

Electronic supplementary information

FACILE TWO-STEP SYNTHESIS OF ISOQUINOLONES FROM BENZOIC ACIDS AND ALKYNES AND THEIR COMPARATIVE PHOTOLUMINESCENT STUDY VS ISOCOUMARINS

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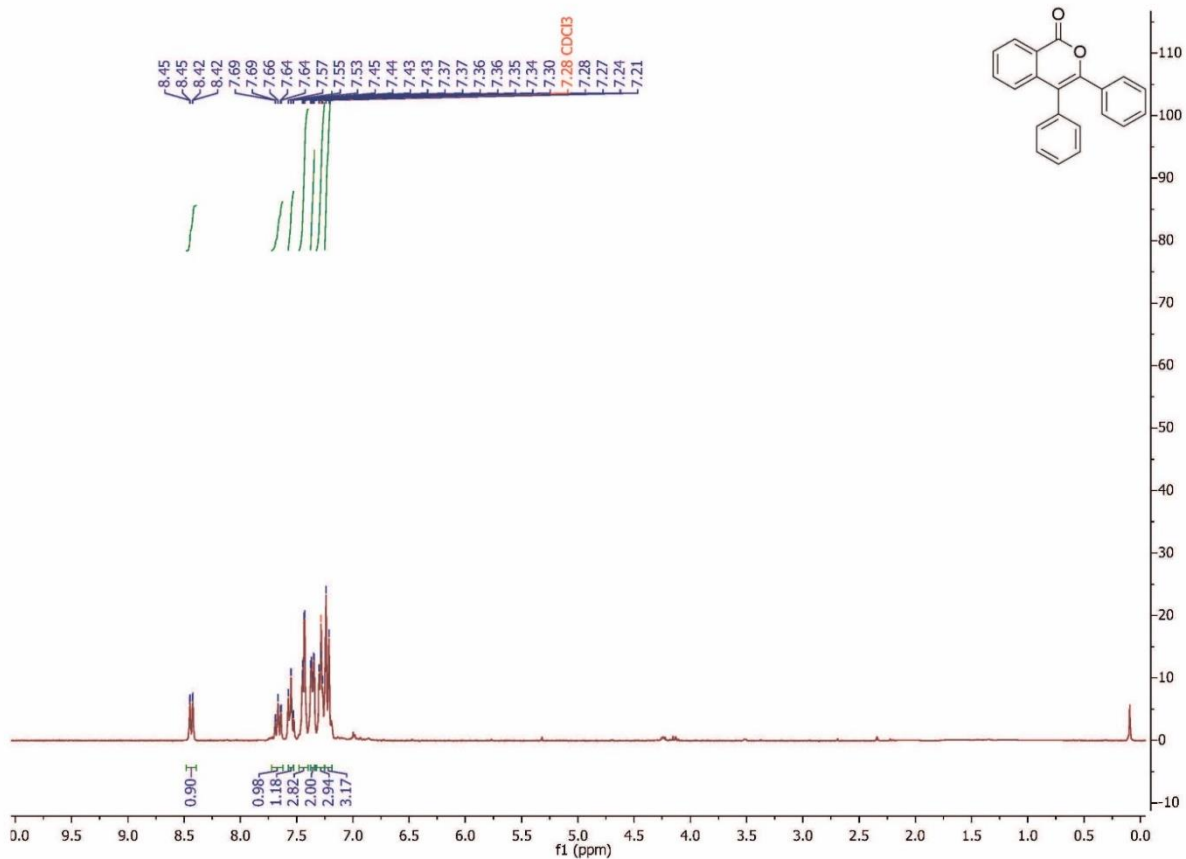
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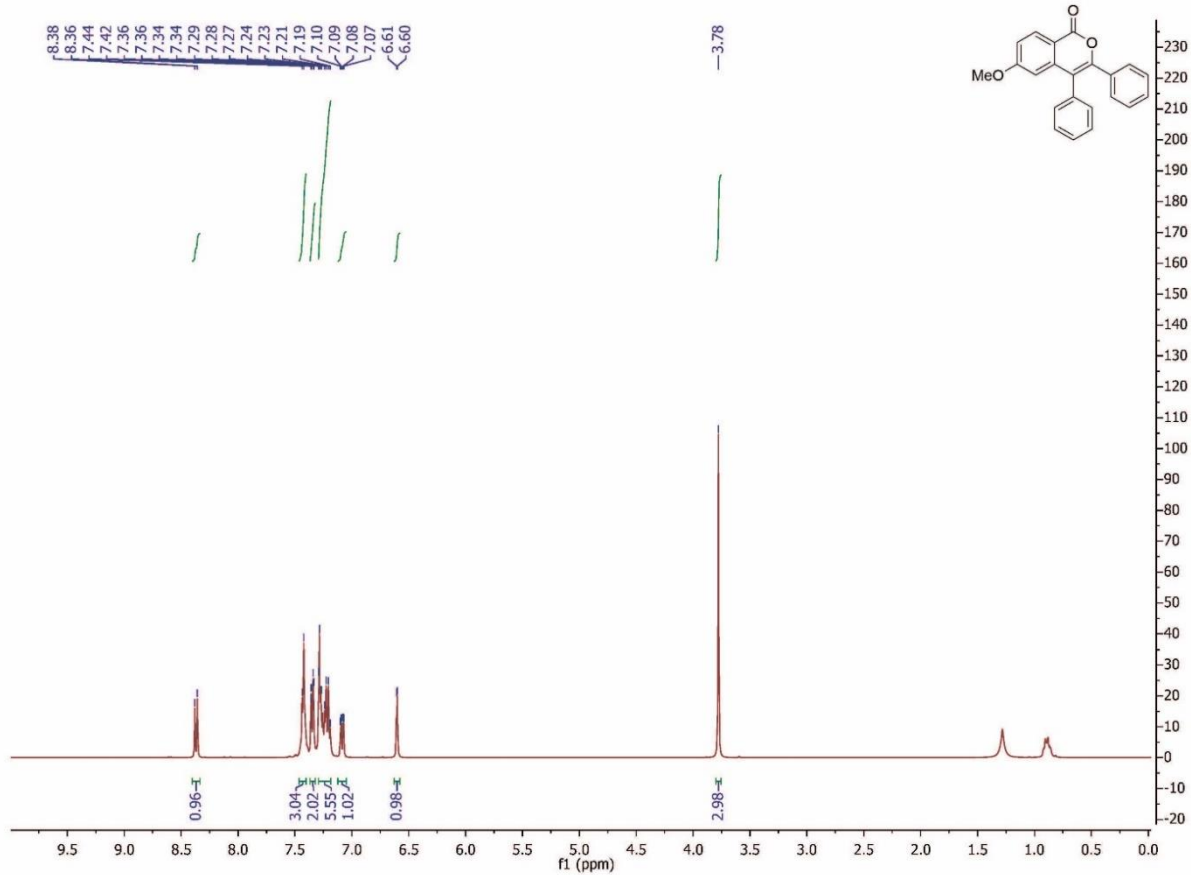
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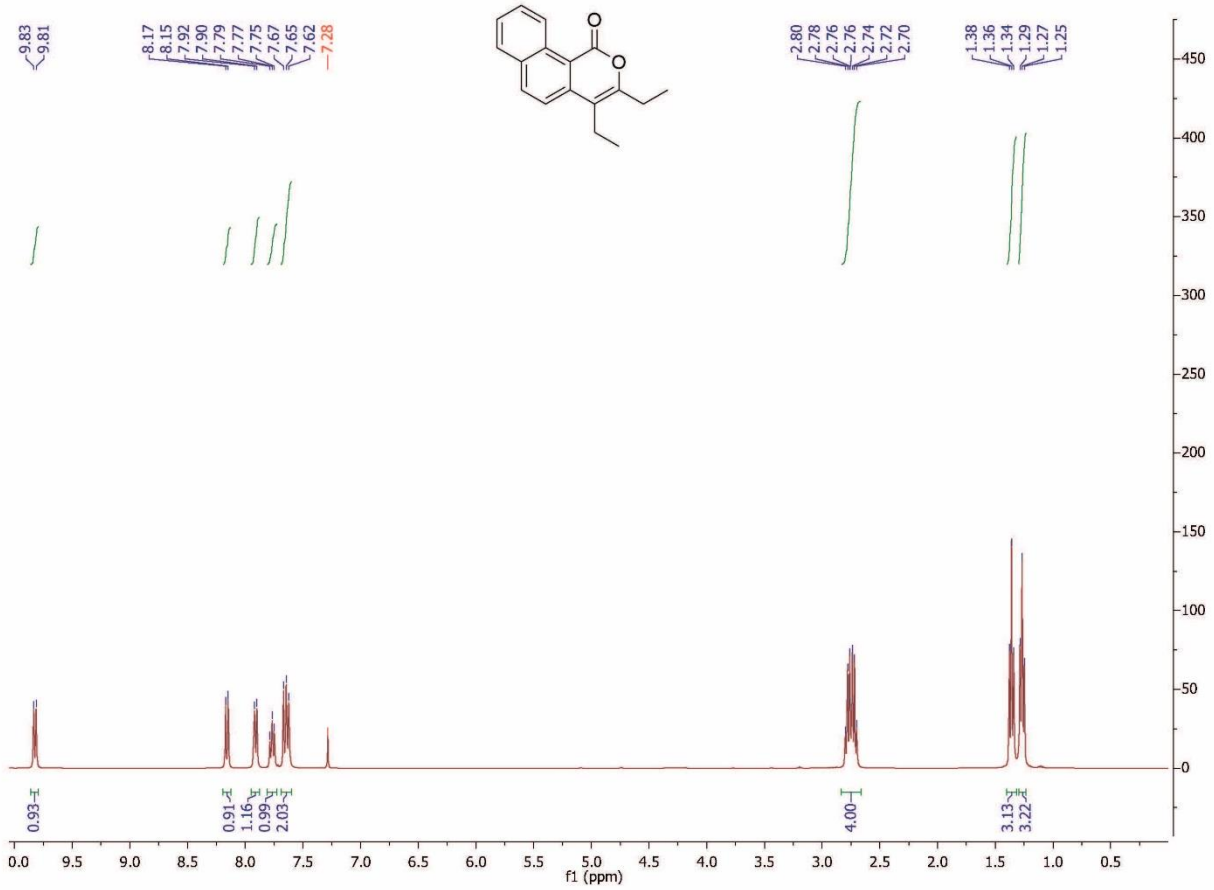
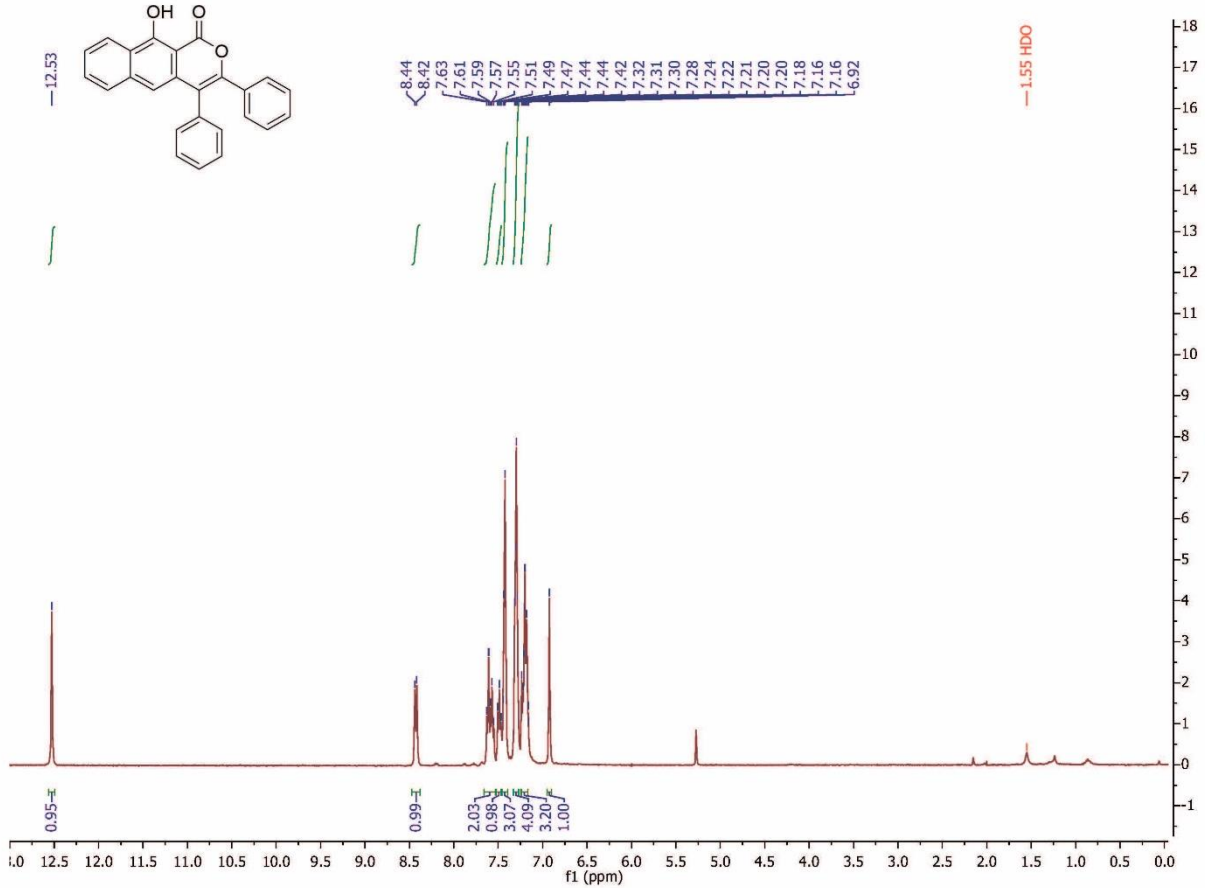
1. NMR spectra

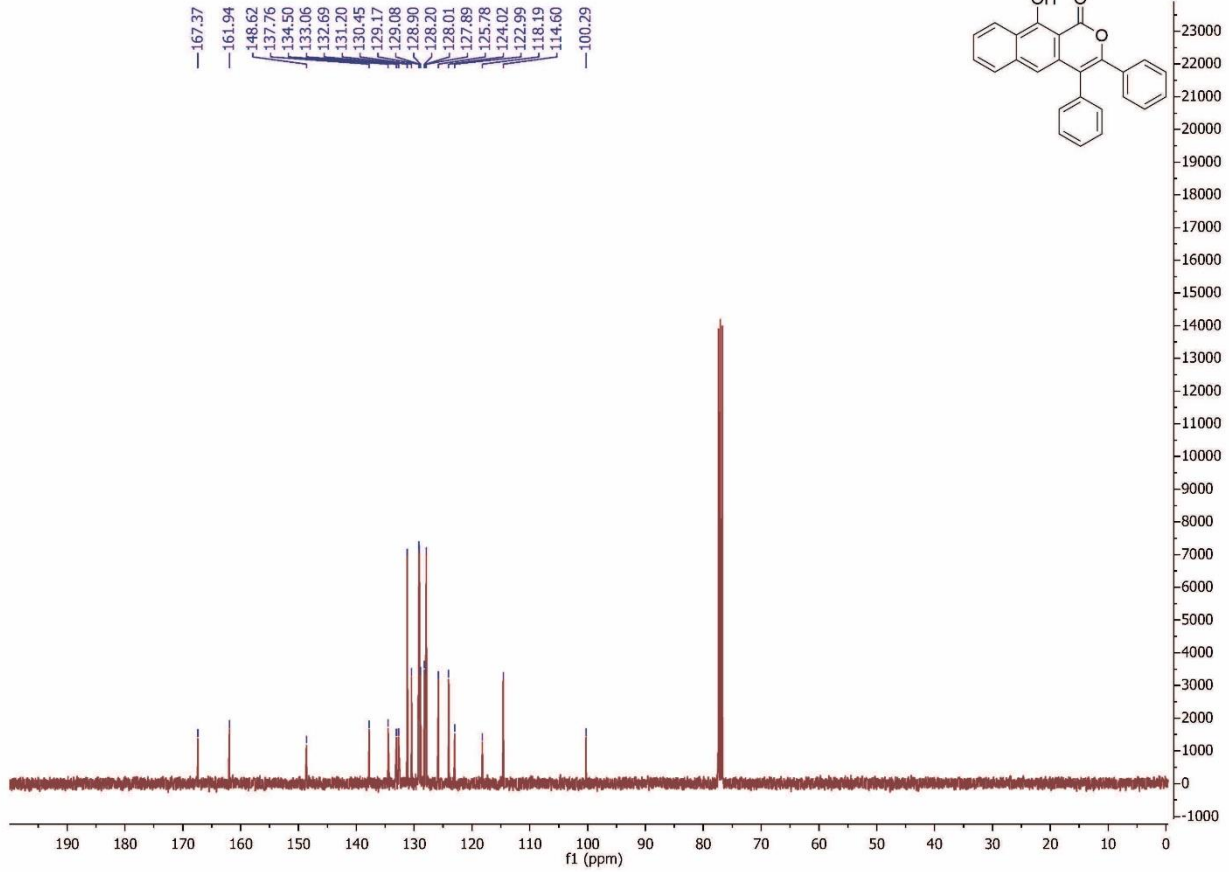
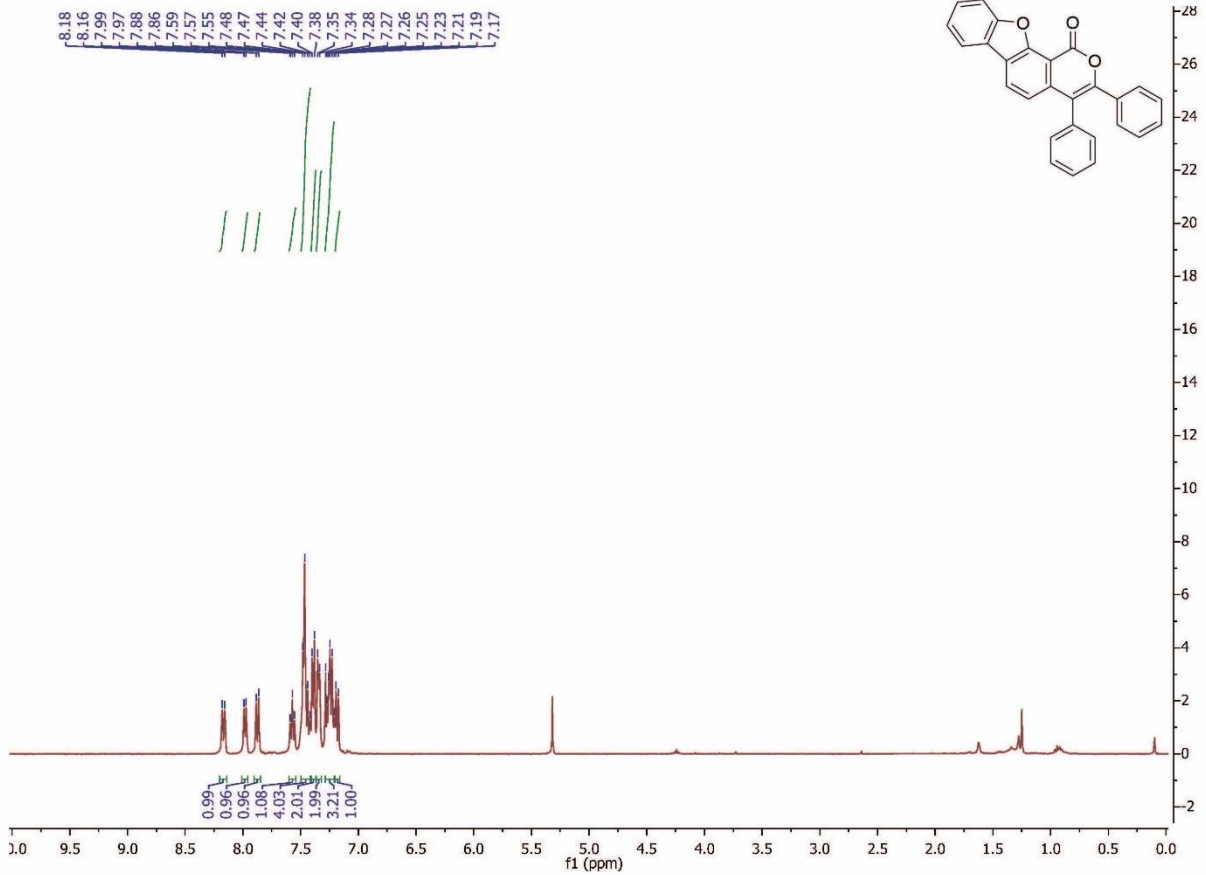
^1H NMR (400 MHz) spectrum of **1a** in CDCl_3

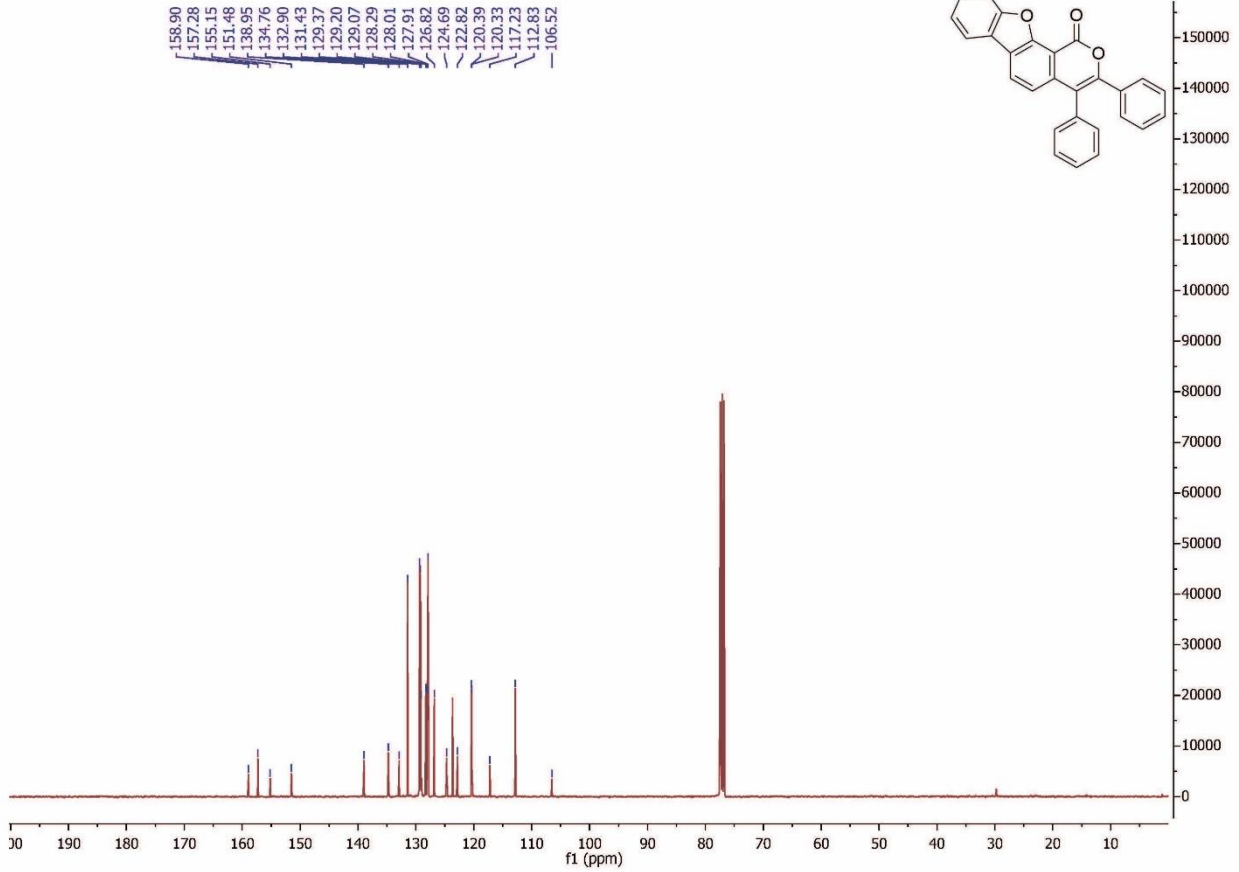
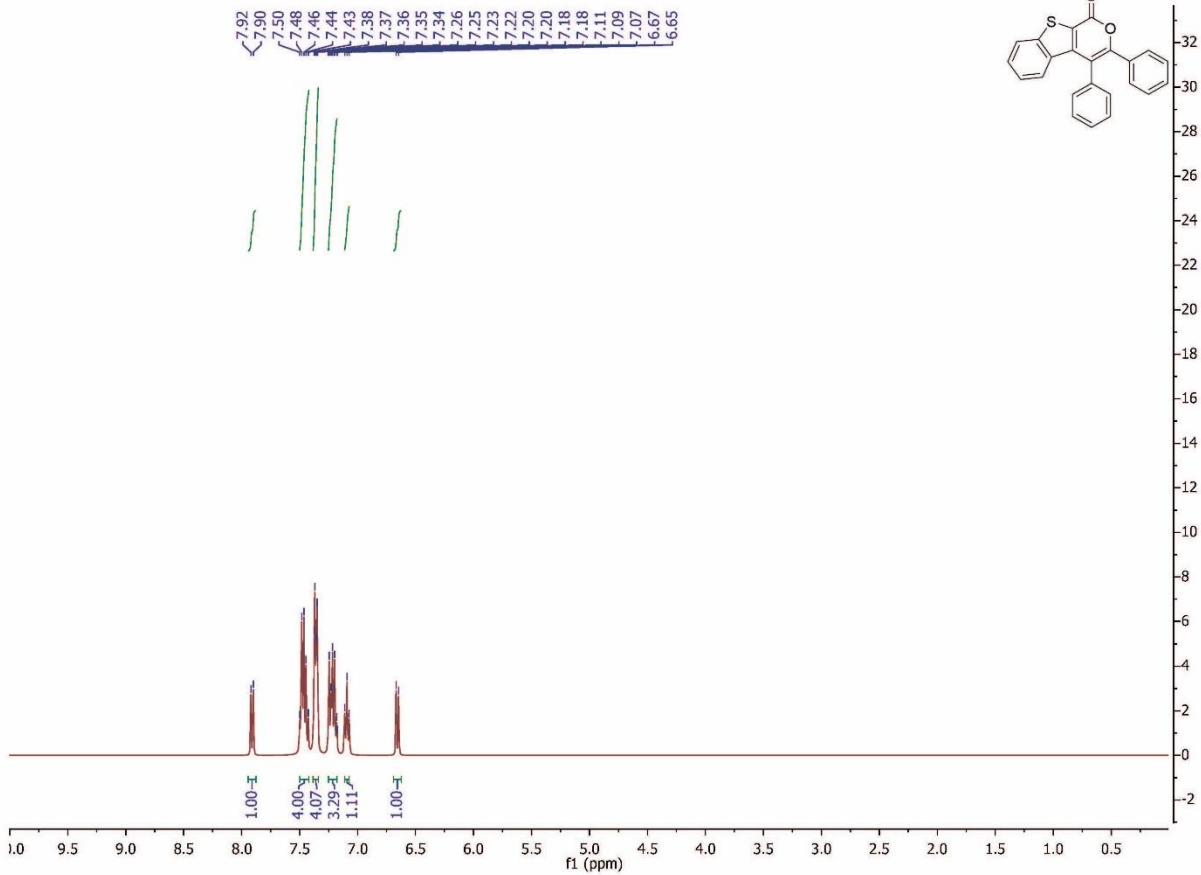


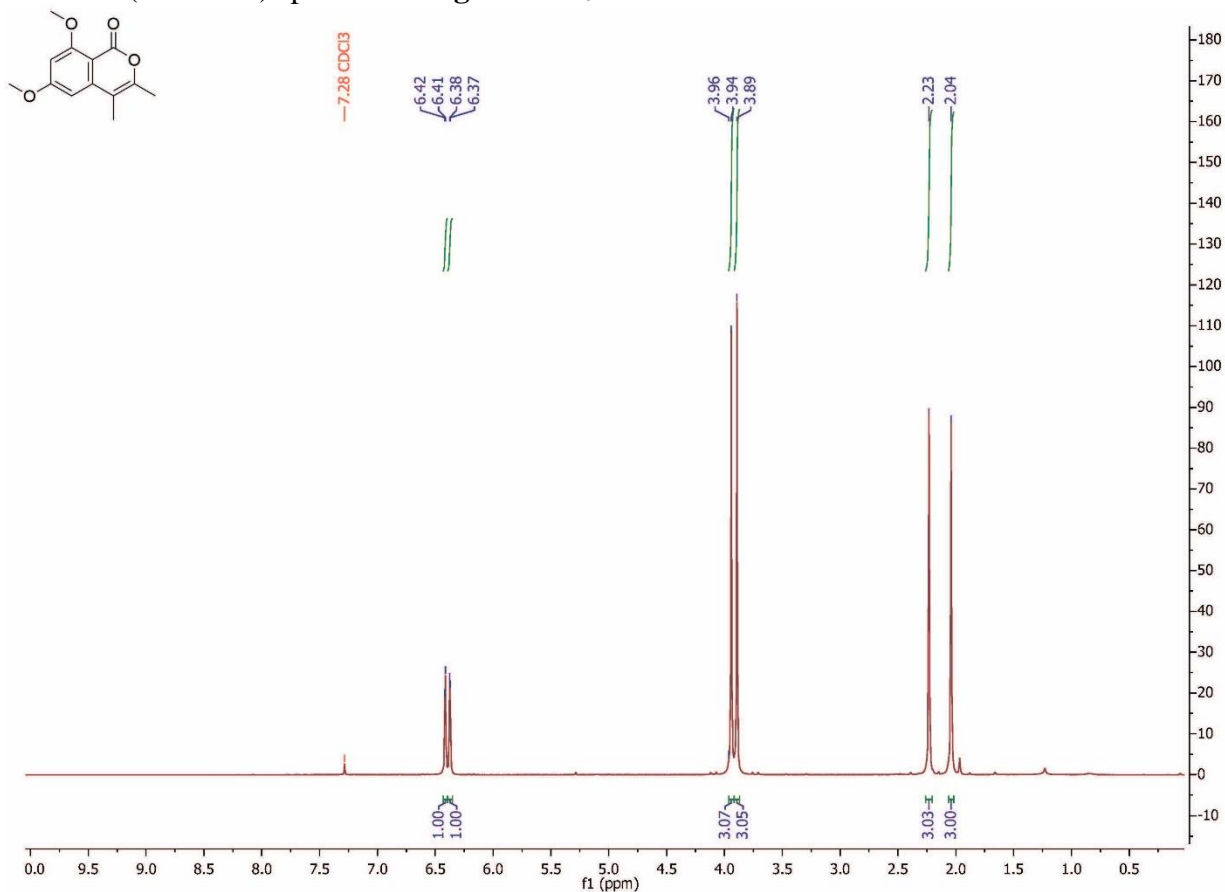
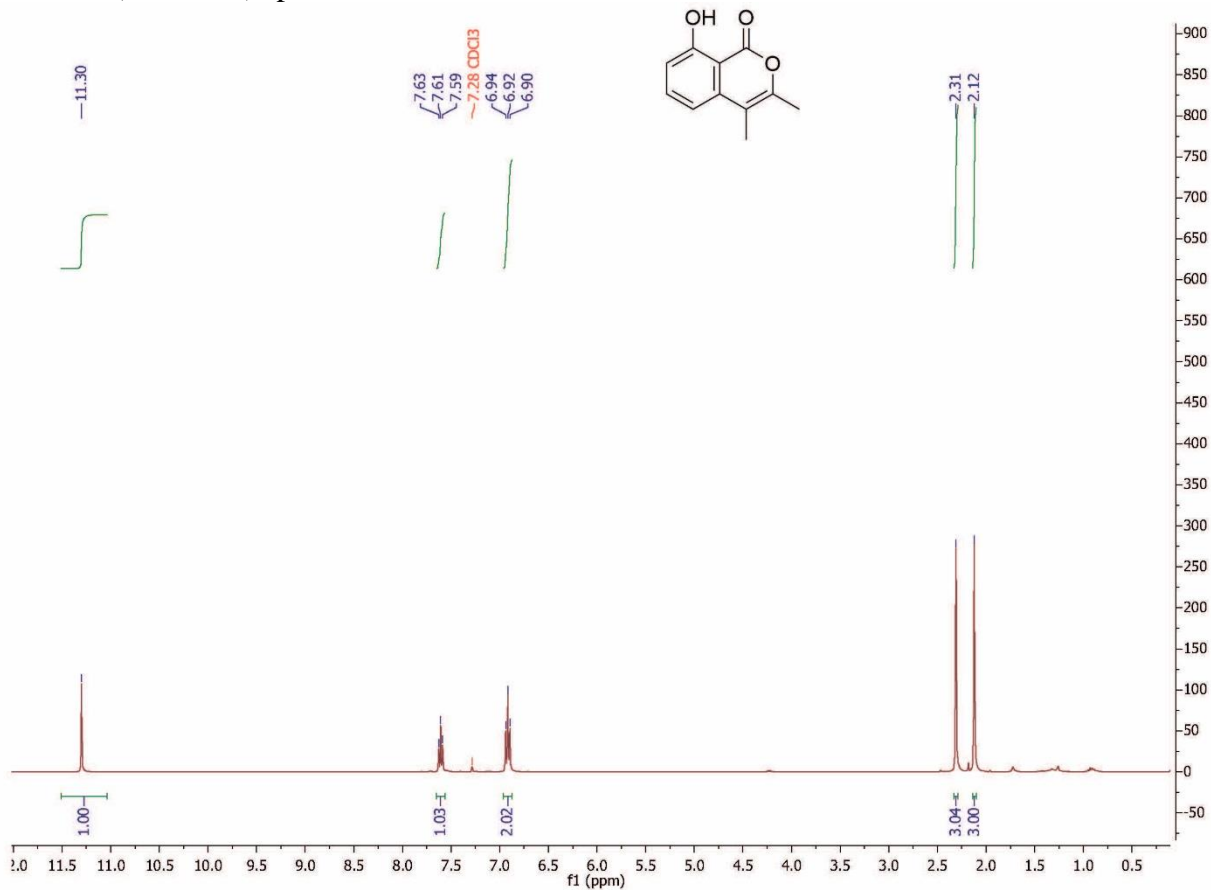
^1H NMR (400 MHz) spectrum of **1b** in CDCl_3



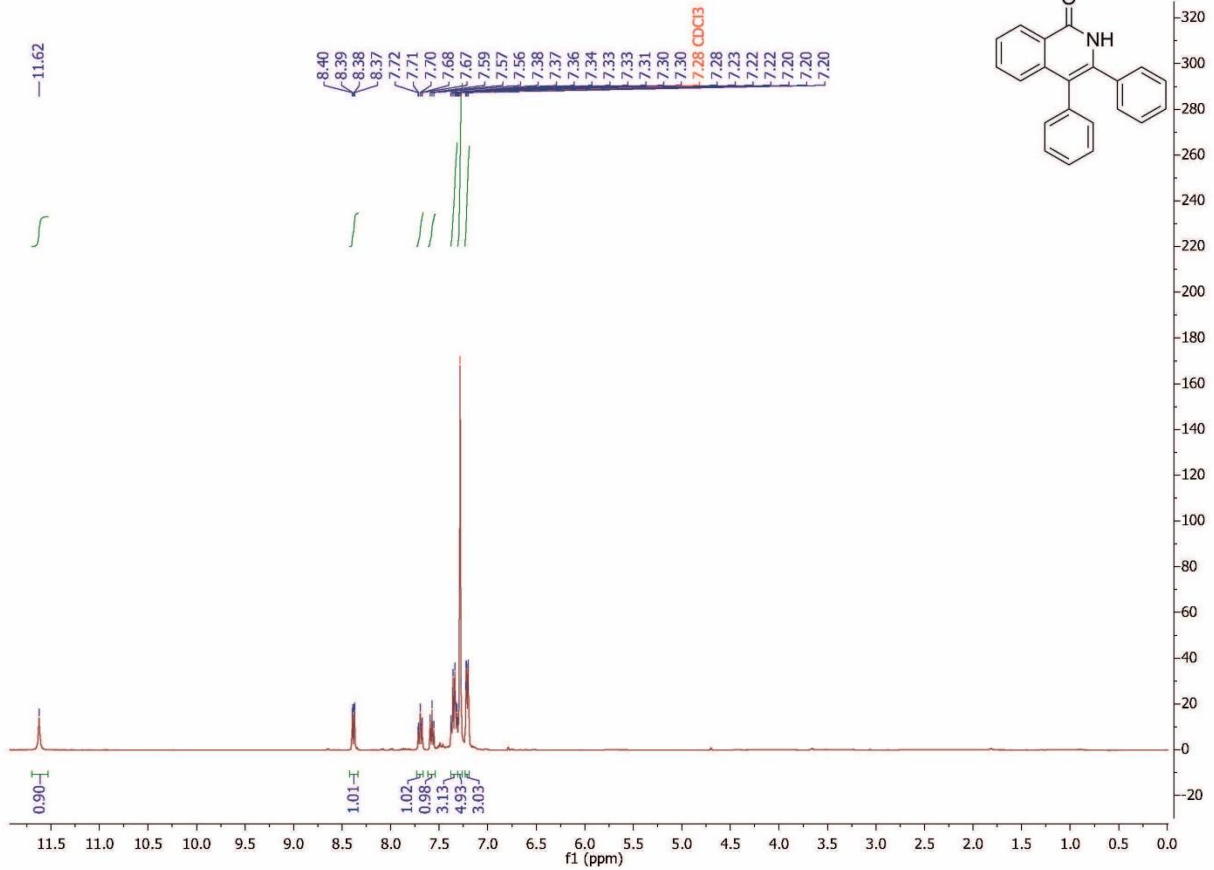
^1H NMR (400 MHz) spectrum of **1c** in CDCl_3  ^1H NMR (400 MHz) spectrum of **1d** in CDCl_3 

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **1d** in CDCl_3  ^1H NMR (400 MHz) spectrum of **1e** in CDCl_3 

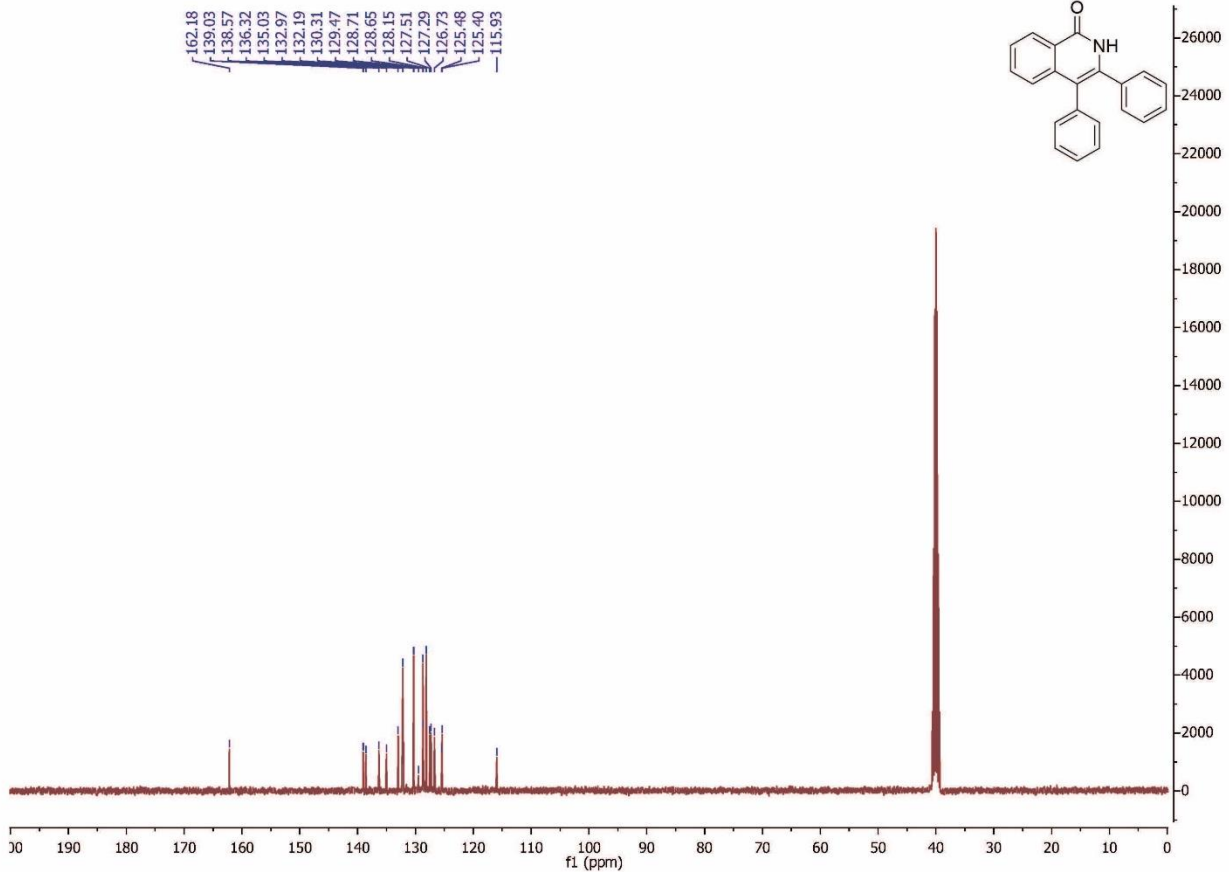
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **1e** in CDCl_3  ^1H NMR (400 MHz) spectrum of **1f** in CDCl_3 

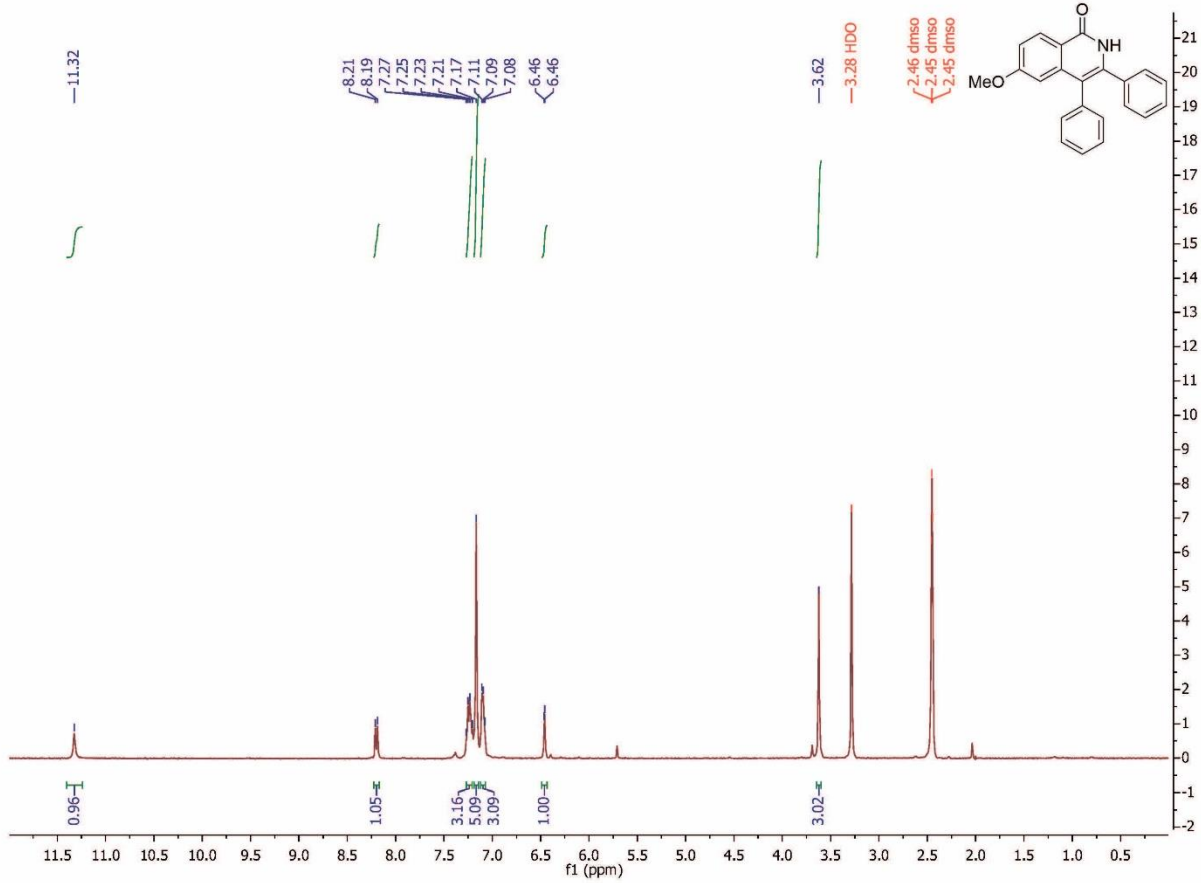
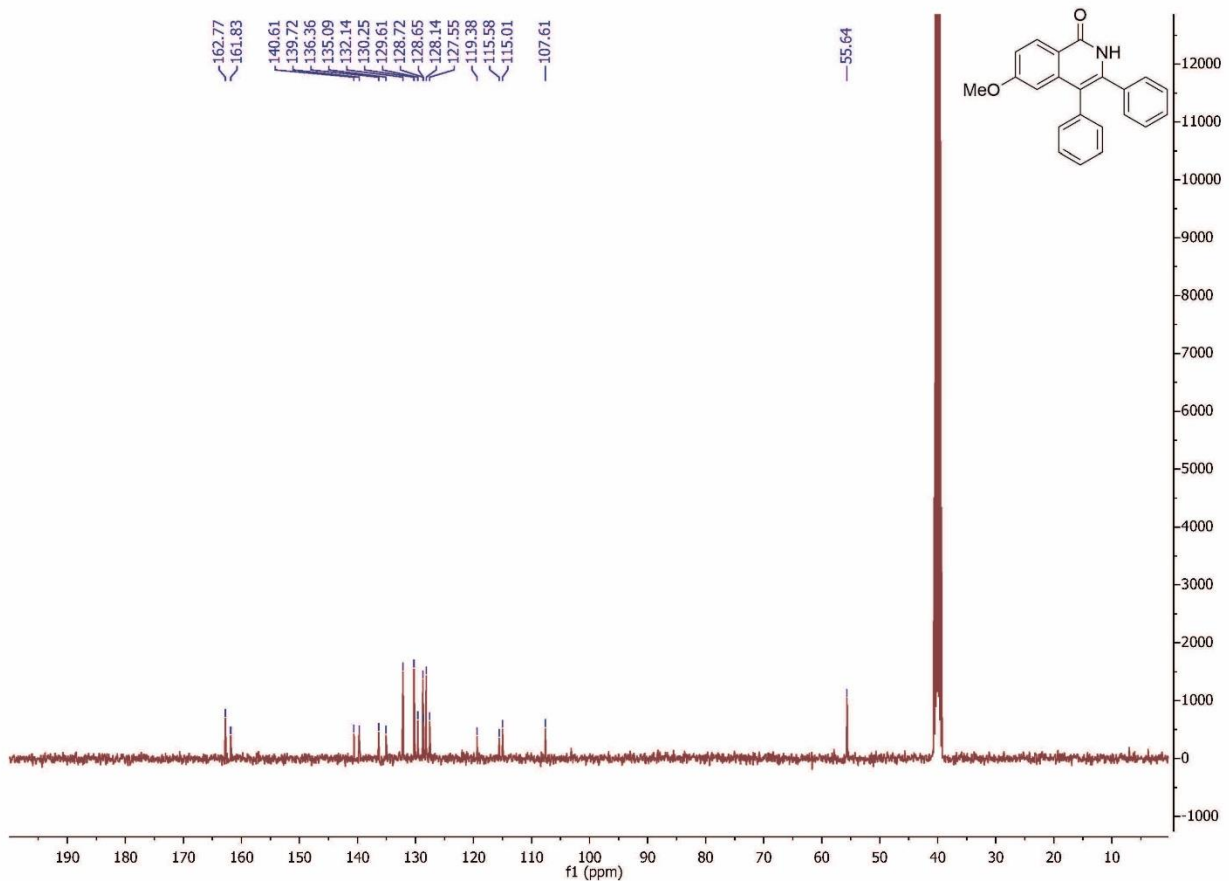
^1H NMR (400 MHz) spectrum of **1g** in CDCl_3  ^1H NMR (400 MHz) spectrum of **1h** in CDCl_3 

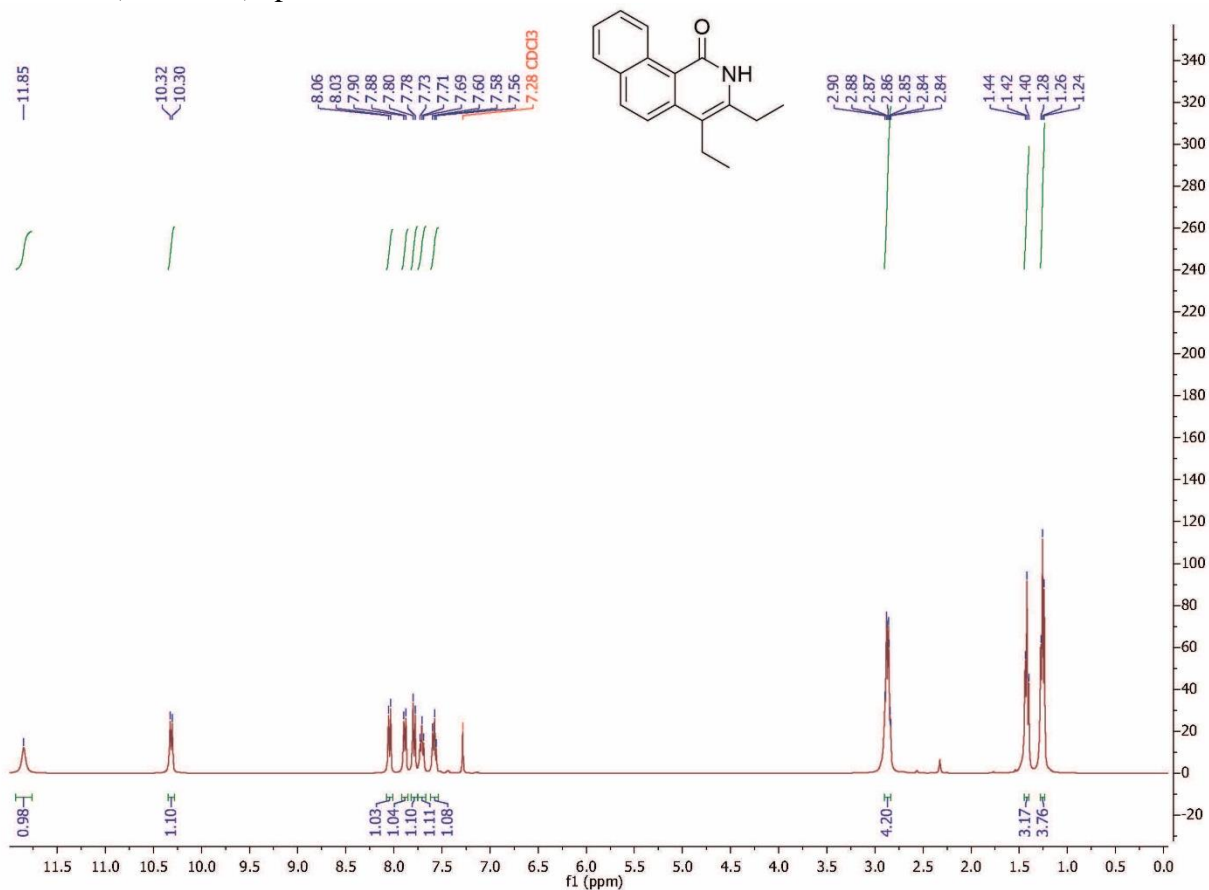
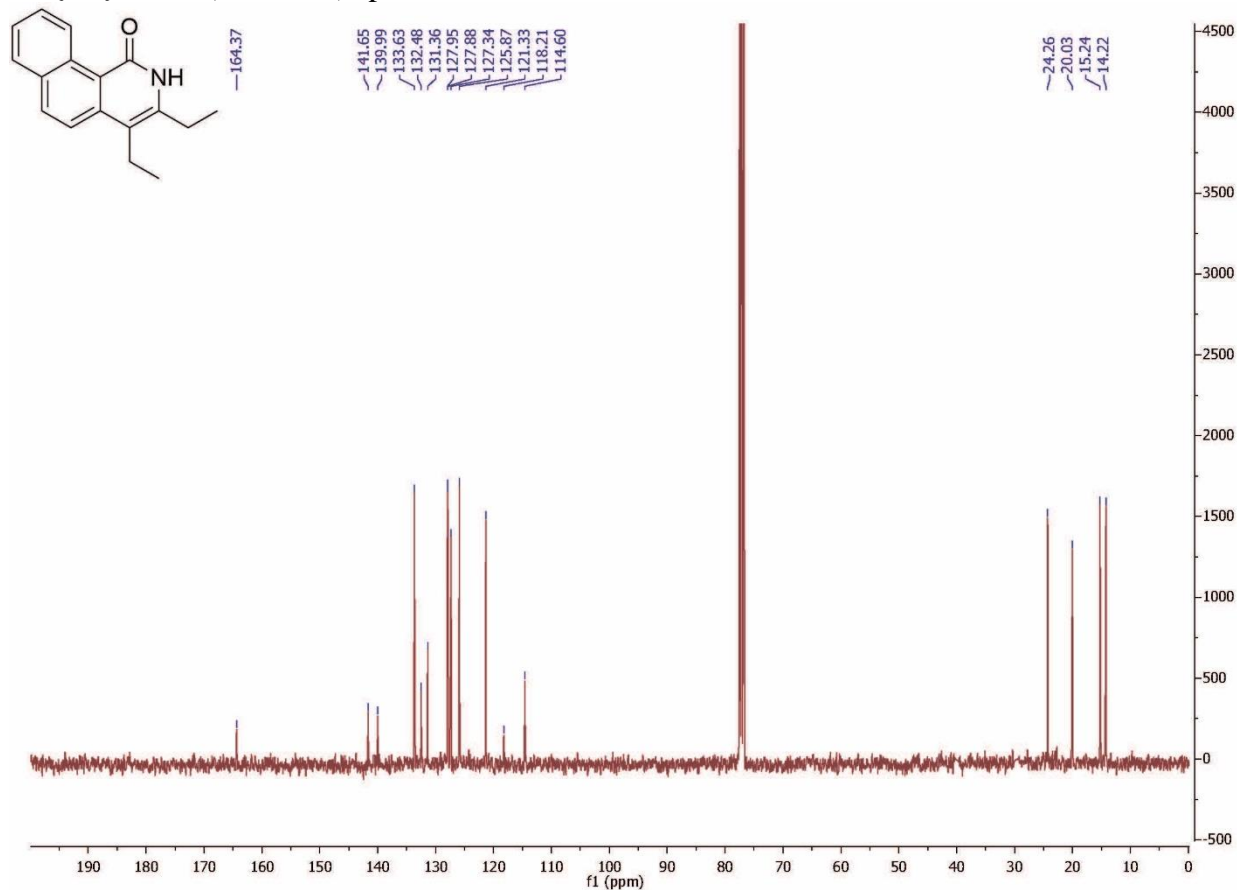
^1H NMR (400 MHz) spectrum of **2a** in CDCl_3



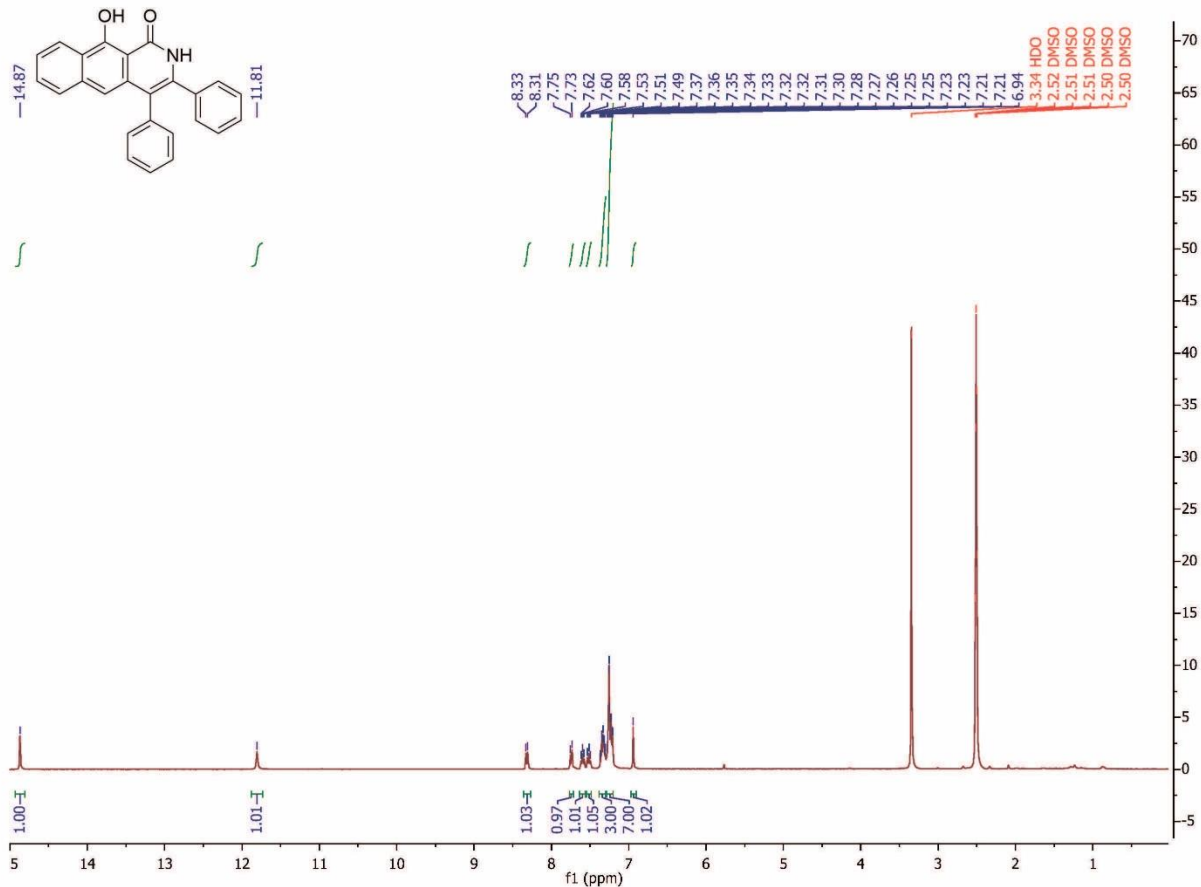
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2a** in $\text{dms}\text{-}d_6$



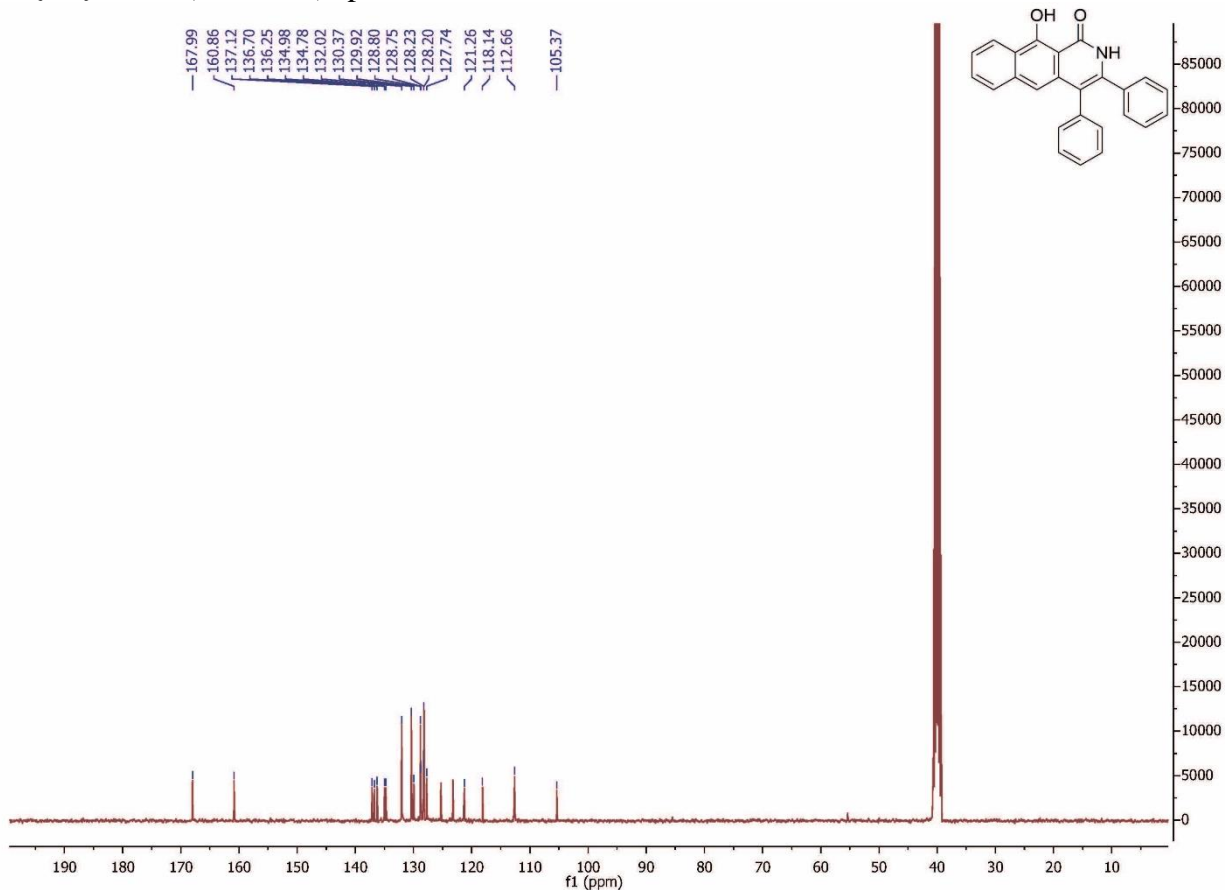
^1H NMR (400 MHz) spectrum of **2b** in $\text{dms}\text{-d}_6$  $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2b** in $\text{dms}\text{-d}_6$ 

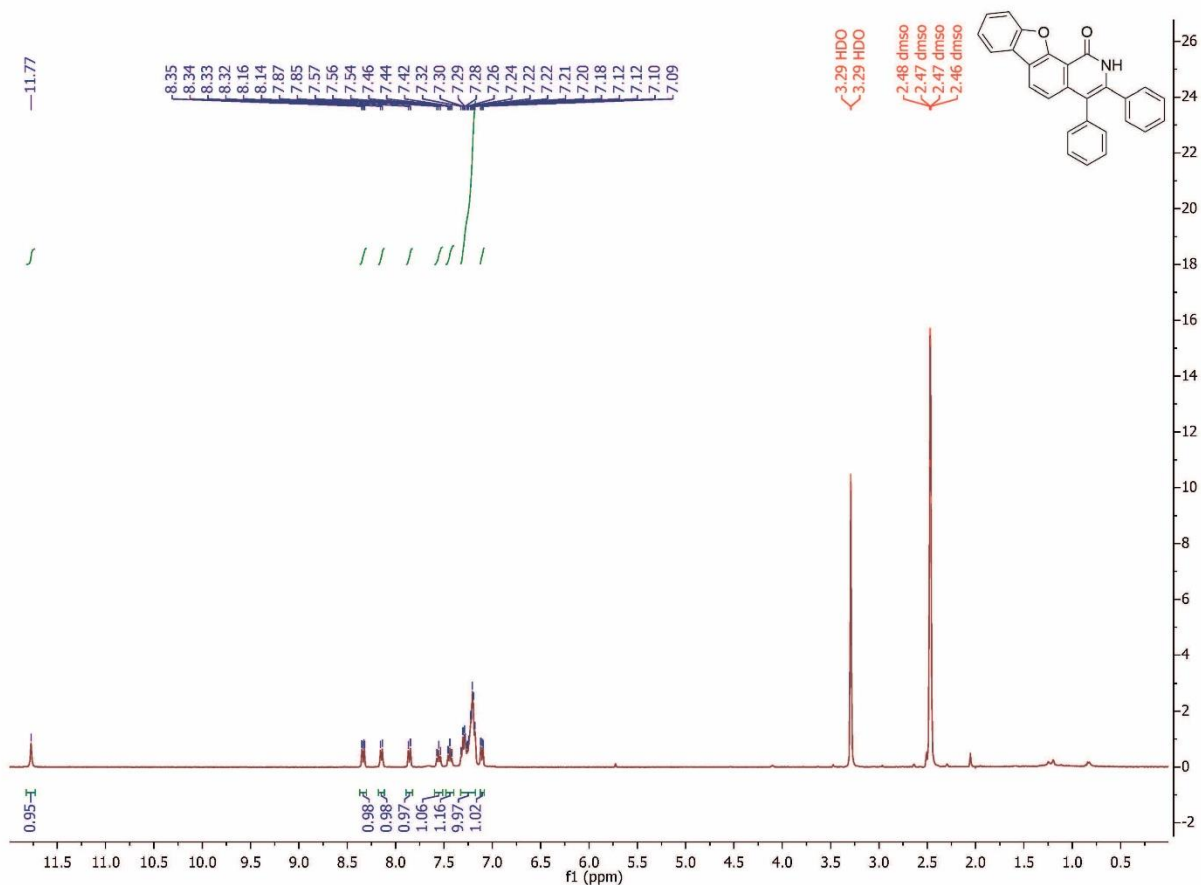
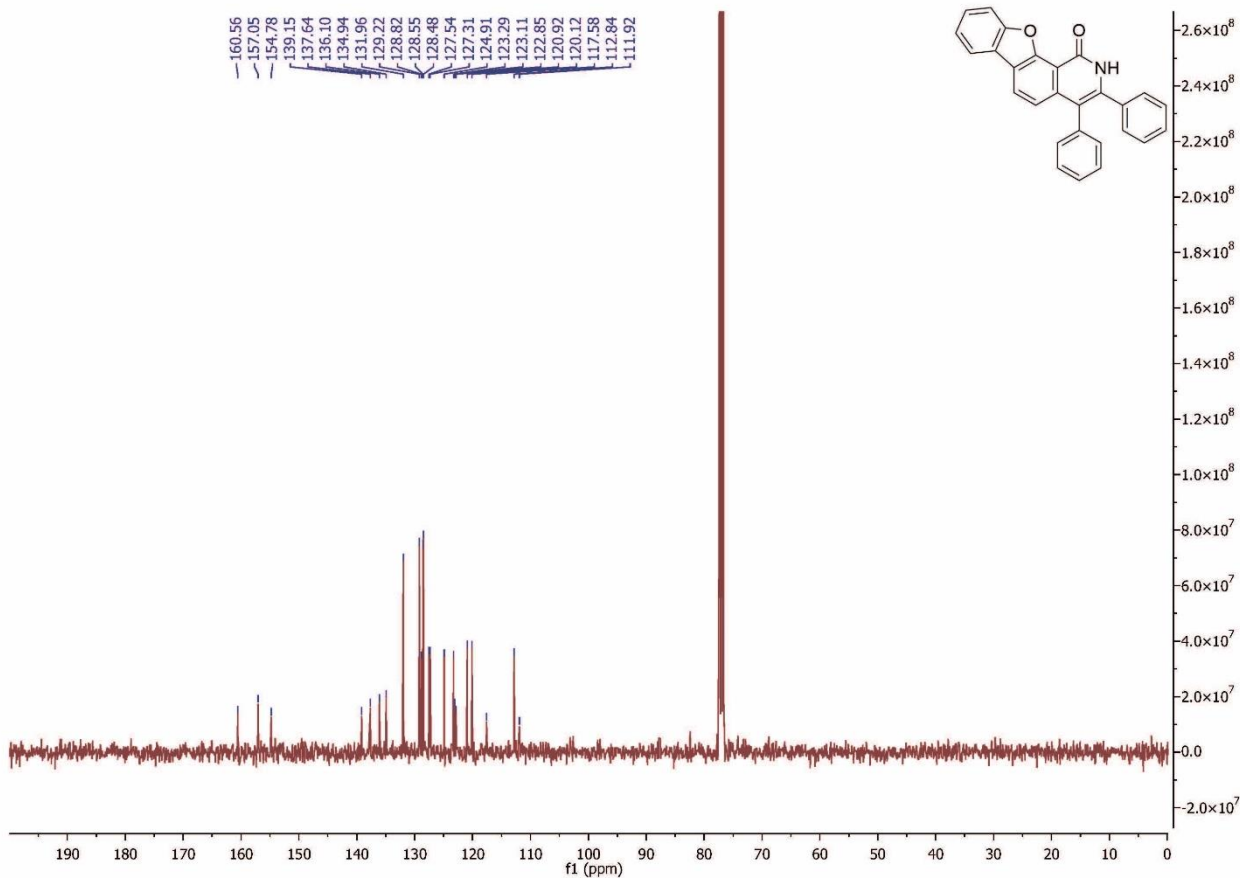
^1H NMR (400 MHz) spectrum of **2c** in CDCl_3  $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2c** in CDCl_3 

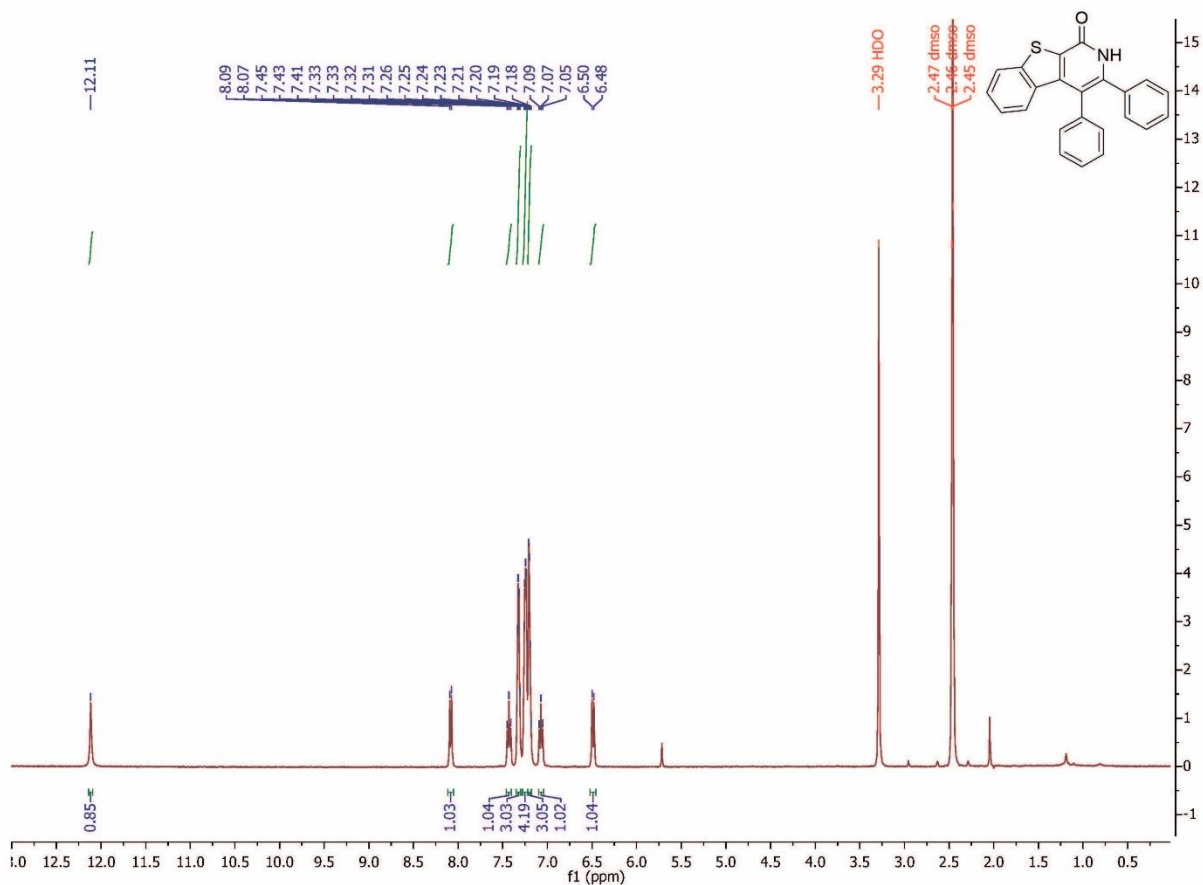
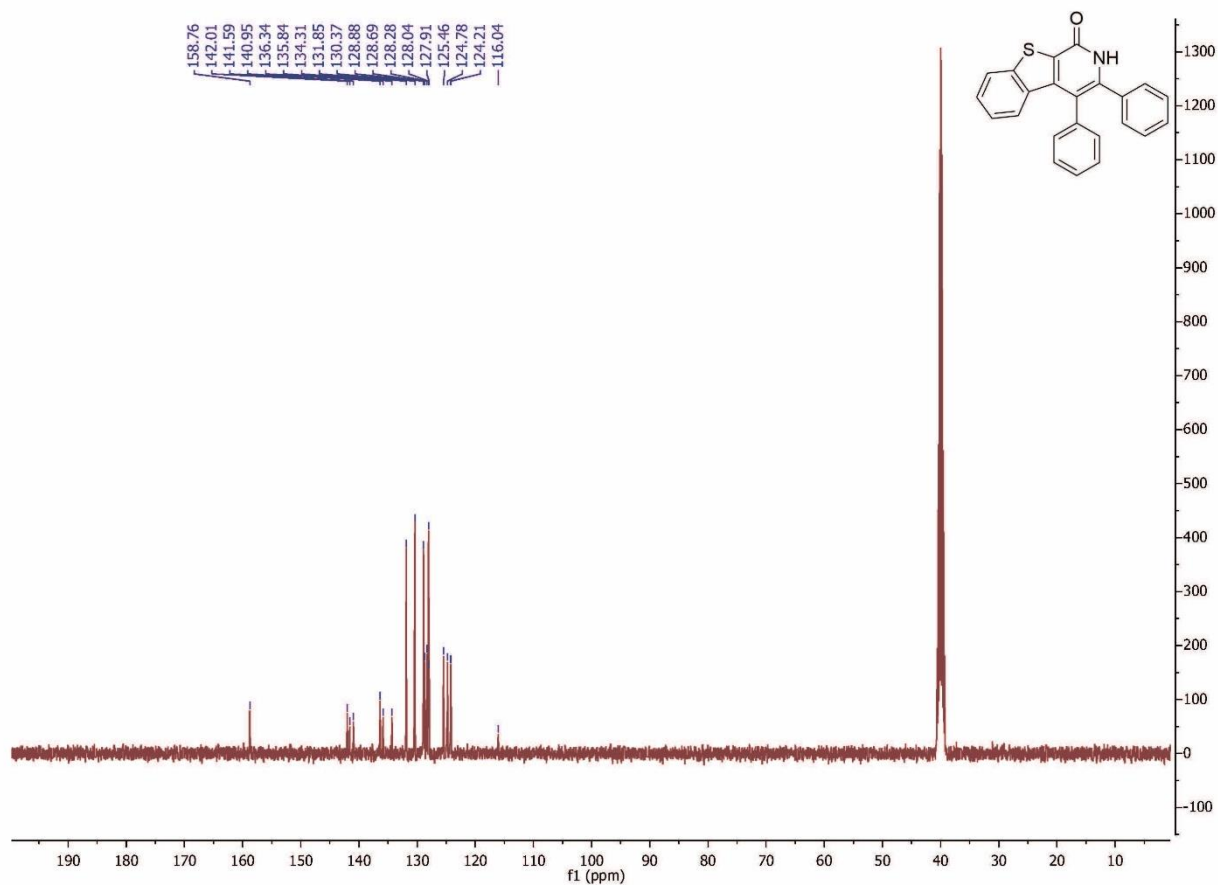
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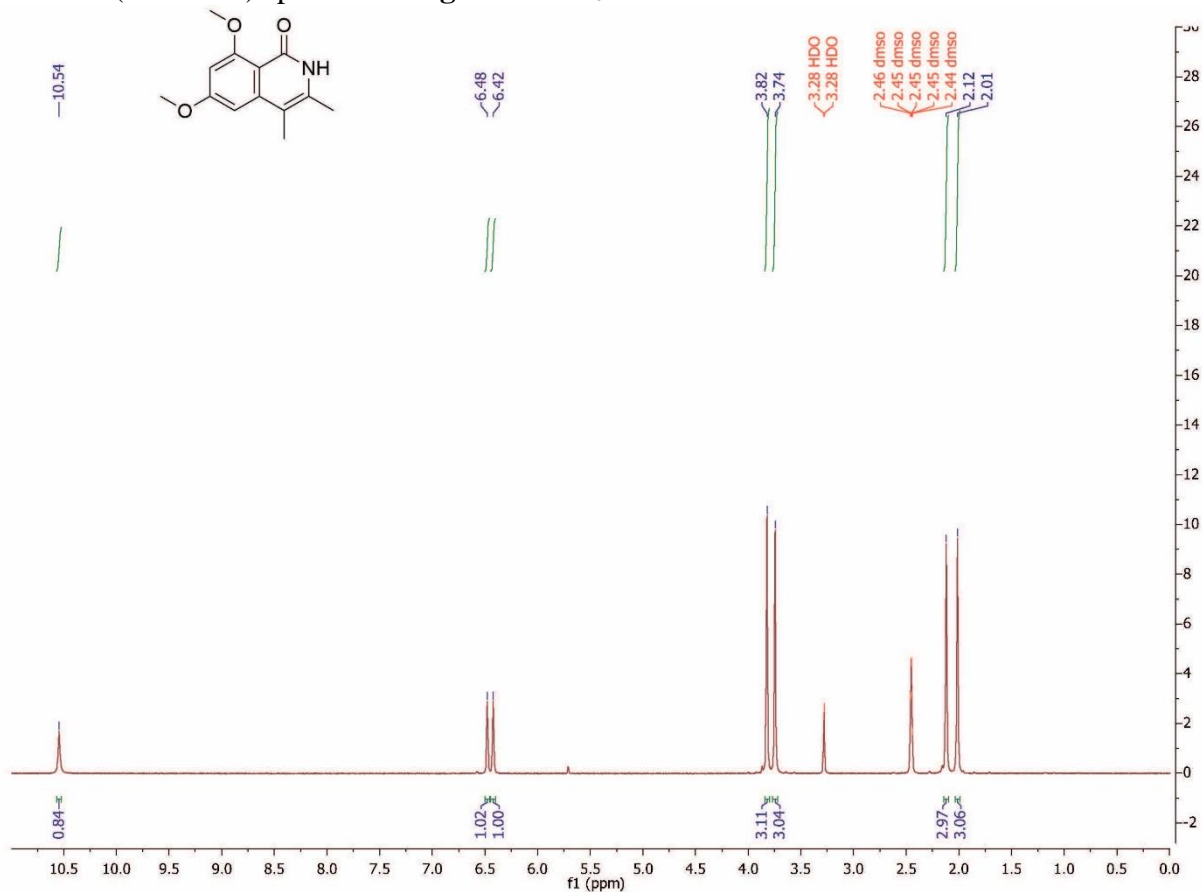
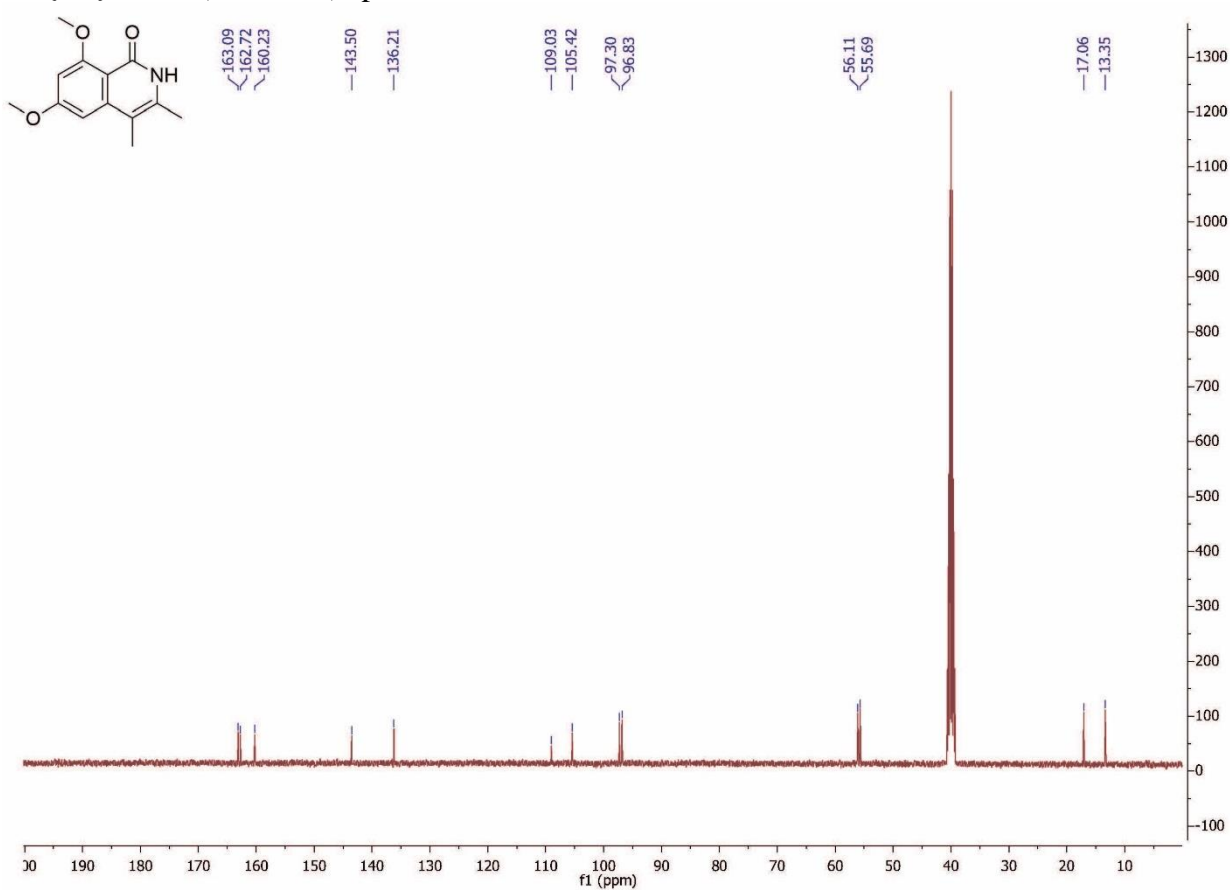


$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2d** in $\text{dms}\text{-d}_6$

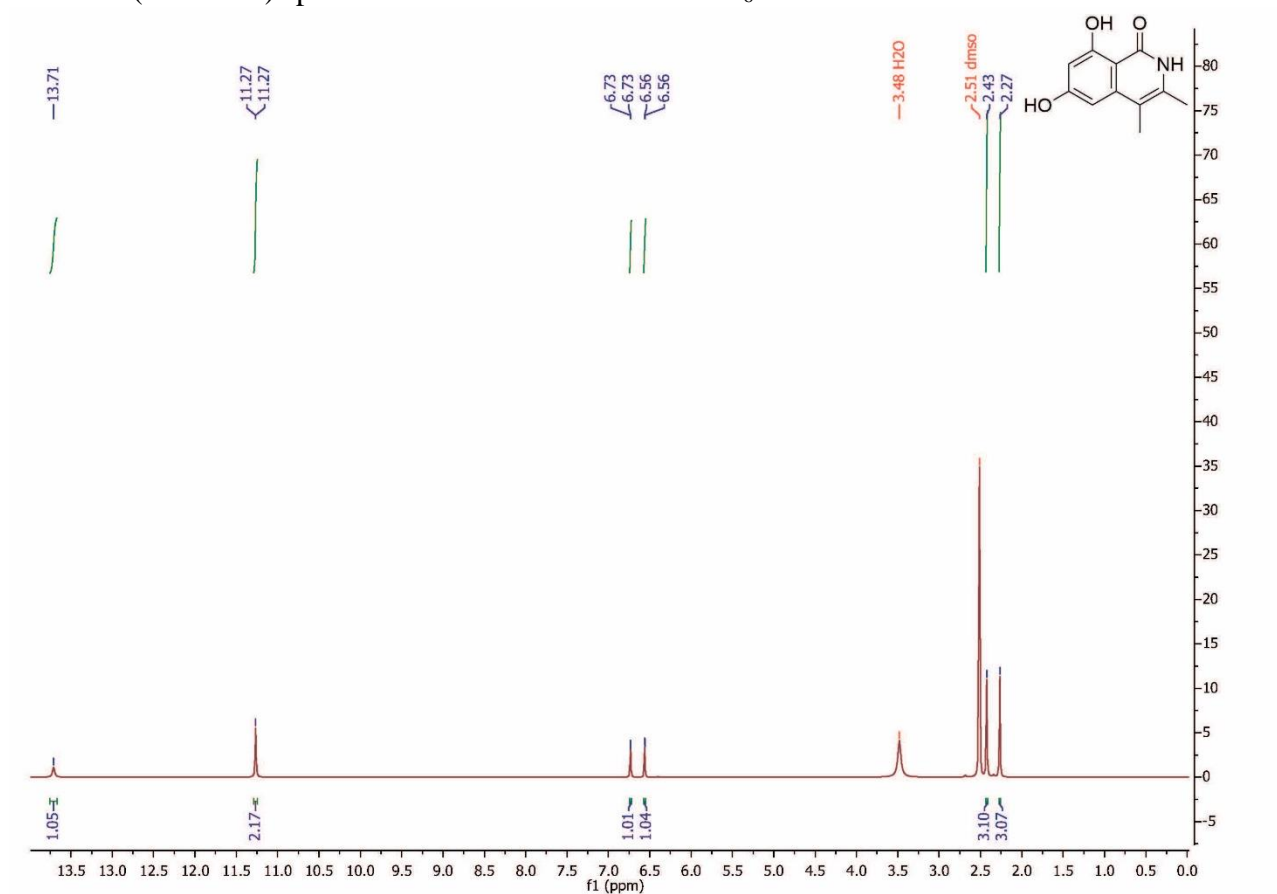


^1H NMR (400 MHz) spectrum of **2e** in $\text{dms}\text{-d}_6$  $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2e** in CDCl_3 

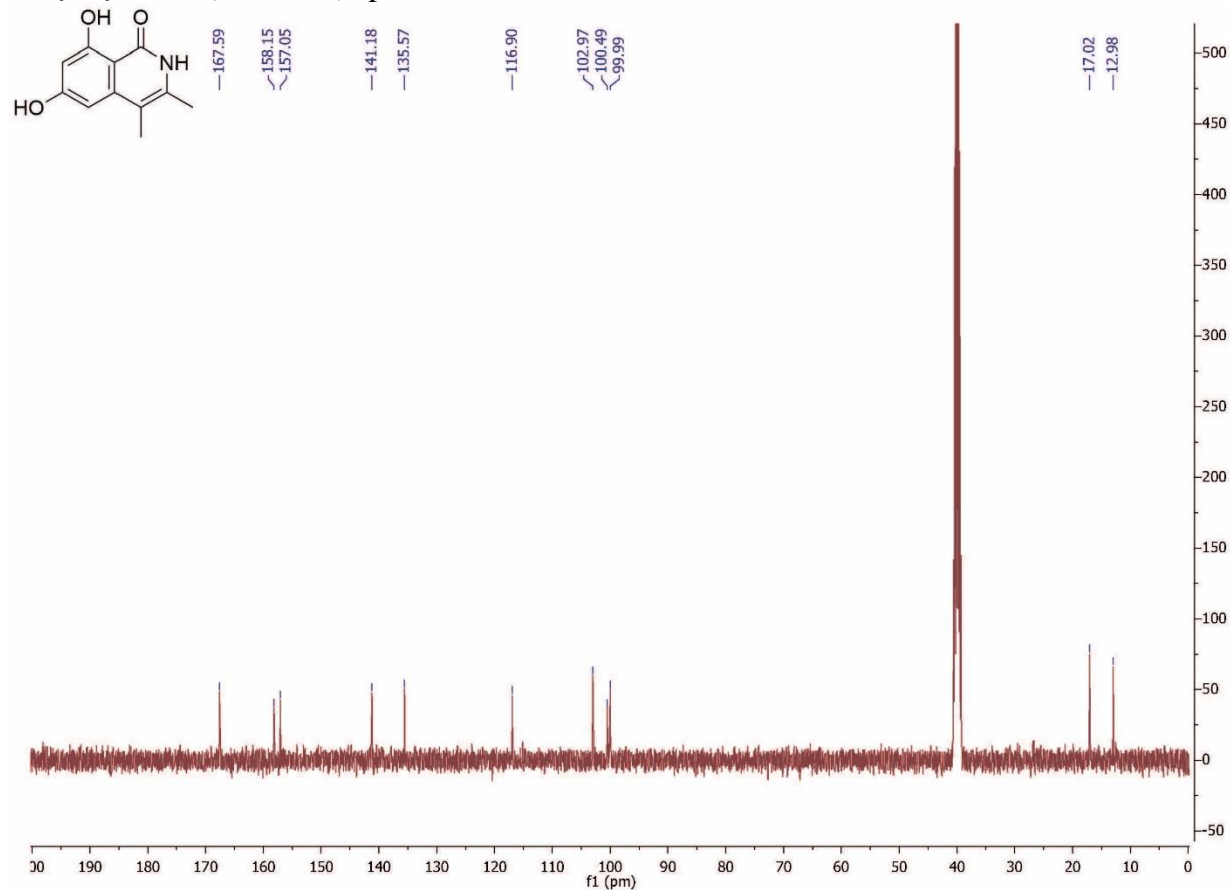
^1H NMR (400 MHz) spectrum of **2f** in $\text{dms}\text{-d}_6$  $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2f** in $\text{dms}\text{-d}_6$ 

^1H NMR (400 MHz) spectrum of **2g** in $\text{dms}\text{-d}_6$  $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2f** in $\text{dms}\text{-d}_6$ 

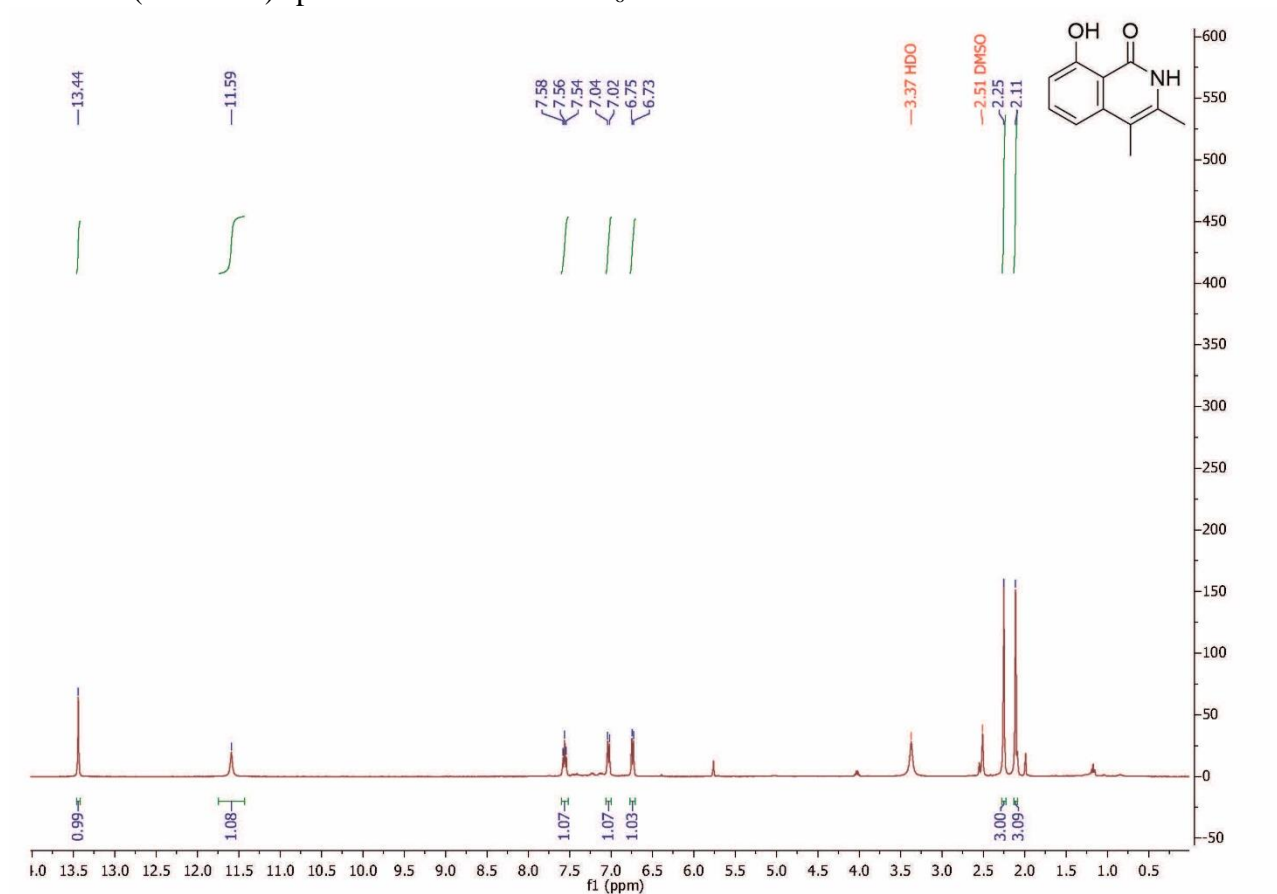
^1H NMR (400 MHz) spectrum of **siaminine A** in $\text{dms}\text{-d}_6$



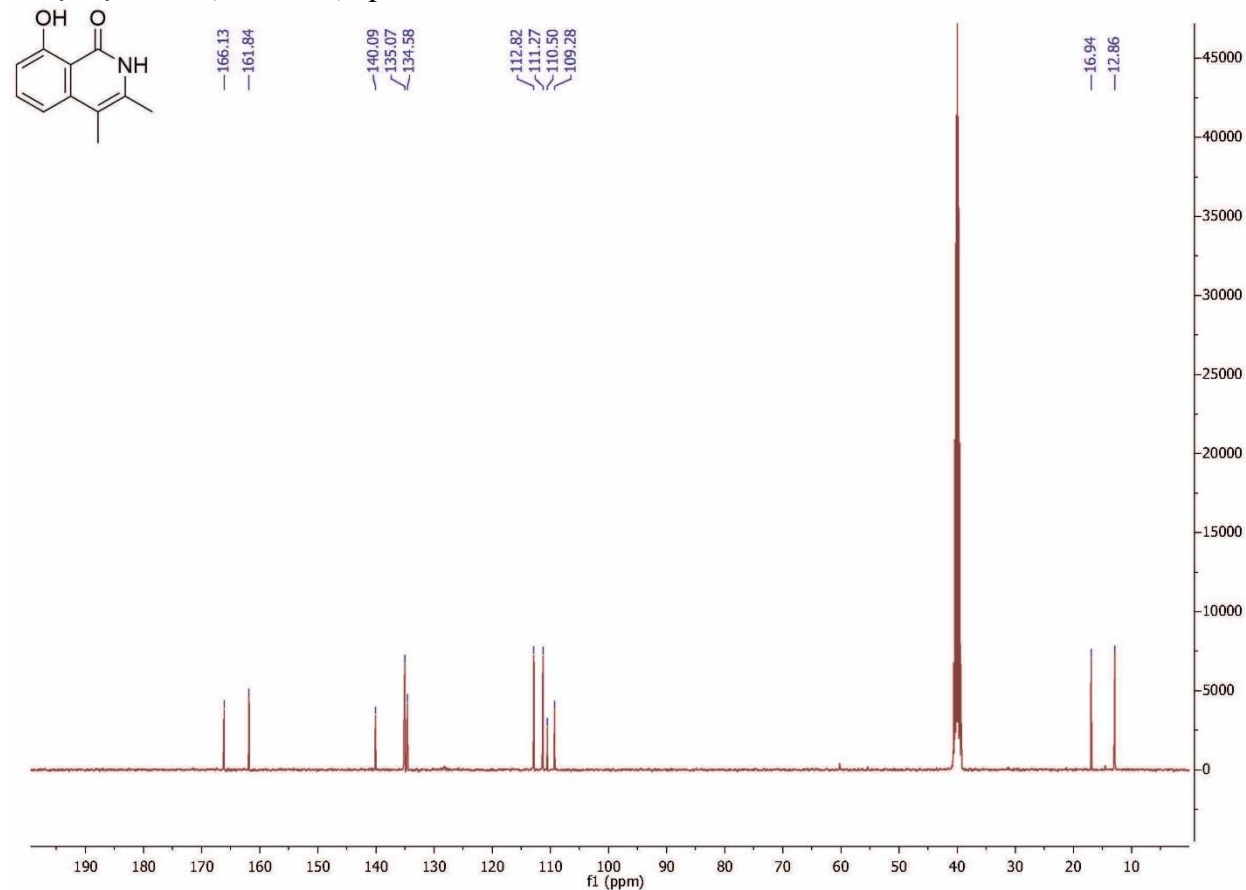
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **siaminine A** in $\text{dms}\text{-d}_6$



^1H NMR (400 MHz) spectrum of **2h** in $\text{dms}\text{-d}_6$



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz) spectrum of **2h** in $\text{dms}\text{-d}_6$



2. Absorption and fluorescence spectra

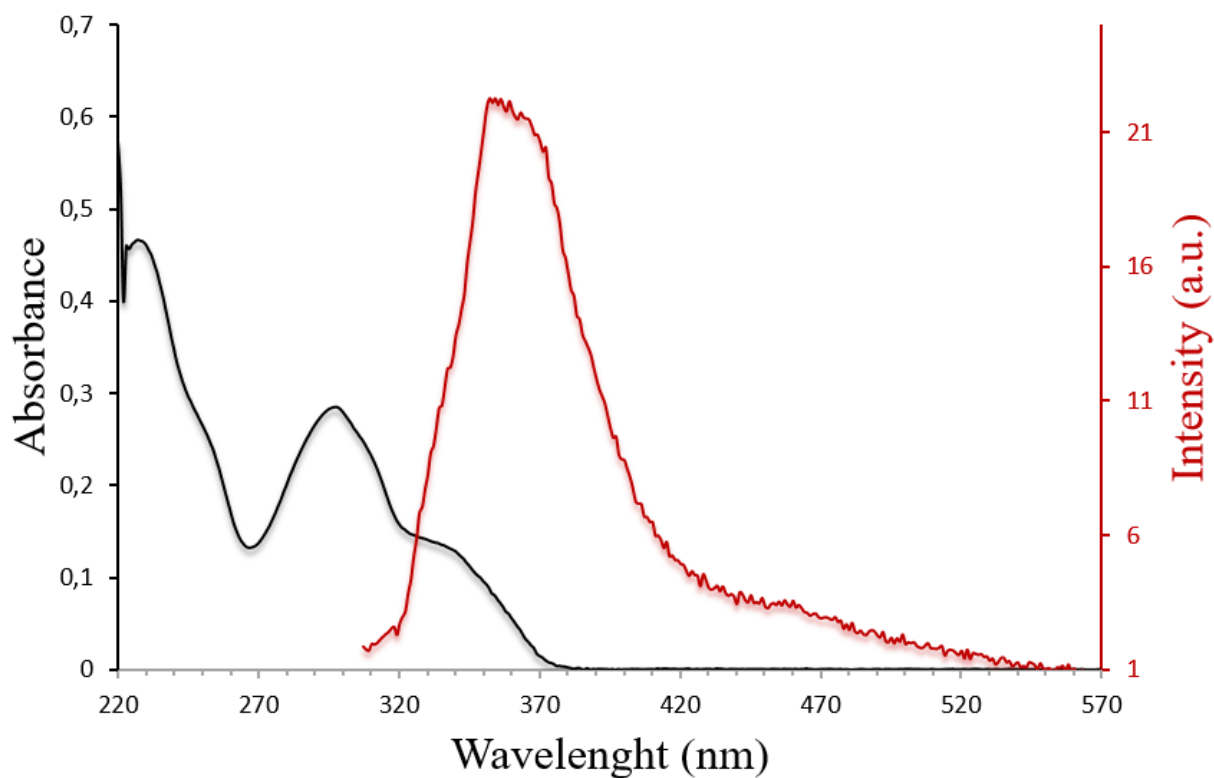


Figure S1. Absorption ($C = 3.1 \cdot 10^{-5}$ M) and fluorescence ($C = 3.1 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 297$ nm) spectra of 3,4-diphenyl-1*H*-isochromen-1-one (**1a**) in CH_2Cl_2 .

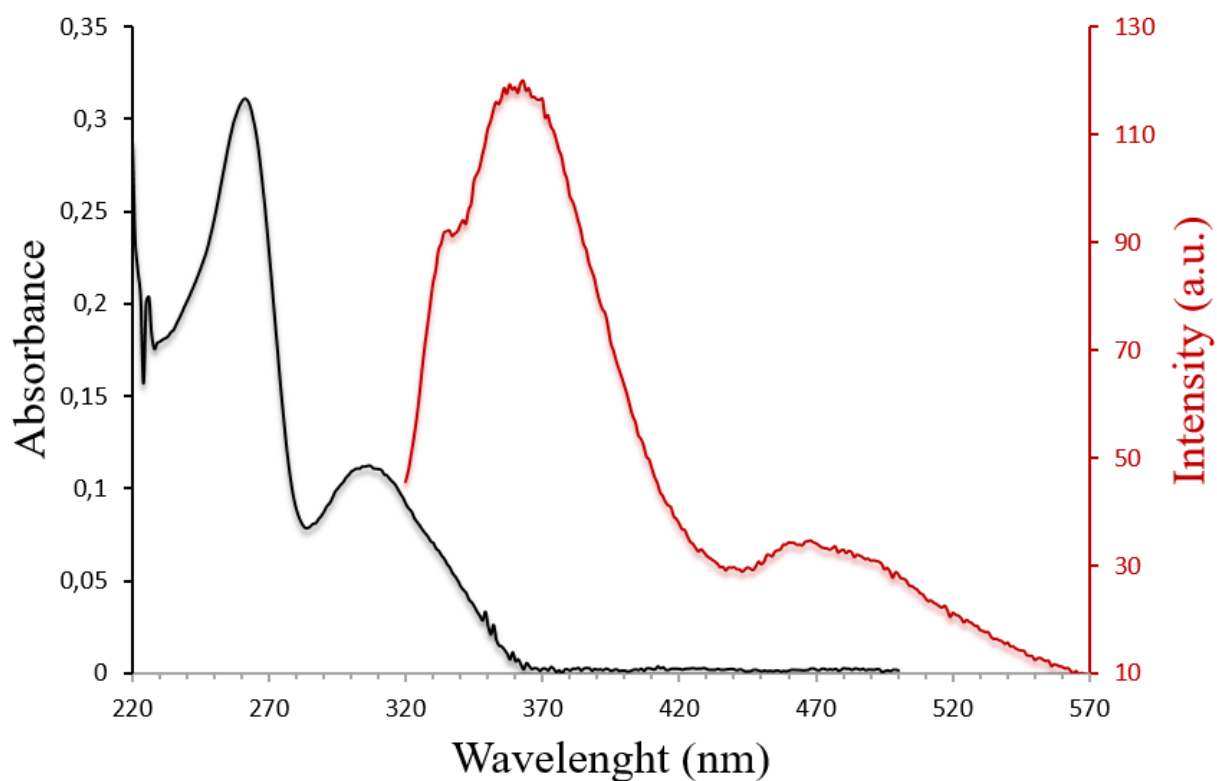


Figure S2. Absorption ($C = 1.1 \cdot 10^{-5}$ M) and fluorescence ($C = 1.1 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 300$ nm) spectra of 6-methoxy-3,4-diphenyl-1*H*-isochromen-1-one (**1b**) in CH_2Cl_2 .

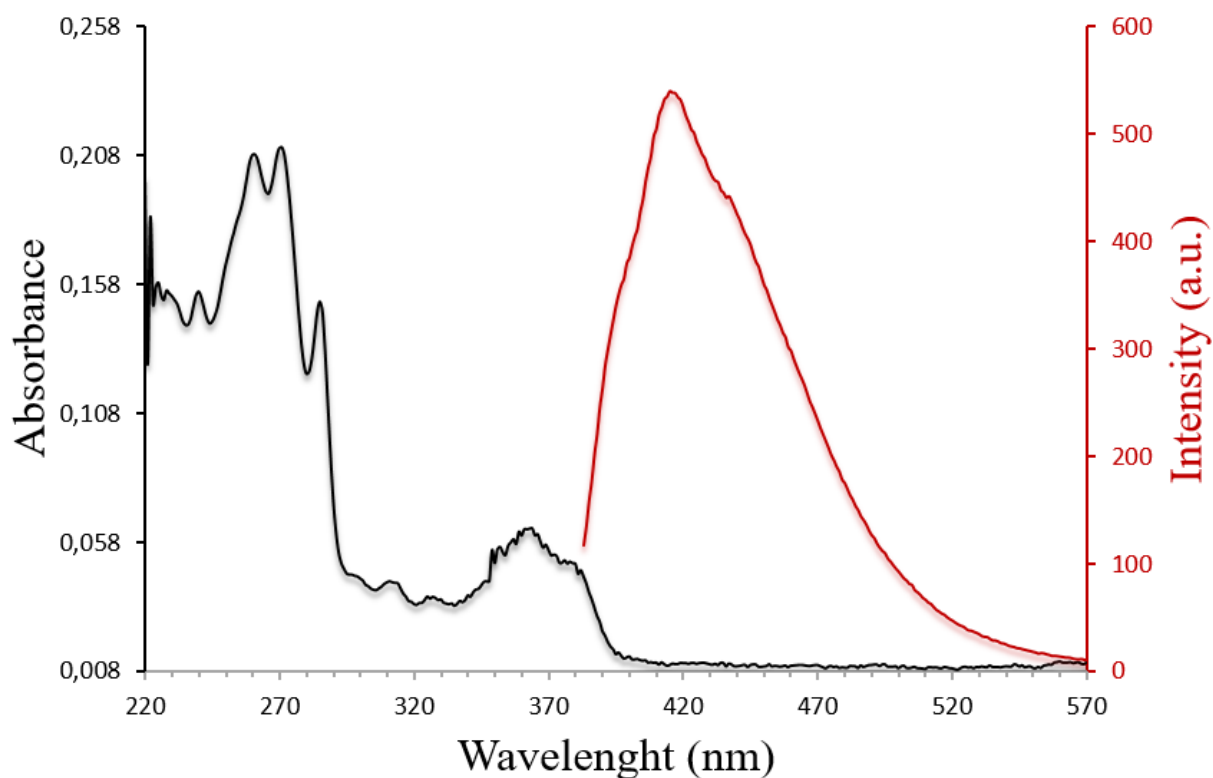


Figure S3. Absorption ($C = 2.6 \cdot 10^{-5}$ M) and fluorescence ($C = 2.6 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 363$ nm) spectra of 3,4-diethyl-1*H*-benzo[*h*]isochromen-1-one (**1c**) in CH_2Cl_2 .

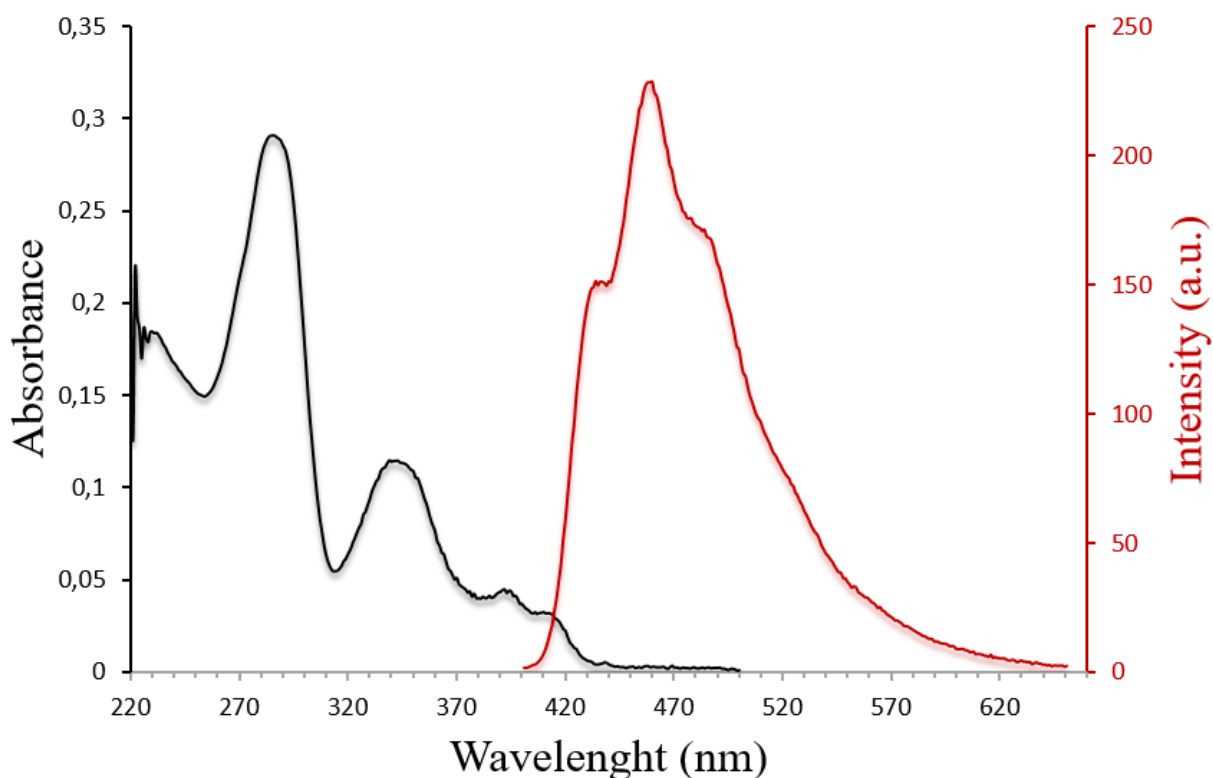


Figure S4. Absorption ($C = 0.7 \cdot 10^{-5}$ M) and fluorescence ($C = 0.7 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 391$ nm) spectra of 10-hydroxy-3,4-diphenyl-1*H*-benzo[*g*]isochromen-1-one (**1d**) in CH_2Cl_2 .

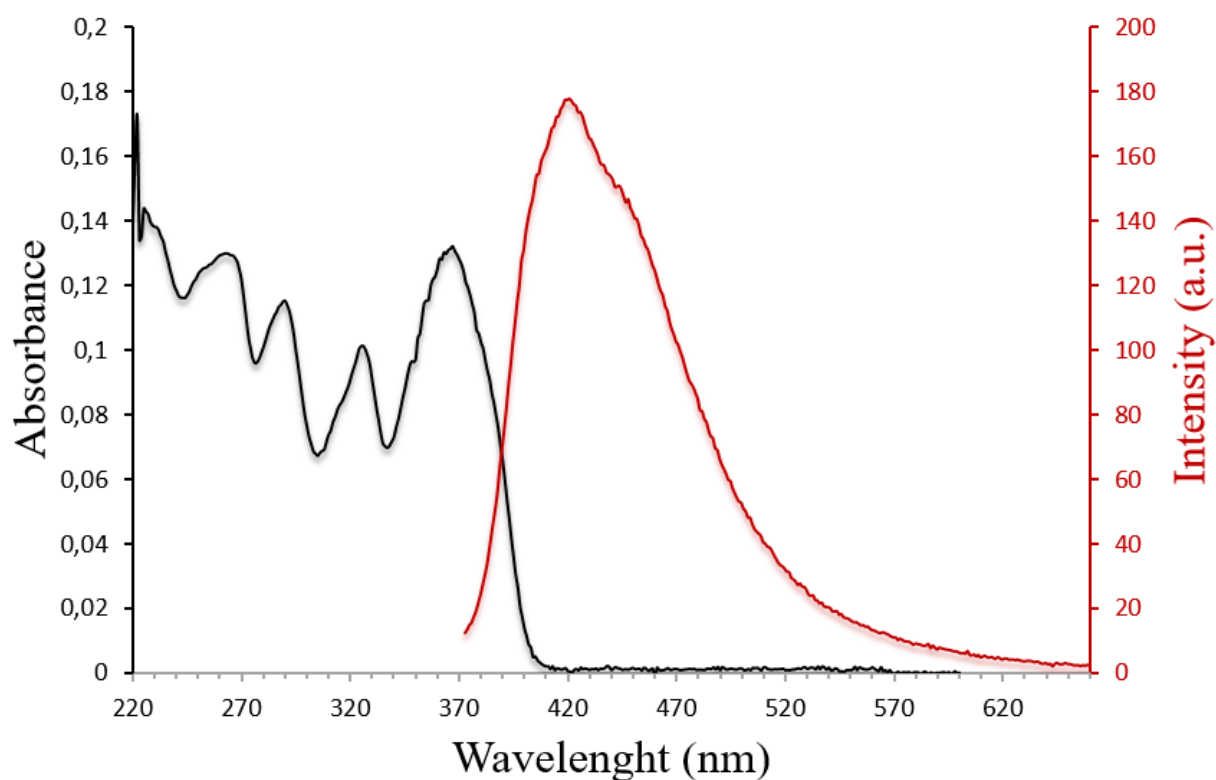


Figure S5. Absorption ($C = 1.2 \cdot 10^{-5}$ M) and fluorescence ($C = 1.2 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 355$ nm) spectra of 3,4-diphenyl-1H-benzofuro[3,2-*h*]isochromen-1-one (**1e**) in CH_2Cl_2 .

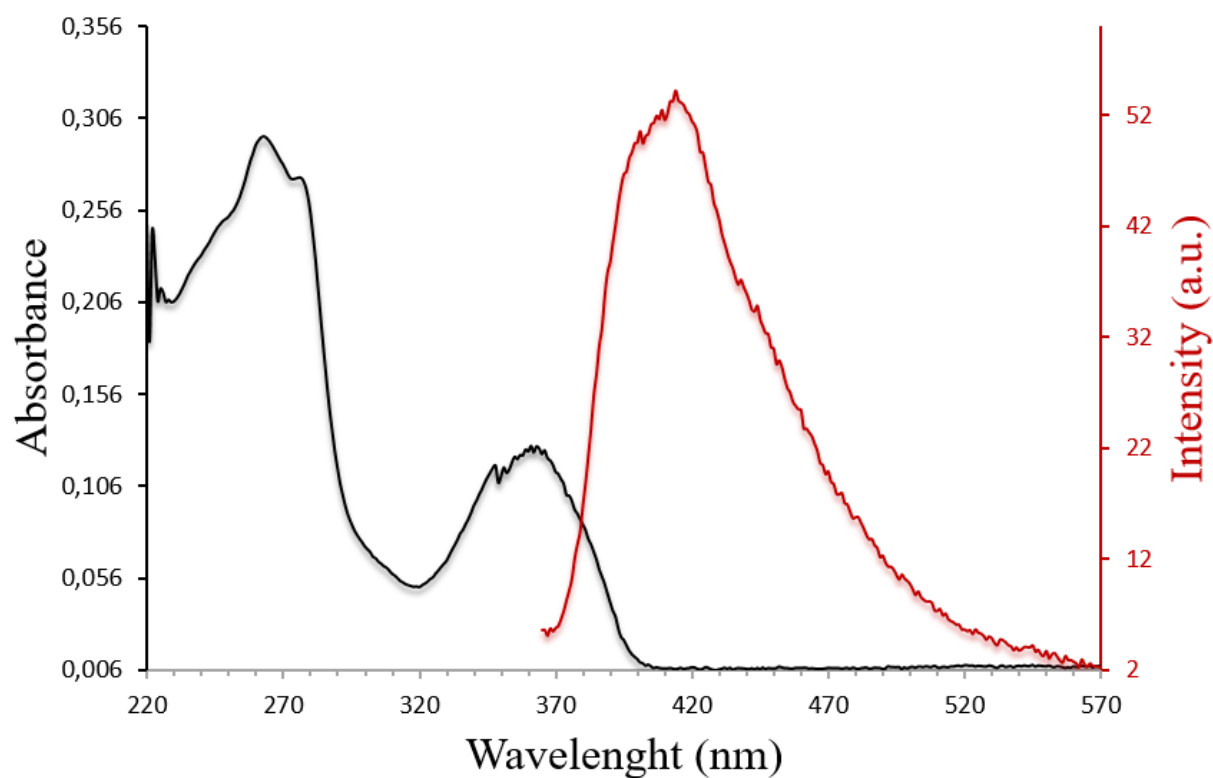


Figure S6. Absorption ($C = 1.2 \cdot 10^{-5}$ M) and fluorescence ($C = 1.2 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 345$ nm) spectra of 3,4-diphenyl-1H-benzo[4,5]thieno[2,3-*c*]pyran-1-one (**1f**) in CH_2Cl_2 .

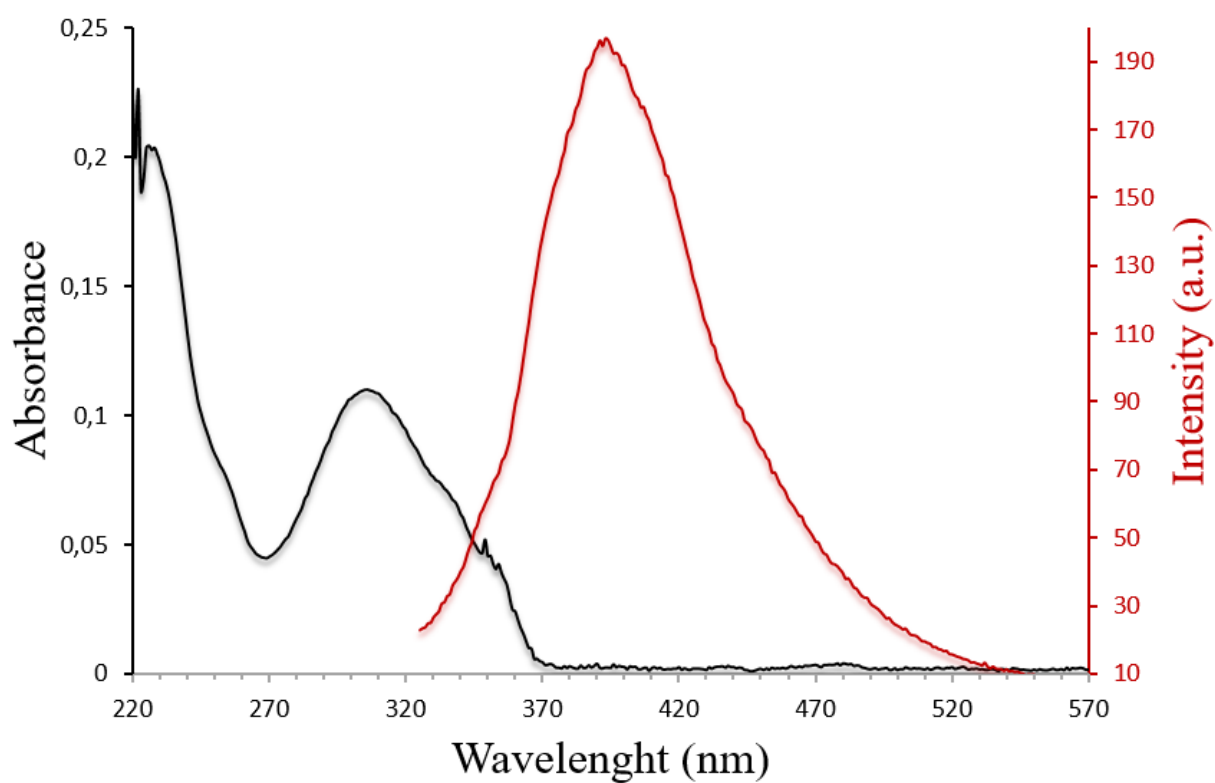


Figure S7. Absorption ($C = 1.2 \cdot 10^{-5}$ M) and fluorescence ($C = 1.2 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 305$ nm) spectra of 3,4-diphenylisoquinolin-1(2H)-one (**2a**) in CH_2Cl_2 .

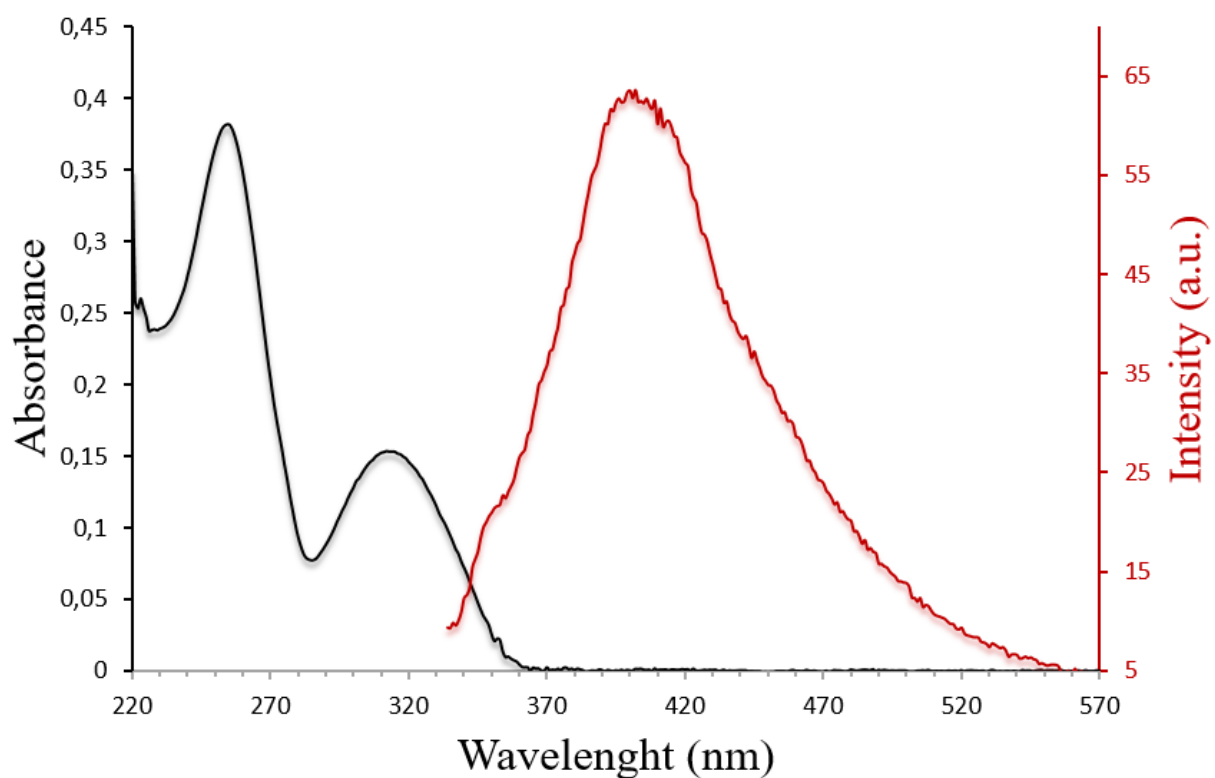


Figure S8. Absorption ($C = 1.0 \cdot 10^{-5}$ M) and fluorescence ($C = 1.0 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 314$ nm) spectra of 6-methoxy-3,4-diphenylisoquinolin-1(2H)-one (**2b**) in CH_2Cl_2 .

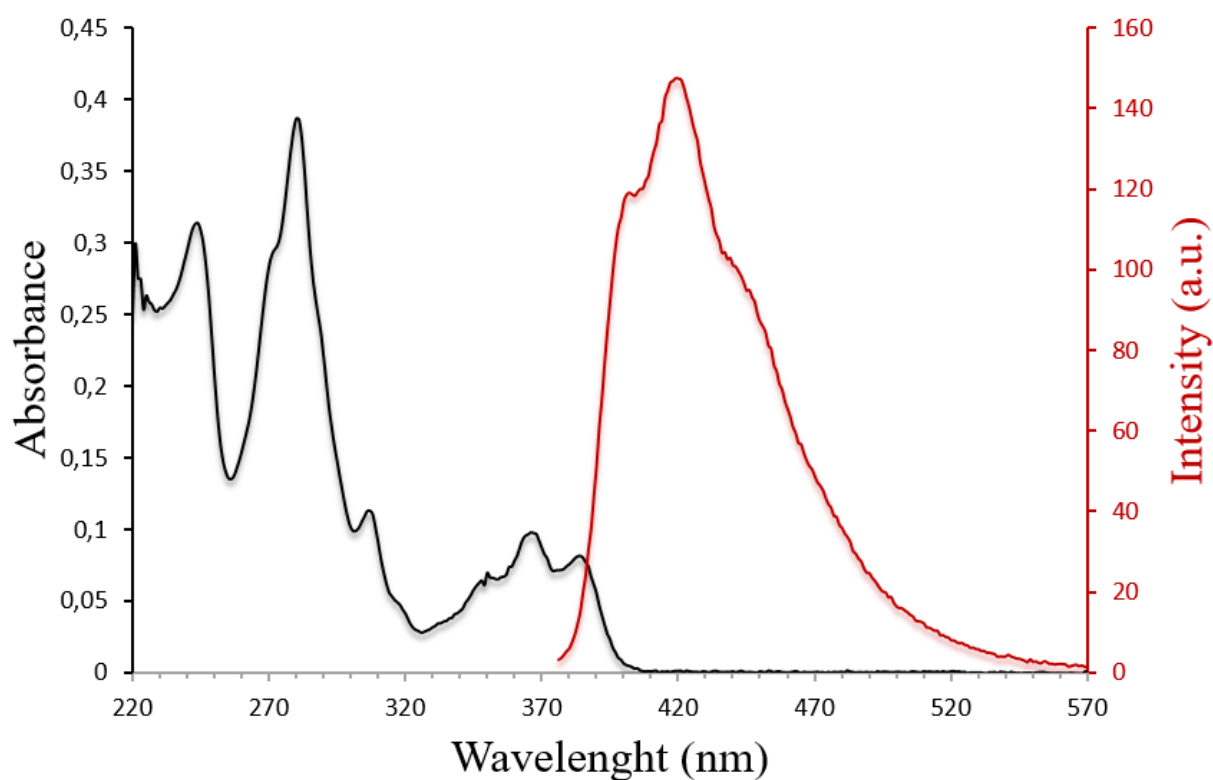


Figure S9. Absorption ($C = 1.2 \cdot 10^{-5}$ M) and fluorescence ($C = 1.2 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 366$ nm) spectra of 3,4-diethylbenzo[*h*]isoquinolin-1(2*H*)-one (**2c**) in CH_2Cl_2 .

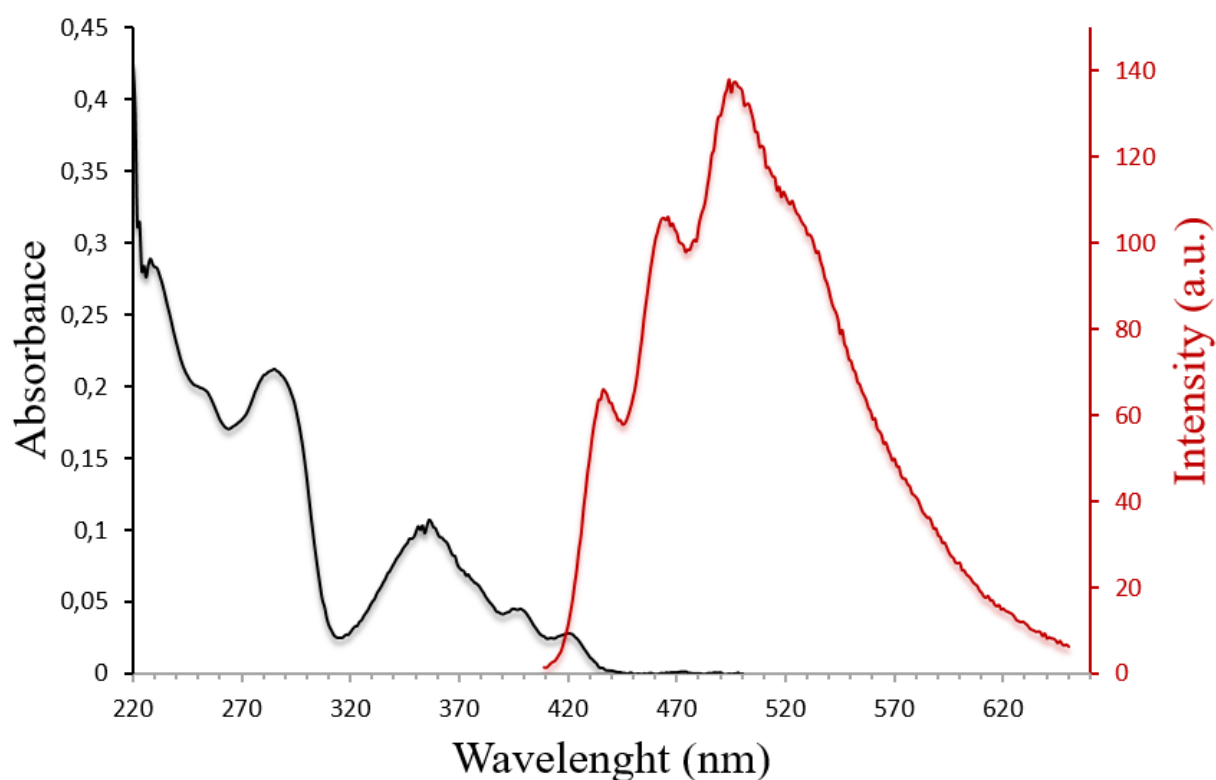


Figure S10. Absorption ($C = 0.7 \cdot 10^{-5}$ M) and fluorescence ($C = 0.7 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 399$ nm) spectra of 10-hydroxy-3,4-diphenylbenzo[*g*]isoquinolin-1(2*H*)-one (**2d**) in CH_2Cl_2 .

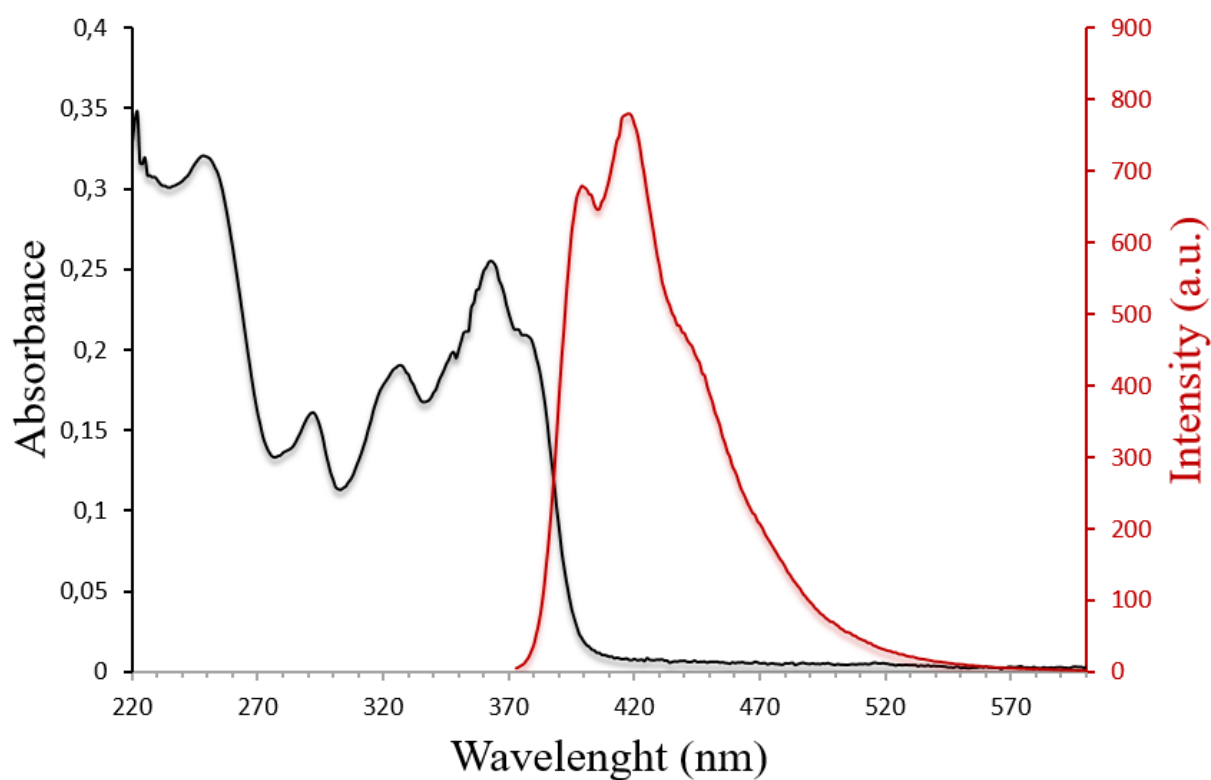


Figure S11. Absorption ($C = 1.2 \cdot 10^{-5}$ M) and fluorescence ($C = 1.2 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 363$ nm) spectra of 3,4-Diphenylbenzofuro[3,2-*h*]isoquinolin-1(2*H*)-one (**2e**) in CH_2Cl_2 .

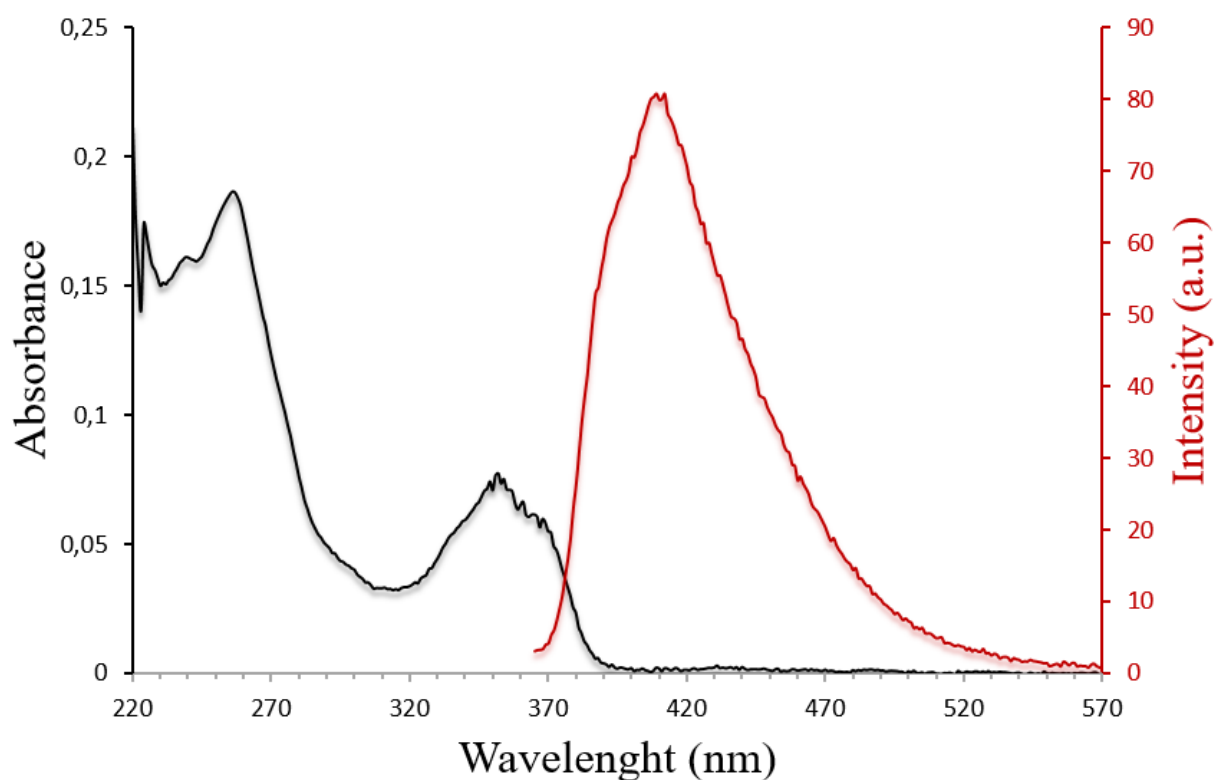
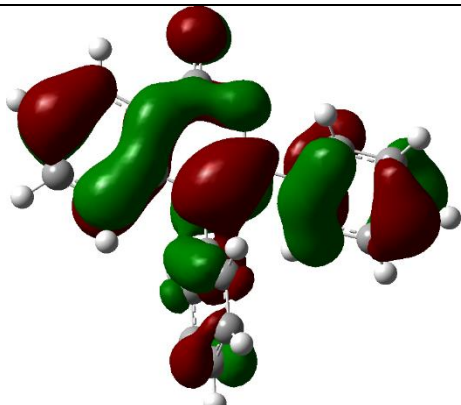
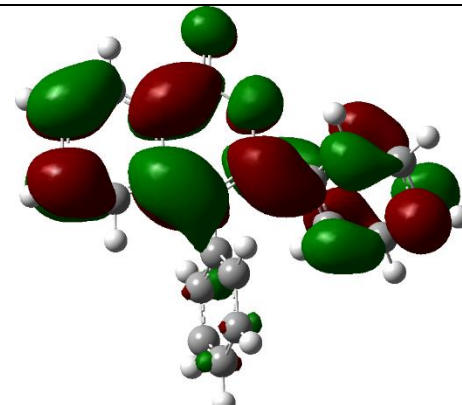
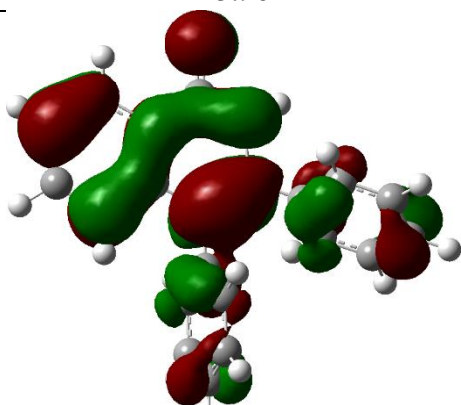
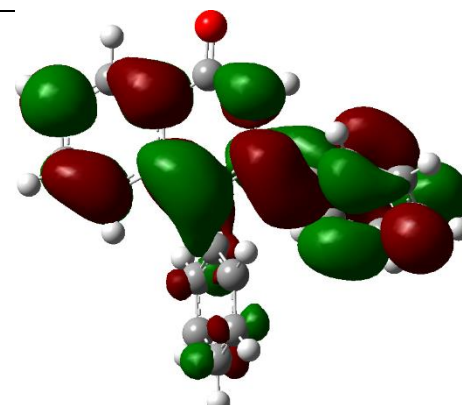
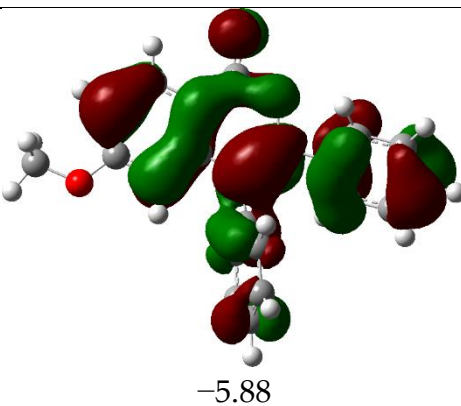
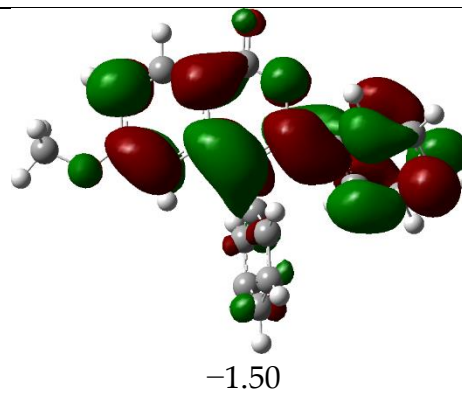
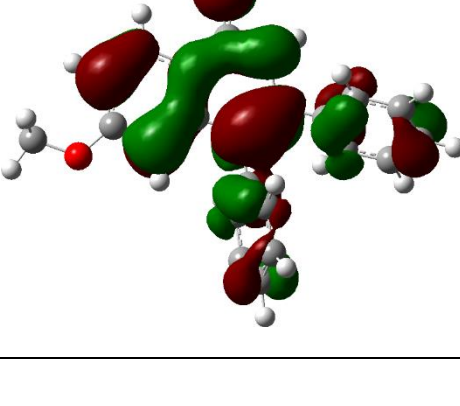
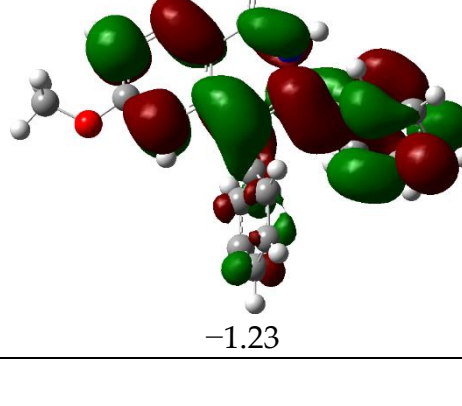
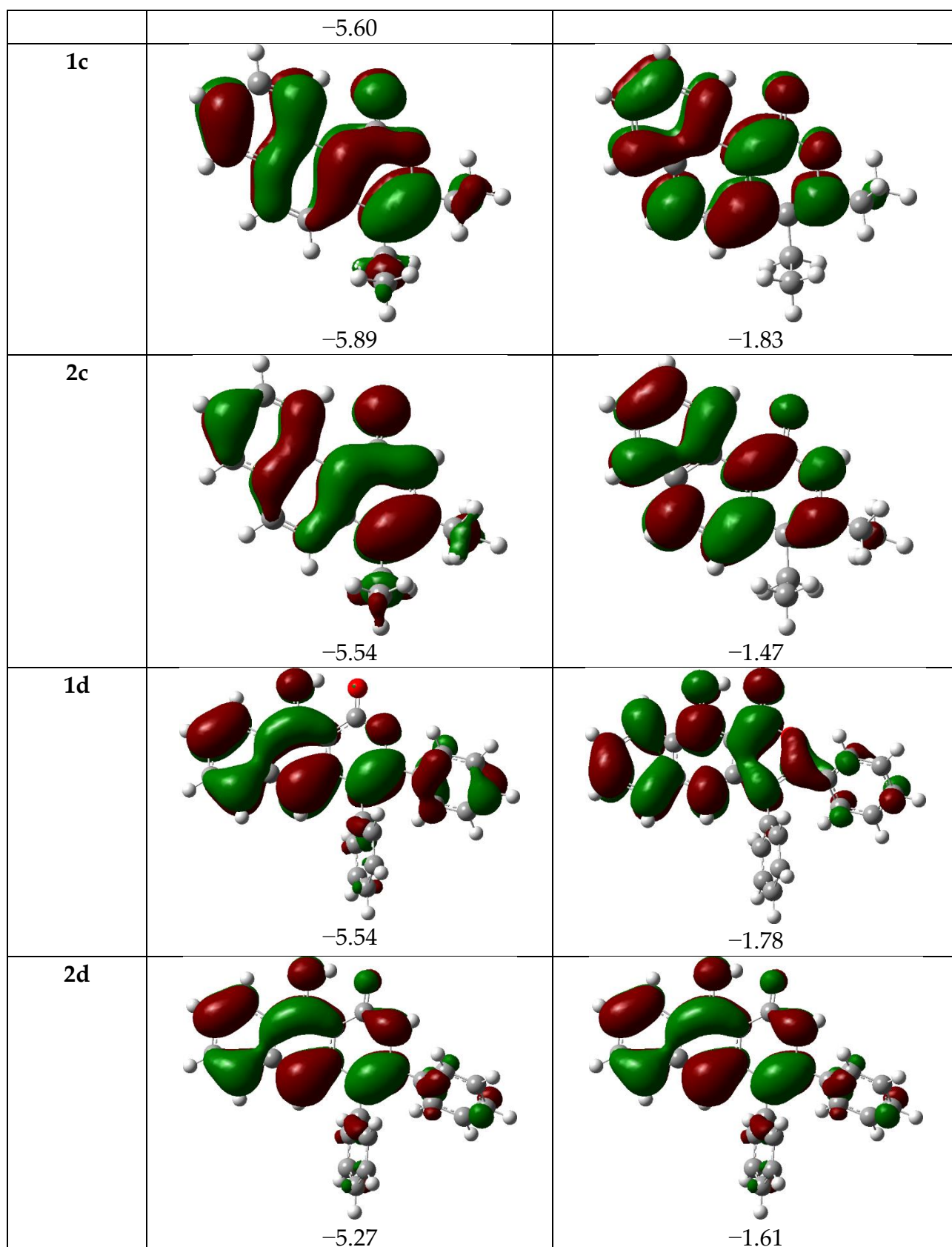


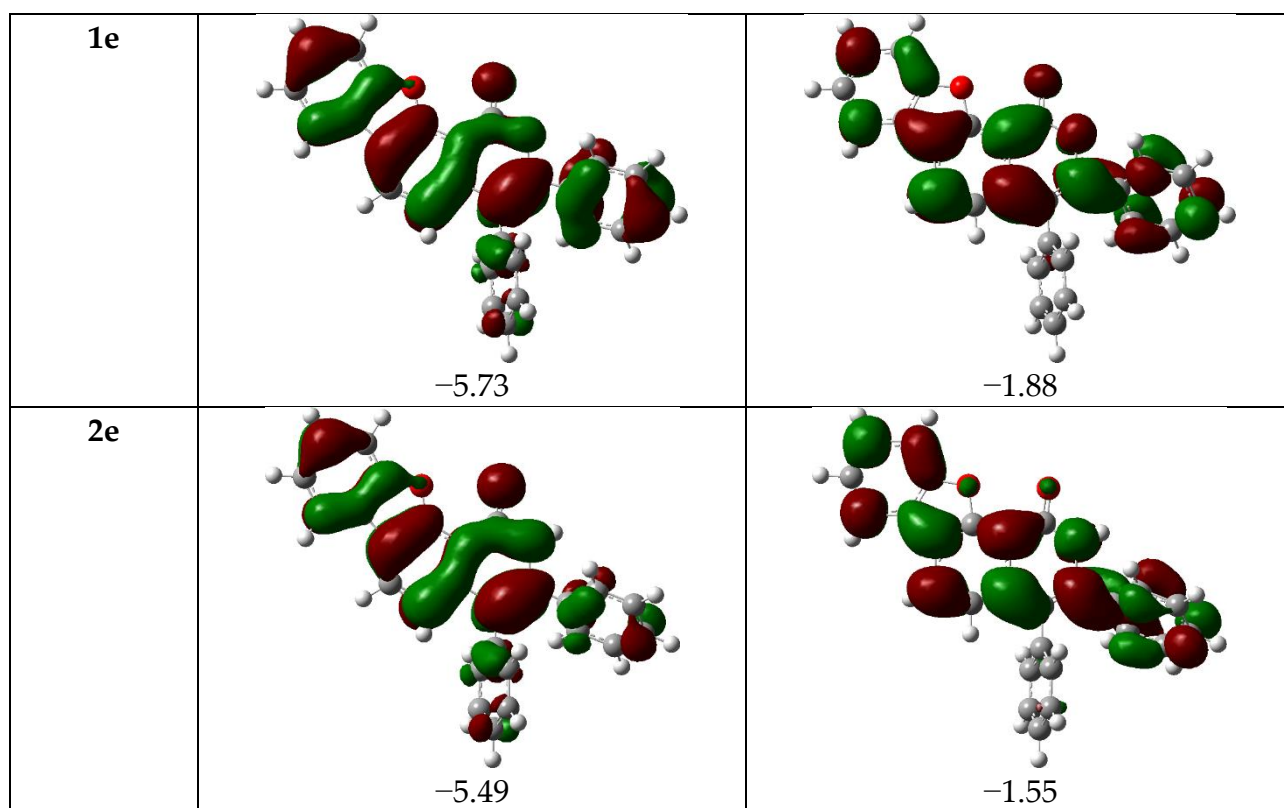
Figure S12. Absorption ($C = 1.1 \cdot 10^{-5}$ M) and fluorescence ($C = 1.1 \cdot 10^{-5}$ M, $\lambda_{\text{ex}} = 355$ nm) spectra of 3,4-Diphenyl-4b,8a-dihydrobenzo[4,5]thieno[2,3-*c*]pyridin-1(2*H*)-one (**2f**) in CH_2Cl_2 .

3. Frontier molecular orbitals

Table S1. Frontier molecular orbitals at the B3LYP/6-31G(d) level (isovalue = 0.02 a.u.). Energies of the orbitals are given in parentheses in eV

Compound	HOMO	LUMO
1a	 -5.90	 -1.63
2a	 -5.62	 -1.25
1b	 -5.88	 -1.50
2b	 -5.88	 -1.23





4. Optimized geometries

1a

$S_0 E = -959.1416373$ Hartree

6	4.710043000	0.121931000	0.011287000
6	3.974489000	-1.052624000	-0.024844000
6	4.037774000	1.354019000	0.044311000
6	2.650495000	1.410763000	0.032260000
6	1.879752000	0.229788000	-0.019478000
6	2.571005000	-1.005800000	-0.037145000
6	0.419561000	0.235217000	-0.029886000
6	-0.235352000	-0.959598000	-0.067107000
8	0.454393000	-2.153923000	-0.065074000
6	1.828333000	-2.263177000	-0.046018000
6	-0.313219000	1.534729000	0.066834000
6	-1.692211000	-1.218848000	-0.101073000
6	-0.995769000	1.878374000	1.243304000
6	-1.667840000	3.097439000	1.345768000
6	-1.662184000	3.994303000	0.275298000
6	-0.978058000	3.666806000	-0.897878000
6	-0.306118000	2.447541000	-1.000524000
6	-2.209998000	-2.322058000	0.602206000
6	-3.574479000	-2.603288000	0.575977000
6	-4.444160000	-1.798842000	-0.164210000
6	-3.937215000	-0.712667000	-0.881283000
6	-2.573913000	-0.423171000	-0.852373000
8	2.298559000	-3.384068000	-0.040014000
1	4.607610000	2.278263000	0.082415000
1	2.152281000	2.372620000	0.062772000
1	-0.999670000	1.183934000	2.078704000
1	-2.193448000	3.346681000	2.263525000
1	-2.185387000	4.943179000	0.354997000
1	-0.968403000	4.358964000	-1.735434000
1	0.220974000	2.195466000	-1.917021000
1	-1.537991000	-2.954902000	1.172020000
1	-3.957813000	-3.453469000	1.133238000
1	-5.507464000	-2.020623000	-0.187471000
1	-4.602976000	-0.091115000	-1.473488000
1	-2.192193000	0.412730000	-1.426620000
1	4.460109000	-2.022558000	-0.039892000
1	5.795155000	0.089746000	0.020399000

$S_1 E = -959.023902472$ Hartree

6	-2.994735000	0.717356000	0.186258000
6	-2.366368000	-0.499129000	-0.019359000
6	-2.235606000	1.910857000	0.125293000
6	-0.869229000	1.872236000	-0.068787000
6	-0.168531000	0.632733000	-0.172211000
6	-0.975877000	-0.566073000	-0.223855000
6	1.246249000	0.503391000	-0.265268000
6	1.755337000	-0.849637000	-0.404080000
8	0.952266000	-1.776267000	-1.035299000
6	-0.411763000	-1.817435000	-0.684681000
6	2.172113000	1.635600000	-0.260573000
6	2.989325000	-1.371069000	0.069871000

6	3.270651000	1.652365000	-1.159037000
6	4.151037000	2.727836000	-1.197253000
6	3.990081000	3.803493000	-0.318449000
6	2.935505000	3.789713000	0.603184000
6	2.037627000	2.728676000	0.631861000
6	3.398342000	-2.692812000	-0.308350000
6	4.605417000	-3.213185000	0.118542000
6	5.458120000	-2.463777000	0.949715000
6	5.068231000	-1.180981000	1.357445000
6	3.864524000	-0.636152000	0.938332000
8	-0.985728000	-2.872649000	-0.872735000
1	-2.733844000	2.871331000	0.221196000
1	-0.320332000	2.802725000	-0.144937000
1	3.398065000	0.825024000	-1.849735000
1	4.968994000	2.725801000	-1.912178000
1	4.686388000	4.636752000	-0.339265000
1	2.822309000	4.605451000	1.311691000
1	1.255718000	2.711524000	1.383296000
1	2.751285000	-3.274800000	-0.953311000
1	4.896963000	-4.212367000	-0.193954000
1	6.403826000	-2.881454000	1.282899000
1	5.706465000	-0.607583000	2.024423000
1	3.564821000	0.334874000	1.309347000
1	-4.067310000	0.760396000	0.349115000
1	-2.936769000	-1.421763000	-0.059619000

1b

$S_0 E = -1073.6679031$ Hartree

6	4.026459000	-1.202278000	-0.018886000
6	3.004701000	-2.137416000	-0.046168000
6	3.695773000	0.167763000	0.012748000
6	2.357342000	0.574121000	0.008734000
6	1.318294000	-0.364613000	-0.033982000
6	1.659196000	-1.742500000	-0.051672000
6	-0.092672000	0.017092000	-0.036438000
6	-1.032309000	-0.969676000	-0.066328000
8	-0.679512000	-2.302319000	-0.063049000
6	0.623582000	-2.762851000	-0.051243000
6	-0.466517000	1.460999000	0.059832000
6	-2.507151000	-0.839906000	-0.094739000
6	-1.055326000	1.965369000	1.229190000
6	-1.393352000	3.315680000	1.330698000
6	-1.142377000	4.184154000	0.266141000
6	-0.548964000	3.695092000	-0.900136000
6	-0.210862000	2.344543000	-1.001622000
6	-3.291714000	-1.760561000	0.623554000
6	-4.682538000	-1.676787000	0.601249000
6	-5.315061000	-0.683617000	-0.150426000
6	-4.545227000	0.223332000	-0.882409000
6	-3.153484000	0.148062000	-0.856900000
8	0.784198000	-3.968918000	-0.043622000
1	2.146487000	1.636106000	0.037740000
1	-1.250632000	1.292299000	2.059215000
1	-1.850654000	3.688878000	2.243030000
1	-1.405586000	5.235336000	0.345039000
1	-0.350472000	4.363686000	-1.733364000

1	0.246166000	1.968306000	-1.913078000
1	-2.805453000	-2.539142000	1.201675000
1	-5.272363000	-2.390079000	1.170161000
1	-6.399520000	-0.621063000	-0.170879000
1	-5.028330000	0.988844000	-1.483174000
1	-2.568115000	0.848829000	-1.440554000
1	3.232519000	-3.198028000	-0.060406000
1	5.058348000	-1.531084000	-0.016324000
8	4.608540000	1.169152000	0.050485000
6	5.997921000	0.836022000	0.061431000
1	6.256815000	0.241805000	0.945044000
1	6.282962000	0.291358000	-0.845802000
1	6.527749000	1.788479000	0.095401000

$S_1 E = -1073.54847978$ Hartree

6	3.945164000	-1.275194000	-0.234620000
6	2.893423000	-2.132566000	0.041598000
6	3.700279000	0.121915000	-0.234042000
6	2.419137000	0.617756000	-0.026650000
6	1.305329000	-0.245888000	0.151088000
6	1.591127000	-1.658242000	0.250955000
6	-0.047152000	0.184175000	0.298160000
6	-1.043072000	-0.865838000	0.468186000
8	-0.649995000	-2.048171000	1.061649000
6	0.605602000	-2.583490000	0.777125000
6	-0.465234000	1.581324000	0.337875000
6	-2.399178000	-0.850146000	0.058589000
6	-1.462279000	1.996431000	1.263918000
6	-1.860610000	3.325865000	1.347180000
6	-1.316449000	4.282662000	0.485438000
6	-0.366899000	3.888778000	-0.467824000
6	0.056196000	2.567730000	-0.540665000
6	-3.289566000	-1.901049000	0.468632000
6	-4.622136000	-1.885657000	0.107591000
6	-5.142369000	-0.847865000	-0.690985000
6	-4.288666000	0.171710000	-1.131880000
6	-2.948738000	0.184787000	-0.776164000
8	0.769976000	-3.756234000	1.054717000
1	2.300283000	1.692565000	-0.005588000
1	-1.884233000	1.264116000	1.944378000
1	-2.604009000	3.616179000	2.084415000
1	-1.639107000	5.318240000	0.540702000
1	0.033329000	4.616852000	-1.167978000
1	0.750084000	2.275616000	-1.320787000
1	-2.902701000	-2.701217000	1.088069000
1	-5.275675000	-2.685818000	0.445179000
1	-6.191170000	-0.847224000	-0.973525000
1	-4.673101000	0.958741000	-1.775465000
1	-2.301426000	0.952720000	-1.177830000
1	3.070410000	-3.199927000	0.127045000
1	4.938527000	-1.672307000	-0.401638000
8	4.668609000	1.056456000	-0.421709000
6	6.013898000	0.624756000	-0.627940000
1	6.388408000	0.060154000	0.233602000
1	6.102926000	0.014867000	-1.534278000
1	6.599921000	1.536907000	-0.746358000

1c $S_0 E = -807.9358419$ Hartree

6	-4.753834000	0.017847000	0.080130000
6	-3.935095000	1.114859000	0.235988000
6	-2.802501000	-1.414902000	-0.167472000
6	-4.173952000	-1.252117000	-0.123191000
6	-2.524687000	0.980476000	0.194551000
6	-1.925817000	-0.305438000	-0.009977000
6	-1.688433000	2.119432000	0.354536000
6	-0.326278000	2.017679000	0.318567000
6	0.318651000	0.759133000	0.118265000
6	-0.480363000	-0.394000000	-0.045403000
6	1.772538000	0.678111000	0.086700000
6	2.337106000	-0.535713000	-0.134534000
8	1.568483000	-1.654749000	-0.290497000
6	0.186283000	-1.679369000	-0.249184000
8	-0.316486000	-2.781367000	-0.394348000
1	-5.834102000	0.126863000	0.112494000
1	-4.357037000	2.104428000	0.393118000
1	-2.379067000	-2.395622000	-0.323949000
1	-4.815118000	-2.120739000	-0.247697000
1	-2.155375000	3.089324000	0.507579000
1	0.271172000	2.912002000	0.441484000
6	3.793486000	-0.896955000	-0.223696000
1	3.916558000	-1.565536000	-1.084364000
1	4.389463000	-0.005114000	-0.429602000
6	4.312963000	-1.600748000	1.044504000
1	3.732676000	-2.504787000	1.254577000
1	4.245534000	-0.941350000	1.916550000
1	5.360922000	-1.889906000	0.914183000
6	2.630030000	1.918158000	0.267523000
1	2.202262000	2.546805000	1.056306000
1	3.616523000	1.629753000	0.640313000
6	2.801053000	2.746035000	-1.018977000
1	1.835731000	3.074957000	-1.418656000
1	3.297640000	2.156164000	-1.797400000
1	3.409358000	3.636755000	-0.826147000

 $S_1 E = -807.813366192$ Hartree

6	-4.771294000	0.000564000	0.086195000
6	-3.942443000	1.109402000	0.260969000
6	-2.824073000	-1.410547000	-0.192691000
6	-4.209191000	-1.261910000	-0.141786000
6	-2.537869000	0.996527000	0.214242000
6	-1.945369000	-0.308048000	-0.018432000
6	-1.707229000	2.138429000	0.391456000
6	-0.319015000	2.028685000	0.351539000
6	0.309150000	0.797334000	0.132970000
6	-0.500758000	-0.407397000	-0.061560000
6	1.742458000	0.671137000	0.092769000
6	2.319453000	-0.574788000	-0.167336000
8	1.586379000	-1.682316000	-0.340044000
6	0.143252000	-1.667143000	-0.282874000
8	-0.322539000	-2.784146000	-0.448197000
1	-5.850599000	0.121799000	0.126781000

1	-4.377188000	2.090099000	0.437000000
1	-2.399477000	-2.387947000	-0.368599000
1	-4.847498000	-2.129614000	-0.279766000
1	-2.174679000	3.103476000	0.561082000
1	0.277746000	2.922066000	0.489168000
6	3.781779000	-0.882752000	-0.255190000
1	3.913923000	-1.607580000	-1.066965000
1	4.351584000	0.010744000	-0.517803000
6	4.331191000	-1.495401000	1.055266000
1	3.774177000	-2.398497000	1.321558000
1	4.258718000	-0.786167000	1.885877000
1	5.383760000	-1.763837000	0.921270000
6	2.636048000	1.872466000	0.284725000
1	2.194108000	2.531626000	1.037566000
1	3.601855000	1.562553000	0.692348000
6	2.868058000	2.669116000	-1.018712000
1	1.919299000	3.007519000	-1.445906000
1	3.377655000	2.057413000	-1.770647000
1	3.488915000	3.547505000	-0.813997000

1d

$S_0 E = -1188.0153144$ Hartree

6	3.684426000	-0.449959000	-0.009690000
6	2.775125000	-1.548339000	-0.039192000
6	3.146838000	0.876323000	0.022921000
6	1.743132000	1.084340000	0.016873000
6	0.861068000	0.019534000	-0.028573000
6	1.388991000	-1.317581000	-0.048264000
6	-0.593232000	0.181714000	-0.033487000
6	-1.386585000	-0.923076000	-0.061349000
8	-0.842887000	-2.201683000	-0.054277000
6	0.493755000	-2.449547000	-0.050278000
6	-1.172495000	1.556948000	0.056346000
6	-2.862564000	-1.014408000	-0.088548000
6	-1.819152000	1.979031000	1.227302000
6	-2.348928000	3.266853000	1.322024000
6	-2.234711000	4.153543000	0.249120000
6	-1.585243000	3.746417000	-0.918887000
6	-1.055064000	2.458634000	-1.013762000
6	-3.501213000	-2.043115000	0.628468000
6	-4.888968000	-2.166623000	0.607634000
6	-5.663026000	-1.276169000	-0.140093000
6	-5.037235000	-0.262824000	-0.869976000
6	-3.649730000	-0.131136000	-0.847156000
8	0.836060000	-3.635752000	-0.050683000
1	1.370812000	2.101520000	0.047236000
1	-1.907803000	1.291889000	2.063978000
1	-2.848649000	3.577283000	2.235567000
1	-2.647227000	5.155975000	0.322830000
1	-1.492304000	4.429936000	-1.758421000
1	-0.553279000	2.144877000	-1.925189000
1	-2.905016000	-2.742723000	1.204673000
1	-5.365315000	-2.961189000	1.175121000
1	-6.744748000	-1.375216000	-0.159386000
1	-5.629459000	0.424273000	-1.467834000
1	-3.175910000	0.649581000	-1.430603000

8	3.292509000	-2.784630000	-0.053150000
1	2.525264000	-3.418427000	-0.060254000
6	5.089451000	-0.645757000	-0.003955000
6	5.942272000	0.435742000	0.032538000
6	4.058899000	1.967035000	0.061781000
6	5.419586000	1.752144000	0.066045000
1	7.017369000	0.282431000	0.036136000
1	5.477060000	-1.658255000	-0.028621000
1	6.100616000	2.598238000	0.095237000
1	3.660750000	2.977969000	0.087372000

$S_1 E = -1187.90621686$ Hartree

6	3.693419000	-0.446815000	-0.039893000
6	2.784778000	-1.543824000	-0.068270000
6	3.163025000	0.890555000	0.034715000
6	1.744814000	1.063188000	0.068430000
6	0.855896000	-0.016112000	0.003598000
6	1.371438000	-1.357192000	-0.039352000
6	-0.575354000	0.159922000	0.010128000
6	-1.394519000	-0.977200000	0.000293000
8	-0.888007000	-2.219789000	0.026663000
6	0.519232000	-2.473322000	-0.002344000
6	-1.160773000	1.526222000	0.066517000
6	-2.863639000	-1.013059000	-0.037374000
6	-1.917977000	1.935210000	1.177823000
6	-2.446445000	3.223740000	1.239107000
6	-2.234732000	4.121393000	0.189157000
6	-1.483615000	3.726310000	-0.920522000
6	-0.943744000	2.441324000	-0.979661000
6	-3.526864000	-2.067578000	0.627313000
6	-4.913268000	-2.162225000	0.593018000
6	-5.662844000	-1.227662000	-0.128808000
6	-5.015672000	-0.196372000	-0.815501000
6	-3.629794000	-0.081238000	-0.767945000
8	0.824389000	-3.685574000	-0.009187000
1	1.354491000	2.070525000	0.154122000
1	-2.082570000	1.241647000	1.997045000
1	-3.022678000	3.527316000	2.108492000
1	-2.652053000	5.123201000	0.236028000
1	-1.317772000	4.417288000	-1.742108000
1	-0.366824000	2.133881000	-1.847062000
1	-2.944349000	-2.796897000	1.178476000
1	-5.410933000	-2.967205000	1.125346000
1	-6.745541000	-1.307461000	-0.162011000
1	-5.592020000	0.517776000	-1.395831000
1	-3.140240000	0.709372000	-1.322183000
8	3.300614000	-2.790535000	-0.116808000
1	2.524591000	-3.417364000	-0.095696000
6	5.093130000	-0.614889000	-0.067959000
6	5.945511000	0.498744000	-0.027768000
6	4.040787000	1.982375000	0.078045000
6	5.435031000	1.795982000	0.045176000
1	7.020657000	0.341011000	-0.051650000
1	5.505878000	-1.616286000	-0.117336000
1	6.101643000	2.651727000	0.077523000
1	3.626143000	2.985713000	0.135825000

1e $S_0 E = -1264.2192962$ Hartree

6	6.852466000	0.814492000	0.026377000
6	5.602363000	1.431213000	0.044620000
6	4.460122000	0.620682000	0.016840000
6	4.614905000	-0.776234000	-0.027780000
6	5.847478000	-1.412435000	-0.046876000
6	6.973279000	-0.585898000	-0.018799000
6	3.028083000	0.843372000	0.020769000
6	2.443340000	-0.433215000	-0.022237000
8	3.391769000	-1.418424000	-0.050179000
6	2.194737000	1.969957000	0.064145000
6	0.818676000	1.801738000	0.051497000
6	0.222888000	0.517722000	-0.007914000
6	1.055495000	-0.635183000	-0.031768000
6	-1.225020000	0.340482000	-0.022027000
6	-1.731170000	-0.925483000	-0.059000000
8	-0.902532000	-2.024204000	-0.054283000
6	0.477625000	-1.971814000	-0.038253000
6	-2.116938000	1.537957000	0.064495000
6	-3.145793000	-1.359201000	-0.093051000
6	-2.841200000	1.799428000	1.236943000
6	-3.666636000	2.921447000	1.327587000
6	-3.775857000	3.801937000	0.249129000
6	-3.053105000	3.555650000	-0.920836000
6	-2.227841000	2.433506000	-1.011633000
6	-3.525189000	-2.514457000	0.615144000
6	-4.844325000	-2.962240000	0.587415000
6	-5.804340000	-2.275540000	-0.159768000
6	-5.433502000	-1.138725000	-0.881657000
6	-4.116799000	-0.682164000	-0.850650000
8	1.072076000	-3.030199000	-0.031085000
1	7.750437000	1.424917000	0.047177000
1	5.517878000	2.513408000	0.079000000
1	5.925609000	-2.493768000	-0.081690000
1	7.961223000	-1.036616000	-0.032220000
1	2.618958000	2.968669000	0.109644000
1	0.179169000	2.674625000	0.089096000
1	-2.757162000	1.117247000	2.078186000
1	-4.224220000	3.107938000	2.242461000
1	-4.418542000	4.675072000	0.319973000
1	-3.132578000	4.235088000	-1.765023000
1	-1.671102000	2.243745000	-1.925594000
1	-2.781712000	-3.056577000	1.189744000
1	-5.121439000	-3.850174000	1.148710000
1	-6.831959000	-2.627276000	-0.184498000
1	-6.169282000	-0.607769000	-1.479120000
1	-3.840022000	0.192120000	-1.427745000

 $S_1 E = -1264.10893320$ Hartree

6	6.796889000	0.712924000	-0.405520000
6	5.568587000	1.362043000	-0.322858000
6	4.409836000	0.581243000	-0.146880000
6	4.543474000	-0.823927000	-0.058543000
6	5.753786000	-1.487385000	-0.139013000

6	6.891823000	-0.689137000	-0.316021000
6	3.007593000	0.841680000	-0.018322000
6	2.390739000	-0.417649000	0.134811000
8	3.314315000	-1.427482000	0.117176000
6	2.205936000	2.015109000	0.036842000
6	0.845087000	1.888710000	0.184203000
6	0.189706000	0.612354000	0.254789000
6	1.013129000	-0.590935000	0.301069000
6	-1.216861000	0.463382000	0.295751000
6	-1.747750000	-0.866233000	0.431540000
8	-0.932976000	-1.846587000	0.955417000
6	0.447643000	-1.859864000	0.680885000
6	-2.129240000	1.624689000	0.241602000
6	-3.047029000	-1.347612000	0.079352000
6	-3.133423000	1.780222000	1.220937000
6	-3.988854000	2.878269000	1.197202000
6	-3.879308000	3.834812000	0.183331000
6	-2.902028000	3.686156000	-0.805328000
6	-2.032516000	2.597794000	-0.775428000
6	-3.465052000	-2.641060000	0.529805000
6	-4.717359000	-3.136845000	0.212254000
6	-5.605822000	-2.388854000	-0.577555000
6	-5.207424000	-1.132835000	-1.056833000
6	-3.960093000	-0.615695000	-0.745363000
8	1.011993000	-2.922962000	0.848487000
1	7.702358000	1.297022000	-0.541972000
1	5.504892000	2.443756000	-0.394065000
1	5.813766000	-2.568024000	-0.066463000
1	7.865875000	-1.164205000	-0.384384000
1	2.664034000	2.997180000	-0.021309000
1	0.239796000	2.784112000	0.250926000
1	-3.222010000	1.040169000	2.010445000
1	-4.744534000	2.987167000	1.970022000
1	-4.554699000	4.685209000	0.159549000
1	-2.821671000	4.415518000	-1.606427000
1	-1.294053000	2.475352000	-1.561621000
1	-2.790467000	-3.225014000	1.143679000
1	-5.013063000	-4.115411000	0.580925000
1	-6.586019000	-2.785437000	-0.826092000
1	-5.874554000	-0.560299000	-1.695580000
1	-3.662348000	0.333395000	-1.170159000

2a $S_0 E = -939.290321$ Hartree

6	4.716992000	0.307776000	0.058063000
6	4.040057000	-0.898506000	-0.008959000
6	3.983532000	1.505751000	0.108541000
6	2.597616000	1.492340000	0.082347000
6	1.879717000	0.275215000	-0.000159000
6	2.635382000	-0.927927000	-0.032904000
6	0.423108000	0.225979000	-0.022218000
6	-0.188823000	-1.001172000	-0.064825000
7	0.582925000	-2.154679000	-0.084126000
6	1.965196000	-2.231197000	-0.085017000
6	-0.370289000	1.489787000	0.065631000
6	-1.654893000	-1.252993000	-0.089499000

6	-1.115620000	1.788390000	1.216705000
6	-1.850542000	2.971848000	1.305464000
6	-1.847361000	3.881397000	0.245773000
6	-1.103976000	3.600032000	-0.903059000
6	-0.370699000	2.415520000	-0.991108000
6	-2.221057000	-2.175619000	0.807130000
6	-3.588183000	-2.451764000	0.772298000
6	-4.407399000	-1.818221000	-0.164094000
6	-3.851900000	-0.905632000	-1.064655000
6	-2.486927000	-0.624027000	-1.029372000
8	2.530972000	-3.327718000	-0.131699000
1	4.506104000	2.456482000	0.171748000
1	2.052832000	2.428305000	0.127845000
1	-1.118009000	1.085539000	2.045122000
1	-2.422879000	3.183870000	2.204625000
1	-2.418710000	4.803068000	0.314674000
1	-1.096600000	4.300993000	-1.733472000
1	0.202010000	2.200024000	-1.889474000
1	-1.593769000	-2.662034000	1.549570000
1	-4.011628000	-3.159479000	1.479399000
1	-5.471529000	-2.034963000	-0.193434000
1	-4.481483000	-0.415531000	-1.802016000
1	-2.060293000	0.078443000	-1.737189000
1	0.108933000	-3.046872000	-0.169359000
1	5.802567000	0.329279000	0.077800000
1	4.570615000	-1.844487000	-0.039863000

$S_1 E = -939.168662389$ Hartree

6	4.733705000	0.281678000	-0.250518000
6	4.030519000	-0.907574000	-0.089463000
6	4.017160000	1.495327000	-0.251090000
6	2.639966000	1.516581000	-0.149287000
6	1.871933000	0.307253000	-0.076374000
6	2.636520000	-0.909073000	0.007007000
6	0.446608000	0.274933000	0.019917000
6	-0.227360000	-1.018297000	0.173344000
7	0.584876000	-2.107374000	0.431017000
6	1.963978000	-2.175910000	0.291701000
6	-0.347033000	1.502761000	0.074326000
6	-1.627496000	-1.272333000	0.032762000
6	-1.352949000	1.673257000	1.064247000
6	-2.076427000	2.857311000	1.157755000
6	-1.862462000	3.892534000	0.243028000
6	-0.907648000	3.729269000	-0.770701000
6	-0.159114000	2.561799000	-0.851523000
6	-2.240452000	-2.411866000	0.660328000
6	-3.588104000	-2.679169000	0.511314000
6	-4.409680000	-1.848519000	-0.276029000
6	-3.836941000	-0.734570000	-0.906093000
6	-2.490433000	-0.437691000	-0.759417000
8	2.524709000	-3.268563000	0.415989000
1	4.555151000	2.437513000	-0.315446000
1	2.135885000	2.473028000	-0.102541000
1	-1.522595000	0.881097000	1.785293000
1	-2.817164000	2.970047000	1.944562000
1	-2.442032000	4.808932000	0.305894000

1	-0.757766000	4.513445000	-1.507621000
1	0.546744000	2.435237000	-1.665898000
1	-1.662284000	-3.041927000	1.331338000
1	-4.018319000	-3.535770000	1.024265000
1	-5.466542000	-2.068754000	-0.392434000
1	-4.450316000	-0.094959000	-1.536252000
1	-2.070709000	0.390465000	-1.315095000
1	0.149790000	-3.021253000	0.493792000
1	5.815635000	0.278092000	-0.336870000
1	4.546637000	-1.859739000	-0.018993000

2b

$S_0 E = -1053.8156764$ Hartree

6	4.070370000	-1.102266000	-0.001799000
6	3.082324000	-2.071254000	-0.052545000
6	3.690194000	0.255099000	0.043032000
6	2.341271000	0.611790000	0.027681000
6	1.328868000	-0.361738000	-0.037023000
6	1.722111000	-1.730186000	-0.065623000
6	-0.088514000	-0.013891000	-0.044938000
6	-1.010059000	-1.029702000	-0.070495000
7	-0.584378000	-2.350759000	-0.085781000
6	0.726843000	-2.799909000	-0.099686000
6	-0.506983000	1.418140000	0.042280000
6	-2.489668000	-0.872427000	-0.076880000
6	-1.142286000	1.909714000	1.193183000
6	-1.527447000	3.248482000	1.280958000
6	-1.277549000	4.121937000	0.220303000
6	-0.639576000	3.647719000	-0.928467000
6	-0.256518000	2.308283000	-1.015513000
6	-3.273364000	-1.610424000	0.827004000
6	-4.664369000	-1.504068000	0.812483000
6	-5.293414000	-0.667163000	-0.111186000
6	-4.522986000	0.063417000	-1.019569000
6	-3.132520000	-0.037348000	-1.004513000
8	0.969843000	-4.010725000	-0.141284000
1	2.093309000	1.665568000	0.067840000
1	-1.335940000	1.234505000	2.021933000
1	-2.019932000	3.609140000	2.180097000
1	-1.576330000	5.164431000	0.288413000
1	-0.442225000	4.319286000	-1.759775000
1	0.235013000	1.944316000	-1.914010000
1	-2.791376000	-2.253162000	1.559105000
1	-5.254299000	-2.072943000	1.525615000
1	-6.376654000	-0.585700000	-0.124823000
1	-5.005592000	0.709588000	-1.747493000
1	-2.541452000	0.524795000	-1.719383000
1	3.345378000	-3.123705000	-0.078918000
1	5.113580000	-1.393806000	0.008415000
8	4.570224000	1.289906000	0.105344000
6	5.967311000	1.000925000	0.133698000
1	6.233874000	0.404250000	1.013891000
1	6.285309000	0.475967000	-0.774654000
1	6.467594000	1.968708000	0.186728000
1	-1.284390000	-3.080149000	-0.159302000

$S_1 E = -1053.69390517$ Hartree

6	4.088700000	-1.112831000	-0.110501000
6	3.076795000	-2.059240000	0.021706000
6	3.725295000	0.250880000	-0.132286000
6	2.388679000	0.635952000	-0.069690000
6	1.331593000	-0.316833000	-0.017838000
6	1.731933000	-1.695748000	0.076626000
6	-0.056655000	0.035703000	0.052046000
6	-1.055630000	-1.030749000	0.180487000
7	-0.573708000	-2.300422000	0.427409000
6	0.740982000	-2.736527000	0.324553000
6	-0.493327000	1.428162000	0.107627000
6	-2.470964000	-0.898123000	0.018205000
6	-1.453272000	1.851481000	1.069441000
6	-1.832812000	3.185561000	1.168694000
6	-1.315658000	4.137247000	0.285184000
6	-0.405175000	3.735662000	-0.703681000
6	0.004503000	2.411785000	-0.788203000
6	-3.376544000	-1.829835000	0.633782000
6	-4.743981000	-1.725516000	0.465299000
6	-5.301064000	-0.705138000	-0.331567000
6	-4.441115000	0.213208000	-0.949293000
6	-3.066073000	0.138389000	-0.781910000
8	0.981912000	-3.942150000	0.444691000
1	2.185162000	1.697646000	-0.041332000
1	-1.853592000	1.125434000	1.768237000
1	-2.542857000	3.483056000	1.935405000
1	-1.628205000	5.175280000	0.351796000
1	-0.025267000	4.460251000	-1.418589000
1	0.676957000	2.111366000	-1.584713000
1	-2.997729000	-2.592052000	1.309954000
1	-5.395742000	-2.434440000	0.969894000
1	-6.376456000	-0.633281000	-0.463329000
1	-4.850843000	0.994073000	-1.585636000
1	-2.431414000	0.823005000	-1.329152000
1	3.321763000	-3.113671000	0.098777000
1	5.123725000	-1.426266000	-0.160762000
8	4.621243000	1.272182000	-0.198653000
6	6.013440000	0.961351000	-0.241317000
1	6.328172000	0.416013000	0.656016000
1	6.264663000	0.375641000	-1.133248000
1	6.528685000	1.921874000	-0.281788000
1	-1.240524000	-3.063740000	0.462005000

2c

$S_0 E = -788.0833608$ Hartree

6	4.765849000	0.096627000	-0.114091000
6	3.919677000	1.176140000	-0.253221000
6	2.849363000	-1.379337000	0.143538000
6	4.217049000	-1.186842000	0.085879000
6	2.513931000	1.010220000	-0.198113000
6	1.945336000	-0.288933000	0.003420000
6	1.648657000	2.131771000	-0.341432000
6	0.292446000	1.995496000	-0.292558000
6	-0.330303000	0.719245000	-0.095634000
6	0.502389000	-0.420148000	0.053647000

6	-1.777919000	0.625260000	-0.057427000
6	-2.340417000	-0.606268000	0.151605000
7	-1.516338000	-1.696998000	0.295423000
6	-0.129221000	-1.727657000	0.261325000
8	0.426219000	-2.826735000	0.412363000
1	5.843080000	0.231242000	-0.157175000
1	4.317945000	2.176181000	-0.407557000
1	2.442569000	-2.367603000	0.297592000
1	4.878695000	-2.042119000	0.197096000
1	2.090876000	3.113821000	-0.491973000
1	-0.325526000	2.877518000	-0.403335000
1	-1.931590000	-2.608722000	0.455050000
6	-3.817701000	-0.922506000	0.206451000
1	-3.973565000	-1.735485000	0.927020000
1	-4.368293000	-0.063453000	0.597302000
6	-4.397647000	-1.335384000	-1.160228000
1	-3.878854000	-2.211566000	-1.564035000
1	-4.304362000	-0.523973000	-1.889667000
1	-5.459080000	-1.585725000	-1.060914000
6	-2.649524000	1.858332000	-0.218890000
1	-2.240688000	2.502415000	-1.005418000
1	-3.637479000	1.563802000	-0.583732000
6	-2.820381000	2.674430000	1.075940000
1	-1.855295000	3.012931000	1.468234000
1	-3.300349000	2.072267000	1.855748000
1	-3.442963000	3.558666000	0.897617000

$S_1 E = -787.961056621$ Hartree

6	4.784251000	0.080491000	-0.124763000
6	3.933337000	1.173079000	-0.273749000
6	2.864953000	-1.375151000	0.154742000
6	4.250962000	-1.195733000	0.089905000
6	2.525255000	1.028795000	-0.212676000
6	1.964122000	-0.293011000	0.009007000
6	1.668178000	2.147715000	-0.363597000
6	0.276618000	2.012269000	-0.313510000
6	-0.323560000	0.763479000	-0.106560000
6	0.517551000	-0.419863000	0.066359000
6	-1.761616000	0.624813000	-0.066274000
6	-2.345258000	-0.635364000	0.167602000
7	-1.538834000	-1.705816000	0.330243000
6	-0.118160000	-1.693024000	0.294216000
8	0.401718000	-2.807188000	0.472720000
1	5.861092000	0.223604000	-0.175545000
1	4.342971000	2.166477000	-0.440359000
1	2.464484000	-2.364084000	0.320354000
1	4.908209000	-2.052880000	0.206902000
1	2.111757000	3.126101000	-0.524919000
1	-0.335395000	2.896830000	-0.436250000
1	-1.930747000	-2.623722000	0.513100000
6	-3.823719000	-0.916896000	0.211351000
1	-3.996904000	-1.751916000	0.900833000
1	-4.358204000	-0.058574000	0.625625000
6	-4.404744000	-1.276370000	-1.174310000
1	-3.901909000	-2.152692000	-1.595844000
1	-4.293689000	-0.448471000	-1.881493000

1	-5.470822000	-1.505343000	-1.078258000
6	-2.656520000	1.827186000	-0.229688000
1	-2.232422000	2.493574000	-0.986704000
1	-3.633582000	1.523706000	-0.613673000
6	-2.858161000	2.614523000	1.085792000
1	-1.899562000	2.945991000	1.495425000
1	-3.354554000	1.998001000	1.842752000
1	-3.480511000	3.496372000	0.901094000

2d

$S_0 E = -1168.1644273$ Hartree

6	3.701977000	-0.400549000	0.000639000
6	2.821999000	-1.519082000	-0.047084000
6	3.130323000	0.912244000	0.046734000
6	1.725818000	1.083921000	0.034915000
6	0.863658000	-0.003516000	-0.025814000
6	1.429277000	-1.328567000	-0.055119000
6	-0.591429000	0.141530000	-0.034877000
6	-1.375618000	-0.980141000	-0.058831000
7	-0.778685000	-2.241311000	-0.068556000
6	0.566741000	-2.494804000	-0.082976000
6	-1.193735000	1.507399000	0.045966000
6	-2.861886000	-1.023933000	-0.069508000
6	-1.867517000	1.923828000	1.204018000
6	-2.424670000	3.201204000	1.285503000
6	-2.310830000	4.086414000	0.211477000
6	-1.635117000	3.686854000	-0.944240000
6	-1.079497000	2.408997000	-1.025105000
6	-3.541944000	-1.872469000	0.821755000
6	-4.934283000	-1.957200000	0.799690000
6	-5.667896000	-1.202891000	-0.117953000
6	-5.000423000	-0.362688000	-1.012809000
6	-3.609396000	-0.273227000	-0.991219000
8	0.974334000	-3.680748000	-0.122011000
1	1.328368000	2.091315000	0.074734000
1	-1.955709000	1.239185000	2.042902000
1	-2.944825000	3.504912000	2.190012000
1	-2.743719000	5.081044000	0.274620000
1	-1.542443000	4.368522000	-1.785486000
1	-0.557201000	2.101940000	-1.927381000
1	-2.981794000	-2.451217000	1.551635000
1	-5.443715000	-2.610125000	1.502743000
1	-6.751975000	-1.270260000	-0.137332000
1	-5.563434000	0.220223000	-1.736334000
1	-3.098279000	0.372809000	-1.696576000
1	-1.374361000	-3.057993000	-0.142981000
8	3.366701000	-2.745781000	-0.079240000
1	2.599559000	-3.389753000	-0.106631000
6	5.112948000	-0.559721000	0.010347000
6	5.938063000	0.541146000	0.064006000
6	4.017485000	2.025727000	0.103472000
6	5.381735000	1.845255000	0.111402000
1	7.016866000	0.415147000	0.070602000
1	5.524945000	-1.562443000	-0.024899000
1	6.041652000	2.707549000	0.154426000
1	3.593879000	3.026166000	0.139510000

$S_1 E = -1168.05570682$ Hartree

6	3.724704000	-0.392158000	-0.043247000
6	2.819232000	-1.506480000	-0.062287000
6	3.162711000	0.926806000	0.034663000
6	1.747718000	1.078237000	0.072785000
6	0.855827000	-0.013862000	0.007433000
6	1.415269000	-1.334663000	-0.021574000
6	-0.572830000	0.147954000	0.021008000
6	-1.397674000	-1.009874000	0.038310000
7	-0.804494000	-2.231117000	0.067542000
6	0.571460000	-2.484518000	0.016229000
6	-1.180483000	1.500904000	0.065729000
6	-2.869794000	-1.033966000	-0.003282000
6	-2.024850000	1.880177000	1.126563000
6	-2.583935000	3.155936000	1.173221000
6	-2.319356000	4.079241000	0.157857000
6	-1.486467000	3.716901000	-0.904134000
6	-0.919710000	2.443509000	-0.948316000
6	-3.578128000	-1.955305000	0.798444000
6	-4.966155000	-2.037866000	0.729349000
6	-5.677765000	-1.211446000	-0.145200000
6	-4.987095000	-0.296974000	-0.946946000
6	-3.600600000	-0.200397000	-0.875578000
8	0.957631000	-3.690853000	-0.009306000
1	1.349222000	2.081847000	0.164529000
1	-2.230765000	1.171273000	1.922992000
1	-3.224905000	3.430849000	2.006441000
1	-2.759408000	5.071858000	0.193298000
1	-1.280714000	4.424437000	-1.702655000
1	-0.283931000	2.163379000	-1.783368000
1	-3.041323000	-2.581431000	1.505924000
1	-5.493189000	-2.742758000	1.365892000
1	-6.760484000	-1.277265000	-0.199733000
1	-5.531350000	0.341785000	-1.636727000
1	-3.077014000	0.501010000	-1.514608000
1	-1.385540000	-3.060018000	-0.002065000
8	3.353061000	-2.739017000	-0.109679000
1	2.575882000	-3.378803000	-0.090642000
6	5.117794000	-0.550099000	-0.081548000
6	5.963977000	0.577804000	-0.044666000
6	4.031990000	2.033733000	0.076941000
6	5.428529000	1.858942000	0.034950000
1	7.040777000	0.436436000	-0.076047000
1	5.537795000	-1.548193000	-0.134936000
1	6.081642000	2.726150000	0.065783000
1	3.608683000	3.032806000	0.138807000

2e

$S_0 E = -1244.3677979$ Hartree

6	6.858079000	0.865227000	0.079092000
6	5.598717000	1.463090000	0.097680000
6	4.468074000	0.637388000	0.044808000
6	4.643020000	-0.756589000	-0.024257000
6	5.885931000	-1.373617000	-0.044117000
6	6.999772000	-0.532262000	0.009141000

6	3.033522000	0.839038000	0.040320000
6	2.465262000	-0.441735000	-0.032004000
8	3.431778000	-1.414549000	-0.069549000
6	2.185653000	1.956675000	0.098366000
6	0.815625000	1.770112000	0.072866000
6	0.229474000	0.477382000	-0.013900000
6	1.079800000	-0.668926000	-0.055037000
6	-1.215802000	0.304177000	-0.030862000
6	-1.728034000	-0.969185000	-0.068115000
7	-0.865266000	-2.051319000	-0.093489000
6	0.521937000	-2.020850000	-0.109979000
6	-2.114246000	1.497117000	0.052477000
6	-3.168541000	-1.340217000	-0.074135000
6	-2.860217000	1.751632000	1.213310000
6	-3.696874000	2.866237000	1.294645000
6	-3.796533000	3.749713000	0.217761000
6	-3.053995000	3.511626000	-0.941463000
6	-2.219351000	2.395732000	-1.022193000
6	-3.640682000	-2.311893000	0.825291000
6	-4.980269000	-2.701146000	0.811088000
6	-5.865188000	-2.133544000	-0.107614000
6	-5.402748000	-1.173170000	-1.011087000
6	-4.065804000	-0.778214000	-0.996192000
8	1.161460000	-3.072804000	-0.170474000
1	7.746838000	1.488254000	0.119053000
1	5.498406000	2.543315000	0.151284000
1	5.980178000	-2.453004000	-0.098235000
1	7.994270000	-0.968557000	-0.003879000
1	2.597841000	2.959351000	0.166110000
1	0.164677000	2.633977000	0.124266000
1	-2.783536000	1.068845000	2.054878000
1	-4.268302000	3.045159000	2.201528000
1	-4.447058000	4.617713000	0.281238000
1	-3.126164000	4.192293000	-1.785503000
1	-1.647296000	2.213106000	-1.928256000
1	-2.962699000	-2.748190000	1.554220000
1	-5.330969000	-3.445192000	1.520686000
1	-6.907899000	-2.438097000	-0.120943000
1	-6.083154000	-0.733619000	-1.735030000
1	-3.712059000	-0.039049000	-1.706693000
1	-1.261617000	-2.981034000	-0.175442000

$S_1 E = -1244.25381579$ Hartree

6	6.850998000	0.868232000	-0.100497000
6	5.596364000	1.472090000	-0.086542000
6	4.454671000	0.644782000	-0.042208000
6	4.636045000	-0.759214000	-0.011436000
6	5.871480000	-1.375988000	-0.025526000
6	6.992651000	-0.531431000	-0.071271000
6	3.042076000	0.848675000	-0.014782000
6	2.456144000	-0.441166000	0.028497000
8	3.419664000	-1.414841000	0.034389000
6	2.188248000	1.984131000	0.020327000
6	0.828452000	1.805464000	0.053955000
6	0.208948000	0.500889000	0.028496000
6	1.084089000	-0.665233000	0.064802000

6	-1.195044000	0.333541000	0.037098000
6	-1.763435000	-0.996061000	0.113174000
7	-0.875318000	-2.041898000	0.287708000
6	0.516586000	-1.995283000	0.206517000
6	-2.093700000	1.512146000	0.064384000
6	-3.155740000	-1.352817000	0.016931000
6	-3.004827000	1.693453000	1.124162000
6	-3.827089000	2.816623000	1.172469000
6	-3.776064000	3.772131000	0.152971000
6	-2.889355000	3.598751000	-0.913090000
6	-2.052621000	2.484352000	-0.955050000
6	-3.643790000	-2.536267000	0.658769000
6	-4.966034000	-2.931569000	0.532415000
6	-5.867652000	-2.187571000	-0.244225000
6	-5.410995000	-1.027543000	-0.889173000
6	-4.094921000	-0.610594000	-0.765520000
8	1.142893000	-3.056534000	0.257847000
1	7.741660000	1.489341000	-0.134886000
1	5.498566000	2.553342000	-0.110355000
1	5.965482000	-2.456453000	-0.000854000
1	7.985952000	-0.969997000	-0.083405000
1	2.608281000	2.985129000	0.039424000
1	0.190097000	2.677405000	0.115285000
1	-3.049857000	0.954552000	1.918174000
1	-4.510946000	2.945858000	2.006723000
1	-4.425902000	4.641979000	0.186796000
1	-2.851426000	4.329772000	-1.715891000
1	-1.375887000	2.346897000	-1.793221000
1	-2.992531000	-3.103294000	1.318430000
1	-5.305913000	-3.822240000	1.054779000
1	-6.901064000	-2.505350000	-0.345640000
1	-6.090974000	-0.450647000	-1.510937000
1	-3.763969000	0.260750000	-1.315852000
1	-1.238281000	-2.987899000	0.247503000