

Electronic Supplementary Information

Expanding the spectrum of polydopamine antioxidant activity by nitroxide conjugation

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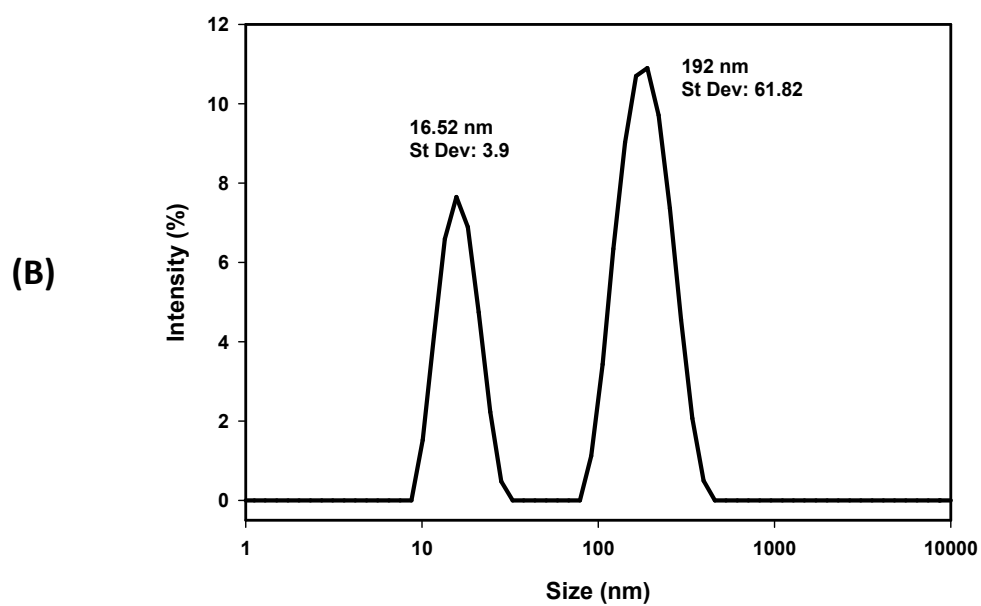
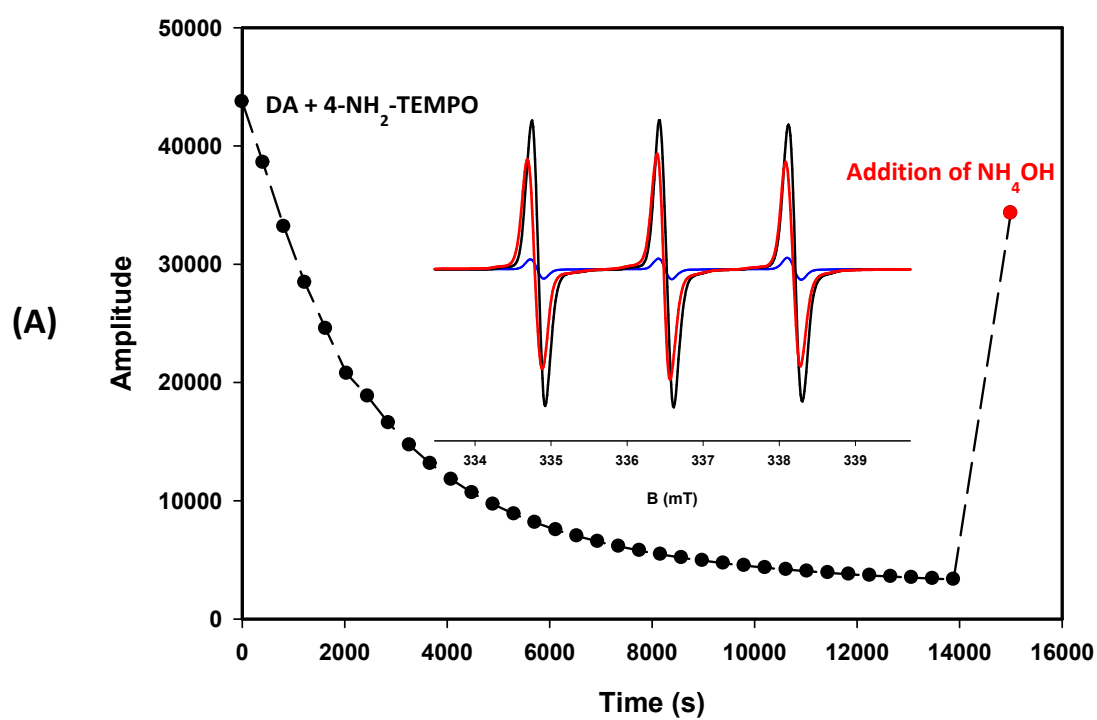


Figure S1. (A) EPR signal measured after mixing dopamine and 4-NH₂TEMPO. The red dot represents the signal after NH₄OH addition. (B) DLS spectrum of polydisperse particles obtained by the sequential mixing of 4-NH₂TEMPO and NH₄OH.

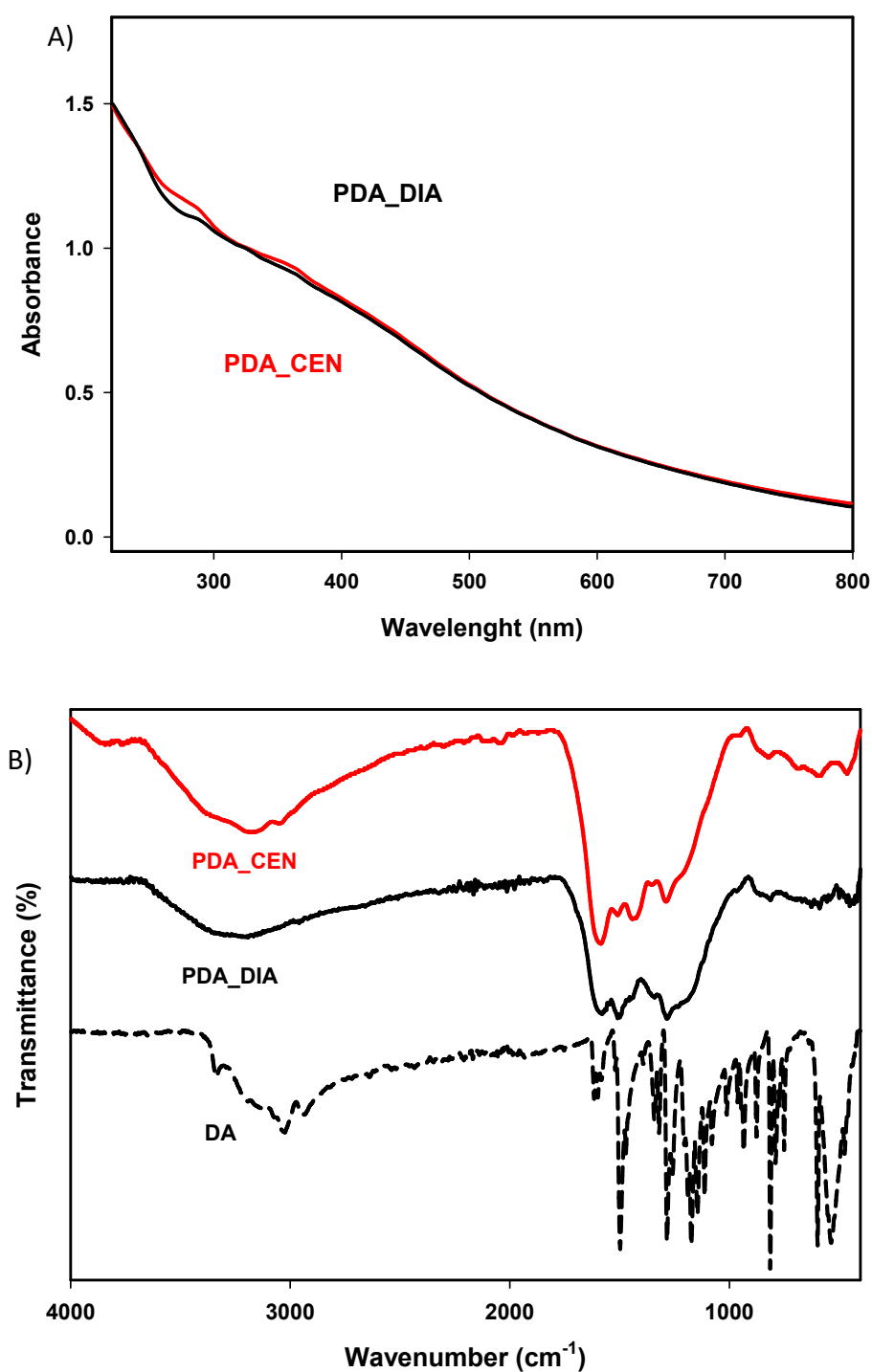


Figure S2. Chemical and morphological characterization of PDAn purified only by centrifugation (PDA_CEN) or by centrifugation and dialysis (PDA_DIA). A) UV-vis spectrum in water of (—) PDA_CEN and (—) PDA_DIA (30 $\mu\text{g/mL}$); B) FTIR-ATR spectra on solid samples of (—) PDA_CEN, (—) PDA_DIA and (- - -) DA;

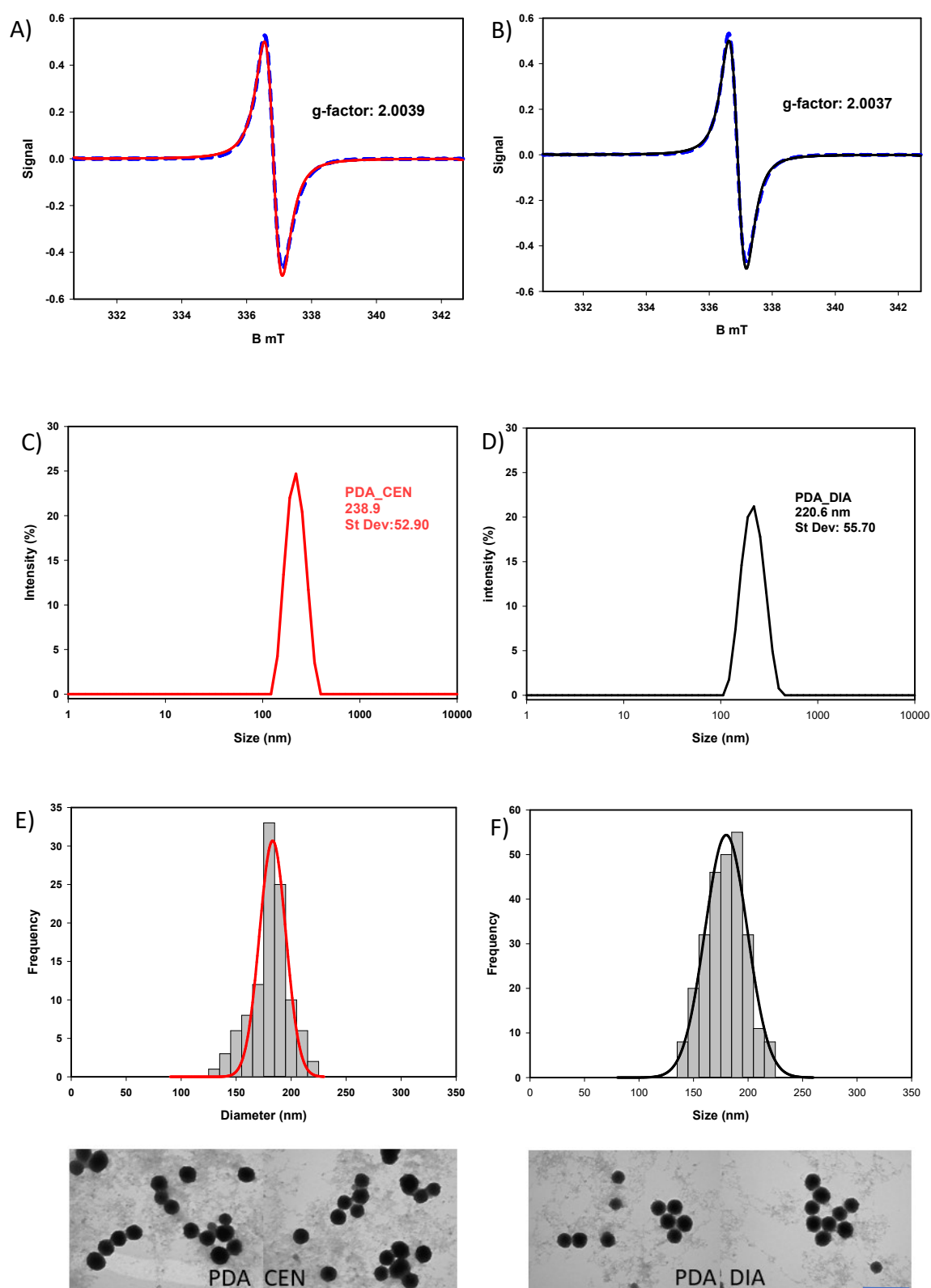


Figure S3. Chemical and morphological characterization of PDAn purified only by centrifugation (PDA_CEN) or by centrifugation and dialysis (PDA_DIA). A,B) Experimental (---) and simulated EPR spectra on solid samples of (—) PDA_CEN and (—) PDA_DIA; C,D) DLS spectra; E,) Gaussian distribution and TEM images of (—) PDA_CEN and (—) PDA_DIA. The blue bar is equivalent to 500 nm.

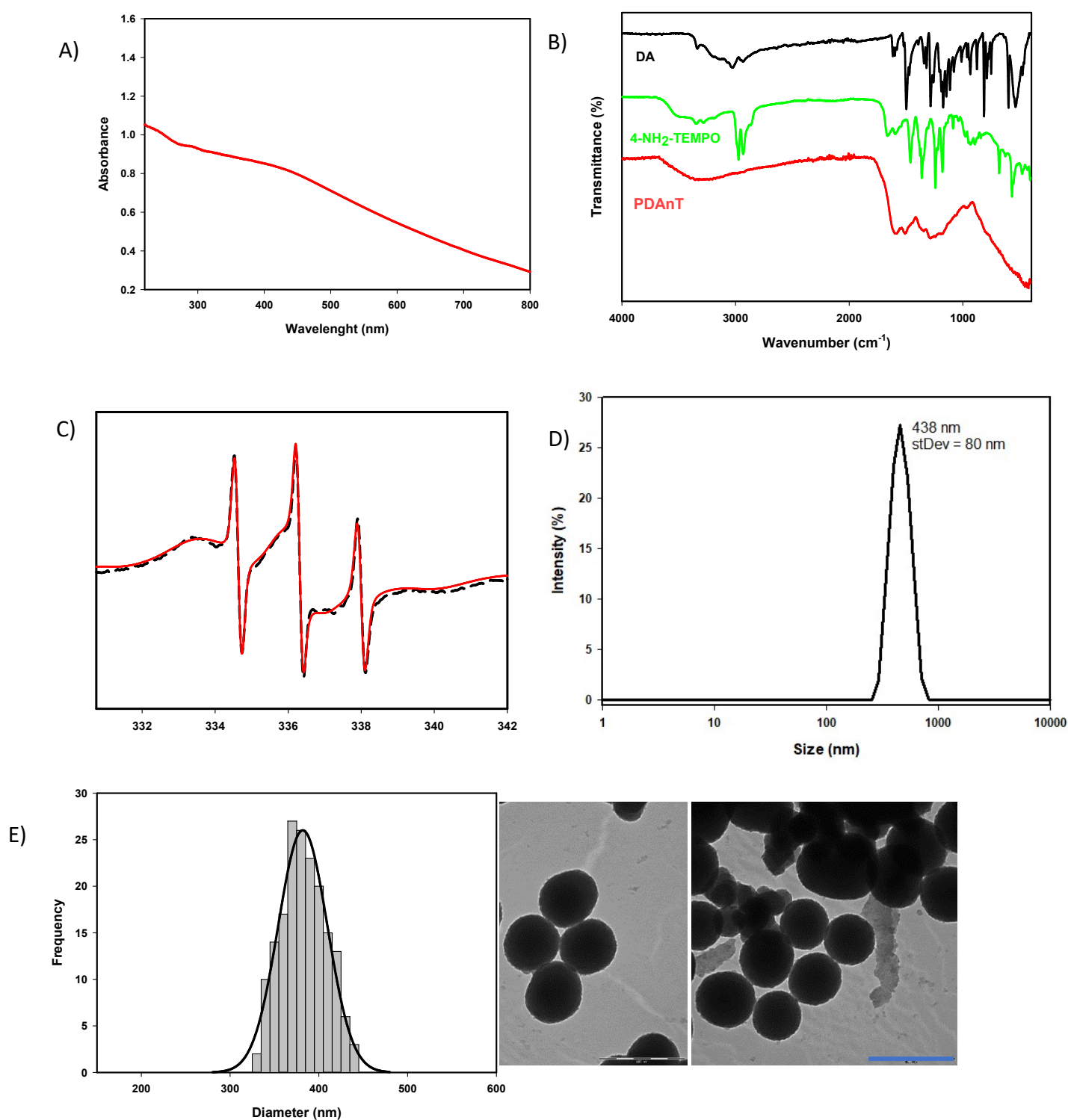


Figure S4. Chemical and morphological characterization of functionalized polydopamine nanoparticles. A) UV-vis spectrum in water of (—) PDAnT (30 $\mu\text{g/mL}$); B) FTIR-ATR spectra on solid samples of (—) DA (Dopamine-HCl), (—) 4-NH₂-TEMPO and (—) PDAnT; C) experimental (---) and simulated (—) EPR spectrum of PDAnT in water (0.9 mg/mL); D) DLS spectra and E) Gaussian distribution and TEM images (Bar=500 nm).

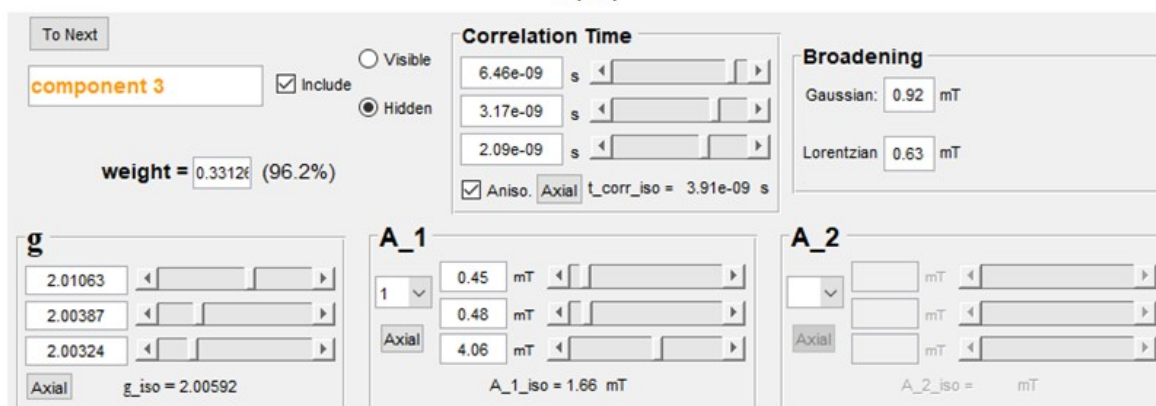
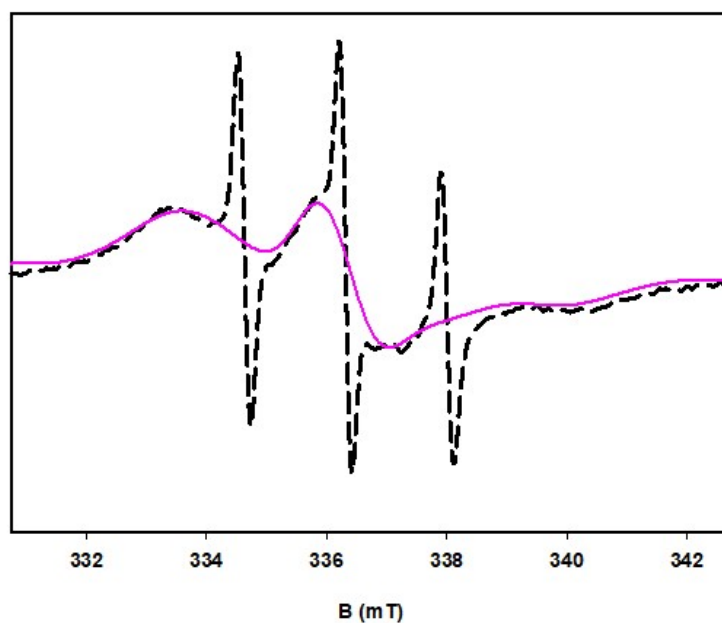


Figure S5. Simulation of the EPR spectrum of PDnT. Slow component, accounting for 96,2% of the signal.

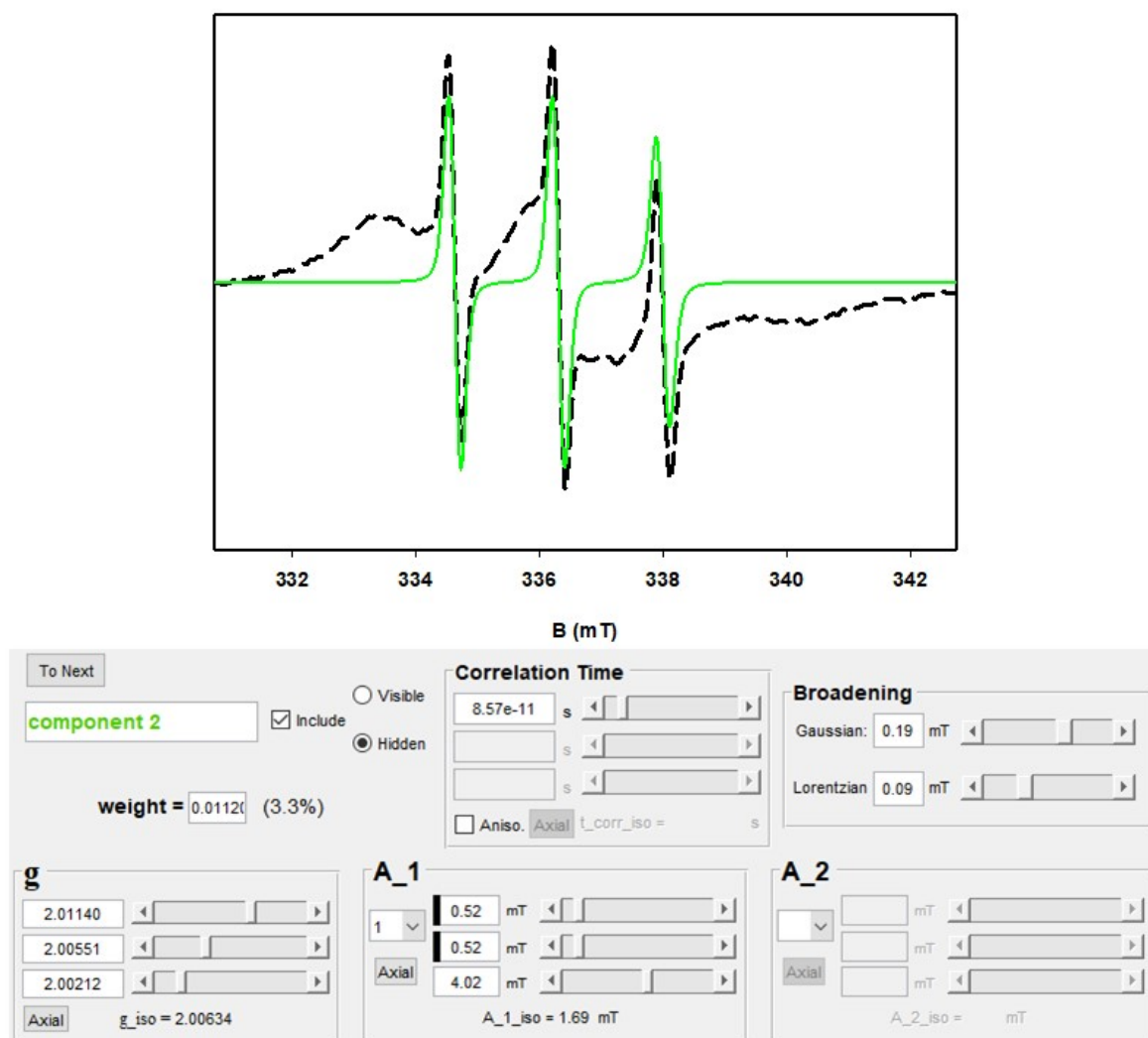


Figure S6. Simulation of the EPR spectrum of PDTnT. Fast component, accounting for 3.3% of the signal.

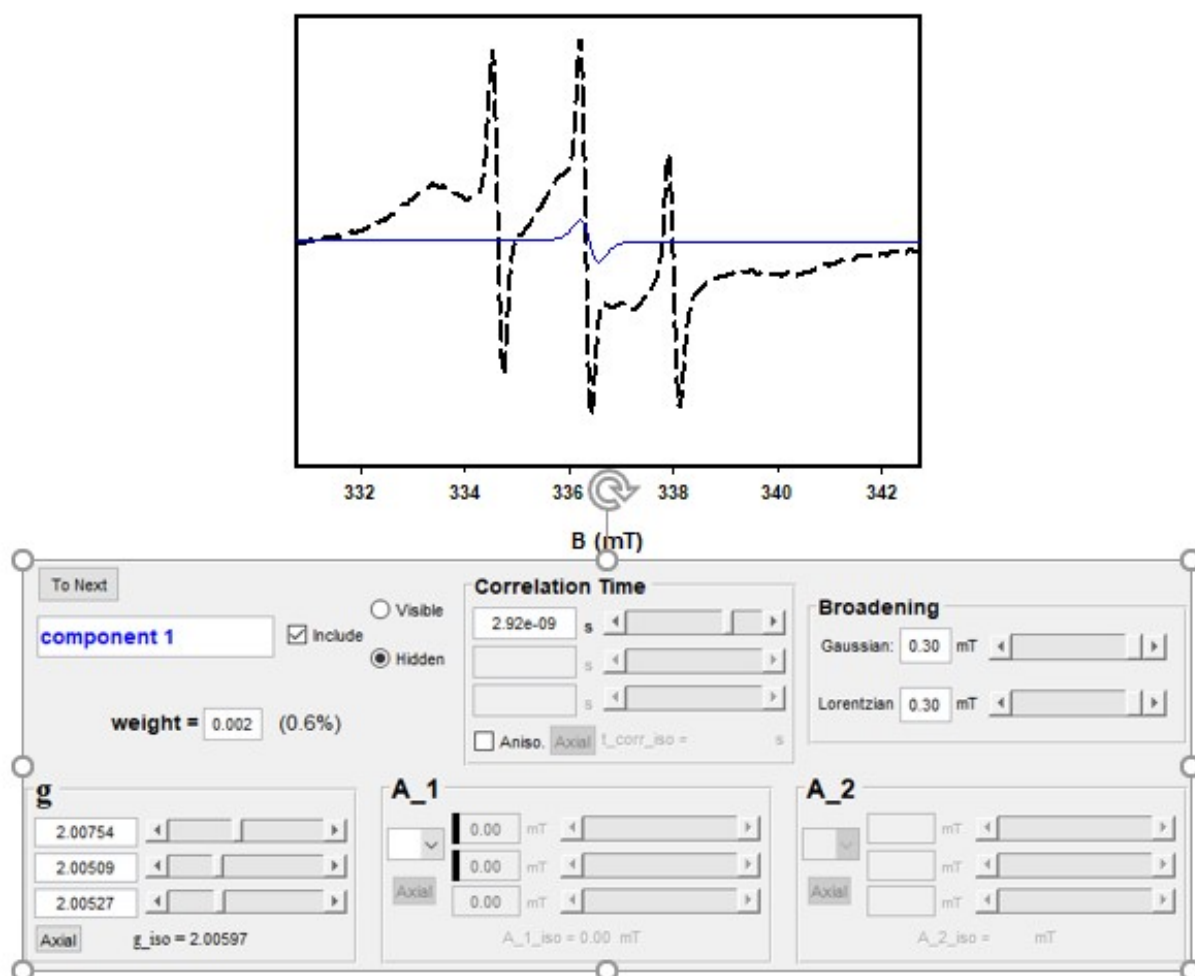


Figure S7. Simulation of the EPR spectrum of PDTnT. Slow component, accounting for 0.6% of the signal.

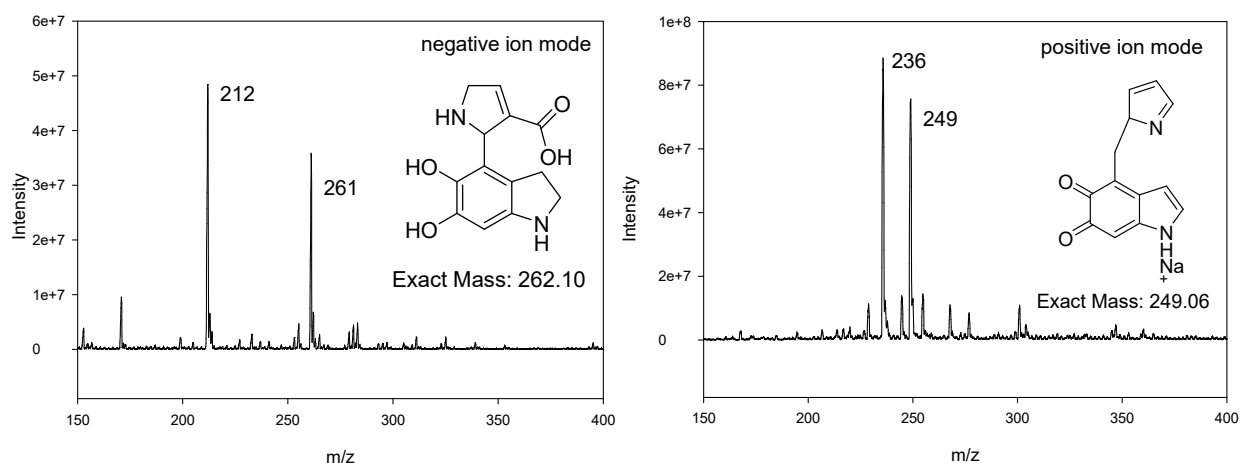


Figure S8. ESI-MS spectra of dialysate. Direct infusion, ESI type, desolvation gas (N₂), 242 L/h; cone gas (skimmer), 33 L/h; desolvation temperature, 120 °C, source block temperature, 80 °C; capillary voltage, 3.00 kV; cone voltage, 22 V; hexapole extractor, 3 V. The tentative identification of some peaks is reported, based on the structures reported in reference 4.

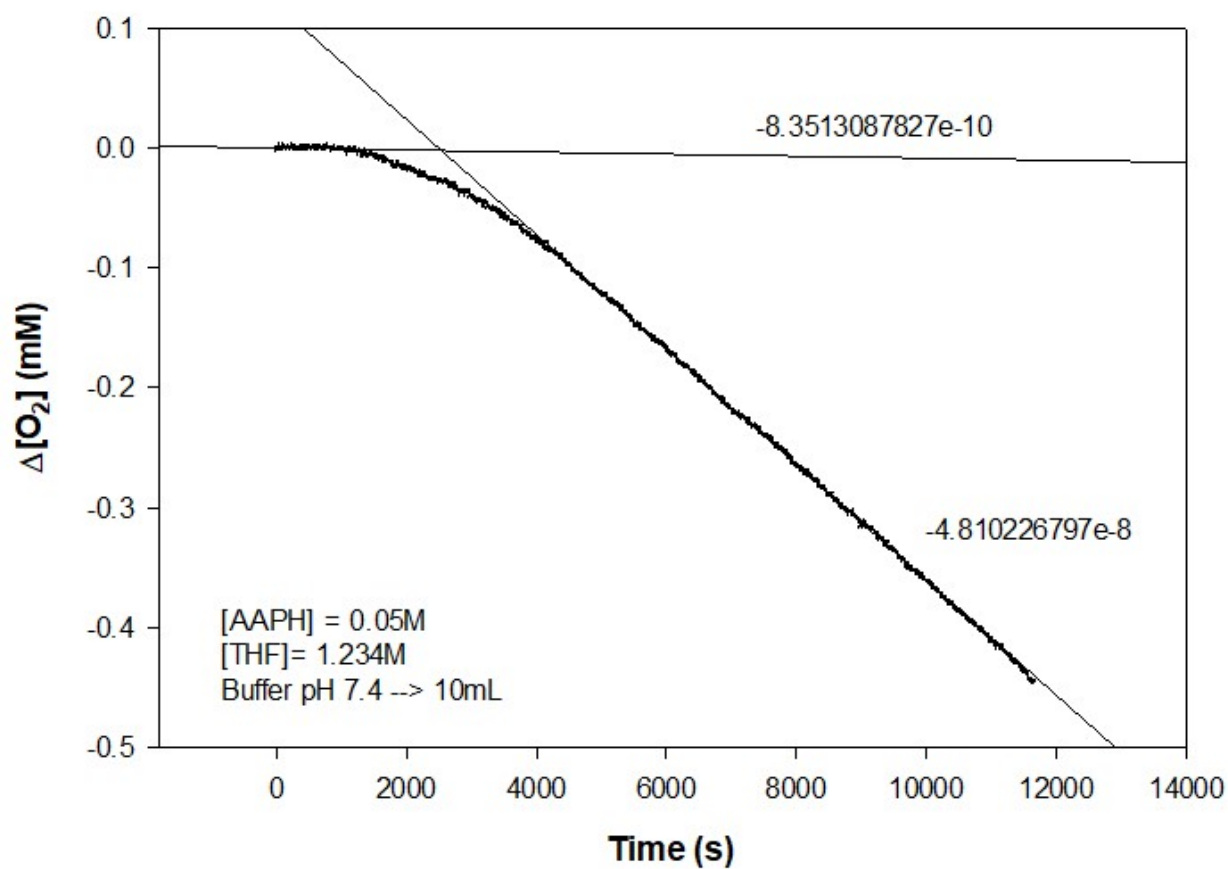


Figure S9. O_2 consumption measured during the autoxidation of THF initiated by AAPH at 30 °C in the presence of PDAn purified by only one centrifugation.

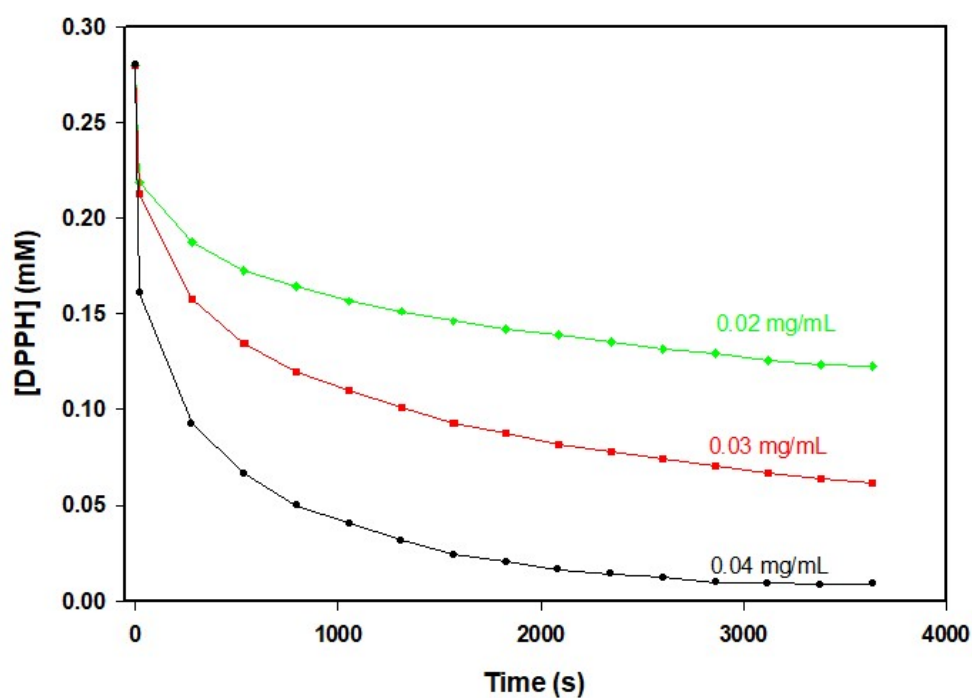


Figure S10. Reaction between DPPH• (0.28 mM) and PDAn (see concentration on each plot) purified by centrifugation and dialysis, in ethanol, studied by EPR spectroscopy.

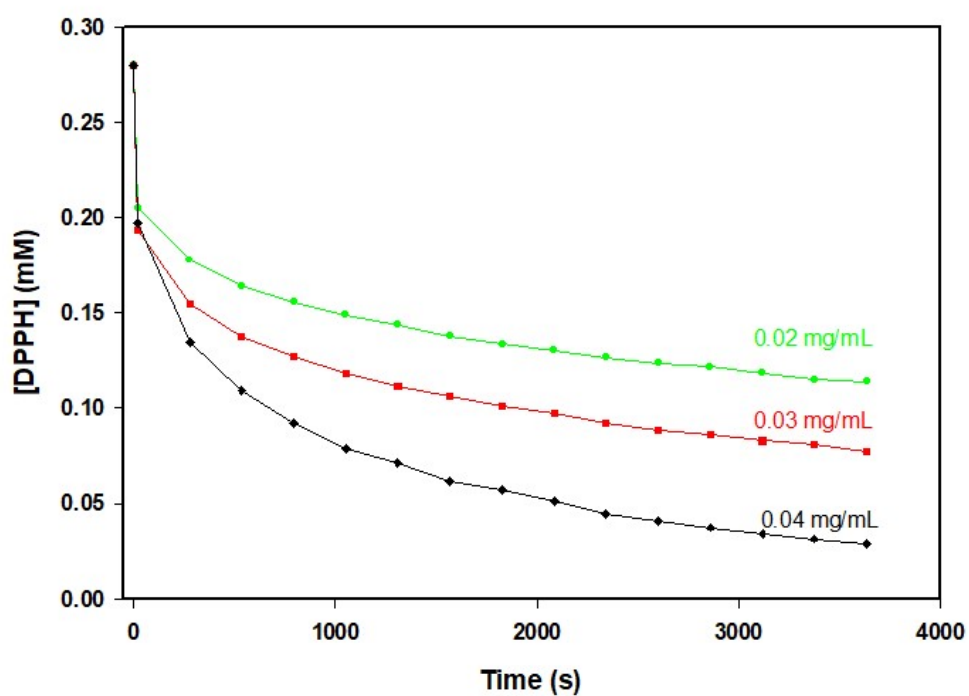


Figure S11. Reaction between DPPH• (0.28 mM) and PDAn (see concentration on each plot) purified by centrifugation, in ethanol, studied by EPR spectroscopy.

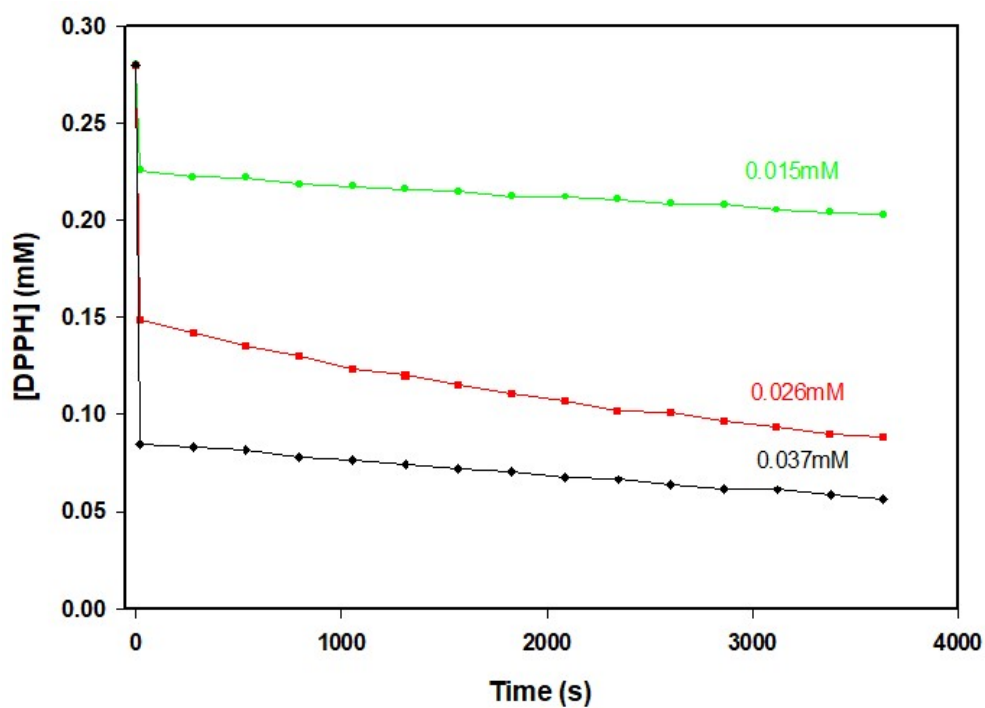


Figure S12. Reaction between DPPH• (0.28 mM) and DA (see concentration on each plot), in ethanol, studied by EPR spectroscopy.

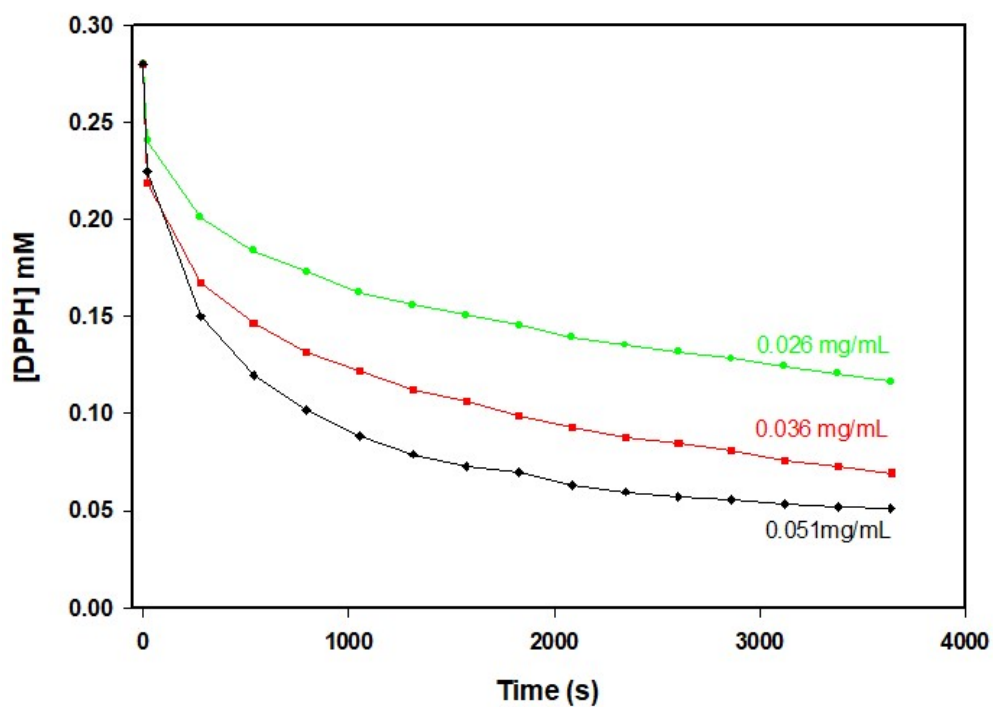


Figure S13. Reaction between DPPH• (0.28 mM) and PDAnT (see concentration on each plot), in ethanol, studied by EPR spectroscopy.

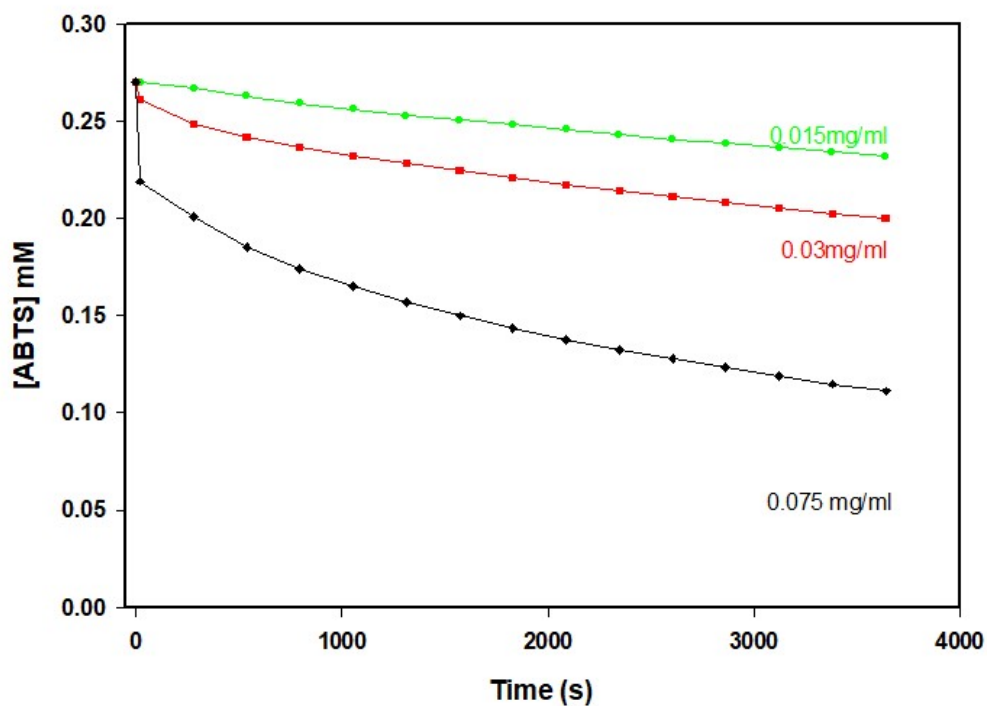


Figure S14. Reaction between ABTS+• (0.27 mM) and PDAnT (see concentration on each plot), in water, studied by EPR spectroscopy.

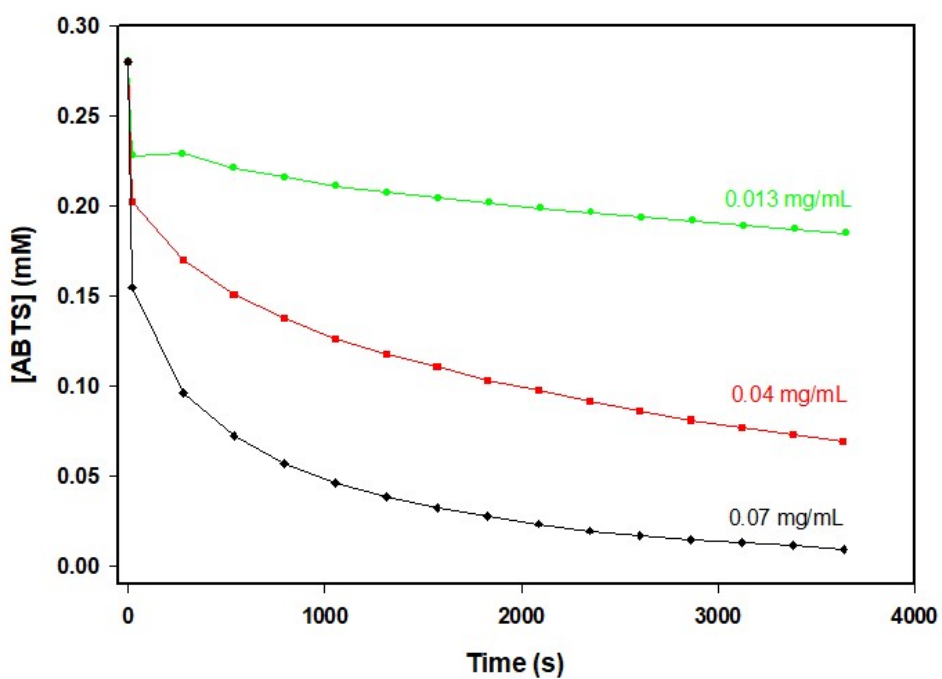


Figure S15. Reaction between ABTS+• (0.28 mM) and PDAn (see concentration on each plot) purified by centrifugation and dialysis, in water, studied by EPR spectroscopy.

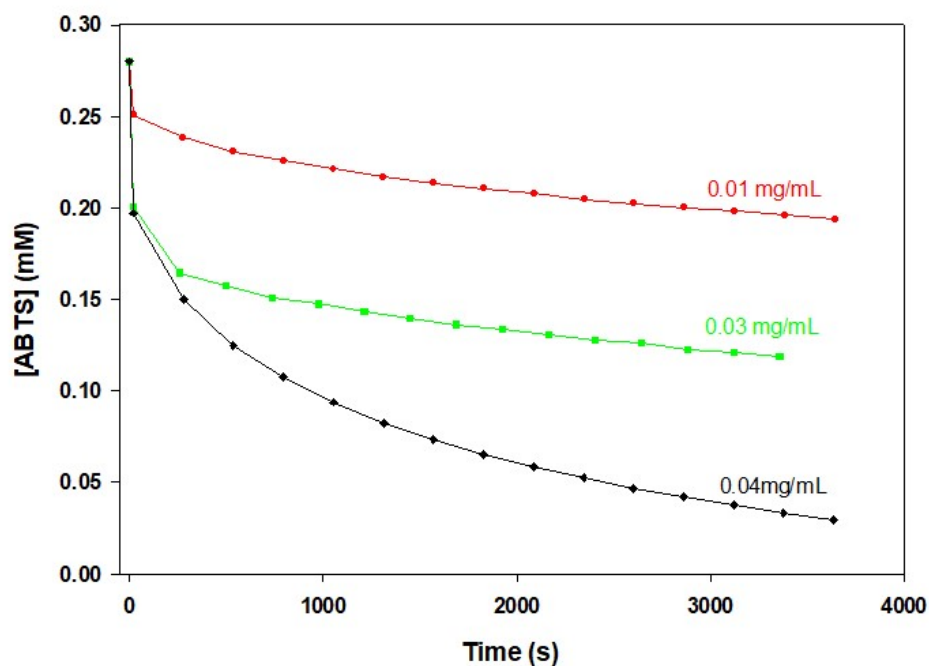


Figure S16. Reaction between ABTS+• (0.28 mM) and PDAn (see concentration on each plot) purified by centrifugation, in water, studied by EPR spectroscopy.

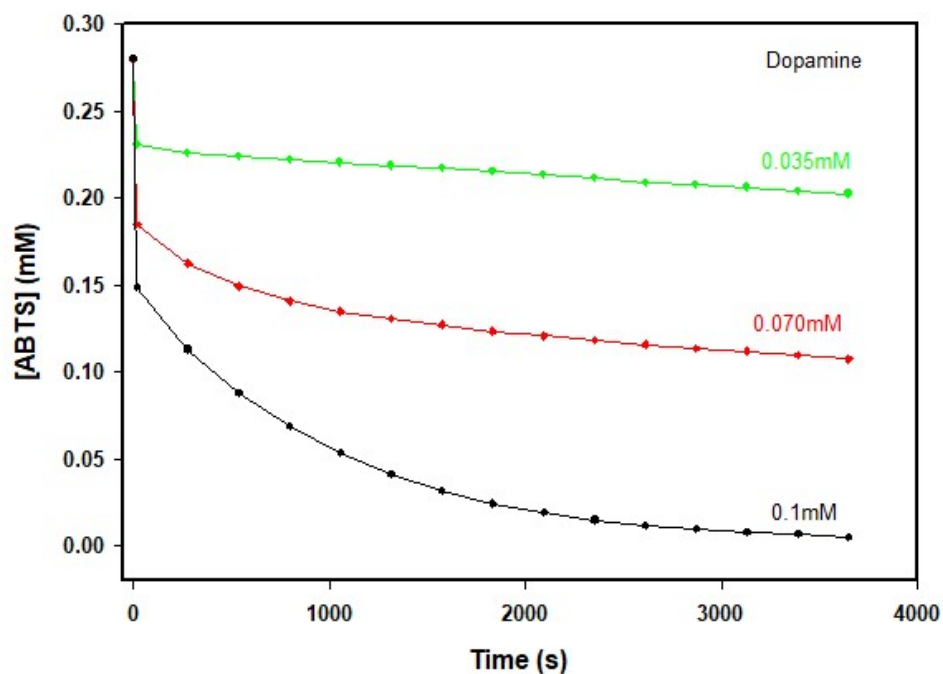


Figure S17. Reaction between ABTS+• (0.28 mM) and DA (see concentration on each plot), in water, studied by EPR spectroscopy.

Results of theoretical calculations

ROOH

b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

0,1

C,-0.0141778255,0.1533631361,0.1473633286\O,-0.220420026,-0.1143688699,1.5343469555\
H,1.0533586283,0.2364294202,-0.0796152573\H,-0.5442527706,1.060152293,-0.1637512249\
H,-0.4369583161,-0.7184070592,-0.360523779\O,0.375600412,0.9847911469,2.2809691345\
H,-0.4128704939,1.495046969,2.5369545767\\

ROO⁻

b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

-1,1

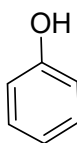
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ROO[•]

b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

0,2

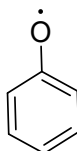
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b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

0,1

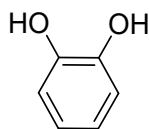
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b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

0,2

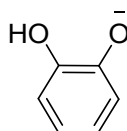
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0,1

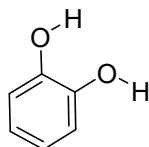
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b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

-1,1

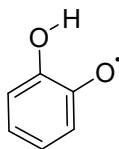
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b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

0,1

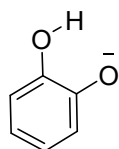
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0,2

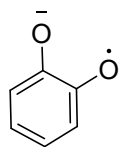
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b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

-1,1

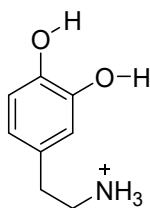
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-1,2

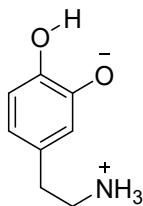
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b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

1,1

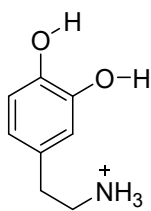
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b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

0,1

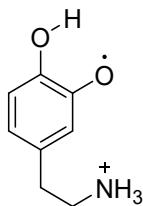
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b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

1,1

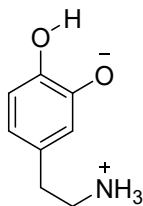
C,0.1016754149,0.0035932659,0.0257121823\C,0.0584094813,0.1175868861,1.4230990749\
 C,1.2338896444,0.2234119394,2.1707239414\C,2.4724908436,0.2202268479,1.5318224411\
 C,2.5281415382,0.1105082581,0.1331518203\C,1.3538382708,0.0012788867,-0.6111084468\
 H,-0.8978917682,0.1336955654,1.9382668971\H,1.2010165181,0.3159501375,3.2517667815\
 O,3.6195093623,0.3289095955,2.2707038127\O,3.7916651436,0.1228572147,-0.4057104015\
 H,1.4172699475,-0.0738351435,-1.6944101006\C,-1.1747075184,-0.1230539797,-0.7858764504\
 C,-1.8909450316,-1.465535507,-0.6119164244\H,-0.9689683235,0.0479238769,-1.8481503753\
 H,-1.896233806,0.6435280319,-0.4824656416\N,-1.0134236036,-2.6162842635,-1.0486369362\
 H,-2.1449923051,-1.6583093926,0.4308938064\H,-2.7973780347,-1.5191263965,-1.2158982583\
 H,-0.1171197764,-2.6028727724,-0.5501800561\H,-0.8076679646,-2.5771734813,-2.0513397752\
 H,3.7621894889,0.0587782325,-1.3706072713\H,4.3821461719,0.3201655618,1.6706837532\
 H,-1.4589081734,-3.5194080125,-0.8640681796\\



b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

1,2

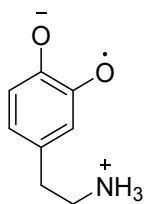
C,0.162975587,0.0003556264,0.018404659\C,0.0716998344,0.1622887368,1.4406360641\
 C,1.1963320385,0.2734027602,2.2488605216\C,2.4561988943,0.22737443,1.6546026204\
 C,2.6086384775,0.0670457761,0.2056453005\C,1.4033955071,-0.0435314233,-0.5784326731\
 H,-0.9103782276,0.2099771702,1.9017984083\H,1.1062064294,0.4006669034,3.3223229559\
 O,3.5779495149,0.3314909856,2.371887985\O,3.7793441213,0.0376401748,-0.2669464587\
 H,1.51556082,-0.1504916804,-1.6534836842\C,-1.1094402127,-0.1177704036,-0.7971482353\
 C,-1.8409914831,-1.452912008,-0.6273148017\H,-0.8973378564,0.0545786208,-1.8571895349\
 H,-1.8204796665,0.657276959,-0.4908084849\N,-1.0168229156,-2.6090170153,-1.1470756497\
 H,-2.0551507482,-1.6764176642,0.4185419876\H,-2.7745211992,-1.4623193682,-1.1903109974\
 H,-0.1003074034,-2.6544772673,-0.6898964645\H,-0.8532667909,-2.5346622476,-2.1556877207\
 H,4.3208867538,0.2758581293,1.7329682487\H,-1.4868063102,-3.5035418435,-0.9799713608\\



b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

O,1

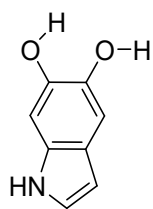
C,0.1045950248,0.0274783725,0.0490450257\C,0.1794141431,-0.0893410325,1.443601919\
 C,1.4343676416,-0.0286713396,2.0914617499\C,2.580737728,0.1382851317,1.339102835\
 C,2.559220011,0.2612200865,-0.0964247562\C,1.2839956062,0.1975632875,-0.7052445437\
 H,-0.7256477967,-0.1912542681,2.037779123\H,1.5020105339,-0.1079268462,3.1738532765\
 O,3.834190172,0.20908732,1.8979603399\O,3.7032719152,0.4225414639,-0.699996559\
 H,1.2255004655,0.2915185362,-1.7886313054\C,-1.2326939086,-0.0886785745,-0.6605287764\
 C,-1.4679652482,-1.4811847707,-1.2577744231\H,-1.2967634379,0.6185862412,-1.4947375698\
 H,-2.0540250253,0.1543394564,0.0236562556\N,-1.4050675552,-2.5294105918,-0.1706403664\
 H,-2.4465588309,-1.5733186912,-1.7308156632\H,-0.6921028958,-1.742963924,-1.9784807921\
 H,-2.219602662,-2.4788256419,0.4476832173\H,-0.5707872469,-2.3711862098,0.411659883\
 H,4.4013839591,0.3330558809,1.0996168389\H,-1.363787428,-3.4780985352,-0.5507430235\\



b3lyp/6-31+g(d,p) SCRF=(Solvent= Water)

0,2

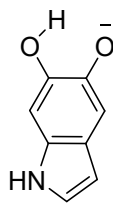
C,0.119839961,0.0434425178,0.0441493922\C,0.0089710556,0.2552302971,1.454879538\
 C,1.127268239,0.3077640525,2.2563839918\C,2.4621943381,0.1505554169,1.7337385823\
 C,2.5936914729,-0.0585888713,0.2532451354\C,1.3757999313,-0.105227021,-0.5185649139\
 H,-0.9777987652,0.3830645008,1.8944551044\H,1.032475667,0.4756773867,3.3267126258\
 O,3.4860240499,0.1909703468,2.4823247407\O,3.7327130247,-0.1880363263,-0.2905780148\
 H,1.4868983041,-0.2429203803,-1.5930133013\C,-1.1337539316,-0.0603161811,-0.8013969278\
 C,-1.8263973954,-1.4237232163,-0.6811593797\H,-0.9037263597,0.1412023642,-1.8533913392\
 H,-1.872732756,0.6864235911,-0.4901246116\N,-0.901446506,-2.5309072872,-1.1323351714\
 H,-2.092770055,-1.6507970403,0.3517650193\H,-2.7194435943,-1.4851765343,-1.3042572951\
 H,0.0116645043,-2.4429823181,-0.6692234456\H,-0.7354465667,-2.496847903,-2.1423200132\
 H,-1.2801210749,-3.4559920433,-0.9144981024\\



b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

0,1

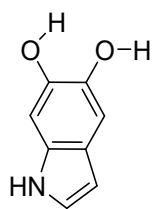
C,-0.0166784156,-0.0370478008,-0.0292847655\C,-0.0427415894,0.0672968009,1.3505417407\
 C,1.1848590145,0.1633227345,2.013541951\C,2.4250692267,0.1563276238,1.3226190693\
 C,2.4207711762,0.0490693718,-0.0813365114\C,1.2084577267,-0.0458861723,-0.7391651852\
 N,1.4624074005,0.2763777127,3.3597110301\C,2.8296149785,0.3400334784,3.5370065415\
 C,3.4562771718,0.2701307331,2.3182214847\H,4.5224045647,0.2966952934,2.1510052104\
 H,3.2451416094,0.430945353,4.5285411471\H,0.7762981254,0.3063965159,4.0991058648\
 H,3.3438676616,0.0398731237,-0.6518519951\H,-0.9879707433,0.0729768438,1.8803857712\
 O,1.0883696822,-0.1551912075,-2.1169849979\O,-1.2147606863,-0.1335979543,-0.7160880884\
 H,-1.0264321858,-0.1994089729,-1.6631093016\H,1.9652868762,-0.1552361066,-2.5228149028\\



b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

-1,1

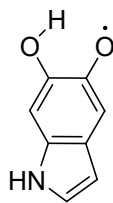
C,-0.0383776067,-0.0328985853,-0.0062710921\C,-0.0671126565,0.0624937086,1.3687264883\
 C,1.1737202778,0.1608949431,2.0204512761\C,2.3984104927,0.1626411395,1.3091834332\
 C,2.386674393,0.0627699055,-0.1032846549\C,1.1719843153,-0.0368552102,-0.7913079218\
 N,1.468746755,0.2683290408,3.3692391744\C,2.8367839522,0.3373250122,3.5283097412\
 C,3.4426268048,0.276231378,2.2952509227\H,4.5071628816,0.3085633828,2.1143968791\
 H,3.2676097184,0.424878875,4.5137542952\H,0.7930694827,0.2924119018,4.117661067\
 H,3.3155689173,0.0619899264,-0.6662374952\H,-1.0062918473,0.0604047851,1.911449817\
 O,1.0282156554,-0.1358547821,-2.1068948517\O,-1.2099068335,-0.1341837957,-0.7422166774\
 H,-0.8776609091,-0.1846761889,-1.6642570505\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,1

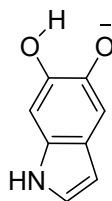
C,-0.0203048227,-0.0379245701,-0.0311202504\C,-0.0483227028,0.0666239978,1.3520140391\
 C,1.1833613793,0.1633627182,2.0164921641\C,2.4266557222,0.1570156587,1.3251763099\
 C,2.4248364605,0.0497253653,-0.0823920647\C,1.2095012538,-0.0459654529,-0.7404543681\
 N,1.4625441226,0.276847967,3.364129199\C,2.8317025262,0.3409665053,3.5435333074\
 C,3.4586881033,0.2711519099,2.3211309089\H,4.5264258981,0.2981763637,2.1528347489\
 H,3.2483534751,0.432072371,4.5363197323\H,0.77850162,0.3054417898,4.1050238564\
 H,3.3549538883,0.0419145987,-0.645037367\H,-0.9971038479,0.0715871866,1.8788812098\
 O,1.0692455541,-0.1555482401,-2.1121603361\O,-1.2031031133,-0.1352230781,-0.7254283994\
 H,-0.9985751323,-0.1992577267,-1.6717437367\H,1.9328812093,-0.1578899935,-2.5471548904\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

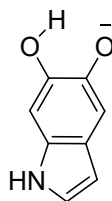
C,-0.075847987,-0.0326301314,0.0006915062\C,-0.0920971248,0.0647927415,1.3726750207\
 C,1.1634510495,0.1605292701,2.0069154609\C,2.4214604621,0.1602359438,1.2929095555\
 C,2.425913794,0.0617112161,-0.0880873648\C,1.1774860839,-0.0384786156,-0.7868818555\
 N,1.4560450379,0.2665408319,3.3320115713\C,2.8400811815,0.3362903207,3.5079577493\
 C,3.4599556649,0.2748061638,2.2939104573\H,4.5252407536,0.3058424465,2.1167569498\
 H,3.2525733351,0.4239948547,4.5023082194\H,0.7784110992,0.2936620264,4.0805998277\
 H,3.3442343812,0.0579346451,-0.66659656\H,-1.0229307837,0.0673317059,1.9298251783\
 O,1.062867915,-0.1333774304,-2.047919248\O,-1.2096309586,-0.1299171372,-0.7220072711\
 H,-0.9159901109,-0.1848034152,-1.6571158466\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

-1,1

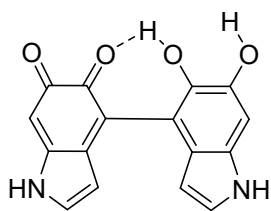
C,-0.0535920645,-0.0342878283,-0.0027522884\C,-0.0802213223,0.0609058003,1.3751283322\
C,1.1695690103,0.1605181583,2.0242151985\C,2.3940076383,0.1633532241,1.3082136676\
C,2.3820165792,0.0636322383,-0.1095608726\C,1.1628376959,-0.0373125651,-0.7980566872\
N,1.4704036837,0.2682108091,3.3749720215\C,2.8411601194,0.3382474147,3.5330143117\
C,3.4415869959,0.2773852541,2.2923953752\H,4.5075415673,0.3103207584,2.1068798515\
H,3.2764383648,0.4261899893,4.5183922926\H,0.7981026312,0.2912176298,4.1260211793\
H,3.3131583871,0.0640978336,-0.6732673813\H,-1.0198962725,0.0580280914,1.9216747908\
O,0.9903718957,-0.135810775,-2.1000257524\O,-1.1973509316,-0.1367656272,-0.758960357\
H,-0.8049101849,-0.1834649691,-1.6703303312\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

-1,2

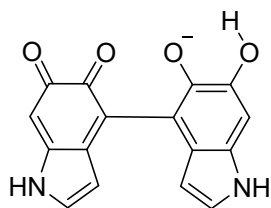
C,-0.1126204086,-0.1092352571,-0.0544006702\C,-0.0658769369,0.0147810466,1.3719015222\
C,1.157384629,0.1396983303,2.0063472673\C,2.4178057492,0.15217429,1.294015486\
C,2.4216969348,0.0319948338,-0.0928004971\C,1.2015705586,-0.1037424308,-0.8266524371\
N,1.4548713696,0.2724464298,3.3518972304\C,2.829818655,0.3671621326,3.514601248\
C,3.4499431388,0.2986898633,2.2918967938\H,4.5163933907,0.3466742923,2.1195558447\
H,3.2532228255,0.4768344471,4.503167651\H,0.7796521113,0.2966891024,4.1003805692\
H,3.3538728328,0.0370299997,-0.653645101\H,-1.0021945182,0.0086128685,1.9243586434\
O,1.1824254065,-0.2189776529,-2.0959577771\O,-1.2118730925,-0.2225243339,-0.6823785575\\



b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

0,1

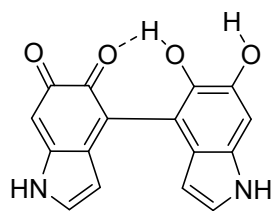
N,-0.0056292713,0.0187195129,0.0082858205\C,0.0023572062,0.0066309298,1.3759752217\
 C,1.4359838794,0.0067748956,1.7863701604\C,2.1902015884,0.0392568182,0.5651888706\
 C,1.2970307432,0.0501654375,-0.4626454051\C,-1.054364684,-0.0156316834,2.2296477652\
 C,-0.7597264718,-0.0044753796,3.6318059608\C,0.7460695112,0.0937286816,4.0896815245\
 C,1.8176761968,-0.0005372193,3.1089329089\C,3.2343431541,-0.0999708413,3.5350107603\
 C,4.0568607061,-1.1579119329,3.061233267\C,5.4219872166,-1.2129902353,3.4524556045\
 C,6.0043443935,-0.274812756,4.305900946\C,5.180897447,0.7285309328,4.7844427892\
 C,3.8186943028,0.8127287766,4.4156156456\N,5.9765824536,-2.3316259122,2.8707083539\
 C,5.0086795429,-2.9898893105,2.1429018622\C,3.8217712664,-2.3087114718,2.2324105417\
 O,5.6993778188,1.6751047113,5.6448974667\O,3.1370315831,1.8979039894,4.9549882445\
 O,-1.6101236775,-0.0536012345,4.5186285868\O,0.9403819131,0.2679487526,5.2939404674\
 H,6.9330827564,-2.6348925677,2.980208996\H,2.8973218148,-2.5965491289,1.7582795308\
 H,5.2485777565,-3.8990562282,1.6138716715\H,-0.8362905486,0.0370580545,-0.5667058513\
 H,3.2622915538,0.0593141159,0.4697543899\H,1.4798911173,0.0813309834,-1.5264156387\
 H,4.9705554794,2.2624537372,5.9009886917\H,2.2941832551,1.5670768057,5.3162061248\
 H,7.0442192156,-0.327548404,4.6049258554\H,-2.0829347897,-0.0526699237,1.8932139417\\



b3lyp/6-311++g(d,p) SCRF=(SMD, Solvent=Water)

-1,1

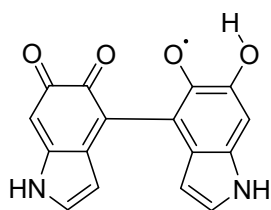
N,0.0275085151,0.0308986907,-0.0005442268\C,0.0103303443,0.0165553118,1.358087451\
C,1.4164979863,0.0749688131,1.7934439707\C,2.2068976695,0.1479880767,0.5788818832\
C,1.3454832406,0.1216885241,-0.4646884796\C,-1.0924526411,0.0328162957,2.1890155283\
C,-0.8612036636,0.0838211771,3.5788334563\C,0.6181803016,-0.0544021029,4.0722502044\
C,1.756677459,0.1186502956,3.1234087466\C,3.1100890562,0.1933403913,3.6593261414\
C,4.1604449169,-0.6879736542,3.2528304658\C,5.4365548822,-0.5730483886,3.848411421\
C,5.7410901241,0.3938070308,4.8261722865\C,4.7280018304,1.242724149,5.1933010432\
C,3.3939699892,1.1920468334,4.6358570384\N,6.2349790464,-1.5781109483,3.33979549\
C,5.5026377523,-2.3297618552,2.4490795857\C,4.2274367863,-1.8210193958,2.3688096565\
O,4.9298112014,2.2410921638,6.1288774811\O,2.556718239,2.108394697,5.0300403264\
O,-1.7363373839,0.2093844552,4.4595266942\O,0.7849773308,-0.4293027764,5.2233664712\
H,7.1977703954,-1.7448084194,3.5925417043\H,3.4390382127,-2.2118480208,1.7450953125\
H,5.9523460197,-3.1661607775,1.9371526062\H,-0.7947609154,0.045962257,-0.5878206559\
H,3.2800230686,0.2100426505,0.5140713561\H,1.5355032966,0.1617842299,-1.5261421306\
H,4.0623266918,2.6942381268,6.1650710874\H,-2.1021400389,0.0733159193,1.7980692548\
H,6.7278971722,0.4698245772,5.2693888422\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,1

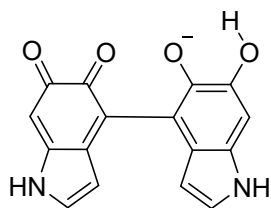
N,-0.1484941199,0.1264636637,0.00159293\C,-0.1657279945,0.033839703,1.3718149229\
 C,1.2589006481,-0.068273303,1.8015524183\C,2.0364896292,-0.0048756487,0.5938264172\
 C,1.162004191,0.1158612399,-0.4485271954\C,-1.2368340173,0.0183605596,2.2121232663\
 C,-0.9628503423,-0.0665887128,3.6254828235\C,0.5410543987,-0.0510601498,4.104686529\
 C,1.622768101,-0.1709352921,3.1312283276\C,3.0287028725,-0.3773521368,3.5595559498\
 C,3.8064835036,-1.4376277103,3.0080471806\C,5.1672767985,-1.586959154,3.400162882\
 C,5.7914377653,-0.7426161889,4.3255030693\C,5.0102002259,0.2597210997,4.8812822353\
 C,3.6510522439,0.4337182322,4.5159595742\N,5.6715750273,-2.6874451486,2.7389551312\
 C,4.6781636358,-3.247515285,1.9618029526\C,3.5224349924,-2.5146082794,2.0973043232\
 O,5.5543535653,1.1090973074,5.8095960738\O,3.0246412046,1.492028062,5.1470108595\
 O,-1.8342487356,-0.1351867262,4.4907871399\O,0.7288659585,0.0917576105,5.3194669276\
 H,6.6089150145,-3.0482286527,2.8346865182\H,2.586745317,-2.7221092701,1.5999602017\
 H,4.8771656158,-4.1286567919,1.3691151699\H,-0.9639064935,0.2290850625,-0.5849363268\
 H,3.1113209788,-0.0420706731,0.5187269098\H,1.3666882585,0.2012913844,-1.5068018054\
 H,4.8411611291,1.7010145499,6.1061340565\H,2.1440702568,1.1731819071,5.4409728582\
 H,6.8271680756,-0.866007765,4.6241068026\H,-2.2648001544,0.0496512923,1.8684889851\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

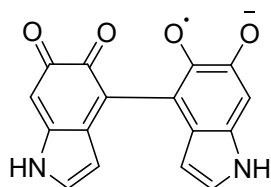
N,-0.0551313158,0.1830309696,0.0069369345\C,-0.0231924732,0.0864805011,1.3744178018\
C,1.4164055154,0.0078990179,1.7499476289\C,2.1536577138,0.0812708667,0.5113271957\
C,1.2410089528,0.1850630754,-0.4954021176\C,-1.0617325024,0.0884667452,2.2590217974\
C,-0.7456874878,0.0062605225,3.6625006926\C,0.7662567454,-0.1592875635,4.0880211614\
C,1.8186243435,-0.0872957589,3.0590921329\C,3.2338150189,-0.1699381541,3.4676964641\
C,4.078314216,-1.2084466323,3.0757917272\C,5.4506155991,-1.2364445594,3.5257586551\
C,6.026083091,-0.2537617379,4.3555819496\C,5.1988456973,0.7735860641,4.7392916909\
C,3.7849051878,0.868188009,4.3155344274\N,6.0175019656,-2.3649910411,3.0177419562\
C,5.077381132,-3.0698977116,2.2670332854\C,3.8874219107,-2.4004780627,2.2796570376\
O,5.6274746524,1.7802585022,5.5256769154\O,3.1437962721,1.8886017456,4.7001219472\
O,-1.5900537938,0.052063043,4.5589280379\O,1.0021070805,-0.3935197312,5.2678821308\
H,6.9712640244,-2.6595950464,3.1726365271\H,2.9790495927,-2.7098492339,1.7848731026\
H,5.3532732192,-3.9983256673,1.789097402\H,-0.8923563867,0.271057514,-0.5504128113\
H,3.226237927,0.056751326,0.3984645405\H,1.4017182083,0.2649356817,-1.5615414014\
H,4.8532268443,2.3748724755,5.6300072403\H,-2.0983774204,0.1771809099,1.9521930455\
H,7.0611035046,-0.3010984182,4.6763189002\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

-1,1

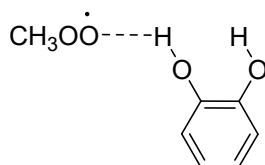
N,-0.1281244583,0.0322388946,0.0484449512\C,-0.0215016429,0.0635148859,1.4101602867\
C,1.4007501725,-0.1224900932,1.7193707536\C,2.0804683521,-0.2228120899,0.4385512725\
C,1.1351790119,-0.127449716,-0.5331597811\C,-1.0263292195,0.330541712,2.329644229\
C,-0.6674282094,0.4005548196,3.6984549974\C,0.7791925804,-0.0574691849,4.0666523088\
C,1.8609328325,-0.082917824,3.0234320643\C,3.239853123,-0.1790811128,3.4579014732\
C,4.1682687192,-1.1621656636,2.9757100716\C,5.4883625295,-1.1872846112,3.484196131\
C,5.9689843684,-0.2659459113,4.4466891524\C,5.0805937448,0.6812716682,4.8910010683\
C,3.7031045895,0.7798561244,4.4206172557\N,6.1368546398,-2.2727254477,2.9281736993\
C,5.2696341092,-2.9453877818,2.0926340253\C,4.0521469202,-2.2980751591,2.0980274188\
O,5.42565697,1.6426472449,5.8035621205\O,3.0215477206,1.7805166791,4.8672899034\
O,-1.4148827178,0.7651089938,4.6319346088\O,0.9537791864,-0.5475345795,5.176803387\
H,7.0888721032,-2.5460194678,3.1198619133\H,3.1817050431,-2.6015834467,1.5347191055\
H,5.5920883081,-3.825662828,1.5556604188\H,-0.9840869568,0.1801509747,-0.4656168871\
H,3.1392902609,-0.3591774757,0.2842159017\H,1.2330215326,-0.1579292262,-1.6087812938\
H,4.595420666,2.1715283414,5.8707745202\H,-2.0394031606,0.5676160645,2.0199356503\
H,6.989605916,-0.3007971331,4.8173352714\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

-1,2

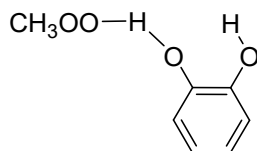
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C,1.3961855336,-0.082400953,1.7239952346\C,2.1016238018,-0.1230927705,0.4571909011\
C,1.1691029131,-0.0438722198,-0.5300248429\C,-1.0554514903,0.2159130972,2.2995949632\
C,-0.7154752955,0.2524456616,3.682224299\C,0.7640400336,-0.0858764283,4.0731515931\
C,1.8327001943,-0.079265271,3.0331381226\C,3.2258995263,-0.1663290194,3.460635784\
C,4.1165221814,-1.1587641763,3.0170158685\C,5.4768932935,-1.1835806302,3.5134735846\
C,5.9867236852,-0.2751231411,4.4245917982\C,5.1418533243,0.7625147498,4.9197300148\
C,3.7117357109,0.8578523204,4.3753171429\N,6.0930142739,-2.2819828711,2.9466009119\
C,5.1907544071,-2.9538573886,2.1405125832\C,3.9798759925,-2.3046652924,2.157181307\
O,5.5270465986,1.6059901257,5.778603563\O,3.0114627073,1.8534218142,4.6866246628\
O,-1.5102955158,0.5160237351,4.6039398707\O,0.9751280285,-0.469551004,5.2199310419\
H,7.0417262953,-2.5743329851,3.1257521906\H,3.0976697274,-2.608745833,1.614034306\
H,5.4903096856,-3.8490156858,1.6142170741\H,-0.9613887068,0.1629615757,-0.5069449865\
H,3.1681337906,-0.2084628863,0.3190338675\H,1.2919297386,-0.0409463069,-1.6036949548\
H,7.0071533715,-0.3416571336,4.7916934252\H,-2.0816400512,0.3896235521,1.9919925442\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

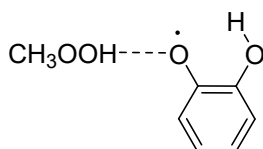
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 C,1.9662246988,1.9926020639,-0.078919262\C,3.2042266587,1.3648992889,0.0798469858\
 C,3.2771601281,-0.0313207663,0.1663431808\C,2.1131108862,-0.7927856827,0.0937661852\
 O,2.1849621463,-2.1601941802,0.1785019765\O,-0.2117319448,-1.0080464794,-0.1251175323\
 O,-2.7864660362,0.0664278095,-0.4454687065\O,-2.8054131182,1.3849800907,-0.52064224\
 C,-4.161651471,1.8958634519,-0.6857361795\H,-0.1724749776,1.7091982866,-0.2755182337\
 H,1.9033967744,3.0743070797,-0.1465549022\H,4.1144571694,1.9537447955,0.1369675368\
 H,4.2295883964,-0.5379578819,0.2898108835\H,1.2844423442,-2.5165952296,0.1088297498\
 H,-4.7530513794,1.5933004339,0.1792415842\H,-4.5722927916,1.4940358544,-1.6127705039\
 H,-4.0454384818,2.977883252,-0.7339492983\H,-1.0598591906,-0.5275750552,-0.2379707619\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2\

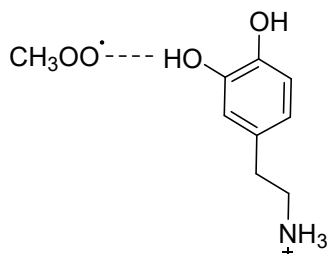
C,0.4430815506,0.7848707838,0.3916324855\C,0.3949608531,0.283839565,1.6915202466\
 C,1.3865974591,-0.6386091756,2.1515524257\C,2.4258527681,-1.0282067894,1.2773331794\
 C,2.4700307063,-0.5159490066,-0.0118267369\C,1.4797594279,0.3859179172,-0.4534732049\
 O,-0.5909563468,0.6571677277,2.537897269\O,1.230856923,-1.0983839832,3.388859881\
 O,3.1594250292,-0.9598417883,4.7982560127\O,4.1548871922,-0.4257132936,3.9980206075\
 C,4.711835431,0.7334274954,4.6378698005\H,3.1731491351,-1.7297588563,1.6319324287\
 H,3.2660839739,-0.8151670194,-0.6857036167\H,1.5215708074,0.7766778539,-1.4651868139\
 H,-0.3199710046,1.4810480032,0.0596073915\H,-0.434906402,0.2048908969,3.3879584042\
 H,5.135868425,0.4528153299,5.6059325678\H,3.9374058505,1.4950925456,4.7637902927\
 H,5.4934040216,1.0831718098,3.9608954032\H,2.158585728,-1.1432999804,3.9925892062\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

C,3.0568657991,-0.0609352012,-0.2625097367\C,1.9913926579,-0.9529728145,-0.1554357095\
 C,0.6190694968,-0.4805854753,0.0504484247\C,0.4052955332,0.9397036039,0.138824812\
 C,1.4716086178,1.7980971548,0.0301412224\C,2.7949698803,1.3025556141,-0.1698345325\
 O,2.1731547847,-2.2741063784,-0.2352402412\O,-0.2922427377,-1.3607535499,0.1376256068\
 O,-2.9506750278,-0.8816150653,0.6218127083\O,-3.0800826426,0.5559720819,0.4238914967\
 C,-3.7525686071,0.7540288605,-0.8173697119\H,-0.6110794357,1.2902950266,0.2887190607\
 H,1.3164516127,2.8701743992,0.0953413624\H,3.6154803084,2.0080051828,-0.251489676\
 H,4.0632034,-0.4359336809,-0.4145216048\H,1.2907183958,-2.6888795659,-0.1329490119\
 H,-4.7400703655,0.280411867,-0.8068002557\H,-3.158787959,0.3729069535,-1.6558080509\
 H,-3.8625384487,1.8394490441,-0.9016498117\H,-1.9859652627,-1.0169980569,0.4356636489\

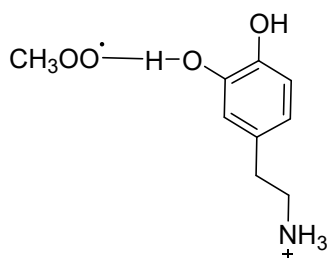


b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

1,2

C,0.0045990223,0.0214821804,0.0114217973\C,0.0122918429,-0.0048802191,1.4131750702\
 C,1.2169581705,0.0168177805,2.1222811928\C,2.4292478891,0.0653197626,1.4380698161\
 C,2.4380554051,0.0950249122,0.032340766\C,1.2323004807,0.0722177403,-0.6716056348\
 H,-0.9250400259,-0.0331753601,1.9617494128\H,1.2254121323,0.0024787269,3.2077551523\
 O,3.6077611744,0.0905228612,2.1352497529\O,3.6763851651,0.1503558511,-0.5438527194\
 H,1.2530798214,0.1104343245,-1.7578490589\C,-1.3003107923,-0.0255485535,-0.7617747221\
 C,-1.946286713,-1.4142256059,-0.7994539142\H,-1.149183642,0.3345496433,-1.7852261482\
 H,-2.0399870073,0.6394947021,-0.3032749802\N,-1.0290123581,-2.4243908287,-1.4498235759\
 H,-2.1512078506,-1.7933292199,0.2026401222\H,-2.8704609153,-1.4142337324,-1.3785040928\

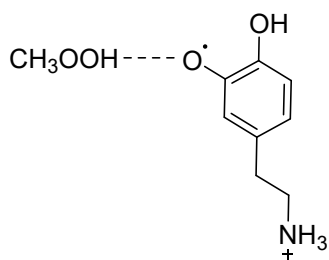
H,-0.1142558178,-2.4364846469,-0.9856396648\H,-0.868718884,-2.2098034157,-2.4382281425\
H,3.6361556207,0.168683667,-1.5250101995\H,4.3392112808,0.1288682993,1.497690331\
H,-1.4166041698,-3.3704972691,-1.4002405572\O,3.8792915682,0.2058545758,-3.3354522714\
O,2.7096668656,0.1594978893,-3.9472904294\C,2.8590349782,0.1835869674,-5.398334393\
H,1.8402722692,0.1412354446,-5.7816597621\H,3.4391264894,-0.689042404,-5.7007478446\
H,3.3559611118,1.1127913917,-5.6794296266\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

1,2

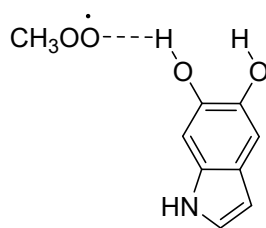
C,0.0095027603,0.0762076637,-0.0033519962\C,0.0114975467,-0.0004675885,1.3867288614\
C,1.2500665146,-0.0671151187,2.0737501007\C,2.4616056695,-0.0632406829,1.3883249154\
C,2.4606308864,0.0079518106,-0.003914888\C,1.2256472068,0.0808274473,-0.724779867\
C,-1.2906577441,-0.0210324729,2.1631156592\C,-1.6648768907,-1.3978173017,2.7216873667\
N,-1.8844406926,-2.4045630148,1.6156675562\O,3.621568651,0.0150331063,-0.6926836944\
O,1.3318783957,0.1539371668,-2.0375094444\O,-0.5252374691,0.178194459,-3.5524714072\
O,-1.7162982487,0.1345739963,-2.8411483466\C,-2.8096387208,0.0635477344,-3.7656178547\
H,1.2586232823,-0.1122270457,3.158863277\H,3.4068756669,-0.1090748231,1.918607489\
H,-0.9215817692,0.1436268298,-0.5575679984\H,-2.1087553286,0.3577791507,1.5420244934\
H,-1.2217872975,0.6459855958,3.0293549473\H,-0.8788446644,-1.8099644912,3.3555566972\
H,-2.5949161585,-1.3537553084,3.2890462015\H,-1.0568745166,-2.4869175925,1.0160255429\
H,-2.6735465999,-2.1449730411,1.0161672338\H,0.397533304,0.1713243089,-2.671575104\
H,3.4064192818,0.0720207915,-1.6421872749\H,-2.0832374451,-3.3350352108,1.9936835927\
H,-3.7051731178,0.0349725044,-3.1424504281\H,-2.7275449475,-0.8456755439,-4.367961597\
H,-2.8118276288,0.9500367028,-4.4061851591\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

1,2

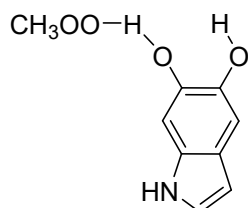
C,0.0140717425,0.1616915149,0.004637066\C,0.0239547763,0.0199830432,1.3741086191\
 C,1.2732748083,-0.1729897925,2.0548480291\C,2.4845439154,-0.2280800358,1.3800398895\
 C,2.4859622601,-0.0913631826,-0.008351427\C,1.2392476962,0.1115003994,-0.7478364801\
 C,-1.2612072864,0.0552239091,2.1764094274\C,-1.7245534675,-1.3181981908,2.6738955367\
 N,-2.0729931965,-2.240322674,1.5277823412\O,3.6158460296,-0.1341471899,-0.7151841336\
 O,1.320429281,0.2317312802,-2.0080887813\O,-0.7833718593,0.7637615549,-3.6992030061\
 O,-1.9490066034,0.4455304043,-2.8849972455\C,-2.4901969802,-0.7767341503,-3.3805451922\
 H,1.2713337911,-0.26909719,3.1365188806\H,3.4195366228,-0.3687001182,1.9111810004\
 H,-0.9054427106,0.320852576,-0.5521157111\H,-2.0581287658,0.5245938961,1.5911464302\
 H,-1.1246329422,0.6711636128,3.0718542229\H,-0.9524844594,-1.8274645396,3.2519645385\
 H,-2.6238677803,-1.2290491945,3.2834005662\H,-1.281932293,-2.3609126175,0.886847151\
 H,-2.8613057472,-1.8846385551,0.9787895195\H,-0.046232716,0.558149855,-3.0693629948\
 H,3.369301498,-0.0136615283,-1.656608985\H,-2.3337389326,-3.1701109513,1.8686928128\
 H,-3.3806638811,-0.9522435884,-2.7693193767\H,-1.7822833687,-1.6037901753,-3.2557568795\
 H,-2.7761956212,-0.679242664,-4.4332249997\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

C,-0.0261012336,0.000504937,0.076873705\C,-0.0024506034,0.0001904771,1.4635728915\
 C,1.2474699137,-0.0002114755,2.1214488684\C,2.4378260587,-0.0002960376,1.34320559\
 C,2.4190527751,0.0000102959,-0.0600828915\C,1.1779561287,0.0004131583,-0.6788894199\
 O,1.1040505227,0.0007347629,-2.0521634563\O,-1.1701919632,0.0009406092,-0.6889629185\
 O,-3.6768531231,0.0012088079,0.5875704587\O,-3.6018993533,0.0009171898,1.9064507032\
 C,-4.9243817014,0.0010248904,2.5214338307\H,-0.9315093564,0.0002701286,2.0264916227\
 H,3.3260657678,-0.0000515391,-0.6560519613\H,0.1649665132,0.0009852434,-2.2993087072\
 H,-5.452139713,-0.9006664662,2.2083782743\H,-5.4518351729,0.9030117806,2.2087179419\
 H,-4.7307998956,0.0007895501,3.5934442128\H,-1.9826012948,0.0009732067,-0.1404465756\
 C,1.6525504901,-0.0005842172,3.5024287119\C,3.0282037739,-0.0009005185,3.5189652159\
 N,3.5044382132,-0.0007093563,2.2211160891\H,4.4793973332,-0.0008598026,1.9617540843\
 H,1.0077292651,-0.0006269002,4.3704851511\H,3.7157625323,-0.0012350668,4.3525490515\\

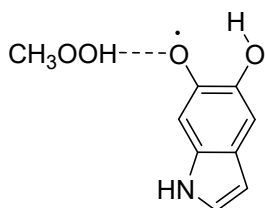


b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

N,-0.3857155176,-0.6891890608,-0.1384682946\C,-0.1604571644,-0.2166510333,1.1264566727\
 C,1.2516976682,0.021630127,1.2454650855\C,1.8395509179,-0.3371613664,-0.0201891719\
 C,0.8191024115,-0.7630310665,-0.8290465567\C,-1.0664572212,0.0264144885,2.1714698975\
 C,-0.5384269905,0.5099240073,3.3546143505\C,0.872464656,0.7690932588,3.5025754428\
 C,1.7607120778,0.525344371,2.4466386594\O,1.2367590478,1.2621155326,4.6944862534\
 O,-1.3473082641,0.754682534,4.4196519588\O,3.3559140573,0.3704438949,5.5235255898\

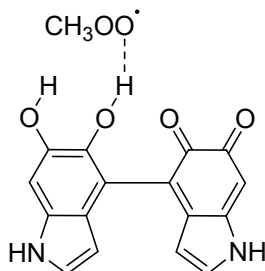
O,3.9574930085,1.4126717813,6.2044730382\C,4.5548223498,0.9173413738,7.4114424844\
H,2.8175794616,0.7353324057,2.5752472881\H,-2.1304526561,-0.1601814743,2.0744244722\
H,-0.7809983157,1.0633292615,5.1500650321\H,5.3054890392,0.1595129144,7.1696572953\
H,3.7822641351,0.4971669623,8.0619699489\H,5.0215066265,1.7870506975,7.8780241764\
H,2.2033212734,0.9401239886,4.9976117171\H,-1.2853557822,-0.9487648568,-0.516049318\
H,2.8852446972,-0.2841474376,-0.2875565457\H,0.8372639475,-1.1180093285,-1.8491543737\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

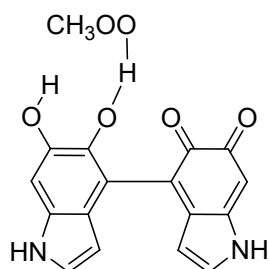
N,0.4502812157,0.6473097376,0.3953160744\C,0.1437816214,0.2137692104,1.6465542393\
C,1.3868626724,-0.1883704965,2.27369683\C,2.4298846013,0.0431028119,1.298396594\
C,1.8284370543,0.5457122553,0.1821436574\C,-1.1096794297,0.137799714,2.2845513994\
C,-1.1100908916,-0.348296183,3.5717414511\C,0.1269055667,-0.7719974689,4.260123946\
C,1.3757038368,-0.6763708925,3.5680186127\O,-0.0092344757,-1.2042215803,5.4533228789\
O,-2.2461853759,-0.4676226534,4.2847690686\O,1.9716662722,-2.1683819933,7.0434367343\
O,3.1996896019,-1.798829456,6.3522968111\C,3.7845005996,-0.7188497974,7.0753621912\
H,2.2772113809,-0.9890580944,4.0857674416\H,-2.0277000701,0.4433690459,1.7948173049\
H,-1.980312683,-0.831714505,5.1551665657\H,4.0024847219,-1.012000599,8.1080115861\
H,3.1367175731,0.1649861615,7.0620464726\H,4.7178824016,-0.5044014762,6.5459444123\
H,1.2816921508,-1.7954024711,6.4312429623\H,-0.2134399467,0.994664487,-0.2825450048\
H,3.4857115614,-0.1457046433,1.4268425514\H,2.2498911443,0.8489458544,-0.7649727132\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

N,3.71854,-2.43098,-0.98772\C,2.50038,-2.38883,-0.36072\C,2.01446,-0.98652,-0.49456\
 C,3.03152,-0.28458,-1.24225\C,4.02093,-1.17915,-1.51549\C,1.81719,-3.3971,0.25531\
 C,0.53364,-3.08141,0.82495\C,0.01167,-1.59041,0.73974\C,0.81358,-0.5801,0.0293\
 C,0.33065,0.81843,-0.05502\C,1.06352,1.88472,0.52996\C,0.57064,3.21629,0.41768\
 C,-0.61696,3.53357,-0.25247\C,-1.32218,2.47492,-0.80888\C,-0.86774,1.13537,-0.69813\
 N,1.45737,4.04009,1.07818\C,2.4824,3.27933,1.60773\C,2.2795,1.95619,1.2965\
 O,-2.48614,2.72074,-1.48933\O,-1.63484,0.19253,-1.36872\O,-0.19051,-3.90655,1.37761\
 O,-1.06614,-1.32458,1.30115\H,1.36879,5.0408,1.17138\H,2.9225,1.13545,1.57918\
 H,3.27928,3.74867,2.16633\H,4.29308,-3.25526,-1.08649\H,3.01455,0.75546,-1.52764\
 H,4.94642,-1.03586,-2.05565\H,-2.79889,1.86233,-1.82594\H,-2.17625,-0.34882,-0.75685\
 H,-0.98477,4.55058,-0.34038\H,2.19325,-4.41255,0.31905\C,-5.90485,-1.38812,0.38004\
 H,-5.68189,-1.96208,1.2804\H,-6.18806,-2.03852,-0.44855\O,-4.71301,-0.64049,-0.00178\
 H,-6.66204,-0.62753,0.56809\O,-3.69779,-1.44314,-0.26869\\

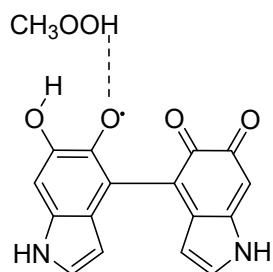


b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

C,-0.0507292975,-0.03628833,0.0413914938\C,-0.0373041673,-0.0125058651,1.4811294169\
 C,1.3422176732,-0.0400920832,1.8801162362\N,2.0944237142,-0.0778189541,0.7357240909\
 C,1.2557046551,-0.0757227339,-0.3704514304\C,1.7505598424,-0.019175946,3.2185443218\
 C,0.7487364174,0.0119852965,4.174925095\C,-0.6473810379,-0.003288424,3.8157351869\
 C,-1.044136112,0.0069412498,2.4622334018\C,-2.4818411556,0.0609159422,2.1020968546\
 C,-3.0465046728,1.1454803252,1.4819329819\C,-4.4911842101,1.1802750772,1.1155060982\
 C,-5.3816013464,0.1777651137,1.3628213661\C,-4.8895953653,-1.0047453374,2.0245250856\
 C,-3.348602352,-1.0958129216,2.3643584156\C,-2.5012096683,2.4161276927,1.0668019932\
 C,-3.5194490884,3.1275471203,0.5070128822\N,-4.7045755105,2.400126944,0.5269305145\
 O,-5.6020595939,-1.9588412244,2.3410637777\O,-2.9258600509,-2.1586867228,2.8072963729\

O,1.0902517479,0.0870197051,5.4878004897\O,-1.5487784951,0.0820247469,4.8101555071\
O,-1.6255766006,-2.0028300752,6.0915844811\O,-0.5838562994,-2.7011198263,5.5240194442\
C,-1.056827237,-3.9635173301,5.0166808813\H,3.1030528736,-0.1022841121,0.6972733402\
H,-0.9186412163,-0.0283810332,-0.6013194537\H,1.6718122568,-0.1047380513,-1.3669436356\
H,-5.5941668584,2.733418013,0.1853387696\H,-1.478699249,2.7427047033,1.1749961608\
H,-3.5093175511,4.121404391,0.0815866708\H,0.2783341783,0.1805009105,6.0145740271\
H,-1.5996502156,-0.8030305784,5.4027004942\H,2.7948358761,-0.0079093566,3.5110279554\
H,-6.4330641276,0.2438442461,1.1045522686\H,-1.8074454091,-3.7832431385,4.2446470666\
H,-1.4708657119,-4.5528088332,5.8392980219\H,-0.1723984836,-4.4502821672,4.6011132614\\



b3lyp/6-31+g(d,p) SCRF=(Solvent=Water)

0,2

C,0.041403423,1.2984421824,-0.0859562228\C,0.3546946561,0.452282028,1.0436743702\
C,1.7819142096,0.5656854392,1.252803783\N,2.2582345631,1.4251440394,0.3132435928\
C,1.2115408803,1.867676935,-0.4970438863\C,2.4848902695,-0.1319609912,2.2525708496\
C,1.7342111442,-0.9576738592,3.0543902895\C,0.2725497061,-1.1130503616,2.8984281862\
C,-0.4102877523,-0.38586102,1.8524614774\C,-1.8679894563,-0.5476175334,1.673608772\
C,-2.75844739,0.4872680006,1.8200641842\C,-4.2223339325,0.2975807299,1.6178618047\
C,-4.8151894235,-0.8823004878,1.282256928\C,-3.964682401,-2.0348654539,1.105561447\
C,-2.4047315069,-1.8565708692,1.2681198716\C,-2.5854720413,1.8702133887,2.1897124282\
C,-3.8232226001,2.4426358058,2.1992130314\N,-4.8013952633,1.5192179033,1.8557467772\
O,-4.3870725396,-3.1559843888,0.8216664349\O,-1.6897230326,-2.8181168519,1.0059772833\
O,2.2889075634,-1.673069159,4.0501034081\O,-0.2956905615,-1.8741995565,3.7436483129\
O,-2.8765270731,-2.5226438657,4.3353061116\O,-3.2491775994,-1.4939221649,5.2960402294\
C,-3.1959237887,-2.0851433665,6.5918560757\H,3.2263919997,1.6921497608,0.2035235833\
H,-0.9315870518,1.4562468787,-0.5261171372\H,1.4084723195,2.5579483653,-1.3039900749\

H,-5.7915992636,1.7122009466,1.8165113446\H,-1.6540550212,2.3647522642,2.4170374021\
H,-4.105145743,3.4606445847,2.4296660689\H,1.5505633026,-2.1595805208,4.4740736697\
H,-1.9531589503,-2.246878558,4.1005053849\H,3.5557105075,-0.0289205752,2.3881148657\
H,-5.8872622826,-0.9906680588,1.1580944464\H,-2.1764769981,-2.3981974118,6.8442044894\
H,-3.8815025322,-2.9364931934,6.6629698823\H,-3.5196566586,-1.2906453954,7.2711478078\\