Supporting Information

Designing New Togni Reagents by Computation

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1. The scan of I-C bond of Togni's reagent II.

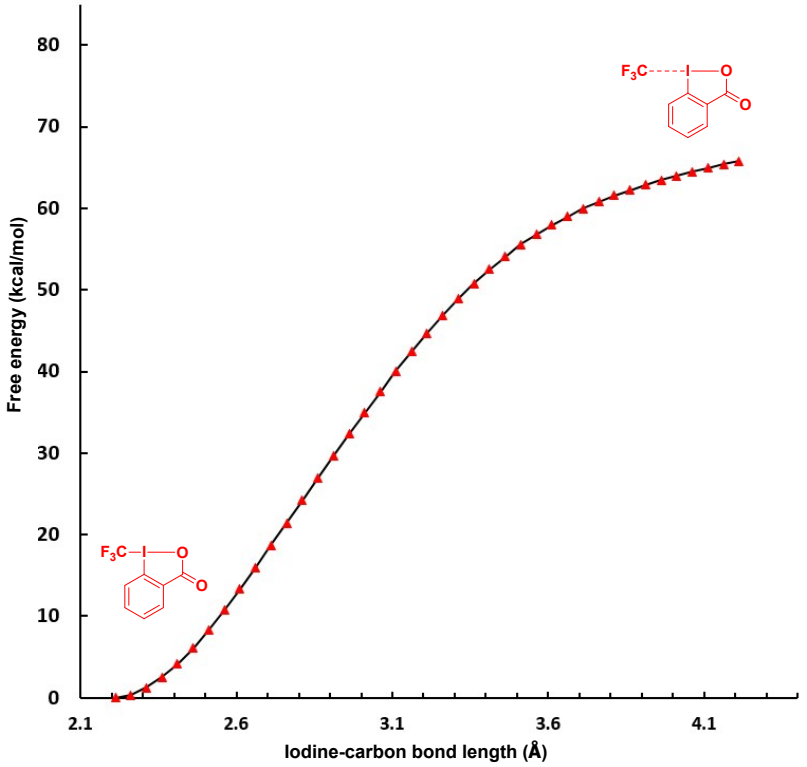


Figure S1. The scan of I-C bond of Togni's reagent II..

3. The protocol of synthetic route to product 1.

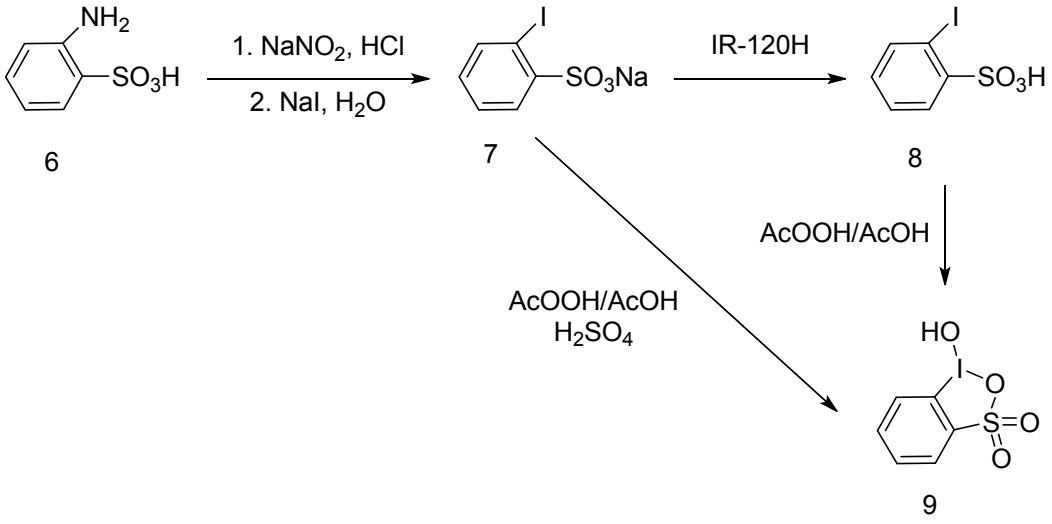


Figure S2. The synthetic route of reagent **9**.[1-3]

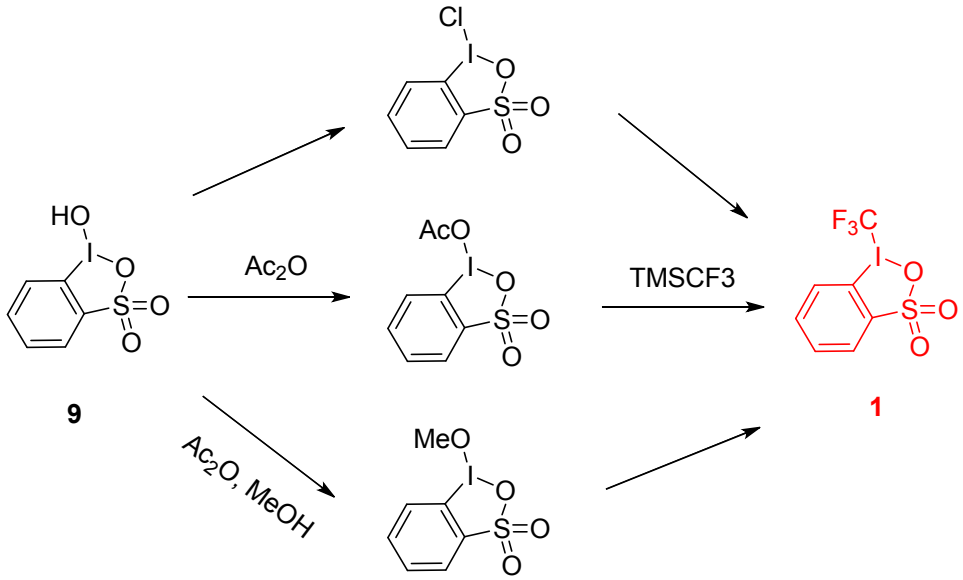
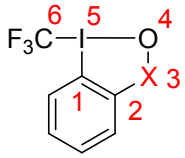


Figure S3. The protocol of synthetic method to the product (**1**).[4-5]

Due to interest, we investigate the possibility of synthesize the compound **1** and **1'** (see **Figure S2** & **S3**), the most reactive reagents from the computational results, and we look forward to finish this synthesis by synthetic chemists who are interested of it.

4. The computational geometries and the known crystal structure data[6-7] of Togni I and Togni II



	Togni I		Togni II	
	expt.	Cal.	expt.	cal.
bond (Å) 5-4	2.283	2.263	2.118	2.105
bond (Å) 5-6	2.219	2.212	2.267	2.257
angle (°) 2-1-5-4	0.3	0.0	11.6	14.3

Figure S4. The computational geometries and the known crystal structure data of Togni I and Togni II.

REFERENCES

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(5) Charpentier, J.; Früh, N.; Togni, A. *Chem. Rev.* **2015**, *115*, 650.

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Cartesian coordinates (in Å) of related structures which calculated at the M06-2X/ cc-pVQZ(-pp) level of theory.

CF_3

C	0.00000000	0.00000000	-0.00008700
F	0.00000000	1.22642200	0.00001900
F	1.06211300	-0.61321100	0.00001900
F	-1.06211300	-0.61321100	0.00001900

1

C	0.19822700	2.12804400	-0.28326600
C	-0.35503200	0.86793400	-0.15518400
C	-1.71057200	0.66968800	0.03053600
C	-2.54060700	1.77820200	0.11859800
C	-2.00792400	3.05390000	0.02031700
C	-0.64790900	3.22533300	-0.18620200
H	-3.60294300	1.62792600	0.25167400
H	-2.65851600	3.91364000	0.08793500
H	-0.22955100	4.21628900	-0.28726500
I	0.86044300	-0.87096200	-0.26782800
H	1.24814400	2.28450100	-0.47157800
C	2.71421800	0.18332700	0.24707200
F	2.54241000	0.97620500	1.29092100
F	3.19213100	0.90133700	-0.75654400
F	3.60700200	-0.74361000	0.55778200
O	-1.42400500	-1.75291500	-0.64476100
S	-2.39760400	-0.97245000	0.15029900
O	-2.36919000	-1.31822100	1.55069200
O	-3.70371000	-0.92462500	-0.45234400

1’

C	0.09692800	2.14289700	-0.33371300
C	-0.41343300	0.86167000	-0.16615300
C	-1.73215300	0.60170100	0.18543400
C	-2.56831100	1.66443900	0.47049100
C	-2.07671900	2.96086800	0.39633600
C	-0.77895400	3.18783700	-0.01555000
H	-3.60050000	1.46766900	0.72113000
H	-2.72316300	3.79607900	0.62473000
H	-0.41581100	4.20063800	-0.12626200
I	0.78768500	-0.85809500	-0.53514600
C	2.55573000	-0.21203600	0.59957400
F	2.20490100	0.64982500	1.53303400
F	3.49001000	0.32112100	-0.16003500
F	3.04605500	-1.29777000	1.16839600
O	-1.70935300	-1.63352800	-1.01232300
S	-2.39370800	-1.06470500	0.15796400
O	-1.98383700	-1.67976800	1.40104600
O	-3.81751500	-0.92762700	-0.01771800
C	1.46271000	2.48397500	-0.84866300
H	1.83632000	1.73934100	-1.54822000
H	2.17963300	2.59297200	-0.03595100
H	1.41769100	3.43830500	-1.36725200

1- anion

C	0.26497300	2.32789700	0.00006500
C	0.11755700	0.94683700	0.00007000
C	-1.14989000	0.36914100	0.00005200
C	-2.26175100	1.20561700	-0.00001100
C	-2.12185700	2.58514300	-0.00004500
C	-0.85547600	3.14709200	0.00000700
H	-3.24176800	0.75226100	-0.00003200
H	-3.00034200	3.21481400	-0.00011400
H	-0.72907600	4.22059200	-0.00000700
I	1.90059300	-0.17269600	-0.00001000
H	1.25354100	2.76362600	0.00009900
O	-0.80910800	-1.89485400	-1.21693600
S	-1.43623400	-1.40963700	0.00000500
O	-2.88115900	-1.55199100	-0.00001500
O	-0.80915400	-1.89497900	1.21690800

1’- anion

C	1.24567600	1.80824800	-0.00000400
C	0.42018300	0.67801300	-0.00004800
C	-0.97013700	0.79558500	0.00004400
C	-1.54011400	2.06334700	-0.00017100
C	-0.74131600	3.19480500	-0.00018400
C	0.63484400	3.06190900	0.00004300
H	-2.61612700	2.14466600	-0.00013000
H	-1.19328300	4.17688300	-0.00039600
H	1.26367500	3.94220200	0.00009500
I	1.36772500	-1.20885600	-0.00044700
O	-1.80988900	-1.34353800	-1.21705700
S	-2.10619300	-0.60847600	0.00052800
O	-3.42978600	-0.01026000	-0.00000200

O	-1.81032600	-1.34238600	1.21890700
C	2.74462400	1.72987500	0.00029000
H	3.10971100	1.19513100	0.87719300
H	3.11014100	1.19576900	-0.87682200
H	3.17298500	2.72908900	0.00073300

2

C	1.69379400	0.73216400	0.03086000
C	0.32103600	0.89579900	0.06934300
I	-0.83086000	-0.90065600	0.13094800
C	2.47881300	1.88440000	0.00424700
C	1.89675300	3.14055500	0.00806400
C	0.51558300	3.26161500	0.04826700
C	-0.29440400	2.13400600	0.08321600
H	3.55569600	1.78020800	-0.01159000
H	2.51738500	4.02477100	-0.01140100
H	0.05153200	4.23746300	0.06215300
H	-1.36249100	2.26059100	0.13176100
P	2.45907900	-0.91196400	0.04101100
O	3.67238600	-0.93574500	0.87594800
C	-2.76433700	0.13386400	-0.11662300
F	-3.09851400	0.90218700	0.91731200
F	-2.83412800	0.87728200	-1.21699800
F	-3.68051800	-0.82805100	-0.21604900
O	1.28344200	-1.81660700	0.35656800
O	2.80841500	-1.19909100	-1.49812300
H	3.70833700	-0.93443900	-1.72413300

2’

C	-1.71407100	0.69163800	0.19201800
C	-0.38293100	0.90448600	-0.14424000
I	0.71352600	-0.91395900	-0.45659000
C	-2.49481100	1.80061700	0.48242300
C	-1.94148700	3.07252900	0.42823100
C	-0.63544100	3.23890000	0.00965200
C	0.19069700	2.15604900	-0.31917800
H	-3.53949000	1.65783000	0.72180200
H	-2.54394300	3.93746100	0.66714000
H	-0.22779100	4.23467600	-0.10435400
P	-2.45424300	-0.96249600	0.01349900
O	-3.90163300	-0.86322400	-0.24147200
C	2.57226600	-0.24340100	0.52344400
F	3.50739400	0.21781800	-0.29448900
F	2.33272300	0.67109800	1.45394800
F	3.06722700	-1.32406000	1.12337900
O	-1.52145500	-1.61323100	-0.98568500
O	-2.15229100	-1.70603800	1.40637300
H	-2.83089800	-1.53321600	2.07000500
C	1.55249400	2.43964200	-0.87984400
H	1.88072200	1.66269900	-1.56715700
H	2.29801200	2.55420900	-0.09510100
H	1.51680200	3.37710100	-1.42984800

2- anion

C	-1.11846700	0.45304300	-0.03955200
C	0.17667300	0.96879800	-0.00808300
I	1.88977100	-0.26517900	-0.00124800
C	-2.16662100	1.37733500	-0.03599300
C	-1.94174000	2.74560000	-0.00524700
C	-0.64212800	3.22635400	0.02902500
C	0.42207400	2.33583100	0.02962200
H	-3.17576300	0.99036200	-0.05562400
H	-2.77747200	3.43148400	-0.00536800
H	-0.44755900	4.28955500	0.05651200
H	1.43651900	2.70610200	0.05882000
P	-1.57057600	-1.32944100	-0.11783900
O	-0.86850000	-1.95328600	-1.26598600
O	-3.04994000	-1.40594700	0.02452900
O	-0.89634100	-1.92209800	1.23851400
H	-1.49546100	-1.81249300	1.98432200

2’- anion

C	-0.89215900	0.87893000	-0.03330000
C	0.48846600	0.66973800	-0.01319600
I	1.28043600	-1.29616100	-0.00372700
C	-1.34162000	2.20065300	-0.02723400
C	-0.45563800	3.26496300	-0.00735400
C	0.90612200	3.02098800	0.01151900
C	1.41091200	1.72110400	0.01181600
H	-2.40830200	2.37091700	-0.03805000
H	-0.82491300	4.28133000	-0.00556400
H	1.60585300	3.84624200	0.02769000
P	-2.19492800	-0.42326100	-0.11626900
O	-1.90650500	-1.32033400	-1.26209100
O	-3.50560700	0.27063000	0.01397200
O	-1.94011200	-1.27613900	1.24584800
H	-2.42345400	-0.88140000	1.97920800
C	2.89793100	1.51796100	0.03604400

H	3.20483200	0.95373600	0.91675700
H	3.23333200	0.95666600	-0.83615400
H	3.40713700	2.47865700	0.04609600

3

C	0.08198100	2.07388800	-0.00024000
C	0.52141300	0.76225500	-0.00006200
C	1.85718500	0.42468000	0.00008200
C	2.80276200	1.44278900	0.00007800
C	2.39554100	2.76533900	-0.00008400
C	1.04163900	3.07640600	-0.00024900
H	3.85346900	1.18660900	0.00020800
H	3.13139400	3.55651400	-0.00009000
H	0.71953900	4.10788300	-0.00038600
I	-0.77933700	-0.90756200	-0.00002600
H	-0.96165400	2.34146400	-0.00036700
C	-2.60553800	0.33201700	-0.00005600
F	-2.73295100	1.10722900	1.07513800
F	-2.73309400	1.10710000	-1.07533300
F	-3.62693700	-0.52737300	0.00006400
O	1.27290200	-1.86568400	0.00033200
C	2.25738400	-1.03690400	0.00019100
F	3.11668200	-1.24406200	-1.08180200
F	3.11682300	-1.24389600	1.08209000

3’

C	-.26694000	2.07535800	-0.26336100
C	-0.62406400	0.74175900	-0.11474700
C	-1.91742700	0.32261300	0.14990800
C	-2.89451900	1.26978100	0.40016900
C	-2.56371500	2.61539400	0.34950600
C	-1.28282000	3.00086500	-0.00128700
H	-3.90673300	0.95092600	0.60337400
H	-3.31827900	3.36569700	0.53746200
H	-1.04820800	4.05134000	-0.10994600
I	0.69482600	-0.92072100	-0.35461800
C	2.54891600	0.03185000	0.40096500
F	2.32594700	0.87244400	1.40685700
F	3.30707200	0.64695300	-0.49867700
F	3.26410500	-0.99137100	0.87868300
O	-1.39518600	-1.81222600	-0.68794300
C	-2.22929700	-1.16009500	0.04399000
F	-3.53414500	-1.30414800	-0.40094300
F	-2.31190300	-1.67618000	1.35140700
C	1.05846300	2.57655800	-0.75140200
H	1.50024000	1.88814600	-1.46866700
H	1.76216400	2.73212700	0.06369500
H	0.91526800	3.53400800	-1.24601900

3- anion

C	0.01839300	2.16978700	-0.00418100
C	-0.00179600	0.77507000	-0.01013900
C	-1.20423800	0.07960700	-0.01435100
C	-2.38515100	0.82937000	-0.00401200
C	-2.37738200	2.21071300	0.00271200
C	-1.16392700	2.88679700	0.00061700
H	-3.32531500	0.29678000	-0.00298300
H	-3.30942800	2.75809500	0.00919700
H	-1.13354800	3.96740400	0.00411700
I	1.91046900	-0.11932800	0.00084100
H	0.96441500	2.69070000	-0.00259800
O	-0.36678900	-2.19359000	-0.11044400
C	-1.33560800	-1.44857900	-0.01949700
F	-2.17243400	-1.72062900	1.16720400
F	-2.36294700	-1.70786400	-1.04227400

3’- anion

C	0.39323500	2.01771400	0.01760400
C	0.02779400	0.66835000	-0.01775900
C	-1.30846100	0.26158300	-0.04787000
C	-2.29175400	1.24656700	-0.05494300
C	-1.95659800	2.59080900	-0.03158200
C	-0.62739100	2.96780400	0.00729400
H	-3.32855900	0.95095300	-0.07963200
H	-2.73471700	3.34163700	-0.04104800
H	-0.35976700	4.01588900	0.03061500
I	1.59706000	-0.75018100	-0.01496300
O	-1.35058500	-1.87255200	-1.12825500
C	-1.70782400	-1.21562800	-0.15066000
F	-1.30494000	-1.79934500	1.14384300
F	-3.14748500	-1.25695300	0.07348400
C	1.81932300	2.48450700	0.06488000
H	2.33108700	2.09885900	0.94672500
H	2.37651500	2.13830000	-0.80587900
H	1.85783700	3.57083300	0.09057300

4

C	-1.64319400	1.15612500	0.00000000

C	-0.27799100	0.94438300	0.00000000
C	0.64425400	1.97297400	0.00000000
C	0.17213100	3.28011500	0.00000000
C	-1.18962100	3.52947400	0.00000000
C	-2.08986500	2.47187700	0.00000000
H	-2.36247900	0.35409800	0.00000000
H	0.89302400	4.08514900	0.00000000
H	-1.55327400	4.54673000	0.00000000
H	-3.15356100	2.66195600	0.00000000
C	2.12178000	1.67301400	0.00000000
O	2.39511700	0.41687300	0.00000000
I	0.60966300	-0.97158900	0.00000000
C	-1.34218900	-2.03031400	0.00000000
F	-2.08986500	-1.78266600	1.07524200
F	-1.06124100	-3.33476000	0.00000000
F	-2.08986500	-1.78266600	-1.07524200
O	2.93751600	2.57828400	0.00000000

4’

C	-0.72943200	1.90680900	-0.24696200
C	-0.90058900	0.53922600	-0.07933800
C	-2.12763700	-0.05820900	0.16614800
C	-3.23207400	0.75503400	0.36838200
C	-3.09652500	2.13087800	0.29302200
C	-1.87151600	2.68526300	-0.03407200
H	-4.18764700	0.28619100	0.55431600
H	-3.95253300	2.77211400	0.44761400
H	-1.78026300	3.75632300	-0.15731600
C	-2.29386100	-1.55744400	0.07553800
O	-1.26220500	-2.16012300	-0.39205400
I	0.65183200	-0.92335500	-0.23176100
C	2.44387200	0.26880100	0.32626600
F	3.02559600	0.97342500	-0.63734700
F	3.31816900	-0.67413300	0.69812200
F	2.25287400	1.06814400	1.37159000
O	-3.34911900	-2.08113900	0.39031300
C	0.53204700	2.57536300	-0.69826300
H	1.21360600	2.76333600	0.12864600
H	1.04506000	1.97325900	-1.44470200
H	0.28979700	3.53546700	-1.14688100

4- anion

C	-0.93180100	-1.87772300	-0.00497700
C	-0.42832500	-0.58321300	-0.00483300
C	-1.25953600	0.52868700	-0.00454800
C	-2.63699200	0.30692500	-0.00213700
C	-3.15924800	-0.97705700	-0.00556500
C	-2.30540300	-2.07273100	-0.00736800
H	-0.26100300	-2.72473600	-0.00317100
H	-3.30203400	1.16141200	0.00212500
H	-4.23034600	-1.12453200	-0.00571400
H	-2.70183300	-3.07838100	-0.00925400
C	-0.73817800	1.96451600	-0.00990000
O	-0.49283200	2.44280600	-1.13285500
O	-0.63552200	2.50407400	1.10728100
I	1.66564000	-0.33104200	0.00861500

4’- anion

C	0.99783300	-1.66645600	0.00402000
C	0.45088600	-0.38034300	0.00393500
C	1.23242800	0.76797200	0.00376900
C	2.61850300	0.62036100	0.00145300
C	3.19340800	-0.63901700	0.00443100
C	2.38744700	-1.76845800	0.00603800
H	3.24103500	1.50600100	-0.00215900
H	4.26964800	-0.74517200	0.00455800
H	2.83469500	-2.75366800	0.00769600
C	0.64966700	2.18061300	0.01011100
O	0.52182100	2.71568800	-1.10677600
O	0.39112500	2.65079900	1.13365100
I	-1.65270600	-0.16003700	-0.00846400
C	0.15854500	-2.90981500	0.00247100
H	-0.49243900	-2.94432400	0.87634200
H	-0.48545900	-2.94696000	-0.87647400
H	0.79006400	-3.79497800	0.00625200

5

C	-0.38312000	1.99718800	0.00000900
C	-0.75833000	0.66747000	-0.00013100
C	-2.06866300	0.22667700	0.00001700
C	-3.06212500	1.20694600	0.00029000
C	-2.73434800	2.55387900	0.00039900
C	-1.40123000	2.94362900	0.00025800
H	-4.09975500	0.89977400	0.00041500
H	-3.51368100	3.30308900	0.00062200
H	-1.13992500	3.99262700	0.00035000
I	0.64488600	-0.94284400	-0.00047300
H	0.64223200	2.32663400	-0.00009200

B	-2.30423000	-1.33577700	-0.00012200
O	-3.59693900	-1.79961900	0.00031700
H	-3.63232800	-2.76159900	0.00044400
C	2.38050500	0.45975300	0.00034900
F	2.46947000	1.25223400	-1.07564700
F	2.46842100	1.25225600	1.07642200
F	3.47553500	-0.31577800	0.00085100
O	-1.21197300	-2.09319900	-0.00004800

5’

C	-0.56431500	1.95028700	-0.31317000
C	-0.83711000	0.60895600	-0.07979300
C	-2.08772200	0.09434200	0.22931100
C	-3.11267300	1.00707500	0.45987400
C	-2.87430800	2.36937100	0.35265200
C	-1.63107300	2.81990100	-0.05650200
H	-4.10191800	0.63878400	0.69660100
H	-3.66737100	3.08099200	0.53549100
H	-1.46885500	3.87732000	-0.22090200
I	0.60045600	-0.98579300	-0.25478800
B	-2.29852200	-1.46656500	0.05651300
O	-3.53144200	-1.98688800	0.37249100
H	-3.57625900	-2.93129000	0.19227600
C	2.39099200	0.19889400	0.37898500
F	3.11031500	0.81558100	-0.56112400
F	2.12873900	1.09014400	1.34038000
F	3.20392300	-0.72599200	0.92035400
O	-1.27302300	-2.14629600	-0.44155500
C	0.69782600	2.51129600	-0.89728700
H	1.42044500	2.78816700	-0.13275700
H	1.16453700	1.80272800	-1.57792000
H	0.45710500	3.41028000	-1.45996800

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C	0.95912000	-1.90993400	-0.02335300
C	0.46158300	-0.61307700	-0.00316800
C	1.26479800	0.52184100	0.01255700
C	2.64600500	0.28220400	0.00178300
C	3.17961300	-0.99841100	-0.02455100
C	2.33362900	-2.09984900	-0.03587900
H	3.32020500	1.13086300	0.01688500
H	4.25198500	-1.13959200	-0.03445000
H	2.73497600	-3.10381200	-0.05294100
I	-1.64850200	-0.39172100	0.02089500
H	0.29069000	-2.75887200	-0.02886300
B	0.71454100	2.04387500	0.09866000
O	0.36223000	2.51995600	-1.19212700
H	0.04418200	3.42327100	-1.10221600
O	0.64869300	2.71671300	1.19669400

5’- anion

C	-1.14295700	1.62016200	-0.01344700
C	-0.51166300	0.37350500	0.00534500
C	-1.17725800	-0.84727100	0.02226500
C	-2.57625100	-0.78394700	0.01428400
C	-3.25088600	0.42632100	-0.00793400
C	-2.53683800	1.61552000	-0.02059200
H	-3.14316100	-1.70758200	0.02770300
H	-4.33253500	0.44848500	-0.01504800
H	-3.05954000	2.56317100	-0.03628900
I	1.61731900	0.33151000	0.01574700
B	-0.45211300	-2.29439900	0.10217300
O	-0.12984100	-2.76142500	-1.20016500
H	0.29350100	-3.62095500	-1.11443700
O	-0.24705600	-2.93055300	1.20500200
C	-0.40129000	2.92465100	-0.02626400
H	0.23212200	3.02551000	0.85583700
H	0.25058700	2.99804700	-0.89734600
H	-1.10029400	3.75746900	-0.04649500

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C	0.39060100	1.96977700	0.38875600
C	0.69003200	0.64670000	0.15200600
C	1.96876600	0.19120100	-0.16176100
C	2.98513000	1.14541900	-0.25693800
C	2.69756400	2.48422300	-0.03656600
C	1.41625000	2.90401300	0.29392400
H	3.99298000	0.84215600	-0.49678300
H	3.49609200	3.20953100	-0.10921300
H	1.20856200	3.94670900	0.48333700
I	-0.68403000	-0.94510300	0.15114000
H	-0.60740100	2.28564500	0.65151000
C	-2.38147400	0.47399800	-0.19242600
F	-2.72376200	1.23761700	0.85492000
F	-2.18083700	1.30105100	-1.22665800
F	-3.45810100	-0.26983400	-0.49023500
N	2.12668800	-1.17113600	-0.39534700
O	1.22979800	-1.90883600	0.40304600

C	3.45506700	-1.73062100	-0.26879200
H	4.11694200	-1.26817300	-0.99684700
H	3.86298200	-1.59234500	0.73792600
H	3.39092100	-2.79218700	-0.48875400

6’

C	-0.53384600	1.93789700	-0.38599400
C	-0.75205400	0.59763200	-0.11565400
C	-1.98595700	0.07336700	0.28215400
C	-3.02055900	0.96462600	0.55623000
C	-2.80345400	2.32391600	0.38128100
C	-1.59963000	2.80113400	-0.10682800
H	-3.98552200	0.60217500	0.87559000
H	-3.60833600	3.01660400	0.58493100
H	-1.47161400	3.85650100	-0.30456900
I	0.62236600	-0.99965500	-0.30061100
C	2.37854400	0.19984700	0.44567700
F	3.14901200	0.79985700	-0.46901100
F	2.04860500	1.12264800	1.35812800
F	3.17214800	-0.68949000	1.07070300
N	-2.08620500	-1.31460900	0.36004300
O	-1.30400800	-1.89682700	-0.66291700
C	-3.41103500	-1.89419200	0.34059000
H	-3.96846400	-1.55977300	1.21218600
H	-3.95966600	-1.62993900	-0.56967500
H	-3.30219400	-2.97336400	0.39451300
C	0.71573800	2.49555600	-1.00097200
H	1.42778400	2.82399800	-0.24588900
H	1.20418500	1.76478900	-1.64196900
H	0.45952300	3.36176200	-1.60696000

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C	-0.46192300	-1.99705300	0.19721700
C	-0.24279500	-0.63168400	0.11930600
C	-1.31870500	0.29181400	-0.02488000
C	-2.61327700	-0.30108900	-0.13057100
C	-2.80785700	-1.66377100	-0.06072700
C	-1.74006000	-2.53797800	0.12576600
H	-3.47352800	0.34065300	-0.23994200
H	-3.81675700	-2.04921300	-0.13422400
H	-1.88925800	-3.60509900	0.19663200
I	1.77941900	-0.06249400	-0.07420800
H	0.38957100	-2.65709400	0.29480100
N	-1.15381500	1.62645200	-0.05475900
O	-0.11377100	2.20855000	0.61322800
C	-2.28626000	2.50253600	-0.21553100
H	-2.93433200	2.19059800	-1.03319900
H	-2.88373500	2.57360200	0.70393000
H	-1.88902500	3.48849500	-0.44099200

6’- anion

C	0.23223100	1.91636800	0.12709700
C	0.20953600	0.52630000	0.05417300
C	1.38505000	-0.25431700	-0.05451400
C	2.59881500	0.45374300	-0.15554400
C	2.63136000	1.83624500	-0.10860700
C	1.46721900	2.56751700	0.05517800
H	3.52593500	-0.09038800	-0.24531600
H	3.58379900	2.34567900	-0.17790700
H	1.49687400	3.64687600	0.11198100
I	-1.66016800	-0.43026600	-0.11782100
N	1.33501100	-1.63167600	-0.07291200
O	0.60458800	-2.20964000	0.96284600
C	2.57758500	-2.33637300	-0.26313300
H	3.09896100	-2.00172900	-1.16042400
H	3.24924500	-2.23016700	0.60231100
H	2.33461200	-3.39061300	-0.37251200
C	-1.01364800	2.74716100	0.25261200
H	-1.63862500	2.65855500	-0.63642500
H	-1.61887200	2.42998600	1.10165800
H	-0.75371300	3.79492100	0.38518900

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C	-0.98518500	1.71530700	-0.27718600
C	-1.00613000	0.34811700	-0.07614800
C	-2.16053700	-0.36674000	0.16048800
C	-3.36067400	0.33192800	0.21380600
C	-3.37767000	1.70568500	0.02463800
C	-2.19684200	2.39355800	-0.22558300
H	-4.27990500	-0.20982100	0.39687100
H	-4.31540800	2.24219100	0.05937400
H	-2.21134700	3.46123300	-0.39142500
I	0.69334100	-0.92205800	-0.10248700
H	-0.07645800	2.25730800	-0.48530700
C	2.04843700	0.86517800	0.12104100
F	2.15822800	1.65393900	-0.96136400
F	1.74594300	1.66984600	1.15232500

F	3.28141400	0.38462300	0.36145100
O	-0.88479100	-2.32503500	-0.27077500
C	-2.04210000	-1.86475400	0.34434600
H	-2.92314300	-2.34662900	-0.08900500
H	-2.04853000	-2.08026300	1.42338500

7’

C	-1.18878400	1.58181900	-0.36633400
C	-1.05617700	0.23428300	-0.06203500
C	-2.10157000	-0.57465100	0.34900400
C	-3.33444400	0.00963900	0.58945600
C	-3.49572600	1.37313600	0.38549300
C	-2.44866900	2.13309600	-0.10732700
H	-4.16499600	-0.60808000	0.90520900
H	-4.45638600	1.83651500	0.56289400
H	-2.60359100	3.17917400	-0.33681500
I	0.70104400	-0.96258800	-0.26720900
C	2.09026700	0.70394800	0.38747300
F	2.65668900	1.47106300	-0.55542500
F	1.55536900	1.52928400	1.30005100
F	3.11173900	0.07235400	1.00217300
O	-0.85654200	-2.38565400	-0.52409700
C	-1.83533500	-2.06442800	0.41355000
H	-2.76247100	-2.60307300	0.20440700
H	-1.52348500	-2.32698800	1.43689600
C	-0.14036400	2.43416700	-1.01673500
H	0.47113700	2.96029100	-0.28625800
H	0.51379200	1.84011100	-1.65089800
H	-0.62636400	3.18407000	-1.63703500

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C	-1.08135700	-1.63907200	-0.17874200
C	-0.50714800	-0.39260900	0.02636900
C	-1.26151800	0.75783400	0.23233300
C	-2.64831100	0.60138600	0.21675100
C	-3.25125700	-0.63175400	0.00955600
C	-2.46537600	-1.75751700	-0.18932000
H	-3.26248500	1.48093700	0.37156500
H	-4.32972600	-0.71405900	0.00401100
H	-2.91881800	-2.72596600	-0.34980600
I	1.60590000	-0.30275100	0.03255600
H	-0.46004600	-2.51081000	-0.32851500
O	-0.20808400	2.64397400	-0.79873100
C	-0.64748800	2.15246800	0.37329600
H	0.13934600	2.05481600	1.16156500
H	-1.44154600	2.76469000	0.86408200

7’- anion

C	-1.16860800	-1.39989900	-0.08749000
C	-0.51279800	-0.17603900	0.06470000
C	-1.17833500	1.03733700	0.22044900
C	-2.57245700	0.99739500	0.21695600
C	-3.26371900	-0.19395700	0.06371400
C	-2.56399400	-1.37989800	-0.08792100
H	-3.11325700	1.92890800	0.33358400
H	-4.34545100	-0.20101100	0.06147100
H	-3.09575300	-2.31449800	-0.20936500
I	1.61033300	-0.17875100	0.06378700
O	-0.00463000	2.80422900	-0.89719400
C	-0.46669600	2.39238900	0.29691400
H	0.31685700	2.27897400	1.08550000
H	-1.21498400	3.07717900	0.76262100
C	-0.45131600	-2.70901800	-0.24840000
H	0.19738700	-2.69736700	-1.12448700
H	0.18029800	-2.92309200	0.61418700
H	-1.16817000	-3.51897500	-0.36019200

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C	-0.02110800	2.09743300	-0.21247500
C	-0.50046200	0.80378900	-0.12659100
C	-1.83784200	0.49182900	0.01410500
C	-2.73681500	1.55112500	0.10095700
C	-2.29123800	2.86237300	0.02476600
C	-0.94018500	3.13618200	-0.13892200
H	1.02507200	2.31954300	-0.34785900
H	-3.79145500	1.34853900	0.22749200
H	-3.00277000	3.67383800	0.08635200
H	-0.59276200	4.15663200	-0.21461300
C	-2.24025700	-0.98245400	0.09259100
C	-3.52647000	-1.24572600	-0.68288700
H	-3.72737900	-2.31640400	-0.67147800
H	-4.37914900	-0.73542400	-0.23714100
H	-3.42135500	-0.92095600	-1.71738000
C	-2.41757900	-1.36496100	1.56544900
H	-2.68205700	-2.42020700	1.63355500
H	-1.48873100	-1.20330600	2.11438100
H	-3.20324000	-0.77352200	2.03543100
O	-1.21704600	-1.73695700	-0.49345300

I	0.70603200	-0.93522100	-0.19391100
C	2.56099900	0.30274600	0.15332300
F	2.94934200	1.08687000	-0.86754300
F	3.56350000	-0.57264000	0.35581900
F	2.51896100	1.08795300	1.24219900

8’

C	-0.16218800	2.09452900	-0.28703800
C	-0.58298900	0.78023600	-0.12113600
C	-1.88665600	0.41361100	0.17217000
C	-2.79331100	1.42268800	0.46847700
C	-2.39598900	2.75037800	0.40932500
C	-1.11329100	3.07575000	0.00535200
H	-3.81437400	1.17316200	0.72119100
H	-3.10461000	3.53595600	0.63202300
H	-0.83147200	4.11311500	-0.11818500
C	-2.26831800	-1.06846700	0.08712300
C	-3.64010300	-1.23834000	-0.55715100
H	-3.82933700	-2.30295200	-0.69066800
H	-4.43494700	-0.82667500	0.06283700
H	-3.66559000	-0.75474700	-1.53292200
C	-2.27188700	-1.67974400	1.49229000
H	-2.51246200	-2.74065800	1.42344700
H	-1.29675400	-1.57474800	1.96867300
H	-3.01430600	-1.19159600	2.12360700
O	-1.32744200	-1.69609500	-0.74302400
I	0.61597500	-0.96858800	-0.37010900
C	2.53085200	-0.01165500	0.39184400
F	3.36972800	0.58128800	-0.47011200
F	3.21599700	-1.06411500	0.89122200
F	2.35292300	0.83853400	1.41633300
C	1.16921400	2.51888600	-0.83246000
H	1.90181200	2.68390800	-0.04530400
H	1.56569100	1.78211800	-1.52708400
H	1.04935900	3.45844300	-1.36740600

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C	0.05596800	2.20058600	0.02285700
C	0.07869400	0.81103000	-0.01536700
C	1.26774900	0.07782000	-0.03193500
C	2.44149900	0.84207300	-0.00315500
C	2.44243600	2.22967200	0.02738100
C	1.24184300	2.91923500	0.03873100
H	-0.88950300	2.72358300	0.03866700
H	3.39489800	0.33564300	-0.00909300
H	3.38192600	2.76563900	0.04168600
H	1.21756600	3.99982000	0.06091400
C	1.30759900	-1.48409700	-0.09221900
O	0.43466000	-1.96373500	-0.99683300
I	-1.85305200	-0.06448000	-0.01801200
C	2.74396600	-1.95741200	-0.42241800
H	3.49746300	-1.71026100	0.32867900
H	2.70027700	-3.04307200	-0.50876200
H	3.06606000	-1.55646100	-1.38535500
C	1.01412200	-1.97828900	1.35227800
H	1.05203000	-3.06988100	1.35383600
H	1.73495400	-1.60585400	2.08522700
H	0.01557400	-1.67555900	1.66657200

8’- anion

C	-0.64278300	-1.96368700	0.00947600
C	-0.10286100	-0.67115300	-0.01578500
C	1.27336900	-0.41286800	-0.02190800
C	2.10529800	-1.53707500	0.01158600
C	1.60781000	-2.82992200	0.03324600
C	0.24231200	-3.04064300	0.02840800
H	3.17551000	-1.40209300	0.01303400
H	2.28862200	-3.67047000	0.05049500
H	-0.15753500	-4.04579300	0.03972900
C	1.88037600	1.03028700	-0.09524700
C	3.39852100	0.94813500	-0.39386000
H	3.75089700	1.97607800	-0.48118900
H	3.99827200	0.45282900	0.37283200
H	3.57268400	0.45264900	-1.35067900
C	1.76974000	1.62901000	1.33671400
H	2.19237900	2.63604400	1.31673200
H	0.73100700	1.70815800	1.65407300
H	2.31212000	1.04214400	2.08294800
O	1.26460200	1.77300400	-1.03280800
I	-1.52781500	0.91140000	-0.01724100
C	-2.11678400	-2.25789100	0.01323300
H	-2.60482000	-1.84028600	0.89357200
H	-2.61109700	-1.82965600	-0.85833900
H	-2.28064200	-3.33301100	0.00786600

INT1

C	-5.99690100	-1.07480100	-2.23643500
C	-5.12919900	-1.62328200	-1.30294000

C	-3.85135500	-1.10722500	-1.10386900
C	-3.41881800	-0.02452800	-1.86498700
C	-4.26921500	0.52112000	-2.82499600
C	-5.54656000	-0.00067300	-3.00754000
H	-7.01077500	-1.43422700	-2.36538200
H	-2.43434600	0.39939700	-1.68015600
H	-3.93536200	1.36708100	-3.41724600
H	-6.21953500	0.43439100	-3.73946800
O	-1.94537400	-0.63224900	0.58374200
O	-3.71262700	-2.25923200	1.18716900
I	-5.76759100	-3.24667300	-0.08894400
C	-7.20767200	-4.02153600	-1.54770800
F	-7.49895900	-5.25646800	-1.16290900
F	-8.32698000	-3.31177600	-1.58677200
F	-6.67646500	-4.05324900	-2.76108100
Zn	-0.11485100	-0.69085400	1.42177300
C	1.17638000	5.91161300	-0.44886800
C	0.30494900	4.83937200	-0.32012700
C	0.76971500	3.53938100	-0.14532000
C	2.13931500	3.29502800	-0.14058700
C	3.02964600	4.35393400	-0.30062600
C	2.54892500	5.65233400	-0.44511500
H	0.82795400	6.93480800	-0.52500200
H	2.48633500	2.27647300	-0.00044900
H	4.09840400	4.16615600	-0.29778600
H	3.23772000	6.48510400	-0.54511600
O	0.33635700	1.26719900	1.02777600
O	-1.55519800	2.82644600	0.67897400
I	-1.79423300	5.15912800	-0.34430900
C	-1.69117200	7.01288600	-1.50425800
F	-2.92663700	7.25576800	-1.92622400
F	-1.27631100	8.05105400	-0.78875100
F	-0.89257800	6.87175900	-2.55349100
C	0.60687900	-1.76220200	-2.44817700
C	5.01598400	0.53767300	-1.24781200
F	1.07000000	-1.44004100	-3.65348600
F	0.30291400	-3.05326200	-2.43032100
F	-0.46897600	-1.04212700	-2.18499700
F	5.12166500	-0.59784600	-0.56721600
F	6.12492700	0.72559100	-1.95857500
F	4.87868100	1.54660200	-0.39171400
N	2.35548100	0.07206300	-1.41647800
O	2.93836300	-2.45974900	-1.43822400
O	1.21791800	-1.53889500	0.09302100
O	3.92837800	-0.54180600	-3.38704400
O	3.37827000	1.84640400	-2.82934900
S	1.93416100	-1.43926900	-1.19274300
S	3.56515000	0.47146100	-2.40237500
C	3.35366500	0.47833900	2.57386100
C	-0.41629500	-1.33676100	5.50574900
F	2.87892000	1.61725000	3.05918000
F	4.67592700	0.45719200	2.70787900
F	3.04001900	0.37712200	1.28988000
F	0.64405100	-1.74172900	6.18696500
F	-1.32198800	-0.84624100	6.34386600
F	-0.93631100	-2.36273100	4.84498600
N	1.03359900	-0.74586900	3.24525100
O	3.01260800	-0.78309100	4.87965300
O	3.05659900	-2.12709200	2.73987100
O	0.63435900	1.06149900	5.09873000
O	-1.16450100	0.21774700	3.52008600
S	2.63660900	-0.96213800	3.49027700
S	0.05178300	-0.00016200	4.30730400
C	6.86142300	-4.33997800	-2.90233100
C	8.04027300	-4.30985400	-1.93161700
H	7.22457200	-4.23383600	-3.93361300
H	6.35186100	-5.31108900	-2.83831500
C	9.05569300	-5.42165900	-2.19183100
H	8.54636500	-3.33595900	-1.99985400
H	7.66755000	-4.39662400	-0.90072900
C	10.23020800	-5.38180200	-1.21721000
H	8.55036600	-6.39424800	-2.12100700
H	9.42752000	-5.33683200	-3.22179800
H	10.94629300	-6.18640300	-1.41644500
H	10.76726100	-4.42865400	-1.29086300
H	9.88317900	-5.49000200	-0.18269500
C	5.85338800	-3.24099800	-2.61970800
H	6.34187700	-2.25695800	-2.69513700
H	5.46430800	-3.34415200	-1.59630600
O	4.79290200	-3.33616800	-3.55959500
H	4.15957600	-2.63165000	-3.34243000
S	-0.36259300	2.17675300	0.06420500
S	-2.77095100	-1.80533200	0.13060700
O	-0.60856000	1.57304200	-1.24323900
O	-1.96095100	-2.86552500	-0.46521100

INT2

C	4.66752700	2.56485800	-3.33640200

C	4.19968300	2.08218000	-2.12367000
C	2.96389400	1.45352500	-1.99496700
C	2.16836000	1.29748200	-3.13159300
C	2.61221000	1.77116900	-4.36209700
C	3.85253600	2.40066100	-4.45954900
H	5.62220000	3.06280700	-3.44692600
H	1.20496400	0.80786500	-3.02812100
H	1.99188300	1.65344400	-5.24465700
H	4.20276400	2.77573400	-5.41612900
C	2.50659400	0.97793600	-0.65584600
O	1.42840700	0.32917600	-0.58888000
O	3.23770900	1.26335400	0.33018300
I	5.29847100	2.23935500	-0.31996500
C	7.08829000	3.07587700	-1.27840000
F	8.00370200	3.20959200	-0.31604400
F	7.59188800	2.27899100	-2.22151700
F	6.88063300	4.27638000	-1.82015100
Zn	0.74895200	-0.45735000	1.10848500
C	-4.05693700	-4.68680900	-0.41655400
C	-3.13935900	-3.65103100	-0.50715200
C	-2.39403100	-3.21581600	0.58531500
C	-2.57176400	-3.84993300	1.81611600
C	-3.48192500	-4.89551400	1.93502200
C	-4.21854900	-5.30702600	0.82500600
H	-4.64666700	-5.02844900	-1.25737200
H	-1.99008000	-3.50897200	2.66704300
H	-3.61991600	-5.38873000	2.89173800
H	-4.93265300	-6.12006500	0.91226900
C	-1.43984700	-2.08186000	0.41985600
O	-0.79482400	-1.68110100	1.43021400
O	-1.33593200	-1.58491100	-0.73026900
I	-2.76716700	-2.58922700	-2.30082500
C	-4.17792900	-3.77133600	-3.50226800
F	-4.07550600	-3.31065400	-4.75292700
F	-3.88784900	-5.07410700	-3.51918800
F	-5.44942100	-3.63812300	-3.11830000
C	-0.16310900	3.58601400	0.52972700
C	-4.24326000	0.59290300	0.33403600
F	-1.01753800	4.40999400	-0.06012800
F	0.48332500	4.23512000	1.49181600
F	0.71189000	3.14663300	-0.36578200
F	-4.32823800	1.07576900	1.56779800
F	-5.43063200	0.68995600	-0.25750500
F	-3.89643400	-0.68947000	0.39296500
N	-1.61298300	1.27818500	0.09021000
O	-2.06355800	2.79097800	2.16546000
O	-0.00561300	1.38660600	1.93416100
O	-3.48008100	2.94814200	-0.50886000
O	-2.99439500	0.93718200	-1.95169300
S	-1.08590200	2.16608400	1.29004600
S	-3.01424400	1.57260900	-0.64753500
C	1.65413300	-2.71756900	4.16311500
C	3.99349700	-2.64496800	-0.34745800
F	1.28491000	-3.89101700	3.66574500
F	2.06596700	-2.88029800	5.41638900
F	0.61423400	-1.89036200	4.14726600
F	5.02791400	-2.62161100	0.48252100
F	4.19501800	-3.57371500	-1.27665200
F	3.88020500	-1.45911700	-0.93569700
N	2.34507800	-1.87438200	1.68733900
O	4.12087700	-2.95890200	3.22154500
O	3.20111800	-0.65438600	3.68840400
O	2.64631600	-4.39357300	1.09557000
O	1.36218000	-2.78207500	-0.36944000
S	3.03826900	-1.99635500	3.16225700
S	2.43671800	-3.05793000	0.57335500
C	-6.81537100	5.08725900	1.75087600
C	-8.04061000	5.22192800	0.84901400
H	-6.44736100	6.08432700	2.02884600
H	-7.09269400	4.57510700	2.68224700
C	-9.18640800	5.98563300	1.51157200
H	-7.75596600	5.73465900	-0.08114600
H	-8.39431600	4.22192900	0.55883400
C	-10.40381000	6.12239200	0.60047100
H	-9.47441600	5.47039800	2.43776400
H	-8.83203500	6.98265700	1.80599200
H	-11.21511000	6.66971800	1.09245900
H	-10.14525800	6.66062000	-0.31918200
H	-10.78973800	5.13709800	0.31306600
C	-5.68859700	4.31857900	1.08477100
H	-5.39732800	4.81664300	0.14867100
H	-6.02830400	3.30382700	0.82869100
O	-4.58809700	4.26229500	1.98100800
H	-3.88049600	3.72882500	1.58208900

TS1

C	-3.47441100	4.23730400	-1.92352500
C	-3.86860800	2.94891600	-1.58656000

C	-3.01411000	2.07479400	-0.92192600
C	-1.74430000	2.50778800	-0.55101900
C	-1.33968000	3.80483300	-0.85684400
C	-2.19902000	4.65927400	-1.54304200
H	-4.11222500	4.90849300	-2.48651600
H	-1.06925600	1.82739600	-0.04108000
H	-0.34619300	4.13372100	-0.57032900
H	-1.88259200	5.66404300	-1.80433700
O	-2.28778200	-0.41910500	-0.70743500
O	-4.03996900	0.39844300	0.83878700
I	-5.80745300	2.25148500	-2.11061900
C	-6.69180200	4.25044500	-2.19682100
F	-8.00779300	4.08021500	-2.13826100
F	-6.30563400	4.99070100	-1.16585500
F	-6.39766900	4.89459900	-3.31934000
Zn	-1.50378600	-1.90426800	0.46591800
C	3.23849000	-3.82070300	-4.29254000
C	2.89067900	-3.70519700	-2.94824700
C	1.65798000	-3.15576700	-2.57968300
C	0.77536900	-2.72570200	-3.57080400
C	1.12045800	-2.84198200	-4.91625200
C	2.34797700	-3.39031100	-5.27621600
H	4.19877700	-4.24257600	-4.57019700
H	-0.17746600	-2.29693200	-3.28110100
H	0.42623600	-2.50198200	-5.67818800
H	2.62418500	-3.48386100	-6.32199500
O	-0.12660500	-2.22633000	-0.96363500
O	0.90724500	-4.39186100	-0.37219200
I	4.32049900	-4.35766500	-1.55417500
C	5.03463900	-1.66450900	-0.99862500
F	4.79492100	-1.73494500	0.23043600
F	6.22212600	-1.81154200	-1.39618000
F	4.17127700	-1.22530500	-1.79390200
C	2.10713400	0.40598000	1.79530600
C	3.73624600	5.02178300	0.52573500
F	2.00516300	1.04664500	2.95829100
F	0.98343800	-0.27389000	1.58486600
F	3.13187900	-0.43406500	1.86008400
F	2.55625400	4.99033000	-0.08667000
F	3.85382900	6.17894200	1.17559000
F	4.69771000	4.94648400	-0.39131300
N	3.75134200	2.32742000	0.80184400
O	1.17153600	2.47453300	0.47821900
O	2.60994900	0.82006800	-0.75939700
O	2.77708400	3.84173000	2.66633500
O	5.24921700	3.71106800	2.21471000
S	2.35537900	1.62910500	0.42551400
S	3.87760400	3.62724600	1.73831400
C	-4.52817900	-4.47070600	1.69738200
C	-2.67509800	-0.19925100	3.75846100
F	-4.38178600	-4.83121800	2.96459500
F	-5.71078300	-4.88831200	1.25564200
F	-3.56784700	-5.03381500	0.97067800
F	-3.91751700	0.22453800	3.61131800
F	-2.23729500	0.13817500	4.97044300
F	-1.88999400	0.36081800	2.84503400
N	-2.92209700	-2.29898400	2.02336800
O	-5.50361000	-2.09988600	2.35042500
O	-4.44575100	-2.42708300	0.07319300
O	-3.62005700	-2.55783600	4.50027100
O	-1.19758600	-2.36965600	3.83938700
S	-4.44771600	-2.62580400	1.51283800
S	-2.59456200	-2.04629900	3.61357900
C	7.20774700	2.29079000	-0.10332600
C	8.24511900	2.74613200	0.91961000
H	6.39347000	3.02552100	-0.14497500
H	7.65704200	2.24145300	-1.10418500
C	8.78992200	4.14134900	0.61652300
H	7.78868100	2.74774200	1.91883200
H	9.07742700	2.02799600	0.94885400
C	9.82159200	4.60550900	1.64141400
H	9.23732500	4.14563000	-0.38666900
H	7.95247600	4.85196700	0.58810100
H	10.19706800	5.60777900	1.40823000
H	9.38607800	4.63593800	2.64727300
H	10.67995900	3.92377700	1.66956100
C	6.61202600	0.93517400	0.23653900
H	6.17369400	0.94829900	1.24326700
H	7.37772700	0.15208900	0.20263800
O	5.61140600	0.55609900	-0.71498300
H	4.83569600	1.12873500	-0.56509500
S	-3.52678200	0.40918700	-0.52945800
S	1.15821300	-3.02932500	-0.85874300
O	-4.52594400	0.12226500	-1.59475700
O	2.20106800	-2.28436200	-0.14855700

TS2

C	3.56563100	4.65445800	0.97540300

C	3.64214300	3.27062200	1.01575600
C	2.54164600	2.45201300	0.77324100
C	1.31428500	3.05033100	0.48344200
C	1.20618300	4.43632600	0.43573900
C	2.32658100	5.22929300	0.68065900
H	4.41477400	5.29889800	1.16210900
H	0.45608300	2.40918300	0.31169700
H	0.24956400	4.89439200	0.20668500
H	2.24974200	6.31159700	0.64601200
C	2.69080500	0.96851600	0.82937100
O	1.68897500	0.24710200	0.56305100
O	3.82763200	0.52394700	1.14360800
I	5.43714400	2.23683300	1.45602200
C	6.65415800	4.05629400	1.67033300
F	7.89151100	3.64117000	1.95319200
F	6.70759100	4.78616900	0.55527400
F	6.24987100	4.85075400	2.66312700
Zn	1.85763600	-1.76917200	0.53440600
C	-3.92046100	-4.86435800	1.32262100
C	-2.87776600	-4.20795400	0.67037700
C	-1.62098400	-4.05819800	1.26421500
C	-1.43321600	-4.58204200	2.54814400
C	-2.45834300	-5.25959400	3.20394500
C	-3.70172000	-5.40294400	2.59029500
H	-4.89268100	-4.95390600	0.84859000
H	-0.46414000	-4.46027500	3.02329300
H	-2.28665500	-5.67184800	4.19360600
H	-4.50913200	-5.92493200	3.09492200
C	-0.43878400	-3.42123000	0.57022400
O	0.20711100	-2.56928400	1.29328300
O	-0.15253700	-3.75400000	-0.57907200
I	-3.32635800	-3.33046600	-1.18930500
C	-4.50554400	-1.06167100	-0.00066000
F	-4.81606700	-0.56330800	-1.11872700
F	-5.35748400	-1.73985300	0.63605800
F	-3.43119700	-0.71561200	0.55897500
C	-1.71988300	1.30239000	-2.03176100
C	-5.16178000	4.75124700	-0.67505200
F	-2.16096900	1.71024800	-3.21564800
F	-0.39041200	1.28346000	-2.04282900
F	-2.16578500	0.06625500	-1.80816100
F	-4.04681400	5.37838900	-0.31878400
F	-5.95317100	5.60327200	-1.32214700
F	-5.78698500	4.32745100	0.42110100
N	-3.89940800	2.36596900	-0.81875300
O	-1.69308400	3.72621900	-1.00951800
O	-1.92581500	1.75902600	0.53917500
O	-4.07079300	3.88804300	-2.91445300
O	-6.06280900	2.66257000	-1.97445100
S	-2.29886600	2.44280900	-0.69033900
S	-4.77715600	3.31523300	-1.78091100
C	3.98025100	-4.80706400	-0.16494900
C	4.89749600	-0.13748400	-1.99661900
F	3.73112800	-5.04554300	-1.44537500
F	4.75725500	-5.76947900	0.32004600
F	2.83305700	-4.78731800	0.50883200
F	5.87800100	-0.35887800	-1.13135200
F	5.41720900	0.08254300	-3.19934700
F	4.21290500	0.93669200	-1.62249600
N	3.69674200	-2.16112400	-0.56566900
O	6.04060500	-3.24091900	-0.76750600
O	4.91268900	-2.98542200	1.47108600
O	4.39896100	-2.52188700	-3.03474600
O	2.45194400	-1.05281800	-2.39614900
S	4.83527800	-3.17542700	0.03477600
S	3.75932500	-1.61457700	-2.10324600
C	-7.49324100	0.35590900	2.08359200
C	-9.01360800	0.46860300	1.98701300
H	-7.13184600	0.90198200	2.96458500
H	-7.20771300	-0.69632500	2.21476300
C	-9.72722600	-0.07772300	3.22269400
H	-9.29322600	1.52225400	1.84427500
H	-9.36565900	-0.07250200	1.09711700
C	-11.24570800	0.04216500	3.12062600
H	-9.44837200	-1.13053400	3.36394600
H	-9.37306900	0.46186600	4.11118400
H	-11.74084400	-0.35471900	4.01335700
H	-11.54830300	1.08986700	3.00672700
H	-11.62420100	-0.51085500	2.25278300
C	-6.80896000	0.91479000	0.85017500
H	-7.04747500	1.97708900	0.73043800
H	-7.14846500	0.39112100	-0.05552900
O	-5.38738500	0.76175600	0.98511900
H	-4.93023500	1.46434400	0.47372500