

Supplementary Information

Studies Directed Towards Nonylacridine Orange Analogues Having the Potential to Act as FRET Donors with the PDT Drug Pc 4

Ping Zhang,^a Yang Yang,^a Yun Liu,^a Myriam E. Rodriguez^b and Malcolm E. Kenney^{a*}

^a*Department of Chemistry, Case Western Reserve University, Cleveland, OH 44106, USA*

^b*Department of Radiation Oncology, School of Medicine, Case Western Reserve University, OH 44106, USA*

* E-mail: mek9@case.edu

Telephone: +1-216-368-3739

The optimized geometry of 1

C	-5.10702500	-2.26663500	0.21506600
C	-3.72669500	-2.21423700	0.37327400
C	-3.00058800	-0.99970200	0.24124300
C	-3.71878900	0.21833100	-0.05328900
C	-5.13407800	0.14535100	-0.19840000
C	-5.80615800	-1.03810100	-0.06941400
C	-2.98428300	1.39971200	-0.17432500
C	-1.59859300	1.38048500	-0.01098400
C	-0.97167200	0.11443900	0.28859400
C	0.44508700	0.06958600	0.44682200
H	0.86914700	-0.90705300	0.64308800
C	1.22993600	1.20442800	0.33751200
C	0.58299200	2.46093400	0.05486500
C	-0.76973000	2.53751000	-0.11461500
H	-3.13978700	-3.09275400	0.60698000
H	-5.68555500	1.05807600	-0.41423600
H	-6.88310600	-1.04437900	-0.18540700
H	-3.49363900	2.33665000	-0.39651700
H	1.17424400	3.36920200	0.01519000
H	-1.23760100	3.49867300	-0.31730000
N	-1.66277800	-1.03316800	0.40720600
N	-5.81470700	-3.45775600	0.31053600
N	2.61647700	1.18910500	0.55789200
C	3.48036000	1.93255700	-0.35384000
H	3.05513300	2.90679300	-0.59562800
H	4.45091300	2.09990100	0.12522100
H	3.65230600	1.39237700	-1.30112000
C	3.21342600	-0.05764900	1.00578900
H	2.66792600	-0.44352900	1.87112700
H	3.22703600	-0.83982900	0.22642400
H	4.24660500	0.13734400	1.30977300
C	-5.10771300	-4.65562700	0.73037900
H	-5.79000200	-5.50734800	0.69284700
H	-4.27176200	-4.86552500	0.05361600
H	-4.70346400	-4.57639600	1.75250900
C	-7.26302000	-3.43925900	0.44664800
H	-7.74085200	-2.98469700	-0.42889700
H	-7.62372800	-4.46749900	0.51456600
H	-7.60437600	-2.89766500	1.34304700

The optimized geometry of 2

C	-5.15829400	-2.27898300	0.28510000
C	-3.76301100	-2.22106100	0.42570500
C	-3.06942200	-1.01854400	0.22809200
C	-3.73672300	0.18566000	-0.11233000
C	-5.14136700	0.10008800	-0.24022300
C	-5.83790800	-1.07176000	-0.05160400
C	-3.00038300	1.42926000	-0.31046000
C	-1.55464800	1.34505400	-0.13585800
C	-0.92431300	0.12111400	0.20489700
C	0.46421300	0.02316100	0.37362900
H	0.88404700	-0.94353500	0.62949600
C	1.28953600	1.14748400	0.21544600
C	0.66488600	2.38112600	-0.13200900
C	-0.69936400	2.45858700	-0.29539700
H	-3.19312900	-3.10496600	0.69025000
H	-5.66970300	1.01231700	-0.49624100
H	-6.91524200	-1.06391600	-0.16033100
H	1.26111800	3.27398000	-0.27318500
H	-1.16329700	3.40288900	-0.55983600
N	-1.69905100	-1.00614300	0.37280600
N	-5.85160900	-3.45936100	0.46220500
N	2.65557400	1.06780700	0.39133700
H	-1.23658600	-1.87179500	0.61428100
S	-3.77255300	2.87395300	-0.71567800
C	3.49675400	2.22714400	0.13791200
H	3.22066100	3.07107100	0.78244400
H	4.53435800	1.96820500	0.35528100
H	3.44061500	2.56373400	-0.90743600
C	3.27481500	-0.21711200	0.66060800
H	2.89013900	-0.65953300	1.58960600
H	3.10620500	-0.93799100	-0.15378900
H	4.35136100	-0.08224200	0.77659700
C	-5.14814800	-4.64768100	0.91008600
H	-5.85159700	-5.47905700	0.97874000
H	-4.36047500	-4.93445200	0.20079000
H	-4.68201700	-4.51004700	1.89794900
C	-7.30615600	-3.46499400	0.43257700
H	-7.74452500	-2.84270200	1.22652200
H	-7.68705000	-3.10572800	-0.53118400
H	-7.66042800	-4.48830500	0.56799100

The optimized geometry of 3

C	-5.08565400	-2.22087100	0.20696800
C	-3.70387200	-2.15776600	0.33053900
C	-2.99265900	-0.93017000	0.24006600
C	-3.71885800	0.30024700	0.01599100
C	-5.13924400	0.21236100	-0.07635700
C	-5.79645100	-0.98338900	0.01565600
C	-2.97977600	1.49606300	-0.09147300
C	-1.58048300	1.45795300	0.06029200
C	-0.96213100	0.17291400	0.30870700
C	0.45452300	0.09600600	0.45544700
H	0.85504000	-0.89721600	0.61334800
C	1.26317400	1.21538200	0.38197700
C	0.63174200	2.48720300	0.14399100
C	-0.72027900	2.59698100	-0.01260700
H	-3.09870300	-3.03665500	0.50978600
H	-5.70849200	1.12778600	-0.20046600
H	-6.87779500	-0.98670700	-0.05031400
H	1.23391600	3.38897100	0.12631400
H	-1.16699400	3.57160900	-0.17634400
N	-1.65489200	-0.97444000	0.38288100
N	-5.77951700	-3.42208400	0.25678700
N	2.64789000	1.16435300	0.59446000
S	-3.81915000	3.06444900	-0.39625000
C	-4.12353700	2.92533300	-2.20251900
H	-4.64659300	3.83820900	-2.50099100
H	-3.18092600	2.85446700	-2.75061600
H	-4.75040200	2.05940500	-2.42892100
C	3.52634000	1.94876800	-0.26706300
H	3.11925500	2.94378600	-0.44691700
H	4.49801100	2.06885500	0.22350700
H	3.69206500	1.46673700	-1.24614200
C	3.22473400	-0.11251800	0.97933600
H	2.67813800	-0.52869300	1.82986300
H	3.21845000	-0.85714900	0.16410800
H	4.26309200	0.04904900	1.28473200
C	-5.05006100	-4.63261900	0.59425000
H	-5.72230200	-5.48985500	0.51894500
H	-4.22461100	-4.79090200	-0.10867000
H	-4.62807800	-4.60756200	1.61198300
C	-7.22292100	-3.42550700	0.44096300
H	-7.53831300	-2.95068600	1.38350600
H	-7.73099200	-2.91520800	-0.38510500
H	-7.57433300	-4.45921400	0.44785500

The optimized geometry of 4

C	-5.11750300	-2.24454000	0.19074400
C	-3.73552500	-2.18833700	0.33258400
C	-3.01206000	-0.97221700	0.20015000
C	-3.73988600	0.24039800	-0.08797700
C	-5.15679700	0.17106100	-0.20548300
C	-5.82316200	-1.01554300	-0.07062400
C	-3.00399800	1.42600200	-0.22250600
C	-1.61519100	1.41449000	-0.04011300
C	-0.99018500	0.14694500	0.25205900
C	0.42636900	0.10850100	0.41524500
H	0.85285700	-0.86900400	0.60139500
C	1.20690900	1.24827300	0.32953500
C	0.55461900	2.50642200	0.07105700
C	-0.79726400	2.58067800	-0.10905300
H	-3.14335200	-3.06525200	0.55862000
H	-5.70995600	1.08816600	-0.38211800
H	-6.90296800	-1.02037800	-0.15619400
H	1.13925200	3.41992900	0.06652300
H	-1.27540200	3.54163900	-0.27122800
N	-1.67319400	-1.00667400	0.35585500
N	-5.81957500	-3.43912800	0.28693500
N	2.59208700	1.23492600	0.55714300
C	-3.77245200	2.90500000	-1.89601500
H	-4.30022300	3.85907400	-1.96367800
H	-2.78588500	2.99704100	-2.36713100
H	-4.34783900	2.12937300	-2.41675800
O	-3.65341300	2.61015100	-0.50114500
C	3.45708600	2.00231200	-0.33310700
H	3.02454200	2.97658400	-0.56127200
H	4.42196000	2.17001200	0.15726400
H	3.64251100	1.48080700	-1.28838000
C	3.19347800	-0.01684500	0.98428300
H	2.64653400	-0.42169500	1.83998500
H	3.21445300	-0.78421000	0.19046000
H	4.22433200	0.17766500	1.29638100
C	-5.10404400	-4.63579100	0.69593900
H	-5.78277400	-5.49043000	0.65883900
H	-4.27221800	-4.83832800	0.01201600
H	-4.69278900	-4.56003300	1.71554400
C	-7.26576700	-3.42586000	0.44516700
H	-7.59512300	-2.89946500	1.35507600
H	-7.75664100	-2.95811600	-0.41589700
H	-7.62345500	-4.45592400	0.50138500

The optimized geometry of 5

C	-5.10864900	-2.26475300	0.22838400
C	-3.72933300	-2.19339300	0.38048000
C	-3.01507700	-0.97300100	0.24349900
C	-3.74657100	0.24063600	-0.05264800
C	-5.16137300	0.14841900	-0.19128600
C	-5.81695400	-1.04329400	-0.05606800
C	-2.99469500	1.41584500	-0.17506100
C	-1.60436900	1.41306700	-0.01600600
C	-0.98841100	0.13843600	0.28492700
C	0.42726500	0.07892300	0.44219500
H	0.83355000	-0.90495000	0.63807900
C	1.22972600	1.20092800	0.33307000
C	0.59308100	2.46111400	0.04987900
C	-0.75828900	2.55742100	-0.11894500
H	-3.12826700	-3.06227800	0.61343700
H	-5.72772400	1.04786000	-0.40658900
H	-6.89426900	-1.05729100	-0.16767600
H	1.18939900	3.36545400	0.00577100
H	-1.20607700	3.52436600	-0.32055700
N	-1.67957500	-1.00576000	0.40615800
N	-5.80127700	-3.46048000	0.33168300
N	2.61259000	1.16418200	0.55248200
Cl	-3.81927600	2.93343000	-0.53962700
C	3.49239700	1.93573500	-0.31967500
H	3.08251900	2.92524100	-0.52192100
H	4.46017000	2.07010000	0.17457200
H	3.66607300	1.43480500	-1.28752400
C	3.19645700	-0.09760300	0.97565200
H	2.65029000	-0.49267300	1.83645500
H	3.19686900	-0.86485600	0.18193900
H	4.23270600	0.07946500	1.27905400
C	-5.07980500	-4.65268600	0.74341800
H	-5.75555700	-5.50969100	0.71560900
H	-4.24958400	-4.85703700	0.05754100
H	-4.66529300	-4.56759400	1.76052900
C	-7.25254000	-3.46304300	0.43576000
H	-7.61999600	-2.91779200	1.31901700
H	-7.71800800	-3.02426800	-0.45452000
H	-7.59883700	-4.49578700	0.50734500

The optimized geometry of 6

C	-5.09745200	-2.24561600	0.21234500
C	-3.71524500	-2.18379100	0.33745200
C	-2.99300700	-0.96325700	0.23199500
C	-3.71817500	0.25708500	-0.01498200
C	-5.13564100	0.17618500	-0.11174600
C	-5.80582900	-1.01308200	-0.00063700
C	-2.98224900	1.46022100	-0.14441900
C	-1.58114200	1.41581100	0.04876800
C	-0.96936900	0.13562200	0.29762100
C	0.44878600	0.07128100	0.44654100
H	0.85657400	-0.92031800	0.59718200
C	1.25136300	1.19622300	0.39331000
C	0.61825500	2.46927000	0.18516000
C	-0.73574800	2.56381200	0.01684800
H	-3.11467800	-3.06285600	0.53094700
H	-5.72623200	1.08016500	-0.23983800
H	-6.88678600	-1.01060000	-0.06797000
H	1.21279100	3.37595700	0.21161900
H	-1.16850300	3.55548900	-0.09182900
N	-1.65367300	-1.01899700	0.37320700
N	-5.79365500	-3.44805200	0.27932900
N	2.64001400	1.15134200	0.60660200
N	-3.62484300	2.66030700	-0.40813600
H	-3.05112800	3.37811000	-0.82888800
H	-4.51977700	2.58318000	-0.87123600
C	3.50357100	1.91825600	-0.28536400
H	3.08847900	2.90726900	-0.48131500
H	4.48271000	2.05255800	0.18690200
H	3.65593100	1.41537900	-1.25660100
C	3.21979100	-0.12538900	0.98698900
H	2.67499100	-0.54490600	1.83697500
H	3.21479000	-0.86868000	0.17009700
H	4.25848500	0.03773500	1.29146300
C	-5.06704600	-4.64907400	0.65474500
H	-5.73838700	-5.50837400	0.59261000
H	-4.23470900	-4.82393900	-0.03561900
H	-4.65505500	-4.60013200	1.67601400
C	-7.23313600	-3.44118800	0.48822400
H	-7.75125600	-2.93361900	-0.33318400
H	-7.59136400	-4.47263300	0.50748400
H	-7.53139300	-2.95745500	1.43244300

The optimized geometry of 7

C	-5.04232500	-2.25781400	0.23250000
C	-3.66062100	-2.21278000	0.37005800
C	-2.93346400	-0.99543700	0.26956500
C	-3.64693800	0.23661700	0.03131900
C	-5.06540600	0.16939800	-0.09560100
C	-5.73781500	-1.01684300	0.00208000
C	-2.91732300	1.43739200	-0.06116000
C	-1.51637800	1.38591000	0.08461100
C	-0.90101700	0.09945200	0.32439600
C	0.51756400	0.01976500	0.45956100
H	0.91819800	-0.97475700	0.61006100
C	1.32789200	1.13734000	0.38687000
C	0.69946700	2.41288100	0.16860700
C	-0.65432400	2.52456500	0.02187600
H	-3.07004100	-3.09868700	0.56307000
H	-5.60333400	1.09435900	-0.27262200
H	-6.81653500	-1.01445200	-0.09939400
H	1.30484400	3.31288100	0.15938200
H	-1.08473600	3.50745900	-0.12872100
N	-1.59532300	-1.04746200	0.41174400
N	-5.75236000	-3.44997700	0.29639300
N	2.71731200	1.08442600	0.58506700
N	-3.65209600	2.64839900	-0.29927400
C	-3.75713900	3.57407000	0.82068900
H	-2.85011200	4.17572800	1.00807200
H	-4.58489900	4.26956100	0.63189400
H	-3.98508300	3.01488300	1.73295400
C	-3.47715500	3.27507400	-1.60259900
H	-4.31685200	3.95810400	-1.78458400
H	-2.54416600	3.85475900	-1.71599100
H	-3.49214100	2.50512400	-2.37957800
C	3.58020300	1.84403700	-0.31407800
H	3.17173400	2.83591100	-0.50886900
H	4.56323700	1.97170200	0.15165700
H	3.72211500	1.33828400	-1.28515900
C	3.29239900	-0.19358000	0.96863500
H	2.75320800	-0.60355200	1.82685900
H	3.27401900	-0.94208300	0.15686200
H	4.33507600	-0.03549700	1.26157700
C	-5.04243200	-4.66318400	0.66368300
H	-5.72585100	-5.51263300	0.60061500
H	-4.21389500	-4.84726100	-0.02931100
H	-4.62726500	-4.62354000	1.68389800

C	-7.19700600	-3.43108300	0.46786000
H	-7.51440500	-2.92597100	1.39394000
H	-7.69267600	-2.93805800	-0.37614200
H	-7.56125300	-4.45989600	0.50104900

The optimized geometry of 8

C	-5.09356200	-2.32785600	0.05244000
C	-3.71848100	-2.24714500	0.23570800
C	-3.02536300	-1.00656300	0.20528600
C	-3.76839000	0.20984000	-0.00875500
C	-5.17630000	0.10849800	-0.17951200
C	-5.81771800	-1.09979300	-0.14926000
C	-3.05884200	1.43556100	-0.03328000
C	-1.65611000	1.41096700	0.15489100
C	-1.01974400	0.13575700	0.36847300
C	0.39470600	0.09025700	0.54734000
H	0.82067200	-0.89657900	0.67639300
C	1.17263200	1.23427200	0.53834000
C	0.51462300	2.49884600	0.33983300
C	-0.83707500	2.57612000	0.15338200
H	-3.10694400	-3.12195100	0.41320600
H	-5.74822100	1.01834400	-0.33485100
H	-6.89260700	-1.12182400	-0.28214000
H	1.09345400	3.41524600	0.37659800
H	-1.31058400	3.54347600	0.01544300
N	-1.69021400	-1.02945100	0.38999500
N	-5.76795400	-3.54138100	0.04595500
N	2.55465000	1.21274900	0.78137400
C	-3.74125400	2.66459400	-0.24397400
C	-4.32527400	3.71802500	-0.42506100
C	-5.00830700	4.94963300	-0.63704200
C	-6.40375200	4.97111400	-0.83810300
C	-4.30154700	6.16963300	-0.64970600
C	-7.06720500	6.17697800	-1.04481900
H	-6.95358400	4.03498700	-0.82974800
C	-4.97349500	7.37068100	-0.85715100
H	-3.22695700	6.15986000	-0.49530900
C	-6.35663000	7.38000400	-1.05526400
H	-8.14293600	6.17865600	-1.19847200
H	-4.41621100	8.30352400	-0.86428900
H	-6.87777500	8.31958600	-1.21682900
C	3.15590300	-0.06123700	1.13735700
H	2.60179300	-0.51919900	1.96116000
H	3.18757500	-0.77849200	0.29839800
H	4.18274800	0.11657400	1.47164400
C	3.42732800	2.03838200	-0.04726600
H	2.99719600	3.02628800	-0.21247100
H	4.38727900	2.17218100	0.46262100
H	3.62182400	1.58300200	-1.03386700

C	-5.03257000	-4.74780400	0.38459300
H	-5.68820400	-5.61309300	0.26709900
H	-4.17954200	-4.87939300	-0.29048000
H	-4.64833100	-4.73802200	1.41743600
C	-7.21795500	-3.57280100	0.16149000
H	-7.58590500	-3.11520000	1.09345500
H	-7.69673900	-3.06161600	-0.68159900
H	-7.55027500	-4.61257400	0.14037400

The optimized geometry of 9

C	-5.11239200	-2.26739100	0.24949300
C	-3.73050200	-2.20518600	0.39442700
C	-3.01629800	-0.98570300	0.25885200
C	-3.74365600	0.22760800	-0.02720200
C	-5.15812100	0.14917100	-0.16083200
C	-5.81774200	-1.04105000	-0.02752400
C	-3.00093000	1.41886900	-0.15250500
C	-1.60120100	1.39925100	0.00163200
C	-0.98197100	0.12914600	0.29311400
C	0.43360400	0.07016100	0.44254100
H	0.84582400	-0.91224700	0.63273500
C	1.23044000	1.19784900	0.33238200
C	0.58652500	2.45724900	0.05567300
C	-0.76665500	2.54931400	-0.10520300
H	-3.13353000	-3.07892000	0.61944800
H	-5.71887200	1.05573700	-0.37052500
H	-6.89552800	-1.05173500	-0.13436700
H	1.17898000	3.36365400	0.00814200
H	-1.22363700	3.51471300	-0.30383400
N	-1.67767100	-1.01476400	0.41319900
N	-5.81035800	-3.45714000	0.35477400
N	2.61248200	1.16572200	0.54468200
C	-3.67188100	2.65252500	-0.43847300
N	-4.21743800	3.65447200	-0.67065700
C	3.20627300	-0.09632700	0.95389800
H	2.66719000	-0.50255600	1.81402100
H	3.20705100	-0.85577700	0.15306200
H	4.24267300	0.08442500	1.25375600
C	3.48987300	1.96376900	-0.30606900
H	3.07685800	2.95650500	-0.48396100
H	4.45548000	2.09015800	0.19398200
H	3.66794000	1.48802200	-1.28538300
C	-5.09250400	-4.66004400	0.74134200
H	-5.77750900	-5.50959500	0.72367800
H	-4.27854800	-4.86892400	0.03698300
H	-4.65647900	-4.58460600	1.74972900
C	-7.26380400	-3.45914100	0.42659400
H	-7.64837400	-2.90149900	1.29406600
H	-7.71110600	-3.03336500	-0.47955500
H	-7.61122700	-4.49057700	0.50722500

The optimized geometry of 10

C	-5.11401400	-2.33047800	0.22613000
C	-3.73737600	-2.24329200	0.38994800
C	-3.04423100	-1.00801300	0.28118000
C	-3.78299700	0.20418800	0.01046700
C	-5.19901900	0.09201300	-0.14253400
C	-5.83623600	-1.11260300	-0.03922600
C	-3.06912800	1.41621400	-0.05209100
C	-1.66733500	1.39905100	0.09172100
C	-1.02988000	0.12733800	0.34922000
C	0.38861000	0.06999500	0.48691700
H	0.80190900	-0.91558500	0.65918600
C	1.18484100	1.19544100	0.37725000
C	0.53752700	2.45266700	0.10958400
C	-0.81857500	2.54535600	-0.02789300
H	-3.12445100	-3.10808700	0.60735200
H	-5.77439600	0.98152700	-0.37073300
H	-6.91128500	-1.14158200	-0.17012300
H	1.13077200	3.35780300	0.04157600
H	-1.26231400	3.51364000	-0.23384000
N	-1.70831500	-1.02645300	0.45253600
N	-5.79095500	-3.53756900	0.29767900
N	2.57292200	1.16392400	0.57418000
C	-3.82975300	2.70305200	-0.28141400
O	-4.58111800	2.87728800	-1.23209100
N	-3.63356100	3.66546700	0.67279400
H	-4.19333000	4.50549700	0.61578900
H	-3.12466800	3.47500800	1.52323500
C	3.43135700	1.93216300	-0.32228100
H	3.02093100	2.92422700	-0.51116400
H	4.41343700	2.06094200	0.14454100
H	3.57488200	1.43207000	-1.29554400
C	3.16601900	-0.09983500	0.97855100
H	2.63418700	-0.50238900	1.84488800
H	3.15531300	-0.86163800	0.17956400
H	4.20677900	0.07703600	1.26664100
C	-5.05557400	-4.72995600	0.68200700
H	-5.71842000	-5.59567400	0.62560900
H	-4.21729600	-4.90314000	-0.00268100
H	-4.64941100	-4.66727600	1.70425800
C	-7.24284000	-3.56367400	0.38636000
H	-7.62746100	-3.04229900	1.27675200
H	-7.70607000	-3.11311800	-0.49917000
H	-7.57431600	-4.60274200	0.43323500

The optimized geometry of **18**

C	-5.11006800	-2.29079200	0.18308200
C	-3.72702000	-2.23343400	0.30845300
C	-3.02156900	-0.99965700	0.28613300
C	-3.75999400	0.23167200	0.14393600
C	-5.17758200	0.15187200	0.03141800
C	-5.83051900	-1.04982000	0.05158700
C	-3.04418400	1.43233100	0.12908800
C	-1.65406700	1.41899300	0.25021500
C	-1.01083200	0.13765500	0.39384200
C	0.41259800	0.10619900	0.49904100
H	0.86227600	-0.87603200	0.57654700
C	1.18946000	1.24494700	0.48591400
C	0.51443300	2.53112100	0.37862100
C	-0.84886300	2.59837800	0.24971300
H	-3.12198700	-3.12215400	0.43167300
H	-5.74745500	1.07310700	-0.07049900
H	-6.91022600	-1.05974000	-0.03586700
H	-3.57421700	2.37796700	0.02241400
H	-1.35055500	3.55673900	0.17161100
N	-1.67834600	-1.02715900	0.41021300
N	-5.80090200	-3.49795500	0.16603500
N	2.58548800	1.21382500	0.66090900
C	3.41364600	1.80604900	-0.39155800
H	2.99833800	2.76050700	-0.70811900
H	4.42110200	1.98053100	0.00244700
H	3.49752000	1.14101400	-1.26895100
C	3.15557500	-0.02443800	1.16622700
H	2.59849400	-0.36179200	2.04438100
H	3.16496400	-0.84226300	0.42333000
H	4.19182400	0.16815100	1.46401200
C	-5.06506200	-4.72052500	0.43885800
H	-5.73360400	-5.57591800	0.32043500
H	-4.24125400	-4.83848200	-0.27374600
H	-4.63934400	-4.74735700	1.45538700
C	-7.24004900	-3.51529300	0.37922400
H	-7.76719200	-2.96918500	-0.41140300
H	-7.58855300	-4.54950500	0.34450900
H	-7.53817300	-3.08623200	1.34927800
O	1.33034200	3.62558100	0.45013700
C	0.73129400	4.91015100	0.42431900
H	1.55085700	5.62438600	0.52348200
H	0.20228400	5.09071200	-0.52102800
H	0.02967800	5.03961300	1.25870900

The optimized geometry of **20**

C	-5.11742900	-2.29100400	0.18234300
C	-3.73611600	-2.21094800	0.29931100
C	-3.04744300	-0.96769600	0.27236900
C	-3.79225000	0.26103300	0.12518700
C	-5.21104500	0.15418200	0.03881900
C	-5.84782100	-1.05686100	0.06774000
C	-3.07319000	1.47530700	0.08013500
C	-1.67215800	1.45311300	0.21808300
C	-1.03845400	0.16567100	0.38438900
C	0.38372200	0.11328200	0.50315000
H	0.81090200	-0.87745600	0.59581200
C	1.18184000	1.23548800	0.48424400
C	0.52141600	2.52581300	0.35442500
C	-0.83903200	2.61326800	0.20924500
H	-3.11420200	-3.08776200	0.42345300
H	-5.79714200	1.06492400	-0.02906200
H	-6.92955300	-1.07354300	0.00917900
H	-1.32337700	3.57620500	0.11854000
N	-1.70629700	-0.99524600	0.40059900
N	-5.79157700	-3.50666600	0.16551800
N	2.57344100	1.18291300	0.67432900
C	3.42676200	1.76835400	-0.36172800
H	3.02719300	2.72735200	-0.68424900
H	4.42854900	1.93140800	0.05098600
H	3.51960600	1.10334100	-1.23813400
C	3.11932200	-0.06284500	1.18790100
H	2.54871200	-0.38967800	2.06133400
H	3.12298900	-0.88186300	0.44641600
H	4.15533700	0.11433400	1.49550000
C	-5.03843400	-4.71895900	0.43757800
H	-5.69466800	-5.58364500	0.31761900
H	-4.21264400	-4.82417800	-0.27467100
H	-4.61337400	-4.74088500	1.45444000
C	-7.22952100	-3.54373100	0.38513200
H	-7.76477900	-2.98726500	-0.39234300
H	-7.56698800	-4.58078700	0.33038200
H	-7.52813400	-3.13765200	1.36489300
O	1.34616100	3.61219700	0.42310400
C	0.75989900	4.90410900	0.38576700
H	1.58678900	5.60911700	0.48952800
H	0.24172600	5.08479700	-0.56505900
H	0.05145600	5.04342200	1.21206000
S	-3.94108000	3.04215200	-0.13017400

C	-4.26118300	2.99847800	-1.93885800
H	-4.87805200	2.13660800	-2.20503300
H	-4.80018700	3.91812900	-2.18352800
H	-3.32320800	2.96973200	-2.49866800

The optimized geometry of 23

C	-5.09806600	-2.43364100	0.15725100
C	-3.72215400	-2.33398000	0.31153400
C	-3.04355300	-1.08488700	0.26656800
C	-3.79818700	0.13210200	0.07366800
C	-5.21179800	0.00308700	-0.07015500
C	-5.83695600	-1.21390100	-0.02943500
C	-3.10005900	1.35881400	0.03998700
C	-1.70116400	1.33989200	0.18968800
C	-1.04983600	0.06973800	0.38026100
C	0.37178000	0.04858500	0.51230400
H	0.82217700	-0.92999800	0.62347000
C	1.14392600	1.18958400	0.48294700
C	0.45981600	2.46544300	0.33021900
C	-0.90053800	2.52182700	0.17500600
H	-3.09469100	-3.20045900	0.47480300
H	-5.81445800	0.89173400	-0.21650300
H	-6.91384400	-1.24660400	-0.14418700
H	-1.41968300	3.46428100	0.06270400
N	-1.70415300	-1.09992200	0.41815000
N	-5.75976300	-3.65817200	0.16068800
N	2.53641300	1.17005600	0.68291400
C	3.38081500	1.75081100	-0.36279900
H	2.96347300	2.69549400	-0.70477300
H	4.37852000	1.94137400	0.04835900
H	3.48857300	1.07078600	-1.22605600
C	3.10514200	-0.05479400	1.22086200
H	2.53547600	-0.37910600	2.09588200
H	3.13143700	-0.88644300	0.49380500
H	4.13520100	0.14946700	1.53215600
C	-5.00183000	-4.85018400	0.50043400
H	-5.64429600	-5.72680200	0.39204300
H	-4.15351700	-4.97092000	-0.18202500
H	-4.60776800	-4.83030000	1.52996700
C	-7.20044100	-3.70164300	0.35924000
H	-7.72891400	-3.17806400	-0.44522100
H	-7.52765600	-4.74323700	0.33503900
H	-7.51880900	-3.26469300	1.31959300
O	1.26518700	3.56950600	0.38942400
C	0.65280700	4.84629600	0.31982300
H	1.46298500	5.57179700	0.41581000
H	0.13860700	4.99638800	-0.63870800
H	-0.06637600	4.98836700	1.13680400
N	-3.73612600	2.63458200	-0.13969200

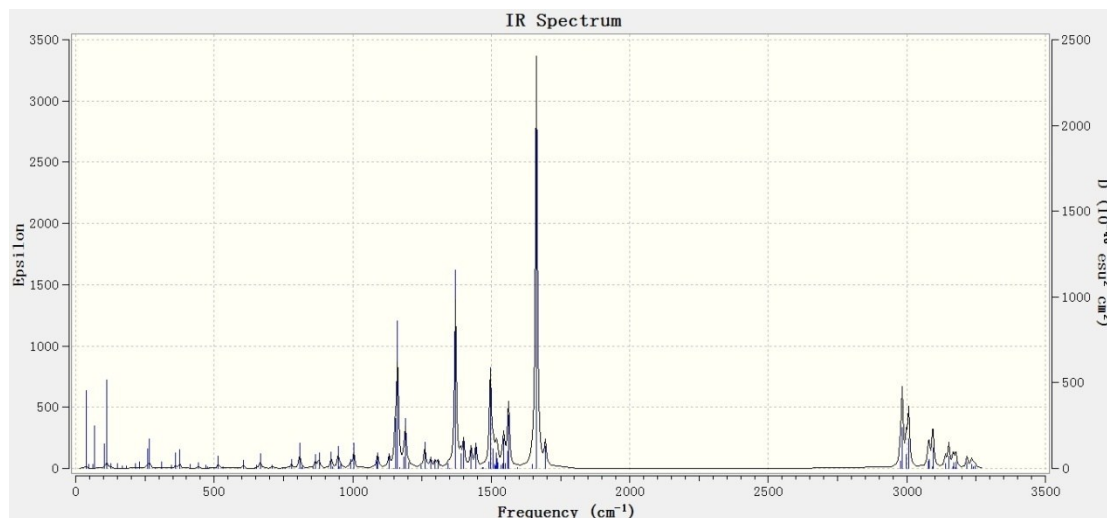
C	-4.56086000	3.11480400	0.96118700
H	-4.70316300	4.19794700	0.85367900
H	-5.56121000	2.65184600	1.02673800
H	-4.04297300	2.93256800	1.90742800
C	-4.26037700	2.91692200	-1.46930900
H	-5.21711500	2.41720500	-1.70324500
H	-4.41727900	3.99870400	-1.56940400
H	-3.52728500	2.60883000	-2.22071000

The optimized geometry of 34

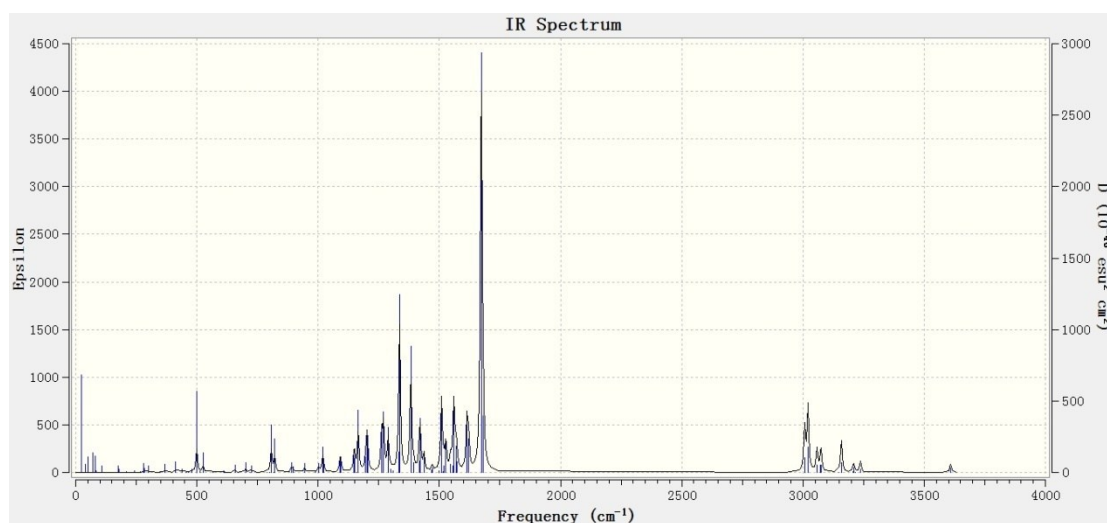
C	-5.07234200	-2.27992400	0.18573500
C	-3.69402700	-2.18918600	0.36402600
C	-3.01178100	-0.95012000	0.27076400
C	-3.75481100	0.24912000	-0.00121500
C	-5.16267300	0.14041900	-0.16936200
C	-5.80152700	-1.06733100	-0.07858500
C	-3.05223800	1.45960000	-0.07721600
C	-1.67325900	1.49338400	0.10612300
C	-1.02499900	0.23361200	0.36708300
C	0.40544800	0.19685800	0.50345800
H	0.83887000	-0.78757400	0.63606700
C	1.17977100	1.31813100	0.42270000
C	0.54440600	2.62620000	0.26588400
C	-0.86544900	2.70980600	0.07507300
H	-3.08247800	-3.05471900	0.58279400
H	-5.73926500	1.04091300	-0.37025900
H	-6.87624300	-1.10158200	-0.20979900
H	-3.61306200	2.36753900	-0.28213700
N	-1.67070500	-0.93520800	0.44757900
N	-5.74216200	-3.49358900	0.24494900
N	2.59527000	1.27987800	0.53087800
C	3.31473300	1.56034700	-0.71597400
H	2.87738700	2.42120100	-1.22410100
H	4.36320900	1.78530900	-0.48921700
H	3.28633500	0.70138900	-1.40934400
C	3.16287100	0.13060100	1.22163100
H	2.64055000	-0.02712700	2.16881000
H	3.11711000	-0.80512000	0.63600100
H	4.21770600	0.33750900	1.43438000
C	-5.00520100	-4.67982300	0.64605800
H	-5.66253700	-5.54938100	0.58407200
H	-4.15680100	-4.85246500	-0.02603700
H	-4.61392500	-4.61059600	1.67372200
C	-7.19379600	-3.52561800	0.33120200
H	-7.65690800	-3.07457000	-0.55433800
H	-7.52171600	-4.56598300	0.37419400
H	-7.58270400	-3.00779400	1.22209200
C	-1.43996900	3.98820000	-0.09510200
C	1.29696600	3.81713000	0.35406900
C	-0.67482200	5.14166500	-0.05033300
H	2.35369100	3.74378000	0.58479400
C	0.70400800	5.05797500	0.19365200

H	-2.51008500	4.07941100	-0.24981500
H	1.30304300	5.96144000	0.26942200
H	-1.14966500	6.11025200	-0.18252500

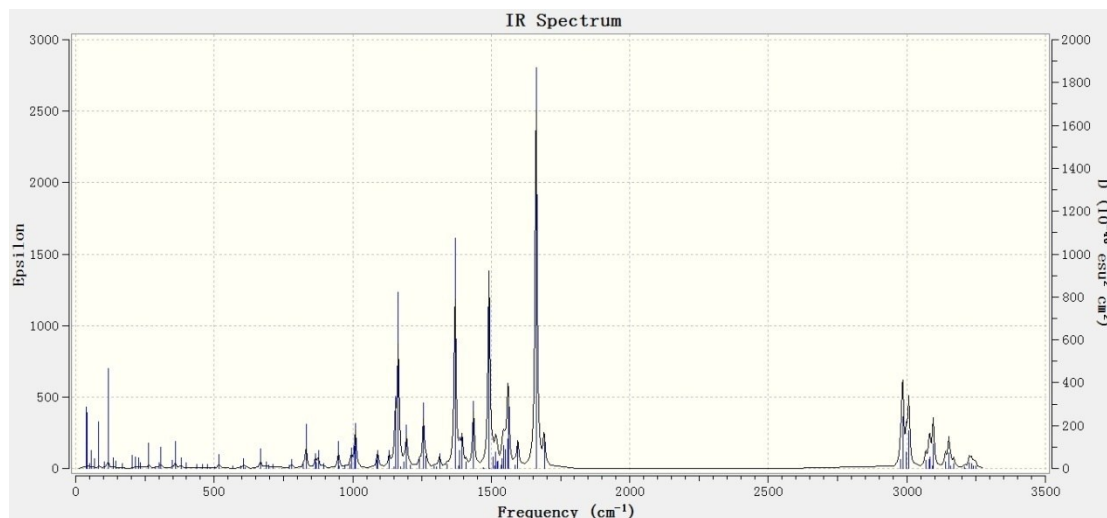
The calculated IR spectrum of **1**:



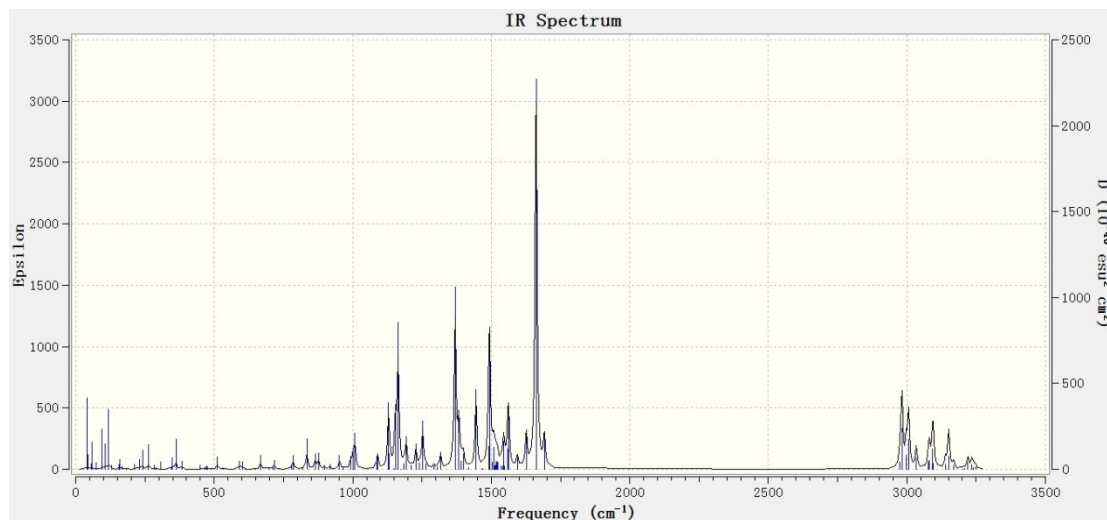
The calculated IR spectrum of **2**:



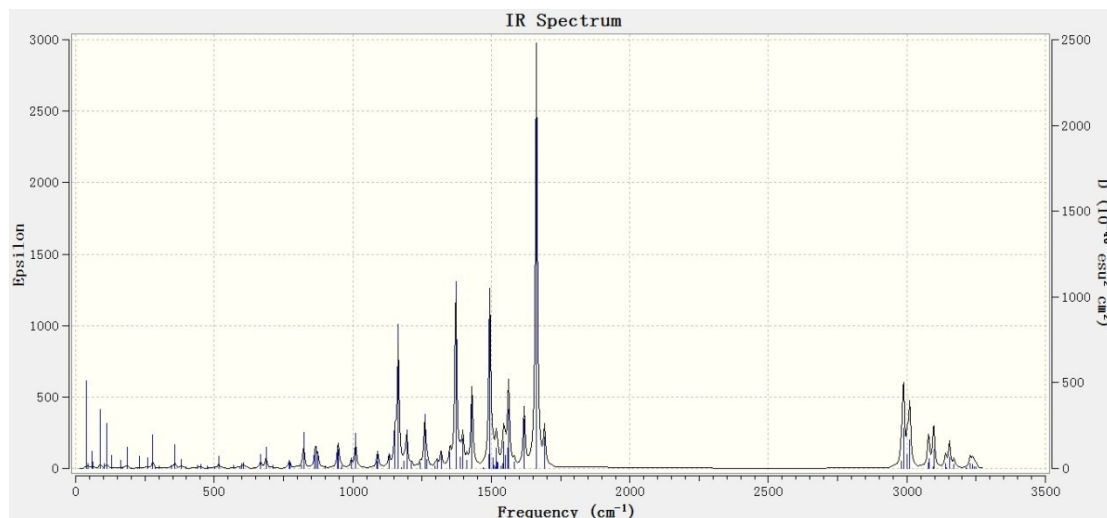
The calculated IR spectrum of **3**:



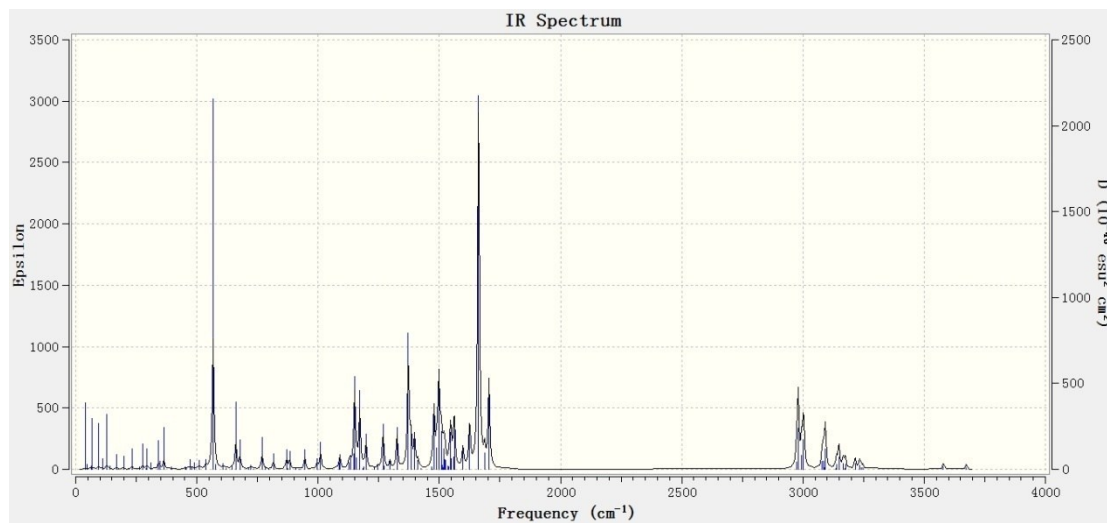
The calculated IR spectrum of **4**:



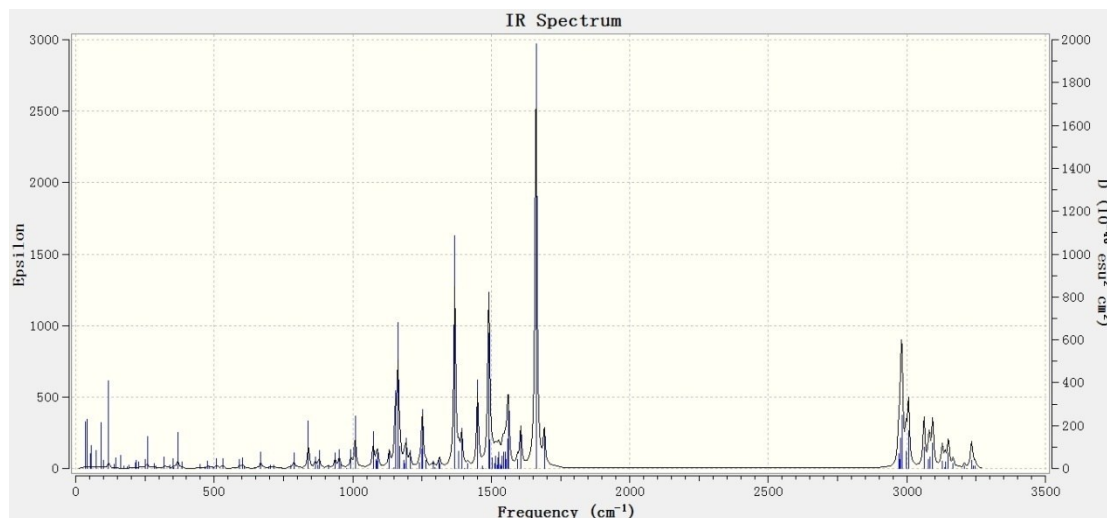
The calculated IR spectrum of **5**:



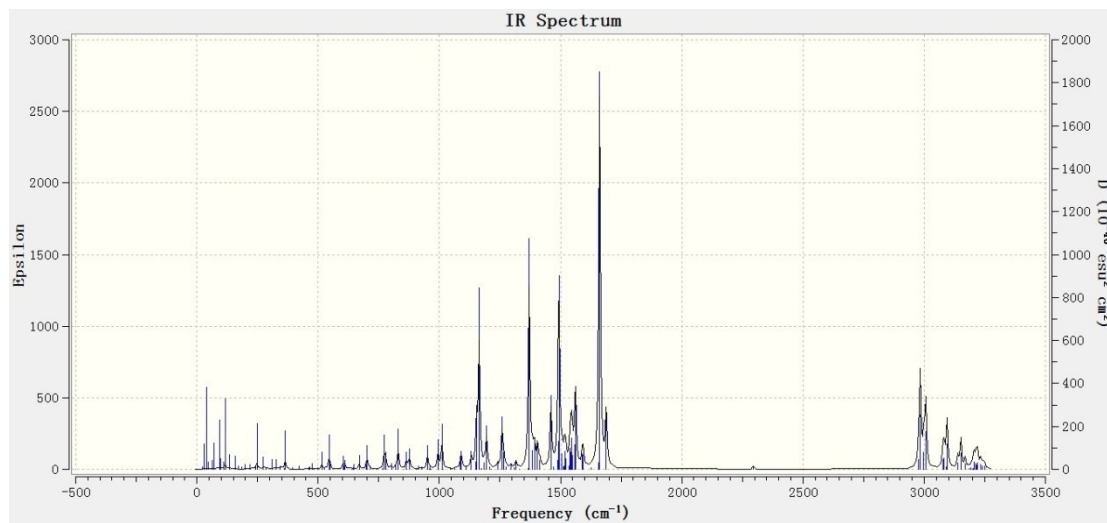
The calculated IR spectrum of **6**:



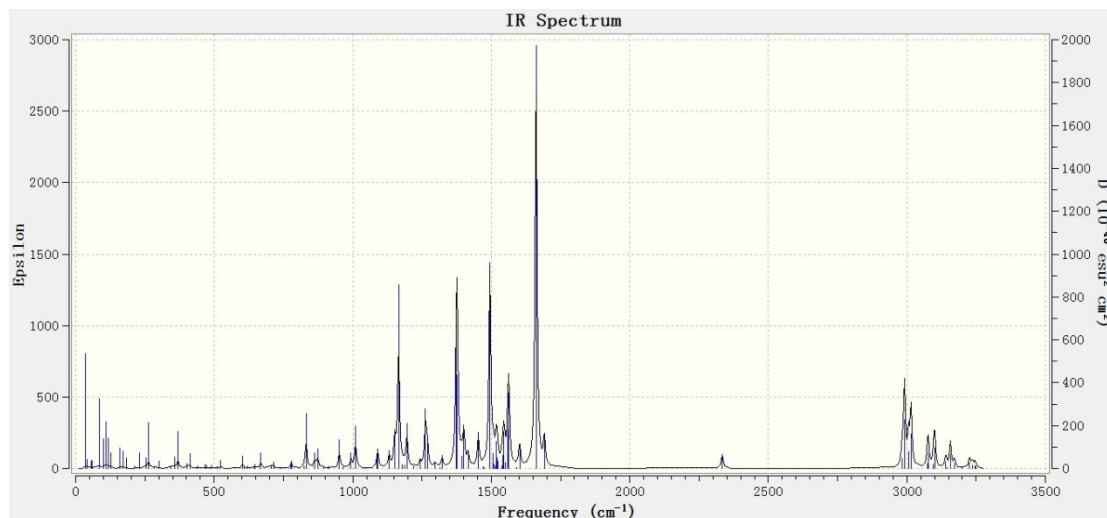
The calculated IR spectrum of **7**:



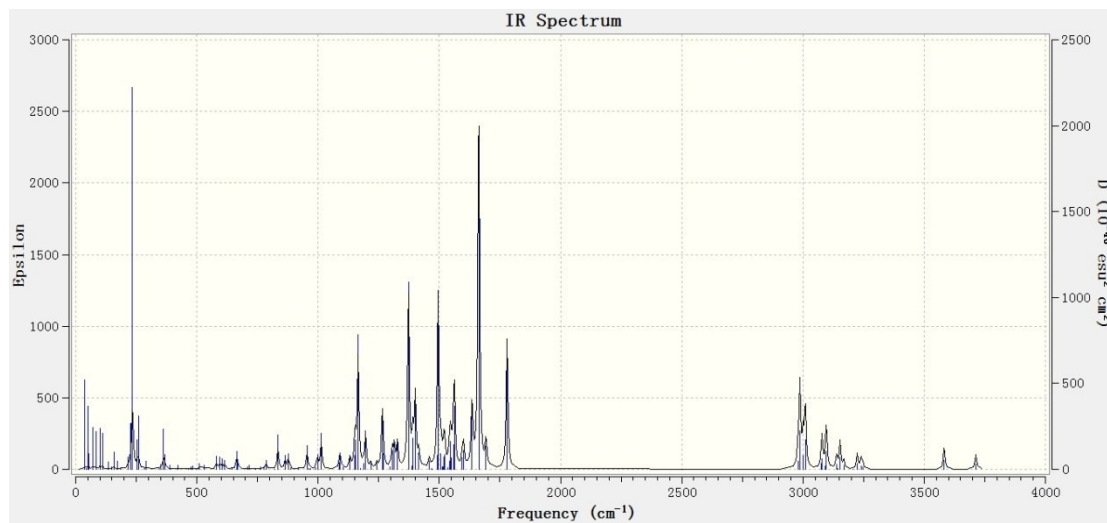
The calculated IR spectrum of **8**:



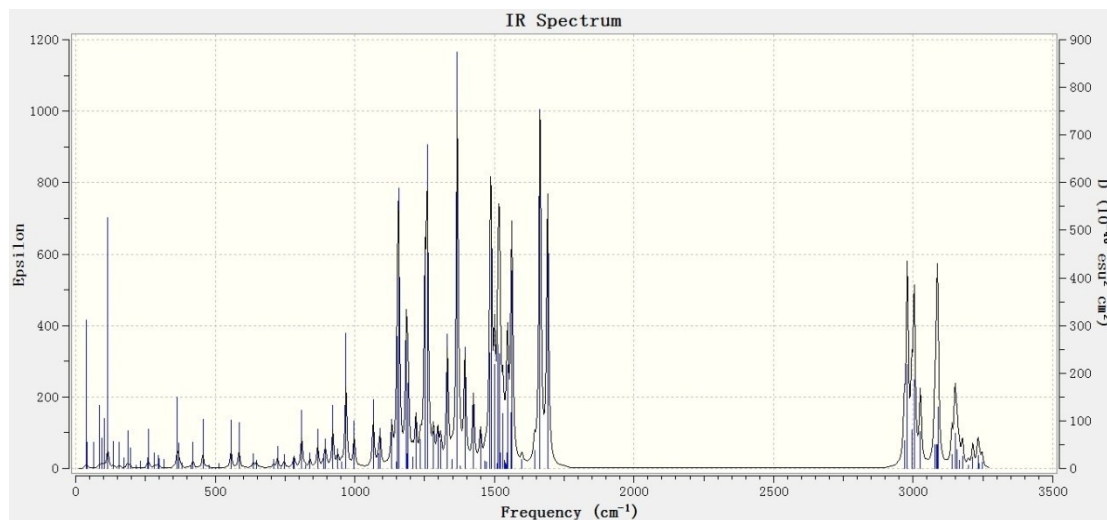
The calculated IR spectrum of **9**:



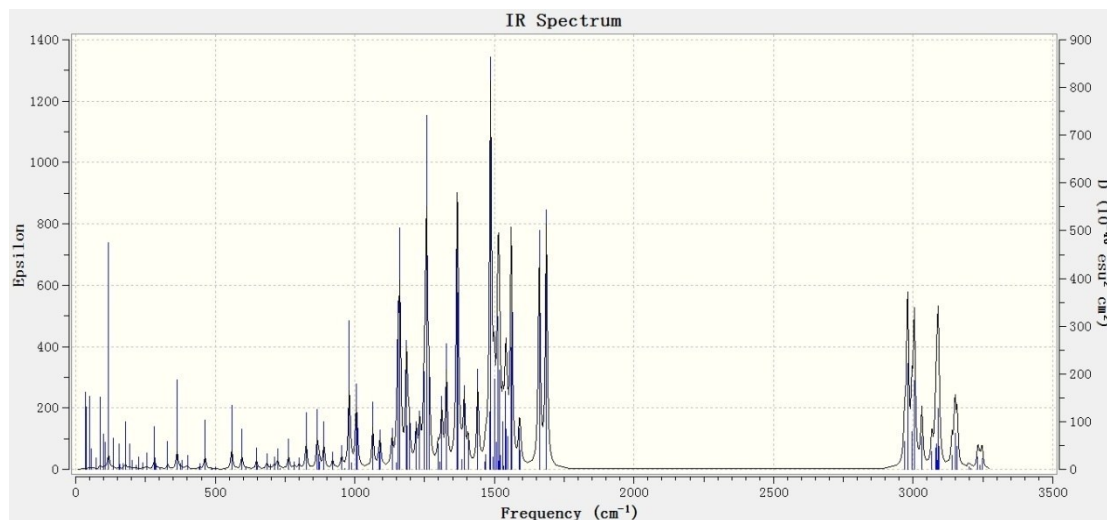
The calculated IR spectrum of **10**:



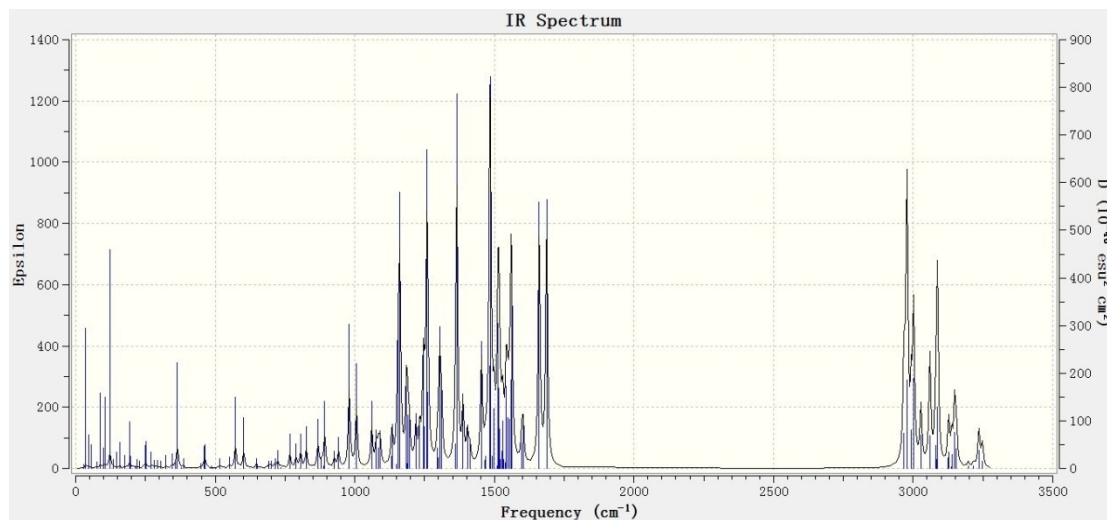
The calculated IR spectrum of **18**:



The calculated IR spectrum of **20**:



The calculated IR spectrum of **23**:



The calculated IR spectrum of **34**:

