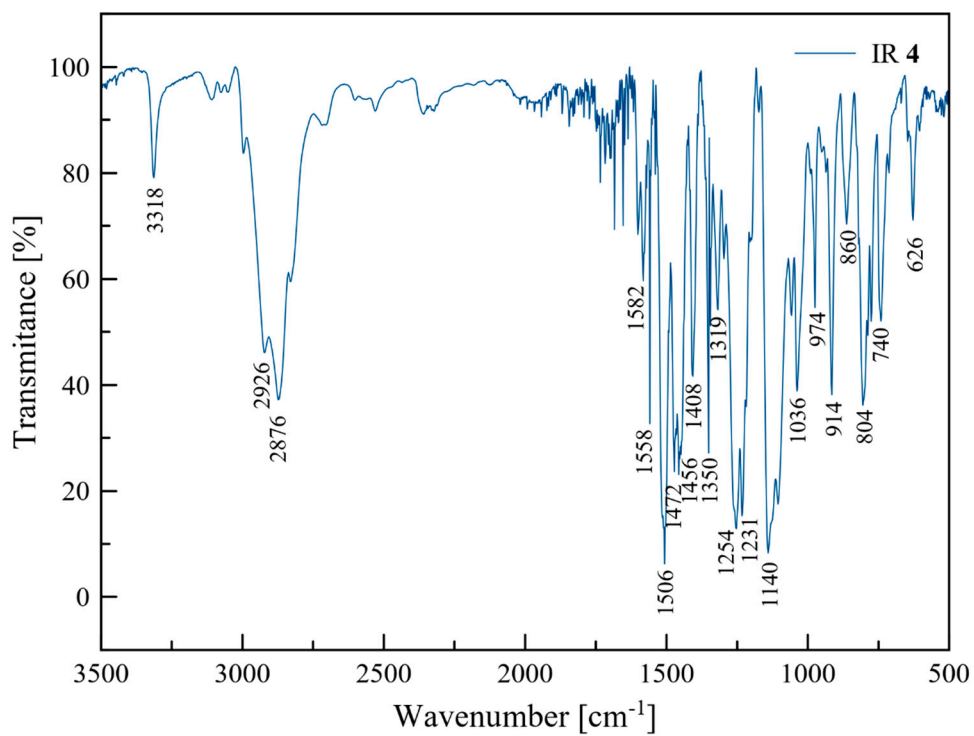


Figure S45. IR spectrum of porphyrin 4.

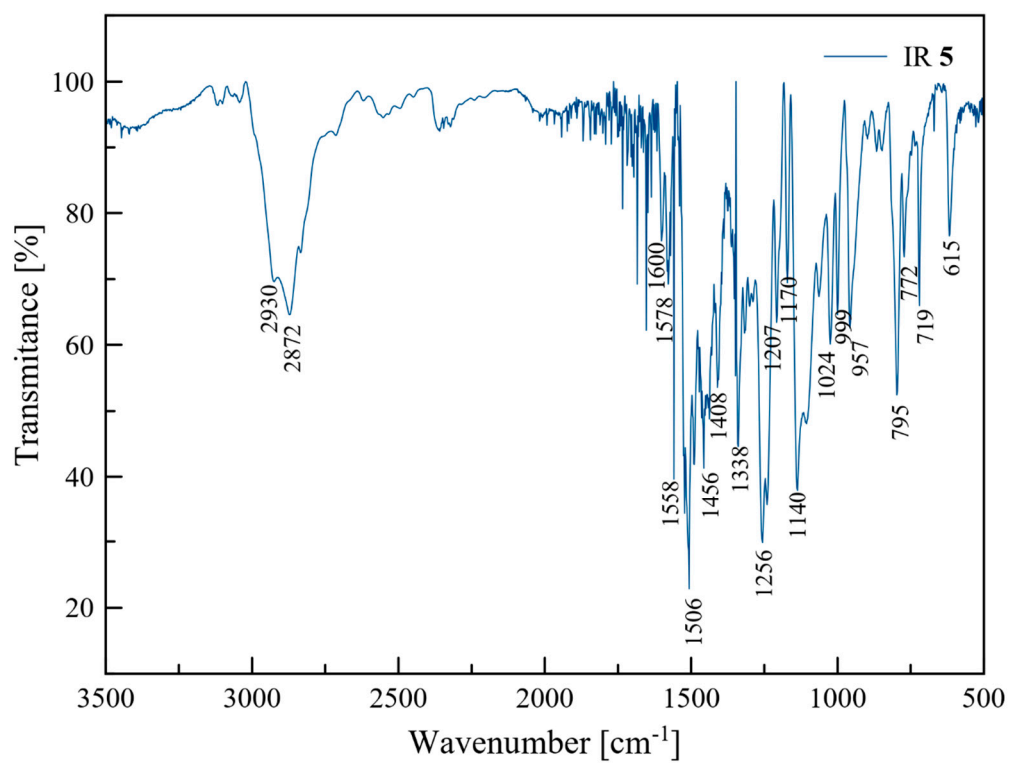


Figure S46. IR spectrum of porphyrin 5.

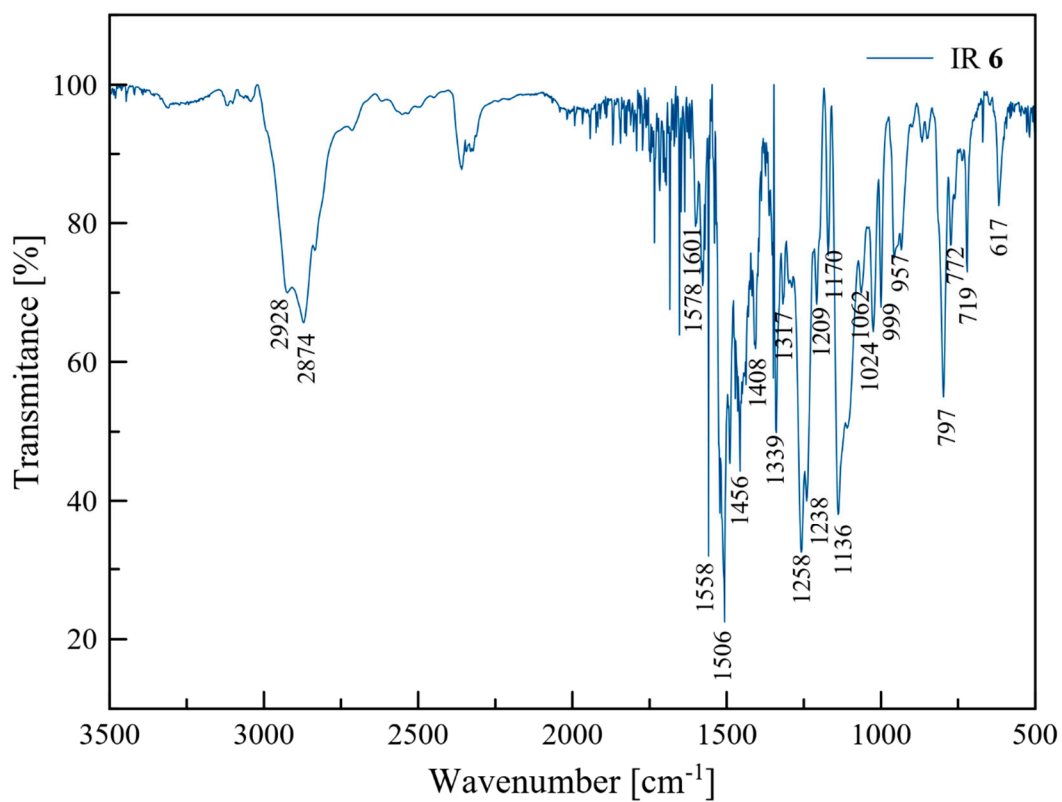


Figure S47. IR spectrum of porphyrin 6.

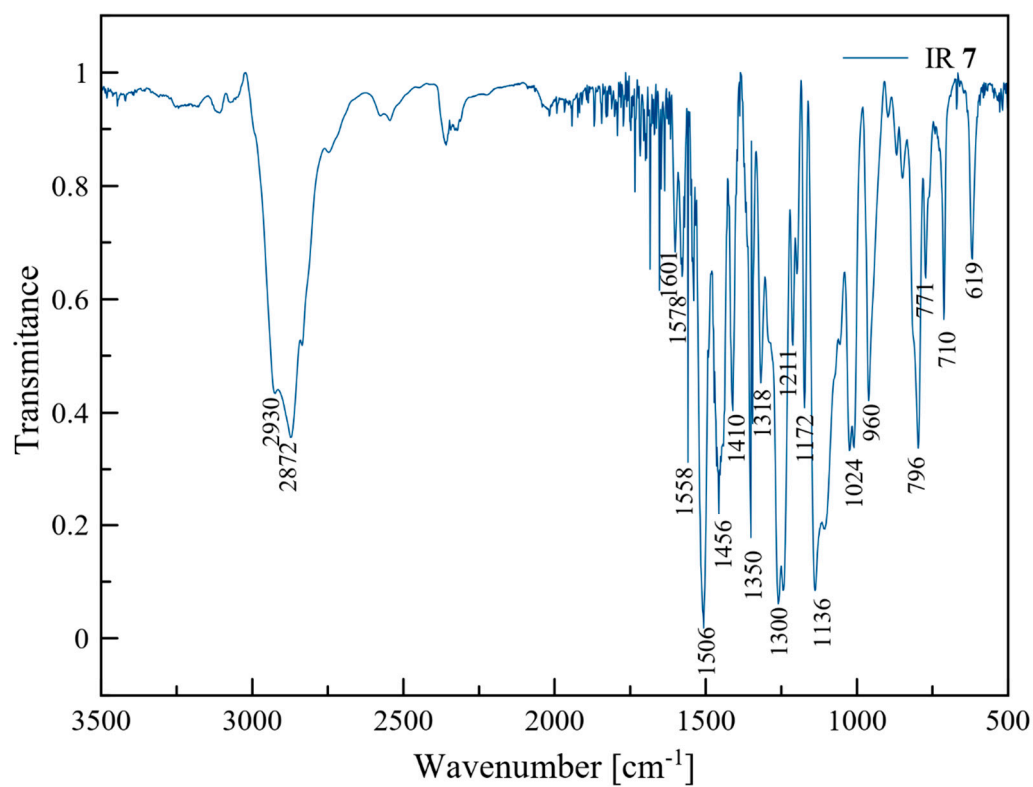


Figure S48. IR spectrum of porphyrin 7.

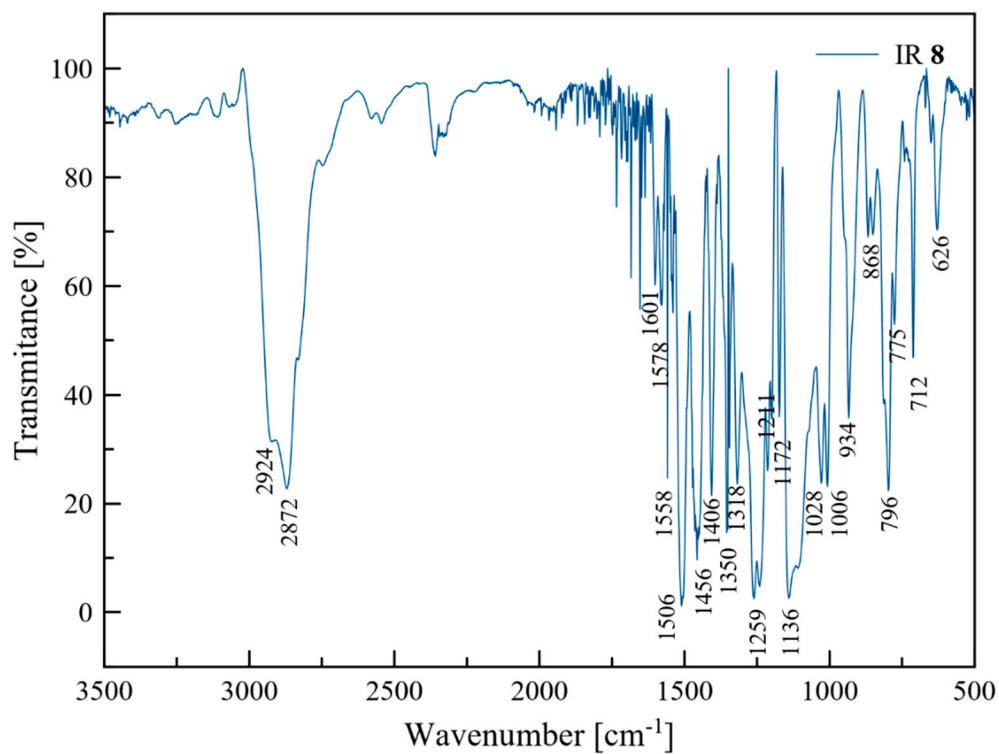


Figure S49. IR spectrum of porphyrin 8.

4. UV-vis data

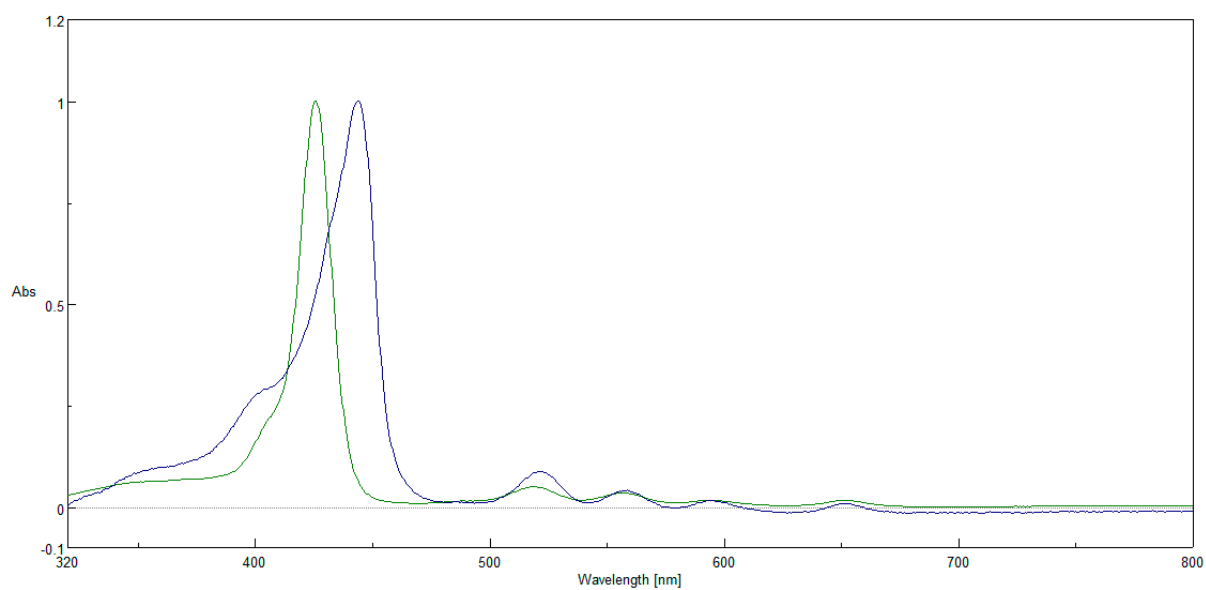


Figure S50. UV-vis spectrum of porphyrin **3** normalized in DMF (green) and water (blue).

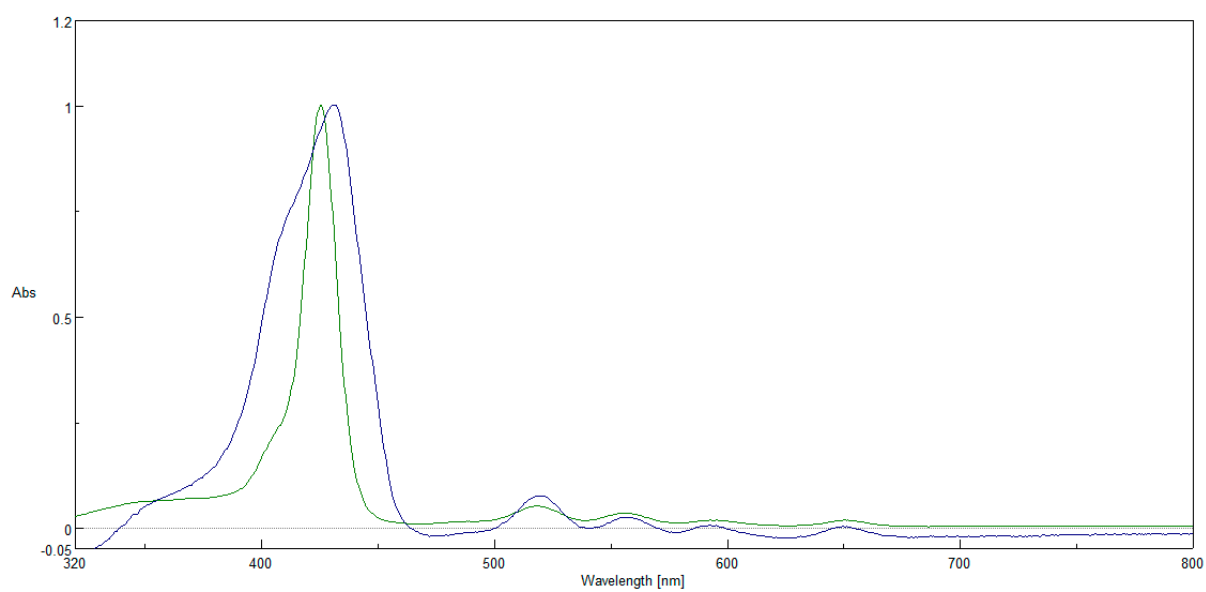


Figure S51. UV-vis spectrum of porphyrin **4** normalized in DMF (green) and water (blue).

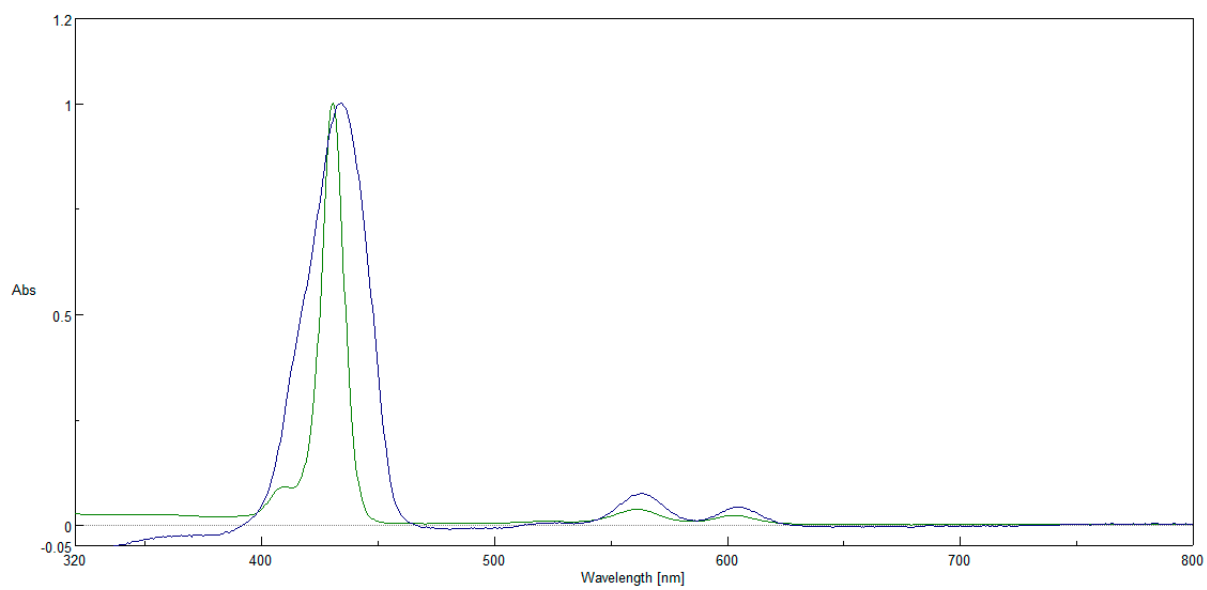


Figure S52. UV-vis spectrum of porphyrin 5 normalized in DMF (green) and water (blue).

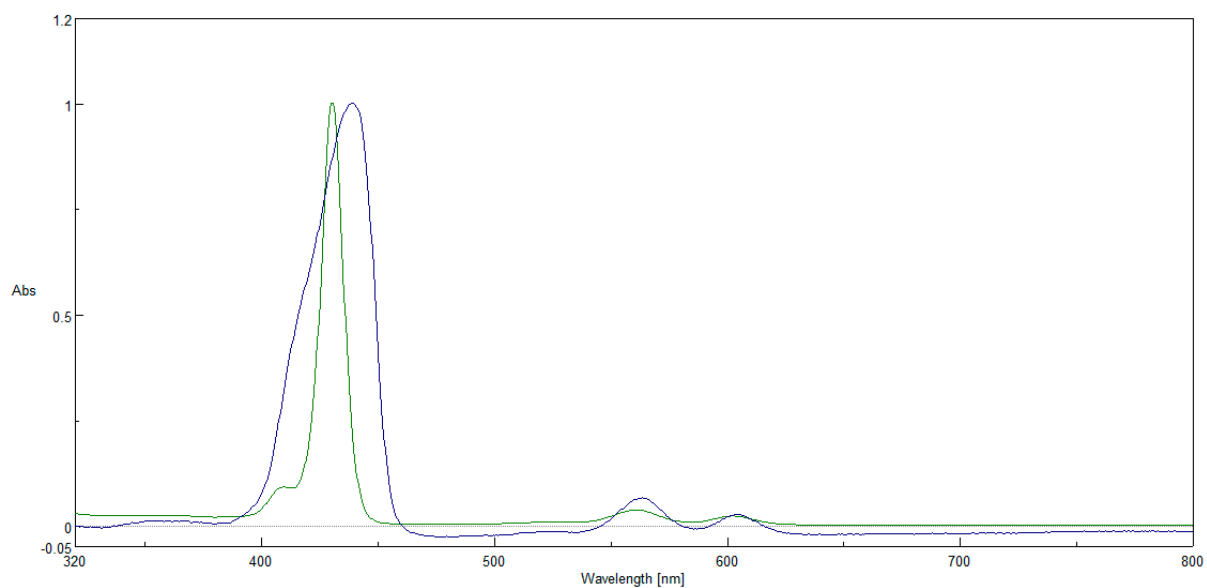


Figure S53. UV-vis spectrum of porphyrin 6 normalized in DMF (green) and water (blue).

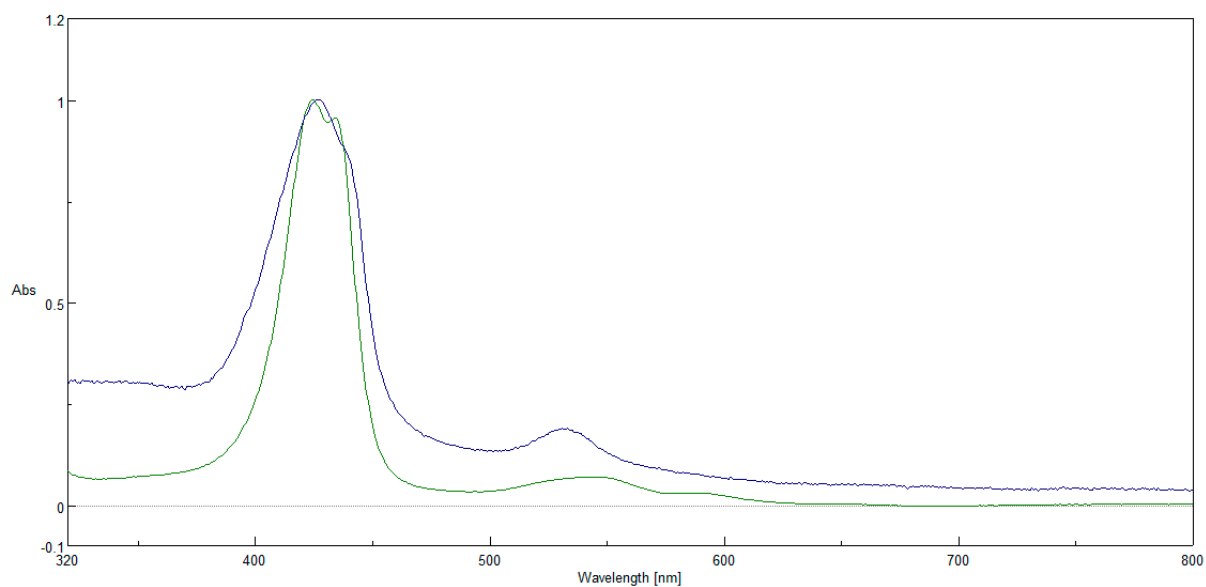


Figure S54. UV-vis spectrum of porphyrin 7 normalized in DMF (green) and water (blue).

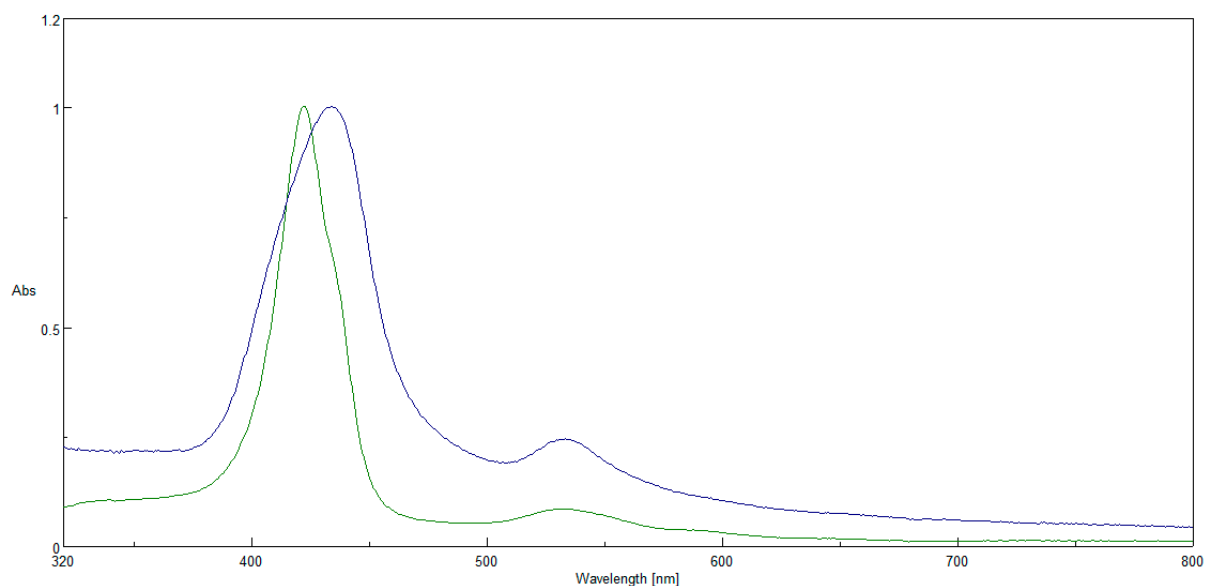


Figure S55. UV-vis spectrum of porphyrin 8 normalized in DMF (green) and water (blue).

4 HPLC data

Chromatograph HPLC: Agilent 1260 Infinity II

Column: Luna 5 μm C18(2) 100 Å 150 x 4.6 mm, Phenomenex

Solvent: Acetonitrile

Column temp.: 35°C

Mobile phase: A – H₂O, B – acetonitrile

Table S1. Gradient 3.

Time, min	A	B
0	50	50
5	40	60
10	30	70
20	0	100
30	50	50

Flow: 1.0 ml/min

Termostat: 20°C

Injection: 10 µl

Analysis time: 30 min

Detector DAD, ELSD

Table S2. Analysis date: 13.12.2021

Symbol	C, mg/ml	λ_{max} , nm	Method		
			t_R , min	%	ELSD, %
3	0.2	424	17.71	96.78	96.52
4	0.2	423	16.95	95.30	95.12
5	0.2	426	14.94	96.72	96.49
6	0.2	425	15.20	96.00	96.00
7	0.2	436	16.70	96.12	96.02
8	0.2	436	16.02	96.10	96.05

6 Computational data

The first twenty vertical excitations of **3** at the PCM/TD-DFT/PBE1PBE/6-31+G(d,p)//PBE1PBE/6-31G(d,p) of theory.

Excited state 1 ($E=2.0952$ eV, oscillator strength $f=0.106$) the transitions: 369 \rightarrow 370 0.85 (73%), 368 \rightarrow 371 0.49 (24%)

Excited state 2 ($E=2.2234$ eV, oscillator strength $f=0.157$) the transitions: 369 \rightarrow 371 0.85 (73%), 368 \rightarrow 370 -0.50 (25%)

Excited state 3 ($E=2.8783$ eV, oscillator strength $f=1.023$) the transitions: 368 \rightarrow 371 0.65 (43%), 367 \rightarrow 371 0.46 (21%), 369 \rightarrow 370 -0.38 (15%), 364 \rightarrow 370 -0.38 (15%), 368 \rightarrow 370 -0.20 (4%)

Excited state 4 ($E=2.9093$ eV, oscillator strength $f=1.061$) the transitions: 368 \rightarrow 370 0.61 (37%), 367 \rightarrow 370 -0.51 (26%), 364 \rightarrow 371 0.40 (16%), 369 \rightarrow 371 0.38 (14%), 368 \rightarrow 371 0.21 (4%)

Excited state 5 ($E=2.9474$ eV, oscillator strength $f=0.000$) the transitions: 365 \rightarrow 370 0.69 (47%), 366 \rightarrow 371 0.58 (34%), 366 \rightarrow 370 -0.39 (15%), 365 \rightarrow 371 -0.15 (2%)

Excited state 6 ($E=2.9528$ eV, oscillator strength $f=0.000$) the transitions: 366 \rightarrow 370 0.78 (61%), 366 \rightarrow 371 0.41 (17%), 365 \rightarrow 371 0.41 (17%), 365 \rightarrow 370 0.19 (3%)

Excited state 7 ($E=2.9591$ eV, oscillator strength $f=0.191$) the transitions: 367 \rightarrow 370 0.84 (70%), 368 \rightarrow 370 0.42 (18%), 369 \rightarrow 371 0.23 (5%), 364 \rightarrow 371 0.16 (3%), 367 \rightarrow 371 0.15 (2%)

Excited state 8 ($E=3.0029$ eV, oscillator strength $f=0.000$) the transitions: 365 \rightarrow 370 0.69 (48%), 366 \rightarrow 371 -0.68 (46%), 366 \rightarrow 370 0.22 (5%)

Excited state 9 ($E=3.0099$ eV, oscillator strength $f=0.160$) the transitions: 367 \rightarrow 371 0.87 (75%), 368 \rightarrow 371 -0.30 (9%), 364 \rightarrow 370 0.25 (6%), 369 \rightarrow 370 0.23 (5%), 367 \rightarrow 370 -0.15 (2%)

Excited state 10 ($E=3.0301$ eV, oscillator strength $f=0.002$) the transitions: 365 \rightarrow 371 0.89 (80%), 366 \rightarrow 370 -0.42 (17%)

Excited state 11 ($E=3.2612$ eV, oscillator strength $f=0.405$) the transitions: 364 \rightarrow 370 0.84 (70%), 368 \rightarrow 371 0.37 (14%), 362 \rightarrow 370 -0.24 (6%), 358 \rightarrow 370 -0.18 (3%), 369 \rightarrow 370 -0.15 (2%)

Excited state 12 ($E=3.3446$ eV, oscillator strength $f=0.554$) the transitions: 364 \rightarrow 371 0.88 (78%), 368 \rightarrow 370 -0.36 (13%), 369 \rightarrow 371 -0.21 (4%)

Excited state 13 ($E=3.4633$ eV, oscillator strength $f=0.000$) the transitions: 363 \rightarrow 370 0.90 (81%), 360 \rightarrow 370 -0.37 (14%)

Excited state 14 (E=3.6407 eV, oscillator strength f=0.413) the transitions: 362 -> 370 0.84 (71%), 359 -> 370 0.32 (10%), 364 -> 370 0.23 (5%), 358 -> 370 0.21 (4%), 362 -> 371 -0.17 (3%), 368 -> 371 0.15 (2%)

Excited state 15 (E=3.6864 eV, oscillator strength f=0.000) the transitions: 363 -> 371 0.97 (94%), 360 -> 371 -0.18 (3%)

Excited state 16 (E=3.7131 eV, oscillator strength f=0.039) the transitions: 362 -> 371 0.94 (88%), 358 -> 371 0.18 (3%), 359 -> 371 0.17 (3%)

Excited state 17 (E=3.8032 eV, oscillator strength f=0.001) the transitions: 361 -> 370 0.61 (37%), 361 -> 371 -0.57 (32%), 360 -> 370 0.37 (14%), 369 -> 372 0.27 (7%), 363 -> 370 0.25 (6%)

Excited state 18 (E=3.8148 eV, oscillator strength f=0.000) the transitions: 369 -> 372 0.89 (80%), 361 -> 370 -0.33 (11%), 360 -> 371 0.24 (6%)

Excited state 19 (E=3.8292 eV, oscillator strength f=0.001) the transitions: 360 -> 370 0.63 (40%), 360 -> 371 0.54 (29%), 361 -> 370 -0.44 (19%), 369 -> 372 -0.25 (6%), 363 -> 370 0.20 (4%)

Excited state 20 (E=3.8515 eV, oscillator strength f=0.023) the transitions: 359 -> 370 0.74 (55%), 359 -> 371 0.41 (17%), 362 -> 370 -0.40 (16%), 358 -> 370 0.31 (10%)

The first twenty vertical excitations of **4** at the PCM/TD-DFT/PBE1PBE/6-31+G(d,p)//PBE1PBE/6-31G(d,p) of theory.

Excited state 1 (E=2.0787 eV, oscillator strength f=0.150) the transitions: 369 -> 370 0,87 (76%), 368 -> 371 -0,47 (22%)

Excited state 2 (E=2.1992 eV, oscillator strength f=0.227) the transitions: 369 -> 371 0,88 (77%), 368 -> 370 0,47 (22%)

Excited state 3 (E=2.8914 eV, oscillator strength f=1.177) the transitions: 368 -> 371 0,70 (48%), 366 -> 371 0,43 (19%), 369 -> 370 0,37 (14%), 364 -> 370 0,35 (12%), 368 -> 370 -0,21 (4%)

Excited state 4 (E=2.9281 eV, oscillator strength f=1.273) the transitions: 368 -> 370 0,69 (48%), 366 -> 370 -0,40 (16%), 369 -> 371 -0,38 (15%), 364 -> 371 -0,38 (14%), 368 -> 371 0,22 (5%)

Excited state 5 (E=2.9719 eV, oscillator strength f=0.001) the transitions: 367 -> 371 0,65 (42%), 365 -> 370 -0,65 (42%), 367 -> 370 -0,36 (13%)

Excited state 6 (E=2.9784 eV, oscillator strength f=0.000) the transitions: 367 → 370 0,82 (67%), 367 → 371 0,39 (15%), 365 → 371 -0,39 (15%)

Excited state 7 (E=2.9787 eV, oscillator strength f=0.094) the transitions: 367 → 370 0,82 (67%), 367 → 371 0,39 (15%), 365 → 371 -0,39 (15%)

Excited state 8 (E=3.0203 eV, oscillator strength f=0.000) the transitions: 365 → 370 0,74 (55%), 367 → 371 0,63 (40%), 367 → 370 -0,20 (4%)

Excited state 9 (E=3.0344 eV, oscillator strength f=0.141) the transitions: 366 → 371 0,88 (78%), 368 → 371 -0,30 (9%), 364 → 370 -0,23 (5%), 369 → 370 -0,22 (5%)

Excited state 10 (E=3.0537 eV, oscillator strength f=0.000) the transitions: 365 → 371 0,91 (83%), 367 → 370 0,39 (15%)

Excited state 11 (E=3.3119 eV, oscillator strength f=0.353) the transitions: 364 → 370 0,86 (73%), 368 → 371 -0,34 (11%), 362 → 370 -0,25 (6%), 358 → 370 0,17 (3%)

Excited state 12 (E=3.3924 eV, oscillator strength f=0.473) the transitions: 364 → 371 0,91 (82%), 368 → 370 0,33 (11%), 369 → 371 -0,17 (3%)

Excited state 13 (E=3.5034 eV, oscillator strength f=0.000) the transitions: 363 → 370 0,88 (78%), 360 → 370 0,39 (16%), 369 → 372 -0,15 (2%)

Excited state 14 (E=3.6611 eV, oscillator strength f=0.371) the transitions: 362 → 370 0,85 (72%), 359 → 370 0,33 (11%), 364 → 370 0,24 (6%), 362 → 371 -0,18 (3%), 358 → 370 -0,16 (3%)

Excited state 15 (E=3.7156 eV, oscillator strength f=0.000) the transitions: 363 → 371 0,97 (93%), 360 → 371 0,19 (4%)

Excited state 16 (E=3.7378 eV, oscillator strength f=0.032) the transitions: 362 → 371 0,94 (89%), 359 → 371 0,18 (3%), 358 → 371 -0,15 (2%)

Excited state 17 (E=3.7601 eV, oscillator strength f=0.000) the transitions: 369 → 372 0,97 (94%)

Excited state 18 (E=3.8339 eV, oscillator strength f=0.000) the transitions: 361 → 370 0,65 (43%), 361 → 371 -0,57 (33%), 360 → 370 -0,40 (16%), 363 → 370 0,25 (6%)

Excited state 19 (E=3.8635 eV, oscillator strength f=0.000) the transitions: 360 → 370 0,61 (37%), 360 → 371 0,57 (33%), 361 → 370 0,48 (23%), 363 → 370 -0,21 (4%)

Excited state 20 (E=3.8904 eV, oscillator strength f=0.032) the transitions: 359 → 370 0,79 (62%), 362 → 370 -0,39 (15%), 359 → 371 0,38 (14%), 358 → 370 -0,24 (6%)

The first twenty vertical excitations of **5** at the PCM/TD-DFT/PBE1PBE/6-31+G(d,p)//PBE1PBE/6-31G(d,p) of theory.

Excited state 1 (E=2.2021 eV, oscillator strength f=0.139) the transitions: 383 → 384 0.84 (71%), 382 → 385 -0.49 (24%), 383 → 385 -0.18 (3%)

Excited state 2 (E=2.2021 eV, oscillator strength f=0.139) the transitions: 383 → 385 0.84 (71%), 382 → 384 0.49 (24%), 383 → 384 0.18 (3%)

Excited state 3 (E=2.9538 eV, oscillator strength f=1.429) the transitions: 382 → 385 0.62 (38%), 382 → 384 -0.51 (26%), 383 → 384 0.37 (14%), 383 → 385 0.29 (8%), 378 → 384 0.26 (7%), 381 → 385 0.22 (5%)

Excited state 4 (E=2.9538 eV, oscillator strength f=1.429) the transitions: 382 → 384 0.62 (38%), 382 → 385 0.51 (26%), 383 → 385 -0.37 (14%), 383 → 384 0.29 (8%), 378 → 385 -0.26 (7%), 381 → 384 -0.22 (5%)

Excited state 5 (E=3.1049 eV, oscillator strength f=0.001) the transitions: 379 → 384 0.67 (46%), 380 → 385 0.67 (46%), 379 → 385 -0.19 (4%), 380 → 384 0.19 (4%)

Excited state 6 (E=3.1168 eV, oscillator strength f=0.000) the transitions: 380 → 384 0.53 (28%), 379 → 385 0.53 (28%), 380 → 385 0.46 (21%), 379 → 384 -0.46 (21%)

Excited state 7 (E=3.1289 eV, oscillator strength f=0.031) the transitions: 381 → 384 0.95 (91%), 381 → 385 -0.18 (3%), 382 → 384 0.15 (2%)

Excited state 8 (E=3.1289 eV, oscillator strength f=0.031) the transitions: 381 → 385 0.95 (91%), 381 → 384 0.18 (3%), 382 → 385 -0.15 (2%)

Excited state 9 (E=3.1538 eV, oscillator strength f=0.000) the transitions: 380 → 385 0.53 (28%), 379 → 384 -0.53 (28%), 380 → 384 -0.46 (21%), 379 → 385 -0.46 (21%)

Excited state 10 (E=3.1792 eV, oscillator strength f=0.001) the transitions: 379 → 385 0.68 (46%), 380 → 384 -0.68 (46%), 379 → 384 0.19 (4%), 380 → 385 0.19 (4%)

Excited state 11 (E=3.4021 eV, oscillator strength f=0.086) the transitions: 378 → 384 0.81 (65%), 376 → 384 -0.52 (27%), 382 → 385 -0.18 (3%)

Excited state 12 (E=3.4021 eV, oscillator strength f=0.086) the transitions: 378 → 385 0.81 (65%), 376 → 385 -0.52 (27%), 382 → 384 0.18 (3%)

Excited state 13 (E=3.6027 eV, oscillator strength f=0.268) the transitions: 376 → 384 0.82 (68%), 378 → 384 0.46 (21%), 382 → 385 -0.19 (4%)

Excited state 14 (E=3.6027 eV, oscillator strength f=0.268) the transitions: 376 -> 385 0,82 (68%), 378 -> 385 0,46 (21%), 382 -> 384 0,19 (4%)

Excited state 15 (E=3.7907 eV, oscillator strength f=0.000) the transitions: 374 -> 384 0,48 (23%), 375 -> 385 0,48 (23%), 372 -> 384 0,37 (14%), 373 -> 385 0,37 (14%), 373 -> 384 0,30 (9%), 372 -> 385 -0,30 (9%), 375 -> 384 0,18 (3%), 374 -> 385 -0,18 (3%)

Excited state 16 (E=3.7975 eV, oscillator strength f=0.000) the transitions: 383 -> 386 0,83 (70%), 375 -> 385 -0,24 (6%), 374 -> 384 0,24 (6%), 372 -> 385 0,21 (5%), 373 -> 384 0,21 (5%)

Excited state 17 (E=3.8278 eV, oscillator strength f=0.047) the transitions: 377 -> 384 0,89 (79%), 370 -> 384 -0,35 (12%), 377 -> 385 -0,19 (4%)

Excited state 18 (E=3.8279 eV, oscillator strength f=0.047) the transitions: 377 -> 385 0,89 (79%), 370 -> 385 -0,35 (12%), 377 -> 384 0,19 (4%)

Excited state 19 (E=3.8391 eV, oscillator strength f=0.000) the transitions: 383 -> 386 0,52 (27%), 372 -> 385 -0,33 (11%), 373 -> 384 -0,33 (11%), 375 -> 385 0,32 (10%), 374 -> 384 -0,32 (10%), 375 -> 384 -0,29 (9%), 374 -> 385 -0,29 (9%), 373 -> 385 0,25 (6%), 372 -> 384 -0,25 (6%)

Excited state 20 (E=3.9223 eV, oscillator strength f=0.001) the transitions: 375 -> 384 0,57 (32%), 374 -> 385 0,57 (32%), 372 -> 384 -0,29 (8%), 373 -> 385 0,29 (8%), 374 -> 384 -0,28 (8%), 375 -> 385 0,28 (8%)

Atomic coordinates of global minimum of compound 3

6	-3.471933000	-0.029052000	0.026489000
6	-0.001281000	3.473278000	0.013832000
6	3.471933000	0.029052000	0.026489000
6	0.001281000	-3.473278000	0.013832000
7	1.434225000	1.447246000	-0.003665000
7	-1.501973000	1.490147000	0.037710000
7	-1.434225000	-1.447246000	-0.003665000
7	1.501973000	-1.490147000	0.037710000
6	-1.240094000	-2.799699000	0.088491000
6	-2.787915000	-1.264751000	0.096559000
6	-2.852840000	1.232528000	-0.041750000
6	-1.257411000	2.843073000	-0.049741000

6	1.257411000	-2.843073000	-0.049741000
6	2.852840000	-1.232528000	-0.041750000
6	2.787915000	1.264751000	0.096559000
6	1.240094000	2.799699000	0.088491000
6	-2.507003000	-3.493043000	0.289049000
6	-3.469459000	-2.538547000	0.294949000
6	-3.497539000	2.501579000	-0.210586000
6	-2.533355000	3.474955000	-0.215920000
6	2.507003000	3.493043000	0.289049000
6	3.469459000	2.538547000	0.294949000
6	2.533355000	-3.474955000	-0.215920000
6	3.497539000	-2.501579000	-0.210586000
1	-2.629265000	-4.557044000	0.426167000
1	-4.531545000	-2.669913000	0.437332000
1	-4.561681000	2.637433000	-0.324679000
1	-2.679196000	4.537138000	-0.334702000
1	2.629265000	4.557044000	0.426167000
1	4.531545000	2.669913000	0.437332000
1	2.679196000	-4.537138000	-0.334702000
1	4.561681000	-2.637433000	-0.324679000
6	-4.968063000	-0.045804000	0.018699000
6	-5.677312000	-0.651703000	-1.019679000
6	-5.693341000	0.555221000	1.068400000
1	-5.141176000	-1.112558000	-1.842571000
1	-5.149431000	1.016785000	1.883084000
6	-7.077258000	-0.661446000	-1.023498000
6	-7.084724000	0.548452000	1.077728000
1	-7.600741000	-1.131839000	-1.846744000
6	-7.793471000	-0.068596000	0.014706000
6	0.001281000	4.969393000	-0.001635000
6	-0.598445000	5.706794000	1.020582000
6	0.615320000	5.666028000	-1.063260000
1	-1.067628000	5.193708000	1.853528000
1	1.073421000	5.099623000	-1.864250000

6	-0.587792000	7.106709000	0.998076000
6	0.628936000	7.056716000	-1.098613000
1	-1.052658000	7.652264000	1.810026000
6	0.018718000	7.794303000	-0.051293000
6	4.968063000	0.045804000	0.018699000
6	5.693341000	-0.555221000	1.068400000
6	5.677312000	0.651703000	-1.019679000
1	5.149431000	-1.016785000	1.883084000
1	5.141176000	1.112558000	-1.842571000
6	7.084724000	-0.548452000	1.077728000
6	7.077258000	0.661446000	-1.023498000
1	7.600741000	1.131839000	-1.846744000
6	7.793471000	0.068596000	0.014706000
6	-0.001281000	-4.969393000	-0.001635000
6	-0.615320000	-5.666028000	-1.063260000
6	0.598445000	-5.706794000	1.020582000
1	-1.073421000	-5.099623000	-1.864250000
1	1.067628000	-5.193708000	1.853528000
6	-0.628936000	-7.056716000	-1.098613000
6	0.587792000	-7.106709000	0.998076000
1	1.052658000	-7.652264000	1.810026000
6	-0.018718000	-7.794303000	-0.051293000
8	0.082696000	9.149606000	-0.169732000
6	-0.517962000	9.937808000	0.855589000
1	-1.594028000	9.743675000	0.931876000
1	-0.047747000	9.755497000	1.828735000
1	-0.357637000	10.976466000	0.565677000
8	-9.151636000	-0.025264000	0.107584000
6	-9.911095000	-0.635201000	-0.933801000
1	-9.717262000	-0.160038000	-1.902309000
1	-9.699471000	-1.708057000	-1.008588000
1	-10.957377000	-0.491027000	-0.663483000
8	-0.082696000	-9.149606000	-0.169732000
6	0.517962000	-9.937808000	0.855589000

1	1.594028000	-9.743675000	0.931876000
1	0.047747000	-9.755497000	1.828735000
1	0.357637000	-10.976466000	0.565677000
8	9.151636000	0.025264000	0.107584000
6	9.911095000	0.635201000	-0.933801000
1	9.717262000	0.160038000	-1.902309000
1	9.699471000	1.708057000	-1.008588000
1	10.957377000	0.491027000	-0.663483000
8	1.192954000	7.805202000	-2.091501000
6	1.832233000	7.127729000	-3.170572000
1	2.655339000	6.500850000	-2.805034000
1	1.120238000	6.487535000	-3.706584000
1	1.541353000	8.838866000	-4.456535000
6	2.368311000	8.205839000	-4.100769000
1	3.075650000	8.851238000	-3.558275000
8	3.004369000	7.543536000	-5.178904000
6	3.553912000	8.438338000	-6.132570000
1	4.307489000	9.093193000	-5.669141000
1	2.772097000	9.080993000	-6.565181000
6	4.198841000	7.600538000	-7.226577000
1	4.979453000	6.956587000	-6.793109000
1	3.444503000	6.945621000	-7.689207000
8	4.748322000	8.494797000	-8.178916000
6	5.386558000	7.832032000	-9.257737000
1	6.211254000	7.197770000	-8.897791000
1	4.677963000	7.184271000	-9.796500000
1	6.634216000	9.548922000	-9.656488000
6	5.927843000	8.899279000	-10.197324000
1	5.102073000	9.533826000	-10.556389000
8	6.566363000	8.236966000	-11.273649000
6	7.111229000	9.139815000	-12.220404000
1	6.333330000	9.775282000	-12.669017000
1	7.579180000	8.543465000	-13.006892000
1	7.871652000	9.792853000	-11.767051000

8	7.859610000	-1.097871000	2.058570000
6	7.211381000	-1.737445000	3.155189000
1	6.569829000	-1.030668000	3.696425000
1	6.591012000	-2.573392000	2.808109000
1	8.959704000	-2.951951000	3.523493000
6	8.313644000	-2.248925000	4.070804000
1	8.940584000	-1.409532000	4.407687000
8	7.679616000	-2.884463000	5.166167000
6	8.598738000	-3.409912000	6.110240000
1	9.236606000	-2.613812000	6.523443000
1	9.256993000	-4.158584000	5.643712000
6	7.789355000	-4.055287000	7.225085000
1	7.130224000	-3.306068000	7.690028000
1	7.150889000	-4.850776000	6.810949000
8	8.707541000	-4.580024000	8.168500000
6	8.072278000	-5.213377000	9.266597000
1	7.422616000	-4.507389000	9.806531000
1	7.444905000	-6.052340000	8.928158000
1	9.791025000	-4.885994000	10.532332000
6	9.162779000	-5.725849000	10.195543000
1	9.813689000	-6.430444000	9.653873000
8	8.527559000	-6.358460000	11.291521000
6	9.453460000	-6.876513000	12.231047000
1	10.110221000	-7.633811000	11.777853000
1	8.876807000	-7.341709000	13.033690000
1	10.084515000	-6.083086000	12.658174000
8	-7.859610000	1.097871000	2.058570000
6	-7.211381000	1.737445000	3.155189000
1	-6.569829000	1.030668000	3.696425000
1	-6.591012000	2.573392000	2.808109000
1	-8.959704000	2.951951000	3.523493000
6	-8.313644000	2.248925000	4.070804000
1	-8.940584000	1.409532000	4.407687000
8	-7.679616000	2.884463000	5.166167000

6	-8.598738000	3.409912000	6.110240000
1	-9.236606000	2.613812000	6.523443000
1	-9.256993000	4.158584000	5.643712000
6	-7.789355000	4.055287000	7.225085000
1	-7.130224000	3.306068000	7.690028000
1	-7.150889000	4.850776000	6.810949000
8	-8.707541000	4.580024000	8.168500000
6	-8.072278000	5.213377000	9.266597000
1	-7.422616000	4.507389000	9.806531000
1	-7.444905000	6.052340000	8.928158000
1	-9.791025000	4.885994000	10.532332000
6	-9.162779000	5.725849000	10.195543000
1	-9.813689000	6.430444000	9.653873000
8	-8.527559000	6.358460000	11.291521000
6	-9.453460000	6.876513000	12.231047000
1	-10.110221000	7.633811000	11.777853000
1	-8.876807000	7.341709000	13.033690000
1	-10.084515000	6.083086000	12.658174000
8	-1.192954000	-7.805202000	-2.091501000
6	-1.832233000	-7.127729000	-3.170572000
1	-2.655339000	-6.500850000	-2.805034000
1	-1.120238000	-6.487535000	-3.706584000
1	-1.541353000	-8.838866000	-4.456535000
6	-2.368311000	-8.205839000	-4.100769000
1	-3.075650000	-8.851238000	-3.558275000
8	-3.004369000	-7.543536000	-5.178904000
6	-3.553912000	-8.438338000	-6.132570000
1	-4.307489000	-9.093193000	-5.669141000
1	-2.772097000	-9.080993000	-6.565181000
6	-4.198841000	-7.600538000	-7.226577000
1	-4.979453000	-6.956587000	-6.793109000
1	-3.444503000	-6.945621000	-7.689207000
8	-4.748322000	-8.494797000	-8.178916000
6	-5.386558000	-7.832032000	-9.257737000

1	-6.211254000	-7.197770000	-8.897791000
1	-4.677963000	-7.184271000	-9.796500000
1	-6.634216000	-9.548922000	-9.656488000
6	-5.927843000	-8.899279000	-10.197324000
1	-5.102073000	-9.533826000	-10.556389000
8	-6.566363000	-8.236966000	-11.273649000
6	-7.111229000	-9.139815000	-12.220404000
1	-6.333330000	-9.775282000	-12.669017000
1	-7.579180000	-8.543465000	-13.006892000
1	-7.871652000	-9.792853000	-11.767051000
1	-0.783021000	0.778860000	0.102662000
1	0.783021000	-0.778860000	0.102662000

Atomic coordinates of global minimum of compound 4

6	1.398225000	3.160136000	-0.095781000
6	-3.170594000	1.374192000	-0.080152000
6	-1.398225000	-3.160136000	-0.095781000
6	3.170594000	-1.374192000	-0.080152000
7	-1.884652000	-0.736715000	-0.070236000
7	-0.767087000	1.962532000	-0.099022000
7	1.884652000	0.736715000	-0.070236000
7	0.767087000	-1.962532000	-0.099022000
6	3.041628000	0.025528000	-0.183967000
6	2.253033000	2.043169000	-0.191302000
6	0.000942000	3.092057000	0.000008000
6	-2.096831000	2.272080000	0.007605000
6	2.096831000	-2.272080000	0.007605000
6	-0.000942000	-3.092057000	0.000008000
6	-2.253033000	-2.043169000	-0.191302000
6	-3.041628000	-0.025528000	-0.183967000
6	4.173077000	0.903037000	-0.431248000

6	3.680297000	2.163801000	-0.436040000
6	-0.899160000	4.181504000	0.212543000
6	-2.172758000	3.683664000	0.217376000
6	-4.173077000	-0.903037000	-0.431248000
6	-3.680297000	-2.163801000	-0.436040000
6	2.172758000	-3.683664000	0.217376000
6	0.899160000	-4.181504000	0.212543000
1	5.192136000	0.585979000	-0.600425000
1	4.215778000	3.086317000	-0.609523000
1	-0.594839000	5.207289000	0.356899000
1	-3.090671000	4.232575000	0.365938000
1	-5.192136000	-0.585979000	-0.600425000
1	-4.215778000	-3.086317000	-0.609523000
1	3.090671000	-4.232575000	0.365938000
1	0.594839000	-5.207289000	0.356899000
6	2.004262000	4.516235000	-0.087096000
6	2.940885000	4.860412000	0.903725000
6	1.664995000	5.465969000	-1.046807000
1	3.196477000	4.123813000	1.656306000
1	0.953394000	5.214183000	-1.826714000
6	3.525453000	6.118522000	0.931227000
6	2.244406000	6.736239000	-1.029025000
1	1.970010000	7.454841000	-1.792622000
6	3.170594000	7.074621000	-0.050026000
6	-4.536457000	1.957506000	-0.057264000
6	-4.923309000	2.895736000	-1.030630000
6	-5.454775000	1.592342000	0.923273000
1	-4.213086000	3.169779000	-1.801970000
1	-5.169809000	0.876620000	1.687688000
6	-6.193176000	3.455668000	-1.021672000
6	-6.735685000	2.147088000	0.942615000

1	-7.429416000	1.851626000	1.721197000
6	-7.116625000	3.074874000	-0.019244000
6	-2.004262000	-4.516235000	-0.087096000
6	-1.664995000	-5.465969000	-1.046807000
6	-2.940885000	-4.860412000	0.903725000
1	-0.953394000	-5.214183000	-1.826714000
1	-3.196477000	-4.123813000	1.656306000
6	-2.244406000	-6.736239000	-1.029025000
6	-3.525453000	-6.118522000	0.931227000
1	-1.970010000	-7.454841000	-1.792622000
6	-3.170594000	-7.074621000	-0.050026000
6	4.536457000	-1.957506000	-0.057264000
6	5.454775000	-1.592342000	0.923273000
6	4.923309000	-2.895736000	-1.030630000
1	5.169809000	-0.876620000	1.687688000
1	4.213086000	-3.169779000	-1.801970000
6	6.735685000	-2.147088000	0.942615000
6	6.193176000	-3.455668000	-1.021672000
1	7.429416000	-1.851626000	1.721197000
6	7.116625000	-3.074874000	-0.019244000
8	6.648855000	-4.360006000	-1.920009000
6	5.750551000	-4.789296000	-2.925761000
1	4.861768000	-5.265398000	-2.493967000
1	5.437191000	-3.957296000	-3.567926000
1	6.295255000	-5.519522000	-3.524551000
8	-6.648855000	4.360006000	-1.920009000
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1	-4.861768000	5.265398000	-2.493967000
1	-5.437191000	3.957296000	-3.567926000
1	-6.295255000	5.519522000	-3.524551000
8	4.431925000	6.533021000	1.847067000

6	4.836890000	5.600144000	2.831265000
1	3.994718000	5.286810000	3.460030000
1	5.297707000	4.713609000	2.378831000
1	5.574055000	6.114148000	3.448413000
8	-4.431925000	-6.533021000	1.847067000
6	-4.836890000	-5.600144000	2.831265000
1	-3.994718000	-5.286810000	3.460030000
1	-5.297707000	-4.713609000	2.378831000
1	-5.574055000	-6.114148000	3.448413000
8	8.330532000	-3.669810000	-0.089905000
6	9.294940000	-3.321955000	0.885177000
1	8.941300000	-3.570381000	1.894582000
1	9.519319000	-2.247676000	0.850926000
6	10.539140000	-4.121155000	0.561749000
1	10.886071000	-3.875561000	-0.454016000
1	10.307210000	-5.197338000	0.584664000
8	11.503394000	-3.784649000	1.527276000
6	12.722381000	-4.462113000	1.334853000
1	13.157460000	-4.225402000	0.351281000
1	12.582604000	-5.553342000	1.383846000
6	13.665789000	-4.017256000	2.432048000
1	13.230137000	-4.254898000	3.415426000
1	13.802331000	-2.925294000	2.384158000
8	14.884752000	-4.691821000	2.238704000
6	15.848348000	-4.357049000	3.208212000
1	15.497155000	-4.609414000	4.221266000
1	16.069846000	-3.278163000	3.192518000
6	17.104548000	-5.141072000	2.892888000
1	17.453763000	-4.888961000	1.878321000
1	16.880833000	-6.220266000	2.905821000
8	18.066928000	-4.807594000	3.861456000

6	19.282817000	-5.485933000	3.656581000
1	19.726222000	-5.239528000	2.680055000
1	19.153328000	-6.577428000	3.709432000
1	19.970597000	-5.173434000	4.445564000
8	3.788182000	8.274419000	0.057062000
6	3.464149000	9.272450000	-0.892056000
1	3.714129000	8.944126000	-1.909588000
1	2.393599000	9.514196000	-0.858806000
1	4.036494000	10.810959000	0.499205000
6	4.282258000	10.492233000	-0.525735000
1	5.354442000	10.242589000	-0.549941000
8	3.968355000	11.492489000	-1.461774000
6	4.667511000	12.691680000	-1.227053000
1	5.756124000	12.533579000	-1.278736000
1	4.436489000	13.097329000	-0.229640000
6	4.242987000	13.680430000	-2.291894000
1	4.474109000	13.274594000	-3.289485000
1	3.153790000	13.836445000	-2.240686000
8	4.940777000	14.878529000	-2.055348000
6	4.624319000	15.883323000	-2.988465000
1	4.869030000	15.564787000	-4.014107000
1	3.550027000	16.125305000	-2.963092000
1	6.507765000	16.867458000	-2.652094000
6	5.433145000	17.111330000	-2.627939000
1	5.189711000	17.426473000	-1.600174000
8	5.116624000	18.116043000	-3.558430000
6	5.819854000	19.309509000	-3.310241000
1	5.585351000	19.720365000	-2.316695000
1	5.518843000	20.032823000	-4.071426000
1	6.908371000	19.160389000	-3.372059000
8	-8.330532000	3.669810000	-0.089905000

6	-9.294940000	3.321955000	0.885177000
1	-9.519319000	2.247676000	0.850926000
1	-8.941300000	3.570381000	1.894582000
1	-10.307210000	5.197338000	0.584664000
6	-10.539140000	4.121155000	0.561749000
1	-10.886071000	3.875561000	-0.454016000
8	-11.503394000	3.784649000	1.527276000
6	-12.722381000	4.462113000	1.334853000
1	-13.157460000	4.225402000	0.351281000
1	-12.582604000	5.553342000	1.383846000
6	-13.665789000	4.017256000	2.432048000
1	-13.802331000	2.925294000	2.384158000
1	-13.230137000	4.254898000	3.415426000
8	-14.884752000	4.691821000	2.238704000
6	-15.848348000	4.357049000	3.208212000
1	-16.069846000	3.278163000	3.192518000
1	-15.497155000	4.609414000	4.221266000
1	-17.453763000	4.888961000	1.878321000
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1	-16.880833000	6.220266000	2.905821000
8	-18.066928000	4.807594000	3.861456000
6	-19.282817000	5.485933000	3.656581000
1	-19.153328000	6.577428000	3.709432000
1	-19.970597000	5.173434000	4.445564000
1	-19.726222000	5.239528000	2.680055000
8	-3.788182000	-8.274419000	0.057062000
6	-3.464149000	-9.272450000	-0.892056000
1	-3.714129000	-8.944126000	-1.909588000
1	-2.393599000	-9.514196000	-0.858806000
1	-4.036494000	-10.810959000	0.499205000
6	-4.282258000	-10.492233000	-0.525735000

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8	-3.968355000	-11.492489000	-1.461774000
6	-4.667511000	-12.691680000	-1.227053000
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1	-3.153790000	-13.836445000	-2.240686000
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6	-5.433145000	-17.111330000	-2.627939000
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8	-5.116624000	-18.116043000	-3.558430000
6	-5.819854000	-19.309509000	-3.310241000
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1	-5.518843000	-20.032823000	-4.071426000
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Atomic coordinates of global minimum of compound 5

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7	1.443980000	1.444219000	0.043467000

7	-1.444217000	1.443983000	-0.043427000
7	-1.443980000	-1.444219000	0.043467000
6	-2.795944000	1.243665000	0.054133000
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6	1.243664000	2.795947000	-0.054092000
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6	-2.796625000	-1.243165000	-0.038809000
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6	1.243165000	-2.796629000	0.038849000
6	2.795944000	-1.243665000	0.054133000
6	-3.466134000	2.507372000	0.227334000
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6	2.507371000	3.466135000	-0.227294000
6	3.468624000	2.505103000	-0.216820000
6	3.466134000	-2.507372000	0.227334000
6	2.505103000	-3.468626000	0.216857000
6	-3.468624000	-2.505103000	-0.216820000
6	-2.507371000	-3.466135000	-0.227294000
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1	-2.633053000	4.534195000	0.340540000
1	2.637759000	4.530330000	-0.360887000
1	4.534193000	2.633051000	-0.340506000
1	4.530329000	-2.637758000	0.360926000
1	2.633053000	-4.534195000	0.340540000
1	-4.534193000	-2.633051000	-0.340506000
1	-2.637759000	-4.530330000	-0.360887000
6	-0.000597000	4.935664000	-0.026223000
6	-0.638076000	5.649395000	-1.036975000
6	0.651977000	5.649530000	0.994151000
1	-1.139998000	5.115446000	-1.837718000
1	1.139805000	5.094560000	1.787080000

6	-0.628892000	7.045680000	-1.041396000
6	0.669983000	7.036593000	0.999351000
1	-1.126444000	7.576166000	-1.844858000
6	0.018564000	7.751372000	-0.033507000
6	4.935660000	0.000597000	0.026263000
6	5.649391000	0.638055000	1.037027000
6	5.649524000	-0.651957000	-0.994126000
1	5.115443000	1.139962000	1.837780000
1	5.094554000	-1.139769000	-1.787063000
6	7.045677000	0.628870000	1.041447000
6	7.036587000	-0.669963000	-0.999326000
1	7.576164000	1.126406000	1.844919000
6	7.751367000	-0.018566000	0.033544000
6	0.000597000	-4.935664000	-0.026223000
6	-0.651977000	-5.649530000	0.994151000
6	0.638076000	-5.649395000	-1.036975000
1	-1.139805000	-5.094560000	1.787080000
1	1.139998000	-5.115446000	-1.837718000
6	-0.669983000	-7.036593000	0.999351000
6	0.628892000	-7.045680000	-1.041396000
1	1.126444000	-7.576166000	-1.844858000
6	-0.018564000	-7.751372000	-0.033507000
6	-4.935660000	-0.000597000	0.026263000
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1	9.649274000	0.125023000	1.943408000
1	10.901288000	0.386389000	0.700955000
8	0.088379000	9.099455000	0.055661000
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6	-4.631494000	-7.623736000	6.807041000
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8	-7.798057000	1.273796000	-1.944954000
6	-7.131601000	1.979583000	-2.973533000
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