

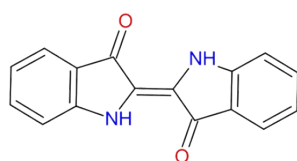
## Supplementary Information

### Indigo-Functionalized BODIPY, Aza-BODIPY, and BOPHY Systems for CYP17A1-Targeted NIR Bioimaging in Prostate Cancer

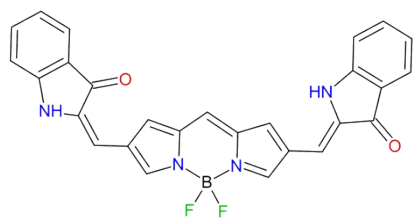
Naveed Khan<sup>a</sup>, Rohith Ramasamy<sup>a</sup>, Rajadurai Vijay Solomon<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, Madras Christian College (Autonomous),

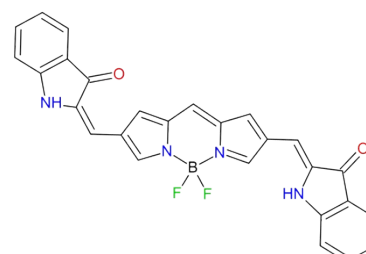
Tambaram East, Chennai – 600 059, Tamil Nadu, India



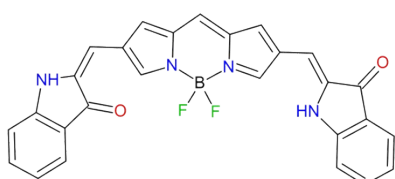
**IB0**



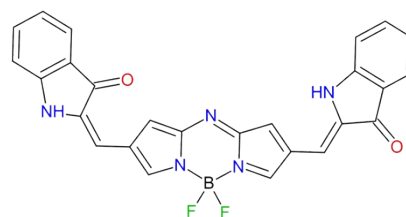
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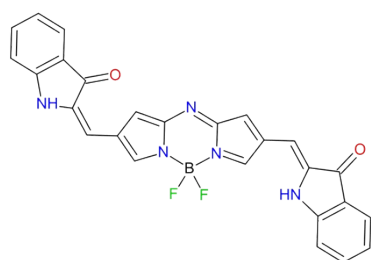
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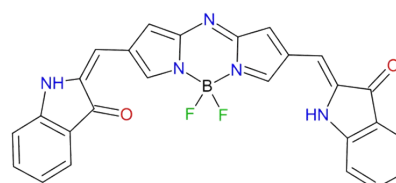
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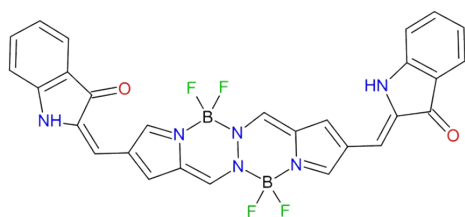
**IB4**



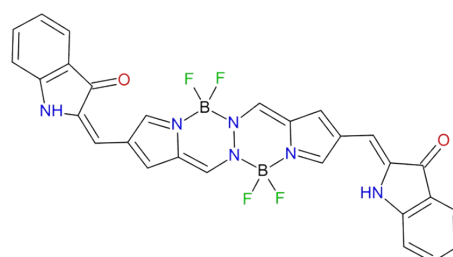
**IB5**



**IB6**

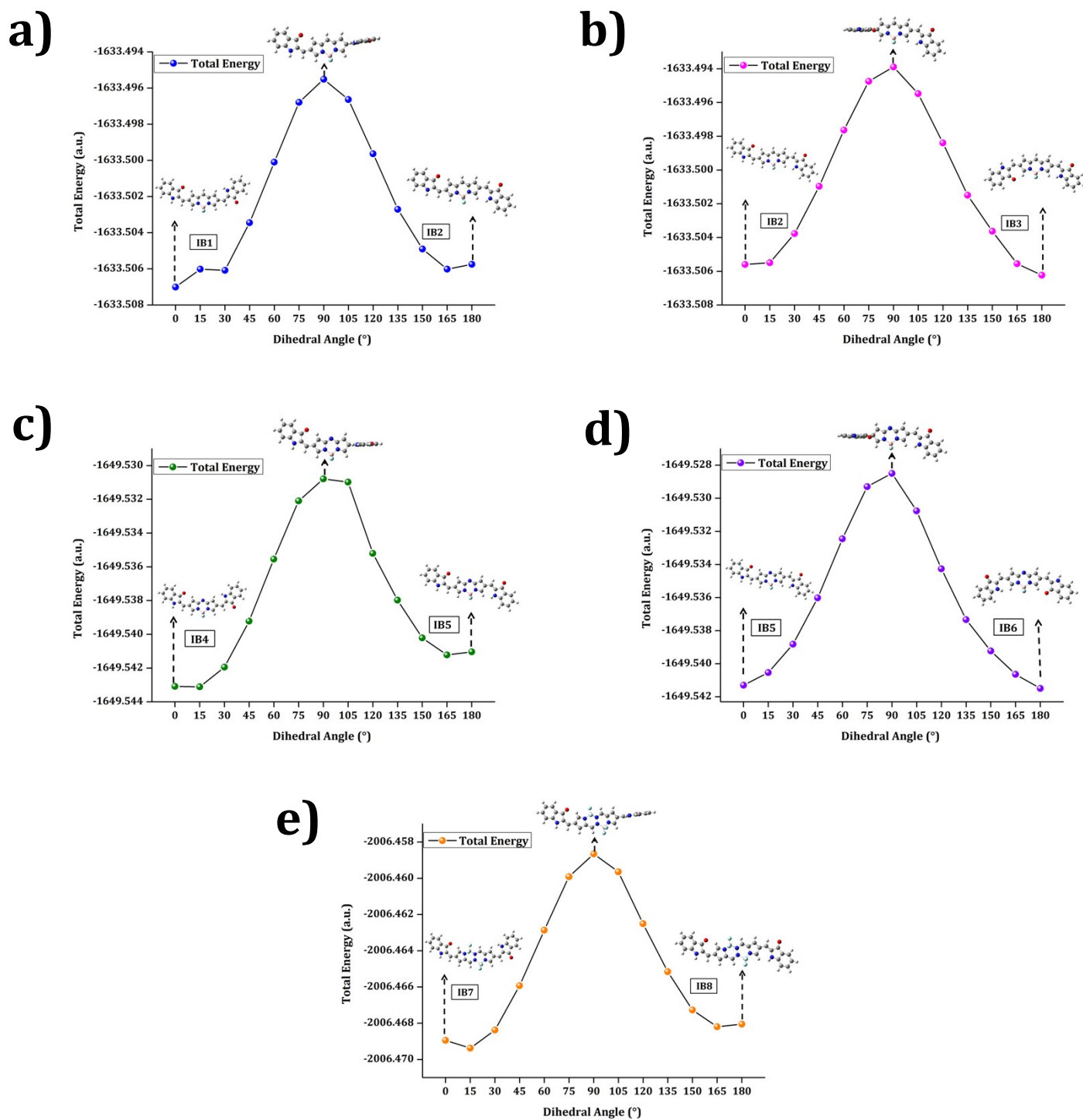


**IB7**



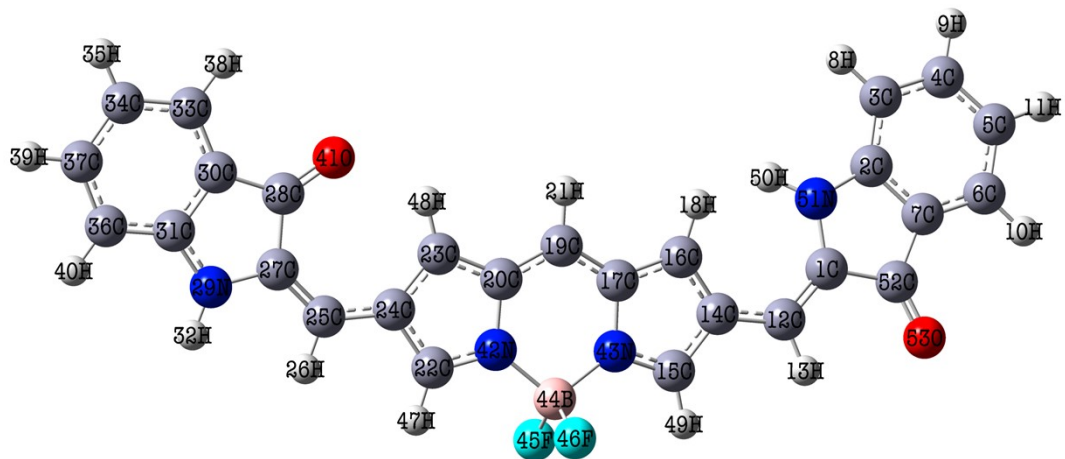
**IB8**

**SIF1.** 2D structural representation of IB0 and designed IBs

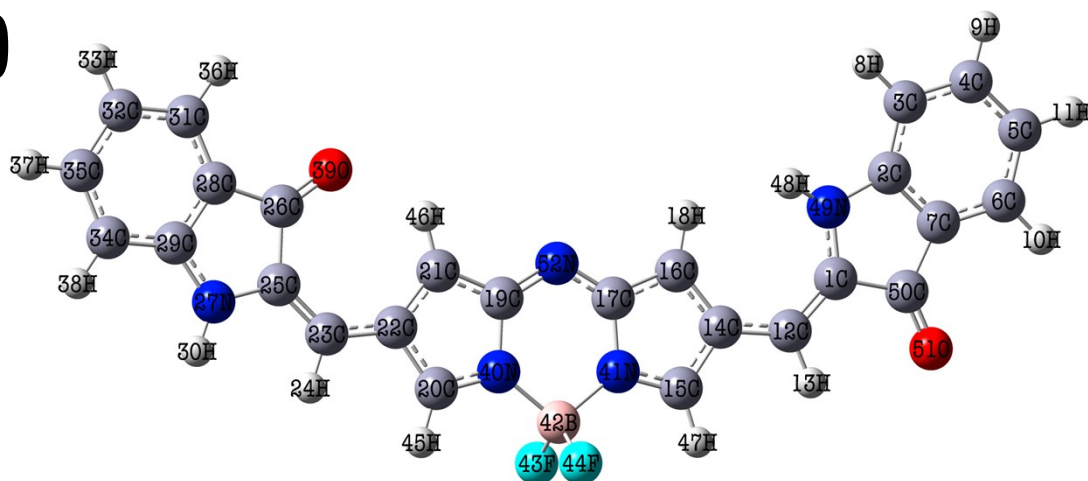


**SIF2.** Potential energy surface (PES) scan performed for the three molecular series: a) and b) BODIPY (IB1–IB3), c) and d) Aza-BODIPY (IB4–IB6), e) and f) BOPHY (IB7–IB8) to determine the barrier to interconversion. The energy profile illustrates the relative stability of each isomer and the transition barriers separating them.

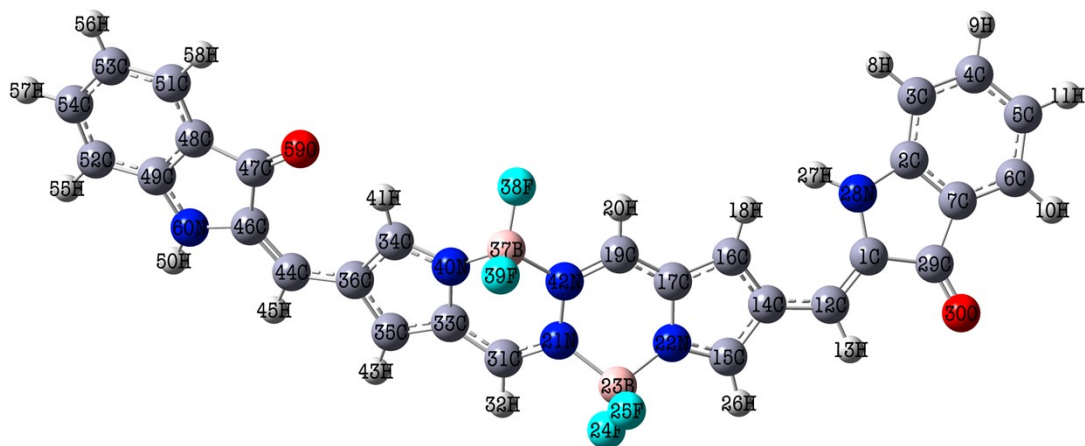
a)



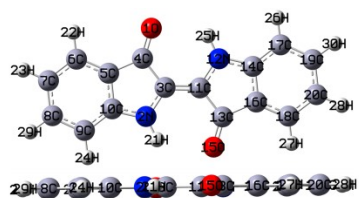
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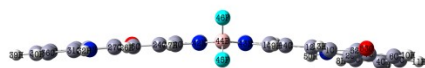
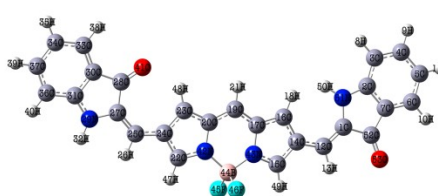
c)



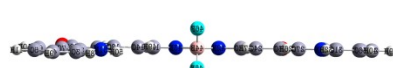
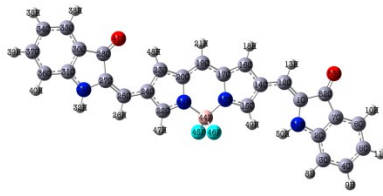
**SIF3.** Labelled molecular diagram of the designed molecular series: a) BODIPY series, b) Aza-BODIPY series, and c) BOPHY series



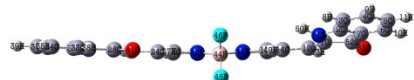
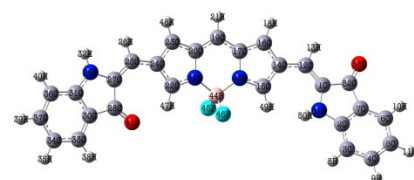
**IB0**



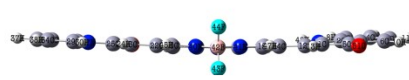
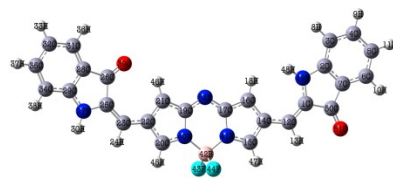
**IB1**



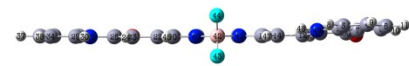
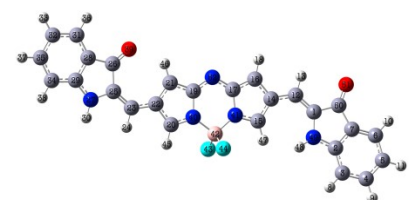
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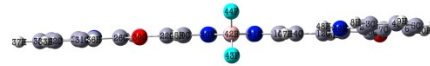
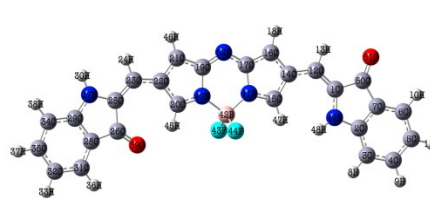
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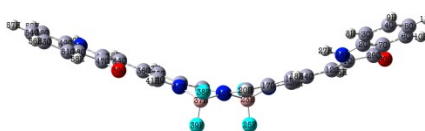
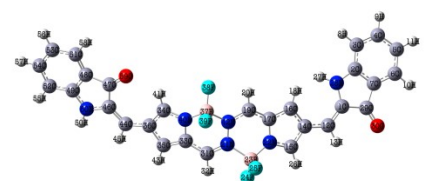
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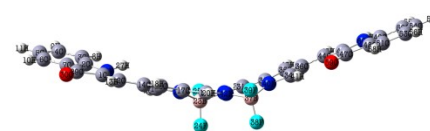
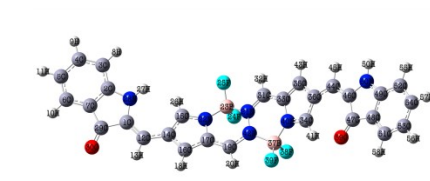
**IB5**



**IB6**



**IB7**



**IB8**

**SIF4.** Excited state Optimized geometry of IB0 and designed IBs at M06L/6-311G(d,p) level

**SIT1.** Computed total thermodynamic energy of IB0 and its designed IBs at M06L/6-311G(d,p) level

Molecules	Total energy (au)
IB0	-875.82
IB1	-1633.51
IB2	-1633.51
IB3	-1633.51
IB4	-1649.54
IB5	-1649.54
IB6	-1649.54
IB7	-2006.47
IB8	-2006.47

**SIT2.** Ground-state optimized coordinates of IB0 and its designed IBs at M06L/6-311G(d,p) level

IB0				IB1			
O	1.13735300	2.36640600	-0.00020000	C	-5.73533700	-0.21973600	-0.05117700
N	1.48206400	-1.11312300	-0.00064500	C	-6.76124800	1.80207700	0.10564700
C	0.68120200	0.00086100	-0.00030200	C	-7.02260400	3.16143300	0.24499000
C	1.54660600	1.20386900	-0.00019300	C	-8.35644600	3.55407600	0.29807900
C	2.90408700	0.67326100	-0.00000100	C	-9.40848200	2.63132100	0.21596700
C	4.14816500	1.29982600	0.00027700	C	-9.13568300	1.27678400	0.08713800
C	5.29150900	0.51312900	0.00045800	C	-7.80697900	0.86511500	0.03760900
C	5.18435300	-0.88434300	0.00035100	H	-6.21991100	3.88807100	0.30745300
C	3.95249800	-1.53106500	0.00002900	H	-8.58653600	4.60957100	0.40487400
C	2.81264400	-0.73492600	-0.00014400	H	-9.93257800	0.54130000	0.03184400
C	-0.68120200	-0.00086200	-0.00008300	H	-10.43344400	2.98203700	0.25725600
N	-1.48206400	1.11312400	0.00022800	C	-4.81805200	-1.21488600	-0.08725100

C	-1.54660600	-1.20386900	0.00001200	H	-5.24824500	-2.21359700	-0.07567200
C	-2.81264300	0.73492600	0.00006700	C	-3.39189800	-1.11414200	-0.12848300
O	-1.13735300	-2.36640600	0.00001000	C	-2.52675000	-2.22850200	0.03124100
C	-2.90408700	-0.67326100	0.00001300	C	-2.54778500	-0.01148400	-0.32855800
C	-3.95249800	1.53106500	0.00006000	C	-1.22430600	-0.47720100	-0.27487500
C	-4.14816500	-1.29982600	-0.00001700	H	-2.81713800	1.01516100	-0.52647000
C	-5.18435300	0.88434400	0.00000300	C	-0.00978500	0.19413700	-0.36843000
C	-5.29150900	-0.51312900	-0.00002300	C	1.20474200	-0.45817200	-0.21014700
H	1.10891000	-2.05268500	0.00038400	H	-0.01215400	1.26353000	-0.54590300
H	4.20898300	2.38360900	0.00036900	C	2.50778300	-2.18589500	0.18824200
H	6.27234200	0.97501800	0.00069300	C	2.52240900	0.02900800	-0.19880000
H	3.88409100	-2.61287700	-0.00006700	C	3.36881500	-1.05882500	0.05806600
H	-1.10891000	2.05268500	-0.00046900	C	4.78530400	-1.19795400	0.20553100
H	-3.88409100	2.61287700	0.00008800	H	5.10588200	-2.21807700	0.41461700
H	-4.20898300	-2.38360900	-0.00004500	C	5.79075600	-0.28245500	0.13499200
H	-6.27234200	-0.97501800	-0.00005100	C	5.77013500	1.19233800	-0.13294500
H	6.08867500	-1.48399300	0.00051100	N	7.12405000	-0.62902900	0.32097600
H	-6.08867500	1.48399300	-0.00001300	C	7.16800100	1.60359100	-0.07489500
				C	7.94730700	0.46548400	0.20266300
				H	7.44110800	-1.56513100	0.51769400
				C	7.76477200	2.85117400	-0.24021600
				C	9.14370100	2.95010400	-0.12597500
				H	9.63627000	3.90788900	-0.24909700
				C	9.33292800	0.55326200	0.31981700
				C	9.90912100	1.80703900	0.15127500
				H	7.14988000	3.72023500	-0.45318500
				H	10.98696800	1.90197200	0.23745500
				H	9.93852500	-0.32012500	0.53413000
				O	4.78657700	1.89445200	-0.35329400
				N	1.23591900	-1.83539300	0.03174600
				N	-1.25176900	-1.85371000	-0.04775900
				B	-0.00124800	-2.78929500	0.01472700
				F	-0.03517200	-3.56108900	1.16315300
				F	0.04301700	-3.59448700	-1.11507000
				H	2.78348100	-3.21394700	0.38705700
				H	2.82715500	1.05179500	-0.34740100
				H	-2.79663600	-3.26243400	0.20279900

				H	-4.68115200	1.57776500	0.31032300
				N	-5.53866300	1.15389400	-0.00994700
				C	-7.20956100	-0.46428800	-0.06158700
				O	-7.75629400	-1.55821300	-0.14255200
<b>IB2</b>				<b>IB3</b>			
C	-5.71517000	0.93153300	0.00017700	C	5.69369200	-0.57471900	0.05412800
C	-7.29505800	-0.70709100	0.00033700	C	6.61609300	1.48541500	-0.19960300
C	-7.94145500	-1.93927600	0.00039600	C	6.80368800	2.84458000	-0.42744000
C	-9.33221100	-1.93058900	0.00048800	C	8.11357100	3.30825400	-0.48658000
C	-10.07041400	-0.73886700	0.00052200	C	9.21291800	2.45390600	-0.32197700
C	-9.41420200	0.48409700	0.00046100	C	9.01365800	1.09847200	-0.10186600
C	-8.02218200	0.49676900	0.00037000	C	7.70840400	0.61479100	-0.04756200
H	-7.38474400	-2.86993100	0.00036900	H	5.96231700	3.51697800	-0.55421200
H	-9.86019400	-2.87914200	0.00053500	H	8.28722400	4.36491800	-0.66401600
H	-9.96396200	1.42049700	0.00048500	H	9.84980800	0.41598800	0.01748400
H	-11.15365800	-0.77946200	0.00059500	H	10.21756400	2.85851600	-0.37119700
C	-4.55903200	1.63829300	0.00004600	C	4.83002900	-1.61495900	0.11452100
H	-4.71570300	2.71441400	0.00002600	H	5.31162800	-2.58849600	0.16323500
C	-3.19813000	1.19561500	-0.00006500	C	3.39790600	-1.59353200	0.10291500
C	-2.68613400	-0.12916000	-0.00010300	C	2.53502200	-0.48062000	0.29419000
C	-2.06927400	2.02770800	-0.00018200	C	2.55174900	-2.69490700	-0.08109000
C	-0.93051700	1.20898600	-0.00021300	C	1.22882000	-2.23257600	-0.01764600
H	-2.06448100	3.10811800	-0.00020100	H	2.85050500	-3.71785600	-0.25980000
C	0.42758700	1.51433900	-0.00026100	C	0.01236800	-2.88852200	-0.17951000
C	1.40245900	0.52658400	-0.00027000	C	-1.19743700	-2.21288400	-0.12866600
H	0.73177500	2.55464600	-0.00030100	H	0.01233300	-3.95620500	-0.36717100
C	2.14545800	-1.54430000	-0.00018200	C	-2.49606500	-0.43408000	0.08069100
C	2.80648600	0.60482000	-0.00033300	C	-2.51903500	-2.64917800	-0.31237500
C	3.29760900	-0.70865300	-0.00018100	C	-3.36053200	-1.53629900	-0.18659300
C	4.60726200	-1.28511000	-0.00007600	C	-4.78327000	-1.59227100	-0.32531000
H	4.60223500	-2.37442000	0.00002800	H	-5.15536800	-2.59272600	-0.54312600
C	5.84365900	-0.71758000	-0.00007900	C	-5.74363400	-0.63137400	-0.23365900
C	6.27198300	0.71994000	-0.00019900	C	-5.66303700	0.83934300	0.05721900
N	7.00852200	-1.47484800	0.00005600	N	-7.09243400	-0.92058700	-0.41096500
C	7.72979000	0.67643600	-0.00011100	C	-7.04475000	1.30248500	0.03668400
C	8.12520400	-0.67368000	0.00005100	C	-7.87093000	0.19959700	-0.24671100
H	7.02765700	-2.48234900	0.00010800	H	-7.45254500	-1.84468300	-0.58866100

C	8.68083600	1.69449000	-0.00015900	C	-7.59367800	2.56601200	0.24653200
C	10.02514200	1.35099100	-0.00003200	C	-8.97078700	2.71432500	0.17324500
H	10.78746100	2.12195200	-0.00005800	H	-9.42636000	3.68479000	0.33329700
C	9.47227600	-1.03006900	0.00017700	C	-9.25509200	0.33749800	-0.32478400
C	10.40474000	0.00022900	0.00013700	C	-9.78270100	1.60514000	-0.10974700
H	8.36203400	2.73228000	-0.00028400	H	-6.94438800	3.40847100	0.46472200
H	11.46059300	-0.25128400	0.00023500	H	-10.85864000	1.73863300	-0.16323800
H	9.78132300	-2.06928800	0.00030300	H	-9.89538900	-0.50988600	-0.54279100
O	5.54430700	1.70907200	-0.00033400	O	-4.65030900	1.50265200	0.26797400
N	1.03102200	-0.82247200	-0.00023300	N	-1.22851200	-0.83606400	0.11191900
N	-1.35344200	-0.12029900	-0.00018000	N	1.25880200	-0.85902800	0.22107800
B	-0.42734300	-1.37601000	-0.00024000	B	0.01037400	0.05471800	0.44711900
F	-0.65018600	-2.13563000	1.13873900	F	-0.04279500	0.45966000	1.77332900
F	-0.65020800	-2.13554000	-1.13927600	F	0.06150100	1.15129100	-0.39664200
H	2.11009500	-2.62656400	-0.00011800	H	-2.78188600	0.59487800	0.24274900
H	3.39739100	1.50645600	-0.00039000	H	-2.81763700	-3.66607800	-0.52383000
H	-3.20498900	-1.07706000	-0.00006500	H	2.78045000	0.54774500	0.52191000
H	-5.23610200	-1.15193300	0.00014900	H	4.57202500	1.13320800	-0.48227400
N	-5.93999500	-0.43401200	0.00024300	N	5.42419700	0.78422700	-0.06915900
C	-7.06025500	1.59596500	0.00029800	C	7.17933700	-0.73712800	0.12056100
O	-7.26155100	2.80474600	0.00025400	O	7.77979900	-1.79275200	0.28497800
<b>IB4</b>				<b>IB5</b>			
C	-5.66647500	-0.16903800	0.04114800	C	-5.62899100	1.00394100	0.02775500
C	-6.70859300	1.85052100	-0.05405800	C	-7.17919400	-0.62373100	-0.30470600
C	-6.97731400	3.21204400	-0.14521500	C	-7.80357000	-1.83079600	-0.59771000
C	-8.31441700	3.59937100	-0.15168200	C	-9.19439000	-1.84873300	-0.59112300
C	-9.36003300	2.67018400	-0.07036600	C	-9.95120100	-0.70486700	-0.30168500
C	-9.07881000	1.31322000	0.01429100	C	-9.31645500	0.49722500	-0.02288900
C	-7.74838200	0.90726100	0.01957800	C	-7.92438900	0.53490800	-0.03126000
H	-6.17959700	3.94402000	-0.20714200	H	-7.23034400	-2.72437000	-0.81869900
H	-8.55119900	4.65640200	-0.22067100	H	-9.70699300	-2.77937300	-0.81355500
H	-9.87105400	0.57310900	0.07228700	H	-9.88188100	1.39869300	0.19278400
H	-10.38704800	3.01687500	-0.07634200	H	-11.03356200	-0.76501000	-0.30110700
C	-4.75273500	-1.17073500	0.05900400	C	-4.47355800	1.70122000	0.14291500
H	-5.19545900	-2.16394600	0.07725300	H	-4.61269300	2.77134500	0.27428500
C	-3.32753200	-1.09702900	0.05390500	C	-3.12738200	1.21761100	0.11446300
C	-2.50751200	-2.26158900	-0.01635800	C	-2.68684200	-0.13454100	0.22971600

C	-2.43907000	-0.01940100	0.11810100	C	-1.96259300	1.98358400	0.02716300
C	-1.13190100	-0.54329000	0.08092200	C	-0.86495900	1.10327600	0.07501900
H	-2.64391200	1.03604300	0.20436600	H	-1.88948300	3.05692000	-0.06333200
C	1.15243900	-0.53946700	0.06015300	C	1.31925600	0.43340800	0.09373800
C	2.52139900	-2.25763900	-0.06959500	C	2.11516600	-1.60946500	0.27988500
C	2.46016800	-0.01277600	0.07279200	C	2.72638400	0.54488700	0.05688300
C	3.34589700	-1.09018800	-0.01029300	C	3.25036400	-0.74398500	0.17290300
C	4.76882300	-1.21512300	-0.04547700	C	4.56867400	-1.29315600	0.19634800
H	5.11841900	-2.24513700	-0.10482300	H	4.59101900	-2.37492500	0.32005800
C	5.75151200	-0.27127400	-0.02069000	C	5.79055300	-0.70103300	0.08138400
C	5.68003900	1.22772400	0.04708300	C	6.17940400	0.73773300	-0.10950400
N	7.09721800	-0.59676300	-0.06628200	N	6.97074400	-1.42402800	0.11796700
C	7.07014800	1.67016500	0.02837000	C	7.63659100	0.72524500	-0.18229100
C	7.88894200	0.52916900	-0.03908900	C	8.06684600	-0.60608800	-0.04300600
H	7.44886600	-1.53996600	-0.11866300	H	7.01614100	-2.42713100	0.20671900
C	7.63025000	2.94457100	0.06657000	C	8.55994700	1.75339100	-0.35544100
C	9.01218200	3.06469600	0.03617200	C	9.91074900	1.43593500	-0.38980900
H	9.47697900	4.04378700	0.06424500	H	10.65211900	2.21503300	-0.52434900
C	9.27638400	0.63678900	-0.06919400	C	9.41852600	-0.93709000	-0.07648500
C	9.81656400	1.91745800	-0.03022000	C	10.32405800	0.10304100	-0.25187500
H	6.98658300	3.81720000	0.11805100	H	8.21653200	2.77787100	-0.46182000
H	10.89584400	2.02976600	-0.05273800	H	11.38431500	-0.12701400	-0.28223400
H	9.91080200	-0.24075800	-0.12047800	H	9.75267400	-1.96308400	0.02936900
O	4.66801600	1.91828700	0.10549500	O	5.42447700	1.70119400	-0.18639200
N	1.23557200	-1.94241600	-0.03011800	N	0.98267200	-0.92773400	0.23190500
N	-1.21935000	-1.94250100	-0.00454700	N	-1.35909800	-0.20268800	0.20430300
B	0.00777300	-2.90797100	-0.05648700	B	-0.47489400	-1.48593200	0.27580900
F	0.01991800	-3.73462800	1.05295900	F	-0.70004900	-2.17435400	1.45382300
F	-0.00527100	-3.64767600	-1.22514500	F	-0.71087800	-2.29478200	-0.82290700
H	2.84436800	-3.28952700	-0.13798400	H	2.11784100	-2.68786800	0.38442000
H	2.71555900	1.03112100	0.13242800	H	3.28217000	1.46180900	-0.04359500
H	-2.83123800	-3.29324900	-0.07513400	H	-3.27318000	-1.03314200	0.37129200
H	-4.61325300	1.65833700	-0.21490300	H	-5.14388000	-0.91830300	-0.69696300
N	-5.48445600	1.19927300	-0.00439400	N	-5.81916100	-0.35205600	-0.20518100
C	-7.14256200	-0.42007400	0.08181000	C	-6.98090700	1.63046700	0.18207000
O	-7.67943500	-1.51821400	0.15468800	O	-7.20036800	2.80694100	0.44141000
N	0.01094900	0.12421200	0.11461600	N	0.42579100	1.40236700	0.02165300

IB6				IB7			
C	5.68918300	-0.56618500	0.00065700	C	6.71734200	0.13800800	-0.31166600
C	6.84108100	1.39734300	0.00027500	C	7.48497200	2.26704400	-0.11748900
C	7.17799800	2.74650100	-0.00015000	C	7.57232500	3.64551000	0.04804000
C	8.53236400	3.06599000	0.00010300	C	8.81701300	4.23579800	-0.14660600
C	9.53005500	2.08143500	0.00076100	C	9.95018500	3.48675700	-0.49306600
C	9.18044600	0.73781300	0.00116400	C	9.84945900	2.11331400	-0.66390700
C	7.83066100	0.39879100	0.00092300	C	8.60948400	1.50669000	-0.48128100
H	6.41755200	3.51966800	-0.00065800	H	6.70568000	4.23829300	0.31840400
H	8.82197900	4.11187200	-0.00021300	H	8.91087900	5.31028400	-0.02491700
H	9.93461400	-0.04341300	0.00166300	H	10.70989200	1.51282500	-0.94232100
H	10.57327000	2.37550600	0.00094000	H	10.90203400	3.98720700	-0.63041300
C	4.74017900	-1.53447400	0.00068900	C	5.93075600	-0.95877700	-0.39229800
H	5.15974300	-2.53814300	0.00103500	H	6.44848000	-1.84861500	-0.74287000
C	3.31357600	-1.45030600	0.00033400	C	4.53482300	-1.08741500	-0.09227300
C	2.48313600	-0.29026100	0.00020000	C	3.77096900	-2.23267000	-0.41977000
C	2.43358000	-2.53578500	0.00011100	C	3.64941300	-0.20935900	0.55835900
C	1.12171700	-2.02816000	-0.00017400	C	2.39695400	-0.83364100	0.58303100
H	2.69088200	-3.58423200	0.00014000	H	3.85713900	0.75778200	0.99078400
C	-1.16152300	-2.04652100	-0.00061600	C	1.16510400	-0.39912700	1.06819200
C	-2.54483000	-0.31980600	-0.00065100	H	1.08327500	0.52426800	1.62855600
C	-2.46955200	-2.57102900	-0.00080000	N	0.03395700	-2.19691900	0.13085500
C	-3.36105400	-1.49750100	-0.00079300	N	2.50287700	-2.07126900	-0.03488600
C	-4.78348700	-1.62765300	-0.00085200	B	1.35610600	-3.09336200	0.04680700
H	-5.12142900	-2.66293500	-0.00100600	F	1.27096200	-3.87957700	-1.07603000
C	-5.78002100	-0.69764500	-0.00067400	F	1.44927600	-3.83666100	1.20798200
C	-5.75043100	0.80595500	-0.00036200	H	4.09747600	-3.14272200	-0.90444800
N	-7.11946300	-1.05854700	-0.00068200	H	5.44231800	1.79609600	-0.00873400
C	-7.15063500	1.20853600	-0.00016100	N	6.38355000	1.43773800	0.04791800
C	-7.94083300	0.04603600	-0.00033600	C	8.18018600	0.11713300	-0.62326400
H	-7.44500200	-2.01247200	-0.00074800	O	8.83661400	-0.87212100	-0.92530600
C	-7.73894000	2.47059800	0.00018100	C	-1.09031800	-2.55834900	-0.46648600
C	-9.12326100	2.55763300	0.00036700	H	-1.00621100	-3.44938500	-1.07634700
H	-9.61116600	3.52580500	0.00064800	C	-2.29505100	-1.87067400	-0.37233500
C	-9.33096900	0.12088300	-0.00015700	C	-3.64737600	-0.28477600	0.36819900
C	-9.90030900	1.38974400	0.00020100	C	-3.50122000	-2.02169800	-1.06220200
H	-7.11400300	3.35800900	0.00031200	C	-4.37087900	-1.01273800	-0.61359800

H	-10.98224400	1.47587000	0.00035700	B	-1.34528100	-0.52592600	1.56133100
H	-9.94637000	-0.77139700	-0.00028200	F	-1.21114400	0.80713300	1.86063700
O	-4.76177400	1.53352400	-0.00034000	F	-1.56607400	-1.30500700	2.68119300
N	-1.25910100	-0.64205300	-0.00055600	N	-2.41809300	-0.79124100	0.49397400
N	1.19714200	-0.62714000	-0.00009700	H	-3.99424600	0.54935600	0.95839600
B	-0.03741200	0.33159100	-0.00035700	N	0.01895700	-1.02970500	0.88356700
F	-0.04008300	1.11500200	1.13947100	H	-3.70578500	-2.76285800	-1.82131000
F	-0.03961600	1.11492700	-1.14023900	C	-5.69803200	-0.83289600	-1.12565800
H	-2.89217700	0.70421300	-0.00061300	H	-5.95785800	-1.54636800	-1.90656600
H	-2.71084600	-3.62342300	-0.00087200	C	-6.67430200	0.06174800	-0.81577500
H	2.75680700	0.75569200	0.00037200	C	-6.72700800	1.16626700	0.19840800
H	4.73414100	1.34417400	-0.00047000	C	-8.05009500	1.75572400	0.04352600
N	5.58674400	0.81123000	0.00016000	C	-8.72175000	1.06116600	-0.97907100
C	7.15457800	-0.89534500	0.00119500	H	-8.14622600	-0.54534800	-2.22702000
O	7.63292400	-2.02249700	0.00169000	C	-8.66664700	2.81415300	0.70752300
N	-0.01772900	-2.70489500	-0.00044000	C	-10.01519400	1.41447400	-1.35933400
				C	-9.95450600	3.17236100	0.33874600
				C	-10.61162400	2.47379300	-0.68627100
				H	-10.53581300	0.88402400	-2.14869600
				H	-10.45938300	3.99160100	0.83754400
				H	-11.61905200	2.76799100	-0.96372600
				H	-8.13631200	3.34029400	1.49534500
				O	-5.84467900	1.49559500	0.98830400
				N	-7.90738700	0.06625300	-1.46291700
<b>IBB</b>							
C	6.72859200	0.65659000	0.71887000				
C	8.00174000	-1.22211600	0.62664700				
C	8.43381300	-2.53564100	0.47768900				
C	9.75217600	-2.81863600	0.81869600				
C	10.62566000	-1.83024600	1.29414200				
C	10.18073600	-0.52539700	1.44833400				
C	8.86064300	-0.22520200	1.11866200				
H	7.77015800	-3.30934100	0.10773700				
H	10.11387500	-3.83640200	0.71110100				
H	10.83504400	0.25442800	1.82603400				
H	11.64727900	-2.09320800	1.54387100				
C	5.69397100	1.52650400	0.68641600				

H	5.91715000	2.50600300	1.10157800
C	4.36361000	1.30542100	0.19482800
C	3.90654400	0.25285500	-0.63580700
C	3.24571900	2.12247300	0.42984700
C	2.15848200	1.53559600	-0.22496500
H	3.21395300	3.01756400	1.03348700
C	0.80987500	1.88512500	-0.26862800
H	0.46341400	2.81713100	0.16094100
N	0.21172200	-0.09392800	-1.32501400
N	2.59792100	0.39001600	-0.87165800
B	1.69379700	-0.34813200	-1.87231100
F	1.78623700	0.21467400	-3.13100800
F	1.92448400	-1.70222900	-1.88367900
H	4.46134800	-0.54516400	-1.10847000
H	5.93242200	-1.25668000	0.31974800
N	6.75969000	-0.67798300	0.32360800
C	8.09628300	1.01738700	1.20638700
O	8.45624600	2.12641200	1.58255600
C	-0.72918100	-1.01965400	-1.42111700
H	-0.38201000	-1.97046400	-1.80596000
C	-2.05745900	-0.84436300	-1.05082500
C	-3.80218200	0.30075300	-0.31785100
C	-3.11610000	-1.75150200	-0.95212700
C	-4.23323700	-1.04360900	-0.47609600
B	-1.65991800	1.65861100	-0.90065400
F	-1.85204400	2.12293900	-2.18799900
F	-1.84716300	2.63235400	0.04809000
N	-2.51255900	0.40522700	-0.64839100
H	-4.38750500	1.14790900	0.00510800
N	-0.14456400	1.13813600	-0.79285200
H	-3.06746200	-2.80654400	-1.17986300
C	-5.50628700	-1.65878000	-0.24145500
H	-5.51851700	-2.72150400	-0.47956800
C	-6.68760600	-1.16001800	0.21103100
C	-7.08474900	0.21910600	0.64827600
C	-8.48908000	0.10451400	1.02072900
C	-8.88812300	-1.22944000	0.81615600

H	-7.85595800	-2.93348500	0.10687600
C	-9.39311700	1.05204700	1.49610100
C	-10.19498400	-1.63756000	1.07838500
C	-10.69551200	0.65611300	1.76215000
C	-11.08086200	-0.67691400	1.55037000
H	-10.50861200	-2.66361400	0.92024700
H	-11.42083600	1.37114700	2.13286900
H	-12.10465000	-0.96965600	1.76170400
H	-9.07073000	2.07770200	1.64853900
O	-6.37508100	1.22169300	0.68144700
N	-7.82033800	-1.95648400	0.34989400

**SIT3.** FMO Energies of IB0 and designed IBs from HOMO-2 to LUMO+2 and the HOMO-LUMO energy gap computed at M06L/6-311G(d,p) level

<b>Molecules</b>	<b>HOMO-2 (eV)</b>	<b>HOMO-1 (eV)</b>	<b>HOMO (eV)</b>	<b>LUMO (eV)</b>	<b>LUMO+1 (eV)</b>	<b>LUMO+2 (eV)</b>	<b>HOMO-LUMO Energy gap (eV)</b>
IB0	-6.163	-5.938	-5.012	-3.580	-1.960	-1.029	1.432
IB1	-6.057	-5.267	-4.988	-3.807	-2.950	-2.900	1.181
IB2	-6.042	-5.218	-4.983	-3.796	-2.948	-2.927	1.187
IB3	-6.014	-5.261	-5.014	-3.796	-2.975	-2.934	1.218
IB4	-6.150	-5.352	-5.043	-4.201	-3.034	-2.971	0.842
IB5	-6.124	-5.358	-5.085	-4.220	-3.056	-2.992	0.865
IB6	-6.110	-5.307	-5.060	-4.208	-3.074	-2.986	0.852
IB7	-6.066	-5.203	-5.069	-3.617	-3.063	-2.920	1.452
IB8	-6.049	-5.225	-5.069	-3.611	-3.055	-2.950	1.458

**SIT4.** Excited-state optimized coordinates of IBO and its designed IBs at M06L/6-311G(d,p) level

IB0				IB1			
O	-1.13471500	-2.40585600	0.00000100	C	5.74922200	-0.22085600	-0.02740700
N	-1.48981900	1.08380800	-0.00010400	C	6.83319600	1.77796500	-0.06776900
C	-0.68954500	-0.03784100	-0.00013200	C	7.13550000	3.13675400	-0.10146300
C	-1.53250000	-1.22461100	-0.00003500	C	8.47990300	3.49095200	-0.14674000
C	-2.89696200	-0.69110200	0.00009300	C	9.50151400	2.53060300	-0.16043400
C	-4.14285600	-1.29969300	0.00024500	C	9.18748300	1.17740300	-0.13498300
C	-5.28789000	-0.49596300	0.00033800	C	7.84902400	0.80283600	-0.09138300
C	-5.18764100	0.90004000	0.00027500	H	6.35520500	3.89006700	-0.08950500
C	-3.94733400	1.53505800	0.00012600	H	8.74328100	4.54341400	-0.17132100
C	-2.81390900	0.72584700	0.00004300	H	9.96247700	0.41692800	-0.15261500
C	0.68954500	0.03784300	-0.00017500	H	10.53673700	2.85070000	-0.19358500
N	1.48981900	-1.08380700	-0.00017300	C	4.79217000	-1.18774300	-0.01309800
C	1.53250100	1.22461200	-0.00013600	H	5.19519300	-2.19602600	-0.08284000
C	2.81390800	-0.72584700	-0.00011600	C	3.37770100	-1.06064800	0.07350700
O	1.13471700	2.40585800	-0.00014800	C	2.50685000	-2.16903700	-0.05105800
C	2.89696200	0.69110200	-0.00008800	C	2.54326600	0.05982700	0.28173500
C	3.94733300	-1.53505900	-0.00006200	C	1.21399900	-0.39318100	0.26628200
C	4.14285600	1.29969200	-0.00002700	H	2.82302100	1.08800500	0.45409900
C	5.18764000	-0.90004100	0.00000200	C	0.00260600	0.27823100	0.38119000
C	5.28789000	0.49596100	0.00001200	C	-1.22281100	-0.41133500	0.24168900
H	-1.09304800	2.01941300	-0.00003300	H	-0.00760200	1.34832600	0.54067400
H	-4.22284200	-2.38226900	0.00028800	C	-2.52088700	-2.18306700	-0.11647000
H	-6.26868100	-0.95926300	0.00045600	C	-2.52892100	0.05660000	0.22743900
H	-3.86413900	2.61600600	0.00007400	C	-3.37448000	-1.06924300	-0.00536900
H	1.09304800	-2.01941200	-0.00023600	C	-4.77996500	-1.18487900	-0.14158200
H	3.86413800	-2.61600700	-0.00006300	H	-5.12378300	-2.20249300	-0.32805300
H	4.22284300	2.38226900	-0.00001000	C	-5.78253900	-0.24928300	-0.09021400
H	6.26868200	0.95926100	0.00006200	C	-5.80031000	1.21858400	0.13774500
H	-6.08997500	1.50087400	0.00034300	N	-7.10975900	-0.63382200	-0.28319300
H	6.08997400	-1.50087500	0.00004400	C	-7.21625300	1.59239200	0.04628400
				C	-7.96576400	0.42502200	-0.21211100
				H	-7.39431800	-1.58691400	-0.46701600
				C	-7.84913300	2.81813700	0.16273400
				C	-9.23473000	2.86455000	0.01693100
				H	-9.75539000	3.81146400	0.10151300
				C	-9.35574300	0.45874800	-0.35916100
				C	-9.96987400	1.69636400	-0.24047700
				H	-7.27163200	3.71501000	0.36027400
				H	-11.04658100	1.76312300	-0.34899800
				H	-9.92545100	-0.44127800	-0.55800300
				O	-4.85189400	1.96520500	0.35597700

				N	-1.24286200	-1.79245600	0.02964000
				N	1.23254200	-1.78151100	0.05603100
				B	-0.00503400	-2.72000800	0.05502500
				F	0.01575500	-3.55012600	-1.06428100
				F	-0.00990600	-3.50747100	1.21123300
				H	-2.77633500	-3.21865000	-0.29201900
				H	-2.85154200	1.07741300	0.35304500
				H	2.76566000	-3.20670300	-0.21502300
				H	4.73089600	1.63946600	-0.15550400
				N	5.60067800	1.15691500	0.00523000
				C	7.20803300	-0.51081800	-0.07244200
				O	7.72366400	-1.62602900	-0.08435400
<b>IB2</b>				<b>IB3</b>			
C	5.73000800	0.94074300	0.00819900	C	5.70445400	-0.57939700	0.01910100
C	7.27552900	-0.72652000	-0.07665100	C	6.60305400	1.49622700	-0.19972600
C	7.89113100	-1.97379600	-0.14877600	C	6.77411300	2.86395400	-0.39195200
C	9.28046600	-1.99485700	-0.14865700	C	8.07847100	3.34264400	-0.44633200
C	10.03848600	-0.81752800	-0.08047600	C	9.18583500	2.49350800	-0.31182000
C	9.41083000	0.42256000	-0.01116400	C	9.00250400	1.12906900	-0.12539500
C	8.02305700	0.46538200	-0.01046600	C	7.70436000	0.62978500	-0.07464100
H	7.31133100	-2.88825500	-0.20116400	H	5.92426600	3.52971500	-0.49431100
H	9.79107400	-2.95056200	-0.20342900	H	8.24122400	4.40526900	-0.59540200
H	9.98477600	1.34234600	0.03952000	H	9.84788300	0.45445500	-0.02892000
H	11.12067200	-0.87915600	-0.08273700	H	10.18650200	2.90853600	-0.35703800
C	4.56236000	1.64359500	0.03872500	C	4.83462300	-1.62246100	0.07535000
H	4.72126600	2.72005900	0.06409000	H	5.32238400	-2.59472400	0.10031200
C	3.21076300	1.20273100	0.03668400	C	3.40872900	-1.60813300	0.08371700
C	2.69320600	-0.10959000	0.07914400	C	2.54716600	-0.50364100	0.28448500
C	2.08275500	2.06109100	-0.00530900	C	2.56556400	-2.72623600	-0.09387900
C	0.93876100	1.26340000	0.00610300	C	1.23886400	-2.27934600	-0.01887100
H	2.10148600	3.14051200	-0.04381500	H	2.87719700	-3.74264800	-0.28597700
C	-0.42491900	1.58352300	-0.01713000	C	0.01998000	-2.93512700	-0.17061900
C	-1.39992800	0.57340800	0.01424400	C	-1.19513100	-2.21703000	-0.11072000
H	-0.73048800	2.62047300	-0.05560000	H	0.00004600	-3.99937500	-0.36336500
C	-2.13291200	-1.52437300	0.08708500	C	-2.47610000	-0.39457100	0.11774400
C	-2.79220600	0.63791400	0.00451400	C	-2.50825200	-2.62266200	-0.29645600
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H	-4.59432200	-2.34271100	0.09051200	H	-5.12353900	-2.53881900	-0.51701200
C	-5.82252000	-0.67469600	0.02194600	C	-5.72338500	-0.57589200	-0.20765400
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C	-7.74405700	0.65740700	-0.04319800	C	-7.07169300	1.31753200	0.03016300
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C	-10.40559500	-0.10219800	-0.07179000	C	-9.82887000	1.53495200	-0.18060900
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H	-11.45430700	-0.37850400	-0.08400200	H	-10.90441100	1.64688100	-0.25735700
H	-9.72249300	-2.15235400	-0.00661800	H	-9.87149100	-0.58569800	-0.59611900
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H	-2.08213700	-2.60396400	0.12509700	H	-2.71884300	0.63972600	0.29396200
H	-3.39473100	1.53083700	-0.03033600	H	-2.83921400	-3.62745800	-0.51840500
H	3.19391000	-1.06472400	0.14435400	H	2.78106500	0.52398000	0.52482000
H	5.20811400	-1.11831000	-0.16177100	H	4.54666600	1.13616200	-0.42880400
N	5.93116400	-0.42492600	-0.05390800	N	5.42614900	0.77666300	-0.08878900
C	7.07517800	1.58126000	0.04302200	C	7.18558500	-0.73129800	0.06688100
O	7.29808300	2.78504400	0.10584200	O	7.79996800	-1.78586900	0.20047900
<b>IB4</b>				<b>IB5</b>			
C	5.66409300	-0.17155800	-0.00354400	C	-5.66733700	0.99852100	0.03006700
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C	6.97888200	3.21382800	0.07678300	C	-7.89757700	-1.85874700	-0.24777200
C	8.31618700	3.59749700	0.10147000	C	-9.28330300	-1.84109900	-0.27891300
C	9.35919800	2.66149700	0.09222400	C	-10.00755400	-0.64144500	-0.19952100
C	9.07624800	1.30115500	0.06119900	C	-9.35227100	0.58466600	-0.08666600
C	7.74659100	0.89803600	0.03686400	C	-7.96868200	0.59006900	-0.05395900
H	6.18169900	3.94904000	0.08340500	H	-7.33776900	-2.78450000	-0.30813900
H	8.55599500	4.65548300	0.12807200	H	-9.82139400	-2.77822600	-0.36704000
H	9.86840200	0.55864400	0.05796500	H	-9.90653800	1.51521200	-0.02751100
H	10.38711500	3.00505400	0.11117200	H	-11.09043200	-0.67336900	-0.22806000
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H	5.17751600	-2.16290800	0.01040100	H	-4.55805500	2.71665400	0.14750000
C	3.31823700	-1.09081400	-0.05907600	C	-3.14272400	1.10422500	0.10927500
C	2.49722500	-2.24963600	0.02710000	C	-2.68906200	-0.22584300	0.14449100
C	2.43502500	-0.00584600	-0.17744700	C	-1.97856600	1.91727900	0.06861800
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H	2.64982700	1.04521100	-0.28884300	H	-1.94484800	2.99620700	0.03195700
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C	-2.52757800	-2.28920600	0.06958600	C	2.13631200	-1.61080800	0.13205300
C	-2.45577300	-0.03921400	-0.14804700	C	2.73091800	0.56420400	0.04013500
C	-3.34034400	-1.14024400	-0.01119000	C	3.25813800	-0.73661700	0.08141200
C	-4.75943400	-1.20870500	0.05568000	C	4.57891100	-1.27147800	0.07523400

H	-5.14658900	-2.22308300	0.15384300	H	4.60893500	-2.35998300	0.11912800
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H	-7.40876000	-1.52349900	0.19558200	H	7.00895900	-2.42023300	0.03132200
C	-7.64409800	2.93666800	-0.06662100	C	8.60891200	1.76778500	-0.15780400
C	-9.03225800	3.03313500	0.00644500	C	9.95769100	1.43663100	-0.18842000
H	-9.50955500	4.00592000	-0.02505100	H	10.71005100	2.21543500	-0.24110300
C	-9.26952400	0.61114300	0.16502700	C	9.43468500	-0.94697800	-0.08422200
C	-9.82612500	1.87963700	0.11965700	C	10.35482900	0.09155700	-0.15244900
H	-7.02052300	3.82018800	-0.15453200	H	8.28051100	2.80217700	-0.18550300
H	-10.90409000	1.98388100	0.17409300	H	11.41307500	-0.14775800	-0.17768400
H	-9.88517600	-0.27616400	0.25337500	H	9.75399200	-1.98267300	-0.05650500
O	-4.67605100	1.96714000	-0.17603700	O	5.47411300	1.75132300	-0.05890600
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B	-0.01013400	-2.88526200	0.01655200	B	-0.43945100	-1.49466200	0.14358700
F	-0.00385000	-3.72372900	-1.09794200	F	-0.65527000	-2.25373600	1.29437500
F	0.01229200	-3.65667300	1.17600500	F	-0.66842700	-2.29225500	-0.97932100
H	-2.82606600	-3.32278500	0.17723800	H	2.13879500	-2.69274400	0.17064400
H	-2.73081600	0.99891500	-0.23402100	H	3.28886900	1.48406800	-0.00342200
H	2.81382000	-3.28018000	0.12485500	H	-3.22445700	-1.16104600	0.21476000
H	4.60464700	1.67015400	0.09480800	H	-5.20052700	-1.07241800	-0.17039300
N	5.48894100	1.19779400	-0.00203800	N	-5.91053800	-0.36177600	-0.07290800
C	7.13532600	-0.42916600	0.01170700	C	-6.98733300	1.67870500	0.04830700
O	7.67064500	-1.53180100	0.00161800	O	-7.17844800	2.88400000	0.13337300
N	-0.01420800	0.15452600	-0.22056800	N	0.42930600	1.42659600	0.04014700
<b>IB6</b>				<b>IB7</b>			
C	5.71711700	-0.60056700	0.04777900	C	6.70873700	0.14898900	-0.37584900
C	6.83374000	1.37861800	-0.07060400	C	7.46511100	2.26870000	-0.07254800
C	7.14604000	2.73521800	-0.17263900	C	7.55602500	3.63860100	0.16246400
C	8.49114300	3.07490000	-0.14578700	C	8.79538900	4.24124600	-0.02170100
C	9.49666500	2.10370200	-0.02372400	C	9.92377100	3.51171700	-0.42556600
C	9.17232800	0.75169200	0.07279200	C	9.82033800	2.14957600	-0.66829600
C	7.83525400	0.39147900	0.04839500	C	8.58423900	1.52963200	-0.49920300
H	6.37186200	3.48757100	-0.26560900	H	6.69280600	4.21477700	0.47781100
H	8.77194800	4.11965700	-0.22004200	H	8.89066200	5.30829300	0.15432000
H	9.94155400	-0.00768600	0.16423300	H	10.67693800	1.56658700	-0.99357300
H	10.53508600	2.41317000	-0.00683400	H	10.87337600	4.02005200	-0.55138900
C	4.73381800	-1.54020600	0.08420800	C	5.90470300	-0.93644100	-0.49733100
H	5.12320900	-2.55483600	0.14577800	H	6.40265000	-1.80927200	-0.91487700
C	3.31589600	-1.40825900	0.04920700	C	4.52153200	-1.06930600	-0.16410800
C	2.50013200	-0.26022200	0.05818900	C	3.75627200	-2.19431500	-0.51182200

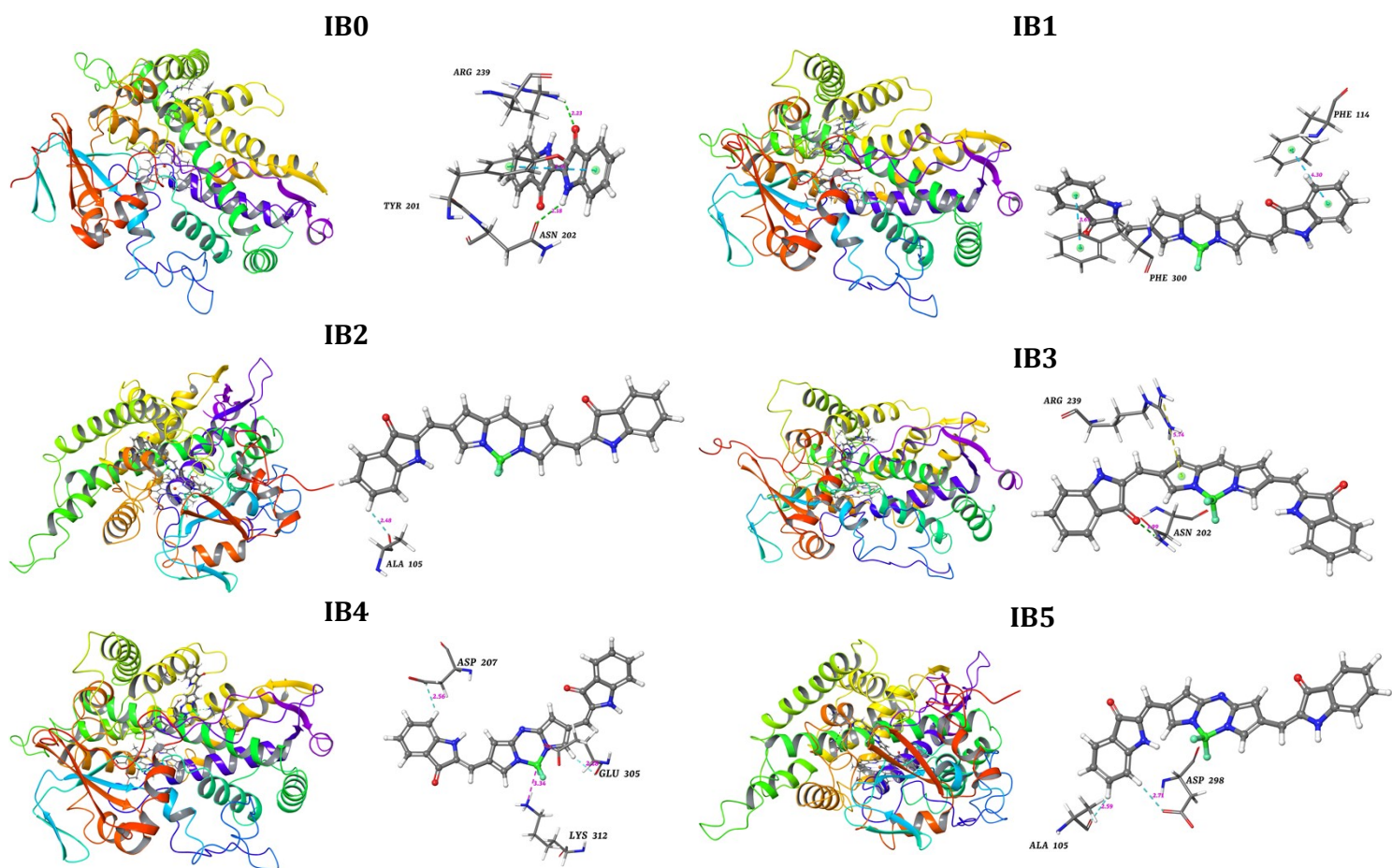
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H	-5.09421200	-2.63144500	-0.13912100	F	1.27950500	-3.86723300	-1.10652500
C	-5.77108000	-0.67438000	-0.05519300	F	1.47746300	-3.82357400	1.17560800
C	-5.76149900	0.81716500	0.02093000	H	4.06411800	-3.08677500	-1.03852800
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C	-7.16971900	1.20091000	0.04418400	N	6.37271200	1.43014100	0.07340800
C	-7.94571100	0.02691300	-0.01431600	C	8.15286300	0.14943900	-0.71416900
H	-7.41809400	-2.01714100	-0.11985700	O	8.81616600	-0.81836300	-1.08816000
C	-7.77735200	2.44930700	0.11005500	C	-1.08913400	-2.62925700	-0.44016200
C	-9.16488800	2.51322500	0.11849400	H	-0.99519500	-3.52792500	-1.03345400
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H	-7.16819400	3.34656700	0.15328400	C	-4.36309800	-1.01041400	-0.55406600
H	-11.01000200	1.40770900	0.07062800	B	-1.32849800	-0.63021800	1.61744600
H	-9.94001200	-0.82219000	-0.04928700	F	-1.24640700	0.70621100	1.95308000
O	-4.78224200	1.55813800	0.05753500	F	-1.54245900	-1.42626400	2.74046600
N	-1.23412200	-0.64060000	-0.03336300	N	-2.44029400	-0.88848100	0.57891500
N	1.20204400	-0.62730000	0.01275500	H	-3.96534900	0.50081100	1.06509600
B	-0.02050400	0.31906400	0.00087400	N	-0.00349800	-1.07625500	0.90845300
F	-0.04778800	1.11534100	1.14585500	H	-3.71865400	-2.75197200	-1.82038900
F	-0.00096400	1.13966600	-1.12782100	C	-5.65820500	-0.81260300	-1.08485800
H	-2.84744700	0.73819300	-0.00401800	H	-5.92500700	-1.50913500	-1.87828600
H	-2.72051600	-3.59543300	-0.14259400	C	-6.63476200	0.10685200	-0.77584700
H	2.75199800	0.78860100	0.11950800	C	-6.71124300	1.20031300	0.23445700
H	4.73672600	1.27835000	-0.19360500	C	-8.03564400	1.80044700	0.03459200
N	5.60116000	0.77556400	-0.06006900	C	-8.67404000	1.10961400	-1.01227300
C	7.16862800	-0.91307400	0.12296500	H	-8.05692300	-0.50652500	-2.22129200
O	7.66297000	-2.02762300	0.22680700	C	-8.67617200	2.84947200	0.66984400
N	-0.01071600	-2.72893500	-0.07919400	C	-9.95352100	1.44321900	-1.45401100
				C	-9.95755600	3.19410300	0.23963200
				C	-10.58074800	2.49882400	-0.80609300
				H	-10.43213500	0.90358500	-2.26191400
				H	-10.48295200	4.01210600	0.71793000
				H	-11.57683700	2.79178900	-1.11708200
				H	-8.18868200	3.38486400	1.47670700
				O	-5.85841800	1.52080100	1.04884800
				N	-7.83264200	0.12486000	-1.46183900

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C	6.74371800	-0.64067900	-0.74985100
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C	8.42211300	2.55643600	-0.38597600
C	9.74127200	2.85810100	-0.70584100
C	10.62383500	1.88922400	-1.20554900
C	10.18649900	0.58802200	-1.40711400
C	8.86492800	0.26911100	-1.10036400
H	7.75095000	3.31391400	0.00407600
H	10.09695100	3.87362200	-0.56175100
H	10.84861600	-0.17537100	-1.80485600
H	11.64665400	2.16489700	-1.43708600
C	5.70158100	-1.50690200	-0.74573200
H	5.92530200	-2.47423200	-1.19033900
C	4.37151500	-1.29893600	-0.25679500
C	3.90766600	-0.25095600	0.55861300
C	3.25671800	-2.13942900	-0.49571100
C	2.15631900	-1.57156400	0.15690000
H	3.24294000	-3.03069500	-1.10528400
C	0.81518800	-1.94018900	0.22817400
H	0.45609100	-2.86910000	-0.18707800
N	0.19965700	0.05788100	1.29651400
N	2.58787800	-0.41523800	0.79904500
B	1.70483400	0.29522200	1.81066800
F	1.79052700	-0.27937900	3.07361600
F	1.93819900	1.65456200	1.85544900
H	4.44632800	0.55360000	1.03661400
H	5.92518700	1.25218600	-0.31093200
N	6.76034400	0.68378700	-0.29971300
C	8.10677700	-0.97487000	-1.23708200
O	8.48591500	-2.06906800	-1.65094100
C	-0.71132400	0.99112700	1.46835000
H	-0.35153900	1.91898300	1.88971000
C	-2.07059500	0.81614900	1.10672700
C	-3.80787700	-0.35453600	0.34456100
C	-3.10933600	1.71421100	0.99188800
C	-4.23441600	0.98290700	0.49541100
B	-1.63233800	-1.68202200	0.90859900
F	-1.82342900	-2.19268400	2.19147100
F	-1.87455200	-2.64047000	-0.05544900
N	-2.52286700	-0.43794200	0.71240200
H	-4.36853200	-1.21391400	0.01691700
N	-0.16033900	-1.15839300	0.76851900
H	-3.07672900	2.77199600	1.20857000
C	-5.48311800	1.60751700	0.26998200

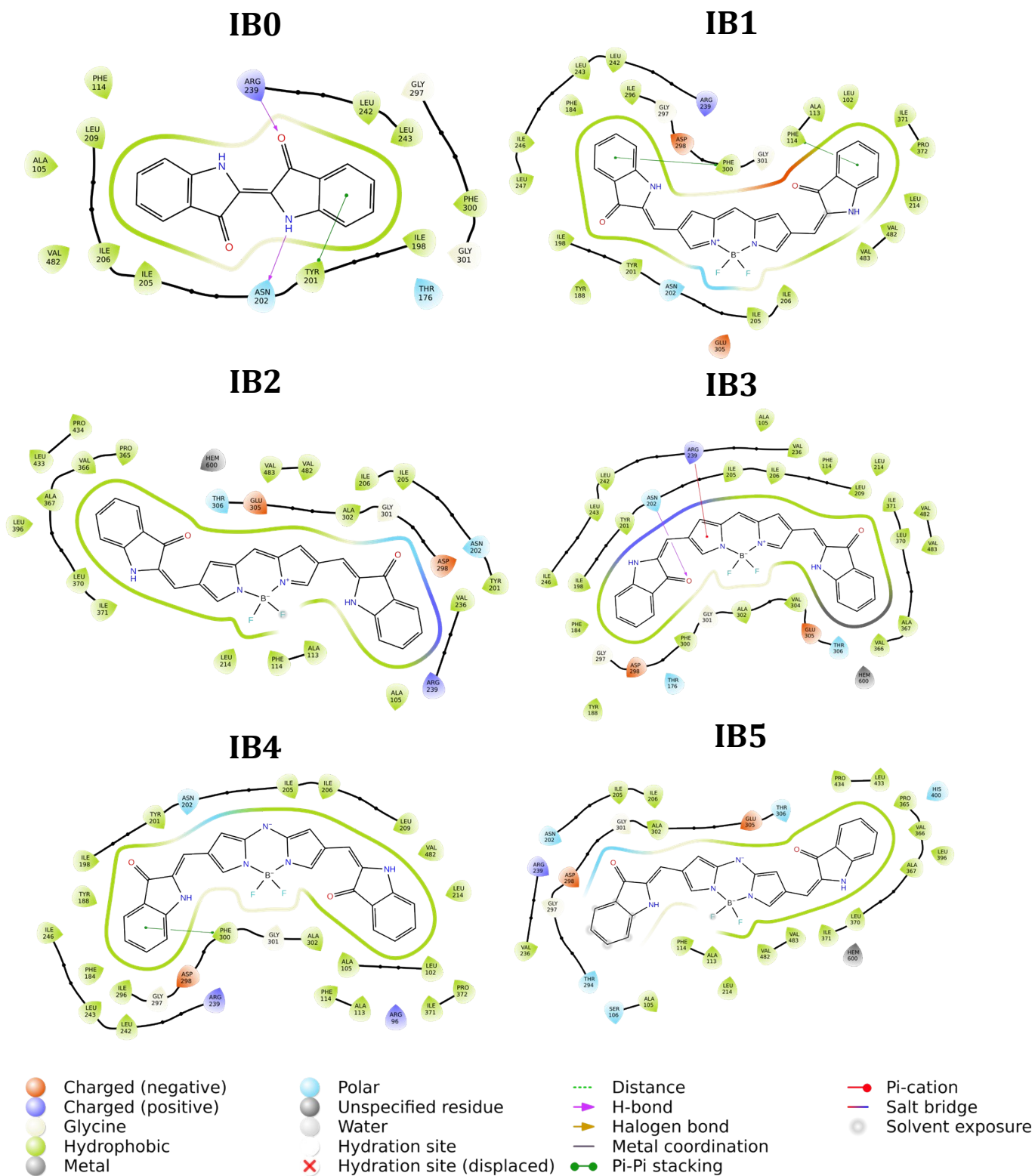
H	-5.49782000	2.66886300	0.51308500
C	-6.67944100	1.11143500	-0.19353700
C	-7.10434600	-0.24072800	-0.64941900
C	-8.51491300	-0.08166200	-1.02419300
C	-8.87795800	1.26003400	-0.79625300
H	-7.78634400	2.91361400	-0.06896600
C	-9.44386100	-0.98147200	-1.51484000
C	-10.16544700	1.73558000	-1.04492600
C	-10.73515700	-0.51959000	-1.77003300
C	-11.08409400	0.81850500	-1.53547800
H	-10.43303600	2.76938100	-0.86312400
H	-11.48357100	-1.20205300	-2.15482800
H	-12.09673000	1.14491200	-1.74234500
H	-9.16853400	-2.01523000	-1.69173200
O	-6.42484400	-1.25505600	-0.69799900
N	-7.78510000	1.93132200	-0.31501100

**SIT5.** Computed Stokes shift for IB0 and designed IBs at M06L/6-311G(d,p) level

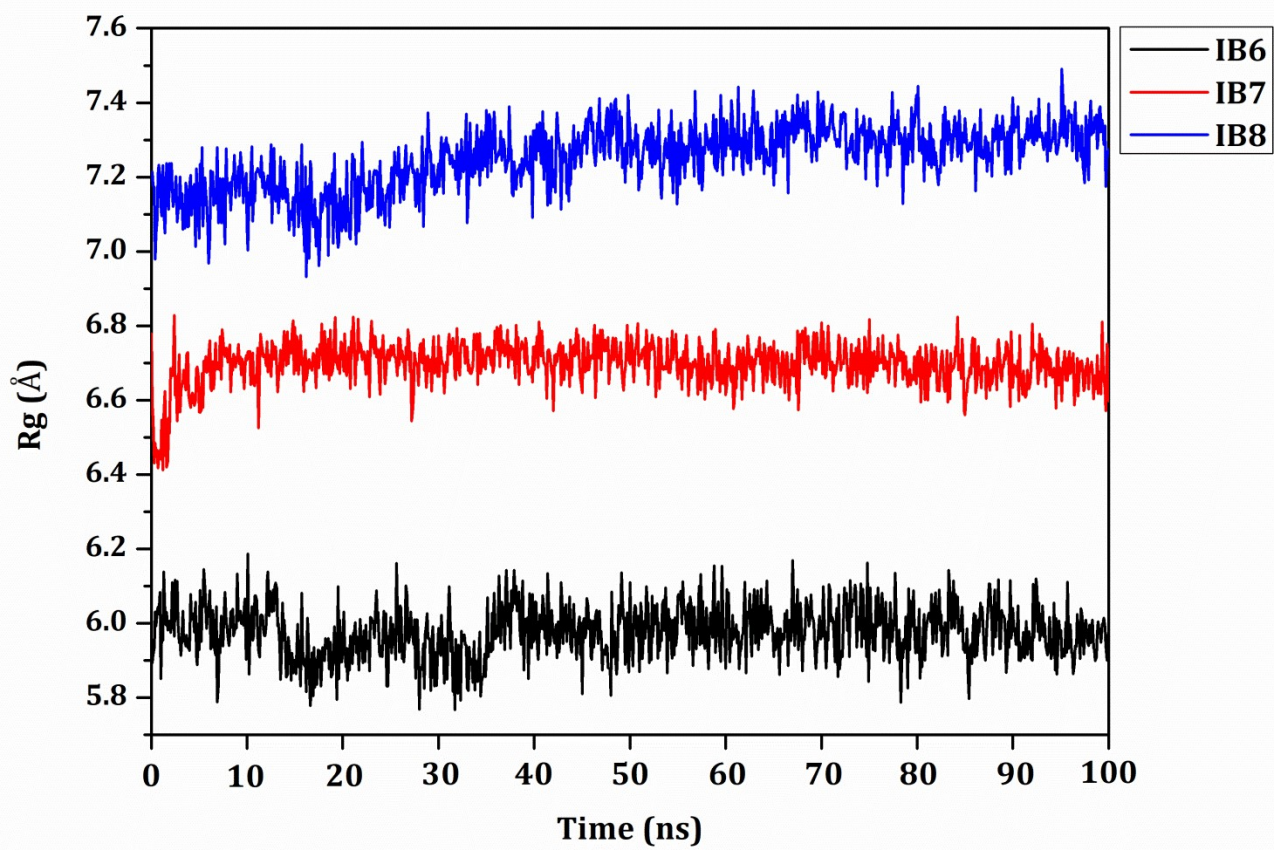
<b>Molecules</b>	<b>Stokes Shift (cm<sup>-1</sup>)</b>
IB0	1396.87
IB1	1432.01
IB2	1184.23
IB3	1571.18
IB4	1358.31
IB5	1850.12
IB6	1428.28
IB7	2618.66
IB8	2611.10



**SIF 5.** 3D binding interaction view of IB0 and designed IBs (IB1-IB5) with CYP17A1 (3RUK) docked complexes



**SIF 6.** 2D binding interaction view of IB0 and designed IBs (IB1-IB5) with CYP17A1 (3RUK) docked complexes



**SIF 7.** Radius of the gyration graph during MD simulation