Supplementary Data for

Evaluation of using the time-dependent density functional theory in studying fluorescence properties of coumarin derivatives

Nguyen Khoa Hien[1], Mai Van Bay[2], Quan V. Vo[3], Ngo Duy Y[4], Duong Tuan Quang[4*], and Pham Cam Nam[5*]

[1]Mientrung Institute for Scientific Research, Vietnam National Museum of Nature Vietnam Academy of Science and Technology, Hue 530000, Vietnam

[2]The University of Danang, University of Science and Education, Danang 550000, Vietnam

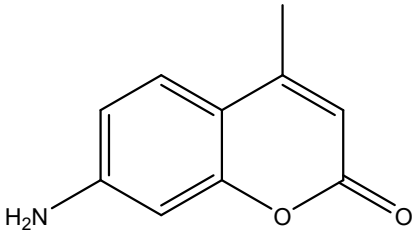
[3]Faculty of Chemical Technology-Environment, The University of Danang - University of Technology and Education, 48 Cao Thang, Danang 550000, Vietnam.

[4]Department of Chemistry, Hue University, Hue 530000, Vietnam

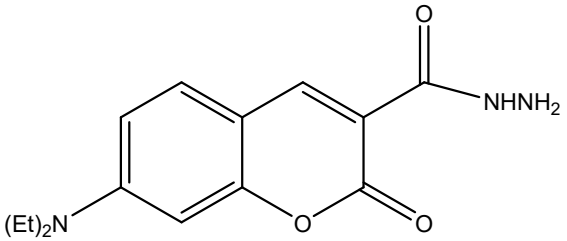
[5]The University of Danang – University of Science and Technology, Danang 550000, Vietnam

*Corresponding author: duongtuanquang@hueuni.edu.vn; pcnam@dut.udn.vn

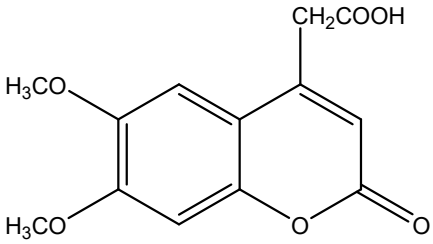
S1. Structures of investigated coumarin derivatives



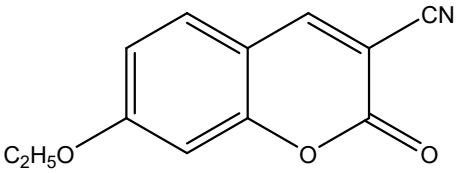
7-Amino-4-methylcoumarin (**F1**)



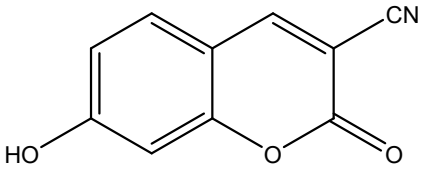
7-Diethylaminocoumarin-3-carboxylic acid hydrazide (**F2**)



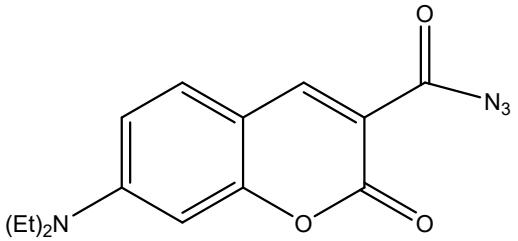
6,7-Dimethoxycoumarin-4-acetic acid **(F3)**



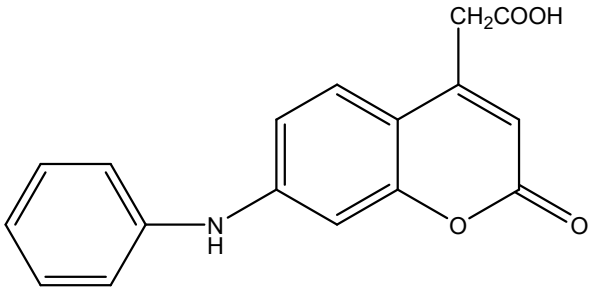
3-Cyano-7-ethoxycoumarin (**F4**)



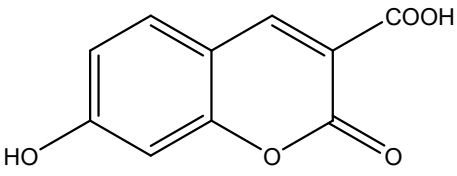
3-Cyano-7-hydroxycoumarin (**F5**)



7-Diethylaminocoumarin-3-carbonyl azide (**F6**)

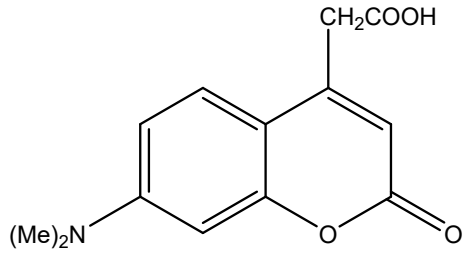


7-Anilinocoumarin-4-acetic acid (**F7**)

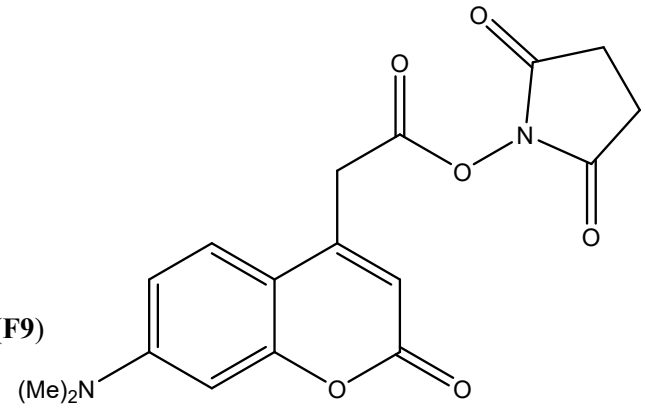


7-hydroxycoumarin-3carboxylic acid (**F8**)

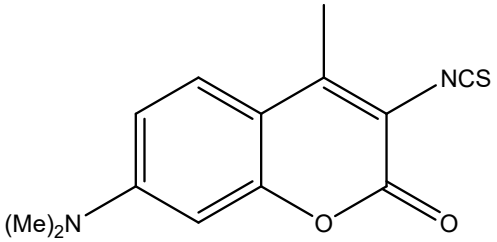
Fig.S1. *Structure of investigated coumarin derivatives **F1**-**F8***



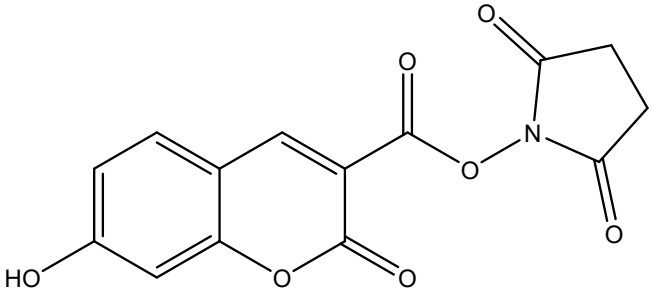
7-Dimethylaminocoumarin-4-acetic acid (**F9**)



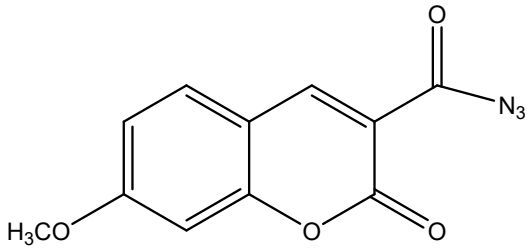
7-Dimethylaminocoumarin-4-acetic acid succinimidyl ester (**F10**)



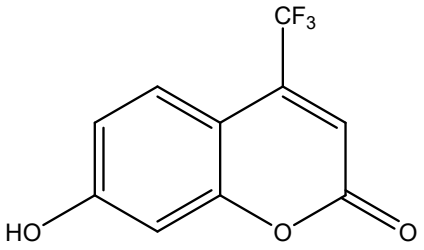
7-Dimethylamino-4-methylcoumarin-3-isothiocyanate (DACITC) (**F11**)



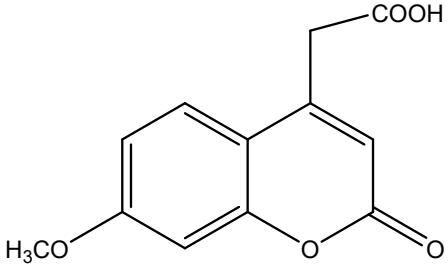
7-Hydroxycoumarin-3-carboxylic acid succinimidyl ester (**F12**)



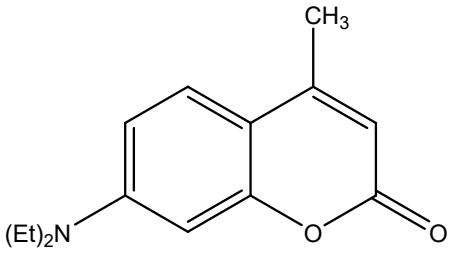
7-Methoxycoumarin-3-carbonyl azide (**F13**)



7-Hydroxy-4-(trifluoromethyl)coumarin (**F14**)

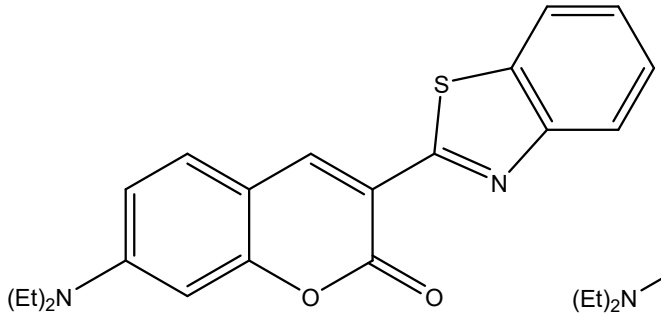


7-Methoxycoumarin-4-acetic acid (**F15**)

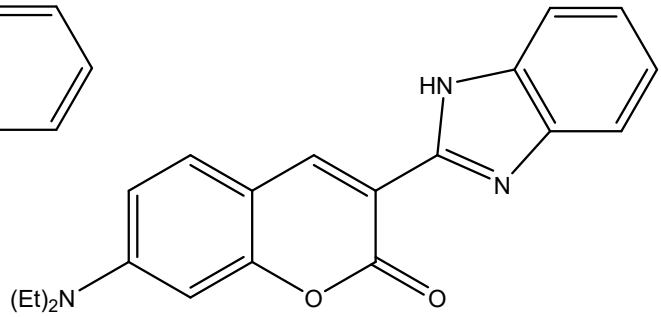


7-(Diethyamino)-4-methylcoumarin (**F16**)

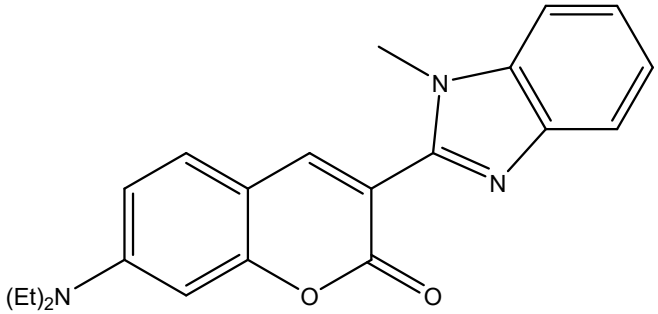
Fig.S2. *Structure of investigated coumarin derivatives **F9**-**F16***



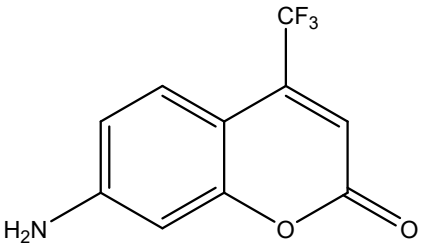
Coumarin 6 (**F17**)



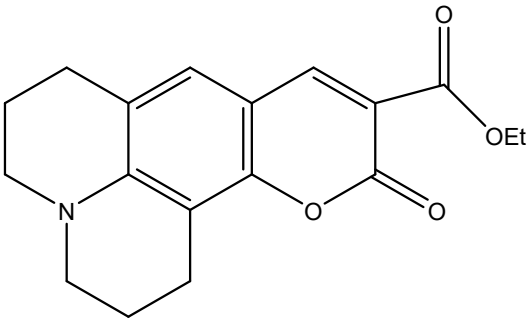
Coumarin 7 (**F18**)



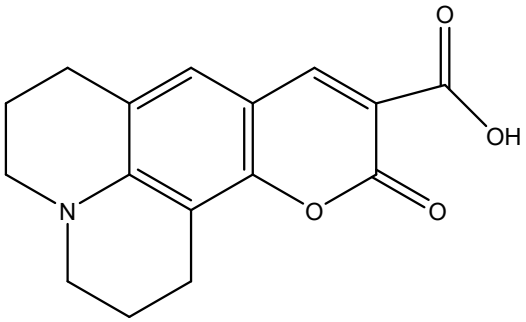
Coumarin 30 (**F19**)



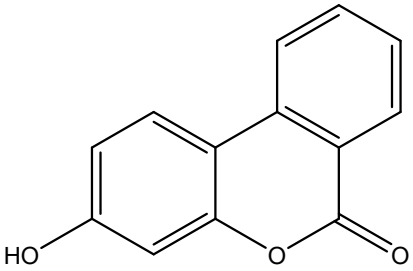
Coumarin 151 (**F20**)



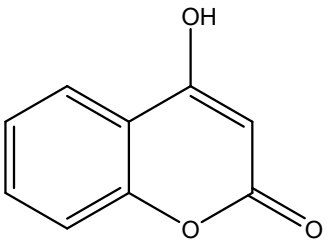
Coumarin 314 (**F21**)



Coumarin 343 (**F22**)

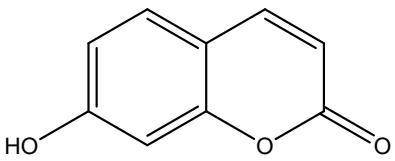


Urolithin B (**F23**)

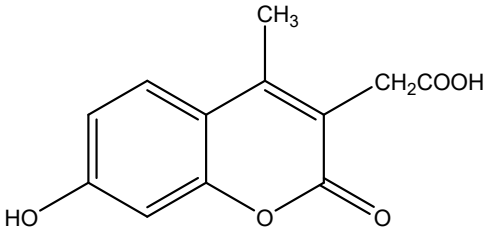


4-Hydroxylcoumarin (**F24**)

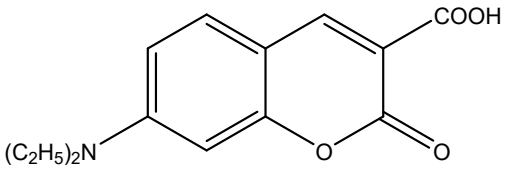
Fig.S3. *Structure of investigated coumarin derivatives **F17-F24***



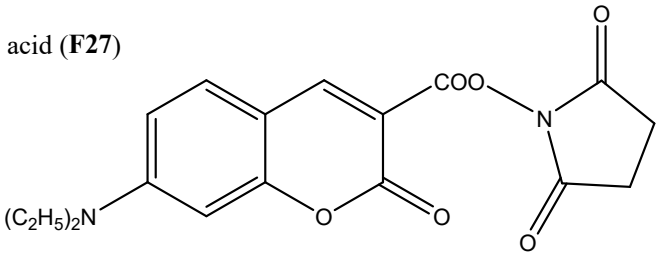
7-Hydroxylcoumarin (**F25**)



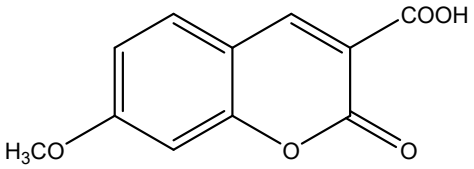
7-hydroxy-4-methylcoumarin-3-acetic acid (**F26**)



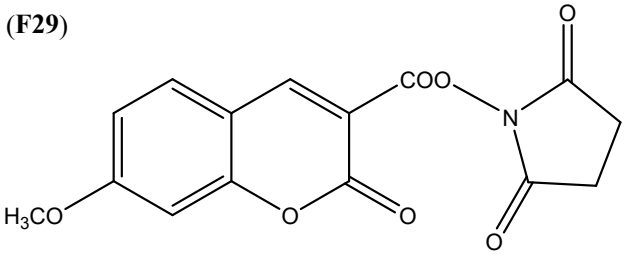
7-diethylaminocoumarin-3-carboxylic acid (**F27**)



7-diethylaminocoumarin-3-carboxylic acid succinimidyl ester (**F28**)



7-methoxycoumarin-3-carboxylic acid (**F29**)



7-methoxycoumarin-3-carboxylic acid succinimidyl ester (**F30**)

Fig.S4. *Structure of investigated coumarin derivatives **F25-F30***

S2. The paired *t*-test method for comparing pairs of values

The following table gives the values of factor determined by two different method for n test samples:

Sample	1	2	3	4	…		n	n samples
Method N°1	x_1	x_2	x_3	x_4	…		x_n	
Method N°2	y_1	y_2	y_3	y_4	…		y_n	

The calculated $|t|$ value is determined according to the expression (1) below:

$$|t| = \frac{|\bar{d}|}{S_d} * \sqrt{n} \quad (1)$$

In there:

$$\bar{d} = \frac{\sum (x_i - y_i)}{n} \quad (2)$$

$$S_d = \sqrt{\frac{\sum (d_i - \bar{d})^2}{n-1}} \quad (3)$$

The results of determining the calculating *t* value for each parameter are as follows:

Samples	1	2	3	4	5	6	7	8	9	10
MAE (1)	58	71	56	75	53	75	70	58	55	77
MAE (2)	58	70	54	80	52	79	70	58	53	81
di=MAE(1)-MAE(2)	0.1	0.6	2.1	-5.2	1.3	-3.6	-0.3	-0.1	2.6	-3.7
$\bar{d}$	-0.62									
$d_i - \bar{d}$	0.76	1.22	2.72	-4.58	1.88	-3.02	0.34	0.56	3.22	-3.08
$\sum (d_i - \bar{d})^2$	63.38									
S_d	2.65									
$\|t\|$ (MEA)	0.74									

Samples	1	2	3	4	5	6	7	8	9	10
RMSM (1)	64	96	61	78	60	78	96	63	62	80
RMSM (2)	64	104	60	82	60	81	105	63	62	83
d_i=RMSM(1)-RMSM(2)	-0.15	-7.85	1.31	-4.77	-0.21	-3.21	-9.72	0.01	-0.17	-3.36
MSE (1)	-46	20	-34	-75	-44	-75	19	-41	-47	-77
MSE (2)	-46	37	-31	-80	-47	-79	39	-40	-51	-81
$d_i - \bar{d}$	2.93	-5.07	4.09	-1.99	2.57	-0.43	-6.94	2.79	2.62	-0.58
d_i=MSE(1)-MSE(2)	-0.14	17.16	-3.14	5.20	2.82	3.64	19.32	-1.46	4.36	3.70
$\sum (d_i - \bar{d})^2$	124.84									
$\bar{d}$	-2.15									
S_d	3.72									
$\lvert t \rvert$ (RMSM)	2.36									
$d_i - \bar{d}$	2.01	15.01	-0.99	7.35	4.97	5.79	17.17	0.69	6.51	5.85
$\sum (d_i - \bar{d})^2$	714.46									
S_d	8.91									
$\lvert t \rvert$ (MSE)	0.76									

S3. The coordinates of the optimized structures for the Ground State (GS) and Excited State (ES) of the studied compounds

S3-F1. The coordinates of the optimized structures for the GS and ES of F1 compound

*** GS of F1 at PBE0/6-311++G(d,p)**

O	0.83407000	-1.55474900	0.00014500
O	2.97798400	-2.07058500	0.00068200
N	-3.83351100	-0.78799000	-0.00135100
C	0.07321700	0.72866700	-0.00006700
C	1.44008300	1.16871300	0.00021000
C	-0.18398300	-0.65198100	-0.00008200
C	-1.04595600	1.58148900	-0.00028100
C	-1.46522100	-1.17234400	-0.00028100
C	-2.56508700	-0.30526400	-0.00049600
C	2.42937300	0.23328800	0.00044700
C	-2.32914600	1.09009700	-0.00050500
C	1.76453300	2.62705600	0.00026000
C	2.15662700	-1.17586600	0.00039700
H	-0.89450600	2.65532400	-0.00025500
H	-1.60065200	-2.24819600	-0.00027600
H	3.47549300	0.51389500	0.00067500
H	-3.17295200	1.77220800	-0.00070800
H	1.33969500	3.11942800	0.88048700
H	1.34013800	3.11938900	-0.88020300
H	2.84289500	2.78729400	0.00052800
H	-4.01490800	-1.77629500	0.00246000
H	-4.62370700	-0.16757600	0.00251800

*** GS of F1 at APFD/6-311++G(d,p)**

O	0.83311300	-1.56035300	-0.00012800
O	2.98716600	-2.06668800	0.00025100
N	-3.83446500	-0.79056200	-0.00093300
C	0.07177600	0.73027900	-0.00010000
C	1.43873300	1.16932100	0.00000900
C	-0.18439400	-0.65368400	-0.00011700
C	-1.04797200	1.58325600	-0.00006900
C	-1.46551500	-1.17475800	-0.00008900
C	-2.56573700	-0.30634100	-0.00007900
C	2.43128500	0.23610100	0.00003800
C	-2.33193600	1.09048300	-0.00007900
C	1.76168200	2.62923700	0.00014700
C	2.15979500	-1.17582100	-0.00020400
H	-0.89621900	2.65730900	-0.00000500
H	-1.60065900	-2.25104800	-0.00009300
H	3.47745200	0.51770200	0.00022800
H	-3.17677500	1.77213600	-0.00010300
H	1.33576900	3.12105200	0.88037300
H	1.33591200	3.12120000	-0.88006500
H	2.83940400	2.79449900	0.00025200
H	-4.01576000	-1.77928100	0.00396400
H	-4.62640700	-0.17175300	0.00426200

*** GS of F1 at B3LYP/6-311++G(d,p)**

O	0.83732500	-1.56285200	0.00010500
O	2.99499000	-2.07573100	-0.00040800
N	-3.85027200	-0.79048400	-0.00134200
C	0.07193700	0.73090700	0.00006600
C	1.44348700	1.17089400	0.00008500
C	-0.18881000	-0.65393900	-0.00003200
C	-1.05156100	1.58595400	0.00003200
C	-1.47269100	-1.17544800	-0.00014100
C	-2.57500400	-0.30560600	-0.00016000
C	2.43701900	0.23479100	0.00014300
C	-2.33776700	1.09310500	-0.00007600
C	1.77357700	2.63675000	-0.00007100
C	2.17024100	-1.17817500	0.00064100
H	-0.90238900	2.65846300	0.00010200

H	-1.60910000	-2.25002300	-0.00020300
H	3.48131900	0.51783400	-0.00011600
H	-3.18047100	1.77482900	-0.00015500
H	1.35229000	3.13124100	0.87997500
H	1.35235200	3.13101000	-0.88027500
H	2.85200400	2.79308400	-0.00005600
H	-4.03317100	-1.77981300	0.00461400
H	-4.64201900	-0.16998100	0.00501000

*** GS of F1 at BP86/6-311++G(d,p)**

O	0.84283500	-1.57600900	-0.00013200
O	3.02538400	-2.08121000	0.00023400
N	-3.86708600	-0.80100100	-0.00153900
C	0.07132500	0.73580900	-0.00010300
C	1.44146700	1.18280200	0.00001900
C	-0.18820700	-0.66090100	-0.00014000
C	-1.06096000	1.59256400	-0.00005400
C	-1.47815100	-1.18654500	-0.00010900
C	-2.58901300	-0.31279200	-0.00009900
C	2.44879400	0.24211800	0.00006200
C	-2.35321600	1.09468900	-0.00007600
C	1.76786000	2.65263700	0.00014300
C	2.19560700	-1.17401400	-0.00013000
H	-0.91098500	2.67437100	0.00005900
H	-1.61428700	-2.27017500	-0.00011700
H	3.49916800	0.53835100	0.00023800
H	-3.20436600	1.78026800	-0.00011500
H	1.34174400	3.15188400	0.88613000
H	1.34192400	3.15200800	-0.88586000
H	2.85408900	2.81477400	0.00026800
H	-4.05050200	-1.79853900	0.00587900
H	-4.66596400	-0.17638200	0.00640200

*** GS of F1 at CAM-B3LYP/6-311++G(d,p)**

O	0.83373600	-1.55564800	0.00017600
O	2.97646700	-2.06935400	-0.00059500
N	-3.83669600	-0.78414600	-0.00135400
C	0.07180800	0.72509400	0.00011200
C	1.44488400	1.16398900	0.00011000

C	-0.18795400	-0.64904200	-0.00000400
C	-1.04398400	1.57928000	0.00005700
C	-1.46809200	-1.16925000	-0.00017200
C	-2.56296500	-0.30243500	-0.00020800
C	2.42907500	0.23410900	0.00016800
C	-2.32581600	1.09028500	-0.00009200
C	1.76830600	2.62585300	-0.00012300
C	2.15413000	-1.17852500	0.00087600
H	-0.89198900	2.65093500	0.00012200
H	-1.60409600	-2.24323100	-0.00025700
H	3.47422600	0.51089700	-0.00020900
H	-3.16770300	1.77191900	-0.00018400
H	1.34451900	3.11572000	0.87937200
H	1.34454100	3.11539200	-0.87981000
H	2.84504200	2.78573200	-0.00014300
H	-4.01966600	-1.77263200	0.00461000
H	-4.62599300	-0.16183600	0.00499000

*** GS of F1 at M06/6-311++G(d,p)**

O	0.83695200	-1.55184700	-0.00011000
O	2.98238700	-2.06210300	0.00022500
N	-3.82955900	-0.79061000	-0.00090200
C	0.07095000	0.72634900	-0.00008100
C	1.43606100	1.16729700	0.00000900
C	-0.18394700	-0.65259900	-0.00010100
C	-1.04684000	1.57816200	-0.00004900
C	-1.46317700	-1.17233100	-0.00008100
C	-2.56069700	-0.30665000	-0.00007900
C	2.42603600	0.23680000	0.00003000
C	-2.32736400	1.08640600	-0.00006400
C	1.75426200	2.62316300	0.00012300
C	2.16058800	-1.17237300	-0.00017900
H	-0.89530000	2.65311700	0.00001500
H	-1.59991100	-2.24928100	-0.00009500
H	3.47248900	0.52143400	0.00019400
H	-3.17531200	1.76498900	-0.00008500
H	1.32715700	3.11568300	0.88025000
H	1.32726900	3.11580700	-0.87998900
H	2.83262800	2.78982400	0.00020700
H	-4.00990000	-1.78130400	0.00372200

H	-4.62214800	-0.16974700	0.00400500

*** GS of F1 at M06-2X/6-311++G(d,p)**

O	0.83608300	-1.55814300	0.00016500
O	2.97815900	-2.06816200	-0.00059900
N	-3.83683400	-0.78698600	-0.00141900
C	0.07240700	0.72484600	0.00008900
C	1.44712700	1.16687800	0.00011200
C	-0.18499400	-0.65263200	-0.00002400
C	-1.04381600	1.58181200	0.00003200
C	-1.46722400	-1.17486000	-0.00018200
C	-2.56384900	-0.30461000	-0.00019900
C	2.43435900	0.23830600	0.00017900
C	-2.32849000	1.09167100	-0.00010600
C	1.75919300	2.63305900	-0.00010100
C	2.15585000	-1.18082300	0.00089700
H	-0.88914700	2.65418400	0.00009400
H	-1.60342200	-2.24930000	-0.00025200
H	3.48064900	0.51289600	-0.00018300
H	-3.17259800	1.77095400	-0.00019900
H	1.32768000	3.11477200	0.88060500
H	1.32772700	3.11446400	-0.88099700
H	2.83482300	2.79998200	-0.00010500
H	-4.01869000	-1.77619200	0.00492000
H	-4.62650000	-0.16430500	0.00534900

*** GS of F1 at PBE/6-311++G(d,p)**

O	0.84174800	-1.57305600	-0.00012800
O	3.02061800	-2.07903500	0.00022600
N	-3.86123300	-0.80035400	-0.00147500
C	0.07150100	0.73530300	-0.00010200
C	1.43974000	1.18192300	0.00001600
C	-0.18688000	-0.65987600	-0.00013600
C	-1.05949000	1.59067000	-0.00005500
C	-1.47563300	-1.18464300	-0.00010100
C	-2.58561900	-0.31270100	-0.00009200
C	2.44533200	0.24149100	0.00005900
C	-2.35014300	1.09303500	-0.00007300
C	1.76530000	2.64864900	0.00014100

C	2.19119400	-1.17276300	-0.00012700
H	-0.90968200	2.67206600	0.00005200
H	-1.61135900	-2.26794700	-0.00010200
H	3.49539500	0.53706000	0.00023100
H	-3.20119900	1.77802600	-0.00010700
H	1.33865200	3.14771300	0.88517700
H	1.33882200	3.14784000	-0.88490500
H	2.85075200	2.81139100	0.00026000
H	-4.04400300	-1.79711300	0.00563100
H	-4.65948100	-0.17635700	0.00612700

*** GS of F1 at PW6B95D3/6-311++G(d,p)**

O	0.83549900	-1.55155600	-0.00011400
O	2.97829200	-2.06216800	0.00021200
N	-3.82597600	-0.78934200	-0.00096800
C	0.07175800	0.72548800	-0.00008800
C	1.43536300	1.16576800	0.00001300
C	-0.18414200	-0.65070300	-0.00010900
C	-1.04450500	1.57650300	-0.00005600
C	-1.46140800	-1.17115100	-0.00009200
C	-2.55836100	-0.30652400	-0.00008500
C	2.42443900	0.23646100	0.00004400
C	-2.32424100	1.08549400	-0.00007500
C	1.75238500	2.62397000	0.00012800
C	2.15619200	-1.17088600	-0.00015300
H	-0.89259100	2.64532600	0.00001200
H	-1.59556300	-2.24208100	-0.00010200
H	3.46492000	0.51873400	0.00020700
H	-3.16518800	1.76311200	-0.00009000
H	1.32523800	3.11027000	0.87662100
H	1.32540200	3.11038500	-0.87638100
H	2.82508000	2.78868300	0.00024100
H	-4.00670500	-1.77451800	0.00402100
H	-4.61396100	-0.17124800	0.00430000

*** GS of F1 at WB97XD/6-311++G(d,p)**

O	0.83301500	-1.55669200	0.00007400
O	2.97401300	-2.07257200	-0.00030300
N	-3.83724900	-0.78474900	-0.00125500

C	0.07308400	0.72574900	0.00003600
C	1.44710300	1.16607400	0.00007500
C	-0.18516300	-0.65036400	-0.00003600
C	-1.04330200	1.58141900	0.00000400
C	-1.46771700	-1.17134300	-0.00012600
C	-2.56374900	-0.30278900	-0.00016200
C	2.43152400	0.23390800	0.00011800
C	-2.32681500	1.09218900	-0.00009800
C	1.76755300	2.62976100	-0.00001400
C	2.15272000	-1.18064300	0.00048000
H	-0.89139000	2.65427000	0.00006200
H	-1.60465400	-2.24593500	-0.00017700
H	3.47797700	0.50945000	-0.00005600
H	-3.16861400	1.77509600	-0.00017700
H	1.34011200	3.11620200	0.88088300
H	1.34015500	3.11606600	-0.88100500
H	2.84456800	2.79389000	0.00000000
H	-4.01926400	-1.77246900	0.00457300
H	-4.62580300	-0.16296900	0.00485200

*** ES of F1 at PBE0/6-311++G(d,p)**

O	0.84036300	-1.57681100	0.00017400
O	3.00549300	-2.07584800	0.00006000
N	-3.80812100	-0.82883700	-0.00025300
C	0.07129600	0.73727800	-0.00001200
C	1.41760500	1.21163300	0.00004200
C	-0.17134900	-0.67174200	0.00002500
C	-1.07334800	1.58785200	-0.00020100
C	-1.44333800	-1.18399000	-0.00004600
C	-2.56543700	-0.31244300	-0.00011000
C	2.42846500	0.23343600	0.00020800
C	-2.35462800	1.08818800	-0.00025200
C	1.72208700	2.66726800	-0.00013800
C	2.18699000	-1.15606100	0.00046900
H	-0.92253400	2.66078600	-0.00030300
H	-1.58471000	-2.25902900	0.00001200
H	3.47304400	0.52647800	0.00013500
H	-3.20766600	1.75815700	-0.00041000
H	1.30271400	3.17562800	0.87968200
H	1.30288300	3.17538500	-0.88017900

H	2.80030900	2.83771900	-0.00006100
H	-3.96109200	-1.82552400	0.00054700
H	-4.62300500	-0.23497800	0.00055900

*** ES of F1 at APFD/6-311++G(d,p)**

O	0.83810000	-1.58156500	0.00018300
O	3.01488900	-2.07302200	-0.00001500
N	-3.81085600	-0.82974600	-0.00022700
C	0.06935900	0.73708600	0.00001000
C	1.41830000	1.21138400	0.00004400
C	-0.17244600	-0.67301700	0.00003400
C	-1.07410200	1.58822100	-0.00017400
C	-1.44541600	-1.18607200	-0.00004200
C	-2.56685700	-0.31279600	-0.00010300
C	2.43166100	0.23718600	0.00021100
C	-2.35727000	1.08851000	-0.00022800
C	1.72008500	2.66854000	-0.00017800
C	2.19196800	-1.15551500	0.00053100
H	-0.92242800	2.66132400	-0.00027000
H	-1.58656800	-2.26149600	0.00000500
H	3.47606800	0.53175000	0.00009400
H	-3.21058500	1.75880100	-0.00037900
H	1.29901200	3.17636300	0.87946100
H	1.29915300	3.17607500	-0.88005100
H	2.79762100	2.84403800	-0.00012400
H	-3.96523200	-1.82660900	0.00043100
H	-4.62666000	-0.23649000	0.00044300

*** ES of F1 at B3LYP/6-311++G(d,p)**

O	0.84100100	-1.58438800	0.00019600
O	3.02343800	-2.08292400	0.00006100
N	-3.82721100	-0.83015800	-0.00027700
C	0.06820500	0.73769200	0.00000600
C	1.42624400	1.21306600	0.00002900
C	-0.17659500	-0.67147500	0.00004000
C	-1.07784400	1.59057900	-0.00016000
C	-1.45336300	-1.18567300	-0.00003600
C	-2.57742900	-0.31095400	-0.00010800
C	2.43781100	0.23506700	0.00018900
C	-2.36443300	1.09184000	-0.00021500

C	1.73395700	2.67541700	-0.00018500
C	2.20258100	-1.15855900	0.00047900
H	-0.92842600	2.66217700	-0.00024000
H	-1.59583100	-2.25929600	0.00001000
H	3.48050600	0.53103300	0.00008800
H	-3.21497900	1.76297900	-0.00035200
H	1.31611400	3.18548500	0.87915100
H	1.31622700	3.18520900	-0.87973600
H	2.81199600	2.84416200	-0.00014500
H	-3.98176300	-1.82791700	0.00043800
H	-4.64368300	-0.23623500	0.00042800

*** ES of F1 at BP86/6-311++G(d,p)**

O	0.82915400	-1.59450900	-0.00009800
O	3.04401100	-2.10600600	0.00047900
N	-3.85421500	-0.83809500	-0.00005200
C	0.06078300	0.73222900	-0.00015400
C	1.46123200	1.22015900	-0.00007200
C	-0.17081900	-0.66191100	-0.00015200
C	-1.07633900	1.58730500	-0.00003900
C	-1.47692000	-1.18144400	-0.00013200
C	-2.59581500	-0.29722000	-0.00004600
C	2.45468300	0.23906300	0.00028900
C	-2.38621600	1.10322200	-0.00000400
C	1.74862400	2.68588700	-0.00038100
C	2.22622700	-1.16529500	0.00035600
H	-0.91669200	2.66759700	0.00003100
H	-1.62184400	-2.26379000	-0.00012900
H	3.50893200	0.53211900	0.00049500
H	-3.23680100	1.78728800	0.00007700
H	1.31832800	3.19840200	0.88427800
H	1.31838500	3.19795500	-0.88532800
H	2.83265500	2.87316200	-0.00039500
H	-3.99746300	-1.84615200	0.00015200
H	-4.68396400	-0.24777700	0.00013800

*** ES of F1 at CAM-B3LYP/6-311++G(d,p)**

O	0.84639700	-1.57878000	0.00014500
O	3.01186700	-2.06641600	0.00008600
N	-3.80557700	-0.82982100	-0.00030600

C	0.07480400	0.74104100	-0.00002000
C	1.39998800	1.20996800	0.00006900
C	-0.17585400	-0.67936500	-0.00000100
C	-1.08127000	1.59124400	-0.00022600
C	-1.43774900	-1.18950500	-0.00007300
C	-2.56213600	-0.31948700	-0.00012400
C	2.42744700	0.23569000	0.00024100
C	-2.34991300	1.08476900	-0.00027500
C	1.71537900	2.66988700	-0.00009500
C	2.19109100	-1.15098400	0.00048000
H	-0.93536100	2.66260500	-0.00033600
H	-1.57863500	-2.26283900	-0.00001600
H	3.46700100	0.53749200	0.00019500
H	-3.20579900	1.74882400	-0.00044600
H	1.30151500	3.17615600	0.87934400
H	1.30174700	3.17591900	-0.87978000
H	2.79311400	2.83138200	0.00002300
H	-3.96297200	-1.82618000	0.00069900
H	-4.61839800	-0.23259600	0.00075500

*** ES of F1 at M06/6-311++G(d,p)**

O	0.84446400	-1.57275700	0.00018500
O	3.01004700	-2.06575300	0.00004200
N	-3.80461100	-0.83248100	-0.00033100
C	0.07068200	0.73660600	0.00000400
C	1.40970200	1.20979100	0.00006900
C	-0.17136000	-0.67400800	0.00002300
C	-1.07469100	1.58689700	-0.00019500
C	-1.43958900	-1.18533300	-0.00006800
C	-2.56129000	-0.31558400	-0.00012900
C	2.42615400	0.23799600	0.00022900
C	-2.35163700	1.08353800	-0.00025900
C	1.70923600	2.66260700	-0.00012800
C	2.19253900	-1.15304100	0.00051300
H	-0.92497300	2.66094200	-0.00029000
H	-1.58138300	-2.26138800	-0.00002100
H	3.47021700	0.53737600	0.00014200
H	-3.20952800	1.74875400	-0.00042700
H	1.28716700	3.17137200	0.87961200

H	1.28734100	3.17110500	-0.88010700
H	2.78745500	2.83934200	-0.00005100
H	-3.95740800	-1.83112800	0.00061600
H	-4.62119000	-0.23774500	0.00066300

*** ES of F1 at M06-2X/6-311++G(d,p)**

O	0.84972200	-1.58147600	0.00012400
O	3.01417300	-2.06375500	0.00001500
N	-3.80413700	-0.83298400	-0.00020500
C	0.07459300	0.73991500	-0.00002200
C	1.40086300	1.21353100	0.00006900
C	-0.17217600	-0.68457400	-0.00000700
C	-1.08160600	1.59307700	-0.00023600
C	-1.43605600	-1.19703900	-0.00007200
C	-2.56224600	-0.32287100	-0.00010000
C	2.43194800	0.24103400	0.00025200
C	-2.35299000	1.08613500	-0.00027100
C	1.70351900	2.67789300	-0.00010800
C	2.19455400	-1.15081300	0.00051400
H	-0.93311500	2.66513100	-0.00036500
H	-1.57763800	-2.27083900	-0.00001300
H	3.47257900	0.54110500	0.00019100
H	-3.21176000	1.74705900	-0.00044000
H	1.28178500	3.17570500	0.88048200
H	1.28203100	3.17545700	-0.88095700
H	2.78008600	2.84671700	0.00001600
H	-3.96108800	-1.83029800	0.00062000
H	-4.61751600	-0.23503200	0.00067100

*** ES of F1 at PBE/6-311++G(d,p)**

O	0.82862900	-1.59143400	-0.00007600
O	3.03877400	-2.10344400	0.00053200
N	-3.84782500	-0.83782400	-0.00008700
C	0.06114300	0.73192800	-0.00006600
C	1.45897300	1.21919300	-0.00006000
C	-0.16931500	-0.66084300	-0.00013000
C	-1.07478800	1.58556200	0.00000300
C	-1.47404600	-1.17956100	-0.00015200
C	-2.59184400	-0.29717100	-0.00006100
C	2.45075500	0.23852600	0.00020800

C	-2.38301500	1.10154900	-0.00000800
C	1.74552700	2.68171600	-0.00040700
C	2.22121300	-1.16411100	0.00035800
H	-0.91532600	2.66544200	0.00005400
H	-1.61856400	-2.26162200	-0.00016300
H	3.50467200	0.53078300	0.00033600
H	-3.23365000	1.78484300	0.00005200
H	1.31466600	3.19400400	0.88335500
H	1.31467700	3.19353500	-0.88445400
H	2.82874200	2.86952000	-0.00045300
H	-3.99016700	-1.84516000	0.00004500
H	-4.67711300	-0.24828000	0.00008400

*** ES of F1 at PW6B95D3/6-311++G(d,p)**

O	0.84312500	-1.57423200	0.00016200
O	3.00831900	-2.06486000	0.00004600
N	-3.79954100	-0.83117400	-0.00024900
C	0.07003500	0.73424500	-0.00002000
C	1.40970300	1.20933700	0.00005400
C	-0.17127100	-0.67229800	0.00001300
C	-1.07326600	1.58300700	-0.00022100
C	-1.43808500	-1.18468800	-0.00005700
C	-2.55825900	-0.31559600	-0.00011100
C	2.42337200	0.23795200	0.00022400
C	-2.34966800	1.08267500	-0.00027100
C	1.70633400	2.66486700	-0.00011000
C	2.18831300	-1.14889300	0.00048000
H	-0.92256800	2.65103600	-0.00033300
H	-1.57836200	-2.25482500	0.00000800
H	3.46159000	0.53506900	0.00015700
H	-3.20059000	1.74728200	-0.00044100
H	1.28370900	3.16635000	0.87602400
H	1.28395200	3.16611800	-0.87649600
H	2.77879500	2.84017200	0.00001100
H	-3.95260300	-1.82463900	0.00061600
H	-4.61192500	-0.23925400	0.00065600

*** ES of F1 at WB97XD/6-311++G(d,p)**

O	0.84623000	-1.57965800	0.00014200
O	3.00931500	-2.06923500	0.00004700

N	-3.80587200	-0.83090100	-0.00030700
C	0.07650800	0.74219000	-0.00001300
C	1.40118600	1.21231200	0.00007600
C	-0.17291300	-0.68140200	-0.00000100
C	-1.08148900	1.59401000	-0.00022400
C	-1.43695100	-1.19214500	-0.00007200
C	-2.56217900	-0.32049300	-0.00011900
C	2.43006900	0.23568500	0.00025500
C	-2.35109400	1.08632800	-0.00027200
C	1.71386000	2.67423200	-0.00010000
C	2.19005300	-1.15300500	0.00051000
H	-0.93599400	2.66658100	-0.00033800
H	-1.57850400	-2.26613400	-0.00001700
H	3.47104100	0.53632200	0.00019400
H	-3.20759800	1.75073600	-0.00044300
H	1.29667800	3.17728800	0.88070600
H	1.29691100	3.17704000	-0.88115800
H	2.79203900	2.83937500	0.00001600
H	-3.96273300	-1.82620800	0.00069700
H	-4.61739500	-0.23382400	0.00073500

S3-F2. The coordinates of the optimized structures for the GS and ES of F2 compound

*** GS of F2 at PBE0/6-311++G(d,p)**

O	-0.82611300	1.37124200	0.23040300
O	-2.87135900	2.14966200	0.37046700
O	-4.42462600	-1.73208600	-0.26452500
N	3.74005900	0.09762100	-0.00284100
N	-4.96497100	0.43019600	0.10427700
N	-6.34148800	0.21939900	0.07589300
C	2.42690300	-0.22778600	-0.05506300
C	4.79355900	-0.87386900	-0.27131300
C	4.18535800	1.44590700	0.32468100
C	1.42165400	0.75115700	0.11504700
C	-0.32586800	-0.93719700	-0.15785900
C	0.09557900	0.38599200	0.06364700
C	2.00937500	-1.57587100	-0.28097000
C	0.68307500	-1.90795100	-0.32925400
C	5.22723400	-1.65179600	0.96338000
C	4.28633400	2.36028800	-0.88872500
C	-1.70762600	-1.18987500	-0.19085600

C	-2.63351700	-0.19359300	-0.01854200
C	-2.18142400	1.16017800	0.20296200
C	-4.07411000	-0.56838000	-0.07095700
H	4.47219400	-1.54960100	-1.06721800
H	5.64228000	-0.31757000	-0.67825000
H	3.52235600	1.87193600	1.08194400
H	5.16405000	1.35212700	0.80291000
H	1.65716300	1.79514000	0.26798200
H	2.74551800	-2.35908900	-0.39900300
H	0.39321600	-2.94073500	-0.49517900
H	5.59002300	-0.97592000	1.74277800
H	4.40081100	-2.23525600	1.37743600
H	6.03759900	-2.33989400	0.70741200
H	4.98650100	1.95486700	-1.62444400
H	3.31614100	2.48591900	-1.37617800
H	4.64691600	3.34694600	-0.58531600
H	-2.07238200	-2.19941000	-0.35719300
H	-4.63265500	1.37445400	0.25686200
H	-6.58657500	-0.20556600	-0.81459000
H	-6.58073300	-0.46261800	0.79091200

*** GS of F2 at APFD/6-311++G(d,p)**

O	-0.82189300	1.37808800	0.23283300
O	-2.87787800	2.14858100	0.37207100
O	-4.42361300	-1.73491900	-0.26663100
N	3.74128800	0.09786600	-0.00290200
N	-4.96324500	0.43103000	0.10481000
N	-6.34053900	0.21750800	0.07591900
C	2.42876300	-0.22763100	-0.05501900
C	4.79507700	-0.87289700	-0.27273500
C	4.18634600	1.44604200	0.32564500
C	1.42409000	0.75315900	0.11640500
C	-0.32327900	-0.93663400	-0.15797800
C	0.09813700	0.38905900	0.06483900
C	2.01199900	-1.57680700	-0.28202200
C	0.68480500	-1.90864300	-0.33025200
C	5.21966200	-1.64771300	0.96983900
C	4.27771300	2.35415000	-0.89606400
C	-1.70433200	-1.19079000	-0.19159200
C	-2.63295800	-0.19562500	-0.01899000

C	-2.18240400	1.16130600	0.20411500
C	-4.07246000	-0.56993500	-0.07184400
H	4.47155200	-1.54787600	-1.06832000
H	5.64367400	-0.31771100	-0.68125400
H	3.52319100	1.86939200	1.08420800
H	5.16546800	1.35397700	0.80311000
H	1.66185200	1.79657300	0.27118300
H	2.74967700	-2.35883300	-0.40136700
H	0.39232900	-2.94101000	-0.49681700
H	5.58226500	-0.96845900	1.74660200
H	4.38527100	-2.21979500	1.38415900
H	6.02581100	-2.34542000	0.72622300
H	4.97825800	1.94689600	-1.63063900
H	3.30489300	2.46477200	-1.38222200
H	4.63006500	3.34785700	-0.60574100
H	-2.06556700	-2.20167600	-0.35885200
H	-4.63168400	1.37571000	0.25840800
H	-6.58281500	-0.20808600	-0.81529400
H	-6.57663800	-0.46738400	0.78955900

*** GS of F2 at B3LYP/6-311++G(d,p)**

O	-0.83065300	1.38095700	0.23564600
O	-2.88896900	2.15918200	0.37726700
O	-4.44364900	-1.73889100	-0.26975500
N	3.75681600	0.09516700	-0.00328300
N	-4.99408300	0.42849000	0.10453200
N	-6.38393100	0.21489100	0.07468000
C	2.43594400	-0.22934900	-0.05549500
C	4.81843800	-0.88612300	-0.26985900
C	4.21137900	1.45374400	0.32288800
C	1.42717800	0.75281300	0.11683600
C	-0.32953700	-0.93610100	-0.15907000
C	0.09812500	0.38915100	0.06527900
C	2.01161700	-1.58018200	-0.28415900
C	0.68180600	-1.91060000	-0.33307500
C	5.26063600	-1.66415400	0.97280500
C	4.32745200	2.37113900	-0.89816300
C	-1.71428100	-1.18830400	-0.19274000
C	-2.64721800	-0.19227300	-0.01840400
C	-2.19802000	1.16590300	0.20750000

C	-4.09384300	-0.57049100	-0.07319300
H	4.49456300	-1.56601600	-1.05889500
H	5.66562900	-0.33273500	-0.67986500
H	3.54614400	1.88654900	1.07184500
H	5.18585500	1.35675600	0.80564600
H	1.66317100	1.79432300	0.27298800
H	2.74350200	-2.36438800	-0.40537400
H	0.39153800	-2.94168800	-0.50134800
H	5.62742900	-0.98710100	1.74833000
H	4.43850800	-2.24848500	1.39195500
H	6.07028100	-2.35097200	0.71193500
H	5.03032500	1.96218900	-1.62831400
H	3.36254500	2.50478400	-1.39206400
H	4.69268600	3.35436700	-0.58987700
H	-2.07358600	-2.19745600	-0.36143000
H	-4.67064200	1.37527300	0.26040600
H	-6.62845600	-0.20683500	-0.81891900
H	-6.62299600	-0.46942700	0.78933000

*** GS of F2 at BP86/6-311++G(d,p)**

O	-0.83247000	1.39381900	0.23926100
O	-2.91359500	2.16972700	0.38151300
O	-4.46706300	-1.75727200	-0.27530900
N	3.77537300	0.09719400	-0.00342600
N	-5.00931300	0.43215400	0.10661500
N	-6.40829200	0.23014700	0.07582400
C	2.44851300	-0.22954300	-0.05639800
C	4.84014500	-0.88892900	-0.26543000
C	4.22902100	1.46190000	0.31914100
C	1.43554300	0.75887200	0.11826700
C	-0.33053400	-0.94301500	-0.16013400
C	0.09916400	0.39333200	0.06676800
C	2.02535900	-1.58699600	-0.28748400
C	0.68813400	-1.92107400	-0.33619000
C	5.27753600	-1.66250800	0.98662200
C	4.34452300	2.37335700	-0.91145800
C	-1.71760900	-1.19978000	-0.19443000
C	-2.66019700	-0.19654800	-0.01843800
C	-2.21817000	1.16551200	0.20874400
C	-4.10975900	-0.57980800	-0.07416500

H	4.51178300	-1.57570400	-1.05976300
H	5.69356100	-0.33087600	-0.68109200
H	3.55434900	1.89773900	1.07176900
H	5.21008200	1.36482800	0.80962800
H	1.67569100	1.80920000	0.27589000
H	2.76620800	-2.37589000	-0.41050700
H	0.39553200	-2.96060400	-0.50636500
H	5.64445900	-0.97702000	1.76651000
H	4.44628500	-2.24847400	1.40773700
H	6.09386300	-2.35660700	0.73151200
H	5.05450900	1.95845700	-1.64395000
H	3.37193700	2.50195400	-1.41046100
H	4.70972000	3.36712700	-0.60788200
H	-2.08257800	-2.21709300	-0.36481000
H	-4.66701900	1.38522400	0.26327000
H	-6.64452300	-0.20898900	-0.82318000
H	-6.64323800	-0.46855900	0.79238400

*** GS of F2 at CAM-B3LYP/6-311++G(d,p)**

O	-0.82621500	1.37302900	0.23125100
O	-2.87248600	2.14798600	0.37049200
O	-4.42560400	-1.72855700	-0.26465500
N	3.74219100	0.09635400	-0.00289700
N	-4.97007200	0.42937800	0.10350300
N	-6.35067700	0.20889800	0.07362100
C	2.42644600	-0.22739900	-0.05429300
C	4.79744900	-0.87828900	-0.27551500
C	4.19108000	1.44719900	0.32746200
C	1.42361500	0.75011900	0.11497100
C	-0.32426600	-0.93220500	-0.15687000
C	0.09881400	0.38437400	0.06355600
C	2.00635700	-1.57421000	-0.27909400
C	0.68174900	-1.90356600	-0.32769200
C	5.23163500	-1.66145700	0.95824400
C	4.28952600	2.36585900	-0.88553300
C	-1.71007400	-1.18421800	-0.18997300
C	-2.63200800	-0.19383400	-0.01839600
C	-2.17958400	1.16301400	0.20461100
C	-4.07668500	-0.56577000	-0.07111700
H	4.47584800	-1.55113800	-1.07049800

H	5.64589500	-0.32381400	-0.67943700
H	3.53202600	1.87239500	1.08522100
H	5.16970200	1.35279200	0.80052100
H	1.65744300	1.79209300	0.26782700
H	2.73936200	-2.35716600	-0.39682800
H	0.39117300	-2.93445900	-0.49343300
H	5.59527900	-0.98834700	1.73737700
H	4.40574400	-2.24330700	1.37108600
H	6.03950100	-2.34964100	0.70070200
H	4.98651100	1.96142200	-1.62242800
H	3.31969900	2.49253100	-1.36956800
H	4.65084400	3.35056600	-0.58180200
H	-2.07137700	-2.19271800	-0.35657900
H	-4.64630100	1.37530500	0.25770300
H	-6.59896800	-0.20746100	-0.81930100
H	-6.59234200	-0.46883100	0.79097700

*** GS of F2 at M06/6-311++G(d,p)**

O	-0.82456500	1.37486100	0.22741900
O	-2.86827300	2.15597700	0.36883600
O	-4.41741500	-1.72702600	-0.26345200
N	3.73920300	0.09309800	-0.00303900
N	-4.96964900	0.43026700	0.10640400
N	-6.34556400	0.20095800	0.07804600
C	2.42300200	-0.22946700	-0.05623300
C	4.79382800	-0.87999800	-0.27031300
C	4.18995400	1.44087900	0.32673600
C	1.42254300	0.75071500	0.11278500
C	-0.32602500	-0.92968800	-0.15930200
C	0.09673300	0.39026200	0.06139100
C	2.00329000	-1.57443200	-0.28204900
C	0.67798300	-1.90218300	-0.33049000
C	5.21804000	-1.64025300	0.97190800
C	4.29848200	2.33718300	-0.89260100
C	-1.70724000	-1.18004200	-0.19118000
C	-2.63214900	-0.18660100	-0.01907400
C	-2.18257800	1.16861800	0.20126800
C	-4.07079800	-0.56624000	-0.07025200
H	4.47297200	-1.56142400	-1.06352100
H	5.64335300	-0.32583300	-0.68426400

H	3.52488100	1.87369800	1.08038800
H	5.16619600	1.34420700	0.81426600
H	1.65946600	1.79566500	0.26723200
H	2.73911100	-2.35921000	-0.40153400
H	0.38128700	-2.93402200	-0.49667200
H	5.57327100	-0.95170800	1.74541300
H	4.38467800	-2.21396200	1.38929300
H	6.02953400	-2.33566300	0.73966800
H	4.99849800	1.91617300	-1.62151100
H	3.32905800	2.45503500	-1.38650500
H	4.66061600	3.32960200	-0.60989900
H	-2.06954200	-2.19208300	-0.35715200
H	-4.65090900	1.38077100	0.26026600
H	-6.58465200	-0.22590200	-0.81535100
H	-6.57411900	-0.48863000	0.79204000

*** GS of F2 at M06-2X/6-311++G(d,p)**

O	-0.81963600	1.37901700	0.22927200
O	-2.86415500	2.15470400	0.36614300
O	-4.42120800	-1.72619600	-0.26270200
N	3.74814000	0.09836600	-0.00183700
N	-4.97348000	0.42894500	0.10367100
N	-6.35266700	0.19081100	0.07284900
C	2.43384300	-0.22550500	-0.05289800
C	4.80139800	-0.87580600	-0.28458300
C	4.19327000	1.44873600	0.33590700
C	1.43065200	0.75704400	0.11579000
C	-0.31846200	-0.93092800	-0.15477200
C	0.10336400	0.38962100	0.06428100
C	2.01540100	-1.57677500	-0.27603500
C	0.68762100	-1.90557700	-0.32370300
C	5.20702100	-1.67459000	0.95090700
C	4.25454400	2.36677900	-0.88215500
C	-1.70768500	-1.18448700	-0.18831300
C	-2.62831000	-0.19077300	-0.01870100
C	-2.17301100	1.17143700	0.20183400
C	-4.07510300	-0.56453500	-0.07060600
H	4.48205300	-1.53303500	-1.09421600
H	5.65703200	-0.31590900	-0.66691700
H	3.54360800	1.86057100	1.10987300

H	5.18353600	1.35563500	0.78573900
H	1.66336500	1.80087400	0.26579400
H	2.74946300	-2.36056800	-0.39039300
H	0.39360900	-2.93652000	-0.48653700
H	5.56726600	-1.00535100	1.73502100
H	4.36094600	-2.23955700	1.34680200
H	6.00631900	-2.37528400	0.70285900
H	4.94623700	1.96514500	-1.62562000
H	3.27252500	2.46627100	-1.34833400
H	4.60164900	3.35951300	-0.59018900
H	-2.06769000	-2.19503800	-0.35317800
H	-4.66643600	1.37947000	0.25727500
H	-6.58188700	-0.24014200	-0.81982100
H	-6.57280600	-0.50095900	0.78564700

*** GS of F2 at PBE/6-311++G(d,p)**

O	-0.83092200	1.39218000	0.23491200
O	-2.90798500	2.16979100	0.37515800
O	-4.46067700	-1.75532800	-0.27002900
N	3.77007700	0.09661700	-0.00338100
N	-5.00392300	0.43160300	0.10524500
N	-6.39752500	0.22722500	0.07545000
C	2.44517400	-0.22967200	-0.05608000
C	4.83205800	-0.88541800	-0.26970200
C	4.22262600	1.45647300	0.32319400
C	1.43358600	0.75780400	0.11610700
C	-0.33051000	-0.94206800	-0.15827100
C	0.09823400	0.39322400	0.06545200
C	2.02247400	-1.58576400	-0.28406500
C	0.68657100	-1.91927300	-0.33196000
C	5.27215700	-1.66030400	0.97663500
C	4.33730000	2.37079900	-0.90130200
C	-1.71602500	-1.19803400	-0.19172700
C	-2.65688800	-0.19499600	-0.01816900
C	-2.21370200	1.16565900	0.20512600
C	-4.10405600	-0.57830100	-0.07261700
H	4.50339900	-1.57026500	-1.06494800
H	5.68420500	-0.32662800	-0.68598800
H	3.54924700	1.88979300	1.07779400
H	5.20358500	1.35839700	0.81283000

H	1.67325000	1.80844200	0.27017900
H	2.76263800	-2.37520700	-0.40421900
H	0.39356900	-2.95865700	-0.49935200
H	5.63893300	-0.97668400	1.75740400
H	4.44310200	-2.24840600	1.39752600
H	6.08876500	-2.35181500	0.71877500
H	5.04528900	1.95795600	-1.63600100
H	3.36480600	2.50234000	-1.39840200
H	4.70398000	3.36233400	-0.59504300
H	-2.08135700	-2.21527000	-0.35959000
H	-4.66404200	1.38462500	0.25926900
H	-6.63456500	-0.21446100	-0.82103400
H	-6.63253900	-0.46850900	0.79355900

*** GS of F2 at PW6B95D3/6-311++G(d,p)**

O	-0.81911300	1.37495500	0.23067300
O	-2.86207600	2.15402300	0.36835100
O	-4.40346100	-1.72867000	-0.26179400
N	3.73647400	0.09768500	-0.00273300
N	-4.95828000	0.42447200	0.10175300
N	-6.33408500	0.19197600	0.06895700
C	2.42528800	-0.22561500	-0.05360900
C	4.78752500	-0.87306500	-0.27975200
C	4.18159600	1.44390500	0.33040100
C	1.42492000	0.75324000	0.11588700
C	-0.32000000	-0.92939000	-0.15444500
C	0.10232400	0.38952500	0.06517400
C	2.00815300	-1.57076800	-0.27705800
C	0.68479000	-1.90013500	-0.32438400
C	5.19585500	-1.66785300	0.95017500
C	4.24692600	2.36024600	-0.88128700
C	-1.69927400	-1.17946100	-0.18731300
C	-2.62289400	-0.18592600	-0.01699500
C	-2.17416000	1.16594600	0.20283900
C	-4.05901300	-0.56446500	-0.06989500
H	4.47032100	-1.53114500	-1.08527300
H	5.63898500	-0.31500300	-0.66450400
H	3.53329700	1.85694700	1.10039000
H	5.16700300	1.35004900	0.78258600
H	1.66048000	1.79239700	0.26642200

H	2.74044600	-2.35101000	-0.39282800
H	0.39369400	-2.92768500	-0.48763500
H	5.55306800	-1.00311600	1.73500800
H	4.35649000	-2.23761100	1.34461400
H	5.99603200	-2.36259700	0.70177300
H	4.93356500	1.96122400	-1.62609600
H	3.26829700	2.46754300	-1.34536100
H	4.59791800	3.34795900	-0.58847900
H	-2.06267400	-2.18430400	-0.35195000
H	-4.64655900	1.37071300	0.25251900
H	-6.56346100	-0.24311000	-0.81728800
H	-6.56068500	-0.48974600	0.78399300

*** GS of F2 at WB97XD/6-311++G(d,p)**

O	-0.82266300	1.37317300	0.22886300
O	-2.86574400	2.15054800	0.36573900
O	-4.42632600	-1.73239600	-0.26012300
N	3.74509300	0.09827400	-0.00267700
N	-4.97091100	0.42873700	0.10123900
N	-6.35229600	0.21411200	0.07139400
C	2.42937700	-0.22684200	-0.05315500
C	4.79924900	-0.87268300	-0.28349000
C	4.19128300	1.44679400	0.33322100
C	1.42612300	0.75206600	0.11485600
C	-0.32174600	-0.93403800	-0.15377900
C	0.09895400	0.38493500	0.06397000
C	2.01081500	-1.57606100	-0.27525100
C	0.68461800	-1.90670900	-0.32267400
C	5.22602400	-1.66460700	0.94859000
C	4.27017300	2.36970500	-0.87940100
C	-1.70923000	-1.18842400	-0.18674400
C	-2.63063500	-0.19560600	-0.01767400
C	-2.17477000	1.16387300	0.20189000
C	-4.07811900	-0.56936700	-0.07000700
H	4.47969400	-1.53901200	-1.08665500
H	5.65000400	-0.31448800	-0.68058600
H	3.53858000	1.86506400	1.10230000
H	5.17664100	1.35373700	0.79510500
H	1.65907900	1.79590100	0.26479700
H	2.74360600	-2.36121100	-0.39112500

H	0.39402600	-2.93883000	-0.48567200
H	5.58794100	-0.99300700	1.73123800
H	4.39240400	-2.24255700	1.35450000
H	6.03188700	-2.35625100	0.69165300
H	4.96342600	1.96829100	-1.62292300
H	3.29240200	2.48551500	-1.35279500
H	4.62574500	3.35787800	-0.57815200
H	-2.06867400	-2.19918800	-0.35104300
H	-4.64723100	1.37455400	0.25216200
H	-6.59604000	-0.20903900	-0.81944300
H	-6.59150800	-0.46402300	0.78900000

*** ES of F2 at PBE0/6-311++G(d,p)**

O	0.85271100	1.32265500	-0.20131100
O	2.92780500	2.07444000	-0.33474200
O	4.53614000	-1.70724900	0.18557100
N	-3.74692100	0.13508500	-0.00606700
N	4.91928900	0.50130100	-0.03102000
N	6.21462800	0.27197400	-0.20671900
C	-2.43525200	-0.24150000	0.05656600
C	-4.82554000	-0.79910700	0.26942700
C	-4.14359600	1.48913800	-0.35423800
C	-1.39329200	0.70823800	-0.10448000
C	0.32486100	-1.01775200	0.18322000
C	-0.07641600	0.32359100	-0.04254300
C	-2.05397300	-1.58782300	0.28440700
C	-0.72721000	-1.95191500	0.34492300
C	-5.28096900	-1.58305200	-0.95601900
C	-4.22556800	2.42798300	0.84403000
C	1.69281300	-1.31450400	0.22422800
C	2.63256400	-0.26242000	0.03995700
C	2.21529100	1.06371700	-0.17012500
C	4.05012800	-0.58892300	0.07209600
H	-4.52276500	-1.47708700	1.07189700
H	-5.66253200	-0.21788700	0.66764400
H	-3.46070400	1.88548600	-1.11059700
H	-5.12213000	1.42437800	-0.83917700
H	-1.60236500	1.75850100	-0.25914400
H	-2.80657300	-2.35744700	0.39602200
H	-0.47033900	-2.99338300	0.51319100

H	-5.62950600	-0.90795100	-1.74275300
H	-4.46814600	-2.18957800	-1.36366500
H	-6.10674900	-2.24948000	-0.69073000
H	-4.94386300	2.05675300	1.58050700
H	-3.25518300	2.52950600	1.33680200
H	-4.55218800	3.42098800	0.52207300
H	2.04342700	-2.32519100	0.38843200
H	4.47929300	1.42964900	-0.20022400
H	6.83477000	1.02281600	0.06582000
H	6.48028100	-0.68138700	0.02570500

*** ES of F2 at APFD/6-311++G(d,p)**

O	-0.84778100	1.33077200	0.20352000
O	-2.93596200	2.07607000	0.33348300
O	-4.52951500	-1.71628500	-0.18406300
N	3.74878600	0.13497400	0.00684100
N	-4.92244400	0.49686200	0.02561500
N	-6.21809400	0.27172700	0.21198000
C	2.43739300	-0.24087700	-0.05644200
C	4.82714900	-0.79884600	-0.27050100
C	4.14571300	1.48833000	0.35727600
C	1.39668100	0.71117800	0.10597400
C	-0.32167900	-1.01534200	-0.18486000
C	0.07947400	0.32808900	0.04319100
C	2.05653100	-1.58774000	-0.28623600
C	0.72848800	-1.95122300	-0.34777200
C	5.27281700	-1.58165300	0.96204900
C	4.22049700	2.42153600	-0.84870400
C	-1.68972500	-1.31172800	-0.22611200
C	-2.63026900	-0.26092200	-0.04165900
C	-2.21631500	1.06663700	0.16965000
C	-4.04933200	-0.59446100	-0.07405500
H	4.52221000	-1.47510400	-1.07358000
H	5.66457600	-0.21888100	-0.66950300
H	3.46204800	1.88201500	1.11429200
H	5.12390200	1.42445800	0.84288600
H	1.60859500	1.76072900	0.26300700
H	2.81047300	-2.35632400	-0.39923300
H	0.46862600	-2.99215700	-0.51751300
H	5.62181000	-0.90419600	1.74680000

H	4.45126900	-2.17653100	1.36974900
H	6.09397300	-2.25860700	0.70853100
H	4.93983600	2.04841000	-1.58345900
H	3.24865900	2.50886400	-1.34164200
H	4.53907800	3.42125900	-0.53908500
H	-2.03951200	-2.32293600	-0.39105000
H	-4.47974400	1.42583100	0.19435000
H	-6.83725200	1.02549200	-0.05502400
H	-6.49476700	-0.67959900	-0.01488300

*** ES of F2 at B3LYP/6-311++G(d,p)**

O	-0.85503300	1.33699500	0.20572400
O	-2.94670300	2.09095300	0.33554800
O	-4.54630500	-1.71519200	-0.18573600
N	3.76612800	0.13044300	0.00663300
N	-4.96186200	0.49760500	0.01815100
N	-6.26280500	0.25066800	0.21961600
C	2.44480300	-0.24263400	-0.05790800
C	4.85104800	-0.81514900	-0.26684900
C	4.17365900	1.49331300	0.35653000
C	1.40160100	0.71237900	0.10556400
C	-0.32746900	-1.01175300	-0.18726400
C	0.08072500	0.33105300	0.04279800
C	2.05558600	-1.59078300	-0.29016700
C	0.72469000	-1.95169300	-0.35258100
C	5.31103700	-1.60313600	0.96557900
C	4.27236800	2.43865600	-0.84691000
C	-1.69890700	-1.30584600	-0.22805600
C	-2.64623800	-0.25375900	-0.04106100
C	-2.23322800	1.07550400	0.17125200
C	-4.06834400	-0.59035500	-0.07588900
H	4.54655500	-1.49502200	-1.06486800
H	5.68901200	-0.23826500	-0.66528700
H	3.48880200	1.89603100	1.10534800
H	5.14778900	1.42303600	0.84630500
H	1.61350200	1.75959100	0.26412600
H	2.80307800	-2.36234200	-0.40507500
H	0.46575100	-2.99095200	-0.52430000
H	5.66276100	-0.92921100	1.75099900
H	4.50079600	-2.21030400	1.37522800

H	6.13567900	-2.26892100	0.69579700
H	4.99202000	2.06389600	-1.57930700
H	3.30705400	2.55218800	-1.34520700
H	4.60637700	3.42676200	-0.51805800
H	-2.04651900	-2.31565500	-0.39427500
H	-4.54840200	1.43157400	0.19513200
H	-6.89394200	0.99481200	-0.05138000
H	-6.52421900	-0.70505500	-0.01047900

*** ES of F2 at BP86/6-311++G(d,p)**

O	-0.85144500	1.35697300	0.19642400
O	-2.98742300	2.09427200	0.30638100
O	-4.57461600	-1.73924100	-0.14632800
N	3.78387800	0.12924800	0.01529500
N	-4.97940300	0.49928300	-0.00938100
N	-6.28326900	0.26617900	0.29363700
C	2.45862500	-0.24158000	-0.06099200
C	4.87204000	-0.82311800	-0.25101100
C	4.19300600	1.49535500	0.37335300
C	1.41364000	0.72221400	0.10770100
C	-0.32382800	-1.00644200	-0.21385900
C	0.08327000	0.34476700	0.03254700
C	2.06971400	-1.59400600	-0.31084800
C	0.73032900	-1.95266200	-0.38438400
C	5.31477300	-1.61548700	0.98939400
C	4.30166800	2.44252500	-0.83242600
C	-1.70087700	-1.30390200	-0.25769600
C	-2.64826100	-0.26036100	-0.06367700
C	-2.24833700	1.07237000	0.14902700
C	-4.09810500	-0.59822800	-0.08069100
H	4.56755700	-1.50391500	-1.06116100
H	5.72057900	-0.24132900	-0.64537200
H	3.49592200	1.89788700	1.12481500
H	5.17020100	1.41809900	0.87653600
H	1.63234200	1.77609600	0.27753900
H	2.82476700	-2.37102100	-0.42902800
H	0.46566600	-2.99794000	-0.56765900
H	5.66254000	-0.93888500	1.78599600
H	4.48986700	-2.22365000	1.39121200
H	6.14582800	-2.29042100	0.72871700

H	5.03118600	2.06418900	-1.56588500
H	3.33202400	2.55759200	-1.34071500
H	4.63709100	3.43819400	-0.50036400
H	-2.04747400	-2.32454500	-0.42811000
H	-4.50856800	1.43186400	0.17396600
H	-6.92710600	0.97381300	-0.06592600
H	-6.53894100	-0.71369300	0.11813200

*** ES of F2 at CAM-B3LYP/6-311++G(d,p)**

O	-0.82500100	1.38292100	0.20417000
O	-2.87867500	2.14363600	0.36569000
O	-4.43342700	-1.71212600	-0.25558800
N	3.73967300	0.10490400	0.00355300
N	-4.97292000	0.45020200	0.12298600
N	-6.35066900	0.21688800	0.10488200
C	2.43449400	-0.24121200	-0.05754000
C	4.81236800	-0.85449400	-0.25841900
C	4.17423900	1.46186400	0.33518400
C	1.40725400	0.73744400	0.10765600
C	-0.33108300	-0.96277900	-0.17732100
C	0.09507000	0.37860900	0.04610900
C	2.02681100	-1.59281200	-0.28630400
C	0.70675200	-1.93065500	-0.33905400
C	5.23719300	-1.62560800	0.98865900
C	4.28055900	2.36679000	-0.88973600
C	-1.70268900	-1.24332100	-0.22031300
C	-2.63730700	-0.19698500	-0.02880400
C	-2.19192100	1.14514400	0.18875400
C	-4.06913400	-0.54549600	-0.06308600
H	4.50366400	-1.53286800	-1.05266100
H	5.65640800	-0.28461200	-0.64831000
H	3.50077600	1.88579900	1.07886200
H	5.14881900	1.37186400	0.81614000
H	1.63926500	1.77931900	0.26584300
H	2.76641700	-2.37026400	-0.40215100
H	0.42379200	-2.96287400	-0.50381700
H	5.58452200	-0.94641900	1.76901300
H	4.41295000	-2.21698600	1.38947100
H	6.05611900	-2.30178800	0.73656800
H	4.98384900	1.95799500	-1.61717500

H	3.31299800	2.48905500	-1.37839000
H	4.63956300	3.35135200	-0.58451900
H	-2.06345800	-2.24636100	-0.38914000
H	-4.65358000	1.39728800	0.27427600
H	-6.60323100	-0.20354200	-0.78531800
H	-6.58027400	-0.46530600	0.82246700

*** ES of F2 at M06/6-311++G(d,p)**

O	-0.84685600	1.33608200	0.19609100
O	-2.91157100	2.10007700	0.33887800
O	-4.51156700	-1.70354100	-0.17964700
N	3.74634200	0.12467900	0.00583700
N	-4.94328500	0.49595000	0.02771700
N	-6.23554500	0.21900900	0.20095400
C	2.43064000	-0.24352800	-0.05733800
C	4.82277800	-0.81376600	-0.27257700
C	4.15447100	1.47600400	0.35827200
C	1.39651900	0.71203600	0.10209000
C	-0.32865100	-1.00157200	-0.18250400
C	0.07934300	0.33645400	0.04069300
C	2.04214800	-1.58672600	-0.28418300
C	0.71638100	-1.94262800	-0.34394600
C	5.27132700	-1.58095800	0.95914100
C	4.25281500	2.39640100	-0.84599800
C	-1.69403800	-1.29141800	-0.22200600
C	-2.63606800	-0.23850900	-0.03668500
C	-2.21546700	1.09157800	0.17193100
C	-4.04253300	-0.58097400	-0.06812500
H	4.51593500	-1.49667600	-1.07119800
H	5.66053800	-0.23631400	-0.68068500
H	3.46878100	1.88208100	1.10895800
H	5.12895800	1.40277000	0.85505100
H	1.61125700	1.76281700	0.25640400
H	2.79246400	-2.36005900	-0.39682800
H	0.44847600	-2.98258900	-0.51130100
H	5.61646800	-0.89418800	1.73889600
H	4.45219700	-2.17685600	1.37339000
H	6.09637000	-2.25605600	0.71356600
H	4.97090200	2.00549400	-1.57419700
H	3.28520700	2.49619000	-1.34747200

H	4.58630400	3.39332200	-0.54320300
H	-2.04393500	-2.30356800	-0.38636900
H	-4.56383600	1.43921000	0.20359000
H	-6.88179400	0.94001400	-0.09966400
H	-6.45490000	-0.74836400	-0.03565500

*** ES of F2 at M06-2X/6-311++G(d,p)**

O	-0.81835100	1.39153300	0.19209900
O	-2.87031000	2.15066400	0.35966300
O	-4.42884900	-1.71006100	-0.25088000
N	3.74524700	0.10604000	0.00522900
N	-4.97620700	0.44893800	0.12791300
N	-6.35240600	0.19731100	0.11092300
C	2.44122000	-0.23967500	-0.05706400
C	4.81612100	-0.85268900	-0.26625100
C	4.17679600	1.46101500	0.34840300
C	1.41401600	0.74533900	0.10532000
C	-0.32556400	-0.96009700	-0.17953400
C	0.09879800	0.38600400	0.04138600
C	2.03547700	-1.59607000	-0.28406500
C	0.71191600	-1.93219900	-0.33639800
C	5.21171400	-1.63823900	0.98430600
C	4.24822800	2.36692300	-0.88126500
C	-1.70044100	-1.24255200	-0.22398100
C	-2.63302400	-0.19348800	-0.03114800
C	-2.18642000	1.15380400	0.18310600
C	-4.06683100	-0.54455200	-0.06063500
H	4.50923000	-1.51681700	-1.07388700
H	5.66739400	-0.27761300	-0.63416600
H	3.51121200	1.87089200	1.10779900
H	5.16291800	1.37065800	0.80671700
H	1.64580500	1.78941300	0.25879800
H	2.77626600	-2.37484200	-0.39419400
H	0.42510200	-2.96457700	-0.49702200
H	5.55300100	-0.96182100	1.76979900
H	4.36778300	-2.21488100	1.36605900
H	6.02431500	-2.32485600	0.74220000
H	4.94542900	1.96019800	-1.61580700
H	3.26834200	2.46520800	-1.35111900
H	4.59597100	3.35777500	-0.58520300

H	-2.06001600	-2.24781500	-0.39109100
H	-4.67447700	1.40085800	0.27760700
H	-6.58730500	-0.23717800	-0.77890700
H	-6.55935400	-0.49884800	0.82382900

*** ES of F2 at PBE/6-311++G(d,p)**

O	-0.84978200	1.35553300	0.19144400
O	-2.98187800	2.09374500	0.30056700
O	-4.56795500	-1.73827100	-0.14317100
N	3.77818500	0.12853900	0.01434100
N	-4.97274200	0.49656200	-0.00404900
N	-6.27621200	0.26650000	0.28359800
C	2.45504900	-0.24184100	-0.06031400
C	4.86352400	-0.81911600	-0.25860700
C	4.18680800	1.48925800	0.37744100
C	1.41165100	0.72129000	0.10514400
C	-0.32407100	-1.00552200	-0.20896000
C	0.08207800	0.34491100	0.03203100
C	2.06628600	-1.59340300	-0.30499400
C	0.72812800	-1.95128500	-0.37626500
C	5.31269900	-1.61194300	0.97516200
C	4.29606700	2.43980700	-0.82146400
C	-1.69987100	-1.30220000	-0.25146900
C	-2.64484300	-0.25948700	-0.06091400
C	-2.24388500	1.07248600	0.14646800
C	-4.09330900	-0.59729600	-0.07715100
H	4.55698700	-1.49834300	-1.06866400
H	5.70941200	-0.23610700	-0.65592100
H	3.49061700	1.88912200	1.13049700
H	5.16349400	1.41012700	0.88057400
H	1.63003200	1.77577200	0.26961300
H	2.82052900	-2.37119900	-0.41954100
H	0.46273900	-2.99665700	-0.55511500
H	5.66142100	-0.93674100	1.77174100
H	4.49166400	-2.22313000	1.37868300
H	6.14421800	-2.28324000	0.70991600
H	5.02367900	2.06339200	-1.55693300
H	3.32681900	2.55905000	-1.32827100
H	4.63376400	3.43262800	-0.48578100
H	-2.04679300	-2.32297800	-0.41843300

H	-4.50472700	1.42984600	0.17255900
H	-6.91553700	0.97666800	-0.07604500
H	-6.53387900	-0.71143200	0.10652200

*** ES of F2 at PW6B95D3/6-311++G(d,p)**

O	-0.84295000	1.33465800	0.19961400
O	-2.90860900	2.09306600	0.34073800
O	-4.50145600	-1.70694900	-0.18293000
N	3.74293500	0.13118200	0.00479000
N	-4.92374600	0.48862400	0.02793000
N	-6.21843400	0.22189200	0.19536300
C	2.43259800	-0.23972600	-0.05584500
C	4.81669000	-0.80487600	-0.27948300
C	4.14438600	1.48120100	0.36031800
C	1.39788900	0.71362300	0.10342500
C	-0.32171600	-1.00298700	-0.17828200
C	0.08396700	0.33358800	0.04325900
C	2.04835500	-1.58322700	-0.27976100
C	0.72440400	-1.94103600	-0.33790800
C	5.24685200	-1.60514400	0.94211600
C	4.19960800	2.41998500	-0.83698700
C	-1.68700300	-1.29431600	-0.21880100
C	-2.62619700	-0.24288900	-0.03589500
C	-2.20732700	1.08464700	0.17354500
C	-4.03158400	-0.58084200	-0.06860400
H	4.51471800	-1.46556800	-1.08980600
H	5.65692300	-0.22394000	-0.65687600
H	3.47519700	1.86792300	1.12656200
H	5.12795800	1.41190600	0.82249800
H	1.60998700	1.75874700	0.25397000
H	2.79532000	-2.35169600	-0.38858700
H	0.46307800	-2.97674600	-0.50193900
H	5.59266000	-0.94125500	1.73285600
H	4.42041400	-2.19633000	1.33195200
H	6.06110100	-2.27982400	0.68301600
H	4.90467300	2.05116400	-1.58024700
H	3.22316500	2.50834300	-1.30954900
H	4.52157300	3.41168700	-0.52370300
H	-2.04011500	-2.29885000	-0.38140100
H	-4.53960700	1.42491500	0.20220800

H	-6.84957300	0.94737500	-0.10842300
H	-6.44416100	-0.73394100	-0.05507000

*** ES of F1 at WB97XD/6-311++G(d,p)**

O	-0.82133800	1.38405900	0.19876100
O	-2.87168500	2.14711100	0.35885800
O	-4.43243000	-1.71612700	-0.25167200
N	3.74135400	0.10652600	0.00375400
N	-4.97302600	0.44829500	0.12451900
N	-6.35152500	0.22008900	0.10544500
C	2.43753400	-0.24117900	-0.05645200
C	4.81391200	-0.84900400	-0.26548300
C	4.17280400	1.46152500	0.34167300
C	1.40916900	0.73981300	0.10739700
C	-0.32924600	-0.96510100	-0.17578600
C	0.09573900	0.38108000	0.04532100
C	2.03158900	-1.59596100	-0.28301400
C	0.71088900	-1.93530300	-0.33500400
C	5.23135300	-1.62716500	0.98083000
C	4.25697600	2.37117900	-0.88264000
C	-1.69914200	-1.24745500	-0.21880500
C	-2.63571500	-0.19774200	-0.02886300
C	-2.18750100	1.14645000	0.18465000
C	-4.06890500	-0.54921400	-0.06146200
H	4.50745200	-1.52164300	-1.06725800
H	5.65967300	-0.27521400	-0.64900800
H	3.50619900	1.87720800	1.09807200
H	5.15476500	1.37309900	0.81013900
H	1.64132500	1.78336600	0.26248600
H	2.77153400	-2.37520500	-0.39607300
H	0.42766300	-2.96867400	-0.49682100
H	5.57582400	-0.94842600	1.76424600
H	4.39993700	-2.21533900	1.37476100
H	6.04922700	-2.30611100	0.73040900
H	4.95560000	1.96611900	-1.61813200
H	3.28060400	2.48243500	-1.35892100
H	4.61036000	3.35915300	-0.57997800
H	-2.05830100	-2.25291800	-0.38549500
H	-4.65468800	1.39586600	0.27052400
H	-6.59841900	-0.20965400	-0.78175800

H	-6.57950000	-0.46033200	0.82502600

S3-F3. The coordinates of the optimized structures for the GS and ES of F3 compound

*** GS of F3 at PBE0/6-311++G(d,p)**

O	-0.14621900	2.63105000	0.03514500
O	2.39051200	-2.21847600	-0.24167100
O	3.74772400	-0.07605700	0.23347800
O	-3.50520600	-2.74319600	0.15283600
O	-1.88620400	3.98578700	-0.04423600
O	-2.64458600	-1.29018700	1.62107400
C	-0.35260200	0.25755200	-0.29785300
C	-1.77022200	0.43236100	-0.47091400
C	0.41278300	1.39412400	-0.04445000
C	-2.65749200	-0.74472000	-0.73765600
C	0.31359800	-0.98398100	-0.36856900
C	1.67587600	-1.07589300	-0.19033700
C	1.79087700	1.32845400	0.13976500
C	2.43015800	0.10298300	0.07115800
C	-2.29750500	1.68001600	-0.39511800
C	-1.49016700	2.84292300	-0.13216000
C	-2.91033800	-1.59390700	0.48610500
C	1.68817500	-3.42281700	-0.49551100
C	4.55141900	1.06557400	0.49492500
H	-2.25356500	-1.38382300	-1.52831300
H	-3.63606300	-0.40748200	-1.09248500
H	-0.25715600	-1.88069900	-0.57023300
H	2.33364800	2.24408700	0.33349800
H	-3.35779300	1.85931400	-0.52465200
H	2.43788900	-4.21208500	-0.49322300
H	1.19341200	-3.39415100	-1.47202000
H	0.94807200	-3.62161800	0.28674500
H	4.49814700	1.78026400	-0.33188600
H	4.24953900	1.55263900	1.42705400
H	5.57011900	0.69509900	0.59098400
H	-3.68178700	-3.23892300	0.96521500

*** GS of F3 at APFD/6-311++G(d,p)**

O	-0.21435400	2.64584900	0.03863800
O	2.40679400	-2.16417100	-0.25334900

O	3.72474400	-0.01332500	0.21818400
O	-3.34474200	-2.85145300	0.15820900
O	-1.99262700	3.96396200	-0.02327600
O	-2.46675900	-1.38828000	1.61770200
C	-0.38250000	0.26553600	-0.30387100
C	-1.80336100	0.41527600	-0.46465600
C	0.36485500	1.41608700	-0.04848200
C	-2.66279300	-0.78365100	-0.72218500
C	0.30144900	-0.96481600	-0.37914200
C	1.66712300	-1.03535700	-0.20253400
C	1.74398200	1.37320700	0.13179000
C	2.40328600	0.15529400	0.05931800
C	-2.35849800	1.65038600	-0.37655300
C	-1.57019800	2.82997400	-0.11753300
C	-2.79178700	-1.67841900	0.49274900
C	1.72818500	-3.38580900	-0.49966200
C	4.52126300	1.13446100	0.48435100
H	-2.28259500	-1.37889500	-1.55832200
H	-3.67573600	-0.47922800	-1.00241900
H	-0.25770800	-1.86905300	-0.57980300
H	2.27179100	2.29765400	0.32693500
H	-3.42400200	1.80855500	-0.49134800
H	2.49465600	-4.15844000	-0.49410700
H	1.23164300	-3.37297300	-1.47564000
H	0.99385200	-3.59540900	0.28525500
H	4.46189500	1.85236900	-0.33925700
H	4.21695300	1.61457900	1.41930800
H	5.54223100	0.77019100	0.57730400
H	-3.44346000	-3.38300900	0.96170000

*** GS of F3 at B3LYP/6-311++G(d,p)**

O	-0.13205000	2.64043500	0.03329000
O	2.40697700	-2.23687400	-0.23765700
O	3.77535600	-0.08585400	0.24034700
O	-3.58724900	-2.72281800	0.14704600
O	-1.88220800	4.00220700	-0.05294600
O	-2.72530000	-1.27049700	1.63046300
C	-0.34329800	0.25609400	-0.29841100
C	-1.76475800	0.43528500	-0.47477800
C	0.42924200	1.39367000	-0.04438800

C	-2.66435400	-0.74285200	-0.74523200
C	0.32476000	-0.99000400	-0.36715900
C	1.69017100	-1.08451300	-0.18696000
C	1.80985500	1.32574800	0.14191800
C	2.44961400	0.09615700	0.07522500
C	-2.29245900	1.68694500	-0.40212800
C	-1.48707300	2.85445700	-0.13880500
C	-2.96875300	-1.57641000	0.48800300
C	1.70896600	-3.45796900	-0.49535400
C	4.59960800	1.05696300	0.50419400
H	-2.24833500	-1.39983800	-1.51283900
H	-3.62640100	-0.39812200	-1.13367800
H	-0.24589300	-1.88440700	-0.56787600
H	2.35259300	2.23974100	0.33476500
H	-3.35130200	1.86553300	-0.53490900
H	2.46813200	-4.23698100	-0.48947000
H	1.21874600	-3.43217800	-1.47283200
H	0.97000300	-3.66102500	0.28507400
H	4.55331600	1.76992300	-0.32287500
H	4.30278500	1.54477000	1.43609000
H	5.61154300	0.67041500	0.59887200
H	-3.79852200	-3.21206600	0.95856600

*** GS of F3 at BP86/6-311++G(d,p)**

O	-0.13927400	2.65697000	0.03221900
O	2.42857400	-2.24058200	-0.23831500
O	3.79330000	-0.07948000	0.24366200
O	-3.55167800	-2.76941600	0.14826000
O	-1.91561100	4.02201400	-0.05657800
O	-2.74412000	-1.26879600	1.64772100
C	-0.34896600	0.25384700	-0.30259900
C	-1.77147100	0.42658600	-0.48014800
C	0.42615100	1.40491500	-0.04565900
C	-2.66569100	-0.75988800	-0.74808300
C	0.32615000	-0.99635600	-0.37088100
C	1.70069700	-1.08704500	-0.18824700
C	1.81352200	1.33972200	0.14300500
C	2.46026500	0.10334300	0.07660700
C	-2.31216800	1.68713600	-0.40668400
C	-1.51906500	2.86352700	-0.14393700

C	-2.96358300	-1.59361600	0.49393300
C	1.71484700	-3.46320400	-0.50210400
C	4.60591600	1.08369000	0.51045600
H	-2.24525700	-1.42128900	-1.52276600
H	-3.63872800	-0.41910500	-1.13899200
H	-0.24702500	-1.90038600	-0.57395100
H	2.36020500	2.26186600	0.33813800
H	-3.38201700	1.85474900	-0.54169600
H	2.47625700	-4.25201200	-0.49869500
H	1.22121800	-3.42854300	-1.48761000
H	0.96909900	-3.66395600	0.28498200
H	4.55128100	1.79974500	-0.32512100
H	4.29653300	1.57100200	1.44893900
H	5.62963800	0.70490000	0.60862700
H	-3.76034700	-3.24860700	0.97843900

*** GS of F3 at CAM-B3LYP/6-311++G(d,p)**

O	-0.14221700	2.63246000	0.03685600
O	2.38687400	-2.22241700	-0.24444900
O	3.75074000	-0.08126600	0.23265000
O	-3.54745600	-2.72216800	0.15880200
O	-1.88088500	3.98553800	-0.04461600
O	-2.62706400	-1.29928700	1.61672300
C	-0.34864200	0.26108700	-0.29605000
C	-1.77173500	0.43945100	-0.46929800
C	0.41720600	1.38878900	-0.04370000
C	-2.66275500	-0.73860900	-0.73795900
C	0.31462000	-0.98162900	-0.36815900
C	1.67316800	-1.07450800	-0.19125200
C	1.79521700	1.32356800	0.14016500
C	2.42972400	0.10070800	0.07051500
C	-2.29458400	1.68096100	-0.39504300
C	-1.48208000	2.84558600	-0.13105800
C	-2.91848700	-1.58746600	0.48555200
C	1.68789400	-3.43306400	-0.49939400
C	4.56490000	1.05728100	0.49617500
H	-2.25737700	-1.37811500	-1.52431500
H	-3.63743300	-0.40001700	-1.09493900
H	-0.25645900	-1.87520700	-0.56951000
H	2.33584900	2.23800500	0.33357300

H	-3.35215300	1.86514200	-0.52444200
H	2.43991900	-4.21767900	-0.49693500
H	1.19467700	-3.40440600	-1.47431900
H	0.95011000	-3.63294500	0.28179600
H	4.51460600	1.77142900	-0.32862000
H	4.26590800	1.54300200	1.42756600
H	5.57938600	0.68003700	0.59078900
H	-3.72364400	-3.22504800	0.96867800

*** GS of F3 at M06/6-311++G(d,p)**

O	-0.17510700	2.62799700	0.03404500
O	2.39837300	-2.19725300	-0.24340100
O	3.73817000	-0.04716800	0.23031900
O	-3.45193600	-2.77100200	0.16134700
O	-1.92809300	3.96666100	-0.03822400
O	-2.58914500	-1.30840700	1.61819000
C	-0.35913400	0.25669100	-0.30120700
C	-1.77668100	0.42069000	-0.47333000
C	0.39593600	1.39634600	-0.04729000
C	-2.64942100	-0.76428300	-0.73422900
C	0.31481100	-0.97929200	-0.37157300
C	1.67551100	-1.06117000	-0.19310900
C	1.77309300	1.34079400	0.13664500
C	2.42050700	0.12228000	0.06790000
C	-2.31529600	1.65981900	-0.39283800
C	-1.52215000	2.83132500	-0.12928600
C	-2.87022700	-1.61484900	0.49022600
C	1.70998400	-3.40598300	-0.49580200
C	4.53308800	1.09646000	0.49361800
H	-2.24805700	-1.39789800	-1.53304300
H	-3.63870300	-0.44182400	-1.07792200
H	-0.25127300	-1.88091400	-0.57389300
H	2.30646400	2.26300800	0.33112500
H	-3.37901200	1.82774200	-0.52056200
H	2.46241200	-4.19337900	-0.49440500
H	1.21221000	-3.38378100	-1.47239800
H	0.96927600	-3.61234500	0.28575900
H	4.47583500	1.81446700	-0.33168800
H	4.22636700	1.58318200	1.42581900
H	5.55680900	0.73923300	0.59192500

H	-3.61055600	-3.27706700	0.97273100

*** GS of F3 at M06-2X/6-311++G(d,p)**

O	-0.19631500	2.64713000	0.04142900
O	2.37981400	-2.18608300	-0.25636700
O	3.72373000	-0.03708900	0.21235100
O	-3.36269300	-2.83059000	0.16512400
O	-1.95087000	3.97894600	-0.01833700
O	-2.42820700	-1.39353600	1.60181100
C	-0.38073000	0.27324500	-0.29722900
C	-1.80952800	0.43557000	-0.45861000
C	0.37455100	1.41058100	-0.04594900
C	-2.67476600	-0.76268400	-0.72087500
C	0.29011700	-0.96754600	-0.37401700
C	1.65316600	-1.04745600	-0.20237600
C	1.75769800	1.35878900	0.13112900
C	2.40144400	0.13750400	0.05685600
C	-2.34962600	1.67021400	-0.37174300
C	-1.54020200	2.84652300	-0.11162900
C	-2.78645800	-1.66790900	0.48782300
C	1.67676500	-3.39548400	-0.50008900
C	4.51625000	1.11526600	0.47463200
H	-2.29852100	-1.35100000	-1.56153800
H	-3.68921600	-0.45434600	-0.98341400
H	-0.27765000	-1.86567100	-0.57427400
H	2.28980700	2.27953100	0.32375800
H	-3.41094800	1.84506200	-0.48727500
H	2.42592800	-4.18257100	-0.49859800
H	1.17673800	-3.36644200	-1.47181300
H	0.94310700	-3.58472800	0.28818400
H	4.44702600	1.82759000	-0.35078200
H	4.20590800	1.59351000	1.40655700
H	5.53804000	0.75823800	0.56724200
H	-3.44598900	-3.36908600	0.96632400

*** GS of F3 at PBE/6-311++G(d,p)**

O	-0.15059600	2.65683400	0.03262400
O	2.42077600	-2.22917100	-0.24137500
O	3.78054300	-0.06971600	0.23948100
O	-3.49096400	-2.79634700	0.14452900

O	-1.92630700	4.01790300	-0.05084100
O	-2.70511000	-1.29093100	1.64655600
C	-0.35656200	0.25723500	-0.30280600
C	-1.77785000	0.42695100	-0.47641800
C	0.41538900	1.40858700	-0.04652400
C	-2.66710700	-0.75997500	-0.74093700
C	0.31929700	-0.99016100	-0.37234700
C	1.69260800	-1.07894500	-0.19099700
C	1.80157600	1.34505000	0.14058100
C	2.44958800	0.11125800	0.07345700
C	-2.31973700	1.68529500	-0.40003900
C	-1.52814100	2.86104600	-0.13961200
C	-2.92988600	-1.61158100	0.49335900
C	1.70955000	-3.44878500	-0.50254200
C	4.58859100	1.09120400	0.50636900
H	-2.25858500	-1.40644000	-1.53381800
H	-3.65111900	-0.42213600	-1.10459700
H	-0.25226600	-1.89479800	-0.57555500
H	2.34664300	2.26775500	0.33573600
H	-3.38992700	1.85110300	-0.53097900
H	2.46969200	-4.23817300	-0.49909400
H	1.21439900	-3.41651500	-1.48704900
H	0.96378600	-3.64977100	0.28417600
H	4.53314000	1.80874100	-0.32747700
H	4.27901000	1.57836600	1.44450900
H	5.61318600	0.71609300	0.60455000
H	-3.67859400	-3.28588600	0.97253400

*** GS of F3 at PW6B95D3/6-311++G(d,p)**

O	-0.17358600	2.64151300	0.04288400
O	2.35899300	-2.19962100	-0.25568200
O	3.71884900	-0.06009700	0.20972600
O	-3.42454600	-2.78227400	0.15212200
O	-1.91737300	3.98870700	-0.01632000
O	-2.41555300	-1.40459700	1.59470700
C	-0.37546100	0.27402000	-0.29341500
C	-1.79224500	0.44547500	-0.45120200
C	0.38843600	1.40617900	-0.04372600
C	-2.66959400	-0.73707500	-0.71318000
C	0.28683300	-0.96529400	-0.37020000

C	1.64619200	-1.05585300	-0.20063100
C	1.76462400	1.34213500	0.13046700
C	2.40002400	0.11909800	0.05602500
C	-2.32347600	1.68570900	-0.36503400
C	-1.51865200	2.84949500	-0.10975400
C	-2.79975100	-1.64855500	0.48180300
C	1.64499700	-3.40113800	-0.49488200
C	4.51933400	1.08567600	0.46737200
H	-2.30262400	-1.32451000	-1.55443000
H	-3.67440600	-0.41457400	-0.98076300
H	-0.28363900	-1.85722700	-0.56806500
H	2.30574900	2.25339800	0.32151900
H	-3.38116100	1.85953500	-0.48029900
H	2.38444800	-4.19281400	-0.49299000
H	1.14370400	-3.37131800	-1.46237600
H	0.91238000	-3.58223100	0.29177100
H	4.45324600	1.79644300	-0.35529400
H	4.21788300	1.56706000	1.39673400
H	5.53562900	0.72228800	0.55635200
H	-3.51304800	-3.32433900	0.94649200

*** GS of F3 at WB97XD/6-311++G(d,p)**

O	-0.17074300	2.64116300	0.03737100
O	2.38034900	-2.20149700	-0.25200200
O	3.73419900	-0.05662900	0.22456400
O	-3.41483600	-2.79822700	0.15761200
O	-1.91610200	3.98438600	-0.03047800
O	-2.55218100	-1.34004300	1.61756500
C	-0.36663800	0.26944200	-0.30184300
C	-1.79267300	0.43779800	-0.46583500
C	0.39297800	1.40265500	-0.04795700
C	-2.67182400	-0.75086900	-0.72857200
C	0.30186300	-0.97119900	-0.37691400
C	1.66268400	-1.05913000	-0.19962400
C	1.77366700	1.34336700	0.13437700
C	2.41466900	0.12141800	0.06313100
C	-2.32346900	1.67726000	-0.38240400
C	-1.51212700	2.84639700	-0.12167500
C	-2.85033200	-1.63334000	0.48829700
C	1.68197200	-3.41190600	-0.49654900

C	4.54014200	1.08400800	0.49070100
H	-2.28495300	-1.35921100	-1.54982200
H	-3.67010200	-0.42560900	-1.03192500
H	-0.26671200	-1.86779100	-0.58018900
H	2.31046000	2.26102200	0.32936400
H	-3.38419300	1.85558300	-0.50055100
H	2.43468400	-4.19702100	-0.49069200
H	1.18544000	-3.39094900	-1.47172000
H	0.94513200	-3.60738100	0.28889400
H	4.48755400	1.80083000	-0.33361800
H	4.23796300	1.56720000	1.42415200
H	5.55743400	0.71196600	0.58572500
H	-3.54366900	-3.31725100	0.96252000

*** ES of F3 at PBE0/6-311++G(d,p)**

O	-0.00679600	2.63719200	0.02825600
O	2.31577800	-2.26957900	-0.22727500
O	3.78416800	-0.19554400	0.22934600
O	-3.77221200	-2.57723300	0.12428100
O	-1.70836900	4.05823500	-0.01713300
O	-2.75478200	-1.25422900	1.61195900
C	-0.34915000	0.25156100	-0.30537700
C	-1.75492900	0.45300200	-0.48438400
C	0.49111400	1.39022200	-0.04783800
C	-2.67986800	-0.68067200	-0.74863300
C	0.28071700	-0.98815700	-0.36067400
C	1.66693300	-1.12070200	-0.18321600
C	1.86457600	1.27459500	0.13256800
C	2.48043400	0.03484700	0.06964000
C	-2.23377700	1.76698600	-0.37772500
C	-1.41157100	2.87794300	-0.12661300
C	-3.04790800	-1.50337800	0.46939400
C	1.60445900	-3.48510400	-0.46226200
C	4.63578700	0.91379100	0.48576300
H	-2.29127000	-1.37577700	-1.50401700
H	-3.62440400	-0.31005500	-1.16275200
H	-0.30593300	-1.87679900	-0.54997300
H	2.42886500	2.17850600	0.32187400
H	-3.28949100	1.98430900	-0.49307900
H	2.35790700	-4.26835100	-0.44209600

H	1.11876000	-3.45979600	-1.44025700
H	0.86781200	-3.65490000	0.32613200
H	4.60456200	1.62621800	-0.34412200
H	4.35210500	1.41334700	1.41694100
H	5.63789300	0.50126500	0.57959800
H	-4.00000200	-3.05830900	0.93241800

*** ES of F3 at APFD/6-311++G(d,p)**

O	-0.06365700	2.66355700	-0.03917400
O	2.31945600	-2.22193900	-0.23184900
O	3.75536000	-0.14183500	0.22624500
O	-3.59136100	-2.70324400	0.14273500
O	-1.81278200	4.04141700	0.05699000
O	-2.55139800	-1.35412500	1.60316500
C	-0.38013500	0.26723500	-0.33240100
C	-1.79197900	0.44797700	-0.49351300
C	0.44556400	1.41772300	-0.08065500
C	-2.69341300	-0.70805900	-0.73857300
C	0.26065500	-0.96502900	-0.38182000
C	1.65069800	-1.08212300	-0.19589100
C	1.81868500	1.31818600	0.11563000
C	2.44899400	0.08295000	0.06006600
C	-2.29954200	1.74430000	-0.33234600
C	-1.49157900	2.87209700	-0.09911100
C	-2.91594800	-1.59086900	0.47689300
C	1.62869500	-3.45247100	-0.46240000
C	4.60189600	0.97207900	0.48821200
H	-2.34027000	-1.35561400	-1.55222400
H	-3.68379400	-0.36308200	-1.05608800
H	-0.31672500	-1.86012200	-0.56960300
H	2.37190700	2.22965000	0.30329800
H	-3.36498100	1.93677700	-0.39117300
H	2.39560700	-4.22185000	-0.43344300
H	1.14751800	-3.44127800	-1.44279800
H	0.89168300	-3.62875500	0.32414100
H	4.57296700	1.68418300	-0.34204800
H	4.31033700	1.47027700	1.41768300
H	5.60453500	0.56288200	0.58804100
H	-3.72927600	-3.22769200	0.94477100

*** ES of F3 at B3LYP/6-311++G(d,p)**

O	0.00221800	2.64480000	0.02639000
O	2.33564800	-2.28154900	-0.22555600
O	3.81565000	-0.19662300	0.23487800
O	-3.84777700	-2.56040400	0.11794400
O	-1.71903200	4.07051200	-0.02380100
O	-2.81821200	-1.24820500	1.62206000
C	-0.33918800	0.25069800	-0.30627600
C	-1.75558900	0.45220300	-0.48724100
C	0.50299000	1.38902300	-0.04878500
C	-2.68892400	-0.68389600	-0.75311600
C	0.29348200	-0.98911100	-0.36131900
C	1.68718800	-1.12412800	-0.18119500
C	1.88182300	1.27394500	0.13387900
C	2.50204400	0.03404800	0.07265700
C	-2.23793200	1.76754500	-0.38273000
C	-1.42314200	2.88620700	-0.13204400
C	-3.09772000	-1.49403200	0.47232300
C	1.63012700	-3.51712300	-0.46289500
C	4.68281700	0.91659400	0.49465600
H	-2.29113500	-1.39348500	-1.48816200
H	-3.61987800	-0.31095000	-1.19300500
H	-0.28923000	-1.87802100	-0.55071400
H	2.44328200	2.17791200	0.32266800
H	-3.29350600	1.97929800	-0.50045000
H	2.39493100	-4.28776100	-0.43755000
H	1.15006600	-3.49571600	-1.44214500
H	0.89499900	-3.69006100	0.32418600
H	4.65520400	1.62821200	-0.33447400
H	4.40255100	1.41451900	1.42634200
H	5.67961100	0.49299600	0.58632200
H	-4.10269800	-3.03703900	0.92418600

*** ES of F3 at BP86/6-311++G(d,p)**

O	-0.00541100	2.66763900	0.04168200
O	2.34812200	-2.29160800	-0.24095800
O	3.84275700	-0.19432900	0.24162100
O	-3.76067300	-2.64846800	0.12932900
O	-1.75261900	4.09464100	-0.04644000
O	-2.85022600	-1.23356800	1.65062100

C	-0.34421200	0.26525500	-0.30800600
C	-1.78100600	0.45215000	-0.49640500
C	0.49265200	1.39318000	-0.04510500
C	-2.70598200	-0.69626600	-0.74756800
C	0.29483300	-0.97868400	-0.37348400
C	1.70019400	-1.11730400	-0.18853400
C	1.88528400	1.27906800	0.13921200
C	2.51607100	0.03849300	0.07418800
C	-2.26237800	1.77231400	-0.39944600
C	-1.44977700	2.90133200	-0.14417500
C	-3.08779800	-1.51689600	0.48824800
C	1.62327600	-3.52553900	-0.48608300
C	4.68809400	0.94243300	0.51437700
H	-2.31675600	-1.40570800	-1.50114000
H	-3.65765000	-0.32830300	-1.17156600
H	-0.29050000	-1.87522100	-0.57846900
H	2.44772900	2.19216900	0.33553600
H	-3.32618900	1.98586000	-0.52767100
H	2.38826100	-4.30795200	-0.46237000
H	1.14257500	-3.49222100	-1.47423600
H	0.88026200	-3.69326000	0.30653200
H	4.65229400	1.66366200	-0.31849400
H	4.38836200	1.43503800	1.45382900
H	5.70034300	0.53447300	0.61246900
H	-3.99983300	-3.12022100	0.95541200

*** ES of F3 at CAM-B3LYP/6-311++G(d,p)**

O	-0.02106300	2.63710100	0.02886400
O	2.33979100	-2.26359800	-0.22058700
O	3.77538600	-0.17464700	0.22824900
O	-3.82434400	-2.54706000	0.13109200
O	-1.73612700	4.04426800	-0.01591800
O	-2.73499400	-1.26682800	1.60198700
C	-0.34744000	0.24152000	-0.30602600
C	-1.73441700	0.43832000	-0.48474900
C	0.49152900	1.39698100	-0.04579200
C	-2.66253300	-0.69827400	-0.75810000
C	0.29619300	-1.00548900	-0.35702500
C	1.66681400	-1.12127800	-0.18147700
C	1.85637800	1.28799900	0.13350900

C	2.47218900	0.04568300	0.06973000
C	-2.23464400	1.74999400	-0.37918600
C	-1.42703800	2.86817400	-0.12581200
C	-3.05121400	-1.50279700	0.46453900
C	1.64084800	-3.48902600	-0.45495700
C	4.63756900	0.93514000	0.48117900
H	-2.25654600	-1.39983500	-1.49329900
H	-3.59424300	-0.32977000	-1.19499700
H	-0.28739800	-1.89362000	-0.54024800
H	2.41860500	2.19061900	0.32193500
H	-3.29140000	1.95027600	-0.49660200
H	2.40037800	-4.26449500	-0.43599800
H	1.15320800	-3.46932900	-1.43047000
H	0.90747400	-3.66649500	0.33274800
H	4.60452400	1.64315000	-0.34919800
H	4.35855900	1.43337600	1.41160800
H	5.63547000	0.51644300	0.57079800
H	-4.06323000	-3.02589600	0.93921200

*** ES of F3 at M06/6-311++G(d,p)**

O	-0.02698800	2.63677800	-0.02791400
O	2.33046400	-2.25329100	-0.21959200
O	3.77601600	-0.16811400	0.23583500
O	-3.78285000	-2.56298700	0.14388800
O	-1.75338000	4.03058800	0.02633200
O	-2.67571100	-1.27860500	1.60078500
C	-0.35002500	0.24616900	-0.32628900
C	-1.75088300	0.43759100	-0.50097800
C	0.48101900	1.39436600	-0.07234100
C	-2.66705600	-0.70252300	-0.75472400
C	0.28767900	-0.99074600	-0.36857800
C	1.67009000	-1.11114600	-0.18475500
C	1.84989600	1.28771400	0.12214900
C	2.47304400	0.05210100	0.06799200
C	-2.25140000	1.73806400	-0.35206900
C	-1.44363100	2.86229700	-0.11377300
C	-3.01661200	-1.51405700	0.47118400
C	1.63235300	-3.47399000	-0.45379200
C	4.61759000	0.94474700	0.49478200
H	-2.27614300	-1.40308800	-1.50651200

H	-3.61746000	-0.34508400	-1.17129600
H	-0.29539300	-1.88452200	-0.55305600
H	2.40583000	2.19851100	0.30878300
H	-3.31573800	1.93613700	-0.43129300
H	2.38760200	-4.25609300	-0.43015100
H	1.14737100	-3.45651000	-1.43352800
H	0.89186700	-3.64934100	0.33132300
H	4.58853800	1.65673700	-0.33722000
H	4.32286600	1.44869000	1.42161700
H	5.62447700	0.54547400	0.59957600
H	-3.99659500	-3.04937700	0.95423000

*** ES of F3 at M06-2X/6-311++G(d,p)**

O	-0.04445700	2.66698400	-0.10331800
O	2.31269200	-2.24337900	-0.22815100
O	3.73618200	-0.15788900	0.23858200
O	-3.69319800	-2.62257700	0.17680400
O	-1.77548700	4.04234300	0.08751100
O	-2.47777200	-1.37376800	1.57622100
C	-0.37595700	0.26213700	-0.34712400
C	-1.77022100	0.45218800	-0.49714500
C	0.46109000	1.42397000	-0.09769200
C	-2.68701600	-0.69887300	-0.74685800
C	0.26372200	-0.98984700	-0.38964500
C	1.63478300	-1.10412300	-0.19915400
C	1.82488500	1.31441100	0.11635800
C	2.43780500	0.06706600	0.06459800
C	-2.28168600	1.75009800	-0.29917800
C	-1.46422700	2.87799700	-0.08989100
C	-2.91732800	-1.57052700	0.47425100
C	1.60410400	-3.45926400	-0.47135600
C	4.58370300	0.95857400	0.50420700
H	-2.32518900	-1.35342500	-1.54742300
H	-3.66924900	-0.34571600	-1.07178300
H	-0.32332200	-1.87789400	-0.57214900
H	2.38640300	2.21959100	0.29990900
H	-3.34734100	1.93916600	-0.32086800
H	2.35396900	-4.24377200	-0.44720800
H	1.12490600	-3.42873600	-1.45139300
H	0.86063000	-3.62687200	0.30996000

H	4.55709300	1.66215000	-0.33069900
H	4.27787700	1.45654900	1.42674700
H	5.58320100	0.54936800	0.61499800
H	-3.82459500	-3.14696100	0.98049900

*** ES of F3 at PBE/6-311++G(d,p)**

O	-0.01005100	2.67067300	0.02243200
O	2.33561300	-2.28539600	-0.23665600
O	3.82936800	-0.19085200	0.23707400
O	-3.71306800	-2.66724400	0.12269400
O	-1.75821500	4.09083600	-0.01954900
O	-2.80675700	-1.25374100	1.64362700
C	-0.35052000	0.27040500	-0.31311700
C	-1.78520500	0.45647000	-0.49641500
C	0.48582300	1.39751300	-0.05474200
C	-2.70636100	-0.69139900	-0.74613600
C	0.28621700	-0.97316000	-0.37302000
C	1.68923200	-1.11213700	-0.18824200
C	1.87609500	1.28243800	0.13125400
C	2.50521100	0.04229000	0.07006500
C	-2.26740600	1.77320500	-0.38275800
C	-1.45278700	2.90036400	-0.13216200
C	-3.05678800	-1.53003200	0.48286200
C	1.61054700	-3.51492300	-0.47448500
C	4.67286700	0.94264500	0.50588500
H	-2.32732000	-1.38720100	-1.51689800
H	-3.66782100	-0.32380600	-1.14603000
H	-0.30058700	-1.86919500	-0.57418900
H	2.43940200	2.19523600	0.32447200
H	-3.33270800	1.98565700	-0.49439300
H	2.37206000	-4.29999300	-0.44754700
H	1.12849100	-3.48679800	-1.46185100
H	0.86658400	-3.67810400	0.31790800
H	4.63795300	1.66251500	-0.32777100
H	4.37418700	1.43913800	1.44323200
H	5.68504600	0.53614400	0.60530200
H	-3.93195000	-3.14988300	0.94684400

*** ES of F3 at PW6B95D3/6-311++G(d,p)**

O	-0.02384300	2.65790900	-0.02870000

O	2.27260000	-2.25440200	-0.23822700
O	3.74567300	-0.18884000	0.21730700
O	-3.71329200	-2.59575200	0.15195100
O	-1.73694900	4.06323800	0.05739500
O	-2.46221900	-1.40471600	1.56807100
C	-0.37317600	0.27393100	-0.31958600
C	-1.77643200	0.47530000	-0.47473800
C	0.46985800	1.40919200	-0.07204600
C	-2.69540900	-0.66269400	-0.72854000
C	0.24759600	-0.96711400	-0.37294200
C	1.62836000	-1.10300300	-0.19621900
C	1.83773700	1.28821500	0.11668000
C	2.44365500	0.04680500	0.05652900
C	-2.26178000	1.77800400	-0.31946200
C	-1.43969200	2.88960500	-0.09157700
C	-2.92106700	-1.56215000	0.46682900
C	1.54711700	-3.46337500	-0.47084600
C	4.59804600	0.92121500	0.47512200
H	-2.34993200	-1.30330500	-1.54492900
H	-3.67534100	-0.30101100	-1.03945600
H	-0.34185200	-1.84937700	-0.55513300
H	2.40490400	2.18536500	0.30097600
H	-3.31890600	1.98500200	-0.38167600
H	2.28774800	-4.25158300	-0.45053900
H	1.06198300	-3.42975900	-1.44331100
H	0.81217600	-3.61835800	0.31536300
H	4.56601500	1.62764700	-0.35322300
H	4.30795100	1.41910300	1.39925800
H	5.59476400	0.51044200	0.57295400
H	-3.83414500	-3.13724400	0.94211700

*** ES of F3 at WB97XD/6-311++G(d,p)**

O	-0.03920200	2.64858200	0.01754600
O	2.32436900	-2.25140800	-0.22280500
O	3.75792800	-0.16369300	0.22527100
O	-3.68276900	-2.63667800	0.13393200
O	-1.75729800	4.05004400	0.00430900
O	-2.68384200	-1.28220900	1.60421200
C	-0.36448900	0.25297800	-0.31394300
C	-1.75235900	0.44575800	-0.48876800

C	0.47300000	1.41144400	-0.05244200
C	-2.67111300	-0.70085400	-0.75539400
C	0.27918400	-0.99585000	-0.36442700
C	1.65101000	-1.11114300	-0.18613600
C	1.84010300	1.30251800	0.12982000
C	2.45657200	0.05799700	0.06632100
C	-2.25786800	1.75612700	-0.36845500
C	-1.44687900	2.87567400	-0.11721800
C	-2.98947100	-1.54020500	0.46754900
C	1.62143300	-3.47225800	-0.45441900
C	4.61579500	0.94631500	0.47720800
H	-2.28147200	-1.37444000	-1.52640500
H	-3.62906300	-0.33937800	-1.14099100
H	-0.30632600	-1.88399500	-0.54953600
H	2.40234400	2.20615100	0.31927000
H	-3.31750300	1.95393400	-0.47146300
H	2.37810600	-4.25160400	-0.43351200
H	1.13340100	-3.45341000	-1.43136400
H	0.88595700	-3.64577700	0.33425100
H	4.58263500	1.65465500	-0.35479100
H	4.33562400	1.44603500	1.40819300
H	5.61536200	0.52964800	0.56807300
H	-3.88205600	-3.12992300	0.94038400

S3-F4. The coordinates of the optimized structures for the GS and ES of F4 compound

*** GS of F4 at PBE0/6-311++G(d,p)**

O	0.96869600	-1.32516400	-0.00003400
O	-3.44986900	0.39893700	-0.00003000
O	2.98186100	-2.23041400	0.00001300
N	5.42328500	0.39968500	0.00010700
C	0.62723100	1.05109800	-0.00004600
C	0.12716500	-0.25969100	-0.00003400
C	-2.12247000	0.53496900	-0.00003200
C	-1.22989300	-0.53650900	-0.00002600
C	-0.30105100	2.11346800	-0.00005900
C	-1.64737900	1.86518600	-0.00005400
C	2.02917000	1.22504200	-0.00003700
C	2.86245100	0.14130500	-0.00002800
C	-4.01937000	-0.91685800	0.00007200

C	2.33362900	-1.21444500	-0.00005500
C	-5.51815400	-0.76631100	0.00016000
C	4.27373100	0.28128600	-0.00000100
H	-1.55538200	-1.56782000	-0.00002700
H	0.06839100	3.13333800	-0.00006900
H	-2.37093700	2.67167500	-0.00006300
H	2.44266700	2.22850400	-0.00003600
H	-3.67455400	-1.45439000	-0.88990100
H	-3.67443200	-1.45430100	0.89005000
H	-5.98149800	-1.75590100	0.00022300
H	-5.85651000	-0.22846800	0.88882700
H	-5.85661500	-0.22853200	-0.88850500

*** GS of F4 at APFD/6-311++G(d,p)**

O	0.97140600	-1.33335100	0.00007900
O	-3.45317400	0.39654400	0.00000000
O	2.99860500	-2.22620500	-0.00001100
N	5.42630800	0.40875500	-0.00035600
C	0.62686000	1.04991900	0.00001000
C	0.12952000	-0.26515500	0.00003900
C	-2.12330800	0.52654900	0.00000600
C	-1.22650700	-0.54544900	0.00003400
C	-0.30346200	2.11064400	-0.00002200
C	-1.65034200	1.85851900	-0.00002200
C	2.02834400	1.22743200	-0.00001000
C	2.86513300	0.14532700	0.00002100
C	-4.03077300	-0.91763700	0.00005400
C	2.34129200	-1.21470200	0.00014100
C	-5.53080800	-0.75325000	0.00007200
C	4.27612500	0.28892600	-0.00003900
H	-1.54896300	-1.57804100	0.00005400
H	0.06491500	3.13132300	-0.00005000
H	-2.37670000	2.66312200	-0.00004700
H	2.43959700	2.23214700	-0.00006600
H	-3.68767000	-1.45642700	-0.89005200
H	-3.68764200	-1.45636500	0.89018700
H	-6.00661100	-1.73725200	0.00010700
H	-5.86409900	-0.21119600	0.88842000
H	-5.86412600	-0.21124900	-0.88830000

*** GS of F4 at B3LYP/6-311++G(d,p)**

O	0.97778900	-1.33601100	0.00005000
O	-3.46330900	0.39850700	0.00001500
O	3.00413900	-2.24033500	0.00002300
N	5.44249900	0.41744000	-0.00027300
C	0.63219100	1.04967100	-0.00000900
C	0.12809200	-0.26433600	0.00002300
C	-2.12703700	0.53265400	0.00001000
C	-1.23176700	-0.54165800	0.00003100
C	-0.29972000	2.11507200	-0.00003200
C	-1.64928400	1.86615700	-0.00002200
C	2.03729000	1.22384900	-0.00002700
C	2.87904200	0.14114900	-0.00000100
C	-4.05488900	-0.92314600	0.00006100
C	2.35431600	-1.22072000	0.00006500
C	-5.55890300	-0.75087200	0.00008000
C	4.29280900	0.29097200	-0.00002600
H	-1.55759800	-1.57121600	0.00005400
H	0.06844800	3.13413200	-0.00005800
H	-2.37104100	2.67274100	-0.00003900
H	2.44769500	2.22716600	-0.00006400
H	-3.71617100	-1.46139200	-0.88984200
H	-3.71614300	-1.46134300	0.88998400
H	-6.03466700	-1.73440800	0.00011000
H	-5.88988800	-0.20888100	0.88847200
H	-5.88991400	-0.20892400	-0.88832900

*** GS of F4 at BP86/6-311++G(d,p)**

O	0.97517400	-1.34830900	0.00008700
O	-3.48440500	0.41062800	0.00002000
O	3.02252800	-2.25831700	-0.00003300
N	5.47066400	0.42206900	-0.00032700
C	0.63540900	1.05725400	0.00000900
C	0.12535400	-0.26712900	0.00004400
C	-2.14008700	0.54071200	0.00001900
C	-1.24188300	-0.54298400	0.00004600
C	-0.30121100	2.12928000	-0.00002300
C	-1.65871600	1.88121000	-0.00001600
C	2.04205600	1.23321900	-0.00002200
C	2.89286000	0.14047600	0.00000700

C	-4.06744100	-0.92865800	0.00005700
C	2.37263200	-1.22679900	0.00015100
C	-5.57606600	-0.76807500	0.00005900
C	4.30737900	0.29254900	-0.00008200
H	-1.57361300	-1.58036000	0.00007300
H	0.07230600	3.15591700	-0.00005700
H	-2.38553000	2.69529300	-0.00004000
H	2.45664800	2.24454700	-0.00009000
H	-3.71725100	-1.46518900	-0.89781700
H	-3.71724500	-1.46514300	0.89795700
H	-6.04526700	-1.76395000	0.00008400
H	-5.91639500	-0.22695900	0.89558800
H	-5.91640100	-0.22700200	-0.89549400

*** GS of F4 at CAM-B3LYP/6-311++G(d,p)**

O	0.97166400	-1.32712300	0.00014700
O	-3.45043500	0.39691500	0.00000200
O	2.98620300	-2.22717600	0.00000000
N	5.42277400	0.40372000	-0.00073700
C	0.62646800	1.04618400	0.00005300
C	0.12644800	-0.25782400	0.00008400
C	-2.11887400	0.53284800	0.00002100
C	-1.22983400	-0.53609300	0.00006400
C	-0.29960400	2.10833300	0.00000500
C	-1.64375500	1.86113700	-0.00000800
C	2.03333100	1.21954600	0.00002800
C	2.86313600	0.14289800	0.00007500
C	-4.02878600	-0.91835500	0.00003900
C	2.33446600	-1.21525000	0.00026100
C	-5.52841000	-0.75648700	0.00002300
C	4.27943900	0.28421000	-0.00000600
H	-1.55330500	-1.56582900	0.00008700
H	0.06945900	3.12656200	-0.00002900
H	-2.36619800	2.66629200	-0.00004600
H	2.44430800	2.22220000	-0.00005200
H	-3.68811300	-1.45585300	-0.88869400
H	-3.68812700	-1.45579700	0.88881200
H	-6.00042300	-1.74038800	0.00004700
H	-5.86032600	-0.21549100	0.88731300
H	-5.86031100	-0.21554200	-0.88730400

*** GS of F4 at M06/6-311++G(d,p)**

O	0.96997600	-1.32481000	-0.00007600
O	-3.44731200	0.39514800	0.00003800
O	2.98648500	-2.22495300	0.00002500
N	5.41898300	0.40523200	0.00040800
C	0.62411600	1.04766900	-0.00009300
C	0.12637600	-0.26140400	-0.00005600
C	-2.12093400	0.53039800	-0.00000300
C	-1.22896100	-0.53870400	-0.00000900
C	-0.30355700	2.10823900	-0.00008300
C	-1.64724100	1.85918100	-0.00004000
C	2.02471500	1.22252100	-0.00010700
C	2.85900400	0.14293400	-0.00011600
C	-4.01969400	-0.91779100	0.00009300
C	2.33603000	-1.21379100	-0.00018400
C	-5.51285300	-0.75806400	0.00015100
C	4.27027000	0.28565900	-0.00009100
H	-1.55102400	-1.57219500	0.00001600
H	0.06873800	3.12800000	-0.00010400
H	-2.37480000	2.66300300	-0.00003000
H	2.43582700	2.22838700	-0.00009600
H	-3.67331000	-1.45919800	-0.88949400
H	-3.67323600	-1.45915500	0.88967900
H	-5.99030000	-1.74092700	0.00018900
H	-5.84576100	-0.21433500	0.88823200
H	-5.84583200	-0.21436900	-0.88792400

*** GS of F4 at M06-2X/6-311++G(d,p)**

O	0.96761200	-1.32625100	0.00007100
O	-3.45553700	0.39967000	0.00001400
O	2.98330900	-2.22320400	0.00002300
N	5.42751800	0.38605400	-0.00038200
C	0.62380700	1.05153400	0.00000300
C	0.12510800	-0.25572400	0.00003700
C	-2.12402600	0.53693700	0.00001300
C	-1.23425000	-0.53561100	0.00004000
C	-0.30221700	2.11605100	-0.00002500
C	-1.64934400	1.86839200	-0.00002000
C	2.03485000	1.22786100	-0.00001600

C	2.86056600	0.14760300	0.00001600
C	-4.01486100	-0.92087100	0.00005800
C	2.32920200	-1.21537600	0.00010500
C	-5.51832000	-0.77287400	0.00006500
C	4.28162900	0.27880300	-0.00001600
H	-1.55509100	-1.56722200	0.00006500
H	0.06990300	3.13376100	-0.00005400
H	-2.37410700	2.67198700	-0.00004200
H	2.44699700	2.23108100	-0.00006100
H	-3.66752600	-1.45359200	-0.88986100
H	-3.66751300	-1.45353800	0.89000500
H	-5.98126300	-1.76053900	0.00009500
H	-5.84997800	-0.23316900	0.88793900
H	-5.84999000	-0.23321800	-0.88783500

*** GS of F4 at PBE/6-311++G(d,p)**

O	0.97348700	-1.34528400	0.00004900
O	-3.47989100	0.40947600	0.00002900
O	3.01761000	-2.25492400	-0.00003700
N	5.46403800	0.41881800	-0.00010800
C	0.63413600	1.05674900	-0.00001800
C	0.12558300	-0.26645100	0.00002000
C	-2.13801800	0.53987400	0.00001600
C	-1.24027300	-0.54200600	0.00003500
C	-0.30152700	2.12699900	-0.00004000
C	-1.65742100	1.87879000	-0.00002200
C	2.03897700	1.23271000	-0.00004900
C	2.88828300	0.14080200	-0.00003100
C	-4.05967400	-0.92623000	0.00006700
C	2.36770400	-1.22442100	0.00007800
C	-5.56568100	-0.76918300	0.00008000
C	4.30089900	0.29140300	-0.00010800
H	-1.57112100	-1.57933200	0.00006300
H	0.07188400	3.15321600	-0.00007300
H	-2.38444200	2.69214200	-0.00003800
H	2.45345300	2.24368700	-0.00010400
H	-3.70937800	-1.46345800	-0.89697400
H	-3.70935800	-1.46341500	0.89712600
H	-6.03299000	-1.76508300	0.00010800
H	-5.90693200	-0.22890400	0.89499500

H	-5.90695100	-0.22894400	-0.89485100

*** GS of F4 at PW6B95D3/6-311++G(d,p)**

O	0.96515000	-1.32261200	0.00007100
O	-3.44530400	0.40148900	0.00000100
O	2.97731100	-2.22548600	-0.00001000
N	5.41161000	0.39442900	-0.00031500
C	0.62469500	1.04925600	0.00000500
C	0.12377300	-0.25673600	0.00003400
C	-2.11781600	0.53920900	0.00000500
C	-1.23011800	-0.53154000	0.00003200
C	-0.29938800	2.11097900	-0.00002500
C	-1.64284700	1.86540200	-0.00002400
C	2.02465900	1.22151900	-0.00001500
C	2.85526700	0.14126200	0.00001400
C	-4.00769700	-0.91800000	0.00005700
C	2.32855600	-1.21212000	0.00012400
C	-5.50493100	-0.77329400	0.00007500
C	4.26533900	0.27906200	-0.00004200
H	-1.55549500	-1.55764500	0.00005200
H	0.07084900	3.12516000	-0.00005300
H	-2.36290800	2.66822700	-0.00004600
H	2.43630900	2.22023300	-0.00006700
H	-3.65921500	-1.44928000	-0.88595100
H	-3.65918700	-1.44921700	0.88609100
H	-5.96330900	-1.75974100	0.00011100
H	-5.84125500	-0.23790200	0.88489300
H	-5.84128100	-0.23795500	-0.88476500

*** GS of F4 at WB97XD/6-311++G(d,p)**

O	0.96916800	-1.32758600	0.00014200
O	-3.45064900	0.39864400	0.00000200
O	2.98166800	-2.22948300	-0.00000600
N	5.42614700	0.40156800	-0.00069600
C	0.62674800	1.04798700	0.00004900
C	0.12785600	-0.25843600	0.00008000
C	-2.12114700	0.53339300	0.00002000
C	-1.23070700	-0.53709300	0.00006100
C	-0.29988600	2.11127900	0.00000200
C	-1.64575300	1.86371300	-0.00001000

C	2.03489500	1.22340900	0.00002300
C	2.86232600	0.14285100	0.00007000
C	-4.02348900	-0.91619700	0.00004100
C	2.33077600	-1.21669500	0.00025500
C	-5.52556400	-0.76037700	0.00002700
C	4.27995200	0.28229100	-0.00001300
H	-1.55381800	-1.56806500	0.00008400
H	0.06934700	3.13022200	-0.00003100
H	-2.36755700	2.67035300	-0.00004700
H	2.44691300	2.22647900	-0.00005600
H	-3.68243500	-1.45443200	-0.89000100
H	-3.68244500	-1.45437600	0.89012000
H	-5.99104600	-1.74819000	0.00005300
H	-5.85977000	-0.22113500	0.88859000
H	-5.85975900	-0.22118700	-0.88857100

*** ES of F4 at PBE0/6-311++G(d,p)**

O	0.96629100	-1.34009100	-0.00065300
O	-3.44542200	0.38374800	0.00019600
O	2.98118100	-2.23098800	-0.00014900
N	5.42669900	0.37915100	0.00068700
C	0.64238000	1.07736900	-0.00022500
C	0.13053900	-0.26584700	-0.00030900
C	-2.12741800	0.52308300	0.00005100
C	-1.21596300	-0.54323300	-0.00014900
C	-0.31379100	2.12975000	-0.00003600
C	-1.65653500	1.86798000	0.00008500
C	2.03226300	1.28471000	-0.00025800
C	2.87389900	0.13742000	-0.00011800
C	-4.03190000	-0.92802700	0.00025200
C	2.34427200	-1.19850600	-0.00032100
C	-5.52790300	-0.76280200	0.00050100
C	4.27016200	0.25247300	0.00022500
H	-1.53619100	-1.57670900	-0.00022700
H	0.04303700	3.15339200	0.00001800
H	-2.38924300	2.66664800	0.00022100
H	2.45015600	2.28182600	-0.00021100
H	-3.68554100	-1.46423600	-0.89000400
H	-3.68524400	-1.46429400	0.89035800
H	-5.99608300	-1.75002000	0.00051900

H	-5.86196600	-0.22416600	0.88993800
H	-5.86224900	-0.22406500	-0.88877000

*** ES of F4 at APFD/6-311++G(d,p)**

O	0.96834600	-1.34740800	-0.00040600
O	-3.44926200	0.38223500	0.00018600
O	2.99704900	-2.22749100	-0.00011800
N	5.43067100	0.38833900	-0.00025700
C	0.64157800	1.07531700	-0.00009900
C	0.13230500	-0.27094300	-0.00016900
C	-2.12829900	0.51504200	0.00008700
C	-1.21378600	-0.55181200	-0.00005900
C	-0.31496500	2.12615800	0.00003500
C	-1.65900500	1.86129200	0.00011800
C	2.03224500	1.28577400	-0.00012400
C	2.87711200	0.14120100	-0.00000800
C	-4.04346800	-0.92774500	0.00021400
C	2.35187400	-1.19874600	-0.00012300
C	-5.54075800	-0.75016800	0.00037400
C	4.27351600	0.26027000	0.00023200
H	-1.53166200	-1.58629900	-0.00011600
H	0.04112200	3.15047500	0.00007700
H	-2.39389600	2.65855800	0.00021500
H	2.44773500	2.28421600	-0.00010800
H	-3.69821400	-1.46513300	-0.89002600
H	-3.69802600	-1.46517900	0.89035400
H	-6.02018800	-1.73227100	0.00038900
H	-5.87026800	-0.20767200	0.88947900
H	-5.87044900	-0.20761300	-0.88862800

*** ES of F4 at B3LYP/6-311++G(d,p)**

O	0.97491000	-1.35050200	-0.00044200
O	-3.45985500	0.38419900	0.00021600
O	3.00309100	-2.24315000	-0.00029100
N	5.44668800	0.40027200	0.00066400
C	0.64595800	1.07541100	-0.00015800
C	0.13107200	-0.26945400	-0.00020500
C	-2.13243800	0.52109600	0.00009100
C	-1.21904000	-0.54802800	-0.00007200
C	-0.31110200	2.13046400	0.00000300

C	-1.65857600	1.86907700	0.00011600
C	2.04243200	1.28173500	-0.00025000
C	2.89177800	0.13537100	-0.00019900
C	-4.06837900	-0.93371700	0.00024300
C	2.36552700	-1.20574000	-0.00025300
C	-5.56932700	-0.74696400	0.00041800
C	4.29055500	0.26250400	-0.00009100
H	-1.53982200	-1.57968900	-0.00011600
H	0.04475300	3.15325200	0.00003200
H	-2.38881900	2.66831500	0.00022900
H	2.45838900	2.27826900	-0.00026500
H	-3.72765200	-1.47029100	-0.89000900
H	-3.72745000	-1.47034700	0.89038400
H	-6.04992100	-1.72805100	0.00043500
H	-5.89601800	-0.20416200	0.88952400
H	-5.89621500	-0.20409700	-0.88857700

*** ES of F4 at BP86/6-311++G(d,p)**

O	0.97253500	-1.35665300	-0.00035500
O	-3.49202100	0.39782600	0.00009400
O	3.01851100	-2.25845900	-0.00030400
N	5.48376900	0.39185800	-0.00010500
C	0.64471800	1.07959500	0.00003100
C	0.13060900	-0.26251900	-0.00013100
C	-2.14313700	0.52738400	0.00004500
C	-1.23418300	-0.54656700	-0.00011300
C	-0.30244000	2.13491400	0.00006000
C	-1.67093600	1.87691400	0.00008100
C	2.06479700	1.28974300	-0.00002700
C	2.90838100	0.14075700	0.00001400
C	-4.08912800	-0.93039900	0.00022600
C	2.38058500	-1.20776200	-0.00001200
C	-5.59558200	-0.76471200	0.00040600
C	4.31329300	0.25997700	0.00002200
H	-1.55601300	-1.58753400	-0.00023200
H	0.05555700	3.16653900	0.00006300
H	-2.40232600	2.68697200	0.00010600
H	2.48177200	2.29538300	-0.00005500
H	-3.73317500	-1.46980700	-0.89575300
H	-3.73294400	-1.46973800	0.89615400

H	-6.06333500	-1.76111500	0.00053000
H	-5.93486600	-0.22462900	0.89660300
H	-5.93509900	-0.22474100	-0.89577000

*** ES of F4 at CAM-B3LYP/6-311++G(d,p)**

O	0.96883100	-1.34650100	-0.00049500
O	-3.43983800	0.38060000	0.00020000
O	2.98894100	-2.22998200	-0.00003700
N	5.42050800	0.39208500	-0.00009400
C	0.64500500	1.07439500	-0.00014800
C	0.12841700	-0.27180600	-0.00021100
C	-2.12404300	0.52236500	0.00007900
C	-1.21237900	-0.54515200	-0.00007700
C	-0.31960200	2.13101600	0.00000200
C	-1.65285200	1.86862100	0.00010200
C	2.02408900	1.28079100	-0.00013900
C	2.87296000	0.13515600	-0.00003300
C	-4.03672000	-0.93372600	0.00023200
C	2.34979300	-1.20156600	-0.00028900
C	-5.53299000	-0.75349100	0.00041000
C	4.27118500	0.25975600	0.00032700
H	-1.53440200	-1.57588200	-0.00013100
H	0.03884300	3.15230300	0.00004600
H	-2.38738600	2.66326000	0.00021500
H	2.44092300	2.27650100	-0.00006200
H	-3.69576800	-1.46805700	-0.88958400
H	-3.69555900	-1.46810800	0.88993800
H	-6.01202700	-1.73389700	0.00042700
H	-5.85931500	-0.21093300	0.88844900
H	-5.85951700	-0.21086600	-0.88751300

*** ES of F4 at M06/6-311++G(d,p)**

O	0.96752200	-1.34054800	-0.00049400
O	-3.44336800	0.38131100	0.00020400
O	2.98660800	-2.22556700	-0.00015400
N	5.42123500	0.38406100	0.00024500
C	0.63998800	1.07400800	-0.00015900
C	0.12929800	-0.26813800	-0.00022300
C	-2.12648800	0.52000700	0.00007800
C	-1.21492700	-0.54460700	-0.00008900

C	-0.31625000	2.12579700	0.00000000
C	-1.65520200	1.86365700	0.00010500
C	2.02595600	1.28261200	-0.00019000
C	2.86977600	0.13901400	-0.00008500
C	-4.03059700	-0.92946600	0.00023700
C	2.34613000	-1.20000300	-0.00026200
C	-5.52129100	-0.75723900	0.00042300
C	4.26560500	0.25788300	0.00018500
H	-1.53245800	-1.58001700	-0.00014400
H	0.04450600	3.14900000	0.00004100
H	-2.39134700	2.65998300	0.00022100
H	2.44089700	2.28209400	-0.00015300
H	-3.68220200	-1.46887200	-0.88975800
H	-3.68198100	-1.46892500	0.89011300
H	-6.00248400	-1.73817300	0.00044000
H	-5.85072900	-0.21315000	0.88920200
H	-5.85094000	-0.21307900	-0.88823500

*** ES of F4 at M06-2X/6-311++G(d,p)**

O	0.96307000	-1.34690100	-0.00048400
O	-3.44212600	0.38343900	0.00021600
O	2.98382300	-2.22743200	-0.00024700
N	5.42447400	0.37694500	0.00035300
C	0.64249900	1.07921000	-0.00014700
C	0.12688000	-0.27184800	-0.00020500
C	-2.12901800	0.52636900	0.00009500
C	-1.21663600	-0.54600300	-0.00006700
C	-0.32203600	2.13890100	0.00000200
C	-1.65812000	1.87714500	0.00011300
C	2.02426800	1.28888200	-0.00021300
C	2.86938700	0.13943900	-0.00010600
C	-4.02137200	-0.93612100	0.00023300
C	2.34535900	-1.20142500	-0.00018000
C	-5.52137500	-0.76827300	0.00040600
C	4.27255500	0.25520200	0.00008000
H	-1.53730400	-1.57821700	-0.00012100
H	0.03998600	3.15949500	0.00002700
H	-2.39526200	2.67005100	0.00022100
H	2.44184500	2.28533000	-0.00023200
H	-3.67359600	-1.46542700	-0.89085900

H	-3.67339400	-1.46549200	0.89120700
H	-5.99178500	-1.75229500	0.00041600
H	-5.84705200	-0.22692900	0.88909900
H	-5.84724700	-0.22685400	-0.88816900

*** ES of F4 at PBE/6-311++G(d,p)**

O	0.97103200	-1.35375500	-0.00050200
O	-3.48731800	0.39674300	0.00009300
O	3.01342000	-2.25469700	-0.00048200
N	5.47647400	0.38861900	0.00116300
C	0.64357700	1.07873900	-0.00010200
C	0.13096300	-0.26151400	-0.00026400
C	-2.14055400	0.52668300	-0.00001400
C	-1.23233700	-0.54549300	-0.00020200
C	-0.30270100	2.13232500	0.00002900
C	-1.66941700	1.87431800	0.00006600
C	2.06160400	1.28898400	-0.00018200
C	2.90324900	0.14101000	-0.00015800
C	-4.08099700	-0.92753000	0.00030200
C	2.37475100	-1.20512300	-0.00026600
C	-5.58476000	-0.76598300	0.00051900
C	4.30619800	0.25867300	-0.00025000
H	-1.55327000	-1.58632500	-0.00031100
H	0.05526000	3.16346100	0.00007000
H	-2.40094300	2.68364000	0.00014600
H	2.47858300	2.29411600	-0.00010700
H	-3.72453600	-1.46789100	-0.89456900
H	-3.72424800	-1.46772300	0.89515900
H	-6.05020100	-1.76255100	0.00072800
H	-5.92510100	-0.22683500	0.89603600
H	-5.92539000	-0.22707800	-0.89503400

*** ES of F4 at PW6B95D3/6-311++G(d,p)**

O	0.96178800	-1.33875700	-0.00043200
O	-3.43922500	0.38648500	0.00020900
O	2.97664800	-2.22682400	-0.00022200
N	5.41352300	0.37579700	0.00030100
C	0.64027600	1.07558500	-0.00014000
C	0.12715800	-0.26382900	-0.00018900
C	-2.12262900	0.52804900	0.00009400

C	-1.21549400	-0.53824800	-0.00006100
C	-0.31296200	2.12811500	0.00000900
C	-1.65173700	1.86943600	0.00011500
C	2.02616200	1.28137300	-0.00021300
C	2.86601700	0.13637000	-0.00011900
C	-4.01892200	-0.93021500	0.00022800
C	2.33949400	-1.19658300	-0.00018600
C	-5.51333600	-0.76993100	0.00039400
C	4.26043900	0.25062700	0.00004800
H	-1.53647100	-1.56626500	-0.00010700
H	0.04529400	3.14591200	0.00003800
H	-2.38116300	2.66421200	0.00022100
H	2.44245900	2.27367000	-0.00022700
H	-3.66901400	-1.45945700	-0.88634100
H	-3.66882000	-1.45951600	0.88668600
H	-5.97701900	-1.75383600	0.00040400
H	-5.84511400	-0.23354900	0.88598900
H	-5.84530100	-0.23347900	-0.88509000

*** ES of F4 at WB97XD/6-311++G(d,p)**

O	0.96578900	-1.34628200	-0.00052200
O	-3.44007900	0.38273500	0.00020900
O	2.98324200	-2.23216700	-0.00017300
N	5.42399500	0.38775200	0.00035100
C	0.64549600	1.07707700	-0.00016800
C	0.12948600	-0.27243400	-0.00023200
C	-2.12599600	0.52335000	0.00007800
C	-1.21370600	-0.54573500	-0.00009000
C	-0.32003200	2.13489600	-0.00001100
C	-1.65487400	1.87173600	0.00010000
C	2.02532200	1.28545000	-0.00019700
C	2.87211600	0.13535300	-0.00010100
C	-4.02997600	-0.93188900	0.00024000
C	2.34570600	-1.20271700	-0.00028300
C	-5.52894900	-0.75912300	0.00043500
C	4.27142100	0.25682600	0.00017700
H	-1.53570700	-1.57752500	-0.00014600
H	0.03848200	3.15689200	0.00002600
H	-2.38896600	2.66768200	0.00021800
H	2.44316500	2.28174400	-0.00016000

H	-3.68811000	-1.46649700	-0.89084200
H	-3.68788100	-1.46655600	0.89119800
H	-6.00049600	-1.74393100	0.00045200
H	-5.85796700	-0.21858900	0.88974500
H	-5.85818800	-0.21851600	-0.88874900

S3-F5. The coordinates of the optimized structures for the GS and ES of F5 compound

*** GS of F5 at PBE0/6-311++G(d,p)**

O	-0.39588300	1.43174400	-0.00010400
O	4.24234600	0.50032400	0.00014800
O	-2.53319500	1.98265200	-0.00025200
N	-4.49726800	-1.01629600	0.00006500
C	0.34148400	-0.85521500	0.00004900
C	0.61219100	0.52301000	-0.00001300
C	1.43297800	-1.74605900	0.00014000
C	-1.01255000	-1.26297300	0.00001200
C	1.90412300	1.01686900	0.00001700
C	2.95978300	0.10937200	0.00011100
C	2.72237900	-1.27756700	0.00017100
C	-2.01507400	-0.33476800	-0.00008800
C	-1.72241100	1.09178000	-0.00014100
C	-3.38348900	-0.70854800	-0.00014800
H	1.23995300	-2.81339200	0.00018700
H	-1.25181800	-2.32165600	0.00005500
H	2.07307500	2.08796000	-0.00003500
H	3.56910800	-1.95341100	0.00024200
H	4.30793900	1.46139100	0.00010900

*** GS of F5 at APFD/6-311++G(d,p)**

O	-0.39498100	1.43917000	-0.00005000
O	4.24819400	0.49615900	0.00003900
O	-2.54321300	1.97900800	-0.00003000
N	-4.49830400	-1.01868300	-0.00081700
C	0.34241900	-0.85555700	0.00011800
C	0.61238500	0.52596600	0.00002300
C	1.43386800	-1.74659200	0.00018800
C	-1.01133700	-1.26441400	0.00014200
C	1.90399800	1.02081600	-0.00000600
C	2.96151000	0.11134600	0.00006000
C	2.72406400	-1.27662200	0.00015500

C	-2.01536900	-0.33675600	0.00009100
C	-1.72566900	1.09277000	-0.00006300
C	-3.38355500	-0.71161300	0.00020200
H	1.24006500	-2.81418400	0.00026300
H	-1.24989200	-2.32357800	0.00023300
H	2.07177100	2.09248700	-0.00008200
H	3.57190800	-1.95184700	0.00020300
H	4.32039000	1.45715200	-0.00002200

*** GS of F5 at B3LYP/6-311++G(d,p)**

O	-0.39741600	1.44171000	-0.00012400
O	4.26275400	0.49728800	0.00018600
O	-2.54668300	1.99272600	-0.00033600
N	-4.50796100	-1.02979800	0.00037900
C	0.34201500	-0.85508500	0.00002700
C	0.61822100	0.52657400	-0.00002500
C	1.43572000	-1.75044000	0.00012600
C	-1.01605600	-1.26146900	-0.00003400
C	1.91377800	1.01944300	0.00002400
C	2.96940100	0.10680300	0.00012900
C	2.72914500	-1.28286100	0.00017900
C	-2.02499100	-0.33427400	-0.00015200
C	-1.73501800	1.09739900	-0.00016100
C	-3.39488400	-0.71594700	-0.00027900
H	1.24210600	-2.81642200	0.00016300
H	-1.25392400	-2.31911300	-0.00000800
H	2.08598300	2.08881600	-0.00001800
H	3.57335100	-1.96008200	0.00025700
H	4.33497900	1.46072600	0.00015000

*** GS of F5 at BP86/6-311++G(d,p)**

O	-0.39696100	1.45619300	-0.00007100
O	4.28673200	0.49783300	0.00008400
O	-2.56870600	2.00623700	-0.00014500
N	-4.53137700	-1.04320000	-0.00043900
C	0.34315700	-0.86007600	0.00009300
C	0.62149700	0.53300200	0.00000800
C	1.44418700	-1.75958700	0.00017200
C	-1.01533700	-1.27035600	0.00008900
C	1.92407400	1.02763800	0.00000200

C	2.98612400	0.10828100	0.00008200
C	2.74458400	-1.28964400	0.00016600
C	-2.03623700	-0.33620500	0.00001700
C	-1.75366400	1.10033500	-0.00008000
C	-3.40584500	-0.72241100	0.00004100
H	1.24810300	-2.83423000	0.00023600
H	-1.25472500	-2.33686300	0.00015600
H	2.09807000	2.10584000	-0.00006500
H	3.59584700	-1.97230700	0.00022400
H	4.34859900	1.47199300	0.00002800

*** GS of F5 at CAM-B3LYP/6-311++G(d,p)**

O	-0.39579200	1.43323400	-0.00010600
O	4.24542800	0.49717700	0.00015000
O	-2.53307500	1.98084300	-0.00026700
N	-4.49535400	-1.01623100	0.00009200
C	0.34262000	-0.85118300	0.00004900
C	0.61579100	0.52035300	-0.00001300
C	1.43037300	-1.74341200	0.00014200
C	-1.01720700	-1.25776600	0.00001000
C	1.90704900	1.01392800	0.00001700
C	2.95695300	0.10646400	0.00011200
C	2.71876200	-1.27774400	0.00017300
C	-2.01393500	-0.33501900	-0.00009100
C	-1.72051600	1.09378800	-0.00013500
C	-3.38763100	-0.70960700	-0.00016600
H	1.23628800	-2.80886800	0.00018800
H	-1.25512900	-2.31503100	0.00005100
H	2.07674300	2.08312600	-0.00003500
H	3.56355800	-1.95329200	0.00024500
H	4.31997700	1.45883800	0.00010900

*** GS of F5 at M06/6-311++G(d,p)**

O	-0.39628000	1.43179000	-0.00010500
O	4.23888500	0.49691100	0.00015100
O	-2.53578300	1.97812800	-0.00025900
N	-4.49292400	-1.01851300	0.00009500
C	0.34287700	-0.85115100	0.00004700
C	0.61338100	0.52504500	-0.00001400
C	1.43148300	-1.74250900	0.00013900

C	-1.00966900	-1.25878700	0.00000700
C	1.90424600	1.01596800	0.00001800
C	2.95705200	0.10854300	0.00011200
C	2.71909100	-1.27638800	0.00017200
C	-2.01194400	-0.33435700	-0.00009400
C	-1.72420800	1.09173500	-0.00013900
C	-3.38004600	-0.71013200	-0.00016700
H	1.23310400	-2.80973900	0.00018400
H	-1.24637200	-2.31939400	0.00004700
H	2.07513900	2.08759200	-0.00003300
H	3.56837900	-1.95011600	0.00024300
H	4.31205600	1.45882600	0.00010900

*** GS of F5 at M06-2X/6-311++G(d,p)**

O	-0.39630900	1.43373000	-0.00013800
O	4.24729800	0.50137100	0.00022400
O	-2.53485000	1.97560300	-0.00041300
N	-4.50410500	-1.00483800	0.00071700
C	0.34450400	-0.85454100	0.00000000
C	0.61389500	0.52060500	-0.00003600
C	1.43442700	-1.74708900	0.00010500
C	-1.01813800	-1.26625800	-0.00008600
C	1.90700100	1.01781700	0.00003400
C	2.96039900	0.10962500	0.00014600
C	2.72482900	-1.27829800	0.00018100
C	-2.01288600	-0.34030000	-0.00022100
C	-1.71957100	1.09387000	-0.00018400
C	-3.39233400	-0.70795600	-0.00042800
H	1.23923200	-2.81290700	0.00012900
H	-1.25644500	-2.32438100	-0.00008100
H	2.07382700	2.08801900	0.00000300
H	3.57275200	-1.95047000	0.00026500
H	4.31749700	1.46312900	0.00020000

*** GS of F5 at PBE/6-311++G(d,p)**

O	-0.39635600	1.45317900	-0.00008000
O	4.28025300	0.49825400	0.00012600
O	-2.56483100	2.00344400	-0.00027400
N	-4.52658700	-1.04025800	-0.00003600
C	0.34278700	-0.85963600	0.00006900

C	0.61977700	0.53205500	-0.00000100
C	1.44266600	-1.75748100	0.00015200
C	-1.01383100	-1.26960500	0.00003200
C	1.92105900	1.02595700	0.00001300
C	2.98266900	0.10865300	0.00010200
C	2.74142600	-1.28772400	0.00017000
C	-2.03320900	-0.33603200	-0.00006200
C	-1.75007800	1.09849000	-0.00006900
C	-3.40115800	-0.72057700	-0.00014900
H	1.24657200	-2.83168700	0.00020000
H	-1.25314000	-2.33575100	0.00006200
H	2.09446500	2.10390400	-0.00004300
H	3.59265300	-1.96976500	0.00023400
H	4.34038600	1.47149400	0.00007700

*** GS of F5 at PW6B95D3/6-311++G(d,p)**

O	-0.39581500	1.42902000	-0.00012100
O	4.23619900	0.50114800	0.00018800
O	-2.53208200	1.97603900	-0.00034600
N	-4.48873400	-1.01132100	0.00042000
C	0.34207600	-0.85349500	0.00002400
C	0.61264400	0.52029300	-0.00002500
C	1.43094100	-1.74217300	0.00012300
C	-1.01020900	-1.26030800	-0.00004100
C	1.90072100	1.01441600	0.00002500
C	2.95278700	0.10910200	0.00013000
C	2.71723800	-1.27420500	0.00017800
C	-2.00998000	-0.33577600	-0.00016000
C	-1.72017000	1.08879100	-0.00015400
C	-3.37743100	-0.70765800	-0.00030600
H	1.23842400	-2.80452500	0.00015700
H	-1.24752800	-2.31430100	-0.00002200
H	2.06851600	2.08060800	-0.00001600
H	3.56077400	-1.94605500	0.00025600
H	4.30284600	1.45993600	0.00015400

*** GS of F5 at WB97XD/6-311++G(d,p)**

O	-0.39465600	1.43376500	-0.00011600
O	4.24524400	0.49735100	0.00017400
O	-2.53022100	1.98347900	-0.00031700

N	-4.49967500	-1.01560800	0.00028600
C	0.34200100	-0.85305400	0.00003400
C	0.61336000	0.52069200	-0.00002100
C	1.43107100	-1.74578700	0.00013100
C	-1.01859800	-1.26207200	-0.00001900
C	1.90658700	1.01586000	0.00002200
C	2.95921300	0.10789800	0.00012300
C	2.72071600	-1.27880300	0.00017600
C	-2.01392200	-0.33522100	-0.00013000
C	-1.71827800	1.09543300	-0.00014900
C	-3.38911500	-0.70861000	-0.00024500
H	1.23745400	-2.81206800	0.00017000
H	-1.25743700	-2.31990300	0.00001100
H	2.07493300	2.08590200	-0.00002300
H	3.56519100	-1.95579100	0.00025200
H	4.31644300	1.45634900	0.00013700

*** ES of F5 at PBE0/6-311++G(d,p)**

O	0.39537400	-1.44669600	-0.00040400
O	-4.23466200	-0.52089400	0.00033400
O	2.53202700	-1.98434000	-0.00024700
N	4.49954400	1.00534200	0.00050000
C	-0.33224300	0.88343000	-0.00008700
C	-0.60790700	-0.53061300	-0.00014500
C	-1.45435700	1.76018600	0.00007100
C	1.00040200	1.32172000	-0.00014100
C	-1.88938500	-1.02413600	0.00000800
C	-2.96380300	-0.12571000	0.00018300
C	-2.73485400	1.27656500	0.00019600
C	2.02618600	0.33181900	-0.00012000
C	1.73047800	-1.07419200	-0.00028700
C	3.38139000	0.68328400	0.00005800
H	-1.27439700	2.82907700	0.00009800
H	1.24577700	2.37461600	-0.00009500
H	-2.05140500	-2.09660100	-0.00003800
H	-3.59110700	1.94095300	0.00031400
H	-4.30303700	-1.48410600	0.00033400

*** ES of F5 at APFD/6-311++G(d,p)**

O	0.39363100	-1.45344100	-0.00019900

O	-4.24217500	-0.51444500	0.00013300
O	2.54144900	-1.98169900	-0.00014900
N	4.50166000	1.00804400	-0.00050600
C	-0.33318100	0.88283800	0.00005600
C	-0.60877500	-0.53368200	-0.00004300
C	-1.45367800	1.76021800	0.00014600
C	1.00025300	1.32194200	0.00006300
C	-1.89041900	-1.02845900	-0.00000700
C	-2.96598300	-0.12758500	0.00010100
C	-2.73574500	1.27566600	0.00016700
C	2.02721200	0.33346300	0.00008800
C	1.73385800	-1.07523800	-0.00000400
C	3.38247100	0.68657900	0.00021700
H	-1.27257300	2.82932200	0.00020500
H	1.24460700	2.37539300	0.00010400
H	-2.05180000	-2.10142700	-0.00008000
H	-3.59261600	1.94003300	0.00023500
H	-4.31855800	-1.47740400	0.00009500

*** ES of F5 at B3LYP/6-311++G(d,p)**

O	0.39564600	-1.45617300	-0.00022800
O	-4.25633800	-0.51581500	0.00018600
O	2.54455400	-1.99743400	-0.00012500
N	4.51052500	1.02187400	-0.00018300
C	-0.33349100	0.88303800	0.00001200
C	-0.61482100	-0.53381000	-0.00006300
C	-1.45536600	1.76453300	0.00012900
C	1.00576100	1.31860200	0.00000900
C	-1.90072800	-1.02654000	0.00000100
C	-2.97413300	-0.12267700	0.00012100
C	-2.74119700	1.28248200	0.00017800
C	2.03802500	0.32911400	-0.00001000
C	1.74393500	-1.08066900	-0.00018300
C	3.39404400	0.69084600	0.00013800
H	-1.27443900	2.83209800	0.00018500
H	1.25107300	2.37019800	0.00008300
H	-2.06649100	-2.09723600	-0.00005800
H	-3.59441600	1.94884800	0.00026500
H	-4.33246900	-1.48115900	0.00015500

*** ES of F5 at BP86/6-311++G(d,p)**

O	0.38965200	-1.46393600	-0.00006600
O	-4.29152100	-0.50888500	0.00001000
O	2.55447600	-2.01428300	-0.00002900
N	4.54557100	1.01891700	-0.00074600
C	-0.33618500	0.88730900	0.00013700
C	-0.62168600	-0.53072200	0.00002800
C	-1.44905700	1.76991200	0.00023400
C	1.02153100	1.32757400	0.00015600
C	-1.91948800	-1.03141700	0.00003200
C	-2.99224900	-0.12398700	0.00005700
C	-2.75428700	1.28629200	0.00015200
C	2.05209600	0.33381500	0.00006600
C	1.75435700	-1.08111500	-0.00001200
C	3.41407800	0.68937600	0.00002500
H	-1.26855800	2.84662000	0.00031300
H	1.26703900	2.38818800	0.00025500
H	-2.08249300	-2.11154200	-0.00002100
H	-3.61016800	1.96357600	0.00016600
H	-4.36034100	-1.48463400	-0.00005300

*** ES of F5 at CAM-B3LYP/6-311++G(d,p)**

O	0.39717300	-1.45203000	-0.00028500
O	-4.23073300	-0.52082700	0.00024800
O	2.53794000	-1.98200300	-0.00024900
N	4.49102500	1.01501500	0.00024200
C	-0.33058500	0.88112700	-0.00002400
C	-0.61020600	-0.53590600	-0.00008800
C	-1.45997200	1.76071600	0.00010300
C	0.99316600	1.31673500	-0.00007100
C	-1.88736400	-1.02426600	0.00000800
C	-2.95974400	-0.12363900	0.00014900
C	-2.73246000	1.27839400	0.00018500
C	2.02447500	0.32975500	-0.00008200
C	1.73516300	-1.07621000	-0.00018100
C	3.38071400	0.68970800	0.00000500
H	-1.27803300	2.82757000	0.00013700
H	1.23749700	2.36807800	-0.00004500
H	-2.05334800	-2.09436600	-0.00004500
H	-3.58957100	1.93885000	0.00028100

H	-4.30788400	-1.48483000	0.00023100

*** ES of F5 at M06/6-311++G(d,p)**

O	0.39695900	-1.44746600	-0.00019000
O	-4.23163300	-0.51853600	0.00012400
O	2.53707700	-1.97862600	-0.00013900
N	4.49423100	1.00800500	-0.00059400
C	-0.33329500	0.87892900	0.00006100
C	-0.60873500	-0.53336900	-0.00004000
C	-1.45394200	1.75671500	0.00014800
C	0.99571900	1.31786700	0.00007700
C	-1.88865900	-1.02327200	-0.00001200
C	-2.96161400	-0.12480300	0.00009400
C	-2.73157400	1.27553500	0.00016400
C	2.02242800	0.33207200	0.00010900
C	1.73309000	-1.07601100	0.00001700
C	3.37682900	0.68698800	0.00025600
H	-1.26826500	2.82554700	0.00020900
H	1.23743500	2.37268100	0.00012200
H	-2.05277200	-2.09624300	-0.00009000
H	-3.59015500	1.93787900	0.00023100
H	-4.30656300	-1.48278400	0.00008700

*** ES of F5 at M06-2X/6-311++G(d,p)**

O	0.39674200	-1.45392800	-0.00041100
O	-4.23046900	-0.52369200	0.00038900
O	2.53838200	-1.97784700	-0.00034100
N	4.49922700	1.00509200	0.00108900
C	-0.33206600	0.88414700	-0.00013000
C	-0.60792500	-0.53792900	-0.00015500
C	-1.46360100	1.76451100	0.00005400
C	0.99315300	1.32523100	-0.00024500
C	-1.88681400	-1.02933200	0.00002400
C	-2.96272800	-0.12687900	0.00021100
C	-2.73818000	1.28008100	0.00021300
C	2.02259300	0.33506300	-0.00027100
C	1.73513600	-1.07554800	-0.00039000
C	3.38484900	0.68898100	-0.00019300
H	-1.28021900	2.83167200	0.00006800
H	1.23690100	2.37771400	-0.00023100

H	-2.05085000	-2.10029400	-0.00000400
H	-3.59869500	1.93685300	0.00034800
H	-4.30546000	-1.48780200	0.00039100

*** ES of F5 at PBE/6-311++G(d,p)**

O	0.38944900	-1.46092200	-0.00011700
O	-4.28491700	-0.50964800	0.00012800
O	2.55091400	-2.01060200	-0.00005800
N	4.54089500	1.01453100	-0.00010700
C	-0.33598300	0.88649900	-0.00000200
C	-0.61983400	-0.52942000	-0.00005400
C	-1.44771000	1.76745400	0.00016200
C	1.02012400	1.32704900	0.00000700
C	-1.91624300	-1.02979300	-0.00000400
C	-2.98849200	-0.12435700	0.00007200
C	-2.75130900	1.28411300	0.00018900
C	2.04846200	0.33420900	-0.00003600
C	1.75025500	-1.07877800	-0.00014700
C	3.40898200	0.68803700	-0.00011200
H	-1.26732300	2.84373100	0.00027900
H	1.26511500	2.38733400	0.00004400
H	-2.07847700	-2.10963800	-0.00004100
H	-3.60719200	1.96070500	0.00030300
H	-4.35145600	-1.48454900	0.00008600

*** ES of F5 at PW6B95D3/6-311++G(d,p)**

O	0.39501700	-1.44518400	-0.00020700
O	-4.22713300	-0.52161400	0.00013600
O	2.53154800	-1.97838500	-0.00015300
N	4.48941300	1.00322200	-0.00053300
C	-0.33227600	0.88167100	0.00005500
C	-0.60786600	-0.52916900	-0.00004600
C	-1.45313900	1.75649500	0.00014500
C	0.99657300	1.31898500	0.00006500
C	-1.88526800	-1.02191100	-0.00001200
C	-2.95668400	-0.12533000	0.00010000
C	-2.72971600	1.27376400	0.00016500
C	2.02106200	0.33184200	0.00010200
C	1.72937200	-1.07121800	0.00001000
C	3.37446000	0.68311900	0.00024300

H	-1.27344700	2.82031900	0.00020300
H	1.24012100	2.36711500	0.00010400
H	-2.04677500	-2.08928500	-0.00008900
H	-3.58297300	1.93371800	0.00023400
H	-4.29738500	-1.48244500	0.00010200

*** ES of F5 at WB97XD/6-311++G(d,p)**

O	0.39615000	-1.45213800	-0.00032200
O	-4.23069300	-0.52156700	0.00028800
O	2.53491900	-1.98387100	-0.00027200
N	4.49620200	1.01235600	0.00044600
C	-0.32998100	0.88344700	-0.00005200
C	-0.60778800	-0.53649700	-0.00010700
C	-1.46103200	1.76321100	0.00008800
C	0.99423700	1.32194700	-0.00011100
C	-1.88701200	-1.02640000	0.00001200
C	-2.96160100	-0.12538400	0.00016600
C	-2.73471200	1.27907700	0.00019100
C	2.02454400	0.33083400	-0.00012500
C	1.73297900	-1.07722800	-0.00024000
C	3.38235200	0.68839400	-0.00003000
H	-1.27982200	2.83089600	0.00011700
H	1.23878800	2.37418300	-0.00008400
H	-2.05172400	-2.09729100	-0.00003400
H	-3.59173200	1.94066900	0.00029600
H	-4.30384400	-1.48275900	0.00027600

S3-F6. The coordinates of the optimized structures for the GS and ES of F6 compound

*** GS of F6 at PBE0/6-311++G(d,p)**

O	-0.60519600	1.40003400	0.20379800
O	-2.63875000	2.21344700	0.31268800
O	-4.19925800	-1.69257900	-0.30702000
N	3.94586100	0.08054800	0.00938900
N	-4.76294800	0.49075800	0.15582300
N	-5.94523300	0.13305900	0.11783900
N	-7.04565000	-0.07876200	0.10737600
C	2.63316200	-0.23049100	-0.05578800
C	4.40395700	1.42323100	0.34712500
C	4.99395600	-0.90077200	-0.25042600

C	1.63604200	0.76010300	0.10865400
C	0.30772500	0.41113700	0.04611700
C	-0.12241500	-0.91157700	-0.17997100
C	2.20557700	-1.57629300	-0.29004400
C	0.87870800	-1.89464500	-0.34730900
C	4.53113800	2.33816500	-0.86303500
C	5.40688400	-1.68283800	0.98841600
C	-1.49869900	-1.15301200	-0.21404100
C	-2.42898300	-0.15005000	-0.04035400
C	-1.97914300	1.21392400	0.16872800
C	-3.83867600	-0.54976600	-0.08636800
H	5.37526300	1.31456500	0.83675300
H	3.73668900	1.85451900	1.09715600
H	5.85094700	-0.35038700	-0.64746400
H	4.67422700	-1.57183800	-1.05047200
H	1.88270800	1.80088800	0.26504700
H	2.93585200	-2.36523900	-0.40499700
H	0.57832100	-2.92382100	-0.51658000
H	5.23408300	1.92523600	-1.59177800
H	4.90187800	3.31860500	-0.55220800
H	3.56831300	2.47862600	-1.36078500
H	5.76659500	-1.01099300	1.77258500
H	4.57123300	-2.26021500	1.39220100
H	6.21440100	-2.37684900	0.74003900
H	-1.86449100	-2.16221600	-0.37844200

*** ES of F6 at PBE0/6-311++G(d,p)**

O	-0.60688700	1.38808600	0.18428000
O	-2.63858000	2.19058500	0.29902400
O	-4.21783000	-1.70235900	-0.27286400
N	3.95598300	0.09489400	0.01320800
N	-4.76518200	0.50414000	0.14511900
N	-5.95134200	0.16986400	0.12161500
N	-7.06282900	-0.02238100	0.12225800
C	2.63795600	-0.24025900	-0.05766800
C	4.39506100	1.43600800	0.36516200
C	5.01235500	-0.86813000	-0.25520800
C	1.63060200	0.74476700	0.10163800
C	0.30321100	0.38818500	0.03281300
C	-0.11825000	-0.93950500	-0.18873700

C	2.22856600	-1.58520100	-0.28951300
C	0.89621700	-1.91323900	-0.34763400
C	4.52177300	2.35635800	-0.84678200
C	5.42990600	-1.65257200	0.98655000
C	-1.51198300	-1.20822000	-0.22970400
C	-2.43845700	-0.17618700	-0.04524000
C	-1.97880100	1.18939500	0.15596200
C	-3.84798100	-0.54196000	-0.07520500
H	5.36728100	1.33285300	0.85396400
H	3.71476600	1.85722500	1.10791900
H	5.86541400	-0.30311300	-0.63965000
H	4.69570800	-1.54000700	-1.05511300
H	1.86848100	1.78754400	0.26042500
H	2.96345600	-2.37039100	-0.40250900
H	0.60631000	-2.94506900	-0.51405700
H	5.23197200	1.95219600	-1.57221000
H	4.88503000	3.33382300	-0.51952000
H	3.55884600	2.49252300	-1.34420700
H	5.78662200	-0.98183900	1.77193700
H	4.59793100	-2.23871700	1.38332300
H	6.24216800	-2.33520900	0.72435800
H	-1.87508200	-2.21457500	-0.39216900

S3-F7. The coordinates of the optimized structures for the GS and ES of F7 compound

*** GS of F7 at PBE0/6-311++G(d,p)**

O	0.80184600	2.12536300	-0.19881400
O	2.17466600	3.84986600	-0.14542400
O	5.16352500	-2.39811500	0.49919200
O	3.97010100	-0.98894700	1.77344800
N	-2.41198900	-1.39783700	-0.33197600
C	1.60004400	-0.13111300	-0.43359500
C	2.95198100	0.36129200	-0.46440200
C	0.55479400	0.79104800	-0.29337000
C	-1.11586900	-0.93500700	-0.34430600
C	1.23641400	-1.48582200	-0.53832200
C	-0.77996300	0.41714500	-0.25216600
C	4.09777800	-0.58330600	-0.59583200
C	-0.07774600	-1.88297100	-0.49344400
C	3.15377900	1.70445700	-0.37063100
C	2.07684800	2.64164400	-0.23277600

C	-3.59141400	-0.70845900	-0.03326800
C	4.42826900	-1.40360100	0.68810200
C	-4.76078300	-1.05916300	-0.71805100
C	-3.65834800	0.26614600	0.96792800
C	-5.96608300	-0.44145100	-0.41453600
C	-4.86694100	0.89109900	1.25110500
C	-6.02677300	0.54606200	0.56465800
H	2.01001300	-2.23774100	-0.64663400
H	-1.53232100	1.19063100	-0.17481800
H	5.00421500	-0.02564700	-0.84988900
H	3.92515800	-1.28989400	-1.41222400
H	-0.32947900	-2.93605400	-0.56814400
H	4.14989000	2.12969100	-0.39719300
H	-2.53816400	-2.32926000	-0.69808900
H	-4.71688100	-1.81895900	-1.49264100
H	-2.77597900	0.51688600	1.54460400
H	-6.86162400	-0.72869900	-0.95613100
H	-4.90086500	1.64514200	2.03100900
H	-6.96705900	1.03541600	0.79420500

*** ES of F7 at PBE0/6-311++G(d,p)**

O	1.18725800	2.36845200	-0.02015700
O	2.82187600	3.71483200	0.64223300
O	4.27009800	-3.17371700	0.27211400
O	3.41229100	-1.74630600	1.76953900
N	-2.60515900	-0.20919200	-1.34626700
C	1.56406600	0.03567200	-0.57296000
C	2.93452200	0.20056200	-0.29731500
C	0.70219900	1.15803300	-0.41949100
C	-1.21046800	-0.14406900	-1.07236900
C	0.95186500	-1.18347700	-0.99531100
C	-0.65248900	1.08484600	-0.66041100
C	3.88629400	-0.94048400	-0.45284400
C	-0.40352600	-1.26771800	-1.24488200
C	3.39145600	1.46157500	0.12670800
C	2.54972300	2.56658600	0.28076000
C	-3.57188100	-0.23453400	-0.42153900
C	3.83488100	-2.05152100	0.63146300
C	-4.93404300	-0.22571900	-0.84138600
C	-3.25468600	-0.26851200	0.96620200

C	-5.93042100	-0.24258200	0.09854600
C	-4.27426400	-0.28536200	1.88648800
C	-5.60953700	-0.27023800	1.46524300
H	1.56679600	-2.06794900	-1.11535400
H	-1.27103900	1.96674100	-0.53795000
H	4.91400400	-0.55860600	-0.43936700
H	3.75664100	-1.42866700	-1.42510300
H	-0.84698000	-2.20578800	-1.56290600
H	4.44018800	1.61949300	0.34930800
H	-2.90464700	-0.20626100	-2.31764100
H	-5.16067100	-0.20069600	-1.90124000
H	-2.21596100	-0.28770700	1.26902200
H	-6.96812500	-0.23395100	-0.21188900
H	-4.04394200	-0.31365700	2.94456300
H	-6.40448400	-0.28306300	2.20118800

S3-F8. The coordinates of the optimized structures for the GS and ES of F8 compound

*** GS of F8 at PBE0/6-311++G(d,p)**

O	4.07468200	0.23298700	0.09735300
O	-0.03295600	1.53781900	-0.01377000
O	3.31338100	-1.86236200	-0.06835300
O	-4.61777600	0.43896300	0.00815600
O	2.03586900	2.25187300	-0.03296000
C	-0.65859700	-0.76645700	0.00099900
C	1.71191300	-0.13569200	-0.00480500
C	-1.01738800	0.59838500	-0.00448400
C	0.70879800	-1.07841400	-0.00132900
C	3.15708300	-0.61471300	0.00724800
C	-1.71454700	-1.71112300	0.00996900
C	1.33637000	1.25860900	-0.01586400
C	-2.32488100	1.02483500	-0.00235000
C	-3.40468900	0.08251500	0.00629500
C	-3.02281600	-1.31531900	0.01265400
H	1.02086300	-2.11932700	-0.00035800
H	-1.46063600	-2.76843400	0.01499100
H	-2.54930500	2.08675500	-0.00768900
H	-3.82399500	-2.04898700	0.01963900

*** ES of F8 at PBE0/6-311++G(d,p)**

O	-3.71236700	0.57652700	1.13266000

O	0.02178700	-1.52972600	-0.03353100
O	-3.66958600	0.81352200	-1.09015000
O	4.60438200	-0.50963700	0.01266500
O	-2.11112100	-2.16372500	-0.04219300
C	0.67055600	0.81387200	0.00080300
C	-1.68101100	0.18746600	0.00114700
C	0.99388700	-0.56576600	-0.01204600
C	-0.70412200	1.19786200	0.00023500
C	-3.14516800	0.54758200	0.01638700
C	1.76388400	1.72372900	0.01553500
C	-1.34518200	-1.18837100	-0.02179200
C	2.29560700	-1.01014200	-0.00728400
C	3.41015200	-0.09285000	0.00836300
C	3.07347200	1.30708300	0.01840800
H	-0.98134300	2.24538500	0.00854300
H	1.53597200	2.78652300	0.02429600
H	2.50053300	-2.07588600	-0.01633200
H	3.88761800	2.02549700	0.02934600

S3-F9. The coordinates of the optimized structures for the GS and ES of F9 compound

*** GS of F9 at PBE0/6-311++G(d,p)**

O	0.00167500	2.34759700	0.12291000
O	-1.62006300	3.84128100	0.17429100
O	-3.80013300	-2.73096400	-0.02041000
O	-2.78136200	-1.46903900	1.52071200
N	3.72416800	-0.58373200	0.08206400
C	-0.41595900	0.02533600	-0.35201700
C	-1.81082500	0.32566700	-0.47481200
C	0.46318400	1.07718900	-0.04601700
C	2.38899400	-0.38116700	-0.05816800
C	1.82521800	0.89984300	0.09959100
C	0.16211200	-1.24730900	-0.51106100
C	1.51219800	-1.45590600	-0.37188500
C	-2.79883400	-0.75536200	-0.79376500
C	-2.23499400	1.60629800	-0.30655100
C	-1.32686900	2.67590600	0.00482100
C	4.28741500	-1.90813100	-0.08560800
C	4.59632800	0.52746900	0.39930500
C	-3.09779800	-1.66408500	0.37477500

H	2.42948100	1.76547200	0.33509200
H	-0.46803200	-2.09651200	-0.75297900
H	1.90404500	-2.45537200	-0.50500000
H	-2.46441400	-1.37083800	-1.63389100
H	-3.75303100	-0.31669600	-1.10148900
H	-3.27895600	1.87952200	-0.39658400
H	4.10877900	-2.29971300	-1.09348800
H	3.87526800	-2.61810800	0.64034100
H	5.36337700	-1.85578000	0.06898800
H	4.56193000	1.30114300	-0.37669600
H	5.62046100	0.16662100	0.47158500
H	4.32943800	0.98800200	1.35765900
H	-3.99949500	-3.26709000	0.76034600

*** ES of F9 at PBE0/6-311++G(d,p)**

O	0.06261300	2.36764000	0.11936900
O	-1.54838900	3.89847600	0.17944500
O	-3.90830700	-2.68062700	-0.05412000
O	-2.83553600	-1.49737300	1.51008200
N	3.73018600	-0.61641200	0.07580100
C	-0.41452400	0.02474900	-0.33250800
C	-1.81170400	0.32421300	-0.47404800
C	0.48198400	1.08453600	-0.04079400
C	2.38734600	-0.42111800	-0.05538000
C	1.83629100	0.87831200	0.09291100
C	0.15551100	-1.26633800	-0.46566400
C	1.50901000	-1.49470900	-0.33776100
C	-2.80312900	-0.73494400	-0.79640700
C	-2.19703800	1.65784700	-0.29268900
C	-1.30054900	2.70538200	0.00457500
C	4.29342400	-1.93801400	-0.08903400
C	4.61615600	0.48762600	0.37787200
C	-3.15760800	-1.64922400	0.35797100
H	2.45879000	1.73575000	0.31092700
H	-0.49154900	-2.10912200	-0.68003900
H	1.88728300	-2.50172900	-0.44996700
H	-2.47699500	-1.37472500	-1.62741400
H	-3.74551500	-0.28608400	-1.13022700
H	-3.23930800	1.94594700	-0.38039200
H	4.07192200	-2.33435900	-1.08635000

H	3.88646600	-2.63208500	0.65535900
H	5.37166200	-1.88562600	0.03529400
H	4.57719700	1.24920800	-0.40893300
H	5.63465400	0.11559400	0.45031100
H	4.34687300	0.95783500	1.32973400
H	-4.12686200	-3.22055200	0.71860100

S3-F10. The coordinates of the optimized structures for the GS and ES of F10 compound

*** GS of F10 at PBE0/6-311++G(d,p)**

O	2.85943100	0.18925400	1.03759600
O	-2.95819500	2.27154600	-0.45047600
O	4.99735100	1.44358800	-0.24368200
O	2.88594300	-2.53829400	0.46330400
O	1.65689400	0.51188800	-0.85386400
O	-2.41117300	4.40088800	-0.62487200
N	3.78382100	-0.43633200	0.26287400
N	-4.47024700	-2.21204200	-0.20927100
C	-1.45477100	0.63783600	0.47933800
C	-0.48885900	1.67614500	0.67184400
C	5.66878500	-0.78743500	-1.02629700
C	4.96002400	-2.12449200	-0.78815200
C	-2.68956900	0.98450400	-0.09434800
C	0.84992200	1.36840500	1.27556600
C	-3.50085100	-1.28825500	0.01074300
C	4.83911600	0.25357100	-0.32227900
C	3.74553200	-1.80838500	0.04393700
C	-1.27792600	-0.71715600	0.81461500
C	-3.69314200	0.06550800	-0.32812800
C	-2.25639500	-1.65443900	0.59382000
C	-0.79103800	2.95092000	0.31081300
C	1.76943900	0.66030000	0.32158100
C	-2.05970000	3.29459700	-0.27297400
C	-4.25783400	-3.59955700	0.15080500
C	-5.73036300	-1.81380800	-0.80096800
H	5.73505700	-0.52022500	-2.08274300
H	6.68022300	-0.75963600	-0.61576000
H	4.63057800	-2.60479500	-1.71154200
H	5.57480100	-2.84434800	-0.24403500

H	1.35698600	2.29177600	1.57230700
H	0.75784400	0.76647400	2.18441900
H	-0.34627800	-1.04391800	1.26429200
H	-4.61384200	0.41836600	-0.77266000
H	-2.06794700	-2.68276900	0.87156400
H	-0.09116700	3.76647500	0.44331100
H	-3.40922600	-4.03246700	-0.39063800
H	-4.07977300	-3.71615200	1.22581400
H	-5.14770900	-4.17053500	-0.10680700
H	-6.37018400	-2.68874500	-0.89755200
H	-6.25248800	-1.07706700	-0.17931000
H	-5.58811100	-1.38432900	-1.79942400

*** ES of F10 at PBE0/6-311++G(d,p)**

O	2.88867900	0.20125800	1.03801900
O	-3.02110100	2.26773200	-0.42956300
O	5.02720200	1.45843600	-0.24118100
O	2.92524500	-2.52779100	0.46727100
O	1.69480200	0.50216200	-0.86230200
O	-2.48150700	4.41550800	-0.61861100
N	3.81974500	-0.42385300	0.27186900
N	-4.49421400	-2.21881500	-0.20245500
C	-1.46314000	0.62860700	0.46646100
C	-0.48372900	1.66036600	0.67435000
C	5.70605400	-0.77152600	-1.01808200
C	4.99945300	-2.10964600	-0.78117700
C	-2.71753700	0.98830700	-0.08613700
C	0.84691300	1.35585900	1.26222300
C	-3.50622300	-1.30582500	0.01818000
C	4.87170800	0.26738400	-0.31613900
C	3.78397600	-1.79466400	0.05015300
C	-1.27581000	-0.74184400	0.77191600
C	-3.71126100	0.06035500	-0.30406000
C	-2.25734200	-1.68731300	0.56435500
C	-0.83350300	2.95901000	0.28922400
C	1.79253600	0.66281700	0.31353400
C	-2.08556900	3.30689300	-0.26093100
C	-4.28865700	-3.60987100	0.13458200
C	-5.76046900	-1.81981800	-0.77907700
H	5.77491200	-0.50440400	-2.07437700

H	6.71630100	-0.74153100	-0.60466800
H	4.67126900	-2.58997500	-1.70504100
H	5.61484000	-2.82902100	-0.23708500
H	1.35074600	2.27797900	1.57396800
H	0.77995700	0.73782400	2.16742600
H	-0.32978400	-1.06744700	1.18937900
H	-4.64448500	0.40916500	-0.72542600
H	-2.05751800	-2.71956000	0.81771600
H	-0.13237000	3.77795100	0.41036400
H	-3.45331600	-4.03053300	-0.43700800
H	-4.06750500	-3.72350600	1.20167300
H	-5.18945500	-4.17120100	-0.09805600
H	-6.39654500	-2.69528100	-0.87851000
H	-6.26905900	-1.08851400	-0.14118900
H	-5.61766000	-1.37625400	-1.77037800

S3-F11. The coordinates of the optimized structures for the GS and ES of F11 compound

*** GS of F11 at PBE0/6-311++G(d,p)**

S	-5.83687700	-0.36197400	-0.00042100
O	-0.14186900	-1.46350400	0.00040100
O	-2.24903000	-2.11748100	0.00022200
N	4.47429800	-0.40295100	0.00140500
N	-3.19589500	0.47281000	-0.00022600
C	0.46251200	0.86449400	0.00040800
C	0.81742600	-0.49365500	0.00050400
C	3.17933200	0.00056300	0.00079800
C	-0.91916200	1.22581000	0.00014800
C	2.12461100	-0.93386400	0.00058500
C	1.52758500	1.78667700	0.00027000
C	2.83879900	1.38197500	0.00037200
C	-1.84967800	0.21713200	0.00001300
C	-1.33208700	2.65888700	-0.00005600
C	-1.47486200	-1.18804800	0.00021400
C	5.54761200	0.57107000	-0.00134000
C	4.79329600	-1.81558000	-0.00100100
C	-4.31014700	0.05367800	-0.00029600
H	2.30445500	-2.00026700	0.00045400
H	1.30938400	2.84866200	-0.00002600

H	3.61784300	2.13256500	0.00004600
H	-0.93540600	3.17115400	-0.88175700
H	-0.93375000	3.17196900	0.88040100
H	-2.41675400	2.75726400	0.00086800
H	5.51390100	1.20742300	-0.89277300
H	6.50054300	0.04552200	0.00130600
H	5.51254500	1.21327100	0.88573700
H	5.87470100	-1.93596800	0.00130500
H	4.39670200	-2.31626400	-0.89187500
H	4.39282500	-2.31971000	0.88609400

*** ES of F11 at PBE0/6-311++G(d,p)**

S	5.94359400	-0.03780200	-0.00108800
O	0.03421200	-1.58899700	-0.00123600
O	2.10289500	-2.37013200	-0.00359100
N	-4.50720700	-0.26243400	-0.00046500
N	3.17417000	0.15766600	-0.00002400
C	-0.42418800	0.80245700	0.00163000
C	-0.85723700	-0.55108800	0.00042100
C	-3.19423000	0.08785800	0.00064800
C	0.95650300	1.10747500	0.00167300
C	-2.18118000	-0.90739300	0.00030200
C	-1.45663300	1.78324800	0.00265200
C	-2.78936000	1.44845100	0.00192300
C	1.84384500	-0.01017000	0.00019200
C	1.45084800	2.50997800	0.00364300
C	1.39792700	-1.37716700	-0.00172200
C	-5.53560900	0.75602000	-0.01317000
C	-4.90010700	-1.65602700	0.01056300
C	4.35482400	0.04552000	-0.00045700
H	-2.42291300	-1.96180300	-0.00212200
H	-1.17964200	2.83091000	0.00440200
H	-3.52891000	2.23808600	0.00401000
H	1.10000200	3.06194500	0.88582200
H	1.09772300	3.06522400	-0.87553100
H	2.54084000	2.54565400	0.00232500
H	-5.47544200	1.38972200	0.87927000
H	-6.51108100	0.27651700	-0.03164200
H	-5.44542700	1.39593000	-0.89816000
H	-5.98532600	-1.71869700	0.02657600

H	-4.51012900	-2.16957700	0.89636900
H	-4.53521100	-2.17765700	-0.88164600

S3-F12. The coordinates of the optimized structures for the GS and ES of F12 compound

*** GS of F12 at PBE0/6-311++G(d,p)**

O	1.97554100	0.59506200	0.03851000
O	-2.10843100	1.54458800	0.06146300
O	3.52432500	0.26753900	-2.25961200
O	3.48366300	-0.06574500	2.29003400
O	1.48066200	-1.60242000	-0.11440500
O	-6.63570100	0.17067100	0.02760100
O	-0.06057900	2.33525200	0.08456200
N	3.27497000	0.19928900	0.02052300
C	5.39029200	-0.29844300	-0.76510900
C	5.37656900	-0.41164600	0.76222200
C	3.98983100	0.08462200	-1.16507800
C	3.96895100	-0.08829900	1.18904200
C	-2.62419400	-0.78980400	-0.04336200
C	-0.31046500	-0.04685900	-0.01731200
C	-3.02624800	0.55424200	0.02152100
C	-1.23999100	-1.05150700	-0.06156400
C	1.09631500	-0.46879400	-0.04010200
C	-3.62177500	-1.78539100	-0.08374500
C	-0.73942300	1.34336100	0.04617700
C	-4.36106600	0.91884000	0.04681700
C	-5.32097600	-0.08864000	0.00609000
C	-4.94968600	-1.44582800	-0.05989600
H	5.64752100	-1.23581900	-1.26222400
H	6.07678300	0.46755900	-1.13171400
H	6.05632100	0.29001400	1.24999500
H	5.62484600	-1.41280700	1.12007900
H	-0.88911800	-2.07784900	-0.11058100
H	-3.32374000	-2.82721200	-0.13334500
H	-4.63549800	1.96675700	0.09716000
H	-5.72769400	-2.19915200	-0.08971700
H	-6.79885700	1.11877200	0.07724800

*** ES of F12 at PBE0/6-311++G(d,p)**

O	1.98882200	0.62575800	-0.02455300
O	-2.11179200	1.54470400	-0.03150200
O	3.50828900	0.02541200	-2.28653700
O	3.51831800	0.20837700	2.27197200
O	1.49362000	-1.59220100	0.05025000
O	-6.64133400	0.19738200	-0.01320200
O	-0.06428800	2.31299100	-0.05220100
N	3.28111300	0.21883100	-0.01096200
C	5.38061700	-0.40295800	-0.75657700
C	5.38563900	-0.33491200	0.77297900
C	3.98130400	-0.04195700	-1.18137400
C	3.98682400	0.05442100	1.17357500
C	-2.62025600	-0.82316800	0.02482600
C	-0.29881100	-0.06406300	0.00511800
C	-3.03158000	0.55712800	-0.01161800
C	-1.24662400	-1.11987500	0.03530800
C	1.09618300	-0.44829400	0.01400300
C	-3.64590100	-1.80118600	0.04741600
C	-0.73634700	1.30996600	-0.02813100
C	-4.35495200	0.93256600	-0.02547600
C	-5.33456900	-0.06244500	-0.00192400
C	-4.96893700	-1.43761400	0.03509300
H	5.61214700	-1.39807700	-1.14164300
H	6.07665200	0.29925900	-1.21989200
H	6.07922100	0.41108600	1.16661900
H	5.62729700	-1.28971900	1.24401500
H	-0.89866000	-2.14321900	0.06270900
H	-3.36827900	-2.84853800	0.07441900
H	-4.61392300	1.98544300	-0.05284600
H	-5.75839800	-2.18011500	0.05214600
H	-6.81247400	1.14701700	-0.04192200

S3-F13. The coordinates of the optimized structures for the GS and ES of F13 compound

*** GS of F13 at PBE0/6-311++G(d,p)**

O	-0.39539000	-1.39619700	0.01100700
O	-4.88383200	0.13732400	-0.01326600
O	1.62456000	-2.25274300	0.03210900
O	3.25757300	1.67146200	0.02709700

N	3.77888000	-0.56965900	-0.02343600
N	4.97152800	-0.23797700	-0.02766600
N	6.07629000	-0.05698700	-0.03417800
C	-0.83824300	0.95178800	0.00685700
C	-1.28282500	-0.37793500	0.00528900
C	0.55414400	1.17030100	0.00954900
C	-1.80751400	1.97778200	0.00241200
C	-2.62923100	-0.70957300	-0.00171500
C	-3.56121700	0.32607800	-0.00634500
C	1.45621300	0.14027800	0.01128700
C	-3.14252900	1.67547800	-0.00379600
C	0.98111800	-1.23576500	0.01848200
C	2.88286500	0.51496400	0.00818300
C	-5.38768600	-1.19341000	-0.01755500
H	0.93766300	2.18619300	0.00828700
H	-1.47910700	3.01170500	0.00375500
H	-2.91487900	-1.75279200	-0.00301600
H	-3.89949200	2.45071600	-0.00724900
H	-6.47143400	-1.09851400	-0.02342400
H	-5.07168100	-1.73287400	0.87966400
H	-5.06181600	-1.73076200	-0.91251200

*** ES of F13 at PBE0/6-311++G(d,p)**

O	-0.39423600	-1.39704200	0.00062600
O	-4.88108700	0.11677200	-0.00022800
O	1.62483100	-2.23037900	-0.00029200
O	3.26264700	1.67599300	-0.00017300
N	3.78342600	-0.57979300	-0.00005600
N	4.97498000	-0.26267300	-0.00008500
N	6.08811700	-0.08887500	-0.00009800
C	-0.83156300	0.97772000	0.00020100
C	-1.28564100	-0.38333600	0.00028400
C	0.55114700	1.22912900	0.00020500
C	-1.82461400	1.99103100	0.00006300
C	-2.61994800	-0.72310500	0.00010100
C	-3.56853800	0.30484900	-0.00007100
C	1.47092500	0.15846900	0.00004300
C	-3.15482800	1.67035300	-0.00006900
C	0.98561100	-1.20847800	0.00005600
C	2.88301500	0.50229800	-0.00010400

C	-5.40186500	-1.20994300	-0.00025700
H	0.93082700	2.24199100	0.00024900
H	-1.51174600	3.02887300	0.00004700
H	-2.89619700	-1.76921400	0.00017400
H	-3.92247200	2.43547100	-0.00017400
H	-6.48346200	-1.10012200	-0.00053500
H	-5.08124900	-1.74706300	0.89659600
H	-5.08080900	-1.74722100	-0.89685400

S3-F14. The coordinates of the optimized structures for the GS and ES of F14 compound

*** GS of F14 at PBE0/6-311++G(d,p)**

O	0.67438500	2.12757500	-0.00017400
O	4.35990600	-0.83237900	0.00012600
O	-0.95589700	3.61420800	-0.00030400
C	0.25410400	-0.24592400	0.00002700
C	1.13234000	0.84857000	-0.00005900
C	0.82301800	-1.53344100	0.00014700
C	-1.15002100	0.05873200	-0.00001800
C	2.50941600	0.69256400	-0.00003200
C	3.03679300	-0.59213700	0.00008800
C	2.18651100	-1.70846400	0.00017900
C	-1.58760000	1.33576200	-0.00012400
C	-0.65768800	2.44443400	-0.00018700
H	0.18366500	-2.40724600	0.00021800
H	3.14570800	1.57060200	-0.00010100
H	2.62125700	-2.70091900	0.00027200
H	4.85532500	-0.00651500	0.00006500
H	-2.63822200	1.59036300	-0.00016300
C	-2.16147900	-1.06126900	0.00005300
F	-2.01881800	-1.84610600	1.08046300
F	-2.01881400	-1.84624500	-1.08025500
F	-3.41872800	-0.61370200	0.00002100

*** ES of F14 at PBE0/6-311++G(d,p)**

O	0.74541100	2.14501800	-0.00064500
O	4.32918000	-0.90464300	0.00035500
O	-0.86858700	3.66114800	-0.00002700
C	0.23842400	-0.24669600	-0.00008500

C	1.15879500	0.86040500	-0.00027700
C	0.79463100	-1.55036700	0.00017000
C	-1.16523100	0.04597700	-0.00010200
C	2.52147600	0.66633100	-0.00013500
C	3.03018100	-0.63551800	0.00015700
C	2.15063300	-1.75158000	0.00026300
C	-1.55351900	1.39573800	0.00014700
C	-0.62780700	2.46318000	-0.00011000
H	0.13527000	-2.40834000	0.00028800
H	3.18069800	1.52714500	-0.00028900
H	2.57454900	-2.74872700	0.00043800
H	4.85919100	-0.09654000	0.00039800
H	-2.59841800	1.67682100	0.00047700
C	-2.17200300	-1.03124100	-0.00000100
F	-2.06870100	-1.85781200	1.07680400
F	-2.06856300	-1.85810100	-1.07655600
F	-3.42416000	-0.55741200	-0.00012900

S3-F15. The coordinates of the optimized structures for the GS and ES of F15 compound

*** GS of F15 at PBE0/6-311++G(d,p)**

O	0.68212900	2.13188100	0.14030600
O	-0.65554800	3.88437400	0.20815400
O	-3.97769600	-2.17638900	-0.03042200
O	-2.68609400	-1.17995400	1.50158200
C	-0.13188800	-0.07749200	-0.34927900
C	-1.45977300	0.46455300	-0.47004100
C	0.90965000	0.80509200	-0.04063800
C	2.52503400	-0.95669200	-0.07919700
C	2.22898500	0.38998100	0.09671800
C	0.20544000	-1.43320400	-0.52106600
C	1.50117700	-1.86985100	-0.39080300
C	-2.62014800	-0.42467300	-0.79762800
C	-1.64985500	1.79496900	-0.29289800
C	-0.56765400	2.69009900	0.02792100
C	4.83513300	-0.60221100	0.33833500
C	-3.06655300	-1.28187300	0.36318800
H	2.98323700	1.12798500	0.33517800
H	-0.56695800	-2.15445900	-0.76312500

H	1.75735400	-2.91434000	-0.52437500
H	-2.39856200	-1.07887300	-1.64624100
H	-3.48395200	0.17598600	-1.09737600
H	-2.62910600	2.24932600	-0.37985500
H	4.95616300	0.16267200	-0.43466000
H	5.72523900	-1.22734200	0.37319800
H	4.68494300	-0.12590300	1.31186000
H	-4.26052600	-2.68169200	0.74518400
O	3.75906700	-1.47560500	0.02694800

*** ES of F15 at PBE0/6-311++G(d,p)**

O	0.74752800	2.14584900	0.10737000
O	-0.60094100	3.89967500	0.23060400
O	-4.13465100	-2.05573400	-0.03951800
O	-2.74601500	-1.19261800	1.48674100
C	-0.13249500	-0.08952400	-0.34808000
C	-1.44480000	0.42630800	-0.48903800
C	0.95034400	0.81876800	-0.04847200
C	2.54362200	-0.97396300	-0.06867100
C	2.25110400	0.38839000	0.08599000
C	0.21034600	-1.46505700	-0.48068900
C	1.50370400	-1.89909600	-0.35388700
C	-2.60683300	-0.44159500	-0.81724500
C	-1.61476500	1.81212300	-0.26973600
C	-0.55538500	2.69143400	0.02857600
C	4.86718800	-0.64810000	0.32578400
C	-3.14011500	-1.24785800	0.34888900
H	3.01711500	1.12000500	0.30699100
H	-0.56875100	-2.18705600	-0.69242700
H	1.76160300	-2.94632100	-0.46134600
H	-2.38233000	-1.14950000	-1.62507800
H	-3.44177800	0.16283500	-1.18755100
H	-2.59870200	2.26432700	-0.32550600
H	4.99391000	0.09932600	-0.46234400
H	5.73604100	-1.30084600	0.36060600
H	4.73170000	-0.15573100	1.29272300
H	-4.44888000	-2.54179300	0.73610900
O	3.76015100	-1.49669900	0.03696600

S3-F16. The coordinates of the optimized structures for the GS and ES of F16 compound

*** GS of F16 at PBE0/6-311++G(d,p)**

O	-1.86462100	-1.51458000	-0.24225300
O	-3.91148400	-2.32324700	-0.37834300
N	2.66568200	-0.12629400	0.00493900
C	1.33900400	0.17593300	0.03892000
C	3.69200900	0.87063500	0.27120000
C	3.13693400	-1.46979500	-0.29338400
C	0.35401500	-0.81950200	-0.11792900
C	-1.44227900	0.82777600	0.10704300
C	-0.98624700	-0.48545100	-0.08491800
C	0.88862600	1.51207700	0.23141100
C	-0.45129900	1.81312200	0.26368700
C	4.12809300	1.64232400	-0.96741300
C	3.24058000	-2.36600300	0.93416400
C	-2.85630500	1.06649000	0.12926900
C	-3.70126100	0.01033200	-0.03385000
C	-3.22774800	-1.33038500	-0.22675400
H	3.34449300	1.55262100	1.05159000
H	4.54887600	0.34264100	0.69949200
H	2.48967300	-1.92127700	-1.05037800
H	4.11955600	-1.37027300	-0.76341800
H	0.60832400	-1.86257500	-0.24803900
H	1.60207300	2.31814800	0.33791300
H	-0.74848100	2.84640400	0.40725000
H	4.51966500	0.96404300	-1.73087400
H	3.29419000	2.19846800	-1.40373300
H	4.91723700	2.35469500	-0.71033800
H	3.92826800	-1.93937600	1.66993800
H	2.26789600	-2.49730400	1.41532900
H	3.61745200	-3.35272100	0.65039500
H	-4.77694300	0.13663800	-0.02450400
C	-3.38638300	2.44905200	0.32925000
H	-3.04244300	2.86276800	1.28229500
H	-3.03057000	3.11926400	-0.45943200
H	-4.47663300	2.45489200	0.32253700

*** ES of F16 at PBE0/6-311++G(d,p)**

O	-1.85280000	-1.53537400	-0.22826400
O	-3.91350300	-2.35698600	-0.38766300
N	2.66118600	-0.12915000	0.00559300
C	1.33640300	0.19891100	0.03505000
C	3.69799200	0.85418200	0.27225700
C	3.12622900	-1.47493400	-0.29137100
C	0.34455200	-0.80990500	-0.11921700
C	-1.44714100	0.83827300	0.10598300
C	-0.99337600	-0.49388300	-0.08087800
C	0.90266300	1.53347700	0.22016200
C	-0.44472000	1.83251500	0.24886300
C	4.13572800	1.60851500	-0.98089100
C	3.24174700	-2.35045100	0.95399500
C	-2.85718400	1.09520700	0.13662400
C	-3.70202600	-0.00947200	-0.03820400
C	-3.24976700	-1.33144300	-0.22508300
H	3.34940500	1.54470800	1.04273200
H	4.54864600	0.31344400	0.69495100
H	2.46813400	-1.93241400	-1.03189300
H	4.10645200	-1.37398800	-0.76469400
H	0.60855800	-1.85045300	-0.24974100
H	1.61797400	2.33835700	0.32127100
H	-0.74824700	2.86416000	0.38342000
H	4.52529100	0.92136900	-1.73602500
H	3.30453600	2.16695500	-1.41712800
H	4.92862600	2.31355500	-0.71880700
H	3.92764900	-1.90914000	1.68130300
H	2.26964000	-2.48587300	1.43354600
H	3.62918100	-3.33225000	0.67010900
H	-4.77942500	0.11914800	-0.03443100
C	-3.37642700	2.47456800	0.33629700
H	-3.03211600	2.91010300	1.28528200
H	-3.04199100	3.15976400	-0.45617700
H	-4.46821600	2.48213400	0.34302300

S3-F17. The coordinates of the optimized structures for the GS and ES of F17 compound

*** GS of F17 at PBE0/6-311++G(d,p)**

S	-3.63196800	1.47390000	-0.17590800

O	0.87114700	1.60583200	-0.19183700
O	-1.09387000	2.58880700	-0.30685400
N	5.26918000	-0.16658400	0.02783000
N	-3.13455600	-1.06045100	0.11640200
C	3.92756200	-0.35017000	0.04931200
C	6.20753000	-1.25632400	0.26679000
C	5.86258900	1.13820700	-0.23371400
C	1.11180400	-0.75983200	0.09138800
C	1.67776500	0.51867300	-0.06383000
C	3.03618600	0.73842800	-0.08553900
C	3.36342100	-1.65357700	0.20622700
C	2.00831500	-1.84101200	0.22572700
C	-0.28859800	-0.86941700	0.10224900
C	-1.09845200	0.23280400	-0.03010300
C	6.58207400	-2.01974400	-0.99608800
C	6.04465300	1.98248200	1.02042500
C	-2.54625300	0.09271100	-0.01563800
C	-0.49855900	1.53902700	-0.18353600
C	-4.97873700	0.38300800	-0.05115800
C	-4.50127500	-0.93438000	0.10060300
C	-6.34303300	0.66547700	-0.08446100
C	-5.41465700	-1.98916700	0.22085900
C	-7.23122400	-0.39265500	0.03629700
C	-6.76931500	-1.70842700	0.18765400
H	7.10201100	-0.81330000	0.71318500
H	5.79954300	-1.92895900	1.02478200
H	6.83224800	0.95937000	-0.70615500
H	5.26090000	1.66671500	-0.97741700
H	3.38520600	1.75663500	-0.18684600
H	4.00844800	-2.51703700	0.29362500
H	1.60536200	-2.84243000	0.33931000
H	-0.75112200	-1.84480200	0.21852000
H	5.70742800	-2.49268300	-1.45014700
H	7.03008300	-1.35194800	-1.73717600
H	7.30987400	-2.80092000	-0.75999600
H	5.08697300	2.19319200	1.50322700
H	6.68512000	1.47121700	1.74447600
H	6.51564600	2.93562500	0.76496000
H	-6.70229900	1.68197000	-0.20140200
H	-5.05031200	-3.00428100	0.33761800

H	-8.29826000	-0.19818400	0.01325400
H	-7.48673000	-2.51711000	0.27983700

*** ES of F17 at PBE0/6-311++G(d,p)**

S	-3.62861400	1.49609200	-0.18094000
O	0.86168600	1.60017300	-0.18512000
O	-1.10121500	2.57771800	-0.30570200
N	5.26599100	-0.15365300	0.02731900
N	-3.13623700	-1.06649200	0.11927200
C	3.92390000	-0.36081900	0.04802000
C	6.21800200	-1.22867800	0.26636400
C	5.84230500	1.15735200	-0.23248900
C	1.09440300	-0.79345000	0.09187100
C	1.66213200	0.49748900	-0.05974600
C	3.01495800	0.72197700	-0.08311500
C	3.37404800	-1.66804000	0.19998800
C	2.01900500	-1.86686500	0.21852900
C	-0.29801700	-0.93230300	0.10782500
C	-1.11825100	0.22177800	-0.02920300
C	6.60242000	-1.98198300	-1.00248100
C	6.01936200	1.99576200	1.02907900
C	-2.52408000	0.11255400	-0.01798700
C	-0.50959300	1.52378600	-0.18064400
C	-4.96671800	0.39591200	-0.05408400
C	-4.47827200	-0.93324700	0.10171900
C	-6.32753400	0.67186200	-0.08766600
C	-5.40521800	-1.99101600	0.22391200
C	-7.21784600	-0.38918300	0.03508400
C	-6.75488300	-1.70844400	0.18947500
H	7.10691100	-0.77280400	0.71086400
H	5.81487900	-1.90978100	1.01896700
H	6.81369300	0.98977800	-0.70551100
H	5.23028600	1.68301700	-0.96888500
H	3.35587700	1.74344000	-0.18409200
H	4.02573500	-2.52734200	0.28378300
H	1.62739100	-2.87295300	0.32734200
H	-0.76341700	-1.90195800	0.22267600
H	5.73338100	-2.46465400	-1.45613500
H	7.04362800	-1.30655800	-1.74009800
H	7.33952700	-2.75295700	-0.76271300

H	5.05992400	2.19563500	1.51231900
H	6.66668100	1.48742300	1.74842800
H	6.48152500	2.95249000	0.77160000
H	-6.69026900	1.68694800	-0.20636600
H	-5.04094800	-3.00581700	0.34258400
H	-8.28491700	-0.19533400	0.01134800
H	-7.47485000	-2.51482000	0.28264200

S3-F18. The coordinates of the optimized structures for the GS and ES of F18 compound

*** GS of F18 at PBE0/6-311++G(d,p)**

O	-0.67650700	1.66101000	-0.05757500
O	1.26950000	2.67976800	-0.04175300
N	-5.07037500	-0.14303100	0.00051000
N	3.37306700	-0.85706100	0.65721900
N	3.61669200	0.90517000	-0.69168700
C	-3.72543900	-0.32150100	0.00509900
C	-0.90864300	-0.71772900	0.01927200
C	-6.00168000	-1.25556300	0.13348600
C	-5.66928300	1.17783500	-0.13066500
C	-1.47820600	0.56431700	-0.02439400
C	-2.83957500	0.77815200	-0.02894000
C	1.30465200	0.29060700	-0.02659400
C	-3.15486100	-1.62938600	0.04085200
C	0.49850300	-0.81581900	0.01205800
C	-1.79679000	-1.81031600	0.04797500
C	2.75923800	0.16030500	-0.03062500
C	4.72243400	-0.75573200	0.42745600
C	0.70220600	1.61391200	-0.04751100
C	4.85361300	0.35895900	-0.42674900
C	-6.37120300	-1.89841800	-1.19644400
C	-5.84928400	1.89587500	1.20033800
C	5.81534800	-1.49703500	0.86687100
C	6.12029500	0.74758700	-0.87137900
C	7.06376300	-1.09167500	0.41640900
C	7.21373500	0.01222800	-0.44096100
H	-6.89977500	-0.86347300	0.61888600
H	-5.59027000	-1.99541900	0.82435300
H	-5.07293800	1.77942000	-0.82151300

H	-6.64044200	1.04304700	-0.61472500
H	-3.19282300	1.79996500	-0.04011300
H	-3.79443900	-2.50137400	0.04502400
H	0.94298500	-1.80766500	0.01413300
H	-1.38967500	-2.81645800	0.06895400
H	2.92363300	-1.49570300	1.29424100
H	-7.09344300	-2.70393600	-1.03706100
H	-5.49299800	-2.31933700	-1.69295700
H	-6.82383800	-1.16593500	-1.87067700
H	-6.48696700	1.31499800	1.87266000
H	-4.89025500	2.05899700	1.69874000
H	-6.32198900	2.86903600	1.04148800
H	5.70036200	-2.34990200	1.52690000
H	6.23631900	1.60062200	-1.53172000
H	7.94485200	-1.64042000	0.73240400
H	8.20914100	0.29215400	-0.77001000

*** ES of F18 at PBE0/6-311++G(d,p)**

O	-0.66904000	1.63899700	-0.22506200
O	1.26438600	2.65602000	-0.37423700
N	-5.07324100	-0.11826000	0.03899300
N	3.34998000	-1.07985900	0.13551600
N	3.66901000	1.12532000	-0.16786900
C	-3.72816800	-0.32267400	0.04326700
C	-0.89745500	-0.74611600	0.05993600
C	-6.01851600	-1.19498100	0.29225900
C	-5.65488100	1.19115300	-0.21306400
C	-1.46808500	0.54303300	-0.08792600
C	-2.82300200	0.76187700	-0.09724200
C	1.33048100	0.27903000	-0.06876300
C	-3.17393100	-1.62752400	0.18644400
C	0.49505200	-0.87372100	0.06748900
C	-1.81666500	-1.82286000	0.19221500
C	2.74124600	0.15919200	-0.04114900
C	4.69790600	-0.89712500	0.12246600
C	0.72343900	1.58226000	-0.23147200
C	4.86630000	0.50649500	-0.07216900
C	-6.41900400	-1.95286100	-0.96898300
C	-5.81599400	2.03114800	1.04971900
C	5.77153000	-1.77135900	0.25411400

C	6.16620800	1.04335900	-0.13666500
C	7.04024000	-1.21180400	0.18634300
C	7.23178700	0.17487200	-0.00650900
H	-6.90303900	-0.74182600	0.74853300
H	-5.60329700	-1.87399900	1.04051900
H	-5.05390100	1.71780900	-0.95800900
H	-6.63261500	1.02281500	-0.67290300
H	-3.16784900	1.78241000	-0.19537800
H	-3.82221500	-2.48919500	0.27389200
H	0.91458600	-1.86517300	0.17430500
H	-1.42272700	-2.82884800	0.29591600
H	2.88508800	-1.96281800	0.26680900
H	-7.14957500	-2.72655700	-0.71771500
H	-5.55478200	-2.43282300	-1.43465200
H	-6.87352800	-1.28057200	-1.70147800
H	-6.45305400	1.52276300	1.77827300
H	-4.85020700	2.23184900	1.51986700
H	-6.28228700	2.98766700	0.79851300
H	5.62802600	-2.83579900	0.40230700
H	6.31336600	2.10771300	-0.28419200
H	7.90895700	-1.85435900	0.28355600
H	8.24513600	0.56003400	-0.05211800

S3-F19. The coordinates of the optimized structures for the GS and ES of F19 compound

*** GS of F19 at PBE0/6-311++G(d,p)**

O	-0.80155900	1.67349200	0.06936200
O	1.15786300	2.66566200	0.19360000
N	-5.20424600	-0.10598400	-0.05097200
N	3.34743200	-0.61112700	0.73222000
N	3.38404100	0.79819200	-1.01328700
C	-3.86023200	-0.29134100	-0.06874100
C	-1.04574100	-0.70148700	-0.10880700
C	-6.14179200	-1.22093300	-0.02704300
C	-5.79609100	1.22453800	-0.05140100
C	-1.60794200	0.58117400	-0.01378300
C	-2.96834000	0.80108000	0.00952900
C	1.16784300	0.29534800	-0.06070100

C	-3.29702200	-1.59861100	-0.17028200
C	0.36254300	-0.80644400	-0.13631300
C	-1.93967200	-1.78616000	-0.18835400
C	2.62950600	0.18958500	-0.12509500
C	4.66407400	-0.50841000	0.34917100
C	0.57473000	1.61329300	0.06992500
C	4.66755400	0.38285500	-0.74223600
C	-6.52298100	-1.72248000	-1.41328200
C	-5.97205300	1.81053200	1.34328900
C	5.82827300	-1.08976000	0.84643000
C	5.87267000	0.70851500	-1.37036400
C	7.01410200	-0.75187400	0.20980100
C	7.03576100	0.13331700	-0.88223300
H	-7.03465800	-0.87527600	0.50137900
H	-5.73131700	-2.02992600	0.58196800
H	-5.19681300	1.88747800	-0.68088300
H	-6.76818100	1.14268700	-0.54544400
H	-3.31631000	1.82005600	0.10808700
H	-3.94141000	-2.46304900	-0.25342100
H	0.80727800	-1.79311700	-0.23701700
H	-1.53791100	-2.79102600	-0.27387800
H	-7.25097200	-2.53450900	-1.33230300
H	-5.65092800	-2.09762600	-1.95527800
H	-6.97315600	-0.92194000	-2.00704300
H	-6.61130500	1.16949100	1.95688500
H	-5.01207100	1.92156200	1.85409000
H	-6.44144300	2.79616100	1.28009000
H	5.81569900	-1.77626100	1.68608700
H	5.89043500	1.39284000	-2.21230400
H	7.94599700	-1.18189800	0.56189200
H	7.98589300	0.36888300	-1.35053800
C	2.87259100	-1.36970800	1.86973200
H	1.87090000	-1.03610900	2.13538900
H	2.84817200	-2.43956000	1.64659700
H	3.53438700	-1.19780600	2.72077200

*** ES of F19 at PBE0/6-311++G(d,p)**

O	-0.80667800	1.69736400	0.05995500
O	1.12823600	2.72072100	0.19334000
N	-5.20455400	-0.09100700	-0.05733200

N	3.31833300	-0.85904800	0.47539700
N	3.44086600	1.14069400	-0.57292400
C	-3.85757600	-0.29226200	-0.05613200
C	-1.02533500	-0.70672800	-0.04371500
C	-6.14955700	-1.19551300	-0.00904300
C	-5.78667800	1.24081600	-0.11022400
C	-1.59969700	0.58849500	0.00885900
C	-2.95573700	0.80233300	0.00714400
C	1.19345700	0.33242700	0.02410400
C	-3.30008500	-1.60056500	-0.12533000
C	0.37091200	-0.83183500	-0.03817400
C	-1.94089200	-1.79105900	-0.12328200
C	2.61534200	0.24636800	-0.00445000
C	4.63663500	-0.64476100	0.18537200
C	0.58615100	1.64055400	0.08474600
C	4.68112200	0.61434700	-0.47555400
C	-6.52389700	-1.72854000	-1.38824500
C	-5.97999300	1.86893800	1.26637700
C	5.77998600	-1.39458700	0.44296000
C	5.91600700	1.12438400	-0.91713300
C	6.98596800	-0.86385300	0.00228800
C	7.05028300	0.37533400	-0.67058800
H	-7.04458600	-0.82696100	0.50010400
H	-5.74503400	-1.99137100	0.62036400
H	-5.17207300	1.88034800	-0.74799600
H	-6.75342100	1.14653500	-0.61256400
H	-3.30432100	1.82462000	0.06707300
H	-3.94527500	-2.46576000	-0.20012600
H	0.81226500	-1.80967700	-0.17363100
H	-1.54347300	-2.79907300	-0.18504000
H	-7.25691800	-2.53321900	-1.28500500
H	-5.64986900	-2.12308400	-1.91216400
H	-6.96696900	-0.94168800	-2.00441600
H	-6.63040500	1.25022000	1.89029200
H	-5.02575400	1.99384900	1.78387900
H	-6.44556000	2.85242800	1.15940600
H	5.73942600	-2.35162500	0.95099800
H	5.96431100	2.08006300	-1.42785000
H	7.90276200	-1.41769600	0.17508700
H	8.01744400	0.74354200	-0.99667300

C	2.86086800	-1.90087100	1.37470100
H	1.94816500	-1.58063000	1.87373700
H	2.67228200	-2.83710900	0.84273100
H	3.62831800	-2.07339600	2.13139100

S3-F20. The coordinates of the optimized structures for the GS and ES of F20 compound

*** GS of F20 at PBE0/6-311++G(d,p)**

O	0.63811500	2.13895300	-0.00017300
O	-1.00724300	3.60874300	-0.00029300
C	0.24377700	-0.23950100	0.00002300
C	1.11676000	0.86462700	-0.00004100
C	0.83514900	-1.51950300	0.00014500
C	-1.15624200	0.04864400	-0.00004100
C	2.49004300	0.72864300	0.00001800
C	3.05787600	-0.55227900	0.00014100
C	2.19703300	-1.67723800	0.00020200
C	-1.61394300	1.32344500	-0.00018000
C	-0.69916200	2.43903900	-0.00028100
H	0.20885400	-2.40316900	0.00019600
H	3.11041700	1.61769200	-0.00003400
H	2.62642900	-2.67330100	0.00029500
H	-2.66788200	1.56263500	-0.00021900
C	-2.15445400	-1.08265700	0.00003200
F	-2.00527900	-1.86748200	1.08059300
F	-2.00503400	-1.86783100	-1.08024100
F	-3.41825600	-0.65100100	-0.00017900
N	4.40000100	-0.71962800	0.00020100
H	4.80700600	-1.63855800	0.00027600
H	5.02429700	0.06802800	0.00014500

*** ES of F20 at PBE0/6-311++G(d,p)**

O	0.69549400	2.15738000	-0.00028100
O	-0.94291100	3.65598700	-0.00058900
C	0.24392500	-0.23653200	0.00017500
C	1.12600000	0.86998300	-0.00004300
C	0.82416100	-1.53083400	0.00041600
C	-1.18062600	0.03710500	0.00004000
C	2.49408300	0.70264900	-0.00003900

C	3.04996000	-0.60013100	0.00019700
C	2.18213000	-1.72239900	0.00042500
C	-1.58180300	1.37325600	0.00016500
C	-0.67457100	2.46000500	0.00032800
H	0.17607400	-2.39813900	0.00057300
H	3.13494800	1.57703200	-0.00021200
H	2.59885500	-2.72297700	0.00058400
H	-2.63131100	1.63907800	0.00013100
C	-2.16360400	-1.05399600	-0.00012500
F	-2.04700200	-1.88561200	1.07677400
F	-2.04655800	-1.88565700	-1.07692600
F	-3.42764200	-0.60967400	-0.00038300
N	4.38137400	-0.76006500	0.00017000
H	4.79740200	-1.67933400	0.00027600
H	5.00664700	0.03170300	0.00000400

S3-F21. The coordinates of the optimized structures for the GS and ES of F21 compound

*** GS of F21 at PBE0/6-311++G(d,p)**

O	0.64099500	1.34184100	-0.08652600
O	2.73304300	1.99841300	-0.10867300
O	4.65482500	0.04782700	0.04496000
O	3.96355500	-2.07842700	-0.01690600
N	-4.00318500	0.36875000	-0.05130100
C	-2.71127300	-0.05239200	-0.06662400
C	-4.33131100	1.77572800	-0.22436900
C	-1.65471900	0.89624400	-0.06792400
C	-5.11833100	-0.56254400	-0.14228400
C	-2.41346700	-1.45715300	-0.07132500
C	-1.92820700	2.37474100	-0.06251200
C	-3.32056100	2.66326900	0.47123600
C	-4.79315200	-1.88875400	0.51164400
C	-3.53417500	-2.45989300	-0.11595700
C	-0.35693600	0.42137200	-0.06960900
C	-1.10718200	-1.86606200	-0.05077300
C	-0.03774700	-0.94780000	-0.05357500
C	1.31766000	-1.30094500	-0.03570800
C	2.32890800	-0.36769900	-0.03905300
C	1.99548600	1.04228300	-0.07764500

C	3.71094600	-0.88783700	-0.00579700
C	6.01496200	-0.42214700	0.08286400
C	6.91412700	0.78629200	0.12328800
H	-5.33057400	1.93238100	0.18874900
H	-4.38032400	2.01990300	-1.29607800
H	-5.39288800	-0.71667700	-1.19663400
H	-5.97517600	-0.09273100	0.34791000
H	-1.16935100	2.88611500	0.53458000
H	-1.83219500	2.77061200	-1.08192800
H	-3.35835200	2.47397800	1.54947000
H	-3.58586800	3.71139500	0.31235000
H	-5.63829000	-2.56983200	0.38455900
H	-4.64693800	-1.73999300	1.58716800
H	-3.74374200	-2.72522600	-1.16061200
H	-3.22359800	-3.38102400	0.38433000
H	-0.88092200	-2.92874100	-0.04261100
H	1.59787000	-2.35013500	-0.01470800
H	6.14289700	-1.05473200	0.96529100
H	6.19828100	-1.03714500	-0.80210800
H	7.95726900	0.46103200	0.15369500
H	6.77578400	1.40947300	-0.76353700
H	6.71892000	1.39265200	1.01112000

*** ES of F21 at PBE0/6-311++G(d,p)**

O	0.64358800	1.33204900	-0.09287000
O	2.73882000	1.98035200	-0.10457100
O	4.66675600	0.06597400	0.04172100
O	3.98343300	-2.07224500	0.00103000
N	-4.01322200	0.39131600	-0.06396900
C	-2.72123600	-0.05819100	-0.06642500
C	-4.31291300	1.79914900	-0.23890000
C	-1.64770600	0.88518600	-0.05734500
C	-5.13191600	-0.52810300	-0.14865600
C	-2.44442800	-1.45912000	-0.07085300
C	-1.90677900	2.36120500	-0.03817100
C	-3.30100900	2.66886900	0.47764800
C	-4.82615800	-1.85479400	0.51459200
C	-3.57188300	-2.44875700	-0.10177700
C	-0.35098200	0.39975900	-0.07174300
C	-1.13203300	-1.87995700	-0.05816900

C	-0.04608200	-0.97525500	-0.06014300
C	1.32204800	-1.36160800	-0.04158300
C	2.33570900	-0.38782700	-0.03702600
C	2.00405200	1.01450300	-0.07611800
C	3.71605800	-0.87675400	0.00043100
C	6.02111200	-0.40622000	0.07980500
C	6.92545300	0.79959400	0.11102000
H	-5.32422300	1.97045100	0.13490100
H	-4.31860900	2.03503400	-1.31691400
H	-5.38367600	-0.68631500	-1.21141900
H	-5.99318900	-0.04019200	0.31413800
H	-1.14273800	2.85846000	0.56324000
H	-1.79329900	2.75510900	-1.05798100
H	-3.36051400	2.47871900	1.55451400
H	-3.55096700	3.71952000	0.31359200
H	-5.68209300	-2.52095400	0.38440900
H	-4.68653600	-1.70140800	1.59015500
H	-3.77737800	-2.73047300	-1.14382600
H	-3.27148200	-3.36445000	0.41423600
H	-0.91850600	-2.94456900	-0.05024900
H	1.59834900	-2.40749800	-0.02498800
H	6.15432000	-1.03474200	0.96528800
H	6.20600700	-1.02822100	-0.80088200
H	7.96813800	0.47243700	0.14140700
H	6.78686200	1.41828000	-0.77909700
H	6.73347000	1.41249100	0.99524800

S3-F22. The coordinates of the optimized structures for the GS and ES of F22 compound

*** GS of F22 at PBE0/6-311++G(d,p)**

O	1.33444700	1.36272400	-0.04363400
O	3.43475000	2.00548600	-0.01431500
O	5.34171900	0.26106900	0.03395300
O	4.80885400	-1.88731500	0.05286300
N	-3.29283500	0.32786500	-0.08432700
C	-1.99994700	-0.07821100	-0.07654400
C	-3.63639600	1.73275700	-0.25438200
C	-0.95238200	0.88321900	-0.06210100
C	-4.40030400	-0.61485200	-0.17164200

C	-1.68546500	-1.48064000	-0.07611400
C	-1.24282700	2.35836200	-0.06196700
C	-2.64457400	2.62981300	0.45534800
C	-4.06392900	-1.93636800	0.48530800
C	-2.79510400	-2.49394500	-0.13415900
C	0.34603100	0.42049100	-0.04500900
C	-0.37679600	-1.87585000	-0.03967700
C	0.68547800	-0.94735500	-0.02806700
C	2.04113800	-1.29147600	-0.00178900
C	3.02647200	-0.33018000	0.00463900
C	2.65610100	1.05657100	-0.01664700
C	4.45012400	-0.72790900	0.03253500
H	-4.64173300	1.87470200	0.14837900
H	-3.67667700	1.97805300	-1.32566600
H	-4.67195700	-0.77169800	-1.22578900
H	-5.26059900	-0.15070200	0.31744600
H	-0.49783500	2.88045800	0.54291600
H	-1.14055300	2.75194600	-1.08149700
H	-2.69337200	2.43898100	1.53273800
H	-2.91949700	3.67490000	0.29393400
H	-4.90067000	-2.62653600	0.35312600
H	-3.92611200	-1.78587500	1.56161100
H	-2.99232700	-2.75605100	-1.18190800
H	-2.47928500	-3.41367700	0.36496300
H	-0.13933400	-2.93580300	-0.03002800
H	2.33739000	-2.33634800	0.01447600
H	4.84851800	1.12031700	0.01625300

*** ES of F22 at PBE0/6-311++G(d,p)**

O	1.33446500	1.35735000	-0.04033800
O	3.43823900	1.99828100	-0.00830600
O	5.34797100	0.28828800	0.03024100
O	4.83546300	-1.87027000	0.03959700
N	-3.30428600	0.34745800	-0.09809200
C	-2.00871600	-0.08823800	-0.07174100
C	-3.61688500	1.75142100	-0.28418400
C	-0.94708700	0.86959600	-0.04573600
C	-4.41122200	-0.58601000	-0.18698900
C	-1.71384900	-1.48330500	-0.06759600
C	-1.22334800	2.34149300	-0.03049300

C	-2.63198800	2.63417200	0.45332200
C	-4.09718100	-1.90422000	0.48919000
C	-2.82815000	-2.48778900	-0.10652200
C	0.35634600	0.39659500	-0.04117600
C	-0.39589200	-1.88582300	-0.03970000
C	0.67986600	-0.97064600	-0.03029200
C	2.05793700	-1.34765400	-0.00663200
C	3.03346900	-0.34491900	0.00245900
C	2.66337600	1.03581100	-0.01327700
C	4.45930800	-0.70966200	0.02556500
H	-4.63852800	1.91138000	0.06505500
H	-3.59966100	1.98290800	-1.36274400
H	-4.64906600	-0.75347800	-1.25129300
H	-5.28291500	-0.10416800	0.26242500
H	-0.47822100	2.84846200	0.58610600
H	-1.09167800	2.73416800	-1.04879600
H	-2.71353700	2.44657100	1.52903400
H	-2.88910900	3.68140900	0.27993400
H	-4.94348000	-2.58114900	0.35272200
H	-3.97359100	-1.74166500	1.56529700
H	-3.01549100	-2.78081600	-1.14858500
H	-2.52342600	-3.39479200	0.42193000
H	-0.16906300	-2.94758600	-0.02869800
H	2.35222400	-2.38870300	0.00073300
H	4.84053100	1.14113600	0.01678900

S3-F23. The coordinates of the optimized structures for the GS and ES of F23 compound

*** GS of F23 at PBE0/6-311++G(d,p)**

O	0.27406900	1.82610100	0.00000200
O	4.60899800	-0.06851000	-0.00001100
O	-1.65867100	2.86561200	-0.00006200
C	-0.97164800	-0.69376800	0.00001400
C	0.47733500	-0.58161100	0.00001100
C	-1.73423300	0.48860200	0.00000300
C	1.04235200	0.69535400	0.00000200
C	1.36766500	-1.66681100	0.00000900
C	-1.65517600	-1.91831900	0.00002700
C	-1.08766700	1.80146700	0.00000000

C	2.41427500	0.90817600	-0.00000500
C	-3.13275700	0.44294100	-0.00000300
C	2.73422800	-1.48537100	0.00000200
C	3.26353600	-0.18937200	-0.00000500
C	-3.03789200	-1.95422300	0.00002300
C	-3.78645600	-0.77334800	0.00000800
H	0.97981200	-2.67867900	0.00001300
H	-1.10354000	-2.85082200	0.00003800
H	2.79491800	1.92389800	-0.00001200
H	-3.68316300	1.37674300	-0.00001300
H	3.40978200	-2.33287900	0.00000100
H	-3.54494100	-2.91356600	0.00003200
H	-4.86990400	-0.81308400	0.00000500
H	4.86049100	0.86045800	-0.00001500

*** ES of F23 at PBE0/6-311++G(d,p)**

O	0.30810200	1.86050400	0.00022900
O	4.57545500	-0.09501900	-0.00024700
O	-1.65390900	2.91367600	-0.00064100
C	-0.96412900	-0.69873000	0.00022700
C	0.46397000	-0.57319300	0.00019600
C	-1.72798100	0.53203500	0.00024300
C	1.04428300	0.74003000	0.00011900
C	1.36138100	-1.67596500	0.00006000
C	-1.62867600	-1.92574900	0.00012400
C	-1.12082400	1.80935000	0.00050500
C	2.41142900	0.91710600	-0.00001600
C	-3.13807600	0.42887500	-0.00004200
C	2.71672300	-1.51002900	-0.00005500
C	3.25413100	-0.19803700	-0.00009000
C	-3.02606900	-2.00538200	-0.00006500
C	-3.76425800	-0.81114300	-0.00017900
H	0.95939300	-2.68076300	0.00004400
H	-1.05667800	-2.84680700	0.00016600
H	2.81579500	1.92311500	-0.00006300
H	-3.72635800	1.33936800	-0.00010000
H	3.39550400	-2.35413600	-0.00014800
H	-3.52234000	-2.96744800	-0.00014800
H	-4.84944700	-0.85083700	-0.00035700
H	4.85552400	0.82921600	-0.00028500

S3-F24. The coordinates of the optimized structures for the GS and ES of F24 compound

*** GS of F24 at PBE0/6-311++G(d,p)**

O	-0.86408500	-1.43943400	-0.00008000
O	-3.06929600	-1.37066800	0.00017600
C	0.48067900	0.55791500	0.00001200
C	0.35113600	-0.83418400	-0.00010600
C	1.76241100	1.12368600	-0.00003600
C	-0.73718500	1.33113100	0.00018800
C	1.47227200	-1.65729500	-0.00026800
C	2.73074700	-1.07958900	-0.00031300
C	2.87992500	0.31067100	-0.00019700
C	-1.94351000	0.70423400	0.00019300
C	-2.04302400	-0.72568300	0.00001400
H	1.85915600	2.20300800	0.00005800
H	1.33915800	-2.73294000	-0.00036000
H	3.87080800	0.75026200	-0.00023200
H	-2.87702600	1.25424100	0.00032600
H	3.60807500	-1.71736400	-0.00044100
O	-0.57777700	2.65451700	0.00031800
H	-1.43161900	3.10215100	0.00041300

*** ES of F24 at PBE0/6-311++G(d,p)**

O	-0.84024300	-1.45879400	0.00046700
O	-3.05038600	-1.42025000	-0.00036800
C	0.46447400	0.60132100	0.00018700
C	0.34970900	-0.85018500	0.00001900
C	1.77180500	1.14834600	0.00005400
C	-0.71135100	1.34841400	0.00028100
C	1.47747300	-1.66705200	-0.00043000
C	2.74389500	-1.09438100	-0.00056500
C	2.87642700	0.31575100	-0.00030000
C	-1.96986800	0.68678800	0.00012400
C	-2.05684600	-0.71075600	0.00045000
H	1.88733000	2.22464800	0.00019800
H	1.33562000	-2.74153900	-0.00056100
H	3.86995000	0.75151100	-0.00040400
H	-2.90292100	1.23744800	-0.00021900
H	3.62660300	-1.72265300	-0.00085900

O	-0.61022700	2.68998700	0.00025900
H	-1.48403200	3.09355500	0.00007000

S3-F25. The coordinates of the optimized structures for the GS and ES of F25 compound

*** GS of F25 at PBE0/6-311++G(d,p)**

O	-1.19965400	-1.11187600	-0.00003100
O	-3.40082400	-1.25866200	0.00001000
C	-0.06004400	1.00202100	0.00005300
C	-0.04201600	-0.40030400	0.00004100
C	1.17021300	1.67528400	0.00004700
C	-1.33429900	1.64811500	0.00003200
C	1.14097300	-1.12009100	0.00003800
C	2.34390100	-0.42337900	0.00006800
C	2.36044700	0.98007600	-0.00006000
C	-2.47573400	0.92431300	-0.00003300
C	-2.44300000	-0.51904000	-0.00004800
H	1.17636200	2.76039100	-0.00010300
H	1.12805800	-2.20324300	-0.00003600
H	3.30720100	1.51057800	-0.00031300
H	-3.45620900	1.38248900	-0.00007700
H	-1.37207300	2.73347600	0.00005700
O	3.47642200	-1.15542900	-0.00003400
H	4.24646900	-0.57792600	0.00007700

*** ES of F25 at PBE0/6-311++G(d,p)**

O	-1.20002300	-1.13360700	0.00042000
O	-3.41360000	-1.26381600	-0.00048200
C	-0.06296600	1.02828600	0.00010300
C	-0.05257200	-0.41720700	0.00016300
C	1.20349800	1.68562200	-0.00031000
C	-1.29990100	1.69717500	0.00050500
C	1.12208700	-1.12760000	0.00013900
C	2.34478900	-0.43993200	-0.00004400
C	2.37770800	0.97841500	-0.00024200
C	-2.47804100	0.92073000	-0.00002800
C	-2.46172900	-0.49039400	-0.00010300
H	1.22082700	2.76965300	-0.00048800
H	1.10779600	-2.21083900	0.00024900

H	3.33340800	1.49299900	-0.00034400
H	-3.45741300	1.38411800	-0.00045400
H	-1.34105000	2.77856800	0.00063800
O	3.45565800	-1.17821700	0.00001300
H	4.24291400	-0.61994300	-0.00029900

S3-F26. The coordinates of the optimized structures for the GS and ES of F26 compound

*** GS of F26 at PBE0/6-311++G(d,p)**

O	0.58777600	-1.73893100	-0.11641000
O	5.03023800	-0.28296000	0.45688800
O	-1.42641000	-2.57980100	-0.34575900
C	1.01799200	0.61809600	-0.19717200
C	-1.24832100	-0.21507200	-0.49828400
C	1.47700800	-0.70382600	-0.04895200
C	-0.37518500	0.84543300	-0.42025200
C	2.00474300	1.62800500	-0.10871400
C	-0.75600700	-1.55740700	-0.32375700
C	2.79917600	-1.02965800	0.16685600
C	3.80475700	-0.01850300	0.25731500
C	3.32732100	1.33522300	0.10558500
H	1.70544800	2.66625700	-0.21506900
H	3.08142800	-2.07270400	0.27238500
H	4.06050100	2.13485000	0.16800800
C	-0.85278600	2.25958100	-0.55709000
H	-1.93195400	2.32190600	-0.68073800
H	-0.58181400	2.84118200	0.32954300
H	-0.37966600	2.74836300	-1.41516200
C	-2.72205800	-0.07430700	-0.72450000
H	-2.93706500	0.66847400	-1.49767100
H	-3.11109100	-1.02328600	-1.10488600
C	-3.58941000	0.27584400	0.51222100
O	-3.06152400	0.22361600	1.64541400
O	-4.78372500	0.56988900	0.25537600

*** ES of F26 at PBE0/6-311++G(d,p)**

O	0.60860600	1.76839300	-0.07224300
O	5.02223200	0.27503000	0.43206700
O	-1.40751300	2.63684800	-0.37215400

C	1.01190900	-0.62138900	-0.18209400
C	-1.24260200	0.25301500	-0.48192800
C	1.47024500	0.71173400	-0.03265900
C	-0.38891600	-0.87023600	-0.37293400
C	2.00750500	-1.64140700	-0.12549400
C	-0.75979300	1.57978400	-0.32311600
C	2.79563100	1.01273200	0.16787200
C	3.80676800	-0.01732400	0.24034100
C	3.34140600	-1.36679100	0.08022800
H	1.69216300	-2.67267900	-0.24544200
H	3.10102100	2.04788700	0.28129300
H	4.07371800	-2.16728400	0.12423200
C	-0.86729300	-2.27636000	-0.47631100
H	-0.55270200	-2.87435600	0.39253300
H	-1.95413200	-2.33726900	-0.53647900
H	-0.45775400	-2.79348800	-1.35947800
C	-2.69814000	0.10325100	-0.73704900
H	-3.10150800	1.05294700	-1.10063400
H	-2.89097700	-0.64618200	-1.51114400
C	-3.59566300	-0.28275100	0.48845500
O	-3.14547900	-0.09048900	1.63720900
O	-4.72736700	-0.72917300	0.18552700

S3-F27. The coordinates of the optimized structures for the GS and ES of F27 compound

*** GS of F27 at PBE0/6-311++G(d,p)**

O	-5.12849700	0.30720300	1.04705300
O	-1.22752300	1.40576600	-0.27410600
O	-4.97218600	-1.49574100	-0.27954500
O	-3.27033600	2.20777600	-0.31330100
C	-0.74663700	-0.92996200	-0.13751600
C	-3.05345400	-0.15378500	0.00921400
C	-0.31603600	0.39901300	-0.24152500
C	-2.14132100	-1.16453600	-0.01842400
C	-4.52221700	-0.46289800	0.27020400
C	0.25082000	-1.92017400	-0.12405500
C	-2.59771400	1.20882400	-0.18306300
C	1.01765500	0.75187500	-0.31929300
C	2.01360600	-0.24662800	-0.31386400

C	1.58432200	-1.60088200	-0.20532900
H	-2.49970400	-2.18654000	0.07117900
H	-0.04468000	-2.96149500	-0.03731100
H	1.25881900	1.80379400	-0.38577900
H	2.30994900	-2.40207100	-0.17582200
N	3.33594700	0.07056800	-0.42477200
C	3.77033400	1.45992800	-0.45851000
H	4.76948700	1.47135300	-0.89965600
H	3.13104600	2.01824900	-1.15052300
C	4.36423400	-0.96083000	-0.41761300
H	5.23693000	-0.54325700	-0.92544600
H	4.03257600	-1.79976200	-1.03668300
C	3.80455100	2.14895600	0.90146600
H	2.82378300	2.13610700	1.38382700
H	4.51850100	1.66313600	1.57085900
H	4.10823900	3.19290200	0.78101100
C	4.76644200	-1.45241100	0.96834300
H	3.91016900	-1.85729400	1.51413600
H	5.51637300	-2.24380200	0.87850500
H	5.19771600	-0.64426600	1.56409400

*** ES of F27 at PBE0/6-311++G(d,p)**

O	-5.36977400	0.45637500	0.19404200
O	-1.22797900	1.38689600	-0.15550800
O	-4.95780100	-1.56752200	0.23828000
O	-3.27346300	2.20295200	-0.03883900
C	-0.74685700	-0.98994500	-0.10209000
C	-3.04121800	-0.16416100	0.03613300
C	-0.31768100	0.35313100	-0.18210600
C	-2.12561800	-1.25520900	0.00911600
C	-4.43974100	-0.41055100	0.15383800
C	0.28557900	-1.95192700	-0.13139300
C	-2.59878300	1.17823800	-0.04801600
C	1.00854600	0.71786600	-0.28384400
C	2.02950800	-0.25796800	-0.32520200
C	1.62085400	-1.60777500	-0.23338600
H	-2.48708600	-2.27375700	0.07744800
H	0.01629700	-3.00220300	-0.06404400
H	1.23071700	1.77615700	-0.32879300
H	2.35466900	-2.40352500	-0.23865500

N	3.35576300	0.09594400	-0.47487400
C	3.75561300	1.49053400	-0.49091200
H	4.74003500	1.53740400	-0.96449600
H	3.08154400	2.04929500	-1.15003400
C	4.39900700	-0.91233000	-0.45212600
H	5.27533400	-0.47925700	-0.94227300
H	4.09382600	-1.75705700	-1.07965200
C	3.81934800	2.16530400	0.87710500
H	2.85652600	2.11508000	1.39251900
H	4.57045600	1.69286900	1.51512400
H	4.08714000	3.22024700	0.76273300
C	4.79081100	-1.41271400	0.93589300
H	3.93049500	-1.82832800	1.46722300
H	5.54857300	-2.19785700	0.85164200
H	5.20706000	-0.60524400	1.54353700

S3-F28. The coordinates of the optimized structures for the GS and ES of F28 compound

*** GS of F28 at PBE0/6-311++G(d,p)**

O	3.26168800	0.59442900	0.02427900
O	-0.84115500	1.42768800	0.23230100
O	4.72569000	0.30665600	-2.33364300
O	4.87163300	-0.03784900	2.21234000
O	2.81969200	-1.61694000	-0.11462200
O	1.18211100	2.27497100	0.18756600
N	4.56641100	0.22698900	-0.04606600
C	6.65946900	-0.22678500	-0.91603900
C	6.70805600	-0.34463400	0.61004900
C	5.23674600	0.12945800	-1.25794700
C	5.31223600	-0.04924000	1.09186200
C	-1.29578900	-0.92012700	0.11590400
C	0.99415400	-0.11118300	0.06078100
C	-1.74104900	0.41347300	0.21631500
C	0.07997600	-1.14499700	0.03861100
C	2.39996200	-0.49444000	-0.02058600
C	-2.28469900	-1.92955800	0.09610900
C	0.53098300	1.26022400	0.16039000
C	-3.07130700	0.74849300	0.29596200
C	-4.05654000	-0.26819100	0.29059300

C	-3.61314000	-1.62487700	0.17435800
H	6.91535000	-1.15746200	-1.42630300
H	7.31581700	0.55372900	-1.30637000
H	7.39334700	0.36808900	1.07337100
H	6.98877000	-1.34209800	0.95408800
H	0.45514400	-2.16098200	-0.03922800
H	-1.97308000	-2.96579800	0.01301400
H	-3.32780500	1.79647500	0.35736200
H	-4.33261000	-2.43078600	0.14480200
N	-5.37046900	0.02793200	0.40376000
C	-5.82499600	1.41212200	0.50356400
H	-6.80452800	1.39057800	0.98489900
H	-5.16499100	1.95203700	1.18841300
C	-6.39350200	-1.01476000	0.36439700
H	-7.27792500	-0.60573300	0.85619800
H	-6.06893400	-1.85637700	0.98220300
C	-5.92201100	2.13909700	-0.83196000
H	-4.96150100	2.15531900	-1.35318300
H	-6.65704000	1.66555500	-1.48671200
H	-6.23419100	3.17356100	-0.66436400
C	-6.75642200	-1.48676300	-1.03778700
H	-5.88726600	-1.88684100	-1.56604300
H	-7.50867300	-2.27792600	-0.97486200
H	-7.17153300	-0.67130500	-1.63434900

*** ES of F28 at PBE0/6-311++G(d,p)**

O	-3.26769500	0.62193000	-0.01116100
O	0.84667900	1.40933900	-0.18566300
O	-4.70202400	0.23448200	2.35034600
O	-4.90729200	0.07917600	-2.20392400
O	-2.84701000	-1.60956200	0.03697400
O	-1.17600100	2.24998400	-0.10645900
N	-4.56956900	0.25394400	0.05932200
C	-6.65012100	-0.24975500	0.93694300
C	-6.71901500	-0.30216700	-0.59151100
C	-5.22441700	0.10036900	1.27314900
C	-5.33019200	0.01957000	-1.07751100
C	1.30227900	-0.96048100	-0.17001300
C	-0.99938100	-0.13965900	-0.08242500
C	1.73924600	0.37941000	-0.21304900

C	-0.09406300	-1.21593000	-0.10534700
C	-2.40531600	-0.48284600	-0.01287300
C	2.30636700	-1.95749800	-0.19246600
C	-0.52779300	1.22767500	-0.12244000
C	3.07073800	0.72469600	-0.28223000
C	4.06722700	-0.28396200	-0.31330200
C	3.64270200	-1.64036400	-0.26101500
H	-6.89272800	-1.20351000	1.40973200
H	-7.30591000	0.50829200	1.37009900
H	-7.41304700	0.42692100	-1.01481700
H	-7.00071200	-1.28509900	-0.97438300
H	-0.46988300	-2.22958200	-0.06998600
H	2.00643000	-2.99927000	-0.15879800
H	3.31775200	1.77714500	-0.29956300
H	4.36531000	-2.44412600	-0.28572200
N	5.39242600	0.04410000	-0.39826000
C	5.82434600	1.42552900	-0.53839600
H	6.78189300	1.40789800	-1.06293400
H	5.12097800	1.95107400	-1.18816500
C	6.42592600	-0.97380000	-0.28407700
H	7.34525700	-0.53689000	-0.67529000
H	6.17304500	-1.81294600	-0.94026900
C	5.98101500	2.16585800	0.79027000
H	5.04540500	2.17598600	1.35407700
H	6.75507100	1.70807800	1.40911700
H	6.27361800	3.19925300	0.58654200
C	6.65606000	-1.47081700	1.14332700
H	5.74733500	-1.89992600	1.57084200
H	7.42692600	-2.24561800	1.12678100
H	6.99636600	-0.66176100	1.79218600

S3-F29. The coordinates of the optimized structures for the GS and ES of F29 compound

*** GS of F29 at PBE0/6-311++G(d,p)**

O	4.43729300	-0.54821700	-0.00439800
O	0.22091000	-1.42542700	0.00101500
O	3.90057600	1.62462900	0.00044000
O	-4.24623800	0.20429200	-0.00031600
O	2.21211200	-2.33552400	0.00181500

C	-0.16956200	0.92379700	0.00055700
C	2.12710200	0.07337300	0.00023000
C	-0.64542500	-0.38946700	0.00062200
C	1.24054300	1.10548500	0.00030500
C	3.62702000	0.40029100	-0.00125000
C	-1.11350700	1.96790900	0.00036400
C	1.61155600	-1.28890500	0.00130600
C	-2.00362900	-0.69028400	0.00034000
C	-2.91143400	0.36398000	0.00007300
C	-2.46015700	1.69901500	0.00015800
H	1.65245200	2.11030600	-0.00010500
H	-0.76211800	2.99470100	0.00031800
H	-2.31286700	-1.72707600	0.00032600
H	-3.19575500	2.49502900	-0.00002300
C	-4.77042600	-1.11540600	-0.00055400
H	-4.45888300	-1.66195700	-0.89580900
H	-4.45930800	-1.66212900	0.89474100
H	-5.85322900	-1.00564100	-0.00080300

*** ES of F29 at PBE0/6-311++G(d,p)**

O	-4.41980700	-0.56328000	-0.00013700
O	-0.24226100	-1.39724500	-0.00011600
O	-4.05935100	1.47117100	-0.00008600
O	4.28074000	0.13826700	0.00019400
O	-2.27208000	-2.26100900	0.00019200
C	0.17552200	0.99177400	-0.00005500
C	-2.10109500	0.11097100	-0.00017500
C	0.63833500	-0.34113400	-0.00001500
C	-1.21452000	1.22207300	-0.00016000
C	-3.51270800	0.32606200	-0.00014700
C	1.17306200	1.99555000	0.00006500
C	-1.62253400	-1.22239300	-0.00020400
C	1.98415100	-0.67061000	0.00007900
C	2.93660300	0.35047700	0.00015000
C	2.51813400	1.68644500	0.00016600
H	-1.60336600	2.23250200	-0.00016700
H	0.86194800	3.03571300	0.00007300
H	2.25878100	-1.71791900	0.00007200
H	3.26847300	2.46985400	0.00024600
C	4.73885200	-1.19956700	0.00013700

H	4.40324200	-1.73696700	0.89391700
H	4.40335700	-1.73684500	-0.89375900
H	5.82682800	-1.14745100	0.00020900

S3-F30. The coordinates of the optimized structures for the GS and ES of F30 compound

*** GS of F30 at PBE0/6-311++G(d,p)**

O	-2.30463300	-0.60294600	0.03888400
O	1.81165200	-1.39322400	0.04792700
O	-3.86620600	-0.33312200	-2.25762900
O	-3.83714800	-0.00772300	2.29270400
O	-1.89610800	1.61296700	-0.10665700
O	6.28663000	0.17388400	0.00424100
O	-0.20419900	-2.26306600	0.07013900
N	-3.61841900	-0.25809600	0.02244100
C	-5.75210600	0.15750100	-0.76158600
C	-5.74201300	0.26922800	0.76585700
C	-4.33790200	-0.16996100	-1.16259000
C	-4.32289800	-0.00088800	1.19165600
C	2.23761300	0.95799000	-0.04320100
C	-0.04593400	0.12740700	-0.01820500
C	2.69130800	-0.36835100	0.01152400
C	0.84553100	1.16724800	-0.05725700
C	-1.46723500	0.49491200	-0.03722900
C	3.19936800	1.99099300	-0.07965300
C	0.43576200	-1.24505600	0.03628600
C	4.03939500	-0.68953100	0.03000400
C	4.96389300	0.35264300	-0.00760200
C	4.53580400	1.69848900	-0.06230000
H	-6.04600400	1.08474600	-1.25738100
H	-6.40837700	-0.63420200	-1.12885800
H	-6.39464600	-0.45803800	1.25310500
H	-6.02770800	1.25994300	1.12493300
H	0.45648800	2.18007000	-0.09915800
H	2.86306100	3.02143900	-0.12174600
H	4.33293700	-1.72963600	0.07220600
H	5.28752000	2.47825700	-0.08989100
C	6.80142700	-1.15218100	0.05563400
H	6.48214100	-1.65878800	0.97056200

H	6.48726100	-1.72590600	-0.82065200
H	7.88428300	-1.04803700	0.05489200

*** ES of F30 at PBE0/6-311++G(d,p)**

O	-2.31670300	-0.63388900	0.03709100
O	1.81382600	-1.39190200	0.05466500
O	-3.85465100	-0.31862700	-2.26960500
O	-3.86573100	-0.05329700	2.28472300
O	-1.91158200	1.60116200	-0.06777600
O	6.29214100	0.15205300	-0.01234300
O	-0.20291100	-2.23757900	0.08091800
N	-3.62417500	-0.27980700	0.01370300
C	-5.74637100	0.17728900	-0.78510000
C	-5.74900000	0.27179400	0.74300300
C	-4.33204900	-0.16353200	-1.17508700
C	-4.33760200	-0.02516900	1.17724400
C	2.23260900	0.99121800	-0.02519300
C	-0.05835000	0.14619900	0.00171600
C	2.69675000	-0.36833000	0.01857400
C	0.84708100	1.23604600	-0.03323800
C	-1.46721800	0.47524600	-0.01526500
C	3.21911900	2.00732000	-0.05896900
C	0.43176900	-1.21057400	0.04776400
C	4.03321800	-0.69925500	0.02475500
C	4.97667100	0.33218900	-0.01184800
C	4.55381400	1.69380100	-0.05251200
H	-6.02377900	1.11354600	-1.27344800
H	-6.40897300	-0.60197300	-1.16747100
H	-6.41753800	-0.45009800	1.21650500
H	-6.02206800	1.26305300	1.11045400
H	0.46168000	2.24570300	-0.06676800
H	2.90184100	3.04329300	-0.09076400
H	4.31480600	-1.74347900	0.05722000
H	5.31570800	2.46430800	-0.07855900
C	6.81844800	-1.17109800	0.01975000
H	6.50512100	-1.68677700	0.93195800
H	6.49429600	-1.73372800	-0.86040200
H	7.89968200	-1.05743000	0.01041700

S4. The specific data of the calculated emission energies of the studied compounds

Table S.1. The calculated emission energies of coumarin derivatives using 11 DFT functionals (eV)

Compounds	PBE0	PBE	B3LYP	CAM-B3LYP	M06	M06-2X	BP86	LC-ωPBE	APFD	PW6B95D3	ωB97XD
F1	3.54	3.17	3.45	3.68	3.51	3.68	3.18	3.83	3.51	3.52	3.71
F2	2.48	1.86	2.37	3.03	2.53	3.02	1.87	3.32	2.43	2.53	3.06
F3	3.22	2.79	3.13	3.43	3.20	3.45	2.80	3.62	3.19	3.22	3.45
F4	3.46	3.16	3.39	3.55	3.41	3.56	3.16	3.65	3.43	3.44	3.56
F5	3.52	3.25	3.45	3.60	3.46	3.62	3.25	3.69	3.50	3.50	3.62
F6	3.01	2.59	2.92	3.21	3.01	3.19	2.59	3.39	2.97	3.00	3.25
F7	2.63	1.76	2.44	3.45	2.70	3.36	1.77	4.03	2.56	2.67	3.63
F8	3.10	2.61	3.01	3.25	3.06	3.26	2.62	3.39	3.07	3.09	3.28
F9	3.25	2.77	3.16	3.48	3.25	3.47	2.78	3.68	3.21	3.24	3.52
F10	3.20	2.73	3.12	3.46	3.21	3.44	2.73	3.67	3.17	3.20	3.50
F11	3.01	2.65	2.93	3.19	3.00	3.16	2.68	3.35	2.98	3.00	3.21
F12	3.48	2.88	3.41	3.57	3.43	3.58	2.90	3.67	3.46	3.45	3.59
F13	3.33	2.95	3.25	3.48	3.30	3.49	2.95	3.62	3.31	3.32	3.50
F14	3.46	3.16	3.39	3.58	3.41	3.62	3.16	3.75	3.44	3.44	3.62
F15	3.65	3.34	3.41	3.72	3.56	3.73	3.34	3.84	3.59	3.59	3.75
F16	3.32	2.85	3.21	3.54	3.32	3.52	2.85	3.73	3.28	3.30	3.58
F17	2.70	2.44	2.64	2.86	2.68	2.84	2.43	3.00	2.68	2.70	2.89
F18	2.75	2.45	2.68	2.92	2.72	2.91	2.45	3.09	2.73	2.74	2.96
F19	2.86	2.52	2.78	3.05	2.82	3.03	2.52	3.23	2.83	2.85	3.09
F20	3.12	2.73	3.03	3.33	3.10	3.35	2.73	3.55	3.09	3.11	3.37
F21	3.05	2.71	2.97	3.20	3.03	3.19	2.71	3.36	3.02	3.03	3.24
F22	3.00	2.65	2.92	3.16	2.98	3.15	2.66	3.32	2.97	2.98	3.20
F23	3.40	2.89	3.29	3.68	3.35	3.70	2.89	3.94	3.37	3.40	3.72
F24	3.92	3.59	3.84	4.04	3.85	4.07	3.59	4.16	3.90	3.90	4.05
F25	3.76	3.49	3.69	3.83	3.68	3.85	3.49	3.92	3.75	3.73	3.85
F26	3.13	2.67	3.04	3.29	3.09	3.27	2.68	3.44	3.10	3.11	3.32
F27	3.17	2.82	3.06	3.35	3.17	3.35	2.82	3.50	3.13	3.16	3.38
F28	3.09	2.74	3.02	3.26	3.09	3.23	2.75	3.41	3.07	3.08	3.29
F29	3.61	3.27	3.53	3.67	3.56	3.71	3.28	3.82	3.59	3.60	3.68
F30	3.43	2.91	3.35	3.53	3.39	3.54	2.93	3.64	3.41	3.41	3.55

Table S.2. The difference between the calculated emission energies and the experimental emission energies of coumarin derivatives using 11 DFT functionals (eV)

Compounds	PBE0	PBE	B3LYP	CAM-B3LYP	M06	M06-2X	BP86	LC-ωPBE	APFD	PW6B95D3	ωB97XD
F1	0.66	0.29	0.57	0.80	0.63	0.80	0.30	0.94	0.63	0.64	0.83
F2	-0.16	-0.79	-0.28	0.38	-0.12	0.37	-0.78	0.67	-0.22	-0.12	0.41
F3	0.23	-0.20	0.14	0.45	0.21	0.47	-0.19	0.63	0.20	0.23	0.47
F4	0.45	0.15	0.37	0.54	0.39	0.55	0.15	0.63	0.42	0.43	0.55
F5	0.77	0.49	0.70	0.85	0.71	0.86	0.49	0.93	0.75	0.75	0.86
F6	0.42	0.00	0.32	0.62	0.42	0.59	0.00	0.79	0.38	0.40	0.66
F7	0.02	-0.85	-0.17	0.84	0.09	0.75	-0.85	1.42	-0.05	0.06	1.02
F8	0.33	-0.16	0.24	0.48	0.29	0.49	-0.15	0.62	0.30	0.32	0.51
F9	0.54	0.07	0.45	0.78	0.55	0.77	0.08	0.98	0.51	0.54	0.82
F10	0.55	0.08	0.47	0.81	0.56	0.79	0.08	1.02	0.52	0.55	0.85
F11	0.40	0.04	0.33	0.58	0.39	0.56	0.07	0.75	0.38	0.39	0.61
F12	0.71	0.11	0.63	0.80	0.66	0.81	0.13	0.89	0.69	0.68	0.82
F13	0.35	-0.04	0.26	0.50	0.31	0.51	-0.04	0.63	0.32	0.34	0.51
F14	0.99	0.69	0.92	1.11	0.94	1.15	0.69	1.28	0.97	0.97	1.15
F15	0.38	0.08	0.14	0.46	0.30	0.47	0.08	0.58	0.33	0.33	0.48
F16	0.54	0.08	0.44	0.77	0.54	0.75	0.08	0.96	0.51	0.52	0.81
F17	0.22	-0.04	0.16	0.38	0.20	0.36	-0.05	0.52	0.20	0.22	0.41
F18	0.19	-0.11	0.12	0.36	0.16	0.35	-0.11	0.53	0.16	0.18	0.40
F19	0.26	-0.07	0.19	0.46	0.23	0.44	-0.07	0.64	0.24	0.26	0.50
F20	0.56	0.16	0.47	0.77	0.54	0.79	0.17	0.99	0.53	0.55	0.81
F21	0.44	0.10	0.36	0.59	0.42	0.58	0.10	0.75	0.41	0.42	0.63
F22	0.31	-0.03	0.23	0.48	0.30	0.46	-0.03	0.64	0.28	0.30	0.51
F23	0.44	-0.06	0.34	0.73	0.40	0.75	-0.06	0.98	0.42	0.44	0.77
F24	0.52	0.19	0.43	0.63	0.44	0.66	0.19	0.75	0.49	0.49	0.65
F25	0.55	0.29	0.49	0.62	0.48	0.65	0.29	0.72	0.54	0.53	0.65
F26	0.40	-0.06	0.32	0.57	0.37	0.55	-0.04	0.72	0.38	0.38	0.60
F27	0.55	0.20	0.44	0.73	0.55	0.73	0.20	0.88	0.51	0.54	0.76
F28	0.52	0.17	0.46	0.70	0.52	0.66	0.18	0.84	0.50	0.51	0.72
F29	0.53	0.19	0.45	0.59	0.48	0.63	0.19	0.74	0.50	0.52	0.60
F30	**0.40**	**-0.11**	**0.33**	**0.51**	**0.36**	**0.52**	**-0.09**	**0.61**	**0.38**	**0.38**	**0.53**
MSE	**0.44**	**0.03**	**0.34**	**0.63**	**0.41**	**0.63**	**0.03**	**0.80**	**0.41**	**0.43**	**0.66**
MAE	**0.45**	**0.20**	**0.37**	**0.63**	**0.42**	**0.63**	**0.20**	**0.80**	**0.42**	**0.43**	**0.66**
RMSE	**0.49**	**0.29**	**0.41**	**0.65**	**0.46**	**0.65**	**0.29**	**0.83**	**0.46**	**0.47**	**0.69**

S5. The specific data of the calculated excited energies of the studied compounds

Table S.3. The calculated excited energies of coumarin derivatives using 11 DFT functionals (eV)

Compounds	PBE0	PBE	B3LYP	CAM-B3LYP	M06	M06-2X	BP86	LC-ωPBE	APFD	PW6B95D3	ωB97XD
F1	3.79	3.32	3.69	4.00	3.76	4.00	3.33	4.20	3.76	3.77	4.03
F2	3.32	2.92	3.23	3.50	3.31	3.48	2.92	3.66	3.29	3.30	3.53
F3	3.68	3.16	3.58	3.94	3.65	3.96	3.16	4.15	3.65	3.68	3.95
F4	3.70	3.33	3.63	3.85	3.66	3.88	3.34	4.00	3.68	3.69	3.88
F5	3.79	3.45	3.71	3.92	3.72	3.95	3.45	4.07	3.77	3.77	3.94
F6	3.11	2.69	3.02	3.31	3.11	3.29	2.69	3.47	3.08	3.10	3.34
F7	3.49	2.56	3.37	3.80	3.49	3.79	2.60	4.06	3.46	3.49	3.86
F8	3.43	2.61	3.36	3.54	3.39	3.53	2.64	3.65	3.41	3.41	3.56
F9	3.47	2.95	3.37	3.75	3.47	3.75	2.96	3.99	3.43	3.47	3.79
F10	3.43	2.91	3.33	3.72	3.44	3.71	2.92	3.96	3.40	3.43	3.77
F11	3.23	2.78	3.14	3.47	3.23	3.46	2.79	3.69	3.21	3.23	3.51
F12	3.71	3.35	3.63	3.85	3.67	3.86	3.35	3.97	3.69	3.69	3.86
F13	3.52	3.05	3.42	3.71	3.48	3.73	3.05	3.90	3.49	3.51	3.75
F14	3.90	3.48	3.80	4.09	3.84	4.13	3.46	4.31	3.86	3.89	4.12
F15	4.01	3.57	3.92	4.20	3.96	4.23	3.58	4.40	3.99	4.00	4.23
F16	3.53	3.01	3.43	3.80	3.53	3.79	3.02	4.01	3.49	3.52	3.84
F17	2.95	2.61	2.87	3.16	2.94	3.13	2.61	3.34	2.92	2.95	3.19
F18	3.15	2.73	3.07	3.29	3.12	3.27	2.82	3.43	3.12	3.12	3.32
F19	3.26	2.82	3.17	3.51	3.25	3.48	2.82	3.72	3.24	3.26	3.55
F20	3.48	3.03	3.38	3.71	3.45	3.73	3.03	3.95	3.44	3.47	3.76
F21	3.18	2.84	3.11	3.33	3.16	3.32	2.84	3.49	3.16	3.16	3.37
F22	3.14	2.82	3.07	3.29	3.12	3.27	2.82	3.43	3.12	3.12	3.32
F23	4.41	3.97	4.31	5.61	4.29	4.41	3.97	5.88	4.38	4.41	5.66
F24	4.41	4.00	4.32	4.58	4.34	4.61	4.00	4.75	4.38	4.40	4.59
F25	4.13	3.73	4.04	4.28	4.05	4.32	3.73	4.46	4.11	4.12	4.31
F26	3.36	2.85	3.27	3.57	3.32	3.55	2.87	3.75	3.33	3.35	3.60
F27	3.44	2.63	3.34	3.70	3.42	3.71	2.65	3.92	3.40	3.45	3.73
F28	3.23	2.88	3.16	3.38	3.22	3.35	2.89	3.51	3.20	3.21	3.41
F29	3.52	2.26	3.34	4.09	3.53	4.12	2.29	4.26	3.43	3.61	4.11
F30	3.64	3.27	3.55	3.79	3.59	3.80	3.12	3.94	3.62	3.63	3.82

Table S.4. The difference between the calculated Stokes shift and the experimental Stokes shift of coumarin derivatives using 11 DFT functionals (eV)

Compounds	PBE0	PBE	B3LYP	CAM-B3LYP	M06	M06-2X	BP86	LC-ωPBE	APFD	PW6B95D3	ωB97XD
F1	0.40	0.50	0.41	0.33	0.40	0.33	0.50	0.27	0.40	0.40	0.34
F2	-0.53	-0.76	-0.56	-0.17	-0.48	-0.16	-0.75	-0.04	-0.55	-0.46	-0.17
F3	0.20	0.30	0.21	0.16	0.21	0.15	0.29	0.13	0.20	0.20	0.16
F4	0.24	0.31	0.24	0.18	0.22	0.16	0.30	0.12	0.23	0.23	0.16
F5	0.01	0.08	0.03	-0.04	0.02	-0.05	0.08	-0.09	0.02	0.02	-0.04
F6	0.15	0.15	0.15	0.16	0.15	0.15	0.15	0.16	0.15	0.15	0.16
F7	-0.17	-0.11	-0.23	0.34	-0.09	0.26	-0.14	0.67	-0.20	-0.13	0.47
F8	0.11	0.44	0.10	0.16	0.11	0.17	0.43	0.18	0.11	0.12	0.16
F9	0.42	0.47	0.44	0.39	0.43	0.38	0.47	0.34	0.43	0.41	0.38
F10	0.42	0.46	0.43	0.39	0.42	0.38	0.46	0.36	0.42	0.42	0.38
F11	0.28	0.36	0.29	0.21	0.26	0.19	0.39	0.16	0.26	0.26	0.19
F12	-0.04	-0.28	-0.03	-0.09	-0.05	-0.09	-0.26	-0.12	-0.04	-0.05	-0.08
F13	0.27	0.35	0.29	0.23	0.27	0.21	0.35	0.17	0.27	0.27	0.21
F14	0.31	0.42	0.33	0.24	0.32	0.23	0.44	0.19	0.33	0.31	0.25
F15	0.20	0.33	0.05	0.08	0.17	0.07	0.32	0.01	0.17	0.16	0.08
F16	0.33	0.39	0.34	0.29	0.33	0.28	0.38	0.27	0.34	0.33	0.30
F17	-0.02	0.05	-0.01	-0.08	-0.04	-0.07	0.04	-0.12	-0.02	-0.03	-0.08
F18	-0.12	0.00	-0.11	-0.08	-0.12	-0.08	-0.09	-0.05	-0.11	-0.10	-0.07
F19	0.04	0.15	0.05	-0.01	0.02	-0.01	0.15	-0.05	0.04	0.03	-0.02
F20	0.31	0.36	0.32	0.29	0.31	0.28	0.37	0.27	0.32	0.30	0.28
F21	0.10	0.10	0.10	0.10	0.10	0.11	0.10	0.10	0.10	0.10	0.10
F22	-0.04	-0.07	-0.05	-0.02	-0.04	-0.02	-0.07	0.00	-0.05	-0.04	-0.02
F23	0.49	0.42	0.49	-0.42	0.57	0.80	0.42	-0.43	0.50	0.49	-0.43
F24	0.53	0.62	0.54	0.49	0.54	0.48	0.62	0.43	0.54	0.52	0.48
F25	0.22	0.36	0.25	0.15	0.23	0.13	0.36	0.06	0.24	0.21	0.14
F26	0.48	0.53	0.49	0.45	0.49	0.44	0.53	0.41	0.49	0.48	0.44
F27	0.13	0.60	0.13	0.07	0.15	0.05	0.58	0.00	0.13	0.13	0.06
F28	0.10	0.09	0.11	0.12	0.11	0.12	0.10	0.13	0.10	0.10	0.12
F29	0.70	1.61	0.80	0.19	0.63	0.19	1.60	0.17	0.76	0.60	0.18
F30	0.23	0.08	0.24	0.18	0.23	0.18	0.25	0.14	0.23	0.22	0.18
MSE	**0.19**	**0.28**	**0.19**	**0.14**	**0.20**	**0.18**	**0.28**	**0.13**	**0.19**	**0.19**	**0.14**
MAE	**0.25**	**0.36**	**0.26**	**0.20**	**0.25**	**0.21**	**0.37**	**0.19**	**0.26**	**0.24**	**0.20**
RMSE	**0.31**	**0.47**	**0.32**	**0.24**	**0.31**	**0.26**	**0.47**	**0.24**	**0.32**	**0.29**	**0.25**

S6. The optimized complex configurations between F1 and MeOH and their coordinates

S6.1. The complex configurations with an F1: MeOH molar ratio of 1:1

S6.1.1. F1-MeOH-1

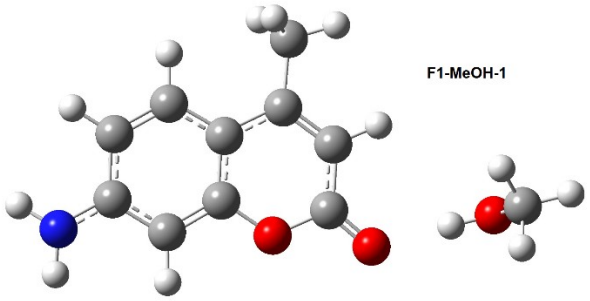


Fig.S5. The optimized complex configuration of F1-MeOH-1

The coordinates of F1-MeOH-1

O	0.11208100	-1.27378700	-0.14508900
O	2.30052900	-1.36690100	-0.30287700
N	-4.60588000	-1.44675700	0.22723300
C	-1.07920500	0.81339900	-0.02487500
C	0.17179800	1.51324800	-0.09754800
C	-1.06147400	-0.58992800	-0.05071000
C	-2.34077800	1.42970300	0.07070200
C	-2.21215100	-1.35407600	0.01532600
C	-3.45516200	-0.72004200	0.11195600
C	1.32207400	0.78857100	-0.19023300
C	-3.49838200	0.69292000	0.13829700
C	0.20723000	3.00578100	-0.07077300
C	1.32014400	-0.64224200	-0.21878700
H	-2.40318000	2.51199900	0.09096200
H	-2.13355400	-2.43540300	-0.00831300
H	2.29157800	1.26783500	-0.24915800
H	-4.45811700	1.19355600	0.21293800
H	-0.24292500	3.38736000	0.85083200
H	-0.36516100	3.42203700	-0.90542500
H	1.23129300	3.37383200	-0.13493400
H	-4.58594800	-2.41981900	-0.03218700
H	-5.48079000	-0.98093700	0.04829800
C	5.42139100	-0.33312800	0.82086200

H	6.45993200	0.00052400	0.76363000
H	4.84907500	0.42707600	1.36876800
H	5.39432200	-1.26753700	1.39637800
O	4.94863400	-0.50697300	-0.49815400
H	4.02177400	-0.79718100	-0.44877100

S6.1.2. F1-MeOH-2

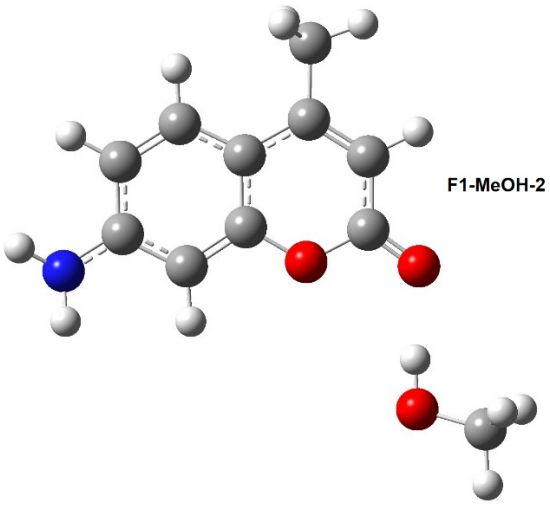


Fig.S6. The optimized complex configuration of F1-MeOH-2

The coordinates of F1-MeOH-2

O	0.74472500	0.26743400	0.05527500
O	2.61636500	-0.89055900	0.08024500
N	-3.08393200	3.05495900	0.04509700
C	-1.41326500	-0.79438600	-0.00703800
C	-0.76480000	-2.07526300	-0.00848300
C	-0.61363700	0.35875800	0.02605300
C	-2.80647300	-0.59863800	-0.03896300
C	-1.14227800	1.63639300	0.02863300
C	-2.53010800	1.80709100	-0.00314500
C	0.59668200	-2.11983200	0.02177100
C	-3.35653300	0.66054100	-0.03658000
C	-1.57134800	-3.33141400	-0.04228500
C	1.39572400	-0.93343400	0.05369900
H	-3.46339600	-1.46080600	-0.06734500
H	-0.47244900	2.48871800	0.05496000
H	1.13606800	-3.05875100	0.02223900
H	-4.43436100	0.78357200	-0.06092000
H	-2.20121400	-3.36362900	-0.93661200

H	-2.23807200	-3.38695400	0.82372600
H	-0.92640100	-4.21019200	-0.04052000
H	-2.49974500	3.84576200	-0.17419200
H	-4.04795700	3.15544100	-0.22878500
C	5.46889100	1.02192000	-0.15865900
H	6.11329800	1.90399200	-0.15197700
H	5.56408600	0.53777300	-1.13942300
H	5.83549100	0.32605600	0.60726200
O	4.14802100	1.44810400	0.09836500
H	3.57216600	0.66405300	0.09481000

S6.1.3. F1-MeOH-3

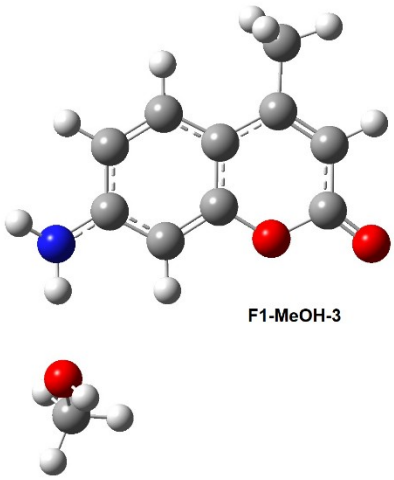


Fig.S7. The optimized complex configuration of F1-MeOH-3

The coordinates of F1-MeOH-3

O	0.78915800	1.55138300	-0.02610400
O	2.30031700	3.15684900	-0.04721700
N	-2.70316200	-1.63888200	0.04773300
C	1.40207500	-0.77598700	0.01586700
C	2.78619100	-0.39576600	0.01679600
C	0.43035800	0.23833400	-0.00538600
C	0.93238200	-2.10264000	0.03300600
C	-0.92612400	-0.02779800	-0.00793100
C	-1.37401400	-1.35599400	0.01232700
C	3.10245700	0.92877900	-0.00384000
C	-0.41058900	-2.39319800	0.03177000
C	3.85623200	-1.43825800	0.04006900
C	2.10293800	1.95818800	-0.02698800

H	1.64758000	-2.91785400	0.04679300
H	-1.63137800	0.79559700	-0.02542700
H	4.13155100	1.26656000	-0.00402300
H	-0.74381100	-3.42593300	0.04530000
H	3.77466400	-2.09811700	-0.82921100
H	3.76604700	-2.06751800	0.93091300
H	4.84647400	-0.98215400	0.03695300
H	-3.37614600	-0.90631000	-0.16410700
H	-2.99653400	-2.58598000	-0.12521200
C	-4.98603900	1.45412500	0.48633500
H	-5.97268900	1.88280400	0.28365300
H	-5.02880600	0.90883500	1.42983200
H	-4.25379400	2.26291600	0.57997700
O	-4.61086700	0.52003200	-0.51782600
H	-4.56510000	0.97451800	-1.36253400

S6.1.4. F1-MeOH-4

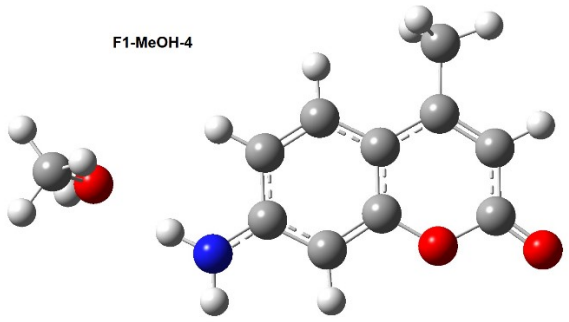


Fig.S8. The optimized complex configuration of F1-MeOH-4

The coordinates of F1-MeOH-4

O	2.14601700	-1.46611200	0.02690400
O	4.34359100	-1.64381400	0.05765200
N	-2.59233300	-1.42557900	-0.00699800
C	1.03984300	0.67155800	-0.00866500
C	2.32150700	1.31748800	0.00315200
C	0.99955200	-0.73250700	0.00401800
C	-0.19882400	1.34067800	-0.03517600
C	-0.18539600	-1.44520600	-0.00666600
C	-1.40768000	-0.76032200	-0.03100500
C	3.44444800	0.54694200	0.02591500
C	-1.38960500	0.65603000	-0.04592300

C	2.41694700	2.80855200	-0.00938600
C	3.39341200	-0.88679000	0.03813300
H	-0.21517800	2.42510900	-0.04888200
H	-0.15265500	-2.52930000	0.00447300
H	4.43435500	0.98639000	0.03552300
H	-2.33267400	1.19191900	-0.06962000
H	1.90899000	3.23763200	0.85984000
H	1.93396200	3.22122600	-0.90053300
H	3.45750100	3.13371300	0.00229000
H	-2.59596400	-2.41811900	-0.17318000
H	-3.45097000	-0.92082600	-0.21234600
C	-5.92760200	0.39660300	0.53502700
H	-5.36349200	0.48007400	1.46471500
H	-6.62111200	-0.44657100	0.61846100
H	-6.49770300	1.31918600	0.38629600
O	-4.98273900	0.19751000	-0.50861700
H	-5.45329900	0.11977900	-1.34211800

S6.2. The complex configurations with an F1: MeOH molar ratio of 1:2

S6.2.1. F1-2MeOH-1

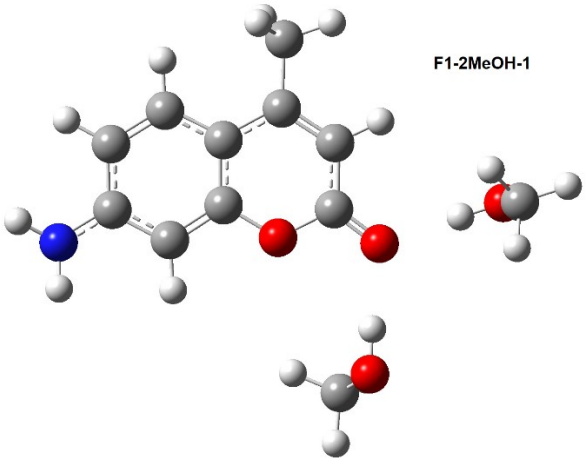


Fig.S9. The optimized complex configuration of F1-2MeOH-1

The coordinates of F1-2MeOH-1

O	-0.00247800	-0.67007000	-0.03052900
O	-2.16786700	-0.34119300	0.08906500
N	4.59747400	-1.75854200	-0.27882000
C	1.58245500	1.13624600	0.07253500

C	0.49451100	2.06004800	0.20515000
C	1.28752200	-0.23143000	-0.04240800
C	2.94423300	1.49382900	0.04554900
C	2.26221200	-1.20198600	-0.17419000
C	3.60882300	-0.82328600	-0.19642200
C	-0.78090100	1.57397400	0.21250700
C	3.93247600	0.54954200	-0.08441400
C	0.75464000	3.52435100	0.33248700
C	-1.05397700	0.17975200	0.09248200
H	3.22099500	2.53891900	0.12792200
H	1.96961100	-2.24269400	-0.25815900
H	-1.63909900	2.22703500	0.31094700
H	4.97441900	0.85179200	-0.10207100
H	1.29358000	3.89874100	-0.54324600
H	1.37799300	3.73152500	1.20762700
H	-0.17743900	4.08074700	0.43039100
H	4.35899000	-2.68906700	-0.58119700
H	5.52567400	-1.45480700	-0.52403600
C	-1.91781800	-3.80494500	0.67983200
H	-2.06882800	-4.87089500	0.49511100
H	-0.83783600	-3.60999600	0.69838300
H	-2.32899500	-3.56847000	1.66998300
O	-2.56744700	-3.09069200	-0.35036600
H	-2.40919800	-2.14320400	-0.20405800
C	-5.04610400	1.37291600	-0.87851900
H	-5.98659600	1.91761600	-0.77014900
H	-4.34154900	2.01381700	-1.42459300
H	-5.23805400	0.47640000	-1.48198000
O	-4.58012400	1.05268300	0.41579900
H	-3.74109100	0.57244200	0.32157200

S6.2.2. F1-2MeOH-2

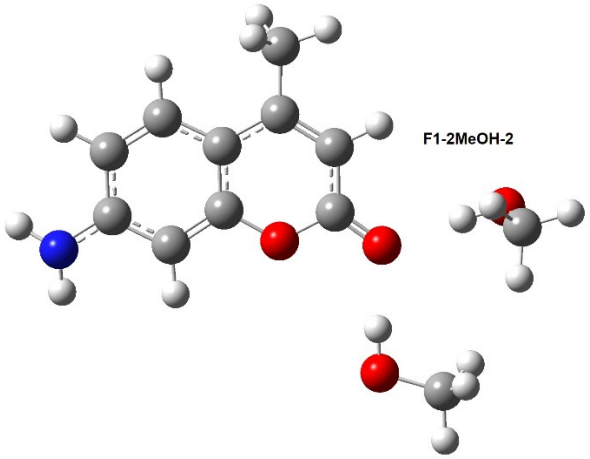


Fig.S10. The optimized complex configuration of F1-2MeOH-2

The coordinates of F1-2MeOH-2

O	0.10637000	0.69999800	-0.05480500
O	-2.01529000	0.16224200	-0.19637400
N	4.57287700	2.22595400	0.29755400
C	1.85595100	-0.95075000	-0.05088100
C	0.86244700	-1.97860100	-0.15549000
C	1.43144800	0.38646700	-0.00204200
C	3.24487100	-1.17570600	0.00564400
C	2.30809700	1.44973700	0.09782400
C	3.68388100	1.20217400	0.15383000
C	-0.45264400	-1.61652600	-0.20330700
C	4.13753300	-0.13720500	0.10547100
C	1.26099900	-3.41606100	-0.21098400
C	-0.85784400	-0.25041400	-0.15531100
H	3.62010000	-2.19222100	-0.03146900
H	1.91787000	2.46073700	0.13069000
H	-1.24316100	-2.35223300	-0.28267200
H	5.20290000	-0.33832900	0.14808600
H	1.82487900	-3.69613800	0.68400900
H	1.90912700	-3.60431100	-1.07240500
H	0.38631300	-4.06201200	-0.28687400
H	4.26297300	3.16540000	0.10851600
H	5.54467800	2.04947100	0.10147900
C	-4.14688600	2.88025800	-0.21851600
H	-4.48212500	3.91980700	-0.20730700
H	-4.61979400	2.36027700	0.62492800
H	-4.49777800	2.41824800	-1.15038600

O	-2.73811200	2.87899900	-0.12182400
H	-2.43615000	1.95586700	-0.14285300
C	-4.84774800	-1.50877900	0.93101500
H	-5.75398100	-2.11695800	0.88819300
H	-4.14763000	-1.98794700	1.62770200
H	-5.11656200	-0.52331700	1.33316400
O	-4.32174000	-1.42343800	-0.37697200
H	-3.51225500	-0.88799000	-0.33940100

S6.2.3. F1-2MeOH-3

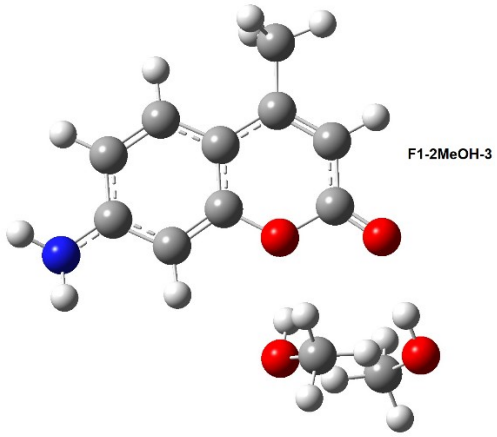


Fig.S11. The optimized complex configuration of F1-2MeOH-3

The coordinates of F1-2MeOH-3

O	-0.44126100	0.12814400	-0.08228200
O	-2.06811400	1.58180000	-0.39068600
N	2.80815700	-3.24224900	0.65080500
C	1.87032200	0.79133300	-0.02250000
C	1.46809400	2.15121600	-0.24359500
C	0.87828300	-0.19833700	0.05172700
C	3.20258600	0.36201500	0.12520200
C	1.16376400	-1.53458900	0.25699700
C	2.49611800	-1.93763700	0.40184100
C	0.14014500	2.43148300	-0.37054500
C	3.51462000	-0.95956300	0.33264400
C	2.48872900	3.23751800	-0.33016700
C	-0.86380300	1.41817400	-0.29008400
H	4.00410500	1.09034000	0.07338700
H	0.35414400	-2.25488700	0.30050400
H	-0.21570200	3.44052100	-0.53640100
H	4.55044400	-1.26261500	0.44457100

H	3.19229000	3.04413800	-1.14570200
H	3.07299700	3.29431000	0.59340300
H	2.01641200	4.20479800	-0.50157700
H	2.11142300	-3.94659900	0.46944500
H	3.75980100	-3.54056300	0.51062200
C	-2.93051700	-1.82241100	-2.14514900
H	-3.44936300	-2.73150300	-2.45469500
H	-2.20697100	-1.55561100	-2.92516000
H	-3.66836200	-1.01585400	-2.05913100
O	-2.29911700	-2.09496700	-0.90759300
H	-1.83424900	-1.29957800	-0.62626600
C	-3.93249700	-0.00383200	2.12860000
H	-4.82367400	-0.34902500	2.65729200
H	-3.25978200	-0.86107700	1.99689700
H	-3.42830500	0.74054700	2.75841100
O	-4.34763100	0.53962900	0.89268600
H	-3.55838000	0.84933300	0.42194200

S6.2.4. F1-2MeOH-4

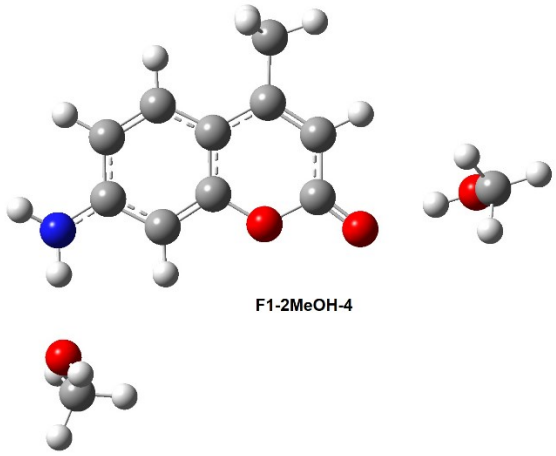


Fig.S12. The optimized complex configuration of F1-2MeOH-4

The coordinates of F1-2MeOH-4

O	0.45434200	-0.80845000	-0.14285200
O	2.46361900	-1.68137800	-0.29696700
N	-4.01121700	0.71822500	0.15714200
C	0.08929400	1.56852700	-0.04388300
C	1.50532400	1.77254600	-0.12530900
C	-0.39833300	0.25084400	-0.05545000
C	-0.86906000	2.59636200	0.05100600

C	-1.74409300	-0.05099900	0.02013600
C	-2.68242800	0.98702800	0.11250100
C	2.32168600	0.68286600	-0.21013200
C	-2.21246900	2.32368400	0.12625800
C	2.07351200	3.15383700	-0.11733600
C	1.80817900	-0.65140600	-0.22219200
H	-0.53920300	3.62935500	0.06517200
H	-2.06133200	-1.08767300	0.00761600
H	3.39811000	0.78380000	-0.27457500
H	-2.92964400	3.13498900	0.19818000
H	1.79225400	3.68342000	0.79809800
H	1.68602800	3.73669100	-0.95859100
H	3.16137500	3.13020000	-0.18408600
H	-4.33115200	-0.23395600	0.31727300
H	-4.64885300	1.46219000	0.38582400
C	-4.95815700	-2.96017000	-0.52173300
H	-5.68428000	-3.75516200	-0.32439700
H	-5.28791700	-2.39373200	-1.39335800
H	-3.98333300	-3.40806300	-0.74092900
O	-4.88316200	-2.04606100	0.56486400
H	-4.59223300	-2.51842900	1.34873000
C	5.72971200	-1.83943400	0.85441900
H	6.81954500	-1.89819100	0.80934000
H	5.46022800	-0.92791600	1.40415400
H	5.36451400	-2.70556600	1.42156300
O	5.24079300	-1.82623300	-0.46994100
H	4.27066900	-1.76466400	-0.43055200

S6.2.5. F1-2MeOH-5

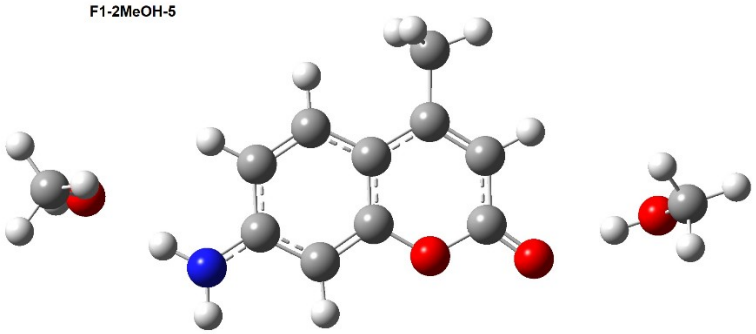


Fig.S13. The optimized complex configuration of F1-2MeOH-5

The coordinates of F1-2MeOH-5

O	1.20442500	-1.28160100	-0.16968200
O	3.39824600	-1.34994200	-0.24208000
N	-3.52437900	-1.50194500	-0.00048700
C	-0.01707800	0.79111100	-0.11042300
C	1.22516100	1.50431600	-0.14004600
C	0.01801300	-0.61317900	-0.12627300
C	-1.29115700	1.39129000	-0.06805200
C	-1.12311300	-1.39186000	-0.10006000
C	-2.38107000	-0.77483900	-0.05652700
C	2.38943600	0.79421600	-0.18328500
C	-2.44053000	0.64171100	-0.04159100
C	1.24257000	2.99780000	-0.12378300
C	2.40649100	-0.63503200	-0.20127000
H	-1.36707100	2.47308800	-0.05732100
H	-1.02947500	-2.47220600	-0.11351500
H	3.35367000	1.28680400	-0.20856200
H	-3.41201700	1.12375500	-0.01205600
H	0.75307000	3.38146100	0.77662800
H	0.69815400	3.40122800	-0.98308100
H	2.26415200	3.37735800	-0.15154900
H	-3.48576200	-2.49412300	-0.16301000
H	-4.42142000	-1.04089700	-0.13115800
C	-6.92515200	0.11554200	0.78300100
H	-6.32926500	0.17224500	1.69468200
H	-7.58584100	-0.75514500	0.84763900
H	-7.53139700	1.02340600	0.70270700
O	-6.01439900	0.00327300	-0.30311700
H	-6.51313300	-0.05167700	-1.12191600
C	6.46019500	-0.27773900	0.98658700
H	7.49684100	0.06596700	0.96488800
H	5.86099900	0.48020800	1.50832500
H	6.42143300	-1.20854200	1.56733700
O	6.03720100	-0.46496900	-0.34725000
H	5.11133000	-0.76340500	-0.32927200

S6.2.6. F1-2MeOH-6

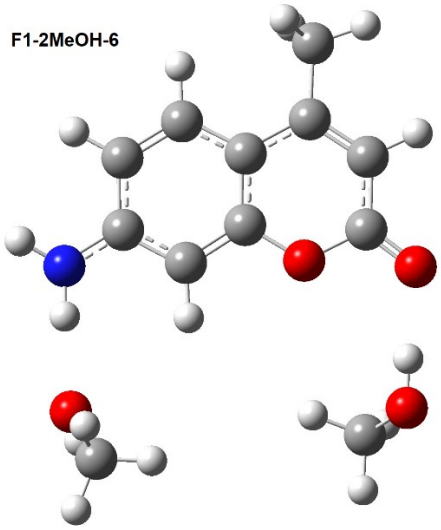


Fig.S14. The optimized complex configuration of F1-2MeOH-6

The coordinates of F1-2MeOH-6

O	0.71755300	0.93538700	-0.11469400
O	2.04114400	2.69279200	-0.16872900
N	-2.41175400	-2.60646100	0.01901000
C	1.57524800	-1.30810200	0.03372500
C	2.90769200	-0.77975500	0.04487000
C	0.49951400	-0.40801600	-0.04699100
C	1.24967900	-2.67697000	0.09695900
C	-0.81987400	-0.81570000	-0.06426700
C	-1.12297500	-2.18317200	0.00177700
C	3.07914000	0.57187900	-0.02246400
C	-0.05359300	-3.10902000	0.08270900
C	4.08473100	-1.69546000	0.12869600
C	1.97309200	1.47351900	-0.10507500
H	2.04707200	-3.40945200	0.15823200
H	-1.60789600	-0.07412000	-0.13042100
H	4.06381100	1.02215800	-0.01680900
H	-0.27607000	-4.16991000	0.13396900
H	4.09404100	-2.39277000	-0.71464100
H	4.04422900	-2.29609200	1.04255300
H	5.01885800	-1.13349600	0.12412900
H	-3.16023600	-1.95501500	-0.20386000
H	-2.60246700	-3.58707800	-0.10121000
C	-1.13795100	4.03410400	0.55782100
H	-1.98923600	4.70870100	0.44065900

H	-1.50092900	3.00308400	0.45659400
H	-0.73987500	4.16125500	1.57327900
O	-0.18636300	4.36102900	-0.43187200
H	0.56878500	3.75392400	-0.33869700
C	-4.90645300	0.30008000	0.43744500
H	-5.92780200	0.65375000	0.26437200
H	-4.87281600	-0.21584600	1.39767400
H	-4.22902900	1.15984700	0.47564700
O	-4.50823300	-0.63839400	-0.55377100
H	-4.53046200	-0.21054100	-1.41325400

S6.2.7. F1-2MeOH-7

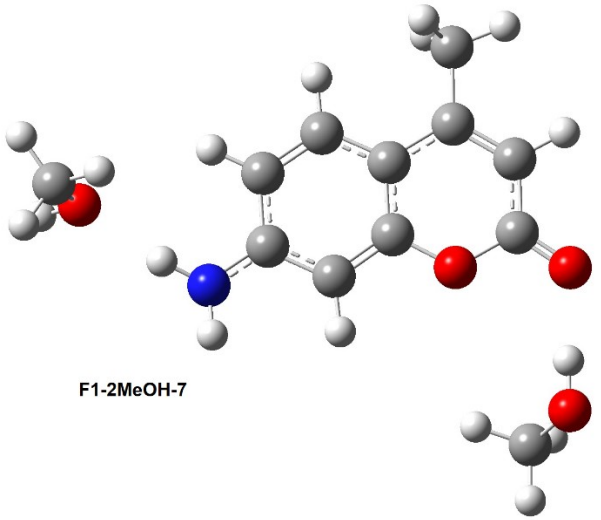


Fig.S15. The optimized complex configuration of F1-2MeOH-7

The coordinates of F1-2MeOH-7

O	-1.76674500	-0.27833500	-0.13141400
O	-3.88970800	0.24923200	-0.37630200
N	2.70379300	-1.75096000	0.40987000
C	-0.05499600	1.39309100	0.12541000
C	-1.05894600	2.41149800	0.02964600
C	-0.45521300	0.04937200	0.03920000
C	1.32252600	1.63246200	0.29907300
C	0.43469700	-1.00462900	0.11901000
C	1.80081000	-0.74466800	0.29395000
C	-2.36001400	2.03799200	-0.13979100
C	2.22802700	0.60419000	0.38187300

C	-0.68420300	3.85491900	0.11444700
C	-2.74984700	0.66571100	-0.22546500
H	1.67793200	2.65475400	0.36806700
H	0.06347200	-2.02093800	0.04474100
H	-3.15668200	2.76719300	-0.21734100
H	3.28507000	0.80978300	0.51430200
H	0.02394600	4.11896000	-0.67697500
H	-0.19614200	4.07328700	1.06929500
H	-1.56289500	4.49323200	0.02028800
H	2.42181000	-2.69015900	0.18389300
H	3.69698200	-1.53809300	0.35784600
C	6.16259100	-0.79995900	-0.98732100
H	5.42431600	-0.44694000	-1.70836700
H	6.54750400	-1.76846300	-1.32291600
H	6.98539300	-0.07921500	-0.94610400
O	5.50197700	-0.90414500	0.26744600
H	6.13034200	-1.21379100	0.92438800
C	-4.03757700	-3.13937600	0.51738200
H	-4.29671000	-4.19561200	0.41399500
H	-2.94553900	-3.06061100	0.59530800
H	-4.47757600	-2.77071400	1.45351600
O	-4.53911000	-2.45670300	-0.61149700
H	-4.28622500	-1.51996500	-0.53336500

S6.2.8. F1-2MeOH-8

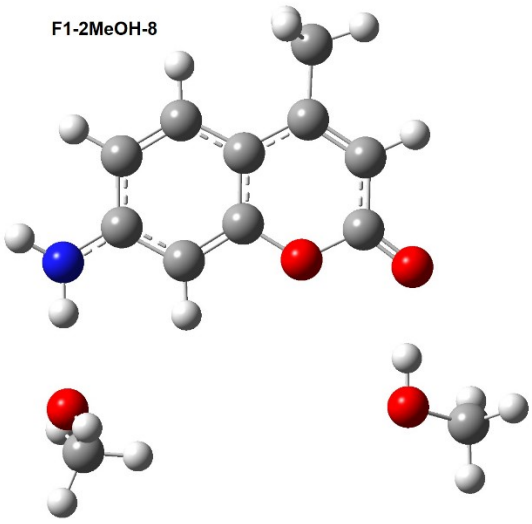


Fig.S16. The optimized complex configuration of F1-2MeOH-8

The coordinates of F1-2MeOH-8

O	0.97971300	0.27810900	-0.11047800
O	3.09930500	0.86558300	-0.19903500
N	-3.65714100	-0.62968000	0.08750800
C	0.29698600	-2.02507700	0.03215600
C	1.67556500	-2.41726700	0.01707400
C	-0.01008100	-0.65567200	-0.03415600
C	-0.79294900	-2.91375000	0.10649900
C	-1.30547300	-0.17663900	-0.02825800
C	-2.37693900	-1.07812900	0.04778600
C	2.63301500	-1.44895000	-0.06125800
C	-2.09027900	-2.46400700	0.11519600
C	2.05334500	-3.86074100	0.08540400
C	2.30316500	-0.05969500	-0.12756700
H	-0.60468500	-3.98050700	0.15741100
H	-1.48077400	0.89189500	-0.08296900
H	3.68822200	-1.69125400	-0.07627400
H	-2.91052800	-3.17214400	0.17373100
H	1.62510200	-4.41372100	-0.75628900
H	1.66854000	-4.31949500	1.00137500
H	3.13645200	-3.98278800	0.06520100
H	-3.85871400	0.34127900	-0.13925300
H	-4.40600500	-1.29150100	-0.02999600
C	3.56681500	4.22447600	0.34287200
H	3.37364100	5.29968800	0.33528000
H	4.48849500	4.03972800	-0.22436600
H	3.73387400	3.91578600	1.38318100
O	2.45056100	3.57890000	-0.23107700
H	2.62184400	2.62091300	-0.22596000
C	-4.02401400	3.20518600	0.44459700
H	-4.64359800	4.07714900	0.21216100
H	-4.35257000	2.78628900	1.39638400
H	-2.97954500	3.51971500	0.53996200
O	-4.17751100	2.18521400	-0.53427200
H	-3.89125200	2.52587800	-1.38531400

S6.2.9. F1-2MeOH-9

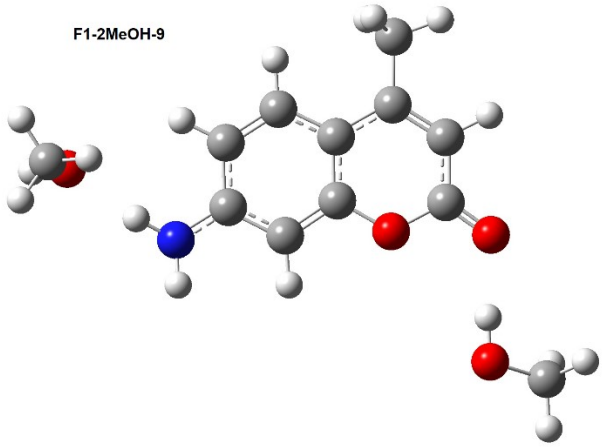


Fig.S17. The optimized complex configuration of F1-2MeOH-9

The coordinates of F1-2MeOH-9

O	1.62180100	-0.30219800	0.03548200
O	3.74116700	0.24813100	0.26095600
N	-2.83625100	-1.81998400	-0.48110300
C	-0.12105900	1.35129200	-0.10088900
C	0.86883700	2.38015700	0.02334100
C	0.30177700	0.01170300	-0.09029600
C	-1.50568900	1.57606400	-0.23279200
C	-0.57324200	-1.05160700	-0.20303900
C	-1.94683300	-0.80602500	-0.33560400
C	2.17901400	2.02037600	0.14620900
C	-2.39680700	0.53833200	-0.34700200
C	0.47026800	3.81970800	0.01822900
C	2.59186600	0.65221800	0.15505500
H	-1.87826100	2.59449800	-0.24320900
H	-0.18487400	-2.06401100	-0.18780300
H	2.96558000	2.75818900	0.24289900
H	-3.45964700	0.73242700	-0.44603200
H	-0.22059000	4.03371800	0.83953300
H	-0.04609300	4.07596100	-0.91198000
H	1.34156500	4.46684700	0.12062000
H	-2.53478500	-2.76563000	-0.31554800
H	-3.83196400	-1.62691800	-0.40650200
C	5.88901800	-2.41639500	-0.07141700
H	6.24684400	-3.44859000	-0.06844500
H	6.48050400	-1.84851300	0.65869900
H	6.07368500	-1.99478200	-1.06822600

O	4.51563300	-2.43231100	0.25359200
H	4.19519600	-1.51333500	0.25328000
C	-6.32727300	-1.07670000	0.98009000
H	-5.60414200	-0.80110300	1.74863500
H	-6.70620100	-2.08079300	1.19685300
H	-7.15754000	-0.36390200	1.00763800
O	-5.64654200	-1.03096900	-0.26736200
H	-6.26125400	-1.27013800	-0.96535300

S6.2.10. F1-2MeOH-10

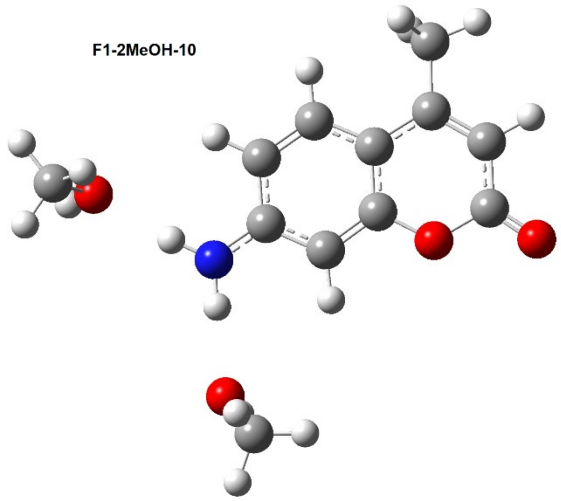


Fig.S18. The optimized complex configuration of F1-2MeOH-10

The coordinates of F1-2MeOH-10

O	2.18394500	1.37431100	-0.24025600
O	4.26261600	2.09387000	-0.39399100
N	-2.38121300	0.15901400	0.03993300
C	1.65960600	-0.95018000	0.10360700
C	3.06118400	-1.24806700	0.11359900
C	1.26080600	0.38589600	-0.07734500
C	0.63123500	-1.90052700	0.26216900
C	-0.06468400	0.77376400	-0.10091200
C	-1.07662800	-0.18771500	0.05864600
C	3.95233900	-0.22951600	-0.05295600
C	-0.69369000	-1.54247300	0.24178800
C	3.53467300	-2.65281500	0.30403200
C	3.53771100	1.13011100	-0.23809300
H	0.89240200	-2.94376500	0.40435500
H	-0.31188700	1.81993400	-0.24371700
H	5.02110800	-0.40505900	-0.05282900

H	-1.46851400	-2.29188800	0.36624200
H	3.14102200	-3.30577900	-0.48106200
H	3.18587900	-3.05397100	1.26067200
H	4.62353900	-2.70460500	0.28356600
H	-2.65517100	1.12671000	-0.09735700
H	-3.09815200	-0.55093000	0.15143300
C	-5.02729100	-2.54264600	-0.77430600
H	-4.32233800	-2.54657700	-1.60655600
H	-5.88294100	-1.91360500	-1.04117900
H	-5.37291300	-3.56716000	-0.60268100
O	-4.33332600	-2.03277300	0.35668500
H	-4.93369300	-2.01603900	1.10603200
C	-2.87025300	3.94145800	0.70467400
H	-3.55041900	4.79710600	0.64287000
H	-3.03171100	3.43491500	1.65695800
H	-1.83619400	4.30009400	0.66812300
O	-3.13419000	2.99349400	-0.32119300
H	-2.99392500	3.41256800	-1.17378400

S6.3. The complex configurations with an F1: MeOH molar ratio of 1:3

S6.3.1. F1-3MeOH-1

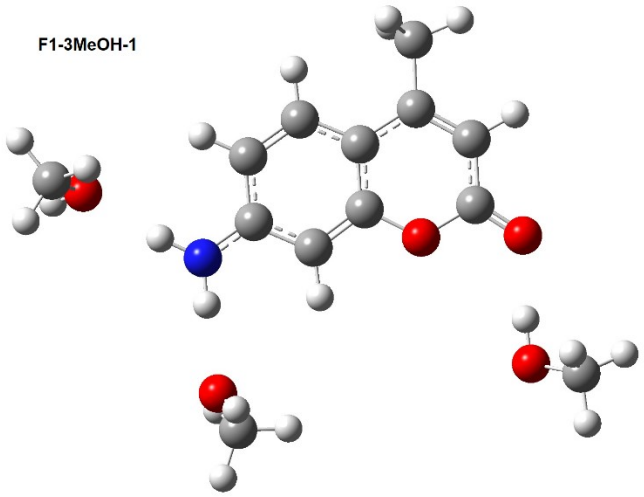


Fig.S19. The optimized complex configuration of F1-3MeOH-1

The coordinates of F1-3MeOH-1

O	-1.85580000	-0.02916300	-0.07082600
O	-4.04546500	-0.25772000	-0.05929900
N	2.80007300	0.81310800	-0.07957500
C	-0.37213200	-1.92276000	-0.15124300

C	-1.50953500	-2.79072600	-0.17376600
C	-0.58946800	-0.53446800	-0.09949900
C	0.97144000	-2.34986400	-0.17622600
C	0.43837300	0.38618300	-0.07493800
C	1.77110900	-0.05857500	-0.10038500
C	-2.75932400	-2.24093900	-0.14273300
C	2.01289200	-1.45750900	-0.15145200
C	-1.33122500	-4.27313200	-0.23049300
C	-2.96339300	-0.82873300	-0.08942500
H	1.18815000	-3.41189600	-0.21564100
H	0.20750200	1.44488000	-0.03542600
H	-3.65183300	-2.85376800	-0.15740800
H	3.03944800	-1.80855900	-0.17189800
H	-0.75888900	-4.62857100	0.63185900
H	-0.77507900	-4.56279500	-1.12737800
H	-2.29476400	-4.78311600	-0.24079300
H	2.62676400	1.81201600	-0.02330800
H	3.75601600	0.47083900	-0.07693500
C	-5.56386100	2.64640900	0.95885700
H	-5.78988600	3.71297800	1.02870100
H	-5.35502500	2.27566600	1.97103800
H	-6.45757500	2.13277200	0.58081900
O	-4.45717600	2.49251300	0.09669400
H	-4.25665200	1.54199000	0.03194600
C	6.18311400	-0.52425000	1.19036100
H	5.43812800	-0.80606600	1.93549000
H	6.65994300	0.40973400	1.50548500
H	6.93923000	-1.31393900	1.13434500
O	5.49848900	-0.37289200	-0.04627400
H	6.13294800	-0.12271400	-0.72239400
C	1.73708000	4.40234500	-1.08300000
H	1.96961200	5.47065600	-1.02688500
H	2.23679800	3.98135100	-1.95622100
H	0.65590200	4.27466300	-1.20087000
O	2.22751600	3.70433000	0.05426000
H	1.79780700	4.05168700	0.83971700

S6.3.2. F1-3MeOH-2

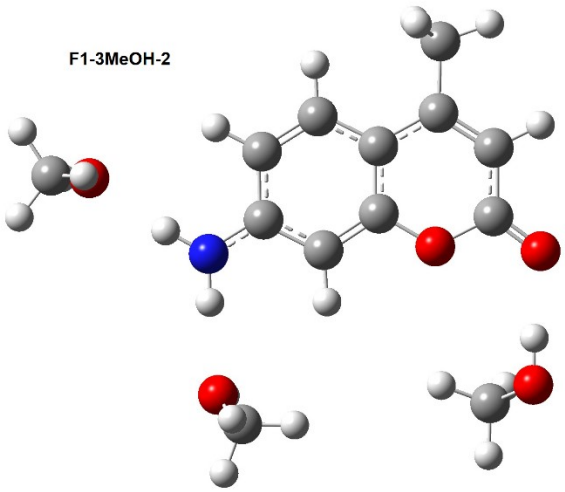


Fig.S20. The optimized complex configuration of F1-3MeOH-2

The coordinates of F1-3MeOH-2

O	1.98775400	0.01912700	-0.19387000
O	4.18287200	-0.10647400	-0.28918400
N	-2.69733800	0.64850900	-0.01600600
C	0.60450300	-1.92777700	0.10392400
C	1.78323900	-2.73859000	0.13399400
C	0.75079900	-0.53943500	-0.06385000
C	-0.71387000	-2.41174800	0.23056800
C	-0.32092300	0.32897500	-0.10615300
C	-1.62737200	-0.17184500	0.02277300
C	3.00189200	-2.13640400	0.00092600
C	-1.79782900	-1.57187300	0.19256700
C	1.68103900	-4.21899100	0.30828100
C	3.13357000	-0.72457100	-0.16659100
H	-0.87604400	-3.47611300	0.36211300
H	-0.14445600	1.39044600	-0.23898900
H	3.92292900	-2.70541800	0.01769400
H	-2.80402600	-1.96542600	0.29322800
H	1.09048800	-4.66471800	-0.49805900
H	1.17887700	-4.46527100	1.24886200
H	2.66823500	-4.68160500	0.31110300
H	-2.57070900	1.65089600	-0.11498300
H	-3.63215200	0.27022300	0.10208100
C	-6.21804000	-0.79896100	-0.76388600
H	-5.61548900	-0.99471100	-1.65168300
H	-6.80351200	0.11134900	-0.92985500

H	-6.89886300	-1.64215900	-0.60905800
O	-5.31753100	-0.65240300	0.32624200
H	-5.82308100	-0.47795600	1.12382500
C	3.53090800	3.28775900	0.36024700
H	3.60175500	4.36772700	0.21110200
H	2.47194500	3.00307100	0.30910100
H	3.90107700	3.05825500	1.36832400
O	4.29786900	2.65978900	-0.64423800
H	4.22575200	1.69631400	-0.52230200
C	-1.54882300	4.28015000	0.74691400
H	-1.81558300	5.34150100	0.71780300
H	-1.87766400	3.86308800	1.69950300
H	-0.46027100	4.18070600	0.67663200
O	-2.21032600	3.55030800	-0.27793900
H	-1.93750000	3.89733500	-1.13077000

S6.3.3. F1-3MeOH-3

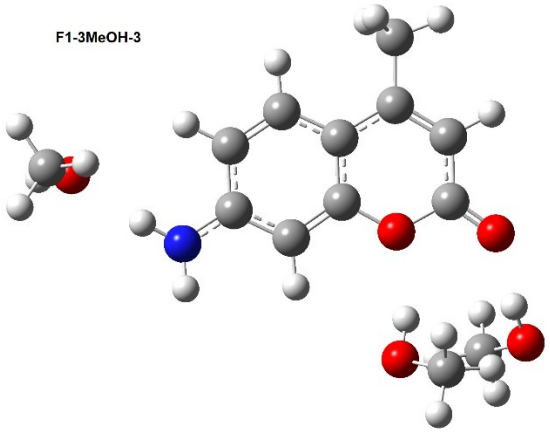


Fig.S21. The optimized complex configuration of F1-3MeOH-3

The coordinates of F1-3MeOH-3

O	-1.33477800	0.10602300	-0.11309700
O	-3.40962100	0.77609000	-0.43098000
N	3.00557600	-1.65467800	0.61927900
C	0.51034300	1.64773600	-0.03397800
C	-0.40542000	2.72680000	-0.25466800
C	0.00447100	0.33910500	0.02999600
C	1.90306200	1.79300400	0.12515000
C	0.80330500	-0.76796400	0.23569400
C	2.18738100	-0.60036400	0.39208100
C	-1.73456300	2.44763400	-0.39164100

C	2.72193700	0.71175300	0.33213000
C	0.08756700	4.13453600	-0.33141000
C	-2.24228000	1.11605300	-0.32122800
H	2.34022300	2.78449700	0.08187000
H	0.35272600	-1.75380500	0.27317000
H	-2.46601900	3.22833800	-0.55816600
H	3.79200100	0.84524500	0.45097800
H	0.81464100	4.24691200	-1.14144900
H	0.59265800	4.41927800	0.59666700
H	-0.73538700	4.82792600	-0.50514900
H	2.64826200	-2.59130000	0.53675100
H	4.01456900	-1.52765900	0.60931200
C	-2.93002100	-2.75043600	-2.05286200
H	-3.02625800	-3.80391300	-2.32213700
H	-2.47160500	-2.21964600	-2.89621900
H	-3.93422400	-2.34362100	-1.88471600
O	-2.13081900	-2.68218000	-0.88626200
H	-2.03282700	-1.75555200	-0.64095200
C	6.68777300	-1.30932700	-0.53171400
H	6.08670500	-1.08355800	-1.41327700
H	7.01154900	-2.35389400	-0.58409000
H	7.56768400	-0.65827000	-0.53051900
O	5.86624800	-1.07137300	0.60424000
H	6.37133100	-1.26306200	1.39825600
C	-4.51585400	-1.35462400	2.12955100
H	-5.20534900	-2.00926100	2.66711700
H	-3.55719000	-1.87916500	2.02624200
H	-4.35598000	-0.45424700	2.73684400
O	-5.09426800	-1.05454100	0.87648000
H	-4.48684400	-0.46809200	0.39886000

S6.3.4. F1-3MeOH-4

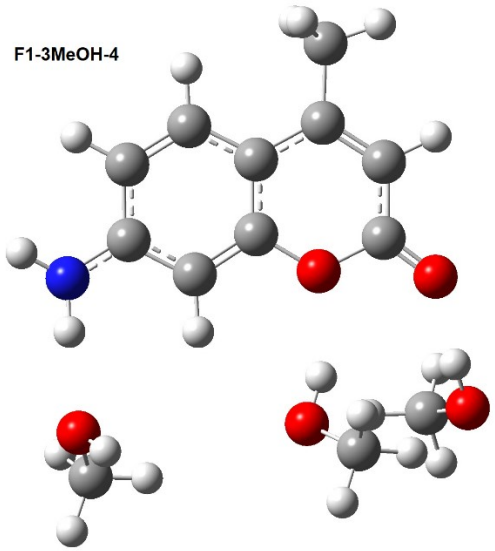


Fig.S22. The optimized complex configuration of F1-3MeOH-4

The coordinates of F1-3MeOH-4

O	0.88306300	-0.30470300	0.14147800
O	2.59929300	-1.67653600	0.31210400
N	-3.01311400	2.34898100	-0.25277500
C	1.16314200	2.08053800	-0.01162700
C	2.58216800	1.90120900	0.07055500
C	0.33841000	0.94415800	0.02873100
C	0.51371800	3.32516300	-0.12908500
C	-1.03829000	1.01008100	-0.03848000
C	-1.66481000	2.26004100	-0.15679400
C	3.08182200	0.63584200	0.18067100
C	-0.85375500	3.42107600	-0.20115800
C	3.49799800	3.08047800	0.03496900
C	2.23755300	-0.51464500	0.21663300
H	1.10790100	4.23166100	-0.16383000
H	-1.62383000	0.09866800	0.00522700
H	4.14611500	0.44763000	0.24368200
H	-1.32700000	4.39326700	-0.29327200
H	3.28221700	3.76348700	0.86232000
H	3.36588300	3.64605500	-0.89246200
H	4.54019600	2.76886800	0.10575600
H	-3.59200100	1.53094400	-0.07852800
H	-3.45094000	3.25222400	-0.19015600
C	-0.67284500	-3.22838200	2.13330200
H	-1.53960700	-3.82381800	2.42622100

H	-0.34275600	-2.64899300	3.00424600
H	0.13243200	-3.90994900	1.83584500
O	-1.07498100	-2.39212700	1.06318500
H	-0.31467900	-1.86890700	0.78693300
C	1.21861100	-3.93129400	-1.97579900
H	0.94548100	-4.89950600	-2.40118900
H	0.31510100	-3.30914200	-1.93522100
H	1.93979400	-3.45274100	-2.65108300
O	1.76269500	-4.16110600	-0.69309100
H	2.00486200	-3.30197100	-0.31287600
C	-4.77236600	-1.01310700	-0.86292300
H	-5.67234100	-1.61651600	-0.70742800
H	-4.89108900	-0.43821300	-1.78204700
H	-3.90769100	-1.67621800	-0.97058500
O	-4.58773400	-0.07779300	0.19232900
H	-4.47306900	-0.55851800	1.01585100

S6.3.5. F1-3MeOH-5

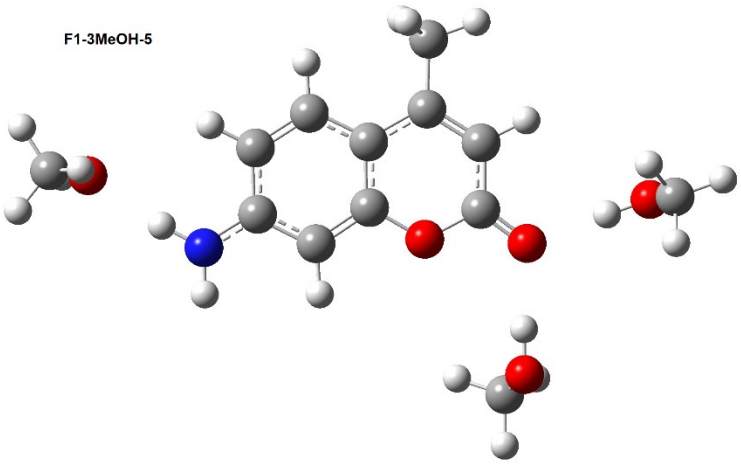


Fig.S23. The optimized complex configuration of F1-3MeOH-5

The coordinates of F1-3MeOH-5

O	0.90672800	-0.63031700	0.03348600
O	3.08879600	-0.39926200	0.00882400
N	-3.74855600	-1.49054900	0.14772900
C	-0.58970400	1.24052800	-0.18734800
C	0.54142000	2.11067400	-0.28467600
C	-0.36317200	-0.13690200	-0.02629700
C	-1.93591300	1.65641600	-0.24076900

C	-1.38391300	-1.06055900	0.07904300
C	-2.71603200	-0.62505600	0.02575500
C	1.79508800	1.57035300	-0.21791100
C	-2.96998300	0.76152100	-0.13881200
C	0.35508800	3.58243600	-0.45523700
C	1.99943300	0.17040500	-0.05748400
H	-2.16029000	2.70991200	-0.36626600
H	-1.14176000	-2.11038300	0.20209100
H	2.68435400	2.18429500	-0.28681200
H	-3.99932500	1.10118100	-0.18437800
H	-0.20969800	4.00064900	0.38355900
H	-0.21302300	3.79770800	-1.36534700
H	1.31545400	4.09448600	-0.51650900
H	-3.57386200	-2.48094100	0.15806200
H	-4.70246700	-1.17477700	-0.00923200
C	-7.33006800	-0.24641700	0.80704300
H	-6.74662200	-0.00725600	1.69688800
H	-7.87720000	-1.17802900	0.98430600
H	-8.04437100	0.56324700	0.62731400
O	-6.41140800	-0.37485600	-0.27074400
H	-6.89867900	-0.58640600	-1.07076900
C	3.19144100	-3.80031400	-0.79595600
H	3.35162200	-4.87035800	-0.64572700
H	2.15774300	-3.65462600	-1.13605200
H	3.86808600	-3.46235500	-1.59170800
O	3.44423500	-3.14775200	0.43008800
H	3.28734000	-2.19719100	0.30076700
C	5.97605200	1.20882400	1.10166200
H	6.94145900	1.71546200	1.03560200
H	5.27208100	1.88109700	1.60949400
H	6.10336300	0.31035700	1.71922400
O	5.56016500	0.89674900	-0.21143100
H	4.69912800	0.44981700	-0.15446600

S6.3.6. F1-3MeOH-6

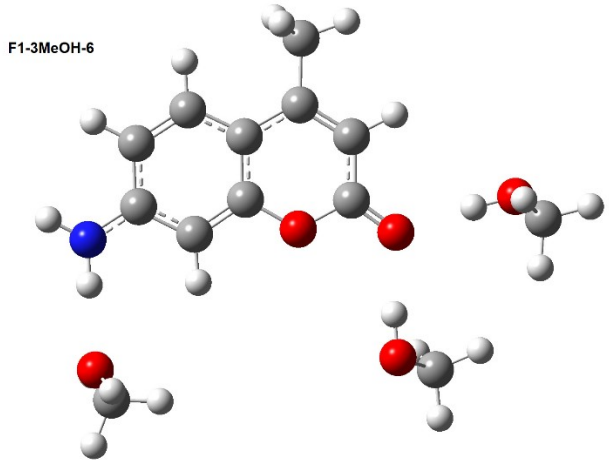


Fig.S24. The optimized complex configuration of F1-3MeOH-6

The coordinates of F1-3MeOH-6

O	0.26731400	0.12261400	-0.02865600
O	2.43458800	0.45224400	0.06034600
N	-4.44163700	-0.20578100	-0.24620300
C	-0.70817700	-2.07320800	0.09657700
C	0.60443400	-2.63028700	0.21033800
C	-0.83622500	-0.67854400	-0.02295100
C	-1.90437900	-2.81868800	0.09283900
C	-2.05486300	-0.04184600	-0.14032600
C	-3.23416000	-0.80270200	-0.14156800
C	1.68024100	-1.78741300	0.19871600
C	-3.12945900	-2.21235200	-0.02155800
C	0.79465200	-4.10580700	0.33865600
C	1.52536000	-0.37690200	0.07850400
H	-1.85660000	-3.89829600	0.18255900
H	-2.08892800	1.03793700	-0.23031600
H	2.69445700	-2.15726000	0.28189200
H	-4.03492800	-2.81032100	-0.02123300
H	0.37311200	-4.62690300	-0.52633500
H	0.28020600	-4.48647800	1.22629100
H	1.85204900	-4.35936700	0.41498700
H	-4.52133600	0.79881300	-0.38063700
H	-5.27622100	-0.76441300	-0.29448400
C	3.00550100	3.76816300	0.79882200
H	2.98720300	4.85632600	0.70524300
H	2.65430500	3.50609500	1.80537800
H	4.04650000	3.43426300	0.69806400

O	2.17552700	3.23252100	-0.21024900
H	2.19844200	2.26409200	-0.13292500
C	-4.28053500	3.58325500	0.46356700
H	-4.78522900	4.54616700	0.33624000
H	-4.63415500	3.12218500	1.38643400
H	-3.20121900	3.74941800	0.54361400
O	-4.59655000	2.68928500	-0.59623400
H	-4.29533000	3.07044400	-1.42465800
C	5.71824600	0.33919700	-1.03462000
H	6.79915200	0.18615800	-0.99889300
H	5.31299900	-0.27545200	-1.84889500
H	5.53036500	1.39461300	-1.27117000
O	5.18748200	-0.02592600	0.22219000
H	4.22592100	0.10934300	0.19111700

S6.3.7. F1-3MeOH-7

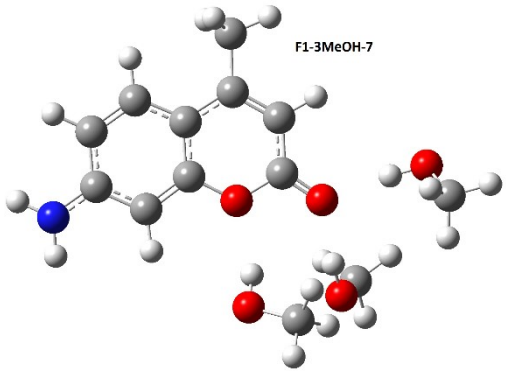


Fig.S25. The optimized complex configuration of F1-3MeOH-7

The coordinates of F1-3MeOH-7

O	0.25096300	-0.34354500	0.09100400
O	-1.82302500	0.37202600	0.09865800
N	4.58951600	-2.24464100	0.05299100
C	2.13238700	1.15271800	0.03868200
C	1.22623400	2.26209400	0.01830300
C	1.60281800	-0.14656200	0.07480200
C	3.53656700	1.26105600	0.02592600
C	2.38910200	-1.28142000	0.09614600
C	3.78272000	-1.14856900	0.07908000
C	-0.11696000	2.01542300	0.03797400
C	4.34296000	0.15060700	0.04485400

C	1.74259000	3.66189600	-0.02182500
C	-0.63703200	0.69118300	0.07828700
H	3.99257900	2.24434000	0.00142900
H	1.91956200	-2.25841900	0.12471900
H	-0.84311200	2.81837300	0.02642600
H	5.42219200	0.26165200	0.03279400
H	2.35794700	3.82098100	-0.91260400
H	2.37494900	3.86563300	0.84771900
H	0.92373200	4.38111100	-0.03207600
H	4.20116400	-3.14478700	0.28234100
H	5.56829700	-2.13053200	0.25922300
C	-2.03084300	-2.89412400	-1.81323600
H	-2.17011600	-3.86124300	-2.29987100
H	-2.05963900	-2.11354600	-2.58309600
H	-2.86084000	-2.73378100	-1.11549700
O	-0.78149900	-2.93388000	-1.14643100
H	-0.63878800	-2.08463200	-0.71656200
C	-3.52659600	-1.11582300	2.73374700
H	-4.09123200	-1.86306500	3.29538800
H	-2.63951100	-0.84510600	3.32057700
H	-4.15552300	-0.22335300	2.62238500
O	-3.18490700	-1.68342900	1.48543700
H	-2.68213900	-1.02326800	0.98479600
C	-4.75488300	1.38832800	-1.43849400
H	-5.64413100	1.98525900	-1.65241700
H	-4.15548400	1.32699900	-2.35597700
H	-5.07962600	0.37533600	-1.16806900
O	-4.05376200	2.01930700	-0.38651400
H	-3.26345300	1.48986200	-0.19526200

S6.4. The complex configurations with an F1: MeOH molar ratio of 1:4

S6.4.1. F1-4MeOH-1

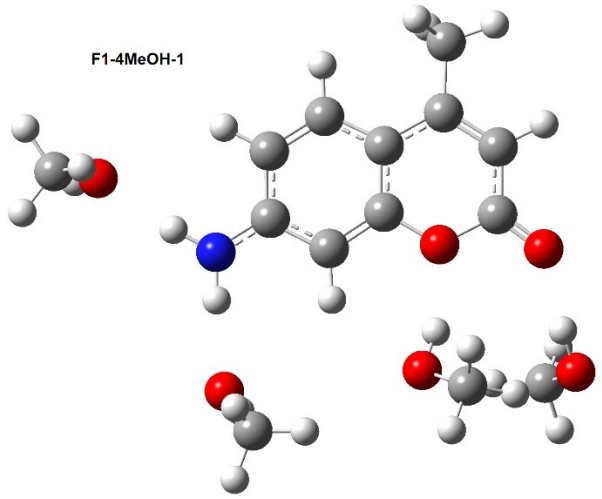


Fig.S26. The optimized complex configuration of F1-4MeOH-1

The coordinates of F1-4MeOH-1

O	1.57191200	0.46824100	0.12011600
O	3.72632500	0.90712700	0.27060600
N	-2.97080900	-0.81829200	-0.22238800
C	-0.07909700	2.20868600	-0.07476700
C	0.96739400	3.18198000	-0.01734400
C	0.26324400	0.84722800	-0.00266300
C	-1.45220200	2.50548900	-0.19928500
C	-0.66905900	-0.16775700	-0.04759600
C	-2.03329600	0.14864800	-0.17202700
C	2.26100500	2.75782200	0.10047200
C	-2.40283100	1.51817900	-0.24719100
C	0.65072600	4.64021700	-0.08841600
C	2.60224700	1.37526400	0.16863500
H	-1.76554400	3.54214100	-0.25874600
H	-0.34589100	-1.20072300	0.01669300
H	3.08715100	3.45622700	0.14460200
H	-3.45395700	1.76967800	-0.34322900
H	-0.01489600	4.93288400	0.72934000
H	0.13615700	4.87986900	-1.02401000
H	1.55832300	5.24103100	-0.02845800
H	-2.70278600	-1.79488400	-0.14686200
H	-3.95353900	-0.57149000	-0.29170800
C	2.99651700	-2.33708700	2.33811100
H	2.92882700	-3.33025500	2.78624400
H	2.91739100	-1.59190400	3.13917100

H	3.97602800	-2.23804000	1.85655400
O	1.93909900	-2.22181100	1.40264900
H	1.99269600	-1.35280800	0.98999100
C	-6.63158300	-0.02576300	0.72739400
H	-6.03242400	0.16536600	1.61847100
H	-7.06061800	-1.03047200	0.80080200
H	-7.44125200	0.70979800	0.68459000
O	-5.76289900	0.09340600	-0.39163700
H	-6.26489400	-0.07620500	-1.19254400
C	4.31473200	-1.75933200	-1.92124000
H	4.83068500	-2.62806300	-2.33615300
H	3.26126400	-2.02856000	-1.76960600
H	4.36277400	-0.94870900	-2.66000600
O	4.95417900	-1.41431800	-0.71044900
H	4.49935500	-0.64028600	-0.34088400
C	-1.34704700	-4.24621800	-1.06430800
H	-1.46159900	-5.33456600	-1.03418000
H	-1.76184700	-3.87697700	-2.00299400
H	-0.28167500	-3.99531600	-1.02712200
O	-2.07109600	-3.61931700	-0.01369600
H	-1.71872100	-3.92044400	0.82740100

S6.4.2. F1-4MeOH-2

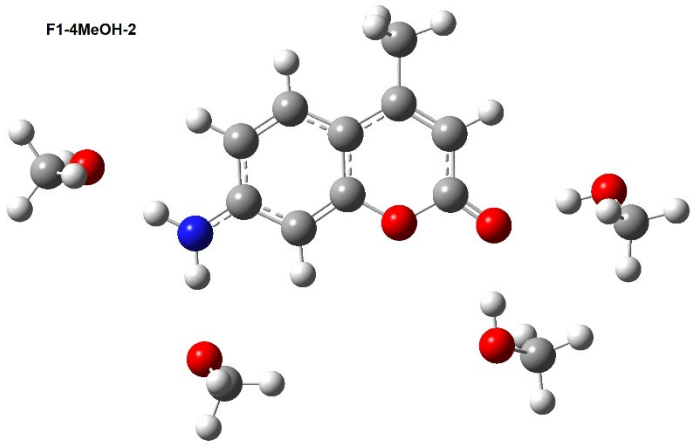


Fig.S27. The optimized complex configuration of F1-4MeOH-2

The coordinates of F1-4MeOH-2

O	-1.10878300	0.16349800	0.00760300
O	-3.30229400	0.12065400	0.00689700

N	3.59807800	0.63279800	0.05247200
C	0.22108400	-1.82798400	-0.23025900
C	-0.97963900	-2.59671900	-0.31730100
C	0.11519200	-0.43511500	-0.06592200
C	1.52765900	-2.35677500	-0.29546100
C	1.21036400	0.39776000	0.02948000
C	2.50382000	-0.14798600	-0.03751300
C	-2.18384700	-1.95205900	-0.23768100
C	2.63465700	-1.55385500	-0.20324400
C	-0.92273200	-4.07897100	-0.49223300
C	-2.26666200	-0.54145900	-0.07281200
H	1.65981200	-3.42584800	-0.42156000
H	1.06340500	1.46456300	0.15512300
H	-3.12182600	-2.48952800	-0.29817300
H	3.63114100	-1.98005600	-0.25583400
H	-0.38397900	-4.54659400	0.33749200
H	-0.38876600	-4.34019200	-1.41095800
H	-1.92449600	-4.50616800	-0.54003700
H	3.50543500	1.63689700	0.17418500
H	4.52337000	0.21744000	-0.00045800
C	7.03759400	-0.91237500	1.00040600
H	6.40391100	-1.04930900	1.87744900
H	7.65212800	-0.01799400	1.14655600
H	7.69008500	-1.78553500	0.89914200
O	6.17352500	-0.77794200	-0.12044700
H	6.70700700	-0.65471700	-0.90937100
C	-4.42650100	3.31340500	-0.62095300
H	-4.57911100	4.38788600	-0.49657300
H	-4.06658900	3.13585200	-1.64280600
H	-5.39801700	2.81513200	-0.50546800
O	-3.49409600	2.89245300	0.35209400
H	-3.36191000	1.93524000	0.24505700
C	2.79928800	4.35561800	-0.68275200
H	3.12383600	5.39388200	-0.55978400
H	3.23815200	3.95844400	-1.59878200
H	1.70843200	4.32743300	-0.77422500
O	3.25779600	3.53893900	0.38680900
H	2.88364400	3.86575100	1.20867800
C	-6.50693400	-0.39722700	1.18528200
H	-7.54924000	-0.72372300	1.19629400

H	-5.99949000	-0.84560200	2.04930700
H	-6.48981200	0.69425400	1.30229600
O	-5.93677100	-0.80932200	-0.03922400
H	-5.00874300	-0.52087000	-0.04892500

S6.4.3. F1-4MeOH-3

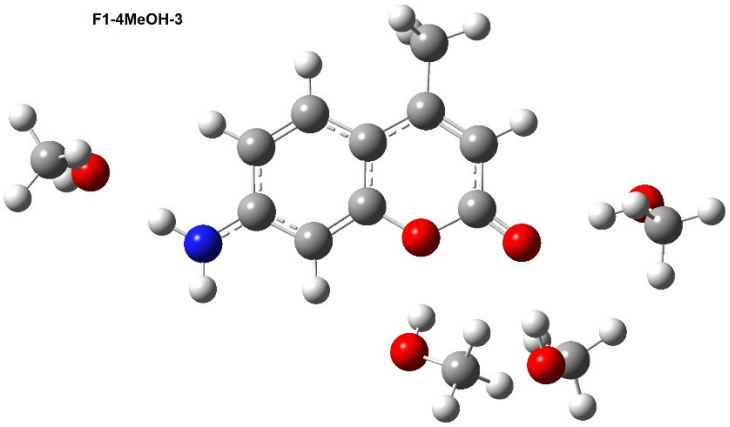


Fig.S28. The optimized complex configuration of F1-4MeOH-3

The coordinates of F1-4MeOH-3

O	-0.61105300	-0.23747200	0.10878200
O	-2.76675900	0.16212600	0.00739400
N	3.95716600	-1.46060600	0.38699600
C	1.02976400	1.52121000	0.11906200
C	-0.02614000	2.48071800	0.03106100
C	0.69749300	0.15654100	0.15670800
C	2.40371300	1.83549900	0.17192700
C	1.63860400	-0.84848500	0.24009500
C	3.00045100	-0.51272000	0.29273000
C	-1.32008400	2.03878700	-0.00826600
C	3.36254600	0.85946800	0.25614600
C	0.27779900	3.94179600	-0.01494700
C	-1.64016300	0.65471000	0.03495600
H	2.71051000	2.87526000	0.14559500
H	1.31766500	-1.88410900	0.26431600
H	-2.15438400	2.72604700	-0.07096000
H	4.41442400	1.12201200	0.29603100
H	0.90946500	4.17823700	-0.87659800
H	0.82502100	4.25143500	0.88060900

H	-0.63710900	4.53016300	-0.08326900
H	3.71033500	-2.43497000	0.36262900
H	4.94221200	-1.20766400	0.37133800
C	-2.34514200	-3.19655100	-1.78329500
H	-2.28497600	-4.17991400	-2.25344000
H	-2.54446700	-2.45305800	-2.56464400
H	-3.18151900	-3.19947800	-1.07515100
O	-1.10713300	-2.96307300	-1.13481300
H	-1.14210500	-2.09836300	-0.71314400
C	7.54034600	-0.67644700	-0.81260700
H	6.90193000	-0.53795900	-1.68587200
H	7.99103800	-1.67305500	-0.85986600
H	8.33186800	0.07928200	-0.83268500
O	6.71345800	-0.52904000	0.33496900
H	7.25040700	-0.64845800	1.12220300
C	-4.21127800	-1.63774900	2.60124500
H	-4.67074300	-2.47424300	3.13219500
H	-3.34832400	-1.29422000	3.18606200
H	-4.94312100	-0.82151200	2.54928300
O	-3.83527400	-2.09616700	1.31857200
H	-3.42625500	-1.35562500	0.84467800
C	-5.78165800	1.00853900	-1.50715600
H	-6.72922400	1.52724000	-1.66843700
H	-5.16706100	1.13173300	-2.40826200
H	-5.99485500	-0.06020900	-1.37629300
O	-5.16966200	1.57140200	-0.36508500
H	-4.32701300	1.11156500	-0.21979400

S6.4.4. F1-4MeOH-4

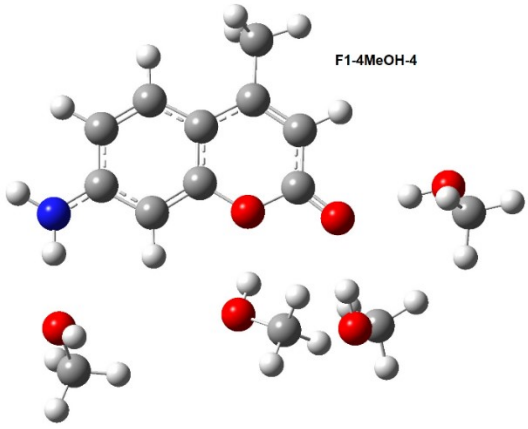


Fig.S29. The optimized complex configuration of F1-4MeOH-4

The coordinates of F1-4MeOH-4

O	-0.17559000	0.18237500	0.02023700
O	-2.35847500	-0.04511700	0.04383600
N	4.55087600	0.28188300	-0.00445500
C	0.89945800	2.33414600	0.06615300
C	-0.38829200	2.95549400	0.09153300
C	0.96873900	0.93113900	0.02976000
C	2.12906700	3.02374600	0.07169500
C	2.15777900	0.23385400	-0.00108600
C	3.37070700	0.94056200	0.00542900
C	-1.50393700	2.16457200	0.08404200
C	3.32776200	2.35771200	0.04337600
C	-0.51318100	4.44283500	0.12809200
C	-1.41722200	0.74577100	0.05108900
H	2.12894600	4.10774800	0.09903300
H	2.14860200	-0.84972800	-0.03258500
H	-2.50068400	2.58680400	0.10533000
H	4.25953200	2.91387900	0.04916200
H	-0.03191600	4.89271100	-0.74561400
H	-0.01830000	4.85081000	1.01465600
H	-1.55944200	4.74786600	0.14344400
H	4.57804500	-0.72571800	-0.14166600
H	5.40766800	0.79832100	-0.10704300
C	-0.98906200	-3.10606100	-1.91151000
H	-0.65910500	-4.03286700	-2.38457000
H	-1.35050500	-2.42917200	-2.69522400
H	-1.81791400	-3.33751300	-1.23289400
O	0.12317900	-2.56655500	-1.21894100
H	-0.15179500	-1.74778800	-0.79348900
C	-3.22676400	-2.30736400	2.52747400
H	-3.40790000	-3.26481500	3.02062200
H	-2.53578600	-1.72648400	3.15177900
H	-4.17998600	-1.76660000	2.46835100
O	-2.68897800	-2.57660700	1.24874300
H	-2.52402700	-1.72830600	0.80911700
C	4.18972300	-3.48550300	0.72415200
H	4.63464000	-4.47504300	0.57915700
H	4.61110700	-3.04104600	1.62649600
H	3.10789100	-3.59195600	0.85520500
O	4.50391800	-2.61413600	-0.35509000

H	4.13478500	-2.97612200	-1.16451100
C	-5.57081500	-0.23396000	-1.25297800
H	-6.63724200	-0.02930600	-1.37035400
H	-5.07630800	-0.03060300	-2.21161300
H	-5.45062800	-1.29987600	-1.02016200
O	-5.08324400	0.59370700	-0.21703100
H	-4.13607300	0.41061800	-0.10879900

S6.4.5. F1-4MeOH-5

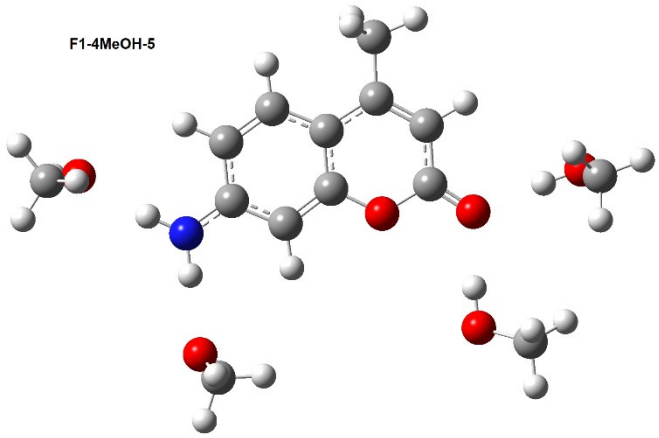


Fig.S30. The optimized complex configuration of F1-4MeOH-5

The coordinates of F1-4MeOH-5

O	-1.09559800	0.24250700	-0.15220300
O	-3.28875700	0.26251300	-0.20079700
N	3.62105600	0.57878500	-0.02053700
C	0.17866300	-1.79743200	-0.22931500
C	-1.04236100	-2.53548400	-0.29780300
C	0.11123200	-0.39438100	-0.15706000
C	1.46976600	-2.36660300	-0.22682300
C	1.22852200	0.41118300	-0.08759600
C	2.50613300	-0.17466400	-0.08607700
C	-2.22806800	-1.85286400	-0.28895700
C	2.59805900	-1.59150900	-0.15725600
C	-1.02608300	-4.02690700	-0.37761300
C	-2.27194900	-0.43288400	-0.21458000
H	1.57252900	-3.44494500	-0.28064900
H	1.11085900	1.48766600	-0.03434100
H	-3.18028500	-2.36581200	-0.33920100

H	3.58186000	-2.04921700	-0.15652300
H	-0.52213100	-4.45599000	0.49378100
H	-0.47806500	-4.36128800	-1.26375800
H	-2.03882600	-4.42751600	-0.42473900
H	3.55591000	1.59032200	0.04471300
H	4.53412700	0.13431300	-0.00267400
C	-4.59472500	3.32868200	0.62780000
H	-4.68978600	4.41286900	0.72170400
H	-4.68425900	2.89034300	1.63047800
H	-5.43019900	2.96461600	0.01567400
O	-3.34269400	3.05290600	0.03638500
H	-3.26068100	2.08845600	-0.05513800
C	6.88398100	-1.00178000	1.28750700
H	6.14629300	-1.10403400	2.08432600
H	7.48693400	-0.10805500	1.47883900
H	7.53319200	-1.88317500	1.29523600
O	6.16496800	-0.89794600	0.06547200
H	6.79228800	-0.80474900	-0.65567200
C	2.99196300	4.27293900	-0.99790500
H	3.35405100	5.30355000	-0.92593100
H	3.44927200	3.80185500	-1.86876900
H	1.90526900	4.28116600	-1.13238300
O	3.37455000	3.50840800	0.13802700
H	2.97886200	3.89821000	0.92143400
C	-6.40084900	-0.71663100	0.97637200
H	-7.43248600	-1.07433300	0.94664900
H	-5.82006900	-1.40234000	1.60711800
H	-6.39669700	0.27478400	1.44793300
O	-5.91797200	-0.67612000	-0.34999000
H	-4.99703700	-0.36633000	-0.32367400

S6.5. The complex configurations with an F1: MeOH molar ratio of 1:5

S6.5.1. F1-5MeOH-1

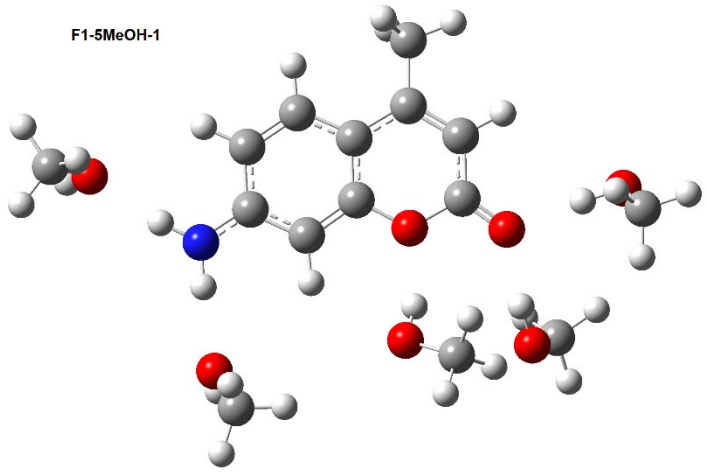


Fig.S31. The optimized complex configuration of F1-5MeOH-1

The coordinates of F1-5MeOH-1

O	0.90392500	-0.09415300	0.04515900
O	3.09540300	-0.21923000	0.03165300
N	-3.78358100	0.55640300	0.07924900
C	-0.50146300	-2.04071400	0.20453500
C	0.66853200	-2.85805300	0.24102900
C	-0.34652500	-0.64656800	0.10592300
C	-1.82692000	-2.52240000	0.26004300
C	-1.40791900	0.23119200	0.06343500
C	-2.72097600	-0.26913500	0.11900700
C	1.89832500	-2.25891700	0.18298600
C	-2.90333900	-1.67541300	0.21953700
C	0.55507800	-4.34362900	0.34440100
C	2.03951000	-0.84902600	0.08696400
H	-1.99823100	-3.59049900	0.33706800
H	-1.22570200	1.29721700	-0.01337000
H	2.81384100	-2.83613200	0.21094900
H	-3.91469100	-2.06592100	0.26385600
H	-0.00849900	-4.74857600	-0.50162900
H	0.01872500	-4.62821000	1.25472900
H	1.53952400	-4.81134000	0.36128900
H	-3.64928700	1.56056000	0.00480700
H	-4.72440900	0.17568800	0.12247800
C	2.26680400	2.81879400	-2.14999900
H	2.10672300	3.73747900	-2.71750400
H	2.54076000	2.02297700	-2.85329300

H	3.09898900	2.97946700	-1.45522500
O	1.05954500	2.52870700	-1.46751900
H	1.18427200	1.72084400	-0.95868200
C	-7.25804200	-0.85703500	-0.91875700
H	-6.61876300	-1.00129100	-1.79054800
H	-7.84309500	0.05780000	-1.05898000
H	-7.93804500	-1.71100900	-0.83701900
O	-6.40320400	-0.76480400	0.21346700
H	-6.94150000	-0.63584200	0.99819600
C	4.29529400	2.00590600	2.40322900
H	4.62565200	2.94780400	2.84650000
H	3.51797200	1.57810800	3.04938400
H	5.14982000	1.31739000	2.38532000
O	3.81230500	2.28648100	1.10532600
H	3.51750300	1.45161800	0.70917400
C	-2.75988100	4.17806400	0.99768500
H	-3.00714700	5.24153100	0.91836500
H	-3.24199400	3.77251400	1.88795500
H	-1.67552700	4.06718900	1.10295100
O	-3.25693600	3.44595900	-0.11518400
H	-2.84407900	3.78033300	-0.91528400
C	6.19354500	-0.81945400	-1.41055500
H	7.20467100	-1.21646500	-1.52462800
H	5.60241700	-1.13546100	-2.27984100
H	6.25434700	0.27653600	-1.41268000
O	5.66668000	-1.31948400	-0.19904100
H	4.76693800	-0.96861900	-0.09674500

S7. The calculated results of the Enthalpies variation (ΔH_{298}) and Gibbs free energy variation (ΔG_{298}) for reactions forming complexes from F1 and MeOH

Complexes	**ΔH_{298} (Kcal/mol)**	**ΔG_{298} (Kcal/mol)**
F1: MeOH molar ratio of 1:1		
F1-1-MeOH-1	-2.99	4.50
F1-1-MeOH-2	-3.06	4.01
F1-1-MeOH-3	-2.15	5.32
F1-1-MeOH-4	-2.09	4.65

F1: MeOH molar ratio of 1:2		
F1-2-MeOH-1	-6.38	8.84
F1-2-MeOH-2	-6.43	8.46
F1-2-MeOH-3	-3.85	12.16
F1-2-MeOH-4	-5.70	9.17
F1-2-MeOH-5	-5.67	9.02
F1-2-MeOH-6	-5.95	9.57
F1-2-MeOH-7	-5.88	9.31
F1-2-MeOH-8	-5.83	9.22
F1-2-MeOH-9	-5.79	8.90
F1-2-MeOH-10	-4.42	9.81
F1: MeOH molar ratio of 1:3		
F1-3-MeOH-1	-8.20	14.07
F1-3-MeOH-2	-8.33	14.09
F1-3-MeOH-3	-6.65	16.05
F1-3-MeOH-4	-7.39	18.12
F1-3-MeOH-5	-9.20	12.38
F1-3-MeOH-6	-11.04	16.26
F1-3-MeOH-7	-6.91	15.62
F1: MeOH molar ratio of 1:4		
F1-4-MeOH-1	-9.19	21.40
F1-4-MeOH-2	-11.66	18.07
F1-4-MeOH-3	-9.84	19.33
F1-4-MeOH-4	-9.90	20.38
F1-4-MeOH-5	-11.68	18.52
F1: MeOH molar ratio of 1:5		

F1-5-MeOH-1	-12.41	25.30

S8. The coordinates of the optimized geometry for the ES of F1-1-MeOH-2

O	0.77200300	-0.28280800	-0.09082600
O	2.64747700	0.90299000	-0.13368600
N	-3.02716400	-3.06117100	0.00763400
C	-1.41177600	0.79484300	0.01109500
C	-0.79961400	2.08942200	0.01378600
C	-0.58440400	-0.36484900	-0.04091600
C	-2.81976800	0.57972800	0.05852100
C	-1.11164200	-1.63101100	-0.04370900
C	-2.52085100	-1.81581000	0.00711600
C	0.60312200	2.11602000	-0.03624500
C	-3.36701900	-0.68200700	0.05713600
C	-1.62036000	3.32758500	0.06951500
C	1.40962500	0.96393100	-0.08805500
H	-3.47517000	1.44163700	0.09741800
H	-0.44568200	-2.48571500	-0.08468800
H	1.13538600	3.06120700	-0.03622300
H	-4.44220700	-0.81832300	0.09503400
H	-2.24405300	3.36646500	0.97390400
H	-2.30831500	3.40335600	-0.78447700
H	-0.98468800	4.21493900	0.06489500
H	-2.42933300	-3.87271200	-0.02599500
H	-4.02254200	-3.22000700	0.04387100
C	5.42782000	-1.01477100	0.20809500
H	6.06409500	-1.90298900	0.22611500
H	5.50225500	-0.52360900	1.18757600
H	5.82435300	-0.32805200	-0.55169200
O	4.11078900	-1.42696700	-0.08226600
H	3.54309600	-0.63219600	-0.10297600