

## Supplementary Information

### Symmetric Cytotoxicity Trimeric and Dimeric Indole

#### Alkaloids from *Bousigonia angustifolia*

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## Spectroscopic data

### UPLC-MS analysis of the crude alkaloid extract and polymeric alkaloids

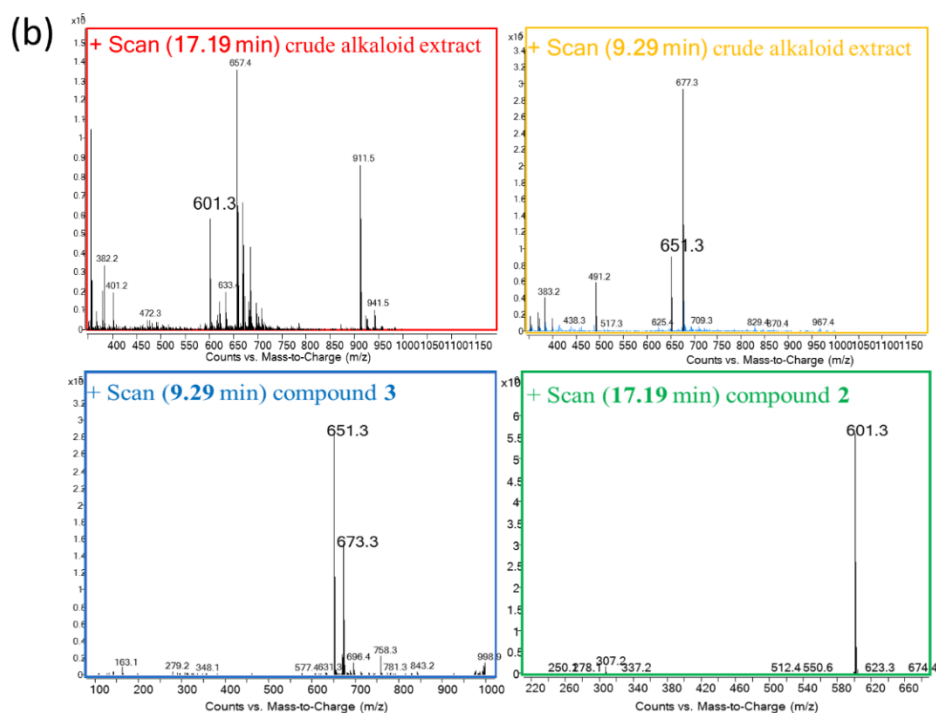
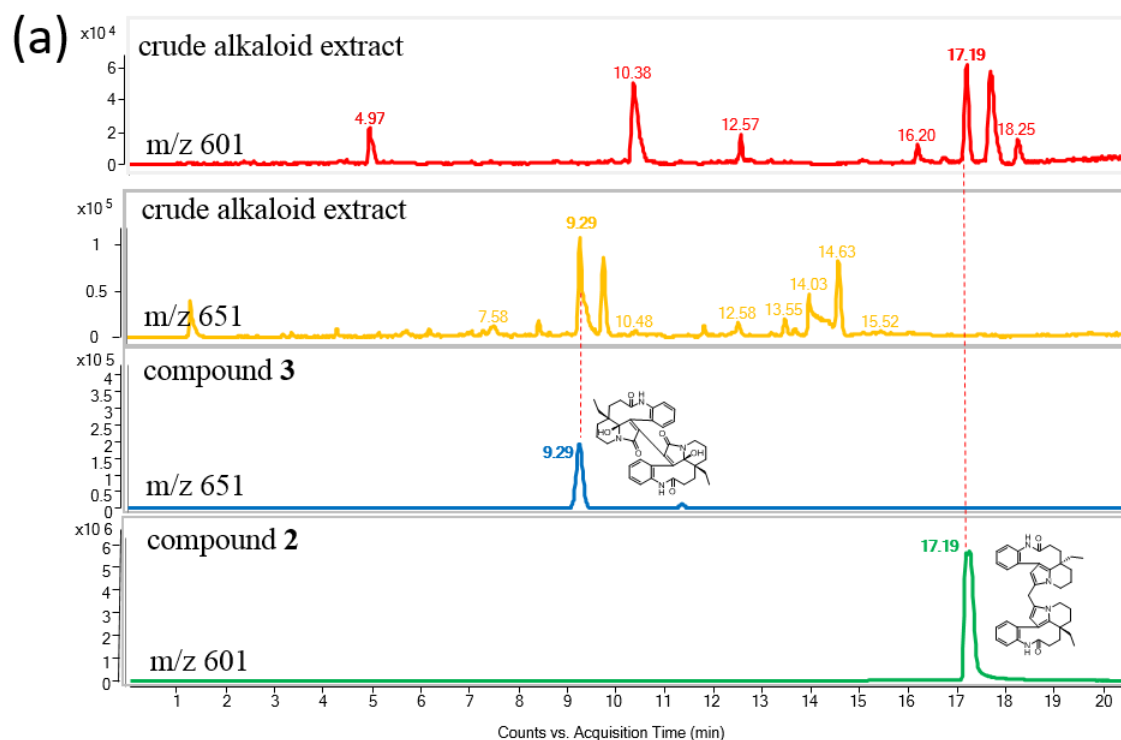


Figure S1A. (a) Positive-ion mode LC-MS analysis of the crude alkaloid extract and polymeric alkaloids (extracted ion chromatogram at  $m/z$  601 and 651 respectively) (b) Mass spectra of peaks at 9.29 and 17.19 min for crude alkaloid extract and compound 2 and 3 respectively. (Conditions: YMC-pack ODS-A C18 4.6×150mm, flow rate 1 mL/min, a linear gradient of 10%-100% CH<sub>3</sub>CN containing 0.01% NH<sub>4</sub>OH over 20 min, then eluting with 100% CH<sub>3</sub>CN for additional 10 min)

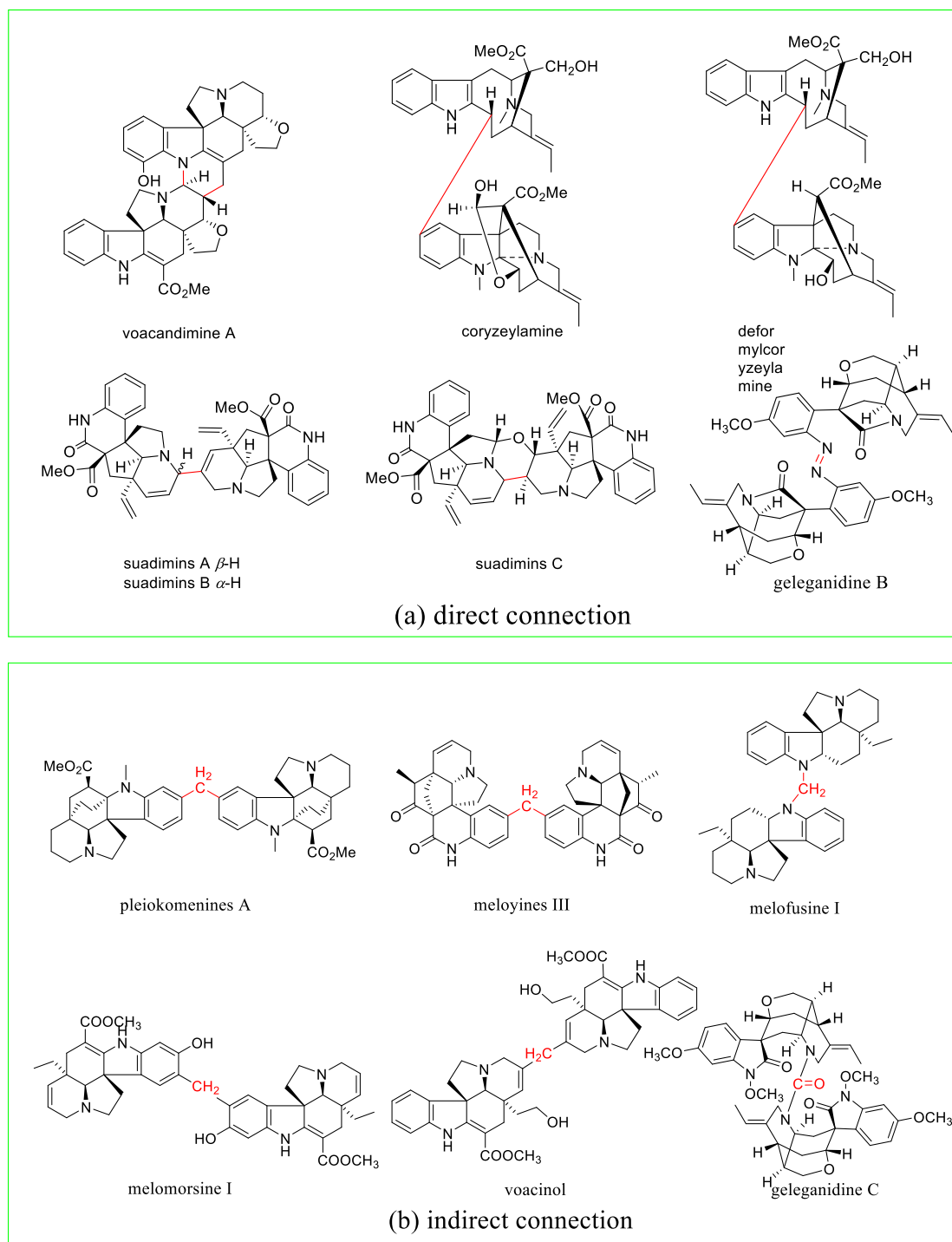
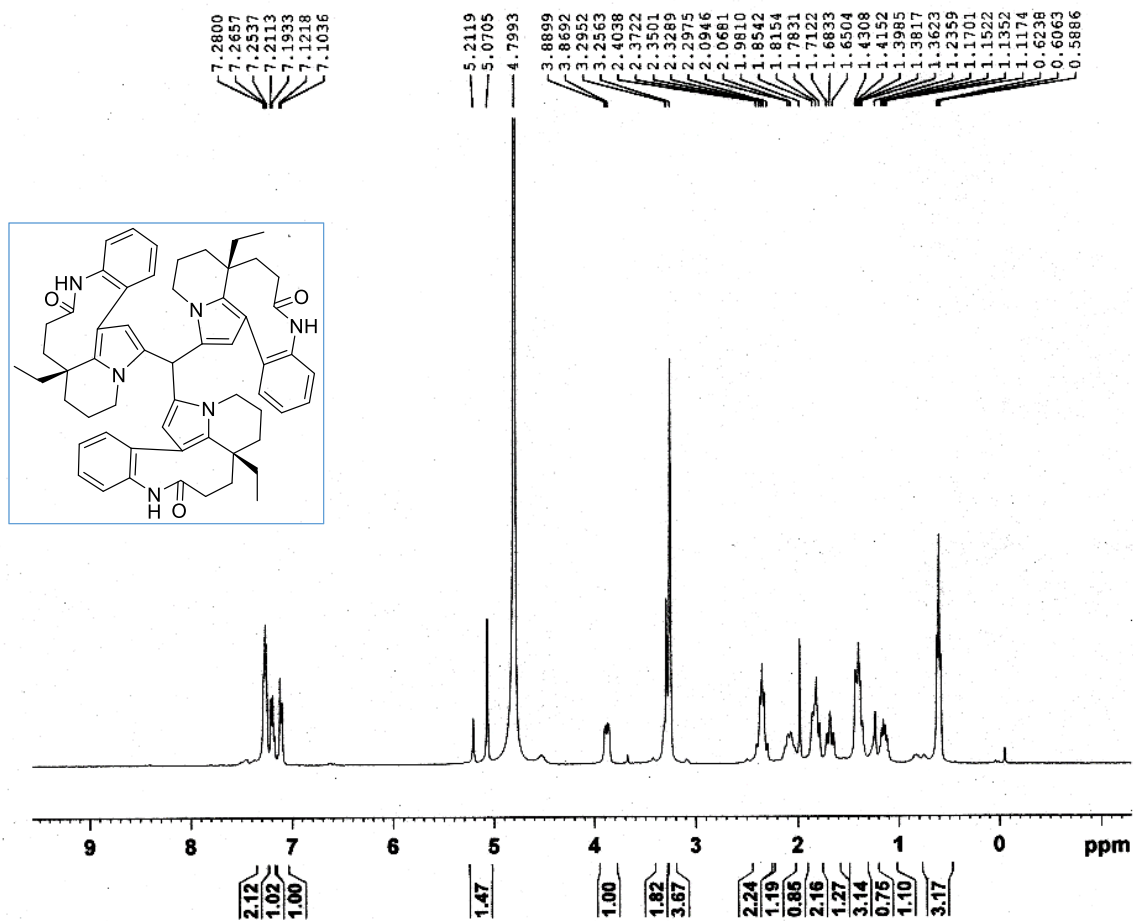


Figure S1B. Two forms of dimeric MIAs: direct connection (a) and indirect connection (b).

Figure S2. <sup>1</sup>H NMR spectrum of **1** in CD<sub>3</sub>OD

wbmp-56d



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Figure S3 <sup>13</sup>C NMR spectrum of 1 in CD<sub>3</sub>OD

wbmp56d

c13 and dept

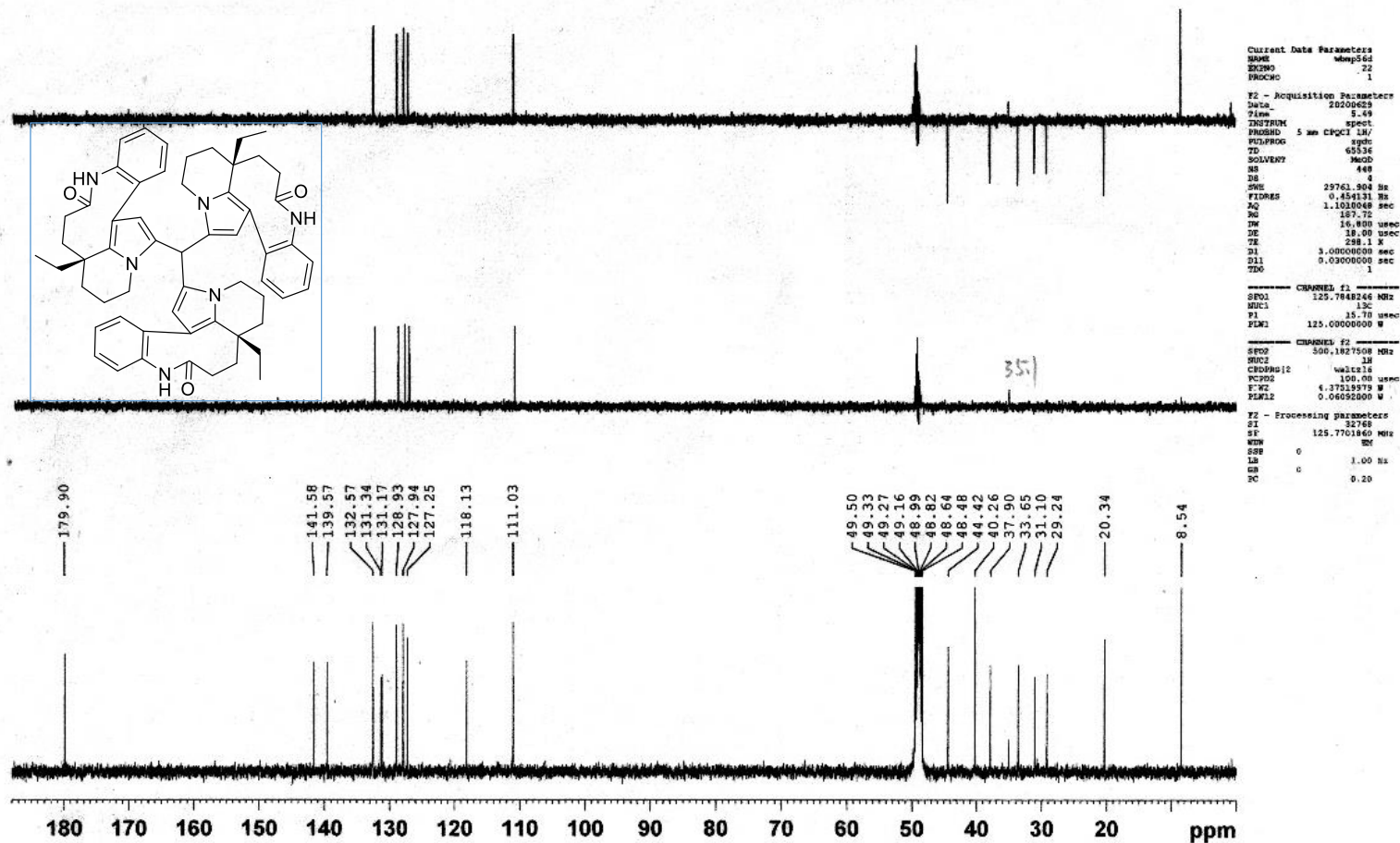


Figure S4 HSQC spectrum of **1** in CD<sub>3</sub>OD

wbmp56d hsqc

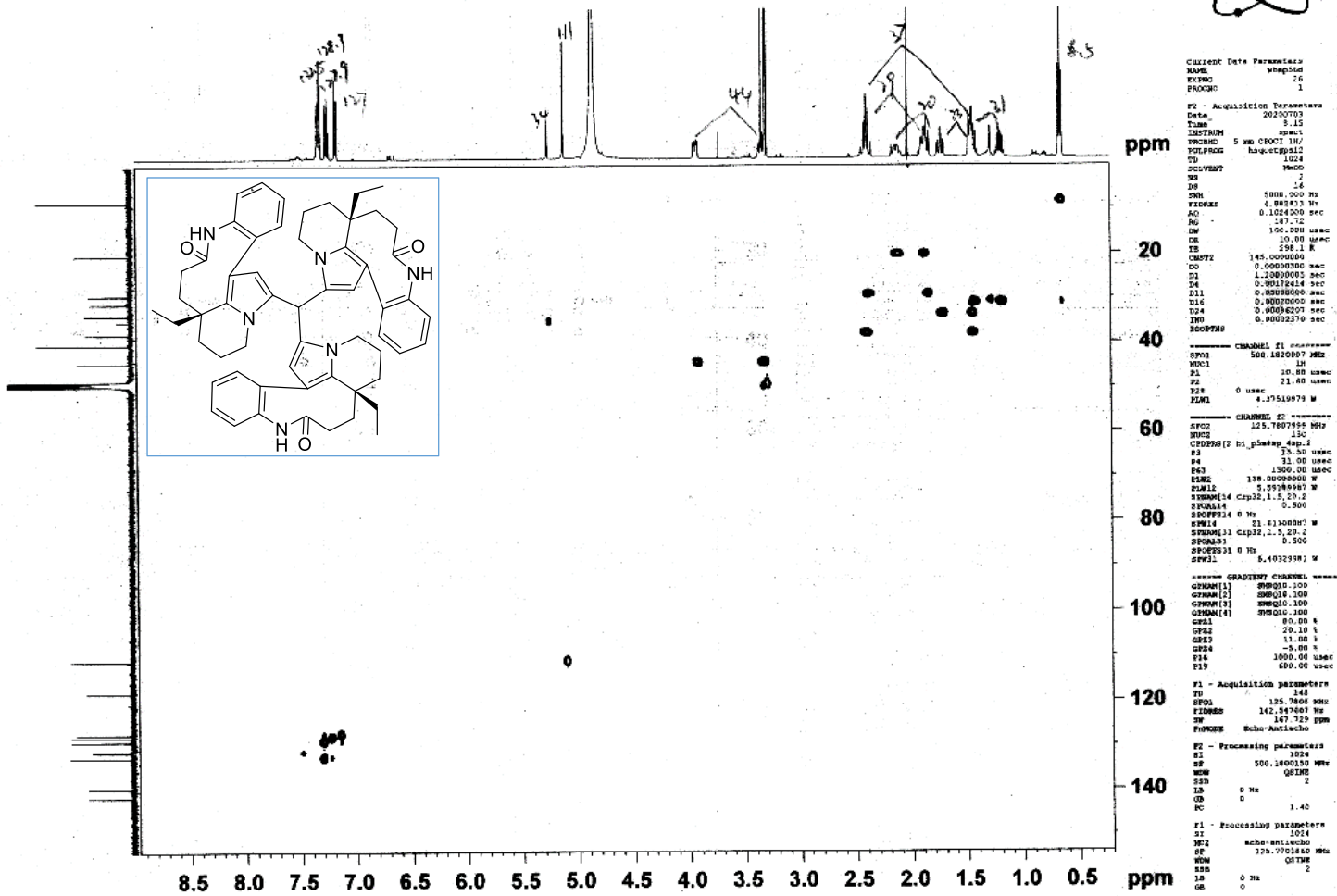




Figure S5 HMBC spectrum of 1 in CD<sub>3</sub>OD

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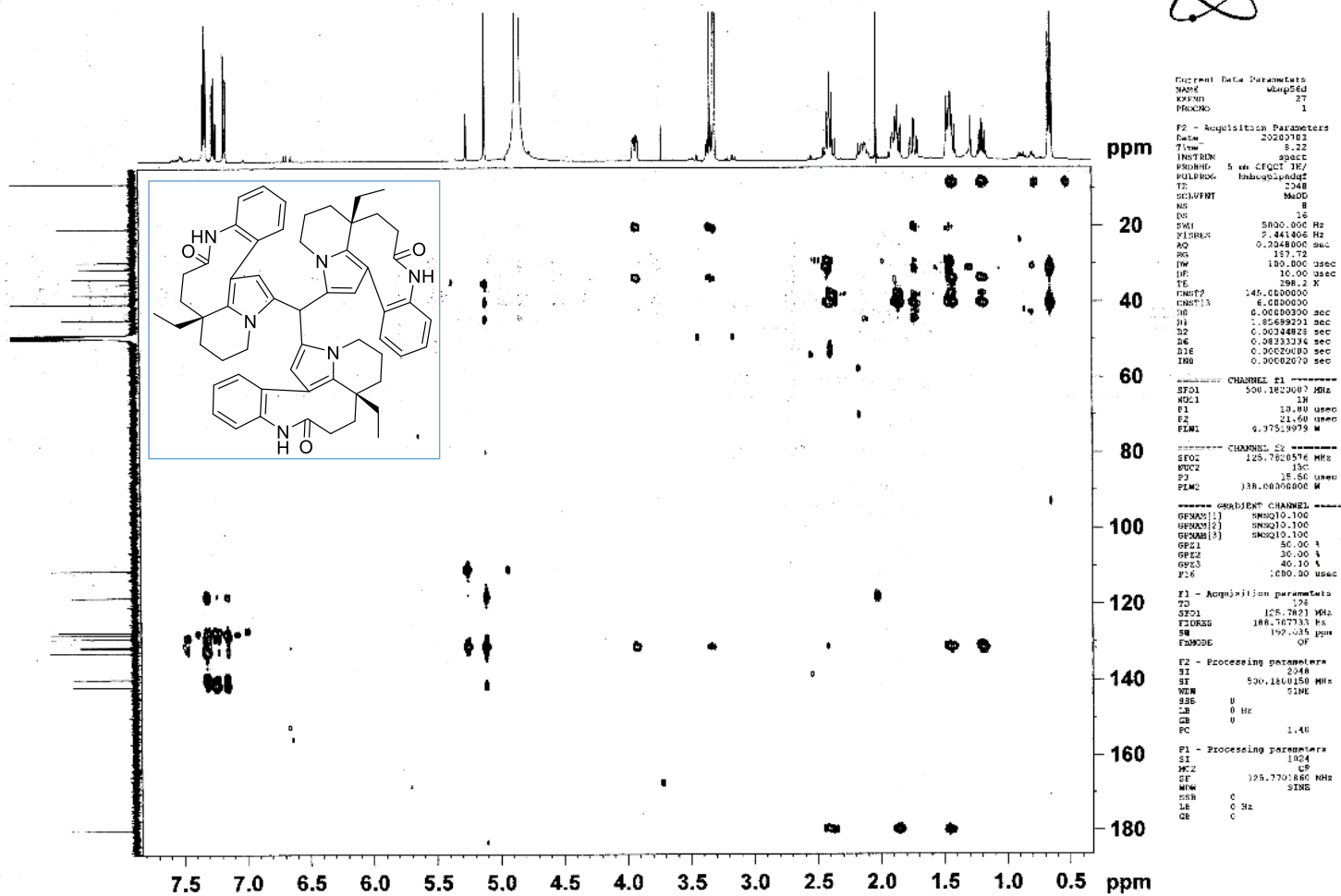


Figure S6 COSY spectrum of **1** in CD<sub>3</sub>OD

wbmp56d cosy

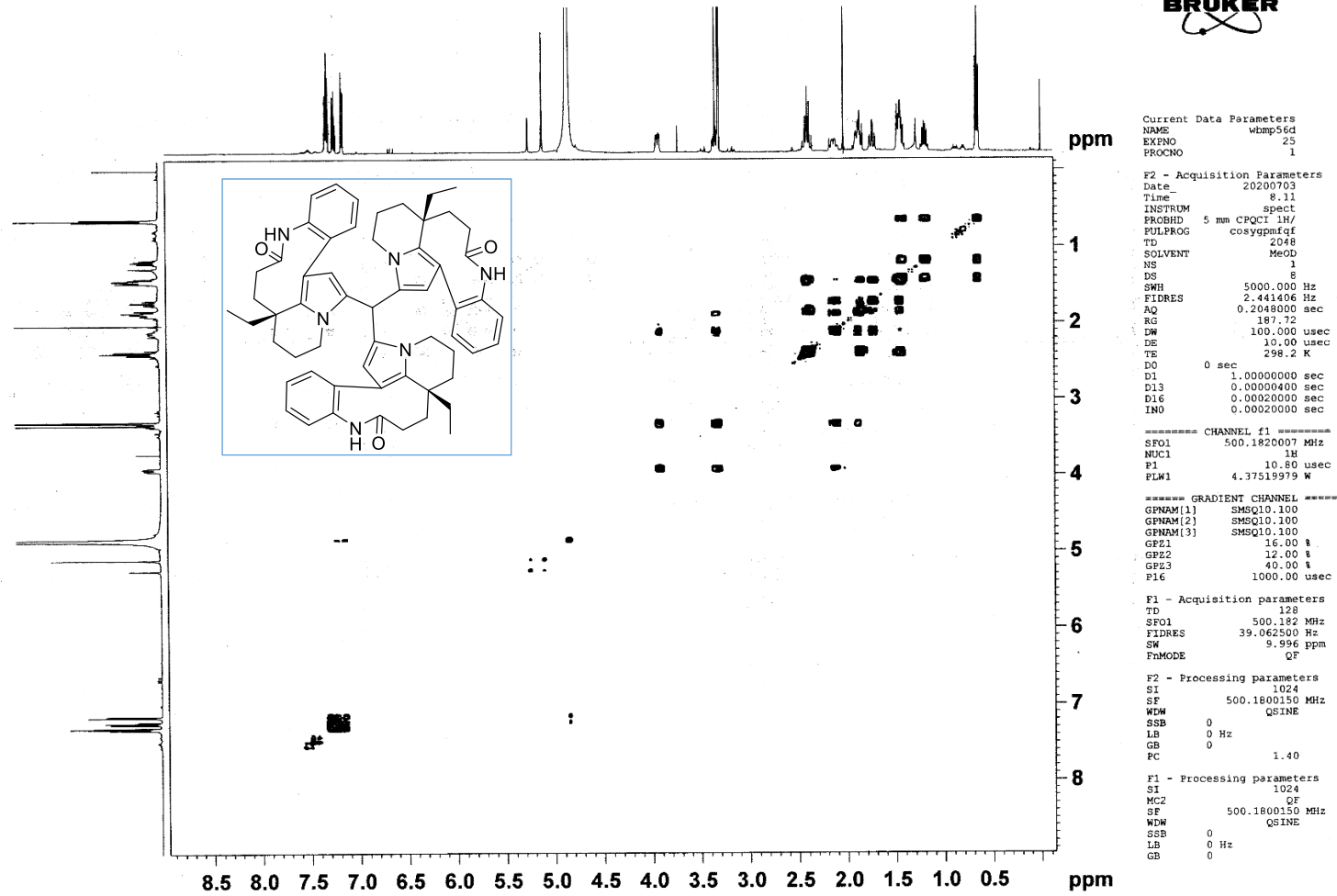
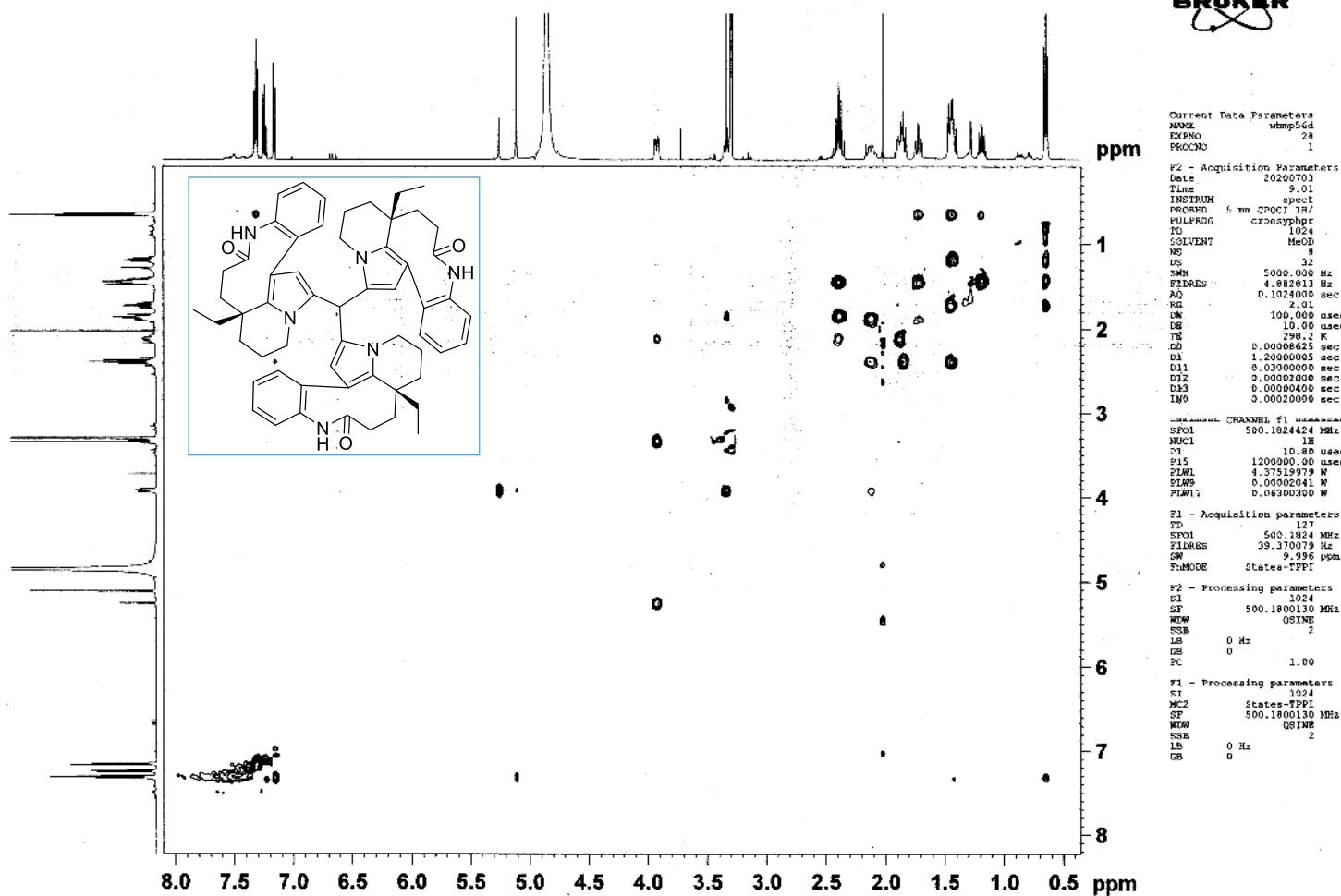


Figure S7 ROESY spectrum of 1 in CD<sub>3</sub>OD

wbmp56d roesy



# Figure S8 HRMS spectrum of 1

Formula Predictor Report - wbmp-56d.lcd

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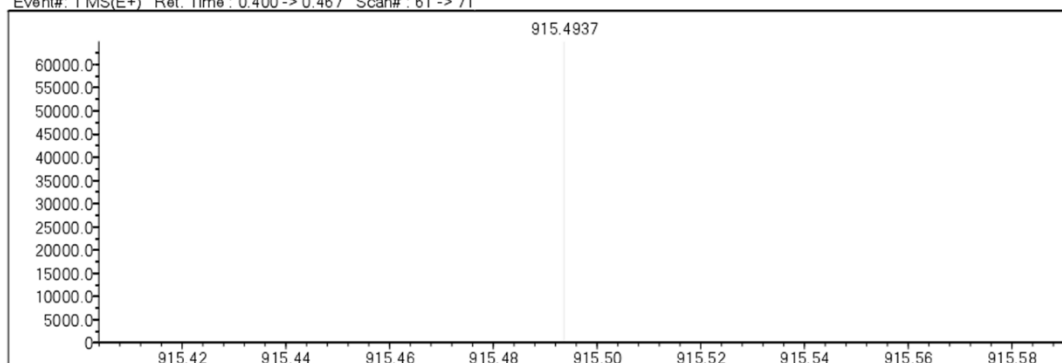
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C	4	10	60	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
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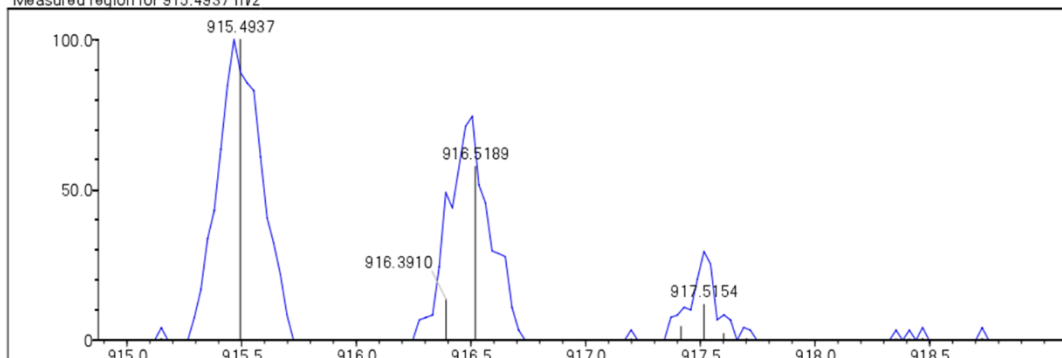
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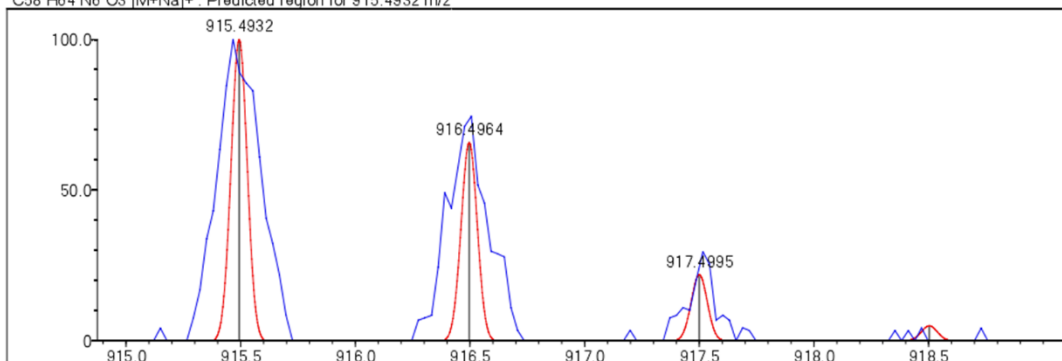
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Measured region for 915.4937 m/z



C58 H64 N6 O3 [M+Na]+ : Predicted region for 915.4932 m/z



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C58 H64 N6 O3	[M+Na]+	915.4937	915.4932	0.5	0.55	30.0

Figure S9 CD and UV spectrum of **1** in MeOH

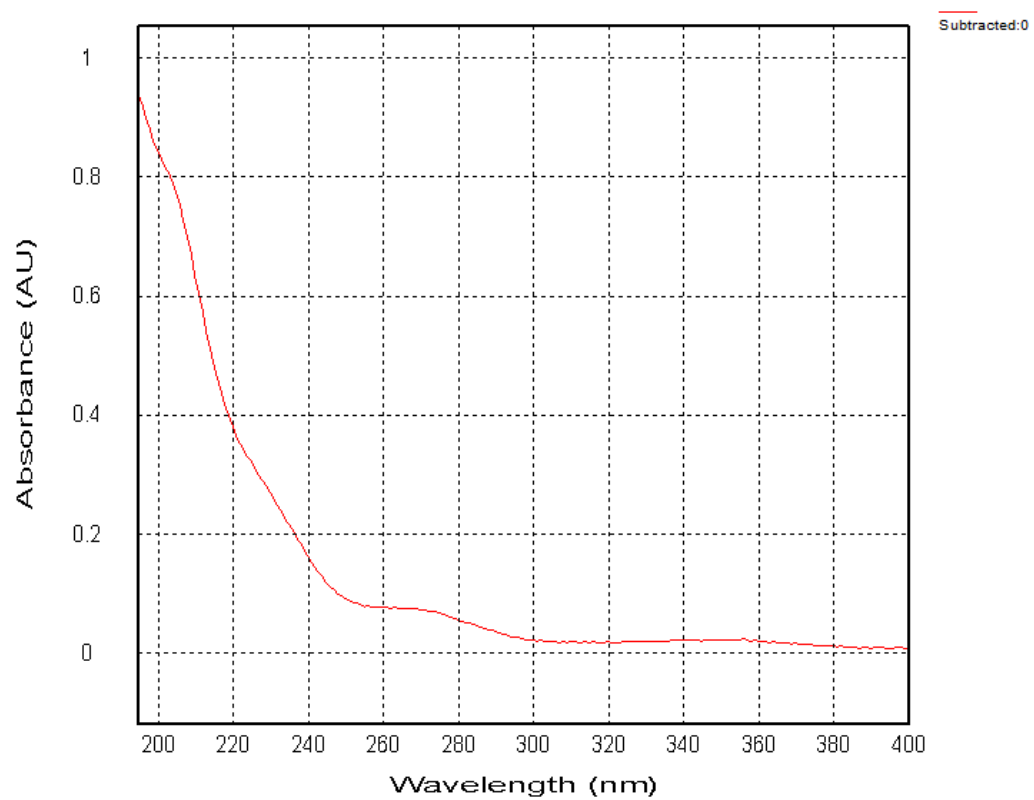
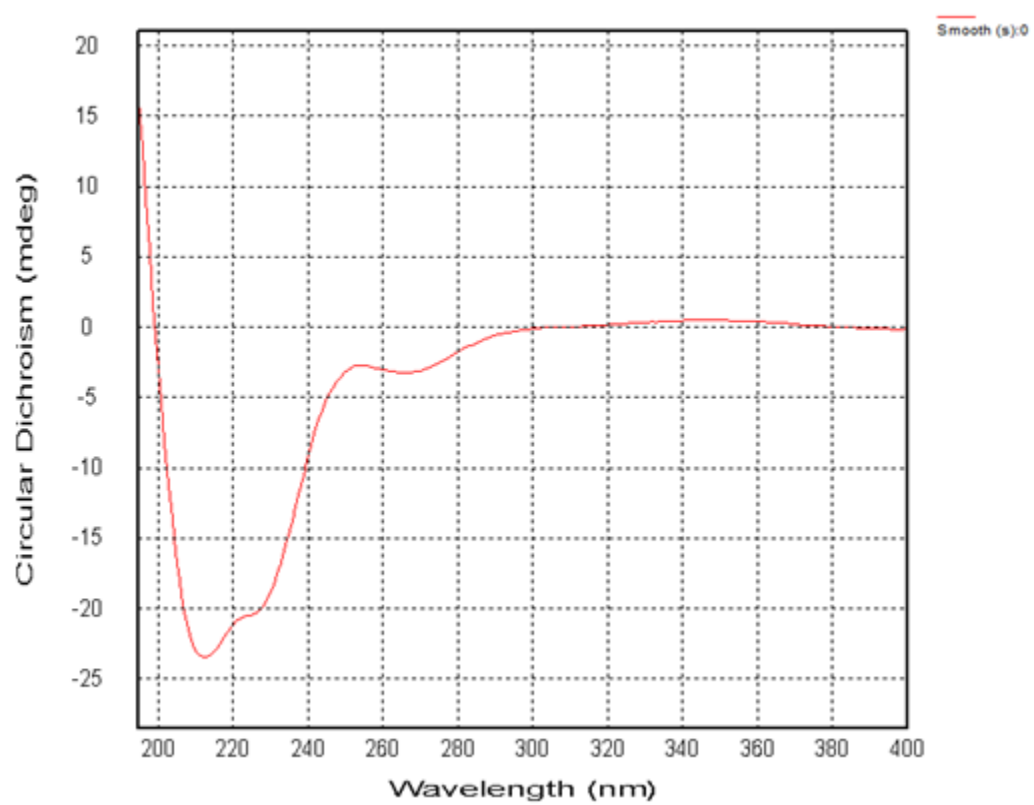
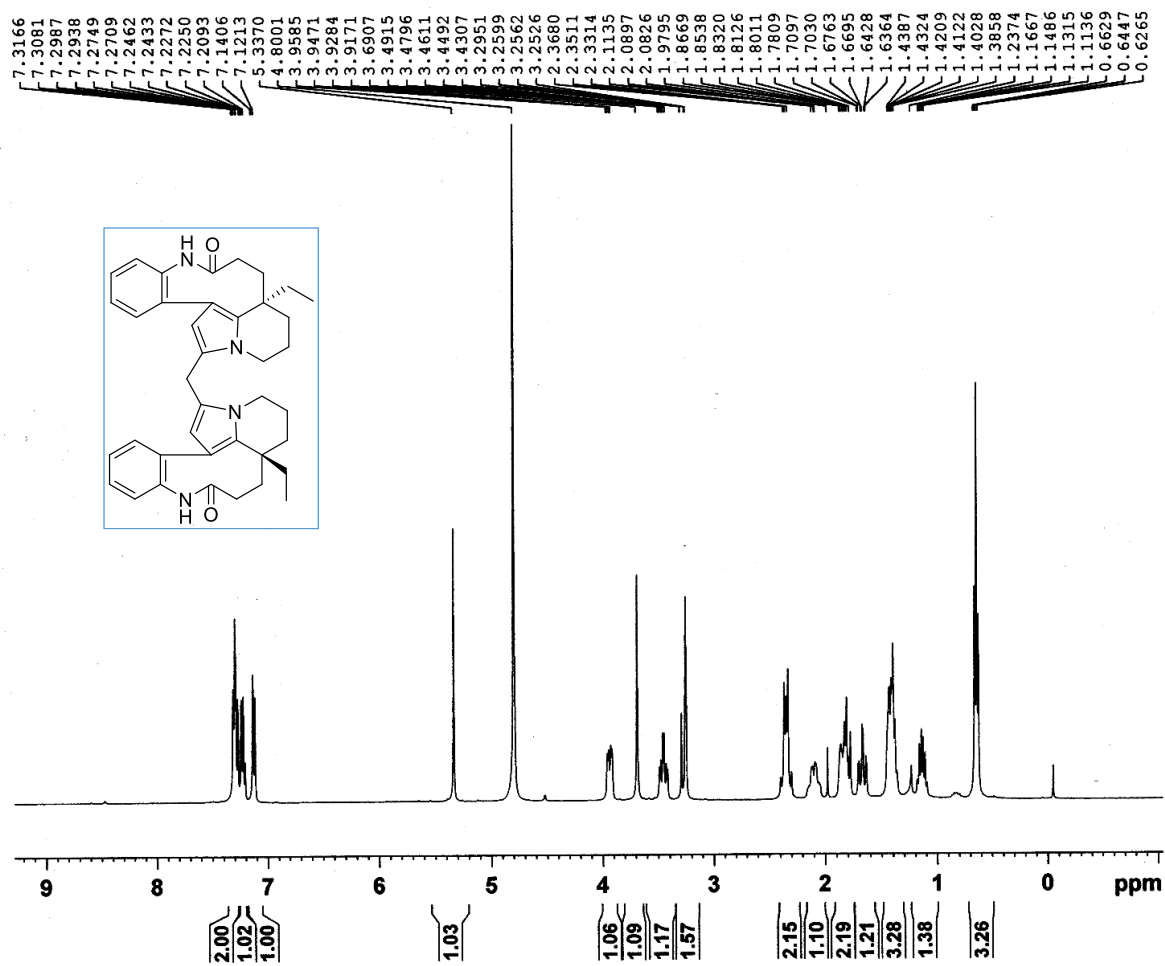


Figure S10 <sup>1</sup>H NMR spectrum of 2 in CD<sub>3</sub>OD

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Figure S11 <sup>13</sup>C NMR spectrum of **2** in CD<sub>3</sub>OD

wbmp38 c13 and dept

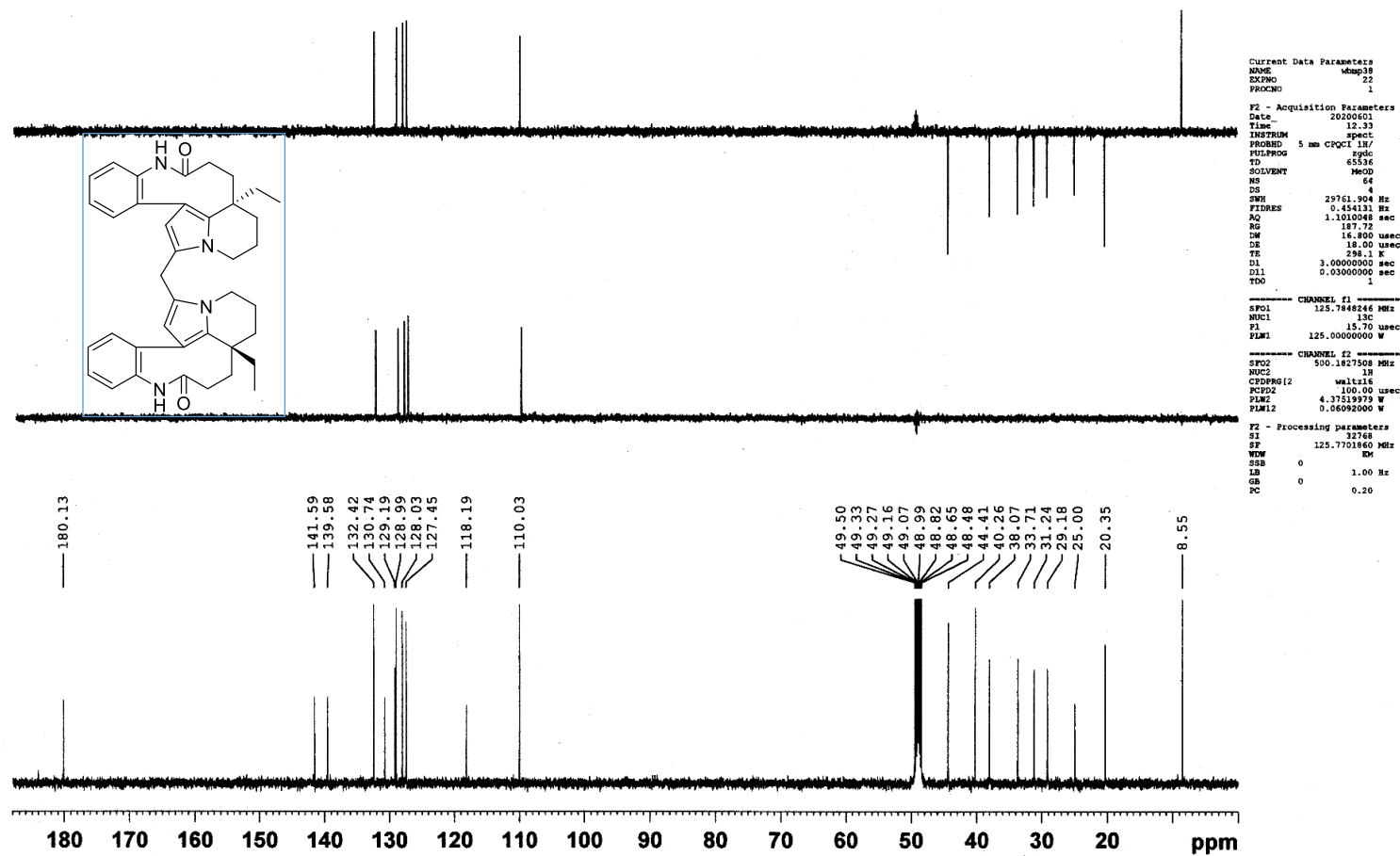


Figure S12 HSQC spectrum of 2 in CD<sub>3</sub>OD

wbmp38 hsqc

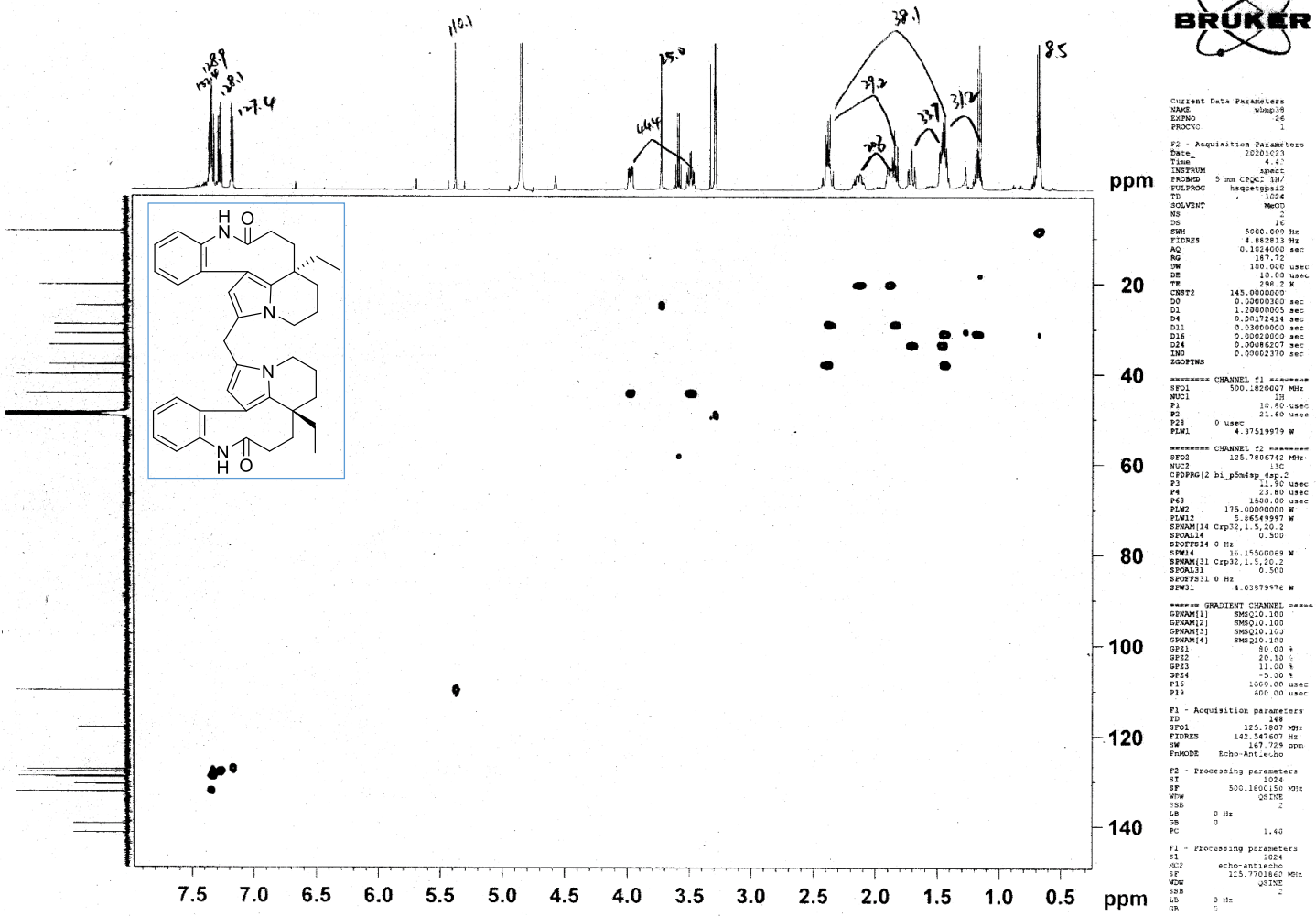




Figure S13 HMBC spectrum of 2 in CD<sub>3</sub>OD

wbmp38 hmbc

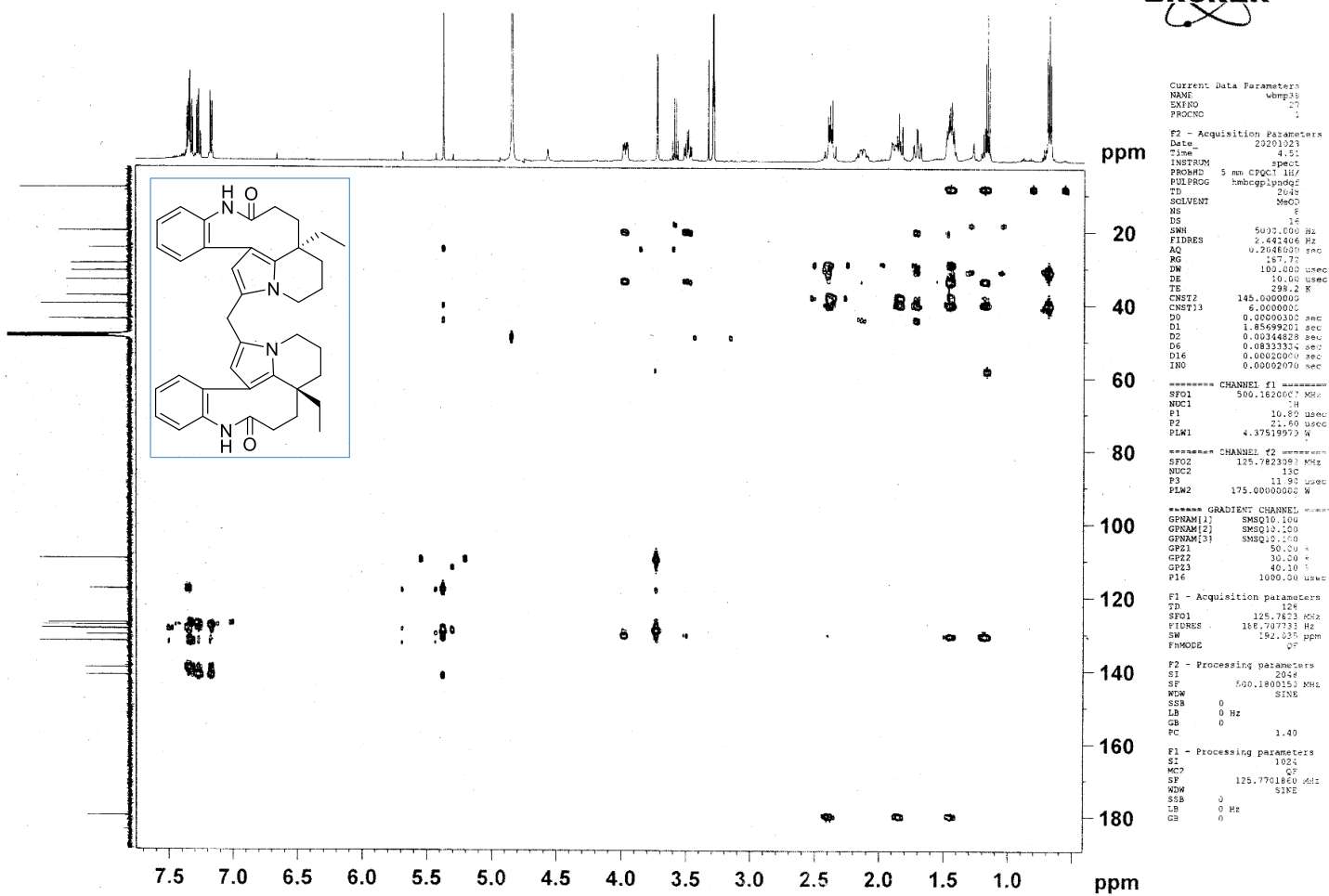


Figure S14 COSY spectrum of **2** in CD<sub>3</sub>OD

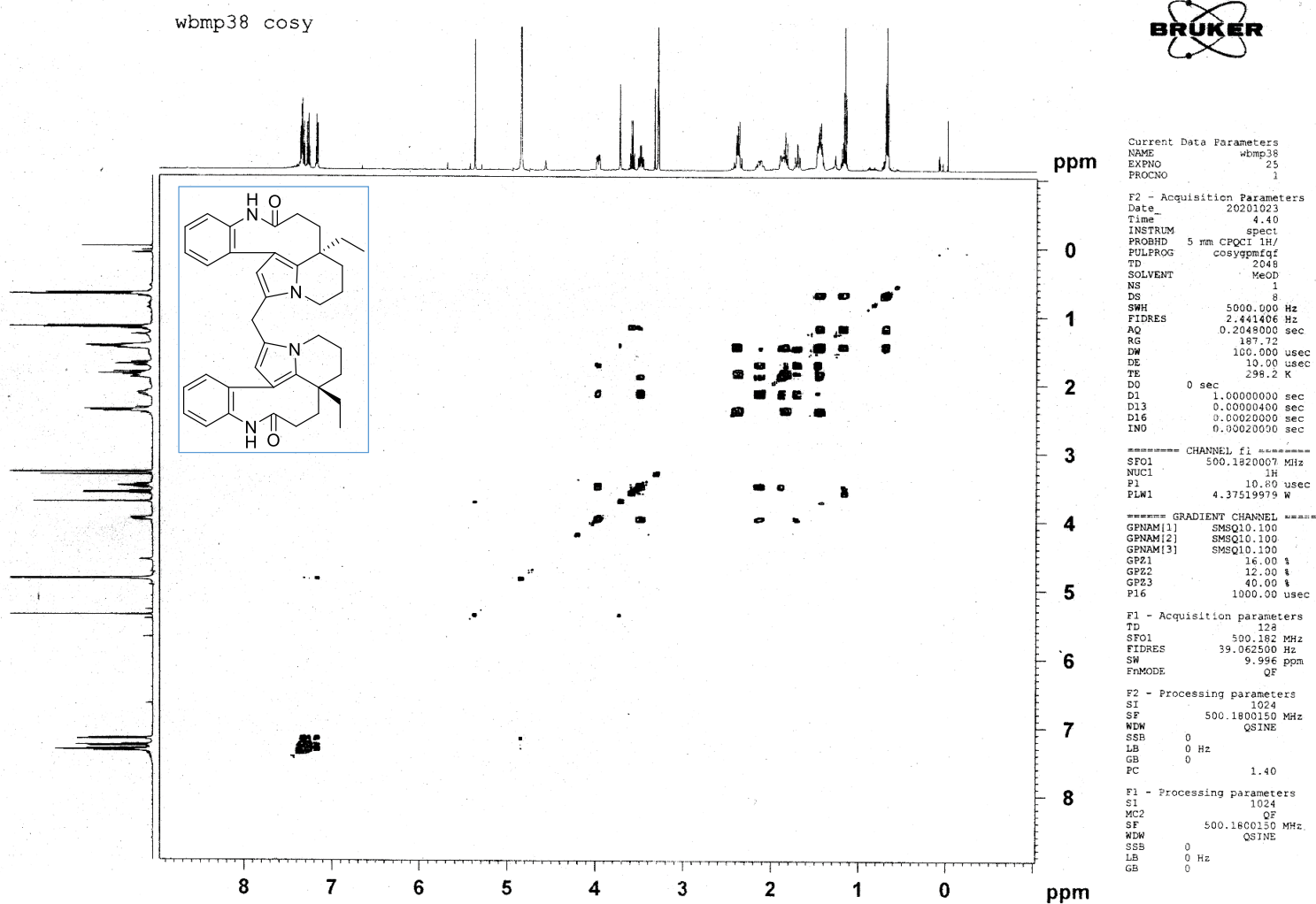


Figure S15 Roesy spectrum of 2 in CD<sub>3</sub>OD

wbmp38 roesy

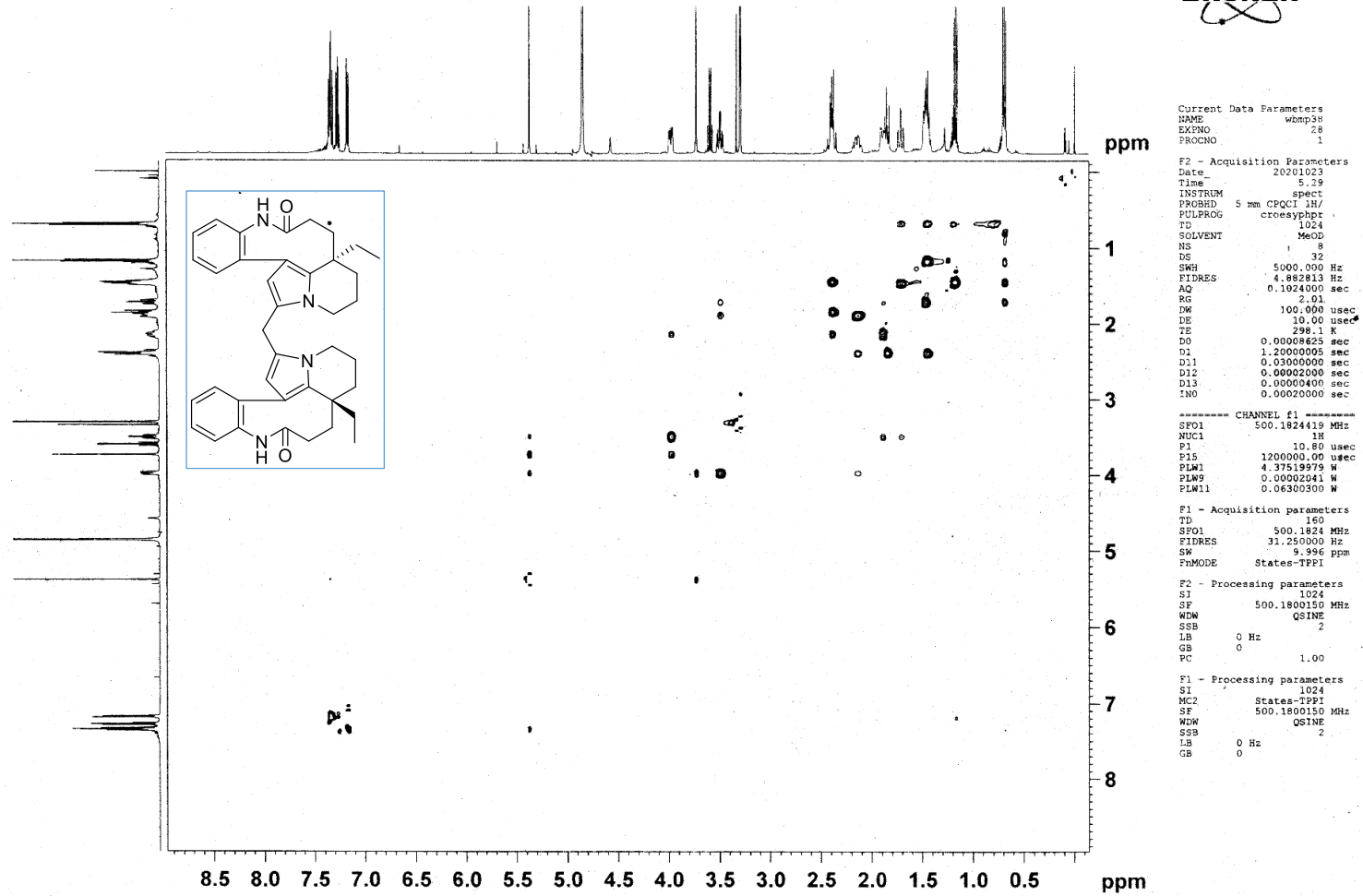


Figure S16 HRMS spectrum of 2

Formula Predictor Report - wbmp-381cd

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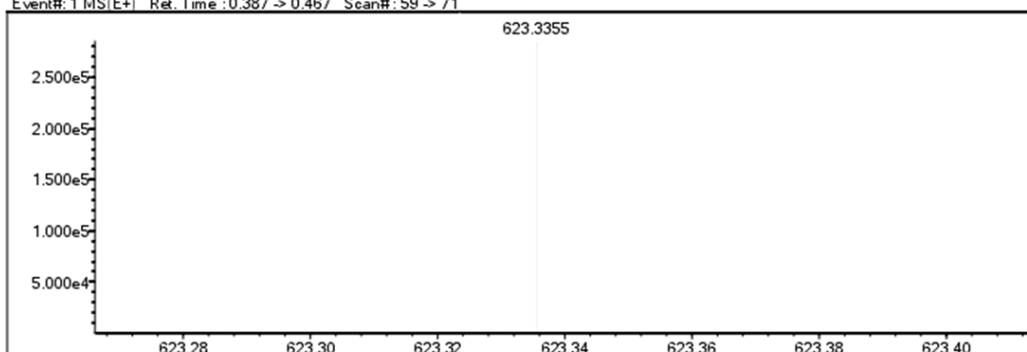
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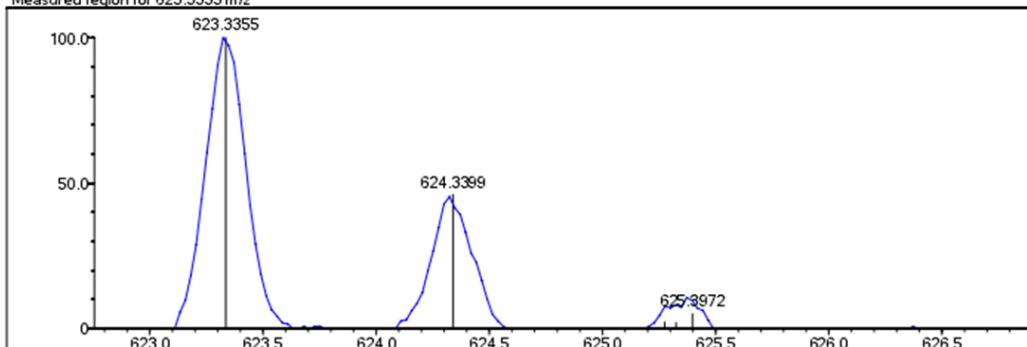
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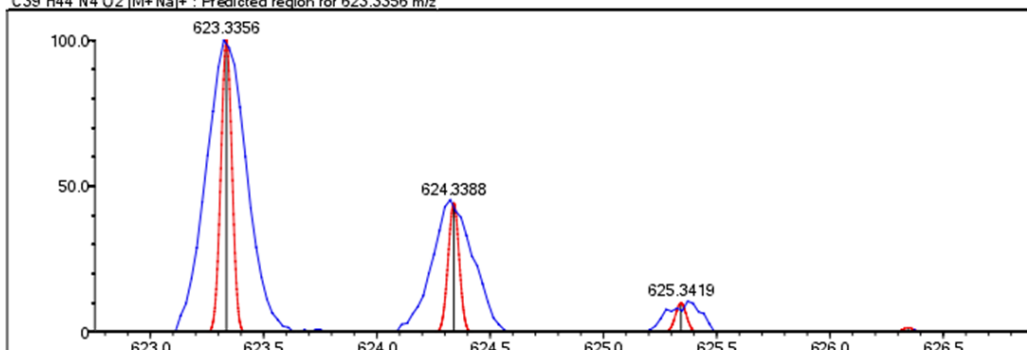
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Measured region for 623.3355 m/z



C39 H44 N4 O2 [M+Na]+ : Predicted region for 623.3356 m/z



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Figure S17 UV and CD spectrum of **2** in MeOH

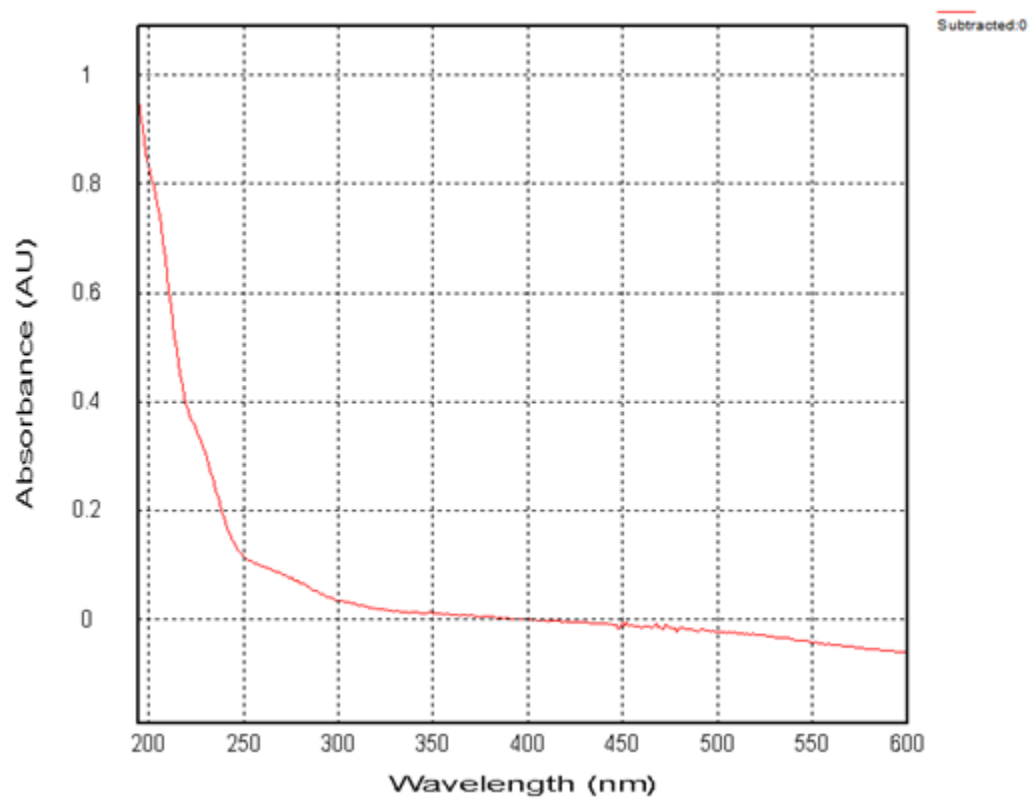
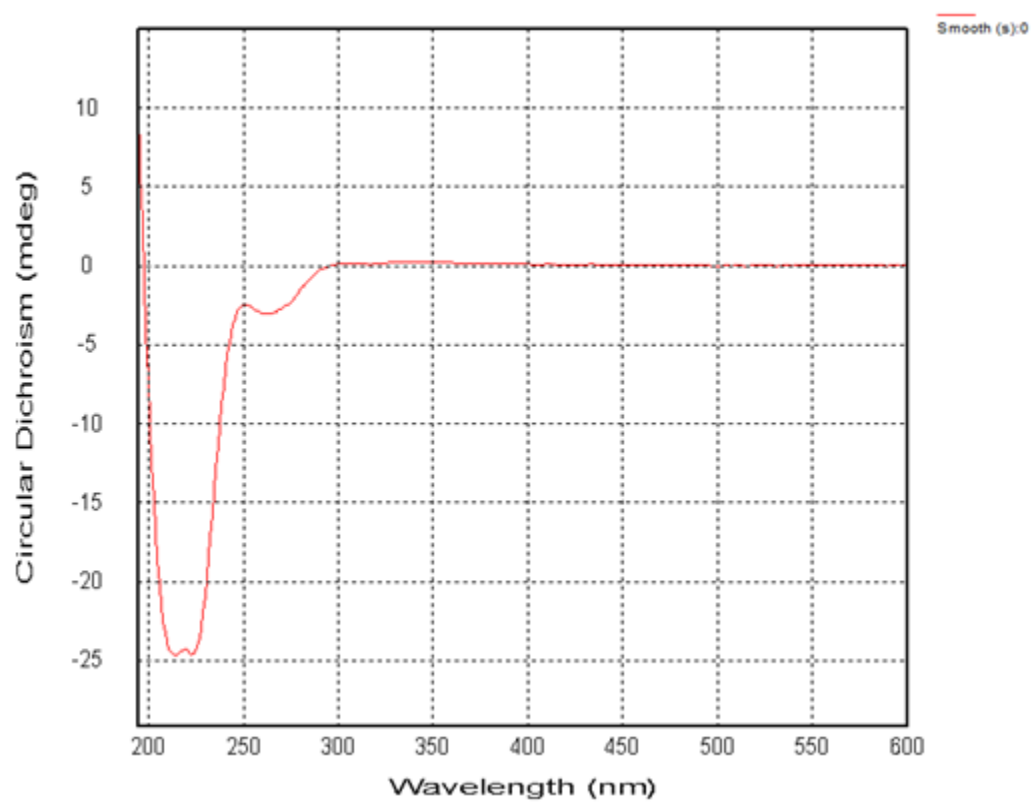
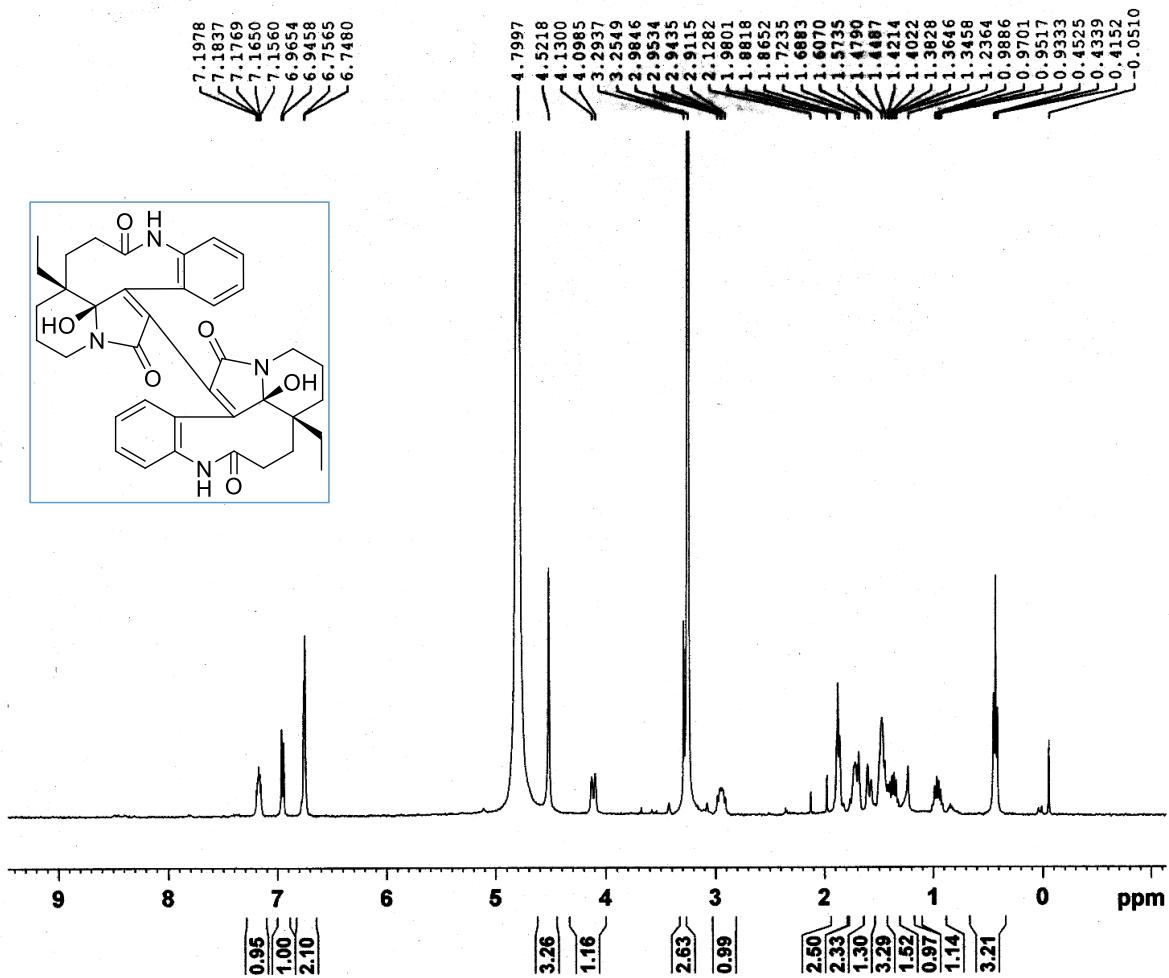


Figure S18 <sup>1</sup>H NMR spectrum of 3 in CD<sub>3</sub>OD

wbmp-59b



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Figure S19 <sup>13</sup>C NMR spectrum of **3** in CD<sub>3</sub>OD

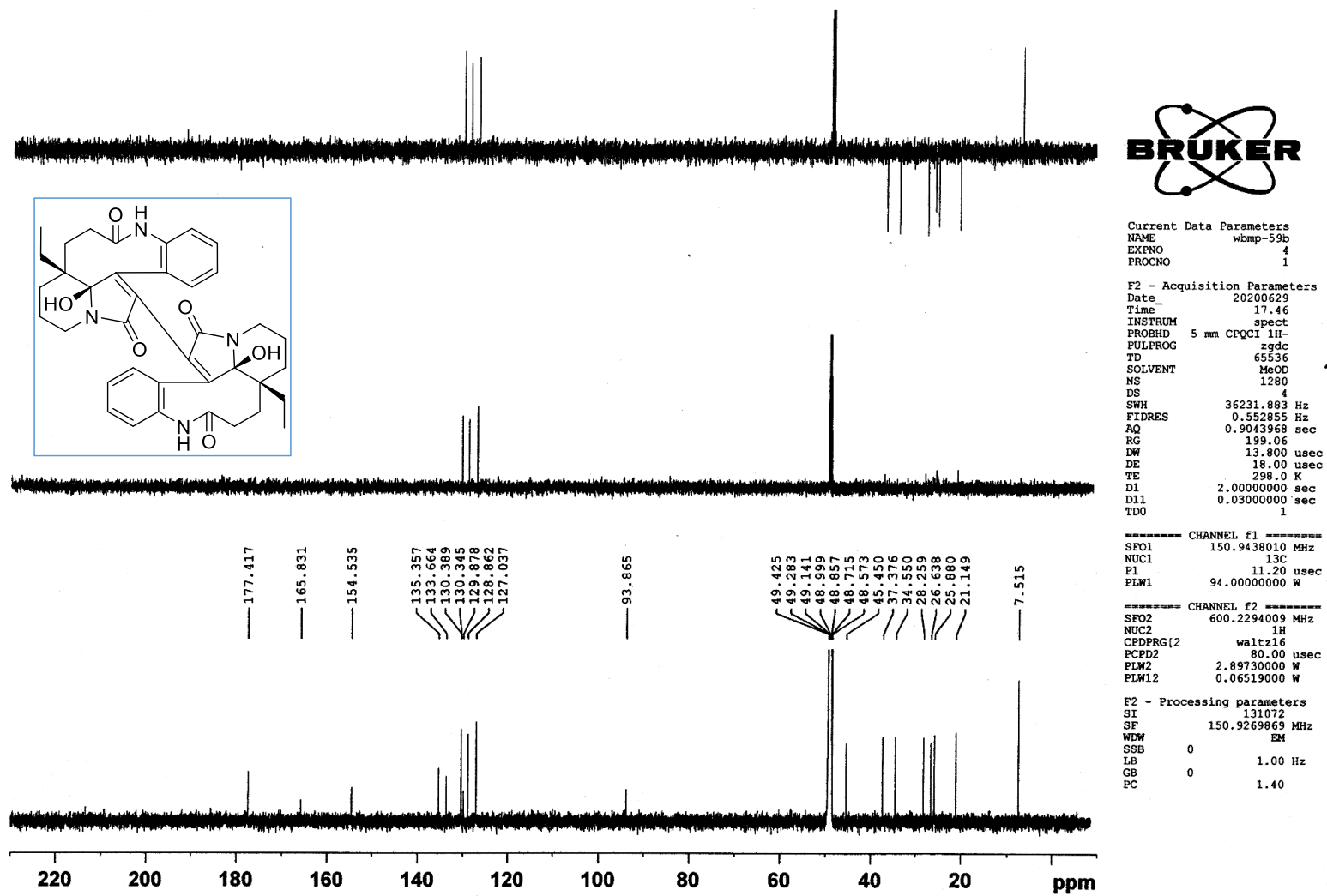


Figure S20 HSQC spectrum of 3 in CD<sub>3</sub>OD

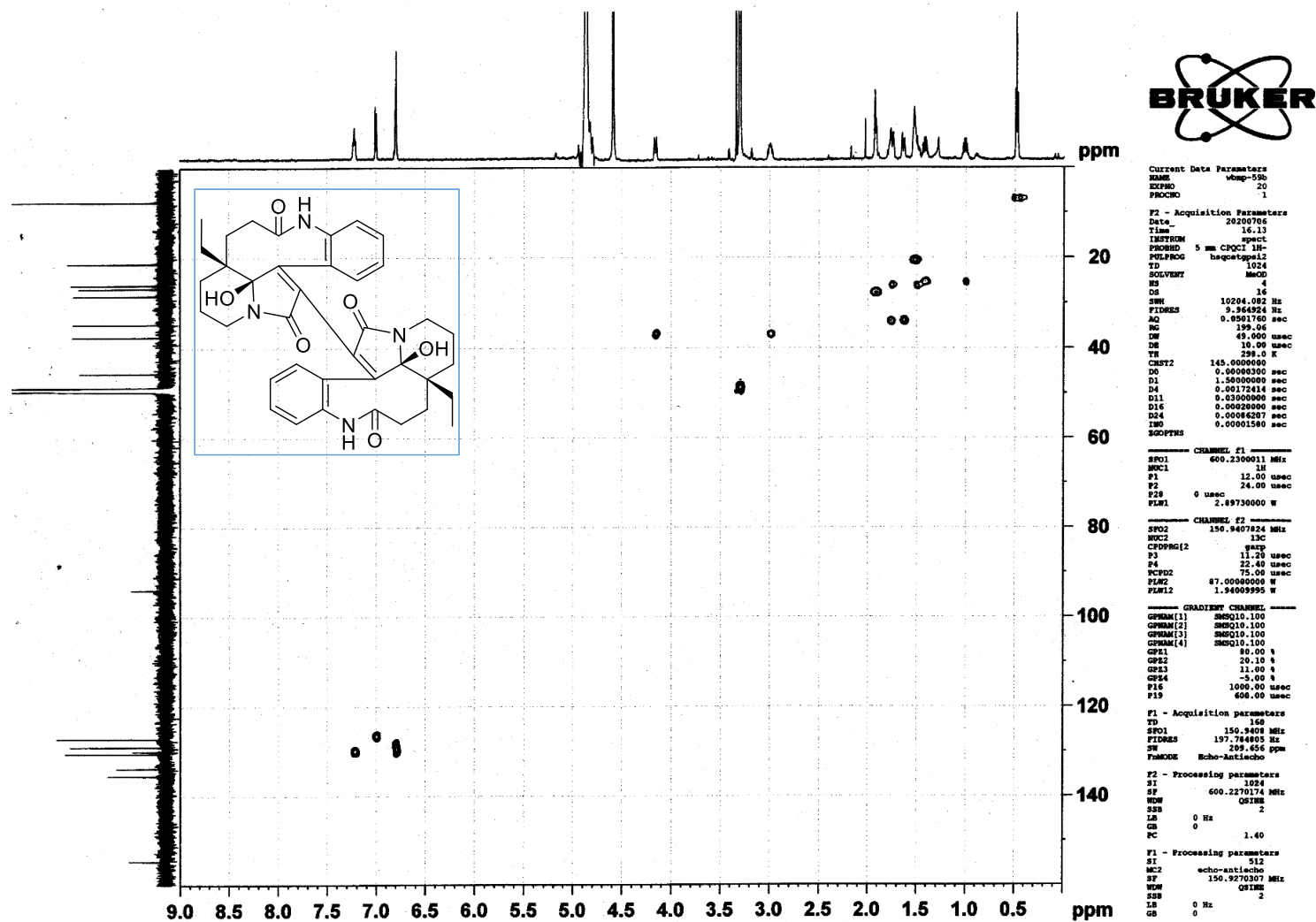




Figure S21 HMBC spectrum of 3 in CD<sub>3</sub>OD

hmbch MeOD D:\ root 11

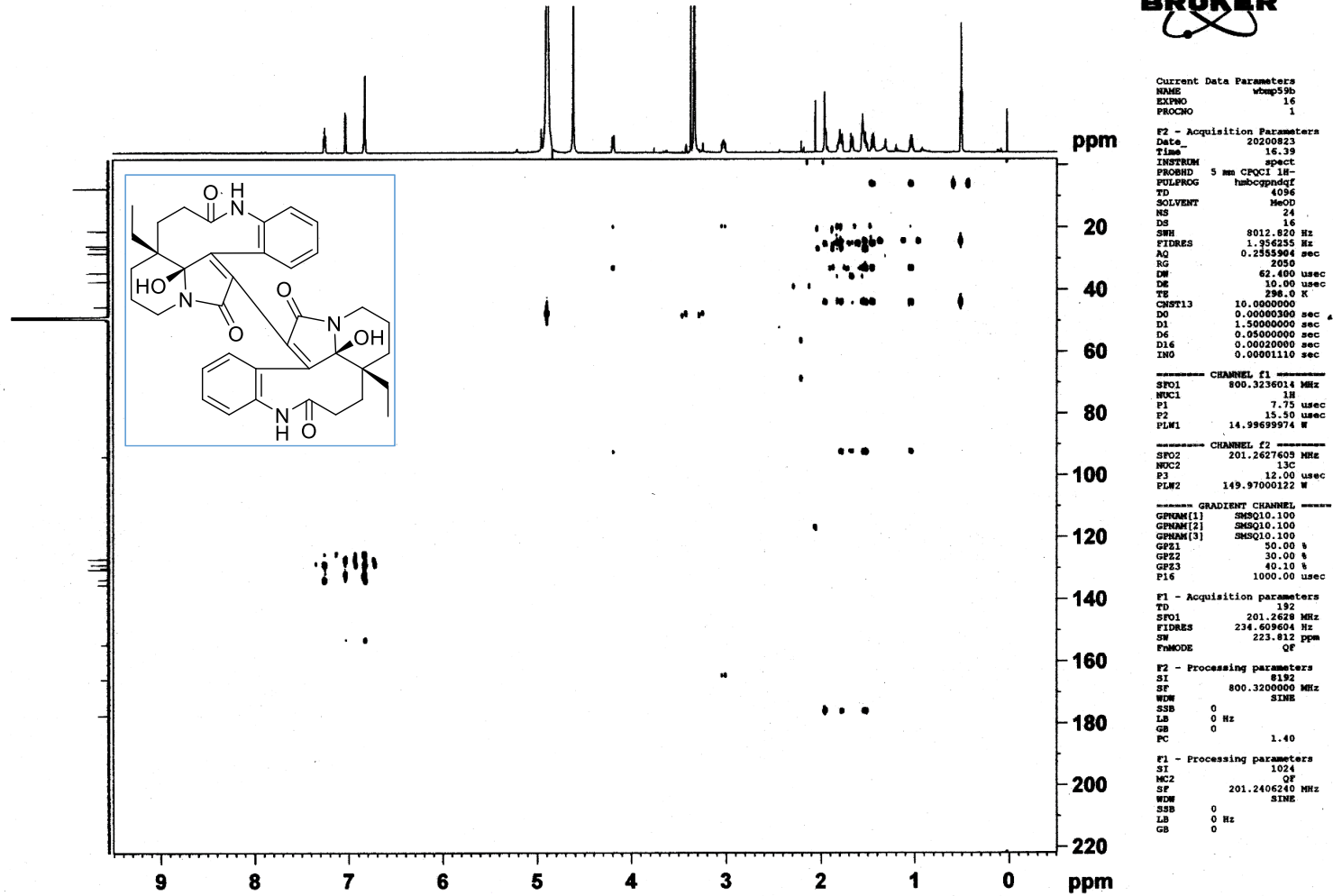


Figure S22 COSY spectrum of 3 in CD<sub>3</sub>OD

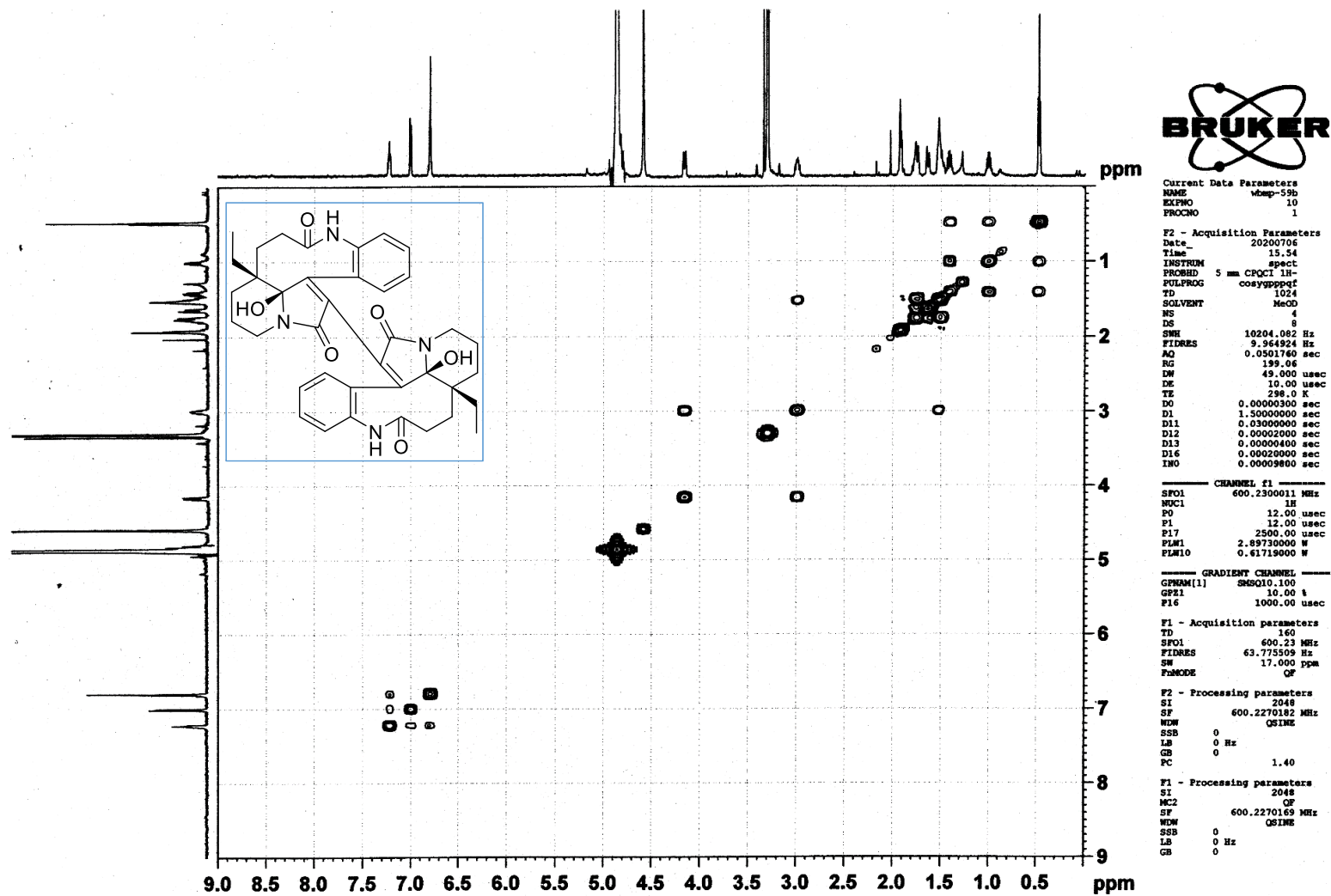


Figure S23 ROESY spectrum of 3 in CD<sub>3</sub>OD

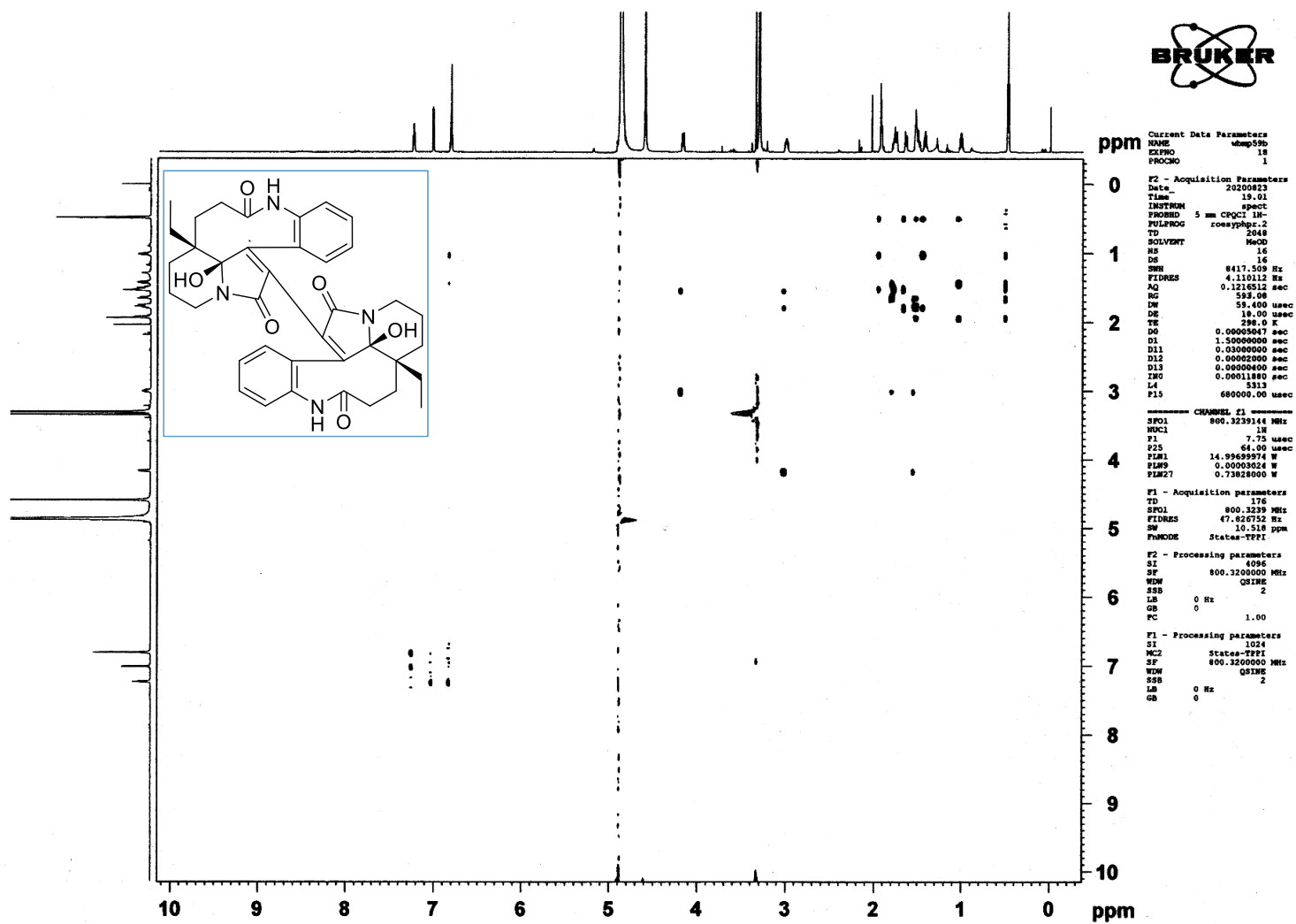


Figure S24 HRMS spectrum of 3

Formula Predictor Report - wbmp-59b.lcd

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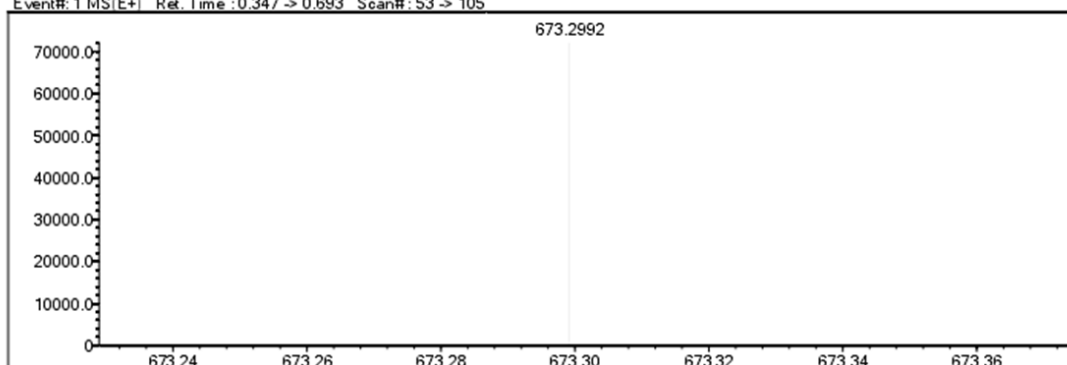
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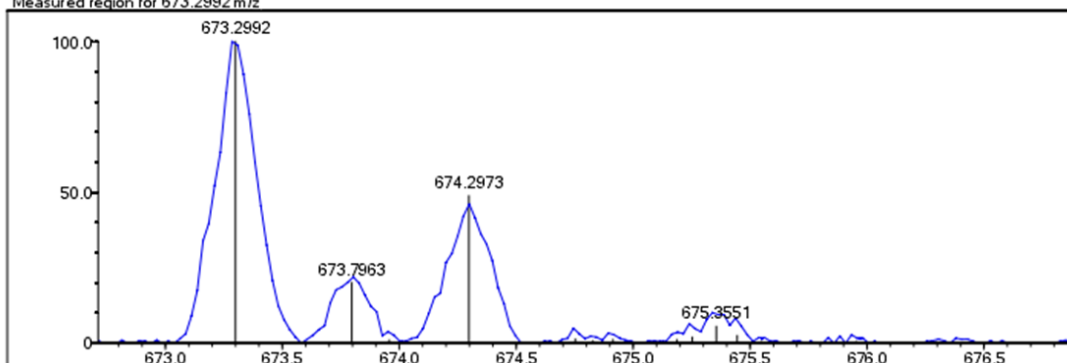
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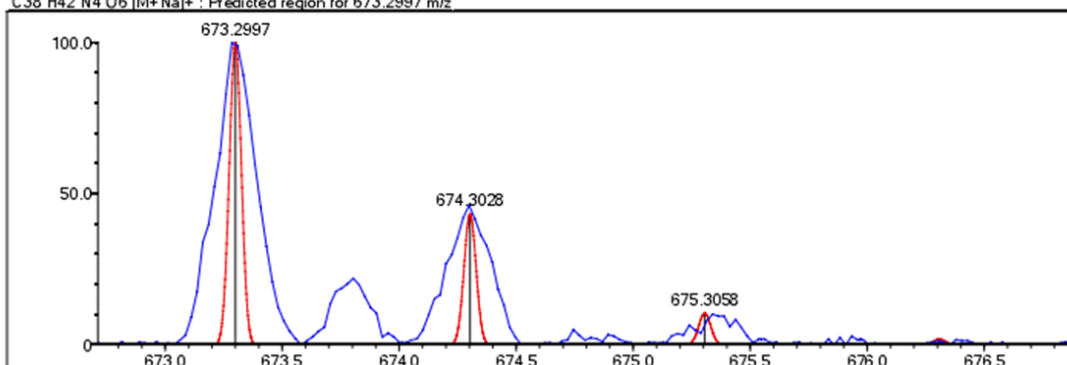
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Measured region for 673.2992 m/z



C38 H42 N4 O6 [M+Na]+ : Predicted region for 673.2997 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
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Figure S25 UV and CD spectrum of **3** in MeOH

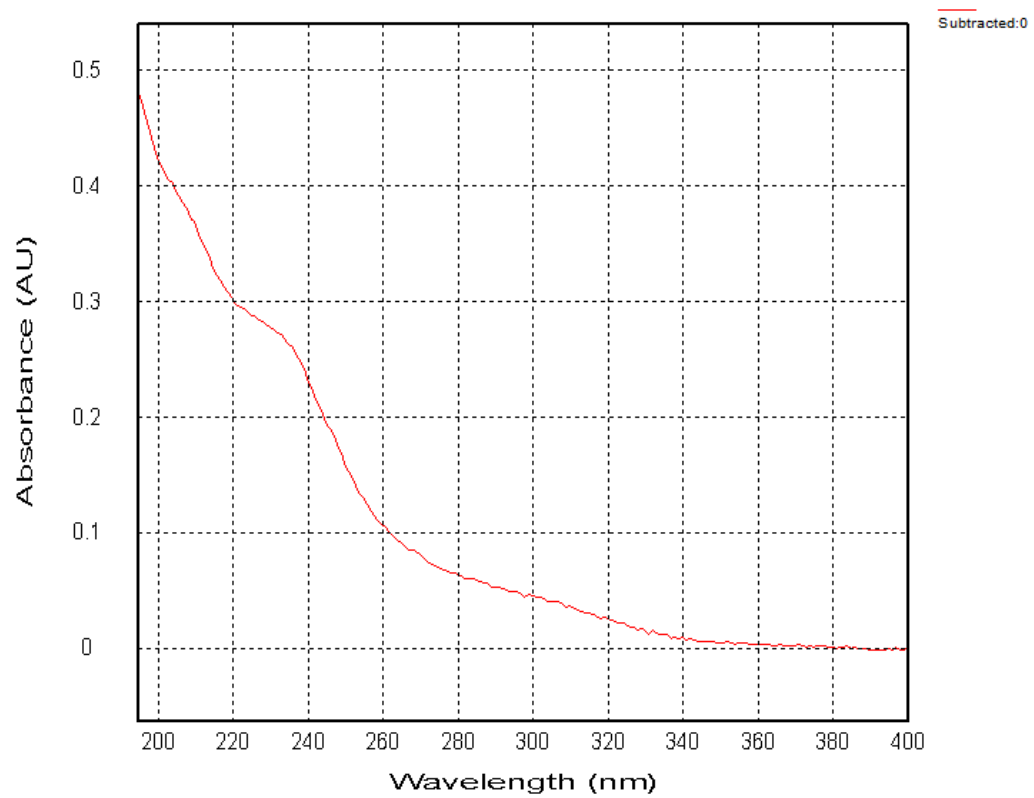
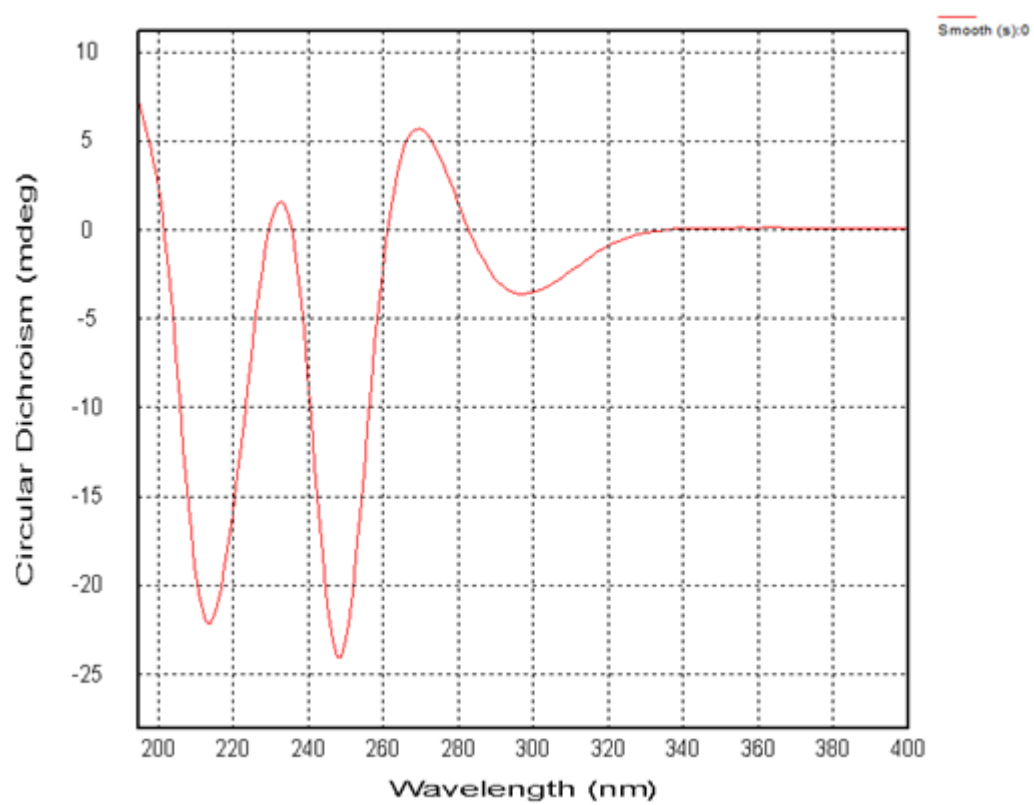
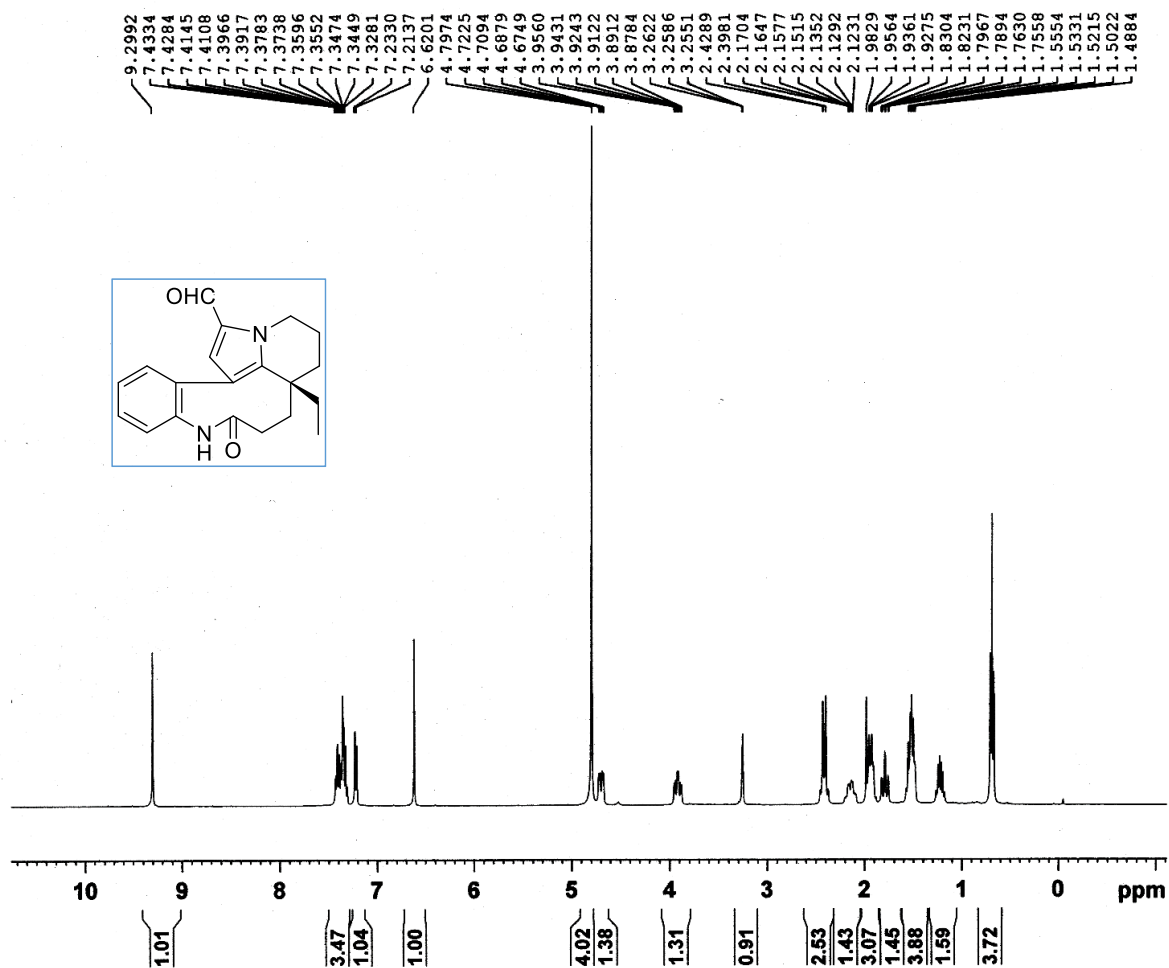


Figure S26 <sup>1</sup>H NMR spectrum of 4 in CD<sub>3</sub>OD

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 Date\_ 20200627  
 Time\_ 13.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg  
 TD 65536  
 SOLVENT MeOD  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.089465 sec  
 RG 32.52  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 2.0000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 SFO1 400.1318812 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 11.69999981 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300283 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

Figure S27 <sup>13</sup>C NMR spectrum of 4 in CD<sub>3</sub>OD

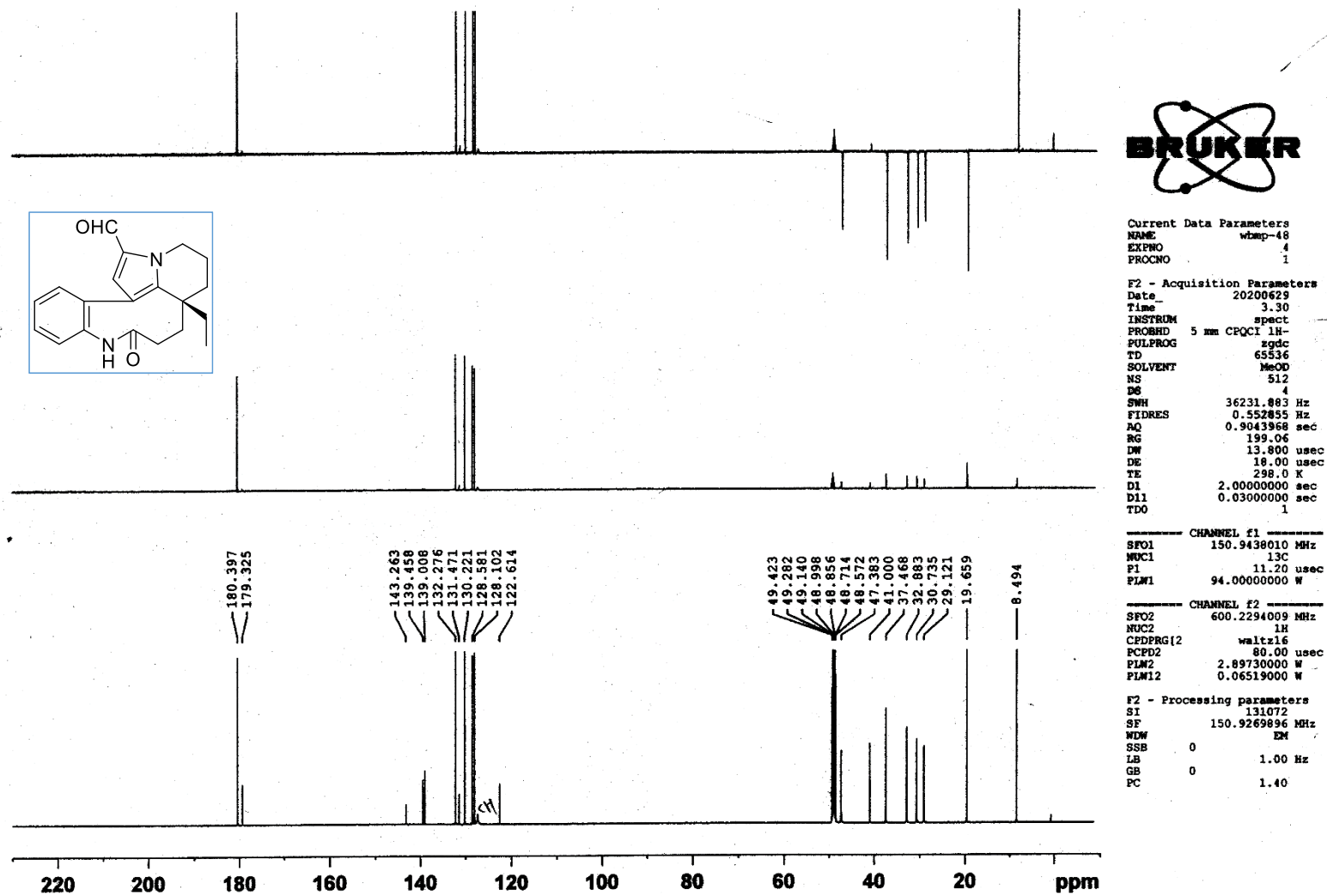


Figure S28 MS spectrum of 4

==== LCMSsolution Data Report ====

Acquired by	: Admin	Sample Information	System Configuration
Date Acquired	: 2020/7/6 14:58:40		<<Instrument>> : LC-IT-TOF
Sample Name	: wbmp-48		
Data File	: wbmp-48.lcd		
Method File	: 阻尼管一级100-1500.lcm		

<Spectrum>

Retention Time:0.480(Scan#:74)

Spectrum:Averaged 0.360-0.613(55-93)

Background:Averaged 0.000-0.362(1-55) MS Stage:MS Polarity:Pos Segment1 - Event1 Precursor:----- Cutoff:

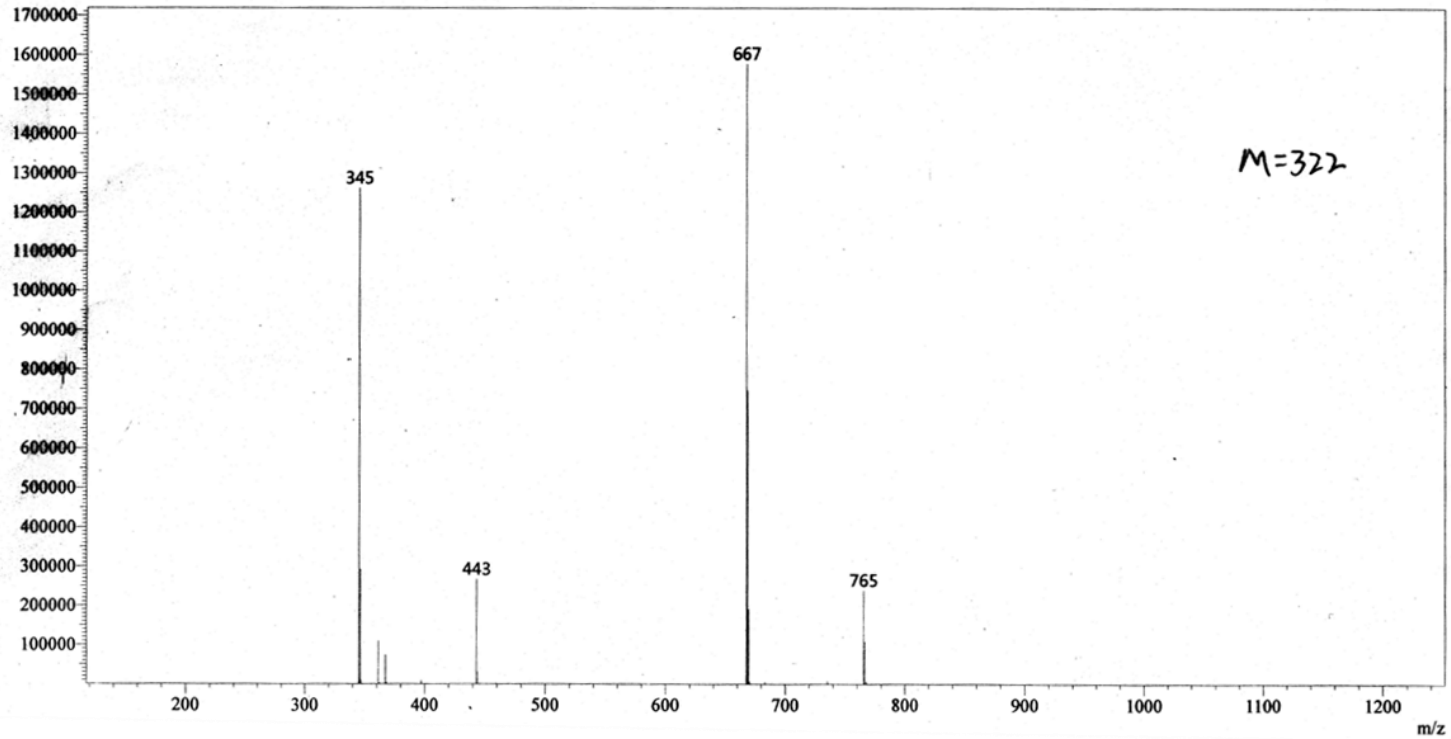




Figure S29 UV and CD spectrum of **4** in MeOH

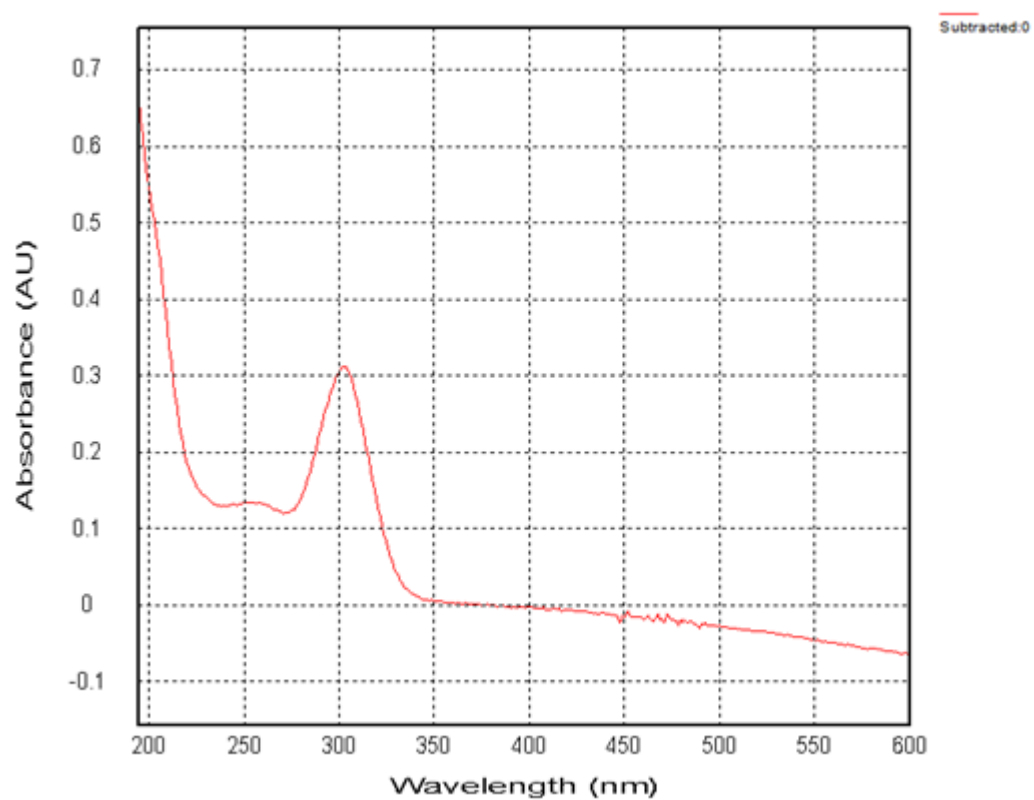
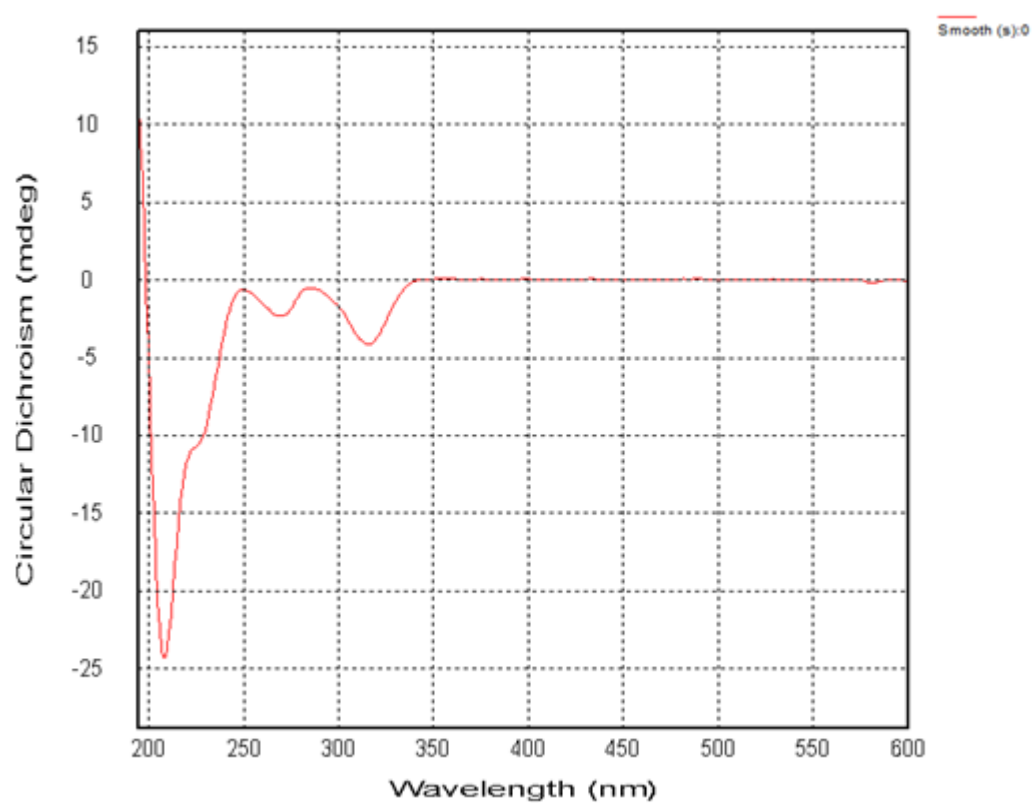


Figure S30 X-ray diffraction of **4**

Crystal data for **4**:  $C_{20}H_{22}N_2O_2 \cdot C_3H_6O$ ,  $M = 380.47$ ,  $a = 12.9963(3) \text{ \AA}$ ,  $b = 12.9963(3) \text{ \AA}$ ,  $c = 10.4728(2) \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 120^\circ$ ,  $V = 1531.91(8) \text{ \AA}^3$ ,  $T = 100.(2) \text{ K}$ , space group  $P31$ ,  $Z = 3$ ,  $\mu(\text{Cu K}\alpha) = 0.655 \text{ mm}^{-1}$ , 23168 reflections measured, 3982 independent reflections ( $R_{int} = 0.0351$ ). The final  $R_I$  values were 0.0427 ( $I > 2\sigma(I)$ ). The final  $wR(F^2)$  values were 0.1105 ( $I > 2\sigma(I)$ ). The final  $R_I$  values were 0.0429 (all data). The final  $wR(F^2)$  values were 0.1106 (all data). The goodness of fit on  $F^2$  was 1.046. Flack parameter = -0.01(6). The CCDC number of **4** is 2048765

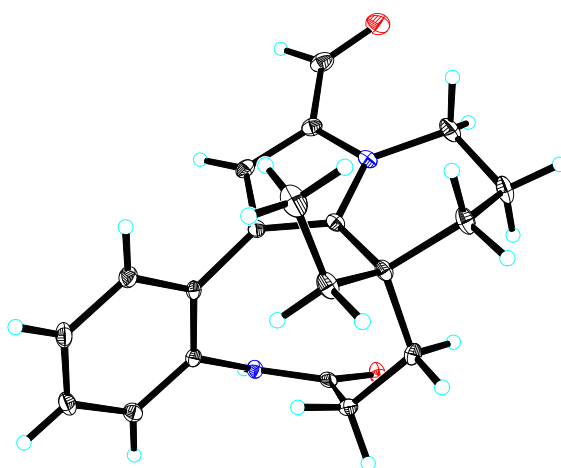
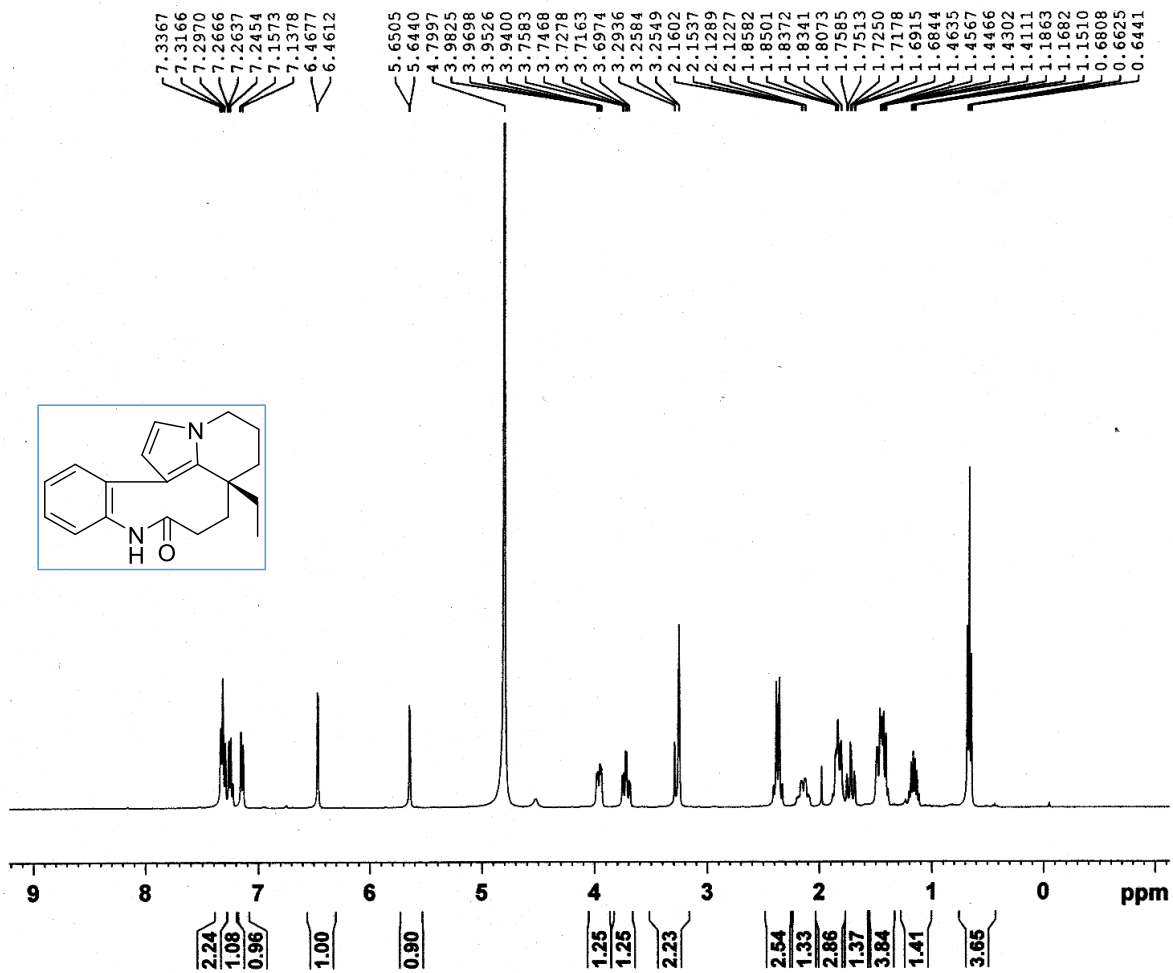


Figure S31 <sup>1</sup>H NMR spectrum of **5** in CD<sub>3</sub>OD

wbmp-60



Current Data Parameters  
 NAME wbmp-60  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200627  
 Time\_ 21.39  
 INSTRUM spect  
 PROBRHD 5 mm PABBO BB/  
 PULPROG zg  
 TD 65536  
 SOLVENT MeOD  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 40.68  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 2.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 400.1318812 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 11.69999981 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300298 MHz  
 .WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

Figure S32  $^{13}\text{C}$  NMR spectrum of **5** in  $\text{CD}_3\text{OD}$

wbmp60 c13 and dept

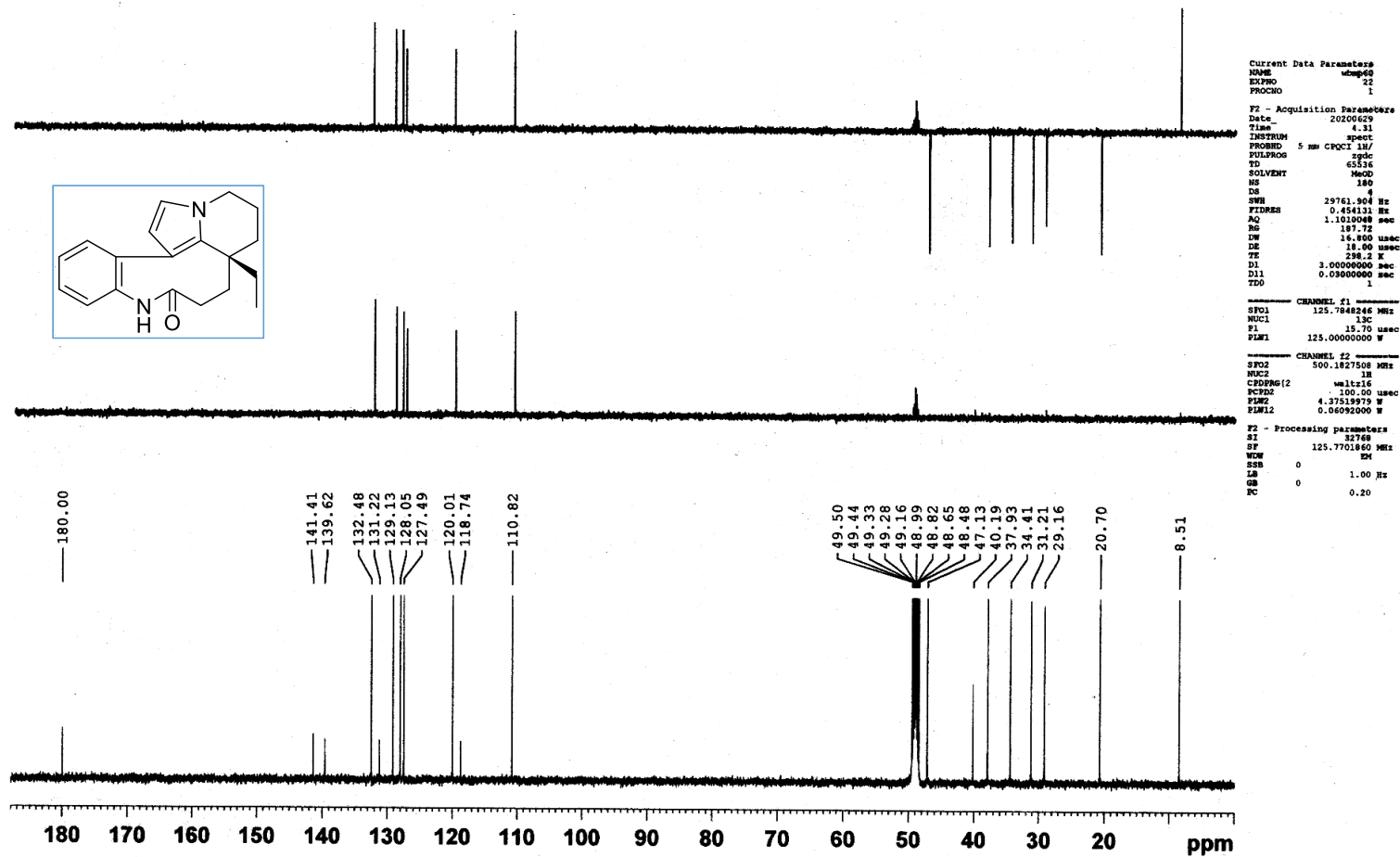


Figure S33 MS spectrum of 5

==== LCMSsolution Data Report ====

Sample Information		System Configuration
Acquired by	: Admin	<<Instrument>> : LC-IT-TOF
Date Acquired	: 2020/6/30 14:24:08	
Sample Name	: wbrmp-60	
Data File	: wbrmp-60.lcd	
Method File	: 阻尼管一級100-1500.lcm	

<Spectrum>

Retention Time:0.440(Scan#:67)

Spectrum:Averaged 0.347-0.533(53-81)

Background:Averaged 0.000-0.344(1-53) MS Stage:MS Polarity:Pos Segment1 - Event1 Precursor:---- Cutoff:

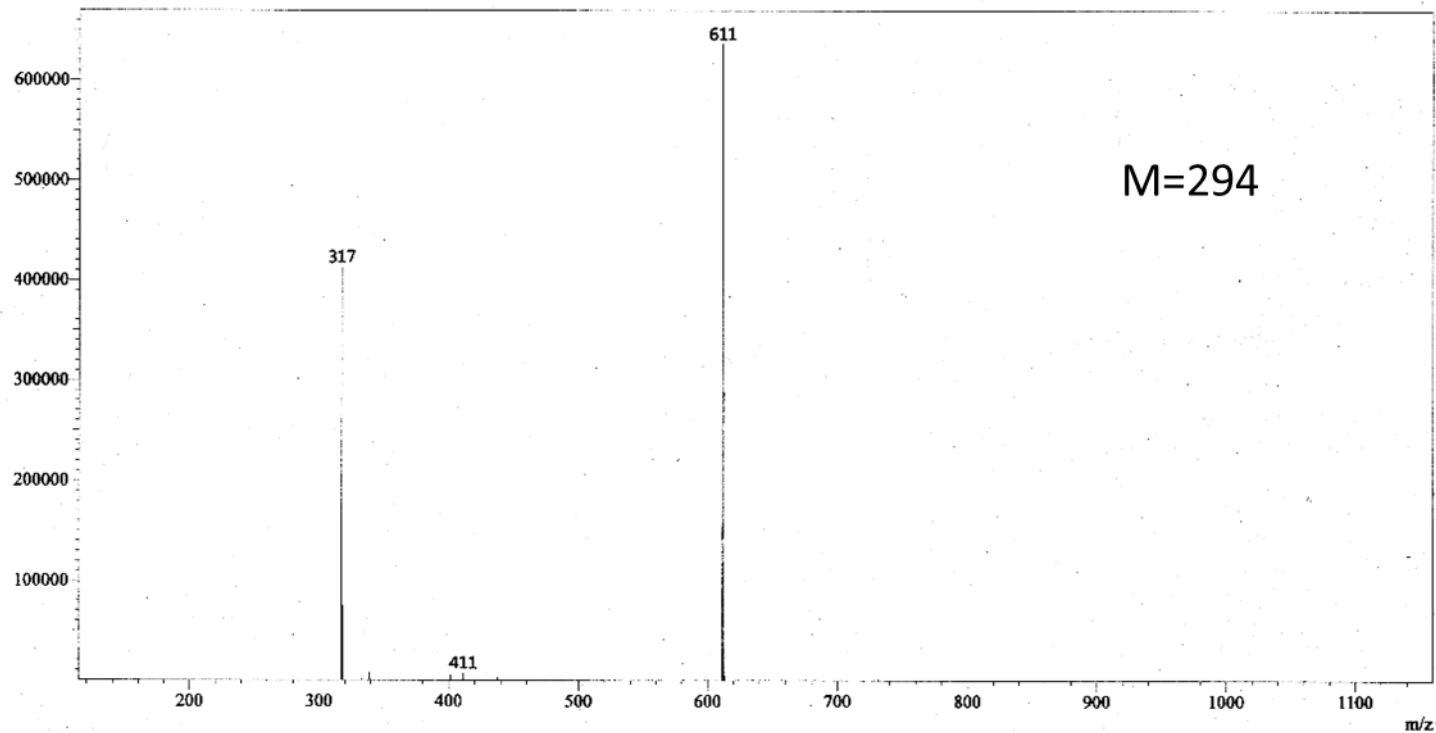


Figure S34 UV and CD spectrum of **5** in MeOH

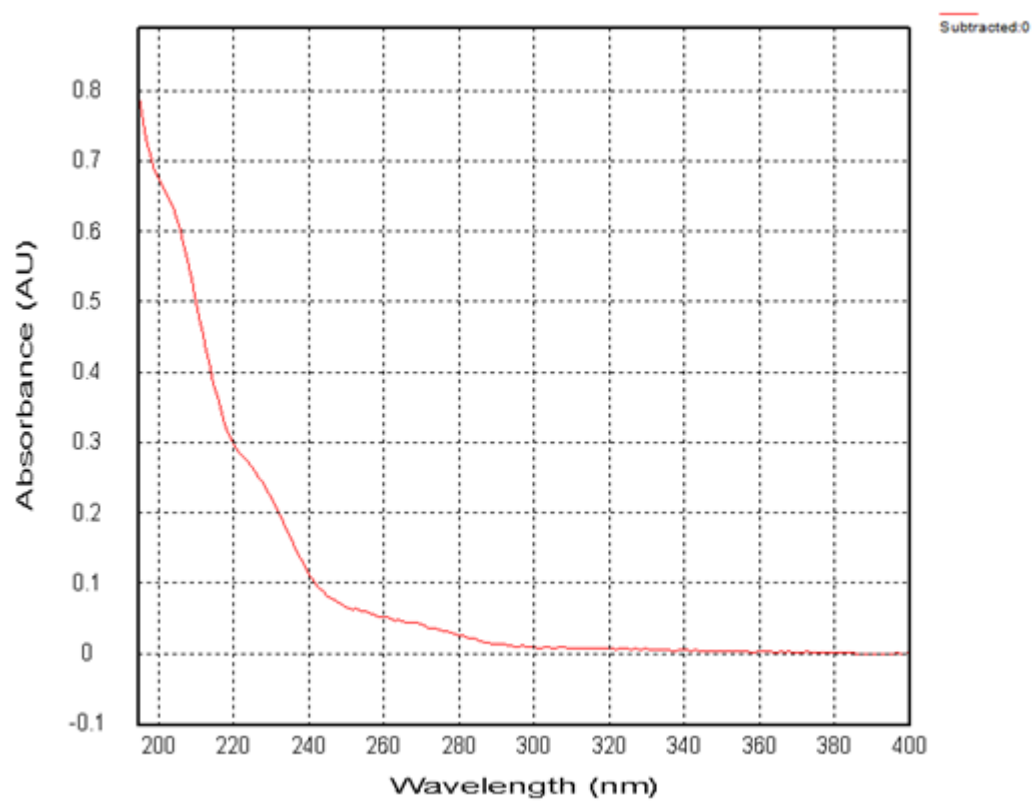
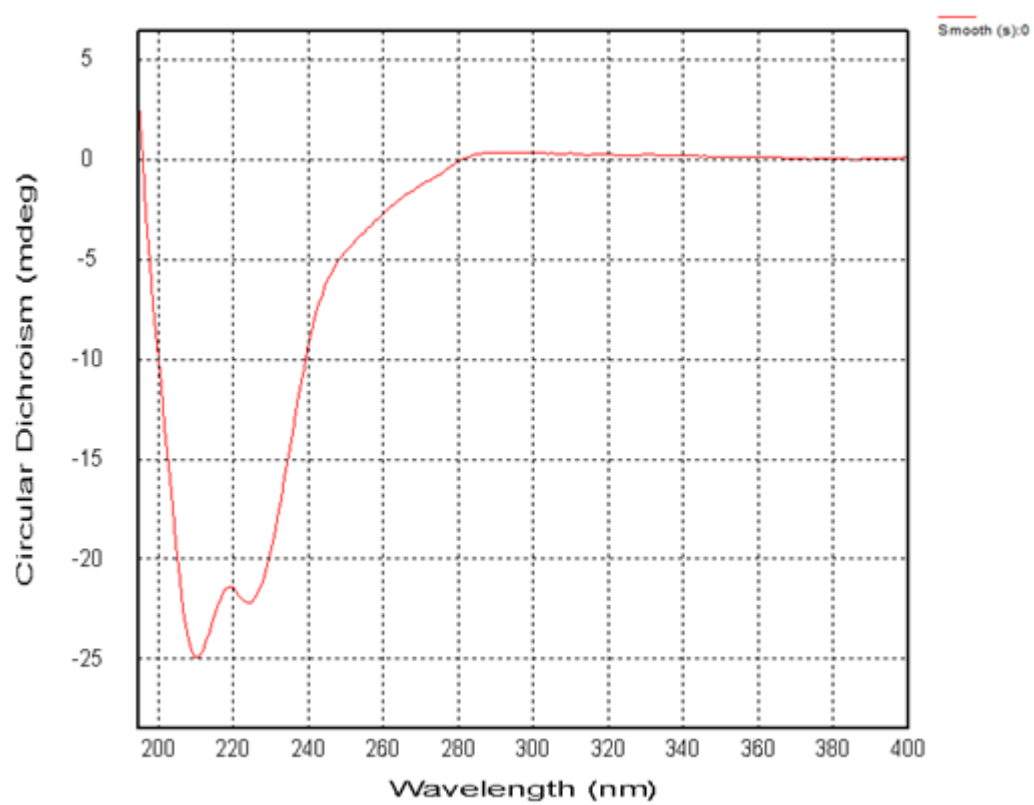
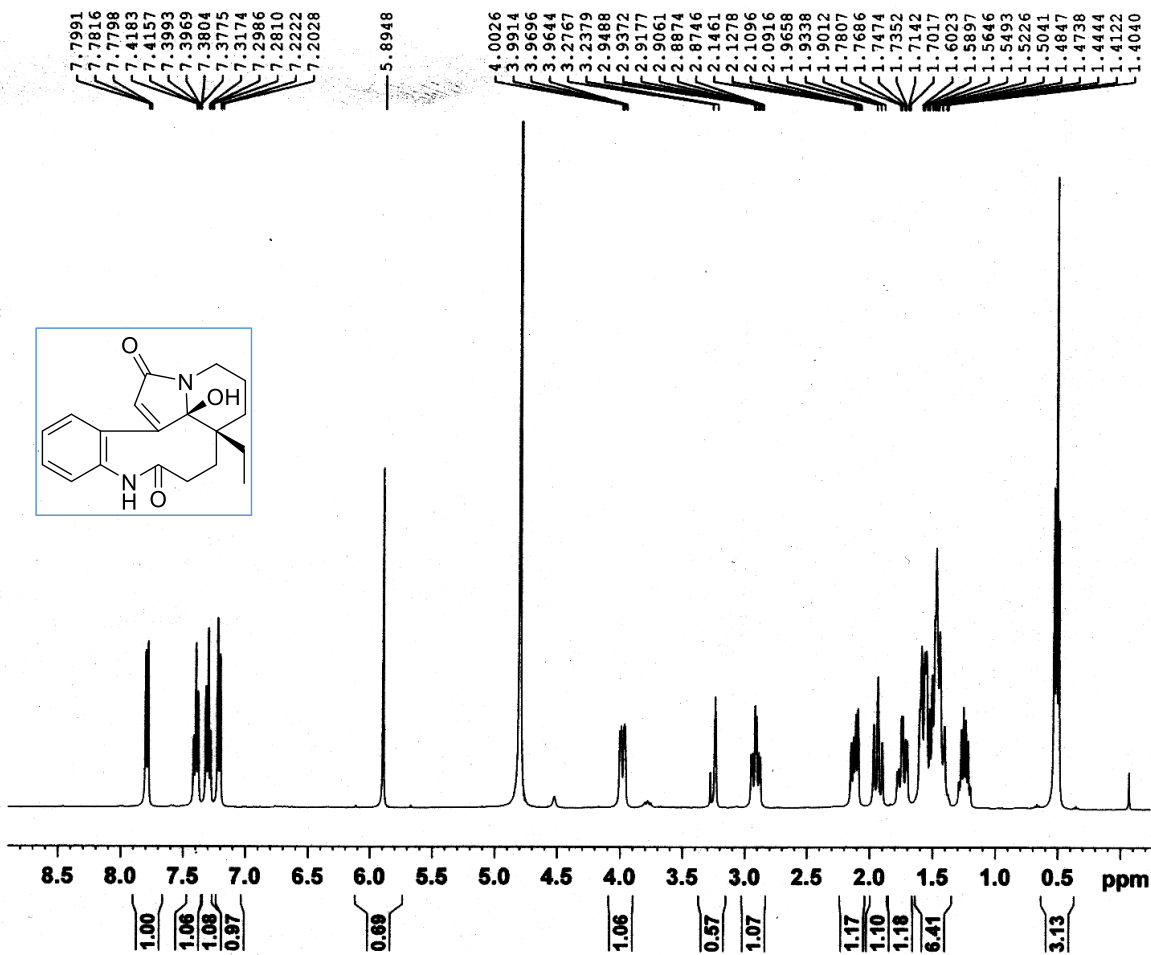


Figure S35 <sup>1</sup>H NMR spectrum of 6 in CD<sub>3</sub>OD

wbmp-106c



Current Data Parameters  
 NAME wbmp-106c  
 EXPNO 1  
 PROCNO 1

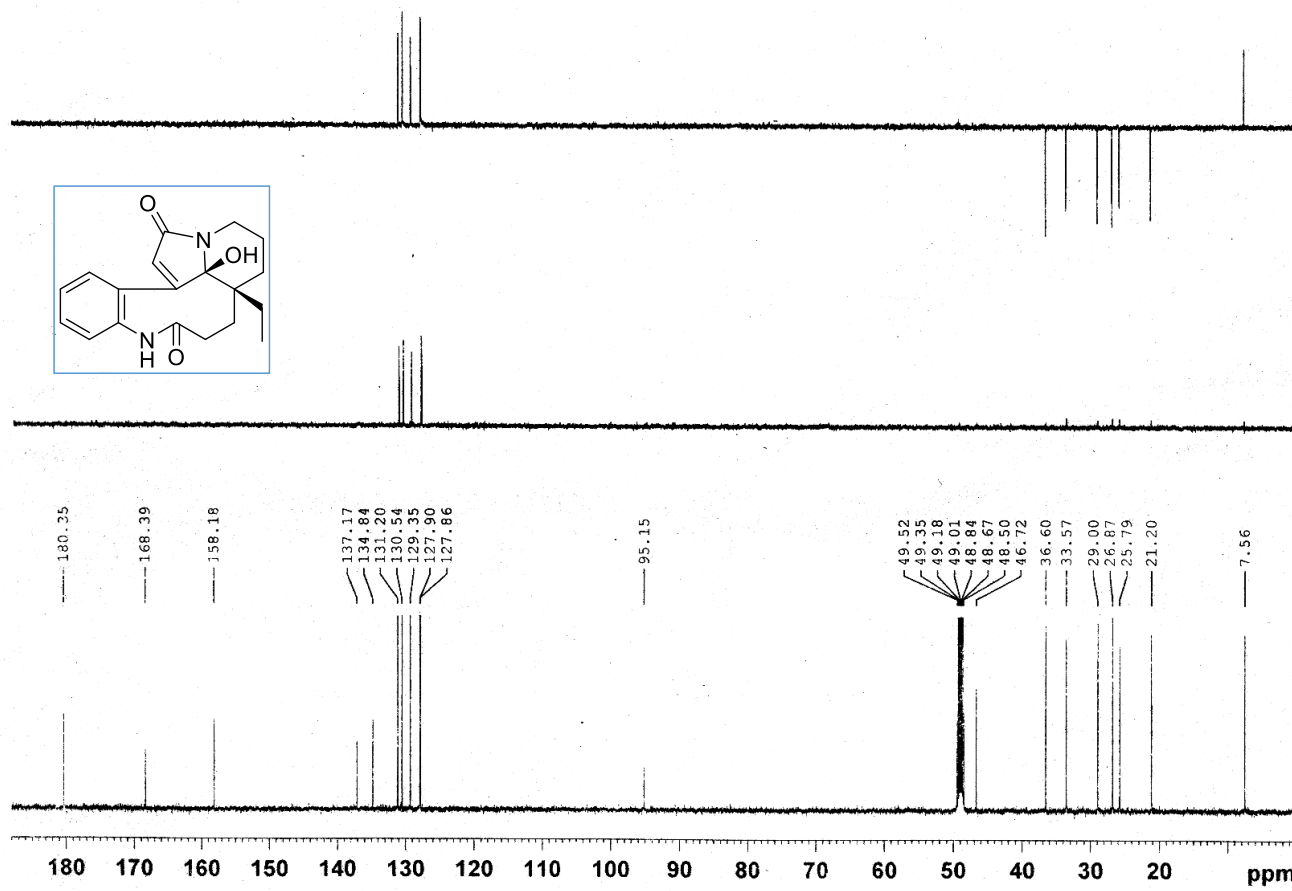
F2 - Acquisition Parameters  
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 Time 12.35  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg  
 TD 65536  
 SOLVENT MeOD  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 14.09  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.00000000 sec  
 TD0 1

CHANNEL f1  
 SFO1 400.1318812 MHz  
 NUC1 1H  
 P1 10.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300364 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

Figure S36 <sup>13</sup>C NMR spectrum of 6 in CD3OD

wbmp106c c13 and dept



```

Current Data Parameters
NAME      wbmpl06c
EXPNO    22
PROCNO   1

F2 - Acquisition Parameters
Date_    20201102
Time     15.20
INSTRUM spect
PROBHD   5 mm CPDQ1 1H/
PULPROG zgpg
TD        65536
SOLVENT  MeOD
NS        18
DS         4
SWH       29761.904 Hz
FIDRES    0.454121 Hz
AQ         1.1010948 sec
RG         197.72
IM        16.800 usec
DE         18.000 usec
TE         298.3 K
D1         3.00000000 sec
D11        0.05000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1     125.7644413 MHz
NUC1      13C
P1        18.70 usec
PLW1     125.0000000 W

===== CHANNEL f2 =====
SFO2     500.1427500 MHz
NUC2      1H
CPDPRG12 waltz16
PCPD2    100.00 usec
PLW2     4.37519970 W
PLW12    0.05696000 W

F2 - Processing parameters
SI        32768
SF        125.761860 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.20
    
```



Figure S37 MS spectrum of 6

==== LCMSsolution Data Report ====

	Sample Information	System Configuration
Acquired by	: Admin	<<Instrument>> : LC-IT-TOF
Date Acquired	: 2020/11/17 15:03:49	
Sample Name	: wbmp-106c	
Data File	: wbmp-106c.lcd	
Method File	: 阻尼管一级100-1500.lcm	

<Spectrum>

Retention Time:0.600(Scan#:91)  
Spectrum:Averaged 0.333-0.867(51-131)  
Background:Averaged 0.000-0.361(1-55) MS Stage:MS Polarity:Pos SegmentI - EventI Precursor:---- Cutoff:

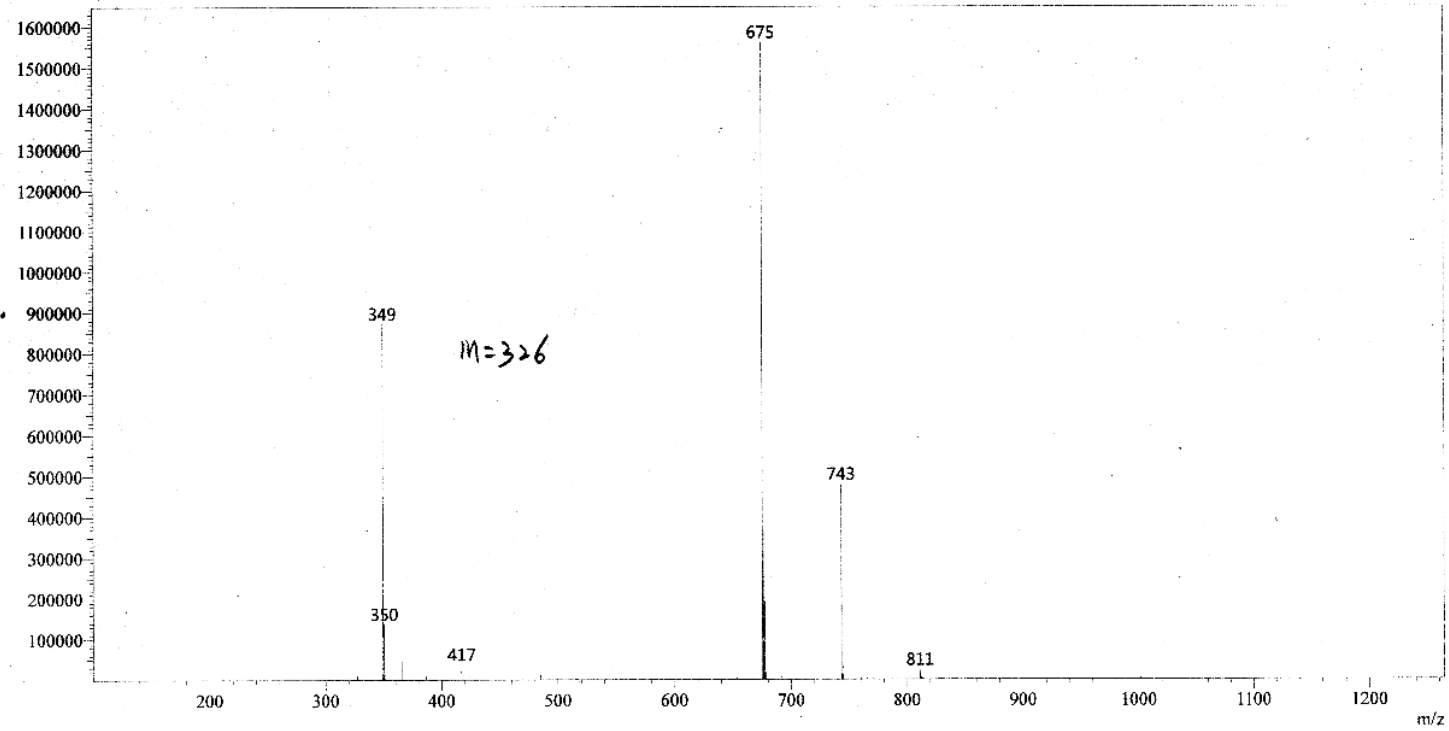
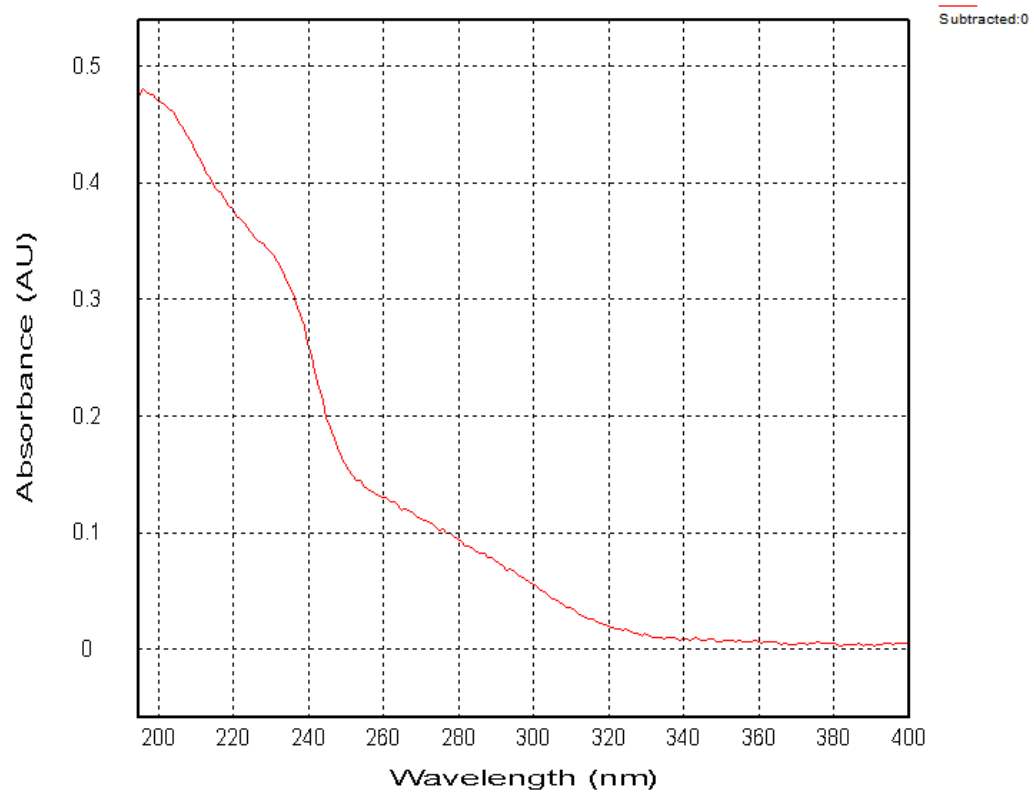
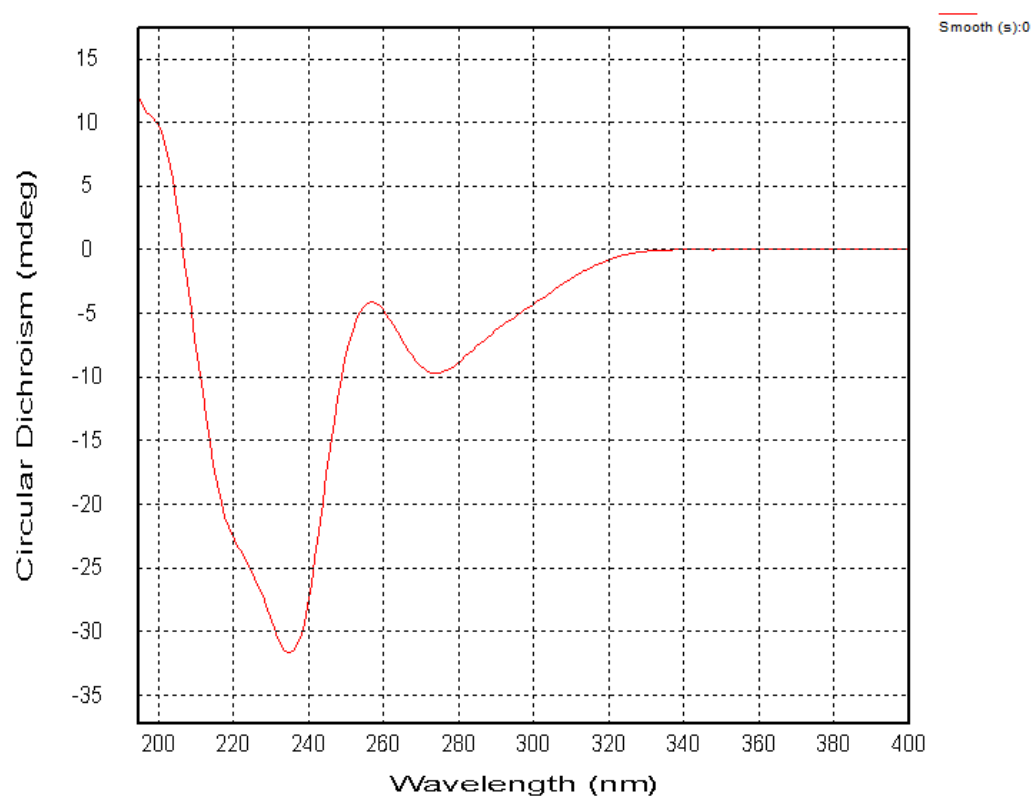


Figure S38 UV and CD spectrum of **6** in MeOH



## Quantum chemical calculation

The initial conformational analysis of the compounds **1-3** and **6** were executed by employing Monte Carlo searching algorithm via the MMFF94 molecular mechanics force field<sup>[1]</sup>, with the aid of the SPARTAN'16 program package, leading to afford a panel of relatively favored conformations in an energy range of 3 kcal/mol above the global minimum. The force field minimum energy conformers thus obtained were subsequently optimized by applying the density functional theory (DFT) with the M06-2X/Def2SVP level in vacuum, implemented in the Gaussian 09 software package<sup>[2]</sup>. Harmonic vibrational frequencies were also performed to confirm no imaginary frequencies of the finally optimized conformers. These predominant conformers were subjected to theoretical calculation of ECD by utilizing Time-dependent density functional theory (TDDFT) calculations at the M06-2X/Def2SVP level in MeOH using the Polarizable Continuum Model (PCM) solvent model. The energies, oscillator strengths, and rotational strengths of each conformers were carried out with Gaussian 09 software package. The oretical calculations of ECD spectra for each conformer were then approximated by the Gaussian distribution. The final ECD spectrum of the individual conformers was summed up on the basis of Boltzmann-weighed population contribution by the SpecDisv1.64<sup>[3]</sup>.

### ECD Computational details of compound **1**

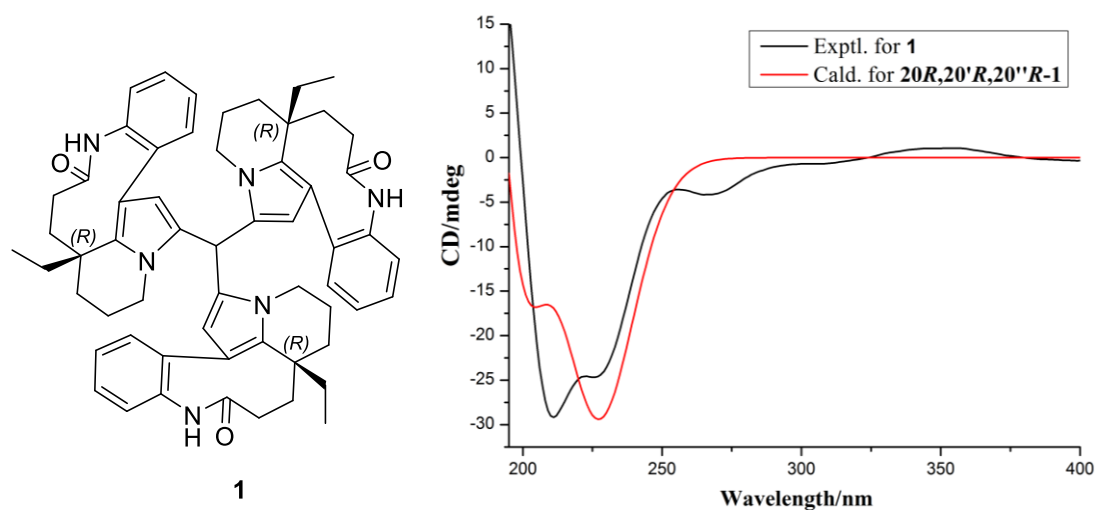
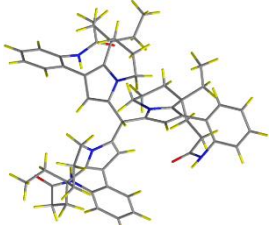
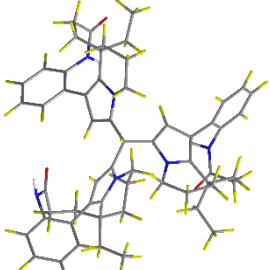
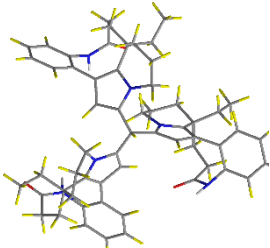
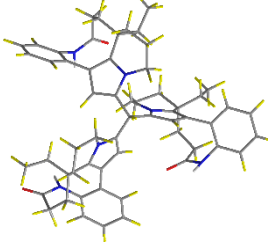
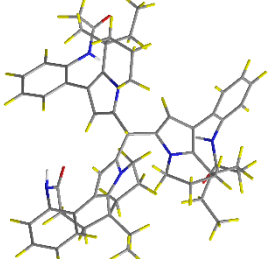


Figure S39. Experimental and calculated ECD of compound **1**

Table S1. M06-2X/Def2SVP optimized lowest energy 3D conformers and energy analysis for **1a-1e**

NO.	3D conformers	G (Hartree)	$\Delta G$ (KJ/mol)	Boltzmann distribution
1a		-2798.766268	0.000000	63.60%
1b		-2798.764952	0.825794	15.76%
1c		-2798.764886	0.867209	14.70%
1d		-2798.764005	1.420039	5.78%
1e		-2798.760619	3.544764	0.16%

## ECD Computational details of compound 2

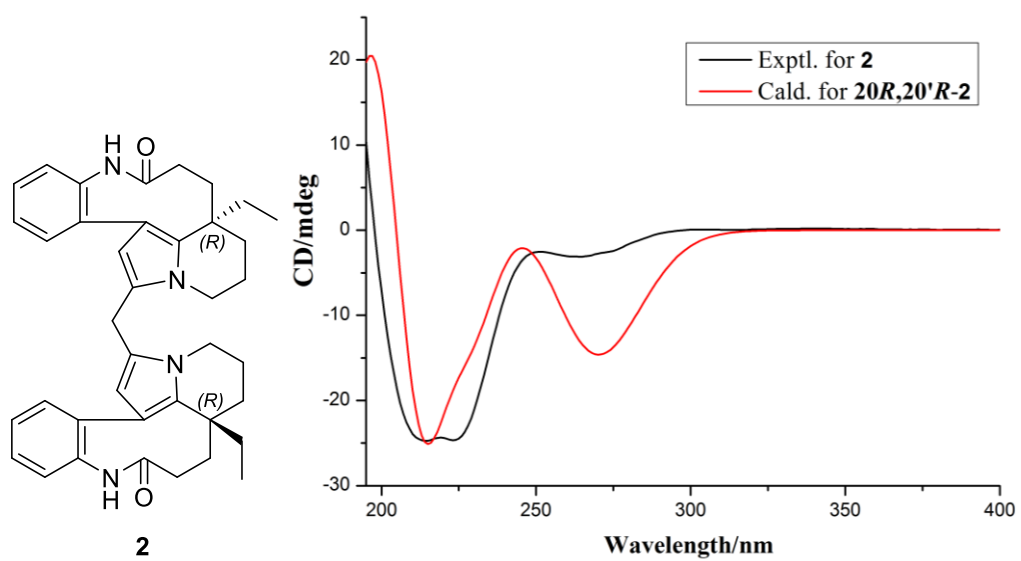
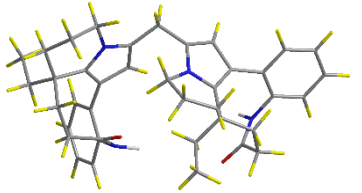
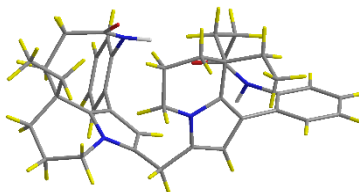
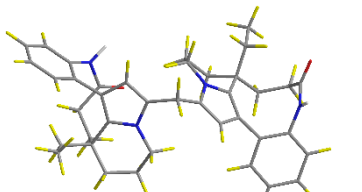
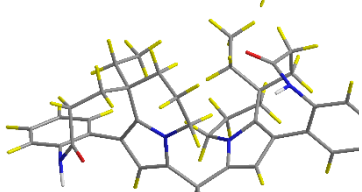
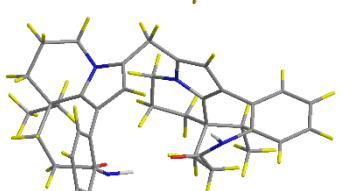


Figure S40. Experimental and calculated ECD of compound **2**

Table S2. M06-2X/Def2SVP optimized lowest energy 3D conformers and energy analysis for 2a-2e

NO.	3D conformers	G (Hartree)	$\Delta G$ (KJ/mol)	Boltzmann distribution
2a		-1879.321776	0.000000	64.15%
2b		-1879.320501	0.001275	16.61%
2c		-1879.320077	0.001699	10.60%
2d		-1879.319321	0.002455	4.76%
2e		-1879.319130	0.002646	3.88%

### ECD Computational details of compound **3**

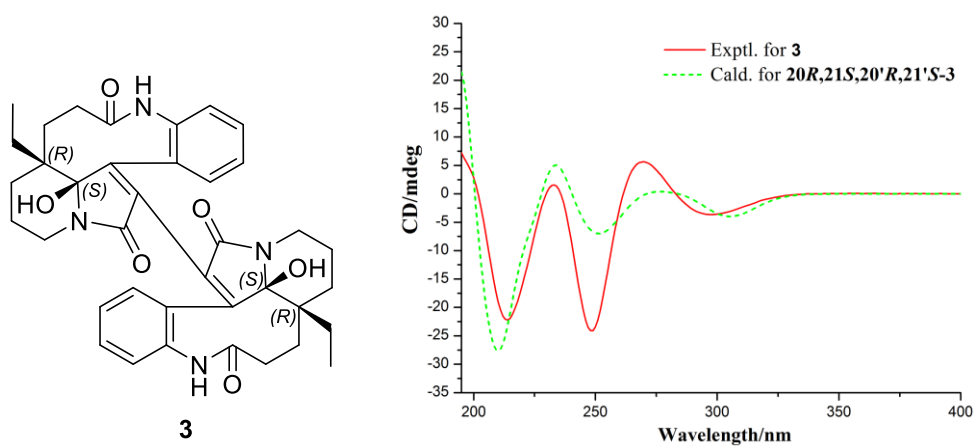


Figure S41. Experimental and calculated ECD of compound **3**

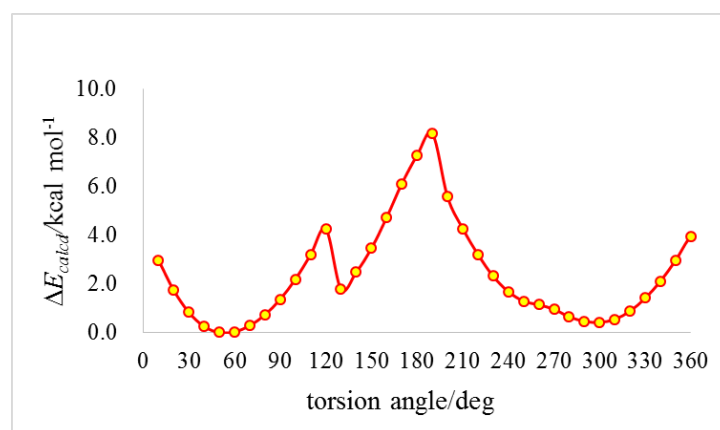
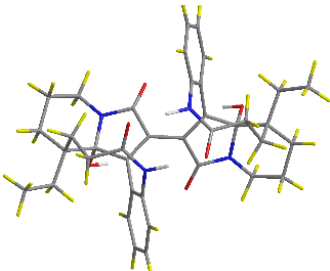
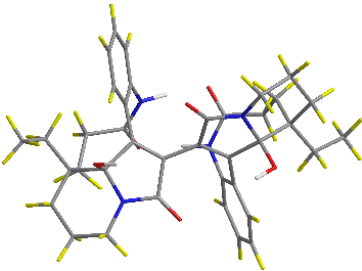
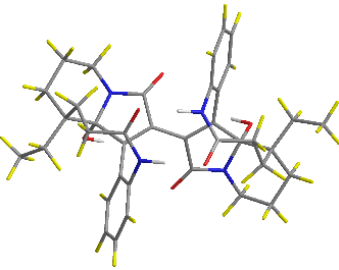
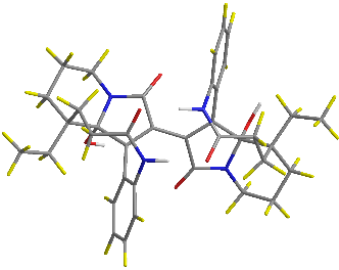
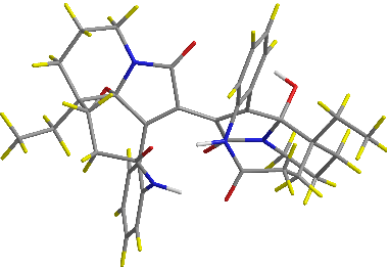


Figure S42. Energy profiles are displayed for the torsion angles of compounds **3**

Table S3. M06-2X/Def2SVP optimized lowest energy 3D conformers and energy analysis for **3a-3e**

NO	3D conformers	G (Hartree)	$\Delta G$ (KJ/mol)	Boltzmann distribution
3a		-2140.681567	0.000000	85.45%
3b		-2140.679151	0.002416	6.60%
3c		-2140.679134	0.002433	6.49%
3d		-2140.677361	0.004206	0.99%
3e		-2140.676651	0.004916	0.47%



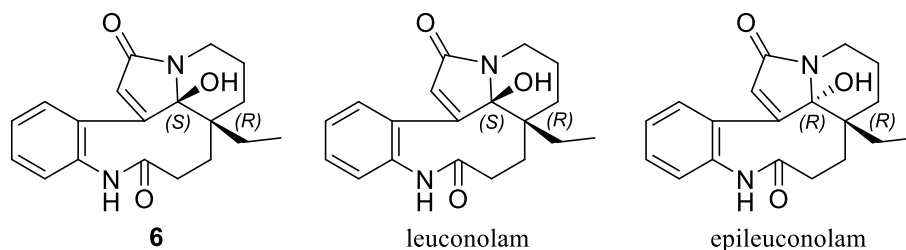


Figure S43. Experimental ECD spectra of **6** and calculated ECD spectra of leuconolam and epileuconolam

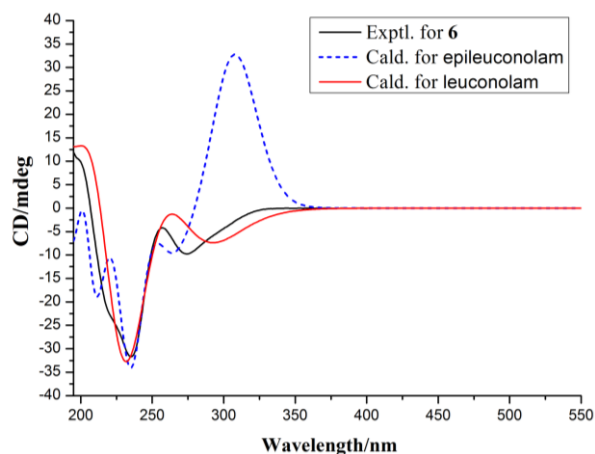


Table S4.  $^{13}\text{C}$  NMR spectroscopic data for compounds **6**, leuconolam and epileuconolam

No.	compound <b>6</b> <sup>a</sup>	leuconolam <sup>b</sup>	epileuconolam <sup>b</sup>
2	180.4 (s)	177.8 (s)	175.8 (s)
3	36.6 (t)	35.3 (t)	37.0 (t)
5	168.4 (s)	166.5 (s)	173.2 (s)
6	<b>129.4 (d)</b>	<b>128.1 (d)</b>	<b>118.1 (d)</b>
7	<b>158.2 (s)</b>	<b>155.6 (s)</b>	<b>164.1 (s)</b>
8	<b>134.8 (s)</b>	<b>133.1 (s)</b>	<b>123.4 (s)</b>
9	130.5 (d)	129.3 (d)	124.2 (d)
10	127.9 (d)	126.6 (d)	121.4 (d)
11	131.2 (d)	129.4 (d)	131.4 (d)
12	<b>127.8 (d)</b>	<b>126.3 (d)</b>	<b>115.8 (d)</b>
13	<b>137.2 (s)</b>	<b>135.0 (s)</b>	<b>148.6 (s)</b>
14	21.2 (t)	19.7 (t)	16.8 (t)
15	33.6 (t)	32.1 (t)	34.1 (t)
16	29.0 (t)	24.5 (t)	26.1 (t)
17	26.9 (t)	25.4 (t)	30.4 (t)
18	7.6 (q)	6.9 (q)	8.2 (q)
19	25.8 (t)	27.3 (t)	33.0 (t)
20	46.7 (s)	44.9 (s)	44.5 (s)
21	95.2 (s)	93.6 (s)	93.6 (s)

<sup>a</sup> recorded in  $\text{CD}_3\text{OD}$ ; <sup>b</sup> in  $\text{CDCl}_3$

Table S5. Cartesian coordinates for the low-energy optimized conformers of **1a-3e** at M06-2X/Def2SVP level

Conformer <b>1a</b>							
C	-6.078091	4.065219	1.992653	C	3.230699	5.141233	-1.649386
C	-5.651631	5.387254	1.871732	H	-7.068774	3.844393	2.392719
C	-4.384779	5.660587	1.36061	H	-6.30664	6.206439	2.171381
C	-3.542771	4.617015	0.974893	H	-4.030535	6.685696	1.244848
C	-3.961146	3.276045	1.092032	H	-5.561443	1.985887	1.717884
C	-5.236182	3.022003	1.610219	H	-1.494498	4.972453	1.146731
N	-2.243744	4.904344	0.461041	H	-3.854206	4.461228	-1.46843
C	-1.799267	4.389619	-0.737314	H	-2.58672	5.022166	-2.559183
C	-2.999203	2.190829	0.767339	H	-3.272188	2.967356	-3.521705
C	-2.84463	4.235162	-1.832745	H	-1.701584	2.705211	-2.748206
C	-2.766168	2.888169	-2.54585	H	-1.913695	2.089209	2.730288
C	-3.37612	1.669706	-1.803401	H	-3.627292	-0.449151	-2.236742
C	-2.746612	1.527322	-0.429993	H	-3.418533	0.573375	-3.666523
N	-1.654883	0.708034	-0.229327	H	-1.421103	-0.854017	-3.223587
C	-1.205168	0.847423	1.062287	H	-0.972742	0.854726	-3.043723
C	-2.013666	1.758536	1.69832	H	-0.053329	-0.288629	-1.121492
C	-3.065508	0.410428	-2.63597	H	-1.52301	-1.268053	-0.930012
C	-1.587712	0.048302	-2.618821	H	-5.124292	2.786446	-1.166514
C	-1.146291	-0.268327	-1.201387	H	-5.288118	1.988963	-2.726304
C	-4.904948	1.850779	-1.70093	H	-5.687072	-0.19587	-1.649707
C	-5.658799	0.708088	-1.02518	H	-5.186951	0.439038	-0.067427
O	-0.622949	4.172664	-0.941858	H	-6.698844	0.999117	-0.819858
O	-2.236866	-3.41638	-2.860246	H	-5.817801	-3.484732	-0.533266
C	-5.066816	-4.031693	0.053809	H	-5.022372	-5.055022	-0.348346
C	-3.717356	-3.321684	-0.031272	H	-5.44181	-4.097068	1.086093
C	-2.486835	-1.629964	2.242826	H	-3.832225	-2.304166	0.36522
C	-3.252329	-2.845642	2.831325	H	-3.446939	-3.184266	-1.08457
C	-2.916752	-4.209175	2.200646	H	-2.079224	-1.011403	3.052216
C	0.736018	-2.234661	0.715654	H	-3.163567	-0.970338	1.678044
C	-0.147582	-1.386502	1.340401	H	-3.072144	-2.897493	3.91357
N	-1.362376	-2.028047	1.403216	H	-4.326629	-2.647482	2.70826
C	-1.298231	-3.228533	0.736302	H	-3.768588	-4.893348	2.334166
C	-2.561757	-4.05617	0.705605	H	-2.055598	-4.670215	2.70868
C	-2.297954	-5.413169	0.036904	H	1.769039	-2.004853	0.461287
C	-2.290638	-5.414756	-1.510557	H	-1.363211	-5.835257	0.430916
C	0.026204	-3.419286	0.347973	H	-3.092969	-6.111774	0.34177
C	-1.605973	-4.285294	-2.287167	H	-1.843275	-6.363545	-1.844409
N	-0.247529	-4.351161	-2.405471	H	-3.325375	-5.39116	-1.876434
C	1.613616	-5.307639	0.655042	H	0.154375	-3.564436	-2.909505
C	0.726032	-4.617334	-0.183707	H	1.727759	-4.963353	1.684526

C	0.598906	-5.059257	-1.510576	H	1.189117	-6.471867	-3.008442
C	1.31965	-6.163433	-1.97021	H	2.751058	-7.701223	-1.484544
C	2.188413	-6.841109	-1.119824	H	3.019175	-6.92521	0.8714
C	2.33635	-6.406285	0.197041	H	-0.10651	0.261565	2.735747
C	-0.036998	0.090688	1.644829	H	7.553918	-0.006479	1.961082
O	6.420248	-0.338236	-1.768717	H	6.631264	-0.745608	3.283705
C	6.801006	-0.772998	2.197107	H	7.244768	-1.749012	1.957127
C	5.511398	-0.569536	1.402729	H	4.778529	-1.323915	1.721759
C	2.710383	-0.491177	2.836633	H	5.704423	-0.789464	0.346398
C	3.799238	0.130754	3.74041	H	1.753618	-0.553761	3.369375
C	4.668298	1.178088	3.032525	H	2.970182	-1.525655	2.568065
C	1.470199	1.586338	0.147695	H	3.330465	0.589488	4.621934
C	1.262095	0.665556	1.143486	H	4.434243	-0.685106	4.115079
N	2.49198	0.290195	1.632134	H	5.633476	1.263349	3.554124
C	3.499149	0.943873	0.94426	H	4.191523	2.16941	3.084274
C	4.897702	0.848221	1.535691	H	0.701006	2.102488	-0.425993
C	5.844062	1.91666	0.943523	H	5.272796	2.84041	0.779888
C	6.661834	1.550759	-0.311902	H	6.586987	2.167693	1.717229
C	2.879318	1.776541	0.011747	H	7.046309	2.486962	-0.747833
C	6.004971	0.753289	-1.431223	H	7.529789	0.940092	-0.034011
N	4.943694	1.32538	-2.062037	H	4.535304	0.750089	-2.793205
C	2.809021	4.103542	-0.824993	H	1.984034	4.262435	-0.129189
C	3.401997	2.83038	-0.886628	H	5.620162	3.467577	-3.397987
C	4.405562	2.62337	-1.847937	H	4.603116	5.74567	-3.210953
C	4.836341	3.672323	-2.666591	H	2.744659	6.115281	-1.577562
C	4.261992	4.935043	-2.565759				

Conformer <b>1b</b>							
C	6.116145	-4.084926	1.962969	C	-3.129527	-5.073836	-1.68193
C	5.680369	-5.405352	1.858935	H	7.113293	-3.866689	2.34811
C	4.405335	-5.675345	1.366797	H	6.334385	-6.225916	2.156949
C	3.564571	-4.629941	0.98328	H	4.043655	-6.699288	1.264472
C	3.992085	-3.290572	1.083735	H	5.608026	-2.004927	1.677794
C	5.275376	-3.039944	1.582923	H	1.516327	-4.977637	1.183461
N	2.257463	-4.913926	0.488623	H	3.847196	-4.493708	-1.463557
C	1.800823	-4.413751	-0.710089	H	2.56635	-5.059953	-2.53592
C	3.032378	-2.20185	0.764241	H	3.242691	-3.015016	-3.521746
C	2.833974	-4.268449	-1.817972	H	1.683328	-2.741657	-2.730181
C	2.749882	-2.926483	-2.539975	H	1.980424	-2.075257	2.74393
C	3.37386	-1.704104	-1.815945	H	3.62907	0.408596	-2.274288
C	2.765156	-1.547044	-0.434589	H	3.390427	-0.626471	-3.69033
N	1.683029	-0.717263	-0.222867	H	1.406625	0.814679	-3.229305
C	1.254262	-0.841658	1.077575	H	0.953478	-0.889277	-3.020255

C	2.066163	-1.75349	1.707914	H	0.076224	0.288784	-1.096715
C	3.055724	-0.451454	-2.655676	H	1.559222	1.25348	-0.941511
C	1.580359	-0.080984	-2.616677	H	5.127086	-2.821965	-1.195083
C	1.167275	0.255069	-1.195383	H	5.271888	-2.037016	-2.763119
C	4.903522	-1.889649	-1.733605	H	5.692565	0.155007	-1.707717
C	5.671087	-0.744896	-1.077084	H	5.215156	-0.468407	-0.113775
O	0.621681	-4.201405	-0.90613	H	6.713322	-1.037874	-0.886169
O	2.197376	3.408103	-2.909997	H	5.488897	4.109456	0.959608
C	5.09107	4.038715	-0.063729	H	5.829361	3.489557	-0.664684
C	3.740804	3.326969	-0.115366	H	5.036701	5.060002	-0.469822
C	2.56269	1.644756	2.193931	H	3.865798	2.311582	0.283597
C	3.340106	2.863911	2.759051	H	3.447322	3.184085	-1.161724
C	2.989027	4.223982	2.129536	H	2.174031	1.02989	3.015257
C	-0.69586	2.242701	0.742506	H	3.22719	0.982949	1.6173
C	0.203274	1.396779	1.347655	H	3.184174	2.920785	3.844798
N	1.419122	2.037939	1.377925	H	4.411565	2.666077	2.612893
C	1.338912	3.235406	0.706649	H	3.842837	4.909679	2.240681
C	2.600922	4.063596	0.643488	H	2.138918	4.686552	2.654499
C	2.321202	5.417653	-0.024662	H	-1.736687	2.010822	0.523633
C	2.278788	5.412956	-1.571504	H	1.395445	5.840915	0.388858
C	0.005122	3.424897	0.350733	H	3.122443	6.117936	0.259314
C	1.578556	4.278794	-2.326798	H	1.822329	6.359579	-1.899146
N	0.217462	4.341457	-2.413738	H	3.304961	5.389432	-1.960768
C	-1.577896	5.313174	0.681344	H	-0.193873	3.550611	-2.903482
C	-0.707465	4.619165	-0.172287	H	-1.66942	4.97477	1.714995
C	-0.609792	5.05352	-1.504254	H	-1.233637	6.457136	-2.996857
C	-1.341673	6.154368	-1.954363	H	-2.763627	7.693851	-1.446537
C	-2.192702	6.836025	-1.089331	H	-2.980111	6.930654	0.919017
C	-2.311697	6.408417	0.232855	H	0.171853	-0.234263	2.760539
C	0.09481	-0.078293	1.668218	H	-7.479113	0.382322	1.184478
O	-7.102442	-0.2171	-1.626337	H	-6.713166	1.404101	2.425262
C	-6.694139	1.130598	1.359164	H	-6.971238	2.021722	0.779853
C	-5.323054	0.626751	0.923256	H	-4.560895	1.37803	1.180883
C	-2.496396	0.290002	3.071343	H	-5.270478	0.564558	-0.167498
C	-3.925353	0.515576	3.550563	H	-1.992687	-0.403075	3.767436
C	-4.845003	-0.601411	3.078444	H	-1.923981	1.229251	3.072071
C	-1.443724	-1.565086	0.189569	H	-3.912832	0.565915	4.648707
C	-1.21092	-0.655617	1.186677	H	-4.303751	1.486602	3.201898
N	-2.423228	-0.303573	1.7381	H	-5.867398	-0.430243	3.446793
C	-3.444546	-0.979869	1.089442	H	-4.511804	-1.566197	3.498559
C	-4.873806	-0.726819	1.535548	H	-0.689513	-2.056079	-0.424489
C	-5.79391	-1.946175	1.209709	H	-5.144655	-2.829184	1.132388
C	-6.777248	-1.928205	0.017602	H	-6.419904	-2.129463	2.09618

C	-2.85722	-1.77565	0.108774	H	-6.926997	-2.9699	-0.307749
C	-6.399564	-1.108648	-1.200523	H	-7.759729	-1.544176	0.315679
N	-5.184676	-1.398684	-1.764738	H	-4.980694	-0.838734	-2.58853
C	-2.714508	-4.038754	-0.853406	H	-1.818276	-4.165442	-0.244461
C	-3.402223	-2.810496	-0.799753	H	-5.79593	-3.535083	-3.119366
C	-4.506992	-2.649274	-1.652617	H	-4.595629	-5.72467	-3.13872
C	-4.930764	-3.701722	-2.474295	H	-2.563313	-6.006221	-1.697851
C	-4.256371	-4.916365	-2.489605				

Conformer <b>1c</b>							
C	-6.508321	3.253626	2.202942	C	2.424512	5.482357	-1.684205
C	-6.237072	4.619415	2.122311	H	-7.46032	2.907966	2.608503
C	-5.020265	5.052414	1.601087	H	-6.975113	5.348086	2.460288
C	-4.071552	4.12519	1.16671	H	-4.787572	6.114646	1.515759
C	-4.332685	2.742818	1.243405	H	-5.764152	1.257298	1.836827
C	-5.561355	2.327723	1.769832	H	-2.081244	4.726838	1.333089
N	-2.821862	4.57812	0.650865	H	-4.377294	4.002151	-1.29988
C	-2.327035	4.16651	-0.565835	H	-3.18794	4.749851	-2.368823
C	-3.265178	1.779718	0.867548	H	-3.564198	2.666216	-3.413035
C	-3.34695	3.915354	-1.667606	H	-2.015728	2.537542	-2.577583
C	-3.101045	2.607543	-2.416107	H	-2.148765	1.737448	2.81508
C	-3.607727	1.317223	-1.720436	H	-3.708363	-0.793306	-2.213894
C	-2.957537	1.186989	-0.353864	H	-3.545403	0.272519	-3.618969
N	-1.780524	0.484568	-0.188778	H	-1.457102	-1.003809	-3.209852
C	-1.332172	0.630193	1.102296	H	-1.160178	0.731235	-3.007844
C	-2.227683	1.425697	1.775419	H	-0.106356	-0.336175	-1.124625
C	-3.197259	0.111212	-2.588435	H	-1.463374	-1.460145	-0.911696
C	-1.694886	-0.131757	-2.584756	H	-5.422808	0.438256	-0.976129
C	-1.197396	-0.424539	-1.18139	H	-5.44147	2.19119	-0.94578
C	-5.143942	1.330714	-1.560847	H	-5.765668	0.465285	-3.476352
C	-5.945204	1.356826	-2.85955	H	-7.020751	1.389903	-2.636607
O	-1.133696	4.111047	-0.781969	H	-5.712921	2.242693	-3.468806
O	-1.884304	-3.934541	-2.817301	H	-4.710504	-5.053418	1.311715
C	-4.401248	-4.949454	0.260927	H	-5.26645	-4.568659	-0.299256
C	-3.212117	-4.005275	0.094925	H	-4.185413	-5.958065	-0.122285
C	-2.192981	-2.063166	2.284138	H	-3.493034	-3.017851	0.48509
C	-2.705731	-3.381226	2.923535	H	-3.022962	-3.844999	-0.972826
C	-2.156802	-4.674537	2.295977	H	-1.869999	-1.363789	3.065178
C	1.028307	-2.140072	0.643843	H	-2.997056	-1.546551	1.738114
C	0.041071	-1.447954	1.304196	H	-2.47336	-3.377335	3.997075
N	-1.050601	-2.277372	1.403921	H	-3.802385	-3.380488	2.84681
C	-0.812843	-3.456152	0.73508	H	-2.861326	-5.499255	2.48293

C	-1.907672	-4.497519	0.781685	H	-1.202555	-4.958675	2.76613
C	-1.435147	-5.805592	0.129685	H	2.002144	-1.745703	0.359318
C	-1.506206	-5.858415	-1.414499	H	-0.420978	-6.039132	0.481734
C	0.509825	-3.425322	0.296317	H	-2.073251	-6.625451	0.495325
C	-1.0787	-4.649427	-2.251813	H	-0.911147	-6.721529	-1.750508
N	0.262093	-4.461875	-2.428031	H	-2.545118	-6.033339	-1.722825
C	2.424912	-4.989889	0.537566	H	0.488274	-3.631197	-2.969336
C	1.383211	-4.491069	-0.259261	H	2.530362	-4.604429	1.55334
C	1.266612	-4.98301	-1.56949	H	2.019705	-6.306429	-3.075295
C	2.14841	-5.952823	-2.05132	H	3.856249	-7.198266	-1.624427
C	3.169139	-6.442658	-1.241901	H	4.107557	-6.324416	0.699185
C	3.307452	-5.953602	0.056829	H	-0.129275	0.155596	2.736138
C	-0.060154	0.022157	1.640078	H	7.418344	-0.755199	1.879712
O	6.427233	0.568579	-1.808432	H	7.467708	1.013555	1.910481
C	6.837368	0.141031	2.137254	H	6.672469	0.126691	3.224868
C	5.526728	0.164488	1.351397	H	4.912819	-0.691665	1.664734
C	2.751003	-0.177311	2.80213	H	5.74322	-0.014341	0.292007
C	3.748677	0.581478	3.706392	H	1.818645	-0.383033	3.34179
C	4.449428	1.752024	3.005908	H	3.152982	-1.160226	2.51528
C	1.207918	1.725555	0.139832	H	3.228423	0.956111	4.598733
C	1.138283	0.78227	1.133702	H	4.498568	-0.13939	4.06307
N	2.412605	0.581552	1.611395	H	5.395585	1.972343	3.522602
C	3.312819	1.373149	0.91991	H	3.832952	2.662156	3.072027
C	4.714265	1.476007	1.503876	H	0.369605	2.133087	-0.423875
C	5.490125	2.68013	0.922917	H	4.785886	3.508285	0.765908
C	6.357537	2.456115	-0.332504	H	6.184729	3.033509	1.701498
C	2.575376	2.111994	-0.005941	H	6.589836	3.444114	-0.761801
C	5.837462	1.572181	-1.45812	H	7.310957	1.988706	-0.056739
N	4.689952	1.963445	-2.076248	H	4.384072	1.338794	-2.816969
C	2.162461	4.398553	-0.852993	H	1.320403	4.436908	-0.16057
C	2.938529	3.22747	-0.908433	H	5.038193	4.174875	-3.423884
C	3.962493	3.167139	-1.868602	H	3.691298	6.2758	-3.250763
C	4.232075	4.264227	-2.693448	H	1.797354	6.372585	-1.617828
C	3.475145	5.427327	-2.600216				

Conformer <b>1d</b>							
C	-6.536887	3.310519	2.15093	C	2.44628	5.445005	-1.597278
C	-6.25055	4.674184	2.088641	H	-7.499125	2.97068	2.53676
C	-5.02077	5.099802	1.592375	H	-6.986859	5.407009	2.421359
C	-4.074384	4.167128	1.164757	H	-4.776016	6.160386	1.521493
C	-4.350502	2.786792	1.223297	H	-5.806867	1.310321	1.7776
C	-5.592082	2.379201	1.72473	H	-2.080477	4.747486	1.367911
N	-2.812014	4.611948	0.673235	H	-4.344627	4.06896	-1.306015

C	-2.303936	4.208808	-0.540223	H	-3.133523	4.818006	-2.349352
C	-3.286226	1.816604	0.856399	H	-3.510658	2.747507	-3.419768
C	-3.309591	3.977737	-1.659188	H	-1.975362	2.599514	-2.563795
C	-3.062328	2.67569	-2.416984	H	-2.207148	1.742102	2.823914
C	-3.588155	1.382235	-1.74178	H	-3.695405	-0.722044	-2.260595
C	-2.962356	1.233426	-0.365434	H	-3.49902	0.35809	-3.650389
N	-1.795681	0.516995	-0.185887	H	-1.427096	-0.937092	-3.218814
C	-1.370191	0.643987	1.115103	H	-1.121214	0.792617	-2.987589
C	-2.269556	1.442172	1.779691	H	-0.113157	-0.313553	-1.09895
C	-3.170925	0.182735	-2.615587	H	-1.487649	-1.422713	-0.92698
C	-1.670727	-0.071696	-2.586726	H	-5.420766	0.507443	-1.036708
C	-1.20389	-0.387231	-1.177969	H	-5.429023	2.26009	-0.988667
C	-5.126791	1.404001	-1.607596	H	-5.721015	0.562339	-3.542281
C	-5.906182	1.448246	-2.919047	H	-6.985106	1.484705	-2.713668
O	-1.108079	4.144675	-0.74071	H	-5.659258	2.339257	-3.514867
O	-1.880503	-3.893274	-2.877914	H	-4.269915	-5.90104	-0.251751
C	-4.483591	-4.892184	0.132022	H	-4.820702	-4.998636	1.173955
C	-3.279556	-3.961292	0.002102	H	-5.329703	-4.497875	-0.447631
C	-2.292991	-2.046262	2.231155	H	-3.558488	-2.973086	0.391805
C	-2.838535	-3.362585	2.846412	H	-3.061969	-3.796486	-1.059527
C	-2.287977	-4.657583	2.224295	H	-1.981508	-1.357319	3.025853
C	0.969214	-2.152566	0.675837	H	-3.076175	-1.515122	1.668857
C	-0.026717	-1.452271	1.314173	H	-2.635716	-3.369127	3.925904
N	-1.130988	-2.267994	1.378608	H	-3.932576	-3.348276	2.739654
C	-0.890805	-3.444743	0.706468	H	-3.005959	-5.475687	2.387563
C	-1.998642	-4.473313	0.718006	H	-1.349092	-4.955452	2.71642
C	-1.525029	-5.783073	0.070078	H	1.956758	-1.767739	0.427874
C	-1.558957	-5.827519	-1.475562	H	-0.522442	-6.029959	0.44536
C	0.443496	-3.427845	0.303612	H	-2.180961	-6.597556	0.415635
C	-1.097497	-4.619053	-2.295052	H	-0.965402	-6.69556	-1.801456
N	0.249398	-4.443384	-2.434035	H	-2.59178	-5.989184	-1.8104
C	2.335375	-5.014559	0.578583	H	0.49757	-3.611743	-2.964086
C	1.317837	-4.499354	-0.238885	H	2.42115	-4.636858	1.599081
C	1.226859	-4.981327	-1.55493	H	2.000693	-6.303425	-3.051305
C	2.109283	-5.957779	-2.022277	H	3.792551	-7.2253	-1.563734
C	3.105288	-6.464186	-1.192523	H	3.998893	-6.368828	0.770932
C	3.218451	-5.984857	0.112293	H	-0.191926	0.133402	2.763869
C	-0.113846	0.016292	1.666722	H	6.818375	-0.65556	2.313206
O	6.950297	1.07707	-1.7197	H	7.123548	-1.205579	0.651849
C	6.753576	-0.364426	1.253568	H	7.444887	0.472777	1.08715
C	5.327795	-0.013277	0.844161	H	4.660582	-0.851826	1.095988
C	2.519847	-0.050213	3.036891	H	5.253122	0.062194	-0.244547
C	3.972829	-0.11186	3.492693	H	1.94759	0.565055	3.752848

C	4.74643	1.114037	3.029122	H	2.064566	-1.051466	3.026801
C	1.20919	1.714969	0.20396	H	3.983383	-0.182127	4.589769
C	1.101629	0.766328	1.185856	H	4.458167	-1.024912	3.120538
N	2.355346	0.553538	1.716269	H	5.787734	1.058446	3.37959
C	3.278511	1.358949	1.068274	H	4.308765	2.025309	3.4722
C	4.734772	1.268166	1.488601	H	0.393057	2.123605	-0.390823
C	5.50166	2.591345	1.171787	H	4.753608	3.39441	1.120071
C	6.460659	2.707037	-0.034636	H	6.116979	2.831457	2.052179
C	2.586037	2.09597	0.111052	H	6.486708	3.765077	-0.34006
C	6.157656	1.873701	-1.264327	H	7.484977	2.430767	0.241202
N	4.908106	2.033943	-1.803803	H	4.754107	1.469929	-2.6356
C	2.167569	4.349384	-0.789734	H	1.274309	4.35735	-0.163768
C	2.992099	3.207527	-0.779461	H	5.245579	4.258547	-3.11437
C	4.093069	3.194963	-1.652019	H	3.801293	6.294905	-3.059044
C	4.37846	4.308567	-2.452543	H	1.776945	6.306372	-1.579904
C	3.568787	5.437536	-2.426027				

Conformer <b>1e</b>							
C	-5.811176	4.580184	2.054594	C	3.234603	5.313699	-1.359558
C	-5.340654	5.787061	1.541615	H	-6.75013	4.552002	2.609559
C	-4.130967	5.81938	0.847321	H	-5.909281	6.706181	1.688873
C	-3.405165	4.646552	0.654396	H	-3.730066	6.752252	0.448604
C	-3.886335	3.412775	1.144341	H	-5.455684	2.458189	2.259846
C	-5.085668	3.403489	1.860337	H	-1.33638	4.549276	0.564506
N	-2.151189	4.680167	-0.033266	H	-3.68623	4.965534	-2.1372
C	-1.974233	4.038803	-1.241932	H	-2.763228	3.858912	-3.173393
C	-3.045256	2.21321	0.903682	H	-4.910782	3.231923	-1.091191
C	-3.182859	3.987519	-2.167944	H	-4.855163	2.80144	-2.791889
C	-4.233676	2.895306	-1.886095	H	-1.842332	2.170568	2.799541
C	-3.698214	1.488719	-1.556154	H	-3.448851	0.869958	-3.612433
C	-2.88127	1.492762	-0.275405	H	-2.062338	1.77071	-2.951373
N	-1.782952	0.671245	-0.11601	H	-2.770699	-1.110381	-2.148426
C	-1.244911	0.866135	1.135697	H	-1.486975	-0.635963	-3.235713
C	-2.008293	1.806195	1.787597	H	-0.277847	0.562623	-1.553363
C	-2.814874	1.000155	-2.721181	H	-0.735672	-1.002079	-0.854024
C	-2.079937	-0.286546	-2.379174	H	-5.460225	0.561495	-2.376786
C	-1.131067	-0.048602	-1.219002	H	-4.52008	-0.507159	-1.340383
C	-4.905494	0.520011	-1.423871	H	-6.312018	1.770389	-0.294811
C	-5.86256	0.766899	-0.264491	H	-6.683683	0.036083	-0.290124
O	-0.890078	3.601688	-1.57215	H	-5.345149	0.659817	0.70013
O	-2.265836	-3.706816	-3.008964	H	-5.746212	-3.636683	-0.632998
C	-4.993001	-4.131564	-0.00398	H	-4.921343	-5.175799	-0.343597
C	-3.656458	-3.400883	-0.114615	H	-5.38094	-4.143254	1.0254



C	-2.514962	-1.619896	2.158508	H	-3.788496	-2.368421	0.238149
C	-3.268606	-2.840951	2.745368	H	-3.384908	-3.308997	-1.172871
C	-2.86638	-4.200578	2.153734	H	-2.146072	-0.97822	2.967309
C	0.770441	-2.187581	0.757926	H	-3.187907	-0.987358	1.559071
C	-0.14561	-1.355557	1.358063	H	-3.127295	-2.866837	3.834329
N	-1.356589	-2.007241	1.359958	H	-4.342836	-2.677875	2.578212
C	-1.254592	-3.203811	0.687368	H	-3.691817	-4.91622	2.287423
C	-2.490977	-4.07584	0.659651	H	-1.997074	-4.614718	2.687994
C	-2.180728	-5.457418	0.059977	H	1.809555	-1.942026	0.548032
C	-2.196094	-5.564166	-1.48178	H	-1.226188	-5.818921	0.466498
C	0.087008	-3.372463	0.345162	H	-2.943241	-6.165448	0.421267
C	-1.582109	-4.455331	-2.337441	H	-1.705051	-6.510025	-1.759215
N	-0.220675	-4.38859	-2.389279	H	-3.234305	-5.616579	-1.83387
C	1.767458	-5.174242	0.643263	H	0.132626	-3.616589	-2.948614
C	0.822838	-4.547314	-0.184042	H	1.897528	-4.796338	1.658968
C	0.673762	-5.032354	-1.493799	H	1.279959	-6.462699	-2.967975
C	1.427988	-6.119216	-1.943078	H	2.937658	-7.581944	-1.462131
C	2.35122	-6.735241	-1.103564	H	3.247867	-6.722955	0.860981
C	2.522717	-6.254053	0.194168	H	-0.12623	0.253411	2.790981
C	-0.058953	0.117977	1.694618	H	6.712039	-1.496692	2.18545
O	6.922623	0.26826	-1.847095	H	6.86807	-2.067292	0.510493
C	6.651498	-1.187081	1.130814	H	7.453457	-0.460585	0.942013
C	5.279701	-0.622898	0.779666	H	4.505898	-1.359863	1.043131
C	2.558317	-0.289114	3.042235	H	5.18011	-0.515195	-0.304451
C	3.995393	-0.570236	3.464522	H	2.102312	0.405532	3.769328
C	4.933987	0.53461	2.999923	H	1.957887	-1.210067	3.046277
C	1.452248	1.693011	0.273481	H	4.016882	-0.658245	4.560189
C	1.235075	0.724906	1.218218	H	4.332611	-1.539395	3.070892
N	2.456622	0.334081	1.723356	H	5.963164	0.315436	3.321086
C	3.469158	1.034945	1.087469	H	4.65027	1.492393	3.469477
C	4.905661	0.719253	1.463147	H	0.692335	2.212215	-0.311483
C	5.858571	1.911819	1.140274	H	5.2488	2.825992	1.151513
C	6.764718	1.912997	-0.112987	H	6.547481	2.018251	1.992053
C	2.867628	1.894772	0.174627	H	6.940331	2.962733	-0.396691
C	6.28615	1.170498	-1.346483	H	7.745502	1.475514	0.106302
N	5.064438	1.548836	-1.839134	H	4.7885	1.041611	-2.675875
C	2.812667	4.239515	-0.586408	H	1.989418	4.366138	0.117793
C	3.416373	2.971607	-0.680645	H	5.693891	3.741644	-3.099396
C	4.454532	2.817475	-1.613785	H	4.62897	5.988748	-2.873159
C	4.883645	3.90448	-2.385834	H	2.740056	6.280659	-1.257096
C	4.285773	5.152657	-2.262657				

Conformer <b>2a</b>							
C	3.592077	3.609541	-2.362448	H	4.047583	4.038428	-3.256165
C	3.189742	4.437776	-1.315227	H	3.330862	5.517361	-1.38039
C	2.605195	3.880495	-0.18132	H	2.284758	4.505369	0.653227
C	2.418523	2.49967	-0.090672	H	3.692828	1.583424	-3.101937
C	2.817115	1.651246	-1.14147	H	0.786151	1.988413	1.123101
C	3.400143	2.232397	-2.274835	H	4.349454	1.702566	1.239927
N	1.802589	1.950685	1.069152	H	4.152579	1.218626	2.926235
C	2.378385	1.004893	1.870199	H	5.454847	-0.526978	2.072946
C	2.508805	0.197489	-1.095829	H	3.805385	-1.157218	2.183087
C	3.897588	0.945002	1.890854	H	0.476873	0.235623	-2.052196
C	4.448455	-0.45699	1.629244	H	5.436904	-2.621057	-0.866281
C	4.572171	-0.903859	0.14862	H	5.978979	-2.40955	0.805426
C	3.22664	-0.86337	-0.555131	H	4.456753	-4.371475	0.629552
N	2.466761	-2.005361	-0.742803	H	3.650605	-3.116443	1.575836
C	1.293377	-1.689603	-1.385785	H	2.040252	-3.922912	-0.029005
C	1.29271	-0.332387	-1.609675	H	3.212345	-3.862786	-1.358807
C	5.098195	-2.353447	0.14713	H	5.255048	1.049837	-0.496456
C	4.036337	-3.357382	0.57419	H	6.538175	-0.04244	0.010554
C	2.895357	-3.360325	-0.428783	H	4.928566	-0.431581	-2.58786
C	5.596794	0.00741	-0.563437	H	6.447104	0.489369	-2.499922
C	5.869743	-0.318634	-2.028857	H	6.448175	-1.245285	-2.150748
O	1.717357	0.297303	2.609526	H	-2.652903	1.711672	3.76429
O	-3.006444	3.218761	0.199829	H	-1.333925	0.591945	4.177376
C	-1.650091	1.369327	3.467134	H	-0.961863	2.21711	3.592472
C	-1.611	0.874554	2.02284	H	-0.593814	0.5098	1.824165
C	-0.246575	-1.829052	1.216165	H	-1.775179	1.721713	1.345269
C	-0.899968	-1.880714	2.616606	H	0.20241	-2.802092	0.974305
C	-2.37003	-1.4466	2.647201	H	0.571134	-1.093793	1.211083
C	-2.294249	-1.735467	-1.761235	H	-0.81389	-2.89609	3.027408
C	-1.121257	-2.046718	-1.116748	H	-0.305263	-1.223063	3.266214
N	-1.197151	-1.529349	0.152349	H	-2.64671	-1.17764	3.678058
C	-2.369558	-0.831741	0.318627	H	-3.032088	-2.273672	2.34444
C	-2.625676	-0.253457	1.696075	H	-2.548405	-1.982394	-2.78977
C	-4.077758	0.239993	1.849096	H	-4.749634	-0.467392	1.343124
C	-4.3928	1.692502	1.427803	H	-4.340295	0.180338	2.917368
C	-3.10641	-0.980932	-0.856392	H	-5.487402	1.787846	1.343553
C	-3.78144	2.283281	0.160635	H	-4.064202	2.384272	2.213235
N	-4.183342	1.762526	-1.033185	H	-3.722584	2.171717	-1.841035
C	-5.39893	-1.722878	-1.435815	H	-5.006412	-2.740204	-1.389108
C	-4.521326	-0.661023	-1.159923	H	-6.738354	1.89633	-1.577892
C	-5.03581	0.644516	-1.229632	H	-8.286465	-0.017395	-2.03008
C	-6.381974	0.865773	-1.536197	H	-7.393436	-2.349333	-1.950677

C	-7.2379	-0.200667	-1.792325	H	0.031772	-2.868143	-2.691968
C	-6.737054	-1.501656	-1.747524	H	0.359939	-3.621089	-1.13851
C	0.15646	-2.652256	-1.620968				

Conformer <b>2b</b>							
C	6.740141	0.709463	-1.079432	H	7.728445	0.30556	-1.304014
C	6.59535	2.053297	-0.735892	H	7.467644	2.706215	-0.684705
C	5.328807	2.560859	-0.457386	H	5.187269	3.607248	-0.183708
C	4.208461	1.730203	-0.520073	H	5.729659	-1.16815	-1.424246
C	4.34064	0.368956	-0.8573	H	2.426573	2.690967	-1.053547
C	5.621712	-0.119333	-1.143246	H	3.780327	1.187528	1.880537
N	2.915691	2.274259	-0.264622	H	2.40479	1.871875	2.74961
C	2.063731	1.816105	0.702799	H	2.314946	-0.399915	3.335829
C	3.128285	-0.478307	-0.98905	H	1.024466	-0.144878	2.162149
C	2.684859	1.185465	1.935256	H	2.619616	-0.084652	-3.142998
C	2.11898	-0.194948	2.270843	H	2.450118	-3.5508	1.53594
C	2.68615	-1.393406	1.46404	H	2.012223	-2.714737	3.035633
C	2.438529	-1.200231	-0.022179	H	-0.016026	-3.583597	1.867331
N	1.314201	-1.721363	-0.627534	H	-0.072942	-1.822409	1.87907
C	1.266144	-1.337852	-1.945457	H	-0.603963	-2.494541	-0.363169
C	2.378566	-0.570009	-2.19969	H	0.703415	-3.706354	-0.40726
C	1.942808	-2.65889	1.937943	H	4.711958	-0.61611	1.482284
C	0.488258	-2.683368	1.486502	H	4.298148	-1.620347	2.865634
C	0.418564	-2.707414	-0.031169	H	4.648232	-2.763203	0.027953
C	4.191815	-1.540656	1.770121	H	5.982868	-2.624934	1.195929
C	4.891824	-2.719901	1.100294	H	4.606501	-3.681708	1.548956
O	0.863037	2.005877	0.619602	H	-5.531553	-3.214612	1.126978
O	-1.676878	-0.280688	2.640541	H	-4.349552	-3.513959	2.40861
C	-4.751317	-2.740065	1.739606	H	-5.24073	-1.988137	2.374723
C	-3.619851	-2.148635	0.899204	H	-3.176928	-2.964924	0.315859
C	-2.862658	-2.570314	-2.087009	H	-2.822672	-1.796672	1.566315
C	-4.356381	-2.252224	-2.279243	H	-2.427911	-2.843365	-3.057413
C	-5.035558	-1.491459	-1.110176	H	-2.706275	-3.429121	-1.418108
C	-1.126787	0.559388	-1.872659	H	-4.42661	-1.635883	-3.18707
C	-1.096733	-0.769112	-2.216687	H	-4.886846	-3.190318	-2.496559
N	-2.174754	-1.37824	-1.60586	H	-5.796054	-2.119866	-0.625198
C	-2.845579	-0.462623	-0.8195	H	-5.56875	-0.62065	-1.520332
C	-4.033444	-0.979791	-0.043997	H	-0.366016	1.300431	-2.106977
C	-4.64001	0.152463	0.801105	H	-4.766693	1.041509	0.168432
C	-3.884957	0.515585	2.104215	H	-5.656734	-0.14739	1.102647
C	-2.249665	0.775051	-1.014721	H	-4.274759	1.484057	2.453459
C	-2.352148	0.59948	2.130586	H	-4.115519	-0.229411	2.876442
N	-1.780576	1.740454	1.663696	H	-0.757462	1.708614	1.577597

C	-3.250368	3.008937	-1.491071	H	-3.42544	2.655972	-2.509095
C	-2.661103	2.131889	-0.570724	H	-2.579093	4.214429	2.124065
C	-2.423975	2.595899	0.732371	H	-3.659128	5.760974	0.473331
C	-2.783539	3.892692	1.102017	H	-4.071592	4.96809	-1.854651
C	-3.379596	4.748437	0.179013	H	0.292308	-1.219249	-3.821156
C	-3.610099	4.303655	-1.12241	H	-0.21556	-2.622719	-2.873723
C	0.049157	-1.555643	-2.803891				

Conformer <b>2c</b>							
C	-7.092724	-1.330797	-1.477336	H	-7.950636	-1.127775	-2.119951
C	-7.140912	-2.375865	-0.555341	H	-8.036736	-2.991948	-0.467378
C	-6.038894	-2.630371	0.257389	H	-6.052231	-3.437258	0.991241
C	-4.889389	-1.845815	0.150171	H	-5.897686	0.259832	-2.317761
C	-4.828527	-0.784319	-0.77398	H	-3.102211	-2.821703	0.61699
C	-5.94459	-0.548393	-1.586127	H	-4.07912	-0.372209	3.453405
N	-3.760278	-2.13145	0.97182	H	-5.101407	-0.22404	2.022881
C	-3.161282	-1.192731	1.777136	H	-3.97769	1.936812	2.970786
C	-3.565551	-0.018009	-0.939013	H	-2.440611	1.227728	2.448133
C	-4.06827	-0.131515	2.37882	H	-2.561488	-1.295848	-2.488801
C	-3.514157	1.281726	2.215475	H	-3.347034	3.923353	0.002131
C	-3.722711	1.950988	0.832152	H	-3.364972	3.865152	1.771327
C	-3.102694	1.109388	-0.270074	H	-1.047422	4.214994	0.914197
N	-1.828479	1.366319	-0.735945	H	-1.135948	2.631583	1.691258
C	-1.471551	0.434414	-1.678042	H	0.001669	2.311535	-0.428639
C	-2.52918	-0.43576	-1.822748	H	-1.208295	3.282557	-1.297155
C	-3.027242	3.327348	0.871536	H	-5.737706	1.17623	0.632117
C	-1.508068	3.219627	0.83962	H	-5.627858	2.728396	1.452213
C	-1.06215	2.575656	-0.460998	H	-6.697297	2.75899	-0.888652
C	-5.235293	2.15309	0.596194	H	-5.377332	3.921489	-0.693058
C	-5.616887	2.848987	-0.707432	H	-5.091695	2.397736	-1.562765
O	-1.988237	-1.262293	2.079935	H	4.673915	-3.930484	1.489977
O	6.474806	-2.038005	-1.432772	H	2.99098	-4.471802	1.34482
C	3.876074	-4.163625	0.769255	H	4.210038	-5.032366	0.185249
C	3.581468	-2.985956	-0.158721	H	2.747882	-3.25907	-0.820639
C	0.645645	-1.928384	-0.636182	H	4.437706	-2.832182	-0.825466
C	0.835789	-2.468018	0.801737	H	-0.393469	-1.608664	-0.775679
C	2.05134	-1.887725	1.531992	H	0.84701	-2.715336	-1.379381
C	2.10996	1.272476	-1.488125	H	-0.068977	-2.25504	1.384032
C	1.105001	0.342277	-1.617803	H	0.937529	-3.561513	0.740687
N	1.491261	-0.77439	-0.916321	H	2.33868	-2.561557	2.353265
C	2.743232	-0.588871	-0.367037	H	1.794155	-0.920722	1.992378
C	3.249411	-1.662626	0.579227	H	2.125126	2.26326	-1.939414
C	4.464963	-1.173828	1.394239	H	4.308184	-0.122169	1.670157

C	5.873215	-1.381206	0.794778	H	4.46751	-1.7255	2.347644
C	3.143634	0.709149	-0.68153	H	6.574746	-0.745003	1.358391
C	6.127936	-1.141694	-0.690235	H	6.18898	-2.421759	0.940305
N	6.006824	0.136755	-1.149721	H	6.176244	0.241369	-2.145932
C	3.933738	2.718563	0.52998	H	2.879351	2.938374	0.708083
C	4.256667	1.546903	-0.175649	H	7.648838	1.884038	-0.104524
C	5.616689	1.273948	-0.39662	H	7.043215	3.950908	1.168606
C	6.604938	2.135793	0.089731	H	4.631676	4.476521	1.558482
C	6.264068	3.286322	0.793398	H	-0.214168	-0.363687	-3.159647
C	4.917342	3.578065	1.009164	H	-0.076787	1.382057	-3.005672
C	-0.163126	0.451865	-2.421398				

Conformer <b>2d</b>							
C	-5.705488	2.717051	-0.447237	H	-5.763184	3.796883	-0.302686
C	-6.870463	1.969302	-0.614653	H	-7.845862	2.457418	-0.597494
C	-6.784734	0.591613	-0.799006	H	-7.680403	-0.018737	-0.921704
C	-5.540898	-0.04273	-0.821915	H	-3.548515	2.67011	-0.360107
C	-4.356099	0.700943	-0.655308	H	-5.450244	-1.77778	-1.984901
C	-4.463528	2.085567	-0.473257	H	-5.254881	-0.913181	1.472066
N	-5.472889	-1.450367	-1.021932	H	-5.436574	-2.637235	1.799213
C	-4.815629	-2.301237	-0.159968	H	-3.491652	-2.083355	3.011955
C	-3.03143	0.040484	-0.794228	H	-2.966337	-2.940566	1.5553
C	-4.791661	-1.893291	1.305847	H	-2.71323	0.361105	-2.991466
C	-3.397443	-1.996371	1.917501	H	-0.400136	-0.324635	2.303204
C	-2.418445	-0.826983	1.637378	H	-1.233312	-1.51719	3.30927
C	-2.228578	-0.600648	0.145978	H	0.593965	-2.557514	1.994795
N	-1.11254	-1.06789	-0.518956	H	-0.953959	-3.198695	1.397874
C	-1.184656	-0.733663	-1.851128	H	0.350703	-2.555849	-0.563364
C	-2.366712	-0.057354	-2.04854	H	0.856811	-1.046377	0.223335
C	-1.06268	-1.204348	2.267593	H	-3.964155	0.670733	1.926366
C	-0.340597	-2.289929	1.482875	H	-3.09633	0.215264	3.388991
C	0.01956	-1.75386	0.109754	H	-1.854644	1.891345	1.122512
C	-2.96109	0.449064	2.319135	H	-2.625306	2.578959	2.56977
C	-2.096145	1.697847	2.179565	H	-1.148575	1.610063	2.729874
O	-4.367583	-3.363071	-0.529017	H	1.412647	4.104275	1.601709
O	2.596815	-0.776082	2.681351	H	0.873513	3.133765	2.981563
C	1.626958	3.195571	2.183745	H	2.604006	3.335861	2.670498
C	1.58934	1.932675	1.325875	H	0.589074	1.837906	0.883054
C	0.371711	1.813608	-1.508366	H	1.694187	1.053337	1.9723
C	1.069163	3.18005	-1.27178	H	-0.082385	1.787922	-2.506254
C	2.503677	3.105135	-0.720345	H	-0.457712	1.663246	-0.799265
C	2.459031	-1.074947	-2.106632	H	1.074588	3.751077	-2.20996
C	1.251737	-0.430374	-2.234398	H	0.44442	3.749482	-0.568545

N	1.298082	0.688236	-1.435627	H	2.74118	4.04015	-0.190373
C	2.470497	0.712457	-0.71871	H	3.231436	3.010115	-1.541081
C	2.672663	1.885705	0.211898	H	2.735362	-2.014442	-2.580945
C	4.070322	1.837439	0.846018	H	4.813351	1.607317	0.0701
C	4.229212	0.887327	2.056961	H	4.322058	2.845704	1.210753
C	3.254005	-0.350127	-1.165585	H	5.305969	0.756001	2.244563
C	3.592387	-0.505433	2.035915	H	3.794141	1.360508	2.946856
N	4.253188	-1.47629	1.338398	H	3.768557	-2.370384	1.335894
C	5.60251	-0.485341	-1.970847	H	5.238108	-0.071876	-2.912917
C	4.684308	-0.673466	-0.926831	H	6.838095	-1.960175	1.384187
C	5.161739	-1.21898	0.276356	H	8.462434	-1.590851	-0.486819
C	6.511662	-1.5414	0.431157	H	7.640809	-0.649892	-2.646822
C	7.409218	-1.337168	-0.612917	H	0.095129	-1.970442	-3.104517
C	6.94817	-0.810337	-1.819229	H	-0.322311	-0.381615	-3.74354
C	-0.04586	-0.915578	-2.820188				

Conformer <b>2e</b>							
C	6.722034	0.647616	-1.290175	H	7.694909	0.238653	-1.566855
C	6.612536	1.976947	-0.881787	H	7.497158	2.613283	-0.833264
C	5.366592	2.489675	-0.531032	H	5.253928	3.523234	-0.200902
C	4.229999	1.680416	-0.591145	H	5.665222	-1.19854	-1.674214
C	4.326094	0.336168	-0.998826	H	2.460307	2.723514	-0.996434
C	5.58815	-0.159357	-1.349608	H	3.848652	0.951339	1.775003
N	2.958585	2.231021	-0.258662	H	2.532023	1.639432	2.730799
C	2.122095	1.725507	0.6983	H	2.309235	-0.645803	3.186326
C	3.096866	-0.485304	-1.141992	H	1.050219	-0.29601	2.013834
C	2.755814	0.993301	1.867412	H	2.549012	0.067999	-3.250376
C	2.141856	-0.381925	2.130958	H	2.438737	-3.700156	1.238016
C	2.680304	-1.545973	1.25866	H	1.971546	-2.931738	2.765733
C	2.415708	-1.262764	-0.211992	H	-0.040289	-3.734163	1.555967
N	1.27096	-1.723818	-0.829408	H	-0.081847	-1.97409	1.661801
C	1.201645	-1.248564	-2.116015	H	-0.633454	-2.54291	-0.612517
C	2.319566	-0.480409	-2.33924	H	0.692912	-3.72893	-0.72838
C	1.922865	-2.825012	1.672495	H	4.516366	-2.560998	0.790057
C	0.468582	-2.818751	1.219875	H	4.743717	-0.863719	1.157645
C	0.392717	-2.758196	-0.294614	H	5.706017	-2.248097	2.94749
C	4.194677	-1.760398	1.47668	H	4.359981	-1.311772	3.61312
C	4.616785	-2.109761	2.901071	H	4.152612	-3.040725	3.255888
O	0.92534	1.951869	0.663166	H	-5.160348	-2.086784	2.353115
O	-1.582405	-0.418529	2.606944	H	-5.500542	-3.236827	1.046385
C	-4.697309	-2.802842	1.659359	H	-4.279359	-3.616541	2.268579
C	-3.589453	-2.168841	0.818626	H	-3.169814	-2.951255	0.174523
C	-2.939841	-2.413449	-2.216243	H	-2.76973	-1.860404	1.479798

C	-4.42894	-2.051256	-2.349094	H	-2.534208	-2.633089	-3.21246
C	-5.065042	-1.385368	-1.101868	H	-2.787091	-3.315578	-1.606073
C	-1.164755	0.678434	-1.873414	H	-4.501124	-1.353716	-3.196168
C	-1.156271	-0.628544	-2.292186	H	-4.985586	-2.954278	-2.637833
N	-2.216794	-1.266115	-1.678964	H	-5.800448	-2.055085	-0.633847
C	-2.854505	-0.391592	-0.820792	H	-5.621185	-0.492907	-1.426095
C	-4.023525	-0.943963	-0.04083	H	-0.407571	1.427364	-2.093865
C	-4.594724	0.140327	0.887567	H	-4.733741	1.065448	0.31167
C	-3.798342	0.422991	2.185766	H	-5.604161	-0.170847	1.20191
C	-2.255621	0.8513	-0.96541	H	-4.169354	1.372364	2.601536
C	-2.264963	0.494467	2.16947	H	-4.011776	-0.363714	2.920635
N	-1.697735	1.655963	1.750415	H	-0.677569	1.622664	1.634051
C	-3.2485	3.116156	-1.280483	H	-3.456791	2.824231	-2.311511
C	-2.640716	2.182683	-0.43036	H	-2.46001	4.104719	2.376442
C	-2.360911	2.568449	0.889822	H	-3.573671	5.752547	0.850894
C	-2.697501	3.844354	1.344094	H	-4.061609	5.099193	-1.505936
C	-3.312431	4.756704	0.490258	H	0.189756	-0.978582	-3.9554
C	-3.585129	4.389945	-0.827283	H	-0.319186	-2.441998	-3.104155
C	-0.036479	-1.386974	-2.960936				

Conformer <b>3a</b>							
C	-1.392524	4.667838	-0.272155	C	1.348635	-3.543648	1.858787
C	-1.841452	4.555875	1.045492	C	1.841452	-4.555875	1.045492
C	-1.348635	3.543648	1.858787	C	1.392524	-4.667838	-0.272155
C	-0.420221	2.623376	1.359622	H	-1.768867	5.463986	-0.915204
C	0.000851	2.70147	0.020569	H	-2.567548	5.266784	1.442082
C	-0.479516	3.751379	-0.776101	H	-1.661374	3.450098	2.899374
N	0.080663	1.617137	2.215057	H	-0.149193	3.822548	-1.810705
C	1.392524	1.361224	2.4336	H	-0.606955	0.934351	2.590736
C	0.90358	1.671215	-0.550942	H	1.910189	3.409772	1.950753
C	2.404478	2.455452	2.162048	H	2.91126	2.562412	3.132528
C	3.463699	2.0917	1.103687	H	4.452548	2.369862	1.496822
C	3.33222	2.761454	-0.281402	H	3.486681	0.995756	0.996247
C	2.279897	2.016159	-1.155763	H	4.608604	3.212488	-1.967306
N	2.772592	0.704988	-1.53104	H	5.461154	3.140181	-0.41734
C	1.829013	-0.273772	-1.435109	H	5.280026	0.640971	-0.421437
C	0.635955	0.363036	-0.762248	H	6.074793	1.225624	-1.891868
C	4.689537	2.646678	-1.025203	H	4.013857	1.002203	-3.191678
C	5.12026	1.217062	-1.345863	H	4.211344	-0.537302	-2.312205
C	4.048412	0.54113	-2.188413	H	3.008839	4.685561	-1.18454
C	2.981709	4.262069	-0.171295	H	1.94263	4.383464	0.164367
C	3.898062	5.069398	0.746217	H	3.868308	4.709482	1.785374
O	1.772264	0.2971	2.913345	H	4.945422	5.046794	0.414139

O	1.920832	-1.403029	-1.856837	H	3.584221	6.122276	0.757461
O	2.08268	2.809649	-2.308824	H	1.453382	2.348577	-2.880348
O	-2.08268	-2.809649	-2.308824	H	-1.453382	-2.348577	-2.880348
O	-1.920832	1.403029	-1.856837	H	-4.945422	-5.046794	0.414139
O	-1.772264	-0.2971	2.913345	H	-3.584221	-6.122276	0.757461
C	-3.898062	-5.069398	0.746217	H	-3.868308	-4.709482	1.785374
C	-2.981709	-4.262069	-0.171295	H	-3.008839	-4.685561	-1.18454
C	-4.048412	-0.54113	-2.188413	H	-1.94263	-4.383464	0.164367
C	-5.12026	-1.217062	-1.345863	H	-4.211344	0.537302	-2.312205
C	-4.689537	-2.646678	-1.025203	H	-4.013857	-1.002203	-3.191678
C	-0.635955	-0.363036	-0.762248	H	-6.074793	-1.225624	-1.891868
C	-1.829013	0.273772	-1.435109	H	-5.280026	-0.640971	-0.421437
N	-2.772592	-0.704988	-1.53104	H	-5.461154	-3.140181	-0.41734
C	-2.279897	-2.016159	-1.155763	H	-4.608604	-3.212488	-1.967306
C	-3.33222	-2.761454	-0.281402	H	-3.486681	-0.995756	0.996247
C	-3.463699	-2.0917	1.103687	H	-4.452548	-2.369862	1.496822
C	-2.404478	-2.455452	2.162048	H	-2.91126	-2.562412	3.132528
C	-0.90358	-1.671215	-0.550942	H	-1.910189	-3.409772	1.950753
C	-1.392524	-1.361224	2.4336	H	0.606955	-0.934351	2.590736
N	-0.080663	-1.617137	2.215057	H	0.149193	-3.822548	-1.810705
C	0.479516	-3.751379	-0.776101	H	1.661374	-3.450098	2.899374
C	-0.000851	-2.70147	0.020569	H	2.567548	-5.266784	1.442082
C	0.420221	-2.623376	1.359622	H	1.768867	-5.463986	-0.915204

Conformer <b>3b</b>							
C	-2.631574	-4.104307	-0.012719	C	1.858178	3.410116	1.751832
C	-2.228683	-4.329828	1.305343	C	2.270316	4.425442	0.898506
C	-1.75715	-3.272932	2.073141	C	2.601205	4.127921	-0.425195
C	-1.667755	-1.986778	1.528994	H	-3.007529	-4.927534	-0.62098
C	-2.032417	-1.760433	0.19031	H	-2.292694	-5.329427	1.737262
C	-2.535706	-2.832674	-0.561529	H	-1.459242	-3.416229	3.11238
N	-1.201278	-0.925965	2.33753	H	-2.824272	-2.662531	-1.59701
C	-1.856026	0.241534	2.543755	H	-0.21814	-0.98594	2.669493
C	-1.867749	-0.418494	-0.42126	H	-3.768385	-0.720909	2.200645
C	-3.355893	0.284173	2.336012	H	-3.720649	0.653054	3.305473
C	-3.821021	1.270434	1.246472	H	-4.679599	1.833012	1.64325
C	-4.287955	0.675623	-0.103723	H	-3.022941	2.012417	1.089108
C	-3.057795	0.368923	-1.005257	H	-5.497567	1.305519	-1.784553
N	-2.419186	1.604518	-1.416957	H	-6.012888	1.970457	-0.227537
C	-1.057938	1.548232	-1.368573	H	-4.018992	3.532345	-0.274446
C	-0.718933	0.241536	-0.689407	H	-5.017468	3.72063	-1.724559
C	-5.128969	1.744254	-0.845543	H	-3.513525	2.327392	-3.050435
C	-4.362533	3.020437	-1.186056	H	-2.472264	3.502192	-2.204396



C	-3.165316	2.663741	-2.057392	H	-4.55032	-1.423141	0.420396
C	-5.183058	-0.563256	0.16347	H	-5.759277	-0.333201	1.076474
C	-6.172137	-0.999264	-0.917095	H	-6.687572	-1.912455	-0.586926
O	-1.279615	1.24014	2.965285	H	-6.945299	-0.239777	-1.099036
O	-0.289434	2.360897	-1.826887	H	-5.667968	-1.212748	-1.86628
O	-3.538712	-0.328771	-2.136975	H	-2.784026	-0.510901	-2.714259
O	3.402488	0.23743	-2.399608	H	2.622591	0.392402	-2.94995
O	0.134228	-2.388242	-1.764647	H	7.065838	-0.385972	0.202927
O	1.487569	-1.04976	2.923027	H	6.993301	1.35383	0.51116
C	6.407061	0.425138	0.54336	H	6.157507	0.233988	1.597642
C	5.161521	0.565035	-0.3299	H	5.459367	0.800007	-1.360825
C	2.984944	-2.727982	-2.19323	H	4.583316	1.435608	0.008997
C	4.227859	-3.073732	-1.386164	H	2.274763	-3.561193	-2.272472
C	5.034799	-1.804	-1.123138	H	3.274056	-2.422653	-3.214707
C	0.664315	-0.236759	-0.736238	H	4.841012	-3.801259	-1.937588
C	0.941691	-1.569782	-1.390451	H	3.931304	-3.550637	-0.43926
N	2.294727	-1.642556	-1.535696	H	5.93378	-2.04944	-0.540061
C	2.973959	-0.402289	-1.214247	H	5.37606	-1.393968	-2.0873
C	4.257283	-0.686625	-0.377483	H	3.075656	-1.932156	0.974116
C	3.889307	-1.192277	1.034311	H	4.763058	-1.745314	1.409082
C	3.505423	-0.13073	2.083123	H	3.950384	-0.423075	3.045724
C	1.833647	0.425122	-0.587148	H	3.895378	0.862859	1.837517
C	2.025505	-0.076528	2.403156	H	0.397317	1.156743	2.5858
N	1.351899	1.077197	2.181692	H	2.722242	2.59834	-1.932853
C	2.489343	2.826039	-0.894323	H	1.62011	3.61023	2.797119
C	2.040406	1.79517	-0.055745	H	2.345908	5.448935	1.268122
C	1.753503	2.094229	1.287519	H	2.9324	4.918025	-1.099748

Conformer <b>3c</b>							
C	2.601205	4.127921	-0.425196	C	-1.757143	-3.272932	2.073141
C	2.270321	4.425442	0.898506	C	-2.228675	-4.329829	1.305343
C	1.858183	3.410116	1.751832	C	-2.63157	-4.104308	-0.012718
C	1.753506	2.09423	1.28752	H	2.9324	4.918025	-1.09975
C	2.040405	1.79517	-0.055745	H	2.345915	5.448935	1.268121
C	2.489341	2.826039	-0.894324	H	1.620118	3.610231	2.79712
N	1.351902	1.077198	2.181694	H	2.722237	2.59834	-1.932855
C	2.025508	-0.076527	2.403156	H	0.397319	1.156745	2.5858
C	1.833646	0.425123	-0.587148	H	3.89538	0.862859	1.837516
C	3.505425	-0.13073	2.083122	H	3.950387	-0.423076	3.045723
C	3.889308	-1.192277	1.03431	H	4.763059	-1.745314	1.40908
C	4.257282	-0.686624	-0.377485	H	3.075657	-1.932156	0.974115
C	2.973958	-0.402289	-1.214247	H	5.376057	-1.393967	-2.087303
N	2.294725	-1.642556	-1.535696	H	5.933779	-2.04944	-0.540065

C	0.941689	-1.569782	-1.39045	H	3.931303	-3.550637	-0.439262
C	0.664314	-0.236759	-0.736237	H	4.84101	-3.801258	-1.93759
C	5.034797	-1.804	-1.123141	H	3.274052	-2.422653	-3.214708
C	4.227857	-3.073732	-1.386165	H	2.27476	-3.561192	-2.272472
C	2.984941	-2.727982	-2.193231	H	5.459365	0.800007	-1.360828
C	5.16152	0.565035	-0.329902	H	4.583315	1.435608	0.008995
C	6.407061	0.425138	0.543356	H	6.993301	1.35383	0.511156
O	1.48757	-1.04976	2.923027	H	6.157508	0.233989	1.597638
O	0.134226	-2.388242	-1.764646	H	7.065837	-0.385972	0.202923
O	3.402485	0.23743	-2.399608	H	2.622587	0.392403	-2.94995
O	-3.538715	-0.328773	-2.136974	H	-2.784029	-0.510903	-2.714257
O	-0.289436	2.360897	-1.826887	H	-6.687574	-1.912454	-0.586923
O	-1.279613	1.240141	2.965282	H	-6.945302	-0.239776	-1.099031
C	-6.17214	-0.999263	-0.917092	H	-5.667972	-1.212746	-1.866278
C	-5.183059	-0.563256	0.163472	H	-4.550322	-1.423141	0.420397
C	-3.165318	2.663739	-2.057392	H	-5.759277	-0.333201	1.076477
C	-4.362534	3.020437	-1.186055	H	-2.472267	3.50219	-2.204398
C	-5.12897	1.744254	-0.845542	H	-3.513528	2.32739	-3.050435
C	-0.718934	0.241537	-0.689406	H	-5.01747	3.720629	-1.724559
C	-1.05794	1.548232	-1.368572	H	-4.018993	3.532345	-0.274446
N	-2.419188	1.604517	-1.416957	H	-6.012889	1.970457	-0.227535
C	-3.057797	0.368922	-1.005257	H	-5.497569	1.305519	-1.784551
C	-4.287957	0.675623	-0.103721	H	-3.022941	2.012417	1.089109
C	-3.821021	1.270434	1.246473	H	-4.679599	1.833011	1.643252
C	-3.355891	0.284172	2.336012	H	-3.768383	-0.72091	2.200645
C	-1.867751	-0.418494	-0.421259	H	-3.720647	0.653053	3.305473
C	-1.856024	0.241534	2.543754	H	-0.218138	-0.985939	2.669493
N	-1.201275	-0.925965	2.337531	H	-2.824276	-2.662532	-1.597007
C	-2.535707	-2.832675	-0.561527	H	-1.459231	-3.41623	3.112379
C	-2.032417	-1.760433	0.190311	H	-2.292682	-5.329428	1.737261
C	-1.667752	-1.986778	1.528995	H	-3.007525	-4.927535	-0.620978

Conformer <b>3d</b>							
C	2.557864	4.151279	-0.369232	C	-1.662712	-3.367276	1.853306
C	2.331538	4.416799	0.982541	C	-2.091705	-4.417164	1.051601
C	1.936169	3.390153	1.831767	C	-2.511143	-4.165692	-0.256548
C	1.771867	2.088914	1.344888	H	2.84021	4.956977	-1.047737
C	1.998757	1.814495	-0.014874	H	2.454866	5.427846	1.372779
C	2.387193	2.863326	-0.861404	H	1.748868	3.572697	2.890468
N	1.33855	1.068626	2.225739	H	2.472486	2.668646	-1.930949
C	1.99323	-0.093136	2.454876	H	0.356893	1.12906	2.564241
C	1.812859	0.449654	-0.564047	H	3.879236	0.842075	1.959627
C	3.47762	-0.15519	2.169261	H	3.901671	-0.479012	3.131028

C	3.86532	-1.191336	1.096642	H	4.725746	-1.766567	1.469211
C	4.25716	-0.648965	-0.293785	H	3.043982	-1.918458	0.999159
C	2.989919	-0.35452	-1.165718	H	5.428395	-1.294942	-1.993557
N	2.34219	-1.586242	-1.53306	H	5.953443	-1.991009	-0.451743
C	0.980787	-1.518965	-1.467887	H	3.956618	-3.510912	-0.458746
C	0.658524	-0.213042	-0.781396	H	4.919059	-3.705982	-1.933268
C	5.067216	-1.735946	-1.050355	H	3.376761	-2.281459	-3.21299
C	4.280356	-3.002252	-1.380013	H	2.36422	-3.471012	-2.349503
C	3.062932	-2.63536	-2.215679	H	5.542148	0.844716	-1.187452
C	5.15988	0.603536	-0.181992	H	4.571146	1.475528	0.141093
C	6.368316	0.452051	0.741958	H	6.072241	0.248307	1.780542
O	1.435513	-1.069647	2.946066	H	7.035132	-0.358249	0.417164
O	0.203147	-2.329724	-1.91193	H	6.957577	1.37916	0.745068
O	3.378171	0.275593	-2.3746	H	3.873144	1.074321	-2.158381
O	-3.536788	-0.347287	-2.284773	H	-2.780628	-0.496336	-2.869372
O	-0.326125	2.433853	-1.786171	H	-7.067115	0.239704	0.518556
O	-1.352984	1.14384	2.856666	H	-6.926432	-1.490059	0.858962
C	-6.366066	-0.545266	0.835071	H	-6.05836	-0.322852	1.867652
C	-5.171773	-0.67116	-0.108897	H	-5.522863	-0.941248	-1.114245
C	-3.194	2.639919	-2.156918	H	-4.547888	-1.515353	0.215265
C	-4.408331	2.965588	-1.299147	H	-2.512076	3.491014	-2.281386
C	-5.160598	1.677632	-0.970972	H	-3.521344	2.310563	-3.159106
C	-0.732298	0.246701	-0.771046	H	-5.069398	3.660859	-1.836741
C	-1.082349	1.570205	-1.408946	H	-4.084283	3.473402	-0.377735
N	-2.441529	1.584278	-1.519908	H	-6.038316	1.907063	-0.350025
C	-3.066429	0.333464	-1.139553	H	-5.533704	1.234701	-1.908381
C	-4.310423	0.604105	-0.241132	H	-4.749147	1.69279	1.545551
C	-3.879408	1.160529	1.133086	H	-3.097842	1.926023	1.00654
C	-3.395043	0.142254	2.181909	H	-3.768944	-0.869312	1.989697
C	-1.872482	-0.445762	-0.553824	H	-3.785443	0.448711	3.163825
C	-1.896589	0.138778	2.408555	H	-0.241449	-1.054505	2.567634
N	-1.209361	-1.0086	2.193379	H	-2.770548	-2.680738	-1.79187
C	-2.469882	-2.873972	-0.763837	H	-1.356443	-3.53226	2.886946
C	-2.005454	-1.807559	0.019973	H	-2.1114	-5.432308	1.450407
C	-1.629231	-2.061399	1.351176	H	-2.856173	-4.983571	-0.889793

Conformer <b>3e</b>							
C	-2.511143	-4.165692	-0.256548	C	1.936169	3.390153	1.831767
C	-2.091705	-4.417164	1.051601	C	2.331538	4.416799	0.982541
C	-1.662712	-3.367276	1.853306	C	2.557864	4.151279	-0.369232
C	-1.629231	-2.061399	1.351176	H	-2.856173	-4.983571	-0.889793
C	-2.005454	-1.807559	0.019973	H	-2.1114	-5.432308	1.450407
C	-2.469882	-2.873972	-0.763837	H	-1.356443	-3.53226	2.886946

N	-1.209361	-1.0086	2.193379	H	-2.770548	-2.680738	-1.79187
C	-1.896589	0.138778	2.408555	H	-0.241449	-1.054505	2.567634
C	-1.872482	-0.445762	-0.553824	H	-3.785443	0.448711	3.163825
C	-3.395043	0.142254	2.181909	H	-3.768944	-0.869312	1.989697
C	-3.879408	1.160529	1.133086	H	-4.749147	1.692789	1.545551
C	-4.310423	0.604105	-0.241132	H	-3.097842	1.926023	1.00654
C	-3.066429	0.333464	-1.139553	H	-5.533704	1.2347	-1.908381
N	-2.441529	1.584278	-1.519908	H	-6.038316	1.907063	-0.350025
C	-1.082349	1.570205	-1.408946	H	-4.084283	3.473402	-0.377735
C	-0.732298	0.246701	-0.771046	H	-5.069398	3.660859	-1.836741
C	-5.160598	1.677632	-0.970972	H	-3.521344	2.310563	-3.159106
C	-4.408331	2.965588	-1.299147	H	-2.512076	3.491014	-2.281386
C	-3.194	2.639919	-2.156918	H	-5.522863	-0.941248	-1.114246
C	-5.171773	-0.67116	-0.108897	H	-4.547888	-1.515353	0.215265
C	-6.366066	-0.545266	0.835071	H	-6.05836	-0.322852	1.867652
O	-1.352984	1.14384	2.856666	H	-7.067115	0.239704	0.518556
O	-0.326124	2.433853	-1.786171	H	-6.926432	-1.49006	0.858962
O	-3.536788	-0.347287	-2.284773	H	-2.780628	-0.496336	-2.869372
O	3.378171	0.275593	-2.3746	H	3.873144	1.074321	-2.158381
O	0.203147	-2.329724	-1.91193	H	6.072241	0.248307	1.780542
O	1.435513	-1.069647	2.946066	H	7.035132	-0.358249	0.417165
C	6.368316	0.452051	0.741958	H	6.957577	1.37916	0.745068
C	5.15988	0.603536	-0.181992	H	5.542148	0.844716	-1.187452
C	3.062932	-2.63536	-2.215679	H	4.571146	1.475528	0.141093
C	4.280356	-3.002252	-1.380013	H	2.36422	-3.471012	-2.349503
C	5.067216	-1.735946	-1.050355	H	3.376761	-2.281459	-3.21299
C	0.658524	-0.213042	-0.781396	H	4.919059	-3.705982	-1.933268
C	0.980787	-1.518965	-1.467887	H	3.956618	-3.510912	-0.458746
N	2.34219	-1.586242	-1.53306	H	5.953443	-1.991009	-0.451743
C	2.989919	-0.35452	-1.165718	H	5.428395	-1.294942	-1.993557
C	4.25716	-0.648965	-0.293785	H	3.043982	-1.918458	0.999159
C	3.86532	-1.191336	1.096642	H	4.725746	-1.766567	1.469211
C	3.477619	-0.15519	2.169261	H	3.879236	0.842075	1.959627
C	1.812859	0.449654	-0.564047	H	3.901671	-0.479012	3.131028
C	1.99323	-0.093136	2.454876	H	0.356893	1.12906	2.564241
N	1.338549	1.068626	2.225739	H	2.472486	2.668646	-1.930949
C	2.387193	2.863326	-0.861404	H	1.748868	3.572697	2.890468
C	1.998757	1.814495	-0.014874	H	2.454866	5.427846	1.372779
C	1.771867	2.088914	1.344888	H	2.84021	4.956977	-1.047737

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