

Supplementary Information: Coordinates for DFT and TD-DFT

**Protomers of DNA-binding dye fluoresce different colours: intrinsic photophysics of Hoechst 33258**

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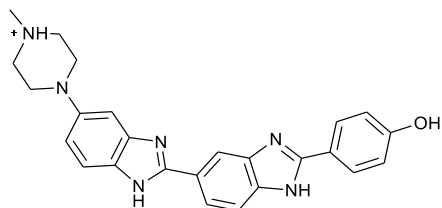
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## Ground State (S<sub>0</sub>) of 1+ Charge State at B3LYP/6-31G(d)

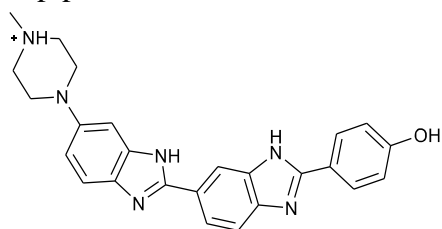
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C, 0, 7.408737, 0.028319, -0.003801  
N, 0, 6.31335, 0.176318, -0.947017  
C, 0, 6.232252, 1.530372, -1.45202  
C, 0, 6.113888, 2.598458, -0.349038  
C, 0, 5.103381, -0.559546, -0.687881  
C, 0, 3.858992, 0.064659, -0.57018  
C, 0, 2.725383, -0.732486, -0.361873  
C, 0, 2.85735, -2.13726, -0.246121  
C, 0, 4.09272, -2.771428, -0.361204  
C, 0, 5.205628, -1.968406, -0.596188  
N, 0, 1.569364, -2.583006, -0.026028  
C, 0, 0.736959, -1.474963, -0.028284  
N, 0, 1.411342, -0.352028, -0.219916  
C, 0, -0.711811, -1.563269, 0.155123  
C, 0, -1.486816, -0.429789, -0.128325  
C, 0, -2.869008, -0.511628, 0.033457  
C, 0, -3.459121, -1.723943, 0.478642  
C, 0, -2.702147, -2.85823, 0.773549  
C, 0, -1.325691, -2.758623, 0.606049  
N, 0, -3.840812, 0.445691, -0.182733  
C, 0, -4.985961, -0.137375, 0.112539  
N, 0, -4.808399, -1.453452, 0.522808  
C, 0, -6.296755, 0.503778, 0.024036  
C, 0, -6.379684, 1.808492, -0.49997  
C, 0, -7.59745, 2.459605, -0.607718  
C, 0, -8.772992, 1.818227, -0.190782  
C, 0, -8.708998, 0.522545, 0.335485  
C, 0, -7.480712, -0.12305, 0.440295  
O, 0, -9.938819, 2.506331, -0.321919  
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H, 0, 6.271928, 3.29445, 2.315239  
H, 0, 8.058236, 3.317547, 2.401035  
H, 0, 8.125208, 2.588769, 0.13006  
H, 0, 6.378699, 0.851971, 1.737161  
H, 0, 8.15991, 0.947259, 1.851996  
H, 0, 7.425053, -0.984335, 0.401384  
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H, 0, 5.378857, 1.627976, -2.1268019  
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H, 0, 5.192987, 2.495848, 0.228178

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H,0,-0.717222,-3.62221,0.860236  
H,0,-5.537206,-2.107808,0.763748  
H,0,-5.464937,2.295037,-0.820399  
H,0,-7.664968,3.463985,-1.012836  
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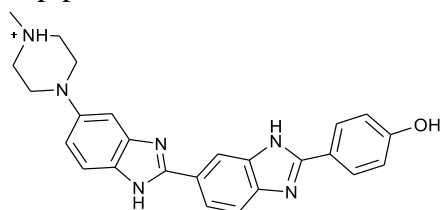
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C,0,9.511816,0.476646,1.748258  
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C,0,7.294281,0.54775,-1.405584  
N,0,6.076466,1.068317,-0.824093  
C,0,6.351862,2.05054,0.209111  
C,0,7.256013,1.495074,1.320425  
C,0,4.928673,0.215537,-0.66257  
C,0,3.671476,0.830868,-0.566129  
C,0,2.564564,0.002969,-0.406289  
C,0,2.663114,-1.413967,-0.367863  
C,0,3.917725,-2.011642,-0.498411  
C,0,5.038202,-1.192473,-0.630321  
N,0,1.41806,-1.983487,-0.218831  
C,0,0.567808,-0.975349,-0.171987  
N,0,1.214893,0.252422,-0.288854  
C,0,-0.878816,-1.100407,-0.013267  
C,0,-1.740553,-0.011582,-0.231251  
C,0,-3.10052,-0.231251,-0.050283  
C,0,-3.628606,-1.491267,0.337212  
C,0,-2.756832,-2.569755,0.546169  
C,0,-1.398511,-2.364019,0.367427  
N,0,-4.2116,0.580572,-0.177496  
C,0,-5.325812,-0.188008,0.122328  
N,0,-4.999049,-1.42962,0.436456  
C,0,-6.692135,0.327853,0.090154  
C,0,-7.757834,-0.561036,0.33323  
C,0,-9.071928,-0.124263,0.311814  
C,0,-9.357169,1.222811,0.04505  
C,0,-8.310462,2.121089,-0.196035  
C,0,-6.993437,1.672901,-0.171782  
O,0,-10.665594,1.593118,0.036029  
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H,0,9.052322,-0.373942,2.253642  
H,0,8.997905,1.793462,0.251625  
H,0,7.861902,-0.910396,0.139954  
H,0,9.237252,-0.30337,-0.820857  
H,0,7.058094,-0.223172,-2.142364  
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H,0,5.420587,2.384791,0.668516  
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H,0,6.792108,0.639103,1.817946  
H,0,7.523407,2.251458,2.06398  
H,0,3.573983,1.909051,-0.65558

H, 0, 4.013252, -3.092556, -0.48785  
H, 0, 6.008243, -1.669658, -0.726812  
H, 0, 0.779183, 1.158672, -0.210969  
H, 0, -1.371728, 0.956452, -0.561054  
H, 0, -3.14776, -3.538706, 0.839075  
H, 0, -0.694055, -3.174187, 0.517473  
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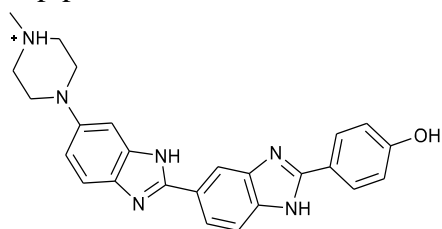
## H-pipN2-II



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C,0,7.416014,-1.17113,0.450354  
N,0,6.560384,-0.745151,-0.643896  
C,0,7.031271,0.490369,-1.232546  
C,0,7.189915,1.639868,-0.22047  
C,0,5.145853,-0.981097,-0.519764  
C,0,4.205428,0.04871,-0.603693  
C,0,2.84491,-0.276107,-0.516194  
C,0,2.447873,-1.620639,-0.318317  
C,0,3.376116,-2.656224,-0.23251  
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N,0,1.069816,-1.562979,-0.256952  
C,0,0.697552,-0.237856,-0.424918  
N,0,1.74959,0.553032,-0.574349  
C,0,-0.693548,0.207532,-0.432805  
C,0,-1.741456,-0.644651,-0.043393  
C,0,-3.031138,-0.130855,-0.0941  
C,0,-3.311942,1.197095,-0.512157  
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N,0,-4.269695,-0.662149,0.210506  
C,0,-5.21628,0.321196,-0.03123  
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C,0,-6.649816,0.126334,0.170162  
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C,0,-8.896608,1.04563,0.015737  
C,0,-9.425867,-0.151908,0.518818  
C,0,-8.567235,-1.207819,0.848425  
C,0,-7.194352,-1.064523,0.674301  
O,0,-10.775779,-0.224502,0.663604  
H,0,8.684474,3.151828,1.464172  
H,0,7.299472,2.50901,2.395166  
H,0,8.951461,1.909196,2.726655  
H,0,8.995383,0.970982,0.533439  
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H,0,8.243163,-0.388127,2.335932  
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H,0,8.415985,-1.419589,0.062053  
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H,0,7.665409,2.519318,-0.664313  
H,0,4.475241,1.088468,-0.753093

H,0,3.0769,-3.69261,-0.107599  
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## H-pip1-d

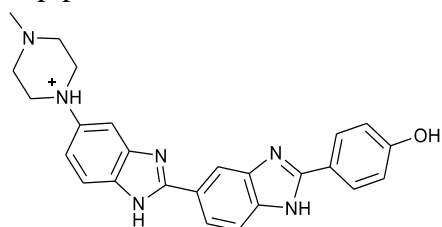


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C, 0, 8.06718957, -1.258333856, -0.4936852511  
C, 0, 7.4392139391, -0.063667717, -1.2353229025  
N, 0, 6.4274897054, 0.6316802714, -0.4708167997  
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C, 0, 7.4913368768, -0.1032827242, 1.6501973165  
C, 0, 5.0475307293, 0.2337525619, -0.5640703932  
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C, 0, 2.741121012, 0.7957574785, -0.3132908484  
C, 0, 2.3444245775, -0.4957061759, -0.7531142187  
C, 0, 3.3247366506, -1.420224858, -1.1169429429  
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N, 0, 0.9711839107, -0.6047678346, -0.7620092475  
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C, 0, -9.0987026392, 0.1656064629, 0.471392294  
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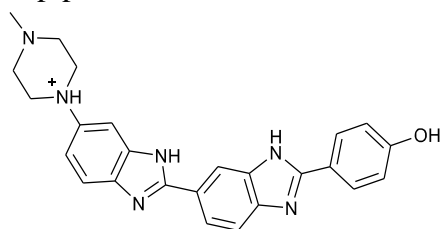
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C, 0, -6.7947474735, -0.6970887539, 1.2519011987  
N, 0, -5.9752974693, -0.6789344247, -0.0294535818  
C, 0, -6.8754105094, -0.4280617667, -1.2296952371  
C, 0, -8.0089881975, -1.4472746618, -1.2510276819  
C, 0, -4.784595233, 0.2112097801, 0.0279693554  
C, 0, -3.5359491719, -0.3918420592, -0.079119571  
C, 0, -2.4167506175, 0.444704016, -0.0256199028  
C, 0, -2.5969984981, 1.8484087307, 0.1293100302  
C, 0, -3.8548954537, 2.4367577429, 0.2356317951  
C, 0, -4.9663107958, 1.5945265137, 0.1836420854  
N, 0, -1.3169565314, 2.3491721676, 0.1364611369  
C, 0, -0.4401669711, 1.280095439, -0.0028036913  
N, 0, -1.0870566883, 0.1279697269, -0.1038392677  
C, 0, 1.0104555601, 1.4313336608, -0.0272381838  
C, 0, 1.7953458026, 0.2677995572, 0.003332587  
C, 0, 3.1814346662, 0.402321, -0.012934242  
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C, 0, 1.6199515735, 2.7106361731, -0.0815624783  
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C, 0, 5.3079920185, 0.0817609922, -0.0178808678  
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C, 0, 9.055816204, -0.4545610887, -0.0647051764  
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O, 0, 10.2878102533, -2.5391848267, 0.0521571605  
H, 0, -10.6122766081, -1.8716394366, -0.8993007188  
H, 0, -10.5553630423, -2.0624322879, 0.8599287287  
H, 0, -9.7771199028, -3.2778963993, -0.1879478714  
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H, 0, 3.451992328, 3.8488598397, -0.1480358015  
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H, 0, 11.0333107209, -1.9207690207, -0.0066084866

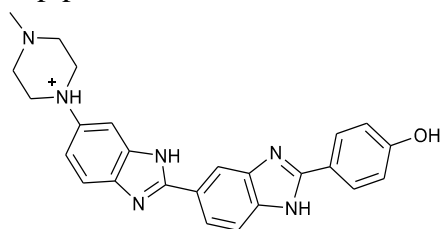
## H-pip2-b



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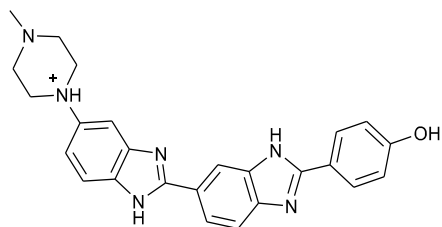
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C,0,-8.2978495715,-0.1370840378,1.10797761  
C,0,-4.7173658917,0.794384537,0.061245441  
C,0,-3.8973933796,-0.3364803762,0.0349559395  
C,0,-2.5302720092,-0.0854972173,0.087274575  
C,0,-1.9905298027,1.2326865254,0.1618261168  
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H,0,-8.5497281126,-0.5220384993,-2.2028581355  
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## H-pip2-d

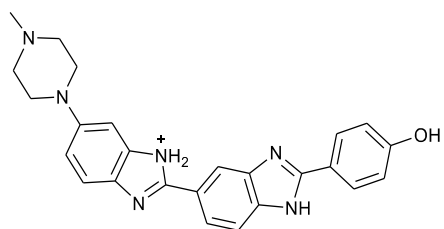


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C, 0, -7.389569, -0.660276, 1.216876  
N, 0, -6.43839, -0.992266, 0.046329  
C, 0, -7.116973, -0.722755, -1.291043  
C, 0, -7.600827, 0.724229, -1.413622  
C, 0, -5.056605, -0.432254, 0.155781  
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N, 0, 4.953232, -1.458967, -0.06657  
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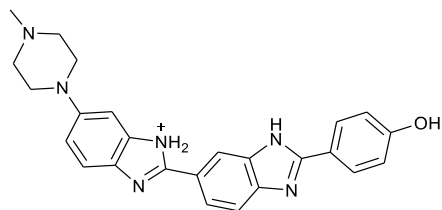
## H-bz1-aI



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C,0,-6.9509702929,0.9364818764,0.6760192012  
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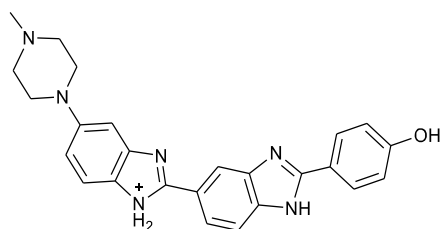
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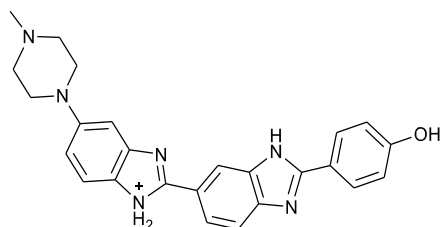
H-bz1-bI



C	0	-9.53671	2.89545	0.29184
N	0	-8.47399	1.99871	-0.14798
C	0	-7.16056	2.62343	-0.07937
C	0	-6.10471	1.70634	-0.69144
N	0	-6.09883	0.38216	-0.04551
C	0	-7.43287	-0.2249	0.03154
C	0	-8.45462	0.75607	0.60928
C	0	-4.97207	-0.41305	-0.07791
C	0	-3.67015	0.16634	-0.08126
C	0	-2.56752	-0.66359	-0.05842
C	0	-2.70755	-2.05543	-0.03808
C	0	-3.94537	-2.66601	-0.04818
C	0	-5.06679	-1.83561	-0.07691
N	0	-1.34922	-2.61785	-0.01286
C	0	-0.46613	-1.31001	-0.01884
N	0	-1.21426	-0.27879	-0.04325
C	0	0.96842	-1.45505	0.00009
C	0	1.73875	-0.27353	-0.01247
C	0	3.1228	-0.39229	0.00456
C	0	3.72477	-1.68451	0.03398
C	0	2.97486	-2.86259	0.047
C	0	1.59306	-2.73105	0.02972
N	0	4.08847	0.58834	-0.0029
C	0	5.24427	-0.04788	0.02059
N	0	5.07006	-1.4326	0.04364
C	0	6.55413	0.58951	0.02257
C	0	7.75766	-0.14006	0.04889
C	0	8.98514	0.50356	0.0497
C	0	9.03595	1.9051	0.02393
C	0	7.84531	2.64686	-0.00244
C	0	6.62165	1.99418	-0.00302
O	0	10.26364	2.47812	0.02602
H	0	-10.50549	2.39899	0.17624
H	0	-9.53857	3.79412	-0.33324
H	0	-9.43187	3.20825	1.34771
H	0	-7.17748	3.55814	-0.65088
H	0	-6.87286	2.87283	0.962
H	0	-6.31103	1.58489	-1.76583
H	0	-5.12918	2.17955	-0.58719
H	0	-7.39273	-1.0919	0.6944
H	0	-7.76375	-0.56056	-0.964
H	0	-8.2237	0.92853	1.67997
H	0	-9.44399	0.28818	0.55757
H	0	-3.51332	1.23601	-0.07009
H	0	-4.07059	-3.74473	-0.05314

H	0	-6.03571	-2.31224	-0.12663
H	0	-1.12566	-3.2004	-0.82946
H	0	-1.14934	-3.17753	0.82538
H	0	1.2592	0.6982	-0.03514
H	0	3.43976	-3.84295	0.06971
H	0	1.00078	-3.64251	0.04013
H	0	5.80448	-2.12502	0.06349
H	0	7.75378	-1.22704	0.06933
H	0	9.91484	-0.05478	0.06994
H	0	7.88186	3.73385	-0.02244
H	0	5.6972	2.56078	-0.02335
H	0	10.17832	3.44495	0.00707

# H-bz1-bII

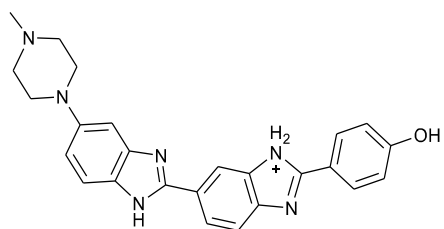


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N	0	9.14755	-0.48094	-0.10034
C	0	8.12741	-1.51679	-0.01953
C	0	6.82771	-1.03139	-0.65643
N	0	6.3612	0.22404	-0.04249
C	0	7.4049	1.25382	0.02064
C	0	8.69508	0.69679	0.62506
C	0	5.03004	0.58243	-0.09339
C	0	4.00683	-0.40897	-0.07818
C	0	2.68518	-0.00932	-0.07452
C	0	2.33921	1.34659	-0.09144
C	0	3.29174	2.34492	-0.12073
C	0	4.63055	1.95059	-0.13013
N	0	0.86978	1.40947	-0.07722
C	0	0.48881	-0.12312	-0.04543
N	0	1.5484	-0.83484	-0.04495
C	0	-0.90375	-0.47886	-0.02454
C	0	-1.9316	0.49235	-0.0285
C	0	-3.23562	0.02957	-0.00714
C	0	-3.55761	-1.36062	0.01816
C	0	-2.52463	-2.31344	0.02194
C	0	-1.21703	-1.86837	0.00072
N	0	-4.46237	0.66087	-0.00363
C	0	-5.43925	-0.32181	0.02243
N	0	-4.90993	-1.54037	0.0357
C	0	-6.86522	-0.03983	0.03356
C	0	-7.38585	1.26897	0.01878
C	0	-8.7522	1.49538	0.03011
C	0	-9.63793	0.40666	0.05675
C	0	-9.13561	-0.90358	0.07174
C	0	-7.76644	-1.12073	0.06024
O	0	-10.96122	0.69064	0.0667
H	0	11.18949	-0.15245	0.23868
H	0	10.76519	-1.80593	-0.23757
H	0	10.44575	-1.25378	1.42773
H	0	8.4701	-2.40139	-0.56784
H	0	7.93153	-1.82656	1.02694
H	0	6.99179	-0.86947	-1.73277
H	0	6.07233	-1.80805	-0.54409
H	0	7.06296	2.06977	0.66092
H	0	7.61087	1.659	-0.98271
H	0	8.526	0.48047	1.69935
H	0	9.4645	1.47441	0.56343
H	0	4.22774	-1.46658	-0.03759



H	0	3.03864	3.40051	-0.15454
H	0	5.37704	2.72971	-0.1949
H	0	0.46683	1.85844	-0.90901
H	0	0.48628	1.88829	0.74686
H	0	-1.72596	1.56013	-0.04712
H	0	-2.75982	-3.37209	0.04114
H	0	-0.39579	-2.57607	0.0029
H	0	-4.62405	1.65662	-0.0172
H	0	-6.72649	2.13326	-0.00191
H	0	-9.15842	2.50102	0.01881
H	0	-9.82015	-1.74859	0.09237
H	0	-7.36996	-2.12992	0.07167
H	0	-11.4781	-0.13108	0.08525

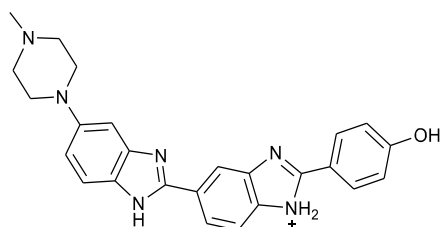
H-bz2-a



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C	0	8.77832	0.73711	0.36413
C	0	7.32963	0.88371	0.8219
N	0	6.41646	0.21904	-0.12141
C	0	6.77708	-1.18337	-0.32273
C	0	8.23845	-1.3007	-0.75687
C	0	5.05239	0.54652	-0.05853
C	0	4.04735	-0.42436	-0.00904
C	0	2.70662	-0.00754	-0.01793
C	0	2.37654	1.36855	-0.05486
C	0	3.3648	2.35698	-0.10005
C	0	4.68029	1.92869	-0.10977
N	0	0.9956	1.40507	-0.03954
C	0	0.55664	0.09343	0.01769
N	0	1.5602	-0.76783	0.02873
C	0	-0.84104	-0.31133	0.05378
C	0	-1.90802	0.61354	-0.04208
C	0	-3.18133	0.09099	0.00417
C	0	-3.47974	-1.26953	0.13493
C	0	-2.42937	-2.18411	0.22647
C	0	-1.13053	-1.69194	0.1843
N	0	-4.48009	0.79116	-0.07504
C	0	-5.4995	-0.41009	0.03735
N	0	-4.85694	-1.50712	0.14996
C	0	-6.90826	-0.12349	-0.00012
C	0	-7.81209	-1.2094	0.10292
C	0	-9.17464	-0.99637	0.0727
C	0	-9.68116	0.31043	-0.06171
C	0	-8.79741	1.39775	-0.16504
C	0	-7.4283	1.17875	-0.13414
O	0	-11.02	0.44404	-0.0838
H	0	10.75177	-1.93401	-0.16094
H	0	11.15288	-0.41879	0.66774
H	0	10.81248	-0.40892	-1.08251
H	0	9.43546	1.18568	1.11834
H	0	8.92043	1.29806	-0.58181
H	0	7.22288	0.44326	1.82782
H	0	7.0794	1.94375	0.89466
H	0	6.14058	-1.59963	-1.10932
H	0	6.62193	-1.77656	0.59575
H	0	8.35133	-0.85224	-1.76444
H	0	8.49771	-2.36277	-0.83695
H	0	4.26955	-1.48191	0.05192
H	0	3.12641	3.41539	-0.14766

H	0	5.46398	2.67312	-0.19596
H	0	0.43562	2.24336	-0.01556
H	0	-1.73338	1.67886	-0.15638
H	0	-2.6294	-3.24513	0.32728
H	0	-0.2849	-2.36705	0.25072
H	0	-4.61246	1.29594	-0.95967
H	0	-4.62487	1.46097	0.68991
H	0	-7.41706	-2.21418	0.20621
H	0	-9.87432	-1.82143	0.15092
H	0	-9.18407	2.40814	-0.26902
H	0	-6.77517	2.04481	-0.21706
H	0	-11.27539	1.37656	-0.17894

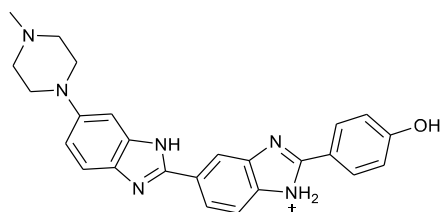
H-bz2-bI



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C	0	-7.26813	-0.9833	0.82498
N	0	-6.38956	-0.27889	-0.12214
C	0	-6.79148	1.11613	-0.29107
C	0	-8.26158	1.20034	-0.70269
C	0	-5.01409	-0.56638	-0.07651
C	0	-4.03864	0.43256	-0.00913
C	0	-2.68571	0.05636	-0.03703
C	0	-2.31558	-1.30778	-0.1074
C	0	-3.27483	-2.3239	-0.17142
C	0	-4.60221	-1.93479	-0.16408
N	0	-0.93473	-1.30438	-0.09758
C	0	-0.53462	0.01598	-0.02045
N	0	-1.56111	0.84921	0.01721
C	0	0.85465	0.45586	0.01573
C	0	1.93954	-0.4443	-0.04124
C	0	3.22532	0.07413	-0.00047
C	0	3.4256	1.45414	0.09431
C	0	2.3904	2.37053	0.15195
C	0	1.09843	1.84689	0.11094
N	0	4.44114	-0.62919	-0.04389
C	0	5.41997	0.18589	0.01517
N	0	4.88522	1.66298	0.11402
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C	0	7.31258	-1.36509	-0.08529
C	0	8.66517	-1.63519	-0.09959
C	0	9.59485	-0.58031	-0.02395
C	0	9.14394	0.74771	0.06616
C	0	7.78333	1.01367	0.08013
O	0	10.89683	-0.91618	-0.043
H	0	-10.7836	1.75061	-0.06347
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H	0	-6.17774	1.56498	-1.07799
H	0	-6.64053	1.69685	0.63634
H	0	-8.3766	0.76604	-1.71619
H	0	-8.55184	2.25591	-0.76049
H	0	-4.29254	1.48117	0.07827
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H	0	-5.36477	-2.69934	-0.26373
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H	0	5.2252	2.22517	-0.67657
H	0	6.59207	-2.17364	-0.14334
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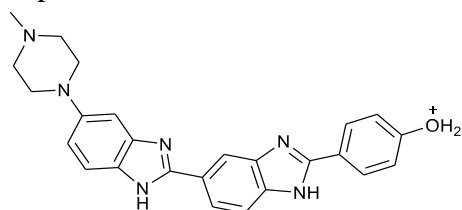
H-bz2-bII



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C	0	-6.19344	1.77986	0.21413
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C	0	-7.29418	-0.11367	-0.84279
C	0	-8.63978	0.41222	-0.35113
C	0	-4.98699	-0.35727	0.01207
C	0	-3.75507	0.31873	-0.0037
C	0	-2.59598	-0.45689	0.03233
C	0	-2.60405	-1.87357	0.06404
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C	0	-4.99614	-1.79152	0.05676
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C	0	-0.53408	-1.30496	0.05284
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C	0	0.91714	-1.38584	0.05311
C	0	1.74312	-0.24067	0.01283
C	0	3.11766	-0.42197	0.01694
C	0	3.66027	-1.70917	0.05991
C	0	2.88733	-2.85764	0.09992
C	0	1.506	-2.67419	0.0959
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C	0	5.27023	0.02033	-0.00158
N	0	5.12526	-1.54539	0.05214
C	0	6.59297	0.58936	-0.02302
C	0	6.71191	1.9994	-0.07168
C	0	7.95322	2.60083	-0.09395
C	0	9.1188	1.81143	-0.06827
C	0	9.01688	0.41078	-0.02
C	0	7.76671	-0.18859	0.00219
O	0	10.29484	2.46389	-0.09217
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H	0	-9.4154	0.12171	-1.06915
H	0	-3.70078	1.39812	-0.07125
H	0	-3.87966	-3.62745	0.12272

H	0	-5.94995	-2.3024	0.11771
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H	0	5.57853	-1.97895	-0.76241
H	0	5.58108	-1.92238	0.89299
H	0	5.81072	2.60249	-0.0913
H	0	8.05504	3.68	-0.13122
H	0	9.91417	-0.20209	-0.00007
H	0	7.72697	-1.27496	0.0396
H	0	11.03987	1.84057	-0.07175

## H-phe-al

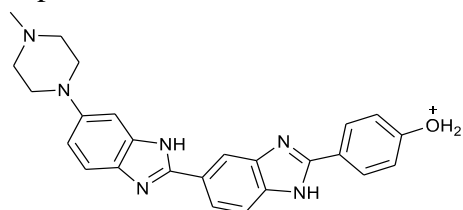


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H,0,5.5674452667,2.37333657,-0.3441596978  
H,0,7.7174960145,1.8571364092,1.7822396088  
H,0,7.24855048,3.4197372544,1.0721280869  
H,0,3.5225828227,1.2383958441,0.1386831325  
H,0,4.1082682988,-3.7482215326,-0.1241686633



H, 0, 6.0652232059, -2.2575999301, -0.02984614  
H, 0, 1.1683351457, -3.5525725048, -0.121773484  
H, 0, -1.1572475515, 0.5153207291, -0.0525546267  
H, 0, -3.4015802872, -3.9856892272, 0.2440046988  
H, 0, -0.9581299496, -3.786280406, 0.2362842832  
H, 0, -5.7589467661, -2.2531747108, 0.1398376097  
H, 0, -5.4345027831, 2.4148554387, -0.1423223775  
H, 0, -7.5395732806, 3.7622287986, -0.2111083006  
H, 0, -9.8490215442, 0.1053483718, 0.0142433116  
H, 0, -7.7556699357, -1.212050687, 0.0810505493  
H, 0, -10.2009972739, 3.23085263, -0.9709841859  
H, 0, -10.1936957512, 3.3232824075, 0.6330035464

## H-phe-aII



C,0,-10.5942524139,0.2889092019,0.186627111  
N,0,-9.1815437436,0.2672387054,-0.1631252847  
C,0,-8.3598240362,0.9392485708,0.8370010988  
C,0,-6.8969000472,0.9927620471,0.3945234512  
N,0,-6.3951478672,-0.3528267115,0.1334365944  
C,0,-7.236339811,-1.0608225439,-0.8427518139  
C,0,-8.6904961225,-1.0897824854,-0.3801547881  
C,0,-5.0019464239,-0.5398210288,0.0513467344  
C,0,-4.1070613965,0.5402292176,0.0248431779  
C,0,-2.7423758332,0.2438891951,0.0018291846  
C,0,-2.2317315156,-1.0736420401,-0.0161861137  
C,0,-3.1351977201,-2.1488777525,0.0054384688  
C,0,-4.4888003329,-1.8727798745,0.0462197947  
N,0,-0.8528616098,-1.0600260876,-0.0490722458  
C,0,-0.5114446298,0.2131242825,-0.0554981705  
N,0,-1.6197595434,1.0486431497,-0.0301111906  
C,0,0.872663603,0.6893318336,-0.0884619633  
C,0,1.90027677,-0.2520002254,0.0097406099  
C,0,3.2226177056,0.201555451,-0.024829783  
C,0,3.5057838736,1.5872320861,-0.1548017293  
C,0,2.4919692494,2.5428755273,-0.2567765856  
C,0,1.1878806992,2.0712211005,-0.2229253735  
N,0,4.3975312795,-0.5146646185,0.0527188656  
C,0,5.3653344913,0.3789983349,-0.0256234854  
N,0,4.8832763258,1.6702181982,-0.1519757157  
C,0,6.7762946446,0.0170669444,0.017902455  
C,0,7.0930910838,-1.3544087783,0.1476038598  
C,0,8.4127027397,-1.7843540572,0.1959621238  
C,0,9.3843675908,-0.7994246658,0.1104546943  
C,0,9.1566410725,0.5556443957,-0.0169264036  
C,0,7.8213543923,0.9573761948,-0.0627389104  
O,0,10.8347702936,-1.2101628278,0.1574780092  
H,0,-11.1778147048,-0.1822552498,-0.611681952  
H,0,-10.9324603263,1.3258466961,0.2885106069  
H,0,-10.8178724563,-0.2399641544,1.1335946428  
H,0,-8.7286671609,1.9637551739,0.9664824587  
H,0,-8.4181205929,0.4357000317,1.822987899  
H,0,-6.8130842807,1.6404308509,-0.497329646  
H,0,-6.3025706355,1.4396141132,1.1974984797  
H,0,-6.8749028725,-2.0828866913,-0.9668055348  
H,0,-7.1811292001,-0.563342782,-1.8267131165  
H,0,-8.768755548,-1.7077580399,0.537084663  
H,0,-9.301821546,-1.5664878384,-1.1556032432  
H,0,-4.4561421537,1.565618444,-0.0006148161  
H,0,-2.7717723895,-3.171790905,0.0106078652  
H,0,-5.1906846575,-2.6968902526,0.1147658934

H, 0, -1.6189032092, 2.0557381285, 0.0177645948  
H, 0, 1.6613547613, -1.3042917124, 0.1082749185  
H, 0, 2.7009437784, 3.6028086506, -0.3630855273  
H, 0, 0.3866917305, 2.7979695024, -0.3174856336  
H, 0, 5.4187902179, 2.5216678905, -0.2319441141  
H, 0, 6.2768717641, -2.0653864815, 0.208380452  
H, 0, 8.652895645, -2.8391267177, 0.2954542615  
H, 0, 9.9703549283, 1.2697277659, -0.0780896312  
H, 0, 7.6132769311, 2.0173897857, -0.1623336429  
H, 0, 11.1085953609, -1.7792022015, -0.5951907044  
H, 0, 11.0983528485, -1.6323747462, 1.0045571502

## Ground State ( $S_0$ ) of 1+ Charge State at B3LYP/6-311+G(d,p)

### H-pipN2-I

C, 0, 7.2293997664, 3.4274807447, 1.7740666011  
N, 0, 7.2706732217, 2.4250463011, 0.6600292528  
C, 0, 7.3294727038, 0.9953013612, 1.1689210398  
C, 0, 7.4130519033, 0.0271676289, -0.0184873126  
N, 0, 6.3037795542, 0.1887206238, -0.9431314075  
C, 0, 6.2199603785, 1.5486650897, -1.4319221939  
C, 0, 6.1202930635, 2.6019600271, -0.3162987618  
C, 0, 5.0977188848, -0.549752797, -0.6835051701  
C, 0, 3.8538109956, 0.0719510109, -0.5747504198  
C, 0, 2.7214337219, -0.7246650013, -0.368128533  
C, 0, 2.8512848394, -2.1259019219, -0.2497928665  
C, 0, 4.0858552438, -2.7580403171, -0.3586048487  
C, 0, 5.1988604266, -1.9565136241, -0.5879149072  
N, 0, 1.5622257925, -2.5728809341, -0.0378784829  
C, 0, 0.7306165679, -1.4663840613, -0.0424927414  
N, 0, 1.4068042139, -0.3477248669, -0.2334109956  
C, 0, -0.7183171388, -1.5542084158, 0.1390234315  
C, 0, -1.4942695095, -0.4248198081, -0.1469184039  
C, 0, -2.8740104688, -0.5091625833, 0.0170470219  
C, 0, -3.4621690891, -1.7169831572, 0.4671214198  
C, 0, -2.7043216832, -2.847619478, 0.7630304547  
C, 0, -1.329700452, -2.7472388748, 0.5931420581  
N, 0, -3.8487084591, 0.4441305113, -0.1995577045  
C, 0, -4.9909425528, -0.1349155536, 0.0996717757  
N, 0, -4.811719507, -1.4481558971, 0.5144782899  
C, 0, -6.3034361893, 0.5028499601, 0.0146539021  
C, 0, -6.408779301, 1.7700897885, -0.5848703444  
C, 0, -7.630755782, 2.410424585, -0.6898030883  
C, 0, -8.7855278149, 1.7965473894, -0.1929996773  
C, 0, -8.6999660687, 0.5397165198, 0.4102332773  
C, 0, -7.4677829453, -0.0960037944, 0.5118720995  
O, 0, -9.9580956658, 2.4744213932, -0.3259124064  
H, 0, 7.2293823258, 4.4301814419, 1.3484621038  
H, 0, 6.31986952, 3.2676227649, 2.3506377586  
H, 0, 8.1031624057, 3.2874353925, 2.4091897107  
H, 0, 8.1347746395, 2.5858141189, 0.1325924209  
H, 0, 6.4190881049, 0.8337770735, 1.7487118912  
H, 0, 8.1983376442, 0.9222511371, 1.825765416  
H, 0, 7.4363358612, -0.9873555997, 0.3749253447  
H, 0, 8.360013905, 0.1850428852, -0.5531624315  
H, 0, 5.3633713703, 1.6589232944, -2.0967013909  
H, 0, 7.1150474363, 1.7594720546, -2.034453608  
H, 0, 5.2082800172, 2.4966287642, 0.2709381727  
H, 0, 6.1833534791, 3.6189592, -0.7080873006  
H, 0, 3.7152930229, 1.141795391, -0.6611331771  
H, 0, 4.1906897629, -3.8348330282, -0.2974989171  
H, 0, 6.1617135586, -2.4297565736, -0.7384387115  
H, 0, 1.2657364355, -3.5339438744, 0.0120707086  
H, 0, -1.0261154306, 0.4871234914, -0.492198806  
H, 0, -3.1539773172, -3.7670437163, 1.1184091447  
H, 0, -0.7237210443, -3.6098578572, 0.8457761879

H, 0, -5.5396932325, -2.1041009178, 0.7457764222  
H, 0, -5.5109736602, 2.2383254341, -0.9673673431  
H, 0, -7.7146686753, 3.3852160416, -1.1541668018  
H, 0, -9.5911923712, 0.0619161711, 0.8046667633  
H, 0, -7.4341221463, -1.0628857072, 1.0021888476  
H, 0, -10.686195262, 1.9637287688, 0.0445942362

## H-pipN2-II

C,0,-8.2855858018,-2.1966413598,2.0372059601  
N,0,-8.0812031821,-1.1592787853,0.974182842  
C,0,-7.5642447091,0.1531718418,1.5371158116  
C,0,-7.4188392795,1.1795259776,0.4057966432  
N,0,-6.5503327125,0.7091733684,-0.6598543238  
C,0,-7.0172780514,-0.5484858588,-1.2034692176  
C,0,-7.1846119208,-1.6538481958,-0.1479746982  
C,0,-5.1387731428,0.9521092956,-0.5373527885  
C,0,-4.1978373141,-0.0744605818,-0.6182083976  
C,0,-2.8389966778,0.2529231773,-0.5387173059  
C,0,-2.4419657274,1.5956359777,-0.3544548994  
C,0,-3.3704525724,2.6285142382,-0.2740395187  
C,0,-4.7156115354,2.2916999683,-0.380039705  
N,0,-1.0630327239,1.5415241748,-0.302996531  
C,0,-0.6905682282,0.2169317851,-0.4619493032  
N,0,-1.7419610642,-0.5722150388,-0.598649605  
C,0,0.7013006757,-0.2256148726,-0.4747542827  
C,0,1.7404025178,0.6168330329,-0.049125577  
C,0,3.0322414641,0.1133362335,-0.1070153093  
C,0,3.3217893759,-1.1952930046,-0.5670600495  
C,0,2.2753236746,-2.0287669076,-0.9796618158  
C,0,0.9827966928,-1.5370635045,-0.9283114123  
N,0,4.2647711107,0.6404470518,0.2285389061  
C,0,5.2181541046,-0.3275416146,-0.0424683624  
N,0,4.6748427594,-1.4319197911,-0.5151839162  
C,0,6.6484048548,-0.1281687808,0.1762209798  
C,0,7.5503739906,-1.1057247513,-0.2803809087  
C,0,8.9138857198,-0.9583710273,-0.0993788549  
C,0,9.4135464329,0.1764375984,0.548584035  
C,0,8.5327835813,1.1562908913,1.0132935164  
C,0,7.164164542,0.9995581122,0.8278188339  
O,0,10.7629434237,0.266031075,0.6962345177  
H,0,-8.6935907708,-3.097026108,1.5796316074  
H,0,-7.3235157991,-2.4157674954,2.4972394553  
H,0,-8.9761733103,-1.8072269993,2.7841253856  
H,0,-8.9963509393,-0.9610273641,0.5571690567  
H,0,-6.6007360802,-0.0654812221,2.000657425  
H,0,-8.2722137019,0.4770397839,2.3023360486  
H,0,-7.0305126636,2.101244656,0.8349605396  
H,0,-8.4104786501,1.4115964791,-0.0069061661  
H,0,-6.3361549376,-0.9016799448,-1.9774673109  
H,0,-7.9877369075,-0.3797858849,-1.691753526  
H,0,-6.2382590565,-1.9246797796,0.3198409239  
H,0,-7.6521689704,-2.5483020161,-0.5639962907  
H,0,-4.4643395448,-1.1138349051,-0.7592717034  
H,0,-3.0736669575,3.6646226364,-0.1617307659  
H,0,-5.4540780825,3.0843523082,-0.3835285297  
H,0,-0.4381139232,2.3305771406,-0.2756328895  
H,0,1.5500225321,1.6116737351,0.3385079849  
H,0,2.4830643887,-3.0317803542,-1.3313712801  
H,0,0.1502590042,-2.1522106111,-1.2427438833  
H,0,4.4455663141,1.5787606344,0.5446447197  
H,0,7.1562089625,-1.9808430548,-0.7807011113

H, 0, 9.6102419944, -1.7088677225, -0.4524471368  
H, 0, 8.9144778736, 2.0349091737, 1.523691405  
H, 0, 6.5073301312, 1.7703878375, 1.2164448817  
H, 0, 10.9990458172, 1.0805163519, 1.1533608975

## H-pipN5-I

C,0,-9.9891425101,-2.1992435842,-0.0862422279  
N,0,-8.7765170897,-1.3821718261,-0.0253349279  
C,0,-7.9294252465,-1.7179488679,1.1086999713  
C,0,-6.7924552494,-0.7146603224,1.2473298279  
N,0,-5.9784952564,-0.6715155868,-0.0353411392  
C,0,-6.8817672203,-0.3982511421,-1.2265990202  
C,0,-8.0148230067,-1.4145021072,-1.2643827525  
C,0,-4.7862620782,0.2144882374,0.0344238319  
C,0,-3.5424625664,-0.3892584341,-0.0906077965  
C,0,-2.4208768594,0.4409404051,-0.0262315233  
C,0,-2.5933193365,1.838918201,0.157077758  
C,0,-3.8466907573,2.4281432057,0.2814615906  
C,0,-4.960257894,1.5922977665,0.2181746959  
N,0,-1.3118921366,2.3358575322,0.1682861513  
C,0,-0.4407974901,1.2678357994,0.0027127761  
N,0,-1.0932130336,0.1241622447,-0.1171229598  
C,0,1.0098316277,1.416467725,-0.0259950277  
C,0,1.7951364819,0.2562495345,0.0088568504  
C,0,3.1789311968,0.3938159072,-0.0107212981  
C,0,3.7625317288,1.684866732,-0.0701301737  
C,0,2.9958135165,2.8477728038,-0.1122135597  
C,0,1.6167253672,2.6943445437,-0.0889977564  
N,0,4.1618135201,-0.5730127037,0.0206512637  
C,0,5.3057444815,0.0748319594,-0.018339943  
N,0,5.1169516199,1.4512317447,-0.0763743755  
C,0,6.6259320229,-0.5497849816,-0.0030965115  
C,0,6.7199561783,-1.9392211639,0.1921331645  
C,0,7.9484366161,-2.5742295235,0.2160142707  
C,0,9.1217591699,-1.8317276162,0.0423982771  
C,0,9.0479311001,-0.4507748643,-0.1567151133  
C,0,7.8092484074,0.1788828269,-0.1795584717  
O,0,10.2985841724,-2.5114068394,0.076418242  
H,0,-10.6168287862,-1.8566285164,-0.9103571149  
H,0,-10.553954398,-2.0805037463,0.8397364611  
H,0,-9.7747998961,-3.2704537228,-0.2309614021  
H,0,-8.5193525881,-1.6832905798,2.0274088601  
H,0,-7.5154441361,-2.7438651236,1.032833376  
H,0,-6.1039039346,-0.9780232817,2.0501201277  
H,0,-7.1735112988,0.2916731848,1.4115111161  
H,0,-5.6097669407,-1.6175053228,-0.1696399329  
H,0,-6.2542587737,-0.4450809329,-2.1165222581  
H,0,-7.2643003204,0.6135599447,-1.1050042345  
H,0,-8.6680322151,-1.1556840064,-2.1007883681  
H,0,-7.6056155222,-2.422716073,-1.4781655228  
H,0,-3.4209553492,-1.4585954144,-0.232464987  
H,0,-3.9721636867,3.4945943748,0.4220928575  
H,0,-5.9489527002,2.0233292368,0.3117679418  
H,0,-1.046761576,3.2947232245,0.3274052371  
H,0,1.33076079,-0.7196100798,0.0538631006  
H,0,3.4438129146,3.8324779569,-0.1681197075  
H,0,1.0085784031,3.5900296355,-0.1447251476  
H,0,5.8400310687,2.1520905377,-0.0795955738  
H,0,5.8082311347,-2.5071039762,0.3254928465



H, 0, 8.023748308, -3.6437704692, 0.3682387032  
H, 0, 9.9542338266, 0.1293051184, -0.2983310548  
H, 0, 7.7883703548, 1.2497487125, -0.3505411149  
H, 0, 11.0405343134, -1.9105197674, -0.0533050672

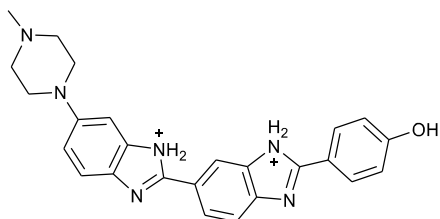
## H-pipN5-II

C, 0, -10.318626232, -1.0078048622, -0.2979626645  
N, 0, -8.8765903828, -0.7686303902, -0.2221524897  
C, 0, -8.3802873883, 0.0277266367, -1.333899299  
C, 0, -6.8586224662, 0.0770137646, -1.3236497503  
N, 0, -6.3644573032, 0.6386835612, -0.0001979333  
C, 0, -6.9518299971, -0.1483233928, 1.1602647854  
C, 0, -8.4696713994, -0.1882019676, 1.0482746558  
C, 0, -4.8914882267, 0.8159355875, 0.0710530529  
C, 0, -4.0583157915, -0.2996958499, 0.0027271518  
C, 0, -2.6959651552, -0.0359852402, 0.0764478902  
C, 0, -2.1750477575, 1.2818854583, 0.2114960194  
C, 0, -3.0464666847, 2.3705224561, 0.2784567368  
C, 0, -4.4134110197, 2.1244812018, 0.206364882  
N, 0, -0.8068397985, 1.250284059, 0.2574743245  
C, 0, -0.4659657277, -0.0202890032, 0.1571767103  
N, 0, -1.5833958111, -0.8417709237, 0.048282339  
C, 0, 0.9006022409, -0.5293057762, 0.1523944243  
C, 0, 1.9493335124, 0.3959650354, 0.0603858488  
C, 0, 3.2545789131, -0.083847822, 0.0501909984  
C, 0, 3.4988010991, -1.4784119548, 0.1340895909  
C, 0, 2.4676006042, -2.4105386006, 0.2334941417  
C, 0, 1.1705816616, -1.9165453009, 0.2415243839  
N, 0, 4.4461542758, 0.6047408051, -0.0339661821  
C, 0, 5.3927758149, -0.307606115, -0.0035516648  
N, 0, 4.8679094746, -1.591723231, 0.0961695763  
C, 0, 6.8258678024, -0.0328289538, -0.0643608589  
C, 0, 7.2634481678, 1.3036749241, -0.0562915954  
C, 0, 8.6103597839, 1.6130735301, -0.1100465701  
C, 0, 9.5602984698, 0.5876359633, -0.1751781207  
C, 0, 9.1443591316, -0.7461755591, -0.187378894  
C, 0, 7.7888654694, -1.0478400573, -0.1332139856  
O, 0, 10.8684116603, 0.9539537058, -0.225310162  
H, 0, -10.6208885307, -1.6660286958, 0.5180490705  
H, 0, -10.5549031649, -1.5068722299, -1.2390269564  
H, 0, -10.9087373192, -0.0792872566, -0.2360259979  
H, 0, -8.6936482526, -0.4265721546, -2.2765925123  
H, 0, -8.787629915, 1.0589912569, -1.325059122  
H, 0, -6.4597908514, 0.7197675574, -2.1082843405  
H, 0, -6.4325693208, -0.920175039, -1.419650723  
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H, 0, -6.6167308721, 0.3401976893, 2.0750921078  
H, 0, -6.5275507306, -1.1494551799, 1.1069335835  
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H, 0, -4.4419090375, -1.3074653751, -0.1003046746  
H, 0, -2.6622842931, 3.3770059943, 0.3828052075  
H, 0, -5.1096899326, 2.9565752665, 0.25541414  
H, 0, -1.5689223241, -1.8393288402, -0.0903425863  
H, 0, 1.7417445306, 1.4556443046, -0.0033321813  
H, 0, 2.6571029529, -3.4744374652, 0.3092420259  
H, 0, 0.3600080132, -2.6294531073, 0.3427802023  
H, 0, 5.3947664924, -2.4471756028, 0.1639589481  
H, 0, 6.5230537372, 2.0915502962, -0.0055972551

H, 0, 8.9499418834, 2.6413539632, -0.1020839145  
H, 0, 9.8764549706, -1.5454836985, -0.2428385498  
H, 0, 7.5015864534, -2.0935119708, -0.1558258053  
H, 0, 11.4363544952, 0.1767825285, -0.2672700029

Ground State (S<sub>0</sub>) of 2+ Charge State at B3LYP/6-31G(d)

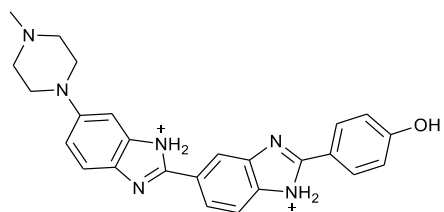
H-bz1-bz2-a



C	0	10.51402	0.62931	0.73227
N	0	9.24158	0.26889	0.11041
C	0	8.66592	-0.93859	0.67842
C	0	7.43691	-1.38708	-0.11815
N	0	6.4403	-0.30228	-0.2172
C	0	7.03416	0.97593	-0.65778
C	0	8.2664	1.34407	0.16867
C	0	5.10201	-0.54571	-0.22781
C	0	4.14899	0.53362	-0.21494
C	0	2.82597	0.19294	-0.18222
C	0	2.31169	-1.11214	-0.17128
C	0	3.2266	-2.17145	-0.20313
C	0	4.57834	-1.883	-0.23592
N	0	0.93052	-1.12551	-0.14113
C	0	0.46597	0.07057	-0.12723
N	0	1.64246	1.09306	-0.15231
C	0	-0.90352	0.53011	-0.08886
C	0	-1.92037	-0.46366	-0.0625
C	0	-3.21349	-0.01092	-0.02754
C	0	-3.58715	1.34461	-0.01597
C	0	-2.59072	2.31853	-0.04156
C	0	-1.26267	1.89622	-0.07804
N	0	-4.47118	-0.78154	0.00514
C	0	-5.55713	0.37939	0.03534
N	0	-4.96489	1.51602	0.02091
C	0	-6.93817	0.02436	0.07157
C	0	-7.89328	1.07723	0.09772
C	0	-9.24066	0.80036	0.13307
C	0	-9.68556	-0.5393	0.14366
C	0	-8.75045	-1.59517	0.11805
C	0	-7.39808	-1.31263	0.08257
O	0	-11.00687	-0.73096	0.17837
H	0	10.92575	1.51148	0.23296
H	0	11.22473	-0.19305	0.60833
H	0	10.421	0.85001	1.81088
H	0	9.4038	-1.74656	0.63482
H	0	8.3802	-0.80724	1.74145
H	0	7.73871	-1.69497	-1.12836
H	0	6.9971	-2.2412	0.39532
H	0	6.30475	1.78135	-0.59062
H	0	7.32676	0.86819	-1.71121
H	0	7.95768	1.58063	1.20729

H	0	8.70298	2.25221	-0.2608
H	0	4.465	1.56803	-0.19983
H	0	2.88068	-3.19929	-0.22162
H	0	5.26257	-2.71693	-0.30213
H	0	1.59408	1.70088	-0.98012
H	0	1.63041	1.69933	0.67818
H	0	-1.64739	-1.5136	-0.07082
H	0	-2.84871	3.37148	-0.03363
H	0	-0.49507	2.6652	-0.09875
H	0	-4.55529	-1.38029	0.83642
H	0	-4.59944	-1.37847	-0.82181
H	0	-7.54594	2.10457	0.08941
H	0	-9.9796	1.59398	0.15324
H	0	-9.09232	-2.62641	0.12618
H	0	-6.70615	-2.15176	0.06356
H	0	-11.23734	-1.67603	0.18352

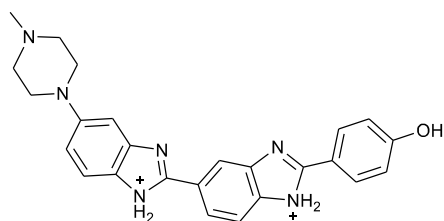
H-bz1-bz2-b



C	0	9.71622	2.63529	0.58597
N	0	8.64842	1.82477	0.00421
C	0	8.52899	0.5225	0.63846
C	0	7.53184	-0.36424	-0.11334
N	0	6.21963	0.30057	-0.2439
C	0	6.33241	1.6809	-0.75612
C	0	7.36028	2.49563	0.02943
C	0	5.04907	-0.39049	-0.21119
C	0	3.78061	0.29213	-0.23259
C	0	2.658	-0.48246	-0.15202
C	0	2.63008	-1.88255	-0.0618
C	0	3.85523	-2.56093	-0.05997
C	0	5.02228	-1.82502	-0.13847
N	0	1.34193	-2.37217	0.00046
C	0	0.48848	-1.41672	-0.03686
N	0	1.2354	-0.04985	-0.14179
C	0	-0.96006	-1.46519	0.00915
C	0	-1.76128	-0.30505	-0.04482
C	0	-3.14248	-0.45789	0.00483
C	0	-3.69617	-1.7384	0.10514
C	0	-2.94383	-2.89766	0.16027
C	0	-1.5577	-2.74546	0.11092
N	0	-4.1158	0.54298	-0.03419
C	0	-5.28434	0.02143	0.03294
N	0	-5.15737	-1.55384	0.13385
C	0	-6.58944	0.60241	0.03055
C	0	-6.68932	2.01661	-0.06145
C	0	-7.91927	2.63424	-0.06841
C	0	-9.09726	1.86127	0.0164
C	0	-9.01506	0.45655	0.10825
C	0	-7.77737	-0.15901	0.11484
O	0	-10.25391	2.52947	0.00398
H	0	9.79531	3.57945	0.03879
H	0	10.66852	2.10589	0.48806
H	0	9.55261	2.86348	1.65459
H	0	9.50165	0.01983	0.619
H	0	8.21664	0.59971	1.69927
H	0	7.91978	-0.59772	-1.11393
H	0	7.41795	-1.29125	0.44695
H	0	5.36871	2.18563	-0.71522
H	0	6.64442	1.62687	-1.80805
H	0	6.98911	2.66243	1.06119
H	0	7.45339	3.47591	-0.45036
H	0	3.71895	1.37103	-0.27869
H	0	3.88546	-3.64434	-0.01757

H	0	5.95306	-2.37276	-0.1774
H	0	0.97521	0.45493	-0.99877
H	0	1.01525	0.55967	0.65653
H	0	-1.35309	0.69747	-0.1238
H	0	-3.38532	-3.88629	0.23817
H	0	-0.91759	-3.61901	0.15054
H	0	-5.5914	-1.89947	0.99998
H	0	-5.63768	-2.00913	-0.65358
H	0	-5.78152	2.60627	-0.12646
H	0	-8.00934	3.71278	-0.13824
H	0	-9.92083	-0.13984	0.17361
H	0	-7.75368	-1.24406	0.18695
H	0	-11.01931	1.93221	0.06534

### H-bz1-bz2-c

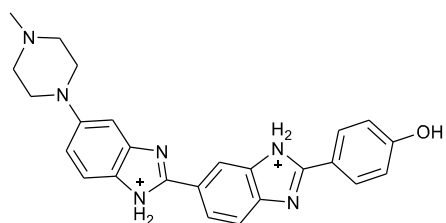


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N,0,14.7786401787,1.8127734727,-0.3381806591  
C,0,16.14009198,1.2458719516,-0.2700137896  
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C,0,12.3646708548,1.540528124,-0.0981015065  
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C,0,12.7063905408,-1.2898321302,-0.2381883592  
C,0,13.8000308606,-0.426881515,-0.2742941706  
N,0,10.1043077666,-1.3083929159,-0.0652302549  
C,0,9.2179096741,-0.0387641929,0.0667863721  
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C,0,7.1136437576,-1.4087790735,0.1643828675  
C,0,5.7261256712,-1.4233845336,0.2727884316  
C,0,5.0305975408,-0.2145422832,0.3873185438  
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O,0,-0.9646393773,-5.2374686537,0.6085845726  
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H,0,3.170822797,-0.2662224994,1.3640918657  
H,0,3.4734139488,-4.7804566023,0.2819802176  
H,0,1.3967955929,-6.1458136186,0.3769147592  
H,0,-0.9502073178,-2.5456846211,0.7428231152  
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H,0,-1.79437159,-4.7374386921,0.6990619849

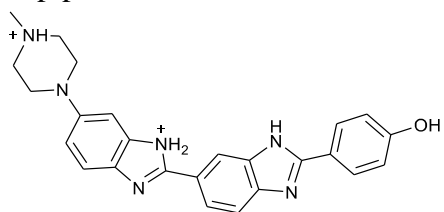
H-bz1-bz2-d



C	0	-9.65374	2.84404	0.09786
N	0	-8.49646	2.01494	-0.23101
C	0	-7.24826	2.59983	0.22706
C	0	-6.05347	1.81237	-0.30856
N	0	-6.14499	0.37109	-0.00385
C	0	-7.48192	-0.22151	-0.20731
C	0	-8.60285	0.67389	0.31869
C	0	-5.02644	-0.41524	-0.03506
C	0	-3.71334	0.15334	-0.04927
C	0	-2.6209	-0.69072	-0.01854
C	0	-2.76169	-2.08149	0.00619
C	0	-4.00418	-2.68501	-0.02001
C	0	-5.11594	-1.84579	-0.05005
N	0	-1.39829	-2.65013	0.0234
C	0	-0.52944	-1.36362	0.00282
N	0	-1.2626	-0.32187	-0.02128
C	0	0.92107	-1.4611	0.01305
C	0	1.64992	-0.24312	-0.0052
C	0	3.01669	-0.35278	0.00384
C	0	3.71905	-1.57117	0.02973
C	0	3.00168	-2.76609	0.04782
C	0	1.60928	-2.69174	0.03906
N	0	4.04058	0.70884	-0.01016
C	0	5.3837	-0.14262	0.01227
N	0	5.09495	-1.39257	0.03362
C	0	6.63115	0.54409	0.00611
C	0	7.8187	-0.23957	0.0266
C	0	9.05514	0.36257	0.02189
C	0	9.15351	1.77127	-0.00348
C	0	7.98465	2.56301	-0.02402
C	0	6.74506	1.95438	-0.0192
O	0	10.38479	2.28394	-0.00657
H	0	-10.55994	2.37877	-0.30137
H	0	-9.54228	3.82693	-0.36994
H	0	-9.7868	2.98871	1.18542
H	0	-7.16575	3.62538	-0.14861
H	0	-7.19272	2.64636	1.33359
H	0	-5.97976	1.94987	-1.397
H	0	-5.15643	2.22478	0.15531
H	0	-7.54221	-1.1673	0.33308
H	0	-7.63592	-0.41852	-1.27798
H	0	-8.5807	0.67803	1.4271
H	0	-9.55469	0.22761	0.01209
H	0	-3.54164	1.21888	-0.08625
H	0	-4.14184	-3.76188	-0.02866

H	0	-6.08291	-2.32454	-0.09699
H	0	-1.19743	-3.24512	-0.79302
H	0	-1.20571	-3.21286	0.86426
H	0	1.11829	0.70249	-0.02512
H	0	3.51773	-3.71924	0.06792
H	0	1.05982	-3.62902	0.05312
H	0	3.98907	1.32919	0.80813
H	0	3.99761	1.29907	-0.85091
H	0	7.73673	-1.32078	0.04604
H	0	9.96838	-0.22228	0.03731
H	0	8.06092	3.64657	-0.04354
H	0	5.86633	2.59525	-0.03548
H	0	10.37656	3.25677	-0.02452

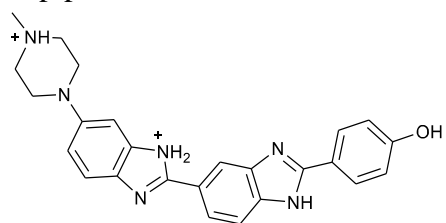
# H-pip1-bz1-aI



C	0	-9.85251	-2.55437	0.23575
N	0	-8.78384	-1.55793	-0.12958
C	0	-8.40801	-0.65952	1.03436
C	0	-7.34018	0.34521	0.60894
N	0	-6.16274	-0.35594	0.10966
C	0	-6.49571	-1.1715	-1.06054
C	0	-7.54467	-2.22113	-0.7007
C	0	-4.94532	0.39194	0.02984
C	0	-3.72378	-0.31837	0.04847
C	0	-2.56811	0.43124	-0.00789
C	0	-2.53408	1.83264	-0.05688
C	0	-3.73963	2.52971	-0.06184
C	0	-4.92865	1.79764	-0.02872
N	0	-1.24032	2.33916	-0.08351
C	0	-0.38321	1.38537	-0.04846
N	0	-1.1628	-0.01287	0.00926
C	0	1.03899	1.3653	-0.04847
C	0	1.793	0.16168	-0.00305
C	0	3.16705	0.28198	-0.00647
C	0	3.83044	1.55268	-0.05399
C	0	3.06929	2.73708	-0.09928
C	0	1.69549	2.63548	-0.09596
N	0	4.19958	-0.63187	0.02893
C	0	5.39095	0.07589	0.0035
N	0	5.17554	1.39304	-0.04673
C	0	6.69873	-0.53991	0.02862
C	0	6.88619	-1.93799	0.08079
C	0	8.1548	-2.48616	0.10367
C	0	9.28005	-1.64206	0.0747
C	0	9.11129	-0.24796	0.02261
C	0	7.83712	0.29265	-0.00002
O	0	10.48771	-2.23885	0.09932
H	0	-10.10734	-3.13847	-0.65
H	0	-9.46536	-3.20686	1.01959
H	0	-10.7294	-2.01359	0.5952
H	0	-9.16936	-0.9526	-0.86576
H	0	-8.04239	-1.31718	1.82639
H	0	-9.31963	-0.15757	1.36771
H	0	-7.07129	0.93281	1.49093
H	0	-7.77199	1.04396	-0.13258
H	0	-5.60745	-1.69977	-1.41478
H	0	-6.85631	-0.55246	-1.90382
H	0	-7.17851	-2.90084	0.07251
H	0	-7.85485	-2.79637	-1.57655
H	0	-3.7165	-1.40072	0.13439

H	0	-3.74772	3.61325	-0.1015
H	0	-5.86317	2.34735	-0.05241
H	0	-0.90864	-0.59648	-0.7963
H	0	-0.90793	-0.52709	0.86087
H	0	1.3241	-0.81922	0.03361
H	0	3.56514	3.70089	-0.13521
H	0	1.0796	3.52697	-0.12939
H	0	4.11163	-1.63642	0.06833
H	0	6.03693	-2.61648	0.10403
H	0	8.30812	-3.55902	0.14371
H	0	9.98042	0.40498	0.00016
H	0	7.69769	1.36713	-0.04011
H	0	11.19752	-1.57576	0.07624

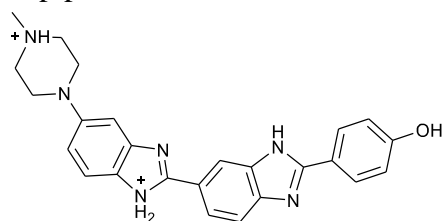
# H-pip1-bz1-aII



C	0	10.56014	0.65241	0.22969
N	0	9.22242	0.08548	-0.16815
C	0	8.58854	-0.7336	0.94073
C	0	7.24698	-1.30341	0.48571
N	0	6.35541	-0.2234	0.07834
C	0	6.92284	0.5322	-1.04103
C	0	8.25891	1.15573	-0.64454
C	0	4.96	-0.52107	-0.0002
C	0	4.0428	0.55216	0.07629
C	0	2.7037	0.23001	0.02303
C	0	2.20792	-1.07715	-0.07667
C	0	3.1115	-2.13296	-0.13874
C	0	4.47719	-1.83805	-0.10979
N	0	0.81492	-1.12306	-0.08841
C	0	0.3267	0.05459	0.0037
N	0	1.52653	1.112	0.09299
C	0	-1.01231	0.55157	0.04191
C	0	-2.05511	-0.40424	-0.03195
C	0	-3.3639	0.0518	0.00431
C	0	-3.62536	1.45352	0.1139
C	0	-2.60487	2.40869	0.18757
C	0	-1.30075	1.94252	0.15024
N	0	-4.54051	-0.65404	-0.04947
C	0	-5.50423	0.24617	0.02186
N	0	-4.98441	1.54422	0.12236
C	0	-6.92791	-0.03617	0.00194
C	0	-7.90737	0.97452	0.07949
C	0	-9.25617	0.66478	0.05774
C	0	-9.66174	-0.67625	-0.04309
C	0	-8.69814	-1.69514	-0.12134
C	0	-7.3501	-1.37583	-0.09888
O	0	-10.99068	-0.91356	-0.05937
H	0	10.9806	1.19253	-0.6201
H	0	10.41346	1.32963	1.07225
H	0	11.21865	-0.16884	0.51691
H	0	9.38369	-0.55067	-0.95956
H	0	8.46567	-0.05894	1.79119
H	0	9.29132	-1.52806	1.20352
H	0	6.81342	-1.83704	1.33581
H	0	7.41746	-2.04568	-0.31691
H	0	6.25093	1.34495	-1.32581
H	0	7.05448	-0.10189	-1.93801
H	0	8.14107	1.8535	0.18803
H	0	8.72864	1.66839	-1.4876
H	0	4.39361	1.57166	0.20356

H	0	2.75912	-3.15526	-0.21925
H	0	5.17535	-2.66474	-0.17973
H	0	1.4683	1.782	-0.68301
H	0	1.46448	1.64442	0.96915
H	0	-1.83257	-1.46182	-0.11393
H	0	-2.8146	3.47007	0.27057
H	0	-0.50134	2.67725	0.20701
H	0	-5.52399	2.39571	0.19043
H	0	-7.62881	2.02248	0.15802
H	0	-10.01438	1.43795	0.11701
H	0	-9.01013	-2.73397	-0.19944
H	0	-6.60115	-2.15779	-0.15882
H	0	-11.16411	-1.86645	-0.13125

# H-pip1-bz1-bl

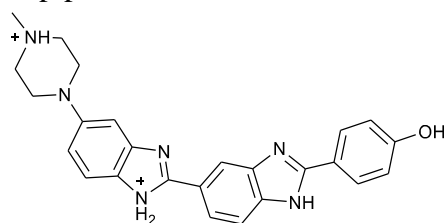


C	0	10.542	-0.66006	0.25671
N	0	9.10684	-0.58335	-0.19376
C	0	8.15859	-1.2524	0.78309
C	0	6.71614	-1.16676	0.28652
N	0	6.34124	0.22344	0.06925
C	0	7.20564	0.86106	-0.924
C	0	8.66031	0.84127	-0.46389
C	0	4.9601	0.55876	0.05181
C	0	3.96521	-0.43185	-0.0303
C	0	2.62909	-0.03661	0.008
C	0	2.30685	1.32082	0.10554
C	0	3.25757	2.32018	0.18003
C	0	4.59619	1.9195	0.161
N	0	0.83702	1.39784	0.11168
C	0	0.43557	-0.13569	-0.00707
N	0	1.50318	-0.85164	-0.0596
C	0	-0.94576	-0.47239	-0.03431
C	0	-1.9753	0.50502	0.04078
C	0	-3.2763	0.04997	0.00554
C	0	-3.60508	-1.34203	-0.10239
C	0	-2.57377	-2.29945	-0.17634
C	0	-1.26817	-1.86216	-0.14185
N	0	-4.50259	0.67929	0.0542
C	0	-5.48194	-0.29776	-0.02129
N	0	-4.94731	-1.51907	-0.11617
C	0	-6.90096	-0.0245	0.00059
C	0	-7.42769	1.28148	0.10169
C	0	-8.79223	1.49946	0.11988
C	0	-9.67443	0.40643	0.03655
C	0	-9.16691	-0.90018	-0.06474
C	0	-7.79875	-1.10956	-0.08221
O	0	-10.99179	0.68652	0.05951
H	0	11.17472	-0.20064	-0.50436
H	0	10.63831	-0.12304	1.20139
H	0	10.81362	-1.70842	0.38989
H	0	9.03754	-1.09522	-1.08263
H	0	8.27956	-0.73015	1.73508
H	0	8.48113	-2.29066	0.8932
H	0	6.08604	-1.60185	1.06642
H	0	6.59509	-1.78879	-0.62023
H	0	6.9179	1.9036	-1.06714
H	0	7.11822	0.36864	-1.91066
H	0	8.79006	1.38723	0.47369
H	0	9.3275	1.25523	-1.22399
H	0	4.1939	-1.48467	-0.13927



H	0	3.00231	3.37133	0.27208
H	0	5.3645	2.6763	0.27361
H	0	0.45342	1.93185	-0.67775
H	0	0.45339	1.80282	0.97463
H	0	-1.76471	1.56886	0.1232
H	0	-2.81611	-3.35335	-0.25804
H	0	-0.45052	-2.57181	-0.19627
H	0	-4.66495	1.67234	0.13284
H	0	-6.77223	2.14635	0.16754
H	0	-9.20557	2.4991	0.19733
H	0	-9.84823	-1.74508	-0.12918
H	0	-7.39845	-2.11418	-0.15993
H	0	-11.51647	-0.1289	-0.00274

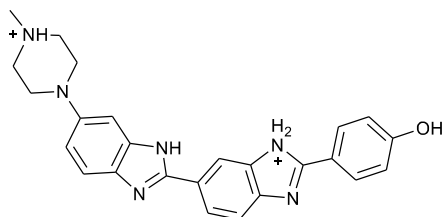
### H-pip1-bz1-bII



C	0	-9.76481	2.58283	0.23748
N	0	-8.4301	2.04607	-0.20917
C	0	-7.32834	2.33176	0.79352
C	0	-5.98855	1.78514	0.30219
N	0	-6.09434	0.35663	0.03949
C	0	-7.10691	0.07331	-0.97804
C	0	-8.47892	0.56277	-0.52394
C	0	-4.90647	-0.42172	0.02421
C	0	-3.63435	0.17936	-0.00677
C	0	-2.51202	-0.64384	0.03142
C	0	-2.66286	-2.03215	0.07855
C	0	-3.89511	-2.65648	0.10217
C	0	-5.02049	-1.82852	0.08363
N	0	-1.30466	-2.59632	0.09824
C	0	-0.41162	-1.28363	0.04567
N	0	-1.17221	-0.25253	0.00923
C	0	1.00939	-1.43215	0.04931
C	0	1.78453	-0.24705	0.00803
C	0	3.16549	-0.36758	0.01115
C	0	3.76484	-1.66533	0.05539
C	0	3.01198	-2.84478	0.09629
C	0	1.63336	-2.71273	0.09265
N	0	4.13254	0.60745	-0.02273
C	0	5.28845	-0.03098	-0.00132
N	0	5.10422	-1.41992	0.04637
C	0	6.5998	0.59126	-0.02307
C	0	7.79711	-0.15223	0.00331
C	0	9.02936	0.47756	-0.01849
C	0	9.0946	1.8798	-0.06768
C	0	7.91074	2.6352	-0.09451
C	0	6.68154	1.99617	-0.07237
O	0	10.32536	2.43427	-0.08679
H	0	-10.50279	2.3826	-0.54093
H	0	-10.04823	2.08106	1.16375
H	0	-9.67434	3.65747	0.40346
H	0	-8.18135	2.53181	-1.08044
H	0	-7.63111	1.852	1.72723
H	0	-7.28827	3.41441	0.93634
H	0	-5.2633	1.96171	1.10056
H	0	-5.65175	2.35798	-0.58207
H	0	-7.18078	-1.00057	-1.1551
H	0	-6.84529	0.53802	-1.94703
H	0	-8.7973	0.06365	0.39447
H	0	-9.234	0.41702	-1.30039
H	0	-3.49336	1.25072	-0.07652

H	0	-4.00926	-3.73469	0.15523
H	0	-6.00011	-2.28762	0.15652
H	0	-1.1007	-3.20103	-0.70721
H	0	-1.09688	-3.13574	0.94807
H	0	1.30722	0.72538	-0.02473
H	0	3.4774	-3.82437	0.12949
H	0	1.04079	-3.62352	0.12397
H	0	5.83679	-2.11543	0.06968
H	0	7.78361	-1.2386	0.04162
H	0	9.95384	-0.0891	0.00169
H	0	7.95932	3.72094	-0.13263
H	0	5.76376	2.57345	-0.09284
H	0	10.2608	3.40271	-0.12058

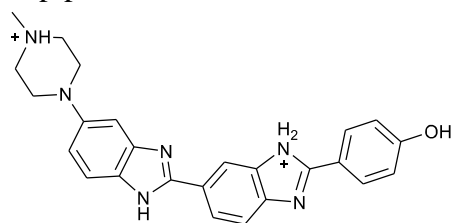
## H-pip1-bz2-aI



C,0,10.112918967,-1.9543350444,-0.1838210404  
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C,0,8.502237214,-0.271980903,0.7574139568  
C,0,7.0390627003,-0.0423546764,1.1218341915  
N,0,6.1877728831,-0.2523816764,-0.0448715165  
C,0,6.2881803651,-1.6139521368,-0.5339151683  
C,0,7.7260282513,-1.9061645202,-0.9620753029  
C,0,4.897898678,0.3710073924,-0.0146085001  
C,0,3.7127601294,-0.3702411194,-0.0481982987  
C,0,2.5165696437,0.3557479624,-0.0545647887  
C,0,2.4786284535,1.7695898558,-0.0041495321  
C,0,3.678207208,2.4953603964,0.0392254498  
C,0,4.8680456204,1.7894019408,0.0208377159  
N,0,1.1782789987,2.2181506977,-0.01813547  
C,0,0.4283341865,1.1374306938,-0.0709344019  
N,0,1.1881081699,-0.025326232,-0.0872562078  
C,0,-1.0357942676,1.1852485102,-0.1028046388  
C,0,-1.8462417381,0.0348446135,0.018510604  
C,0,-3.2108931985,0.2358427499,-0.0232393575  
C,0,-3.8212809328,1.4859028288,-0.1722590088  
C,0,-3.0223945756,2.6222635031,-0.2875730061  
C,0,-1.6420703654,2.4535288343,-0.2507237037  
N,0,-4.3072396478,-0.7471257331,0.0845389402  
C,0,-5.5867047561,0.1855541147,-0.0377437528  
N,0,-5.2160987325,1.3985834019,-0.1766830063  
C,0,-6.8854051526,-0.4188944635,0.021099342  
C,0,-8.0165165082,0.429909211,-0.0915904549  
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C,0,-9.4825048472,-1.476323902,0.1225530285  
C,0,-8.3698449685,-2.3313045179,0.2358163076  
C,0,-7.0901522945,-1.8047958365,0.185135769  
O,0,-10.7502226043,-1.9100028791,0.162279433  
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H,0,10.4075212611,-1.2634109582,-0.9749461579  
H,0,8.4244586197,-2.3281699196,0.9365463014  
H,0,8.8301967219,0.4201224131,-0.0217522554  
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H,0,5.653428078,-1.7348316316,-1.4160065604  
H,0,5.965906557,-2.3702371286,0.2098831188  
H,0,8.0397646641,-1.2350038799,-1.7648156104  
H,0,7.8529277962,-2.9441376636,-1.2802567465  
H,0,3.7137658364,-1.4552613564,-0.0551743539

H, 0, 3.6644454947, 3.5798514566, 0.0598612325  
H, 0, 5.8089397172, 2.330710434, -0.0020894869  
H, 0, 0.8508839912, -0.97015901, -0.1954660202  
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H, 0, -3.4707248871, 3.6028624586, -0.4021106745  
H, 0, -0.9858949175, 3.3123710251, -0.334364952  
H, 0, -4.3144659597, -1.2498901496, 0.980382788  
H, 0, -4.3009968601, -1.4476872332, -0.6666216621  
H, 0, -7.8644916264, 1.49631986, -0.2176774143  
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H, 0, -8.5143862258, -3.4007538403, 0.3627908447  
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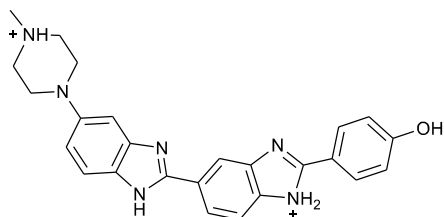
## H-pip1-bz2-aII



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C,0,7.0969055711,0.6002415346,1.059101952  
N,0,6.3109422166,0.2376367997,-0.116912553  
C,0,6.6718492289,-1.0843999006,-0.5991489341  
C,0,8.1406528794,-1.1017577243,-1.016068442  
C,0,4.9107113657,0.5559784472,-0.0509026671  
C,0,3.9257608361,-0.4272691645,-0.0037734846  
C,0,2.5834982376,-0.0159395543,0.0203984309  
C,0,2.2569560767,1.3602563182,0.0198072465  
C,0,3.238007768,2.3543371782,-0.0180842763  
C,0,4.5585371639,1.9307897817,-0.0652587165  
N,0,0.8756585592,1.391514724,0.0524783536  
C,0,0.438818259,0.0786963047,0.0842864775  
N,0,1.4394364567,-0.781179476,0.0628480672  
C,0,-0.9686335433,-0.3273062261,0.1298428571  
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C,0,-3.3073087434,0.0698349386,0.0283376353  
C,0,-3.6012324456,-1.2828110522,0.2325069409  
C,0,-2.5533687606,-2.1888184622,0.3871962001  
C,0,-1.2529175653,-1.6959761869,0.3329576553  
N,0,-4.6060695059,0.7574306531,-0.1101350179  
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O,0,-11.1380502421,0.3531042827,-0.1798960749  
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H,0,8.785418855,1.383102242,-0.0662420848  
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H,0,6.8069194961,1.5933720509,1.4091410206  
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## H-pip1-bz2-bl

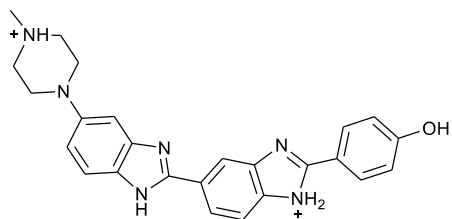


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C,0,3.7904559698,-2.5303074925,0.1166360736  
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N,0,1.2796856326,-2.3388448104,0.0947801859  
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C,0,-0.9688349857,-1.3638702525,0.0587599514  
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H,0,10.358457425,1.5697183638,0.9817461558  
H,0,8.3568353814,2.4117424468,-1.0193503498  
H,0,8.8698437551,-0.2443624057,0.1285842591  
H,0,9.1965092157,0.2628265157,-1.5535816439  
H,0,7.0283345016,-0.9933169434,-1.3526140248  
H,0,6.7782980395,0.6465132042,-1.9560799015  
H,0,5.5813468321,1.8551919421,1.3338855713  
H,0,5.8916849471,2.3928642024,-0.326968988  
H,0,7.9825355342,1.4847479209,1.7448230518  
H,0,7.7277992756,3.1480773572,1.1451443782  
H,0,3.6853418891,1.4170257407,-0.0410031391



H,0,3.8158863434,-3.6137167055,0.1655006818  
H,0,5.9128136598,-2.2858985507,0.1917028806  
H,0,0.8406651628,0.8405099338,0.0097172298  
H,0,-1.3958500262,0.7867986352,-0.0238732142  
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H,0,-0.8779692508,-3.5065994828,0.1383099576  
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H,0,-5.6140695677,-1.9808595798,-0.7637628225  
H,0,-5.8763620566,2.6076870759,-0.1054859915  
H,0,-8.1275240664,3.6681242944,-0.1511683625  
H,0,-9.9608565929,-0.2288068177,-0.012339896  
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H,0,-11.1011960878,1.8149717484,-0.0910208922

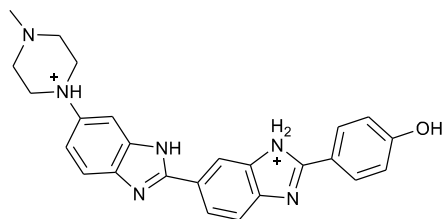
## H-pip1-bz2-bII



C,0,10.574355,0.489136,0.096403  
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C,0,8.60346,-0.850425,-0.697912  
C,0,7.116306,-0.771005,-1.028661  
N,0,6.364938,-0.29647,0.129672  
C,0,6.784342,1.039903,0.513494  
C,0,8.259289,1.026841,0.908819  
C,0,4.953159,-0.566809,0.109395  
C,0,4.002281,0.445513,0.011344  
C,0,2.645958,0.081376,0.039846  
C,0,2.273761,-1.28021,0.136912  
C,0,3.221036,-2.303805,0.227478  
C,0,4.554989,-1.924533,0.224823  
N,0,0.893883,-1.267404,0.125145  
C,0,0.499331,0.052894,0.024118  
N,0,1.526275,0.880409,-0.029654  
C,0,-0.900311,0.492026,-0.017845  
C,0,-1.97379,-0.416838,0.043349  
C,0,-3.266676,0.089004,-0.001039  
C,0,-3.472767,1.467544,-0.104184  
C,0,-2.446617,2.39109,-0.167077  
C,0,-1.147908,1.877454,-0.121879  
N,0,-4.472283,-0.624318,0.04574  
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N,0,-4.933668,1.667088,-0.125939  
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C,0,-7.339281,-1.381622,0.087759  
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C,0,-9.626189,-0.61059,0.021597  
C,0,-9.183956,0.722418,-0.074384  
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O,0,-10.920796,-0.956243,0.041559  
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H,0,11.131946,0.149443,-0.777927  
H,0,8.977857,1.154326,-1.023707  
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H,0,9.200647,-1.141584,-1.56573  
H,0,6.781031,-1.773,-1.305158  
H,0,6.96358,-0.126526,-1.917003  
H,0,6.210273,1.367915,1.384399  
H,0,6.626738,1.792951,-0.284256  
H,0,8.435577,0.355467,1.752326  
H,0,8.624227,2.027848,1.152586  
H,0,4.267981,1.4921,-0.088554

H,0,2.940423,-3.348135,0.320895  
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H,0,-2.617325,3.46016,-0.247005  
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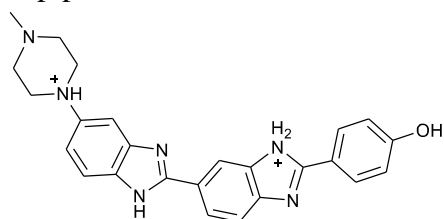
## H-pip2-bz2-aI



C, 0, -9.4990613162, -2.8045178426, 0.1070801409  
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C, 0, -7.9719080098, -1.4190536534, -1.1783223219  
C, 0, -6.5366975829, -0.9077070016, -1.2408463037  
N, 0, -6.2698599328, 0.0220556219, -0.060862136  
C, 0, -6.6100135906, -0.6758003948, 1.2527815012  
C, 0, -8.0418133965, -1.1978297608, 1.2020373949  
C, 0, -4.9271738893, 0.6570033251, -0.0800988506  
C, 0, -3.7877065775, -0.138997052, 0.0262575007  
C, 0, -2.5736183255, 0.547385566, 0.0005999419  
C, 0, -2.4962291081, 1.9608138286, -0.1223004319  
C, 0, -3.6645907681, 2.7232241244, -0.2306459958  
C, 0, -4.88319679, 2.0560480367, -0.207506036  
N, 0, -1.1841289733, 2.3702180434, -0.1125095726  
C, 0, -0.4677664423, 1.2727092932, 0.0092597024  
N, 0, -1.2586139698, 0.1333223856, 0.0739701967  
C, 0, 0.9990553458, 1.277548952, 0.0651838871  
C, 0, 1.7739946614, 0.1026480123, -0.0463289832  
C, 0, 3.1433274108, 0.2618202747, 0.0128607209  
C, 0, 3.7875936068, 1.4953144123, 0.1705464026  
C, 0, 3.0221959558, 2.6551150333, 0.2758173492  
C, 0, 1.6373358186, 2.5276630905, 0.2201828407  
N, 0, 4.211719171, -0.7512622438, -0.0849323005  
C, 0, 5.5175449667, 0.1472020393, 0.0546561566  
N, 0, 5.177504097, 1.3706033571, 0.1916547317  
C, 0, 6.7969509727, -0.4915177009, 0.0100394535  
C, 0, 7.9497577347, 0.3276164491, 0.1379831651  
C, 0, 9.2104778091, -0.2252615203, 0.1023215716  
C, 0, 9.365568354, -1.6173946927, -0.0628099279  
C, 0, 8.2310644858, -2.4433324914, -0.1911592231  
C, 0, 6.9664577572, -1.8834486613, -0.1545969013  
O, 0, 10.6196556436, -2.0833415447, -0.0883200768  
H, 0, -9.5907044993, -3.3589088703, 1.0450848824  
H, 0, -9.5390255522, -3.5225864519, -0.7165644351  
H, 0, -10.359276393, -2.1197202946, 0.0182208059  
H, 0, -8.1114298419, -2.1170459513, -2.0101831128  
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H, 0, -6.3345241792, -0.3329303532, -2.1471566378  
H, 0, -5.8236037288, -1.7289662534, -1.1572946767  
H, 0, -6.9478536054, 0.7886646744, -0.1521002261  
H, 0, -6.4580779175, 0.0573338338, 2.0478067552  
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H, 0, -8.2331902204, -1.7314789749, 2.1386465082  
H, 0, -8.7497809879, -0.3427838417, 1.171538623  
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H, 0, -3.6139318516, 3.802051105, -0.327537245  
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H, 0, 3.4983784882, 3.6217473342, 0.396045038  
H, 0, 1.0081300503, 3.4074072122, 0.2938341357  
H, 0, 4.2157866025, -1.2517618219, -0.9823342611  
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H, 0, 7.8248966939, 1.3974979141, 0.2643824547  
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H, 0, 8.3491181739, -3.5158805436, -0.3186518788  
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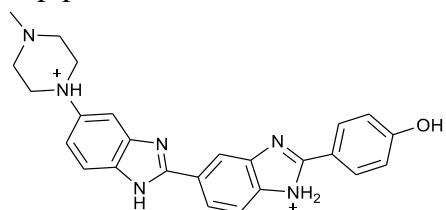
## H-pip2-bz2-aII



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C,0,8.4263487385,0.2767108525,1.2842359517  
C,0,7.0237408062,-0.3208293642,1.2558182756  
N,0,6.2708918116,0.1907406292,0.0307093116  
C,0,7.0745056814,-0.0818660545,-1.2379155327  
C,0,8.4746359979,0.5050746514,-1.0957987997  
C,0,4.8579877144,-0.2635136422,-0.0418399202  
C,0,3.8645428872,0.7029670142,0.0290733216  
C,0,2.5384654949,0.2578443535,-0.042721298  
C,0,2.2617416792,-1.1266871796,-0.1773729095  
C,0,3.2704230981,-2.0889503318,-0.248184943  
C,0,4.5848731122,-1.6381367132,-0.1786914154  
N,0,0.8848256623,-1.1988224823,-0.2097426727  
C,0,0.4017796202,0.0961260156,-0.1070711328  
N,0,1.372146667,0.9831092919,-0.0028345682  
C,0,-1.0207936223,0.4564961699,-0.1100747008  
C,0,-2.0504946273,-0.506134476,-0.0257568031  
C,0,-3.3434858903,-0.0259404062,-0.0338912587  
C,0,-3.6806209332,1.3308310275,-0.1156732711  
C,0,-2.6639402021,2.280901955,-0.1938809563  
C,0,-1.3477737307,1.8276861439,-0.1891719252  
N,0,-4.6187565364,-0.7632730725,0.0487012802  
C,0,-5.6773395234,0.4224539931,-0.0090257121  
N,0,-5.0607306429,1.5376416454,-0.0993953301  
C,0,-7.0701099294,0.1002599716,0.0443496026  
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C,0,-8.9193798626,-1.4695501784,0.1962581797  
C,0,-7.5594870478,-1.2201005986,0.1482882854  
O,0,-11.1575685621,-0.5554062222,0.1818491257  
H,0,11.0628046436,-0.0409057293,-0.7833636254  
H,0,11.027139201,-0.2102341261,0.977855963  
H,0,10.7298105335,1.3844484997,0.2360454868  
H,0,8.9496668564,-0.1493555131,2.1463316271  
H,0,8.362305307,1.3719197458,1.458459605  
H,0,6.4306565399,-0.041632352,2.1292864772  
H,0,7.0615913251,-1.4072745965,1.1675240029  
H,0,6.2402293481,1.2130473355,0.1280891453  
H,0,6.5159174957,0.3601156329,-2.0657277529  
H,0,7.1132419544,-1.1654596784,-1.3558654917  
H,0,9.0339418761,0.2488424504,-2.0013982466  
H,0,8.4131351767,1.613651968,-1.0609621371  
H,0,4.0791034517,1.7633828935,0.1340182676

H, 0, 3.0583547548, -3.1478404592, -0.3528589464  
H, 0, 5.3915451288, -2.3615006038, -0.2307919685  
H, 0, 0.347488365, -2.0399889234, -0.3625796127  
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H, 0, -4.7241463457, -1.2960359392, 0.9210640653  
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# H-pip2-bz2-bl

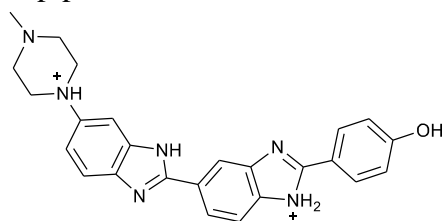


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N	0	9.21156	-0.23043	0.00033
C	0	8.53492	0.24489	1.19628
C	0	7.11181	-0.29982	1.25284
N	0	6.34874	0.12207	0.00031
C	0	7.112	-0.29841	-1.25259
C	0	8.53511	0.24621	-1.1952
C	0	4.91966	-0.28478	-0.00005
C	0	3.96156	0.71911	0.00027
C	0	2.61973	0.31666	-0.00008
C	0	2.29421	-1.06415	-0.00072
C	0	3.26834	-2.06465	-0.00105
C	0	4.59754	-1.6561	-0.00071
N	0	0.91735	-1.09179	-0.00088
C	0	0.47929	0.22049	-0.00037
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C	0	-0.93694	0.61598	-0.00036
C	0	-1.97704	-0.33145	-0.0001
C	0	-3.28722	0.1325	-0.00009
C	0	-3.53652	1.50824	-0.00031
C	0	-2.54284	2.46777	-0.00053
C	0	-1.22667	1.99588	-0.00056
N	0	-4.46646	-0.62163	0.00018
C	0	-5.48359	0.15337	0.00012
N	0	-5.00298	1.66146	-0.00017
C	0	-6.8898	-0.11642	0.00017
C	0	-7.30724	-1.47294	-0.00022
C	0	-8.64624	-1.79542	-0.00013
C	0	-9.61782	-0.77292	0.00039
C	0	-9.2193	0.57825	0.00077
C	0	-7.87287	0.897	0.00066
O	0	-10.89859	-1.16121	0.00051
H	0	11.10882	-0.36555	-0.88441
H	0	11.10868	-0.36654	0.88522
H	0	10.85142	1.16121	0.00123
H	0	9.06304	-0.1174	2.08416
H	0	8.51365	1.35333	1.26696
H	0	6.5497	0.08184	2.1078
H	0	7.1094	-1.39036	1.26721
H	0	6.35612	1.14938	0.0009
H	0	6.55003	0.08423	-2.1072
H	0	7.10955	-1.38894	-1.26819
H	0	9.06336	-0.11513	-2.0834
H	0	8.51388	1.35472	-1.26468
H	0	4.21499	1.77614	0.00077



H	0	3.01756	-3.12017	-0.00155
H	0	5.37836	-2.40912	-0.00095
H	0	0.34571	-1.9246	-0.00149
H	0	-1.80247	-1.40161	0.00017
H	0	-2.74899	3.53348	-0.00069
H	0	-0.39925	2.69552	-0.00074
H	0	-5.35686	2.15615	-0.82908
H	0	-5.35662	2.15642	0.82868
H	0	-6.55651	-2.25555	-0.00062
H	0	-8.97767	-2.82806	-0.00047
H	0	-9.96588	1.36762	0.00116
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H	0	-11.5049	-0.40093	0.00076

# H-pip2-bz2-bII



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N	0	8.1485	-2.25618	0.00079
C	0	7.97918	-1.44503	1.19609
C	0	6.56734	-0.87173	1.2528
N	0	6.29751	-0.04414	-0.00045
C	0	6.56671	-0.87366	-1.25254
C	0	7.97859	-1.44684	-1.19566
C	0	4.98095	0.64356	-0.00058
C	0	3.8111	-0.11301	-0.00014
C	0	2.62423	0.62061	-0.00022
C	0	2.60197	2.0415	-0.00069
C	0	3.80072	2.7638	-0.00112
C	0	4.99254	2.04959	-0.00105
N	0	1.30462	2.49752	-0.00065
C	0	0.54905	1.41966	-0.00018
N	0	1.29601	0.25241	0.00009
C	0	-0.92095	1.46261	0.00005
C	0	-1.70773	0.29647	-0.00022
C	0	-3.09068	0.43861	0.
C	0	-3.65672	1.717	0.00047
C	0	-2.91786	2.884	0.00073
C	0	-1.52781	2.73561	0.00051
N	0	-4.06004	-0.57163	-0.00019
C	0	-5.23076	-0.05668	0.00012
N	0	-5.11801	1.5209	0.00059
C	0	-6.53468	-0.6488	0.00006
C	0	-6.62338	-2.0652	-0.00062
C	0	-7.84985	-2.69193	-0.00069
C	0	-9.03369	-1.9251	-0.00008
C	0	-8.96219	-0.51829	0.00059
C	0	-7.7276	0.10648	0.00066
O	0	-10.18811	-2.6023	-0.00019
H	0	9.44722	-3.64674	-0.88341
H	0	9.44764	-3.64542	0.88646
H	0	10.29734	-2.35171	0.00036
H	0	8.11909	-2.0689	2.08478
H	0	8.71973	-0.62025	1.26524
H	0	6.41728	-0.20839	2.10723
H	0	5.82111	-1.66719	1.2672
H	0	7.00689	0.69911	-0.00123
H	0	6.41619	-0.21167	-2.10793
H	0	5.82052	-1.66919	-1.26534
H	0	8.11809	-2.07205	-2.08347
H	0	8.71909	-0.62215	-1.2664
H	0	3.81804	-1.19801	0.00024

H	0	3.79376	3.84812	-0.0015
H	0	5.93776	2.58761	-0.00139
H	0	0.94271	-0.69364	0.00062
H	0	-1.28505	-0.70218	-0.00067
H	0	-3.36927	3.87115	0.00108
H	0	-0.88806	3.61021	0.00067
H	0	-5.57802	1.91943	-0.82808
H	0	-5.57781	1.91895	0.82961
H	0	-5.71042	-2.65048	-0.00108
H	0	-7.93067	-3.77344	-0.00121
H	0	-9.8726	0.07469	0.00106
H	0	-7.71221	1.19409	0.00119
H	0	-10.95543	-2.00489	0.00025

## Excited State (S<sub>1</sub>) of 1+ Charge State at B3LYP/6-31G(d)

### H-pipN2-I (S<sub>1</sub>)

C, 0, 6.9398488698, 3.3674564141, 1.7820370788  
N, 0, 7.1139419941, 2.4131948649, 0.6410808373  
C, 0, 7.2342567453, 0.9691734578, 1.1066173244  
C, 0, 7.4433659906, 0.0605796431, -0.1127521447  
N, 0, 6.3543789919, 0.1730603986, -1.0686500538  
C, 0, 6.2320389794, 1.5375349414, -1.5339109098  
C, 0, 6.0125872342, 2.5572077755, -0.3992073869  
C, 0, 5.1434571966, -0.558156957, -0.7425887137  
C, 0, 3.8903905358, 0.0803243587, -0.6815433239  
C, 0, 2.7491864655, -0.7171122803, -0.3943729314  
C, 0, 2.912596314, -2.1077805038, -0.1325419955  
C, 0, 4.1538744771, -2.7399461847, -0.1818872145  
C, 0, 5.2708620308, -1.9369353933, -0.5109245288  
N, 0, 1.639159763, -2.5592686555, 0.1363654821  
C, 0, 0.7617762091, -1.4706661265, -0.0035719777  
N, 0, 1.4424186237, -0.353017596, -0.3097095669  
C, 0, -0.6695200698, -1.5435606598, 0.1670027878  
C, 0, -1.4656974247, -0.4210555807, -0.0896204595  
C, 0, -2.8647386357, -0.5351714591, 0.0729323647  
C, 0, -3.4628225636, -1.7637887531, 0.4903585935  
C, 0, -2.6870353719, -2.8938767146, 0.7629743297  
C, 0, -1.3178730612, -2.7598521061, 0.6006776824  
N, 0, -3.8269977526, 0.4066615702, -0.1251920923  
C, 0, -4.9990009424, -0.1966195185, 0.1534367652  
N, 0, -4.8204458556, -1.5082458043, 0.5312970639  
C, 0, -6.2607071667, 0.4795505029, 0.0529757747  
C, 0, -6.266561541, 1.8435557949, -0.3618924848  
C, 0, -7.4451028633, 2.541576443, -0.4790842377  
C, 0, -8.6693787225, 1.9006780801, -0.1848658607  
C, 0, -8.686828956, 0.5478339599, 0.2292462608  
C, 0, -7.501293556, -0.1463166928, 0.3447401563  
O, 0, -9.784845555, 2.6306896537, -0.3174435926  
H, 0, 6.9004369079, 4.3857699103, 1.390637242  
H, 0, 6.0056971232, 3.1261312594, 2.2912999772  
H, 0, 7.780758099, 3.2569310057, 2.4693730672  
H, 0, 7.9987511909, 2.6454026963, 0.1722556136  
H, 0, 6.2959185247, 0.7248531606, 1.6113518979  
H, 0, 8.0633653717, 0.9330225201, 1.8197413319  
H, 0, 7.5289382785, -0.9652994899, 0.2444370655  
H, 0, 8.3941522078, 0.316845104, -0.6063579632  
H, 0, 5.3994409253, 1.6178785304, -2.2361480332  
H, 0, 7.1470911373, 1.8092445232, -2.0832269323  
H, 0, 5.0770020729, 2.3658265646, 0.1297480051  
H, 0, 6.0413111114, 3.5934144616, -0.7502236508  
H, 0, 3.7364349694, 1.1277993994, -0.9089841835  
H, 0, 4.2704524574, -3.805335177, -0.0117559936  
H, 0, 6.2367968369, -2.4147519278, -0.6446870512  
H, 0, 1.3828307279, -3.5312329725, 0.2106547824  
H, 0, -1.0124773558, 0.5075962201, -0.4127154002  
H, 0, -3.1199354164, -3.833250548, 1.092195535  
H, 0, -0.7033578837, -3.6253960898, 0.8297820167

H, 0, -5.5374835305, -2.1714580148, 0.783699781  
H, 0, -5.3139371173, 2.3102081321, -0.5822744969  
H, 0, -7.464122613, 3.578950015, -0.7943667579  
H, 0, -9.6330021871, 0.0623539856, 0.4539796242  
H, 0, -7.5353778043, -1.1829317635, 0.663932652  
H, 0, -10.574445417, 2.107659622, -0.0959240552

## H-pipN2-II (S<sub>1</sub>)

C, 0, 8.1513150965, 2.3358580918, 1.8478713087  
N, 0, 8.0151362436, 1.234611796, 0.8396747881  
C, 0, 7.5412445032, -0.0686811064, 1.4650090361  
C, 0, 7.462777686, -1.1560797729, 0.3832842662  
N, 0, 6.5791397731, -0.7796881909, -0.7076892695  
C, 0, 7.012421416, 0.4585103362, -1.3192073315  
C, 0, 7.1219489104, 1.6311719375, -0.3266498602  
C, 0, 5.1676282078, -1.0109013998, -0.5163470534  
C, 0, 4.2232390931, 0.016024344, -0.6474893578  
C, 0, 2.8532183532, -0.3108659254, -0.4842581872  
C, 0, 2.4796713439, -1.6506892249, -0.16405731  
C, 0, 3.4186163048, -2.6741613341, -0.0284683502  
C, 0, 4.7670574238, -2.3337389775, -0.2256860642  
N, 0, 1.1109292111, -1.6078523602, -0.0579190837  
C, 0, 0.6994157579, -0.2934410599, -0.3146368725  
N, 0, 1.7645833202, 0.4931920015, -0.5673048095  
C, 0, -0.6658938929, 0.1415407958, -0.3050113006  
C, 0, -1.7463898673, -0.7343614419, -0.0194032898  
C, 0, -3.0257041021, -0.1882957968, -0.0488295943  
C, 0, -3.2843549477, 1.188869026, -0.3454044889  
C, 0, -2.1919232926, 2.054154678, -0.6271554141  
C, 0, -0.9257615199, 1.5310801382, -0.604226838  
N, 0, -4.2732062842, -0.7285978595, 0.169562168  
C, 0, -5.2110719003, 0.2898152486, 0.0054965161  
N, 0, -4.6135202136, 1.4497902897, -0.3050461461  
C, 0, -6.630147402, 0.127738465, 0.1470166725  
C, 0, -7.4717831997, 1.2595952318, -0.0501461326  
C, 0, -8.8394320804, 1.1583737716, 0.0729139715  
C, 0, -9.425048667, -0.0832066631, 0.3991904002  
C, 0, -8.6123273332, -1.2171390634, 0.5989614942  
C, 0, -7.2387045289, -1.1111459062, 0.4745515984  
O, 0, -10.7690329523, -0.1187511274, 0.5053344085  
H, 0, 8.5317433449, 3.2286270797, 1.3480271584  
H, 0, 7.1671967525, 2.5360637819, 2.2740532359  
H, 0, 8.8413362163, 2.0162347915, 2.6310232314  
H, 0, 8.9496104918, 1.0531734648, 0.4506503211  
H, 0, 6.5536354385, 0.1313858872, 1.8889317905  
H, 0, 8.2457972233, -0.3132689691, 2.2655958633  
H, 0, 7.1106336265, -2.0738095818, 0.8549752925  
H, 0, 8.4709098578, -1.3567237637, -0.0116191095  
H, 0, 6.3220693072, 0.7410344068, -2.1170409534  
H, 0, 7.9970621697, 0.2978705688, -1.7857849449  
H, 0, 6.1541401904, 1.882298734, 0.1115909861  
H, 0, 7.5662773394, 2.5226858181, -0.779568573  
H, 0, 4.477674038, 1.0378727486, -0.9016463016  
H, 0, 3.1328910761, -3.6986105719, 0.1880848687  
H, 0, 5.514597941, -3.1213593882, -0.2080056194  
H, 0, 0.5109835032, -2.3997082656, 0.1132519125  
H, 0, -1.5910758788, -1.782741275, 0.2147926708  
H, 0, -2.374133407, 3.0993213513, -0.8545583811  
H, 0, -0.0627868919, 2.151567213, -0.8156290988  
H, 0, -4.4653407004, -1.6912549839, 0.4005378624  
H, 0, -7.004089011, 2.2048410116, -0.3007249277

H, 0, -9.486837953, 2.0160808408, -0.0760352763  
H, 0, -9.0669331105, -2.1727651348, 0.8501754104  
H, 0, -6.6352757734, -2.0000280782, 0.6333008612  
H, 0, -11.0686862513, -1.0154166272, 0.730691846

## H-pipN5-I (S<sub>1</sub>)

C, 0, -9.9401349251, -2.2948345777, -0.0479799098  
N, 0, -8.7594244104, -1.4356865994, -0.0263803973  
C, 0, -7.9468247054, -1.6410243933, 1.1652220006  
C, 0, -6.8256193429, -0.6098707925, 1.2357144728  
N, 0, -5.96940554, -0.6807988221, -0.0099782212  
C, 0, -6.8292670491, -0.5424264593, -1.2474632202  
C, 0, -7.9503448434, -1.5759754259, -1.2297533988  
C, 0, -4.7857729357, 0.2291696609, 0.0130036066  
C, 0, -3.5322929746, -0.4054501613, -0.0060292085  
C, 0, -2.4033352922, 0.4702109496, 0.0161139083  
C, 0, -2.6087640255, 1.8718001277, 0.0544602724  
C, 0, -3.8780170863, 2.4818222204, 0.0728446991  
C, 0, -4.9922541901, 1.6033439632, 0.0506046612  
N, 0, -1.3388488542, 2.4002742755, 0.0669859006  
C, 0, -0.4322084576, 1.3423563782, 0.0369448436  
N, 0, -1.0705031432, 0.1744793495, 0.0061598575  
C, 0, 1.0258385484, 1.488950024, 0.0388138159  
C, 0, 1.818170477, 0.3473152229, 0.0063788244  
C, 0, 3.223931284, 0.5011222146, 0.0085285168  
C, 0, 3.8230131221, 1.7916271787, 0.0429909059  
C, 0, 3.0468673087, 2.9462106402, 0.0757630747  
C, 0, 1.6670333554, 2.7689631237, 0.072947002  
N, 0, 4.1848582095, -0.463876683, -0.0193192072  
C, 0, 5.3598467933, 0.1906603312, -0.0031201669  
N, 0, 5.1893250468, 1.5529155914, 0.0344477785  
C, 0, 6.6194730647, -0.5023834807, -0.0239543496  
C, 0, 6.6051959332, -1.9282402901, -0.0630131797  
C, 0, 7.776622541, -2.6444296285, -0.0843552998  
C, 0, 9.0143996885, -1.9586901067, -0.0673691557  
C, 0, 9.050943292, -0.5419320091, -0.0285898978  
C, 0, 7.8714401144, 0.1684254416, -0.0073966551  
O, 0, 10.1189743566, -2.7071525193, -0.0894980564  
H, 0, -10.5473349356, -2.0570491015, -0.926586102  
H, 0, -10.544732357, -2.1051393538, 0.8440178847  
H, 0, -9.6919555307, -3.3714832111, -0.0775867347  
H, 0, -8.5739984089, -1.5232154872, 2.0551422945  
H, 0, -7.5159924912, -2.6644129886, 1.2097063947  
H, 0, -6.1575377873, -0.7762084943, 2.0830011304  
H, 0, -7.2221237494, 0.4044480106, 1.284080185  
H, 0, -5.5754048383, -1.6278109199, -0.0362780635  
H, 0, -6.1636921632, -0.6624744965, -2.1044897942  
H, 0, -7.2258335175, 0.4729896034, -1.2395366753  
H, 0, -8.5801201972, -1.4100833923, -2.1101208407  
H, 0, -7.5197279522, -2.5954067493, -1.3309888571  
H, 0, -3.4107419199, -1.48337146, -0.0354787937  
H, 0, -4.0123819325, 3.5559645932, 0.1021922631  
H, 0, -5.9952918509, 2.0187970615, 0.0633325655  
H, 0, -1.1279755167, 3.3855644878, 0.0933342205  
H, 0, 1.3612989312, -0.6346249453, -0.0198438115  
H, 0, 3.4787330672, 3.9414735661, 0.1024035648  
H, 0, 1.054416367, 3.665137862, 0.0984434034  
H, 0, 5.9107677218, 2.2578647201, 0.0526579186  
H, 0, 5.6431668035, -2.4260312564, -0.0752506713



H, 0, 7.7835020654, -3.7281668817, -0.1140692109  
H, 0, 10.0067280688, -0.0251831886, -0.0158202406  
H, 0, 7.9170019803, 1.251848811, 0.022237695  
H, 0, 10.9229432514, -2.1587230142, -0.0756403066

## H-pipN5-II (S<sub>1</sub>)

C, 0, -10.3367614888, -0.9430727032, -0.2108190139  
N, 0, -8.8927964324, -0.7304653835, -0.1632421938  
C, 0, -8.4125090014, 0.0538352061, -1.2930217844  
C, 0, -6.8896709077, 0.1102720838, -1.3030921648  
N, 0, -6.3605790816, 0.6906192317, -0.0004125949  
C, 0, -6.9436906135, -0.0777764185, 1.1760506451  
C, 0, -8.464403484, -0.1271898883, 1.0916825389  
C, 0, -4.8921046337, 0.8342128782, 0.04249865  
C, 0, -4.0764533519, -0.3412388466, -0.0271456959  
C, 0, -2.6976620034, -0.0730191145, 0.0298518202  
C, 0, -2.1461438861, 1.22584295, 0.1426102592  
C, 0, -3.0083835229, 2.3674893572, 0.2096041371  
C, 0, -4.3762119929, 2.1309245594, 0.1569644176  
N, 0, -0.777780564, 1.1658234978, 0.1684262739  
C, 0, -0.4598012762, -0.1151043443, 0.0772915133  
N, 0, -1.6025122555, -0.9106234132, -0.0018438282  
C, 0, 0.919427246, -0.6260025159, 0.0694364829  
C, 0, 1.9672728699, 0.2830487002, 0.0235814524  
C, 0, 3.291213653, -0.214000781, 0.0221094951  
C, 0, 3.5510772542, -1.6132985597, 0.0602831779  
C, 0, 2.5137619648, -2.5383692264, 0.1075020153  
C, 0, 1.2202789918, -2.0226276268, 0.1157051336  
N, 0, 4.4601385834, 0.4824534991, -0.0157792974  
C, 0, 5.4362886649, -0.4423343285, -0.0019494104  
N, 0, 4.9334762247, -1.7203977645, 0.0427531634  
C, 0, 6.8276448903, -0.0824465905, -0.032043677  
C, 0, 7.1655391734, 1.3030254263, -0.0735279578  
C, 0, 8.4772170498, 1.7075857781, -0.1025803975  
C, 0, 9.507329736, 0.7370440297, -0.0913603897  
C, 0, 9.1931116197, -0.6451609938, -0.0507576116  
C, 0, 7.8750450514, -1.0420597724, -0.0218334219  
O, 0, 10.7617948753, 1.1893649535, -0.120716595  
H, 0, -10.6380984358, -1.5850176287, 0.6224730477  
H, 0, -10.5996323454, -1.4511710492, -1.1435658485  
H, 0, -10.9152070271, -0.0030062985, -0.1521691374  
H, 0, -8.7424973911, -0.4161934398, -2.2257204054  
H, 0, -8.8246555316, 1.085941983, -1.2921926727  
H, 0, -6.500940668, 0.7455357701, -2.1011625252  
H, 0, -6.4538415005, -0.8850734825, -1.3935786278  
H, 0, -6.7354754563, 1.6434151377, 0.0636792652  
H, 0, -6.5920020867, 0.4288811208, 2.0767109605  
H, 0, -6.5084011619, -1.0765990742, 1.1343305939  
H, 0, -8.8328675737, -0.7315545072, 1.9275874072  
H, 0, -8.8796474177, 0.8945141139, 1.2288080142  
H, 0, -4.478888484, -1.3428099686, -0.1156942547  
H, 0, -2.6041400212, 3.3677667004, 0.2954955755  
H, 0, -5.0644888817, 2.9761923251, 0.2053927307  
H, 0, -1.6418731641, -1.9084643261, -0.1379734338  
H, 0, 1.766661282, 1.3473915878, -0.0065385595  
H, 0, 2.6852852755, -3.6093030993, 0.1443224388  
H, 0, 0.4032515108, -2.735737408, 0.1715303758  
H, 0, 5.4582346899, -2.5817553898, 0.065876944  
H, 0, 6.3563760129, 2.0232049536, -0.0810002724

H, 0, 8.7514669695, 2.7559904603, -0.1339309937  
H, 0, 9.991807645, -1.3817935854, -0.0428043976  
H, 0, 7.6516146423, -2.1031448805, 0.0086213987  
H, 0, 11.4062267661, 0.4599791055, -0.110272765