Supporting Information

Rhodomentones A and B, Novel Meroterpenoids with Unique NMR Characteristics from *Rhodomyrtus tomentosa*

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S1. Computational methods.

Calculation Methods: Conformational search was performed with the help of TINKER7.1[1] by using OPLS-AA forcefield.[2] To access the global minimum, conformational search is carried out several times using different initial structures. All these structures were checked by python scripts and then optimized at HF/3-21G theoretical level using Gaussian09.[3] Duplicate conformers were removed manually. Structures within 10 kcal/mol (electronic energy) from the most stable conformer at HF/3-21G theoretical level were further optimized at the b3lyp[4]/6-31G(d) theoretical level in gas phase. Then, single point calculations were performed in pyridine using SMD[5] solvent model at b3lyp[4]/6-31G(d) theoretical level, and structures within 3 kcal/mol (electronic energy) from the most stable conformer at SMD(pyridine)-b3lyp/6-31G(d)//b3lyp/6-31G(d) level were selected. Finally, these selected structures were optimized at the SMD(pyridine)[5]-b3lyp[4]/6-31G(d) theoretical level, and frequency calculations were carried out to get the thermal corrections.

For all these optimized structures, dihedral angles of the nine-membered ring were analyzed. These structures could be classified into two clusters, and the most stable conformers of both clusters were selected. The transition structure connecting these two stable structures was successfully located and optimized at the SMD(pyridine)[5]-b3lyp[4]/6-31G(d) theoretical level.

References:

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1. Conformational sampling by scan program of tinker package.

1.1 Input xyz file for tinker

```
----------------------------------------------------------------------------------------------
79
 1  C  -3.660000  -1.811000   0.793000  222   2   6   8
 2  C  -2.173000  -1.935000   1.086000   84   1   3  11  12
 3  C  -1.355000  -0.825000   0.486000   86   2   4  19
 4  C  -1.833000   0.209000  -0.195000   86   3   5  13
 5  C  -3.244000   0.317000  -0.539000  222   4   6   7
 6  C  -4.161000  -0.860000  -0.270000   84   1   5   9  10
 7  O  -3.685000   1.296000  -1.123000  223   5
 8  O  -4.435000  -2.532000   1.386000  223   1
 9  C  -5.569000  -0.364000   0.094000   80   6  33  34  35
10  C  -4.240000  -1.661000  -1.604000   80   6  36  37  38
11  C  -1.983000  -1.908000   2.622000   80   2  39  40  41
12  C  -1.687000  -3.305000   0.552000   80   2  42  43  44
13  C  -0.952000   1.331000  -0.689000   82   4  14  15  45
14  C   0.535000   0.891000  -0.721000   81  13  20  46  47
15  C  -1.216000   2.659000   0.090000   81  13  16  48  49
16  C  -1.688000   3.818000  -0.814000   82  15  17  18  50
17  C  -2.117000   5.016000   0.054000   80  16  51  52  53
18  C  -0.583000   4.259000  -1.793000   80  16  54  55  56
19  O  -0.047000  -1.000000   0.769000  122   3  20
20  C   1.006000  -0.008000   0.444000  126  14  19  21  28
21  C   1.170000   0.706000   1.816000   81  20  22  57  58
22  C   2.091000   1.952000   1.931000   81  21  23  59  78
23  C   3.344000   1.787000   1.114000   87  22  24  79
24  C   4.372000   1.014000   1.404000   86  23  25  74
25  C   5.320000   0.627000   0.295000   81  24  26  63  64
26  C   4.797000  -0.678000  -0.369000   81  25  27  60  65
27  C   3.361000  -0.594000  -0.922000   82  26  28  29  61
28  C   2.158000  -0.973000   0.043000   82  20  27  30  62
29  C   2.956000  -1.794000  -1.874000   84  27  30  31  32
30  C   1.702000  -2.061000  -0.988000   81  28  29  72  73
31  C   3.910000  -2.992000  -1.905000   80  29  66  67  68
32  C   2.636000  -1.349000  -3.305000   80  29  69  70  71
33  H  -6.233000  -1.208000   0.213000   85   9
34  H  -5.930000   0.286000  -0.689000   85   9
35  H  -5.554000   0.192000   1.024000   85   9
36  H  -4.896000  -2.512000  -1.473000   85  10
37  H  -4.639000  -1.011000  -2.372000   85  10
```

38	H	-3.262000	-2.008000	-1.917000	85	10			
39	H	-2.589000	-2.687000	3.063000	85	11			
40	H	-0.942000	-2.069000	2.859000	85	11			
41	H	-2.294000	-0.953000	3.030000	85	11			
42	H	-1.781000	-3.365000	-0.525000	85	12			
43	H	-0.649000	-3.443000	0.818000	85	12			
44	H	-2.286000	-4.086000	1.001000	85	12			
45	H	-1.240000	1.509000	-1.717000	85	13			
46	H	1.171000	1.762000	-0.764000	85	14			
47	H	0.684000	0.338000	-1.638000	85	14			
48	H	-1.975000	2.485000	0.843000	85	15			
49	H	-0.317000	2.973000	0.602000	85	15			
50	H	-2.546000	3.459000	-1.367000	85	16			
51	H	-2.462000	5.837000	-0.566000	85	17			
52	H	-2.924000	4.738000	0.724000	85	17			
53	H	-1.282000	5.372000	0.651000	85	17			
54	H	-0.266000	3.446000	-2.436000	85	18			
55	H	-0.937000	5.064000	-2.430000	85	18			
56	H	0.283000	4.620000	-1.245000	85	18			
57	H	0.176000	0.988000	2.139000	85	21			
58	H	1.515000	-0.056000	2.503000	85	21			
59	H	2.318000	2.107000	2.981000	85	22			
60	H	4.863000	-1.491000	0.345000	85	26			
61	H	3.210000	0.353000	-1.422000	85	27			
62	H	2.524000	-1.435000	0.949000	85	28			
63	H	5.367000	1.409000	-0.456000	85	25			
64	H	6.325000	0.460000	0.668000	85	25			
65	H	5.463000	-0.923000	-1.189000	85	26			
66	H	4.829000	-2.757000	-2.430000	85	31			
67	H	4.162000	-3.332000	-0.908000	85	31			
68	H	3.429000	-3.815000	-2.426000	85	31			
69	H	3.539000	-1.022000	-3.812000	85	32			
70	H	2.206000	-2.169000	-3.872000	85	32			
71	H	1.930000	-0.527000	-3.312000	85	32			
72	H	1.648000	-3.059000	-0.575000	85	30			
73	H	0.769000	-1.837000	-1.481000	85	30			
74	C	4.604000	0.323000	2.730000	80	24	75	76	77
75	H	5.585000	0.599000	3.108000	85	74			
76	H	3.870000	0.597000	3.475000	85	74			
77	H	4.590000	-0.756000	2.618000	85	74			
78	H	1.561000	2.834000	1.607000	85	22			
79	H	3.324000	2.238000	0.138000	89	23			

1.2 Input parameters for tinker

scan input.xyz

----

oplsaa.prm
2

25 24 23 22
74 24 23 22
74 24 23 79
25 24 23 79

5
50.0
0.1

1.2 Python scripts used to distinguish the structures.

Python2.7 script to calculate the dihedral angles and chiral properties (R or S of each chiral center)

```
Ring_List = [ [20,21,22,23,24,25,26,27,28], [ 1,2,3,4,5,6], [3,4,13,14,20,19] ]
Torsion_List = [ (4,13,15,16), (13,15,16,17) ]
Chir_List = [ (4,14,13,15), (20,27,28,30), (26,28,27,29),(14,19,20,28) ]

import math



class Vec :                                         # general class for vector calculations
    def __init__(self, x, y, z) :
        self.x = x ; self.y = y ; self.z = z
    def Add(self, other) :
        return Vec( self.x + other.x , self.y + other.y , self.z + other.z )
    def Delta(self, other) :
        return Vec( other.x - self.x , other.y - self.y , other.z - self.z )
    def Scalar(self, k) :
        return Vec( self.x * k , self.y * k , self.z * k )
    def Norm(self) :
        temp = self.x * self.x + self.y * self.y + self.z * self.z
        return math.sqrt( temp )
    def Dot(self, other) :
        return ( self.x * other.x + self.y * other.y + self.z * other.z )
    def Cross(self, other) :
        x = self.y * other.z - self.z * other.y
        y = self.z * other.x - self.x * other.z
        z = self.x * other.y - self.y * other.x
```

```
        return Vec( x, y, z )

def Dihed( A1, A2, A3, A4 ) :
    r_12 = A1.Delta( A2 )
    r_23 = A2.Delta( A3 )
    r_34 = A3.Delta( A4 )
    r_123 = r_12.Cross( r_23 )
    r_234 = r_23.Cross( r_34 )
    cosPhi = r_123.Dot(r_234) / r_123.Norm() / r_234.Norm()
    Phi = math.acos(cosPhi*0.9999999999) * 180.0 / math.pi
    if r_12.Dot(r_234) < 0.0 : Phi =   - Phi
    return Phi

def Chir( A1, A2, C1, A4 ) :
    r_12 = A1.Delta( A2 )
    r_23 = A2.Delta( C1 )
    r_34 = C1.Delta( A4 )
    r_123 = r_12.Cross( r_23 )
    r_234 = r_23.Cross( r_34 )
    cosChir = r_123.Dot(r_234) / r_123.Norm() / r_234.Norm()
    Chir = math.acos(cosChir*0.9999999999) * 180.0 / math.pi
    if r_12.Dot(r_234) < 0.0 : Chir =   - Chir
    if Chir > 0:
        return 1;
    else:
        return 0;


def Torsion_Ring(A_list):
    Dih_Ring = []
    Index_End = len(A_list) - 1
    for i in range( len(A_list) ):
        if i+1 > Index_End:
            Dih_Ring.append( Dihed( A_list[i-1], A_list[i],
A_list[i+1-len(A_list)],A_list[i+2-len(A_list)] ) );
        elif i+2 > Index_End:
            Dih_Ring.append( Dihed( A_list[i-1], A_list[i],
A_list[i+1],A_list[i+2-len(A_list)]) );
        else:
            Dih_Ring.append( Dihed( A_list[i-1], A_list[i], A_list[i+1],A_list[i+2] ) );
    return Dih_Ring;

def Print( L ) :
  for each in L :
```

```
        print '%5.0f' %each,
    #print

def Calc( fname ) :
    ifile = file( fname, 'r' )
    read = False
    Atoms = [ '*' ]
    for line in ifile :
        words = line.split()

        if read and len(words) != 4 :
            break
        if read :
            Atoms.append( Vec( float(words[1]), float(words[2]), float(words[3]) ) )

        elif line[0] == '0' :
            read = True

    ifile.close()

    tor_chir = [ ]

    A_list = []
    for RL_i in range( len( Ring_List ) ):
            A_list.append( [] );
            for RL_j in Ring_List[ RL_i ]:
                    A_list[RL_i].append( Atoms[ RL_j ] )
                        tor_chir += Torsion_Ring( A_list[RL_i] )


    for TL_i in range( len(Torsion_List) ):
            tor_chir.append(    Dihed(Atoms[Torsion_List[TL_i][0]],    Atoms[Torsion_List[TL_i][1]],
Atoms[Torsion_List[TL_i][2]], Atoms[Torsion_List[TL_i][3]]))


    for CL_i in range( len( Chir_List ) ) :
            tor_chir.append(    Chir(    Atoms[Chir_List[CL_i][0]],    Atoms[Chir_List[CL_i][1]],
Atoms[Chir_List[CL_i][2]], Atoms[Chir_List[CL_i][3]]));

    Print( tor_chir );

from glob import glob
Files = glob( '*.gjf' )
Files.sort()
```

```
print 'filename ',
for RL_i in range( len( Ring_List ) ):
        for RL_j in range( len( Ring_List[ RL_i ] ) ):
                if RL_j < len( Ring_List[ RL_i ] )-1:
                        print '(' +str(Ring_List[ RL_i ][RL_j]) + ','+ str(Ring_List[ RL_i ][RL_j+1])+')',
                elif RL_j == len( Ring_List[ RL_i ] )-1:
                        print '('+str(Ring_List[ RL_i ][RL_j]) + ','+ str(Ring_List[ RL_i ][0])+')',


for TL_i in range( len(Torsion_List) ):
        print '('+str(Torsion_List[TL_i][0]) + ','+ str(Torsion_List[TL_i][1]) + ','+ str(Torsion_List[TL_i][2]) + ','+ str(Torsion_List[TL_i][3])+')',


for CL_i in range( len( Chir_List ) ) :
        print '('+str(Chir_List[CL_i][0]) + ','+ str(Chir_List[CL_i][1]) + ','+ str(Chir_List[CL_i][2]) + ','+ str(Chir_List[CL_i][3])+')',
print

for fname in Files :
    print fname[:-4],
    Calc( fname )
    print
```

Python2.7 script to find duplicate conformers

```
import sys
import math

Name_list = [ ]

ifile = file('dihed.txt', 'r')
lines = ifile.readlines()
ifile.close()

ofile=file('duplicate_name.txt','w')
duplicate = []

for i in range(1,len(lines)):
    iwords = lines[i].split()
    v_ = 0
    v_list = []
```

```
    index = []
    if len(iwords) > 0:
        for j in range(1,i):
            jwords = lines[j].split()
            v_ = 0
            for k in range(1,len(jwords)):
                #print jwords[k+4],
                v_ += (float(jwords[k])-float(iwords[k]))**2
            if v_ < 50:
                v_list.append(v_)
                add_name = jwords[0]+'.log'
                index.append(jwords[0])
                if add_name not in duplicate:
                    duplicate.append( add_name );
    if len(v_list):
        print iwords[0],index,    v_list

for each in duplicate:
    ofile.write( each + '\n');
ofile.close()
```

----

2. Electronic energies after optimized at HF/3-21G theoretical level in gas phase.

Table S1. Electronic energies at HF/3-21G theoretical level.

Conformers	E_{ele}(Hartree)	E_{ele}(kcal/mol)
RB_15	-1379.70522	0.0
RB_6	-1379.70522	0.0
RB_14	-1379.70512	0.1
RB_7	-1379.70512	0.1
RB_10	-1379.70410	0.7
RB_2	-1379.70410	0.7
RB_5	-1379.70391	0.8
RB_3	-1379.70391	0.8
RB_17	-1379.70372	0.9
RB_25	-1379.70372	0.9
RB_12	-1379.70310	1.3
RB_41	-1379.70310	1.3
RB_46	-1379.70299	1.4
RB_43	-1379.70256	1.7
RB_8	-1379.70218	1.9
RB_35	-1379.70218	1.9
RB_20	-1379.70218	1.9

RB_1	-1379.70218	1.9
RB_40	-1379.70216	1.9
RB_19	-1379.70216	1.9
RB_11	-1379.70209	2.0
RB_18	-1379.70194	2.1
RB_13	-1379.70189	2.1
RB_24	-1379.70075	2.8
RB_57	-1379.70075	2.8
RB_4	-1379.70075	2.8
RB_32	-1379.70075	2.8
RB_22	-1379.70009	3.2
RB_9	-1379.70009	3.2
RB_42	-1379.70002	3.3
RB_64	-1379.70002	3.3
RB_50	-1379.70002	3.3
RB_23	-1379.69988	3.4
RB_27	-1379.69977	3.4
RB_30	-1379.69975	3.4
RB_48	-1379.69934	3.7
RB_56	-1379.69923	3.8
RB_53	-1379.69923	3.8
RB_52	-1379.69923	3.8
RB_31	-1379.69923	3.8
RB_26	-1379.69853	4.2
RB_34	-1379.69853	4.2
RB_49	-1379.69800	4.5
RB_47	-1379.69800	4.5
RB_16	-1379.69792	4.6
RB_60	-1379.69792	4.6
RB_38	-1379.69792	4.6
RB_28	-1379.69792	4.6
RB_21	-1379.69759	4.8
RB_37	-1379.69759	4.8
RB_77	-1379.69759	4.8
RB_155	-1379.69744	4.9
RB_109	-1379.69744	4.9
RB_108	-1379.69744	4.9
RB_66	-1379.69744	4.9
RB_121	-1379.69744	4.9
RB_58	-1379.69733	5.0
RB_45	-1379.69717	5.1
RB_79	-1379.69681	5.3
RB_97	-1379.69681	5.3
RB_112	-1379.69681	5.3

RB_69	-1379.69677	5.3
RB_33	-1379.69677	5.3
RB_76	-1379.69630	5.6
RB_93	-1379.69590	5.9
RB_184	-1379.69590	5.9
RB_100	-1379.69584	5.9
RB_51	-1379.69584	5.9
RB_124	-1379.69584	5.9
RB_131	-1379.69564	6.0
RB_157	-1379.69564	6.0
RB_78	-1379.69564	6.0
RB_63	-1379.69546	6.1
RB_82	-1379.69539	6.2
RB_36	-1379.69492	6.5
RB_70	-1379.69469	6.6
RB_116	-1379.69467	6.6
RB_130	-1379.69467	6.6
RB_71	-1379.69467	6.6
RB_102	-1379.69449	6.7
RB_67	-1379.69448	6.7
RB_132	-1379.69448	6.7
RB_99	-1379.69448	6.7
RB_96	-1379.69448	6.7
RB_68	-1379.69448	6.7
RB_101	-1379.69440	6.8
RB_75	-1379.69440	6.8
RB_59	-1379.69437	6.8
RB_55	-1379.69429	6.9
RB_80	-1379.69420	6.9
RB_85	-1379.69420	6.9
RB_143	-1379.69419	6.9
RB_174	-1379.69418	6.9
RB_126	-1379.69418	6.9
RB_138	-1379.69418	6.9
RB_73	-1379.69413	7.0
RB_88	-1379.69410	7.0
RB_144	-1379.69410	7.0
RB_147	-1379.69410	7.0
RB_142	-1379.69410	7.0
RB_165	-1379.69410	7.0
RB_164	-1379.69410	7.0
RB_62	-1379.69398	7.1
RB_65	-1379.69398	7.1
RB_196	-1379.69398	7.1

RB_86	-1379.69376	7.2
RB_104	-1379.69360	7.3
RB_163	-1379.69360	7.3
RB_92	-1379.69360	7.3
RB_137	-1379.69360	7.3
RB_186	-1379.69360	7.3
RB_44	-1379.69352	7.3
RB_54	-1379.69352	7.3
RB_159	-1379.69341	7.4
RB_152	-1379.69341	7.4
RB_120	-1379.69341	7.4
RB_83	-1379.69341	7.4
RB_113	-1379.69341	7.4
RB_156	-1379.69341	7.4
RB_181	-1379.69341	7.4
RB_61	-1379.69316	7.6
RB_183	-1379.69291	7.7
RB_107	-1379.69291	7.7
RB_91	-1379.69285	7.8
RB_94	-1379.69285	7.8
RB_115	-1379.69275	7.8
RB_81	-1379.69263	7.9
RB_29	-1379.69262	7.9
RB_118	-1379.69262	7.9
RB_119	-1379.69262	7.9
RB_160	-1379.69262	7.9
RB_197	-1379.69262	7.9
RB_169	-1379.69232	8.1
RB_89	-1379.69232	8.1
RB_167	-1379.69230	8.1
RB_162	-1379.69230	8.1
RB_170	-1379.69230	8.1
RB_185	-1379.69230	8.1
RB_114	-1379.69230	8.1
RB_127	-1379.69230	8.1
RB_72	-1379.69215	8.2
RB_74	-1379.69215	8.2
RB_84	-1379.69215	8.2
RB_39	-1379.69215	8.2
RB_106	-1379.69201	8.3
RB_117	-1379.69195	8.3
RB_139	-1379.69195	8.3
RB_153	-1379.69195	8.3
RB_133	-1379.69195	8.3

RB_166	-1379.69190	8.4
RB_87	-1379.69184	8.4
RB_122	-1379.69184	8.4
RB_141	-1379.69151	8.6
RB_179	-1379.69140	8.7
RB_95	-1379.69124	8.8
RB_98	-1379.69124	8.8
RB_136	-1379.69115	8.8
RB_125	-1379.69115	8.8
RB_148	-1379.69100	8.9
RB_103	-1379.69037	9.3
RB_172	-1379.69016	9.5
RB_198	-1379.69016	9.5
RB_176	-1379.69016	9.5
RB_135	-1379.69001	9.6
RB_111	-1379.68988	9.6
RB_123	-1379.68987	9.6
RB_171	-1379.68987	9.6
RB_191	-1379.68987	9.6
RB_145	-1379.68985	9.7
RB_150	-1379.68985	9.7
RB_90	-1379.68935	10.0
RB_105	-1379.68929	10.0
RB_129	-1379.68929	10.0
RB_161	-1379.68918	10.1
RB_194	-1379.68918	10.1
RB_134	-1379.68918	10.1
RB_128	-1379.68918	10.1
RB_192	-1379.68918	10.1
RB_154	-1379.68894	10.2
RB_190	-1379.68894	10.2
RB_193	-1379.68872	10.4
RB_180	-1379.68872	10.4
RB_189	-1379.68854	10.5
RB_199	-1379.68847	10.5
RB_178	-1379.68847	10.5
RB_151	-1379.68841	10.6
RB_175	-1379.68841	10.6
RB_149	-1379.68807	10.8
RB_177	-1379.68799	10.8
RB_195	-1379.68799	10.8
RB_187	-1379.68798	10.8
RB_146	-1379.68796	10.8
RB_158	-1379.68781	10.9

RB_140	-1379.68781	10.9
RB_173	-1379.68736	11.2
RB_168	-1379.68735	11.2
RB_110	-1379.68667	11.6
RB_188	-1379.68639	11.8
RB_182	-1379.65929	28.8

3. Electronic Energies after optimization at b3lyp/6-31G(d) theoretical level.

After removing the duplicate conformers, structures within 10 kcal/mol from the most stable conformer at HF/3-21G theoretical level were further optimized at a higher theoretical level, b3lyp/6-31G(d).

Table S2. Electronic energies at b3lyp/6-31G(d) theoretical level

Conformers	Eele(Hartree)	Eele(kcal/mol)
RB_2	-1396.53440	0.0
RB_6	-1396.53425	0.1
RB_5	-1396.53398	0.3
RB_7	-1396.53388	0.3
RB_8	-1396.53253	1.2
RB_46	-1396.53249	1.2
RB_25	-1396.53249	1.2
RB_13	-1396.53239	1.3
RB_11	-1396.53236	1.3
RB_41	-1396.53224	1.4
RB_43	-1396.53211	1.4
RB_40	-1396.53158	1.8
RB_35	-1396.53140	1.9
RB_57	-1396.53119	2.0
RB_9	-1396.53101	2.1
RB_23	-1396.52999	2.8
RB_31	-1396.52981	2.9
RB_56	-1396.52981	2.9
RB_64	-1396.52968	3.0
RB_34	-1396.52947	3.1
RB_49	-1396.52938	3.2
RB_27	-1396.52935	3.2
RB_48	-1396.52935	3.2
RB_30	-1396.52916	3.3
RB_60	-1396.52907	3.3
RB_77	-1396.52860	3.6
RB_69	-1396.52811	3.9
RB_58	-1396.52790	4.1
RB_97	-1396.52778	4.2

RB_63	-1396.52756	4.3
RB_76	-1396.52733	4.4
RB_66	-1396.52714	4.6
RB_59	-1396.52712	4.6
RB_51	-1396.52697	4.7
RB_78	-1396.52657	4.9
RB_65	-1396.52657	4.9
RB_36	-1396.52634	5.1
RB_45	-1396.52633	5.1
RB_71	-1396.52617	5.2
RB_85	-1396.52614	5.2
RB_159	-1396.52600	5.3
RB_55	-1396.52588	5.4
RB_75	-1396.52586	5.4
RB_82	-1396.52571	5.5
RB_99	-1396.52558	5.5
RB_143	-1396.52554	5.6
RB_70	-1396.52548	5.6
RB_61	-1396.52547	5.6
RB_73	-1396.52544	5.6
RB_88	-1396.52539	5.7
RB_81	-1396.52538	5.7
RB_84	-1396.52521	5.8
RB_29	-1396.52514	5.8
RB_93	-1396.52500	5.9
RB_86	-1396.52497	5.9
RB_54	-1396.52489	6.0
RB_94	-1396.52479	6.0
RB_83	-1396.52448	6.2
RB_92	-1396.52443	6.3
RB_174	-1396.52433	6.3
RB_102	-1396.52398	6.5
RB_103	-1396.52389	6.6
RB_115	-1396.52386	6.6
RB_183	-1396.52385	6.6
RB_87	-1396.52370	6.7
RB_150	-1396.52339	6.9
RB_185	-1396.52334	6.9
RB_98	-1396.52322	7.0
RB_106	-1396.52317	7.1
RB_141	-1396.52275	7.3
RB_153	-1396.52273	7.3
RB_197	-1396.52251	7.5
RB_136	-1396.52234	7.6

RB_166	-1396.52223	7.6
RB_148	-1396.52210	7.7
RB_89	-1396.52191	7.8
RB_179	-1396.52176	7.9
RB_191	-1396.52162	8.0
RB_111	-1396.52123	8.3
RB_90	-1396.52106	8.4
RB_135	-1396.52102	8.4
RB_198	-1396.52097	8.4
RB_18	-1396.51909	9.6

4. Electronic Energies at SMD(pyridine)-b3lyp/6-31G(d)//b3lyp/6-31G(d) theoretical level.

Single point calculations were performed in pyridine using SMD solvent model after optimization in gas phase at b3lyp/6-31G(d) theoretical level.

Conformers RB_25, RB_27, RB_31, RB_61, and RB_81 are duplicate structures of other structures, and are removed from the conformer space.

Table S3. Electronic energies at SMD(pyridine)-b3lyp/6-31G(d)//b3lyp/6-31G(d) theoretical level.

Conformers	E_{ele}(Hartree)	E_{ele}(kcal/mol)
RB_6	-1396.57386	0.0
RB_2	-1396.57374	0.1
RB_7	-1396.57326	0.4
RB_5	-1396.57317	0.4
RB_11	-1396.57148	1.5
RB_40	-1396.57133	1.6
RB_46	-1396.57117	1.7
RB_35	-1396.57093	1.8
RB_8	-1396.57080	1.9
RB_41	-1396.57075	2.0
RB_13	-1396.57062	2.0
RB_43	-1396.57061	2.0
RB_57	-1396.57007	2.4
RB_9	-1396.56976	2.6
RB_23	-1396.56951	2.7
RB_56	-1396.56940	2.8
RB_64	-1396.56892	3.1
RB_34	-1396.56780	3.8
RB_69	-1396.56777	3.8
RB_48	-1396.56764	3.9
RB_49	-1396.56763	3.9
RB_60	-1396.56734	4.1
RB_30	-1396.56726	4.1

RB_58	-1396.56693	4.4
RB_97	-1396.56679	4.4
RB_77	-1396.56676	4.5
RB_78	-1396.56628	4.8
RB_65	-1396.56596	5.0
RB_66	-1396.56577	5.1
RB_63	-1396.56575	5.1
RB_71	-1396.56572	5.1
RB_76	-1396.56549	5.3
RB_51	-1396.56530	5.4
RB_99	-1396.56529	5.4
RB_45	-1396.56528	5.4
RB_75	-1396.56522	5.4
RB_59	-1396.56519	5.4
RB_82	-1396.56457	5.8
RB_86	-1396.56448	5.9
RB_55	-1396.56434	6.0
RB_54	-1396.56425	6.0
RB_83	-1396.56416	6.1
RB_84	-1396.56412	6.1
RB_93	-1396.56412	6.1
RB_29	-1396.56410	6.1
RB_94	-1396.56407	6.1
RB_143	-1396.56402	6.2
RB_159	-1396.56398	6.2
RB_73	-1396.56394	6.2
RB_92	-1396.56391	6.3
RB_36	-1396.56385	6.3
RB_88	-1396.56378	6.3
RB_70	-1396.56368	6.4
RB_103	-1396.56354	6.5
RB_85	-1396.56352	6.5
RB_183	-1396.56338	6.6
RB_115	-1396.56295	6.8
RB_174	-1396.56283	6.9
RB_150	-1396.56278	7.0
RB_185	-1396.56272	7.0
RB_102	-1396.56240	7.2
RB_98	-1396.56225	7.3
RB_87	-1396.56194	7.5
RB_141	-1396.56189	7.5
RB_106	-1396.56178	7.6
RB_153	-1396.56119	8.0
RB_197	-1396.56098	8.1

RB_148	-1396.56072	8.2
RB_135	-1396.56051	8.4
RB_198	-1396.56046	8.4
RB_136	-1396.56041	8.4
RB_179	-1396.56038	8.5
RB_89	-1396.56026	8.5
RB_166	-1396.56003	8.7
RB_191	-1396.56003	8.7
RB_90	-1396.55978	8.8
RB_18	-1396.55944	9.1
RB_111	-1396.55908	9.3

5. Optimization at SMD(pyridine)-b3lyp/6-31G(d) theoretical level.

Structures within 3 kcal/mol at SMD(pyridine)-b3lyp/6-31G(d)//b3lyp/6-31G(d) theoretical level were chosen, then were further optimization at SMD(pyridine)-b3lyp/6-31G(d) theoretical level. Frequency calculations were carried out at the same theoretical level, SMD(pyridine)-b3lyp/6-31G(d), to get thermal correction.

Table S4. Electronic energies and thermal properties after optimized at SMD(pyridine)-b3lyp/6-31G(d) theoretical level and frequency calculations at the same level.

Conformers	E_{ele}	E_0	E	H	G	ΔG(kcal/mol)
RB_5	-1396.57425	-1395.87242	-1395.83753	-1395.83659	-1395.93651	0.0
RB_2	-1396.57472	-1395.87275	-1395.83785	-1395.83690	-1395.93649	0.0
RB_6	-1396.57479	-1395.87265	-1395.83780	-1395.83686	-1395.93627	0.2
RB_7	-1396.57429	-1395.87227	-1395.83734	-1395.83639	-1395.93625	0.2
RB_11	-1396.57248	-1395.87100	-1395.83596	-1395.83501	-1395.93487	1.0
RB_46	-1396.57241	-1395.87049	-1395.83555	-1395.83460	-1395.93465	1.2
RB_43	-1396.57178	-1395.87007	-1395.83504	-1395.83410	-1395.93457	1.2
RB_8	-1396.57192	-1395.87028	-1395.83531	-1395.83436	-1395.93431	1.4
RB_35	-1396.57211	-1395.87008	-1395.83517	-1395.83423	-1395.93390	1.6
RB_57	-1396.57101	-1395.86974	-1395.83470	-1395.83376	-1395.93346	1.9
RB_40	-1396.57231	-1395.87020	-1395.83540	-1395.83446	-1395.93331	2.0
RB_13	-1396.57175	-1395.86978	-1395.83498	-1395.83404	-1395.93331	2.0
RB_9	-1396.57081	-1395.86940	-1395.83439	-1395.83345	-1395.93322	2.1
RB_23	-1396.57066	-1395.86895	-1395.83388	-1395.83294	-1395.93266	2.4
RB_56	-1396.57053	-1395.86886	-1395.83382	-1395.83287	-1395.93234	2.6

Table S5. Dihedral angles in the nine-membered ring of conformers located after optimization at SMD(pyridine)-b3lyp/6-31G(d) level.

Conformers	ΔG (kcal/mol)	9-8-7-6	8-7-6-5	**7-6-5-4**	6-5-4-3	**5-4-3-2**	4-3-2-1	3-2-1-9	2-1-9-8	1-9-8-7
RB_5	0.0	79	-52	**118**	-158	**34**	50	-99	101	-99

RB_2	0.0	78	-51	**119**	-158	**34**	51	-99	101	-99
RB_6	0.2	84	-45	**-72**	157	**-87**	58	-89	114	-94
RB_7	0.2	85	-45	**-74**	157	**-86**	59	-89	112	-94
RB_11	1.0	76	-49	**118**	-158	**33**	51	-98	102	-100
RB_46	1.2	88	-47	**-73**	156	**-87**	60	-89	109	-92
RB_43	1.2	87	-47	**-71**	156	**-87**	59	-90	112	-93
RB_8	1.4	79	-51	**117**	-158	**33**	51	-99	100	-100
RB_35	1.6	84	-44	**-74**	157	**-86**	59	-89	113	-94
RB_57	1.9	81	-52	**117**	-157	**32**	52	-96	98	-102
RB_40	2.0	81	-42	**-74**	158	**-87**	58	-89	115	-95
RB_13	2.0	79	-52	**118**	-157	**33**	51	-99	100	-100
RB_9	2.1	81	-52	**117**	-157	**32**	53	-96	98	-102
RB_23	2.4	92	-51	**-72**	154	**-87**	63	-90	102	-87
RB_56	2.6	92	-51	**-72**	154	**-87**	63	-91	102	-88

So, from the dihedral angle analysis, we could find that these conformers could be classified into two clusters. In cluster α, there are 7 conformers, in which dihedral angle of 7-6-5-4 is in 117°~119°, and dihedral angle of 5-4-3-2 in 32°~34°. However, in cluster β, there are 8 conformers, in which dihedral angle of 7-6-5-4 is in -74°~-71°, and dihedral angle of 5-4-3-2 in -87°~-86°.

RB_5 is the most stable conformer in cluster α, and RB_6 is the most stable conformer in cluster β. Transition state connecting these two conformers were successfully located, referred to α1_TS_β1.

6. Coordinates of stable conformers and transition structure α1_TS_β1.

α1_TS_β1

C	4.077335	-1.501018	-0.444012
C	2.627107	-1.839522	-0.831859
C	1.628275	-0.794456	-0.354367
C	1.923367	0.323980	0.368165
C	3.300648	0.602159	0.758163
C	4.455566	-0.094349	0.015214
O	3.569925	1.443725	1.623439
O	4.934573	-2.364514	-0.556185
C	4.738975	0.755232	-1.263448
C	5.722799	-0.138534	0.881273
C	2.575804	-1.954941	-2.381055
C	2.271578	-3.216224	-0.216367
C	0.839154	1.252618	0.885853
C	-0.539295	0.556691	0.819123
C	0.923683	2.650955	0.217011
C	0.097273	3.777471	0.874713
C	0.534915	4.070663	2.317497
C	0.189875	5.052928	0.022882
O	0.385762	-1.161845	-0.695335
C	-0.795288	-0.301516	-0.429496
C	-0.935462	0.497015	-1.776058
C	-1.975532	1.648001	-1.832227
C	-3.220341	1.128333	-1.181156
C	-4.525380	1.380185	-1.056459
C	-5.269750	0.387828	-0.163380
C	-4.635596	-1.028916	-0.023168
C	-3.246969	-1.245953	0.652487
C	-1.889683	-1.413089	-0.172561
C	-2.976064	-2.670765	1.273725
C	-1.500277	-2.549936	0.808969
C	-3.688743	-3.823751	0.554110
C	-3.203160	-2.770690	2.781755
C	-5.295563	2.520588	-1.661333
H	5.062018	1.759044	-0.961780
H	3.853320	0.859396	-1.899591

H	5.541338	0.292562	-1.850743
H	6.552237	-0.579022	0.320831
H	6.001046	0.873530	1.187044
H	5.566711	-0.737293	1.786642
H	3.302061	-2.703402	-2.716478
H	1.576802	-2.269718	-2.698328
H	2.807471	-1.003006	-2.873344
H	2.265602	-3.172050	0.879905
H	1.284124	-3.540534	-0.554990
H	3.012936	-3.957721	-0.527339
H	1.061791	1.404438	1.953300
H	-1.354241	1.300238	0.909401
H	-0.621069	-0.098908	1.707621
H	1.977881	2.963812	0.223332
H	0.635354	2.570946	-0.838761
H	-0.960198	3.473576	0.898053
H	-0.031989	4.912335	2.735372
H	0.378889	3.213823	2.982744
H	1.600474	4.333600	2.360998
H	-0.155119	4.878639	-1.004110
H	-0.420252	5.861132	0.445716
H	1.225101	5.416284	-0.033811
H	0.066606	0.890499	-2.033623
H	-1.191639	-0.250440	-2.554788
H	-2.117064	1.959860	-2.878344
H	-4.619645	-1.495636	-1.019628
H	-3.104531	-0.500838	1.447363
H	-2.135169	-1.847944	-1.154565
H	-5.411640	0.829290	0.839822
H	-6.289835	0.240699	-0.554692
H	-5.355588	-1.611984	0.570610
H	-4.768327	-3.828690	0.747433
H	-3.545191	-3.789127	-0.532284
H	-3.290324	-4.784872	0.905184
H	-4.268986	-2.678856	3.032868
H	-2.857572	-3.736910	3.174626
H	-2.666349	-1.981400	3.322855
H	-1.049600	-3.445209	0.367279
H	-0.847670	-2.200905	1.616331
H	-5.778588	3.132494	-0.883674
H	-4.651452	3.180786	-2.254775
H	-6.104450	2.158403	-2.314208
H	-1.593893	2.534159	-1.302045
H	-2.958980	0.270069	-0.612745

RB_2

C	4.008933	-1.592386	-0.230874
C	2.567425	-1.957683	-0.624844
C	1.562170	-0.865518	-0.285609
C	1.840037	0.306026	0.356463
C	3.202762	0.605670	0.776118
C	4.380510	-0.161061	0.148225
O	3.448585	1.519586	1.573022
O	4.867435	-2.461348	-0.271004
C	4.743961	0.586237	-1.172994
C	5.598766	-0.157103	1.083940
C	2.558361	-2.233537	-2.153537
C	2.184606	-3.258892	0.126351
C	0.743330	1.275971	0.761451
C	-0.643009	0.598246	0.661676
C	0.880296	2.635091	0.025246
C	0.067415	3.810700	0.609509
C	0.487779	4.174388	2.041939
C	0.194673	5.036129	-0.308053
O	0.333151	-1.247083	-0.651028
C	-0.847370	-0.339937	-0.535258
C	-0.864227	0.343137	-1.932641
C	-1.884284	1.477714	-2.192753
C	-3.245284	0.992530	-1.804854
C	-4.076132	1.473628	-0.870009
C	-5.146067	0.557991	-0.299188
C	-4.698757	-0.915566	-0.205084
C	-3.340755	-1.158665	0.489726
C	-1.984020	-1.393049	-0.293685
C	-3.137092	-2.566191	1.168606
C	-1.650062	-2.510517	0.734178
C	-3.873912	-3.717339	0.470177
C	-3.400969	-2.610107	2.673170
C	-3.979811	2.842999	-0.246168
H	5.577167	0.079352	-1.674521
H	5.052517	1.610741	-0.931994
H	3.897449	0.639100	-1.866634
H	6.448435	-0.652327	0.605637
H	5.878983	0.871072	1.327213
H	5.382508	-0.681737	2.022538
H	2.786506	-1.331185	-2.733801
H	3.306675	-2.997145	-2.391852

H	1.573913	-2.598583	-2.462215
H	2.166181	-3.099289	1.211752
H	1.195977	-3.602564	-0.189116
H	2.917536	-4.040095	-0.094850
H	0.912822	1.482854	1.829446
H	-1.446292	1.358048	0.650354
H	-0.790106	0.006567	1.586223
H	1.940904	2.923310	0.038526
H	0.610411	2.509636	-1.031155
H	-0.995152	3.527178	0.633873
H	-0.073602	5.044981	2.404384
H	0.309118	3.356585	2.749293
H	1.555866	4.425792	2.089173
H	-0.140216	4.812676	-1.328936
H	-0.405323	5.877113	0.062179
H	1.237168	5.377257	-0.370229
H	0.154234	0.732167	-2.130034
H	-1.040360	-0.462742	-2.674591
H	-1.818782	1.726957	-3.265124
H	-4.698247	-1.382400	-1.200041
H	-3.190428	-0.390414	1.260163
H	-2.210242	-1.855902	-1.266162
H	-5.390764	0.912589	0.714620
H	-6.090954	0.625020	-0.865450
H	-5.471578	-1.451195	0.367578
H	-4.956024	-3.684341	0.646263
H	-3.713233	-3.716487	-0.614505
H	-3.511198	-4.680786	0.852601
H	-2.850426	-1.821824	3.201999
H	-4.468403	-2.475817	2.897376
H	-3.095240	-3.573721	3.103867
H	-1.216137	-3.433590	0.334025
H	-1.003534	-2.152181	1.542554
H	-3.764386	2.785938	0.831646
H	-3.221620	3.477810	-0.715981
H	-4.945295	3.365695	-0.334652
H	-1.609210	2.385101	-1.642528
H	-3.476611	0.008117	-2.214189

RB_5

C	4.046130	-1.335600	-0.593677
C	2.602559	-1.768284	-0.895810
C	1.571130	-0.752469	-0.425693
C	1.831486	0.393704	0.270665
C	3.174293	0.683848	0.745638
C	4.352648	-0.259066	0.445044
O	3.405758	1.674399	1.453848
O	4.964730	-1.911470	-1.158790
C	5.568608	0.570750	-0.017304
C	4.709698	-0.988896	1.773016
C	2.466625	-1.971345	-2.425565
C	2.369211	-3.129216	-0.181186
C	0.718722	1.346740	0.673090
C	-0.650112	0.629806	0.609352
C	0.810489	2.692548	-0.096013
C	-0.013070	3.863275	0.484759
C	0.485249	4.317024	1.865044
C	-0.002222	5.046687	-0.494938
O	0.348287	-1.145947	-0.791558
C	-0.868187	-0.302299	-0.589085
C	-0.995746	0.397871	-1.972505
C	-2.078215	1.489128	-2.150538
C	-3.391068	0.934807	-1.695024
C	-4.183951	1.356432	-0.700459
C	-5.178439	0.380957	-0.092662
C	-4.660296	-1.072088	-0.055918
C	-3.255307	-1.266500	0.555191
C	-1.934874	-1.416431	-0.306290
C	-2.946581	-2.676912	1.186580
C	-1.488684	-2.533328	0.679025
C	-3.658666	-3.848062	0.496146
C	-3.132451	-2.768726	2.700643
C	-4.107659	2.713337	-0.047636
H	6.437936	-0.076847	-0.162117
H	5.363340	1.085529	-0.964592
H	5.806625	1.324869	0.737676
H	4.982695	-0.243247	2.527736
H	3.867950	-1.575370	2.161168
H	5.559758	-1.662399	1.614536
H	2.600122	-1.025077	-2.964840
H	3.229093	-2.674131	-2.772154
H	1.479111	-2.372050	-2.669330
H	2.409009	-3.029669	0.909966
H	1.386974	-3.527471	-0.453205
H	3.137404	-3.844966	-0.494537
H	0.895570	1.582034	1.733443
H	-1.474746	1.365732	0.629970
H	-0.750124	0.028047	1.533863

H	1.865065	3.000370	-0.116877
H	0.516140	2.537808	-1.141628
H	-1.058134	3.538128	0.595986
H	-0.118657	5.151348	2.244025
H	0.437482	3.515670	2.611249
H	1.527733	4.659258	1.814786
H	-0.406691	4.764231	-1.475075
H	-0.601848	5.884245	-0.116252
H	1.019410	5.418444	-0.653867
H	-0.008592	0.833528	-2.222812
H	-1.180839	-0.404088	-2.716430
H	-2.086662	1.760012	-3.219566
H	-4.696897	-1.519144	-1.059339
H	-3.097144	-0.510815	1.336315
H	-2.191513	-1.873458	-1.273959
H	-5.383968	0.703964	0.940181
H	-6.154649	0.413723	-0.606272
H	-5.373662	-1.653687	0.547909
H	-4.733487	-3.865527	0.714135
H	-3.541072	-3.822447	-0.593745
H	-3.239148	-4.800562	0.846550
H	-2.757526	-3.724435	3.092761
H	-2.598166	-1.964311	3.221818
H	-4.193059	-2.696397	2.979182
H	-1.027156	-3.424343	0.238969
H	-0.822197	-2.154309	1.461660
H	-3.845183	2.638343	1.018546
H	-3.391306	3.384641	-0.532067
H	-5.092595	3.205308	-0.083033
H	-1.811760	2.397903	-1.598567
H	-3.602751	-0.050405	-2.113501

RB_6

C	3.833557	-1.826478	-0.458904
C	2.338648	-2.047218	-0.748895
C	1.467142	-0.884414	-0.292636
C	1.899689	0.226247	0.370203
C	3.311782	0.377356	0.697503
C	4.359213	-0.444847	-0.076059
O	3.698482	1.209662	1.526381
O	4.603894	-2.766970	-0.583115
C	4.640861	0.328234	-1.402764
C	5.664175	-0.570709	0.722509
C	2.186171	-2.256217	-2.280661
C	1.894815	-3.339700	-0.017235
C	0.934848	1.281492	0.881650
C	-0.516421	0.745858	0.863922
C	1.160504	2.642291	0.170055
C	0.440580	3.865188	0.779720
C	0.870696	4.149179	2.226742
C	0.684150	5.100938	-0.100329
O	0.184790	-1.136764	-0.576383
C	-0.896300	-0.135308	-0.335682
C	-0.968901	0.594792	-1.707613
C	-1.801897	1.895456	-1.834267
C	-3.140661	1.761735	-1.169439
C	-4.185066	1.038978	-1.597205
C	-5.209910	0.613365	-0.575075
C	-4.776050	-0.722513	0.076128
C	-3.401367	-0.739565	0.774421
C	-2.087988	-1.108821	-0.029472
C	-3.144583	-1.974567	1.729577
C	-1.768839	-2.192871	1.042153
C	-4.076486	-3.179132	1.548022
C	-3.070894	-1.598922	3.211417
C	-4.309718	0.435772	-2.973577
H	3.733790	0.474319	-1.999197
H	5.374932	-0.218231	-2.007227
H	5.054072	1.315357	-1.162262
H	6.044747	0.422490	0.975175
H	5.508477	-1.122948	1.657130
H	6.420478	-1.100984	0.136780
H	2.464817	-1.359368	-2.847054
H	2.828379	-3.082715	-2.603584
H	1.148063	-2.504473	-2.522012
H	1.972110	-3.226044	1.071302
H	0.857734	-3.579688	-0.266890
H	2.533913	-4.173376	-0.322375
H	1.196391	1.438256	1.939749
H	-1.235830	1.583619	0.922201
H	-0.658249	0.153428	1.787578
H	2.239657	2.851851	0.182613
H	0.879167	2.554655	-0.887675
H	-0.642737	3.672745	0.783879
H	0.377895	5.051339	2.611118
H	0.616824	3.327098	2.905696
H	1.955438	4.309654	2.292324
H	0.343791	4.936555	-1.130532

H	0.154103	5.979772	0.288369
H	1.753036	5.351590	-0.141525
H	0.071062	0.823598	-2.015719
H	-1.355220	-0.144540	-2.437130
H	-1.892637	2.116730	-2.907959
H	-4.812678	-1.520532	-0.680002
H	-3.274042	0.190773	1.342283
H	-2.356886	-1.585173	-0.984352
H	-5.301683	1.377239	0.211067
H	-6.208541	0.482751	-1.020254
H	-5.537756	-0.984293	0.826293
H	-5.090394	-2.982508	1.918337
H	-4.158024	-3.490469	0.500086
H	-3.684303	-4.036551	2.111405
H	-2.378757	-0.765206	3.382610
H	-4.055021	-1.295375	3.594673
H	-2.726149	-2.445556	3.821112
H	-1.596330	-3.200347	0.647166
H	-0.921236	-1.941552	1.687540
H	-5.261695	0.734344	-3.438597
H	-3.500900	0.737373	-3.647342
H	-4.320541	-0.663710	-2.934324
H	-1.255163	2.737900	-1.394671
H	-3.191932	2.139177	-0.146119

RB_7

C	3.859918	-1.525268	-0.893313
C	2.363702	-1.822805	-1.084899
C	1.473957	-0.749110	-0.473990
C	1.897883	0.319370	0.263726
C	3.292271	0.448283	0.652272
C	4.342691	-0.587424	0.211009
O	3.670186	1.365802	1.394954
O	4.673537	-2.099072	-1.602741
C	5.622518	0.139073	-0.249207
C	4.676638	-1.463383	1.454932
C	2.077255	-1.931747	-2.602762
C	2.072612	-3.197285	-0.417478
C	0.920040	1.352997	0.793144
C	-0.513745	0.774013	0.820225
C	1.086317	2.713445	0.063913
C	0.384374	3.926890	0.712527
C	0.922091	4.245405	2.116051
C	0.521384	5.155701	-0.199337
O	0.194875	-0.999750	-0.762380
C	-0.922346	-0.077311	-0.391364
C	-1.136747	0.703574	-1.719741
C	-2.035477	1.965094	-1.714951
C	-3.300559	1.728446	-0.943231
C	-4.360174	1.002966	-1.326671
C	-5.266667	0.462212	-0.248008
C	-4.722896	-0.893042	0.266109
C	-3.299733	-0.893615	0.859659
C	-2.028574	-1.136330	-0.051985
C	-2.918389	-2.180519	1.696868
C	-1.567288	-2.247121	0.934906
C	-3.777038	-3.425042	1.440459
C	-2.803967	-1.930932	3.201953
C	-4.607197	0.513028	-2.730707
H	5.972771	0.803981	0.544774
H	5.437252	0.742282	-1.146895
H	6.409340	-0.584255	-0.481277
H	3.792902	-1.976916	1.851404
H	5.429163	-2.216131	1.192773
H	5.080159	-0.819874	2.244693
H	2.735384	-2.682773	-3.048004
H	1.038498	-2.226223	-2.773799
H	2.254998	-0.975473	-3.110562
H	2.207242	-3.162868	0.669787
H	1.041206	-3.499253	-0.624800
H	2.747645	-3.956692	-0.828282
H	1.203516	1.526766	1.842222
H	-1.251549	1.588211	0.940917
H	-0.594995	0.149028	1.729753
H	2.161259	2.937101	0.013774
H	0.745282	2.617542	-0.975199
H	-0.689588	3.706001	0.806934
H	0.437546	5.140875	2.525812
H	0.746142	3.428468	2.825093
H	2.003741	4.434971	2.091633
H	0.097223	4.969654	-1.194198
H	0.005461	6.026967	0.223930
H	1.576130	5.430770	-0.336828
H	-0.136534	0.993567	-2.098815
H	-1.549967	-0.021048	-2.449699
H	-2.232688	2.226923	-2.764590
H	-4.782608	-1.636224	-0.542666
H	-3.170572	-0.004197	1.489184

H	-2.339780	-1.585082	-1.007211
H	-5.316344	1.166704	0.595409
H	-6.296175	0.316109	-0.610007
H	-5.411330	-1.245705	1.049677
H	-4.783539	-3.334801	1.867301
H	-3.886497	-3.643275	0.371719
H	-3.304877	-4.301847	1.903804
H	-2.384333	-2.803570	3.721559
H	-2.155399	-1.073402	3.420441
H	-3.786838	-1.724049	3.647728
H	-1.330914	-3.213697	0.475882
H	-0.713191	-1.957350	1.555548
H	-5.609055	0.816921	-3.071384
H	-3.879332	0.899191	-3.451830
H	-4.586710	-0.585541	-2.788393
H	-1.491777	2.814399	-1.284777
H	-3.264168	2.020610	0.108151

RB_8

C	3.608740	-2.026990	-0.287389
C	2.170021	-2.108547	-0.824334
C	1.300562	-0.936297	-0.383461
C	1.707885	0.125769	0.373441
C	3.048905	0.123573	0.949008
C	4.154148	-0.723889	0.291828
O	3.341021	0.829912	1.920379
O	4.327904	-3.011367	-0.371533
C	4.714382	0.114673	-0.899260
C	5.291035	-1.016613	1.281644
C	2.254647	-2.131743	-2.377196
C	1.552168	-3.442105	-0.336648
C	0.733793	1.221691	0.775876
C	-0.713139	0.685295	0.678263
C	0.939661	2.560236	0.009232
C	2.155349	3.435192	0.387010
C	2.291122	4.589674	-0.618677
C	2.060410	3.985742	1.816361
O	0.047748	-1.119685	-0.818579
C	-1.046887	-0.132793	-0.573746
C	-1.071568	0.644559	-1.921529
C	-1.976419	1.893968	-2.045025
C	-3.354822	1.530488	-1.591737
C	-4.056017	2.018090	-0.559163
C	-5.182405	1.180733	0.023503
C	-4.906810	-0.336421	-0.036365
C	-3.547360	-0.792000	0.536425
C	-2.267504	-1.093722	-0.348605
C	-3.464549	-2.270140	1.073908
C	-2.000889	-2.322305	0.565356
C	-4.350603	-3.268892	0.316417
C	-3.664595	-2.430907	2.580504
C	-3.750804	3.307227	0.160584
H	5.480232	-0.459273	-1.435241
H	5.177456	1.029187	-0.509100
H	3.931962	0.402850	-1.609412
H	6.092318	-1.573559	0.787944
H	5.698767	-0.079570	1.669917
H	4.936453	-1.611310	2.131916
H	1.254995	-2.269115	-2.801605
H	2.672964	-1.201828	-2.780476
H	2.889312	-2.964967	-2.698360
H	2.193305	-4.274969	-0.638980
H	1.457334	-3.460364	0.756102
H	0.560345	-3.583790	-0.772491
H	0.909085	1.429312	1.841848
H	-1.433918	1.520490	0.754488
H	-0.885032	0.038432	1.561513
H	0.987002	2.355248	-1.068151
H	0.036993	3.171925	0.166884
H	3.067387	2.828221	0.320173
H	3.154889	5.224069	-0.382210
H	2.422451	4.219649	-1.643646
H	1.399731	5.232420	-0.612071
H	2.039938	3.184360	2.561375
H	2.922028	4.625064	2.048250
H	1.154583	4.594952	1.945035
H	-0.031810	0.937343	-2.162549
H	-1.375066	-0.086951	-2.698435
H	-1.953080	2.201952	-3.103738
H	-5.025348	-0.708572	-1.063567
H	-3.267456	-0.124084	1.362340
H	-2.593360	-1.446875	-1.338510
H	-5.309407	1.470448	1.078811
H	-6.151292	1.401627	-0.456605
H	-5.699688	-0.831394	0.545557
H	-5.414294	-3.136481	0.548872
H	-4.236125	-3.188718	-0.771163
H	-4.081819	-4.296088	0.597052

H	-3.008859	-1.758969	3.148445
H	-4.700273	-2.209038	2.873624
H	-3.446779	-3.458065	2.904793
H	-1.680197	-3.245994	0.071639
H	-1.287568	-2.095971	1.365363
H	-3.459159	3.129313	1.206840
H	-2.959068	3.890415	-0.320724
H	-4.649878	3.941997	0.199683
H	-1.567168	2.728689	-1.465397
H	-3.727021	0.615848	-2.055526

RB_9

C	4.128034	-0.748789	-0.594510
C	2.844120	-1.450713	-1.061687
C	1.594265	-0.639697	-0.742673
C	1.552548	0.514638	-0.009419
C	2.693523	0.848009	0.829145
C	4.093565	0.288671	0.526710
O	2.578448	1.597897	1.809210
O	5.200328	-1.073506	-1.083645
C	4.986658	1.488405	0.124697
C	4.670790	-0.374796	1.803379
C	2.930433	-1.677274	-2.590261
C	2.791304	-2.829955	-0.345414
C	0.257014	1.301077	0.137604
C	-0.773999	0.817669	-0.899726
C	0.498174	2.823133	-0.055966
C	-0.715089	3.748334	0.182601
C	-1.221005	3.695260	1.631805
C	-0.346718	5.190179	-0.199377
O	0.522443	-1.231314	-1.279866
C	-0.862619	-0.691828	-1.121017
C	-1.431346	-1.011119	-2.535450
C	-2.779517	-0.363571	-2.936176
C	-3.777988	-0.641832	-1.857543
C	-4.421669	0.225945	-1.064321
C	-4.960714	-0.258102	0.271141
C	-4.106548	-1.370231	0.913944
C	-2.598047	-1.075078	1.062606
C	-1.487191	-1.548964	0.035928
C	-1.837642	-1.884159	2.179900
C	-0.589838	-1.895491	1.260182
C	-2.373333	-3.304778	2.407490
C	-1.683374	-1.164924	3.519655
C	-4.580362	1.699045	-1.344285
H	6.007176	1.148345	-0.075661
H	5.005016	2.220035	0.938611
H	4.605689	1.984920	-0.777007
H	5.695509	-0.716072	1.619974
H	4.677564	0.357002	2.617063
H	4.071490	-1.235879	2.124590
H	2.079664	-2.268980	-2.937843
H	2.934573	-0.722947	-3.131654
H	3.854170	-2.210190	-2.830719
H	1.914250	-3.390342	-0.685044
H	2.732600	-2.723488	0.744073
H	3.690795	-3.406681	-0.589799
H	-0.130549	1.139274	1.157679
H	-0.511305	1.277873	-1.875734
H	-1.778922	1.188637	-0.635022
H	1.302941	3.144924	0.614278
H	0.861822	2.978375	-1.084300
H	-1.539151	3.435921	-0.475560
H	-2.057345	4.390121	1.781722
H	-1.574128	2.696762	1.914521
H	-0.426665	3.975520	2.337014
H	-0.024460	5.259106	-1.246100
H	-1.199169	5.868692	-0.068305
H	0.474630	5.567609	0.424905
H	-0.663105	-0.692653	-3.267883
H	-1.519947	-2.113518	-2.621260
H	-3.071559	-0.802324	-3.904629
H	-4.250259	-2.320076	0.380474
H	-2.461456	-0.005084	1.272961
H	-1.819122	-2.494732	-0.417928
H	-4.984823	0.602837	0.958310
H	-6.008912	-0.595459	0.195157
H	-4.510106	-1.540376	1.924301
H	-3.340800	-3.303614	2.924558
H	-2.498412	-3.860151	1.470446
H	-1.670866	-3.872707	3.031889
H	-1.017001	-1.719273	4.195018
H	-1.262807	-0.159614	3.392654
H	-2.650268	-1.057684	4.030852
H	-0.027543	-2.834437	1.202375
H	0.104262	-1.094126	1.521730
H	-5.647210	1.972701	-1.331496
H	-4.177755	1.997316	-2.317739

H	-4.100087	2.315394	-0.569370
H	-2.654150	0.713208	-3.103262
H	-3.804597	-1.693171	-1.568203

RB_11

C	-3.934222	-1.718648	0.184804
C	-2.486346	-2.045771	0.588732
C	-1.513372	-0.919345	0.269898
C	-1.825013	0.256704	-0.346490
C	-3.197706	0.542645	-0.736659
C	-4.352193	-0.287941	-0.146502
O	-3.473131	1.495079	-1.477163
O	-4.761478	-2.618179	0.180112
C	-4.753068	0.398972	1.195988
C	-5.563446	-0.292265	-1.092081
C	-2.482537	-2.337622	2.114750
C	-2.055221	-3.326186	-0.171318
C	-0.760240	1.268035	-0.733174
C	0.645847	0.625933	-0.649807
C	-0.927895	2.626830	0.019369
C	-0.944401	3.873362	-0.891466
C	-1.286112	5.127762	-0.075598
C	0.367823	4.078357	-1.661483
O	-0.273526	-1.269119	0.629223
C	0.876572	-0.320508	0.535814
C	0.853074	0.341472	1.943629
C	1.867328	1.465852	2.269643
C	3.236004	1.020252	1.864919
C	4.056288	1.561358	0.953699
C	5.149218	0.699684	0.345050
C	4.749849	-0.783409	0.206580
C	3.398345	-1.051327	-0.491239
C	2.047728	-1.334983	0.287545
C	3.235952	-2.454092	-1.190025
C	1.748858	-2.450667	-0.753402
C	4.007698	-3.592435	-0.508173
C	3.499271	-2.469861	-2.695473
C	3.925956	2.952908	0.387715
H	-5.098366	1.418648	0.986944
H	-3.915110	0.459256	1.899290
H	-5.570449	-0.155712	1.672452
H	-5.876247	0.734216	-1.300420
H	-5.321939	-0.775060	-2.046841
H	-6.399106	-0.833064	-0.639012
H	-1.488940	-2.672669	2.428415
H	-2.746019	-1.450355	2.702984
H	-3.206539	-3.128760	2.338468
H	-2.027893	-3.153748	-1.254566
H	-1.060905	-3.644001	0.153073
H	-2.767008	-4.131608	0.031095
H	-0.935178	1.485923	-1.799346
H	1.426625	1.409229	-0.626808
H	0.807424	0.049583	-1.581928
H	-1.870900	2.614925	0.582760
H	-0.133534	2.746988	0.767174
H	-1.746769	3.722024	-1.628914
H	-1.356347	6.015407	-0.717327
H	-2.245516	5.019725	0.446187
H	-0.517806	5.331200	0.683213
H	0.618246	3.215124	-2.289332
H	0.300962	4.951767	-2.323035
H	1.209322	4.249812	-0.976753
H	-0.170622	0.732234	2.114548
H	0.999521	-0.480994	2.673569
H	1.792773	1.656545	3.353300
H	4.769548	-1.280658	1.186581
H	3.226848	-0.275598	-1.249659
H	2.284671	-1.801814	1.255439
H	5.372660	1.095499	-0.658505
H	6.096735	0.779895	0.905324
H	5.536794	-1.275442	-0.385752
H	5.088118	-3.525622	-0.685046
H	3.848868	-3.610946	0.576651
H	3.672733	-4.560914	-0.903005
H	2.927564	-1.689222	-3.213056
H	4.562526	-2.304441	-2.918690
H	3.218120	-3.435111	-3.138973
H	1.346905	-3.392190	-0.363053
H	1.088630	-2.104859	-1.556053
H	3.706382	2.932916	-0.690553
H	3.155337	3.549967	0.886008
H	4.879495	3.493733	0.493243
H	1.591216	2.400683	1.768953
H	3.488034	0.024850	2.232104

RB_13

C	-3.683018	-1.721673	0.685680
C	-2.198740	-1.973424	0.990084

C	-1.311104	-0.841866	0.484587
C	-1.710336	0.189007	-0.322376
C	-3.017346	0.144630	-0.958830
C	-4.102147	-0.842966	-0.490969
O	-3.302836	0.888657	-1.907711
O	-4.536079	-2.285661	1.355503
C	-5.356212	-0.029535	-0.096582
C	-4.459712	-1.783256	-1.674999
C	-2.026888	-2.133924	2.518764
C	-1.804911	-3.309692	0.296256
C	-0.731235	1.279123	-0.725901
C	0.711015	0.727110	-0.646631
C	-0.923995	2.610710	0.055333
C	-2.146514	3.484912	-0.301316
C	-2.287371	4.619901	0.725360
C	-2.060848	4.062051	-1.720846
O	-0.062815	-1.013661	0.927599
C	1.059691	-0.076118	0.610723
C	1.163958	0.731937	1.936188
C	2.119407	1.947726	1.990123
C	3.466853	1.511042	1.509418
C	4.166240	1.945509	0.452283
C	5.233664	1.041385	-0.141414
C	4.891948	-0.459262	-0.032031
C	3.497432	-0.867313	-0.554727
C	2.229906	-1.093242	0.369640
C	3.336330	-2.351605	-1.055036
C	1.884221	-2.326115	-0.512409
C	4.194444	-3.370495	-0.291745
C	3.496476	-2.555444	-2.561189
C	3.910001	3.236444	-0.282809
H	-5.151271	0.630946	0.755634
H	-6.173027	-0.701890	0.181543
H	-5.673249	0.587082	-0.942622
H	-5.248605	-2.482016	-1.374154
H	-4.820338	-1.180236	-2.514851
H	-3.595152	-2.363009	-2.019483
H	-0.992763	-2.391337	2.760665
H	-2.287104	-1.208624	3.048003
H	-2.682865	-2.929873	2.881273
H	-1.846780	-3.233375	-0.796210
H	-0.784865	-3.586894	0.580481
H	-2.484638	-4.107490	0.617399
H	-0.913296	1.497982	-1.787808
H	1.439024	1.553378	-0.749238
H	0.857902	0.068127	-1.525251
H	-0.959876	2.395181	1.131015
H	-0.023242	3.224440	-0.106422
H	-3.053430	2.869082	-0.243487
H	-3.156428	5.252047	0.502737
H	-2.412803	4.230443	1.743835
H	-1.400695	5.269195	0.727370
H	-2.036135	3.273709	-2.479452
H	-2.928750	4.697845	-1.938662
H	-1.160710	4.681237	-1.841848
H	0.146388	1.070570	2.207919
H	1.470562	0.009781	2.720566
H	2.139533	2.291766	3.037723
H	5.024343	-0.810605	1.000711
H	3.222831	-0.206969	-1.388341
H	2.565976	-1.443053	1.357393
H	5.338741	1.296867	-1.207974
H	6.227105	1.229873	0.300944
H	5.644234	-1.004426	-0.622881
H	5.257740	-3.288585	-0.548005
H	4.106080	-3.260322	0.795701
H	3.877570	-4.391472	-0.543089
H	2.856830	-1.869926	-3.131279
H	4.533824	-2.383145	-2.880507
H	3.230542	-3.579986	-2.856568
H	1.534262	-3.223823	0.009037
H	1.161815	-2.083429	-1.299691
H	3.593849	3.056626	-1.321691
H	3.154518	3.864073	0.201390
H	4.837513	3.826704	-0.346239
H	1.726682	2.778444	1.393171
H	3.804758	0.587074	1.980343

RB_23

C	3.789136	-1.750139	-0.200015
C	2.399573	-2.011569	-0.806591
C	1.423891	-0.859730	-0.589370
C	1.711910	0.337523	0.000097
C	2.982816	0.488482	0.700935
C	4.194330	-0.350292	0.257003
O	3.128186	1.316158	1.607782
O	4.583420	-2.675590	-0.125365
C	4.812258	0.376548	-0.978513

C	5.248124	-0.435757	1.370351
C	2.594331	-2.228612	-2.334577
C	1.844750	-3.316931	-0.183973
C	0.670689	1.442432	0.105397
C	-0.548552	1.124480	-0.783585
C	1.262764	2.813419	-0.321555
C	0.328632	4.035488	-0.184931
C	-0.080018	4.302703	1.271022
C	1.009325	5.275085	-0.784978
O	0.217698	-1.199881	-1.062481
C	-0.992086	-0.338028	-0.896426
C	-1.692903	-0.589136	-2.268164
C	-2.724308	0.451379	-2.772463
C	-3.739250	0.741905	-1.705633
C	-4.712623	-0.080393	-1.290559
C	-5.233354	0.096707	0.112742
C	-4.364139	-0.731137	1.089471
C	-2.872237	-0.361514	1.219885
C	-1.710153	-0.986353	0.335972
C	-2.159293	-0.958589	2.494325
C	-0.879630	-1.151659	1.643701
C	-2.714452	-2.309599	2.967002
C	-2.043813	-0.000355	3.679778
C	-5.173881	-1.309304	-2.032608
H	5.152957	1.374325	-0.675934
H	5.675779	-0.188558	-1.349470
H	4.092815	0.495762	-1.795840
H	6.128332	-0.982502	1.020393
H	5.553697	0.569139	1.673917
H	4.854104	-0.951700	2.254151
H	1.644914	-2.522821	-2.793215
H	2.951217	-1.320462	-2.834511
H	3.325533	-3.027072	-2.501776
H	1.710329	-3.216511	0.899986
H	0.880382	-3.570863	-0.631417
H	2.544676	-4.137220	-0.366648
H	0.361279	1.522775	1.160429
H	-0.299006	1.460721	-1.810998
H	-1.415075	1.728537	-0.459151
H	2.165933	3.012479	0.267160
H	1.582336	2.731425	-1.372657
H	-0.587282	3.852073	-0.765545
H	-0.707355	5.200241	1.345143
H	-0.649549	3.471653	1.702973
H	0.802704	4.462484	1.905166
H	1.263881	5.121510	-1.841382
H	0.358630	6.156754	-0.724661
H	1.939463	5.514750	-0.251864
H	-0.882805	-0.654131	-3.021861
H	-2.177814	-1.584752	-2.229650
H	-3.180944	0.038708	-3.683577
H	-4.458701	-1.797307	0.837480
H	-2.768510	0.732046	1.248718
H	-2.032505	-1.983888	-0.001463
H	-5.194332	1.155938	0.406979
H	-6.280155	-0.231039	0.209558
H	-4.807019	-0.622093	2.092627
H	-3.706935	-2.216422	3.423920
H	-2.788363	-3.038585	2.151385
H	-2.045617	-2.738316	3.725156
H	-1.402448	-0.416968	4.468631
H	-1.614783	0.963746	3.379437
H	-3.026559	0.199645	4.129012
H	-0.350029	-2.103209	1.767385
H	-0.167505	-0.342035	1.809424
H	-6.267429	-1.291490	-2.157540
H	-4.727096	-1.399471	-3.028039
H	-4.945179	-2.231541	-1.478097
H	-2.213657	1.374721	-3.075283
H	-3.517744	1.601709	-1.070384

RB_35

C	-3.815268	-1.590050	0.852890
C	-2.333560	-1.727642	1.244606
C	-1.446409	-0.702545	0.552252
C	-1.883392	0.320848	-0.236939
C	-3.273863	0.398675	-0.650956
C	-4.226472	-0.780570	-0.374187
O	-3.696934	1.355900	-1.312670
O	-4.656586	-2.183458	1.511487
C	-5.675042	-0.289214	-0.227990
C	-4.129175	-1.730531	-1.608163
C	-2.220680	-1.516971	2.777636
C	-1.888975	-3.174270	0.900172
C	-0.935604	1.390650	-0.742464
C	0.510010	0.837443	-0.772368
C	-1.136830	2.745592	0.006065
C	-1.191873	3.990491	-0.904640

C	-1.533576	5.238520	-0.078582
C	0.092955	4.220790	-1.713206
O	-0.169172	-0.898290	0.886386
C	0.945018	-0.002334	0.440512
C	1.221102	0.803893	1.741564
C	2.166194	2.031514	1.687832
C	3.395967	1.744794	0.877502
C	4.444382	0.990296	1.234946
C	5.299609	0.411319	0.134695
C	4.699709	-0.932990	-0.343429
C	3.256594	-0.897947	-0.885073
C	2.016054	-1.090907	0.079404
C	2.805577	-2.183606	-1.689580
C	1.487618	-2.205650	-0.869099
C	3.642025	-3.448135	-1.458296
C	2.630603	-1.946736	-3.190941
C	4.718898	0.504994	2.635461
H	-5.967234	0.275872	-1.116961
H	-5.787924	0.364809	0.645288
H	-6.355478	-1.136962	-0.107624
H	-3.105548	-2.080316	-1.783254
H	-4.778179	-2.602534	-1.463293
H	-4.463185	-1.190464	-2.502098
H	-2.869823	-2.228512	3.296073
H	-1.188969	-1.674578	3.105103
H	-2.524180	-0.501632	3.061921
H	-1.909785	-3.365599	-0.179061
H	-0.870639	-3.348691	1.259784
H	-2.559731	-3.888096	1.390546
H	-1.215306	1.577093	-1.791539
H	1.232444	1.665110	-0.890855
H	0.600332	0.216597	-1.683514
H	-2.083829	2.706054	0.560839
H	-0.352451	2.885546	0.761206
H	-2.012241	3.826549	-1.620607
H	-1.641492	6.123747	-0.718345
H	-2.473696	5.111302	0.473053
H	-0.746124	5.457639	0.655737
H	0.325063	3.376835	-2.373024
H	-0.001557	5.111810	-2.347275
H	0.957368	4.379181	-1.053768
H	0.240301	1.140822	2.134699
H	1.623564	0.081564	2.479836
H	2.406999	2.299501	2.726778

H	4.767295	-1.668076	0.472038
H	3.131379	-0.012332	-1.520503
H	2.353157	-1.529112	1.030803
H	5.342020	1.104467	-0.718413
H	6.335669	0.239248	0.465353
H	5.348636	-1.314561	-1.146772
H	4.629532	-3.389144	-1.932479
H	3.795405	-3.658109	-0.393334
H	3.125636	-4.316800	-1.888541
H	2.160515	-2.811194	-3.680144
H	2.000219	-1.071411	-3.391081
H	3.598125	-1.776441	-3.683270
H	1.247165	-3.158903	-0.385294
H	0.615569	-1.903547	-1.458126
H	5.735388	0.790417	2.947822
H	4.018227	0.910299	3.372785
H	4.677871	-0.592557	2.700754
H	1.637508	2.894907	1.264657
H	3.333931	2.028671	-0.175263

RB_40

C	-3.774643	-1.924223	0.387229
C	-2.278075	-2.117652	0.688723
C	-1.430867	-0.922689	0.273255
C	-1.886127	0.202832	-0.346626
C	-3.302140	0.352754	-0.650763
C	-4.334273	-0.541722	0.059752
O	-3.707735	1.242350	-1.408794
O	-4.521016	-2.888982	0.461432
C	-4.666667	0.155704	1.416008
C	-5.618980	-0.668099	-0.772259
C	-2.136459	-2.361464	2.216671
C	-1.794370	-3.379465	-0.070460
C	-0.949191	1.296920	-0.825486
C	0.518264	0.800065	-0.812735
C	-1.209281	2.650924	-0.096093
C	-1.244309	3.894096	-1.010999
C	-1.653971	5.133765	-0.203042
C	0.074308	4.155255	-1.753581
O	-0.144087	-1.155344	0.551065
C	0.913514	-0.118869	0.353798
C	0.957883	0.556202	1.754916
C	1.806162	1.837544	1.971525
C	3.139338	1.749597	1.290014

C	4.200188	1.027773	1.676345
C	5.225520	0.672634	0.627947
C	4.808083	-0.632490	-0.091331
C	3.430179	-0.634623	-0.783335
C	2.126657	-1.054454	0.012155
C	3.185454	-1.833240	-1.787055
C	1.820978	-2.104117	-1.097196
C	4.139012	-3.028485	-1.665861
C	3.089409	-1.399362	-3.251479
C	4.345292	0.362389	3.021191
H	-5.392718	-0.443585	1.978664
H	-5.107889	1.139451	1.215092
H	-3.775935	0.301103	2.036951
H	-6.370650	-1.247848	-0.229121
H	-6.023394	0.324902	-0.985508
H	-5.427318	-1.169818	-1.728523
H	-2.762167	-3.210261	2.513283
H	-1.095049	-2.591393	2.462201
H	-2.440872	-1.485519	2.802143
H	-1.857405	-3.237637	-1.156616
H	-0.756388	-3.604094	0.189294
H	-2.420238	-4.234378	0.201473
H	-1.208155	1.467438	-1.883534
H	1.212955	1.659821	-0.820929
H	0.692054	0.252852	-1.758832
H	-2.178590	2.599555	0.417599
H	-0.460912	2.806831	0.691196
H	-2.023494	3.713733	-1.767912
H	-1.747848	6.017556	-0.846937
H	-2.617938	4.986424	0.300364
H	-0.908909	5.367673	0.569913
H	0.358948	3.317302	-2.400316
H	-0.009445	5.043844	-2.392581
H	0.900695	4.334063	-1.052014
H	-0.088327	0.789172	2.041209
H	1.309787	-0.221318	2.462275
H	1.905931	1.976083	3.057910
H	4.861356	-1.468415	0.621416
H	3.289508	0.317729	-1.310093
H	2.408083	-1.558649	0.948809
H	5.302097	1.478975	-0.116102
H	6.228027	0.533484	1.061665
H	5.569106	-0.842612	-0.858305
H	5.145989	-2.799732	-2.036401

H	4.235566	-3.384211	-0.633422
H	3.754946	-3.866953	-2.262456
H	2.752680	-2.227193	-3.890825
H	2.381693	-0.571454	-3.382358
H	4.064164	-1.063965	-3.632198
H	1.672901	-3.128993	-0.738622
H	0.962978	-1.847422	-1.726384
H	5.294462	0.656086	3.494934
H	3.534710	0.616326	3.712237
H	4.375704	-0.733524	2.928555
H	1.262932	2.715906	1.601872
H	3.173757	2.173489	0.283937

RB_43

C	3.409377	-2.071428	-0.726479
C	1.970830	-1.887686	-1.238969
C	1.222234	-0.769789	-0.524645
C	1.754364	0.098870	0.385630
C	3.099657	-0.116877	0.900430
C	4.092493	-0.999929	0.122354
O	3.494497	0.438537	1.933402
O	4.025395	-3.075397	-1.052444
C	4.852466	-0.057294	-0.861892
C	5.106142	-1.653921	1.076535
C	2.059821	-1.542830	-2.753859
C	1.227441	-3.235570	-1.077449
C	0.905016	1.212045	0.973183
C	-0.581420	0.784862	0.954757
C	1.157891	2.589827	0.299496
C	2.489437	3.306875	0.611689
C	2.676119	4.489866	-0.351224
C	2.568452	3.787412	2.067263
O	-0.054418	-0.752069	-0.923193
C	-1.090490	0.172099	-0.357845
C	-1.296041	1.165646	-1.538653
C	-2.063420	2.489148	-1.292482
C	-3.330080	2.250036	-0.522651
C	-4.443208	1.655739	-0.975429
C	-5.368290	1.026005	0.035889
C	-4.923996	-0.430948	0.315794
C	-3.490533	-0.629600	0.848322
C	-2.267964	-0.841081	-0.137337
C	-3.195000	-2.046048	1.486783
C	-1.879561	-2.117002	0.664150

C	-4.164657	-3.171912	1.106920
C	-3.010189	-2.015195	3.005319
C	-4.738290	1.377483	-2.427978
H	4.174326	0.459007	-1.550800
H	5.573108	-0.636328	-1.451892
H	5.400024	0.698926	-0.287047
H	5.838801	-2.236918	0.511782
H	5.629934	-0.884554	1.649641
H	4.607838	-2.326482	1.785548
H	2.616427	-2.328126	-3.277175
H	1.052910	-1.482818	-3.179729
H	2.563459	-0.584262	-2.926316
H	1.137660	-3.517845	-0.021540
H	0.224720	-3.169625	-1.506122
H	1.781674	-4.022736	-1.596276
H	1.181262	1.307547	2.033301
H	-1.222191	1.648517	1.214274
H	-0.714540	0.042979	1.765027
H	1.079384	2.474195	-0.789511
H	0.341742	3.266416	0.598670
H	3.318606	2.607675	0.442217
H	3.618070	5.018844	-0.157694
H	2.690344	4.159352	-1.397848
H	1.862052	5.221070	-0.248443
H	2.511536	2.954444	2.775608
H	3.513581	4.312372	2.256597
H	1.751941	4.486417	2.296600
H	-0.294886	1.419564	-1.936596
H	-1.814582	0.601131	-2.339298
H	-2.256902	2.936543	-2.278699
H	-5.064161	-1.032864	-0.594040
H	-3.270504	0.151244	1.587110
H	-2.639208	-1.117745	-1.135556
H	-5.341866	1.590912	0.979337
H	-6.413796	1.016726	-0.309394
H	-5.618688	-0.847104	1.061584
H	-5.144374	-3.060707	1.587819
H	-4.329173	-3.235415	0.024890
H	-3.751762	-4.137224	1.429915
H	-2.653368	-2.983242	3.383547
H	-2.281856	-1.252705	3.308096
H	-3.956314	-1.790527	3.517200
H	-1.747325	-3.024198	0.064884
H	-0.983907	-1.993783	1.281417
H	-5.731750	1.766752	-2.698379
H	-4.007146	1.830232	-3.105678
H	-4.766006	0.297872	-2.638078
H	-1.425716	3.199597	-0.753765
H	-3.254778	2.395508	0.556967

RB_46

C	-3.500552	-1.707269	1.051059
C	-2.036313	-1.577932	1.501324
C	-1.250229	-0.600622	0.638820
C	-1.772095	0.184190	-0.352825
C	-3.083911	-0.105182	-0.904033
C	-3.925390	-1.273757	-0.348988
O	-3.529537	0.508368	-1.883526
O	-4.310385	-2.215826	1.812512
C	-5.417832	-0.897356	-0.350386
C	-3.702241	-2.484574	-1.304847
C	-2.020636	-1.052670	2.960818
C	-1.411397	-2.998353	1.473542
C	-0.923664	1.282122	-0.967698
C	0.557803	0.834501	-0.961573
C	-1.152559	2.665347	-0.298790
C	-2.496843	3.372702	-0.574685
C	-2.672259	4.550177	0.396914
C	-2.613952	3.858432	-2.025952
O	0.021108	-0.549941	1.042062
C	1.085209	0.269095	0.366584
C	1.399756	1.321444	1.469729
C	2.209835	2.587250	1.089134
C	3.417283	2.228396	0.272851
C	4.534812	1.631939	0.710597
C	5.368185	0.875428	-0.293705
C	4.854108	-0.580084	-0.406118
C	3.392911	-0.780038	-0.854758
C	2.184757	-0.832232	0.169351
C	3.027255	-2.248044	-1.311640
C	1.686964	-2.123321	-0.540845
C	3.905550	-3.357477	-0.718014
C	2.906385	-2.432249	-2.824785
C	4.915279	1.476701	2.161400
H	-6.028126	-1.750031	-0.039387
H	-5.720482	-0.590912	-1.354896
H	-5.619050	-0.066407	0.337105
H	-4.269196	-3.354884	-0.953213

H	-4.056625	-2.215443	-2.306690
H	-2.645063	-2.763658	-1.381698
H	-2.612037	-1.715790	3.598419
H	-0.994688	-1.019149	3.338820
H	-2.447448	-0.043848	3.023461
H	-1.376418	-3.414856	0.460515
H	-0.391731	-2.966280	1.868389
H	-2.008440	-3.669142	2.101321
H	-1.211547	1.371739	-2.024896
H	1.204406	1.677461	-1.268553
H	0.661291	0.060176	-1.744947
H	-1.039672	2.557522	0.788061
H	-0.346533	3.339970	-0.628644
H	-3.314049	2.663056	-0.389935
H	-3.621817	5.072931	0.224591
H	-2.662967	4.215099	1.442107
H	-1.865738	5.287769	0.280741
H	-2.564065	3.028615	-2.738447
H	-3.568974	4.373483	-2.191651
H	-1.810606	4.567403	-2.270641
H	0.435222	1.648728	1.902041
H	1.938338	0.787535	2.278291
H	2.478377	3.092958	2.028129
H	5.017875	-1.094500	0.552047
H	3.169680	-0.090037	-1.679072
H	2.564853	-1.081483	1.171764
H	5.301270	1.353966	-1.281938
H	6.432996	0.852440	-0.013966
H	5.494646	-1.097750	-1.137365
H	4.916210	-3.365567	-1.144193
H	4.003529	-3.271960	0.370715
H	3.454526	-4.336809	-0.926984
H	2.498173	-3.421602	-3.073916
H	2.244832	-1.679885	-3.272309
H	3.884642	-2.347412	-3.318291
H	1.431786	-2.961959	0.115554
H	0.836708	-1.947521	-1.208078
H	5.933721	1.857780	2.332670
H	4.241683	2.012253	2.838391
H	4.929385	0.420612	2.469125
H	1.573952	3.286959	0.533437
H	3.280371	2.278221	-0.809255

RB_56

C	3.857460	-1.548837	-0.583543
C	2.415365	-1.953658	-0.923042
C	1.421918	-0.828089	-0.661953
C	1.704571	0.366236	-0.059032
C	2.946928	0.500111	0.686044
C	4.147971	-0.417061	0.401905
O	3.082129	1.363774	1.564769
O	4.785337	-2.184205	-1.063028
C	5.273193	0.473340	-0.182529
C	4.636190	-1.056614	1.727013
C	2.354698	-2.359803	-2.415156
C	2.069215	-3.190676	-0.045119
C	0.657710	1.464225	0.049852
C	-0.574069	1.133177	-0.816089
C	1.240017	2.832512	-0.399425
C	0.304766	4.053645	-0.262367
C	-0.095492	4.327588	1.194706
C	0.979944	5.291093	-0.872982
O	0.211749	-1.182321	-1.106297
C	-1.006007	-0.333730	-0.914249
C	-1.732171	-0.597025	-2.270061
C	-2.789674	0.427905	-2.752478
C	-3.784130	0.706493	-1.663607
C	-4.739488	-0.125617	-1.226639
C	-5.230338	0.048288	0.187950
C	-4.327645	-0.764507	1.146665
C	-2.838431	-0.373630	1.242155
C	-1.688565	-0.987787	0.335135
C	-2.090408	-0.956475	2.503201
C	-0.828143	-1.140700	1.625118
C	-2.620854	-2.310228	2.995964
C	-1.957889	0.009517	3.680654
C	-5.204390	-1.360481	-1.956477
H	6.168177	-0.126733	-0.372718
H	5.518436	1.267872	0.529175
H	4.962973	0.938891	-1.126844
H	3.866359	-1.691223	2.183389
H	5.525288	-1.669427	1.541950
H	4.891190	-0.265897	2.439490
H	3.105945	-3.128275	-2.616219
H	1.367412	-2.756971	-2.664583
H	2.559206	-1.501913	-3.067809
H	2.110475	-2.957077	1.025184
H	1.059989	-3.542438	-0.282565

H	2.778703	-4.000182	-0.251348
H	0.365206	1.554249	1.108643
H	-0.346820	1.466389	-1.849764
H	-1.440210	1.731010	-0.478648
H	2.150571	3.037394	0.175449
H	1.545446	2.740986	-1.453886
H	-0.614510	3.865800	-0.836372
H	-0.720633	5.226692	1.268571
H	-0.664517	3.499461	1.632909
H	0.790845	4.488021	1.823620
H	0.327837	6.171882	-0.814898
H	1.229866	5.131652	-1.929624
H	1.912148	5.535556	-0.345723
H	-0.937597	-0.651617	-3.040960
H	-2.201884	-1.599390	-2.219482
H	-3.260691	0.007075	-3.652402
H	-4.412562	-1.832697	0.899834
H	-2.748995	0.721285	1.263744
H	-2.007157	-1.989428	0.006495
H	-5.199217	1.108779	0.478643
H	-6.270080	-0.293341	0.309593
H	-4.748848	-0.658785	2.159367
H	-3.602546	-2.223814	3.476827
H	-2.708205	-3.044251	2.186221
H	-1.929621	-2.728757	3.739623
H	-1.544205	0.975775	3.365952
H	-2.932374	0.203054	4.150193
H	-1.295623	-0.397020	4.457439
H	-0.287412	-2.087012	1.740851
H	-0.120461	-0.323908	1.772845
H	-6.300814	-1.355840	-2.053972
H	-4.781378	-1.446056	-2.962654
H	-4.950610	-2.279409	-1.407312
H	-2.299091	1.357816	-3.068186
H	-3.557245	1.568563	-1.033264

RB_57

C	4.092295	-1.018688	-0.236322
C	2.829475	-1.533515	-0.948021
C	1.596714	-0.677733	-0.678689
C	1.564394	0.483316	0.040536
C	2.731444	0.845234	0.838516
C	4.126743	0.371038	0.395891
O	2.635733	1.570458	1.835385
O	5.088724	-1.725798	-0.219614
C	4.604549	1.363764	-0.709633
C	5.120756	0.398236	1.566160
C	3.124256	-1.527173	-2.475464
C	2.587856	-2.993824	-0.491018
C	0.275507	1.284017	0.182556
C	-0.747622	0.821417	-0.872519
C	0.528261	2.806522	0.010517
C	-0.681021	3.736949	0.249691
C	-1.193589	3.676797	1.696277
C	-0.302546	5.179371	-0.120178
O	0.524151	-1.246383	-1.244960
C	-0.852654	-0.685178	-1.108710
C	-1.400495	-0.983204	-2.535884
C	-2.733833	-0.315961	-2.953593
C	-3.755377	-0.593316	-1.896478
C	-4.401881	0.274236	-1.105325
C	-4.974430	-0.217354	0.213193
C	-4.143907	-1.343521	0.862275
C	-2.635526	-1.064930	1.040786
C	-1.512067	-1.542829	0.029371
C	-1.904588	-1.892531	2.164240
C	-0.641482	-1.912120	1.266056
C	-2.462003	-3.307993	2.370825
C	-1.763803	-1.186884	3.512652
C	-4.533819	1.752666	-1.369900
H	3.914670	1.401296	-1.559838
H	4.676900	2.371952	-0.283524
H	5.595384	1.067156	-1.074180
H	4.820825	-0.296387	2.359989
H	6.119435	0.113254	1.223554
H	5.167285	1.402407	1.995939
H	2.284014	-1.970422	-3.019419
H	3.283708	-0.511499	-2.857035
H	4.023922	-2.118579	-2.677150
H	3.477920	-3.593947	-0.700421
H	2.384302	-3.046131	0.585255
H	1.738258	-3.424374	-1.027377
H	-0.126433	1.112561	1.195794
H	-0.465742	1.287459	-1.840266
H	-1.751141	1.203269	-0.617891
H	1.328257	3.116862	0.691913
H	0.902563	2.972457	-1.012395
H	-1.503908	3.433911	-0.414154

H	-2.028636	4.373109	1.846541
H	-1.550733	2.677711	1.971585
H	-0.401574	3.950895	2.406512
H	0.023051	5.254485	-1.165442
H	-1.151055	5.862211	0.013898
H	0.519442	5.546750	0.509271
H	-0.616031	-0.666218	-3.251665
H	-1.499888	-2.083571	-2.634687
H	-3.013649	-0.740994	-3.931744
H	-4.286905	-2.287118	0.317648
H	-2.491534	0.001679	1.263209
H	-1.847973	-2.480004	-0.439184
H	-5.005537	0.636726	0.908503
H	-6.023659	-0.544391	0.110716
H	-4.567798	-1.518384	1.863384
H	-3.437006	-3.298604	2.873452
H	-2.580305	-3.853479	1.427134
H	-1.776404	-3.890576	3.000484
H	-1.327636	-0.186352	3.401555
H	-2.737648	-1.071130	4.008603
H	-1.116238	-1.756010	4.194004
H	-0.090987	-2.857865	1.209107
H	0.058884	-1.122277	1.545700
H	-5.596345	2.042809	-1.369543
H	-4.111955	2.056449	-2.333474
H	-4.055891	2.352446	-0.580594
H	-2.592807	0.760936	-3.106925
H	-3.801896	-1.647531	-1.620171

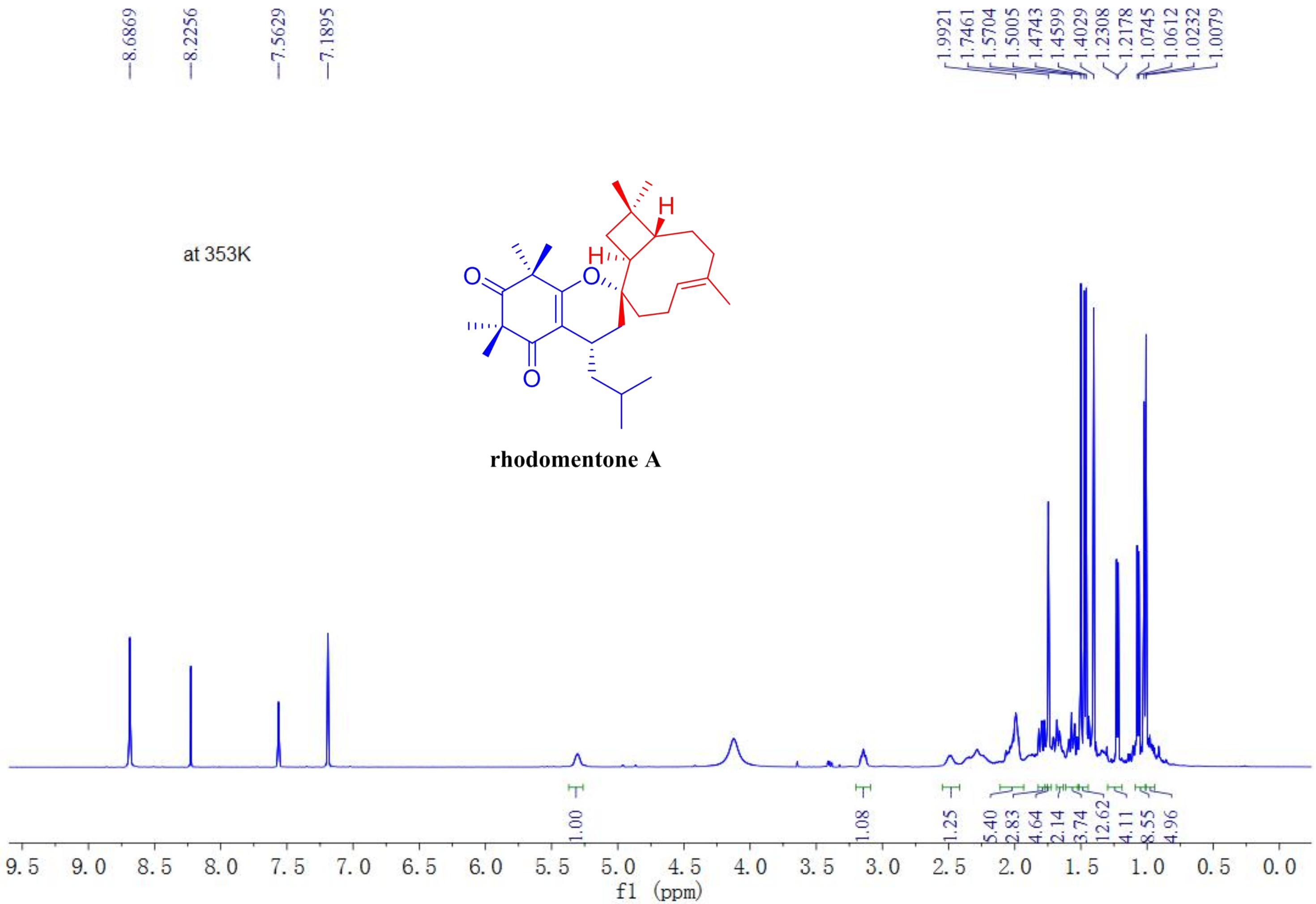


Figure S2. [1]H NMR spectrum (500 MHz, pyridine-d_5, at 353K) of **1**.

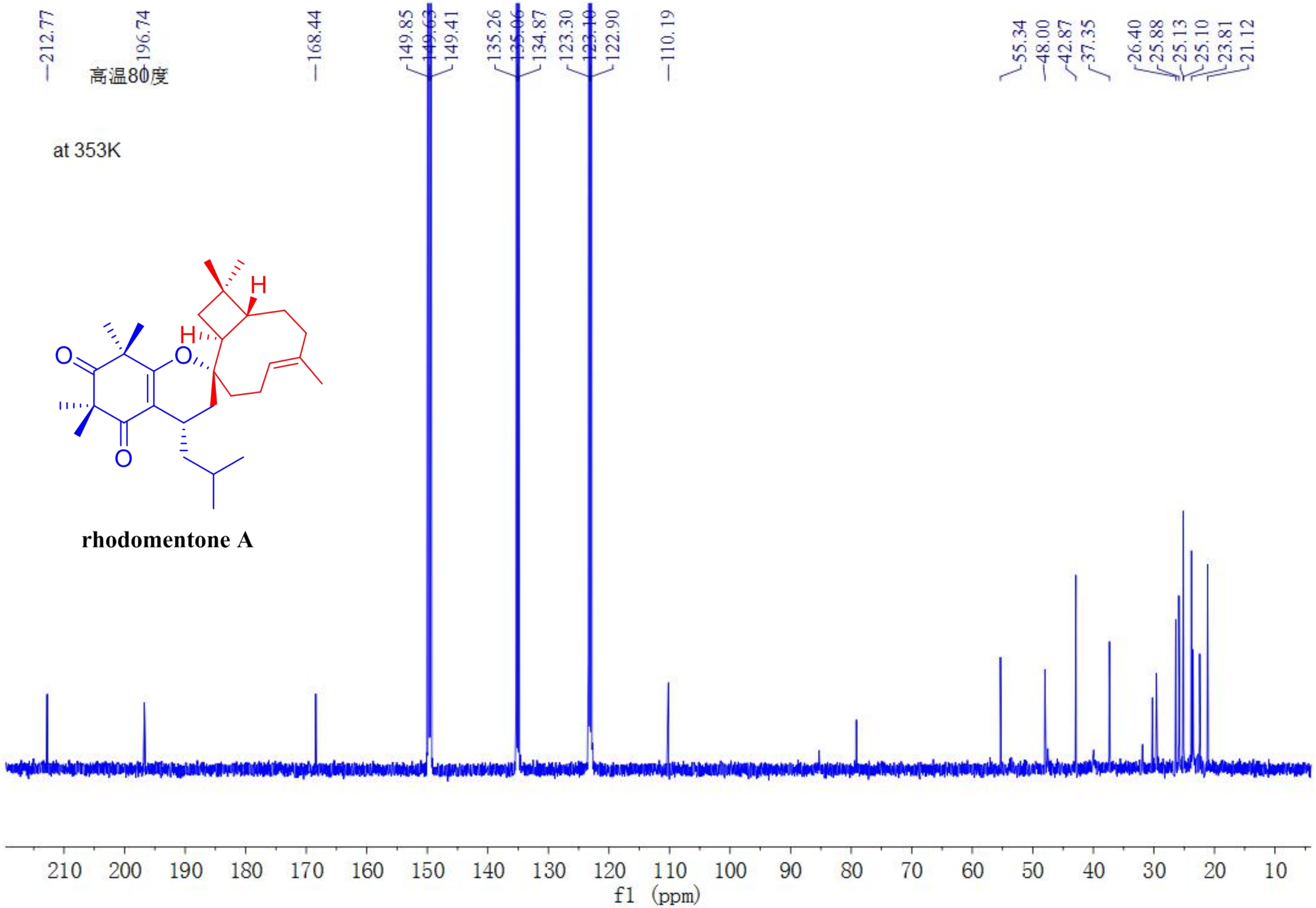


Figure S3. ^{13}C NMR spectrum (125 MHz, pyridine-d_5, at 353K) of **1**.

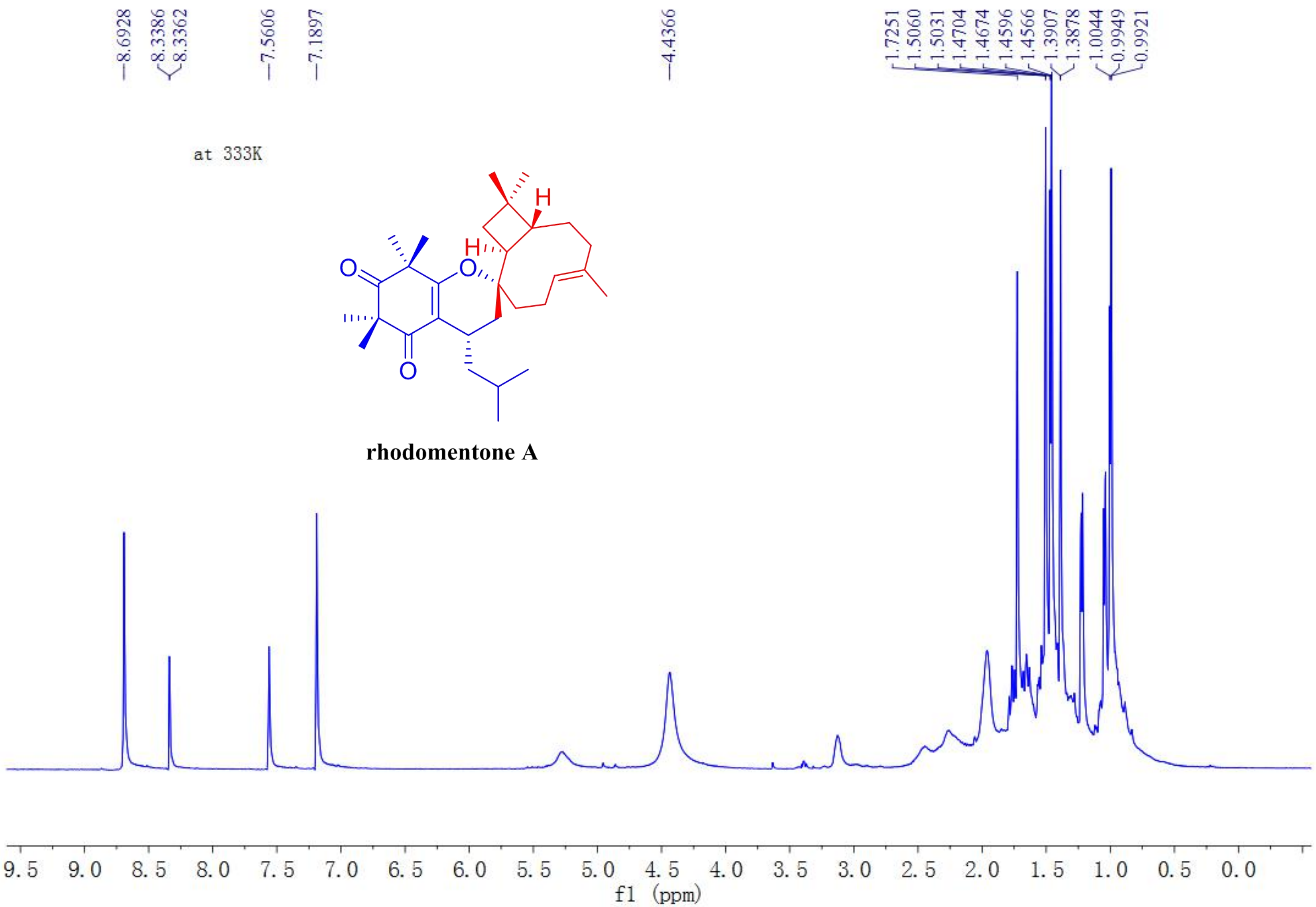


Figure S4. ^{1}H NMR spectrum (500 MHz, pyridine-d_5, at 333K) of **1**.

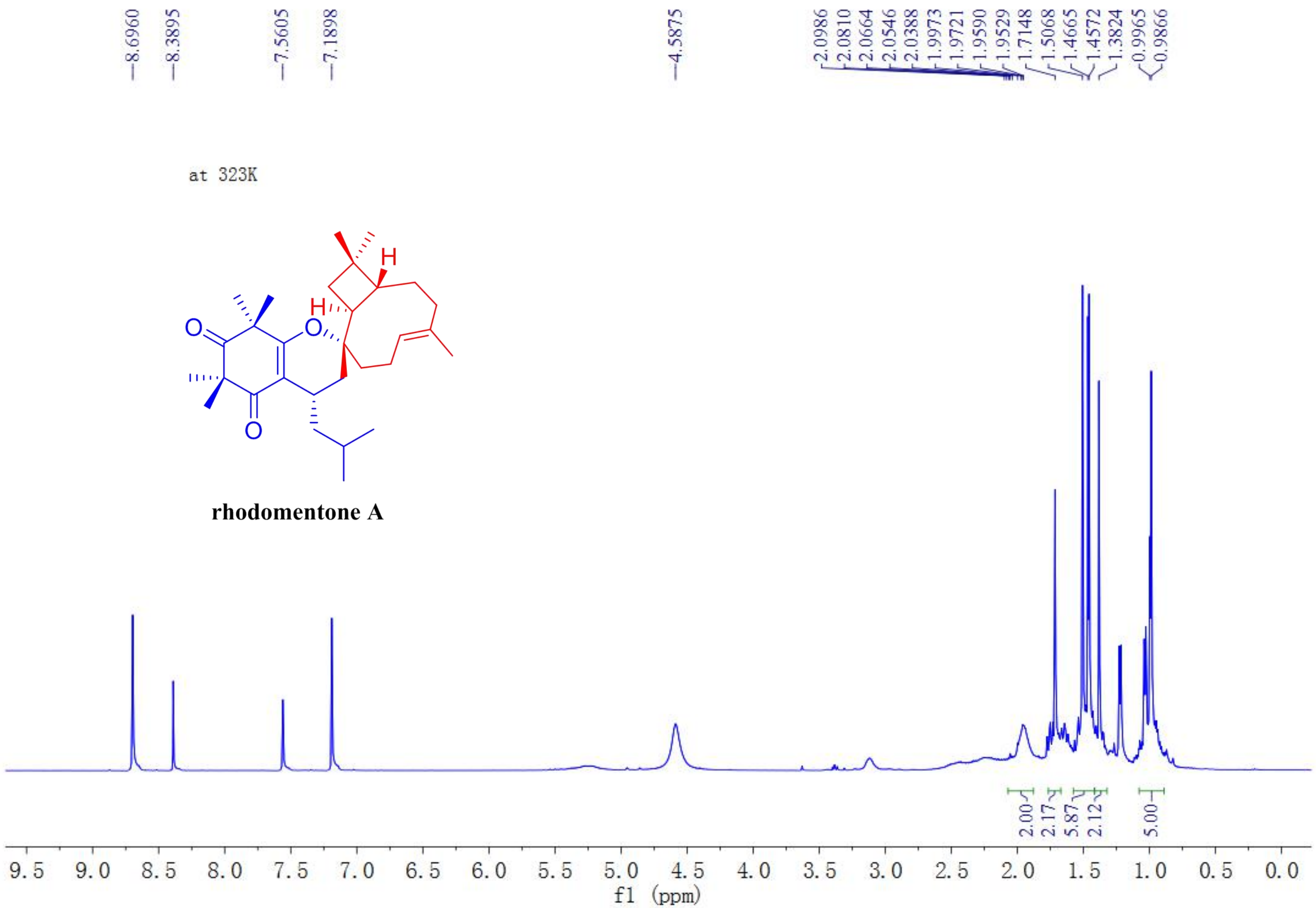


Figure S5. ^{1}H NMR spectrum (500 MHz, pyridine-d_5, at 323K) of **1**.

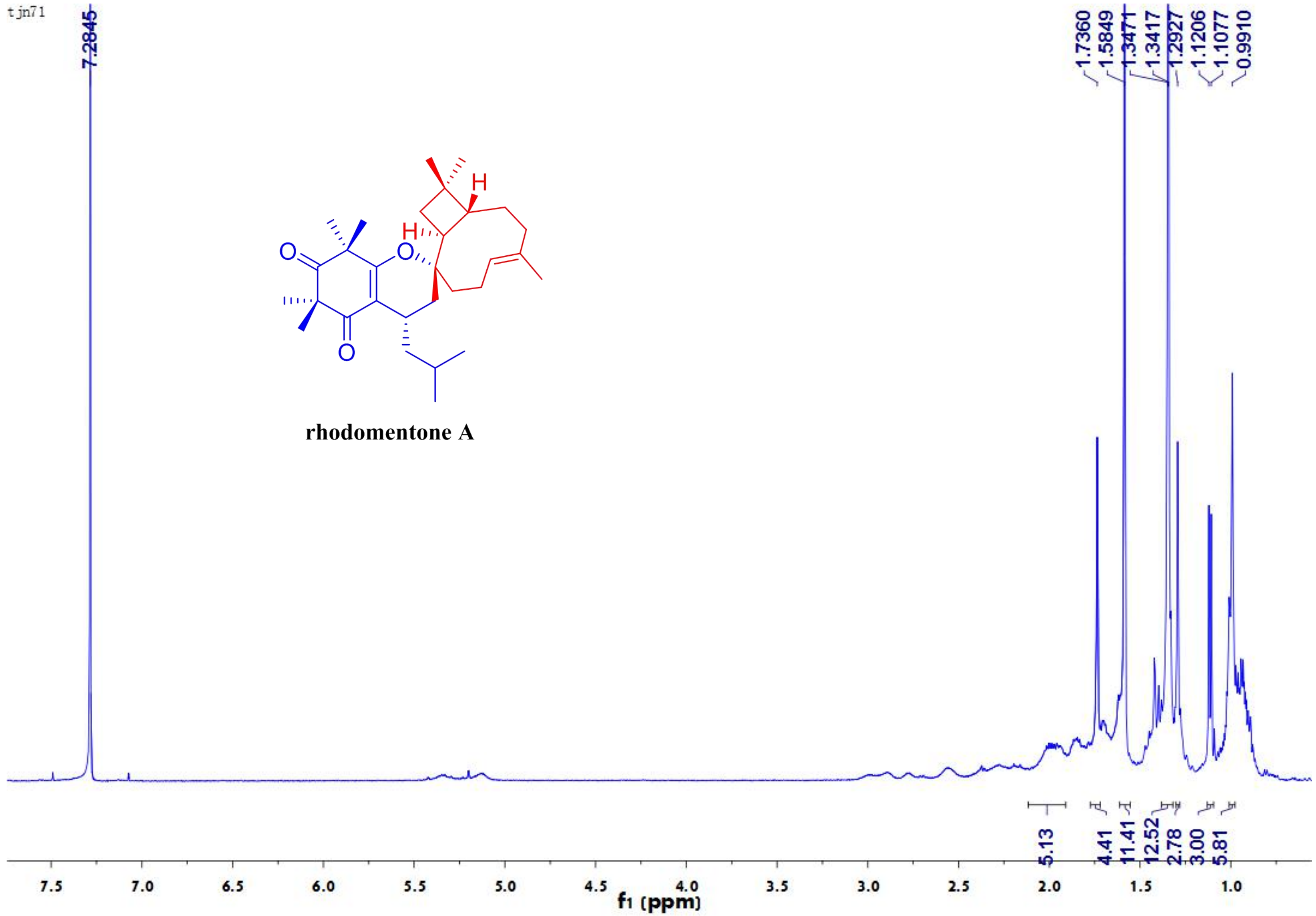


Figure S6. [1]H NMR spectrum (500 MHz, $CDCl_3$, rt) of **1**.

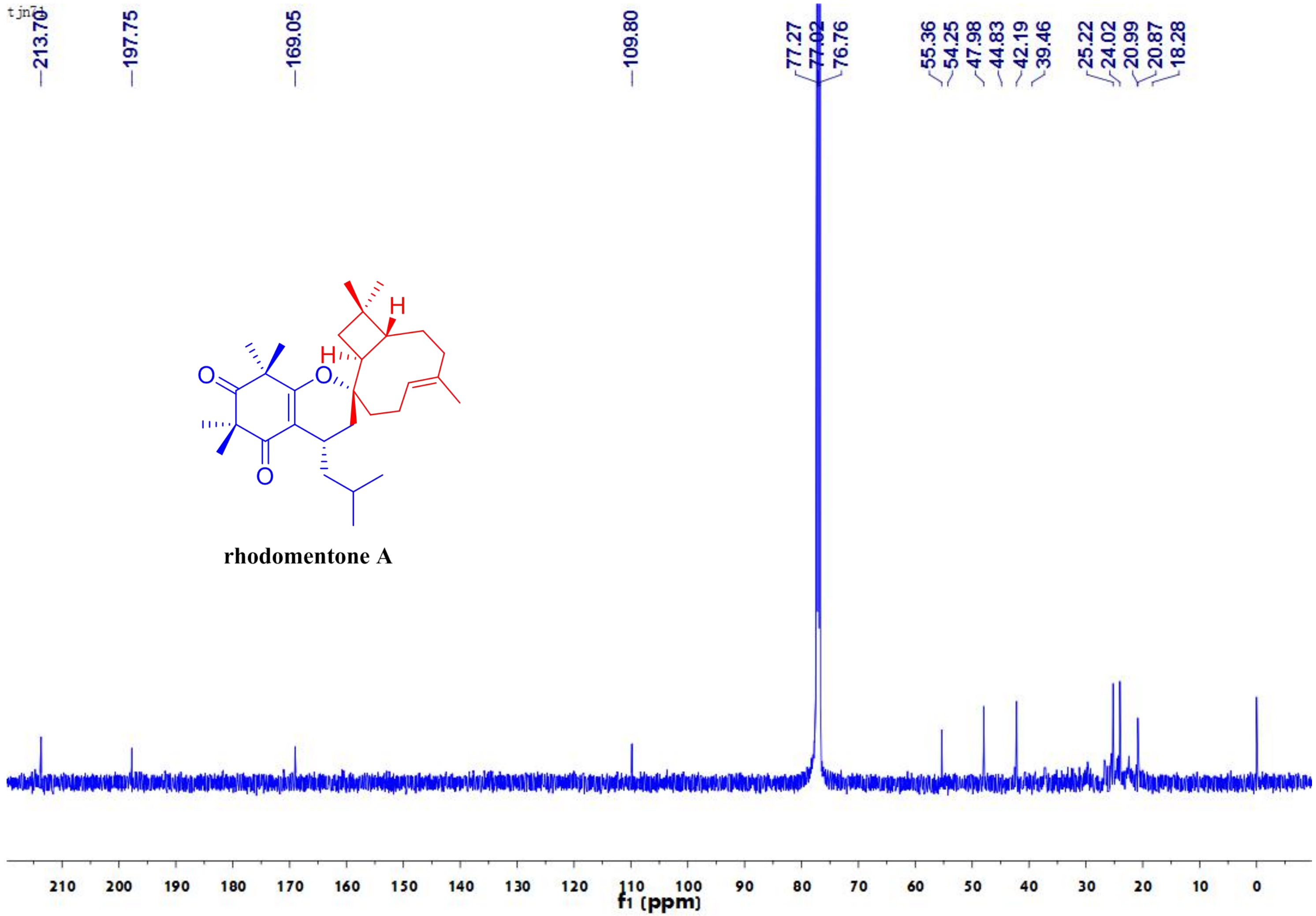


Figure S7. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, rt) of **1**.

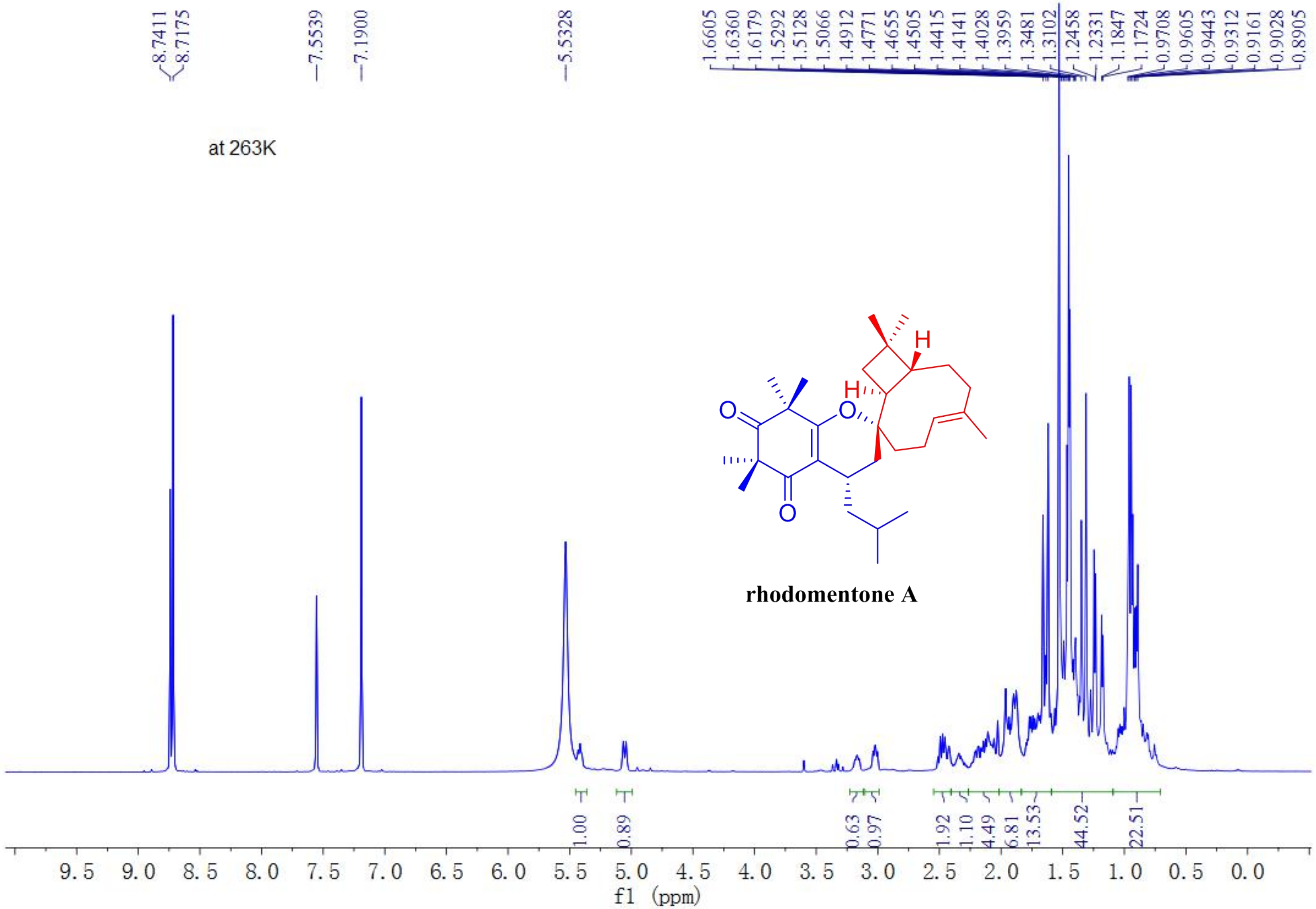


Figure S8. ^{1}H NMR spectrum (500 MHz, pyridine-d_5, at 263K) of **1**.

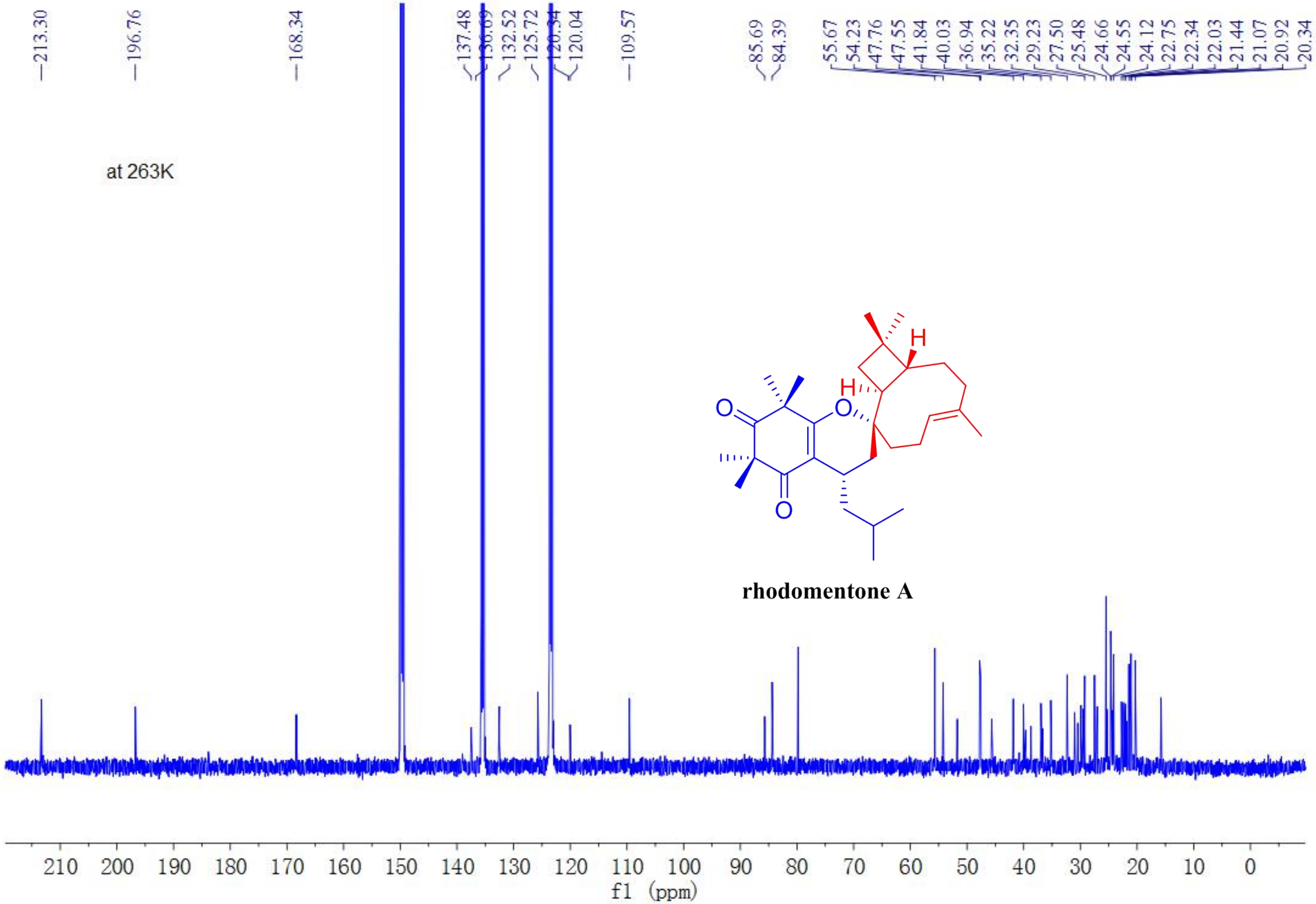


Figure S9. ^{13}C NMR spectrum (125 MHz, pyridine-d_5, at 263K) of **1**.

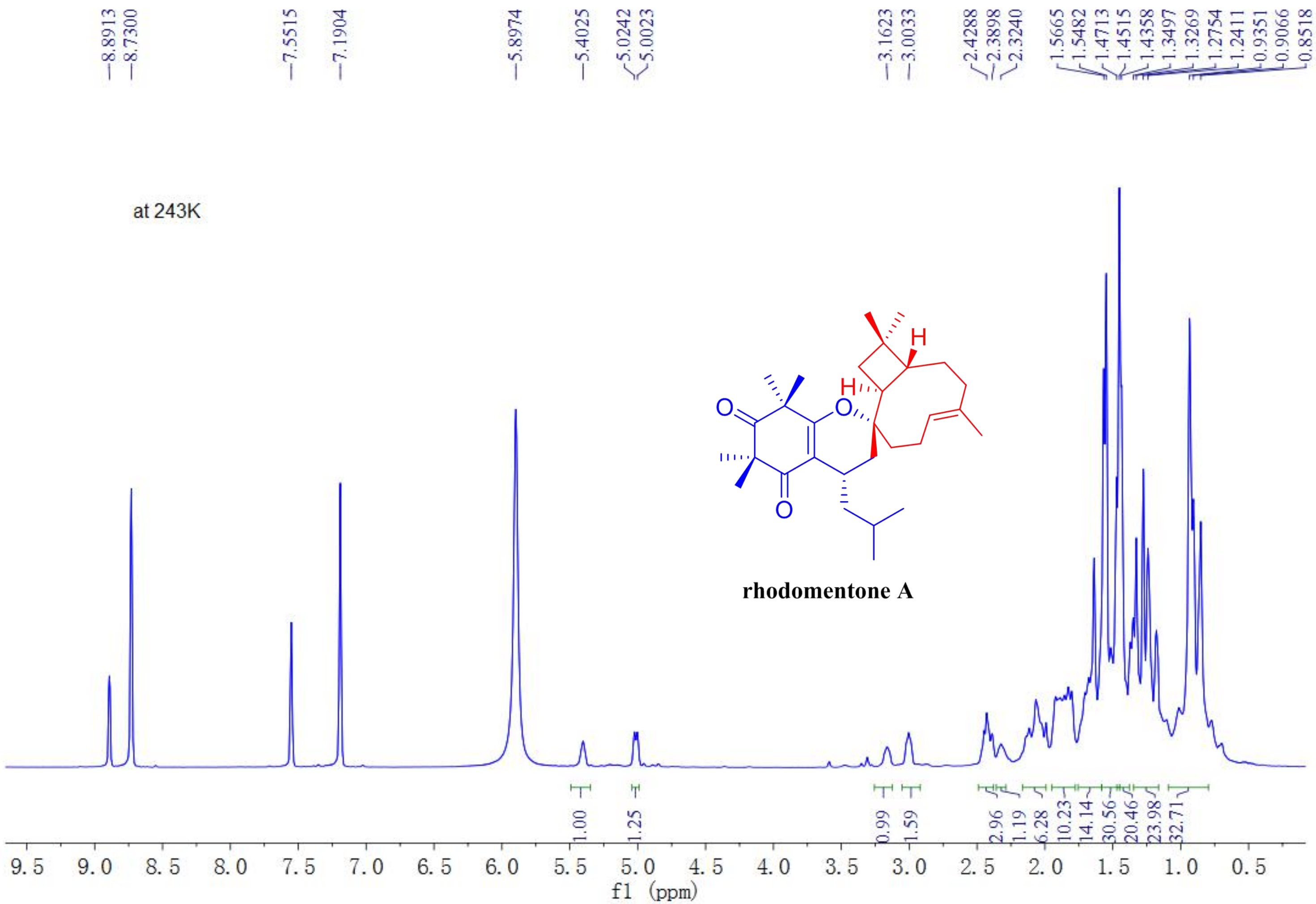


Figure S10. ^{1}H NMR spectrum (500 MHz, pyridine-d_5, at 243K) of **1**.

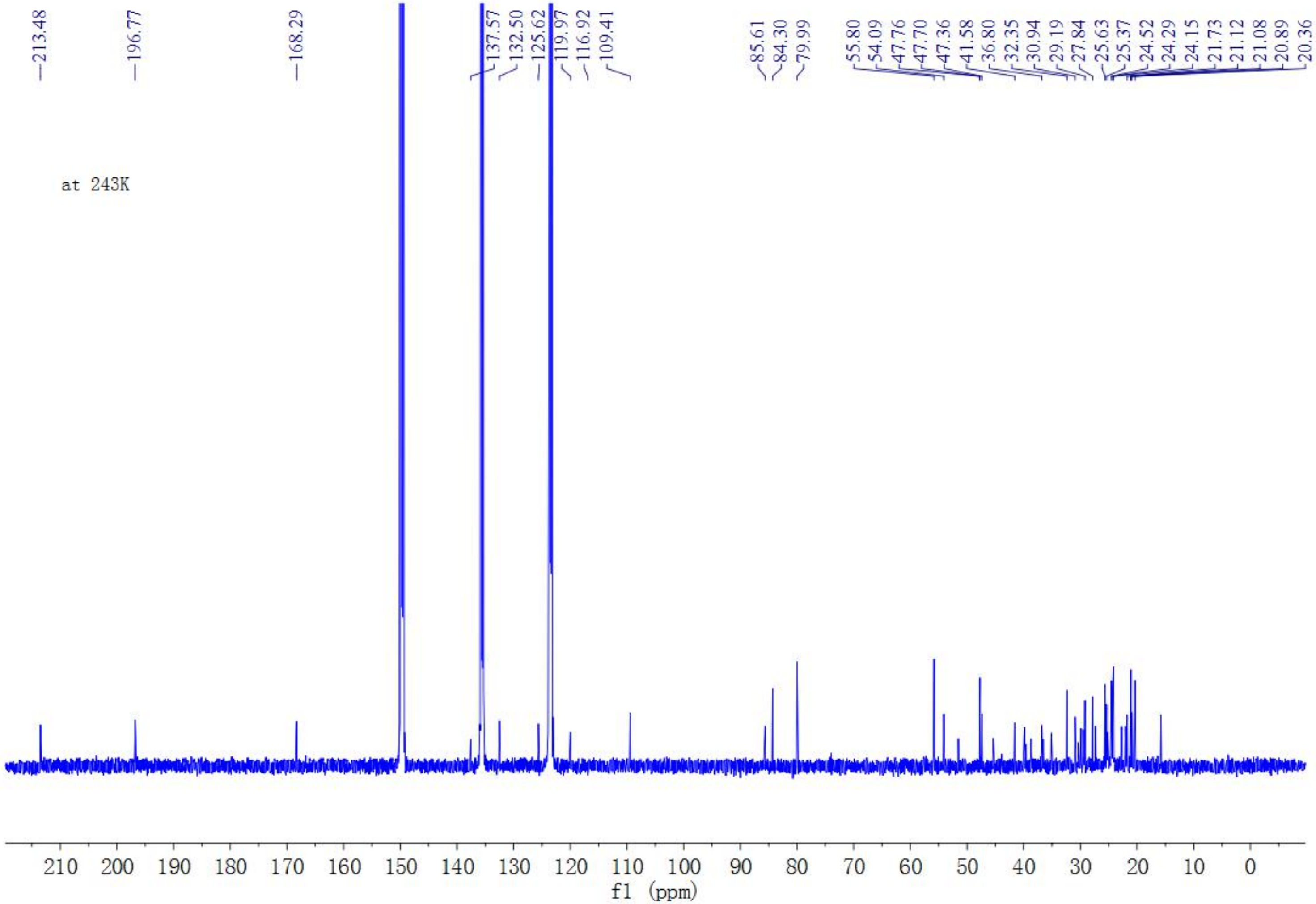


Figure S11. ^{13}C NMR spectrum (125 MHz, pyridine-d_5, at 243K) of **1**.

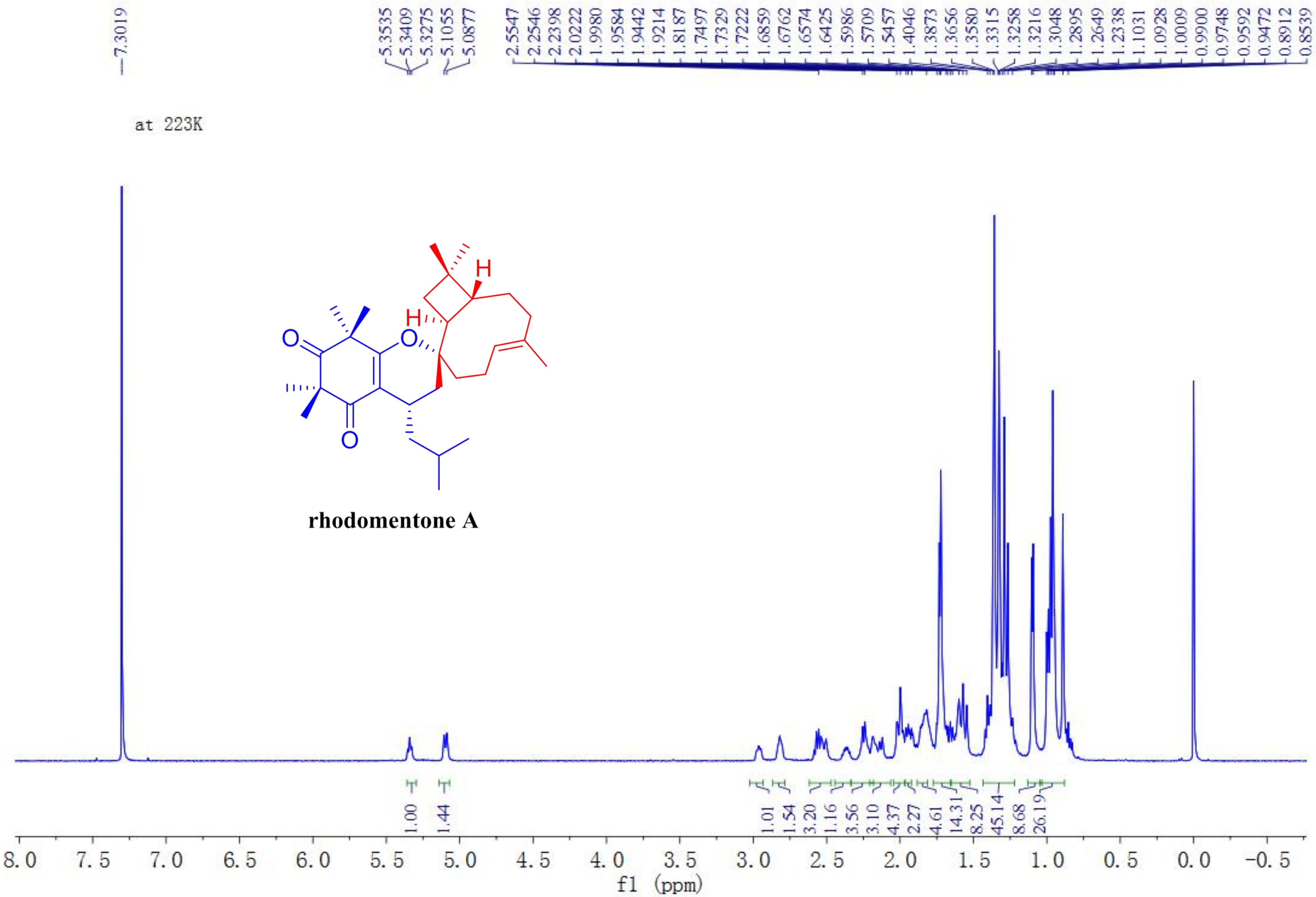


Figure S12. [1]H NMR spectrum (500 MHz, $CDCl_3$, at 223K) of **1**.

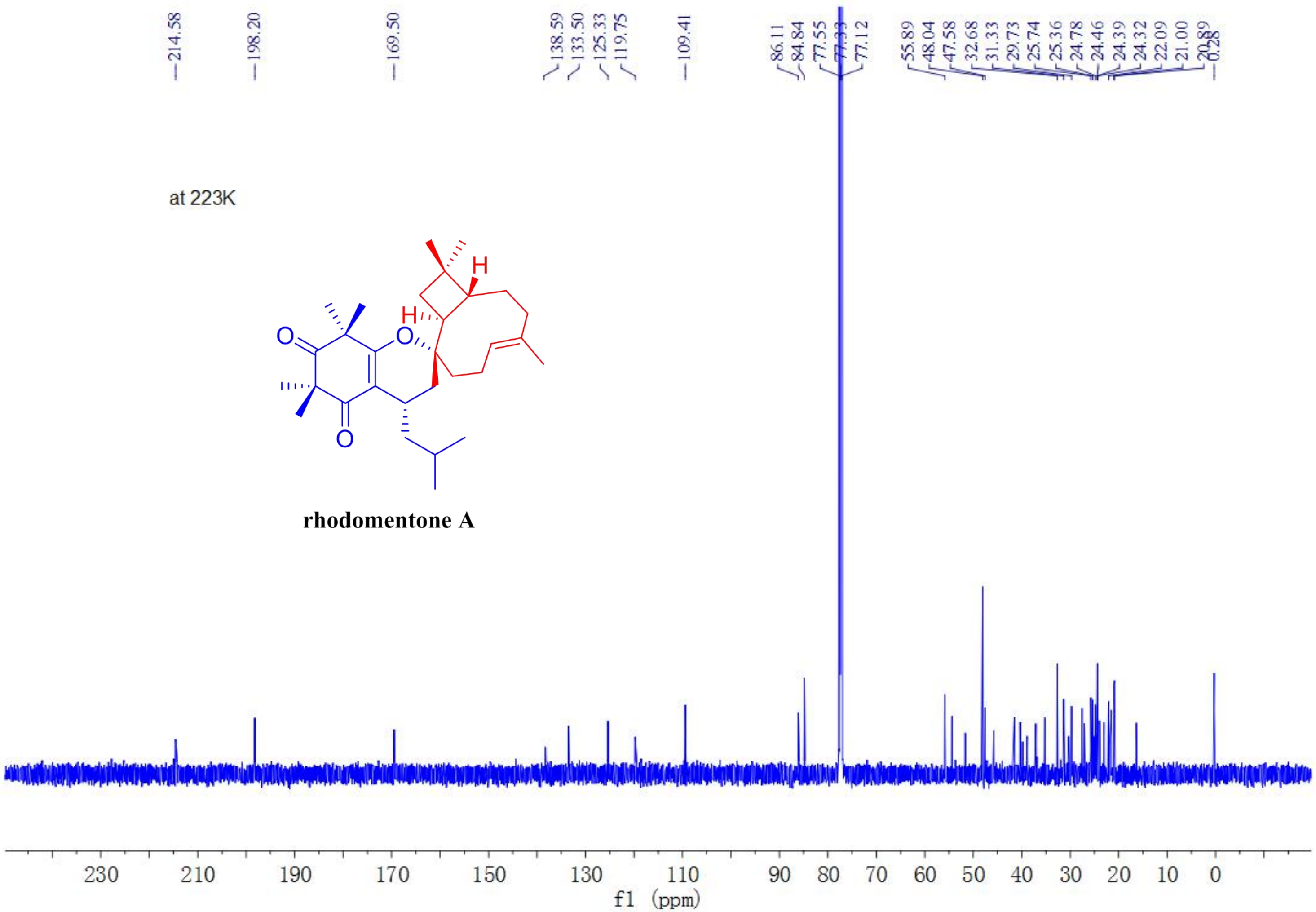


Figure S13. [13]C NMR spectrum (125 MHz, $CDCl_3$, at 223K) of **1**.

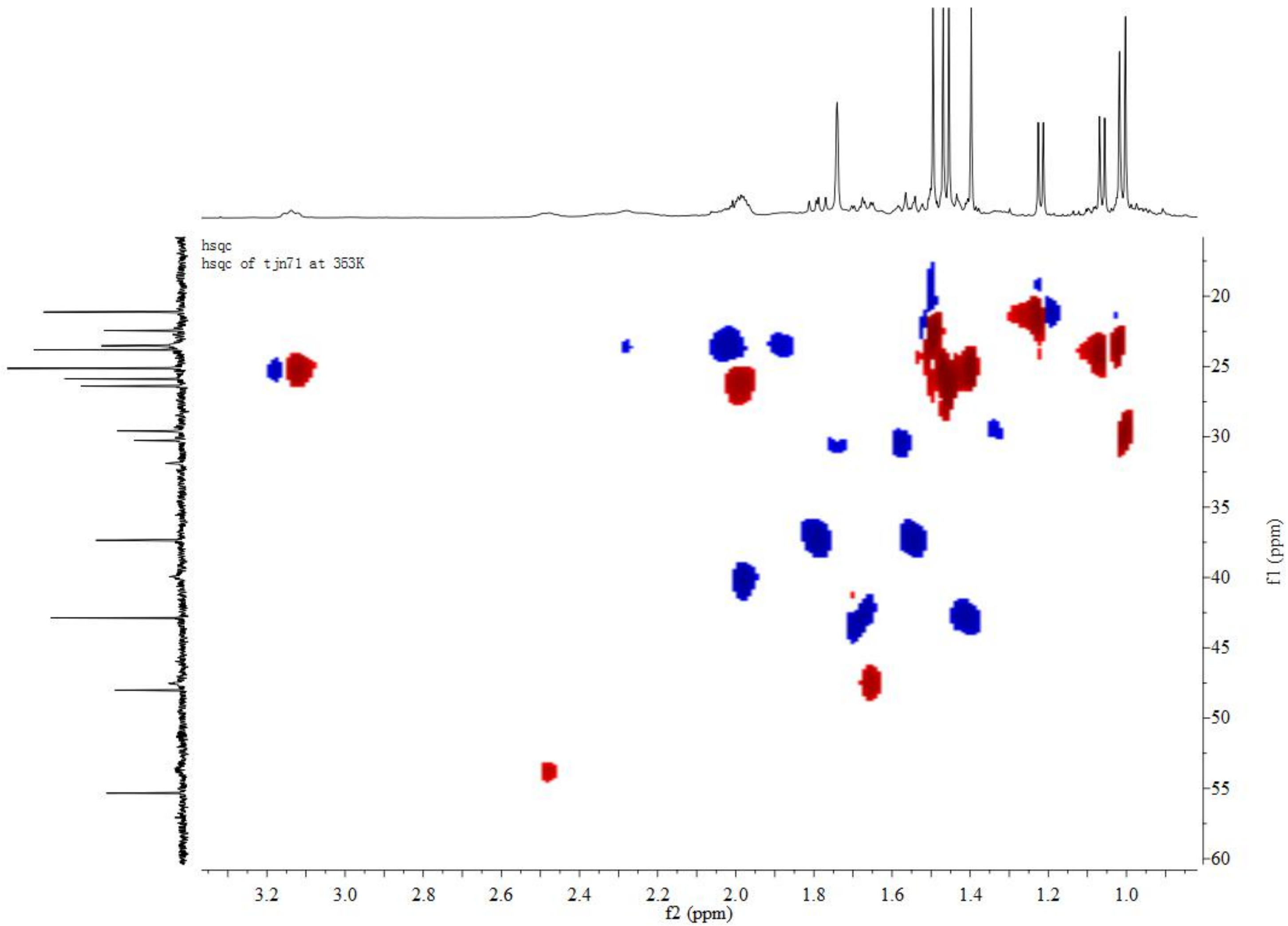


Figure S14. HSQC spectrum (500 MHz, pyridine-d_5, at 353K) of **1**.

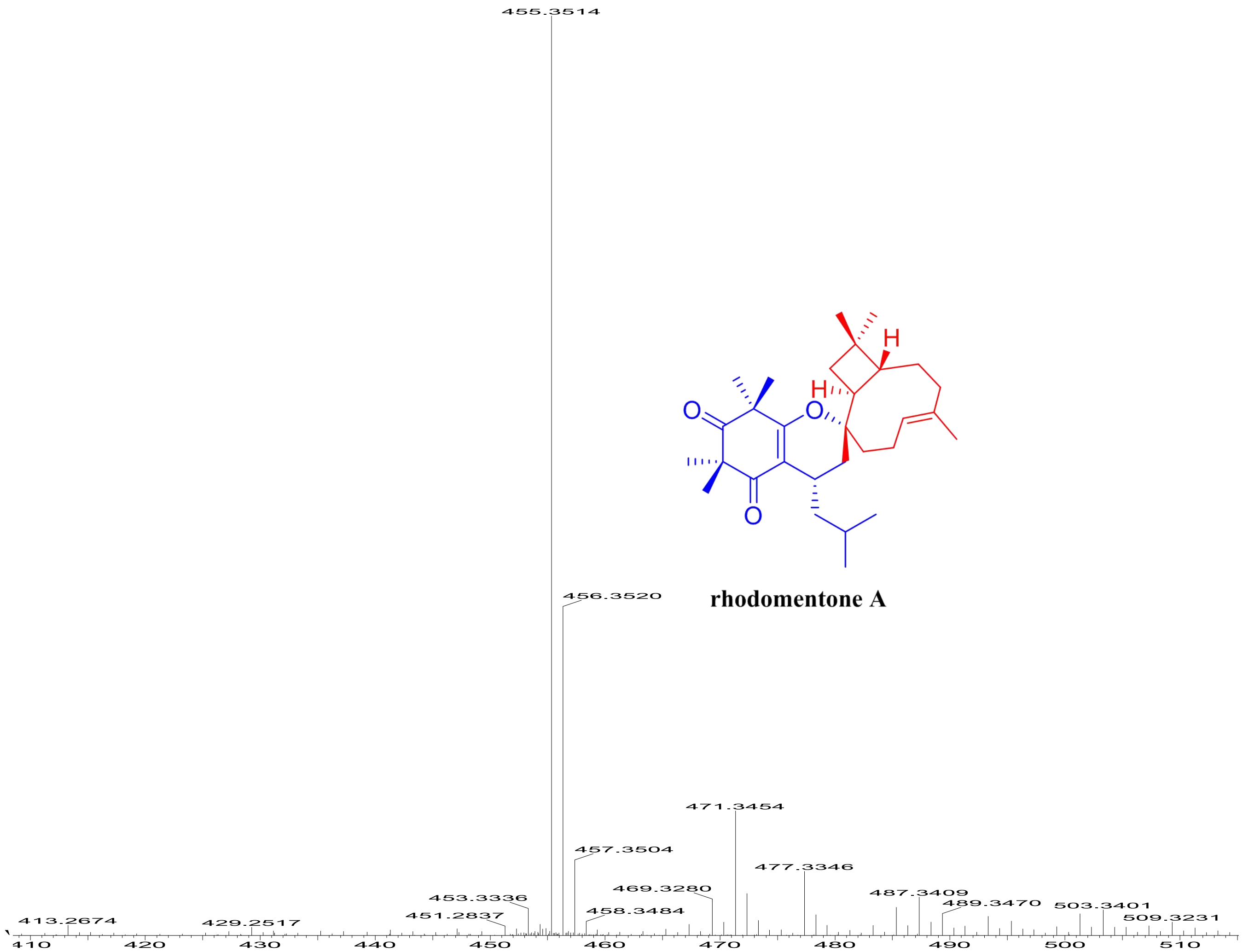

455.3514
456.3520
471.3454
457.3504
477.3346
469.3280
453.3336
487.3409
489.3470
503.3401
451.2837
458.3484
509.3231
413.2674
429.2517
410
420
430
440
450
460
470
480
490
500
510
O
O
O
H
H
rhodomentone A

Figure S15. HRESIMS spectrum of **1**.

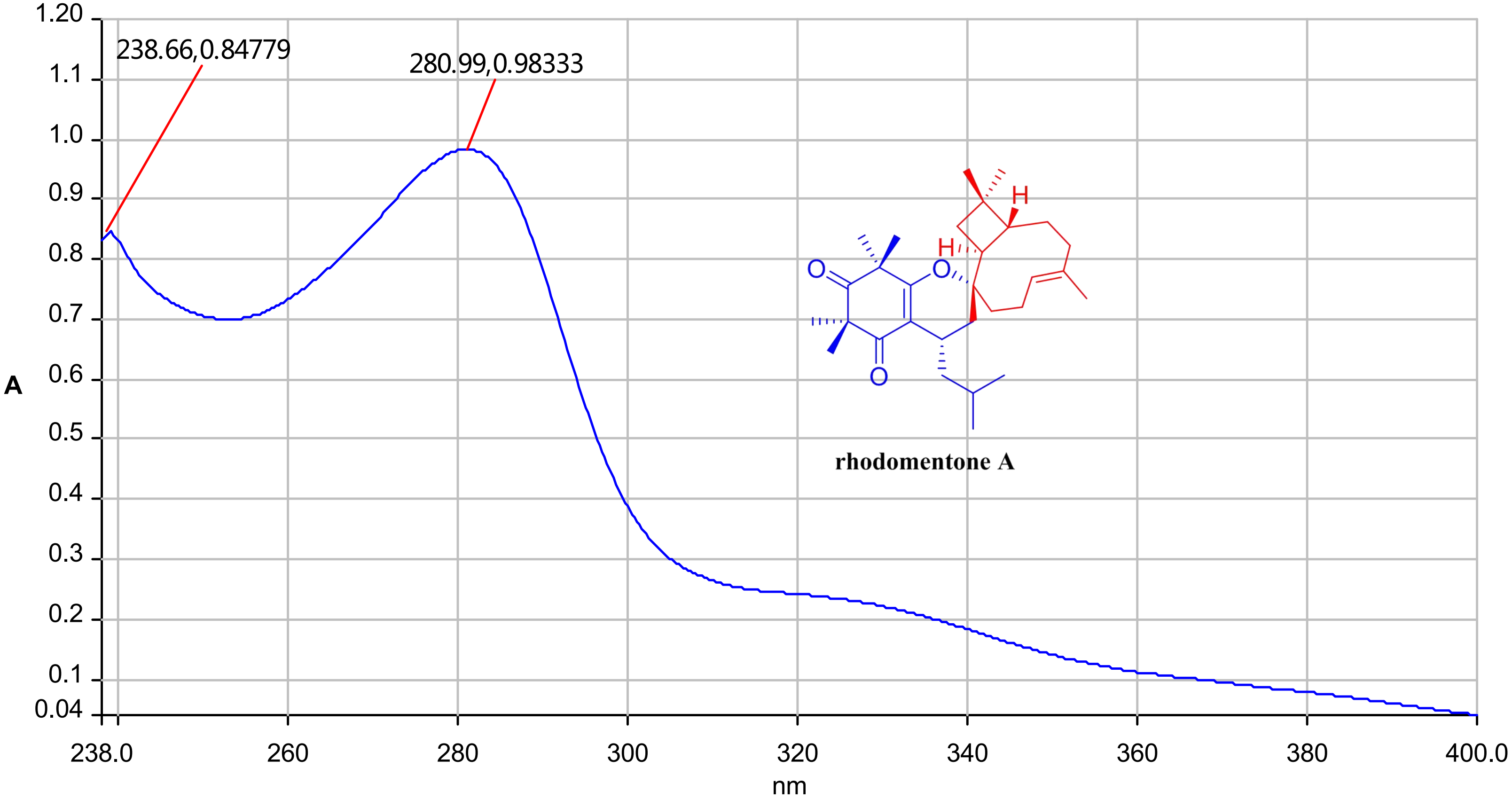


Figure S16. UV spectrum of **1**.

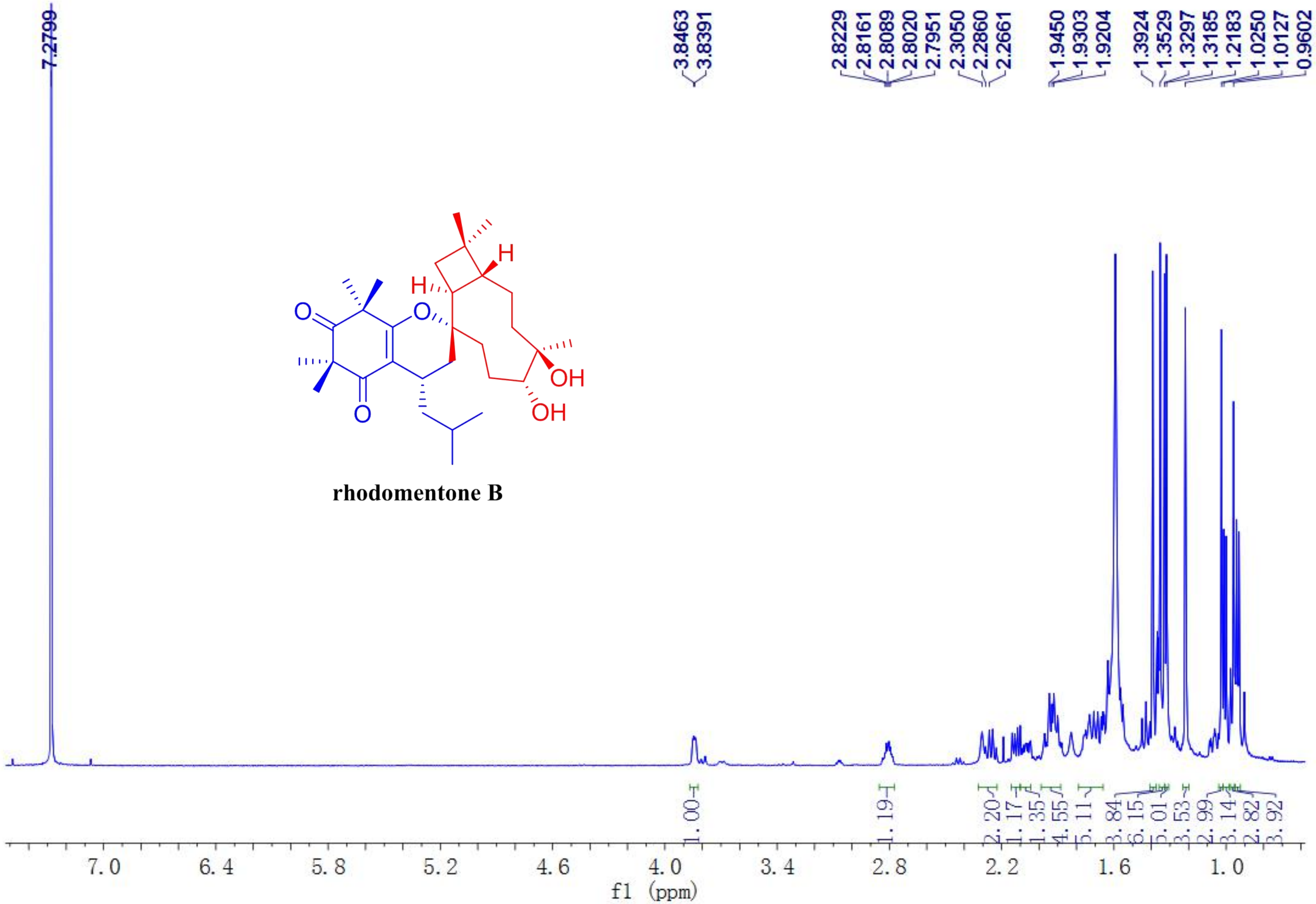


Figure S17. ¹H NMR spectrum (500 MHz, $CDCl_3$) of **2**.

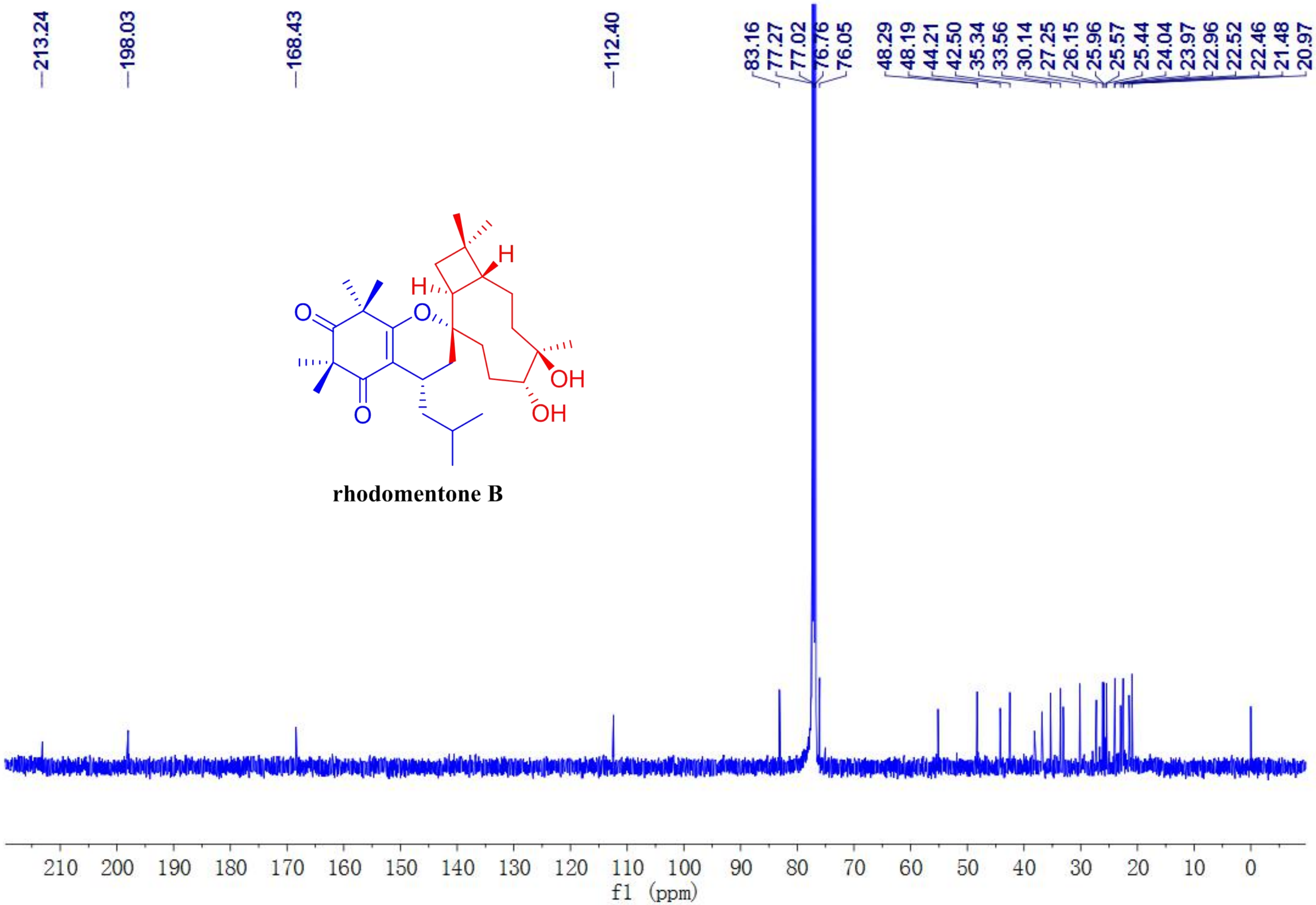


Figure S18. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2**.

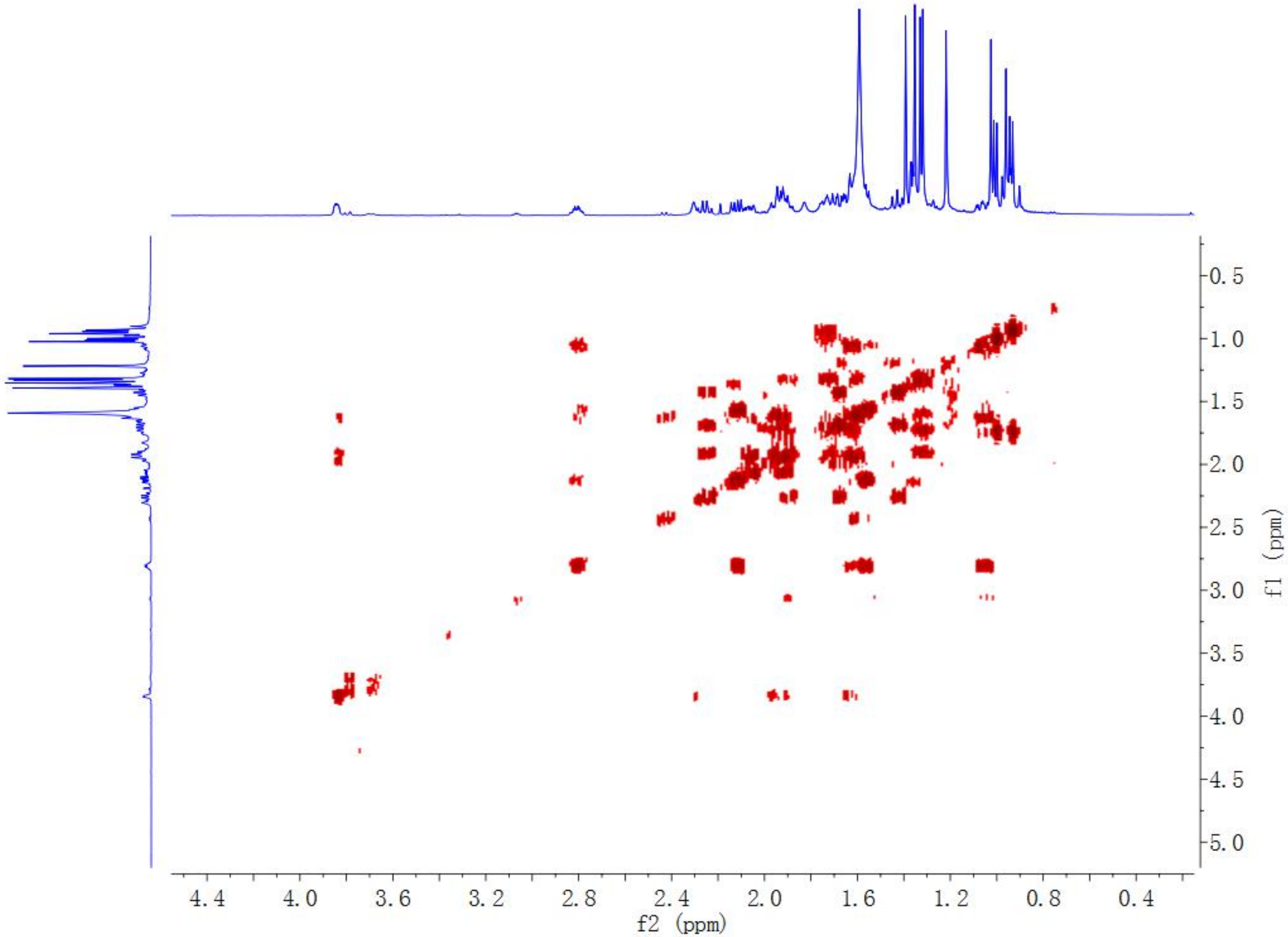


Figure S19. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **2**.

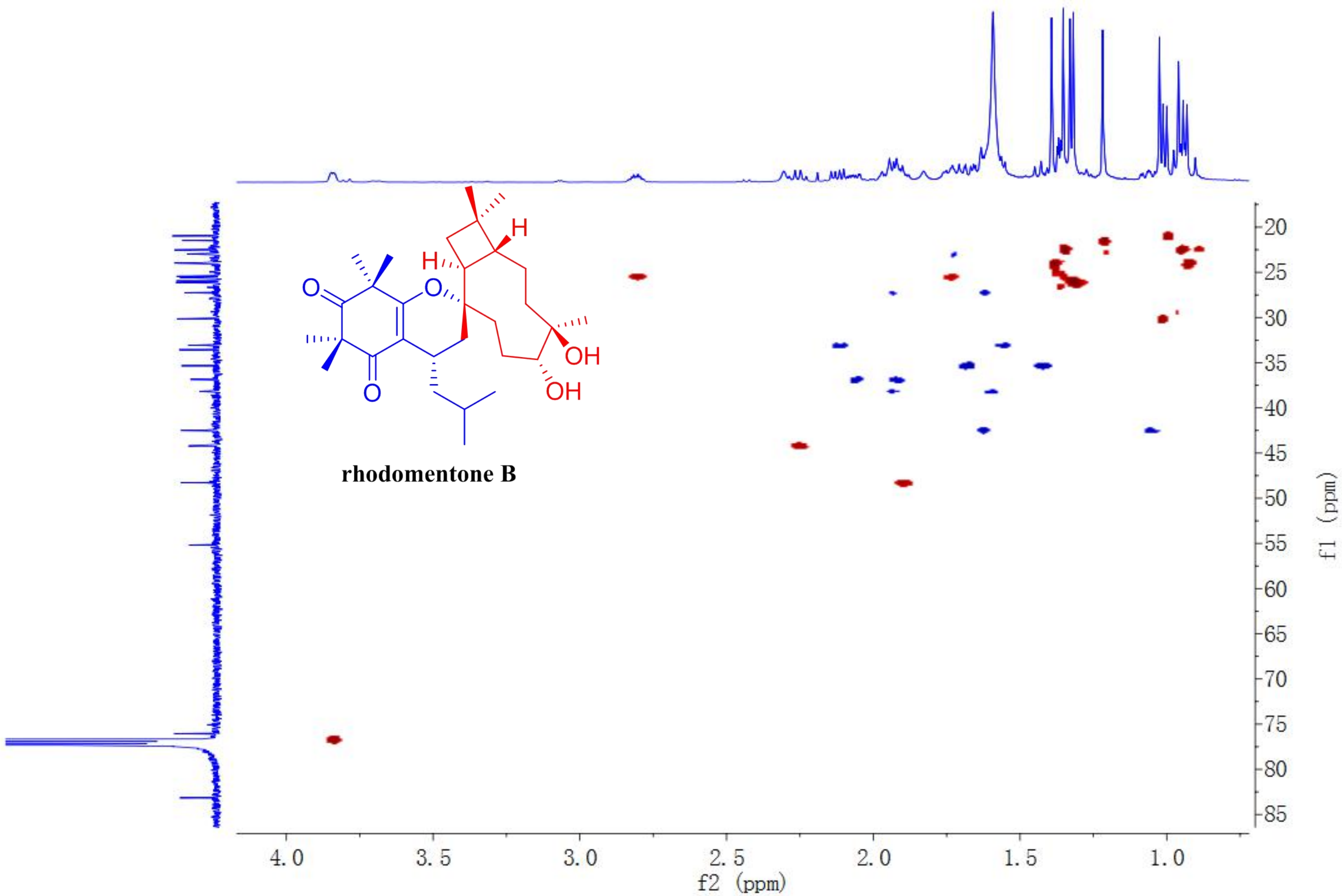


Figure S20. HSQC spectrum of **2**.

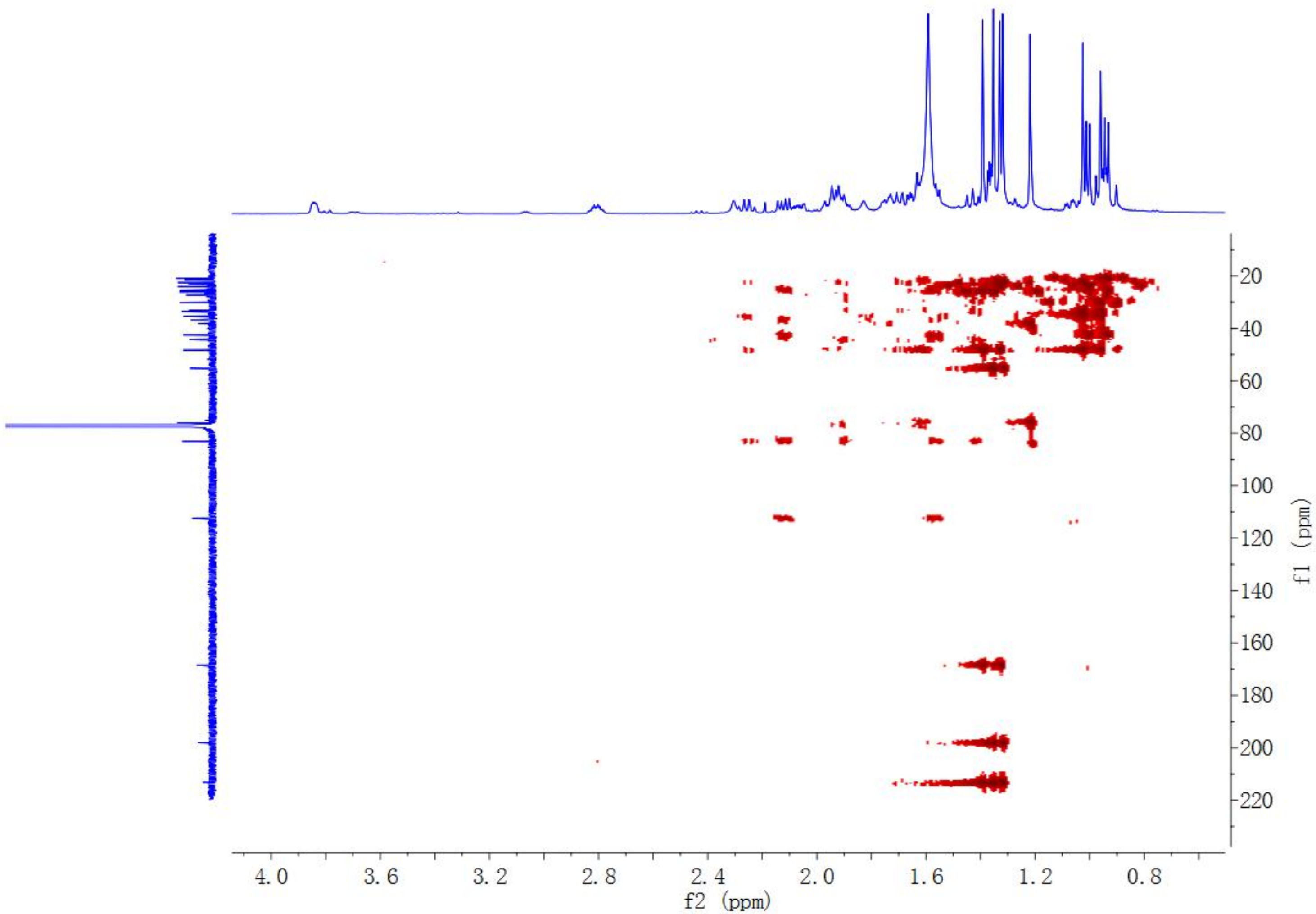


Figure S21. HMBC spectrum of **2**.

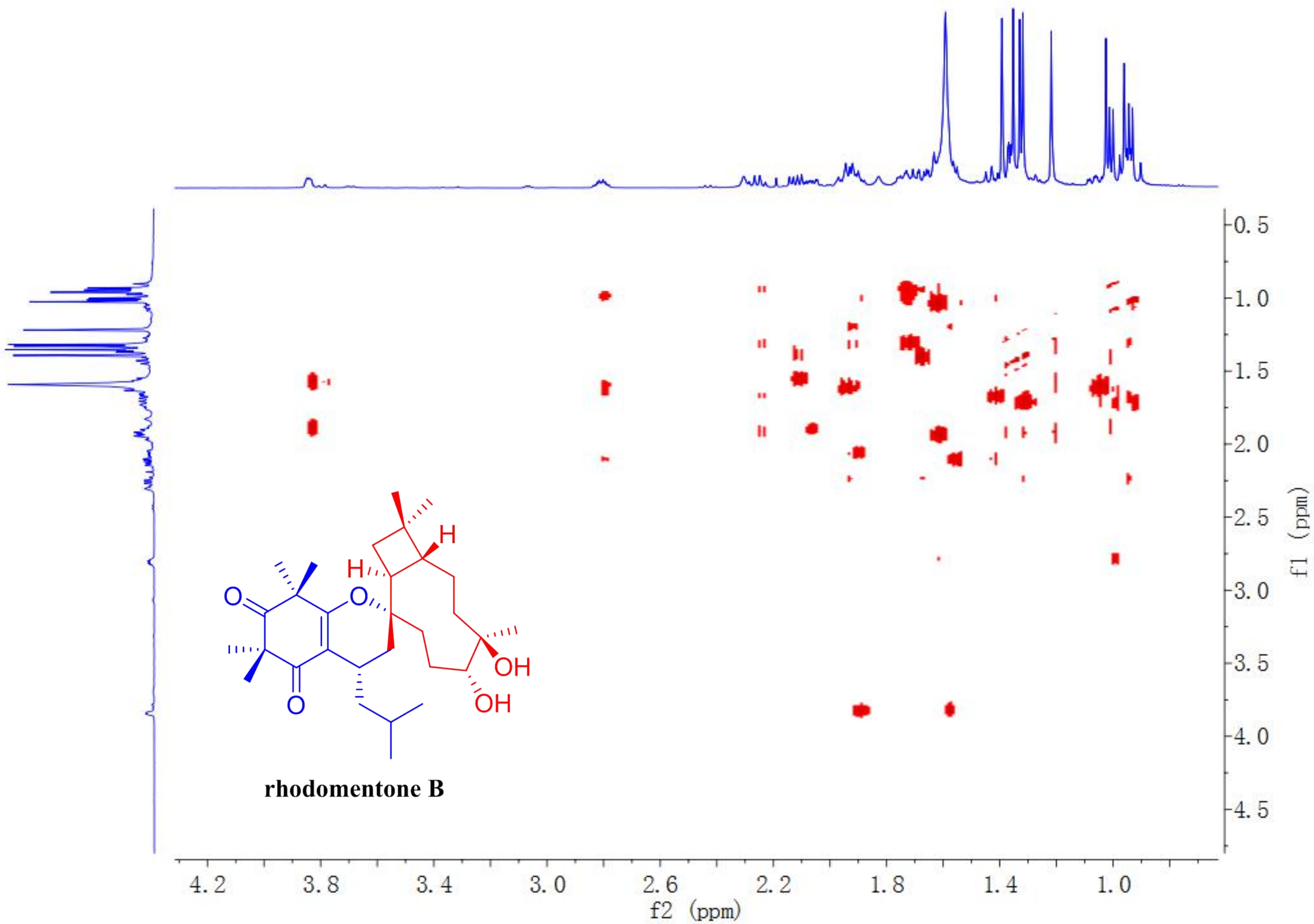
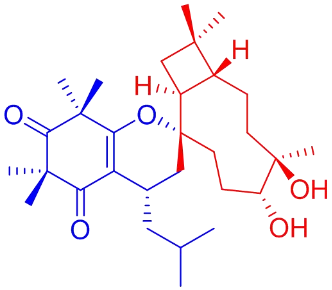


Figure S22. NOESY spectrum of **2**.



rhodomentone B

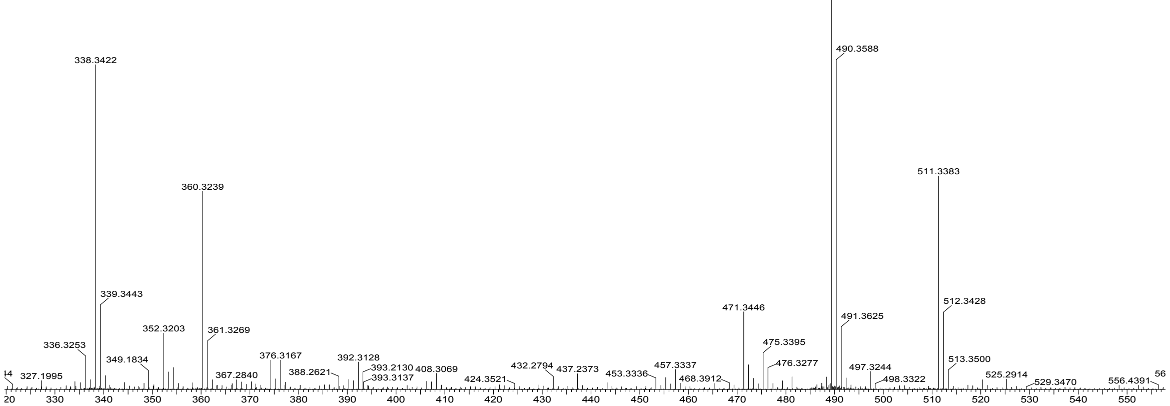


Figure S23. HRESIMS spectrum of **2**.

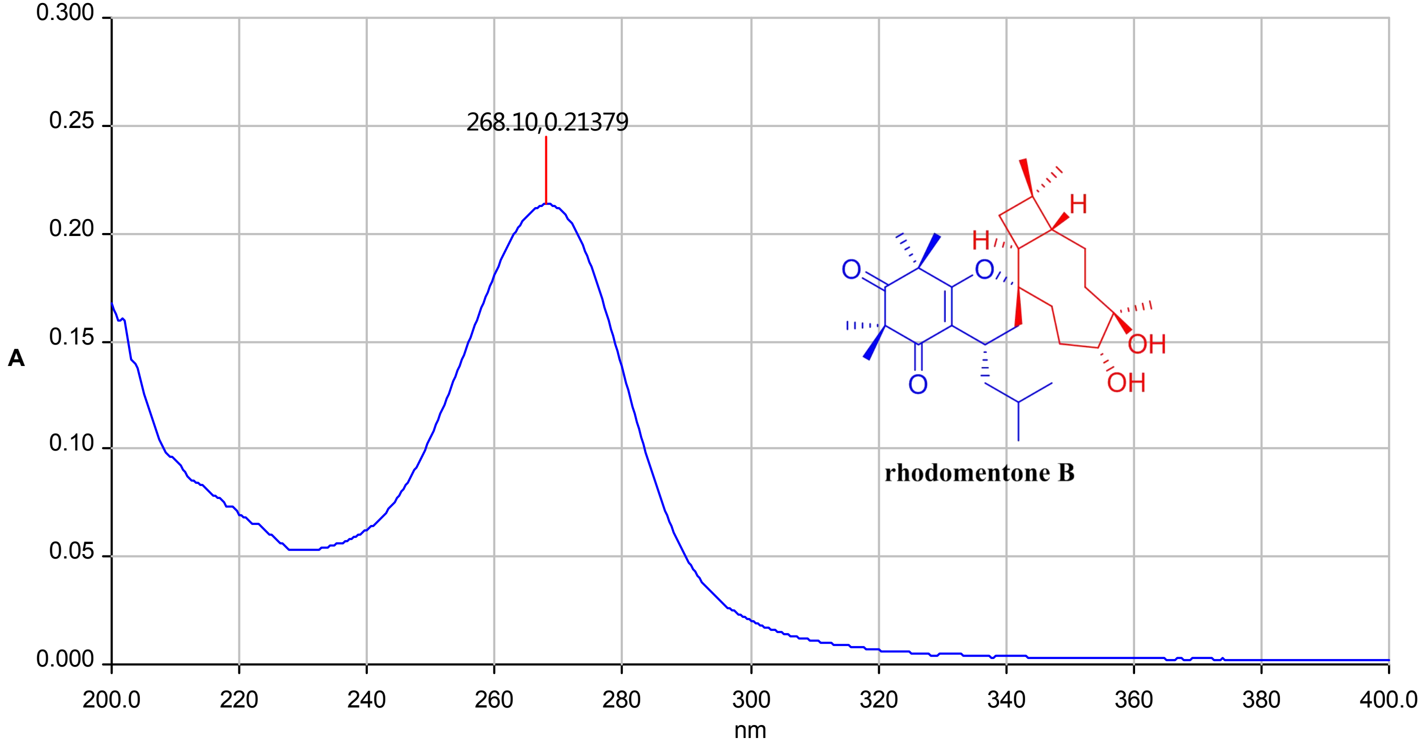


Figure S24. UV spectrum of **2**.

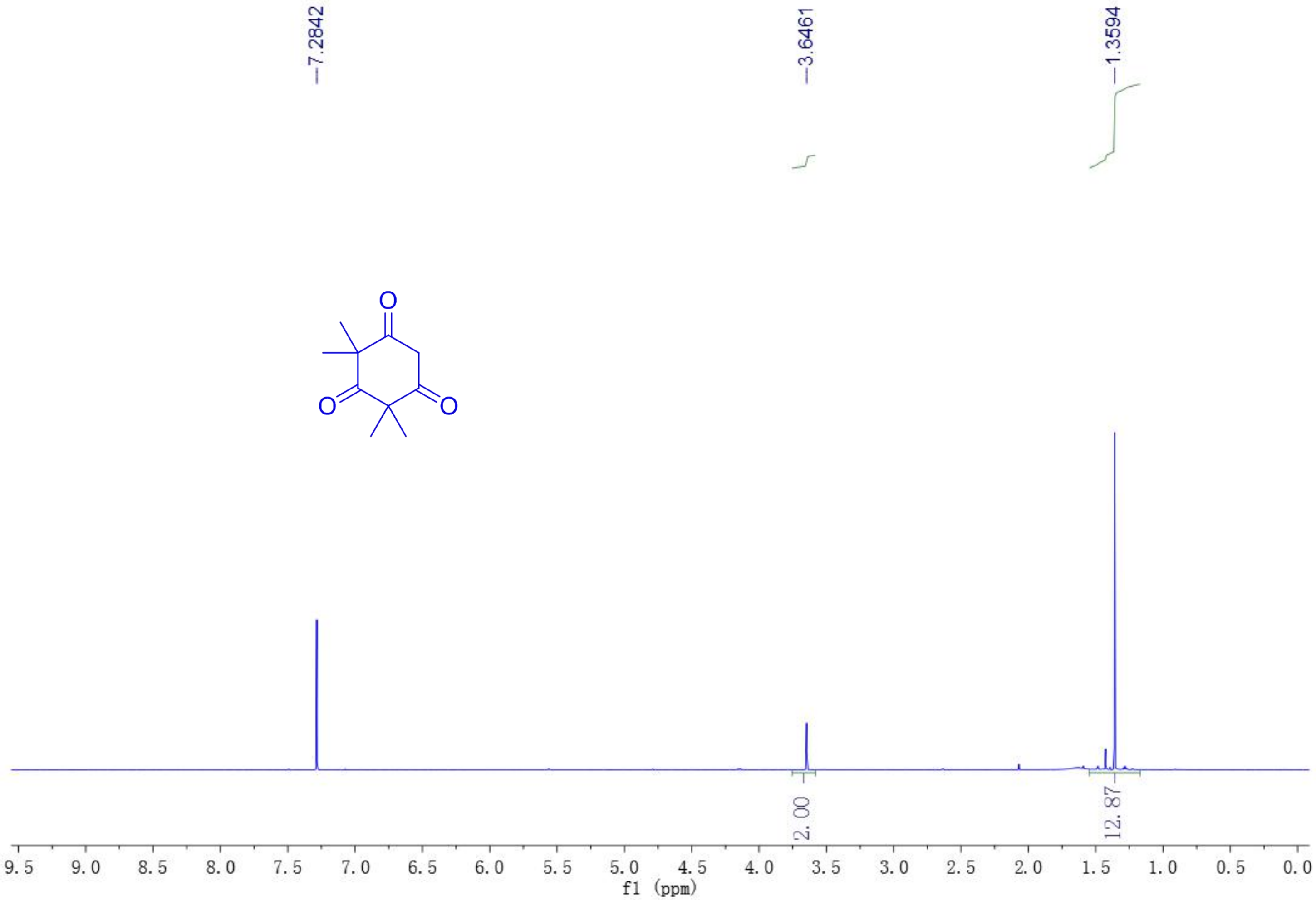


Figure S25. [1]H NMR spectrum (500 MHz, $CDCl_3$) of key intermediate **4**.

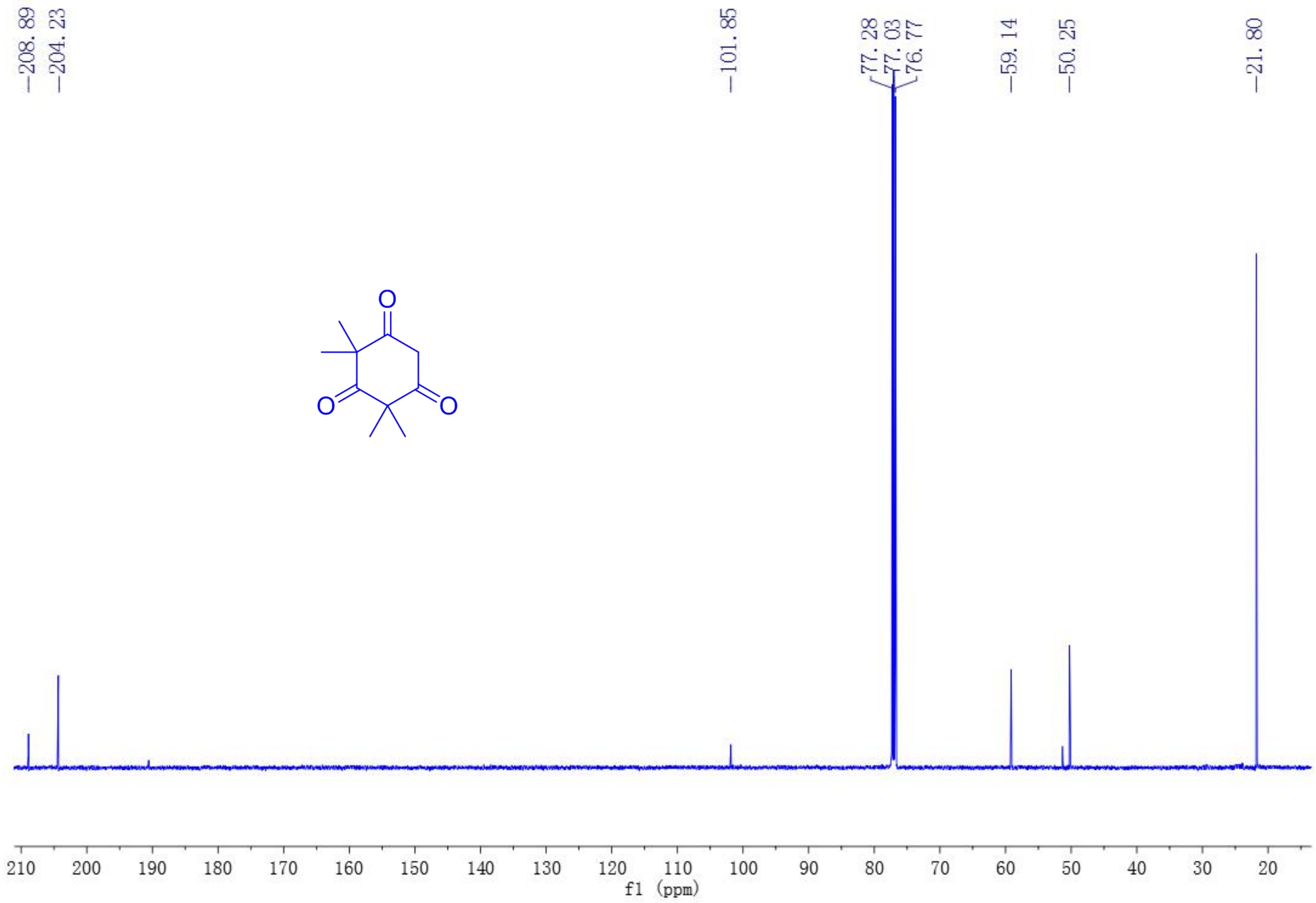


Figure S26. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of key intermediate **4**.

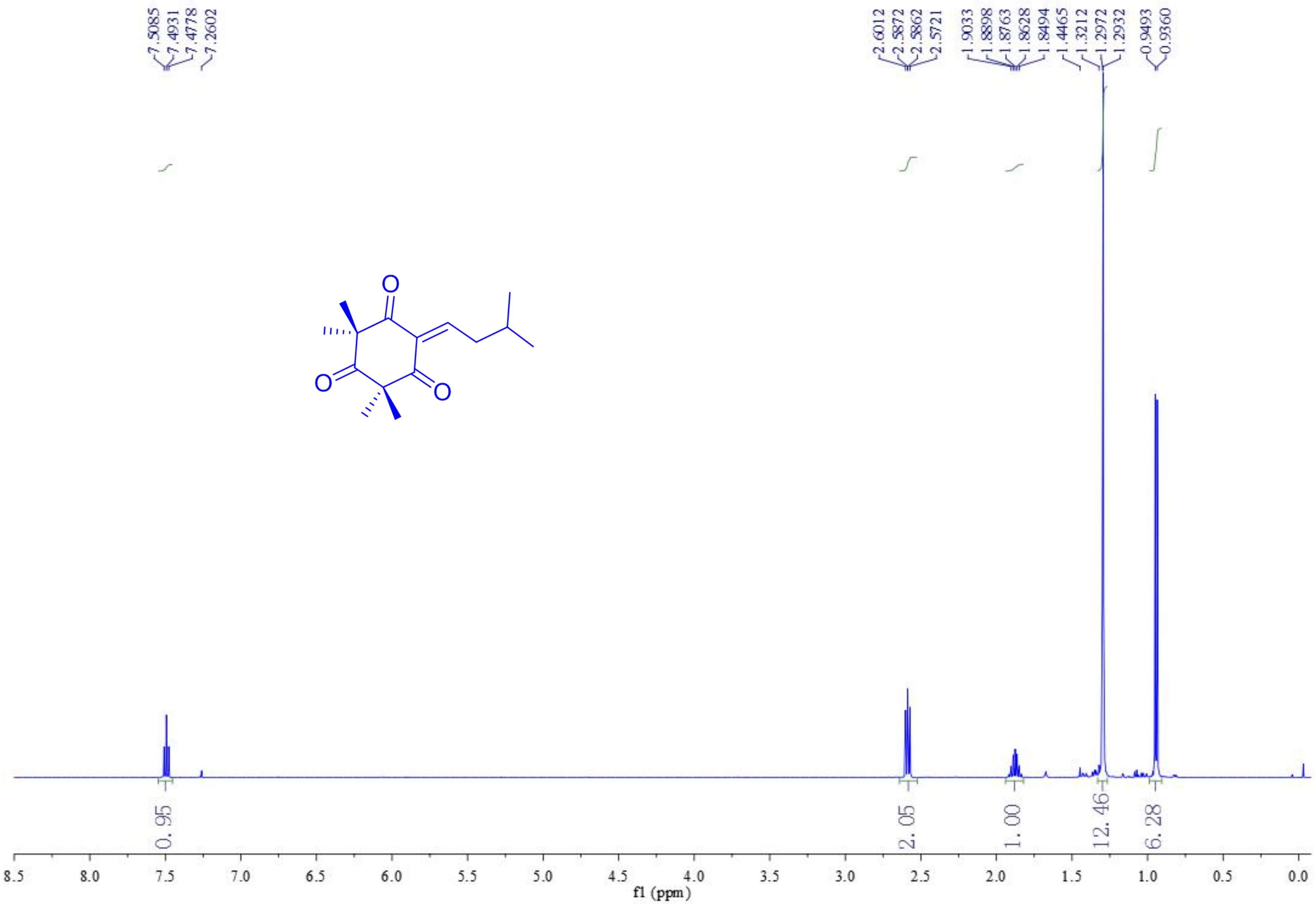


Figure S27. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of key intermediate **i**.

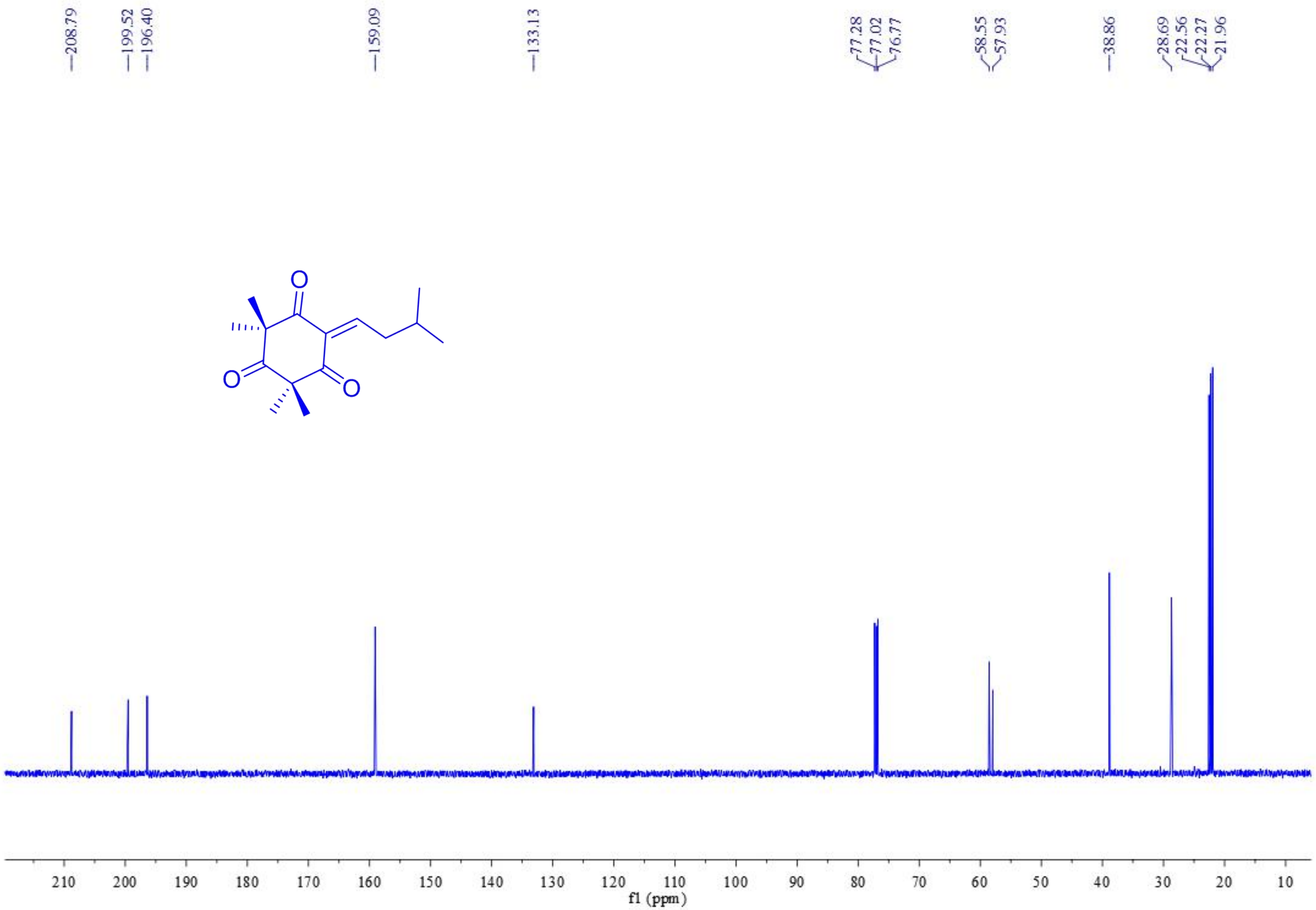


Figure S28. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of key intermediate **i**.

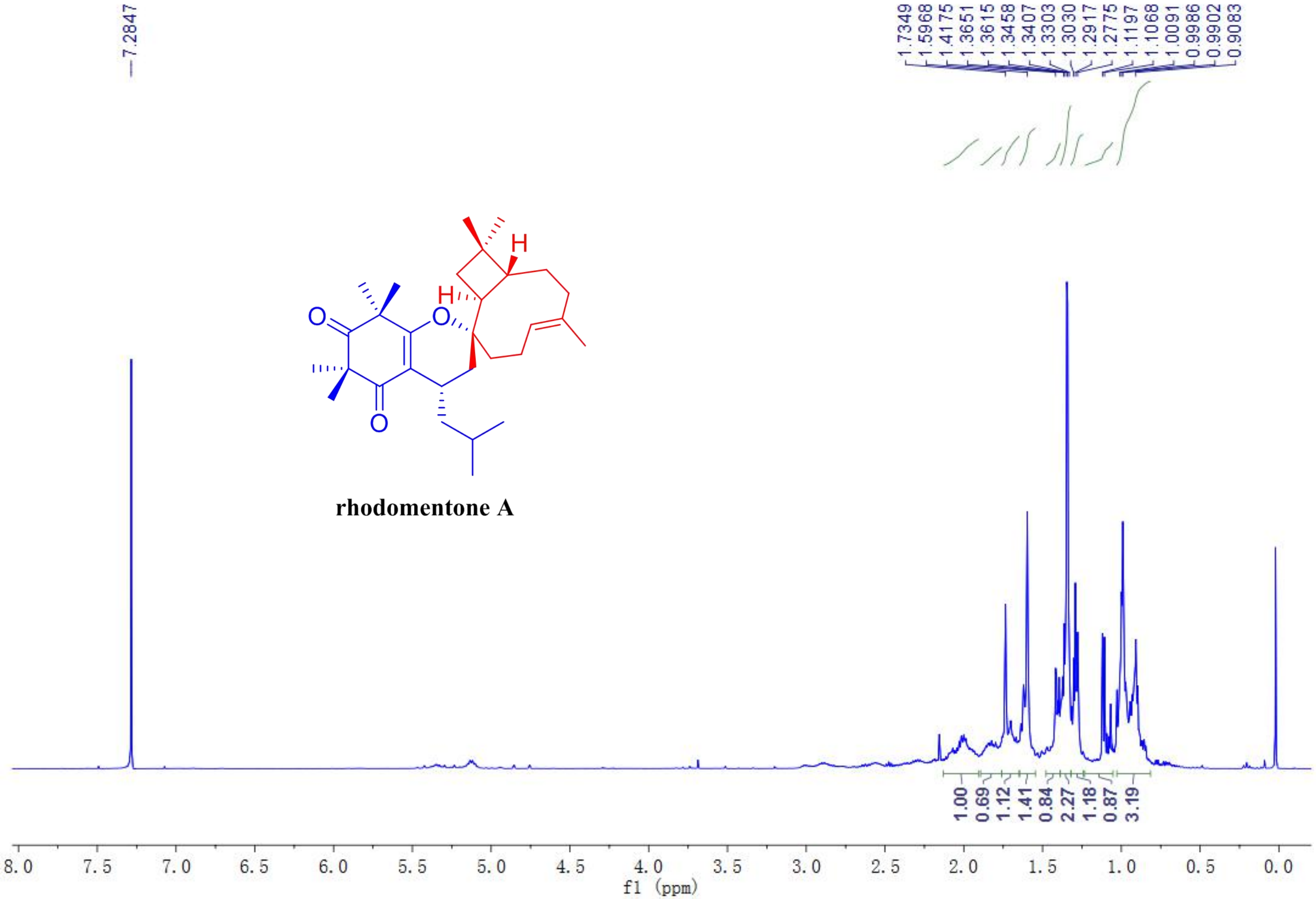


Figure S29. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of synthetic compound **1.**

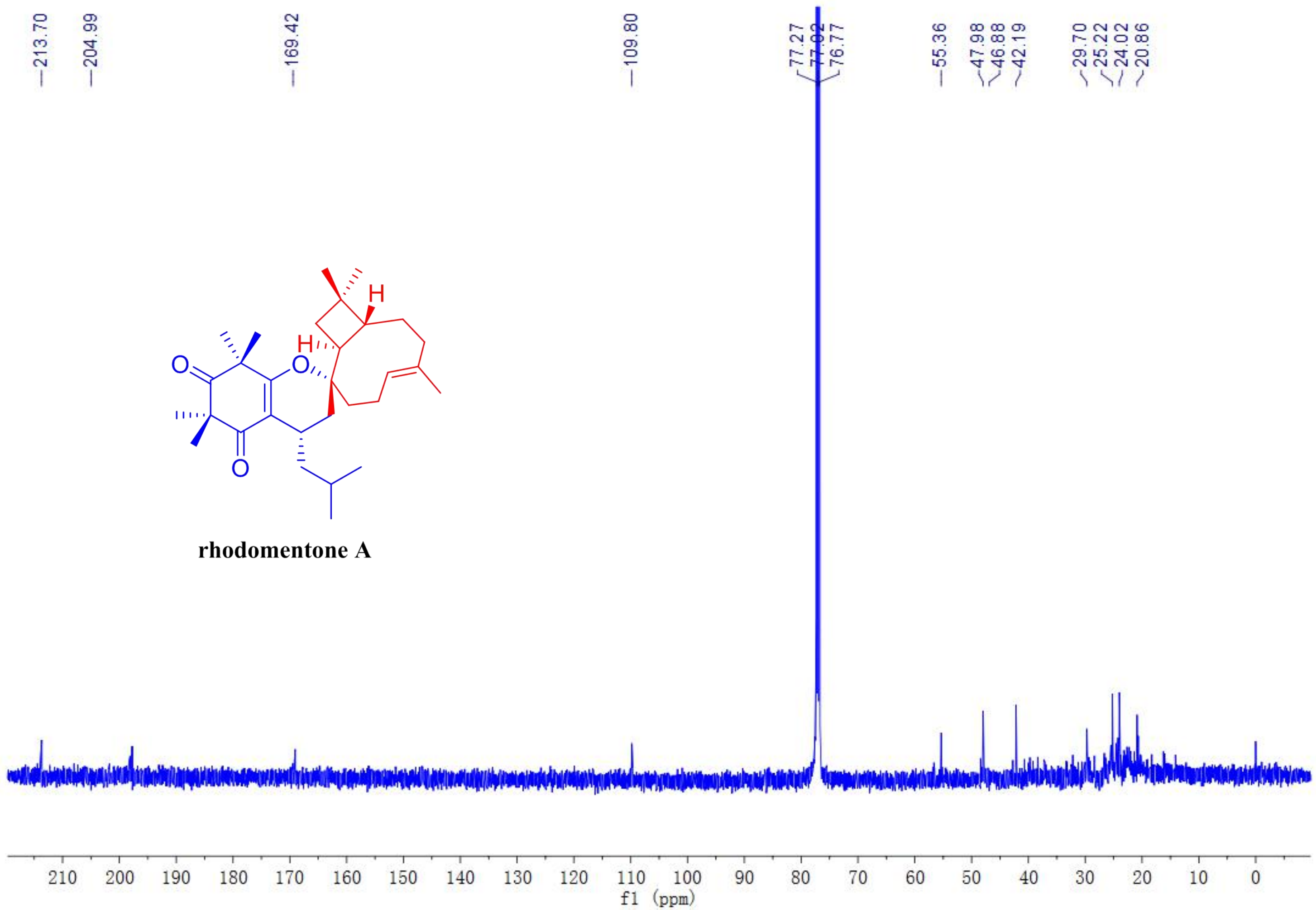


Figure S30. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of synthetic compound **1**.

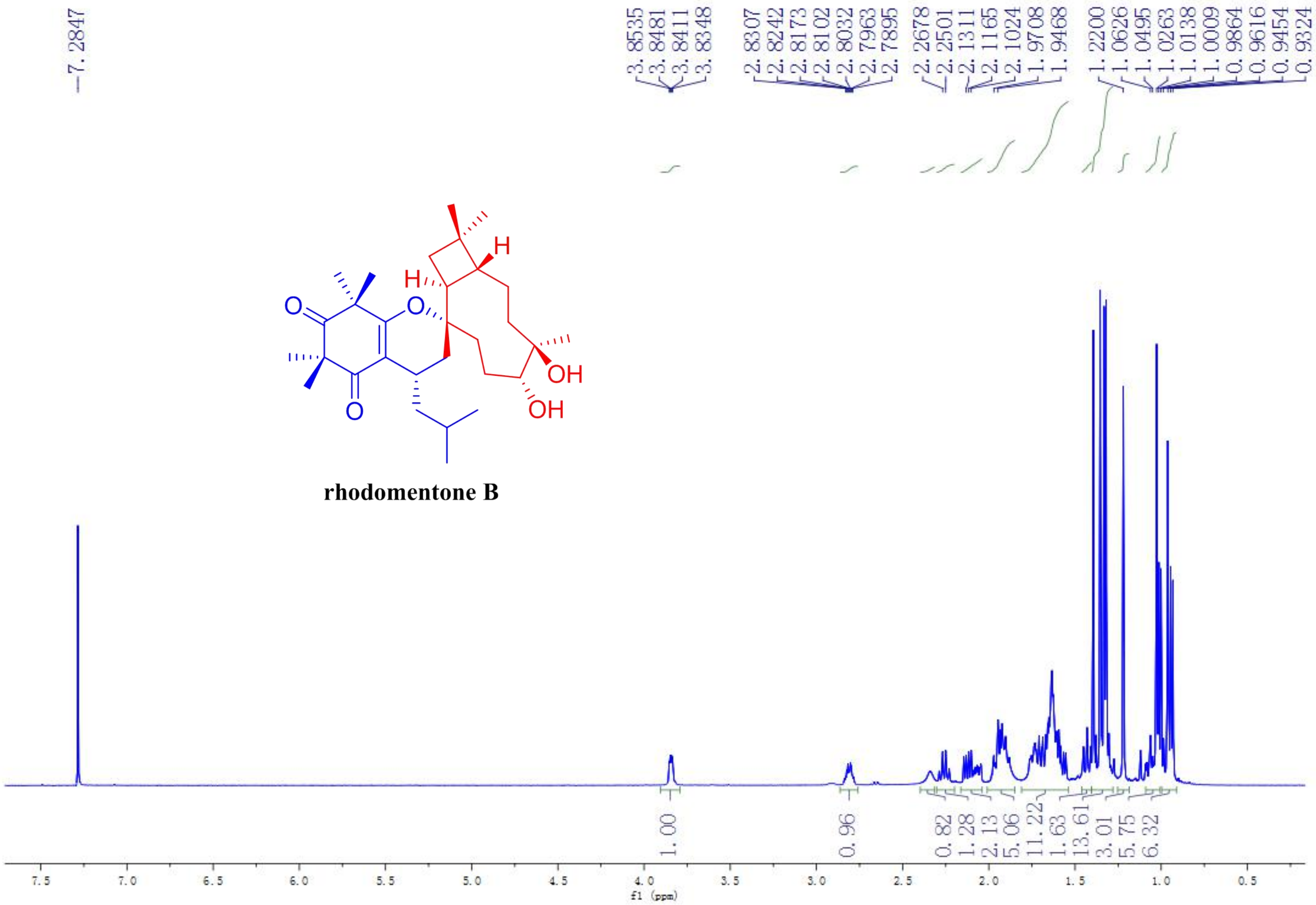


Figure S31. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of synthetic compound **2**.

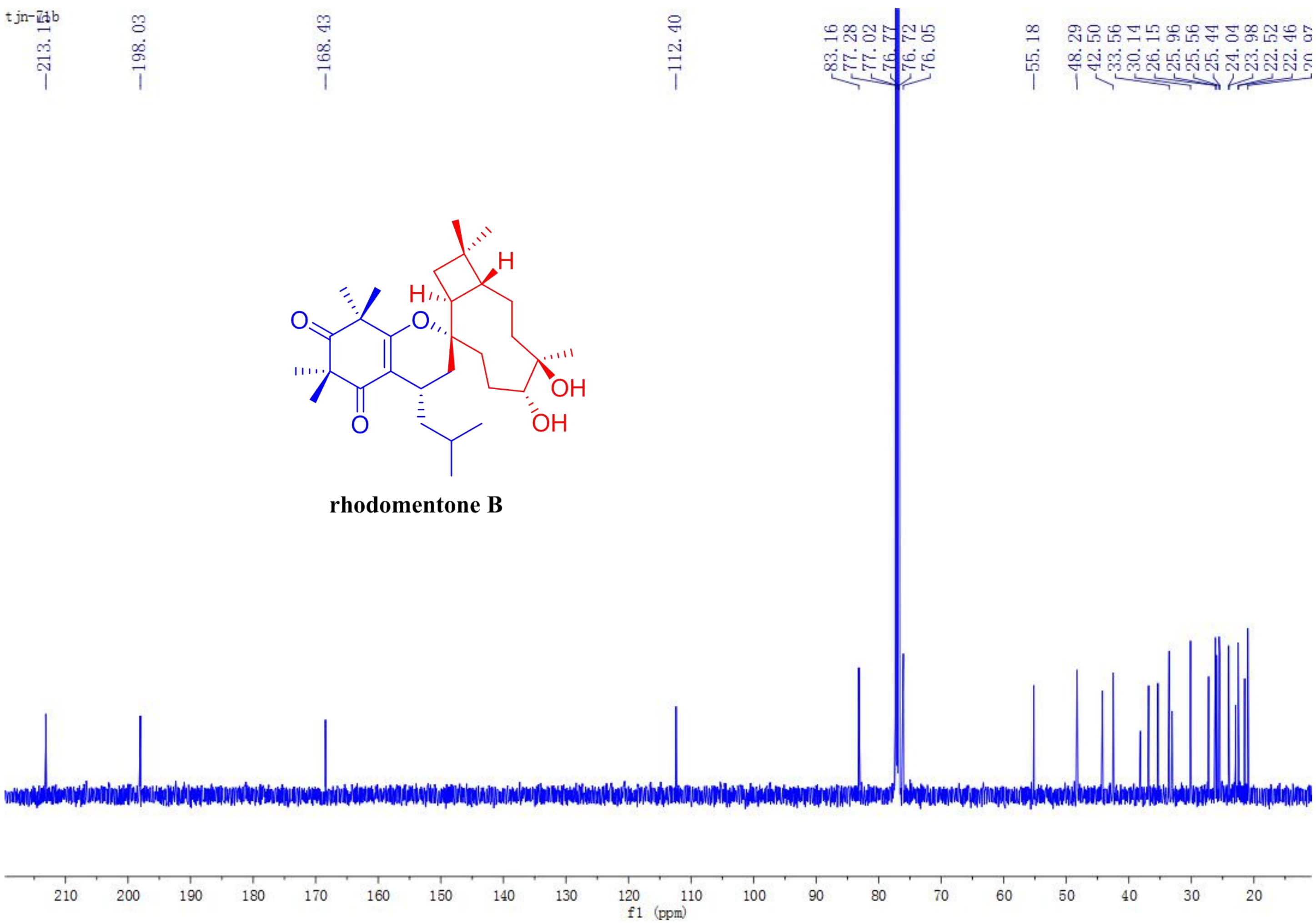


Figure S32. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of synthetic compound **2**.