

Supporting Information

Exploring radiative and nonradiative decay paths in indole, isoindole, quinoline, and isoquinoline

Yu Harabuchi,^{a,b,*} Kenichiro Saita,^a and Satoshi Maeda^{a,*}

^aDepartment of Chemistry, Faculty of Science, Hokkaido University, Kita 10, Nishi 8,
Kita-ku, Sapporo 060-0810, Japan.

^bPrecursory Research for Embryonic Science and Technology (PRESTO), Japan
Science and Technology Agency (JST), 4-1-8 Honcho, Kawaguchi, Saitama 332-0012,
Japan.

Cartesian coordinates (in Å) of $S_{0\text{MIN}}$, $S_{1\text{FCMIN}}$, $S_{1\text{MIN-b}}$, $S_{1\text{TS}}$, $S_{1\text{TS-b}}$ and the optimized S_1/S_0 -MECI at the SF-TDDFT(BHLYP/6-31G*) level for four heteroaromatics, i.e. indole, isoindole, quinoline and isoquinoline. $S_{0\text{MIN}}$ of indole and isoquinoline were optimized at DFT(BHLYP/6-31G*) level. Relative energy in eV and a.u. and the $\langle S^2 \rangle$ values for each state are also shown.

indole

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indole-S0MIN(DFT) FC 4.73 eV S0: -363.583947197300 [0.03] S1: -363.410068 [1.08]

N	1.549898280256	-1.071864881155	0.000000000000
C	2.365440332617	0.032154057085	-0.000000000000
C	1.610906224418	1.159213168859	-0.000000000000
C	-0.984197679290	1.417900016140	-0.000000000000
C	-2.151600319137	0.686602121891	-0.000000000000
C	-2.126456922913	-0.715347007955	0.000000000000
C	-0.935011183623	-1.408373683059	0.000000000000
C	0.239971304673	0.744104039244	-0.000000000000
C	0.241024126225	-0.664956153121	-0.000000000000
H	1.861808044729	-2.020028127668	0.000000000000
H	3.432490082544	-0.081086452502	0.000000000000
H	1.980234625063	2.166676707627	0.000000000000
H	-1.012759433045	2.495981899214	-0.000000000000
H	-3.101778489252	1.195550769108	-0.000000000000
H	-3.056227486938	-1.260811413212	0.000000000000
H	-0.917113596725	-2.486721585826	-0.000000000000

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indole-S1FCMIN 4.53 eV -363.417640807600

N	1.537957345807	-1.075343735979	-0.000000000000
C	2.379603743582	0.032591655083	0.000000000000
C	1.610241630695	1.162860968876	-0.000000000000
C	-0.973574930417	1.478089219988	0.000000000000
C	-2.161551288371	0.684482499658	-0.000000000000
C	-2.137601333161	-0.734249302589	0.000000000000
C	-0.937508646963	-1.462417414320	0.000000000000
C	0.252356253604	0.772390293503	0.000000000000
C	0.245529972183	-0.676024805850	-0.000000000000
H	1.840990507284	-2.027142263185	0.000000000000
H	3.444136307600	-0.089645659897	-0.000000000000

H	1.982331326825	2.169542764998	-0.000000000000
H	-1.014238057376	2.551172286748	0.000000000000
H	-3.120479469611	1.175412982395	-0.000000000000
H	-3.077016195882	-1.261355623012	-0.000000000000
H	-0.910570365463	-2.536606156331	0.000000000000

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indole-01 3.75 eV -363.446071 [0.14] -363.446071 [0.32]

N	1.88411782590400	-0.99474101586100	0.11251765285500
C	2.57251912316600	0.07567945948300	0.19190506345100
C	1.70503128258900	1.24177341392600	0.16384070538800
C	-0.96491404564500	1.41996122736900	-0.02068156737600
C	-2.04451657342600	0.60449911560900	-0.13061519267200
C	-1.93913050640500	-0.79395079283200	-0.16781365810700
C	-0.64080896160700	-1.56068108941900	-0.08262896227900
C	0.33602304341400	0.72305173220800	0.05386364888900
C	0.47816620421500	-0.58359230739600	0.02541278935700
H	-0.50207187802200	-2.20850089225900	-0.95529607046100
H	3.64558994108000	0.08696789091300	0.26848754308200
H	2.00907430374600	2.27412223653900	0.21242405330200
H	-1.03216526406500	2.49216568631300	0.01101945340900
H	-3.03247615199700	1.03496597592100	-0.19360149353400
H	-2.84114046057200	-1.37655347966200	-0.26124050761000
H	-0.63666997279100	-2.24617368619900	0.77240654230100

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indole-02 4.46 eV -363.420070 [0.19] -363.420049 [0.53]

N	1.47893735461200	-1.04136190749100	-0.03497557365100
C	2.25529619117300	0.07247038552800	0.07643373360100
C	1.43768377561600	1.17229056099400	0.13717160812500
C	-1.20430727625200	1.44479945621800	0.07600331047700
C	-2.31772600521200	0.47585874821400	-0.03146250070200
C	-2.25201305788500	-0.85106051067500	-0.13350317315800
C	-0.97417895653900	-1.50373151479700	-0.14659273044500
C	0.10904869423900	0.70898533612500	0.05966844702600
C	0.15520593851600	-0.67915093083200	-0.04762488890800
H	1.81823716593100	-1.97863282321400	-0.09723920529900
H	3.32496798124700	0.00079573974500	0.10416438257400

H	1.76562783770600	2.19072330603400	0.22711669121800
H	-1.25448575855100	2.17066447495500	-0.74094533208200
H	-1.30606880776800	2.04000192724900	0.98814817616700
H	-3.14253172988700	-1.45867156719100	-0.20750823079600
H	-0.89706543734500	-2.57498720618900	-0.22885471414700

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indole-03 4.61 eV -363.414428 [0.33] -363.414428 [0.57]

N	1.54441848254100	-1.45081151081300	-0.06251141379400
C	2.18159494349500	-0.30885210426700	0.33266046078400
C	1.80057960180300	0.80149198668700	-0.58444821122500
C	-0.78971205820800	1.26691620292400	-0.11563164275200
C	-1.99955560894000	0.63349547384200	0.10377072843400
C	-2.07462373420700	-0.76396589040600	0.23858968942700
C	-0.95590562376400	-1.56241389247600	0.19643444542700
C	0.34163087533600	0.47605543136400	-0.23476070852900
C	0.28836164648800	-0.94153440768200	-0.00650699874800
H	2.02382938686200	0.58474409904200	-1.62637922699900
H	2.20651390969000	-0.04937731505800	1.39364932682200
H	2.12741882982100	1.79439908620900	-0.29924822858500
H	-0.74138032831000	2.33710250635900	-0.23763411007800
H	-2.90581705947600	1.21456056633700	0.15081637953100
H	-3.03984836899000	-1.21611371964300	0.40196086949300
H	-1.01087698453300	-2.62670303772900	0.34923864078400

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indole-04 4.62 eV -363.414032 [0.77] -363.414027 [0.20]

N	1.43017283427400	-1.09244062188500	-0.09662812302200
C	2.33476369050400	-0.07018806627700	-0.04857062606200
C	1.67583963302700	1.12541936825600	0.03745377057800
C	-0.88179422193400	1.65778277309200	0.11664876837200
C	-2.07897865222400	1.06245583567800	0.10097433764600
C	-2.30959529834500	-0.39949461253200	0.01578215506700
C	-1.04772462828400	-1.21794202044200	-0.06062273118100
C	0.29281328049400	0.84265361047300	0.04466216820800
C	0.14965970084200	-0.57638290072000	-0.04132254489000
H	1.65735803074900	-2.06249692703700	-0.15880571687800
H	3.38837822001700	-0.27074785154800	-0.07968308409700

H	2.13747429134400	2.09279810838000	0.08952895103800
H	-0.77165799410400	2.73172506138300	0.18154091176600
H	-2.94793765543000	-0.61788978418200	-0.84782205419300
H	-2.91051266171000	-0.72366254968900	0.87301273666900
H	-1.12163065963500	-2.29259594828800	-0.12614891902300

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indole-05 4.72 eV -363.410626 [0.57] -363.410623 [0.09]

N	3.29542215689200	-0.93935845098500	-0.04057650909000
C	2.69082648389900	0.18216322764800	-0.00919098260000
C	1.58856161903000	0.92593946362100	0.01731958404300
C	-0.85753975318700	1.21072974441000	-0.00533459212500
C	-2.14615260668600	0.70755859563900	-0.01566935103900
C	-2.36458711210800	-0.66141602269900	-0.00905077293700
C	-1.27555485449600	-1.52116456414000	0.00845939382900
C	0.24748506929000	0.35624376112600	0.01100545998400
C	0.01305061914400	-1.02072937629200	0.01917711402500
H	0.84495290263400	-1.70881000873100	0.03655491772100
H	3.74187115051700	0.64009846105300	-0.00971938611300
H	1.69754397556800	1.99412110758300	0.03954835873800
H	-0.69843824553000	2.27768618289600	-0.01235989289800
H	-2.98224991003800	1.38831957740300	-0.02953153646400
H	-3.36801148237100	-1.05426875413100	-0.01637165849100
H	-1.43055210293700	-2.58811946972700	0.01573985340900

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indole-06(Fig2a1) 4.81 eV -363.407057 [0.73] -363.407057 [0.23]

N	2.24504217067100	-1.18828386415300	-0.20783063552500
C	2.51394397403100	0.06706246893600	-0.32233034898600
C	1.47056582887400	1.00894636628000	-0.25152221446500
C	-1.00624268473600	1.31005697922400	0.03563825544600
C	-2.24213213139900	0.72294188695300	0.22492061052000
C	-2.36929822319400	-0.66035408997600	0.32677858003100
C	-1.23994162728000	-1.47895030069200	0.24012670997500
C	0.15188757832300	0.51182302127100	-0.05560289279300
C	-0.04485472453800	-0.85297527479400	0.05587262347100
H	3.03683103844500	-1.81333160022800	-0.26885366615300
H	3.52754489220600	0.42731035865500	-0.47348937878800

H	1.66496120907700	2.06293206768400	-0.34452879002000
H	-0.91990085058600	2.38342595014400	-0.04374159146000
H	-3.12080725748100	1.34337482990900	0.29394741142300
H	-3.34231735852100	-1.10357826401300	0.47312828930000
H	-1.32865392430800	-2.55140706052300	0.31748703801800

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indole-S1TS(Fig2a1) 5.82 eV -363.370024135000

N	1.488319123571	-1.184164363774	0.747698641067
C	2.223794435398	-0.106650193278	0.717470567157
C	2.047555463778	0.652396182848	-0.458165462286
C	0.074478005133	0.869726475414	-2.007161074616
C	-1.235626425075	0.375867450923	-2.229207782103
C	-1.637313010307	-0.787028977665	-1.607447937563
C	-0.746074073806	-1.576198313377	-0.848242458926
C	0.919801035825	0.158187269449	-1.178747407853
C	0.569960576318	-1.139448388115	-0.713869349217
H	1.304772133232	-1.654167804377	1.623925203483
H	2.825754874082	0.214785737308	1.553993124508
H	2.558447478487	1.579513921079	-0.646190558893
H	0.385918275261	1.809274864563	-2.436518259041
H	-1.925694981954	0.937638206570	-2.835486604004
H	-2.654385041577	-1.128245595720	-1.734983007231
H	-1.058331835436	-2.554199373446	-0.512698948267

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indole-07 4.90 eV -363.403965 [0.24] -363.403965 [0.28]

N	1.15687055379800	-1.77141957305500	-0.00700917783200
C	2.64665624745300	0.12932218907500	0.00234988971600
C	1.62364345527100	0.96561738381000	0.00549238091800
C	-0.87538035997300	1.27615467883300	0.00227375465100
C	-2.13926057971100	0.72750453859100	-0.00022808031500
C	-2.26966365392500	-0.65775727002400	-0.00302754843000
C	-1.17397359477600	-1.49257320857000	-0.00448189049400
C	0.26293438161300	0.47666381178500	0.00105324262600
C	0.12400788670900	-0.93099271154400	-0.00361072070200
H	2.45680505596400	-0.97735332189200	-0.00641190936300
H	3.69591477059000	0.37147243909800	0.00569948514300

H	1.78650353109000	2.03309107985600	0.01173586672800
H	-0.74793117199300	2.34739036644700	0.00584537810100
H	-3.01082294067400	1.35902663658300	0.00094620537300
H	-3.25063528400200	-1.10567266954200	-0.00401873572200
H	-1.28904038782500	-2.56148089477700	-0.00660814040200

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indole-08(Fig2a2) 5.09 eV -363.396876 [0.66] -363.396876 [0.46]

N	1.41081246007000	-1.51090275251600	-0.03025440509800
C	2.75071501139000	0.54663546054900	-0.01871490270100
C	1.62983464574600	1.21683430462100	-0.00083221176600
C	-0.85609130997300	1.30770576432000	0.02106859895600
C	-2.08851199217400	0.67725137920500	0.02475397240400
C	-2.16280000869500	-0.71749906724500	0.01009662576500
C	-1.01525278480900	-1.46899357715200	-0.00812822837300
C	0.32136212035300	0.57637297935100	0.00326295316700
C	0.26372457283100	-0.85143846113800	-0.01220380085100
H	1.29729967192100	-2.51811442444800	-0.04067473230600
H	3.80741599228400	0.72571471149700	-0.02580632165100
H	1.62559838999700	2.30674920856900	0.01239264625400
H	-0.80503862644400	2.38519628179200	0.03261282469000
H	-2.99218562849900	1.26401847137400	0.03841461113200
H	-3.12458915892200	-1.20397664690700	0.01312885781900
H	-1.06566544551400	-2.54656015720600	-0.01911648742700

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indole-S1TS(Fig2a2) 6.02 eV -363.362579736500

N	1.480692900536	-1.247697972324	-0.020964077835
C	2.588651299468	0.243928908484	-0.054403184213
C	1.626298641262	1.205582821504	0.104429949246
C	-0.909785158877	1.389372795312	-0.169696853047
C	-2.120050376833	0.679798326414	-0.144970975567
C	-2.143224948610	-0.705863954253	0.000914936538
C	-0.959869297993	-1.413169504156	0.127423747698
C	0.292416522385	0.717411059914	-0.090598943355
C	0.270790424445	-0.733019603764	0.008373799053
H	1.605591195697	-2.202687650265	0.289164357020
H	3.547486728754	0.233960464554	0.451026585521

H	1.795507737316	2.175451523811	0.549852783569
H	-0.922674255807	2.464861005939	-0.240467598374
H	-3.048980109525	1.221207069649	-0.217312379181
H	-3.085807090611	-1.226147335393	0.032275639963
H	-0.965847642008	-2.480913411847	0.275765381347

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indole-09(Fig2a3) 5.15 eV -363.394816 [0.74] -363.394816 [0.57]

N	1.54497236080200	-1.04510228337900	-0.00128515901100
C	2.30375356241200	0.00187977634000	-0.00107499253300
C	1.54513625553900	1.22528154945000	0.00106908435900
C	-1.03305341643100	1.49351992350400	0.00281538515600
C	-2.20087511244900	0.73964847044000	0.00106537006200
C	-2.14966097028100	-0.64875972128100	-0.00112534164700
C	-0.93259334896200	-1.33758315589000	-0.00165835745300
C	0.18372426841100	0.82228018839700	0.00198040642200
C	0.21872068711600	-0.59156565329000	0.00011317221800
H	2.39632688571500	-2.79273598282000	-0.00230980881700
H	3.37628225759000	-0.08612105621800	-0.00164409688100
H	1.93998501331500	2.22460540523600	0.00220751138700
H	-1.07517406671200	2.57081271205500	0.00458789492800
H	-3.15702878602500	1.23587343409500	0.00147916307500
H	-3.06997099346000	-1.20964271550800	-0.00266090077400
H	-0.89391668700200	-2.41339741649000	-0.00355933049900

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indole-S1TS(Fig2a3) 5.61 eV -363.377630863300

N	1.459508623556	-1.177290539067	-0.111072583965
C	2.125757783213	-0.595265850001	0.862135275110
C	1.256812652065	-0.201707893719	1.925652476894
C	-1.307242895112	-0.387947219230	2.099119706300
C	-2.404656157206	-0.857362383035	1.381669227911
C	-2.232105594442	-1.480342490405	0.146848570324
C	-0.964062647536	-1.680353175211	-0.444129850518
C	-0.023067766720	-0.521561032596	1.514026240807
C	0.126510253250	-1.175382287101	0.243976215684
H	1.963006439413	-1.052819071060	-1.267535378844
H	3.175189723670	-0.382089920968	0.749466165102

H	1.559686651096	0.280570585424	2.837717820852
H	-1.423748320347	0.037405595021	3.082007175846
H	-3.395783695039	-0.760019292126	1.790666320347
H	-3.102666958699	-1.848456341439	-0.372027667871
H	-0.856957645620	-2.230479800083	-1.361410676384

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indole-10 5.19 eV -363.393306 [0.78] -363.393305 [0.35]

N	1.46091672238900	-1.42673561726600	-0.03801451720000
C	2.76789298927700	0.70220395931300	0.04080421721300
C	1.61659819612300	1.29984529728900	0.05032192408200
C	-0.87212638982600	1.34121499883900	0.03594948975500
C	-2.08821551882300	0.68814789676200	0.00931610561200
C	-2.12834550694800	-0.71205546686700	-0.03421403744600
C	-0.97065318900200	-1.44101249350800	-0.05145034220500
C	0.31983995972800	0.62842066085100	0.02040417464700
C	0.30176624221600	-0.79905069894100	-0.02472558555200
H	1.36647752254200	-2.43442633546000	-0.07144469417900
H	3.57743836592300	0.01925281414600	0.02472995529200
H	1.57130674622500	2.38733374064800	0.08529041095400
H	-0.83969924873000	2.41916756170000	0.06935511116900
H	-3.00540021534700	1.25322942719500	0.02274892984100
H	-3.08037546036300	-1.21765211363000	-0.05372054088800
H	-1.00079330579200	-2.51889015638300	-0.08535060108900

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indole-11(Fig2a4) 5.23 eV -363.391723 [0.74] -363.391722 [0.30]

N	1.57494675679300	-1.11190161415600	0.18654960220400
C	2.38091053274000	0.01729331283800	0.17169581922800
C	1.59932222062300	1.10565865560400	-0.04930585465400
C	-1.02205655787200	1.23822564639500	-0.24636136541100
C	-2.20335905739900	0.53522473445600	0.00500468008700
C	-2.10285979235000	-0.82140415896000	0.32632956014400
C	-0.94778521380600	-1.49705770053100	-0.24259436333000
C	0.25482702767700	0.63025172748800	-0.17937446959100
C	0.29925415265300	-0.76349662264900	-0.02178806012500
H	1.88079018473200	-2.05100358883700	0.34662533376000
H	3.43728806494000	-0.06489598745800	0.33259542071500

H	1.94285610280100	2.12078439184200	-0.11786061057800
H	-1.08053618130700	2.31147847755900	-0.35212053766300
H	-3.11312564919000	1.09703892172700	0.16180700796700
H	-2.81891860636200	-1.28369671606300	0.99311612011100
H	-1.08492607507800	-1.27350600458200	-1.31431828288600

16

indole-S1TS(Fig2a4) 5.69 eV -363.374966515900

N	1.482295927466	-1.069396929952	0.840186773015
C	2.313152288312	0.030211364069	0.639694885330
C	1.552771178861	1.074722389646	0.223450574985
C	-1.046551187020	1.215041580719	-0.075502451920
C	-2.215524402180	0.552383590172	0.278081693451
C	-2.185690849773	-0.735753432146	0.836345859648
C	-0.989261450035	-1.565537191919	0.567852475696
C	0.205924757895	0.608128884190	0.143410489020
C	0.213534900814	-0.760111400116	0.538087072505
H	1.763488247562	-1.963817616781	1.189823864350
H	3.368393626504	-0.044291712007	0.811113786279
H	1.912128794209	2.058494284692	-0.013006552822
H	-1.097757028728	2.238363087307	-0.412015067491
H	-3.155717753770	1.077732673601	0.182953393561
H	-3.061217600866	-1.138088967426	1.320945355032
H	-1.112785552911	-2.047352249270	-0.413672083976

16

indole-12(Fig2a5) 5.35 eV -363.387470 [0.60] -363.387469 [0.50]

N	1.41152203739100	-1.01707640208400	-0.10043753595400
C	2.29178915434400	0.05135144838800	-0.15428062868800
C	1.58612839530600	1.20366251561300	-0.09702449459500
C	-1.01489224865800	1.46590016536900	0.30149791153400
C	-2.19627540305700	0.76596451178600	-0.13215965056200
C	-2.22515139555100	-0.68740162998600	0.16494274679300
C	-1.04729287844300	-1.35340974825600	0.18824006263100
C	0.19687516231600	0.84513202910700	-0.03087796684100
C	0.14098685811300	-0.57358334271000	-0.02207644166700
H	1.68401541128000	-1.97880710562500	-0.07373446249800
H	3.34726282447000	-0.12016371728000	-0.23318207477000

H	1.99322587968000	2.19585928318500	-0.12704628020200
H	-1.03215683601800	2.35917178633000	0.91547585077300
H	-2.00932179750200	0.67707688772000	-1.22242339677500
H	-3.15588549994400	-1.23292778402800	0.23530897481000
H	-0.97420175412400	-2.41175542284200	0.38777738435700

16

indole-S1TS(Fig2a5) 5.62 eV -363.377495161700

N	1.408616415895	-0.979770714830	0.192328053989
C	2.202777557065	0.088257600136	0.628181323329
C	1.438986106998	1.205274178372	0.652725832962
C	-1.008718690069	1.472554165321	-0.334781859810
C	-2.211820992503	0.687595498958	-0.074833515369
C	-2.195633831973	-0.706493441037	-0.335943472216
C	-0.979423704428	-1.344904797685	-0.443889036703
C	0.122840352280	0.836624601864	0.230781840319
C	0.149020215438	-0.572723382147	-0.026888395185
H	1.739793052499	-1.912053870510	0.045637058898
H	3.237700555730	-0.065744085267	0.859093857460
H	1.769952173909	2.188320021447	0.928079392797
H	-0.945114092728	2.260506104809	-1.075291849452
H	-2.767328551491	0.946340706364	0.825737731037
H	-3.105442786508	-1.285800560156	-0.259855225553
H	-0.889100160062	-2.402452383501	-0.622821301260

16

indole-13(Fig2a6) 5.36 eV -363.386930 [0.13] -363.386925 [0.93]

N	1.50392502161100	-1.14761318678500	0.00657859560500
C	2.28222059155600	-0.04729078962400	-0.09421630946000
C	1.49550169717800	1.07881976417400	-0.12339041046900
C	-1.07475512510200	1.39116795054300	0.09211572483100
C	-2.23868484793700	0.70067164554600	0.11569559749200
C	-2.19011984218600	-0.76658184151200	-0.12670780534500
C	-0.99685951814400	-1.43791993371300	0.32648653218700
C	0.15274973535500	0.65555346641500	-0.05678371687600
C	0.17401847550900	-0.76575285579900	0.00703996218800
H	1.83170927089500	-2.09132292840400	-0.00506536860300
H	3.35185611718300	-0.13051096042500	-0.13046850629700

H	1.85440921396200	2.08898455998700	-0.16925829150600
H	-1.03687594664100	2.45859627928800	0.24801048529300
H	-3.17972123312500	1.22646531818200	0.19487109786100
H	-1.94533319679000	-0.67986945474400	-1.20745236244700
H	-0.98741250373800	-2.34440355846100	0.92254477555000

16

indole-S1TS(Fig2a6) 5.72 eV -363.373855319000

N	1.426170359519	-1.226386946274	0.081800069886
C	2.188411511105	-0.151160892705	0.377688244099
C	1.440218094606	0.999290764840	0.253438408999
C	-1.070808321406	1.364633900902	-0.329579523213
C	-2.231467073841	0.639586107168	-0.408756801687
C	-2.173900832622	-0.799263343924	-0.442479500959
C	-0.932548035316	-1.457023634862	-0.842435801976
C	0.134613396832	0.618436264981	-0.109649621094
C	0.148020288362	-0.801442903671	-0.239896842001
H	1.735117632634	-2.176366794040	0.076641123067
H	3.219885808879	-0.264585505553	0.652869919541
H	1.801108976903	1.995639954118	0.423000732065
H	-1.058259816111	2.440926422316	-0.327298653240
H	-3.187521402303	1.133470934451	-0.297985517640
H	-2.604177813922	-1.213768385146	0.474067550352
H	-0.840832743107	-2.195403186944	-1.629669462343

16

indole-14(Fig2a7) 5.40 eV -363.385356 [0.18] -363.385356 [0.75]

N	1.66296991858900	-0.94133128710700	-0.11561770957300
C	2.38219611920900	0.12916069576800	0.28737803135300
C	1.66983047567200	1.27610141278300	-0.22208537255100
C	-0.97739208139200	1.47213621371300	0.19553394351500
C	-2.14376024804900	0.68646023214600	0.16915322441500
C	-2.07718201517400	-0.67384870110200	-0.02840003886600
C	-0.84199441642100	-1.32529310945700	-0.18489518267800
C	0.23731294220700	0.86124461531200	0.06659130847800
C	0.28011759248800	-0.55115319592900	-0.09887673879200
H	1.94192737627400	-1.90124994103700	-0.01053735487000
H	3.11127763606100	0.03704184086500	1.08119032264400

H	1.67158053726200	1.05868396887400	-1.30071583787600
H	-1.03770317876400	2.54176369347300	0.30916142388200
H	-3.10338492020400	1.16073868517800	0.29482227601500
H	-2.98358781126100	-1.25566971289800	-0.06810571633200
H	-0.79558001690000	-2.38579193591200	-0.37459657876400

16

indole-S1TS(Fig2a7) 5.73 eV -363.373327043300

N	1.537982477487	-0.996234564816	0.453922367417
C	2.352693690953	0.029106248170	0.717810212185
C	1.560189961463	1.250258845855	0.447240055132
C	-1.050646020971	1.453287541296	0.305973441299
C	-2.205182026369	0.673844749194	0.069658424610
C	-2.150590455315	-0.691321087676	-0.046567172661
C	-0.903583127464	-1.363284243820	0.058823904146
C	0.171145760354	0.820441817989	0.443129452114
C	0.192828360358	-0.595273014559	0.328419858636
H	1.804861219944	-1.966340734832	0.492965531097
H	3.205383225094	-0.123334577806	1.368400383883
H	1.839133670064	1.780511992384	-0.458198118641
H	-1.124693881428	2.524424838872	0.386597002935
H	-3.156896378836	1.173314659370	-0.019571769310
H	-3.044124449686	-1.260470682071	-0.238951626107
H	-0.825933623641	-2.422876977140	-0.124196055422

16

indole-15(Fig2a8) 5.42 eV -363.384789 [0.83] -363.384789 [0.17]

N	1.53948947257300	-1.01326658124100	-0.12144971745000
C	2.36430560161200	0.03029965679900	0.14088623599200
C	1.63562634089400	1.19849667405300	0.22478766123800
C	-0.99465318346900	1.54251334311800	-0.19057091924300
C	-2.14491280192300	0.80103007262500	0.30608929687300
C	-2.17263624482300	-0.56279895391600	0.05332676462200
C	-0.96109593267300	-1.22378864023200	-0.21485222064000
C	0.29470231418100	0.86710216976200	-0.00618291029000
C	0.24902932058100	-0.53563305936800	-0.21846714460900
H	1.82835166575300	-1.96581576576800	-0.21248576946800
H	3.41927432538600	-0.12566891194300	0.26182551256700

H	2.03267655451200	2.17506906282800	0.42235121022300
H	-1.11269217315200	1.20811361920200	-1.24549366952500
H	-2.96930073641900	1.25825770940400	0.83925747438000
H	-3.04957937129600	-1.16326039639500	0.24829869378700
H	-0.96195724215100	-2.30165652427100	-0.28732049848300

16

indole-S1TS(Fig2a8) 5.87 eV -363.368086372400

N	1.594578646437	-0.907029088197	0.184734642633
C	2.417995507600	0.097446246866	-0.209094841538
C	1.667922893093	1.217240705740	-0.513179551983
C	-0.951556869524	1.610846909561	-0.397906282002
C	-2.078639207991	0.711845434742	-0.718631982090
C	-2.085292506037	-0.565920391013	-0.144732642736
C	-0.903106113580	-1.151304849698	0.301644725868
C	0.322045485598	0.903937752359	-0.287216886665
C	0.296354639890	-0.448562803452	0.154768359836
H	1.882687308388	-1.843948705737	0.381047978178
H	3.480132323214	-0.048769383651	-0.253215401374
H	2.055502177966	2.153077358426	-0.866497191885
H	-1.171786711623	2.032544678919	0.598126991339
H	-2.940193274201	1.049745498636	-1.275500372852
H	-2.995336757497	-1.149148259145	-0.107669502822
H	-0.904927288615	-2.171254712090	0.653135454074

16

indole-16(Fig2a9) 5.69 eV -363.374963 [0.66] -363.374962 [0.36]

N	1.63136847039300	-1.10394013820600	-0.14260679148000
C	2.38748584291300	0.02966176587500	-0.01955050804900
C	1.56772705560500	1.12785111080400	0.09218482290300
C	-1.09279848913100	1.19272191238600	0.04921799775300
C	-2.16202527904500	0.65895433871000	-0.78672646620800
C	-2.03034354498200	-0.44279917609300	0.10296809754500
C	-0.90233854538000	-1.38694678151000	0.05201760423300
C	0.24342554195500	0.65625799274400	0.01775537106800
C	0.30391870004600	-0.74896102332900	-0.07969937158700
H	1.99067986141500	-2.03366604782400	-0.19199719552900
H	3.45876795914200	-0.02334622747400	-0.04113522232900

H	1.90118459067100	2.14468314643600	0.17369319175100
H	-1.29422266537100	2.07550001004400	0.64154346837100
H	-3.09810014232900	1.19398290519100	-0.80818176663600
H	-2.85029686211300	-0.70669874073600	0.76419293510500
H	-1.05780458417200	-2.44426157235500	0.17632383307400

16

indole-17(Fig2a10) 5.69 eV -363.374814 [0.76] -363.374813 [0.32]

N	1.65217663740400	-1.13392296600600	0.69992684671000
C	2.02472262139200	-0.17075889310000	-0.21451514623100
C	1.66479507144800	1.18054974862800	0.21551950156700
C	-0.94003699329200	1.50525371479000	0.27575599313200
C	-2.03487262076000	0.74188207932900	-0.01661945004800
C	-1.97839348547900	-0.65570397248300	-0.26565732026500
C	-0.78269794871100	-1.32918539422200	-0.13325291420600
C	0.33774124974900	0.86996529724800	0.32079443760200
C	0.32844489230500	-0.59586953116800	0.26325849720600
H	1.75272846120800	-2.06619646441500	0.31735584798800
H	2.38414553899900	-0.45661122044500	-1.19703868108000
H	2.21674074495900	2.09369871515200	0.15865470804200
H	-1.02177915109300	2.57006100828500	0.41334324855500
H	-2.99656279048200	1.22703475025800	-0.08411708699400
H	-2.87878341176600	-1.18974034417400	-0.51378061195500
H	-0.73174090626700	-2.40146305301100	-0.23962787001600

16

indole-18 5.70 eV -363.374452 [1.00] -363.374441 [1.01]

N	2.09650599553200	1.00702757018200	-1.82282214579800
C	2.49299090209300	0.62661943458400	-0.61704825090400
C	1.72150857122500	0.10825329521700	0.38113932703700
C	-0.56151173267300	-0.01771848765100	-0.71892544319700
C	-1.92011550755000	-0.25202843531700	-0.59398743456600
C	-2.47966847273700	-0.60431194284600	0.62745576681000
C	-1.66612312444400	-0.73271102581200	1.75244215406800
C	0.29068594267800	-0.12386300833500	0.39490420829000
C	-0.33484120729100	-0.49249100658000	1.57345844932400
H	1.85034148264300	1.92420466099500	-2.14007867133300
H	3.56699351755500	0.63746263902200	-0.40656759118100

H	2.23811630173100	-0.16584452735300	1.28758769816400
H	-0.13285854715900	0.23555956749600	-1.67228682823700
H	-2.55144268089100	-0.16631717406200	-1.46324880280500
H	-3.53993863068300	-0.78488353197800	0.70746478994100
H	-2.07401490043300	-1.00996455290500	2.71051277440300

16

indole-19 5.73 eV -363.373279 [0.37] -363.373277 [0.55]

N	1.45677760316600	-1.73568906914200	0.09868703312400
C	1.71851677486900	0.98009854401100	-0.02405934895700
C	2.15218630692100	2.23209714390600	-0.17489726453100
C	-0.74750307487600	1.18490680864400	-0.14226255402800
C	-1.96418318518500	0.59763181755300	-0.12949500495100
C	-2.06429578520300	-0.83144586302400	-0.02038805036000
C	-0.97298737626700	-1.61298828511700	0.06215139882600
C	0.44571133885000	0.41209732751700	-0.04512855912000
C	0.37254466162800	-1.05231347833900	0.04266668836200
H	1.27151097327200	-2.72731448645900	0.16812821609900
H	2.51003882891400	0.21530529756100	0.01420326320300
H	2.44739739757700	3.04976703838200	0.45483317805400
H	-0.65787871589700	2.25591494331700	-0.23141645943300
H	-2.86211593086600	1.18759139263500	-0.20280231741200
H	-3.04473246203800	-1.28144306231200	-0.00848130040500
H	-1.06435944525800	-2.68522259446700	0.13826108152700

16

indole-20 5.74 eV -363.373156 [0.91] -363.373155 [0.46]

N	1.40700337209200	-1.06045497476300	-0.18052551387500
C	2.25215993259500	0.02781022009800	0.06107939735900
C	1.52201670274300	1.13657264826500	0.26456702246000
C	-1.04890079468900	1.47717863519400	0.02702378046600
C	-2.18659223463200	0.64777806206300	-0.11915400711400
C	-2.03594342719000	-0.67607791043100	0.41501017400500
C	-1.05361062214200	-1.41970763914600	-0.33124621023300
C	0.12934504715500	0.77015854777300	0.15500394443100
C	0.10585737244200	-0.66765555774000	-0.15604295327200
H	1.71503398629100	-1.99172888890800	-0.36648806518900
H	3.31624240803900	-0.10821598674100	0.04563475413500

H	1.90841422254700	2.11669034056900	0.46796792315600
H	-1.05016206720500	2.53020098605600	-0.21652608015600
H	-2.73808002486800	0.76590061186500	-1.04906895771900
H	-2.21851099358500	-0.87302054174400	1.47075818796500
H	-1.02764496999900	-2.48643507773300	-0.48799339640900

16

indole-21 5.75 eV -363.372619 [0.25] -363.372619 [0.27]

N	1.56516773525400	-1.18501501738800	-0.49685866994500
C	2.26075345251100	-0.15075403344400	0.05949974023800
C	1.43841055196900	0.87733401383400	0.35863949073300
C	-1.03740616710100	1.40466944045400	-0.19044290326200
C	-2.26124886951200	0.72611878603500	-0.14483502412000
C	-2.11664536841200	-0.60300349654200	0.12716149317300
C	-0.72498186438900	-1.04713703887600	0.27526056200100
C	0.11421391149300	0.54805196554300	-0.11841428632100
C	0.22714261829800	-0.78887262357600	-0.77530008525500
H	2.01510415241800	-1.88921470060000	-1.04807977371900
H	3.31862729948200	-0.23612376646800	0.23492383656800
H	1.71702303399200	1.79304374156300	0.84517139718100
H	-0.93528742603600	2.47559331525300	-0.21257527246000
H	-3.21234476879300	1.20919480493200	-0.29170963268300
H	-2.93359665077000	-1.29481531066000	0.24812766224900
H	-0.43830373077500	-1.65007660537800	1.12943146561000

16

indole-22 5.76 eV -363.372391 [0.46] -363.372391 [0.38]

N	1.50956836185100	-1.03666711042100	-0.09705655747900
C	2.39037860966900	0.02616044668600	0.02346361048300
C	1.69234203967500	1.18214725354400	0.15536684931100
C	-0.95371066259300	1.40409688774700	-0.02786883707000
C	-2.04897447958500	0.43232598325400	-0.09544607161800
C	-2.14887767053300	-0.70828429479900	0.75156139459200
C	-1.04795945048100	-1.19053646898100	-0.08004195527000
C	0.30304156654700	0.82783105665900	0.11189760070900
C	0.24000673244600	-0.56728713514700	-0.00362676950100
H	1.77500431448300	-1.99963413331800	-0.08488011143900
H	3.44888156801600	-0.14422868874400	-0.00410142941200

H	2.11653552726100	2.16394784513500	0.24142442024300
H	-1.14927420397100	2.45284549868000	-0.16904356479400
H	-2.87329646179500	0.68166428239200	-0.75750953599700
H	-3.06768497370500	-1.27263649790800	0.74010623704900
H	-1.18935290767700	-2.06275145010000	-0.70424527980800

16

indole-23 5.77 eV -363.371776 [0.18] -363.371776 [0.22]

N	1.39293823318200	-0.86115966946600	0.26657097557300
C	2.27160188454600	0.17847979332700	-0.00811878663500
C	1.61834213809700	1.19853689503300	-0.59534412621500
C	-0.73416847595700	1.04878558132500	0.28961765612200
C	-2.12507128337200	0.57962034344700	0.13348176729700
C	-2.24099407304400	-0.75620466603100	-0.12377328016600
C	-1.00259968041200	-1.39961375970100	-0.18702164821200
C	0.22893030922100	0.83372512390000	-0.76339791166800
C	0.11161736287200	-0.49111703725700	-0.12144656696200
H	1.57002062447200	-1.54317639906200	0.97896149877800
H	3.31381070188400	0.07505365725100	0.23289071279900
H	2.06198171707000	2.12591323439000	-0.90842526562800
H	-0.47811132646300	1.66082285101900	1.14706099550300
H	-2.95524101732100	1.26259323915800	0.20723828720900
H	-3.17839697839800	-1.26047827612900	-0.28503609290100
H	-0.85803222674700	-2.46278743650700	-0.26325821488600

16

indole-24 5.78 eV -363.371355 [0.19] -363.371354 [0.37]

N	1.30195957182100	-0.76518933377100	-0.45929173389500
C	2.19020408694400	0.18799106554600	0.03292595424200
C	1.62901535857100	1.41679778305700	0.55184342269500
C	-0.63484006030100	0.80657373660100	-0.31335308894100
C	-2.05084359358500	0.57254667938800	0.13686147957200
C	-2.26765826187200	-0.74528852730900	0.20075647837800
C	-1.04027021281900	-1.48759565824900	-0.06335598834600
C	0.32849931299900	1.58660305742500	0.47278629071100
C	-0.05303386387500	-0.60402268431700	-0.30103902671200
H	1.63108807033100	-1.71228452707400	-0.47992870458900
H	3.23481263592000	0.04694535049900	-0.16206603285300

H	2.29274205698700	2.13249222409200	1.01201013431500
H	-0.65875631975700	1.16263846355700	-1.35123193476400
H	-2.76186566369500	1.36397660354600	0.28459173364800
H	-3.20643835878800	-1.21601492711900	0.43952615694000
H	-0.93798684925000	-2.55717583120000	-0.00103514040300

16

indole-25 5.80 eV -363.370905 [0.49] -363.370905 [0.25]

N	1.23472657136800	-1.11342288014000	0.34945730568700
C	2.15651555803600	-0.07242999920900	0.29894613004600
C	1.57057188865300	1.10988948901700	-0.04149235395800
C	-1.00399424208700	1.56919448476500	-0.17583958496400
C	-2.04186011371200	0.72549618034300	0.12835725180500
C	-1.74307883288500	-0.69077235672400	0.12908325947700
C	-0.93797417414100	-1.32683446356400	-0.93866759581800
C	0.20096200759900	0.85608942330000	-0.25527130254400
C	0.03116412242300	-0.62563667022100	-0.20470854493700
H	1.52842179922000	-2.03898347047300	0.09666664178800
H	3.18104607889100	-0.25852977856900	0.56270021689000
H	2.05519715983600	2.06793258479700	-0.02982005390700
H	-1.08008062627300	2.64082074113800	-0.22384363721600
H	-3.01260811117600	1.08067133389200	0.43620498738200
H	-2.25336754554800	-1.32913743708700	0.83650761920900
H	-0.88901363061800	-2.40535370659300	-0.96828033893800

16

indole-26 5.87 eV -363.368402 [1.02] -363.368402 [0.78]

N	1.47152160186500	-1.03945392218200	0.33661044952900
C	2.27120231370800	0.04992229758800	0.14956234045600
C	1.50344457685300	1.15353563191100	-0.13025912567800
C	-1.13100017839900	1.33983062302600	-0.29742745446500
C	-2.13465379896400	0.68540364017000	0.54411668695400
C	-2.13009257074900	-0.51314902086500	-0.26169341259800
C	-1.00574461833500	-1.38196162362800	-0.08611510366900
C	0.15230833476000	0.74509396152300	-0.10290545047700
C	0.15540124842000	-0.66537806970400	0.15809525005300
H	1.79407296816300	-1.96485407397800	0.52549284804300
H	3.33688344270700	-0.03150682770900	0.24652163945600

H	1.88007347239500	2.14374507802400	-0.30120876577300
H	-1.33066032494700	2.14251925636400	-0.98726061832900
H	-1.98531896734500	0.61476463482400	1.61780766394500
H	-2.83636410998300	-0.66112706696100	-1.06525396871000
H	-1.01444548054100	-2.42839104372500	-0.34608297874800

16

indole-27 5.94 eV -363.365820 [0.07] -363.365809 [0.12]

N	1.58126642596900	-1.25112979523400	0.64378803733500
C	2.05503892954500	-0.27849187060800	-0.35175538285500
C	1.49887118052400	1.02801267906500	-0.13394060554500
C	-0.97379288056300	1.41083801908800	0.50578531818900
C	-2.06828452702300	0.68293465631200	0.13810142589600
C	-1.90857335495700	-0.65861375067300	-0.36552469571200
C	-0.72443849274900	-1.32797698750600	-0.43524831501300
C	0.28593102694700	0.77464938441200	0.47823920770000
C	0.40492039594400	-0.69149068543200	0.16304075031900
H	1.78918538520000	-0.92477358459900	1.58685854773000
H	2.76311873617400	-0.58682919262000	-1.09529941261400
H	1.86496162194100	1.94990826242600	-0.56041570545700
H	-1.06438965646400	2.45215272654600	0.77437932945400
H	-3.05500676386600	1.11152584651000	0.16669416962300
H	-2.79780966047400	-1.16640956582200	-0.70718767299700
H	-0.65437045654500	-2.33531266716500	-0.80751499604200

16

indole-28 5.99 eV -363.363649 [0.32] -363.363649 [0.47]

N	1.53119448177100	-1.05639894016600	-0.24061836131500
C	2.16212590548700	0.08976053101100	0.27753711566100
C	1.32447318279100	1.13079889942000	0.35498765612100
C	-0.96387140103500	1.38193761352400	-0.92610462135600
C	-1.75926505313400	0.70134655050400	0.10782832781500
C	-2.02436848083600	-0.71457774762300	0.09474253577600
C	-0.95596582746800	-1.53628170742400	-0.25758586103800
C	0.03526727113900	0.69213447440200	-0.19690816627000
C	0.19038528942700	-0.77902347689000	-0.33700200383200
H	1.84810225919600	-1.97118183884600	0.01693067609400
H	3.21298762152200	0.05041000384800	0.49639671626900

H	1.58958534519300	2.13846084017500	0.61105964094200
H	-0.94886298225300	2.46024085208100	-0.94948791350700
H	-2.27584425671000	1.31135454509800	0.83654199837700
H	-2.96581947837300	-1.10213726920600	0.44764610817400
H	-1.00349596710700	-2.60784985524600	-0.33596384792800

16

indole-29 6.05 eV -363.361474 [0.61] -363.361474 [0.53]

N	1.55831561918800	-1.33282891207700	-0.02119319295200
C	2.77205063428500	-0.84625413901600	-0.02439806077000
C	1.61028997939200	1.37514037125100	0.00440154813200
C	-0.86959470193400	1.40398824683300	0.01677651255000
C	-2.03540683929300	0.70813666431100	0.01532805095500
C	-2.04740767842700	-0.70909440665200	0.00400949932800
C	-0.86620781739200	-1.39379499435600	-0.00676454478000
C	0.40074993391400	0.73606488439200	0.00503457859100
C	0.33956248085900	-0.68310444903400	-0.00743149006800
H	1.53905406928900	-2.34679847742100	-0.03356779753000
H	2.55917015085000	0.82411565718700	-0.00484165181400
H	1.71959209155300	2.44617990151500	0.01409494929200
H	-0.87488793757500	2.48170437536600	0.02611309553300
H	-2.97297551067600	1.24018119229300	0.02307806917800
H	-2.98339988718800	-1.24111225500500	0.00442398662900
H	-0.85227667726500	-2.47353018491600	-0.01506355227100

16

indole-30 6.18 eV -363.356695 [0.67] -363.356694 [0.53]

N	1.44863240781700	-1.03057014065800	0.35258658363100
C	2.26254519801100	0.06389526262000	0.16644549257300
C	1.49990294115100	1.16297596568500	-0.11188431193400
C	-1.16486494212300	1.27625081540100	-0.32590597134900
C	-2.12405917725900	0.69543988143000	0.60301608043400
C	-2.10835912098100	-0.43514005610300	-0.27217336382300
C	-1.03415668883900	-1.37276212398900	-0.05635289208800
C	0.14448584190700	0.75178614295900	-0.08388317334800
C	0.14454714418800	-0.65939580161100	0.17856530797800
H	1.76966552279400	-1.96075817897200	0.52180234912500
H	3.32657917815100	-0.02604183259500	0.26887452780900

H	1.87550005319000	2.15407972929600	-0.27987924040600
H	-1.41186521685100	1.96281502521100	-1.12052460415900
H	-1.79804479287200	0.53853975017300	1.62361076169700
H	-2.77564132795600	-0.52252998466100	-1.11816322443000
H	-1.05823911072500	-2.40959097951600	-0.34613432171700

16

indole-31 6.31 eV -363.352035 [0.77] -363.352035 [0.10]

N	1.50104139544900	-1.01633788836300	-0.23468670816200
C	2.12974498741700	0.16185034104800	0.22198823999600
C	1.23814943126200	1.14270357331200	0.40583704762400
C	-0.96505022817900	1.22123461275000	-1.07859890665000
C	-1.58335976104000	0.68630630897900	0.20352441007000
C	-2.01850574673800	-0.71151495346300	0.21983871143700
C	-0.99444731889000	-1.57190751848800	-0.11250874115100
C	-0.06731822939000	0.62631656659800	-0.05099669618800
C	0.16738583390800	-0.81291400398800	-0.25008540037000
H	1.94104371328600	-1.91400570306200	-0.23093916028600
H	3.19669922709900	0.17395734333300	0.33820807220300
H	1.46502665827000	2.15627742975700	0.67524480858000
H	-0.87153561462000	2.29405253950600	-1.19631704047900
H	-2.04110376293900	1.40508990524700	0.86664150209900
H	-3.02894277335400	-1.01238623438200	0.43491639027500
H	-1.07219990193200	-2.63972884413600	-0.21206652898300

16

indole-32 6.64 eV -363.339962 [0.25] -363.339962 [0.02]

N	1.61657195669600	-0.92265725276500	0.00774386063600
C	2.34368259796200	0.01120753823700	-0.85106996363800
C	1.64346313807400	1.01370131069000	0.02595733856600
C	-1.01493800862500	1.45597997739500	-0.07720723440100
C	-2.18150491917500	0.68392439722200	-0.08116832926600
C	-2.13526209367200	-0.70065582121100	-0.03718994659000
C	-0.91771445429100	-1.38944149940900	0.00271544268200
C	0.17512791437300	0.77294915100400	-0.04999559790500
C	0.20502382486500	-0.60766569792500	-0.01328083357600
H	1.98362054069100	-1.30870774728500	0.87273131674000
H	3.40356510911300	-0.07967074078300	-0.64002078534400

H	2.01135613538400	1.27596850195500	1.02095587161600
H	-1.06275248988500	2.53229500161600	-0.08803754602100
H	-3.13964605998600	1.17639285577200	-0.11204404587900
H	-3.05651501712100	-1.25971133929200	-0.03226301463900
H	-0.87745026480600	-2.46491516055700	0.05217346702000

16

indole-33 6.73 eV -363.336798 [1.09] -363.336774 [0.85]

N	1.57468131552500	-0.13547534760700	-0.80413355027400
C	2.63178815523100	-0.36539716607200	0.01345873409800
C	2.74191829955100	-0.30087941784700	1.39669536166300
C	-1.89065739866600	1.12884675014700	-1.04993346301700
C	-2.50606122282000	0.46163820984300	0.00796525395100
C	-1.76724608512200	-0.40756451534200	0.79739687770300
C	-0.41872335909200	-0.62518519625400	0.56187671516100
C	-0.55980834265800	0.89083540253900	-1.23674999848900
C	0.22401311136400	0.05400709496500	-0.47541226660000
H	1.77754127316300	-0.03096611546000	-1.78262271597300
H	3.51585060344100	-0.57645197373500	-0.57699566564600
H	1.78623231548800	-0.05697430746200	1.86698476013100
H	-2.44241475578600	1.80273195704900	-1.68425139739600
H	-3.55456901236500	0.61634777366200	0.20366308359400
H	-2.24812469364000	-0.93608762497800	1.60362707333200
H	0.13220770599500	-1.33043204875400	1.15843119778900

16

indole-34 6.78 eV -363.334646 [0.81] -363.334633 [1.17]

N	1.58266684132600	0.10594721845100	-0.68265869977100
C	2.67722997447000	-0.35697108576300	-0.03275512263600
C	2.88711485174900	-0.94558700695300	1.21330164774000
C	-1.96212443715800	0.87465195039700	-1.24743527289400
C	-2.57053759829500	0.40501723161800	-0.08355833174300
C	-1.79315850635100	-0.18216524397500	0.90149764970300
C	-0.41799594652200	-0.31503619228300	0.76877603653400
C	-0.60958691794100	0.73806205057900	-1.32666954208800
C	0.21610380394900	0.15988045451500	-0.38192928771500
H	1.77245129487000	0.50023095649700	-1.58779063020400
H	3.54463240039500	-0.19707506682900	-0.66362346653800

H	1.95974445134100	-1.08702105785100	1.76784852244200
H	-2.53473821205800	1.33192203913300	-2.03726618714800
H	-3.63606198742700	0.50079473090100	0.04556500586000
H	-2.26065789310000	-0.55341934054600	1.79834071342200
H	0.14154579037600	-0.79023816323600	1.54835696507300

16

indole-35 6.84 eV -363.332543 [0.17] -363.332503 [0.53]

N	1.62620836019700	-0.07029476739200	1.09054100339200
C	2.46627897238500	0.54157805541900	0.12517368211300
C	1.52982578069400	0.79994369580300	-0.77918571610100
C	-0.63124451201400	0.89875542158900	0.59601167935900
C	-1.91962866540600	0.58704776691600	0.33544009153400
C	-2.26190513232900	-0.61358108225100	-0.33171058173900
C	-1.25436690335900	-1.54525280768900	-0.67831411665400
C	0.50091255076500	0.06229922487100	0.08879387141400
C	0.03553100517000	-1.21407631061900	-0.48247569215200
H	1.84217157130100	-1.03271543398000	1.31753047811700
H	3.52046120388000	0.73080611594700	0.23872293789700
H	1.44471365656200	1.35482583075000	-1.69271575884600
H	-0.35984665711100	1.77345491471600	1.16564965135100
H	-2.70959953851200	1.24202364582400	0.66695287335000
H	-3.29421825390600	-0.82953859000900	-0.55579187464300
H	-1.53866552872900	-2.49628220521600	-1.10462252839700

16

indole-36 6.98 eV -363.327556 [0.87] -363.327556 [0.57]

N	1.66505703993900	-1.18754606656300	0.18124876191700
C	2.43208939460600	-0.10359359351600	-0.15894261530300
C	1.29602817851200	0.84009482887800	-0.47727103967600
C	-0.95973852095700	1.47794348444600	0.47548602145200
C	-2.06159156067200	0.78759597619800	0.12550013515300
C	-1.99747756233500	-0.60787384664900	-0.25357673248000
C	-0.81752366528600	-1.27477568854800	-0.25962705123600
C	0.33609030812900	0.83414434950100	0.53961215529600
C	0.37907296065500	-0.62264808256200	0.13290316704100
H	1.93223661187800	-1.87126798805400	0.86817717919300
H	3.30253915461500	0.18019614113100	0.41685157449400

H	1.21825717391200	1.37738841953000	-1.41503034382300
H	-1.03239288992000	2.51719983699900	0.75713246083000
H	-3.02252627241700	1.27705473258100	0.12238960061800
H	-2.90526229947600	-1.11338020480400	-0.53697998680900
H	-0.76823014158400	-2.32153882388900	-0.51787328667000

16

indole-37 7.19 eV -363.319765 [1.01] -363.319763 [0.88]

N	2.17188197414900	-0.79074079808800	-0.22342722376400
C	2.70534615803800	0.50502398315200	-0.15966554197700
C	1.67903458943600	1.36938522400000	-0.01766391326300
C	-0.80987822477900	1.09381026750700	0.14090902672900
C	-1.99427726311000	0.41755034842700	0.17195501259000
C	-2.18677032605800	-1.01441625915300	0.06940410327300
C	-3.36347601319400	-1.58717749306000	0.10922626645400
C	0.49379337102700	0.57256019446500	0.00479337918200
C	0.84028591366700	-0.87329101582800	-0.13478401663900
H	2.74977502544900	-1.60204434540600	-0.32899215648000
H	3.76368404796700	0.67970506249000	-0.22202784536300
H	1.74937781819500	2.43793428997100	0.06160501451800
H	-0.87704573103000	2.16872166182600	0.23278880521700
H	-2.89522781502000	1.00044407247800	0.28450973364800
H	-1.27308916383400	-1.60290518959500	-0.04551277090000
H	-3.75678645130900	-2.58556652851900	0.05688212674800

16

indole-38 7.27 eV -363.316908 [1.01] -363.316907 [0.58]

N	0.88821242266400	0.22731751721500	0.40709146415600
C	2.22205694265300	0.27981410459600	0.48099292379500
C	2.78266903304100	-0.29683653196100	-0.66175990356000
C	-1.50197561506500	0.80456067117400	1.58339897586800
C	-2.34568206799300	0.31867727142400	0.64143474215700
C	-2.02862953472200	-0.31280421419600	-0.59783653199500
C	-0.82171963390400	-0.60204007949300	-1.18418573215300
C	1.69674804635700	-0.69203632550100	-1.41287307162600
C	0.50236164476100	-0.37487316435700	-0.76556467347300
H	0.14620818758200	0.56626202079200	1.08853061484500
H	2.71086287694000	0.71836626222100	1.33062510050700

H	3.82687367452900	-0.39806873934300	-0.88267654283000
H	-1.89670924714300	1.26271620207800	2.48410966915000
H	-3.42037685009300	0.39798536176600	0.80857516480100
H	-2.88744374903600	-0.61645282497600	-1.17655322798500
H	-0.87682822094000	-1.09359405677500	-2.14330897166000

16

indole-39 7.29 eV -363.316096 [0.27] -363.316096 [0.06]

N	1.52804471873200	-1.09032514871600	-0.16329281918900
C	2.05162779268900	0.02758585218300	0.34463904423400
C	1.18541246094200	1.11946816575600	-0.16346863613700
C	-0.65507415666500	1.37808803256400	-0.00759291972900
C	-1.85043470545000	0.65433918779400	0.26541442830500
C	-2.05440334334800	-0.67034567422700	-0.00835463688200
C	-0.85016304022900	-1.44407301550200	-0.23922116550600
C	0.23720495123900	0.67045552632300	-1.06604686112600
C	0.23386241244400	-0.80201736322600	-0.68873325865400
H	1.83041841755500	-2.01025364787100	0.09844829968100
H	3.04713251103700	0.08758501822200	0.74085106122500
H	1.47882191339900	2.14921885983500	-0.03839386096700
H	-0.73726469980900	2.45063196905400	-0.05029217568800
H	-2.68656791442300	1.24642205206900	0.61495118636000
H	-3.00257464515000	-1.14446805658600	0.17200967856100
H	-0.75941476336800	-2.43331828298900	0.18908263550700

16

indole-40 7.36 eV -363.313397 [0.23] -363.313355 [0.96]

N	1.47059651028800	-1.06152136201600	0.03370793633600
C	2.17757132293100	0.05154495221100	0.32190597142300
C	1.31601265584100	1.12054143929000	0.38965161575600
C	-1.21517049342500	1.39396039213700	0.12790925414000
C	-1.31577704167000	2.67617599222300	0.38413704725900
C	-2.15362002487500	-1.41363205523800	-0.66667969942500
C	-0.81805300779500	-1.73835798154700	-0.41709658589200
C	0.02307910838800	0.64350977599500	0.13003027590700
C	0.13338951315700	-0.75657992703800	-0.10812440071700
H	1.85109698596500	-1.97684271675200	-0.09627083634300
H	3.24018880217700	0.01420788378100	0.46538310604400

H	1.58144953159800	2.13478859147900	0.61422671402100
H	-2.09226221262900	0.78649544654800	-0.10554929425100
H	-2.11587302898600	3.39273613008300	0.34799145972500
H	-2.67400701679200	-2.32498005382500	-0.98706744983300
H	-0.41199369455800	-2.75305303264300	-0.43415511415600

16

indole-41 7.38 eV -363.312779 [0.35] -363.312765 [0.87]

N	1.23911758591800	-1.03446941310200	-0.34745316223100
C	2.18206681246900	-0.02843633981000	-0.30111611448700
C	1.54913142745700	1.13125676485800	-0.02014679059000
C	-0.87129502962700	1.76646020018500	0.42051777276400
C	-2.20442326769500	1.36838065734300	0.64101043718800
C	-1.19103310853200	-2.65223709066100	-0.40823716184900
C	-1.18151708239800	-1.36839333812400	-0.13854263355300
C	0.14856147383800	0.84495339254500	0.12138255672600
C	0.00830664055000	-0.55065647097800	-0.10710455124300
H	1.41327933201500	-1.99582172648700	-0.56645810158700
H	3.21819877256500	-0.24185008337500	-0.47468947355900
H	2.00504949134700	2.09597570647700	0.09196213880800
H	-0.52576326079500	2.79984768023800	0.45951042178400
H	-2.76287627829500	2.25926970221400	0.95922680723800
H	-1.94724056786200	-3.41539271076700	-0.41511611383000
H	-2.08293503133400	-0.78989345589000	0.08525396840800

16

indole-42 7.41 eV -363.311461 [0.19] -363.311461 [0.10]

N	1.10929944334200	-1.14581680130400	-0.23585617105700
C	1.82020157845800	-0.15091313379700	0.48505939168800
C	1.32192305476100	1.05497649510100	0.11022044567100
C	-0.97917630555000	1.50847652903700	-0.53036464493300
C	-1.82995674587900	0.72464178706500	0.22500929230100
C	-1.48920453928800	-0.59926791311900	0.50550609327200
C	-0.48554822082100	-1.28387193937300	-0.31905466596500
C	0.31130227286200	0.89169384861900	-0.87237870689000
C	0.27191201338900	-0.50666172978900	-1.31175402298500
H	1.57892997665700	-2.00937022137300	-0.45348843934300
H	2.55059123824000	-0.43080967563100	1.21833361740800

H	1.56275306367900	1.98478706488500	0.59831354137200
H	-1.21228410527100	2.54517204562400	-0.72362337058700
H	-2.75016518570400	1.12827557447900	0.61778094783900
H	-2.10332399890800	-1.18573294559000	1.17005623536600
H	-0.68062563036100	-2.33658551014800	-0.48375954317400

16

indole-43 7.62 eV -363.304059 [0.05] -363.304058 [0.53]

N	1.13475249629400	-0.76868837994500	0.35563129132800
C	2.20324914977900	0.19550150430000	0.27724648452300
C	1.72617141589200	1.17161993443800	-0.46963095381000
C	-0.73927552865100	1.23516140524800	0.07609574850400
C	-1.85801527105600	0.47481019689700	0.43359779590600
C	-1.92276089556300	-0.89622282411200	0.10184753794300
C	-0.93995509329500	-1.47461874376500	-0.64744291751400
C	0.32258665106500	0.68080944305300	-0.60004460609300
C	0.39072642524100	-0.87294920857200	-0.88954814565600
H	0.75450920553500	-1.01880194277400	1.26375014159500
H	3.16710789261600	-0.02238266722600	0.70072180206800
H	2.19350284284200	2.03341303803500	-0.90640287980100
H	-0.70384057730200	2.28858759616000	0.30873391200600
H	-2.68891862286500	0.94815476093100	0.92938336211300
H	-2.85350055810900	-1.41930889183400	0.27177605135000
H	-1.18971162281700	-2.36609174616100	-1.20571462446200

16

indole-44 7.96 eV -363.291507 [1.47] -363.291404 [0.43]

N	1.82645673498600	-1.05213229990800	-0.03667729425200
C	1.83933747710200	-0.13612050281600	0.94417300359300
C	0.65734151457200	0.56780423645600	0.92392136077500
C	-1.44229409053800	0.36915169957300	-0.58897234093400
C	-2.39747398175700	1.19854266414700	-0.07567664503400
C	-2.40800267712000	1.91440905097000	1.14291644212900
C	0.25951129420700	-1.79820722203200	-1.79752757453100
C	-0.13025268219300	0.03948330467100	-0.11589529624600
C	0.62980186887400	-0.99456750108900	-0.74250149167900
H	2.56616836362200	-1.69188792726900	-0.24701436653400
H	2.68435469868900	-0.02631513238600	1.59693712221100

H	0.42188242587000	1.38442515367600	1.57374140008500
H	-1.68695071595600	-0.14807505081600	-1.50502240383500
H	-3.28718551585000	1.28619272903400	-0.68681629715000
H	-1.55352823426100	1.75513528546200	1.79577215218300
H	1.01746142940000	-2.47884501299500	-2.18135777079000

16

indole-45 7.99 eV -363.290783 [0.32] -363.290369 [1.33]

N	1.67959460317000	-0.53149227417600	0.67772454212800
C	2.77512668683100	-0.44621300328700	-0.09791192996300
C	2.43929209592500	0.04299433583400	-1.34807709344900
C	-3.61651246843800	0.26315299218600	1.26819084989600
C	-3.06417487657600	0.53372967225100	-0.01373020039300
C	-1.76028309599900	0.41746911469300	-0.40283225912800
C	-0.67383665493100	-0.02381571897000	0.40659667150000
C	1.05874318773100	0.27616670853400	-1.41174295516600
C	0.58965339539500	-0.08673495316500	-0.08054196527300
H	1.66045580222300	-0.84790218348700	1.62682617658800
H	3.73375592473100	-0.74922521146600	0.28773009583900
H	3.15110291174200	0.19259056920700	-2.13953035716200
H	-2.87431310139100	-0.08684850297200	1.99157315107800
H	-3.75026956554700	0.87859572491400	-0.77627970733200
H	-1.48423119980900	0.67247523254400	-1.41461487141400
H	-0.86747573542400	-0.31594902799800	1.42661985228300

16

indole-46 8.03 eV -363.288999 [1.67] -363.288979 [0.26]

N	0.61666270625500	-0.38217412072000	0.89875553910800
C	1.82283691517400	0.26848744678200	0.91867613470300
C	1.86304943067400	1.13964204091400	-0.12212702594700
C	0.14090258957200	1.67925323360200	-1.97095340044500
C	-2.23930947879800	-2.00045025568400	1.26256074532600
C	-2.33153488618200	-1.24381125144000	0.06963975918900
C	-1.45184458880000	-0.36819331099900	-0.50154162496200
C	0.62224327872500	1.02380089440200	-0.83200213538500
C	-0.13908888595300	0.04626101344800	-0.13435094475100
H	0.33909217138700	-1.09115623193900	1.54616955069200
H	2.54856619866400	0.04282090088500	1.67543763660200

H	2.67697192137800	1.79222147864300	-0.37292480071100
H	0.87084441793500	2.36898835290200	-2.39670232533900
H	-1.32646428407000	-1.86100146253800	1.84718648154300
H	-3.25670408866100	-1.35874587730500	-0.48011821835300
H	-1.75959550775500	0.13305062374200	-1.40770537125600

16

indole-47 8.45 eV -363.273585 [0.61] -363.273583 [1.24]

N	1.59639976610200	-1.08450296867300	0.11716482134200
C	2.60909696874500	-0.23393298017300	-0.04109520898600
C	2.12836602974900	1.05065413871100	-0.27591092855100
C	-2.23546120263700	1.96280407291400	0.44448988791100
C	-2.77576735825300	0.69043705479200	0.08052021633500
C	-2.15859347107100	-0.50913395265700	-0.09382733522100
C	-0.78748600950400	-0.97178478422700	0.02044627994100
C	0.72920926009800	1.07797766966600	-0.24356277075000
C	0.39768988210800	-0.33394737949500	-0.03007533929200
H	1.68031159490100	-2.07116961330800	0.26236441582100
H	3.62535136149100	-0.58284402334100	0.04264008199700
H	2.77546334689100	1.89917905866900	-0.41332292361500
H	-1.16487807801900	2.04958924443600	0.23391605374300
H	-3.85635706446300	0.63113251910300	0.01008456328300
H	-2.83421975835100	-1.33879809799900	-0.25618059164300
H	-0.73249735817400	-2.04666648376300	0.14234877769400

16

indole-48 8.69 eV -363.264705 [0.67] -363.264705 [0.87]

N	1.59839229501900	-0.79213577755800	-0.20602796517800
C	2.71220025684900	-0.18241127531000	0.42777914263500
C	2.70498644480100	0.82251063946000	-0.44436571240700
C	-1.33258169622700	1.48211821338200	0.22675591519000
C	-2.38317755421600	0.57190724243800	0.10483614925800
C	-2.10371137040300	-0.76543218024500	-0.14043042839200
C	-0.79629658866000	-1.21185181428100	-0.24053181919000
C	-0.05951667157800	0.98729892225900	0.18429825297600
C	0.26255358300600	-0.31934274845200	-0.07213330484300
H	1.70549888831800	-1.64011841518900	-0.73374456205800
H	2.92558580561700	-0.28980402400800	1.47950041777800

H	2.19477437931800	1.80270557703400	-0.43887578440000
H	-1.53224373554600	2.53043385843100	0.38522447407500
H	-3.40288673049700	0.90742268435500	0.20782274174100
H	-2.91168156256600	-1.46804731713700	-0.26433197578900
H	-0.58526783361000	-2.24626011051600	-0.47577554142000

isoindole

16

isoindole-S0MIN FC 4.52 eV S0: -363.5681646907 [0.03] S1: -363.4021395487 [0.09]

C	-0.000000000000	-0.721705255712	-0.253297671914
C	0.000000000000	-1.428176201898	0.986174883016
C	-0.000000000000	0.721705851561	-0.253297555551
C	-0.000000000000	1.428175324640	0.986175584178
C	0.000000000000	-0.708861962924	2.150597542531
C	-0.000000000000	0.708861284943	2.150598354125
N	-0.000000000000	-0.000000354985	-2.322815229938
H	-0.000000000000	2.506011737563	1.001140354249
H	0.000000000000	-2.506012512397	1.001140123414
H	0.000000000000	-1.226289548439	3.096517973230
H	0.000000000000	1.226291607556	3.096517359380
C	-0.000000000000	-1.121890980683	-1.563829512608
H	-0.000000000000	0.000000030368	-3.323072810510
H	-0.000000000000	-2.096578667995	-2.009885223794
C	0.000000000000	1.121890572601	-1.563829881689
H	0.000000000000	2.096579075803	-2.009883985731

16

isoindole-S1FCMIN 4.20 eV -363.413659182200

C	0.022211537227	-0.717351759984	-0.233208242211
C	0.004651807778	-1.432685037805	0.973940618894
C	0.022210444023	0.717350786801	-0.233207935968
C	0.004650387793	1.432684405990	0.973940598723
C	-0.010596555273	-0.687957134547	2.182208061706
C	-0.010596528349	0.687957118950	2.182208427067
N	-0.074712125575	0.000000234814	-2.393028500417
H	-0.001762915725	2.508729757978	0.986173520567

H	-0.001759934829	-2.508730402200	0.986172086580
H	-0.024277268437	-1.218473995166	3.120369944444
H	-0.024277844909	1.218474648898	3.120369999975
C	0.013365925918	-1.105906399177	-1.565472584924
H	0.335351424750	-0.000000780985	-3.313115182341
H	0.024566441169	-2.093649171376	-1.986311724038
C	0.013368613216	1.105906159620	-1.565472094930
H	0.024570809012	2.093649336710	-1.986310402511

16

isoindole-01(Fig2b1) 4.50 eV -363.402689 [0.79] -363.402688 [0.12]

C	-0.37823065588300	-0.79857090385400	-0.12449618132800
C	-0.26766758512000	-1.45412037464200	1.07053058548100
C	-0.30091220753800	0.60655818125500	-0.16466749785600
C	-0.03470546125000	1.36122101294500	0.95582814309400
C	-0.05068959993200	-0.68993103438700	2.23078789764700
C	0.07593349629700	0.68411510640800	2.17569465650100
N	-1.18036811904600	-0.04093421192100	-2.17567995083400
H	0.09778289130800	2.43044864168400	0.90369420431800
H	-0.31439540364600	-2.52944816505000	1.12126916015200
H	0.03552394428600	-1.19019331787800	3.18199619740000
H	0.26448298265900	1.24153923812000	3.07849694624100
C	-0.43559905883500	-1.24528077255600	-1.55800134589100
H	-1.26706135495900	-0.00783929499100	-3.17592889733200
H	0.59560862668200	-1.17138166166500	-1.92706757405300
C	-0.54003634255900	0.94660259128000	-1.55781179029400
H	-0.23247936257700	1.85716422140600	-2.05130114755400

16

isoindole-S1TS(Fig2b1) 4.70 eV -363.395272638600

C	-0.507804315170	-0.592413567171	-0.264070998957
C	-0.155117933469	-1.302766472840	0.870275607458
C	-0.794388156829	0.805805448224	-0.228264873452
C	-0.789949008499	1.464818539818	0.979868628758
C	-0.167604897316	-0.614640785593	2.109842235659
C	-0.475922016296	0.719814209752	2.150449488871
N	-1.104313746477	-0.018065241897	-2.388080661728
H	-0.995838085889	2.519329118599	1.043465168241

H	0.159032079981	-2.332069840739	0.810426167344
H	0.076188118083	-1.143903316158	3.015655306073
H	-0.472866886451	1.232084160289	3.099799618766
C	-0.576092778996	-0.974732090902	-1.624516934517
H	-0.981954768618	-0.022165136512	-3.383580856775
H	-0.264340066319	-1.918017006399	-2.042604421206
C	-0.926848106571	1.246143981482	-1.601958317191
H	-0.133743057306	1.865770045285	-2.001747550556

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isoindole-02(Fig2b2) 4.54 eV -363.401171 [0.28] -363.401171 [0.84]

C	1.95427867532900	-0.77232744302600	-1.23501653369500
C	2.93749143983000	-1.51550287501900	-0.60154364810500
C	2.00212446177900	0.63910439751100	-1.23484988983700
C	3.03295994083000	1.31381218883200	-0.59999388625700
C	3.96770773191200	-0.83167325736100	0.03053274788700
C	4.01429511064800	0.56163787778900	0.03213882785100
N	0.12416481058600	-0.00400505091000	-2.36361570163800
H	3.07776566161800	2.39085466813900	-0.59177170082800
H	2.90949887002300	-2.59309658985500	-0.59532747876900
H	4.74523150758200	-1.38567130587100	0.53046462001400
H	4.82666075524100	1.06118690839300	0.53401011657400
C	0.76175680470700	-1.10410079562200	-1.96518447846800
H	-0.69315483284100	0.01906920112300	-3.97635187915000
H	0.37841328218800	-2.08069409800100	-2.20088486885400
C	0.83534433132700	1.05095761531300	-1.96586198160200
H	0.51973292946100	2.05087911549700	-2.20410641879100

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isoindole-S1TS(Fig2b2) 4.86 eV -363.389400755200

C	1.948634842482	-0.780498946946	-1.295702223409
C	2.923252249828	-1.518753690037	-0.642441897011
C	1.995333869447	0.645227365774	-1.293635829272
C	3.016197928055	1.315908693605	-0.637893197753
C	3.947591958634	-0.827338956673	0.019913313638
C	3.992843615537	0.556677947324	0.022127695721
N	0.096915007813	-0.004761572413	-2.381886374900
H	3.057547747012	2.392567304425	-0.620517167419

H	2.894005722615	-2.595871506591	-0.628577628130
H	4.708404832020	-1.384169179200	0.541594449949
H	4.788406637698	1.060750353431	0.545461307939
C	0.762029550733	-1.111913282631	-1.987589921469
H	-0.444274879421	0.014363117648	-3.597661440612
H	0.374579497005	-2.086384015046	-2.225485313855
C	0.833042093119	1.055468852595	-1.984815930625
H	0.510390085834	2.053811624150	-2.220472026294

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isoindole-03(Fig2b3) 4.60 eV -363.399294 [0.86] -363.399294 [0.17]

C	0.55175209563200	-0.60534501783100	-0.18213089362400
C	1.03255709610000	-1.05799891278200	1.00653676713000
C	-0.41121818444700	0.44532881446400	-0.20461538838200
C	-0.94838713531300	0.96310495127500	0.95155487808300
C	0.54799136980100	-0.46845349407100	2.19701081988800
C	-0.42781233040600	0.50124826626100	2.17153651268400
N	0.29394411185300	0.14182323240500	-2.35920167188300
H	-1.75383768877100	1.68043706567000	0.93383177887100
H	1.74816341841300	-1.86253770551400	1.04595655487600
H	0.94149354613600	-0.79993154598100	3.14449039445200
H	-0.80456924228700	0.90744813017300	3.09593894272100
C	0.56779194530800	-1.08470283454500	-1.61620982750500
H	0.89401606522000	0.55329939856700	-3.04968225508700
H	-0.37430962025600	-1.63603396168700	-1.68330968442600
C	-0.57267399605800	0.79704111060300	-1.60358873565000
H	-1.27124672467100	1.52527147346300	-1.99308808496100

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isoindole-S1TS(Fig2b3) 4.65 eV -363.397402659600

C	0.557842483385	-0.569268300123	-0.193442458867
C	0.983057658228	-1.080222421655	1.005309832086
C	-0.365762477294	0.527315969864	-0.198872406225
C	-0.901666190285	1.042003166392	0.967830875815
C	0.473729387926	-0.506033766412	2.206989252536
C	-0.436821955125	0.515846099834	2.199252813172
N	0.088068985246	0.064223215527	-2.392926571898
H	-1.685879614135	1.781084839569	0.944282803260

H	1.679836819177	-1.899637394887	1.048245811422
H	0.819007326242	-0.898176816222	3.150651306806
H	-0.816409971760	0.913685750474	3.125385496273
C	0.671615233447	-1.006715015989	-1.575320012011
H	0.581419335978	0.459861786656	-3.179102401235
H	0.198822894909	-1.958033974355	-1.784049171021
C	-0.581620420045	0.856767257595	-1.556321820190
H	-1.195015621175	1.666332388970	-1.922085634801

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isoindole-04(Fig2b4) 5.04 eV -363.383033 [0.44] -363.383033 [0.17]

C	-0.05927306677400	-0.68070438537500	-0.23142447261300
C	-0.21402424790600	-1.44120915839100	0.89192705477700
C	0.06428023529200	0.72925498235300	-0.23022329333400
C	0.02461608426700	1.38494409828100	0.99294836734100
C	-0.22193386922100	-0.77319184678600	2.12472462482200
C	-0.11834110368700	0.60917493680500	2.14696436158100
N	0.80526697171300	-0.17307403827500	-2.31528244512700
H	0.07250400222500	2.45904720373900	1.06103980761100
H	-0.33029877709500	-2.51269308128000	0.84287710823200
H	-0.33453908138100	-1.32608742606700	3.04120354192900
H	-0.15453743895700	1.11397679857400	3.10025440144900
C	-0.09918095151300	-0.89858851069000	-1.67412816743200
H	0.62500445763800	-0.17007726276200	-3.31009468707800
H	-0.74764837803400	-1.60044569273600	-2.18167968099100
C	0.05032608708800	1.06353869310900	-1.61625898464800
H	0.32193978725200	1.97655277476200	-2.11435443876500

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isoindole-05 5.16 eV -363.378679 [0.56] -363.378677 [0.35]

C	0.48768017292700	-1.20453521148000	-0.31266989119400
C	1.19454147635700	-1.82036876582400	0.70779706762100
C	0.69592363719200	0.14584975864400	-0.62517577200600
C	1.64858854668600	0.85320267368800	0.13413297601000
C	2.12631610141900	-1.11008689805100	1.44307063953600
C	2.34578758993100	0.23358257398500	1.14507276267800
N	-0.92684686130200	0.09357363773000	-2.38256281942400
H	1.82799623377700	1.89391864824800	-0.08625133048000

H	1.01220969071100	-2.86063937766300	0.92429882418400
H	2.67531202098500	-1.58931873531000	2.23654943093100
H	3.06974311223900	0.79733636233600	1.71177687088500
C	-1.38663814617200	-1.12729653172600	-2.39862220648900
H	-1.40390613660000	0.61625684539200	-3.11515623556000
H	-0.23415217821000	-1.79475016267500	-0.86662073275100
C	-0.01985129015100	0.78962249683600	-1.66635502830400
H	0.11021240753400	1.81756945010800	-1.93594850048800

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isoindole-06(Fig2b5) 5.16 eV -363.378545 [0.14] -363.378432 [1.01]

C	0.26027816146900	-0.63191820095300	-0.44943651151000
C	0.22757629397900	-1.32773453998400	0.79701385484800
C	-0.00337629000900	0.82841624253700	-0.39350207215800
C	-0.19405066203400	1.48423203590600	0.82998552714500
C	-0.09972584632400	-0.64989375347900	1.93241974860400
C	-0.33086477574000	0.75595048116400	1.97996594724800
N	0.56820158324600	0.19753485369700	-2.59241872274900
H	-0.29708156865200	2.55804082143900	0.84428745418300
H	0.46759416018100	-2.37855193591000	0.82670737299400
H	-0.15382959874000	-1.20329449099900	2.85685901783900
H	-0.58096770082400	1.22938385107200	2.91333131543800
C	0.68930437553300	-0.97727747169800	-1.71332545175100
H	-0.41223484682500	0.31471485612300	-2.84752390371300
H	1.08414017862800	-1.90075415215600	-2.08595932747300
C	0.84139230589000	1.01314220921400	-1.49426167063500
H	1.79143501160400	1.53257210660400	-1.48477363357100

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isoindole-07(Fig2b6) 5.25 eV -363.375157 [0.78] -363.375157 [0.23]

C	-0.06310122305900	-0.59893113701200	-0.03989696640200
C	-0.36663699930100	-1.35246800479400	1.15954603163500
C	-0.27887971602800	0.83867355471400	-0.09662865993600
C	-0.90646785857500	1.41581075630000	1.02404087447700
C	-0.66283826429600	-0.67991825463800	2.28747222517400
C	-0.66103543325000	0.82034398689500	2.29724933438100
N	0.36304315522400	0.15338386989900	-2.08434368731800
H	-1.59993438552800	2.23936191150100	0.88033232394200

H	-0.36974786602900	-2.43099725154600	1.12222955019900
H	-0.80440259046500	-1.21649014095200	3.21437050080200
H	0.45411288391500	0.88572513605600	2.26123286569100
C	0.32902900205300	-0.97587475525600	-1.29100482505000
H	0.63620491033800	0.15600227295600	-3.04684514892400
H	0.57041570845300	-1.93645733409600	-1.70008827794300
C	-0.01648338355300	1.24191046822600	-1.40052606837900
H	-0.03780798882900	2.21419336047400	-1.85224214601900

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isoindole-08(Fig2b7) 5.59 eV -363.362837 [0.39] -363.362837 [0.39]

C	-0.05193737793000	-0.66964154712100	-0.23679291412100
C	-0.07648941335800	-1.23375847287500	1.07102773505400
C	-0.15462440319600	0.77251054935600	-0.29681327995900
C	-0.07484717776400	1.37838162682100	0.94212303283900
C	-0.85401869589300	-0.64382260321700	2.19847229666600
C	0.00558002008000	0.43509464394700	2.09938620831600
N	-0.00263916174100	-0.01278700794700	-2.35022063536500
H	-0.13358419762100	2.43542711874200	1.13601297009500
H	0.49006500412300	-2.12248150564900	1.30101118048700
H	-0.90808980507600	-1.20110009541200	3.12004063540100
H	0.65890873951900	0.73701740438700	2.91634352048200
C	0.07134546791300	-1.11407952517000	-1.52611325358100
H	0.01909199800600	-0.05929607452500	-3.34815911302300
H	0.15597994540000	-2.10029039217000	-1.93645285564700
C	-0.15916634578000	1.13278043795200	-1.64446556342600
H	-0.22180905334300	2.08700345863600	-2.12757067048700

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isoindole-09(Fig2b8) 6.08 eV -363.344850 [0.34] -363.344849 [0.30]

C	-0.52663262324200	-1.04112807642800	0.22641802809600
C	0.16952934100700	-1.63524568969700	1.34856475907300
C	-0.96293833969800	0.36931284238900	0.20646859494200
C	-0.57424104748200	1.21755202070600	1.31620643946700
C	0.99473279267800	-0.46372954935500	1.29445284147000
C	0.43984165700600	0.68295041851800	2.01866864314200
N	-1.71688317396700	-0.63675551152300	-1.61038848961100
H	-1.17579262347000	2.05058381471200	1.64328318044200

H	0.48862234960600	-2.65932757633600	1.26043695604000
H	1.62762881772200	-0.20323320073800	0.43477174770100
H	0.67946577142200	0.91288821568900	3.04558670378000
C	-0.98386502294200	-1.58088905954100	-0.98369684358200
H	-2.21509508702800	-0.78678331904200	-2.46479588445200
H	-0.91502647540800	-2.58146243327800	-1.36130376310100
C	-1.69599009724500	0.55373409312100	-0.93282859976900
H	-2.17065764350300	1.42568521058800	-1.33635461533400

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isoindole-10 6.19 eV -363.340666 [0.21] -363.340662 [0.87]

C	-0.73829514325500	-1.13881655907500	-0.47335553892800
C	1.61149422697400	-1.62330995579300	2.27023233071400
C	-1.05720694088200	0.22671022298600	-0.14048663009700
C	-0.58180575773000	1.01212441832900	0.90246630266000
C	0.96671898705500	-0.52498412354300	2.04914348339300
C	0.35615082681500	0.64009793232000	1.90616811088200
N	-2.21424807023000	-0.34311052087300	-1.94405489490000
H	-0.95753682228000	2.02178792933800	0.97140426581000
H	2.57091511887700	-1.81752969324700	1.81185191655300
H	1.19506382458400	-2.41026315335000	2.88302620366800
H	0.59829985740700	1.40090771194700	2.63601665748100
C	-1.45741778895300	-1.45539377545600	-1.57245453124100
H	-2.83850701721400	-0.29742273233000	-2.72719197001900
H	-1.52658042017900	-2.35608887249500	-2.15139537918500
C	-1.98819086714000	0.66952689679300	-1.10204251907300
H	-2.47615542365100	1.61991646255200	-1.21383810694600

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isoindole-11(Fig2b9) 6.25 eV -363.338330 [0.17] -363.338329 [0.29]

C	-1.49709925213200	-0.52068891173400	-0.21756592063400
C	-0.63993298953400	-1.29195633852500	0.60479516030900
C	-1.12016729206900	0.88967444751000	-0.22445650178600
C	-0.78208769352600	1.55957476696400	0.94993764032700
C	0.02075122119700	-0.61589916742500	1.75530153708700
C	-0.20763387250900	0.70036206643700	1.95952057204200
N	-0.03153532605000	-0.08927564286800	-1.91422276561100
H	-0.57752084869700	2.61666309966900	0.97707466338800

H	-0.81986155905500	-2.35568017475900	0.70567566698600
H	0.58567471178500	-1.20171065436500	2.46000720929700
H	0.16400579905300	1.16048552437200	2.86311943745100
C	-0.56438997188300	-1.16035370315700	-1.16323103774400
H	0.57053767638800	-0.19707977365400	-2.70779692883600
H	-0.76106052372900	-2.07870216019400	-1.69548483020600
C	-0.39092753850900	1.09034244275000	-1.40265010531200
H	0.07356503656600	1.99690741720500	-1.75135125462500

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isoindole-12(Fig2b10) 6.42 eV -363.332307 [0.27] -363.332307 [0.13]

C	-0.07527838772000	-0.69073596352100	0.01803789313000
C	-0.91989222907900	-1.35114837538200	0.84549213749700
C	-0.16603778012700	0.81791506905900	-0.16342865648600
C	-0.26017145866800	1.55209109837900	1.04672897290400
C	-0.04423353804100	-0.66591020509300	1.90235823751600
C	-0.03387027517100	0.72193467696200	2.12097302675800
N	0.39148070682200	-0.16557818452900	-2.12392323037900
H	-0.30956339992200	2.62395268527100	1.09697183119300
H	-0.92646944009500	-2.43134840814000	0.81165938799600
H	0.51034584181300	-1.33832632343800	2.53496845664700
H	0.21536235637300	1.10996139259100	3.09727800070900
C	0.60102319948300	-1.17709985772300	-1.25607919271000
H	0.51429577128000	-0.23780085231300	-3.11287476228000
H	0.64043972124900	-2.19620035887900	-1.59278302327400
C	-0.02209492653300	1.02549410922500	-1.47845316672900
H	-0.13377668232100	1.92041024953500	-2.05953848751100

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isoindole-13 8.14 eV -363.269020 [1.24] -363.268272 [1.05]

C	-0.21450931822700	0.15624338765100	-1.75453182353100
C	-0.39452248538700	-1.62376552268800	1.69490039929600
C	-0.41255066388400	0.37324711225800	-0.37107557635800
C	0.36613066522700	1.12215348391100	0.57661380968900
C	0.28505343946700	-0.61112523905200	2.33454726266300
C	0.60247716094700	0.67977806192200	1.85031744740500
N	-2.02395343701300	-0.93968862308400	-1.22601141414700
H	0.81704167452600	2.04371041738800	0.24702889256200

H	-0.02775728715200	-2.31350786277800	0.94556968306400
H	0.50246885892600	-0.79949377761400	3.38124409733000
H	1.10747858276700	1.34227997242500	2.53601871628000
C	-1.16893365135200	-0.65696604790100	-2.26377701122900
H	-2.86397394993100	-1.47604210086800	-1.29769339083700
H	-1.30487952892200	-1.08032885522200	-3.23922729639900
C	-1.58949201786800	-0.32981558683600	-0.08564657134200
H	-2.21737945286200	-0.26252663190800	0.77721247590200

quinoline

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quinoline-S0MIN FC 4.50 eV S0: -401.6765462208 [0.03] S1: -401.5111631513 [1.06]

C	0.024405389996	-0.681322915268	-0.000000000000
N	1.182431014676	-1.385200120772	-0.000000000000
C	-1.192013746295	-1.387661783843	-0.000000000000
C	-0.005122906731	0.739377210198	-0.000000000000
C	-1.246306226056	1.399417876558	-0.000000000000
C	-2.380809665327	-0.723296392719	-0.000000000000
C	-2.409823797879	0.690476051903	0.000000000000
C	2.392918105658	0.685963304103	0.000000000000
H	-1.262763314534	2.478372664024	0.000000000000
H	-1.143573299168	-2.463557582748	0.000000000000
H	-3.308157442779	-1.272562136439	0.000000000000
H	-3.357489346009	1.203650486150	-0.000000000000
C	2.308481591538	-0.715080667708	0.000000000000
H	3.357511099682	1.165020321620	-0.000000000000
H	3.214557939419	-1.303453040578	-0.000000000000
C	1.233293490481	1.416106477854	-0.000000000000
H	1.251471364034	2.494541354722	0.000000000000

17

quinoline-S1FCMIN 4.309 eV -401.518178263300

C	0.024398801342	-0.710496956705	0.000000000000
N	1.178359231693	-1.415189182631	0.000000000000
C	-1.184037728369	-1.401116811171	0.000000000000
C	-0.009159765848	0.772371258802	0.000000000000
C	-1.243940943626	1.414745711781	-0.000000000000

C	-2.395971839606	-0.728297812193	0.000000000000
C	-2.426995122012	0.694634177349	-0.000000000000
C	2.407204858882	0.685370601424	0.000000000000
H	-1.269092691858	2.492831928421	0.000000000000
H	-1.141743495851	-2.476636270267	0.000000000000
H	-3.320587738381	-1.280124010763	0.000000000000
H	-3.374182224835	1.206542302053	-0.000000000000
C	2.327054461307	-0.720452605087	-0.000000000000
H	3.373827920272	1.159266527741	0.000000000000
H	3.231347026104	-1.307497773418	-0.000000000000
C	1.230612696422	1.450632592072	0.000000000000
H	1.259230812680	2.526488896718	-0.000000000000

17

quinoline-S1TS-b 4.310 eV -401.518150692200

C	0.022311761568	-0.709652034829	0.024889566171
N	1.178632596583	-1.410475130470	0.037813538306
C	-1.185516031297	-1.400294621361	-0.022874622055
C	-0.009897862331	0.771330211819	0.030697019948
C	-1.245128803977	1.413635835719	0.031365606188
C	-2.395514721958	-0.727776914985	-0.017449993414
C	-2.426354178885	0.693837933968	0.013460384826
C	2.408337176980	0.683425247748	-0.046406701277
H	-1.269893026984	2.491720151553	0.037760077319
H	-1.143490552460	-2.475605928978	-0.044799292404
H	-3.320332207789	-1.279220590056	-0.030899502134
H	-3.373649701358	1.205723384015	0.015247513618
C	2.329743731768	-0.719889823781	0.006057733695
H	3.374800545317	1.157670938323	-0.046939999731
H	3.232711509992	-1.305208419013	0.071457565850
C	1.230589549414	1.449130627448	-0.020389497759
H	1.258974473714	2.524721706996	-0.038989397139

17

quinoline-S1MIN-b 3.96 eV -401.531162348200

C	-0.020916608303	-0.702994544493	-0.131852370081
N	1.223449287159	-1.260448462724	-0.227903932606
C	-1.203532089983	-1.410964836407	-0.123409650419

C	0.003532820354	0.722476262014	-0.038304493172
C	-1.229359725818	1.363481489020	0.061693035900
C	-2.402471953777	-0.725001285180	-0.021994381459
C	-2.415478626149	0.660301941433	0.070365630727
C	2.477511926871	0.673980761793	-0.157865076744
H	-1.235311229883	2.440163270308	0.133707089668
H	-1.180909888087	-2.484597596650	-0.196053475193
H	-3.327678464756	-1.277395352525	-0.015389005977
H	-3.351591841002	1.187922244073	0.149203238727
C	2.453932151762	-0.681511076233	-0.247320586939
H	3.432537810559	1.171369639264	-0.170151492276
H	3.311626732897	-1.322210693009	-0.331692919362
C	1.276221938592	1.397978399645	-0.052898941914
H	1.292009108825	2.471086296239	0.018328409883

17

quinoline-01 4.36 eV -401.516321 [0.52] -401.516321 [0.10]

C	-0.18284124114200	-0.69908872175600	-0.23793127905200
N	0.90083407117300	-1.43181750749400	-0.05735061328600
C	-1.44558343601300	-1.44841595844300	-0.63064451427200
C	-0.20405282648800	0.70340235842200	-0.08271871522800
C	-1.40797417198200	1.43850663578800	-0.29188604438100
C	-2.59392618463500	-0.55091336414300	-0.81478135514300
C	-2.60692254171100	0.77808560492400	-0.66470314386700
C	2.12806984862500	0.54833317164700	0.46736934815700
H	-1.39662640552700	2.50936015817300	-0.16469121401700
H	-1.24640871228600	-2.02096636452200	-1.53909837015400
H	-1.65852234314700	-2.20165814132900	0.13116718453800
H	-3.50114425659200	1.36451444824000	-0.81835375202200
C	2.02851222052900	-0.82526047920000	0.28673578304000
H	3.06812819059400	0.99351993008100	0.74672380675300
H	2.88936927142900	-1.46135098064200	0.42481426097700
C	1.00150573755600	1.31713851609500	0.28052656918200
H	1.03576115945900	2.38763347945600	0.40972464066000

17

quinoline-02 4.41 eV -401.514485 [0.32] -401.514482 [0.30]

C	-0.83611945778700	0.77192053846200	-2.36866156312300
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N	-0.03785010090900	0.78407482929100	-3.45033689538600
C	-1.71682823008500	-0.34259985393900	-2.21915265047700
C	-0.81926452927800	1.80436750642700	-1.41070461484000
C	-1.74252043405900	1.75950118652400	-0.20467641893200
C	-2.59349347305100	-0.42866292009500	-1.10547280746800
C	-2.58124280776600	0.55173750563100	-0.19882702848700
C	0.87739020794700	2.86410090247200	-2.72002398109800
H	-1.15483115904500	1.81262746875600	0.71559559687600
H	-1.68391759518200	-1.11115071228100	-2.97203513820900
H	-3.24761761128400	-1.28365021069200	-1.01526297692600
H	-2.37264743390100	2.65320330178300	-0.18728765343800
C	0.78354256299800	1.79865965273800	-3.60994145138200
H	1.56827139502100	3.66977637030000	-2.90185217441200
H	1.40710093393400	1.77390750230800	-4.49158603862400
C	0.06055327355900	2.85506720432800	-1.60462348820100
H	0.10508632384500	3.66053509752900	-0.88709771285800

17

quinoline-03(Fig2c1) 4.57 eV -401.508505 [0.33] -401.508505 [0.08]

C	0.08638388156200	-0.72056545068600	-0.54051433049700
N	1.20820768815600	-1.12901933175600	-1.24124163912100
C	-1.09552690653800	-1.43845623907000	-0.42846510521600
C	0.14787405817500	0.63917304413900	-0.12769304116500
C	-0.99071302586700	1.22211154115100	0.39685471021800
C	-2.20549243323700	-0.84270885509700	0.15394924358300
C	-2.15663210486000	0.48052402267700	0.56172113179400
C	2.53472833613500	0.71745516188800	-0.64018608091500
H	-0.97187445302900	2.26307744871100	0.67954846988200
H	-1.12631609429700	-2.45705640580500	-0.77681381508600
H	-3.11384432932500	-1.41017656095300	0.27339672956600
H	-3.02917879605300	0.94473632360600	0.99084230347300
C	2.36291968714400	-0.74538401439100	-0.59632504722200
H	3.49462892267700	1.20305372806900	-0.70787631519300
H	2.55581519726400	-1.19783347401000	0.37923832232500
C	1.40105576846900	1.37815904889300	-0.36798487001100
H	1.38512065804800	2.45195913416200	-0.25857940585600

17

quinoline-S1TS(Fig2c1) 4.62 eV -401.506750782800

C	0.003431585302	-0.721839093469	-0.186512013184
N	1.229570025501	-1.200515191387	-0.532450720507
C	-1.193786922647	-1.421377551620	-0.146152323683
C	0.011700569645	0.702838219428	-0.067937038317
C	-1.195642246474	1.357692757059	0.086528801410
C	-2.382846985628	-0.729217176712	0.049400662595
C	-2.391896073419	0.649662117822	0.166408747538
C	2.470092596430	0.710717649796	-0.147777887842
H	-1.205404014619	2.436091504973	0.128360577284
H	-1.182543648013	-2.493174810434	-0.247144399755
H	-3.308850480129	-1.278706965767	0.100716211102
H	-3.321271666410	1.177682285358	0.299604919813
C	2.351864007217	-0.719459785264	0.037555371607
H	3.418225665735	1.218784141469	-0.065877203584
H	2.771226337887	-1.175096271050	0.934423928485
C	1.299401997123	1.385089433440	-0.190789574864
H	1.293053510813	2.463901310485	-0.218358058094

17

quinoline-04 4.82 eV -401.499434 [0.58] -401.499430 [0.29]

C	0.51456442817800	-1.79646013906400	1.09689217612300
N	1.26057668364100	-1.78817937218800	-0.00476463872000
C	-0.60357270875600	-2.68193327254500	1.16355027538800
C	0.77479137375600	-0.94523456325400	2.25320057807700
C	-0.10002732541500	-1.03224600035900	3.40263867837800
C	-1.38846491124200	-2.72323874519800	2.26278004466100
C	-1.13644130615200	-1.88458619212900	3.40645992621800
C	2.67464843726600	-0.08700104990900	0.97876156549200
H	0.10706883679000	-0.39539158672000	4.24809907630900
H	-0.78442548318200	-3.30448666092700	0.30458725544700
H	-2.22842478388700	-3.39813812243300	2.29607618592300
H	-1.79039074046500	-1.95359661745900	4.25962237581600
C	2.31644579454800	-1.00899658760300	-0.16658542396300
H	2.72594564445700	0.93164297053200	0.57675995794500
H	3.72025410612400	-0.28262136933500	1.24410583445400
C	1.83052376167600	-0.11406269455200	2.18751569646400

H 2.06093195647000 0.53505986238900 3.02251108982000

17

quinoline-05 4.86 eV -401.498062 [0.77] -401.498052 [0.29]

C 0.00885112124500 -0.79981942787700 0.26726368679400

N 1.21748124723200 -1.40294579087600 0.41431466634300

C -1.15707478483500 -1.55514146323200 0.51932512526600

C -0.10102629417600 0.58346482437100 -0.13734182507600

C -1.32837763607200 1.15370806387100 -0.27253407778800

C -2.41317901504400 -1.03376900151500 0.39838494385800

C -2.57058317924000 0.38055904388600 -0.01461305596600

C 2.30004330886100 0.65894413291700 -0.22339353019700

H -1.41002449151400 2.18864967117600 -0.57474623960300

H -0.99227154956500 -2.58101983868400 0.81742615628600

H -3.21324909591200 0.42258928472200 -0.90326536002100

H -3.17654458109800 0.90611573132700 0.73434991088300

C 2.28920089072800 -0.71100040012400 0.18232377648600

H 3.24098303414200 1.15365284324300 -0.39507444725100

H 3.23137731397100 -1.22490473381500 0.31082469884400

C 1.12232081448400 1.29538414121700 -0.38032832807000

H 1.07274082931300 2.32885458870200 -0.68489209317200

17

quinoline-06(Fig2c2) 5.21 eV -401.485072 [0.62] -401.485072 [0.54]

C -0.00834069645100 -0.74872865702800 0.11762050546300

N 1.19058028075200 -1.33729331967700 0.08479584104900

C -1.23665694039800 -1.42531044276000 0.20788728831500

C 0.02175244456200 0.66752580052900 -0.00617462457200

C -1.16127210337800 1.37566896786800 -0.12339584995000

C -2.40090213878600 -0.69882156143600 0.11299372573800

C -2.36539282230400 0.68988507732500 -0.06215020821500

C 2.37423289855800 0.65671698978900 0.93107986501800

H -1.15156936777200 2.44819755801100 -0.23286490217700

H -1.24127061720000 -2.49653988914900 0.31641201701400

H -3.35319818455400 -1.20081212895100 0.16072700095000

H -3.29074161465200 1.23705877305000 -0.13931715649400

C 2.21663516181100 -0.40298326526500 -0.01300992753600

H 3.32184541432800 1.15689167744600 1.03613710088300

H	3.00894239398100	-0.66176196779400	-0.70380767722100
C	1.38264184475600	1.17700506495200	0.01657125272500
H	1.60692716083300	2.07877307848700	-0.53769594960100

17

quinoline-07(Fig2c3) 5.24 eV -401.483941 [0.35] -401.483941 [0.80]

C	0.20702132126500	-0.56434019102000	0.15153858316000
N	1.35023703029300	-1.29538238433300	0.39068011521600
C	-0.96060188638200	-1.25424224850600	-0.19639664285500
C	0.12704577143100	0.87061737771100	0.24794504851100
C	-1.07284370000900	1.52764360434000	-0.05839113070200
C	-2.11567925830500	-0.57755614201300	-0.51587776488100
C	-2.17809869075400	0.81920823501600	-0.46184894010100
C	2.49041220450500	0.80096112630800	0.70289586622300
H	-1.11197896250800	2.60218155519900	0.02117049297300
H	-0.91544063241800	-2.32877479923200	-0.23479152661500
H	-2.99122893635200	-1.13584571007600	-0.80591909363400
H	-3.09456264944700	1.32951157341400	-0.70657077231300
C	2.45704603158800	-0.65407758065700	0.56372853139000
H	2.67625411680700	0.99223909332800	-0.37628646138700
H	3.37965330862000	-1.19880007468700	0.41817016595500
C	1.23090853141500	1.37426890318300	0.99689833424700
H	1.04738418059600	1.96852297784300	1.88539001404400

17

quinoline-08(Fig2c4) 5.32 eV -401.480928 [0.12] -401.480928 [0.90]

C	-0.00578138666500	-0.44707003382700	-0.04307465723100
N	1.08045497186800	-1.20328946735200	0.17521274920100
C	-1.28958136732300	-1.07630196284800	0.10859319146500
C	0.04088880468200	0.90277462339200	-0.46823653663700
C	-1.25855477578000	1.61902123997400	-0.55724907521900
C	-2.47418066661100	-0.48879910544300	-0.26146847088900
C	-2.37587143496400	0.78376191992300	-0.86449085855600
C	2.41507865465000	0.67981705426700	-0.43597673385300
H	-1.41347921954200	1.56062561955400	0.54995512777300
H	-1.27173753159800	-2.10011236999900	0.44745527751800
H	-3.38486774394200	-1.06927573605300	-0.27013719946400
H	-3.15288092272100	1.07753889087500	-1.56300042770200

C	2.25359361187600	-0.64742540476700	-0.02541967640600
H	3.40690294602000	1.07413441996000	-0.58449917513200
H	3.11865741723400	-1.26674555287000	0.15718928928500
C	1.30120207506100	1.46549759225900	-0.64226699435600
H	1.37644343159000	2.49525295003700	-0.94700601452100

17

quinoline-09(Fig2c5) 5.42 eV -401.477194 [0.47] -401.477193 [0.47]

C	0.00914584120900	-0.59258808223700	-0.03167446695300
N	1.09094402080100	-1.34237789175600	0.15824194430300
C	-1.30854161826600	-1.16968313803000	-0.07553527969900
C	0.04385563019500	0.82585931031500	-0.14457606032700
C	-1.23150945734400	1.37711420209200	-0.04151979251800
C	-2.40087410101400	-0.66127778754600	-0.89015880165900
C	-2.32627442535800	0.39937336621600	0.03513132391900
C	2.41607370624500	0.65102939914700	-0.09843721599200
H	-1.44369963858800	2.43198957720000	-0.00137039020800
H	-1.45284139715200	-2.10837403800500	0.43933397161000
H	-3.30086675670200	-1.24220392875000	-0.99755997384100
H	-3.15023265086300	0.61857221529600	0.70719407050200
C	2.25802905035800	-0.72644400946900	0.11858219993100
H	3.40651527223900	1.07249698183800	-0.13456351937700
H	3.12866412139300	-1.34823349991000	0.26277359315400
C	1.30226944463600	1.44375911803700	-0.22285275736600
H	1.38603706013800	2.51207617088000	-0.34360524755700

17

quinoline-10(Fig2c6) 5.43 eV -401.476855 [0.10] -401.476855 [0.94]

C	0.19517034772700	-1.23624251484700	-0.30585846237000
N	1.15394589148500	-1.54381127869100	0.55756752462100
C	-1.20120195189000	-1.70985095912100	-0.14358923836000
C	0.49304518569300	-0.55748777972400	-1.52901703488800
C	-0.55829720164300	-0.33016833162700	-2.47181565410500
C	-2.17109102158800	-0.99729169228900	-0.90139832299700
C	-1.88108020212900	-0.60047395686000	-2.22494860109700
C	2.76606393768200	-0.40331152243600	-0.82054717673300
H	-0.29170021723000	0.15875747018100	-3.39791572386200
H	-1.03117954371200	-2.52141777802900	-0.89838152034300

H	-3.12689467801700	-0.69739664394500	-0.48141013532700
H	-2.63818039917400	-0.28947931589600	-2.92902259499800
C	2.38486334928500	-1.13061204822000	0.30506425936000
H	3.79028109645400	-0.10006765678400	-0.95325896430800
H	3.12775211537700	-1.39548781077900	1.04344572809100
C	1.80226455830500	-0.13317710058500	-1.76409926695700
H	2.05212649752900	0.36530625034100	-2.68869790397900

17

quinoline-11(Fig2c7) 5.44 eV -401.476685 [0.33] -401.476685 [0.65]

C	0.08852985132600	-0.74562118841400	-0.18018554307400
N	1.25745728012300	-1.40471549817500	-0.28118526352300
C	-1.16251295708900	-1.36167379339400	-0.09648889711300
C	-0.01100331206900	0.66470456903500	-0.03717414261600
C	-1.35447606716400	1.17356730571600	-0.05290856335800
C	-2.30093106804600	-0.44033085313900	0.01238964841000
C	-2.42722790136400	0.64064646113400	-0.88352656650700
C	2.36020027519400	0.70040299026300	0.06990918033600
H	-1.56887026793200	2.07446442331500	0.50602036932900
H	-1.30230992017200	-2.42802405648700	-0.09364065556300
H	-3.10934305587000	-0.71185858517000	0.68415385675500
H	-3.35367846716900	1.18362638826800	-0.96442790440300
C	2.34747636918400	-0.68497089733900	-0.16696813095500
H	3.30052466834400	1.21473929838200	0.17453203693500
H	3.28397281853600	-1.21728598494500	-0.24724040354800
C	1.16560232456900	1.38353550050000	0.14602073160300
H	1.14315184003300	2.45010668518300	0.30588001023500

17

quinoline-12(Fig2c8) 5.55 eV -401.472536 [0.85] -401.472536 [0.26]

C	-0.15543543329000	-0.55063463865900	-0.16809494288300
N	1.04073655949200	-1.14628199733100	0.07777639843000
C	-1.35925861340200	-1.21494399654200	0.12194286470200
C	-0.09735136922900	0.84656432587300	-0.70485762775700
C	-1.26069844014000	1.28024533919000	-0.06706083206900
C	-2.56155616653100	-0.62358768447000	-0.29675403930300
C	-2.50995721339800	0.72023111283700	-0.54449453664400
C	2.28645672080500	0.69666466529800	-0.85435948871900

H	-1.20561819327000	1.79751569201200	0.89061540048300
H	-1.28698564766300	-2.23895942348500	0.44067004625500
H	-3.41717032830300	-1.22279880397600	-0.56936496537300
H	-3.02304811404300	1.18559265191900	-1.37350400842800
C	2.15894742390600	-0.58458147486100	-0.29099688301800
H	3.24989876097000	1.08645307721800	-1.12852678146500
H	3.04642965934700	-1.18553154146900	-0.14536524913000
C	1.13090975748000	1.42354534377700	-0.99766097711100
H	1.15268743977200	2.43959561902500	-1.35887500039300

17

quinoline-13(Fig2c9) 5.57 eV -401.471826 [0.61] -401.471826 [0.47]

C	-0.06135108546000	-0.62226272230900	-0.10921590346900
N	1.07725253404600	-1.27468088204500	0.17086627408900
C	-1.27228949263600	-1.40174633233600	-0.22039263890600
C	-0.06715264268500	0.79309837054500	-0.32810809410500
C	-1.30125194164400	1.30690853833200	-0.82350812478800
C	-2.46929858818500	-0.78364225626000	-0.31995797498300
C	-2.50142180527600	0.70061317951300	-0.38733512236100
C	2.29958331970200	0.79191199209400	0.02684496775000
H	-1.27194452483800	2.09090058994400	-1.57434310339000
H	-1.17139833887700	-2.47274874194900	-0.17091195970800
H	-3.39040268312100	-1.33803892312500	-0.22199597346400
H	-2.28933386914400	0.76822175030800	0.71457713033600
C	2.19425699498800	-0.58701115714000	0.24843602886900
H	3.25794413530800	1.27851792979900	0.08566781318600
H	3.08063750108100	-1.15521723054300	0.49089568010300
C	1.15505203185200	1.48014557607900	-0.27809691222800
H	1.17640173396800	2.54142829929200	-0.46989915757800

17

quinoline-14(Fig2c10) 5.62 eV -401.470050 [0.62] -401.470050 [0.69]

C	-0.09008166261800	-0.48722359303700	0.34071505217800
N	0.97486663605400	-1.24684092210600	0.03340429073900
C	-1.27793044606600	-1.14148873858300	0.81150045574700
C	-0.05754418931800	0.93233749697600	0.44100779908800
C	-1.31959233232800	1.53249655464000	0.67425091201900
C	-2.42587635990700	-0.49891158698000	1.27581984848800

C	-2.43064708121300	0.64092940216500	0.44213288263200
C	2.30108600694700	0.74101331593500	0.14605933428100
H	-1.38484528685200	2.08059302149400	1.61154997739200
H	-1.26676643166900	-2.22275321083700	0.77169498184000
H	-3.27109042609100	-1.04470753256700	1.66033045799000
H	-3.05502182398500	0.69390867368600	-0.44846121116900
C	2.12704830564600	-0.63832917106100	-0.08811703746700
H	3.28729263233100	1.16898187692100	0.06935736759600
H	2.97634491306600	-1.25174507622500	-0.34864503718700
C	1.21949482783500	1.52433403807500	0.44555092128900
H	1.32434919539300	2.58456580415700	0.61106194350200

17

quinoline-15 5.62 eV -401.469982 [0.36] -401.469982 [0.95]

C	-0.03051287727600	-0.87031137433000	0.46642599278500
N	1.16718377773000	-1.48182001073700	0.55719438756500
C	-1.26544621196300	-1.51077406401300	0.70867641195000
C	-0.12618560691300	0.55502798031100	0.33123493549500
C	-1.33113190349400	1.16399204586200	0.79834779267200
C	-2.41288207097300	-0.68654475005500	0.46539513506200
C	-2.45867830653100	0.48430429589900	1.25668204730400
C	2.22115548747000	0.59956299620600	-0.06401522241800
H	-1.39013615789800	2.24569002448100	0.75611425494200
H	-1.28099624939600	-2.03510166915500	1.66062074021200
H	-3.02365763246400	-0.77627918818900	-0.43278351666800
H	-3.33032515851900	1.01146621529800	1.60724227918300
C	2.22763567470800	-0.76672045979000	0.27540087255000
H	3.14313382727700	1.09862470779300	-0.30710507163300
H	3.17227633687800	-1.29142952586700	0.31505241918500
C	1.02988603344800	1.27499434131100	0.00867232939700
H	0.98822655874300	2.34463597413900	-0.13243378980300

17

quinoline-16 5.63 eV -401.469728 [0.88] -401.469728 [0.18]

C	-0.12425162800200	-0.78021823602700	-0.05867890848400
N	0.99336155853100	-1.47367627886100	0.22165280182600
C	-1.24247439110600	-1.40359553380200	-0.70443667450400
C	-0.21271878597000	0.63887803823400	0.03687846059400

C	-1.41459037073800	1.35178391047700	-0.32700186764800
C	-2.51370605201700	-0.80847809943600	-0.54215188701000
C	-2.55329783885100	0.67240833028400	-0.59025735950000
C	2.06450823581000	0.58251129907700	0.78774460627800
H	-1.37880167412400	2.42978331981900	-0.36885075561600
H	-1.04561021458900	-2.26521020199800	-1.33173134520900
H	-2.47152342129900	-0.77399539826200	0.58402854617800
H	-3.49314600583900	1.18922560661300	-0.71317068612500
C	2.04041851956600	-0.81437248207200	0.64505413688900
H	2.96291162727600	1.07037600446900	1.12731162668800
H	2.92112034548500	-1.39558787563100	0.87390702099400
C	0.94476348175000	1.30550762259900	0.47184176044700
H	0.94076506888900	2.38056880759100	0.55499986595900

17

quinoline-17 5.64 eV -401.469254 [0.31] -401.469254 [0.69]

C	0.07106981898200	-0.58004872560400	0.06404003499000
N	1.35486576856600	-1.10092690215800	0.14792088801700
C	-1.06834090120000	-1.35643871742700	0.21598834824900
C	-0.04156009956800	0.81451734556200	-0.14201189736100
C	-1.30634060615300	1.40761225911600	-0.24053202057900
C	-2.30953440161900	-0.75250447383200	0.10786950360500
C	-2.43079157587300	0.62057313041800	-0.12544368142600
C	2.32222192501500	0.49513221199200	-0.07836544457200
H	-1.39228335435300	2.47216061012400	-0.38913213389400
H	-0.97335768603800	-2.41346130033900	0.39700243036000
H	-3.19923310174900	-1.35281444368600	0.20826390841500
H	-3.40988289802400	1.06452850011800	-0.19700267382300
C	2.28950812501700	-0.73601934202000	-0.81384746163600
H	3.19151258324500	0.74284543301200	0.52147597543700
H	3.16445474506900	-1.35384282782900	-0.93658165755900
C	1.23290387707800	1.41729991979900	-0.09807005583300
H	1.39166533114100	2.46906602339700	0.06729751480400

17

quinoline-18 5.69 eV -401.467606 [0.66] -401.467606 [0.22]

C	-0.16951015939500	-0.82138989546300	-0.35415864441800
N	0.74165816536000	-1.78813014084300	-0.19981649665100

C	-1.21918855965300	-0.80267038714700	-1.30960511675700
C	-0.24709072202200	0.34437658357100	0.43456267763500
C	-1.44184012124900	1.11177362287700	0.02759907717900
C	-1.97988248777800	0.38778732479300	-1.16489353645200
C	-2.71508824552300	0.35206136773200	0.27339510236400
C	1.64919058337400	-0.46179867941500	1.58443819489000
H	-1.44564871945300	2.19162798890900	0.07610225713700
H	-1.40643366795100	-1.58930296989300	-2.01879011076100
H	-2.53815705201000	0.84102985347600	-1.96441606428500
H	-3.64026575919900	0.91913222698100	0.21885019650000
C	1.62992047035600	-1.58694139282200	0.75076496235200
H	2.41345225807800	-0.37683154796400	2.33855972731400
H	2.37965042564900	-2.35355759654000	0.87588484658600
C	0.68664610033500	0.52189073364100	1.43723248886600
H	0.67247935545700	1.38843267160200	2.07816990524000

17

quinoline-19 5.69 eV -401.467577 [0.87] -401.467577 [0.31]

C	0.05676815273300	-0.47642646556200	-0.26626297057300
N	1.23381592685200	-1.07309935266800	-0.17281076932800
C	-1.15727640446500	-1.18747050264900	-0.44085991773100
C	-0.01529180396700	0.91342679876600	0.17014605192100
C	-1.18703834745100	1.36103073974300	0.76908339444700
C	-2.32479713447800	-0.64072992839400	0.00854863013100
C	-2.33979043057000	0.61280113117900	0.65143343598600
C	2.18628994644500	0.83972250540200	1.06036337986200
H	-1.21215823089700	2.33713959163300	1.22406188176200
H	-1.11861079255900	-2.16394748296400	-0.89291481146000
H	-3.24843408819700	-1.18478526307900	-0.10385465580900
H	-3.27174426041800	1.01369678893000	1.01359941821600
C	2.24614639930200	-0.41170526610400	0.49786407144200
H	3.00291309755900	1.26748572801000	1.60992332731200
H	3.16183315007800	-0.98445961454100	0.57732997525900
C	1.30289086046500	1.46090483071700	0.09864277965700
H	1.68497357430000	1.67556179383000	-0.90108555310200

17

quinoline-20 5.78 eV -401.464122 [0.12] -401.464122 [0.17]

C	0.09152785541900	-0.79756209102100	-0.55238557808600
N	1.20168877279000	-1.37830516955700	-0.81040783029400
C	-1.03753426983500	-1.07461033346900	0.26190188390300
C	-0.13820051449300	0.53725888756400	-0.00339647924700
C	-1.28490418046300	1.35366251090100	-0.31921223027400
C	-2.38293586617700	-0.65091512046600	-0.14471755499700
C	-2.49257693594600	0.68101534880300	-0.44939604106100
C	2.28372063001700	0.54156286163900	0.12057259107400
H	-1.16491428799100	2.41584124088600	-0.44395860180900
H	-0.90186107816400	-1.72532272758000	1.11590364482400
H	-3.18260086937100	-1.36842942209400	-0.21961272634400
H	-3.39882172405800	1.14607104098300	-0.79648631419800
C	2.31952415277500	-0.62376213737700	-0.66435714884800
H	3.21815442015900	0.99804517074800	0.40867469511200
H	3.24270054793000	-1.03286865253700	-1.03435322443800
C	1.10240857968400	1.07749610117600	0.55516964256200
H	1.07283188685300	1.93105405712100	1.21161817247700

17

quinoline-21 5.79 eV -401.463917 [0.56] -401.463917 [0.61]

C	0.22726707603200	-0.63410630184100	-0.21159834502600
N	1.02856643083700	-1.19572771532100	-1.14156239174100
C	-0.88711582159800	-1.41496767918600	0.35253767106800
C	0.06847059894600	0.87470801342500	-0.13134910831200
C	-1.24433996011100	1.39988220623200	-0.04942245281800
C	-2.07732356479000	-0.83004674318100	0.53278387838800
C	-2.27695697899400	0.58639385489200	0.27650033418600
C	2.31599976252400	0.64111499259700	0.05538824988200
H	-1.39325718027800	2.46227453655800	-0.16251158230700
H	-0.73813535538500	-2.47326430313900	0.48054780370000
H	-2.92475703609200	-1.41318915810000	0.85553465703400
H	-3.26794368338500	0.99334139578800	0.39247678634300
C	1.95923431968300	-0.72994959841900	-0.17740613302000
H	3.31426835558800	0.89900773829500	0.36656825712100
H	2.59376803896600	-1.50389360931200	0.23273227501900
C	1.27871936165700	1.54319195369400	-0.06437290255200
H	1.38049067471500	2.61414523651500	-0.04167274971300

17

quinoline-22 5.82 eV -401.462704 [0.62] -401.462704 [0.29]

C	0.09182685943200	-0.87032376874400	0.31000016772200
N	1.22258814130500	-1.54699452924400	0.13426370272100
C	-1.19934857425400	-1.43802715014700	0.21634765100800
C	0.19436971065100	0.61641465112500	0.47325575721100
C	-0.92217825016500	1.40377393856200	-0.04318230017900
C	-2.25770454442600	-0.63320540644800	-0.06212748164500
C	-2.10059302543600	0.79338233271100	-0.25098155990700
C	1.99550765439200	0.68102421831100	0.35946897855400
H	-0.81185945056300	2.47177547885700	-0.13310847714500
H	-1.29542420719800	-2.50982320729100	0.25842888783000
H	-3.23593146138300	-1.06329710101600	-0.20098999759400
H	-2.96333477979900	1.36835913013000	-0.54575229293100
C	2.21910513764300	-0.68605065415900	0.01876303902900
H	2.59926694804500	1.44710194785300	-0.10511100580600
H	3.15609830532500	-1.01979909365000	-0.39818565518800
C	1.10404790780300	1.06136646988800	1.46075677773400
H	1.07366309820600	2.06956485377700	1.83817648476800

17

quinoline-23 5.87 eV -401.460972 [0.62] -401.460972 [0.39]

C	0.12493420878300	-0.61005300440500	-0.96576885706600
N	1.32943122479500	-1.00627060215600	-1.42815652512900
C	-0.79706964538700	-1.20286014625300	-0.17020799192100
C	-0.00656553907400	0.94268331666800	-0.87777634069900
C	-1.34088479842600	1.48740630038900	-1.08066263132200
C	-1.99772408067300	-0.48115974186100	0.14252473610700
C	-2.29286331009300	0.79159870199700	-0.38911946869300
C	2.02359826217100	0.31484110381800	0.32423353908100
H	-1.57839447572500	2.21869838396800	-1.83551387179500
H	-0.75692722104800	-2.26491012896400	0.01529576017900
H	-2.78407828951600	-1.01780815352400	0.64752596821100
H	-3.31845405639600	1.13056746837200	-0.37454472495400
C	2.20539257481700	-0.83300565809400	-0.43570156250900
H	2.82967814966400	0.65050016782900	0.95602793168300
H	3.15921889750300	-1.34093613665100	-0.45754245251100

C	0.92866645335300	1.27396957909700	0.00879444150700
H	0.93833906865400	2.23679842395000	0.49580306383200

17

quinoline-24 5.90 eV -401.459648 [0.98] -401.459625 [0.13]

C	0.03844678686800	-1.11303301420300	0.34262282452700
N	1.21894803803400	-1.15029011810100	0.65972984854000
C	-1.21756964852500	-1.55414693888000	0.21515575064000
C	-0.10995914653300	0.98955904751700	-0.42329319744300
C	-1.37215949390800	1.43356271660800	-0.20830078054000
C	-2.41146947483300	-0.76507966814900	0.18370104282600
C	-2.48216297810700	0.58455646351900	0.03363613802200
C	2.29148173584400	0.51573738060000	-0.68383547510000
H	-1.53391143120800	2.50493052148500	-0.19192967246000
H	-1.30765360708800	-2.62689839494500	0.12437338629300
H	-3.33319459750500	-1.31380560457100	0.29328918596300
H	-3.45135641024300	1.05252028102000	0.09706019055900
C	2.33273395642300	-0.62480352269900	0.03853464770700
H	3.21864479929700	0.87514757555700	-1.09900961697700
H	3.25405420916100	-1.13828002825100	0.24683877223200
C	1.11315388739400	1.27992132818000	-0.92772551871700
H	1.18973885996700	2.11888746489300	-1.60870074428400

17

quinoline-25 5.98 eV -401.456822 [0.65] -401.456822 [0.44]

C	-0.27293268305800	-0.56813444405800	-0.37209465642500
N	0.63487349484500	-1.35774485480300	0.34306007706900
C	-1.01341626420600	-1.10529521957200	-1.45308376816900
C	-0.14796111825200	0.92420040675600	-0.29369128092000
C	-1.37429170727000	1.57798086820300	-0.27199519420200
C	-2.02141797827900	-0.69635252414300	-0.46414189030600
C	-2.40870908155800	0.66995300956400	-0.23850882139000
C	2.12864834194300	0.55618680585000	0.27660003254000
H	-1.48891493269200	2.64664577825900	-0.21853936080300
H	-0.89836894718400	-2.14969294721100	-1.69183238045900
H	-2.61384628616000	-1.48511434921700	-0.02271052512900
H	-3.42833937888800	0.92761652470000	-0.00555777566100
C	1.76753704603500	-0.81522834612400	0.59243726766400

H	3.13719671251600	0.88254421603200	0.46449162199100
H	2.50094397145800	-1.42742953729100	1.10064270922700
C	1.16271843696800	1.42203381497500	-0.12409160624300
H	1.36425225964400	2.47620811079700	-0.23458912411100

17

quinoline-26 6.04 eV -401.454455 [0.56] -401.454455 [0.42]

C	-0.01205665537100	-0.83537770503800	-0.39306870885600
N	1.22944093306800	-1.37703822525400	-0.46153894189700
C	-1.17725607285100	-1.54476975605500	-0.18313680616600
C	-0.20225048441700	0.66111033917900	-0.40710289933100
C	-1.15077564431200	1.19700725206700	-1.29679112978100
C	-2.23184483231200	-0.68544042934300	0.08627554388600
C	-1.98172388332000	0.68971667234700	-0.18079756802900
C	2.09566050885200	0.77433323511400	0.27278188245600
H	-1.14886966197700	2.25509280553100	-1.50940874441000
H	-1.21473712167100	-2.61805831614900	-0.14245407486900
H	-3.15297686605400	-0.99915880404200	0.54830663094900
H	-2.52810470397800	1.43662425868700	0.37736758998000
C	2.22351860617800	-0.60690810796300	-0.16303401669000
H	2.97698694979800	1.28470875051500	0.62481483626800
H	3.21125978637800	-1.04249854570000	-0.20819473942200
C	0.91041118892000	1.39586562092200	0.19775027723500
H	0.7855777226200	2.43275779953700	0.46424534914200

17

quinoline-27 6.12 eV -401.451753 [0.14] -401.451615 [0.62]

C	0.12081640132200	-0.93228667677000	-0.32233917349600
N	1.16883439866000	-1.35725793725300	0.18912852275900
C	-1.03842463279700	-1.18603739671500	-0.96410132166600
C	0.03410319296700	1.08279869374000	0.06519987792400
C	-1.21695005176100	1.36590880011000	0.40777597757600
C	-2.29929064836800	-0.56866448234100	-0.62818487507400
C	-2.39138525271100	0.59385320503000	0.03242175962100
C	2.45088273851300	0.70444213840300	0.22045946605900
H	-1.36764141632900	2.23115185469900	1.04081176746900
H	-0.97021289643300	-1.79660282452300	-1.85329334570100
H	-3.19412607343200	-1.07609689408100	-0.95332683153600

H	-3.35532904059800	0.99836777422000	0.29160872781100
C	2.35802469901100	-0.63037508326100	0.33136689454700
H	3.42379575408900	1.16349198150000	0.29882420213100
H	3.21377027222100	-1.24313661744000	0.55118507241800
C	1.31641170900400	1.53777499009700	-0.04857934164800
H	1.47816515566700	2.49761658839200	-0.51949947394100

17

quinoline-28 6.31 eV -401.444826 [0.61] -401.444826 [0.32]

C	-0.63327278611300	-0.23240293697500	0.44837014305300
N	-0.07465219135400	-0.28926976466800	1.72185296733500
C	-0.65352717196100	-1.51436848820900	-0.38574962655600
C	-0.31801775810700	0.85126085058800	-0.48784586721900
C	-1.41167031356600	1.07296472779700	-1.35019329573400
C	-1.94976129618100	-0.76252056091300	-0.04055758921800
C	-2.40505144435200	0.18609535307800	-1.05201456792200
C	1.53131138593700	1.32923130635600	0.90338282928600
H	-1.44083771777800	1.81551980275000	-2.12797600762900
H	-0.36400762163400	-2.37659422107200	0.20281442461600
H	-2.63248391437200	-1.28603193110400	0.61015425200100
H	-3.36047436371600	0.12602705986900	-1.54335457208300
C	0.97044581991500	0.43627099953400	1.89560622511000
H	2.44261686148100	1.85104543654700	1.14445816422500
H	1.45727531242400	0.37551107052900	2.85889600019300
C	0.89443889327300	1.54864082255000	-0.27525914080300
H	1.26208490276800	2.26713479216400	-0.99022199490900

17

quinoline-29 6.71 eV -401.429827 [0.25] -401.429827 [0.62]

C	-0.00713217303000	-0.44503277362100	-1.20991258193300
N	0.78416274268600	-1.32857507180400	-0.48252505526200
C	-0.79929744294900	-1.36547271108400	-0.41976786559800
C	0.01493429918100	0.92485141978000	-0.81846053684200
C	-1.25459382612600	1.47994399052500	-0.37993744729700
C	-1.72505866572600	-0.73272329585600	0.53909487239700
C	-2.02266989788900	0.60863753098200	0.39947353871800
C	2.16580298101700	0.47828098269900	0.15769894527500
H	-1.48592705219800	2.53050282327700	-0.43380368362700

H	-1.09965668179200	-2.32277049535500	-0.81564258854500
H	-2.29352714907100	-1.34510754906400	1.21959099974100
H	-2.85146770049500	1.01553720889800	0.95859900484900
C	1.81726991294600	-0.82948390574300	0.26620621990900
H	3.06387220142500	0.83549344423000	0.63289680540500
H	2.37392183363900	-1.53650378786900	0.85883119069900
C	1.19159939451200	1.42162081196200	-0.33445229141000
H	1.28255549264300	2.45533812906000	-0.03950430965200

17

quinoline-30 6.88 eV -401.423644 [0.74] -401.423644 [0.81]

C	0.29511024007300	-0.34590799531300	0.35163528409300
N	1.55082028319000	-0.77497844700200	0.68866774806700
C	-0.82435754512900	-1.00166612095800	0.87181003026400
C	0.13536302720000	0.74795655199200	-0.51379062141000
C	-1.15709246910400	1.14166724513700	-0.84463287358300
C	-2.09450422608100	-0.58513518308800	0.53057080641800
C	-2.26474735011500	0.48987197243500	-0.33379636254500
C	2.53448294492400	1.13047632007400	-0.74265341745600
H	-1.28672962475600	1.97893076805200	-1.51220506315200
H	-0.67134801267900	-1.83080952166700	1.54244409147900
H	-2.95119442747700	-1.09746787867300	0.93706827332200
H	-3.25525680092200	0.81844111411100	-0.60201139701300
C	2.21227947263100	-1.52094330067100	1.36928090341100
H	3.50586212988900	1.49374060783000	-1.02475421429000
H	2.69636233331500	-2.48182485042700	1.30754180876900
C	1.30218005656800	1.44833900241000	-1.04534088694900
H	1.08419247755100	2.27623031773900	-1.71849768125700

17

quinoline-31 6.95 eV -401.421208 [0.96] -401.421200 [0.96]

C	0.30920947126300	-0.54365491177600	0.33812655369500
N	1.51061044055500	-1.17081746100100	0.57365956269000
C	-0.88618366145300	-1.12807292241700	0.76952585197600
C	0.29131537593900	0.68228959093800	-0.34471304867800
C	-0.94157531469300	1.28467774620500	-0.58387193884500
C	-2.09151116592300	-0.50768449916300	0.52162412013100
C	-2.12077965158900	0.70500908893000	-0.15978885835200

C	1.68091165891600	2.36070962111200	-1.52758255439400
H	-0.95543744512000	2.22812295023900	-1.10393354681200
H	-0.84032864429600	-2.06586682799600	1.29791426372200
H	-3.00792595216500	-0.96346993497600	0.85991999116200
H	-3.06070453358300	1.19645125352400	-0.34979956530800
C	2.03526019216300	-2.09656766620200	1.16121734374500
H	2.48637292715300	2.91836175585300	-1.96591483717800
H	2.40338240006600	-3.09372957384400	0.99819343103300
C	1.55051601451900	1.29416681870700	-0.78509057701200
H	2.44829039734600	0.78699557385100	-0.43814976343100

17

quinoline-32 8.50 eV -401.364124 [1.18] -401.364124 [0.56]

C	-0.21194448159100	-0.48555347163000	-0.32490236403500
N	0.65768504006400	-1.50004731021400	-0.30081290396200
C	-1.30064787647300	-0.65395655394200	-1.25349876175600
C	-0.14489453414700	0.60189027327800	0.58778588880300
C	-0.92100388962000	1.77860669667300	0.43501693429000
C	-2.56575259024000	-0.11886871334100	-1.19492775528400
C	-3.12671301139300	0.87560331853100	-0.39768847222400
C	1.63626463062300	-0.58420591184100	1.68015144134900
H	-1.08137383921600	2.07049796735400	-0.59984217580100
H	-1.09963080122300	-1.36826369623500	-2.03508693263800
H	-3.23062258510800	-0.46259399249200	-1.98173131670900
H	-2.99951805045900	0.96044774896900	0.67900670090100
C	1.55925033113300	-1.53288429338000	0.65900249364200
H	2.37676564175000	-0.68399322356400	2.45555151846500
H	2.25770144567300	-2.35549897593900	0.62814268840200
C	0.76605053617000	0.47919272602900	1.65171824115900
H	0.79827589842700	1.25711717524500	2.39599424216400

isoquinoline

17

isoquinoline-S0MIN(DFT) FC 4.56 eV S0: -401.6750102147 [0.03] S1: -401.5074666375 [1.02]

C	1.256785831249	1.322585272156	0.000000000000
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N	2.397419986827	0.695911931650	0.000000000000
C	2.369659436847	-0.656429016222	0.000000000000
C	1.222314015396	-1.392261846584	0.000000000000
C	-1.270704140421	-1.396108755513	0.000000000000
C	-2.432714941248	-0.680087764174	0.000000000000
C	-2.411787803666	0.731311664353	0.000000000000
C	-1.222225794870	1.399381548367	0.000000000000
C	-0.024466631287	-0.729681793866	0.000000000000
C	-0.005788728013	0.683252825380	0.000000000000
H	1.293654792447	2.403952770416	0.000000000000
H	3.333556162806	-1.140312173662	0.000000000000
H	1.262041069531	-2.469489858381	0.000000000000
H	-1.289189701522	-2.474368340816	0.000000000000
H	-3.380712581010	-1.193274029671	0.000000000000
H	-3.341591151052	1.275989484636	0.000000000000
H	-1.195889043176	2.477814603007	0.000000000000

17

isoquinoline-S1FCMIN 4.37 eV -401.514365140200 q2isqn_s1fcminfreq

C	1.258917170709	1.335419565055	-0.000000000000
N	2.425376442239	0.704567571419	-0.000000000000
C	2.387847264273	-0.651706596728	0.000000000000
C	1.212777361208	-1.401177537359	-0.000000000000
C	-1.265648906477	-1.412442330209	-0.000000000000
C	-2.471046968648	-0.683727638305	0.000000000000
C	-2.438096284470	0.732481753280	-0.000000000000
C	-1.208998138086	1.407998003875	0.000000000000
C	-0.027414194167	-0.762184543726	0.000000000000
C	0.002080849313	0.707512120432	0.000000000000
H	1.300506889011	2.415452394728	-0.000000000000
H	3.345099662402	-1.146351604076	-0.000000000000
H	1.267528305987	-2.478014819349	0.000000000000
H	-1.292044132528	-2.490259592940	-0.000000000000
H	-3.413751545927	-1.202049113966	0.000000000000
H	-3.357547877154	1.291609185583	-0.000000000000
H	-1.191377442310	2.486221480314	0.000000000000

17

isoquinoline-S1TS-b 4.46 eV -401.510950566900			
C	1.243823901375	1.356496628075	0.042663828084
N	2.390903217048	0.657976533640	-0.087540359792
C	2.396929279975	-0.669559253587	0.001997365653
C	1.218736072381	-1.413257975396	-0.052748723648
C	-1.258963926115	-1.395951024739	0.008284876201
C	-2.452162243535	-0.677361854534	0.014021574707
C	-2.431701789604	0.729703293208	0.001761000301
C	-1.224589118847	1.411257387751	-0.020677273467
C	-0.030631572404	-0.745591201482	-0.024006679224
C	-0.010205366727	0.713719841831	0.012618980495
H	1.314428494721	2.430926570494	0.015108858012
H	3.355712030320	-1.150543306776	0.111082057236
H	1.264062375557	-2.489036452844	-0.039894539649
H	-1.280500904992	-2.474134442830	0.003463959533
H	-3.393549011951	-1.200203117818	0.015019746157
H	-3.357615815986	1.279513790948	0.024171352770
H	-1.210467165841	2.489392882096	-0.025326023374

17

isoquinoline-S1MIN-b 4.29 eV -401.517531252000			
C	1.195995335054	1.184058089014	0.877054232599
N	2.288662150934	0.583690356248	0.343968431614
C	2.420025574430	-0.518378417731	-0.333564073768
C	1.269442236438	-1.151110503984	-0.723791675486
C	-1.219283708011	-1.122839245810	-0.791215385059
C	-2.431786858541	-0.530137008614	-0.473917674839
C	-2.458915066145	0.646414710209	0.259648398756
C	-1.276141363871	1.230768991913	0.678051621699
C	-0.015323613995	-0.562892337893	-0.383314619109
C	-0.053626520673	0.630731348689	0.383562260445
H	1.287424502906	2.166467716905	1.298804088582
H	3.410467904489	-0.878202883015	-0.558584710185
H	1.331496319994	-2.064498214804	-1.287463848069
H	-1.201998934370	-2.031603048105	-1.372209331385
H	-3.352226986396	-0.984221977159	-0.802942212644
H	-3.399720347974	1.111065250173	0.506375102605

H -1.293024338675 2.145265049149 1.249075218188

17

isoquinoline-01 4.24 eV -401.519218 [0.39] -401.519213 [0.08]

C	1.28756573896300	1.38586567266200	0.46085589006500
N	2.46958704626700	0.80379693182900	0.60289605662900
C	2.64755908784400	-0.46634665091400	0.40797584965000
C	1.50823659387700	-1.36688289209000	0.01219190964700
C	-0.96792467664700	-1.37204586689200	-0.54474073389600
C	-2.17245941162400	-0.70368207005800	-0.68764572318100
C	-2.25206790509200	0.66683361258200	-0.44966792980100
C	-1.12510449569800	1.36075377627000	-0.07124996149400
C	0.17637255018800	-0.68767874236100	-0.16256748330100
C	0.09783535291500	0.69203844568000	0.07507614571000
H	1.23675299755000	2.44876596598800	0.64821757493400
H	1.80064642557500	-1.89198484062900	-0.90019552310000
H	1.44339185499500	-2.15753801609000	0.76432797778500
H	-0.91679737204600	-2.43356252584200	-0.73138050697000
H	-3.05421977292400	-1.24787935923000	-0.98467884452400
H	-3.19283149168600	1.17986299571800	-0.56249892759500
H	-1.17179958976600	2.42220318832800	0.11507401970100

17

isoquinoline-02(Fig2d1) 4.41 eV -401.512921 [0.85] -401.512921 [0.25]

C	1.26975189795300	1.41321276474000	-0.44942926186400
N	2.18971943617800	0.69850362663700	-1.15620351269500
C	2.39638259040500	-0.47439827517300	-0.60399400912700
C	1.34768256597500	-1.07114256729200	0.11398472434200
C	-1.15056558935300	-1.19206498080100	0.32157563287400
C	-2.38883534799400	-0.60339383273100	0.09306272244400
C	-2.47604985438400	0.68015965954100	-0.41626025900000
C	-1.31695087316300	1.41081451369900	-0.67925452810000
C	0.01540243162500	-0.49458525174200	0.02886990816700
C	-0.08966411650100	0.83710927183400	-0.45238412710300
H	1.60585885247600	1.74832454592400	0.53155702358400
H	3.26663044652600	-1.05200296623100	-0.88434821669800
H	1.45313566476500	-2.08850707938100	0.45383844318300
H	-1.09244654830000	-2.18911257659500	0.72952616472500

H	-3.28842022089600	-1.15411951097100	0.31501757519300
H	-3.44084640996200	1.12536057255300	-0.59564867694200
H	-1.37595398212300	2.42185444809100	-1.04691991159300

17

isoquinoline-S1TS(Fig2d1) 4.58 eV -401.506781935100

C	1.214247583030	1.061777248009	0.944386671692
N	2.276731240356	0.714873139239	0.198471170306
C	2.419930043222	-0.499488869121	-0.345993013300
C	1.274447501089	-1.188387685394	-0.615330040736
C	-1.212664239892	-1.136048764696	-0.768463861974
C	-2.429437254481	-0.521256540178	-0.483233702445
C	-2.466982856865	0.661740973217	0.230700346187
C	-1.279703699553	1.245306199667	0.663125367175
C	-0.013733650905	-0.571029014213	-0.356489199449
C	-0.060500537123	0.649995455174	0.376706058858
H	1.327508823432	1.240119733883	2.006040361032
H	3.387408247439	-0.794647313514	-0.717928127726
H	1.324406217405	-2.090541353433	-1.200849679662
H	-1.198955589277	-2.074208703939	-1.300568379984
H	-3.346256893206	-0.978091932563	-0.819051224760
H	-3.409667727490	1.135119279369	0.450534325472
H	-1.296989056355	2.167194079519	1.221539261854

17

isoquinoline-03 4.77 eV -401.499820 [0.41] -401.499811 [0.05]

C	1.30730318074700	1.23475349088300	0.08579747295800
N	2.49898376953700	0.68103580518900	-0.08200946930500
C	2.53221591510000	-0.64809813752700	-0.28297419224600
C	1.43501210081200	-1.45940247851300	-0.32389824371400
C	-1.05128272038900	-1.48873210045700	-0.14775517611500
C	-2.41154890863800	-0.99383337238400	0.02280179304000
C	-2.33267641024200	0.50471654248600	0.24558970354300
C	-1.18211440329900	1.18147347390100	0.26225729680600
C	0.14371437371000	-0.88161963468500	-0.14469510933700
C	0.10434870006000	0.55257931157000	0.07121537304900
H	1.29845235186800	2.30440798816000	0.24789701939300
H	3.51618049978600	-1.07125491688400	-0.41654660129500

H	1.53104057496200	-2.51827675825900	-0.48828877504900
H	-2.91868933048500	-1.47494342767600	0.86578909546500
H	-3.03734929855800	-1.21008004265700	-0.84970217741200
H	-3.27248677819400	1.01297736764200	0.39717027510600
H	-1.19461312180200	2.24877512979300	0.42280640063700

17

isoquinoline-04(Fig2d2) 5.06 eV -401.489109 [0.71] -401.489108 [0.36]

C	1.38717414374300	1.23031329559400	1.10162555406500
N	2.44676232312600	0.52567439744900	1.37024437143800
C	2.33545941844400	-0.61470507416700	0.67877241346500
C	1.31442060514700	-1.53250406387600	1.09544095139600
C	-1.16528730112800	-1.45387668760100	0.71856310404000
C	-2.26513197470700	-0.71707908360200	0.38884178530300
C	-2.16432849381200	0.66605929632000	0.12817448089800
C	-0.95688321173900	1.29804274960800	0.25202130261400
C	0.12331516237200	-0.85674118085600	0.76558428926200
C	0.20475716747000	0.57699985178100	0.58132094894600
H	1.33887310941600	2.25721965527600	1.43673820324500
H	2.58766283914600	-0.53987739145000	-0.38238166982700
H	1.38403603740600	-2.37256750961900	1.76200401412100
H	-1.24894237942600	-2.51246554424500	0.90412330223600
H	-3.22715079552100	-1.19873249602800	0.31584208331000
H	-3.04514917432800	1.22439789503400	-0.14229432879100
H	-0.88776108926200	2.36559028793900	0.10977809594800

17

isoquinoline-05(Fig2d3) 5.08 eV -401.488278 [0.06] -401.488278 [0.90]

C	1.44926232013200	1.01692288397300	0.59391841698100
N	2.52502872704800	0.37972136828800	0.26691217054800
C	2.23601724704200	-0.60741085398400	-0.58787138102800
C	1.31760804173400	-1.62595618667900	-0.24099444959700
C	-1.20876668339300	-1.46558944185200	-0.06163726107800
C	-2.34148241317000	-0.70801350100000	0.14069912446000
C	-2.26128535782500	0.66959679677700	0.36886412707200
C	-1.02726681962100	1.27262458654000	0.43365463883900
C	0.05747485815700	-0.86609739950400	-0.08557493771800
C	0.13336179867100	0.52269634232000	0.21759268945200

H	1.54060535275900	1.87859219133900	1.24011250627100
H	2.50620782002200	-0.39781667496000	-1.62266594057400
H	1.53421632850900	-2.17900386181600	0.67052100641300
H	-1.28051521001500	-2.52337696666900	-0.25171896251100
H	-3.30872893254300	-1.18402202514200	0.10786500156000
H	-3.15924507755800	1.24767304630900	0.51062039554800
H	-0.94659104261200	2.32447467249200	0.66243698800800

17

isoquinoline-06(Fig2d4) 5.18 eV -401.484701 [0.37] -401.484701 [0.50]

C	1.24210526201700	1.11601230159800	0.17995789853200
N	2.36128857136600	0.48976521150600	-0.40498455689900
C	2.21122141439300	-0.35435327328500	0.63175637422200
C	1.11089169240100	-1.33900401011600	0.72606596330500
C	-1.40053297279800	-1.48025365012900	0.45673932707000
C	-2.54555999387000	-0.73115142321800	0.36312213752900
C	-2.47954365547300	0.67092087731700	0.26942328008600
C	-1.26625446309400	1.32635637467400	0.23741070557000
C	-0.15110289815300	-0.82842789828000	0.45563532114900
C	-0.08823590167500	0.58262411596700	0.27489776462000
H	1.39140185576400	2.16670134114100	0.39229129401600
H	3.05802079776200	-0.49334980887700	1.30277096719100
H	1.33357165375600	-2.36486789438000	0.96548614720300
H	-1.44806463185500	-2.55162679647700	0.56720895176900
H	-3.50851751173300	-1.21446334074100	0.37963516059000
H	-3.39329116490500	1.23894421723000	0.20609844685200
H	-1.22722464812300	2.39964400843000	0.14012712561300

17

isoquinoline-07(Fig2d5) 5.29 eV -401.480773 [0.55] -401.480773 [0.48]

C	1.13275742619600	1.19611231114200	-0.33172439678900
N	2.28424309586100	0.61292921088800	-0.07642451083800
C	2.28551138290700	-0.72218686999300	-0.02798804474200
C	1.17419794274800	-1.52115008790100	-0.22896705818200
C	-1.32718081254300	-1.61014719785400	-0.78664423194500
C	-2.49335766347700	-0.82654069634100	-0.52900721205600
C	-2.50985754318100	0.53636676978400	-0.89069655562800
C	-1.29158511274100	1.17081297599200	-0.82299205431600

C	-0.05418639733400	-0.91961615018600	-0.45751855169800
C	-0.06322863300100	0.49931733210600	-0.53056026236600
H	1.14632494287900	2.27481614387500	-0.41657169674800
H	3.23885299326800	-1.17716369352100	0.19552378588600
H	1.24333104802600	-2.59347261394800	-0.17719097817500
H	-1.23430252053700	-1.36851230826200	-1.87315088460300
H	-3.36218602699000	-1.22740864770400	-0.01576302123500
H	-3.41651736806700	1.11678422739100	-0.97201809244500
H	-1.26095625690500	2.24756206740600	-0.90887180819300

17

isoquinoline-08(Fig2d6) 5.42 eV -401.475718 [0.39] -401.475718 [0.50]

C	1.32518073323600	1.34121642150100	-0.24260885269800
N	2.43585828159300	0.65237464242100	-0.13246377280300
C	2.33693940351100	-0.67286062025000	0.06379423842500
C	1.14522391928400	-1.36568388134100	0.12854818626300
C	-1.37523082288800	-1.17864572512200	-0.05568201333600
C	-2.45231130905000	-0.63174435256300	-0.87537414297000
C	-2.33843270168600	0.44785122639700	0.02161792203600
C	-1.19928939009800	1.36984008438300	-0.06524070797000
C	-0.03944415432600	-0.65581220971200	-0.04038131985300
C	0.04839758724600	0.75537685885300	-0.16938978084900
H	1.42375697840000	2.40989145714700	-0.37177637864600
H	3.27336337376000	-1.19967714296000	0.16092545155200
H	1.14427827414700	-2.43465002654800	0.26614557102600
H	-1.57936334999800	-2.09304631628800	0.48376478850800
H	-3.37623830781600	-1.17737025765700	-0.96380007902000
H	-3.15474999616700	0.71786130011400	0.68436313385200
H	-1.35503066813200	2.43393867769500	-0.01658390635800

17

isoquinoline-09(Fig2d7) 5.45 eV -401.474573 [0.49] -401.474573 [0.51]

C	1.18346397061400	1.28566405178200	-0.06253343404700
N	2.35856265507500	0.70052390233100	-0.17035583226700
C	2.41590375508700	-0.63620469219800	-0.04211331363300
C	1.32334045890500	-1.44203237106500	0.16100744756900
C	-1.21829356617400	-1.38534156121300	0.25633975082200
C	-2.31829515526900	-0.40719860832600	0.31781524461600

C	-2.30182613487100	0.60152559761200	1.30176381051900
C	-1.30474788796900	1.14389629942000	0.39107541486300
C	0.06134848244000	-0.82887931066200	0.24332011445600
C	0.00625261041500	0.58629943343300	0.19603407578400
H	1.16867219876200	2.36238405600800	-0.15832109998300
H	3.40080795433000	-1.06848005675200	-0.12680340731900
H	1.43076574572100	-2.51261898639200	0.21680639031900
H	-1.43117182690000	-2.44013374566000	0.22104833462900
H	-3.20283079120700	-0.60126310236700	-0.28039315153400
H	-3.18476940537000	1.16975892147200	1.53987254939200
H	-1.53334327331300	2.09366947712000	-0.07358321813000

17

isoquinoline-10(Fig2d8) 5.52 eV -401.472078 [0.20] -401.472078 [0.90]

C	1.31965566557300	1.38988673296200	0.80867250049800
N	2.44616748177900	0.73717145355800	0.67126291044300
C	2.33191829372000	-0.51487405897300	0.16617425694900
C	1.16457006123000	-1.15429690343400	-0.12763355151600
C	-1.33728894560300	-1.21007426794000	0.03674762060700
C	-2.48819752652200	-0.55031257470600	0.49803538022600
C	-2.36859019514500	0.80317627997200	0.66003223616500
C	-1.15222297852000	1.29699383920300	0.05084805337700
C	-0.09331826900700	-0.56229897998000	0.17610162419000
C	0.05316459584100	0.84088286729400	0.60547244754500
H	1.38589303565000	2.41397765026100	1.14947254242000
H	3.26919930031900	-1.01517807400800	-0.02498580120300
H	1.18507014905800	-2.14437692324300	-0.55245445760200
H	-1.34011082479100	-2.25993599119000	-0.20231884782300
H	-3.33563456336000	-1.10052188018400	0.87843016243400
H	-2.77867656134300	1.31749739789600	1.51816148261800
H	-1.16450443680200	1.77123760602200	-0.92895675615400

17

isoquinoline-11(Fig2d9) 5.55 eV -401.471208 [0.41] -401.471207 [0.68]

C	1.05104734126500	1.41311961728600	-0.29936112563700
N	2.11653173688000	0.77690474708200	-0.72040066338300
C	2.03304327965700	-0.56173066448500	-0.78373776071700
C	0.92402723108500	-1.29515127403700	-0.43544156458000

C	-1.42791340249200	-1.33941957506500	0.39780613328600
C	-2.57329362273700	-0.64785773549300	0.61053365565500
C	-2.53769482182200	0.82939924510000	0.54159582518800
C	-1.25870145270300	1.40896022264400	0.71274328511500
C	-0.23309450467800	-0.63787057783800	0.00201956348200
C	-0.15606012384300	0.78817465520700	0.05574677412000
H	1.12194716185500	2.49012565348300	-0.23733448827000
H	2.92545101027400	-1.06510255885700	-1.12263172951300
H	0.94898087553800	-2.37037410527200	-0.49745700890100
H	-1.39886487557500	-2.41589831660100	0.45540514013500
H	-3.52022629112900	-1.16039378127200	0.69218468186400
H	-2.53771243697000	0.79931780087400	-0.58177560213400
H	-1.07268938280100	2.24085030535700	1.38425546690100

17

isoquinoline-12(Fig2d10) 5.56 eV -401.470535 [0.70] -401.470534 [0.23]

C	1.26825047976200	1.35606623520500	0.73360436735700
N	2.42001586593700	0.70674130680900	0.68786938694100
C	2.40785031571000	-0.55261259352800	0.23896362901900
C	1.27574772348200	-1.24474049637700	-0.12871540582100
C	-1.27347668965500	-1.11370254047100	-0.08219628731900
C	-2.32665766309400	-0.42355121089100	0.62460699641600
C	-2.22087599023800	0.86079276498800	1.10631380840400
C	-1.26694495376000	1.28625228009800	0.13381265723500
C	0.04239497631400	-0.58493552040100	-0.04325432116100
C	0.08467875009000	0.78764723808600	0.30012147414200
H	1.29935421816100	2.37951206208500	1.07564421298000
H	3.37209829925500	-1.03480096052800	0.18475902256400
H	1.33973505787000	-2.27080949775800	-0.45226772123700
H	-1.45036917933800	-2.12770595316900	-0.39783594898400
H	-3.27650105151000	-0.93839979576200	0.71508087480400
H	-3.02430205069200	1.40573560213000	1.56083611285700
H	-1.57390382622800	1.56746525300200	-0.87428105503700

17

isoquinoline-13 5.64 eV -401.467920 [0.73] -401.467920 [0.34]

C	1.27262421636300	1.23511217174100	0.25742980521000
N	2.28861155797400	0.38480143698700	0.50674191559200

C	2.25841426050400	-0.92757407165600	0.51070053381800
C	1.20154070239300	-1.04272321226400	-0.45138517809000
C	-1.30770108943600	-1.35193692446500	0.16625340588500
C	-2.46363115479200	-0.64681158870100	0.45230821181700
C	-2.43390021939900	0.74598970807100	0.55486162439500
C	-1.25625319118700	1.44781622532600	0.41605213274000
C	-0.13215989250700	-0.65169325351800	-0.04420477938500
C	-0.07050285548300	0.75505393676400	0.14087853217200
H	1.46555299775700	2.25951704372800	0.52895762806700
H	3.10095669598000	-1.54476761840600	0.75040569212000
H	1.45573202278900	-0.75187282177600	-1.47541796951700
H	-1.33023295223100	-2.42351263422200	0.05581734597900
H	-3.39585383906300	-1.17351891394000	0.57038845465700
H	-3.34730292443900	1.27973205008200	0.76275319122600
H	-1.23789736316400	2.51951667873800	0.53466520912500

17

isoquinoline-14 5.66 eV -401.466974 [0.73] -401.466974 [0.16]

C	0.78510532097200	1.78181788096900	0.01500327196200
N	1.67825441441800	1.57532293082700	0.95933908514500
C	1.60412588763700	0.43928728731100	1.66043990359700
C	0.64629446423900	-0.54660562170400	1.47325526605900
C	-1.46432115815300	-1.11081512152300	0.03211862106800
C	-2.74528190848300	-0.35782700455700	0.26717832229000
C	-1.99600094757600	-0.36051150946700	-1.14964014253700
C	-1.23637698568700	0.83997942781900	-1.25444551724300
C	-0.28337867155100	-0.34244847901000	0.47464747510800
C	-0.20949415576400	0.84519225900500	-0.28483813604600
H	0.86345985453200	2.70733204020900	-0.53689241121800
H	2.35956491290200	0.31426891360800	2.42091944524200
H	0.64319708447700	-1.42967650388700	2.08984900032100
H	-1.46210780305500	-2.19096242611700	0.06230743022200
H	-3.66113793142700	-0.93785527420100	0.20017269514300
H	-2.52719320726500	-0.80078759137600	-1.97490491266000
H	-1.43183421303200	1.63250805864500	-1.95616068048200

17

isoquinoline-15 5.68 eV -401.466409 [0.31] -401.466409 [0.74]

C	1.14530644323000	1.22310536014400	0.18822102200700
N	2.27899401668000	0.57018812508900	0.26619639180300
C	2.27355458348700	-0.75112067988000	0.03600420892900
C	1.13780962668300	-1.45224244666000	-0.27890266935700
C	-1.32503802624100	-1.30686417995800	-0.83178308517000
C	-2.52297926506900	-0.68818582166800	-0.41542528824200
C	-2.50205132786800	0.79390384827700	-0.32571220637500
C	-1.30517278717500	1.41060298451600	-0.19923916109700
C	-0.08704477114700	-0.77169842860000	-0.34309228119400
C	-0.09663331765600	0.62996333969200	-0.10795742250500
H	1.19055299445400	2.28742075774600	0.36979654995500
H	3.23004310788400	-1.24503787497000	0.09967971193600
H	1.18096507641600	-2.51204107667600	-0.46944223672400
H	-1.28964905725800	-2.12265920736300	-1.54621656959100
H	-2.27500220232400	-0.74291477252600	0.68557845860700
H	-3.42663974976600	1.34518997876400	-0.25013140091800
H	-1.22943412425000	2.48616153680900	-0.15735969867400

17

isoquinoline-16 5.74 eV -401.464233 [0.07] -401.464233 [0.17]

C	1.09082100877800	0.97095598926400	-0.17333802210700
N	2.43412309936300	0.65663354032300	0.05804689910100
C	2.54676431682300	-0.60963136624200	0.38865816310600
C	1.36039841599800	-1.32997357803900	0.37779185367100
C	-0.99015380747800	-1.00955848293000	-0.57023692390400
C	-2.19101928760000	-0.44140709600100	-0.32680684563000
C	-2.32476846434900	0.73617472848300	0.48046633821500
C	-1.20886847327800	1.37199380122000	0.94747852257900
C	0.21355156618800	-0.47453277962000	0.05085627387100
C	0.04768876069800	0.76823302286500	0.81654183832700
H	0.89475378757100	1.63850749948100	-0.99949489442500
H	3.50966840065000	-1.01230897401400	0.65788195313000
H	1.26166749949000	-2.37594554588200	0.60830042143400
H	-0.91654589958400	-1.90278992362700	-1.17110120864500
H	-3.08008704517500	-0.86946453745000	-0.76220708913400
H	-3.30494403984700	1.15131192702900	0.64720365289500
H	-1.28508086099600	2.34410037308800	1.41260619425800

17

isoquinoline-17 5.75 eV -401.463674 [0.11] -401.463673 [0.21]

C	1.22561218013900	1.20871734840900	1.11468740510200
N	2.39263120088100	0.57812287007800	1.12108466950700
C	2.29748402160000	-0.53062689831800	0.42513041137600
C	0.98912600581400	-0.85196909601600	-0.17100153735600
C	-1.38141847608500	-1.48246900475300	0.70089248317300
C	-2.50774798842600	-0.67254856572900	0.66531450858900
C	-2.34817146735900	0.70377759709000	0.33364349567000
C	-1.13438163563000	1.29259825986100	0.18794413756200
C	-0.14623283206700	-0.88627975940300	0.68820484408500
C	0.07201329425400	0.54771103405900	0.54224820914800
H	1.15570309292600	2.21304041612400	1.49708898073300
H	3.14483234291200	-1.19007370154700	0.32611103309700
H	0.92281882350100	-1.21859241206300	-1.18735916467100
H	-1.46556156511900	-2.55830525904300	0.67064952189400
H	-3.49542887440000	-1.09128538593800	0.75057341611600
H	-3.23611246246200	1.29193220134000	0.15889477640300
H	-1.05176046859300	2.33090073302600	-0.09061712759600

17

isoquinoline-18 5.78 eV -401.462725 [0.20] -401.462725 [0.86]

C	1.22646187825600	1.18567410863800	-0.11317317383800
N	2.37777028501600	0.59943517718200	-0.16306203620300
C	2.44990195124600	-0.72145787935600	-0.46438087583300
C	1.33130411503400	-1.48089285463700	-0.64514068038600
C	-1.18583536787500	-1.12129560799700	-0.11496093141800
C	-2.32101344557200	-0.71440488324600	-0.91389754907700
C	-2.37919505884700	0.65490129566200	-1.00248647830900
C	-1.23892187048000	1.32673546823000	-0.55011996348600
C	0.07793194035100	-0.86180958371100	-0.65638264826100
C	-0.03967228000400	0.58434129634400	-0.45004004179000
H	1.21954866380600	2.23727497000600	0.13988911641900
H	3.43686698718900	-1.14981093967600	-0.49864793244400
H	1.40027582864300	-2.54594994556100	-0.79232048798600
H	-1.29436906629300	-1.36638349178400	0.94251382440300
H	-2.69614554175100	-1.37153337470800	-1.68502462896700

H	-3.16532070224700	1.16483307614800	-1.53798618443900
H	-1.18816044646100	2.39900523029100	-0.46946665136100

17

isoquinoline-19 5.99 eV -401.455006 [0.12] -401.455006 [0.10]

C	1.03271596364800	0.92827713362800	0.19700581238000
N	2.19379315654000	0.43670805175400	-0.03637113822800
C	2.31038532904300	-0.68566674874100	-0.82682637503100
C	1.22457780381400	-1.38333509954700	-1.27453901873600
C	-1.11922431985000	-1.12928541004700	-0.22690720432600
C	-2.48113185460900	-0.65424879300400	-0.48328166602700
C	-2.56837922964700	0.69752061017500	-0.71530842180800
C	-1.34029138883200	1.32746482089700	-0.59109505340400
C	-0.04542361884000	-0.82383909082800	-1.12540438093700
C	-0.21169471279300	0.43582771934700	-0.40100919810800
H	0.98270612974700	1.80412400624900	0.83182282868100
H	3.31735903959000	-1.02575940879200	-0.99811713781300
H	1.34282990225000	-2.36109851130600	-1.71656245041000
H	-0.94259624612300	-1.82532471590600	0.58385264701700
H	-3.31815685886900	-1.33075260198300	-0.44785105164700
H	-3.48418102220300	1.21042715263900	-0.95308854067600
H	-1.19857225664000	2.39435849194500	-0.59937266150700

17

isoquinoline-20 6.01 eV -401.454285 [0.78] -401.454285 [0.37]

C	1.21220997095200	0.63933457755400	1.32418229170900
N	2.03041852755500	-0.51520578443000	1.31449707887600
C	2.69497596268900	-0.62302126971500	0.14153572216400
C	1.41071696984700	-1.11447574071600	-0.41322628683700
C	-0.81523122082400	-0.49729414636700	-1.42538497843400
C	-1.79732726168500	0.45531659815500	-1.48924306584500
C	-1.75595543060700	1.61096750751400	-0.66976463855700
C	-0.75387393672200	1.78999589514000	0.23658297457600
C	0.26885069782000	-0.30711145921400	-0.55279141522000
C	0.25303319427000	0.79820955341000	0.34955634720200
H	1.39784191225700	1.31401213464100	2.14331912925200
H	3.55893921055900	-1.27436843319700	0.12949683139200
H	1.36706552852300	-2.17304596587700	-0.62479879830400

H	-0.84085569575900	-1.35660105322500	-2.07607812439500
H	-2.61186869172000	0.33625060941400	-2.18480877324200
H	-2.54267858584500	2.34238820065500	-0.75525871688800
H	-0.74110226753900	2.64844971829600	0.88855722284200

17

isoquinoline-21 6.01 eV -401.454280 [0.72] -401.454279 [0.44]

C	1.26077710839200	1.24313912652400	0.15271732231300
N	2.35702346572300	0.37309723818300	-0.05567661526100
C	2.38915234742500	-0.59531853679800	0.88797452307300
C	1.29887929979800	-1.23299178008200	0.11119285287200
C	-1.18298344549900	-1.35802638599900	-0.31987004237400
C	-2.36521510496100	-0.66706796262400	-0.29833945509000
C	-2.40354671332300	0.71760976397600	0.00173309289800
C	-1.25608015399600	1.41312268512900	0.24094904745700
C	0.01019478614700	-0.68512790919500	-0.00847524703600
C	-0.01562935460400	0.72873273654500	0.18355092168500
H	1.52456210869200	2.28352464106600	0.24650288902700
H	3.32620976476600	-1.12186521679100	1.01208714670000
H	1.57712253010800	-2.11421131520600	-0.44859061180400
H	-1.16996877023400	-2.41780005620300	-0.51792428759300
H	-3.28942310738000	-1.18433424741000	-0.49793176507200
H	-3.35451823502000	1.22423784974800	0.01752100201600
H	-1.27854579647100	2.47414644625900	0.43062964066000

17

isoquinoline-22 6.08 eV -401.451738 [0.35] -401.451738 [0.68]

C	0.75468270162300	1.32317772610800	-0.30747736299400
N	1.87823865199600	0.80553656638100	-0.61897468327300
C	2.09115224101700	-0.54258840967100	-0.33652612253100
C	1.13506638557800	-1.40172559309300	0.09214610752200
C	-1.39582815557100	-1.56498716924500	0.28691389745100
C	-2.44572521285600	-0.65670823924700	0.26384765355700
C	-2.08729187399000	0.69014569159800	0.53674526180100
C	-1.03110386793800	1.09921904637000	1.48934302809700
C	-0.17816462804100	-0.91396585448800	0.30160618547900
C	-0.29121090504100	0.57560538391200	0.41439706502100
H	0.59556689915500	2.37344372682700	-0.51312850752700

H	3.08961238818400	-0.88588581545300	-0.54828786197000
H	1.35094874025700	-2.45435883444700	0.17973986389100
H	-1.50668135345200	-2.63241833154800	0.21084539124900
H	-3.45045789243500	-0.91506985703700	-0.02567802373800
H	-2.68864715966300	1.48973584569000	0.12866727973700
H	-0.92852365502400	2.13676173655200	1.76528284193900

17

isoquinoline-23 6.10 eV -401.450750 [0.31] -401.450750 [0.74]

C	1.22322466087300	1.15221497961400	-1.36308626175400
N	1.88151290505300	0.71732064352800	-0.19494872744800
C	2.21919006607400	-0.59328871632500	-0.04709296975900
C	1.24300880862500	-1.52218662835800	-0.27589327974500
C	-1.26926210547700	-1.47238147056800	-0.46607496248800
C	-2.35640435353400	-0.68462488955600	-0.24172260789900
C	-2.22346684687800	0.73198033922300	-0.06939834148600
C	-1.02784689100900	1.34005869197000	-0.21432717754900
C	0.01526561229900	-0.89031229925900	-0.53336214346100
C	0.11875395352500	0.56610457681300	-0.64485330294400
H	1.21768880879700	2.20480801574800	-1.59879273792800
H	3.23288221142700	-0.81778534086800	0.24741670362000
H	1.37923473777900	-2.58629786957700	-0.20462432711000
H	-1.36414394232300	-2.54560501567500	-0.50126915559200
H	-3.33202262722200	-1.13138833093300	-0.14072665606200
H	-3.10258747100300	1.31443330879600	0.15319514347600
H	-0.92786147281700	2.40965344344300	-0.13730660062800

17

isoquinoline-24 6.14 eV -401.449425 [0.74] -401.449425 [0.45]

C	1.27402101546800	1.27184305096800	-0.17909904354100
N	2.25746947813200	0.54575458619100	0.21464372538300
C	1.98772061952800	-0.77027328305800	0.60247921583700
C	0.80920632099400	-1.39271901106400	0.47217398074100
C	-1.17386870766800	-1.25168380527900	-1.13926532009700
C	-2.01629721691400	-0.72242141409400	-0.04891443056000
C	-2.31976439324100	0.67095676418000	0.12138214360800
C	-1.24692167768900	1.52218535712900	-0.10649475589600
C	-0.28193549258900	-0.68078144682600	-0.19512838892400

C	-0.08045408302700	0.80155379104100	-0.23230701580700
H	1.48005453105800	2.30790011378500	-0.41563959717600
H	2.83907544007500	-1.28749436664800	1.01354430159100
H	0.69310637076800	-2.42901524150900	0.74221076011600
H	-1.15258656339700	-2.31328709009200	-1.32953547656200
H	-2.58301596434600	-1.44796629354900	0.51732810130100
H	-3.28488862896300	0.99659078509200	0.47085778100100
H	-1.30534379365700	2.59677241908900	-0.11302007673800

17

isoquinoline-25 6.27 eV -401.444427 [0.76] -401.444427 [0.18]

C	1.44069995157100	1.28057685141500	0.44463036323300
N	2.56604401020800	0.72346620841400	0.70167776903500
C	2.53090032254100	-0.75479776590300	0.60921518173500
C	1.28839074749700	-1.42019172374000	0.67770312341700
C	-1.04312631003800	-1.46653705680200	-0.31183412821000
C	-2.13382434787700	-0.73055858362400	-0.71152193901800
C	-2.06144166386000	0.66553865457800	-0.73850233489800
C	-0.90852813423700	1.32254394229900	-0.36422303101100
C	0.14513811520900	-0.81916811714500	0.04904166463200
C	0.21646492922000	0.59958972005200	0.03687746798100
H	1.40257138292500	2.36111879702900	0.52079926719900
H	2.28533285472900	-0.67523203336200	-0.50094007485800
H	1.16253070279700	-2.36907778258500	1.19110368449300
H	-1.08832878185000	-2.54333660213400	-0.27802387608100
H	-3.04881250357300	-1.22422295142400	-0.99425025870000
H	-2.92452043528100	1.23476489205500	-1.04296828712100
H	-0.87116875375800	2.39993310094800	-0.37565290228100

17

isoquinoline-26 6.44 eV -401.438248 [0.73] -401.438248 [0.15]

C	1.27262790052300	1.26678570618400	0.38336093806500
N	2.27041379254000	0.47242935026600	0.15859266833200
C	2.02935755364100	-0.83369801980300	-0.21834282517900
C	0.80581586081100	-1.39516977083400	-0.29253063146300
C	-1.13524217475800	-0.97597754478300	1.36864794457200
C	-1.81751682286400	-0.68259303691600	0.02751545427300
C	-2.29772017560400	0.68882661828800	-0.14427625966800

C	-1.27870504142000	1.56680873067700	0.07054628317400
C	-0.32378719914100	-0.58846773405700	0.11940737126600
C	-0.07887575470500	0.84646722547700	0.25925345235500
H	1.50326993237300	2.29447604663100	0.62833004629300
H	2.91396269275600	-1.39982995731400	-0.45819081229500
H	0.67910441548300	-2.43122230116600	-0.55995952489900
H	-0.95200676146500	-1.98803481379300	1.70781975157000
H	-2.31965454986900	-1.52394414898900	-0.42587183316500
H	-3.32715707999300	0.94575439343800	-0.32043446955300
H	-1.36492040887300	2.63821851764300	0.11343403590600

17

isoquinoline-27 6.59 eV -401.432710 [0.52] -401.432710 [0.26]

C	1.11573019059300	1.31652028792900	0.10562800843100
N	2.13042639877000	0.55485117994300	-0.42789695798200
C	1.92143300293700	-0.72196414487900	-0.46413136112500
C	0.84753006055500	-1.42942161129700	0.19138998949600
C	-0.89239195066700	-1.35796076244500	0.26600534314000
C	-1.96764405412700	-0.66222488731900	-0.46114521816900
C	-2.18810150936100	0.65536807120400	-0.21396800650500
C	-1.20630177213500	1.45149109560000	0.43269555198200
C	-0.00207349925700	-0.61992218554300	1.09356198660900
C	0.02278791591300	0.79768071682800	0.73474151586000
H	1.14747479378300	2.36247310735900	-0.16021342502200
H	2.70239597759200	-1.31873445039700	-0.91809893038800
H	1.08382179421100	-2.45463022048500	0.43157549827600
H	-1.10351707530700	-2.39093256119600	0.50674746272100
H	-2.65141996053000	-1.23549771803100	-1.06457755534400
H	-3.07082454453300	1.13563869014300	-0.60488391589500
H	-1.28454781641200	2.52598676973600	0.42070924622600

17

isoquinoline-28 6.75 eV -401.426993 [0.72] -401.426993 [0.84]

C	2.24254026265000	1.68522697799300	-1.75838303414300
N	1.91712696628200	0.81271974698200	-0.99522440879800
C	2.02178477862200	-0.47775531626700	-0.59567315890700
C	1.22794510070300	-1.03910774279600	0.33396121757000
C	-0.63120857440400	-0.96860916874800	1.98983765629200

C	-1.64984848881700	-0.27404789306900	2.61744980917100
C	-1.90668735320900	1.05170198429900	2.28972196652300
C	-1.13402294237400	1.69445935431200	1.32180186552300
C	0.15360248257000	-0.34647431224600	1.00733620174600
C	-0.14788480596000	0.96860712969800	0.71236626685300
H	2.90958619987500	2.52348571543300	-1.84297057398700
H	2.80092138093600	-1.04780788539000	-1.07948964397700
H	1.41247062791500	-2.06947525232900	0.58982182873900
H	-0.42994460883500	-1.99517563779700	2.25897894496700
H	-2.24673881108000	-0.76555229893400	3.36846842812900
H	-2.70643274973200	1.58476300556000	2.78030222307800
H	-1.32690575531700	2.72461142494600	1.06440467809700

17

isoquinoline-29 6.98 eV -401.418374 [0.67] -401.418374 [0.20]

C	1.46264054456300	1.18912209425200	-0.30226148447200
N	2.36214809494800	1.47306591057900	-1.13067065115700
C	1.96855369662700	0.26901880562900	-1.88317947145800
C	0.71073414381700	0.15323137348400	-2.42356627161400
C	-1.72384132723700	0.59020356684200	-2.12555897565800
C	-2.68669683264600	0.80705991003300	-1.18662361813700
C	-2.32161756904000	1.18907077395100	0.15255557448700
C	-1.05795073157900	1.49379984646600	0.48055793695400
C	-0.36573472036600	0.82623894180000	-1.83335422371900
C	-0.01669523730900	1.58521689703200	-0.57795797514800
H	0.13523607764300	2.64969458148400	-0.79517571794300
H	2.74734862622600	-0.45866940886100	-2.02501568731900
H	0.53791150032400	-0.58224630098000	-3.19359881922100
H	-1.98024131173800	0.13999651877300	-3.07247041263100
H	-3.71974042718600	0.60127166009600	-1.41065468461700
H	-3.09105741929500	1.21132943008600	0.90790067212200
H	-0.78905712949500	1.78299351796900	1.48349472760600

17

isoquinoline-30 7.54 eV -401.397768 [0.26] -401.397768 [0.19]

C	1.47011644544500	0.82553400763800	0.91046498107100
N	2.44995506924900	0.01333784143000	0.99118130060800
C	3.46342846088200	-0.65686098150000	0.95208482068500

C	0.97365565642200	-1.50572046583200	-0.89203277863500
C	-1.15614182808200	-0.52269424941900	-1.48141874270600
C	-2.09561278026100	0.46450194136000	-1.36525046521500
C	-1.86952377092800	1.55819217993800	-0.52104393685700
C	-0.69764104253800	1.63274822173200	0.19553014600600
C	0.08181244123300	-0.47897126066600	-0.76611669059000
C	0.28878744560100	0.64638987544700	0.10797450117200
H	1.53447095009500	1.71376969768800	1.52059134709300
H	3.55153161100700	-1.47937477718900	1.66197700208100
H	1.81356655748400	-1.97915763946800	-1.34071649270900
H	-1.32740850611000	-1.36591000902000	-2.12834569582000
H	-3.01208396541900	0.39845817946800	-1.92889170020200
H	-2.60916672995800	2.33587809245700	-0.42872726755300
H	-0.52458710159400	2.47368026585600	0.84911250028400

17

isoquinoline-31 8.38 eV -401.366948 [1.09] -401.366939 [0.80]

C	1.22180858237600	0.56451080119200	1.50125929694600
N	1.27921534549000	-0.62520516386100	2.05827432844700
C	0.51117514335000	-1.57394933457700	1.51954520820400
C	-0.34795441467200	-1.36826600312900	0.45822001740100
C	-1.44210049403500	0.20139843222900	-1.11387012171100
C	-2.51737050614800	-0.58701590735300	-1.41434492383300
C	-2.90819913859900	-1.80749540236700	-0.86385528309500
C	0.36692269240400	2.24965847516200	-0.07925254698400
C	-0.47765323323800	-0.09043241086800	-0.09260556646900
C	0.38649303957100	0.92708155204800	0.42155245199000
H	1.87344222162900	1.31850412178400	1.91855913236700
H	0.60596478944100	-2.55816202968400	1.95230741754500
H	-0.85795641055400	-2.21253878222400	0.02228872529000
H	-1.28608783503400	1.09838497585400	-1.68502189453900
H	-3.08272207264100	-0.29001146054600	-2.29258837349100
H	-3.03676930925400	-1.86380987741900	0.21695597488600
H	1.17336362295300	2.85842467413900	0.33336069585500

17

isoquinoline-32 8.87 eV -401.348984 [0.55] -401.348969 [1.71]

C	1.37779095732800	0.18732550018000	1.16067328914300
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N	2.64821127941700	0.43890366669600	0.99777890805000
C	3.76648155556900	0.81484617794900	0.59404399420500
C	-0.16929312136100	-2.29916696586300	-0.37618048831000
C	-1.36942421718300	-0.57065594462500	-1.46393071110400
C	-1.91116316579300	0.69291465332200	-1.58226172245200
C	-1.45196400764500	1.70321196233200	-0.75958474453300
C	-0.37371376044700	1.46118035815800	0.07484323924700
C	-0.34744308583400	-0.87360625802800	-0.54835076309800
C	0.23881332858400	0.21024754996200	0.17201817244400
H	1.06019748633800	0.23142712102600	2.20056347990300
H	4.70868534648600	0.61382327097300	1.11369141361400
H	0.55780150890300	-2.96081075589600	-0.82590219516500
H	-1.76386144387000	-1.37445392576600	-2.05999284312700
H	-2.70979287077000	0.86791012901600	-2.28239152472800
H	-1.92379307382700	2.67158832142000	-0.77239209303500
H	-0.00237383211800	2.25911608116300	0.69374738921100

17

isoquinoline-33 8.90 eV -401.347841 [0.75] -401.347832 [0.78]

C	0.71807998075300	0.69963243688800	2.04635413202400
N	1.76575188218500	0.04117686480400	2.49596200232100
C	2.01200418901400	-1.16933903815100	2.02607524053800
C	1.20771807437300	-1.78102724413500	1.05259517400200
C	-2.18827070905300	-1.88343607985900	-1.13501903142900
C	-2.39895415840800	-0.58915843416100	-0.84445462499700
C	-2.29186673036400	0.63171979939600	-0.27078399615900
C	-1.31282400715400	1.01186141232100	0.65333550997700
C	0.13735543788300	-1.05273476527700	0.66186383742700
C	-0.20534302731500	0.21238471093000	1.08679381928500
H	0.56607836306400	1.69720055590900	2.43659260304900
H	2.86647065509500	-1.69247724490000	2.42846003697800
H	1.43857825046100	-2.76687683378900	0.68357190571400
H	-1.57291772842800	-2.05102346549000	-2.02860964582300
H	-3.31286426320900	-0.89143160015800	-1.49884602899700
H	-3.04601084523900	1.35819868722700	-0.52258226052200
H	-1.38943089889500	1.99825030442600	1.07780573396500

17

isoquinoline-34 9.60 eV -401.322154 [0.83] -401.322108 [1.36]

C	0.09524637646600	1.37568503286900	0.24447885340000
N	1.02388616104500	1.71938633478000	1.14161106356100
C	1.60279941503300	0.75464859186300	1.79813848956800
C	1.30640818410200	-0.59007815667200	1.56406236701200
C	0.49592595581800	-2.42104718507500	0.36009381460600
C	-3.67119609690500	1.18831088991700	-0.26153242095500
C	-2.71645636952700	0.49701603510000	-1.12537759358700
C	-1.43642585230500	0.09962327091800	-1.08038977658600
C	0.35183077597100	-0.98332948255400	0.62663002318300
C	-0.36585181412400	0.10163683880800	0.00028804711700
H	-0.38558504266900	2.20161841827400	-0.25665480253500
H	2.33688819085300	1.03438233514300	2.53802515433300
H	1.83959027055000	-1.36278619175300	2.08589284242300
H	-0.09781680363500	-2.79109522083200	-0.49658951189900
H	-4.68999920821600	0.84173564165900	-0.44009571285800
H	-3.12600866442400	0.44765711468200	-2.13897112160000
H	-1.00036052087800	-0.05514500056500	-2.06126099919600

Cartesian coordinates (in Å) of S_{1FCMIN}, S_{1MIN-b} and MESXs at the TDDFT(BHLYP/6-31G*) level for four heteroaromatics, i.e. indole, isoindole, quinoline and isoquinoline. Relative energies in eV and a.u., oscillator strength for S₁-minima and spin orbit coupling for MESXs are indicated.

indole

16

indole S1FCMIN 0.00 eV (Osci.Str. 0.17) -363.405119925420

N	1.575068127600	-1.060708127839	0.000000000000
C	2.407282996974	-0.007164256595	0.000000000000
C	1.586013010711	1.156348760504	0.000000000000
C	-0.996076536918	1.452830276856	-0.000000000000
C	-2.179944516261	0.680259504434	-0.000000000000
C	-2.153281352180	-0.691217641248	0.000000000000
C	-0.905809236255	-1.428071951236	0.000000000000
C	0.243691524673	0.751057646500	0.000000000000
C	0.240782479853	-0.660062148734	-0.000000000000
H	1.870003964633	-2.018144396040	0.000000000000
H	3.472572281686	-0.113496427582	-0.000000000000
H	1.959991494703	2.163001803264	-0.000000000000
H	-1.025781732366	2.528398461573	0.000000000000
H	-3.131616334651	1.187228684993	-0.000000000000
H	-3.076122759382	-1.247553491025	-0.000000000000
H	-0.890145503221	-2.503713223151	0.000000000000

16

indole S1T3-MESX 0.06 eV (0.00 cm-1) S -363.403080300705 T -363.403080352491

N	1.588929050602	-1.052221836584	0.000000004707
C	2.415370980044	-0.027716275681	0.000000001173
C	1.570623117834	1.150398432686	-0.000000002164
C	-0.999285666989	1.450759060399	-0.000000006925
C	-2.196416665971	0.677356765756	-0.000000002258
C	-2.160538096285	-0.676659064030	0.000000000023
C	-0.895147043645	-1.418046721172	0.000000000342
C	0.242560985209	0.747815453305	0.000000018474
C	0.244719149627	-0.649831905287	-0.000000006037
H	1.878659735221	-2.012607855581	-0.000000000589
H	3.481730520185	-0.126970602208	-0.000000002744
H	1.953388325882	2.154558268316	-0.000000003400
H	-1.025752569666	2.527140904170	0.000000000099
H	-3.145912045817	1.187806404673	0.000000001231
H	-3.074337437780	-1.248665968330	0.000000000853
H	-0.881964428801	-2.494121585759	-0.000000002786

16

indole S1T4-MESX 0.00 eV (0.07 cm-1) S -363.405003626282 T -363.405003635044

N	1.577965062295	-1.064521078011	-0.000000000164
C	2.402670019243	-0.006767229325	-0.000000000007

C	1.584395362705	1.156360408872	0.000000000043
C	-0.996265231661	1.453679866567	0.000000000320
C	-2.180878664568	0.685386101056	0.000000000069
C	-2.150081889117	-0.693872404985	0.000000000052
C	-0.907547839222	-1.428537282769	-0.000000000061
C	0.242387536020	0.752936564988	-0.000000000798
C	0.240726309900	-0.663430904843	-0.000000000042
H	1.876539438427	-2.020426810207	0.000000000109
H	3.468715170865	-0.109385363137	0.000000000100
H	1.960764099990	2.162069121270	0.000000000169
H	-1.022827569587	2.529511095624	0.000000000086
H	-3.132920222729	1.190544455997	-0.000000000048
H	-3.073044614740	-1.250183553245	-0.000000000066
H	-0.893969058218	-2.504369513173	0.000000000237

16

indole S1T5-MESX 0.04 eV (0.07 cm-1) S -363.403528344568 T -363.403528361260

N	1.566370630000	-1.061912157503	0.000000000071
C	2.401693480495	0.005054388032	-0.000000000048
C	1.600867009454	1.161942267906	0.000000000158
C	-0.988137199943	1.444823049133	-0.000000000006
C	-2.182354615491	0.685461943206	0.000000000084
C	-2.158169988352	-0.712596051296	-0.000000000167
C	-0.918528718012	-1.424036824766	-0.000000000083
C	0.245375995131	0.757590364649	-0.000000000139
C	0.242579197254	-0.658878307359	0.000000000301
H	1.865366876577	-2.017472883451	-0.000000000039
H	3.466475795268	-0.108818363730	-0.000000000051
H	1.978026815955	2.167179922380	-0.000000000058
H	-1.020374571222	2.521313209924	-0.000000000040
H	-3.129374377651	1.198839175582	-0.000000000002
H	-3.079693028427	-1.268794885517	0.000000000093
H	-0.893495391458	-2.500701372484	-0.000000000068

isoindole

16

isoindole S1FCMIN 0.00 eV (Osci.Str. 0.11) -363.425042784598

C	-0.005686267119	-0.718812599521	-0.236972243194
C	0.004456034907	-1.428320693692	0.966292678637
C	-0.005686158314	0.718812595069	-0.236972242953
C	0.004455924186	1.428320694159	0.966292672201
C	0.016477942023	-0.687309006075	2.177664131207
C	0.016477866627	0.687309016587	2.177664129113
N	-0.159624108086	-0.000000014967	-2.398899720001

H	-0.001805341065	2.505038222748	0.980106874579
H	-0.001805186277	-2.505038221164	0.980106889452
H	0.023645591472	-1.221305005425	3.113897397669
H	0.023645456579	1.221305017761	3.113897393305
C	-0.046850254942	-1.110855055018	-1.570451989468
H	0.276080024486	0.000000022405	-3.310168357179
H	-0.048465806800	-2.098827011710	-1.991527664397
C	-0.046850125871	1.110855041636	-1.570451984529
H	-0.048465591802	2.098826997214	-1.991527662054

16

isoindole S1T2-MESX 0.03 eV (0.29 cm⁻¹) S -363.424093841713 T -363.424094062625

C	-0.007420831472	-0.730271641142	-0.233999596927
C	0.005541831763	-1.427328403026	0.957117246708
C	-0.007134689729	0.730266678476	-0.234004002873
C	0.005384469919	1.427327355667	0.957115134314
C	0.017457751054	-0.685825234491	2.172369655728
C	0.017574017599	0.685827494883	2.172367511422
N	-0.172984335190	0.000004591459	-2.398741523489
H	0.000188202110	2.504420329744	0.975373336587
H	0.000173953478	-2.504420524623	0.975371125929
H	0.024780489742	-1.221576174833	3.107488869331
H	0.024771614485	1.221574969479	3.107489715750
C	-0.053467986805	-1.105721835148	-1.561426000792
H	0.298935039461	-0.000008076786	-3.295923215085
H	-0.050115250438	-2.093547985191	-1.985115483125
C	-0.053588721088	1.105730630299	-1.561411311185
H	-0.050095554887	2.093547825230	-1.985121159904

16

isoindole S1T3-MESX 0.09 eV (0.23 cm⁻¹) S -363.421672213118 T -363.421672183076

C	-0.006664916966	-0.729707615783	-0.242055433621
C	0.004785196108	-1.441106307449	0.971528116606
C	-0.006377844074	0.729695510108	-0.242061171936
C	0.004665676864	1.441108454007	0.971515403522
C	0.015138789935	-0.712109746433	2.169231985154
C	0.015204441096	0.712123111123	2.169223985476
N	-0.122456951144	0.000002163039	-2.379595445125

H	-0.000727488813	2.517745267703	0.982393477648
H	-0.000737479903	-2.517743192568	0.982383165134
H	0.018356444213	-1.234720748232	3.111113530084
H	0.018353685292	1.234711381742	3.111118737770
C	-0.037104504664	-1.122187412432	-1.565662563856
H	0.230407031617	-0.000004327006	-3.320375510695
H	-0.047816858582	-2.106588253721	-1.992075785725
C	-0.037218053489	1.122193327671	-1.565651715163
H	-0.047807167485	2.106588388250	-1.992080472921

16

isoindole S1T4-MESX 0.56 eV (0.07 cm-1) S -363.404637951669 T -363.404638022430

C	0.000020142678	-0.763980995081	-0.223679894509
C	0.000135554328	-1.432973616416	0.985182236155
C	-0.000294396587	0.763927753505	-0.223643108279
C	0.000492153010	1.432996502162	0.985184058389
C	0.001485941063	-0.731126062627	2.183998190916
C	0.001272739609	0.731116290633	2.183994378523
N	-0.001156712705	0.000044771685	-2.319912528533
H	-0.000275504061	2.513611887127	0.997465590323
H	-0.000198279944	-2.513592510041	0.997459996054
H	0.001688423150	-1.263953746895	3.117954866205
H	0.001698470983	1.263958180055	3.117942876154
C	-0.000830022968	-1.150388318783	-1.584757557500
H	-0.001610488708	-0.000023726968	-3.325482004747
H	-0.000824511589	-2.104952206934	-2.069017955086
C	-0.000786861507	1.150407723825	-1.584690762521
H	-0.000816646706	2.104928074753	-2.069048079180

16

isoindole S1T5-MESX 1.47 eV (0.19 cm-1) S -363.371069854777 T -363.371069887627

C	-0.206676400286	-0.789734983453	-0.216888889997
C	-0.044651507051	-1.468933087632	0.998968025592
C	-0.206612313474	0.789719551388	-0.216950061865
C	-0.044756147305	1.468953888437	0.998948838445
C	0.020484144954	-0.757048448015	2.160631146583
C	0.020818498640	0.757263052279	2.160669667009
N	0.051194100932	-0.000014088522	-2.271621467299

H	0.010365878832	2.546563989667	1.015774067777
H	0.010194926918	-2.546550857975	1.015473253547
H	0.108210837929	-1.258640279876	3.108781442920
H	0.108158026364	1.258486475461	3.109032390335
C	-0.030669668052	-1.149454317956	-1.607401073455
H	0.192719521179	-0.000114285079	-3.268246557805
H	0.020839404924	-2.093543569487	-2.105242047817
C	-0.029710244073	1.149522662132	-1.607409018757
H	0.020090939551	2.093524298761	-2.105569412872

quinoline

17

quinoline S1MIN-b 0.00 eV (Osci.Str. 0.00) -401.522563316806

C	-0.030707886175	-0.700643590658	-0.017620664405
N	1.190932575589	-1.237991171244	-0.031873696461
C	-1.226326582466	-1.404808555593	-0.012431393362
C	-0.013627122523	0.744015656235	-0.008879087297
C	-1.252332618492	1.379201999917	0.004047923810
C	-2.431934809844	-0.712209056642	0.000899591335
C	-2.445701024944	0.669251774307	0.009033720381
C	2.432240686781	0.683679090647	-0.025743628768
H	-1.264557514229	2.458142276867	0.009751573089
H	-1.198559616884	-2.480387089389	-0.018769664208
H	-3.356176697042	-1.265925990689	0.004674545381
H	-3.382110722357	1.201968270581	0.019110043114
C	2.417151874143	-0.706350577252	-0.033490526142
H	3.391537340585	1.175527161634	-0.028005435609
H	3.278323674727	-1.346386653736	-0.039952163584
C	1.254668633500	1.400531886230	-0.014085904720
H	1.275471969624	2.476816551374	-0.007037929492

17

quinoline S1T2-MESX 0.15 eV (12.63 cm⁻¹) S -401.516999714150 T -401.516999717336

C	-0.020645240027	-0.701945511528	-0.196129861988
N	1.212908816606	-1.168852615664	-0.544660296872
C	-1.201303030282	-1.412077310894	-0.100023066038
C	-0.005467914527	0.727211055313	-0.112332692277

C	-1.226635341116	1.371475106436	0.018264032892
C	-2.390240116011	-0.726944346232	0.076235778350
C	-2.405806250179	0.658795073310	0.127478774949
C	2.447858914104	0.696742387652	-0.073489183945
H	-1.245936919880	2.450415334351	0.010691047021
H	-1.177923277076	-2.487455964530	-0.147773792587
H	-3.311936319215	-1.279698958685	0.156639544380
H	-3.340692827970	1.183288415861	0.236438443712
C	2.356532199368	-0.704758694985	-0.023831064984
H	3.386956060974	1.192324008758	0.116383122417
H	3.002080735766	-1.329647153502	0.576547649795
C	1.275500061034	1.394150299981	-0.175452689147
H	1.283042608273	2.471410857018	-0.135358442585

17

quinoline S1T3-MESX 0.02 eV (8.04 cm⁻¹) S -401.521982570703 T -401.521982609835

C	-0.021118720185	-0.703388353438	-0.017486547147
N	1.190799471369	-1.265951138354	-0.030495473726
C	-1.223250181919	-1.406092664509	-0.012513895487
C	-0.011642831284	0.736677320619	-0.008939595370
C	-1.254740867444	1.382552028259	0.003976293355
C	-2.431010866555	-0.710859897727	0.000565756079
C	-2.444394057372	0.675081469409	0.009035598173
C	2.430455651965	0.685474433623	-0.025565894390
H	-1.263199960585	2.461267469879	0.009911907238
H	-1.196641421633	-2.481567979948	-0.018861011437
H	-3.356281472999	-1.262767366997	0.004486474445
H	-3.381711972090	1.206297234947	0.018999471598
C	2.409350607154	-0.705177706201	-0.033290734783
H	3.389219862108	1.178393975699	-0.028270461781
H	3.278370225735	-1.335929880543	-0.041098265548
C	1.253907088789	1.401987279566	-0.013698083803
H	1.270181604937	2.478435758293	-0.007128234361

17

quinoline S1T4-MESX 0.03 eV (5.76 cm⁻¹) S -401.521363183817 T -401.521362935456

C	-0.021400061257	-0.688639538399	-0.017108934940
N	1.193088537825	-1.270308019168	-0.030014460514

C	-1.222242146914	-1.400250482542	-0.012430725817
C	-0.011740764257	0.749885210401	-0.008655975590
C	-1.253207085240	1.388656130712	0.004041860072
C	-2.427300353497	-0.716913498095	0.000408620444
C	-2.446258846816	0.670208200048	0.008913103402
C	2.432298575136	0.679372295338	-0.025695023997
H	-1.270985768702	2.467087813120	0.010034186692
H	-1.185791478641	-2.475583242034	-0.018915624486
H	-3.350816845792	-1.271816985146	0.004212407897
H	-3.385533989231	1.197891280064	0.018802036503
C	2.398488148377	-0.713009859603	-0.033304036750
H	3.394038323383	1.165911802429	-0.028653327119
H	3.269899477118	-1.342197367881	-0.041440400507
C	1.250033939034	1.409053256722	-0.013514094617
H	1.275722499479	2.485084986680	-0.007052307602

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quinoline S1T5-MESX 0.20 eV (1.62 cm⁻¹) S -401.515138796685 T -401.515138814688

C	-0.008442910612	-0.710006299895	-0.016916102215
N	1.186838236780	-1.319700452558	-0.030117336551
C	-1.224352683334	-1.410453732152	-0.012762737374
C	-0.000580814282	0.761889204111	-0.007730934736
C	-1.242617728551	1.396398116384	0.004168772950
C	-2.425212306220	-0.736079327398	0.000169341963
C	-2.425934663697	0.677917527960	0.008828953496
C	2.426423593076	0.701179305744	-0.026564611062
H	-1.270554660012	2.475168906121	0.009713546531
H	-1.183711491303	-2.486600976458	-0.019408665046
H	-3.354802499255	-1.277548889312	0.004147443042
H	-3.363878040548	1.208630854209	0.018635195623
C	2.358361023028	-0.712349819115	-0.033346231261
H	3.392305664388	1.175626012528	-0.029532735842
H	3.243950812753	-1.326289705982	-0.040183644466
C	1.256277396575	1.419321875613	-0.013195022473
H	1.274223231137	2.497329382808	-0.006277929517

isoquinoline

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isoquinoline S1FCMIN 0.00 eV (Osci.Str. 0.11) -401.517606693104

C	-1.266444680026	-1.317613849239	0.000071681761
N	-2.466589783271	-0.670648088354	0.000032921413
C	-2.400487259552	0.636764998847	0.000009140519
C	-1.198208352433	1.393185048504	0.000020477899
C	1.278313822757	1.387257992598	0.000006912053
C	2.494285174561	0.655037721634	0.000011830051
C	2.442826821898	-0.714486641165	-0.000026779155
C	1.198834191981	-1.397262382997	-0.000087981169
C	0.038783220004	0.739536052378	-0.000014227054
C	-0.013947761709	-0.696350381331	-0.000039774830
H	-1.319559768500	-2.395631439420	0.000188659063
H	-3.341825039465	1.167729261995	-0.000128934415
H	-1.252629737737	2.469483324923	-0.000006215911
H	1.303730159557	2.465264273865	0.000056165856
H	3.435864177593	1.175961377822	0.000050840388
H	3.351074758509	-1.294702013733	-0.000012108707
H	1.187814074746	-2.475296909788	-0.000132607767

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isoquinoline S1FCMIN-b 0.00 eV (Osci.Str. 0.07) -401.517456483318

C	1.216917926822	1.239852680537	0.662173542959
N	2.366752574189	0.560360018174	0.502753200802
C	2.419999347414	-0.506446627179	-0.238112266105
C	1.255683861229	-1.053746325880	-0.812987457308
C	-1.219500749941	-1.105824960564	-0.836389084164
C	-2.452183457253	-0.527703597869	-0.471928737142
C	-2.468572774815	0.603940767296	0.304465448906
C	-1.262620342872	1.182681847203	0.746787543508
C	-0.011242121425	-0.548338809321	-0.426568547826
C	-0.034642817504	0.631271533983	0.391595507294
H	1.283229319188	2.271548252974	0.965693781873
H	3.351203626484	-1.051618875709	-0.281008550796
H	1.325459114448	-1.992943517901	-1.336607932849
H	-1.204498737140	-1.968379817144	-1.483529146494
H	-3.371780155825	-0.981103204536	-0.801629153895

H	-3.404329798514	1.046143362445	0.605045280846
H	-1.288408528884	2.054885148670	1.379782394335

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isoquinoline S1T2-MESX 0.19 eV (0.02 cm-1) -401.510565059213 -401.510565107681

C	-1.250270809983	-1.317902824017	0.000097165036
N	-2.471219534555	-0.667239154726	-0.000012148698
C	-2.390958029005	0.627886820357	-0.000029367651
C	-1.165809077306	1.388563793974	0.000005156607
C	1.257022952303	1.379505557450	0.000009628871
C	2.494761474353	0.655984387879	-0.000070837333
C	2.433024125807	-0.699204061039	0.000128094244
C	1.178279860262	-1.390203724663	-0.000183324547
C	0.042769150353	0.756976374242	0.000044591092
C	-0.026526413544	-0.739466513178	0.000003916160
H	-1.324482691013	-2.395592705249	0.000161543713
H	-3.322476918507	1.177010688799	-0.000121412131
H	-1.229498458346	2.465637853926	0.000024725559
H	1.283706522802	2.458994022780	0.000066574139
H	3.430387184261	1.185496356456	0.000018627003
H	3.335608439963	-1.288810189236	-0.000073841903
H	1.197516241057	-2.469408337150	-0.000069090161

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isoquinoline S1T3-MESX 0.004 eV (0.16 cm-1) -401.517456246511 -401.517456320460

C	-1.264418017789	-1.316852169169	0.000132021817
N	-2.470161268932	-0.665005105555	0.000008252049
C	-2.402886455045	0.634872417585	-0.000092752638
C	-1.199419497919	1.393091441201	0.000028076131
C	1.275622637743	1.385533214089	-0.000148269736
C	2.496908284781	0.650710734087	0.000131871429
C	2.446210442235	-0.712019667454	-0.000168975105
C	1.200123375619	-1.396755041076	0.000103841676
C	0.038695298992	0.737710147502	0.000192624610
C	-0.014045396262	-0.695695303416	-0.000219838699
H	-1.320434193635	-2.394217564154	0.000167386386
H	-3.343535933152	1.168160266605	-0.000086449841
H	-1.253638686009	2.469188485165	0.000008038207

H	1.301810275814	2.463348360178	0.000070294504
H	3.437412594774	1.173877454300	0.000020812562
H	3.354078796634	-1.293111778705	-0.000010326155
H	1.189511761065	-2.474607544640	-0.000136607198

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isoquinoline S1T4-MESX 0.005 eV (0.05 cm-1) -401.517434297677 -401.517434336110

C	-1.266513233652	-1.319581375496	0.000021917119
N	-2.464015885752	-0.672863658255	-0.000027311213
C	-2.394634873978	0.640848407609	0.000128218155
C	-1.199917421280	1.394937837580	-0.000063103095
C	1.278393784626	1.390387283191	0.000042139585
C	2.490851031032	0.659661648105	-0.000083878372
C	2.436880494897	-0.717674471514	0.000112910748
C	1.200712894926	-1.402069627744	-0.000148819279
C	0.040661658461	0.741121788063	0.000018839120
C	-0.015319775951	-0.699658638844	0.000030691436
H	-1.318974760022	-2.397648934612	0.000162595731
H	-3.337313276990	1.169303032277	-0.000162696842
H	-1.253913909923	2.471165304158	0.000034776432
H	1.302091705814	2.468290903694	0.000036867494
H	3.434570000894	1.176340827431	0.000041312196
H	3.347512024176	-1.294483221767	-0.000077036456
H	1.190763561643	-2.479848757341	-0.000067422763

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isoquinoline S1T4T5 0.009 eV (3.33 cm-1, 0.04 cm-1) -401.517258885441 -
401.517258743499

C	-1.264633003145	-1.325925684972	0.000000365806
N	-2.453003172992	-0.664834832656	0.000004681611
C	-2.396158128061	0.648871591295	0.000002607989
C	-1.201578271925	1.396075180868	0.000003211490
C	1.275721751326	1.386128523289	-0.000001139671
C	2.488473523346	0.658270791144	-0.000006153715
C	2.438143359077	-0.716778906894	-0.000001373518
C	1.203024250187	-1.401496378396	-0.000003227433
C	0.038886674255	0.736316739316	0.000001284262
C	-0.012615745835	-0.701023554415	-0.000002514205

H	-1.323144498508	-2.403034657402	-0.000002820319
H	-3.340800616581	1.173127839419	0.000011149250
H	-1.252088520296	2.472449458147	0.000004532713
H	1.298080008005	2.464218059140	-0.000004803438
H	3.430650711540	1.178059821451	-0.000005429653
H	3.349292761049	-1.292790132543	-0.000001817810
H	1.193582937478	-2.479405510260	0.000001446633