Electronic Supplementary Material (ESI) for RSC Advances.
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Supporting Information

Cartesian Coordinates (Å) of optimized ground state of the planar and twisted structures and their corresponding water complexes, where B3LYP/6-311+G* functional and CPCM model (ε= 37.219) were used for optimization.

Planar

C	-4.00873000	-0.23163400	0.00029000
C	-3.35364500	-1.44274300	0.00005100
C	-1.93981500	-1.50696800	-0.00016500
C	-1.18791700	-0.30630800	-0.00011500
C	-1.87350400	0.93650700	0.00010200
C	-3.24947200	0.98784400	0.00029900
H	-3.89574700	-2.37873800	0.00001400
C	0.24344800	-0.46879800	-0.00027300
H	-1.32783200	1.87012800	0.00009400
C	-0.03100900	-2.74112700	-0.00060700
H	0.46199600	-3.71025100	-0.00084000
N	0.79718800	-1.67593100	-0.00053300
N	-1.34262500	-2.74124600	-0.00041900
C	2.44127900	0.79541100	-0.00026100
C	2.92876700	2.11557300	-0.00061100
C	3.35560700	-0.26857400	0.00003200
C	4.29344600	2.36529100	-0.00066000
H	2.23155100	2.94771800	-0.00084100
C	4.71627500	0.02138700	-0.00003800
H	3.00312100	-1.28656300	0.00028100
C	5.21550200	1.31675000	-0.00037800
H	4.64846800	3.39000700	-0.00093300
H	6.28155100	1.50554500	-0.00043000
Cl	5.85338400	-1.33298600	0.00034400
N	1.04431400	0.64485000	-0.00014400
H	0.55372400	1.52463300	0.00002200
O	-5.35014400	-0.07388600	0.00051300
O	-3.98770600	2.12368100	0.00050900
C	-3.30832400	3.38083300	0.00055400
H	-4.09022100	4.13643800	0.00075600
H	-2.69078200	3.49336500	0.89554100
H	-2.69104700	3.49357200	-0.89459000
C	-6.17371300	-1.24422200	0.00057900
H	-7.19833800	-0.88064000	0.00081600
H	-5.99642800	-1.84585800	-0.89405800
H	-5.99606700	-1.84601000	0.89504200

P-1w

C	3.83950400	-0.36301900	-0.00273500
C	3.28032200	0.89583000	-0.00704900
C	1.87654200	1.06642000	-0.00690800
C	1.03299200	-0.07072300	-0.00251000
C	1.62073000	-1.36210300	0.00158300
C	2.98848800	-1.52034000	0.00118500
H	3.89614600	1.78477000	-0.00988900
C	-0.38215700	0.20035900	-0.00325100
H	1.00445100	-2.25018900	0.00451200
C	0.05793200	2.44510600	-0.01373300
H	-0.35510800	3.45038100	-0.01927200
N	-0.84394900	1.44762500	-0.00888000
N	1.36740500	2.34096500	-0.01255500
C	-2.67086300	-0.88837900	0.00218700

C	-3.25548100	-2.16785700	0.00702700
C	-3.50099600	0.24191100	-0.00147500
C	-4.63512800	-2.31402700	0.00815500
H	-2.62178900	-3.04917700	0.00992900
C	-4.87974200	0.05573400	-0.00030300
H	-3.07269600	1.23026500	-0.00526800
C	-5.47489000	-1.19859200	0.00448400
H	-5.06665100	-3.30883500	0.01191300
H	-6.55220900	-1.30621800	0.00530000
Cl	-5.91104600	1.49167200	-0.00500200
N	-1.26512100	-0.84595500	0.00164000
H	-0.84569700	-1.76205400	0.00584800
O	5.16308900	-0.62362400	-0.00231300
O	3.63595300	-2.70917800	0.00457100
C	2.86142100	-3.91072700	0.00927800
H	3.58309600	-4.72394300	0.01158800
H	2.23797000	-3.97228700	0.90512800
H	2.23674000	-3.97853400	-0.88525800
C	6.07720400	0.47818700	-0.00710500
H	7.06940700	0.03392500	-0.00606100
H	5.94765700	1.08829300	-0.90404200
H	5.94888000	1.09513200	0.88532700
O	2.96919600	4.71199900	-0.05042000
H	2.41284400	3.89985500	-0.03365900
H	2.69521600	5.25148300	0.69982600

P-2w

C	-3.85928900	0.17122800	-0.16411700
C	-3.29303300	-1.07210400	0.00905700
C	-1.89294500	-1.21811600	0.14304000
C	-1.06174200	-0.07132100	0.10031000
C	-1.65499900	1.20623500	-0.07962700
C	-3.02056800	1.33553500	-0.21007800
H	-3.89918600	-1.96696600	0.04505500
C	0.35177300	-0.31752200	0.23761300
H	-1.03789900	2.09359400	-0.11605800
C	-0.07046500	-2.56228600	0.41462800
H	0.34833400	-3.55731700	0.54398000
N	0.81839000	-1.55721800	0.38955100
N	-1.37823500	-2.48008700	0.30475900
C	2.65323200	0.64860000	0.27499700
C	3.33868100	1.69230200	0.91422600
C	3.38617400	-0.37573100	-0.34115600
C	4.72913100	1.70768900	0.94375600
H	2.77599900	2.49055700	1.38286500
C	4.77330700	-0.33623500	-0.28443900
H	2.88230600	-1.18301800	-0.84856500
C	5.46998100	0.68676300	0.34954900
H	5.24485300	2.52036500	1.44369300
H	6.55240600	0.68766800	0.37895600
Cl	5.68335800	-1.63845300	-1.06169400
N	1.24330500	0.71959600	0.22373300
H	0.88092500	1.66869300	0.27024500
O	-5.18202500	0.40680100	-0.30314600
O	-3.68106900	2.50606400	-0.38830700
C	-2.92077900	3.71428300	-0.44856100
H	-3.64733900	4.51043900	-0.59381600
H	-2.37237600	3.87964900	0.48155200
H	-2.22090700	3.69615200	-1.28750700
C	-6.08085000	-0.70620200	-0.27220000

H	-7.07392400	-0.28341800	-0.40335300
H	-5.86753400	-1.40345000	-1.08596200
H	-6.02645900	-1.22621400	0.68727300
O	-2.91995800	-4.87762200	0.41008600
H	-2.39300300	-4.04514700	0.38194600
H	-2.83695200	-5.22859300	1.30391000
O	0.60890900	3.60353300	0.17195000
H	0.56242300	4.19787700	0.93022400
H	1.03452600	4.09787400	-0.53859200

P-3w

C	4.13919100	-0.47473200	-0.34781900
C	3.49174600	-1.54626300	0.22823100
C	2.08768900	-1.53713900	0.39859700
C	1.34578300	-0.40252900	-0.01661800
C	2.01772500	0.68681300	-0.62670400
C	3.38301300	0.66437000	-0.79386600
H	4.03236000	-2.42291200	0.55856600
C	-0.06981400	-0.46637500	0.19276200
H	1.45023600	1.53852000	-0.97181400
C	0.17790600	-2.57605200	1.06795100
H	-0.32223300	-3.43759500	1.50260900
N	-0.63283500	-1.54591600	0.73478300
N	1.48131400	-2.63867800	0.94417700
C	-2.24526400	0.61251500	-0.38411500
C	-2.93595500	1.82660400	-0.23664200
C	-2.94363600	-0.51872000	-0.83425400
C	-4.29345200	1.90383300	-0.52520300
H	-2.40044800	2.70533100	0.10340900
C	-4.30072400	-0.40742500	-1.10645800
H	-2.43888200	-1.46353700	-0.96793900
C	-5.00253600	0.78403100	-0.96030700
H	-4.81146000	2.84925800	-0.40496900
H	-6.06158600	0.83794600	-1.17869900
Cl	-5.16273100	-1.84528100	-1.67022600
N	-0.85979500	0.60602400	-0.15561500
H	-0.45373800	1.52530100	0.02615900
O	5.47037900	-0.39342500	-0.55374900
O	4.11547600	1.64900200	-1.36766800
C	3.43452400	2.81013700	-1.84836400
H	4.20788800	3.45435500	-2.25980200
H	2.71976200	2.54824600	-2.63290700
H	2.91986500	3.32775000	-1.03485600
C	6.29386800	-1.49104500	-0.14670600
H	7.31037700	-1.20502500	-0.40532800
H	6.22044400	-1.65544300	0.93092300
H	6.02058900	-2.40341700	-0.68215600
O	-2.28695900	-0.60244900	2.88928700
H	-3.24096100	-0.60061400	2.74961800
H	-1.88043300	-1.02124900	2.09992400
O	-1.13532800	1.83595300	3.44888800
H	-1.55549700	0.96447800	3.26899800
H	-0.61333700	1.74041100	4.25317400
O	0.05068900	2.93719500	1.23082300
H	-0.09022500	3.88766000	1.16181700
H	-0.36153400	2.63195500	2.07015000

P-4w

C	4.19853400	-0.72841500	-0.20374000
C	3.51129600	-1.63165100	0.57772500

C	2.10457500	-1.55981300	0.70353100
C	1.39686800	-0.54069800	0.01747900
C	2.11126400	0.37912600	-0.79179000
C	3.48045100	0.29845000	-0.90659100
H	4.02255600	-2.41911300	1.11457900
C	-0.02950100	-0.54310700	0.18537800
H	1.58182700	1.16926300	-1.30280100
C	0.16573900	-2.37584800	1.56385400
H	-0.35944900	-3.09373900	2.18880700
N	-0.61820200	-1.45025900	0.96815300
N	1.46801600	-2.49259300	1.48195700
C	-2.19912600	0.34058600	-0.65802400
C	-2.90323000	1.55067400	-0.74733600
C	-2.88529500	-0.86639600	-0.86030700
C	-4.26614500	1.55234500	-1.02449700
H	-2.37593100	2.48527800	-0.59900400
C	-4.24795600	-0.83009800	-1.12373200
H	-2.36540800	-1.81175100	-0.81459900
C	-4.96383800	0.35934900	-1.21048700
H	-4.79692500	2.49607400	-1.08862700
H	-6.02676900	0.35557900	-1.41655400
Cl	-5.09663400	-2.36134800	-1.37185500
N	-0.80666900	0.38926400	-0.45128400
H	-0.37506000	1.28806500	-0.67867700
O	5.53720200	-0.71861800	-0.38029900
O	4.24915200	1.13157300	-1.64998400
C	3.60127900	2.16799300	-2.39204500
H	4.39885400	2.71265100	-2.89192300
H	2.92133900	1.74678700	-3.13764800
H	3.05064100	2.84068700	-1.73057900
C	6.32243200	-1.70666800	0.29438700
H	7.35295100	-1.50177200	0.01484400
H	6.21074000	-1.62061300	1.37788200
H	6.04652800	-2.71314500	-0.02928100
O	-0.09198300	3.71715400	1.92455300
H	-0.70724200	3.13499000	2.42695600
H	0.71385900	3.79909700	2.44630500
O	-2.58584000	-0.40118600	2.73481700
H	-3.49777900	-0.50000800	2.43798400
H	-2.01399600	-0.83282200	2.05896200
O	-1.85019000	2.16609100	3.32721000
H	-2.10803500	1.24085100	3.10850800
H	-1.81138000	2.23368800	4.28741700
O	0.24419500	3.06381500	-0.69776300
H	-0.05870300	3.76579800	-1.28374400
H	0.13377900	3.37658000	0.22983900

P-5w

C	-4.07808500	0.03384700	-0.54631500
C	-3.49711600	1.18514300	-0.05878500
C	-2.09637800	1.27391400	0.10454400
C	-1.28232500	0.16350400	-0.23014100
C	-1.88821200	-1.01264400	-0.73950500
C	-3.25332400	-1.08841200	-0.89839300
H	-4.09337800	2.04713900	0.20750600
C	0.13202700	0.33828300	-0.04801700
H	-1.27793900	-1.86960500	-0.98173500
C	-0.25326600	2.47517300	0.71093000
H	0.18419500	3.39090700	1.09935400
N	0.61859000	1.48678200	0.43348400

N	-1.55820800	2.44557800	0.57664000
C	2.39766400	-0.56566700	-0.53895600
C	3.19276700	-1.68035400	-0.23587200
C	2.99917000	0.57712400	-1.08635900
C	4.56386600	-1.64879900	-0.46767000
H	2.73005100	-2.56718900	0.17982600
C	4.37188600	0.58037000	-1.29450400
H	2.40781500	1.44219400	-1.34710600
C	5.17768900	-0.51314300	-0.99469300
H	5.16661400	-2.51773300	-0.22680800
H	6.24608400	-0.48087200	-1.16728300
Cl	5.11439700	2.03001900	-1.98147300
N	1.00297200	-0.66897700	-0.36000400
H	0.65052000	-1.62868600	-0.32154700
O	-5.40189600	-0.14422500	-0.73469900
O	-3.92189300	-2.16551300	-1.37578600
C	-3.16392300	-3.31191200	-1.77226600
H	-3.89457400	-4.04339800	-2.10926800
H	-2.48580500	-3.06458000	-2.59350400
H	-2.59375300	-3.71630900	-0.93293500
C	-6.29203300	0.92673400	-0.40245400
H	-7.28929300	0.55771200	-0.62873000
H	-6.22350000	1.17552100	0.65916200
H	-6.08105100	1.81171900	-1.00735200
O	-3.08802800	4.76060400	1.28292300
H	-2.55889100	3.96729000	1.03897500
H	-2.75868600	5.48952000	0.74515200
O	0.32004500	-3.11284100	2.89280000
H	0.90462900	-2.38499500	3.20638200
H	-0.52224600	-3.02056400	3.35151400
O	2.59917300	1.17363400	2.46885100
H	3.51050800	1.22788500	2.15859200
H	2.02133800	1.33955600	1.69018200
O	2.00267200	-1.15518600	3.78180600
H	2.21000600	-0.31530400	3.31127800
H	1.99107700	-0.96158000	4.72540000
O	0.16534600	-3.36714800	0.18682900
H	0.56457300	-4.18657500	-0.12459200
H	0.21769100	-3.35962800	1.17068900

P-6w

C	-3.75981100	-0.84635400	-0.58348300
C	-3.38401800	0.39983200	-0.12852800
C	-2.02008500	0.72067500	0.05308000
C	-1.02945500	-0.25085700	-0.23457900
C	-1.42582900	-1.52823500	-0.70478000
C	-2.75698500	-1.83214700	-0.87684800
H	-4.11953600	1.16099100	0.09307200
C	0.33458300	0.16301100	-0.05568600
H	-0.67918100	-2.28154300	-0.90641000
C	-0.40623100	2.22729200	0.63647500
H	-0.13073300	3.21267700	1.00236500
N	0.61925200	1.39070100	0.39188600
N	-1.68710400	1.97856300	0.49280400
C	2.72022400	-0.35707100	-0.53351400
C	3.69588400	-1.30997000	-0.20699800
C	3.11488500	0.85532900	-1.11826100
C	5.04040100	-1.05032600	-0.45138300
H	3.39439500	-2.25125600	0.23608500
C	4.46580100	1.08762500	-1.33864400

H	2.38338000	1.59939900	-1.39669300
C	5.44855500	0.15793000	-1.01496600
H	5.78404200	-1.79591500	-0.19178400
H	6.49496800	0.36832200	-1.19713000
Cl	4.94541500	2.62225200	-2.07319300
N	1.36407900	-0.69118200	-0.33931000
H	1.17974000	-1.69522100	-0.26910300
O	-5.03156900	-1.24269100	-0.79224000
O	-3.23316700	-3.02062800	-1.31807400
C	-2.29270400	-4.04205800	-1.66200300
H	-2.88933200	-4.89486000	-1.97698300
H	-1.65086600	-3.71831900	-2.48581700
H	-1.67815400	-4.31704700	-0.80190600
C	-6.09050400	-0.31394900	-0.53493000
H	-7.00830900	-0.84410800	-0.77668800
H	-6.10256800	-0.01747100	0.51646000
H	-5.99664800	0.56948600	-1.17049600
O	-3.51421400	4.01359800	1.19289800
H	-2.87459900	3.30301700	0.93799500
H	-3.05205100	4.85595900	1.11914100
O	1.31109200	-3.15900600	2.99430700
H	1.73099600	-2.31338500	3.27431000
H	0.52049300	-3.27765400	3.53202000
O	2.62884000	1.50590700	2.41476400
H	3.50594400	1.75594400	2.10204600
H	2.02759600	1.53442800	1.63634000
O	2.54755400	-0.85883800	3.79034400
H	2.56926800	-0.00872600	3.29363600
H	2.50998800	-0.64329100	4.72847400
O	1.00855800	-3.47048300	0.30675000
H	1.50634400	-4.22630600	-0.02312000
H	1.12473000	-3.43599700	1.28451600
O	-6.06817900	3.96952200	0.16100500
H	-5.15952300	3.97407100	0.53137800
H	-6.65559600	3.67852800	0.86719500

P-7w

C	-3.57194600	-0.15377800	-0.28739500
C	-3.00530000	1.04922800	0.07606400
C	-1.60070000	1.18235500	0.16045600
C	-0.77257400	0.06807600	-0.12534000
C	-1.36733300	-1.15957800	-0.51088200
C	-2.73464400	-1.27679000	-0.59181400
H	-3.62107500	1.91303500	0.28945900
C	0.64421900	0.28667500	-0.02409700
H	-0.74669800	-2.01920200	-0.71506800
C	0.24073300	2.46819100	0.57972900
H	0.67164000	3.42201900	0.87169700
N	1.12320300	1.47990300	0.34369100
N	-1.06817900	2.40021400	0.50875700
C	2.90974900	-0.60211000	-0.53535600
C	3.74620700	-1.66277500	-0.16019800
C	3.45786300	0.50043100	-1.20664300
C	5.10735000	-1.61675500	-0.44335400
H	3.32439900	-2.51850900	0.35275100
C	4.82219200	0.52113300	-1.46304500
H	2.83227600	1.32152900	-1.52390600
C	5.66911700	-0.51873200	-1.09343500
H	5.74340100	-2.44336300	-0.14594900
H	6.72977700	-0.47437800	-1.30651800

Cl	5.49846200	1.92019400	-2.30520900
N	1.52444700	-0.72222600	-0.29648600
H	1.19694500	-1.68400900	-0.17380000
O	-4.89775500	-0.38525500	-0.39425000
O	-3.39931500	-2.40814300	-0.94524000
C	-2.63426100	-3.57013800	-1.29119300
H	-3.36373900	-4.34312600	-1.51948900
H	-2.01546600	-3.37527500	-2.17037400
H	-2.00572400	-3.88493500	-0.45614100
C	-5.80679500	0.65382000	-0.00009500
H	-6.80185000	0.25551300	-0.18209400
H	-5.68658600	0.87772900	1.06239700
H	-5.65164600	1.56147800	-0.58424000
O	-2.59203600	4.72760900	0.93625400
H	-2.03045600	3.92380000	0.79765800
H	-2.12815200	5.47382900	0.54030900
O	1.06355700	-2.96585700	3.13566400
H	1.64313500	-2.20487700	3.36989900
H	0.24145500	-2.85971300	3.62684700
O	3.17829300	1.35598200	2.33215200
H	4.07941000	1.43983900	1.99949200
H	2.57708100	1.45535200	1.56051600
O	2.72790400	-0.90737800	3.80700100
H	2.88057600	-0.09416900	3.27324700
H	2.75135900	-0.65064100	4.73519300
O	0.77630900	-3.39504100	0.46287400
H	1.19307500	-4.21577800	0.17897400
H	0.88060000	-3.32478500	1.44023500
O	-5.09447000	4.13388100	-0.03927600
H	-4.22767400	4.41679600	0.32461500
H	-5.76552300	4.38860300	0.60372800
H	-5.40244700	-2.55199900	-1.17255200
H	-6.92516600	-2.41239400	-1.41916400
O	-6.20327900	-3.05035100	-1.40284200

Twisted

C	2.89761800	-0.90609000	-0.01708300
C	3.14745400	0.35652100	0.47019600
C	2.18000800	1.38452800	0.35455700
C	0.91855000	1.09067100	-0.23038600
C	0.68735000	-0.20552100	-0.76322500
C	1.64490000	-1.18726800	-0.66829000
H	4.09210100	0.60802600	0.93282600
C	-0.00485100	2.18104400	-0.28082500
H	-0.24615100	-0.41580600	-1.26214300
C	1.60078900	3.57219600	0.57548700
H	1.86348000	4.58850300	0.85788300
N	0.35813000	3.41000200	0.08246900
N	2.51082000	2.64346900	0.77170900
C	-2.24877400	1.06678100	-0.54046900
C	-3.32257300	0.94054200	-1.43141900
C	-2.18253300	0.23441800	0.58357400
C	-4.31089100	-0.01071600	-1.20322400
H	-3.37378100	1.58599300	-2.30143100
C	-3.17203800	-0.72335400	0.77138100
H	-1.38177800	0.33731900	1.30400600
C	-4.24419100	-0.86523800	-0.10226600
H	-5.13898700	-0.10009600	-1.89769000
H	-5.00413300	-1.61699200	0.06997400
Cl	-3.06934200	-1.77547400	2.18536100

N	-1.28952900	2.07766400	-0.78514300
H	-1.68463600	2.98748300	-0.98924900
O	3.75742900	-1.94427800	0.04089100
O	1.52399300	-2.44629400	-1.15332100
C	0.31581100	-2.80217300	-1.82890500
H	0.43950100	-3.84176000	-2.12279500
H	-0.54729000	-2.70883100	-1.16495200
H	0.16842500	-2.18492900	-2.71895800
C	5.03059900	-1.74394400	0.66320200
H	5.54066300	-2.70195400	0.59975100
H	5.60859300	-0.98334700	0.13288600
H	4.91210900	-1.45831500	1.71112800

T-1w

C	3.13934400	-0.69125800	-0.07109600
C	3.19732300	0.56980000	0.47830900
C	2.07770500	1.43475900	0.43274300
C	0.86347100	0.97335500	-0.14374500
C	0.82852100	-0.31459700	-0.74102500
C	1.93208000	-1.13437200	-0.71652400
H	4.10075200	0.94565600	0.93895700
C	-0.22646900	1.90090900	-0.12201300
H	-0.07165300	-0.64859500	-1.23320800
C	1.17457700	3.49156100	0.77902400
H	1.27878000	4.52217200	1.10741900
N	-0.03923800	3.15672600	0.29950600
N	2.22001000	2.70891200	0.91058400
C	-2.24819700	0.43960000	-0.42454400
C	-3.28174200	0.17692700	-1.33289300
C	-2.03734400	-0.43088400	0.65211900
C	-4.08680900	-0.94547000	-1.16965700
H	-3.44444700	0.85233800	-2.16546700
C	-2.84223000	-1.55684700	0.77533600
H	-1.26750900	-0.22869800	1.38510400
C	-3.87146000	-1.83567200	-0.11728600
H	-4.88488000	-1.14019600	-1.87761900
H	-4.48649000	-2.71846200	0.00413000
Cl	-2.55708600	-2.65392500	2.12913000
N	-1.49122000	1.62222100	-0.59551800
H	-2.05101900	2.46202700	-0.74214800
O	4.15363300	-1.58029700	-0.07972400
O	1.99885300	-2.36928900	-1.26844100
C	0.84286900	-2.87767400	-1.93815000
H	1.12131300	-3.86689300	-2.29352800
H	-0.00373100	-2.95892300	-1.25168300
H	0.57273100	-2.24557700	-2.78812300
C	5.38879700	-1.21353100	0.54391700
H	6.04084800	-2.07592800	0.42999600
H	5.83396200	-0.34751400	0.04843600
H	5.24072400	-1.00041700	1.60516400
O	-2.46033200	4.42779600	-0.38351100
H	-1.54515300	4.29620000	-0.05365700
H	-2.43047000	5.10919800	-1.06467500

T-2w

C	3.40734200	0.07485200	-0.11702500
C	3.10035700	1.29507600	0.44174600
C	1.77534000	1.79185100	0.41794400
C	0.74119500	0.99843100	-0.14574700
C	1.07860200	-0.23847800	-0.75646900

C	2.37404400	-0.69913300	-0.75189800
H	3.85990600	1.91827100	0.89379700
C	-0.57744800	1.55935600	-0.10169900
H	0.30990500	-0.81856600	-1.24249800
C	0.31234900	3.48771500	0.79503800
H	0.11499700	4.50171600	1.13322900
N	-0.76094000	2.81265800	0.33219700
N	1.54355800	3.04993500	0.90356800
C	-2.04160000	-0.45127300	-0.37309700
C	-2.92657600	-1.04619400	-1.28260400
C	-1.58249400	-1.19090700	0.72507900
C	-3.33420400	-2.36374700	-1.10118400
H	-3.28577000	-0.47240900	-2.12934000
C	-1.98907000	-2.51160600	0.86642300
H	-0.92805200	-0.74103500	1.46031000
C	-2.86263900	-3.12054600	-0.02828100
H	-4.01850900	-2.81509700	-1.81128900
H	-3.16650100	-4.15090000	0.10730400
Cl	-1.38974600	-3.43557700	2.24726900
N	-1.69768600	0.90535000	-0.55892400
H	-2.49759500	1.50376600	-0.79041300
O	4.63749200	-0.47745200	-0.14561000
O	2.79211500	-1.85796700	-1.31507500
C	1.82794100	-2.67999000	-1.97687300
H	2.37964300	-3.54349100	-2.34073300
H	1.04941600	-3.00748400	-1.28318900
H	1.37576100	-2.15228600	-2.82071000
C	5.72035700	0.23243800	0.46489400
H	6.59442300	-0.40087000	0.33525100
H	5.88519500	1.19276600	-0.02932100
H	5.53264000	0.38855500	1.52978000
O	-3.19632200	4.26136700	0.50850400
H	-2.32273500	3.79995100	0.49096800
H	-3.04684500	5.17621700	0.24447700
O	-4.10864800	2.40786300	-1.23548600
H	-4.94196100	1.97716300	-1.01406600
H	-4.00081500	3.17537300	-0.63117500

T-3w

C	-3.54574500	-0.93880500	-0.14232700
C	-2.90403500	-2.01367700	0.43073400
C	-1.49170500	-2.10390100	0.42081900
C	-0.72796100	-1.04773000	-0.14372000
C	-1.40231300	0.03389600	-0.76898300
C	-2.77545300	0.09762300	-0.77877600
H	-3.45480400	-2.82732700	0.88269100
C	0.69413700	-1.20214900	-0.09230400
H	-0.82681200	0.80662200	-1.25476300
C	0.40126000	-3.29344000	0.82799000
H	0.88460100	-4.19919000	1.18435300
N	1.23452500	-2.33548300	0.36658100
N	-0.90585500	-3.23565700	0.91750400
C	1.56004600	1.12800300	-0.34691700
C	2.30052300	1.95884000	-1.20255600
C	0.87963800	1.69700600	0.73981500
C	2.34252100	3.33062200	-0.98154300
H	2.84268900	1.51680200	-2.03016000
C	0.92578800	3.07354100	0.92053800
H	0.33297500	1.07724000	1.43842100
C	1.64643200	3.91317800	0.07910500

H	2.91803700	3.96182800	-1.65012900
H	1.66789900	4.98281100	0.24550400
Cl	0.05155000	3.77170900	2.28890900
N	1.57779200	-0.25849900	-0.57376400
H	2.45629400	-0.62679500	-0.95554300
O	-4.88240100	-0.76713200	-0.18589800
O	-3.50704200	1.07716700	-1.36067100
C	-2.81674800	2.13103200	-2.03666100
H	-3.59194600	2.78871400	-2.42243200
H	-2.17472800	2.68519700	-1.34737500
H	-2.22142600	1.73970300	-2.86569600
C	-5.71974500	-1.75777000	0.42014200
H	-6.73841100	-1.40657300	0.27588200
H	-5.59175700	-2.72705400	-0.06729900
H	-5.50780800	-1.84646800	1.48822300
O	3.82371300	-2.86732200	1.39447300
H	2.95243400	-2.62324600	0.99843500
H	3.84755000	-2.50133100	2.28556700
O	3.99205800	-0.97422300	-1.96317100
H	4.70206500	-1.45830200	-1.48280700
H	3.85819700	-1.42302800	-2.80539700
O	5.76848500	-2.33005400	-0.40585600
H	5.15401500	-2.53986000	0.33625600
H	6.51101500	-1.83641300	-0.04057700

T-4w

C	-3.85477800	-0.88187600	0.02618000
C	-3.18881000	-1.99534500	0.48707500
C	-1.78632500	-2.11436800	0.34074400
C	-1.05112000	-1.04899800	-0.24288900
C	-1.75463000	0.07530400	-0.75039600
C	-3.12092500	0.16854000	-0.62797800
H	-3.71503800	-2.81888800	0.95024200
C	0.36818900	-1.23429100	-0.32952700
H	-1.21066500	0.85956500	-1.25310900
C	0.09920100	-3.36970700	0.50127000
H	0.58652000	-4.30672100	0.75808500
N	0.91172100	-2.41225700	0.00498100
N	-1.18875500	-3.28305300	0.72812700
C	1.21544500	1.10509500	-0.55325400
C	1.83671700	1.96553100	-1.46898700
C	0.66466500	1.63307600	0.62253000
C	1.89503400	3.33200800	-1.21544700
H	2.26818600	1.55628400	-2.37518800
C	0.71747200	3.00452200	0.83575000
H	0.21152300	0.98465800	1.36108000
C	1.32613800	3.87426500	-0.06273200
H	2.37800900	3.98911900	-1.93042900
H	1.35694400	4.93928600	0.13011700
Cl	0.00458900	3.65610800	2.31486100
N	1.23017700	-0.28125700	-0.81667500
H	2.13795100	-0.62596600	-1.15676000
O	-5.18599400	-0.68391900	0.11221600
O	-3.87749800	1.19300800	-1.08920100
C	-3.22453700	2.26972100	-1.76608700
H	-4.01403300	2.96586000	-2.03896400
H	-2.50645500	2.76793900	-1.10984600
H	-2.71983100	1.91598200	-2.66882900
C	-5.98807900	-1.69097900	0.73827400
H	-7.00819700	-1.31714400	0.69998100

H	-5.92128900	-2.63592200	0.19407000
H	-5.68787800	-1.83767900	1.77841800
O	3.58798900	-3.22368300	-0.14381100
H	2.63218900	-2.96531700	-0.06135000
H	3.62895700	-4.17163100	-0.31319000
O	3.85335200	-0.98960400	-1.80629600
H	4.50899800	-0.45197900	-1.31476100
H	3.94159900	-1.89127200	-1.44804000
O	5.73801300	0.19303600	-0.12534200
O	5.31604100	-1.91757200	1.55975400
H	5.67007000	-0.49179300	0.57767700
H	5.56863500	1.04828800	0.28527900
H	4.72179700	-2.49122900	1.02898700
H	6.04483600	-2.46439700	1.87314000

T-5w

C	-3.77814900	-1.42747800	-0.12862000
C	-2.94792200	-2.36836500	0.43896400
C	-1.54328200	-2.20555800	0.41159800
C	-0.98542700	-1.03316900	-0.16458800
C	-1.84950400	-0.09079100	-0.78188400
C	-3.21215600	-0.27266700	-0.77497800
H	-3.33905500	-3.26550600	0.89913100
C	0.44216400	-0.93306700	-0.13011000
H	-1.42931100	0.77140200	-1.27578900
C	0.53270800	-3.04444100	0.79645100
H	1.17216000	-3.85029500	1.14694700
N	1.18247200	-1.95594300	0.32029100
N	-0.76083400	-3.21437200	0.90516600
C	0.83099100	1.52004900	-0.39271400
C	1.31004700	2.47200000	-1.30272500
C	0.11581400	1.94433500	0.73537200
C	1.06820400	3.82514800	-1.08945700
H	1.86684000	2.14580500	-2.17298300
C	-0.13061900	3.30033900	0.90764700
H	-0.23349700	1.23032100	1.46982300
C	0.33479100	4.25968100	0.01487600
H	1.44387100	4.55402800	-1.79926900
H	0.13317900	5.31133800	0.17535300
Cl	-1.04716400	3.81705000	2.32602300
N	1.13436900	0.15807100	-0.60676300
H	2.08568200	-0.02133300	-0.93238500
O	-5.12336400	-1.49745700	-0.15749700
O	-4.11283800	0.56038700	-1.34635700
C	-3.62970600	1.72094400	-2.02791500
H	-4.51461800	2.23082000	-2.40099800
H	-3.08707100	2.37915900	-1.34485500
H	-2.98597100	1.44223300	-2.86611100
C	-5.76426200	-2.62031000	0.45845400
H	-6.83056500	-2.45731000	0.32376700
H	-5.46942400	-3.55236200	-0.02907400
H	-5.52951400	-2.66594800	1.52436300
O	3.34241400	-1.28227800	2.24399800
H	2.63540600	-1.47516800	1.59620400
H	3.08289400	-1.69737500	3.07459100
O	3.78426800	-0.07572000	-1.95350600
H	4.61734200	0.21682100	-1.50884900
H	3.80119400	0.25328000	-2.85926400
O	6.05689100	0.34106700	-0.55363700
O	5.57026800	-1.98497300	0.75223600

H	5.99435600	-0.47217900	0.00771100
H	6.14471100	1.09900800	0.03492600
H	4.90183400	-1.75121100	1.42883300
H	5.04926100	-2.42130000	0.04509800
H	3.77610700	-1.88875600	-1.68048000
H	2.90455800	-2.69276400	-0.70111300
O	3.72701500	-2.74937000	-1.21661900

T-6w

C	-3.55803300	-1.31548500	-0.14128800
C	-2.59120100	-2.29652400	-0.11654900
C	-1.26218000	-2.01314000	-0.50688100
C	-0.90546000	-0.68707600	-0.86630300
C	-1.91957700	0.30456600	-0.92665800
C	-3.21852500	0.00931900	-0.58449500
H	-2.82334100	-3.31299300	0.17116800
C	0.48001900	-0.47097500	-1.17623400
H	-1.67258300	1.29885100	-1.26456200
C	0.82404400	-2.74580500	-1.03490700
H	1.52765400	-3.56471500	-1.16052800
N	1.29697700	-1.52426600	-1.33822900
N	-0.36406300	-3.04768400	-0.56489200
C	0.70590500	1.97796000	-0.72816700
C	0.90045000	3.17431000	-1.42611600
C	0.26564000	2.01314800	0.60050300
C	0.64557500	4.39365400	-0.80436900
H	1.24527200	3.14213100	-2.45323800
C	-0.00388000	3.24286800	1.18753400
H	0.14124700	1.09896800	1.16621600
C	0.17962400	4.44342200	0.50873900
H	0.79818000	5.31756200	-1.35121700
H	-0.03360100	5.38936200	0.99085400
Cl	-0.57753100	3.27659800	2.85658000
N	1.04588800	0.75747800	-1.37130500
H	2.02305800	0.74078900	-1.68879000
O	-4.84997500	-1.49136300	0.20164000
O	-4.25479100	0.88071400	-0.62867000
C	-4.00295300	2.21472800	-1.07641600
H	-4.96205000	2.72507700	-1.03082400
H	-3.28718500	2.71960700	-0.42273500
H	-3.63390900	2.21928500	-2.10535300
C	-5.26993800	-2.78481600	0.64959600
H	-6.32803900	-2.68493400	0.87824200
H	-5.13184700	-3.53262700	-0.13475100
H	-4.72475700	-3.08144100	1.54859100
O	4.02000400	-1.72884800	-1.89318600
H	3.03256300	-1.68197100	-1.81050800
H	4.24358000	-2.38396100	-2.56375800
O	3.90570300	1.03671300	-1.83566400
H	4.19792000	1.20619000	-0.92219700
H	4.18299000	0.12266200	-2.03212200
O	4.60755100	-1.73026600	0.84171900
H	4.62280800	-0.76679600	0.98406100
H	4.49717800	-1.85567700	-0.12158300
O	2.94713300	-3.20890600	2.43297700
H	3.52648200	-3.69040000	3.03363000
H	3.52697900	-2.66981400	1.84541000
O	4.64544900	1.13886100	0.94185400
H	5.49292900	1.53113200	1.18713600
H	3.97798800	1.55125500	1.50490000

O	0.53314100	-4.56451400	1.89331300
H	1.36366400	-4.06775800	2.03041300
H	0.11244400	-4.19068300	1.10086500

T-7w

C	3.25755100	-1.64035000	-0.32486700
C	3.34998400	-0.26679400	-0.27290100
C	2.22301700	0.54552500	-0.53249900
C	0.96786900	-0.05662300	-0.80621500
C	0.89704200	-1.47246600	-0.89205600
C	2.00475000	-2.25545000	-0.66334500
H	4.28730500	0.22500500	-0.05164000
C	-0.13141700	0.84268600	-1.03594100
H	-0.03605900	-1.94466600	-1.15351500
C	1.33169600	2.61989800	-0.85795700
H	1.46057100	3.69754200	-0.91220000
N	0.08764500	2.16812300	-1.08910500
N	2.39098300	1.90710200	-0.55382000
C	-2.08094900	-0.69666500	-0.75042900
C	-2.88150800	-1.46854500	-1.59662600
C	-2.00593100	-0.99573400	0.61519100
C	-3.59173800	-2.55122300	-1.08288400
H	-2.93500300	-1.22343900	-2.65119000
C	-2.70694900	-2.09585700	1.09320700
H	-1.44339500	-0.35876200	1.28823600
C	-3.50274300	-2.88485400	0.26767200
H	-4.21064000	-3.15111500	-1.74091200
H	-4.04222800	-3.73396600	0.66882900
Cl	-2.60274500	-2.48869300	2.81221300
N	-1.41184800	0.44238800	-1.28131900
H	-2.05231400	1.16411000	-1.63453400
O	4.27560400	-2.49396200	-0.09757600
O	2.03149200	-3.60827200	-0.73352100
C	0.83029100	-4.29446100	-1.09345000
H	1.08478300	-5.35163500	-1.09107700
H	0.03714700	-4.10626600	-0.36549700
H	0.49598900	-4.00014600	-2.09165500
C	5.55883500	-1.95561600	0.24046800
H	6.20573800	-2.81636400	0.39016100
H	5.94886700	-1.33890600	-0.57260200
H	5.50524300	-1.36996500	1.16105900
O	-1.88900600	4.14339700	-0.93097000
H	-1.13453200	3.50786100	-1.03573500
H	-1.57830100	5.02898700	-1.14951400
O	-3.53986800	2.25436800	-2.09007000
H	-4.22943200	2.08746400	-1.42326300
H	-3.13227500	3.10610100	-1.84582000
O	-3.12572200	3.31764300	1.44330900
H	-3.90732800	2.84912900	1.10000600
H	-2.68661300	3.71757500	0.66666100
O	-1.39189300	1.55313300	2.68190200
H	-0.77832800	2.04984800	3.23453200
H	-1.99915800	2.20691900	2.26923000
O	-5.29394400	1.94158300	0.15597700
H	-6.14379600	2.39924200	0.14070800
H	-5.46984500	1.04213600	0.45983400
O	6.08292900	2.86909500	2.35017800
H	5.98027700	3.67208200	2.87275300
H	5.61753000	3.02256600	1.49994500
O	4.79163600	3.27642600	-0.04566600

H	5.32764100	3.25850500	-0.84626200
H	3.95873900	2.77654400	-0.23714000

Table S1. Selected spatial parameters and energies of ground state of four structures of AG1478 rotamers complexed with one water molecule (P-1w) in the gas phase (optimized at B3LYP/6-311+G*).

		P-1w			
Parameter		**(1)**	**(2)**	**(3)**	**(4)**
<R2> (a.u.)		11540.3537	10967.7902	10797.8090	12233.6722
μ (D)		5.1725	7.6347	6.8047	**3.6749**
E_h (a.u.)		-1469.735099	-1469.729833	-1469.731679	-1469.730528
ZPE (kcal/mol)		188.783040	188.576890	188.857020	188.292300
E_h + ZPE (a.u.)		**-1469.434254**	-1469.429317	-1469.430716	-1469.430466
Rotational Const. (GHz)	**A**	0.4173	0.4680	0.4697	0.5160
	B	0.1073	0.1074	0.1116	0.0953
	C	0.0855	0.0930	0.0923	0.0805
HOMO-LUMO gap (eV)		**3.6791**	4.2993	4.2580	4.2942
HOMO (Ha)		-0.20141	-0.2266	-0.2117	-0.2351
LUMO (Ha)		-0.06620	-0.0686	-0.0552	-0.0773
ΔE_{Tot} (kcal/mol)		0.00	3.10	2.22	2.38
		T-1w			
		(1)	**(2)**	**(3)**	**(4)**
<R2> (a.u.)[a]		8841.5171	8532.2868	8230.0944	8864.7514
μ (D)[b]		4.1200	3.0395	**2.0863**	3.5443
E_h (a.u.)[c]		-1469.732375	-1469.734892	-1469.725746	-1469.728043
ZPE (kcal/mol)[d]		189.008020	189.277610	188.681290	188.339290
E_h + ZPE (a.u.)		-1469.431171	**-1469.433259**	-1469.425063	-1469.427905
Rotational Const. (GHz)	**A**	0.3190	0.2687	0.2841	0.2840
	B	0.1548	0.1830	0.1653	0.1659
	C	0.1246	0.1283	0.1463	0.1230
HOMO-LUMO gap (eV)[e]		4.2838	**4.2253**	4.4403	4.3282
HOMO (Ha)		-0.2261	-0.2209	-0.2309	-0.2290
LUMO (Ha)		-0.0687	-0.0657	-0.0677	-0.0699
ΔE_{Tot} (kcal/mol)[f]		1.31	0.00	5.14	3.36

[a] Electronic spatial extent in hatree
[b] Dipole moment in debye
[c] Total molecular energy in hatree
[d] Zero-point energy in kcal/mol
[e] Energy gap between highest occupied molecular orbital and lowest unoccupied molecular orbital in eV
[f] Energy destabilization relative to the most stable isomer in kcal/mol

Table S2. Selected spatial parameters and energies of ground state of six structures of AG1478 rotamers bound to two water molecule (P-2w) in the gas phase (optimized at B3LYP/6-311+G*).

	P-2w					
Parameter	**(1)**	**(2)**	**(3)**	**(4)**	**(5)**	**(6)**
<R2> (a.u.)	12117.2735	12059.9573	13349.7041	11413.1724	12948.6809	12683.1339
μ (D)	6.9528	7.9356	**2.5857**	9.7131	5.2900	5.3348
E_h (a.u.)	-1546.188112	-1546.190484	-1546.188902	-1546.186428	-1546.183234	-1546.186196
ZPE (kcal/mol)	204.034340	204.278200	203.759310	203.966190	203.387380	203.751800
E_h + ZPE (a.u.)	-1545.862963	**-1545.864946**	-1545.864191	-1545.861387	-1545.859116	-1545.861497
Rot. Const. (GHz) A	0.3557	0.3397	0.3604	0.3751	0.4251	0.4228
B	0.1027	0.1068	0.0929	0.1069	0.0906	0.0945
C	0.0838	0.0827	0.0739	0.0908	0.0782	0.0783
HOMO-LUMO gap (eV)	4.3102	4.2993	**4.2672**	4.3021	4.3080	4.2980
HOMO (Ha)	-0.2299	-0.2145	-0.2267	-0.2175	-0.2309	-0.2148
LUMO (Ha)	-0.0715	-0.0565	-0.0698	-0.0594	-0.07258	-0.0568
ΔE_{Tot} (kcal/mol)	1.24	0.00	0.47	2.23	3.66	2.16
	T-2w					
	(1)	**(2)**	**(3)**	**(4)**	**(5)**	**(6)**
<R2> (a.u.)	9783.5510	9782.9577	10014.4313	9663.9626	9825.5268	9476.0802
μ (D)	2.5945	2.5706	2.8414	2.1291	3.1990	**2.0927**
E_h (a.u.)	-1546.192652	-1546.192652	-1546.186083	-1546.199183	-1546.188237	-1546.178980
ZPE (kcal/mol)	204.622710	204.614520	203.800130	205.393300	203.948760	203.389040
E_h + ZPE (a.u.)	-1545.866565	-1545.866578	-1545.861307	**-1545.871868**	-1545.863224	-1545.854859
Rotat. Const. (GHz) A	0.2495	0.2495	0.2420	0.2213	0.2326	0.2403
B	0.1537	0.1537	0.1500	0.1716	0.1600	0.1480
C	0.1118	0.1118	0.1092	0.1128	0.1112	0.1254
HOMO-LUMO gap (eV)	4.2068	4.2065	4.3004	**4.2000**	4.2316	4.4806
HOMO (Ha)	-0.22445	-0.22441	-0.23116	-0.2200	-0.22595	-0.2375
LUMO (Ha)	-0.06985	-0.06982	-0.07312	-0.0656	-0.07044	-0.0728
ΔE_{Tot} (kcal/mol)	3.33	3.32	6.63	0.00	5.42	10.67

[a] Electronic spatial extent in hatree
[b] Dipole moment in debye
[c] Total molecular energy in hatree
[d] Zero-point energy in kcal/mol
[e] Energy gap between highest occupied molecular orbital and lowest unoccupied molecular orbital in eV
[f] Energy destabilization (relative energy difference) relative to the most stable isomer in kcal/mol

Table S3. Selected values of dipole moment (debye) and energies of ground state of four structures of AG1478 rotamers bound to three water molecules (P-3w) in the gas phase (optimized at B3LYP/6-311+G*).

	P-3w			
Parameter	**(1)**	**(2)**	**(3)**	**(4)**
μ (D)	6.6372	6.6376	7.6747	**4.3679**
HOMO-LUMO gap (eV)	4.2683	4.2683	4.2870	**4.1809**
E_h + ZPE (a.u.)	-1622.302610	-1622.302604	-1622.302645	**-1622.310945**
ΔE_{Tot} (kcal/mol)	5.230	5.234	5.208	**0.000**
	T-3w			
	(1)	**(2)**	**(3)**	**(4)**
μ (D)	2.8020	1.3456	3.5662	**1.3473**
HOMO-LUMO gap (eV)	4.1918	**4.0672**	4.1382	4.0675
E_h + ZPE (a.u.)	-1622.298358	-1622.309341	-1622.293538	**-1622.309343**
ΔE_{Tot} (kcal/mol)	6.893	0.001	9.918	**0.000**

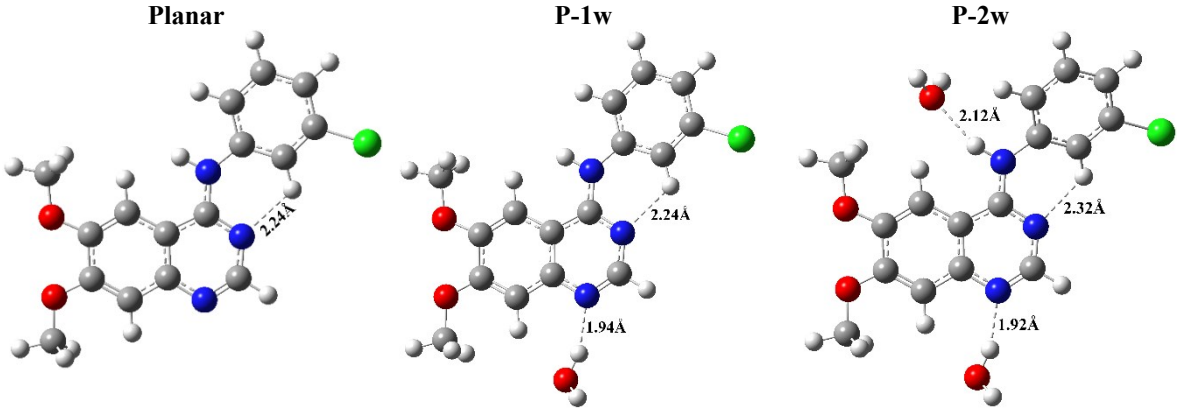
Table S4. Selected values of dipole moment (debye) and energies of ground state of four structures of AG1478 rotamers bound to four water molecules (P-4w) in the gas phase (optimized at B3LYP/6-311+G*).

	P-4w			
Parameter	**(1)**	**(2)**	**(3)**	**(4)**
μ (D)	8.8133	4.8159	5.0003	**3.8824**
HOMO-LUMO gap (eV)	4.2484	4.2846	4.2353	**4.2111**
E_h + ZPE (a.u.)	-1698.73301	-1698.733285	-1698.739464	**-1698.750851**
ΔE_{Tot} (kcal/mol)	11.195	11.023	7.145	**0.000**
	T-4w			
	(1)	**(2)**	**(3)**	**(4)**
μ (D)	2.6920	**1.3674**	2.3107	1.6350
HOMO-LUMO gap (eV)	4.2294	4.1872	4.2772	**4.0759**
E_h + ZPE (a.u.)	-1698.731925	-1698.732469	-1698.739131	**-1698.746396**
ΔE_{Tot} (kcal/mol)	9.081	8.739	4.559	**0.000**

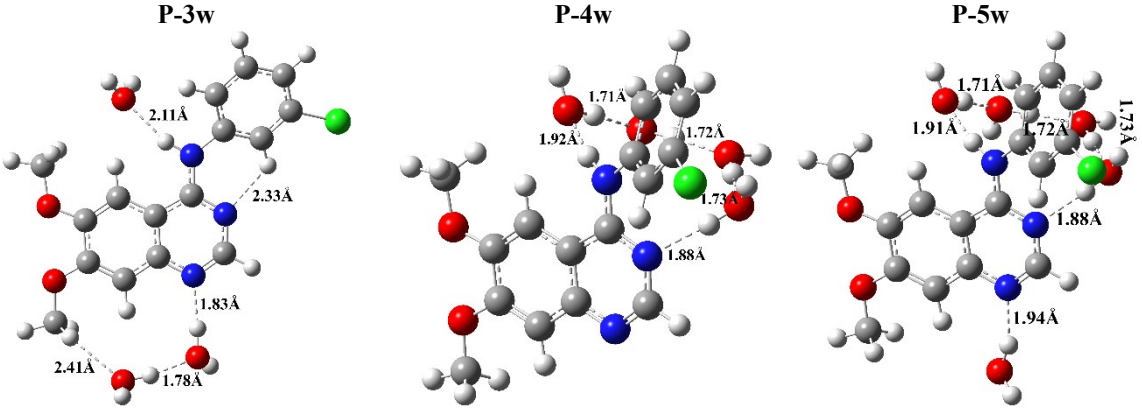
Table S5. Selected values of dipole moment (debye) and energies of ground state of four structures of AG1478 rotamers bound to five water molecules (P-5w) in the gas phase (optimized at B3LYP/6-311+G*).

	P-5w			
Parameter	**(1)**	**(2)**	**(3)**	**(4)**
μ (D)	4.6015	4.0680	**3.4410**	4.3375
HOMO-LUMO gap (eV)	4.2702	4.2887	**4.1888**	4.2503
E_h + ZPE (a.u.)	-1775.170932	-1775.162351	**-1775.184644**	-1775.164725
ΔE_{Tot} (kcal/mol)	8.604	13.989	**0.000**	12.499
	T-5w			
	(1)	**(2)**	**(3)**	**(4)**
μ (D)	4.2740	**2.4043**	6.3786	6.3779
HOMO-LUMO gap (eV)	4.2702	4.2909	4.2332	**4.1192**
E_h + ZPE (a.u.)	-1775.172324	-1775.174615	-1775.172291	**-1775.179012**
ΔE_{Tot} (kcal/mol)	4.197	2.759	4.217	**0.000**

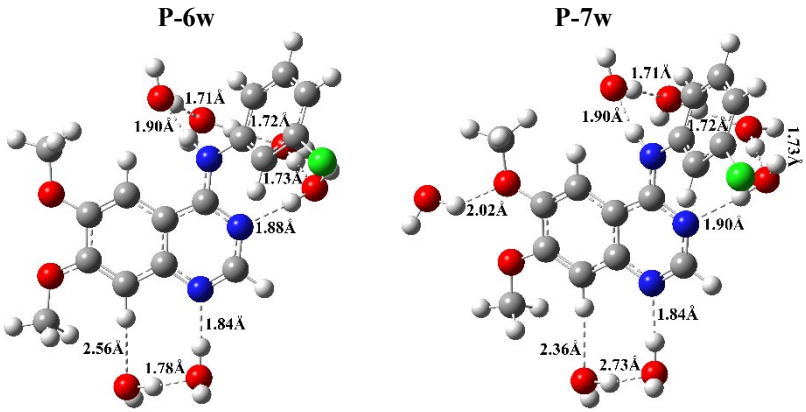
Figure S1. Structural configuration of the most stable planar conformers complexed with n=1-7 water molecules in gas phase at B3LYP/6-311+G*.



	Planar	P-1w	P-2w
H-bond[1]	1 (1+0+0)	2 (1+1+0)	3 (1+2+0)
DM[2]	5.8297	5.1725	7.9356



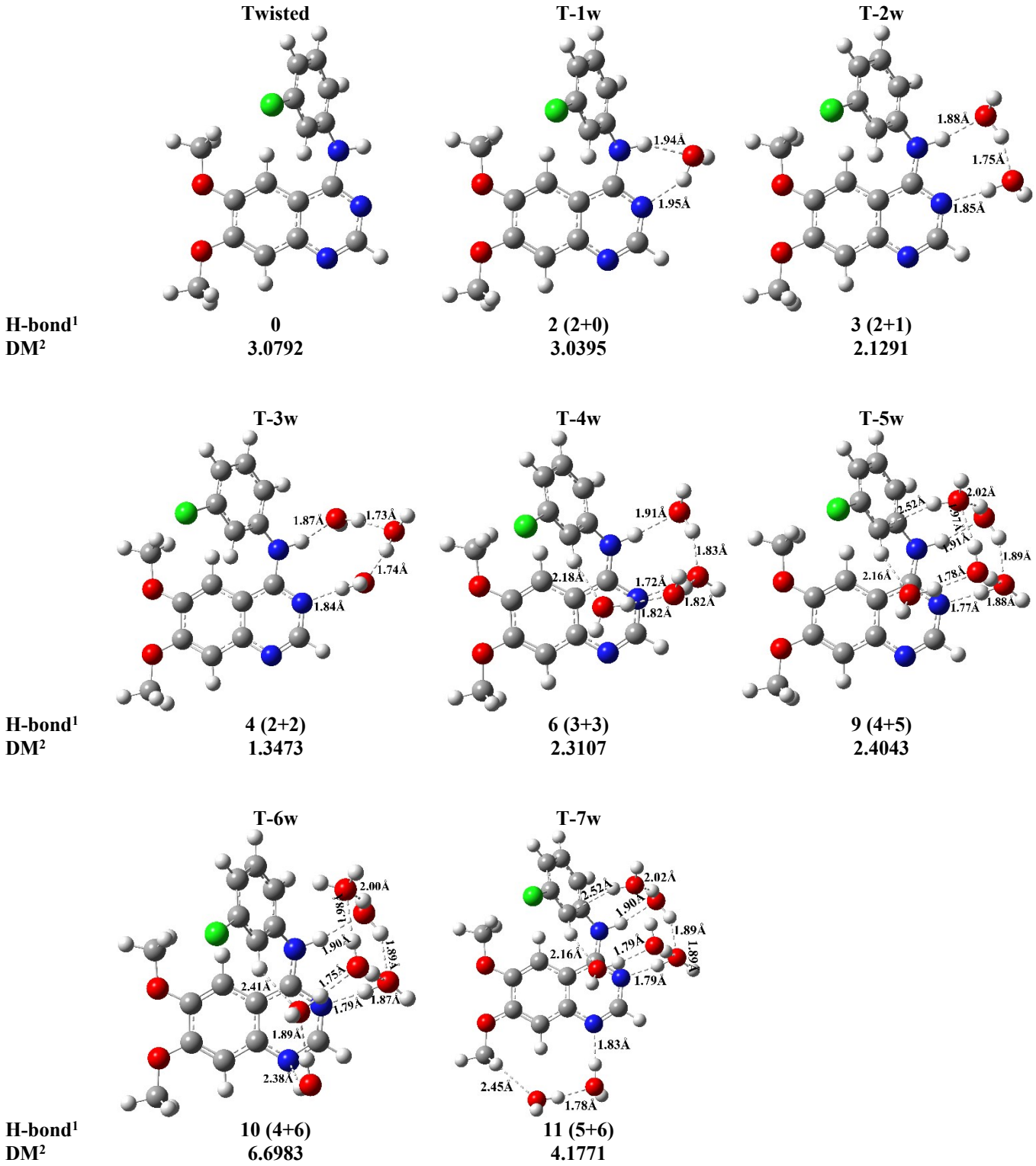
	P-3w	P-4w	P-5w
H-bond[1]	5 (1+3+1)	5 (0+2+3)	6 (0+3+3)
DM[2]	7.6747	3.8824	3.4410



	P-6w	P-7w
H-bond[1]	8 (0+4+4)	9 (0+5+4)
DM[2]	3.6688	2.8834

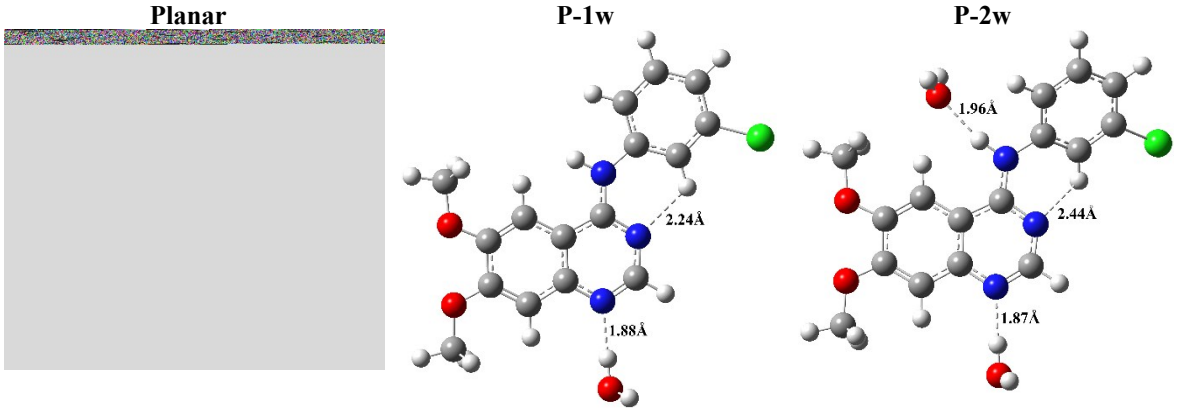
[1] Total number of H-bonds (Intramolecular H-bond + Intermolecular H-bonds between AG1478 and water + Intermolecular H-bonds between two water molecules)
[2] Dipole moment (Debye)

Figure S2. Structural configuration of the most stable twisted conformers complexed with n=1-7 water molecules in gas phase at B3LYP/6-311+G*.

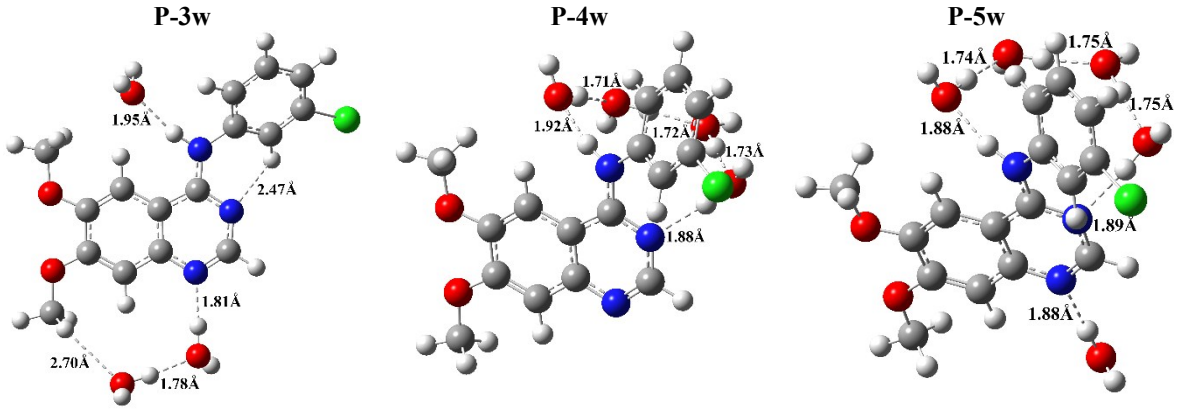


[1] Total number of H-bonds (Intramolecular H-bond + Intermolecular H-bonds between AG1478 and water + Intermolecular H-bonds between two water molecules)
[2] Dipole moment (Debye)

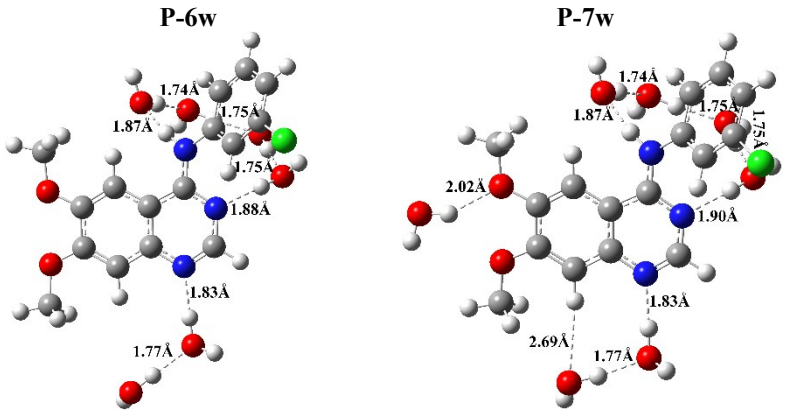
Figure S3. Structural configuration of the most stable planar conformers complexed with n=1-7 water molecules in DMF at B3LYP/6-311+G*.



	Planar	P-1w	P-2w
H-bond[1]	1 (1+0+0)	2 (1+1+0)	3 (1+2+0)
DM[2]	8.0797	9.3541	13.1013



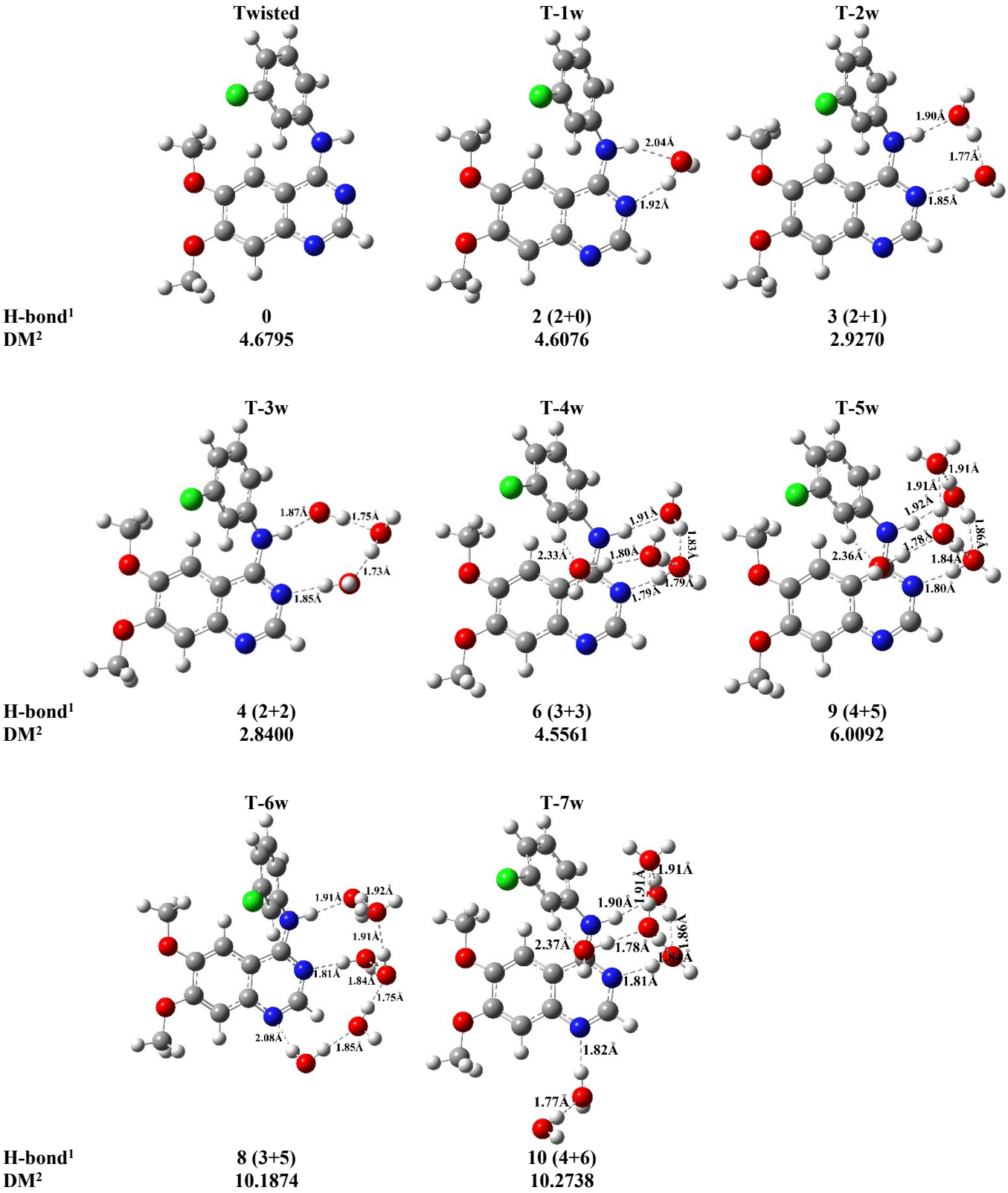
	P-3w	P-4w	P-5w
H-bond[1]	5 (1+3+1)	5 (0+2+3)	6 (0+3+3)
DM[2]	11.0551	3.8824	5.9786



	P-6w	P-7w
H-bond[1]		
DM[2]		

[1] Total number of H-bonds (Intramolecular H-bond + Intermolecular H-bonds between AG1478 and water + Intermolecular H-bonds between two water molecules)
[2] Dipole moment (Debye)

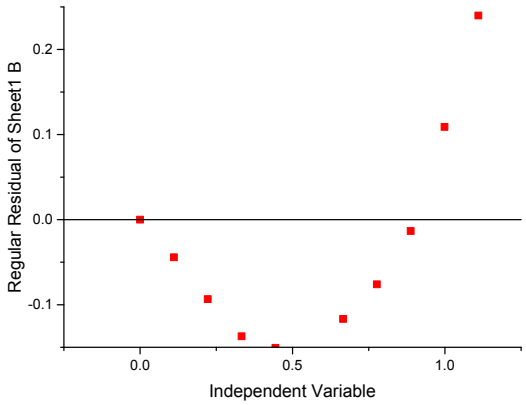
Figure S4. Structural configuration of the most stable twisted conformers complexed with n=1-7 water molecules in DMF at B3LYP/6-311+G*.



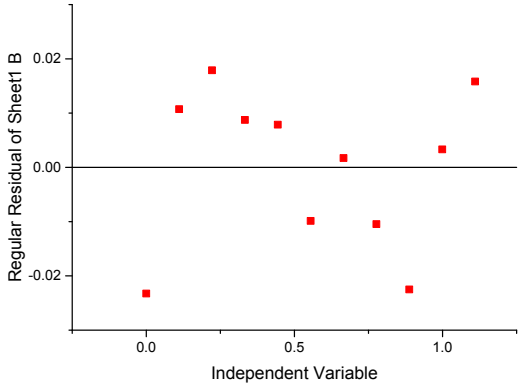
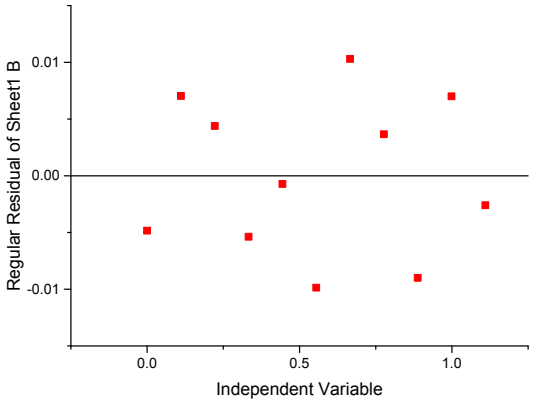
[1] Total number of H-bonds (Intramolecular H-bond + Intermolecular H-bonds between AG1478 and water + Intermolecular H-bonds between two water molecules)
[2] Dipole moment (Debye)

Figure S5. Residual plot for a) linear fitting, b) Quadratic fitting and c) Cubic fitting of Stern-Volmer plot

a)



b)



c)