

## Supporting Information

for

# **Triazine di(carboxy)Porphyrin Dyad versus a Triazine di(carboxy) Porphyrin Triad for sensitizers in DSSC**

*G. E. Zervaki,<sup>1</sup> Vasilitsa Tsaka,<sup>1</sup> Alexandra Vatikioti,<sup>1</sup> Irene Georgakaki,<sup>1</sup>  
Vasilis Nikolaou,<sup>1</sup> G. D. Sharma,<sup>2\*</sup> A. G. Coutsolelos<sup>1\*</sup>*

<sup>1</sup>Department of Chemistry, Laboratory of Bioinorganic Chemistry, University  
of Crete, Voutes Campus, P.O. Box 2208, 71003  
Heraklion, Crete, Greece

<sup>2</sup>R&D Centre for Engineering and Science, JEC Group of Colleges, Jaipur  
Engineering College Campus, Kukas, Jaipur, Raj 303101, India

Corresponding authors: [coutsole@chemistry.uoc.gr](mailto:coutsole@chemistry.uoc.gr), [gdsharma273@gmail.com](mailto:gdsharma273@gmail.com)

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**Table S1.** Cartesian coordinates of gas phase geometry optimized structure of PorZn-(PorCOOH)<sub>2</sub>-(piper)<sub>2</sub> (**2**) calculated by DFT at the B3LYP / 6-31G(d) level. E = - 8169.3356734 Hartree / particle.

|   | x            | y           | z           |
|---|--------------|-------------|-------------|
| C | 10.061832000 | 5.589604000 | 6.965702000 |
| C | 9.889005000  | 4.259634000 | 6.774685000 |
| C | 8.496979000  | 4.079576000 | 6.374229000 |
| N | 7.843823000  | 5.280478000 | 6.325231000 |
| C | 8.775604000  | 6.216973000 | 6.670002000 |
| C | 5.718324000  | 9.838697000 | 6.293822000 |
| C | 7.046597000  | 9.655086000 | 6.574300000 |
| C | 7.319769000  | 8.246212000 | 6.537459000 |
| N | 6.133701000  | 7.626676000 | 6.219349000 |
| C | 5.126042000  | 8.552633000 | 6.063850000 |
| C | 8.553035000  | 7.609675000 | 6.760243000 |
| C | 1.631950000  | 5.502531000 | 5.038190000 |
| C | 1.805328000  | 6.833004000 | 5.224495000 |
| C | 3.225335000  | 7.027031000 | 5.501530000 |
| N | 3.895177000  | 5.836064000 | 5.481748000 |
| C | 2.950274000  | 4.891760000 | 5.191622000 |
| C | 3.782064000  | 8.299422000 | 5.750377000 |
| C | 6.042710000  | 1.291114000 | 5.401641000 |
| C | 4.715885000  | 1.477468000 | 5.113486000 |
| C | 4.417586000  | 2.872207000 | 5.266805000 |
| N | 5.593428000  | 3.484787000 | 5.635775000 |
| C | 6.612658000  | 2.565085000 | 5.732043000 |
| C | 7.949626000  | 2.813539000 | 6.084501000 |
| C | 3.176000000  | 3.502545000 | 5.068091000 |
| C | 2.873703000  | 9.498750000 | 5.680462000 |
| C | 2.024599000  | 2.621790000 | 4.700124000 |
| C | 8.858626000  | 1.614369000 | 6.149622000 |
| C | 9.707256000  | 8.492352000 | 7.116439000 |
| C | 1.518064000  | 1.671538000 | 5.601390000 |
| C | 0.447408000  | 0.854429000 | 5.257555000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | -0.160843000 | 0.955163000  | 3.993308000 |
| C | 0.333214000  | 1.904522000  | 3.084198000 |
| C | 1.408116000  | 2.715307000  | 3.443170000 |
| C | 2.676937000  | 10.164090000 | 4.451380000 |
| C | 1.834912000  | 11.280764000 | 4.409510000 |
| C | 1.177536000  | 11.755191000 | 5.548257000 |
| C | 1.387425000  | 11.081808000 | 6.754857000 |
| C | 2.222181000  | 9.962050000  | 6.843364000 |
| C | 9.590164000  | 1.219622000  | 5.008827000 |
| C | 10.424215000 | 0.099088000  | 5.089582000 |
| C | 10.558993000 | -0.639875000 | 6.268539000 |
| C | 9.823479000  | -0.233043000 | 7.385100000 |
| C | 8.976176000  | 0.880251000  | 7.349042000 |
| C | 9.722498000  | 9.213433000  | 8.323482000 |
| C | 10.792660000 | 10.039715000 | 8.650568000 |
| C | 11.890253000 | 10.157600000 | 7.786970000 |
| C | 11.877483000 | 9.451145000  | 6.575535000 |
| C | 10.799995000 | 8.631719000  | 6.245366000 |
| C | 0.246903000  | 12.943582000 | 5.471076000 |
| C | 2.409340000  | 9.269841000  | 8.175577000 |
| C | 3.360267000  | 9.691613000  | 3.187023000 |
| C | 11.491990000 | -1.826784000 | 6.340356000 |
| C | 8.205250000  | 1.276368000  | 8.589065000 |
| C | 9.484394000  | 1.983842000  | 3.707436000 |
| N | -1.254240000 | 0.114587000  | 3.744009000 |
| C | 13.006811000 | 11.068087000 | 8.199331000 |
| O | 12.883570000 | 11.937494000 | 9.029861000 |
| O | 14.210141000 | 10.878903000 | 7.590271000 |
| C | -1.933968000 | -0.207787000 | 2.593527000 |
| N | -1.539205000 | 0.284416000  | 1.416701000 |
| C | -2.278015000 | -0.129229000 | 0.362613000 |
| N | -3.362917000 | -0.931680000 | 0.446302000 |
| C | -3.649429000 | -1.346255000 | 1.683061000 |
| N | -2.970551000 | -1.037349000 | 2.803206000 |

|   |               |               |              |
|---|---------------|---------------|--------------|
| N | -1.895618000  | 0.287709000   | -0.876145000 |
| C | -9.984001000  | -2.266683000  | -1.484329000 |
| C | -11.098513000 | -1.810145000  | -2.122495000 |
| C | -11.705950000 | -2.944355000  | -2.782684000 |
| N | -10.949163000 | -4.067555000  | -2.541096000 |
| C | -9.885491000  | -3.685426000  | -1.757637000 |
| C | -8.007692000  | -8.051424000  | -1.465937000 |
| C | -7.711489000  | -6.785687000  | -1.055864000 |
| C | -8.791013000  | -5.928541000  | -1.499610000 |
| N | -9.713371000  | -6.684771000  | -2.184102000 |
| C | -9.264788000  | -7.985302000  | -2.177497000 |
| C | -8.863971000  | -4.535028000  | -1.276322000 |
| C | -12.910051000 | -9.737376000  | -4.682101000 |
| C | -11.783703000 | -10.191197000 | -4.062955000 |
| C | -11.112869000 | -9.039493000  | -3.501405000 |
| N | -11.837362000 | -7.906928000  | -3.792735000 |
| C | -12.937899000 | -8.298892000  | -4.518023000 |
| C | -9.910105000  | -9.091044000  | -2.768128000 |
| C | -14.724186000 | -3.908025000  | -4.956961000 |
| C | -15.020040000 | -5.173814000  | -5.367034000 |
| C | -14.009677000 | -6.049876000  | -4.811708000 |
| N | -13.114090000 | -5.301118000  | -4.084909000 |
| C | -13.525097000 | -3.990127000  | -4.152499000 |
| C | -12.891829000 | -2.887951000  | -3.543067000 |
| C | -13.951447000 | -7.446983000  | -5.010390000 |
| C | -9.262220000  | -10.439735000 | -2.597051000 |
| C | -15.054790000 | -8.077609000  | -5.801293000 |
| C | -13.536204000 | -1.538269000  | -3.719290000 |
| C | -7.773678000  | -3.909755000  | -0.464882000 |
| C | -14.814944000 | -8.650655000  | -7.060424000 |
| C | -15.839498000 | -9.249433000  | -7.784957000 |
| C | -17.149422000 | -9.299175000  | -7.276129000 |
| C | -17.406382000 | -8.716804000  | -6.025035000 |
| C | -16.367969000 | -8.122912000  | -5.309882000 |

|   |               |               |               |
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| C | -8.352711000  | -10.917014000 | -3.564715000  |
| C | -7.764004000  | -12.173719000 | -3.385169000  |
| C | -8.048724000  | -12.972076000 | -2.273675000  |
| C | -8.956418000  | -12.482796000 | -1.330152000  |
| C | -9.567229000  | -11.231478000 | -1.469263000  |
| C | -13.156533000 | -0.709695000  | -4.797186000  |
| C | -13.766089000 | 0.541226000   | -4.942414000  |
| C | -14.742579000 | 0.996537000   | -4.051684000  |
| C | -15.100188000 | 0.162538000   | -2.988802000  |
| C | -14.517712000 | -1.097007000  | -2.806826000  |
| C | -6.891658000  | -2.972564000  | -1.023495000  |
| C | -5.871429000  | -2.379393000  | -0.281983000  |
| C | -5.701122000  | -2.719575000  | 1.069204000   |
| C | -6.580855000  | -3.656170000  | 1.642011000   |
| C | -7.594400000  | -4.237061000  | 0.889197000   |
| C | -7.375653000  | -14.312246000 | -2.085225000  |
| C | -10.544120000 | -10.750937000 | -0.418937000  |
| C | -8.010150000  | -10.095586000 | -4.788045000  |
| C | -15.409221000 | 2.338888000   | -4.247512000  |
| C | -14.943380000 | -1.958726000  | -1.638577000  |
| C | -12.105071000 | -1.153203000  | -5.790300000  |
| N | -18.125401000 | -9.905295000  | -8.081753000  |
| N | -4.721348000  | -2.173990000  | 1.910893000   |
| C | -19.385987000 | -10.376711000 | -7.807580000  |
| N | -19.892403000 | -10.269459000 | -6.576576000  |
| C | -21.127288000 | -10.798571000 | -6.431491000  |
| N | -21.851517000 | -11.356635000 | -7.427959000  |
| C | -21.229700000 | -11.389343000 | -8.609476000  |
| N | -19.993231000 | -10.930146000 | -8.872343000  |
| N | -21.678866000 | -10.775421000 | -5.186035000  |
| C | -34.234026000 | -15.049517000 | -12.070306000 |
| C | -33.805795000 | -13.792706000 | -11.802637000 |
| C | -32.370390000 | -13.891234000 | -11.556376000 |
| N | -31.942913000 | -15.185558000 | -11.670688000 |

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| C | -33.057770000 | -15.911927000 | -11.977390000 |
| C | -30.670249000 | -20.011934000 | -12.268065000 |
| C | -31.965249000 | -19.579767000 | -12.380850000 |
| C | -31.977943000 | -18.155644000 | -12.201634000 |
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| C | -29.838591000 | -18.873730000 | -12.002742000 |
| C | -33.097094000 | -17.304671000 | -12.215192000 |
| C | -25.801294000 | -16.615243000 | -10.921187000 |
| C | -26.226293000 | -17.869426000 | -11.206771000 |
| C | -27.657631000 | -17.767023000 | -11.473202000 |
| N | -28.085461000 | -16.474190000 | -11.357569000 |
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| C | -28.452571000 | -18.890595000 | -11.783982000 |
| C | -29.352823000 | -11.645171000 | -10.788248000 |
| C | -28.058894000 | -12.079832000 | -10.666895000 |
| C | -28.049571000 | -13.505149000 | -10.828753000 |
| N | -29.354728000 | -13.881054000 | -11.052207000 |
| C | -30.186234000 | -12.784289000 | -11.041676000 |
| C | -31.574068000 | -12.766994000 | -11.259405000 |
| C | -26.930235000 | -14.356995000 | -10.794126000 |
| C | -27.777155000 | -20.233404000 | -11.879969000 |
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| C | -24.140984000 | -12.514501000 | -8.949945000  |
| C | -23.108716000 | -12.516577000 | -9.901491000  |
| C | -23.346690000 | -13.122325000 | -11.149203000 |
| C | -24.572064000 | -13.711788000 | -11.435019000 |
| C | -27.655949000 | -21.049628000 | -10.735134000 |
| C | -27.028863000 | -22.295288000 | -10.851565000 |
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| C | -26.649230000 | -21.931847000 | -13.189150000 |
| C | -27.268613000 | -20.679157000 | -13.118706000 |

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| C  | -32.372897000 | -10.618529000 | -12.328242000 |
| C  | -32.997227000 | -9.370952000  | -12.222856000 |
| C  | -33.503674000 | -8.896352000  | -11.009230000 |
| C  | -33.365451000 | -9.706816000  | -9.879338000  |
| C  | -32.747793000 | -10.961385000 | -9.938612000  |
| C  | -34.683814000 | -18.537137000 | -13.744878000 |
| C  | -35.912877000 | -19.134468000 | -14.004718000 |
| C  | -36.911555000 | -19.151544000 | -13.021730000 |
| C  | -36.662159000 | -18.560629000 | -11.775135000 |
| C  | -35.429943000 | -17.964491000 | -11.520114000 |
| C  | -25.813433000 | -24.090313000 | -12.161213000 |
| C  | -27.383035000 | -19.827371000 | -14.363682000 |
| C  | -28.189863000 | -20.601078000 | -9.392541000  |
| C  | -34.202648000 | -7.558651000  | -10.928975000 |
| C  | -32.628267000 | -11.798663000 | -8.684277000  |
| C  | -31.846625000 | -11.083556000 | -13.668230000 |
| N  | -21.848347000 | -11.935767000 | -9.708617000  |
| C  | -38.205187000 | -19.802853000 | -13.349912000 |
| O  | -38.470091000 | -20.332523000 | -14.411567000 |
| O  | -39.100046000 | -19.756058000 | -12.328549000 |
| C  | -2.640407000  | -0.059818000  | -2.087378000  |
| C  | -1.712433000  | -0.666616000  | -3.148836000  |
| C  | -0.516777000  | 0.252811000   | -3.434269000  |
| C  | 0.212364000   | 0.602179000   | -2.129280000  |
| C  | -0.755240000  | 1.181311000   | -1.087264000  |
| C  | -23.030114000 | -11.269793000 | -4.917070000  |
| C  | -23.039139000 | -12.218464000 | -3.710338000  |
| C  | -22.392838000 | -11.564729000 | -2.481203000  |
| C  | -20.988285000 | -11.051810000 | -2.826771000  |
| C  | -21.017921000 | -10.127212000 | -4.051329000  |
| Zn | -11.403283000 | -5.990032000  | -3.151239000  |
| H  | 10.958524000  | 6.100598000   | 7.285851000   |
| H  | 10.614394000  | 3.467824000   | 6.899316000   |
| H  | 5.180173000   | 10.773733000  | 6.239376000   |

|   |              |              |             |
|---|--------------|--------------|-------------|
| H | 7.781282000  | 10.418463000 | 6.782437000 |
| H | 6.031369000  | 6.624303000  | 6.096252000 |
| H | 0.712217000  | 4.975421000  | 4.829849000 |
| H | 1.059117000  | 7.614610000  | 5.193331000 |
| H | 6.596816000  | 0.363984000  | 5.384540000 |
| H | 3.998442000  | 0.728296000  | 4.814155000 |
| H | 5.690394000  | 4.484241000  | 5.783898000 |
| H | 1.963568000  | 1.579731000  | 6.587924000 |
| H | 0.072678000  | 0.128625000  | 5.976436000 |
| H | -0.128513000 | 1.997519000  | 2.112101000 |
| H | 1.780160000  | 3.441638000  | 2.725840000 |
| H | 1.690123000  | 11.792687000 | 3.459939000 |
| H | 0.888966000  | 11.436035000 | 7.655242000 |
| H | 10.982700000 | -0.203182000 | 4.205556000 |
| H | 9.909517000  | -0.796322000 | 8.312416000 |
| H | 8.887332000  | 9.113583000  | 9.010436000 |
| H | 10.802182000 | 10.600361000 | 9.579468000 |
| H | 12.682541000 | 9.566704000  | 5.852541000 |
| H | 10.793255000 | 8.103715000  | 5.296683000 |
| H | 0.563007000  | 13.651154000 | 4.696876000 |
| H | 0.202703000  | 13.481088000 | 6.424410000 |
| H | -0.777500000 | 12.631619000 | 5.226298000 |
| H | 3.456956000  | 9.290086000  | 8.498409000 |
| H | 2.114670000  | 8.215172000  | 8.125681000 |
| H | 1.808572000  | 9.752460000  | 8.952663000 |
| H | 3.080763000  | 8.660517000  | 2.941337000 |
| H | 3.090353000  | 10.327009000 | 2.337787000 |
| H | 4.452048000  | 9.707252000  | 3.286852000 |
| H | 11.559263000 | -2.343234000 | 5.376579000 |
| H | 11.161429000 | -2.552011000 | 7.091631000 |
| H | 12.509881000 | -1.517085000 | 6.613516000 |
| H | 8.435108000  | 2.303618000  | 8.894587000 |
| H | 8.445471000  | 0.612667000  | 9.425462000 |
| H | 7.122319000  | 1.231358000  | 8.423208000 |

|   |               |               |              |
|---|---------------|---------------|--------------|
| H | 8.453750000   | 2.005999000   | 3.334295000  |
| H | 9.798708000   | 3.027208000   | 3.827362000  |
| H | 10.112806000  | 1.527945000   | 2.936032000  |
| H | -1.625766000  | -0.379889000  | 4.544759000  |
| H | 14.196347000  | 10.058637000  | 7.071153000  |
| H | -9.295425000  | -1.698386000  | -0.876302000 |
| H | -11.486028000 | -0.801065000  | -2.138002000 |
| H | -7.425989000  | -8.949810000  | -1.313839000 |
| H | -6.837425000  | -6.458507000  | -0.511956000 |
| H | -13.660055000 | -10.321849000 | -5.194866000 |
| H | -11.439545000 | -11.212654000 | -3.980465000 |
| H | -15.259073000 | -2.996190000  | -5.182907000 |
| H | -15.840614000 | -5.487293000  | -5.995887000 |
| H | -13.812036000 | -8.624164000  | -7.477057000 |
| H | -15.624839000 | -9.688480000  | -8.757252000 |
| H | -18.409949000 | -8.737944000  | -5.626074000 |
| H | -16.582975000 | -7.685794000  | -4.338547000 |
| H | -7.064802000  | -12.536968000 | -4.136250000 |
| H | -9.198625000  | -13.091075000 | -0.460592000 |
| H | -13.467586000 | 1.176570000   | -5.774345000 |
| H | -15.853171000 | 0.498988000   | -2.278369000 |
| H | -7.003228000  | -2.702342000  | -2.070036000 |
| H | -5.206794000  | -1.658236000  | -0.733825000 |
| H | -6.468360000  | -3.926618000  | 2.690124000  |
| H | -8.264449000  | -4.951540000  | 1.358788000  |
| H | -8.006195000  | -15.000856000 | -1.512396000 |
| H | -7.144653000  | -14.784155000 | -3.046489000 |
| H | -6.428170000  | -14.209200000 | -1.538945000 |
| H | -11.526362000 | -10.532479000 | -0.853941000 |
| H | -10.680116000 | -11.505113000 | 0.362627000  |
| H | -10.197695000 | -9.827108000  | 0.059365000  |
| H | -7.599753000  | -9.116828000  | -4.513390000 |
| H | -8.896008000  | -9.905261000  | -5.405445000 |
| H | -7.270492000  | -10.610741000 | -5.408933000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -14.723665000 | 3.065864000   | -4.696709000  |
| H | -15.766285000 | 2.751754000   | -3.297903000  |
| H | -16.278408000 | 2.258656000   | -4.914431000  |
| H | -15.692418000 | -1.444995000  | -1.027823000  |
| H | -14.093822000 | -2.209982000  | -0.992849000  |
| H | -15.375816000 | -2.908149000  | -1.976053000  |
| H | -12.389306000 | -2.089450000  | -6.284922000  |
| H | -11.140630000 | -1.334215000  | -5.301227000  |
| H | -11.953921000 | -0.394274000  | -6.564456000  |
| H | -17.848659000 | -10.115028000 | -9.032098000  |
| H | -4.788797000  | -2.428467000  | 2.887894000   |
| H | -35.235777000 | -15.367626000 | -12.320758000 |
| H | -34.385989000 | -12.880736000 | -11.781351000 |
| H | -30.305842000 | -21.025947000 | -12.344579000 |
| H | -32.842126000 | -20.183586000 | -12.559863000 |
| H | -30.381575000 | -16.823397000 | -11.798698000 |
| H | -24.804728000 | -16.298439000 | -10.650020000 |
| H | -25.647333000 | -18.782268000 | -11.225108000 |
| H | -29.714932000 | -10.629382000 | -10.725587000 |
| H | -27.179213000 | -11.478633000 | -10.493606000 |
| H | -29.648530000 | -14.836963000 | -11.225836000 |
| H | -26.146404000 | -13.109731000 | -8.497746000  |
| H | -23.973213000 | -12.050305000 | -7.989572000  |
| H | -22.560671000 | -13.127154000 | -11.901711000 |
| H | -24.731497000 | -14.165935000 | -12.408694000 |
| H | -26.940190000 | -22.921978000 | -9.966085000  |
| H | -26.261762000 | -22.271693000 | -14.147850000 |
| H | -33.089516000 | -8.754316000  | -13.115061000 |
| H | -33.747806000 | -9.355578000  | -8.922743000  |
| H | -33.917860000 | -18.517104000 | -14.514466000 |
| H | -36.121625000 | -19.588819000 | -14.967762000 |
| H | -37.430118000 | -18.575627000 | -11.009597000 |
| H | -35.236604000 | -17.516116000 | -10.550233000 |
| H | -26.194716000 | -24.797358000 | -11.416534000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -24.734000000 | -23.985496000 | -11.986532000 |
| H | -25.938154000 | -24.540992000 | -13.151863000 |
| H | -26.881956000 | -18.860702000 | -14.236235000 |
| H | -26.931791000 | -20.331792000 | -15.223784000 |
| H | -28.429029000 | -19.610108000 | -14.610059000 |
| H | -27.722408000 | -19.664518000 | -9.067120000  |
| H | -28.000053000 | -21.358384000 | -8.625557000  |
| H | -29.270442000 | -20.419033000 | -9.427305000  |
| H | -35.265497000 | -7.648310000  | -11.191462000 |
| H | -34.152065000 | -7.139563000  | -9.918361000  |
| H | -33.760213000 | -6.832382000  | -11.619774000 |
| H | -33.073085000 | -11.282805000 | -7.827584000  |
| H | -31.581374000 | -12.015852000 | -8.441682000  |
| H | -33.132766000 | -12.765407000 | -8.797027000  |
| H | -30.767371000 | -11.273357000 | -13.634969000 |
| H | -32.033434000 | -10.332182000 | -14.441744000 |
| H | -32.321967000 | -12.019635000 | -13.983439000 |
| H | -21.240642000 | -11.920616000 | -10.517566000 |
| H | -39.897562000 | -20.209187000 | -12.659814000 |
| H | -3.109994000  | 0.854140000   | -2.485615000  |
| H | -3.431704000  | -0.754162000  | -1.814583000  |
| H | -2.289508000  | -0.850505000  | -4.063667000  |
| H | -1.354368000  | -1.640808000  | -2.790088000  |
| H | -0.874956000  | 1.178263000   | -3.909645000  |
| H | 0.171493000   | -0.220171000  | -4.145092000  |
| H | 1.013852000   | 1.328575000   | -2.313003000  |
| H | 0.681527000   | -0.299301000  | -1.713118000  |
| H | -1.132802000  | 2.156389000   | -1.435335000  |
| H | -0.258572000  | 1.332565000   | -0.131323000  |
| H | -23.688848000 | -10.408985000 | -4.716348000  |
| H | -23.394594000 | -11.770188000 | -5.811407000  |
| H | -24.074445000 | -12.512047000 | -3.496557000  |
| H | -22.491226000 | -13.132504000 | -3.975238000  |
| H | -23.016298000 | -10.722000000 | -2.147013000  |

|   |               |               |              |
|---|---------------|---------------|--------------|
| H | -22.349090000 | -12.274487000 | -1.646308000 |
| H | -20.324726000 | -11.900579000 | -3.039445000 |
| H | -20.553547000 | -10.505935000 | -1.980162000 |
| H | -20.011803000 | -9.848789000  | -4.356908000 |
| H | -21.567674000 | -9.204373000  | -3.803943000 |

**Table S2.** Coordinates of gas phase geometry optimized structure of (PorZn)<sub>2</sub>-NMe<sub>2</sub> (**5**) calculated by DFT at the B3LYP / 6-31G(d) level. E = - 5328.032313 Hartree / particle.

|   | x            | y            | z            |
|---|--------------|--------------|--------------|
| C | 0.228204000  | 1.907663000  | -1.297364000 |
| C | -0.790721000 | 1.140416000  | -0.817520000 |
| C | -0.195852000 | -0.041594000 | -0.233521000 |
| N | 1.172410000  | 0.028993000  | -0.363245000 |
| C | 1.463066000  | 1.209363000  | -1.004234000 |
| C | 6.174455000  | 0.503620000  | -1.039538000 |
| C | 5.285090000  | 1.457853000  | -1.434048000 |
| C | 3.960635000  | 0.964383000  | -1.116917000 |
| N | 4.069501000  | -0.272615000 | -0.528071000 |
| C | 5.409094000  | -0.581973000 | -0.467481000 |
| C | 2.755060000  | 1.661576000  | -1.351484000 |
| C | 4.814199000  | -4.763239000 | 1.720590000  |
| C | 5.834507000  | -3.994127000 | 1.246149000  |
| C | 5.240302000  | -2.812184000 | 0.661628000  |
| N | 3.872531000  | -2.883787000 | 0.785752000  |
| C | 3.580169000  | -4.066237000 | 1.423984000  |
| C | 5.968062000  | -1.756082000 | 0.075144000  |
| C | -1.129104000 | -3.365891000 | 1.450357000  |
| C | -0.239815000 | -4.325122000 | 1.833315000  |
| C | 1.084738000  | -3.826542000 | 1.527271000  |
| N | 0.976008000  | -2.581167000 | 0.953854000  |
| C | -0.362983000 | -2.273511000 | 0.892643000  |
| C | -0.922429000 | -1.096120000 | 0.354234000  |
| C | 2.288572000  | -4.527278000 | 1.763003000  |
| C | 7.467117000  | -1.892411000 | 0.031137000  |
| C | 2.187274000  | -5.868682000 | 2.418756000  |
| C | -2.421275000 | -0.958583000 | 0.402088000  |
| C | 2.856177000  | 2.994047000  | -2.026506000 |
| C | 8.086532000  | -2.513724000 | -1.074399000 |
| C | 9.480792000  | -2.628653000 | -1.097760000 |

|   |              |               |              |
|---|--------------|---------------|--------------|
| C | 10.280391000 | -2.148311000  | -0.056655000 |
| C | 9.646636000  | -1.533377000  | 1.026691000  |
| C | 8.255368000  | -1.397375000  | 1.091658000  |
| C | 3.284281000  | 3.097719000   | -3.361798000 |
| C | 3.376641000  | 4.335211000   | -3.990242000 |
| C | 3.061889000  | 5.511185000   | -3.295514000 |
| C | 2.622294000  | 5.415586000   | -1.967309000 |
| C | 2.519649000  | 4.173690000   | -1.343499000 |
| C | -3.212674000 | -1.447058000  | -0.658884000 |
| C | -4.603202000 | -1.301407000  | -0.593740000 |
| C | -5.233093000 | -0.687998000  | 0.492434000  |
| C | -4.429659000 | -0.208027000  | 1.531075000  |
| C | -3.036508000 | -0.332988000  | 1.507794000  |
| C | 2.526838000  | -7.041822000  | 1.728598000  |
| C | 2.432782000  | -8.301546000  | 2.317189000  |
| C | 1.982567000  | -8.421236000  | 3.641571000  |
| C | 1.647103000  | -7.251684000  | 4.347010000  |
| C | 1.747591000  | -6.002364000  | 3.745613000  |
| N | 1.867435000  | -9.636736000  | 4.333088000  |
| C | -1.513520000 | -15.385080000 | 10.667619000 |
| C | -2.522420000 | -15.836593000 | 11.465281000 |
| C | -2.050727000 | -15.763916000 | 12.830137000 |
| N | -0.765528000 | -15.274390000 | 12.840081000 |
| C | -0.405364000 | -15.040623000 | 11.533589000 |
| C | 3.929720000  | -13.381775000 | 12.594616000 |
| C | 3.187900000  | -13.656427000 | 11.484601000 |
| C | 1.898589000  | -14.133472000 | 11.939377000 |
| N | 1.886166000  | -14.155777000 | 13.314446000 |
| C | 3.111004000  | -13.700406000 | 13.743299000 |
| C | 0.836451000  | -14.528105000 | 11.095212000 |
| C | 2.184015000  | -14.197897000 | 18.382673000 |
| C | 3.190969000  | -13.743775000 | 17.584602000 |
| C | 2.760336000  | -13.916678000 | 16.214791000 |
| N | 1.501909000  | -14.473219000 | 16.202613000 |

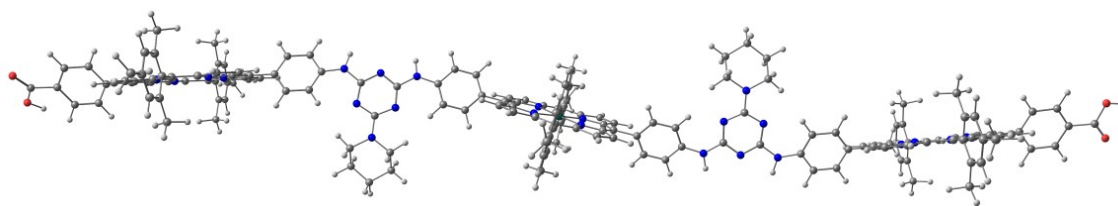
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|---|--------------|---------------|--------------|
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| C | 3.525442000  | -13.566162000 | 15.084768000 |
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| C | -2.406910000 | -16.203495000 | 17.553272000 |
| C | -1.166145000 | -15.607075000 | 17.102673000 |
| N | -1.178090000 | -15.523645000 | 15.730866000 |
| C | -2.380992000 | -16.033685000 | 15.299128000 |
| C | -2.807861000 | -16.136424000 | 13.960203000 |
| C | -0.106571000 | -15.201836000 | 17.943905000 |
| C | 4.901404000  | -13.005213000 | 15.329414000 |
| C | -0.303950000 | -15.358225000 | 19.419782000 |
| C | -4.187236000 | -16.689108000 | 13.716026000 |
| C | 1.043599000  | -14.396613000 | 9.619364000  |
| C | 6.009824000  | -13.870138000 | 15.433094000 |
| C | 7.280332000  | -13.325293000 | 15.658803000 |
| C | 7.482836000  | -11.949778000 | 15.787739000 |
| C | 6.369275000  | -11.109406000 | 15.680663000 |
| C | 5.083870000  | -11.609877000 | 15.454019000 |
| C | 1.087425000  | -15.528243000 | 8.788687000  |
| C | 1.280702000  | -15.406894000 | 7.418016000  |
| C | 1.436308000  | -14.143290000 | 6.819425000  |
| C | 1.395022000  | -13.002760000 | 7.637330000  |
| C | 1.202037000  | -13.142564000 | 9.010743000  |
| C | -4.367690000 | -18.072018000 | 13.503488000 |
| C | -5.659749000 | -18.564507000 | 13.286059000 |
| C | -6.777806000 | -17.726623000 | 13.268598000 |
| C | -6.576741000 | -16.359773000 | 13.483455000 |
| C | -5.303465000 | -15.824823000 | 13.705852000 |
| C | -1.267447000 | -14.596727000 | 20.102971000 |
| C | -1.453023000 | -14.739432000 | 21.475855000 |
| C | -0.673740000 | -15.653890000 | 22.198066000 |
| C | 0.290001000  | -16.418729000 | 21.526982000 |
| C | 0.471683000  | -16.271274000 | 20.155854000 |
| N | 1.628791000  | -14.123058000 | 5.430467000  |

|    |              |               |              |
|----|--------------|---------------|--------------|
| N  | 2.077490000  | -11.232494000 | 2.626536000  |
| C  | 1.902579000  | -10.943350000 | 3.914781000  |
| N  | 1.742947000  | -11.829427000 | 4.923719000  |
| C  | 1.772533000  | -13.103379000 | 4.522827000  |
| N  | 1.933506000  | -13.534648000 | 3.258474000  |
| C  | 2.072108000  | -12.558346000 | 2.346094000  |
| N  | 2.208277000  | -12.918421000 | 1.038930000  |
| Zn | 2.522432000  | -1.427927000  | 0.212497000  |
| Zn | 0.361310000  | -14.856676000 | 14.521502000 |
| C  | -6.738513000 | -0.568831000  | 0.555437000  |
| C  | -2.584388000 | -2.118113000  | -1.860638000 |
| C  | -2.214690000 | 0.204254000   | 2.658576000  |
| C  | 7.622865000  | -0.722032000  | 2.288829000  |
| C  | 7.269149000  | -3.049058000  | -2.229193000 |
| C  | 11.782668000 | -2.311419000  | -0.089921000 |
| C  | 3.182256000  | 6.810429000   | -4.032676000 |
| O  | 3.200301000  | 6.892438000   | -5.238372000 |
| O  | 3.277768000  | 7.938823000   | -3.275774000 |
| C  | 2.351816000  | -14.309595000 | 0.640660000  |
| C  | 2.388839000  | -11.927466000 | -0.009755000 |
| C  | 3.913983000  | -10.656611000 | 15.346913000 |
| C  | 5.848573000  | -15.368706000 | 15.303330000 |
| C  | 8.859197000  | -11.380113000 | 16.044589000 |
| C  | -8.160302000 | -18.275817000 | 13.000779000 |
| C  | -3.192993000 | -19.025388000 | 13.514110000 |
| C  | -5.142806000 | -14.337827000 | 13.932770000 |
| C  | -0.826588000 | -15.849887000 | 23.662142000 |
| O  | -1.790725000 | -15.063263000 | 24.207923000 |
| O  | -0.174029000 | -16.624723000 | 24.334178000 |
| H  | 0.149162000  | 2.852791000   | -1.814884000 |
| H  | -1.851188000 | 1.345059000   | -0.862477000 |
| H  | 7.252269000  | 0.530557000   | -1.117510000 |
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| H  | 4.887990000  | -5.710639000  | 2.234280000  |

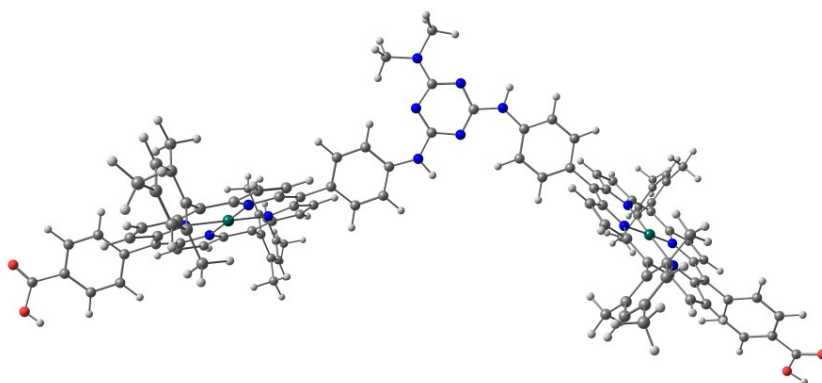
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| H | -0.458707000 | -5.287218000  | 2.272917000  |
| H | 9.953285000  | -3.105343000  | -1.954648000 |
| H | 10.249743000 | -1.146353000  | 1.845967000  |
| H | 3.535141000  | 2.193489000   | -3.908478000 |
| H | 3.689858000  | 4.414123000   | -5.026080000 |
| H | 2.320016000  | 6.301817000   | -1.412869000 |
| H | 2.176448000  | 4.112733000   | -0.315083000 |
| H | -5.208388000 | -1.676867000  | -1.416767000 |
| H | -4.898216000 | 0.278923000   | 2.384394000  |
| H | 2.869496000  | -6.968611000  | 0.700012000  |
| H | 2.700066000  | -9.191025000  | 1.765908000  |
| H | 1.303504000  | -7.325569000  | 5.376841000  |
| H | 1.485603000  | -5.114359000  | 4.313843000  |
| H | 1.675289000  | -9.565017000  | 5.323736000  |
| H | -1.521117000 | -15.282655000 | 9.592342000  |
| H | -3.502958000 | -16.177758000 | 11.164164000 |
| H | 4.943674000  | -13.009554000 | 12.637939000 |
| H | 3.487270000  | -13.554936000 | 10.451716000 |
| H | 2.156651000  | -14.207716000 | 19.462643000 |
| H | 4.138038000  | -13.321178000 | 17.889432000 |
| H | -4.139409000 | -16.905408000 | 16.397205000 |
| H | -2.666239000 | -16.408789000 | 18.581713000 |
| H | 8.132809000  | -13.997411000 | 15.735501000 |
| H | 6.503670000  | -10.033189000 | 15.775146000 |
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| H | -5.793890000 | -19.632998000 | 13.127947000 |
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| H | -2.196061000 | -14.140611000 | 21.991040000 |

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| H | 1.214683000  | -16.872222000 | 19.639885000 |
| H | 1.660820000  | -15.026903000 | 4.976710000  |
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| H | -7.047432000 | 0.345183000   | 1.074486000  |
| H | -7.182870000 | -1.414522000  | 1.097654000  |
| H | -1.884570000 | -1.449515000  | -2.375688000 |
| H | -2.015979000 | -3.010214000  | -1.572155000 |
| H | -3.349904000 | -2.424246000  | -2.580406000 |
| H | -2.858582000 | 0.647103000   | 3.424838000  |
| H | -1.508277000 | 0.973499000   | 2.324596000  |
| H | -1.620328000 | -0.586364000  | 3.131663000  |
| H | 7.055620000  | 0.169400000   | 1.995885000  |
| H | 6.920946000  | -1.389120000  | 2.802948000  |
| H | 8.385819000  | -0.414116000  | 3.010579000  |
| H | 6.558631000  | -3.815553000  | -1.897786000 |
| H | 7.915632000  | -3.494868000  | -2.991527000 |
| H | 6.679827000  | -2.257194000  | -2.706536000 |
| H | 12.164199000 | -2.304531000  | -1.116699000 |
| H | 12.090267000 | -3.263259000  | 0.364002000  |
| H | 12.285332000 | -1.511238000  | 0.464035000  |
| H | 3.405343000  | 7.704563000   | -2.342348000 |
| H | 1.631573000  | -14.548308000 | -0.151975000 |
| H | 2.170842000  | -14.950516000 | 1.500630000  |
| H | 3.363033000  | -14.500690000 | 0.253788000  |
| H | 3.452145000  | -11.780872000 | -0.250370000 |
| H | 1.877236000  | -12.272234000 | -0.915313000 |
| H | 1.963714000  | -10.975397000 | 0.302441000  |
| H | 3.418798000  | -10.735375000 | 14.371903000 |
| H | 4.242001000  | -9.620506000  | 15.476557000 |
| H | 3.152033000  | -10.867833000 | 16.106528000 |
| H | 5.398460000  | -15.643362000 | 14.342218000 |
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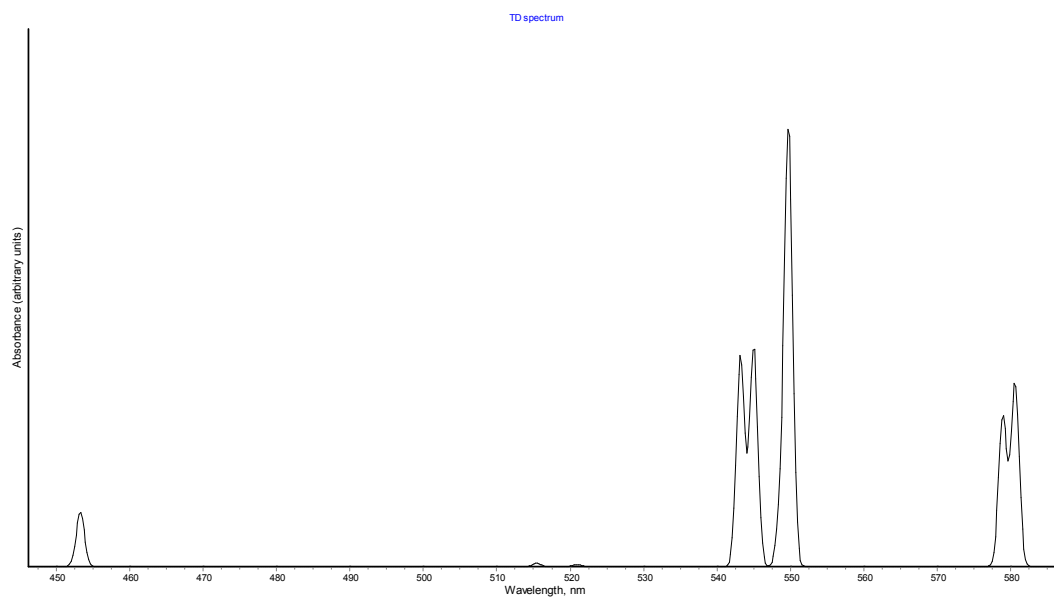
|   |              |               |              |
|---|--------------|---------------|--------------|
| H | 9.630250000  | -12.154856000 | 15.984366000 |
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| H | 9.111739000  | -10.597661000 | 15.318602000 |
| H | -8.228346000 | -19.336577000 | 13.264598000 |
| H | -8.425859000 | -18.186458000 | 11.938649000 |
| H | -8.924450000 | -17.735266000 | 13.570369000 |
| H | -2.461716000 | -18.771049000 | 12.737837000 |
| H | -3.524152000 | -20.054279000 | 13.341982000 |
| H | -2.660122000 | -18.997380000 | 14.471902000 |
| H | -4.472882000 | -13.887995000 | 13.190602000 |
| H | -6.108612000 | -13.826761000 | 13.869543000 |
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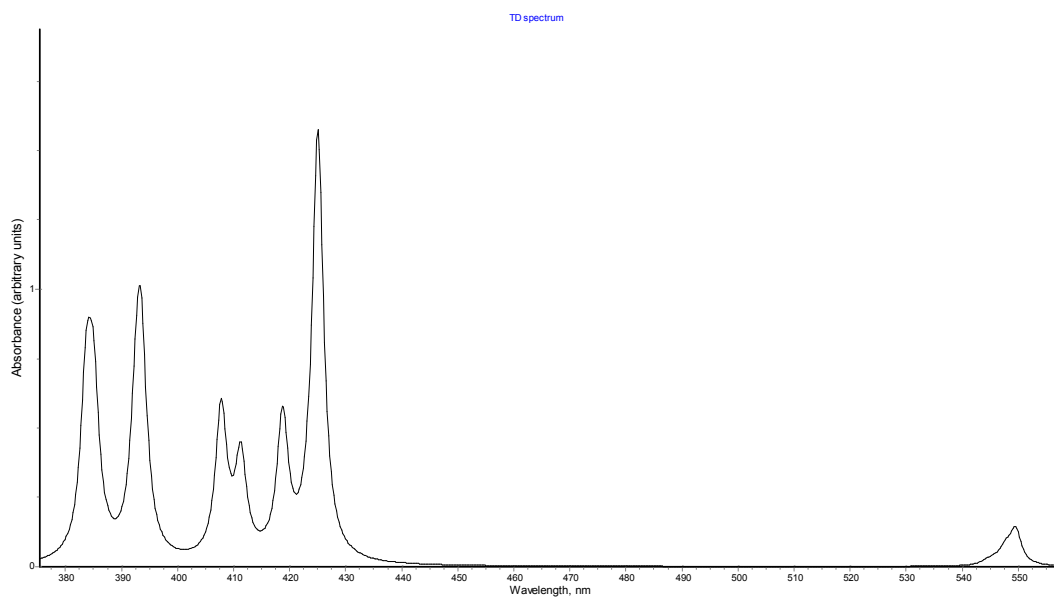
**Figure S1.** Different view perspective of the gas phase geometry optimized structure of  $\text{PorZn}-(\text{PorCOOH})_2-(\text{piper})_2$  (2).



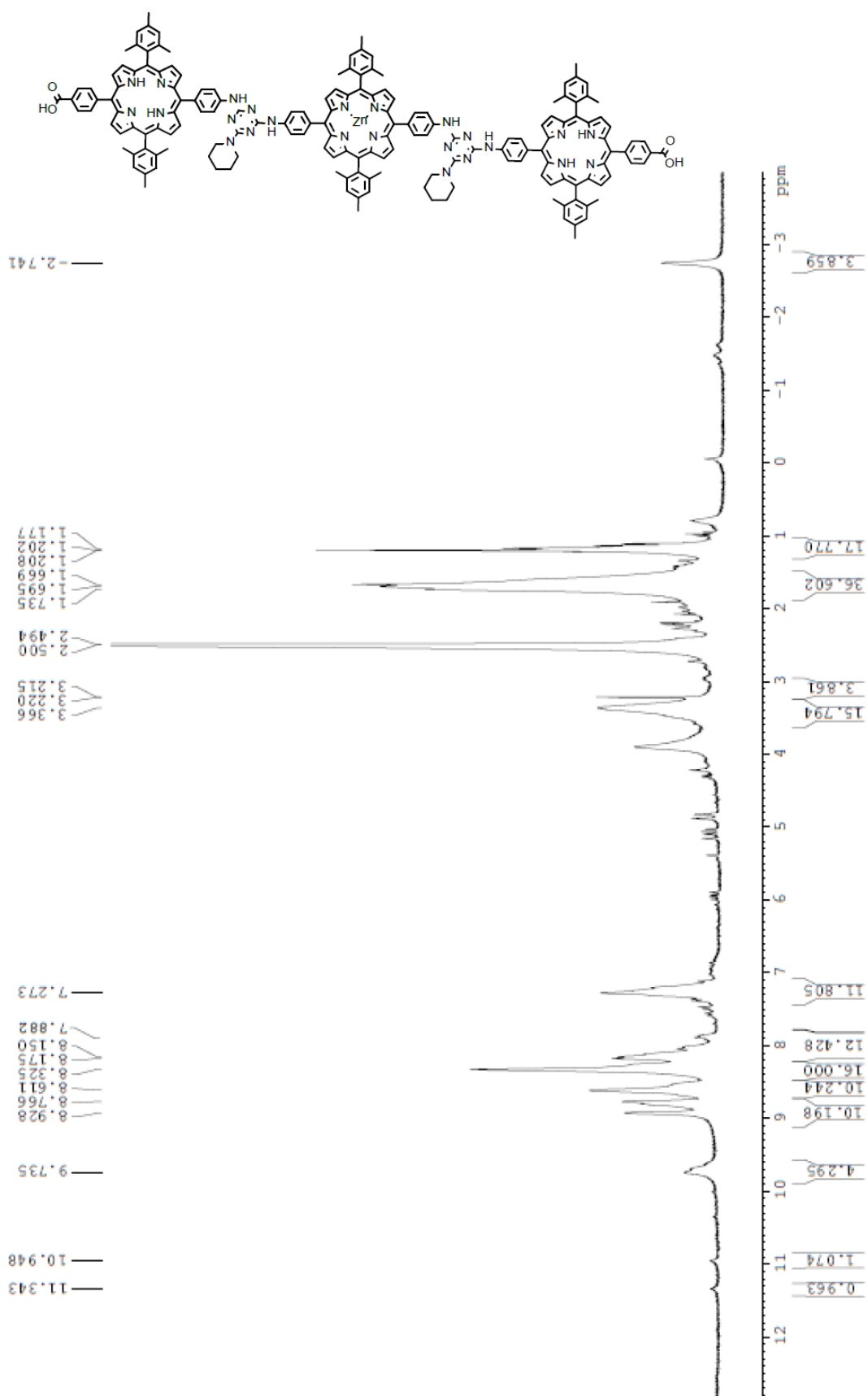
**Figure S2.** Different view perspective of the gas phase geometry optimized structure of  $(\text{PorZn})_2\text{-NMe}_2$  (5).



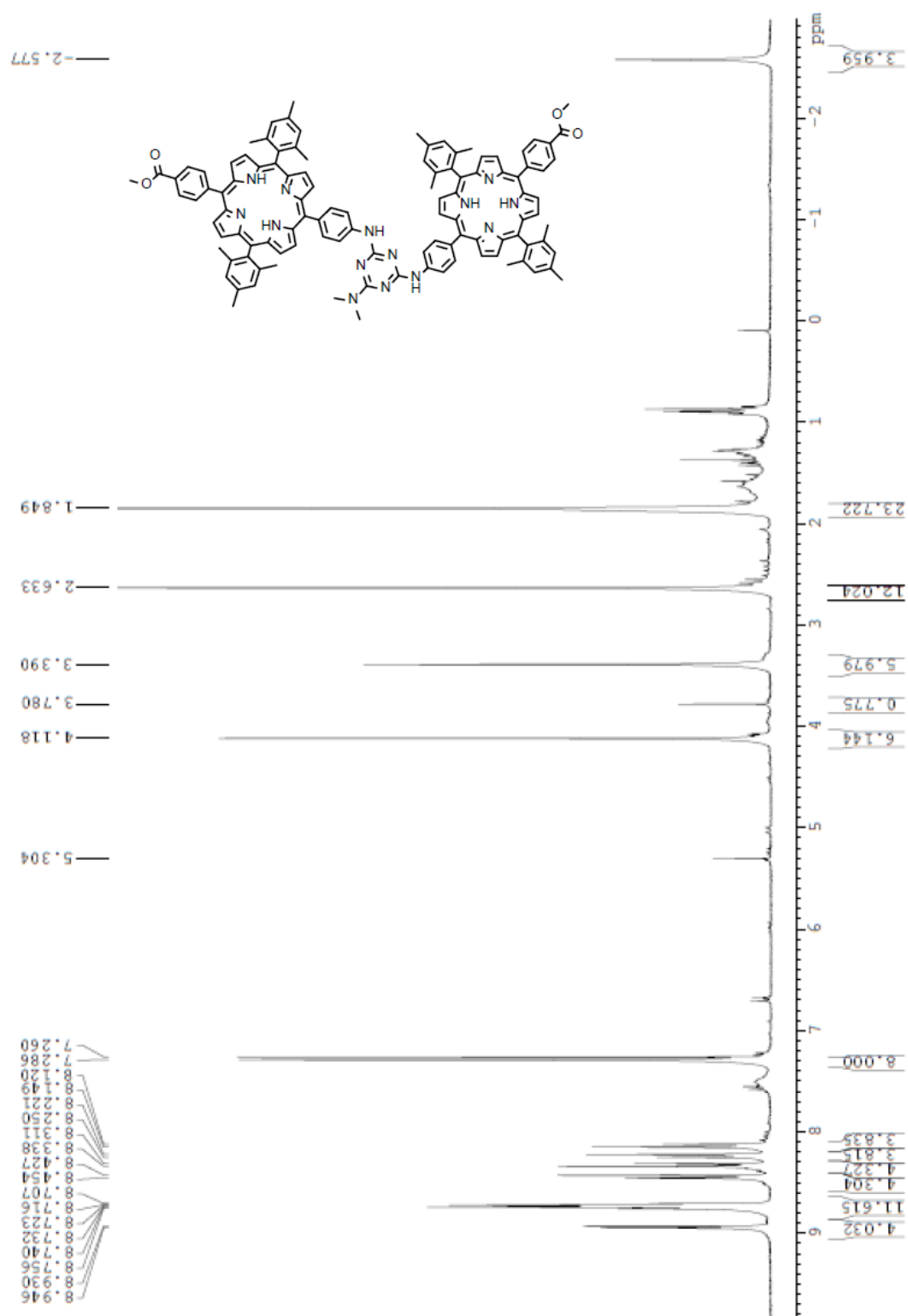
**Figure S3.** Theoretically calculated UV-vis absorption spectrum of **2**.



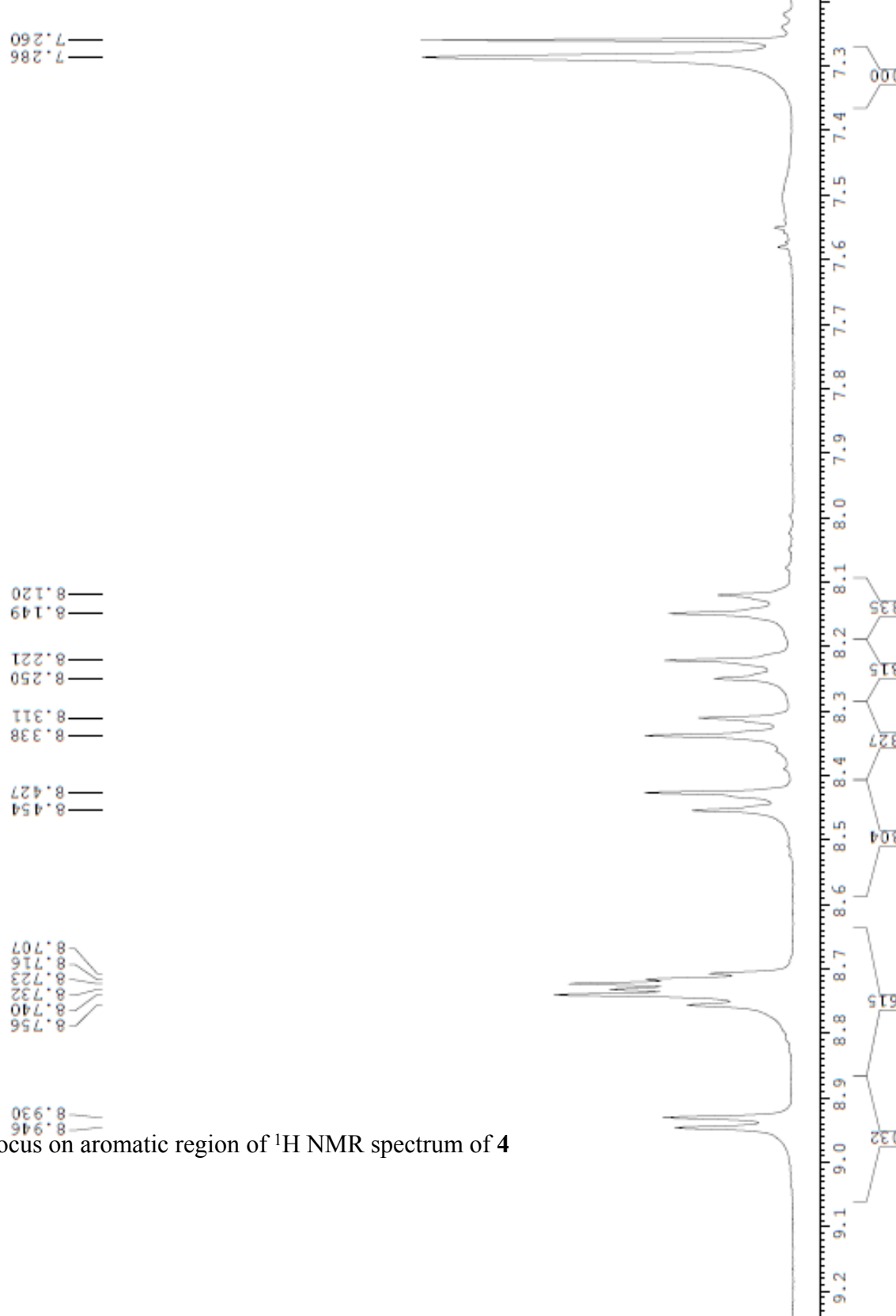
**Figure S4.** Theoretically calculated UV-Vis absorption spectrum of **5**.



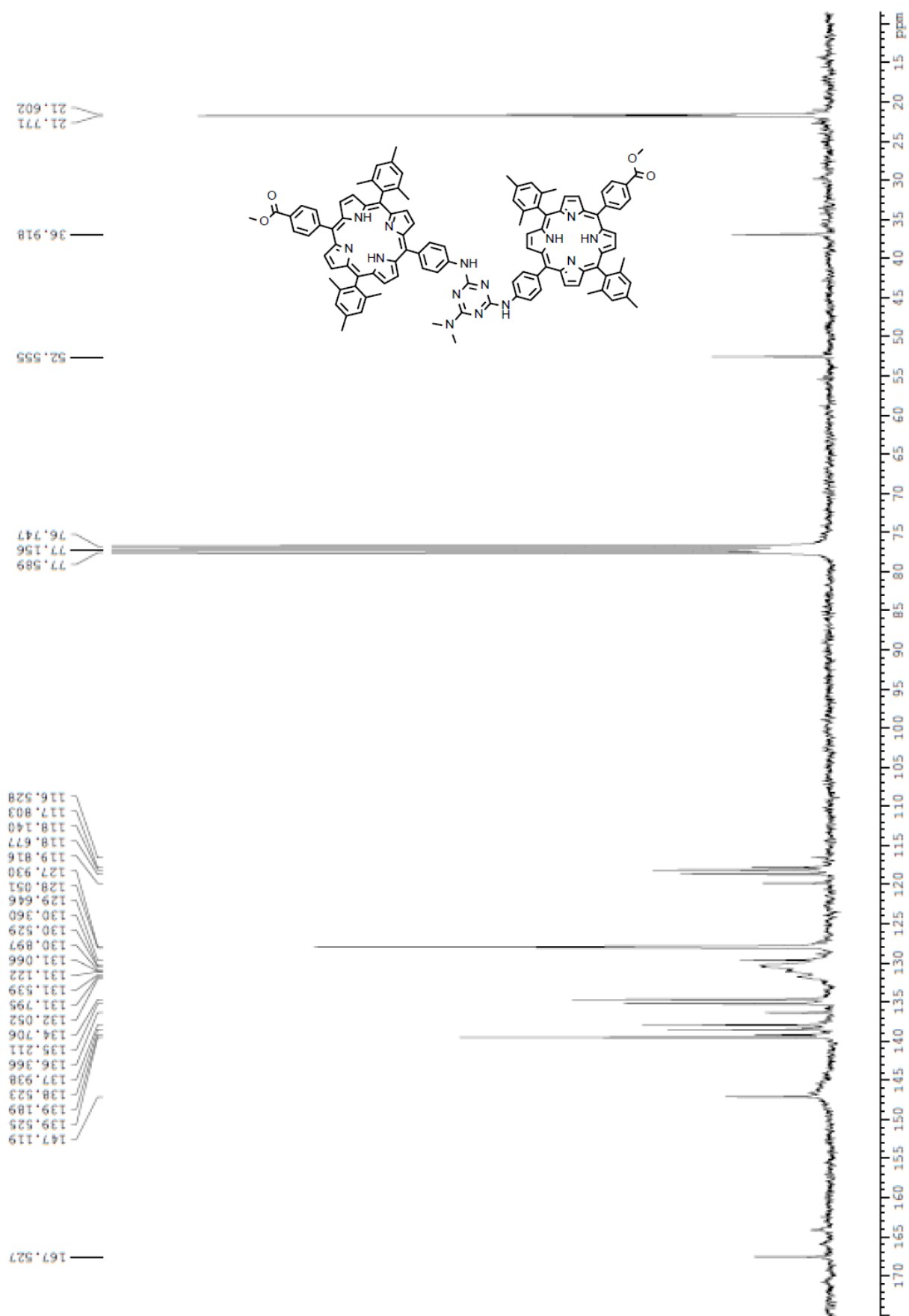
**Figure S5.**  $^1\text{H}$  NMR spectrum of **2** (300 MHz,  $\text{DMSO-d}_6$ ).



**Figure S6.**  $^1\text{H}$  NMR spectrum of **4** (300 MHz,  $\text{CDCl}_3$ ).

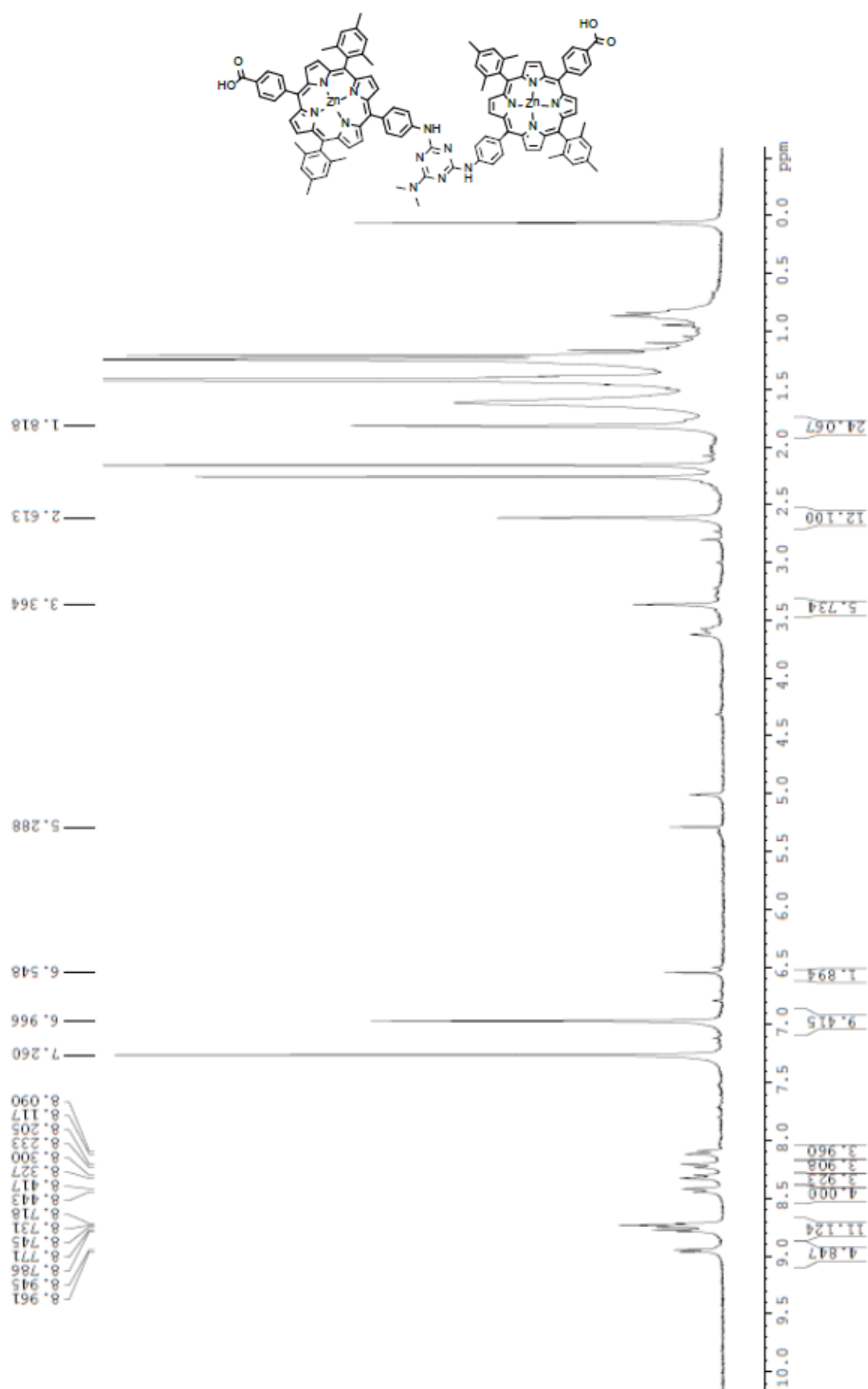


**Figure S7.** Focus on aromatic region of  $^1\text{H}$  NMR spectrum of **4**

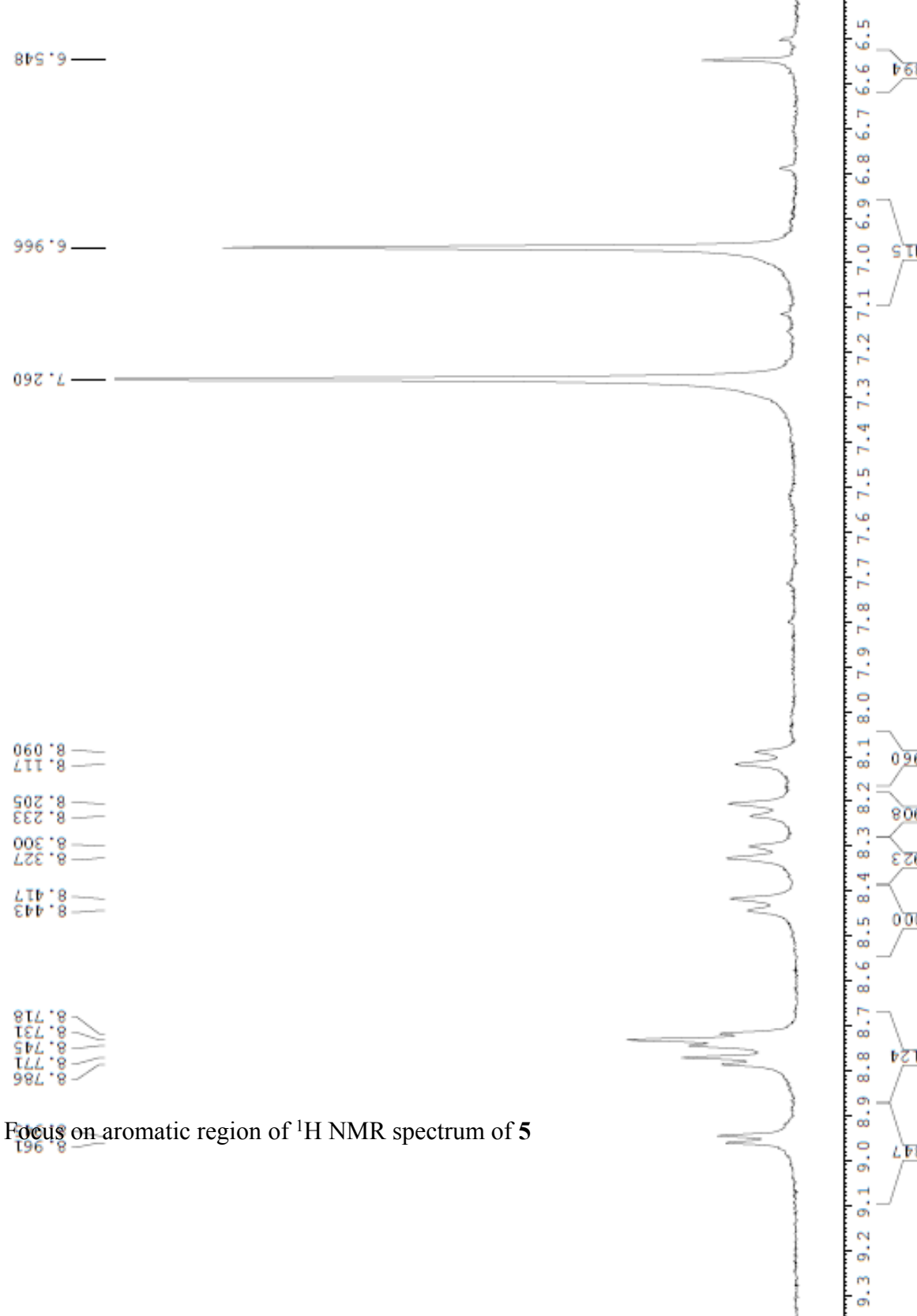




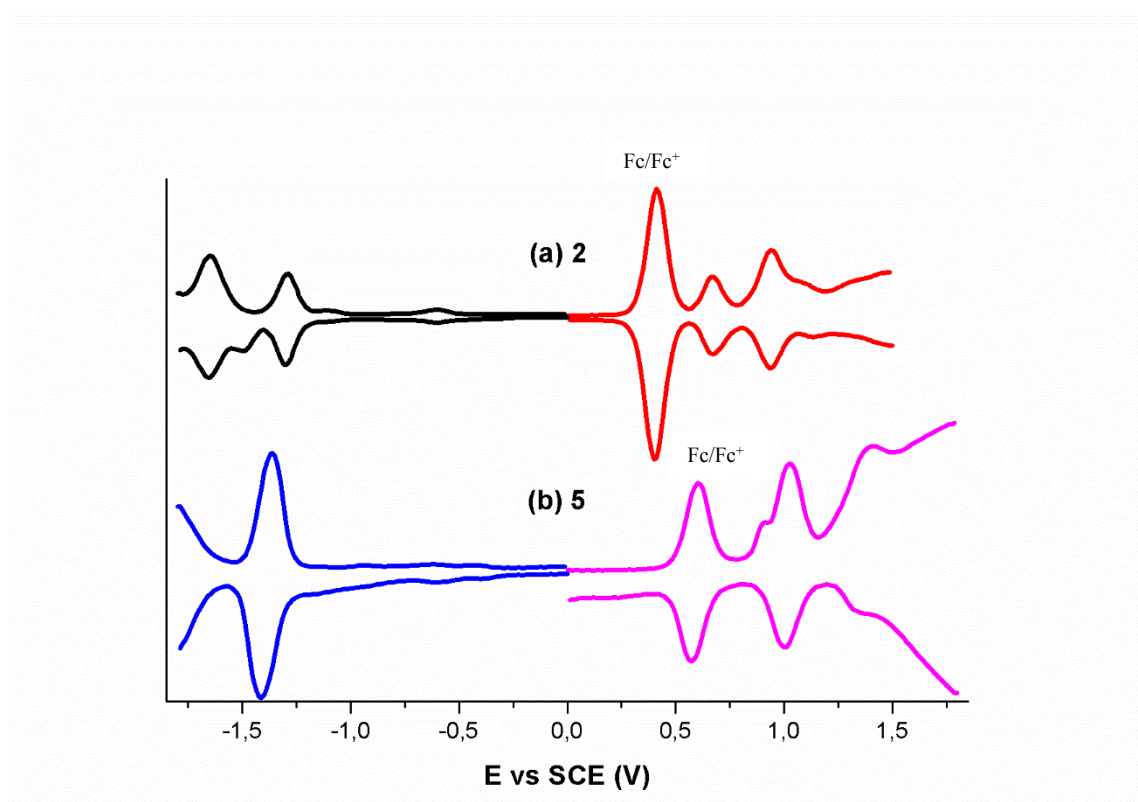
**Figure S9.** Focus on aromatic region of  $^{13}\text{C}$  NMR spectrum of **4**



**Figure S10.** <sup>1</sup>H NMR spectrum of **5** (300 MHz, CDCl<sub>3</sub>:MeOH 1:0.01)



**Figure S11.** Focus on aromatic region of  $^1\text{H}$  NMR spectrum of **5**



**Figure S12.** Square-wave voltammograms in  $\text{CH}_2\text{Cl}_2$  of a)  $\text{PorZn}-(\text{PorCOOH})_2-(\text{piper})_2$  (**2**) and b)  $(\text{PorZn})_2-\text{NMe}_2$  (**5**).