Supporting Information

Strepyrrolins A–E, five pyrrole-sesquiterpene hybrids from Streptomyces sp. KIB 015, revealing a new formation logic of pyrroles by isotope labeling

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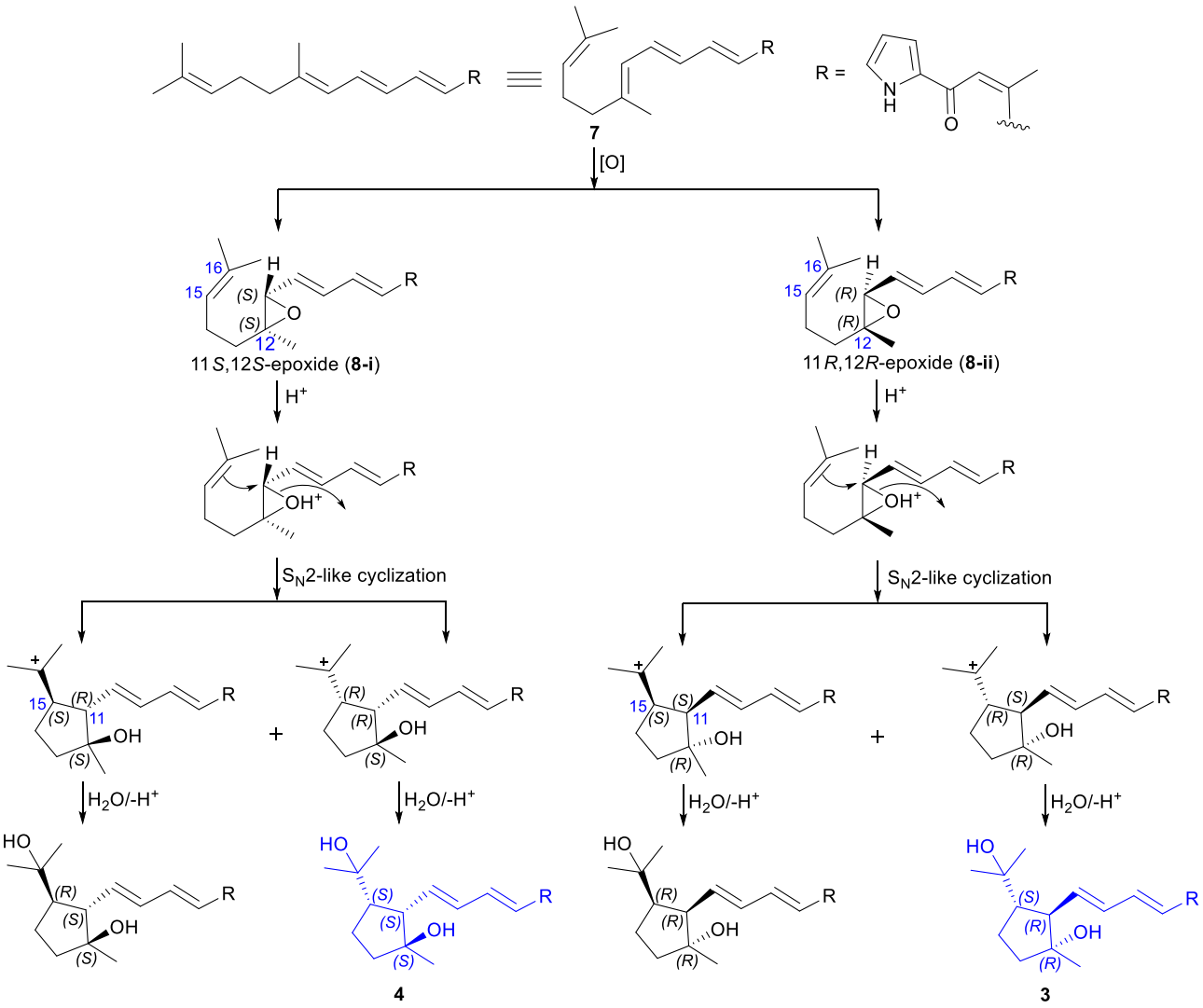
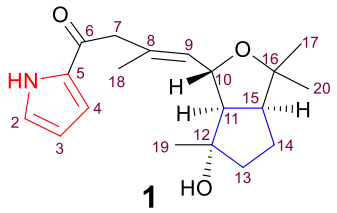
Contents



Scheme S1. Hypothetical formation mechanisms of compounds **3** and **4** from epoxide **8**.

Table S1. Detailed 2D-NMR data of compound **1**.

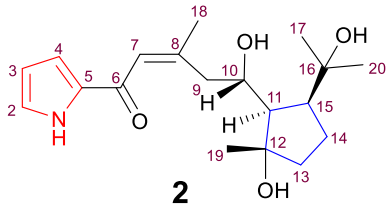
No.	δ_H	δ_C	HMBC	COSY	ROESY
2	7.06 (1H, overlapped)	126.93 (CH)	C-3, C-4, C-5	H-3	
3	6.24 (1H, dd, *J* = 3.6, 2.6 Hz)	111.25 (CH)	C-4, C-2, C-5		
4	7.07 (1H, overlapped)	119.04 (CH)	C-3, C-2, C-5, C-6	H-3	
5		133.00 (C)			
6		189.58 (C)			
7	3.48 (2H, br s)	49.61 (CH_2)	C-6, C-8, C-9, C-18		H-4
8		136.23 (C)			
9	5.41 (1H, dd, *J* = 9.0, 1.4 Hz)	131.53 (CH)	C-18, C-7, C-11, C-10, C-8, C-6	H-7	H-7
10	4.27 (1H, t like, *J* = 8.7 Hz)	77.02 (CH)	C-11, C-12, C-15, C-8, C-9, C-16	H-9	
11	2.41 (1H, td, *J* = 8.7, 1.0 Hz)	65.51 (CH)	C-14, C-13, C-15, C-10, C-12, C-9	H-10	H-9
12		81.37 (C)			
13a	1.83 (1H, m)	40.60 (CH_2)	C-14, C-12		H-10
13b	1.70 (1H, m)		C-14, C-15, C-11, C-12		
14a	1.89 (1H, m)	25.61 (CH_2)	C-15, C-16	H-15	H-10
14b	1.72 (1H, m)		C-15, C-12, C-16	H-15	
15	2.74 (1H, ddd, *J* = 9.5, 8.7, 4.5 Hz)	55.45 (CH)	C-14, C-17, C-13, C-11, C-10	H-11	H-11
16		84.30 (C)			
17	1.26 (3H, s)	31.86 (CH_3)	C-20, C-15, C-16		
18	1.78 (3H, br d, *J* = 1.0 Hz)	17.39 (CH_3)	C-7, C-9, C-8	H-9	H-10
19	1.15 (3H, s)	24.55 (CH_3)	C-11, C-12, C-13		H-10, H-11
20	1.22 (3H, s)	24.07 (CH_3)	C-17, C-15, C-16		H-10



1

Table S2. Detailed 2D-NMR data of compound **2**.

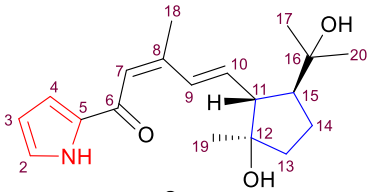
No.	δ_H	δ_C	HMBC	COSY	ROESY
2	7.03 (1H, dd, *J* = 2.1, 1.5 Hz)	126.14 (CH)	C-3, C-4, C-5	H-3	
3	6.22 (1H, dd, *J* = 3.6, 1.2 Hz)	111.03 (CH)	C-4, C-2, C-5		
4	6.96 (1H, dd, *J* = 3.6, 1.2 Hz)	117.01 (CH)	C-3, C-2, C-5	H-3	H-7
5		135.16 (C)			
6		182.13 (C)			
7	6.70 (1H, br t, *J* = 1.2 Hz)	122.84 (CH)	C-18, C-9, C-10, C-8, C-6	H_3-18	
8		157.39 (C)			
9a	3.33 (1H, overlapped)	42.73 (CH_2)	C-18, C-11, C-10, C-7, C-8, C-6	H-7, H-10	H_3-19
9b	2.65 (1H, dd, *J* = 12.9, 9.9 Hz)		C-18, C-11, C-10, C-7, C-8, C-6	H-10	H_3-18
10	3.91 (1H, ddd, *J* = 9.6, 8.1, 3.6 Hz)	81.04 (CH)	C-9, C-11, C-12, C-16, C-8		H_3-19
11	2.42 (1H, t like, *J* = 7.9 Hz)	65.34 (CH)	C-14, C-13, C-9, C-15, C-10, C-12	H-10	
12		82.04 (C)			
13a	1.77 (1H, m)	40.22 (CH_2)	C-14, C-15, C-12		H-10
13b	1.66 (1H, overlapped)		C-14, C-15, C-12	H-11	
14a	1.85 (1H, m)	25.32 (CH_2)	C-13, C-15, C-11, C-12, C-16	H-15	
14b	1.67 (1H, overlapped)		C-13, C-15, C-11, C-12, C-16	H-15, H-11	
15	2.70 (1H, ddd, *J* = 9.6, 7.8, 4.5 Hz)	55.24 (CH)	C-20, C-14, C-17, C-13, C-11, C-10	H-11	H-11
16		84.30 (C)			
17	1.27 (3H, s)	31.89 (CH_3)	C-20, C-15, C-16		H-10
18	2.08 (3H, br d, *J* = 1.2 Hz)	27.59 (CH_3)	C-9, C-10, C-7, C-8, C-6		H-7
19	1.44 (3H, s)	24.69 (CH_3)	C-13, C-11, C-12		
20	1.17 (3H, s)	24.50 (CH_3)	C-17, C-15, C-16		



2

Table S3. Detailed 2D-NMR data of compound **3**.

No.	δ_H	δ_C	HMBC	COSY	ROESY
2	7.06 (1H, dd, *J* = 2.4, 1.2 Hz)	126.57 (CH)	C-3, C-4, C-5, C-6	H-3	
3	6.23 (1H, dd, *J* = 3.8, 2.4 Hz)	111.23 (CH)	C-4, C-2, C-5		
4	6.98 (1H, dd, *J* = 3.8, 1.2 Hz)	117.37 (CH)	C-3, C-2, C-5	H-3	H-7
5		135.40 (C)			
6		182.37 (C)			
7	6.62 (1H, s)	122.22 (CH)	C-8, C-9, C-18		
8		150.63 (C)			
9	7.66 (1H, d, *J* = 15.8 Hz)	130.55 (CH)	C-18, C-11, C-7, C-8		H-11
10	6.08 (1H, dd, *J* = 15.8, 9.7 Hz)	142.37 (CH)	C-15, C-11, C-12, C-8	H-9	
11	2.56 (1H, dd, *J* = 9.7, 7.1 Hz)	57.68 (CH)	C-13, C-15, C-16, C-12, C-19, C-9, C-10	H-10	
12		82.56 (C)			
13a	1.72 (1H, dd, *J* = 8.2, 5.4 Hz)	41.14 (CH_2)	C-14, C-15, C-11, C-12		
13b	1.67 (1H, dd, *J* = 8.2, 4.5 Hz)		C-14, C-15, C-11, C-12	H_2-14	H-10, H-15
14	1.78 (2H, m)	25.17 (CH_2)	C-13, C-15, C-16, C-12	H-15	
15	2.03 (1H, dt, *J* = 9.1, 7.1 Hz)	56.14 (CH)	C-14, C-17, C-13, C-11, C-16, C-12, C-10	H-11	H-10
16		73.25 (C)			
17	1.20 (3H, s)	28.31 (CH_3)	C-20, C-15, C-16		
18	2.11 (3H, br d, *J* = 1.0 Hz)	21.53 (CH_3)	C-7, C-8. C-9		H-7, H-10
19	1.14 (3H, s)	24.17 (CH_3)	C-11, C-12, C-13		H-10
20	1.17 (3H, s)	28.66 (CH_3)	C-17, C-15, C-16		



3

Table S4. Detailed 2D-NMR data of compound **4**.

No.	δ_H	δ_C	HMBC	COSY	ROESY
2	7.06 (1H, dd, *J* = 2.4, 1.4 Hz)	126.46 (CH)	C-3, C-4, C-5	H-3	
3	6.23 (1H, dd, *J* = 3.9, 2.4 Hz)	111.20 (CH)	C-4, C-2, C-5		
4	6.97 (1H, dd, *J* = 3.9, 1.4 Hz)	117.24 (CH)	C-3, C-2, C-5, C-6	H-3	H-7
5		135.48 (C)			
6		182.41 (C)			
7	6.59 (1H, s)	121.63 (CH)	C-18, C-9, C-8, C-6	H-9	
8		150.90 (C)			
9	7.66 (1H, d, *J* = 15.8 Hz)	130.30 (CH)	C-18, C-11, C-12, C-7, C-8		
10	6.12 (1H, dd, *J* = 15.8, 11.1 Hz)	140.34 (CH)	C-15, C-11, C-12, C-9, C-8	H-9	H_3-18
11	2.59 (1H, dd, *J* = 11.1, 5.8 Hz)	60.34 (CH)	C-14, C-13, C-12, C-15, C-9, C-10	H-10	H-9
12		83.04 (C)			
13a	1.83 (1H, m)	38.33 (CH_2)	C-14, C-19, C-15, C-12		H-10
13b	1.78 (1H, m)		C-14, C-11, C-15, C-12		H-15
14	1.91 (2H, m)	23.63 (CH_2)	C-13, C-15, C-11, C-12, C-16	H-13a, b	
15	2.67 (1H, ddd, *J* = 10.2, 9.6, 5.8 Hz)	54.51 (CH)	C-14, C-20, C-17, C-13, C-11, C-16, C-10	H_2-14	H-11
16		72.80 (C)			
17	1.19 (3H, s)	30.45 (CH_3)	C-20, C-15, C-16, C-9		H-10
18	2.09 (3H, br d, *J* = 1.0 Hz)	21.67 (CH_3)	C-6, C-7, C-8, C-9	H-7	H-7
19	1.15 (3H, s)	26.71 (CH_3)	C-11, C-12, C-13		H-10; H-11
20	1.22 (3H, s)	28.25 (CH_3)	C-15, C-16, C-17		

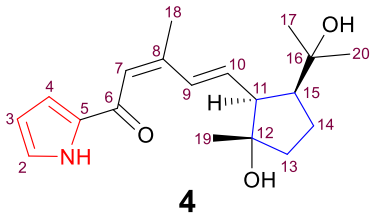


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Table S5. Detailed 2D-NMR data of compound **5**.

No.	δ_H	δ_C	HMBC	COSY	ROESY
2	7.06 (1H, dd, *J* = 2.2, 1.2 Hz)	126.47 (CH)	C-3, C-4, C-5	H-3	
3	6.23 (1H, dd, *J* = 3.7, 2.2 Hz)	111.19 (CH)	C-4, C-2, C-5		
4	6.97 (1H, dd, *J* = 3.7, 1.2 Hz)	117.28 (CH)	C-3, C-2, C-5	H-3	H-7
5		135.48 (C)			
6		182.36 (C)			
7	6.59 (1H, br s)	122.32 (CH)	C-18, C-9, C-8, C-6	H_3-18	H_3-18
8		150.48 (C)			
9	7.66 (1H, d, *J* = 15.8 Hz)	130.26 (CH)	C-18, C-11, C-7, C-8		H-11
10	5.90 (1H, dd, *J* = 15.8, 9.0 Hz)	138.60 (CH)	C-11. C-12, C-15, C-8	H-9	H_3-18
11	3.14 (1H, d, *J* = 9.0 Hz)	60.28 (CH)	C-14, C-13, C-12, C-9, C-10	H-11	H_3-19
12		82.50 (C)			
13	1.75 (2H, m)	38.69 (CH_2)	C-14, C-11, C-12		H-10
14a	2.48 (1H, m)	28.86 (CH_2)	C-13, C-15, C-16	H_2-13	
14b	2.36 (1H, m)		C-13, C-12, C-15, C-16	H_2-13	
15		137.49 (C)			
16		126.86 (C)			
17	1.61 (3H, s)	21.22 (CH_3)	C-15, C-16		
18	2.07 (3H, br d, *J* = 0.9 Hz)	21.44 (CH_3)	C-7, C-8, C-9		
19	1.23 (3H, s)	25.24 (CH_3)	C-11, C-12, C-13		H-10
20	1.65 (3H, s)	21.23 (CH_3)	C-15, C-16		

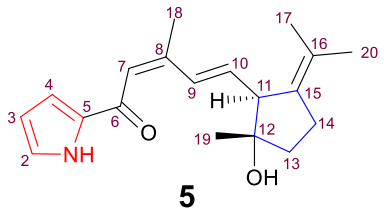

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Table S6. Details of feeding experiments using several isotope labeling substrates.

labeling substrates	Solvent used to dissolve the labeling substrate	Quality of labeling substrate used	Final concentration of the feeding experiment	fermentation medium	fermentation scale in total	yield of compound **3**
[$^{13}C_5$, ^{15}N]-L-Pro	dd H_2O	100 mg	666 mg/L	M15A[a]	150 mL	NP[d]
[$^{13}C_5$, ^{15}N]-L-Glu	0.5N HCl	500 mg	625 mg/L	M15A[a]	800 mL	0.8 mg
$^{13}C_6$-glucose	dd H_2O	1000 mg	1250 mg/L	M15B[b]	800 mL	1.0 mg
$^{13}C_2$-Gly	dd H_2O	500 mg	625 mg/L	M15A[a]	800 mL	0.5 mg
$^{13}C_2$-sodium acetate	dd H_2O	1000 mg	1250 mg/L	M15B[b]	800 mL	0.8 mg
$^{13}C_3$-glycerol	dd H_2O	1000 mg	1250 mg/L	M15B[b]	800 mL	1.0 mg
[$^{13}C_3$, ^{15}N]-L-Ala	dd H_2O	500 mg	714 mg/L	M15A[a]	700 mL	0.6 mg
$^{15}NH_4Cl$	dd H_2O	450 mg	500 mg/L	M15A[a]	900 mL	NP[d]
$^{15}NH_4Cl$	dd H_2O	450 mg	500 mg/L	M15[c]	900 mL	NP[d]

[a] Medium M15A: glucose 30 g/L, beef extract 1 g/L, peptone 1 g/L, NaCl 5 g/L, $CaCO_3$ 3 g/L, pH 7.2

[b] Medium M15B: glucose 12 g/L, beef extract 5 g/L, peptone 1 g/L, NaCl 5 g/L, $CaCO_3$ 3 g/L, pH 7.2

[c] Medium M15: glucose 30 g/L, beef extract 5 g/L, peptone 1 g/L, NaCl 5 g/L, $CaCO_3$ 3 g/L, pH 7.2

[d] NP: Not to be purified.

Table S7. Energies and populations of predominant conformers of (10*S*, 11*R*, 12*S*, 15*R*)-**1** at M06-2X/6-31G(d,p) theory level in gas.

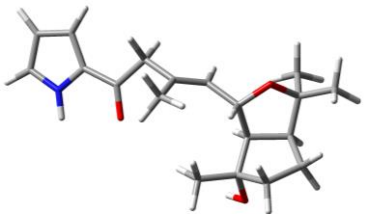
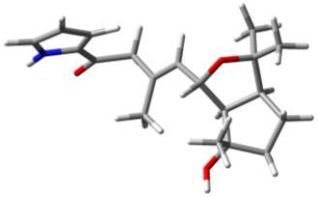
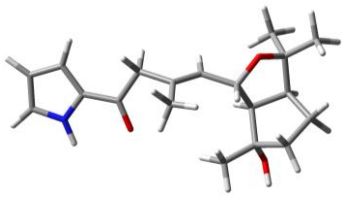
Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
a		−1020.543899	−640400.9603	48.51
b		−1020.540591	−640398.8846	1.46
c		−1020.543929	−640400.9787	50.03

Table S8. Energies and populations of predominant conformers of (11*S*, 12*S*, 15*R*)-**3** at B3LYP/6-31G(d,p) theory level in gas.

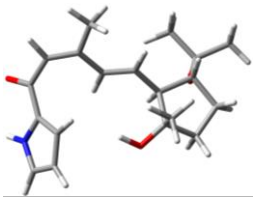
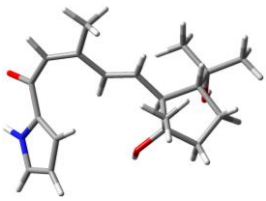
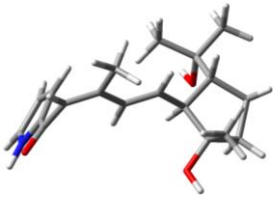
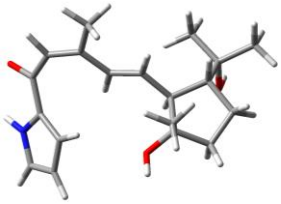
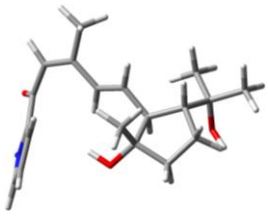
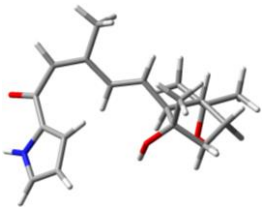
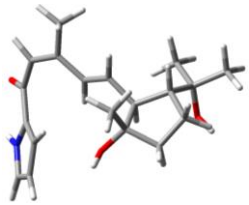
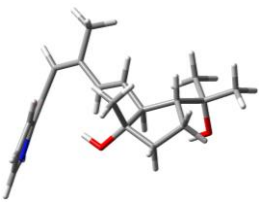
Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
a		−1020.725693	−640515.0377	23.61
b		−1020.725332	−640514.8109	16.10
c		−1020.723932	−640513.9327	3.66
d		−1020.724043	−640514.0023	4.11
e		−1020.725491	−640514.9108	19.06
f		−1020.725034	−640514.624	11.75
g		−1020.72386	−640513.8873	3.39
h		−1020.725453	−640514.8873	18.32

Table S9. Energies and populations of predominant conformers of (11*S*, 12*S*, 15*S*)-**4** at CAM-B3LYP/def2-TZVP theory level in gas.

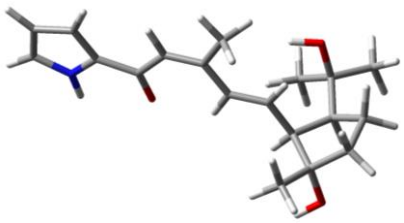
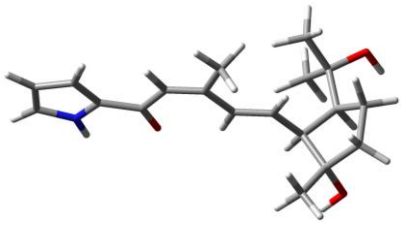
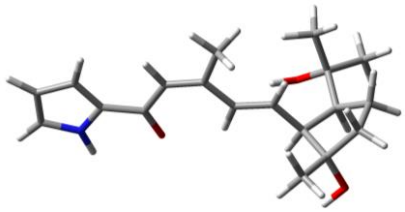
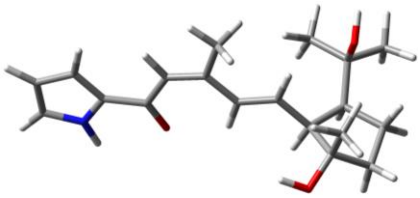
Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
a		−1020.55242	−640406.3074	95.59
b		−1020.548958	−640404.1345	2.44
c		−1020.548691	−640403.967	1.84
d		−1020.546184	−640402.3942	0.13

Table S10. Energies and populations of predominant conformers of (11*S*, 12*S*)-**5** at CAM-B3LYP/def2-TZVP theory level in gas.

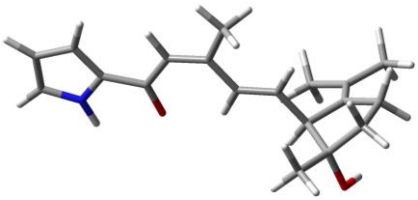
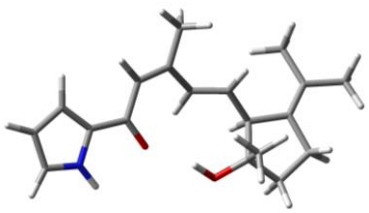
Conformers	Structures	E (Hartree)	E (kcal/mol)	Population (%)
a		−944.0982086	−592430.5656	93.36
b		−944.0957124	−592428.9992	6.64

Table S11. DFT Coordinates of the optimized conformers of (10*S*, 11*R*, 12*S*, 15*R*)-**1** at M06-2X/6-31G(d,p) theory level.

Conformer (10*S*, 11*R*, 12*S*, 15*R*)-**1**-**a**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	6.606840	−0.871758	−0.468339
2	6	0	5.323483	−1.253528	−0.021958
3	6	0	4.489767	−0.156911	−0.176800
4	7	0	5.242940	0.860647	−0.702283
5	6	0	6.520066	0.446116	−0.882735
6	6	0	3.072688	0.084960	0.092269
7	6	0	2.256251	−1.083900	0.630918
8	8	0	2.584705	1.181785	−0.131486
9	6	0	0.894967	−0.652220	1.110620
10	6	0	0.914330	0.169598	2.372040
11	6	0	−0.189781	−0.968926	0.399300
12	6	0	−1.598712	−0.506578	0.623146
13	6	0	−2.078853	0.408263	−0.533105
14	6	0	−3.504627	−0.095355	−0.831988
15	6	0	−3.434465	−1.574046	−0.402874
16	8	0	−2.508120	−1.602316	0.687949
17	6	0	−2.242525	1.886779	−0.158073
18	6	0	−3.529235	1.877240	0.669101
19	6	0	−4.443031	0.869390	−0.052356
20	6	0	−4.734559	−2.183834	0.103082
21	6	0	−2.879493	−2.422775	−1.552954
22	8	0	−2.567671	2.615847	−1.342763
23	6	0	−1.036269	2.514958	0.528274
24	1	0	7.497976	−1.481827	−0.486599
25	1	0	5.032440	−2.218850	0.368866
26	1	0	4.846587	1.769375	−0.900601
27	1	0	7.272969	1.106888	−1.286374
28	1	0	2.831135	−1.560203	1.436842
29	1	0	2.175755	−1.823609	−0.176021
30	1	0	−0.076108	0.302372	2.810650
31	1	0	1.341121	1.158786	2.170573
32	1	0	1.549382	−0.314193	3.123632
33	1	0	−0.063200	−1.582619	−0.494820
34	1	0	−1.673326	0.021948	1.580296
35	1	0	−1.400518	0.308580	−1.390408
36	1	0	−3.727841	−0.035344	−1.900915
37	1	0	−3.305639	1.543833	1.688598
38	1	0	−3.957151	2.881724	0.730146
39	1	0	−5.100476	0.349862	0.648318
40	1	0	−5.082743	1.396035	−0.764269
41	1	0	−5.049679	−1.707610	1.033559
42	1	0	−5.529322	−2.074648	−0.642045
43	1	0	−4.590509	−3.249895	0.303156
44	1	0	−3.621412	−2.533506	−2.350992
45	1	0	−1.981801	−1.967948	−1.986175
46	1	0	−2.614451	−3.416047	−1.179130
47	1	0	−1.793528	2.581611	−1.924472
48	1	0	−0.115072	2.335339	−0.040674

49	1	0	−1.193557	3.593751	0.619672
50	1	0	−0.883958	2.104294	1.530158
Conformer (10*S*, 11*R*, 12*S*, 15*R*)-**1**-**b**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.488302	1.125670	−2.043699
2	6	0	3.562738	1.063472	−0.979671
3	6	0	4.081288	0.191392	−0.034106
4	7	0	5.283814	−0.264244	−0.510762
5	6	0	5.543284	0.289891	−1.719045
6	6	0	3.629180	−0.288567	1.272097
7	6	0	2.297582	0.218648	1.802557
8	8	0	4.310242	−1.084922	1.898772
9	6	0	1.125246	−0.248865	0.965031
10	6	0	1.076971	−1.732936	0.713117
11	6	0	0.224923	0.624430	0.506139
12	6	0	−0.985394	0.291436	−0.342553
13	6	0	−2.054731	−0.589254	0.344388
14	6	0	−3.214320	0.391898	0.687756
15	6	0	−2.710237	1.772203	0.200578
16	8	0	−1.675773	1.469467	−0.744100
17	6	0	−2.693700	−1.711947	−0.513161
18	6	0	−4.154740	−1.697597	−0.037047
19	6	0	−4.478652	−0.206653	0.035759
20	6	0	−3.730160	2.623769	−0.542957
21	6	0	−2.149452	2.565572	1.386702
22	8	0	−2.028407	−2.926576	−0.188752
23	6	0	−2.609799	−1.459705	−2.020865
24	1	0	4.401130	1.708043	−2.949335
25	1	0	2.615071	1.578040	−0.905823
26	1	0	5.851758	−0.913859	0.016015
27	1	0	6.447382	0.056877	−2.261984
28	1	0	2.214513	−0.172113	2.823105
29	1	0	2.317496	1.313601	1.846308
30	1	0	1.947072	−2.037118	0.116908
31	1	0	0.174907	−2.058167	0.190398
32	1	0	1.139529	−2.284810	1.658911
33	1	0	0.369921	1.687080	0.695662
34	1	0	−0.630246	−0.172337	−1.268987
35	1	0	−1.650356	−1.066555	1.241350
36	1	0	−3.370209	0.426138	1.770952
37	1	0	−4.188572	−2.148257	0.962345
38	1	0	−4.822546	−2.266932	−0.693941
39	1	0	−4.631475	0.185579	−0.974373
40	1	0	−5.384371	0.014093	0.607461
41	1	0	−4.019516	2.152418	−1.484870
42	1	0	−4.625513	2.778760	0.067653
43	1	0	−3.295838	3.600657	−0.775442
44	1	0	−2.970012	2.922878	2.018353
45	1	0	−1.583640	3.430163	1.026115
46	1	0	−1.492207	1.949318	2.007739
47	1	0	−2.383965	−3.622387	−0.761193
48	1	0	−1.598778	−1.668166	−2.381203
49	1	0	−3.303182	−2.120533	−2.554867

50	1	0	−2.853527	−0.423595	−2.275401
Conformer (10*S*, 11*R*, 12*S*, 15*R*)-**1**-**c**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	−6.616097	0.904552	−0.489955
2	6	0	−5.325613	1.272205	−0.051606
3	6	0	−4.515896	0.153445	−0.169575
4	7	0	−5.289684	−0.863453	−0.664821
5	6	0	−6.557036	−0.427092	−0.862852
6	6	0	−3.105316	−0.112482	0.114054
7	6	0	−2.263795	1.056719	0.610704
8	8	0	−2.644360	−1.228533	−0.065090
9	6	0	−0.900366	0.623406	1.083149
10	6	0	−0.911691	−0.187490	2.352111
11	6	0	0.181597	0.937634	0.366201
12	6	0	1.593561	0.489930	0.600222
13	6	0	2.104167	−0.403757	−0.557887
14	6	0	3.531300	0.116784	−0.819785
15	6	0	3.434885	1.590653	−0.379928
16	8	0	2.486409	1.598114	0.691953
17	6	0	2.273738	−1.877147	−0.189592
18	6	0	3.541914	−1.857268	0.676367
19	6	0	4.463231	−0.843320	−0.026412
20	6	0	4.716747	2.212268	0.157188
21	6	0	2.891412	2.440703	−1.534313
22	8	0	2.561134	−2.511410	−1.437149
23	6	0	1.057466	−2.524265	0.459929
24	1	0	−7.493864	1.532766	−0.529427
25	1	0	−5.014345	2.242398	0.310469
26	1	0	−4.911205	−1.785254	−0.836116
27	1	0	−7.322672	−1.083255	−1.249660
28	1	0	−2.820847	1.559445	1.413477
29	1	0	−2.186747	1.776553	−0.214197
30	1	0	−1.546131	0.300117	3.101845
31	1	0	0.080910	−0.311567	2.788526
32	1	0	−1.335124	−1.179858	2.160939
33	1	0	0.051744	1.542911	−0.532960
34	1	0	1.661412	−0.046831	1.553250
35	1	0	1.448262	−0.319871	−1.430455
36	1	0	3.777052	0.066466	−1.883906
37	1	0	3.295433	−1.525827	1.691764
38	1	0	3.985935	−2.855971	0.762656
39	1	0	5.107505	−0.323701	0.686245
40	1	0	5.117242	−1.363515	−0.730379
41	1	0	4.554583	3.274211	0.365030
42	1	0	5.527137	2.121368	−0.573487
43	1	0	5.020230	1.731037	1.089095
44	1	0	2.007219	1.977562	−1.985739
45	1	0	2.608423	3.428440	−1.158936
46	1	0	3.645773	2.564707	−2.318572
47	1	0	2.728157	−3.447734	−1.253819
48	1	0	0.873689	−2.122148	1.460070
49	1	0	0.159026	−2.362174	−0.144159
50	1	0	1.218284	−3.604337	0.566358

Table S12. DFT Coordinates of the optimized conformers of (11*S*, 12*S*, 15*R*)-**3** at B3LYP/6-31G(d,p) theory level.

Conformer (11*S*, 12*S*, 15*R*)-**3**-**a**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	−3.629674	−0.104428	−0.373959
2	6	0	−3.241972	−1.074944	0.550792
3	6	0	−3.632281	−2.332501	0.038199
4	6	0	−4.254133	−2.102777	−1.182938
5	7	0	−4.249393	−0.763267	−1.412068
6	6	0	−3.584778	1.357453	−0.406809
7	8	0	−4.224069	1.967431	−1.270052
8	6	0	−2.838803	2.103600	0.643744
9	6	0	−1.548653	1.950190	1.028813
10	6	0	−0.634885	1.002997	0.380670
11	6	0	−0.994470	2.834891	2.122267
12	6	0	0.616779	0.713533	0.787337
13	6	0	1.504601	−0.291302	0.114262
14	6	0	3.034935	−0.040273	0.225135
15	6	0	3.682088	−1.466581	0.208806
16	6	0	2.522888	−2.467346	0.060978
17	6	0	1.296902	−1.756576	0.645914
18	8	0	0.128046	−2.351571	0.096097
19	6	0	1.257273	−1.848260	2.177885
20	6	0	3.614598	0.901355	−0.862547
21	6	0	5.119023	1.134283	−0.635499
22	6	0	2.893176	2.257731	−0.906547
23	8	0	3.414884	0.212771	−2.109177
24	1	0	1.243245	−0.351806	−0.948208
25	1	0	−2.761886	−0.875895	1.498066
26	1	0	−3.483525	−3.298693	0.498466
27	1	0	−4.687295	−2.795263	−1.889619
28	1	0	−4.650265	−0.257373	−2.189336
29	1	0	−3.415363	2.923090	1.067390
30	1	0	−1.000319	0.520110	−0.521741
31	1	0	−1.749992	3.533598	2.487509
32	1	0	−0.650806	2.236087	2.974176
33	1	0	−0.131659	3.409969	1.768153
34	1	0	1.005778	1.179841	1.692106
35	1	0	3.244422	0.441003	1.189813
36	1	0	4.238140	−1.641899	1.135802
37	1	0	4.387605	−1.573543	−0.616541
38	1	0	2.316201	−2.659874	−0.996500
39	1	0	2.716089	−3.430704	0.543676
40	1	0	−0.643810	−1.847512	0.393830
41	1	0	0.400096	−1.300597	2.584126
42	1	0	1.163012	−2.896612	2.475580
43	1	0	2.162489	−1.439896	2.640215
44	1	0	5.527793	1.770944	−1.429348
45	1	0	5.674435	0.193838	−0.641005
46	1	0	5.302798	1.639801	0.318591
47	1	0	3.349059	2.901390	−1.669279
48	1	0	1.836198	2.137577	−1.149493
49	1	0	2.969762	2.783468	0.051180
50	1	0	3.736983	0.786506	−2.817087
Conformer (11*S*, 12*S*, 15*R*)-**3**-**b**					

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	3.579920	0.249300	−0.429173
2	6	0	2.917542	1.312110	0.189068
3	6	0	3.327517	2.500168	−0.455876
4	6	0	4.235684	2.143418	−1.445307
5	7	0	4.375440	0.793538	−1.416936
6	6	0	3.691766	−1.197631	−0.225231
7	8	0	4.535939	−1.821711	−0.883220
8	6	0	2.911618	−1.939265	0.800027
9	6	0	1.599248	−1.881891	1.138110
10	6	0	0.641324	−0.987214	0.489903
11	6	0	1.081580	−2.813587	2.210661
12	6	0	−0.632550	−0.783176	0.873305
13	6	0	−1.529979	0.235988	0.241470
14	6	0	−3.034270	−0.138718	0.109822
15	6	0	−3.808397	1.219179	0.240568
16	6	0	−2.736759	2.314264	0.363665
17	6	0	−1.524009	1.613116	1.000899
18	8	0	−0.299549	2.318526	0.823004
19	6	0	−1.678530	1.476566	2.516819
20	6	0	−3.391301	−0.911196	−1.186523
21	6	0	−4.882185	−1.292356	−1.201311
22	6	0	−2.544417	−2.180561	−1.367589
23	8	0	−3.115110	0.005683	−2.261824
24	1	0	−1.157711	0.461939	−0.767132
25	1	0	2.205054	1.242446	0.996870
26	1	0	3.007302	3.505753	−0.222477
27	1	0	4.779756	2.752624	−2.152412
28	1	0	4.985845	0.206391	−1.968107
29	1	0	3.519356	−2.716359	1.258394
30	1	0	1.006909	−0.434157	−0.369635
31	1	0	1.873244	−3.464383	2.587200
32	1	0	0.678448	−2.247289	3.058673
33	1	0	0.268099	−3.442023	1.830722
34	1	0	−1.032756	−1.315755	1.734958
35	1	0	−3.308379	−0.795247	0.945645
36	1	0	−4.454025	1.204889	1.124638
37	1	0	−4.448023	1.399317	−0.624607
38	1	0	−2.448918	2.665126	−0.635592
39	1	0	−3.063141	3.186659	0.938395
40	1	0	−0.132215	2.396448	−0.126709
41	1	0	−0.822977	0.947233	2.943177
42	1	0	−1.719963	2.472368	2.967424
43	1	0	−2.592769	0.938834	2.784544
44	1	0	−5.134241	−1.798477	−2.140821
45	1	0	−5.523383	−0.412754	−1.112221
46	1	0	−5.122242	−1.979834	−0.383234
47	1	0	−2.846632	−2.705186	−2.282643
48	1	0	−1.482159	−1.944641	−1.444399
49	1	0	−2.680547	−2.876015	−0.532758
50	1	0	−3.295046	−0.453739	−3.092879
Conformer (11*S*, 12*S*, 15*R*)-**3**-**c**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	−3.550694	0.568604	−0.243609
2	6	0	−2.820676	1.595421	0.354280

3	6	0	−3.086627	2.781358	−0.365095
4	6	0	−3.976229	2.456052	−1.381517
5	7	0	−4.246186	1.127449	−1.293719
6	6	0	−3.788426	−0.843372	0.056123
7	8	0	−4.677700	−1.447022	−0.555540
8	6	0	−3.051198	−1.535356	1.147654
9	6	0	−1.717315	−1.613725	1.378586
10	6	0	−0.715288	−0.996225	0.506251
11	6	0	−1.229106	−2.437520	2.549331
12	6	0	0.614789	−1.021728	0.708232
13	6	0	1.626387	−0.448588	−0.241881
14	6	0	2.861683	0.226008	0.429887
15	6	0	4.071066	−0.077570	−0.517568
16	6	0	3.471111	−0.763585	−1.753679
17	6	0	2.221737	−1.497154	−1.235533
18	8	0	1.238085	−1.701301	−2.250298
19	6	0	2.570777	−2.839587	−0.579627
20	6	0	2.684463	1.740952	0.711333
21	6	0	3.900098	2.298492	1.473449
22	6	0	1.405380	2.045187	1.507143
23	8	0	2.601009	2.361865	−0.583400
24	1	0	1.138568	0.287686	−0.890150
25	1	0	−2.182757	1.486512	1.218779
26	1	0	−2.683726	3.765119	−0.170578
27	1	0	−4.422843	3.073588	−2.147074
28	1	0	−4.879989	0.573253	−1.852071
29	1	0	−3.714626	−2.140463	1.762106
30	1	0	−1.085269	−0.499798	−0.385500
31	1	0	−2.063778	−2.864860	3.108896
32	1	0	−0.582190	−3.256846	2.215772
33	1	0	−0.637627	−1.825038	3.240048
34	1	0	1.014369	−1.515296	1.593677
35	1	0	3.037378	−0.247279	1.404739
36	1	0	4.790795	−0.733615	−0.016419
37	1	0	4.603597	0.832658	−0.797567
38	1	0	3.136271	−0.012095	−2.475836
39	1	0	4.175743	−1.432293	−2.262356
40	1	0	1.554000	−2.406867	−2.830573
41	1	0	1.667450	−3.328598	−0.206255
42	1	0	3.042543	−3.505067	−1.313470
43	1	0	3.273557	−2.724950	0.252291
44	1	0	3.790353	3.379469	1.621545
45	1	0	4.829558	2.128655	0.925189
46	1	0	3.993195	1.838783	2.463225
47	1	0	1.342979	3.120415	1.717655
48	1	0	0.513623	1.754219	0.949753
49	1	0	1.396546	1.522425	2.469089
50	1	0	2.432843	3.303807	−0.447546
Conformer (11*S*, 12*S*, 15*R*)-**3**-**d**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	3.628803	0.248448	−0.423554
2	6	0	2.930459	1.346031	0.085430
3	6	0	3.390229	2.494053	−0.595685
4	6	0	4.362168	2.081197	−1.497978
5	7	0	4.492989	0.735306	−1.383817
6	6	0	3.723189	−1.185800	−0.141316

7	8	0	4.596915	−1.842544	−0.726741
8	6	0	2.901567	−1.886583	0.879896
9	6	0	1.583938	−1.811914	1.193878
10	6	0	0.637188	−0.921879	0.522174
11	6	0	1.047256	−2.726374	2.273155
12	6	0	−0.641941	−0.723953	0.890806
13	6	0	−1.559316	0.267706	0.238525
14	6	0	−3.043190	−0.181219	0.074834
15	6	0	−3.889880	1.129512	0.212968
16	6	0	−2.875020	2.274932	0.359768
17	6	0	−1.637158	1.627095	1.003528
18	8	0	−0.427055	2.334574	0.719112
19	6	0	−1.794573	1.474340	2.522229
20	6	0	−3.338290	−0.952720	−1.237666
21	6	0	−4.802294	−1.427413	−1.270670
22	6	0	−2.410826	−2.162263	−1.431066
23	8	0	−3.114229	−0.003624	−2.295273
24	1	0	−1.166575	0.530033	−0.750148
25	1	0	2.158561	1.323570	0.839473
26	1	0	3.049456	3.509622	−0.453820
27	1	0	4.954189	2.648469	−2.201450
28	1	0	5.132494	0.115310	−1.860867
29	1	0	3.490077	−2.661228	1.366642
30	1	0	1.010922	−0.371320	−0.335172
31	1	0	1.831405	−3.373412	2.671228
32	1	0	0.632054	−2.147527	3.106773
33	1	0	0.238447	−3.359045	1.890211
34	1	0	−1.044480	−1.259092	1.750162
35	1	0	−3.296859	−0.864596	0.895851
36	1	0	−4.544488	1.069920	1.088826
37	1	0	−4.527164	1.288421	−0.658068
38	1	0	−2.578656	2.646449	−0.626530
39	1	0	−3.259922	3.122257	0.939488
40	1	0	−0.449181	3.164020	1.215256
41	1	0	−0.911426	0.998042	2.955286
42	1	0	−1.913601	2.460721	2.987693
43	1	0	−2.675851	0.882267	2.789488
44	1	0	−5.014186	−1.934288	−2.219605
45	1	0	−5.498069	−0.590692	−1.175437
46	1	0	−5.005744	−2.140464	−0.464522
47	1	0	−2.679069	−2.696465	−2.351283
48	1	0	−1.366797	−1.855722	−1.506410
49	1	0	−2.499111	−2.873495	−0.603174
50	1	0	−3.236256	−0.465318	−3.135486
Conformer (11*S*, 12*S*, 15*R*)-**3**-**e**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	−3.614745	−0.120902	−0.373832
2	6	0	−3.214114	−1.080372	0.556968
3	6	0	−3.584683	−2.346659	0.050345
4	6	0	−4.207364	−2.132824	−1.173287
5	7	0	−4.222573	−0.794594	−1.409141
6	6	0	−3.592810	1.341922	−0.414996
7	8	0	−4.245712	1.935939	−1.278876
8	6	0	−2.853429	2.106149	0.626759
9	6	0	−1.561577	1.969199	1.012371
10	6	0	−0.639355	1.023870	0.373334

11	6	0	−1.015069	2.869674	2.096674
12	6	0	0.609645	0.739765	0.790586
13	6	0	1.504432	−0.266467	0.127995
14	6	0	3.032942	−0.009336	0.252479
15	6	0	3.676413	−1.436886	0.312700
16	6	0	2.530723	−2.439953	0.103500
17	6	0	1.283784	−1.733929	0.649173
18	8	0	0.139314	−2.334855	0.057436
19	6	0	1.193341	−1.831783	2.178472
20	6	0	3.614841	0.890207	−0.880254
21	6	0	5.118985	1.135838	−0.669048
22	6	0	2.892387	2.238571	−0.967631
23	8	0	3.398916	0.277137	−2.162178
24	1	0	1.259387	−0.322591	−0.939126
25	1	0	−2.740343	−0.868857	1.504712
26	1	0	−3.423629	−3.308001	0.516659
27	1	0	−4.628682	−2.835369	−1.877169
28	1	0	−4.629064	−0.298816	−2.190101
29	1	0	−3.437509	2.924446	1.042291
30	1	0	−0.996350	0.537013	−0.530236
31	1	0	−1.775880	3.567364	2.452681
32	1	0	−0.669274	2.282881	2.956103
33	1	0	−0.155429	3.446078	1.737289
34	1	0	0.991604	1.211101	1.695621
35	1	0	3.234599	0.509188	1.199384
36	1	0	4.157201	−1.591679	1.283907
37	1	0	4.466579	−1.580756	−0.431729
38	1	0	2.361596	−2.620676	−0.963446
39	1	0	2.708276	−3.409183	0.580077
40	1	0	−0.648273	−1.843119	0.334447
41	1	0	0.319273	−1.290091	2.554909
42	1	0	1.095351	−2.881404	2.470538
43	1	0	2.078341	−1.417318	2.673363
44	1	0	5.509700	1.750949	−1.484764
45	1	0	5.689434	0.201227	−0.649928
46	1	0	5.306599	1.656702	0.275786
47	1	0	3.348930	2.849504	−1.751666
48	1	0	1.837256	2.106526	−1.211951
49	1	0	2.963430	2.781423	−0.019858
50	1	0	3.948651	−0.516661	−2.208700

Conformer (11*S*, 12*S*, 15*R*)-**3**-**f**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	3.568826	0.261973	−0.431287
2	6	0	2.906177	1.315583	0.201940
3	6	0	3.298069	2.510910	−0.440894
4	6	0	4.196059	2.167257	−1.444234
5	7	0	4.347307	0.818440	−1.425518
6	6	0	3.692579	−1.185250	−0.236647
7	8	0	4.536456	−1.799822	−0.903311
8	6	0	2.922385	−1.937357	0.788831
9	6	0	1.610886	−1.890531	1.131542
10	6	0	0.645586	−0.998317	0.490485
11	6	0	1.102134	−2.830871	2.200658
12	6	0	−0.627227	−0.801118	0.880058
13	6	0	−1.530540	0.217160	0.254204
14	6	0	−3.032581	−0.165227	0.120707

15	6	0	−3.811404	1.184940	0.300333
16	6	0	−2.746676	2.288876	0.391065
17	6	0	−1.521257	1.594074	1.012668
18	8	0	−0.305423	2.308660	0.818328
19	6	0	−1.655963	1.460323	2.530939
20	6	0	−3.378767	−0.903070	−1.207915
21	6	0	−4.863757	−1.301658	−1.243716
22	6	0	−2.518217	−2.153537	−1.415018
23	8	0	−3.074278	−0.058516	−2.333049
24	1	0	−1.165153	0.444195	−0.757490
25	1	0	2.206168	1.234510	1.019415
26	1	0	2.973324	3.512512	−0.196860
27	1	0	4.725621	2.784925	−2.154977
28	1	0	4.954122	0.239794	−1.989524
29	1	0	3.537128	−2.712362	1.241359
30	1	0	1.004484	−0.442218	−0.369878
31	1	0	1.899008	−3.478556	2.571494
32	1	0	0.697863	−2.271768	3.052945
33	1	0	0.291743	−3.462479	1.819458
34	1	0	−1.022593	−1.337923	1.741191
35	1	0	−3.303227	−0.844073	0.939904
36	1	0	−4.413980	1.154593	1.213356
37	1	0	−4.517892	1.380402	−0.512874
38	1	0	−2.473546	2.633732	−0.614862
39	1	0	−3.068145	3.164615	0.963111
40	1	0	−0.119791	2.341196	−0.130641
41	1	0	−0.792933	0.933862	2.945104
42	1	0	−1.693320	2.456705	2.980738
43	1	0	−2.564113	0.919754	2.813247
44	1	0	−5.092190	−1.788126	−2.196421
45	1	0	−5.526305	−0.435832	−1.139550
46	1	0	−5.104143	−1.999518	−0.434951
47	1	0	−2.825330	−2.661448	−2.333720
48	1	0	−1.461818	−1.897483	−1.505880
49	1	0	−2.631183	−2.849980	−0.578394
50	1	0	−3.736861	0.644346	−2.364739
Conformer (11*S*, 12*S*, 15*R*)-**3**-**g**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	3.626243	0.260044	−0.425006
2	6	0	2.925807	1.352664	0.091339
3	6	0	3.376523	2.505089	−0.588379
4	6	0	4.345153	2.099481	−1.497494
5	7	0	4.482947	0.753941	−1.388130
6	6	0	3.728704	−1.174548	−0.147193
7	8	0	4.604627	−1.824953	−0.735870
8	6	0	2.911991	−1.882825	0.872972
9	6	0	1.594311	−1.817140	1.188394
10	6	0	0.641609	−0.929021	0.522003
11	6	0	1.064026	−2.740063	2.263634
12	6	0	−0.638213	−0.742426	0.893442
13	6	0	−1.564091	0.247093	0.249489
14	6	0	−3.043330	−0.216279	0.083820
15	6	0	−3.903092	1.076895	0.293406
16	6	0	−2.903318	2.237881	0.404645
17	6	0	−1.642788	1.604154	1.019345
18	8	0	−0.451676	2.329971	0.707041

19	6	0	−1.764242	1.448768	2.540891
20	6	0	−3.329165	−0.936644	−1.268765
21	6	0	−4.784620	−1.431768	−1.327050
22	6	0	−2.385348	−2.120748	−1.500955
23	8	0	−3.074636	−0.046024	−2.368483
24	1	0	−1.178456	0.515164	−0.740950
25	1	0	2.158820	1.323172	0.850013
26	1	0	3.032306	3.518784	−0.441471
27	1	0	4.930137	2.671538	−2.202931
28	1	0	5.121750	0.138249	−1.871685
29	1	0	3.505172	−2.656130	1.356215
30	1	0	1.010593	−0.372068	−0.333218
31	1	0	1.852688	−3.383619	2.658353
32	1	0	0.645260	−2.168184	3.100325
33	1	0	0.259597	−3.376457	1.877738
34	1	0	−1.036284	−1.285875	1.749555
35	1	0	−3.284539	−0.934555	0.878493
36	1	0	−4.500461	0.990198	1.206617
37	1	0	−4.622747	1.248424	−0.513815
38	1	0	−2.632020	2.608698	−0.589757
39	1	0	−3.285080	3.083983	0.987765
40	1	0	−0.455521	3.142599	1.230773
41	1	0	−0.864484	0.984542	2.951918
42	1	0	−1.887132	2.432724	3.010656
43	1	0	−2.629113	0.842112	2.828185
44	1	0	−4.972694	−1.909615	−2.292819
45	1	0	−5.503304	−0.613393	−1.210414
46	1	0	−4.985733	−2.162482	−0.536651
47	1	0	−2.655527	−2.627707	−2.431764
48	1	0	−1.349450	−1.789635	−1.583863
49	1	0	−2.450694	−2.841631	−0.680209
50	1	0	−3.767191	0.627984	−2.372870
Conformer (11*S*, 12*S*, 15*R*)-**3**-**h**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	−3.634878	−0.086475	−0.352892
2	6	0	−3.256151	−1.029644	0.603633
3	6	0	−3.661402	−2.299322	0.134035
4	6	0	−4.282756	−2.103788	−1.093373
5	7	0	−4.263402	−0.772943	−1.367487
6	6	0	−3.573152	1.372876	−0.434366
7	8	0	−4.203880	1.961850	−1.317790
8	6	0	−2.817434	2.142687	0.592554
9	6	0	−1.526788	1.987940	0.974396
10	6	0	−0.627150	1.016164	0.342643
11	6	0	−0.956148	2.893702	2.041529
12	6	0	0.622382	0.719506	0.749716
13	6	0	1.498180	−0.304547	0.088907
14	6	0	3.031255	−0.094345	0.223989
15	6	0	3.642400	−1.532000	0.146062
16	6	0	2.458039	−2.508881	0.018697
17	6	0	1.247645	−1.770386	0.603222
18	8	0	0.068103	−2.325875	0.035970
19	6	0	1.195370	−1.873988	2.133370
20	6	0	3.668209	0.885826	−0.807822
21	6	0	5.166830	1.054109	−0.527897
22	6	0	2.990667	2.264506	−0.799975

23	8	0	3.599512	0.330339	−2.131655
24	1	0	1.231003	−0.364491	−0.975567
25	1	0	−2.773653	−0.803986	1.543706
26	1	0	−3.524431	−3.251073	0.626922
27	1	0	−4.725418	−2.814729	−1.775394
28	1	0	−4.660956	−0.289232	−2.160506
29	1	0	−3.385608	2.976956	0.998269
30	1	0	−1.003626	0.519633	−0.547890
31	1	0	−1.701650	3.610048	2.392753
32	1	0	−0.614785	2.313069	2.906853
33	1	0	−0.088987	3.449578	1.668056
34	1	0	1.021794	1.194879	1.644625
35	1	0	3.227216	0.330321	1.218187
36	1	0	4.237497	−1.744155	1.040005
37	1	0	4.305660	−1.623893	−0.715803
38	1	0	2.238435	−2.713157	−1.034534
39	1	0	2.632979	−3.471601	0.509028
40	1	0	−0.699086	−1.839614	0.373122
41	1	0	0.355822	−1.300404	2.540866
42	1	0	1.063415	−2.921350	2.419760
43	1	0	2.112276	−1.502727	2.603310
44	1	0	5.608337	1.722789	−1.272081
45	1	0	5.691743	0.097695	−0.583247
46	1	0	5.330407	1.482241	0.466040
47	1	0	3.488923	2.922559	−1.518119
48	1	0	1.933316	2.197223	−1.074117
49	1	0	3.044494	2.732163	0.188952
50	1	0	2.678113	0.367699	−2.421557

Table S13. DFT Coordinates of the optimized conformers of (11*S*, 12*S*, 15*S*)-**4** at CAM-B3LYP/def2-TZVP theory level.

Conformer (11*S*, 12*S*, 15*S*)-**4**-**a**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	−5.344521	0.165452	−1.397021
2	6	0	−4.649558	0.016348	−0.212347
3	6	0	−5.601013	0.000491	0.795908
4	6	0	−6.879292	0.144946	0.200258
5	6	0	−6.688457	0.244434	−1.156951
6	6	0	−3.198772	−0.087906	−0.210698
7	6	0	−2.500298	−0.240413	1.110041
8	8	0	−2.575599	−0.042721	−1.267800
9	6	0	−1.183154	−0.385760	1.372003
10	6	0	−0.748123	−0.503280	2.817026
11	6	0	−0.138133	−0.438950	0.356125
12	6	0	1.184939	−0.523222	0.576666
13	6	0	2.209389	−0.539897	−0.538578
14	6	0	3.086424	−1.820508	−0.533761
15	6	0	4.164395	−1.529589	0.516462
16	6	0	4.324170	−0.003249	0.545614
17	6	0	3.294719	0.571617	−0.447510
18	6	0	2.852295	2.029378	−0.151384
19	6	0	1.836197	2.531813	−1.185887
20	6	0	4.065049	2.971522	−0.156910
21	8	0	2.279214	2.143328	1.153237
22	8	0	3.738592	−1.944260	−1.807148
23	6	0	2.351104	−3.131935	−0.271908
24	1	0	−4.896302	0.208743	−2.305012
25	1	0	−5.417621	−0.102333	1.857181
26	1	0	−7.834853	0.173026	0.708622
27	1	0	−7.390777	0.364339	−1.971321
28	1	0	−3.177258	−0.218846	1.957350
29	1	0	−0.224628	−1.450321	2.989068
30	1	0	−1.595606	−0.477294	3.511298
31	1	0	−0.086139	0.325711	3.090712
32	1	0	−0.456847	−0.398511	−0.682749
33	1	0	1.582328	−0.567267	1.588284
34	1	0	1.704194	−0.445826	−1.509078
35	1	0	5.117818	−2.012607	0.276164
36	1	0	3.855905	−1.870853	1.511941
37	1	0	4.160766	0.363112	1.565080
38	1	0	5.341408	0.283633	0.255774
39	1	0	3.790397	0.598762	−1.431030
40	1	0	2.255255	2.522669	−2.197238
41	1	0	0.924064	1.927798	−1.186253
42	1	0	1.518407	3.554610	−0.951331
43	1	0	3.752502	4.007095	0.023049
44	1	0	4.765399	2.726328	0.649104
45	1	0	4.601581	2.935468	−1.110504
46	1	0	1.338625	1.901768	1.090990
47	1	0	3.057086	−2.156296	−2.468535
48	1	0	1.920979	−3.177508	0.733462
49	1	0	1.544941	−3.275482	−1.000119
50	1	0	3.031089	−3.983898	−0.387099
Conformer (11*S*, 12*S*, 15*S*)-**4**-**b**					

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	−5.433687	0.178901	−1.381902
2	6	0	−4.706810	0.035764	−0.216119
3	6	0	−5.631918	0.023009	0.817377
4	6	0	−6.926044	0.160798	0.256234
5	6	0	−6.771310	0.254977	−1.105781
6	6	0	−3.255064	−0.069075	−0.247780
7	6	0	−2.533916	−0.205171	1.060371
8	8	0	−2.651910	−0.043944	−1.316982
9	6	0	−1.214682	−0.339222	1.312277
10	6	0	−0.779677	−0.450062	2.759147
11	6	0	−0.166910	−0.377260	0.295486
12	6	0	1.148998	−0.509601	0.538186
13	6	0	2.217653	−0.528698	−0.531905
14	6	0	3.049333	−1.844329	−0.508657
15	6	0	4.102769	−1.619151	0.592458
16	6	0	4.214779	−0.096265	0.776984
17	6	0	3.346724	0.517571	−0.333997
18	6	0	3.003231	2.018866	−0.172368
19	6	0	2.335803	2.558293	−1.444227
20	6	0	2.156888	2.403682	1.042120
21	8	0	4.244928	2.728985	−0.013801
22	8	0	3.749151	−1.968893	−1.758254
23	6	0	2.259578	−3.135131	−0.309533
24	1	0	−5.010836	0.219305	−2.302020
25	1	0	−5.421125	−0.075297	1.874021
26	1	0	−7.867265	0.187582	0.790774
27	1	0	−7.496020	0.369162	−1.901007
28	1	0	−3.200014	−0.188192	1.916279
29	1	0	−0.281816	−1.408926	2.941273
30	1	0	−1.623472	−0.392418	3.455977
31	1	0	−0.096338	0.364768	3.022898
32	1	0	−0.474237	−0.277829	−0.742973
33	1	0	1.507758	−0.615053	1.559065
34	1	0	1.768565	−0.385186	−1.522793
35	1	0	5.075540	−2.040526	0.315116
36	1	0	3.799560	−2.070561	1.544275
37	1	0	3.854211	0.174834	1.774604
38	1	0	5.256157	0.234882	0.706668
39	1	0	3.977883	0.470538	−1.237108
40	1	0	1.353995	2.106005	−1.613871
41	1	0	2.961062	2.368948	−2.324665
42	1	0	2.211480	3.645923	−1.387861
43	1	0	1.109160	2.116437	0.931581
44	1	0	2.547771	1.970464	1.967134
45	1	0	2.174799	3.490692	1.190627
46	1	0	4.802010	2.537211	−0.787918
47	1	0	3.088414	−2.146618	−2.450317
48	1	0	1.768528	−3.180035	0.667173
49	1	0	2.920093	−4.005811	−0.395177
50	1	0	1.496045	−3.245753	−1.087790
Conformer (11*S*, 12*S*, 15*S*)-**4**-**c**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	−5.400573	−0.064358	−1.408822
2	6	0	−4.688628	0.007770	−0.227078

3	6	0	−5.624286	0.204621	0.777215
4	6	0	−6.910473	0.247194	0.182559
5	6	0	−6.740030	0.077077	−1.170224
6	6	0	−3.238845	−0.118549	−0.221881
7	6	0	−2.527392	−0.043583	1.098276
8	8	0	−2.627143	−0.283229	−1.273555
9	6	0	−1.207853	−0.131673	1.372932
10	6	0	−0.772484	−0.019535	2.818269
11	6	0	−0.160916	−0.323258	0.374517
12	6	0	1.159033	−0.419313	0.614732
13	6	0	2.186509	−0.604865	−0.478214
14	6	0	3.017996	−1.908819	−0.316924
15	6	0	4.096796	−1.518092	0.695237
16	6	0	4.437230	−0.058573	0.377432
17	6	0	3.307963	0.474236	−0.528609
18	6	0	2.954014	1.975996	−0.354557
19	6	0	4.166278	2.837816	−0.746899
20	6	0	2.494393	2.409560	1.043810
21	8	0	1.915003	2.310362	−1.282782
22	8	0	3.674986	−2.215399	−1.554470
23	6	0	2.242747	−3.152276	0.105931
24	1	0	−4.967013	−0.203986	−2.314282
25	1	0	−5.425773	0.309723	1.835465
26	1	0	−7.857274	0.387208	0.688736
27	1	0	−7.454083	0.045452	−1.982609
28	1	0	−3.200299	0.101979	1.936546
29	1	0	−1.618492	0.125878	3.499448
30	1	0	−0.257708	−0.931326	3.140166
31	1	0	−0.103227	0.836722	2.956623
32	1	0	−0.477240	−0.392489	−0.664022
33	1	0	1.544217	−0.372323	1.629891
34	1	0	1.682763	−0.612835	−1.454649
35	1	0	4.990254	−2.147429	0.624604
36	1	0	3.717097	−1.582411	1.721987
37	1	0	4.559645	0.505120	1.305410
38	1	0	5.393524	−0.002087	−0.157084
39	1	0	3.693271	0.397725	−1.559714
40	1	0	3.907592	3.903401	−0.737328
41	1	0	4.490960	2.615941	−1.769964
42	1	0	5.013363	2.684743	−0.070918
43	1	0	3.171871	2.077626	1.834241
44	1	0	1.484361	2.065523	1.275506
45	1	0	2.433204	3.503351	1.103303
46	1	0	1.094388	1.880081	−0.984389
47	1	0	2.986953	−2.398203	−2.218066
48	1	0	1.771375	−3.040642	1.087162
49	1	0	2.909011	−4.021752	0.151461
50	1	0	1.466197	−3.392752	−0.628471
Conformer (11*S*, 12*S*, 15*S*)-**4**-**d**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	−5.494402	−0.319635	−1.394579
2	6	0	−4.775859	−0.009759	−0.256064
3	6	0	−5.705413	0.389987	0.691985
4	6	0	−6.994625	0.314314	0.107398
5	6	0	−6.832097	−0.128483	−1.183261
6	6	0	−3.326550	−0.136489	−0.234102

7	6	0	−2.606415	0.205688	1.037983
8	8	0	−2.724130	−0.508788	−1.237073
9	6	0	−1.286685	0.155218	1.320081
10	6	0	−0.833173	0.586822	2.698171
11	6	0	−0.253760	−0.286568	0.389083
12	6	0	1.073686	−0.250399	0.602927
13	6	0	2.098510	−0.684230	−0.415897
14	6	0	2.958139	−1.900186	0.035908
15	6	0	4.155162	−1.826203	−0.908152
16	6	0	4.476895	−0.343457	−0.954137
17	6	0	3.106692	0.377087	−0.978612
18	6	0	3.169080	1.809827	−0.377366
19	6	0	1.846272	2.578988	−0.514824
20	6	0	4.267480	2.636893	−1.072665
21	8	0	3.505428	1.725575	1.009638
22	8	0	2.262171	−3.124152	−0.203461
23	6	0	3.396116	−1.892731	1.503807
24	1	0	−5.065080	−0.643408	−2.253745
25	1	0	−5.500176	0.707164	1.705712
26	1	0	−7.938374	0.556672	0.579337
27	1	0	−7.550439	−0.323905	−1.968428
28	1	0	−3.268848	0.552633	1.823521
29	1	0	−0.182416	1.466009	2.633929
30	1	0	−1.672826	0.858318	3.347784
31	1	0	−0.291985	−0.222657	3.200524
32	1	0	−0.585986	−0.663298	−0.575539
33	1	0	1.476648	0.130086	1.538060
34	1	0	1.531406	−1.029771	−1.295878
35	1	0	5.006718	−2.424256	−0.567203
36	1	0	3.886918	−2.193447	−1.906966
37	1	0	5.059702	−0.065539	−0.068629
38	1	0	5.079167	−0.097177	−1.834929
39	1	0	2.843605	0.501275	−2.040835
40	1	0	1.404090	2.450014	−1.507620
41	1	0	1.116433	2.293733	0.245428
42	1	0	2.001802	3.653166	−0.356171
43	1	0	4.304872	3.655931	−0.669234
44	1	0	4.094839	2.702534	−2.152064
45	1	0	5.263715	2.217334	−0.899059
46	1	0	3.571478	2.633057	1.354760
47	1	0	1.407332	−3.059651	0.258936
48	1	0	2.541310	−2.045905	2.172149
49	1	0	4.080585	−2.726012	1.701888
50	1	0	3.897849	−0.964444	1.789916

Table S14. DFT Coordinates of the optimized conformers of (11*S*, 12*S*)-**5** at CAM-B3LYP/def2-TZVP theory level.

Conformer (11*S*, 12*S*)-**5**-**a**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	−5.132756	0.550009	−1.302236
2	6	0	−4.525131	0.097581	−0.155144
3	6	0	−5.541406	−0.170801	0.767527
4	6	0	−6.773581	0.133336	0.141532
5	6	0	−6.481043	0.578749	−1.145008
6	6	0	−3.056065	0.003228	−0.153256
7	6	0	−2.429778	−0.484077	1.090493
8	8	0	−2.447276	0.334182	−1.175775
9	6	0	−1.101284	−0.668117	1.349834
10	6	0	−0.691327	−1.172145	2.713111
11	6	0	−0.057857	−0.397970	0.361527
12	6	0	1.268228	−0.538723	0.575754
13	6	0	2.324018	−0.229629	−0.449920
14	6	0	3.225385	−1.448198	−0.844882
15	6	0	4.246429	−1.499556	0.309813
16	6	0	4.565558	−0.022133	0.615282
17	6	0	3.354651	0.765732	0.104627
18	6	0	3.224216	2.107741	0.126602
19	6	0	2.009637	2.836256	−0.392871
20	6	0	4.292261	3.013057	0.691184
21	6	0	2.487810	−2.753977	−1.094650
22	8	0	3.887245	−1.135150	−2.069891
23	1	0	−4.583731	0.807822	−2.116056
24	1	0	−5.407047	−0.544951	1.779945
25	1	0	−7.768515	0.040909	0.572849
26	1	0	−7.142030	0.908731	−1.944090
27	1	0	−3.129756	−0.719643	1.895346
28	1	0	−1.563419	−1.340711	3.359789
29	1	0	−0.133903	−2.120428	2.635295
30	1	0	−0.024913	−0.453052	3.218011
31	1	0	−0.413708	−0.052536	−0.610709
32	1	0	1.633220	−0.871714	1.553914
33	1	0	1.833892	0.136536	−1.363834
34	1	0	5.130603	−2.087995	0.022703
35	1	0	3.792271	−1.989086	1.187120
36	1	0	5.487051	0.296470	0.097564
37	1	0	4.751309	0.146706	1.688670
38	1	0	1.235283	2.170552	−0.792756
39	1	0	2.294498	3.551311	−1.185627
40	1	0	1.547267	3.437649	0.410331
41	1	0	4.595857	3.770899	−0.052973
42	1	0	3.904905	3.575938	1.559898
43	1	0	5.193724	2.476571	1.015419
44	1	0	1.967654	−3.105320	−0.191996
45	1	0	1.745494	−2.626123	−1.897191
46	1	0	3.204542	−3.526455	−1.413736
47	1	0	4.214677	−0.226519	−2.016239
Conformer (11*S*, 12*S*)-**5**-**b**					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	−4.740428	−1.239106	−0.324879

2	6	0	−4.238505	0.015701	−0.068725
3	6	0	−5.334043	0.865197	0.119525
4	6	0	−6.504479	0.085859	−0.029863
5	6	0	−6.097130	−1.217458	−0.306067
6	6	0	−2.782352	0.188740	−0.058279
7	6	0	−2.263668	1.529531	0.255102
8	8	0	−2.071407	−0.801667	−0.289755
9	6	0	−0.957235	1.910936	0.172266
10	6	0	−0.526992	3.267925	0.664695
11	6	0	0.062142	1.026229	−0.400251
12	6	0	1.313483	0.849172	0.067796
13	6	0	2.173702	−0.277248	−0.419055
14	6	0	1.705840	−1.665352	0.193836
15	6	0	2.931048	−2.541741	−0.101634
16	6	0	4.141464	−1.642867	0.186393
17	6	0	3.678653	−0.229393	−0.171555
18	6	0	4.494202	0.836860	−0.302383
19	6	0	4.043503	2.198895	−0.773826
20	6	0	5.976572	0.755077	−0.021896
21	6	0	1.422006	−1.588053	1.701063
22	8	0	0.587813	−2.182033	−0.486152
23	1	0	−4.124481	−2.026240	−0.501254
24	1	0	−5.288665	1.929980	0.337167
25	1	0	−7.534552	0.427091	0.052331
26	1	0	−6.684382	−2.115648	−0.486894
27	1	0	−2.991419	2.252512	0.630896
28	1	0	−1.364081	3.833278	1.098256
29	1	0	0.256294	3.171281	1.435501
30	1	0	−0.083741	3.858736	−0.154215
31	1	0	−0.270430	0.378186	−1.214884
32	1	0	1.667086	1.414900	0.937205
33	1	0	1.990967	−0.414199	−1.500713
34	1	0	2.889692	−2.813112	−1.168909
35	1	0	2.925771	−3.477391	0.478470
36	1	0	5.030341	−1.950403	−0.385836
37	1	0	4.425550	−1.703917	1.252872
38	1	0	2.992640	2.227055	−1.088944
39	1	0	4.659182	2.523935	−1.631994
40	1	0	4.186452	2.964446	0.010952
41	1	0	6.563008	0.909957	−0.946435
42	1	0	6.286371	−0.202677	0.416359
43	1	0	6.284211	1.556898	0.673160
44	1	0	2.269091	−1.169330	2.267432
45	1	0	1.212811	−2.599505	2.082483
46	1	0	0.539675	−0.961532	1.901580
47	1	0	−0.214915	−1.679018	−0.256030

Table S15. MIC values (μg/mL) of the active compounds in the antibacterial bioassay.

Compounds	*Xanthomonas oryzae* RS105	methicillin-resistant *Staphylococcus aureus* (shhs A1)	*Staphylococcus aureus* (ATCC 6538)	*Bacillus subtilis* (ATCC 6633)
2	3.125	6.250	3.125	12.50
3	6.250	12.50	6.250	12.50
4	6.250	6.250	3.125	6.250
Acetone [a]	＞50	＞50	＞50	＞50
Kanamycin [b]	0.3906	–	12.50	6.250
Vancomycin [b]	–	1.5625	–	–

[a] Negative control; [b] positive controls

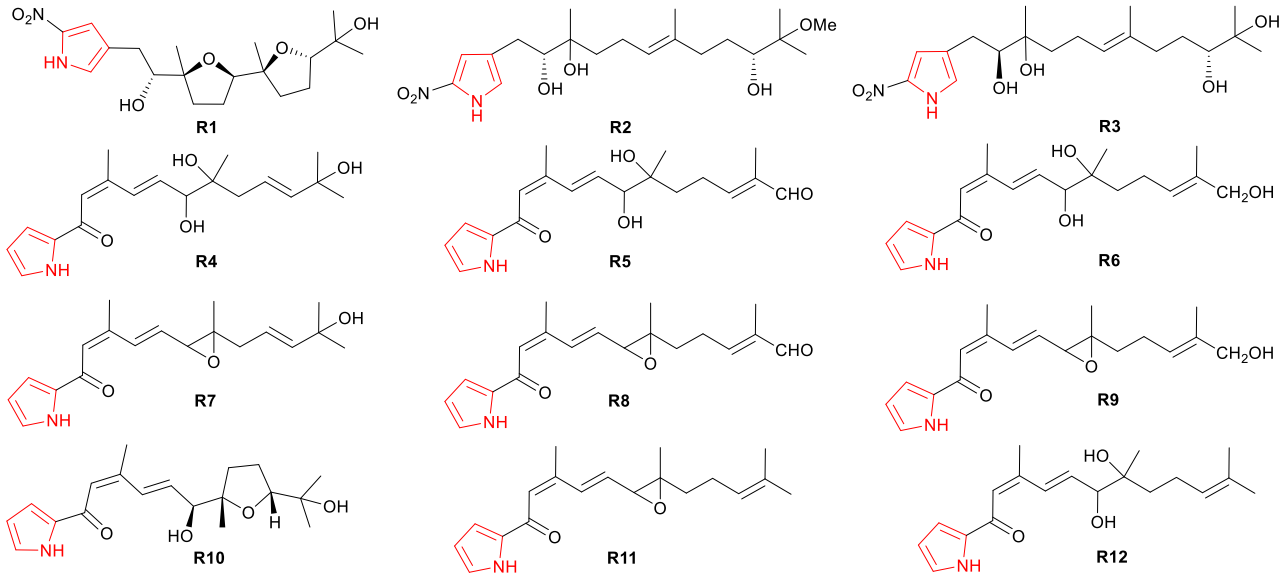


Figure S1. Chemical structures of previously reported pyrrolosesquiterpenes.

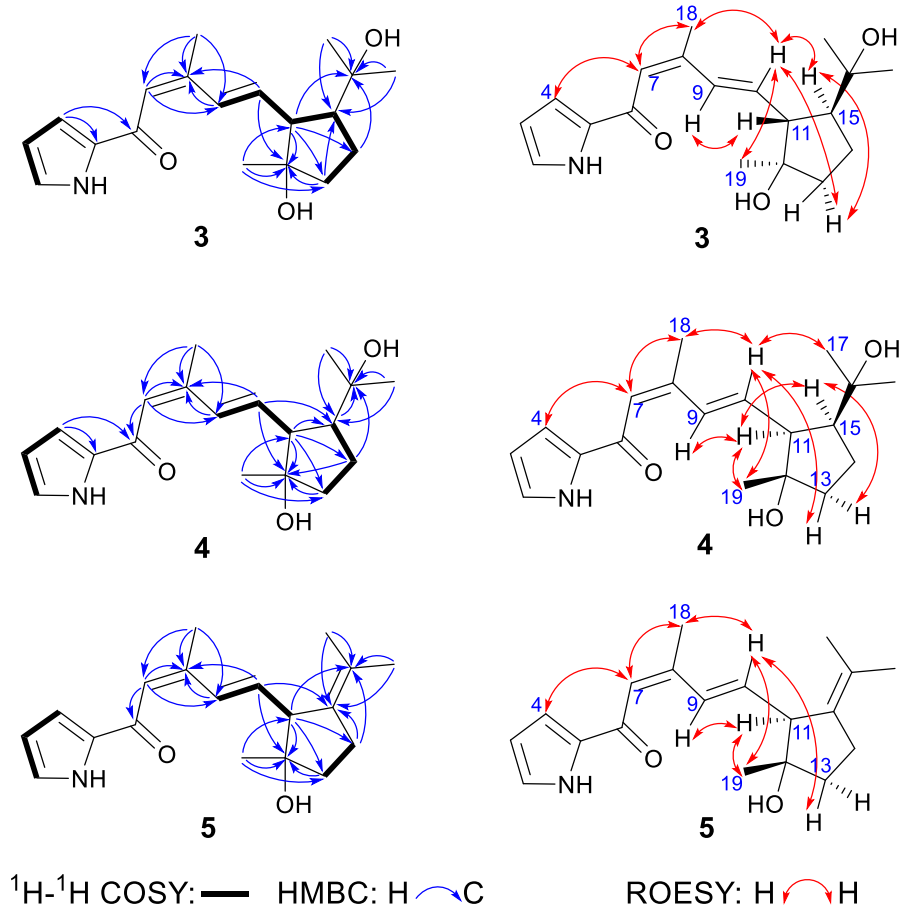


Figure S2. Key 2D NMR correlations of compounds **3**–**5**.

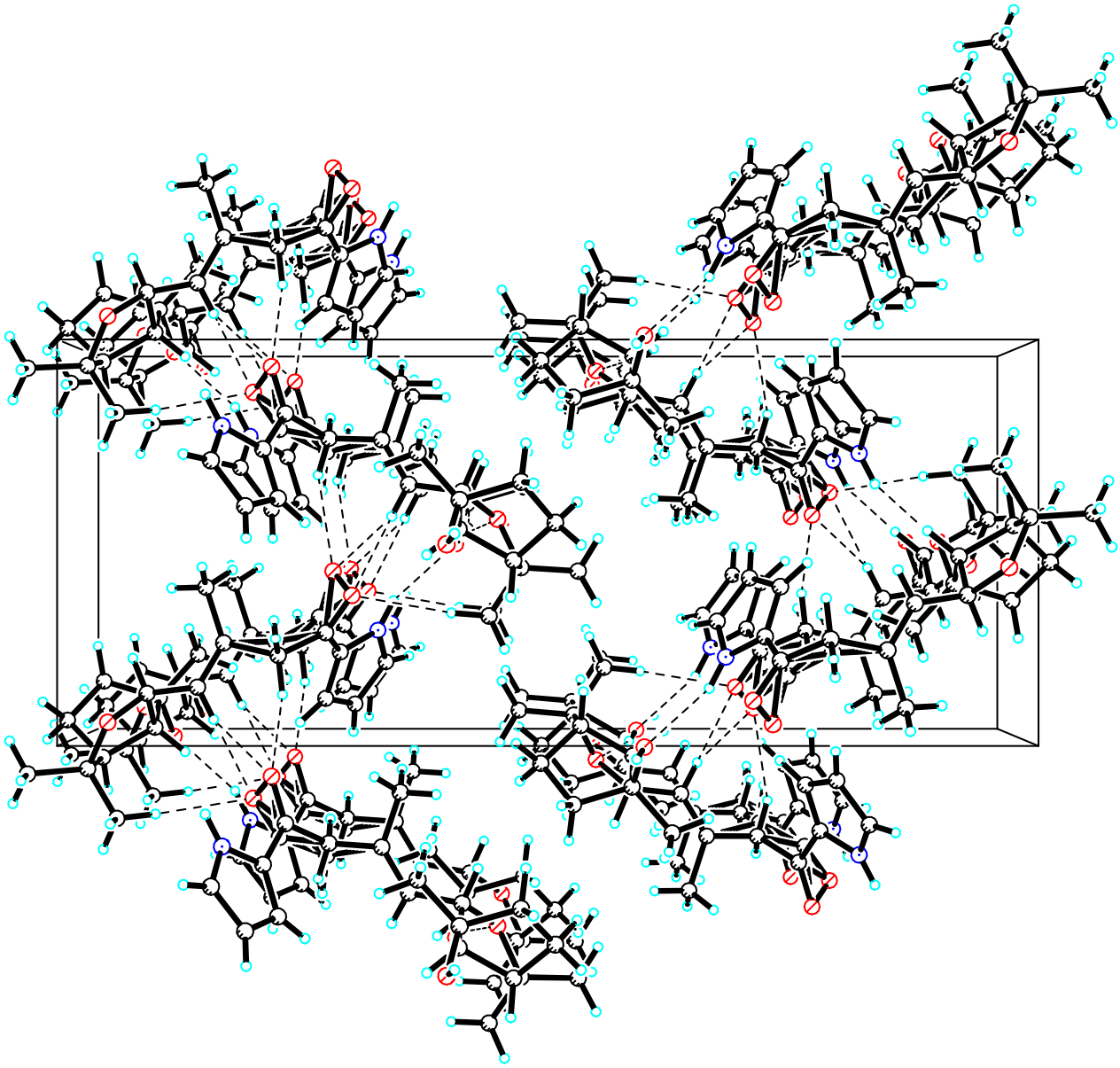


Figure S3. View of the pack drawing of strepyrrolin A (**1**).

Hydrogen-bonds are shown as dashed lines.

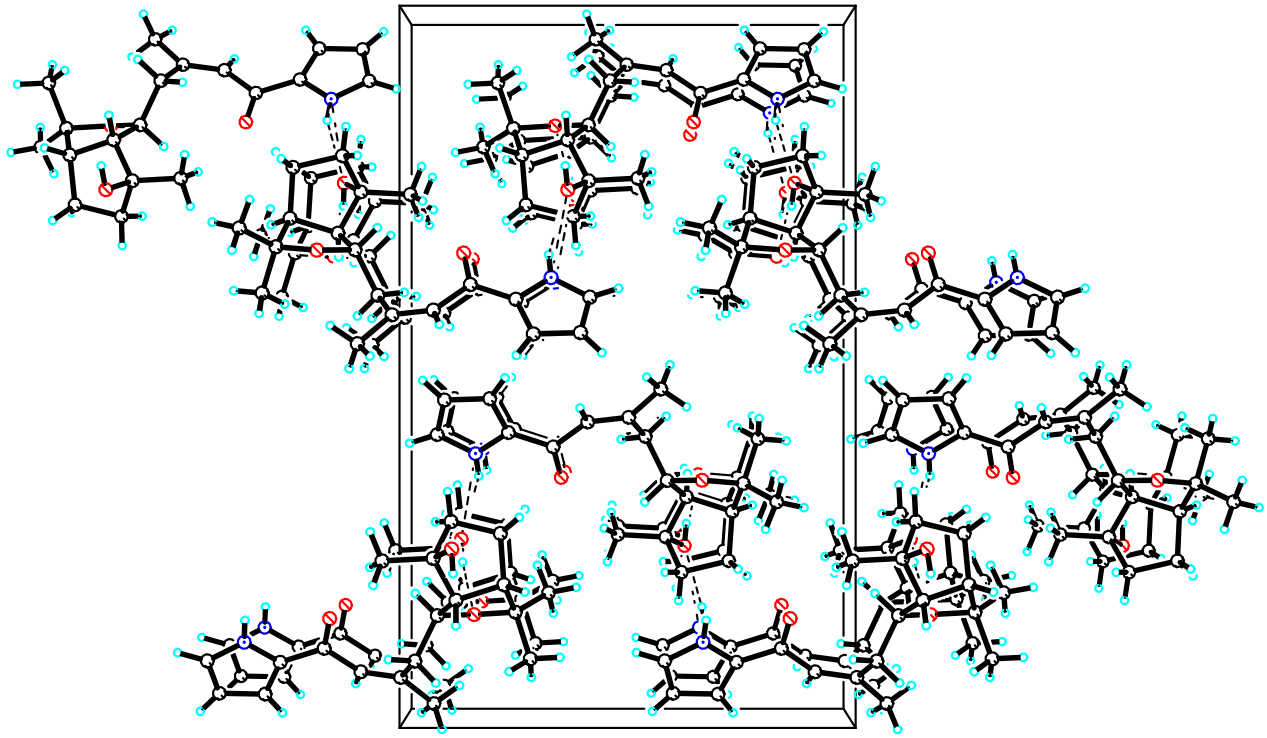


Figure S4. View of the pack drawing of compound **6**.

Hydrogen-bonds are shown as dashed lines.

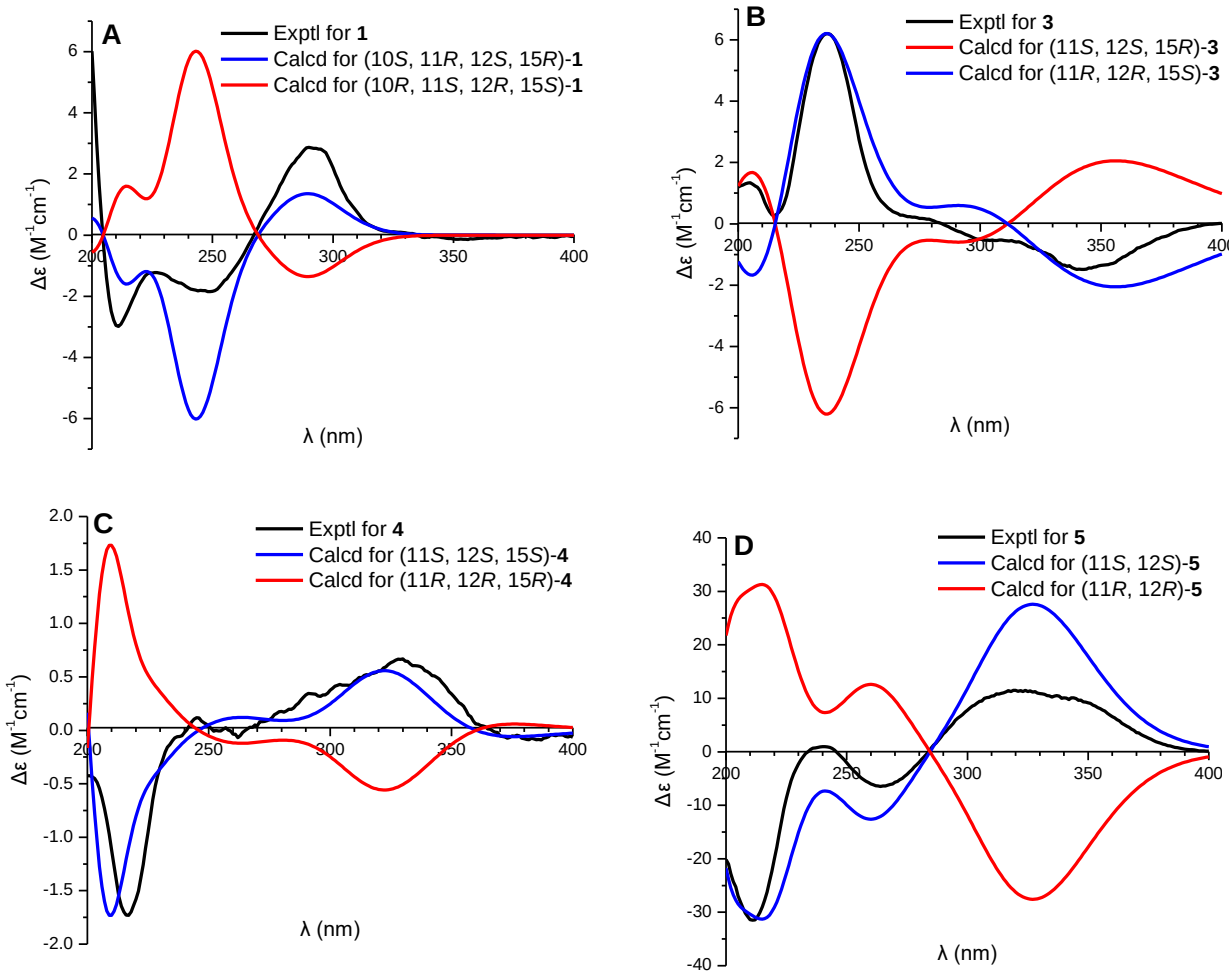


Figure S5. Calculated and experimental ECD spectra of compounds **1**, **3**, **4**, and **5**.

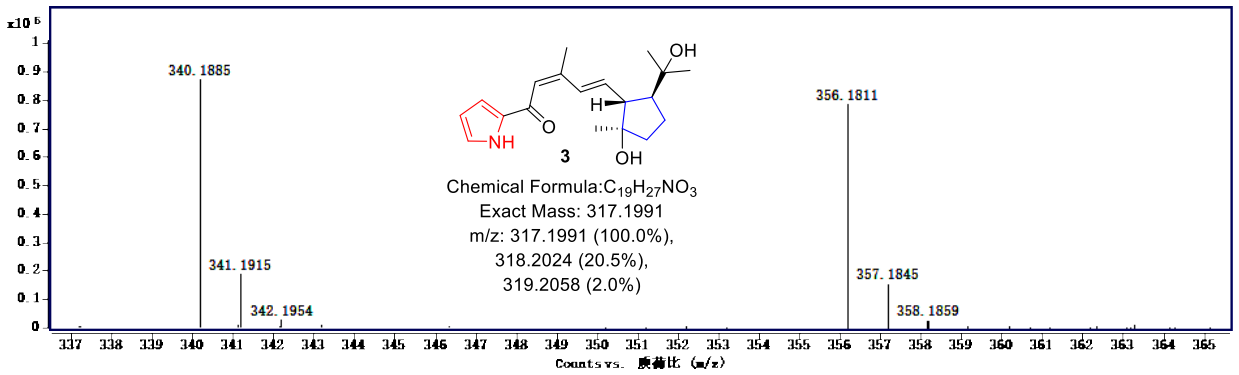


Figure S6. HR-ESI-MS spectrum of compound **3** fed with [$^{13}C_5$, ^{15}N]-L-Pro.
(*m/z* 340.1885 $[M + Na]^+$; *m/z* 356.1811 $[M + K]^+$)

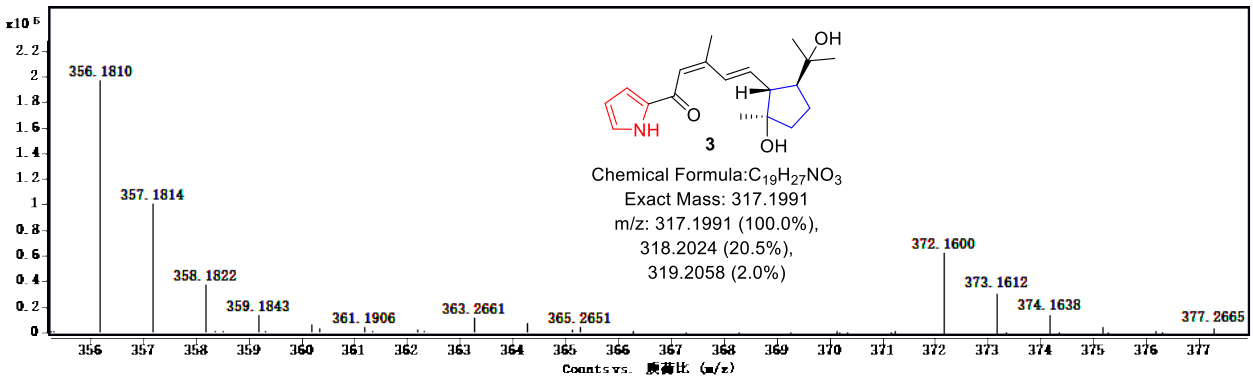


Figure S7. HR-ESI-MS spectrum (*m/z* $[M + K]^+$) of compound **3** fed with [$^{13}C_5$, ^{15}N]-L-Glu.

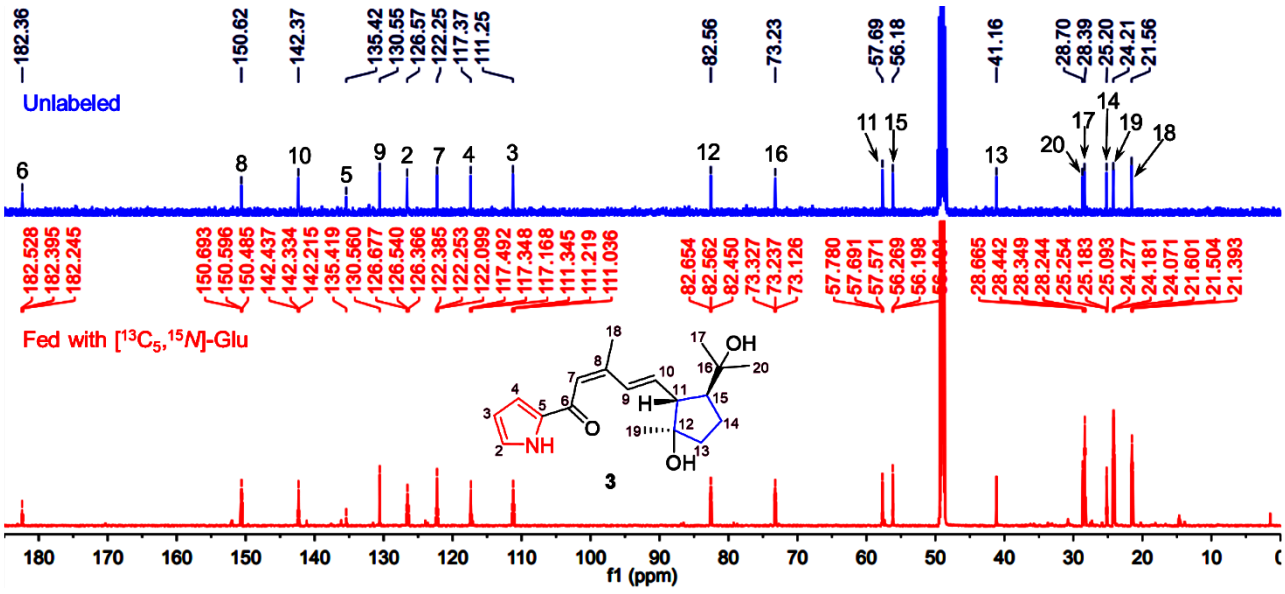


Figure S8. ^{13}C NMR (200 MHz, CD_3OD) spectrum of compound **3** fed with [$^{13}C_5$, ^{15}N]-L-Glu.

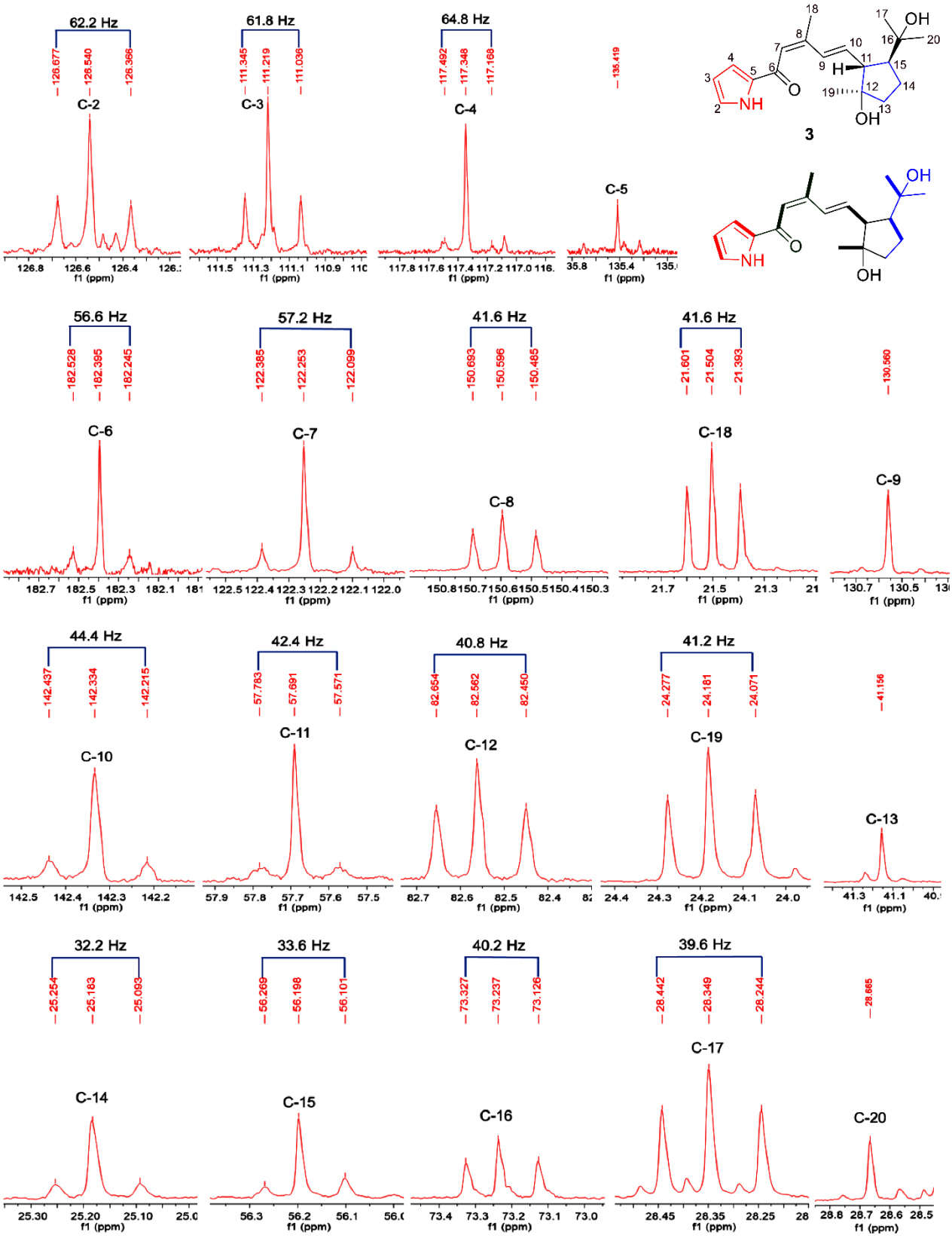


Figure S9. The multiplicity analysis of labeled carbons of compound **3** fed with [$^{13}C_5$, ^{15}N]-L-Glu.
Each pair of coupled carbons was shown in bold bonds. The weak splitting peaks of C-4 were thought to be caused by C-5. The splitting signals of C-5 were not detected because of its long relaxation lifetime, as well as the low involvement of labeled ^{13}C.

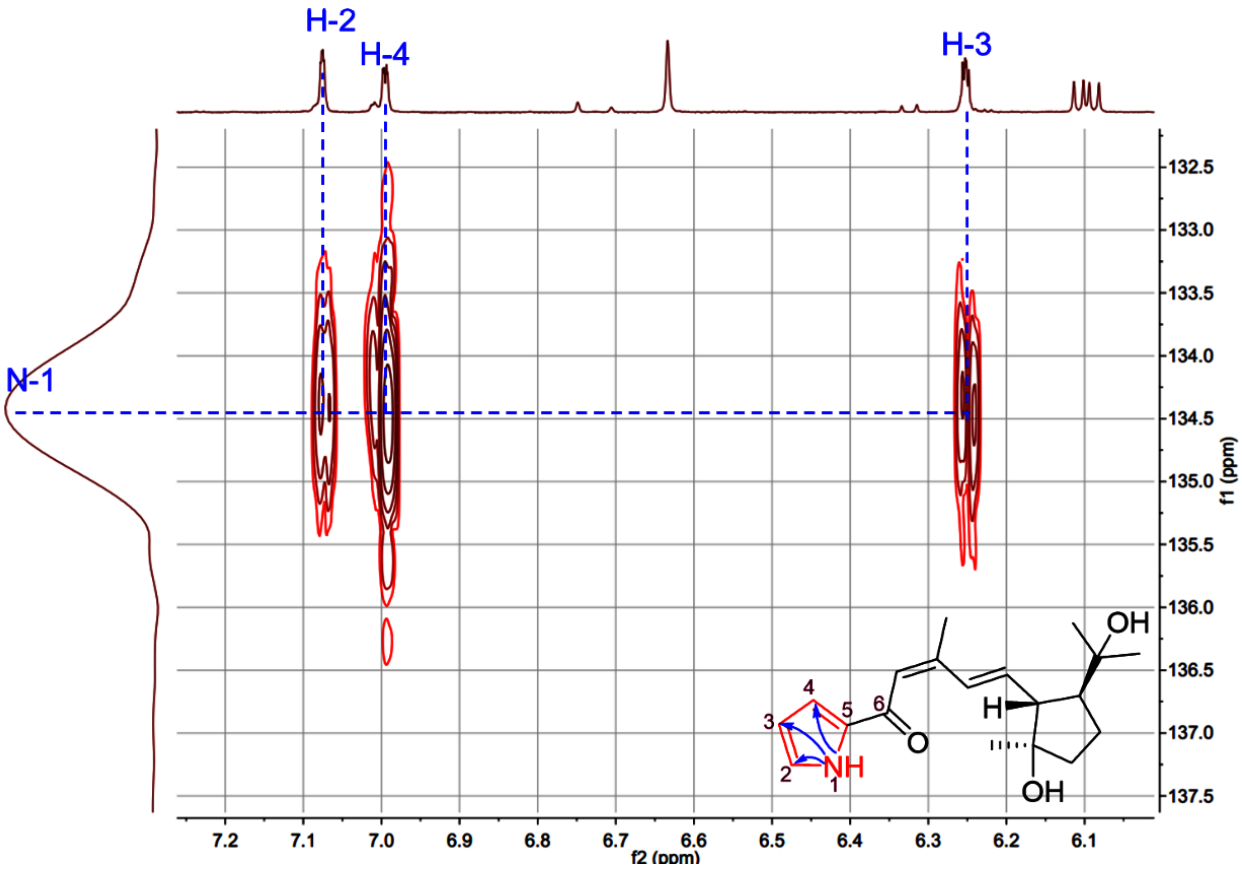


Figure S10. ^{1}H-^{15}N HMBC (800 MHz, CD_3OD) spectrum of compound **3** fed with [$^{13}C_5$, ^{15}N]-L-Glu.

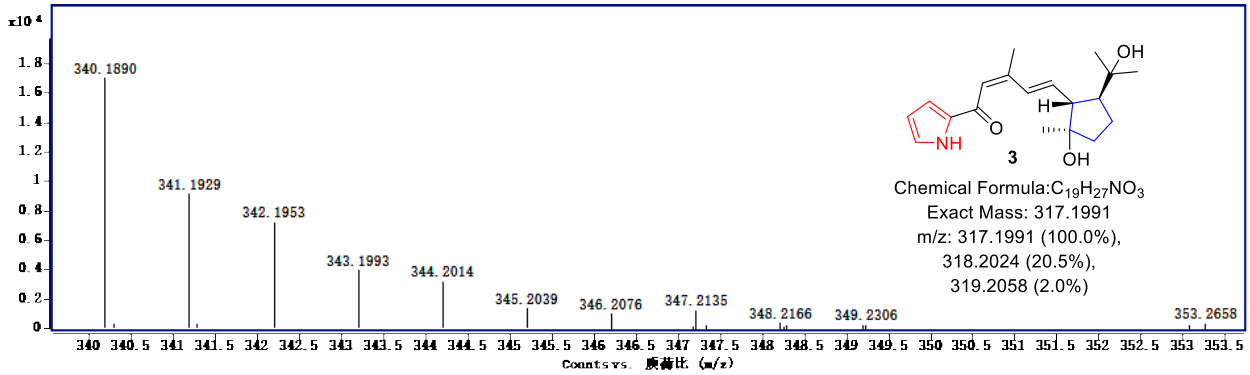


Figure S11. HR-ESI-MS spectrum (*m/z* [M + Na]$^+$) of compound **3** fed with $^{13}C_2$-Gly.

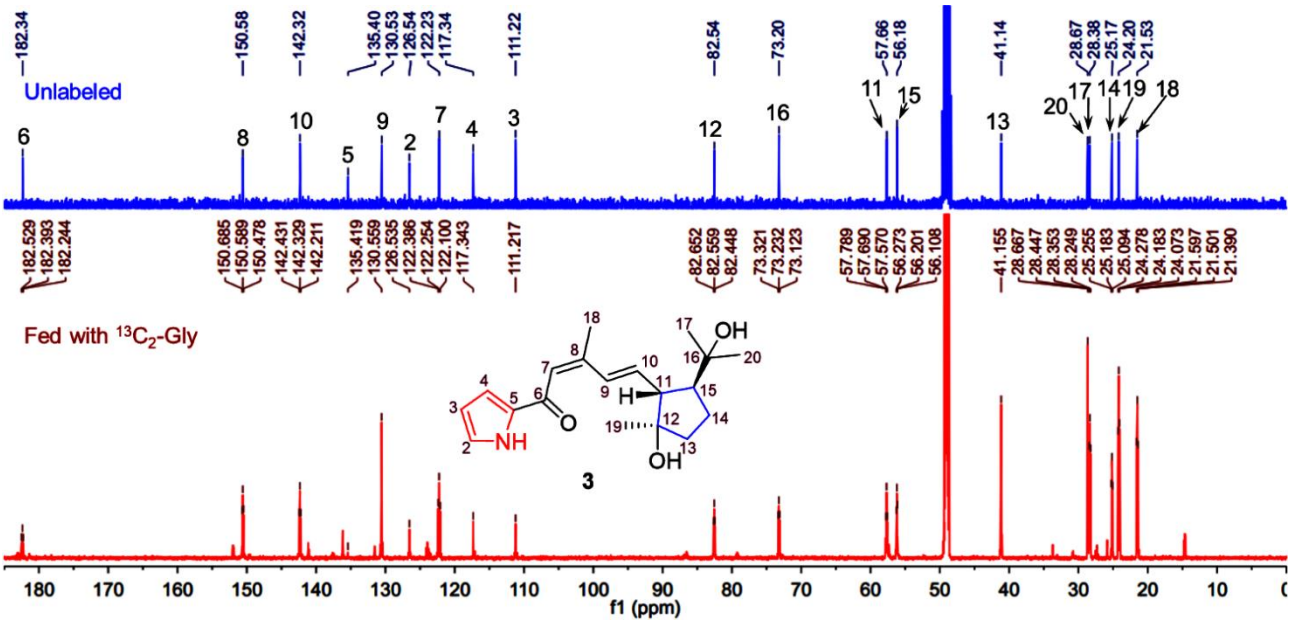


Figure S12. ^{13}C NMR (200 MHz, CD_3OD) spectrum of compound **3** fed with $^{13}C_2$-Gly.

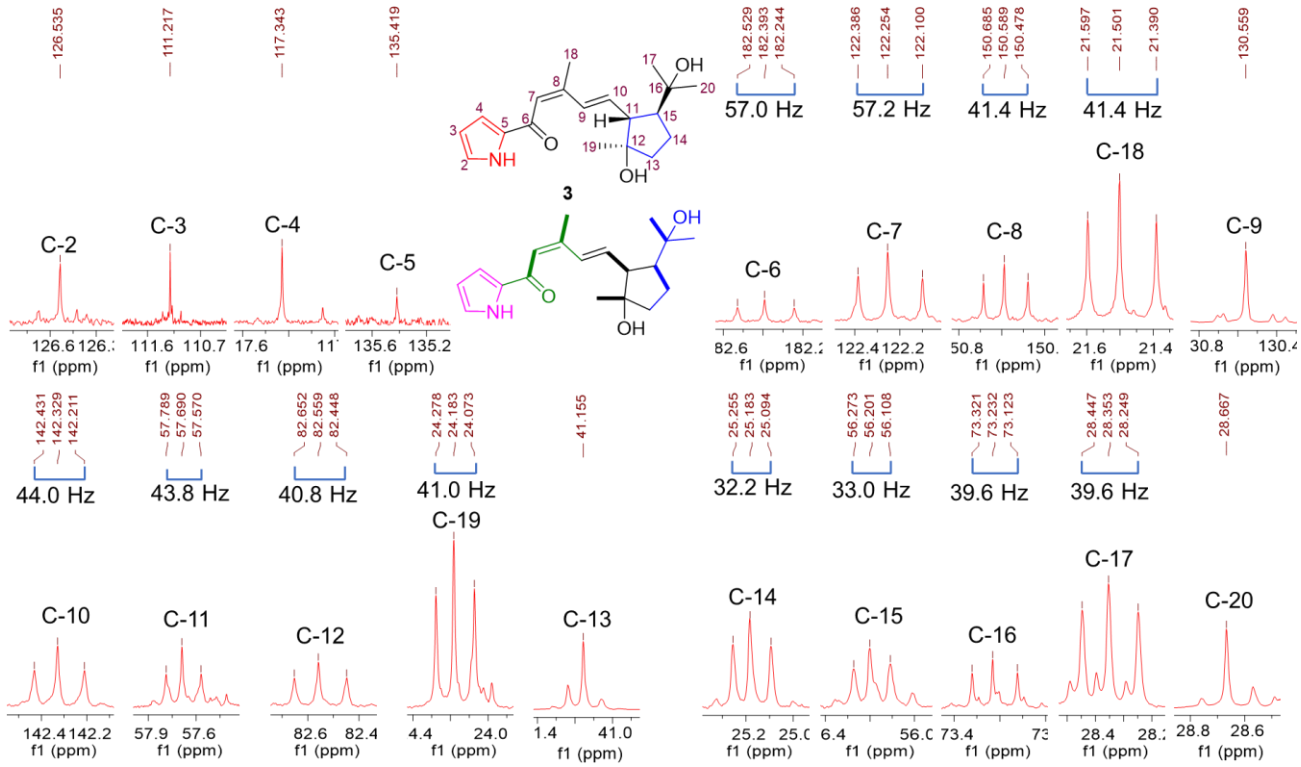


Figure S13. The multiplicity analysis of labeled carbons of compound **3** fed with $^{13}C_2$-Gly.

Each pair of coupled carbons was shown in bold bonds.

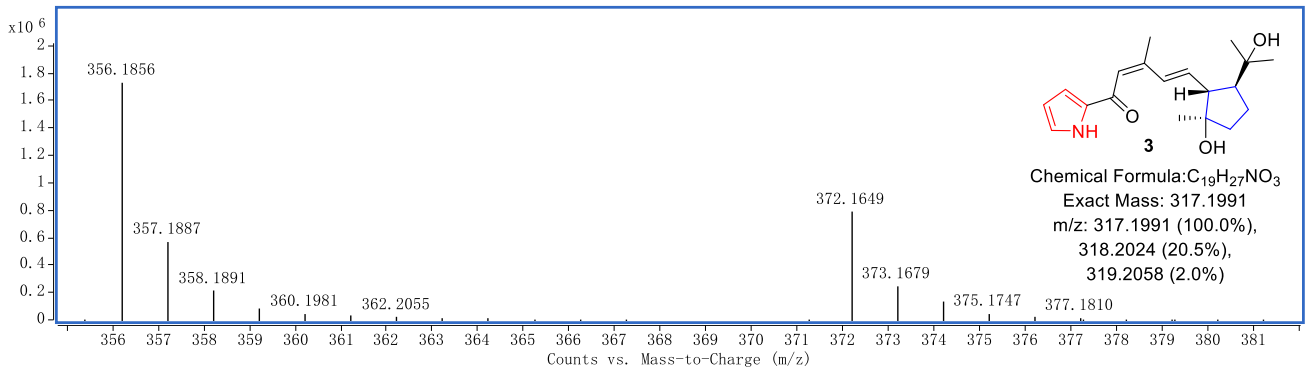


Figure S14. HR-ESI-MS spectrum (*m/z* [M + K]$^+$) of compound **3** fed with $^{13}C_2$-sodium acetate.

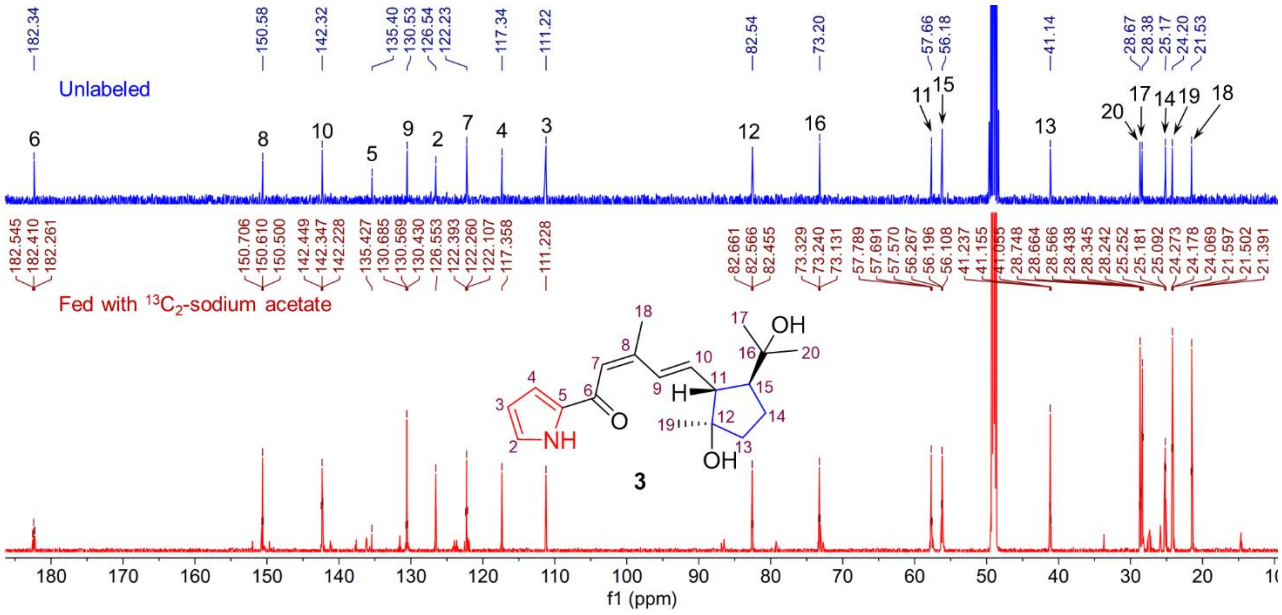


Figure S15. ^{13}C NMR (200 MHz, CD_3OD) spectrum of compound **3** fed with $^{13}C_2$-sodium acetate.

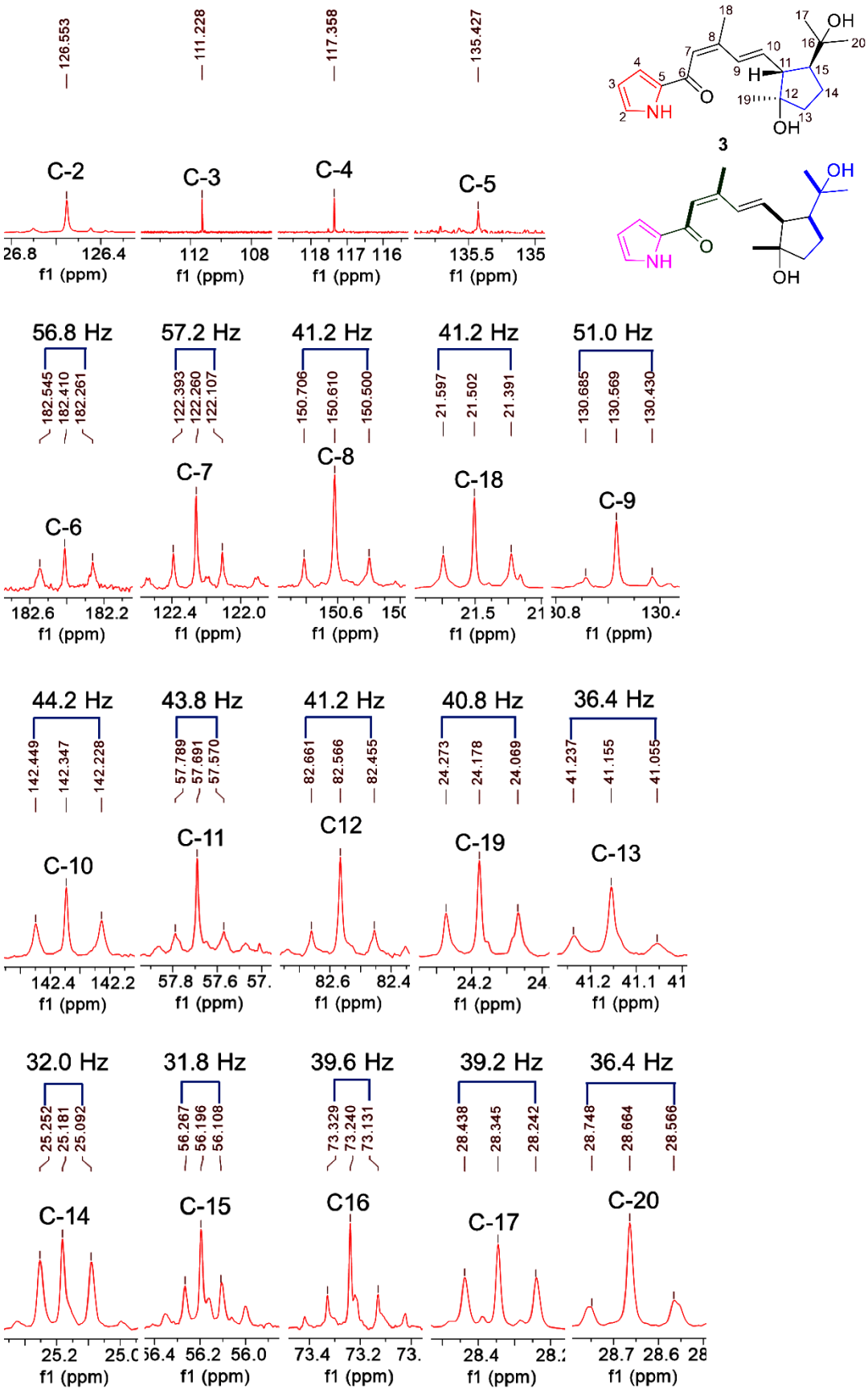


Figure S16. The multiplicity analysis of labeled carbons of compound **3** fed with $^{13}C_2$-sodium acetate. Each pair of coupled carbons was shown in bold bonds.

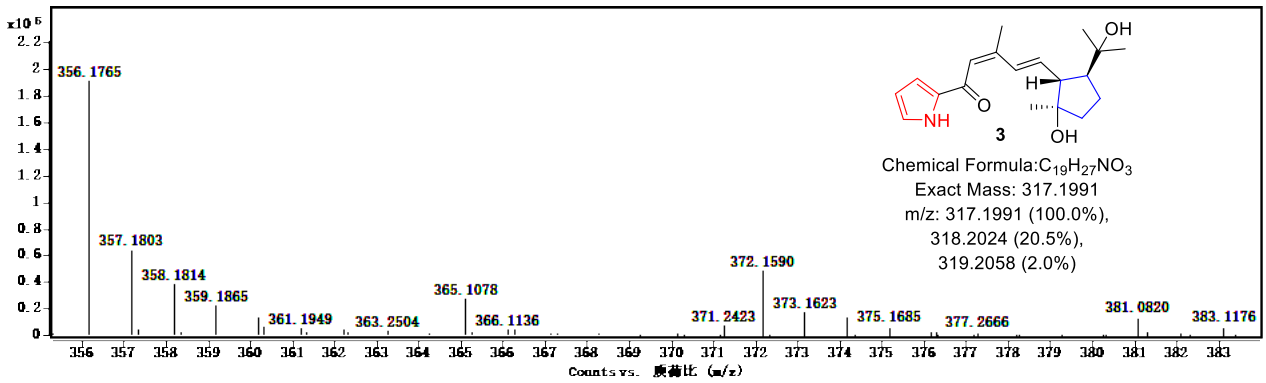


Figure S17. HR-ESI-MS spectrum (*m/z* [M + K]$^+$) of compound **3** fed with $^{13}C_6$-glucose.

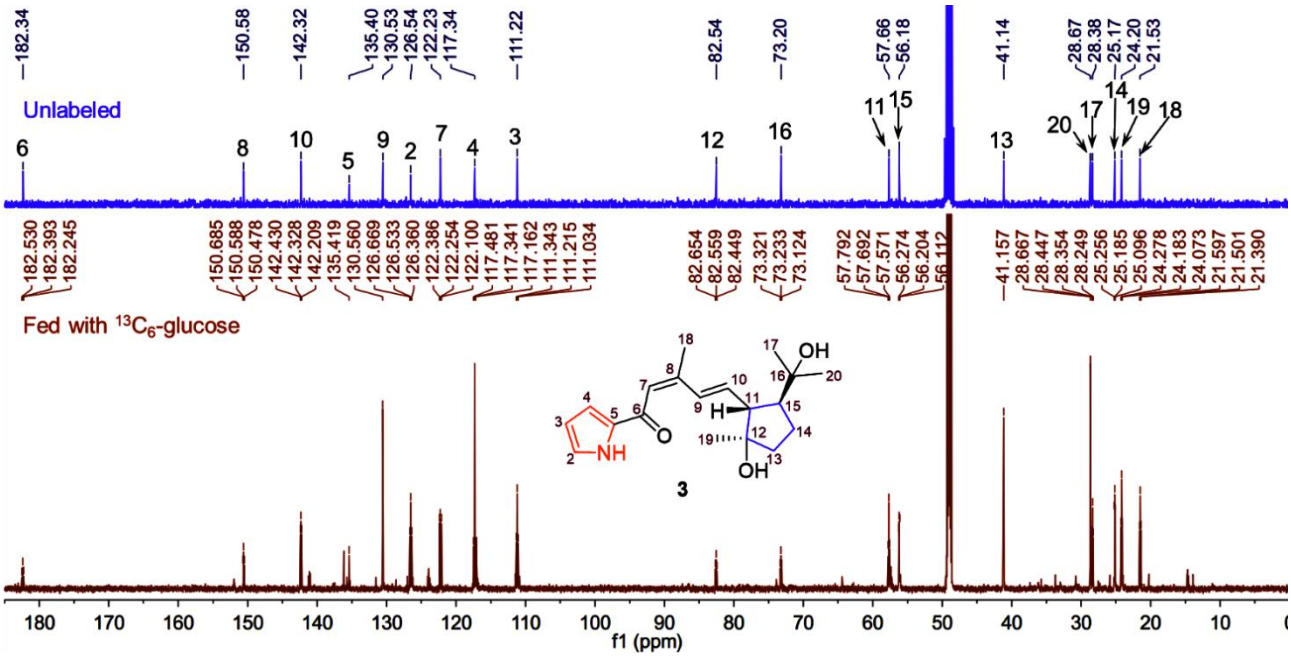


Figure S18. ^{13}C NMR (200 MHz, CD_3OD) spectrum of compound **3** fed with $^{13}C_6$-glucose.

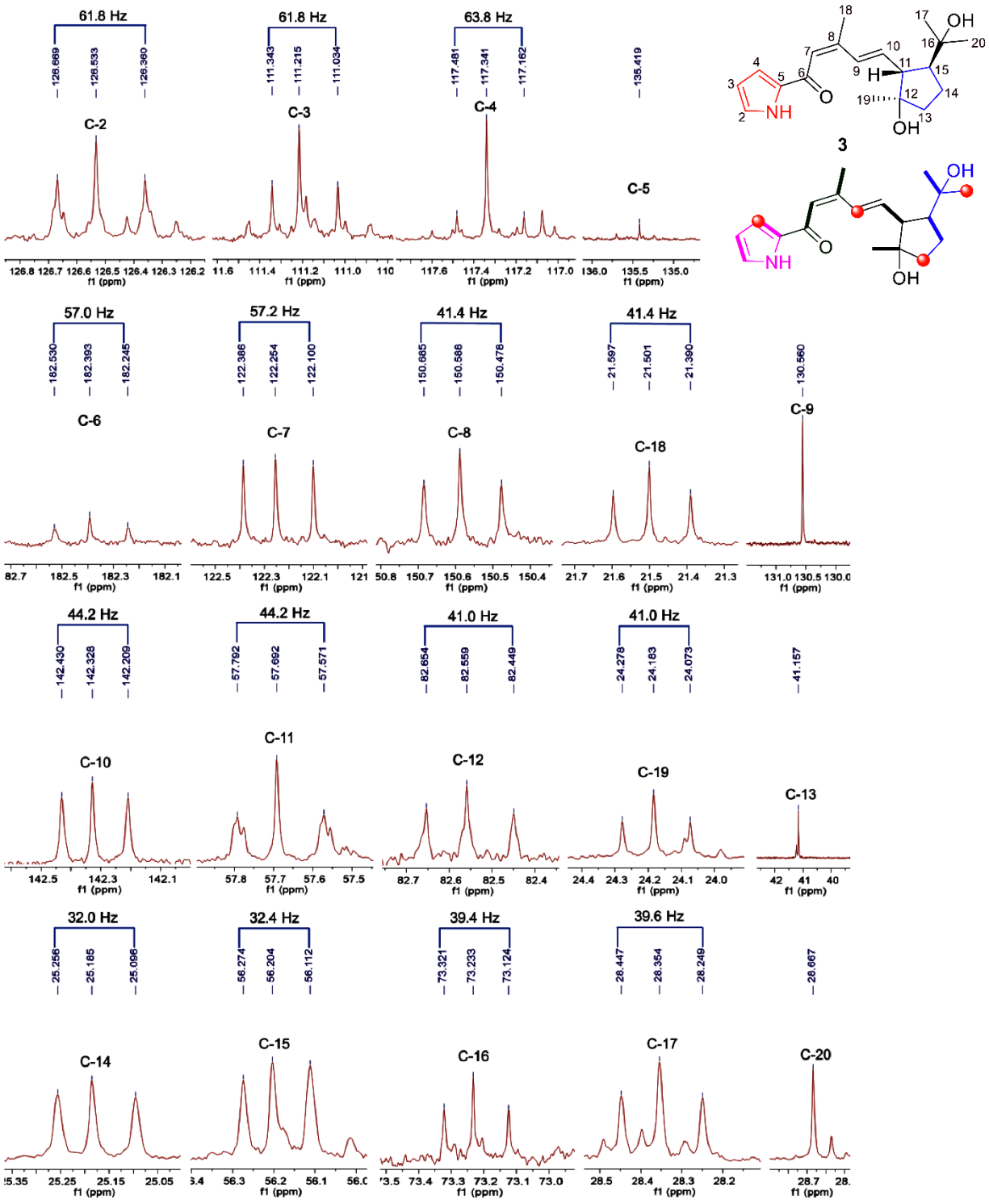


Figure S19. The multiplicity analysis of labeled carbons of compound **3** fed with $^{13}C_6$-glucose.

Each pair of coupled carbons was shown in bold bonds. The red dots represent the carbons showing a singlet with a much higher intensity. The weak splitting peaks of C-4 were thought to be caused by C-5. This deduction was verified by the following selective 1D gradient ^{13}C COSY spectrum targeting C-4 (Figure S19).

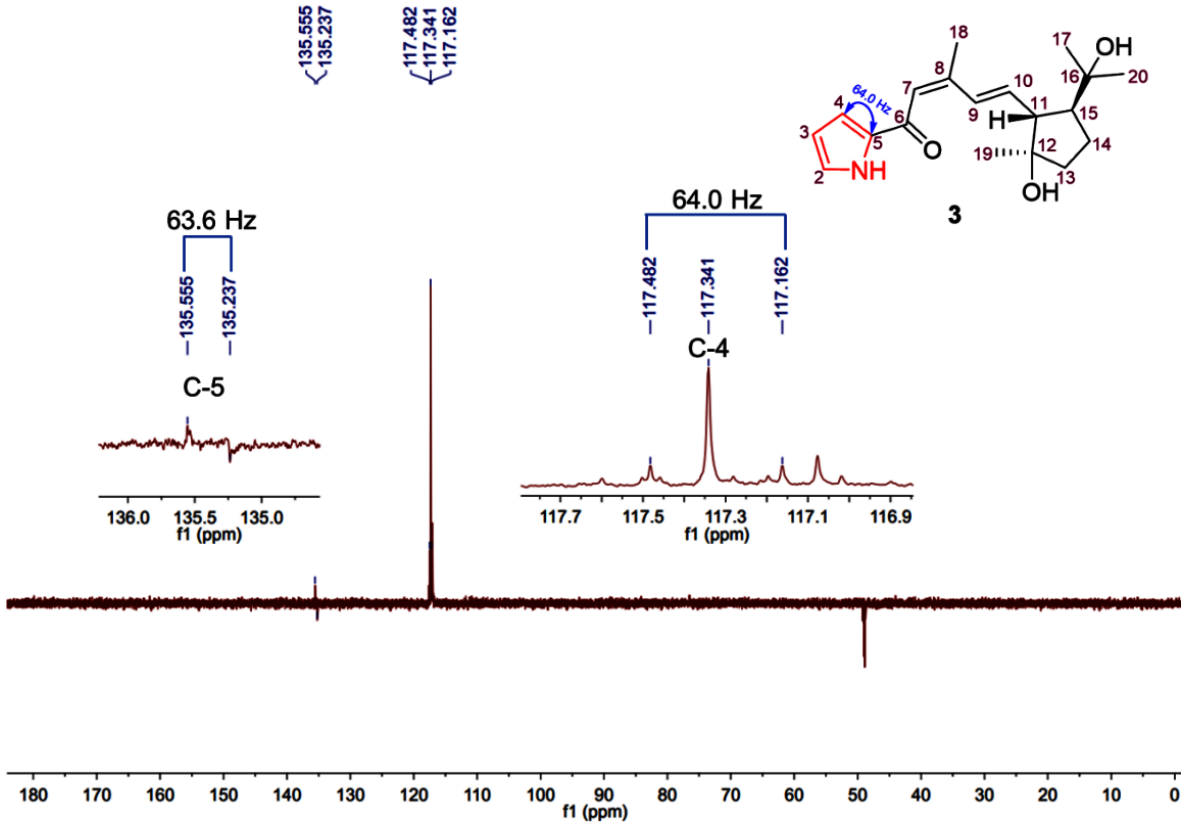


Figure S20. Selective gradient COSY (200 MHz) spectrum targeting C-4 of compound **3** fed with $^{13}C_6$-glucose.

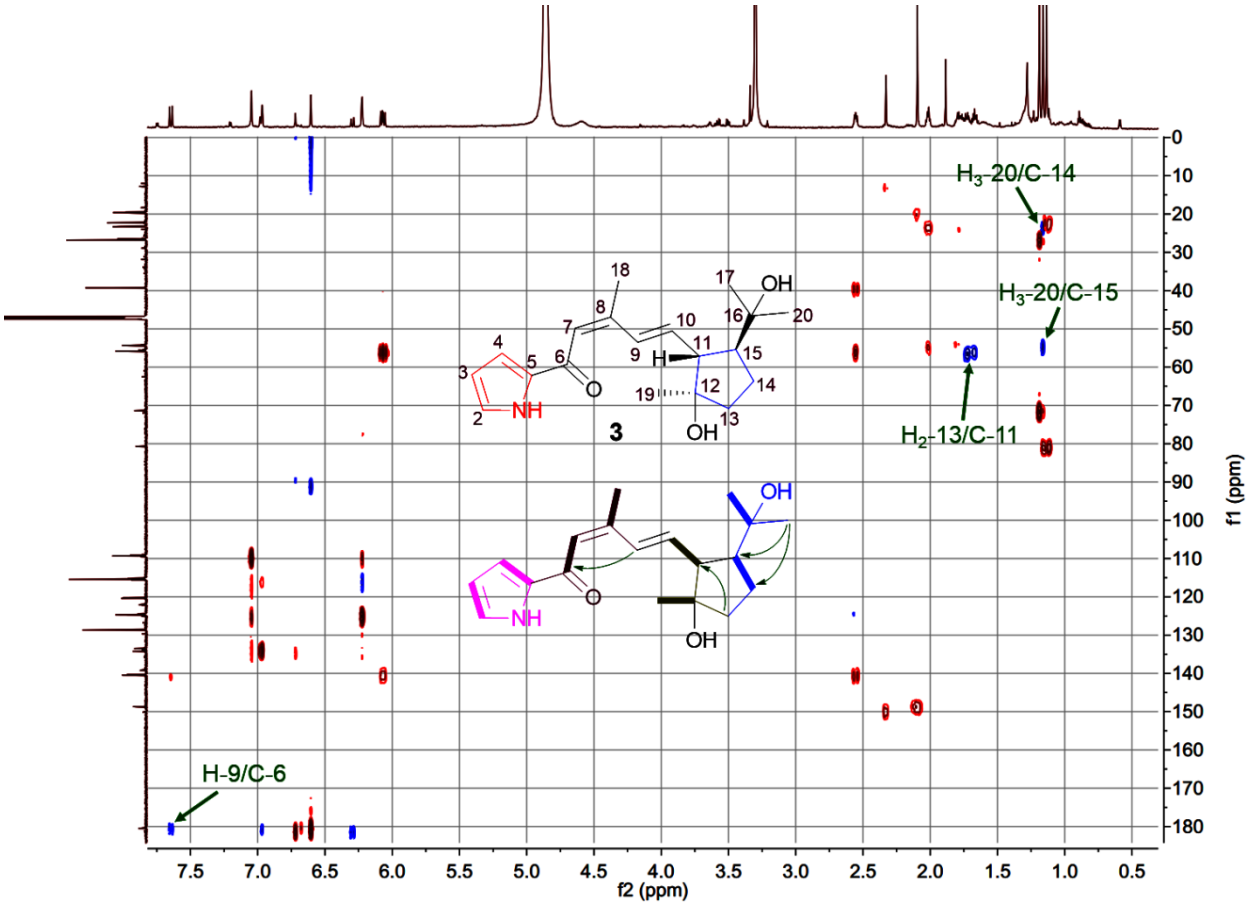


Figure S21. 1,n-ADEQUATE (800 MHz, CD_3OD) spectrum of compound **3** fed with $^{13}C_6$-glucose.

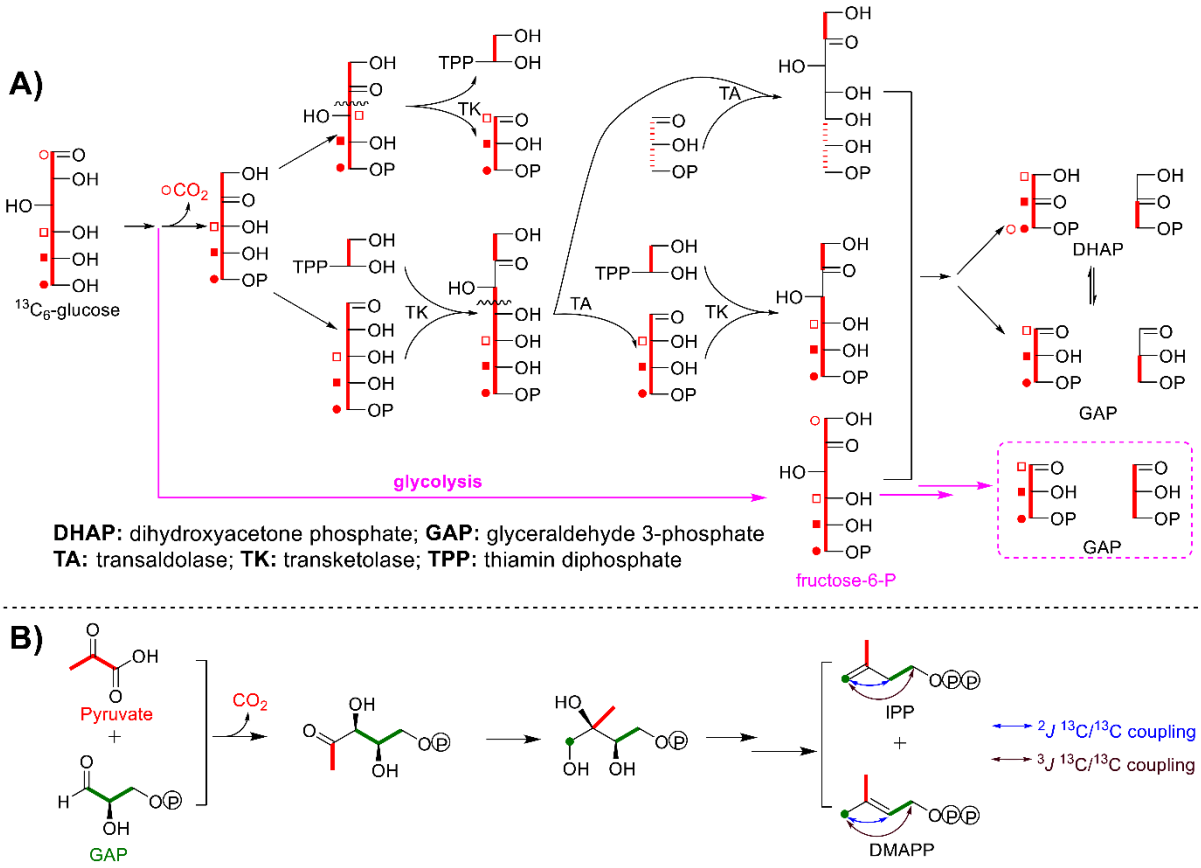


Figure S22. The analyses of labeling pattern of isoprenic units and $^{13}C/^{13}C$ couplings in terpenoid moiety of **3** after incorporation of $^{13}C_6$-glucose.

(A) Involvement of the oxidative pentose phosphate cycle in glucose breakdown. (B) Labeling patterns of terpene precursors, IPP (isopentenyl diphosphate) and DMAPP (dimethylallyl diphosphate), via MEP (methylerythritol phosphate) pathway.

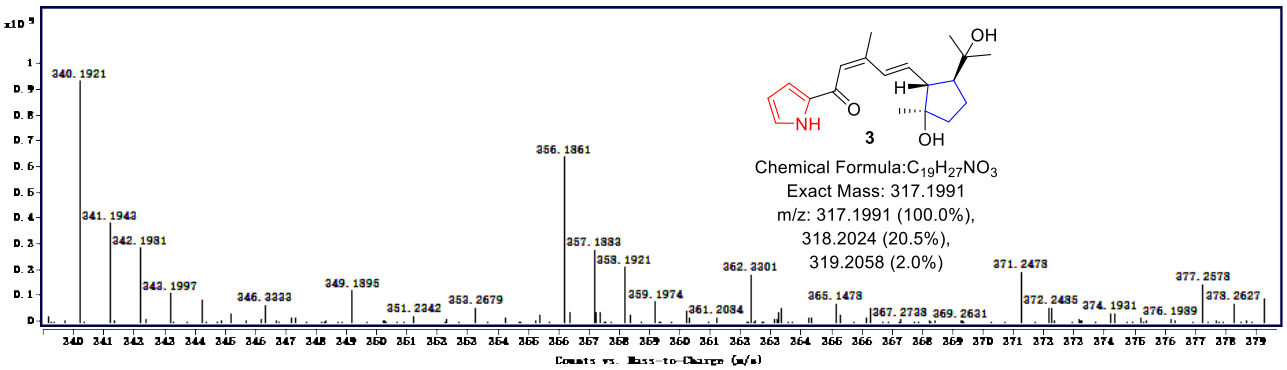


Figure S23. HR-ESI-MS spectrum of compound **3** fed with [$^{13}C_3$, ^{15}N]-L-Ala.

(*m/z* 340.1921 [M + Na]$^+$, *m/z* 356.1861[M + K]$^+$)

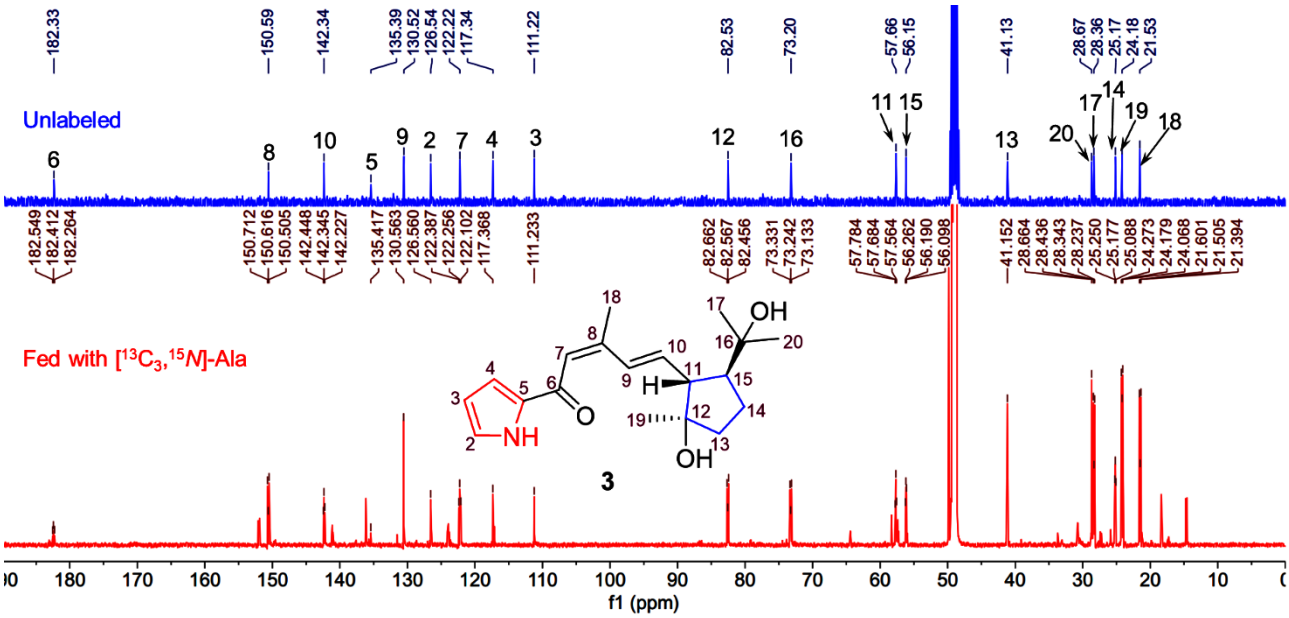


Figure S24. ^{13}C NMR (200 MHz, CD_3OD) spectrum of compound **3** fed with [$^{13}C_3$, ^{15}N]-L-Ala.

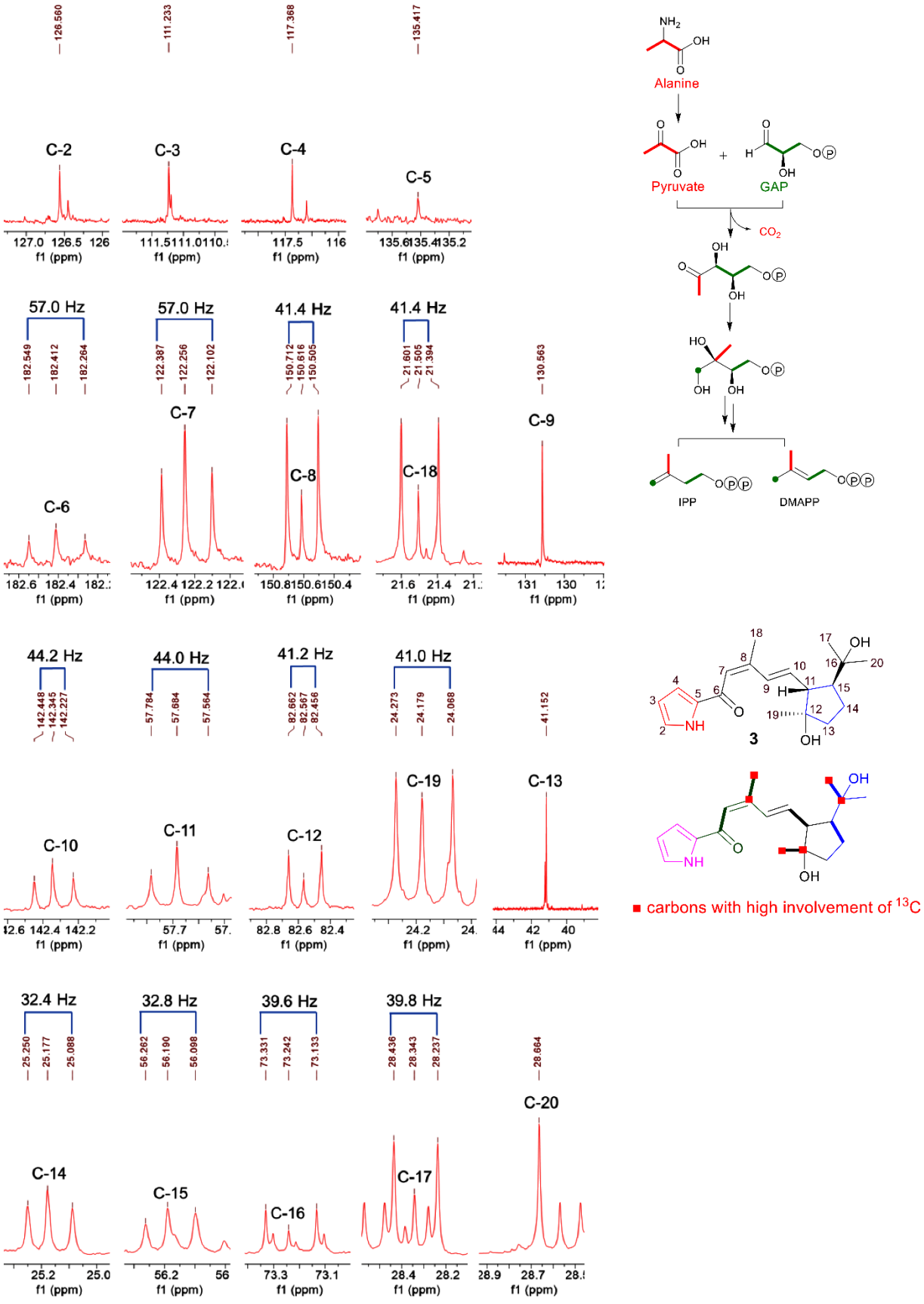


Figure S25. The multiplicity analysis of labeled carbons of compound **3** fed with [$^{13}C_3$, ^{15}N]-L-Ala. Each pair of principally coupled carbons was shown in bold bonds.

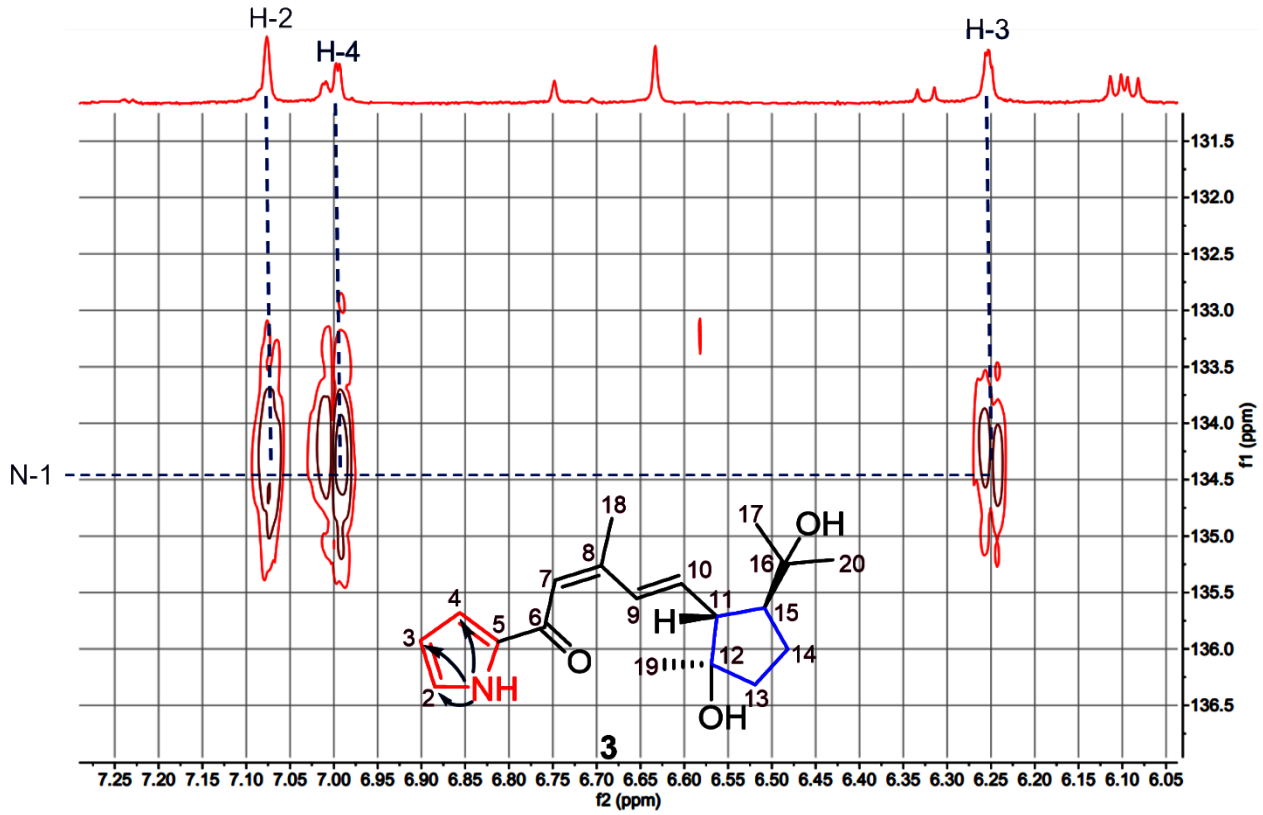


Figure S26. ^{1}H-^{15}N HMBC (800 MHz, CD_3OD) spectrum of compound **3** fed with [$^{13}C_3$, ^{15}N]-L-Ala.

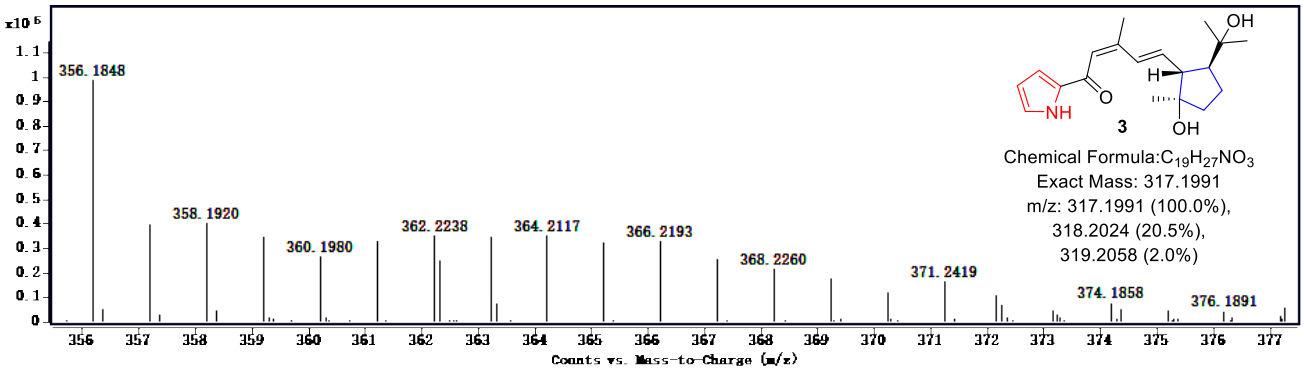


Figure S27. HR-ESI-MS spectrum (*m/z* [M + K]$^+$) of compound **3** fed with $^{13}C_3$-glycerol.

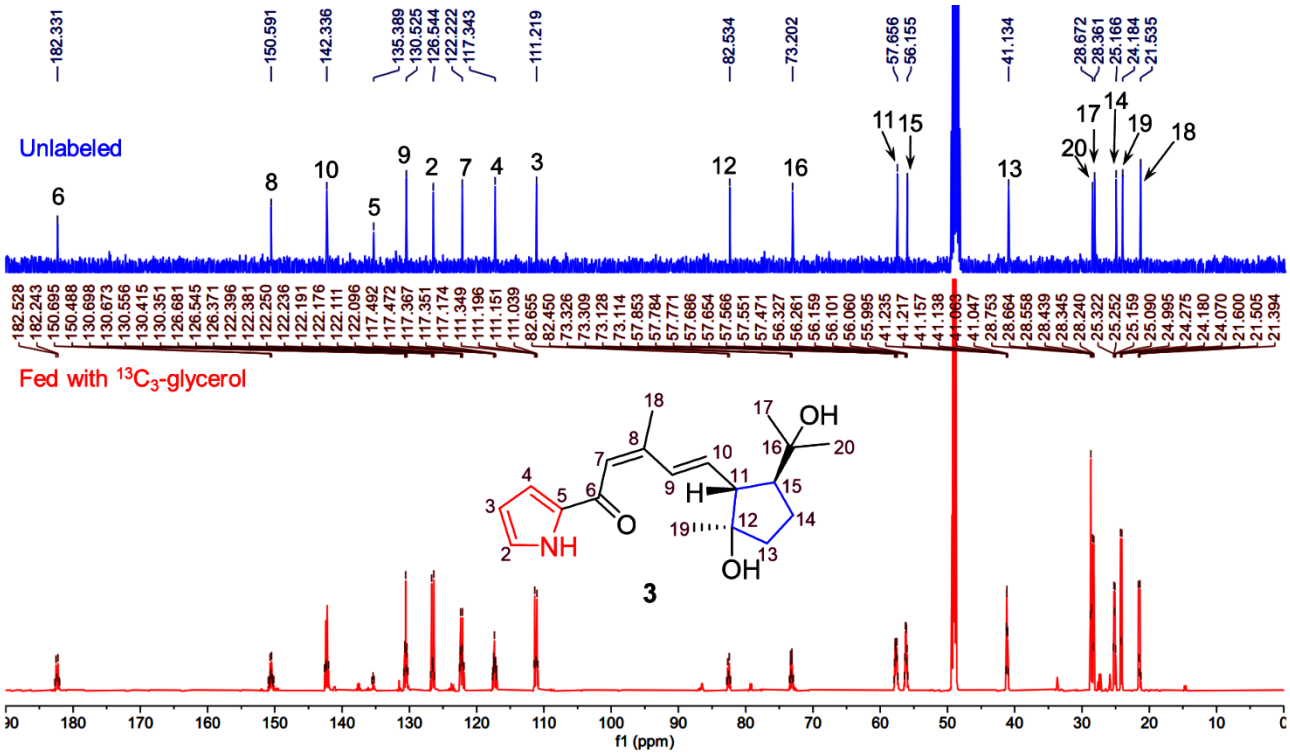


Figure S28. ^{13}C NMR (200 MHz, CD_3OD) spectrum of compound **3** fed with $^{13}C_3$-glycerol.

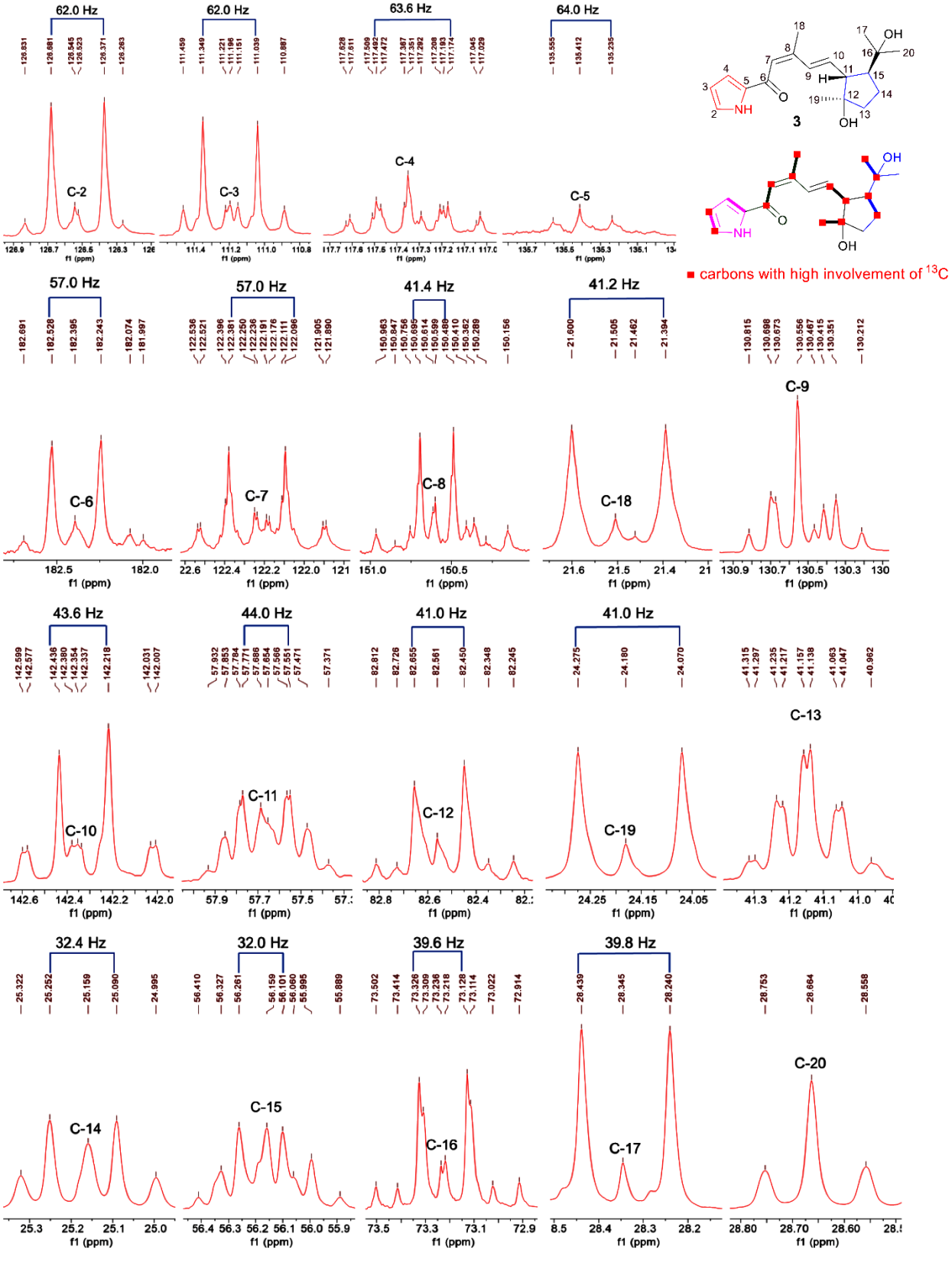


Figure S29. The multiplicity analysis of labeled carbons of compound **3** fed with $^{13}C_3$-glycerol. Each pair of the principally coupled carbons was shown in bold bonds.

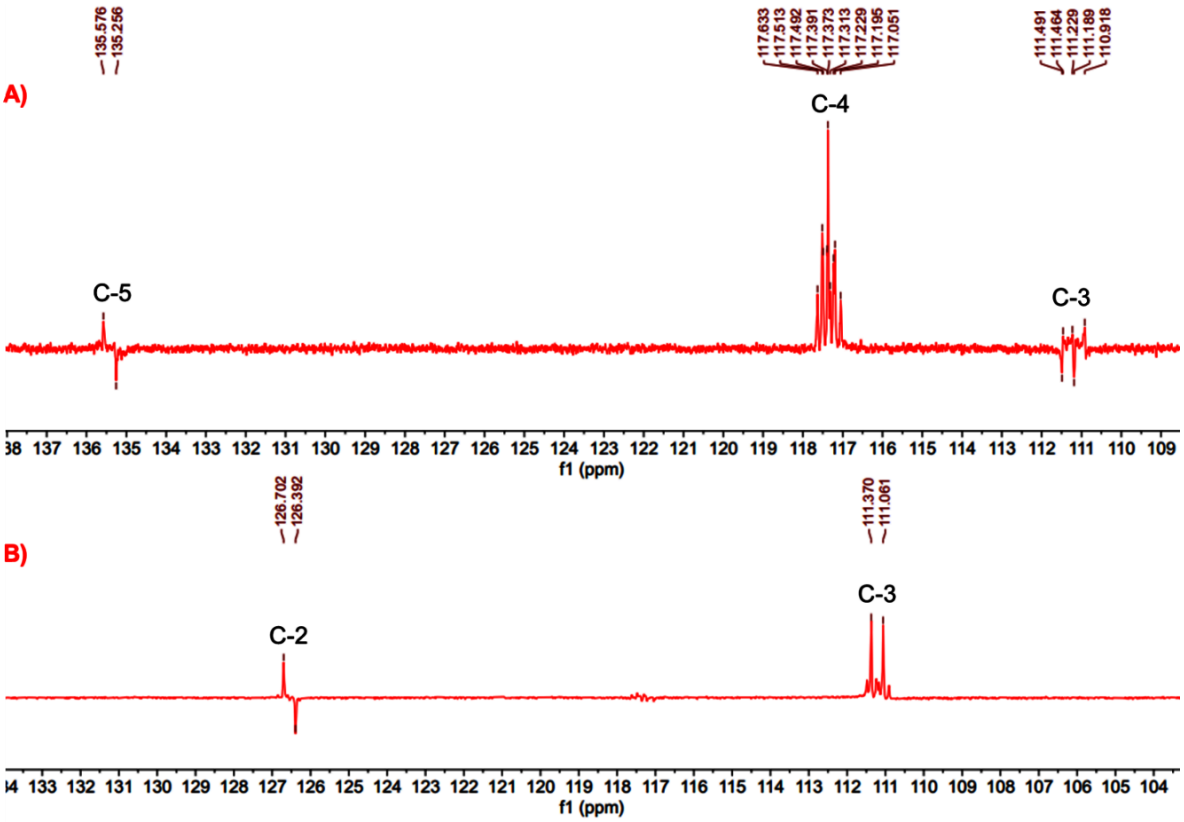


Figure S30. Selective gradient COSY (200 MHz) spectra targeting C-4 (**A**) and C-3 (**B**) of compound **3** fed with $^{13}C_3$-glycerol.

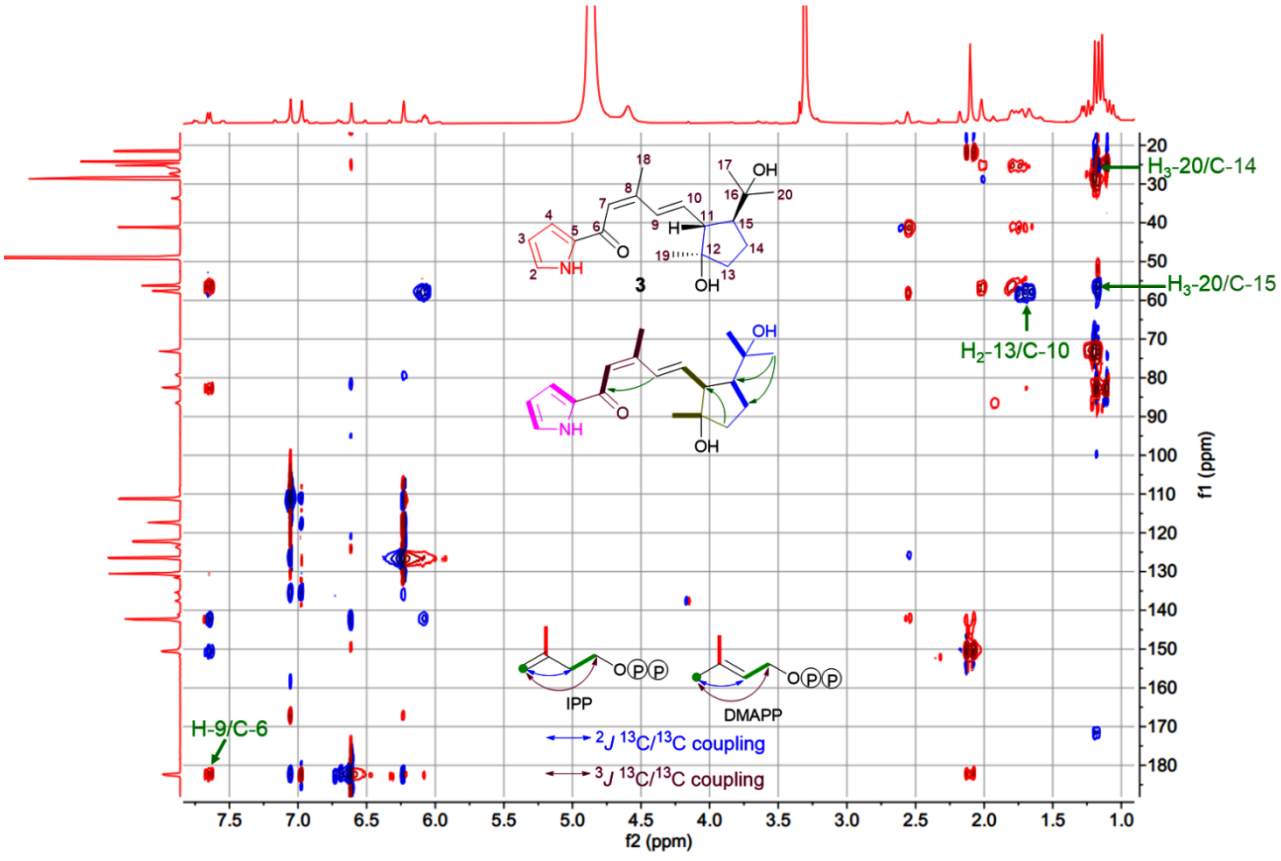
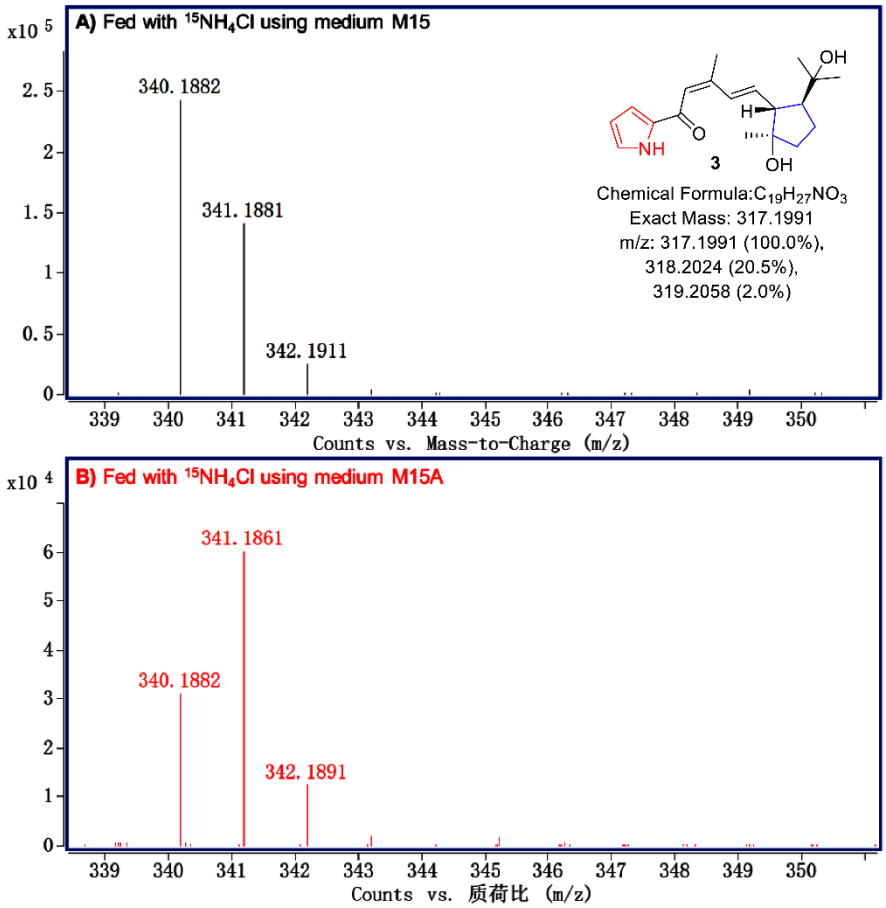


Figure S31. 1,n-ADEQUATE (800 MHz, CD_3OD) spectrum of compound **3** fed with$^{13}C_3$-glycerol.



Medium M15: glucose 30 g/L, beef extract 5 g/L, peptone 1 g/L, NaCl 5 g/L, $CaCO_3$ 3 g/L, pH 7.2

Medium M15A: glucose 30 g/L, beef extract 1 g/L, peptone 1 g/L, NaCl 5 g/L, $CaCO_3$ 3 g/L, pH 7.2

Figure S32. HR-ESI-MS spectra (*m/z* [M + Na]$^+$) of compound **3** fed with $^{15}NH_4Cl$.

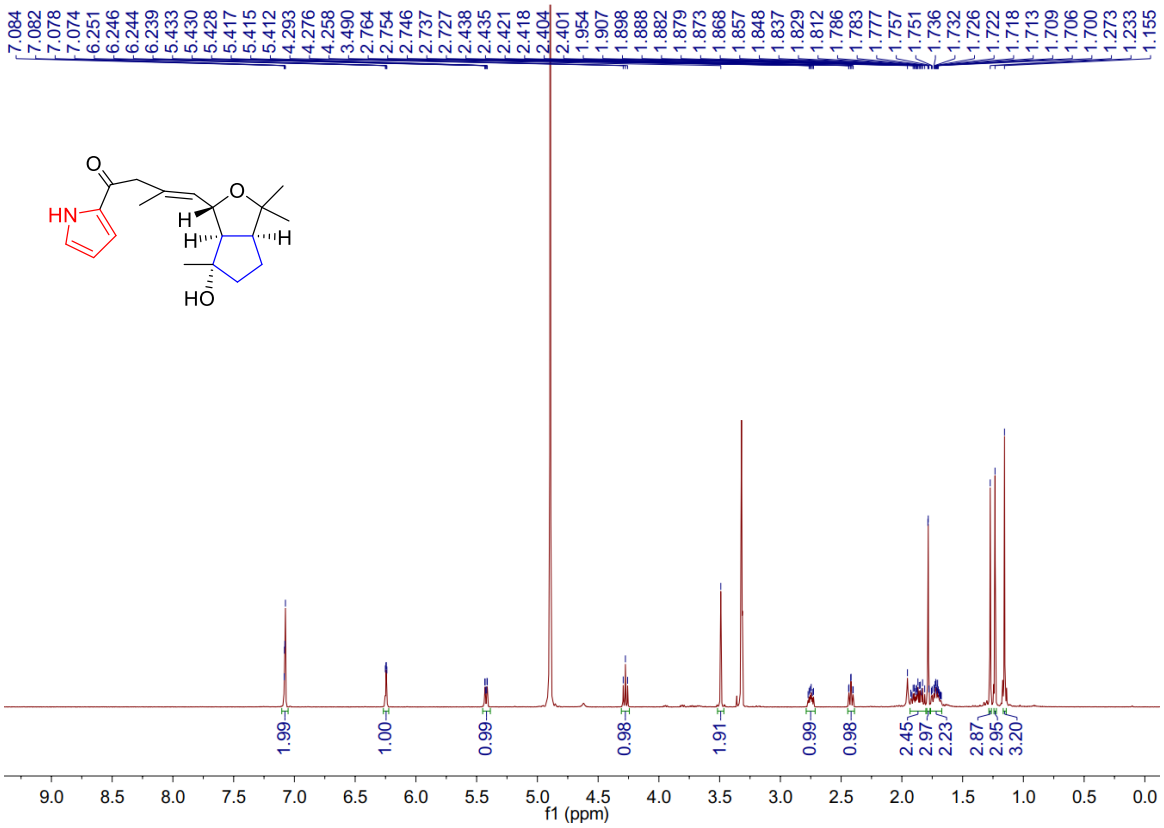


Figure S33. ^{1}H NMR (500 MHz) spectrum of **1** in CD_3OD.

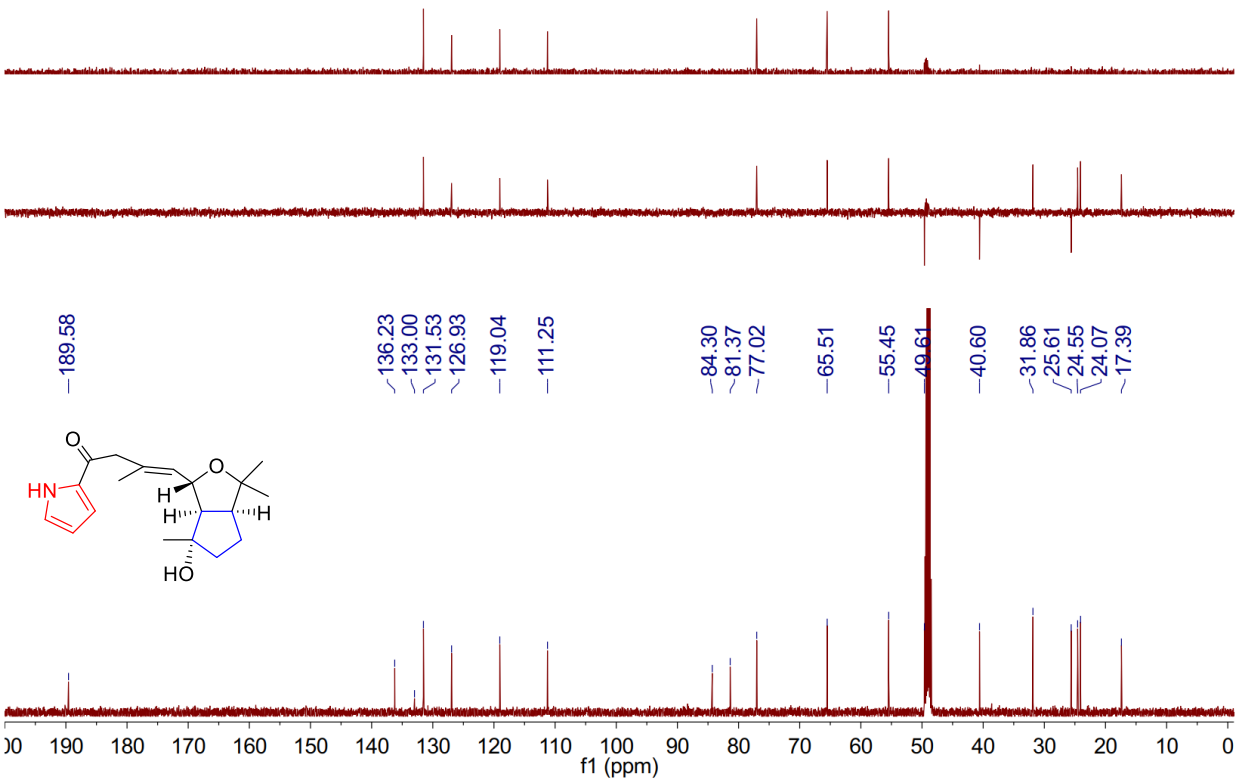


Figure S34. ^{13}C NMR (125 MHz) spectrum of **1** in CD_3OD.

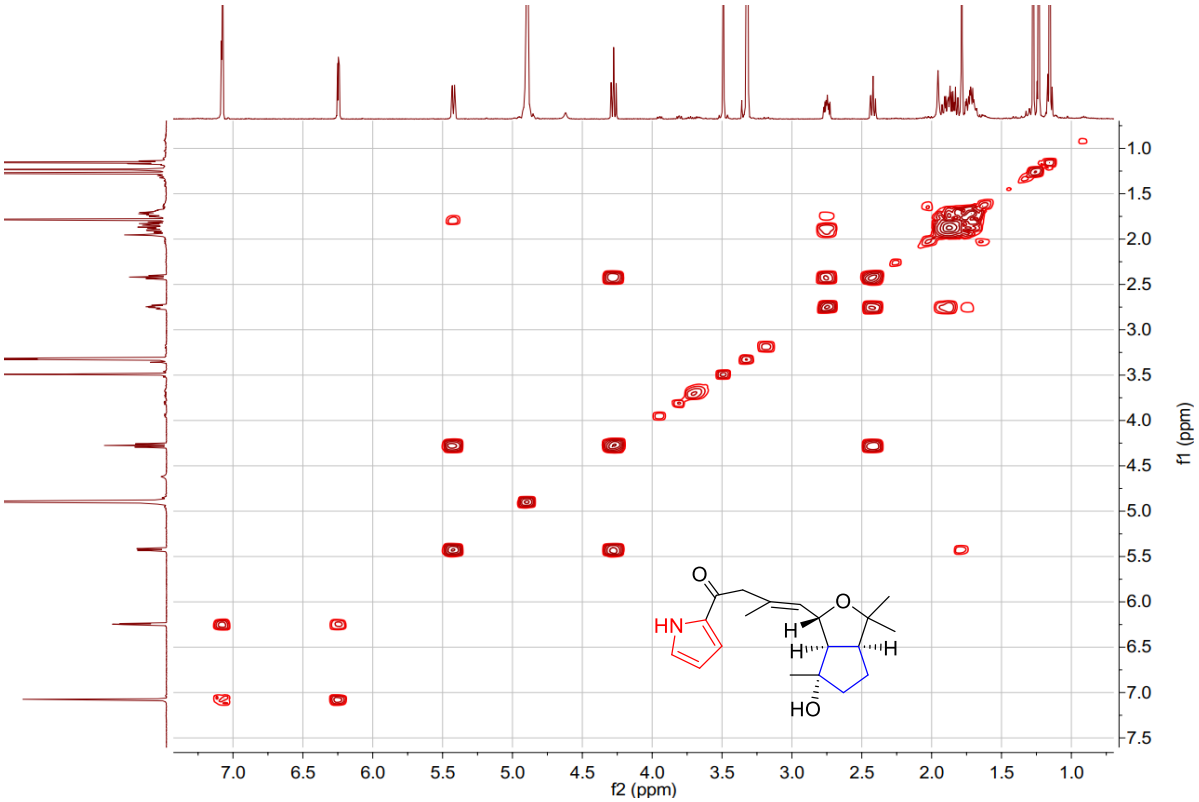


Figure S35. ^{1}H-^{1}H COSY (500 MHz) spectrum of **1** in CD_3OD.

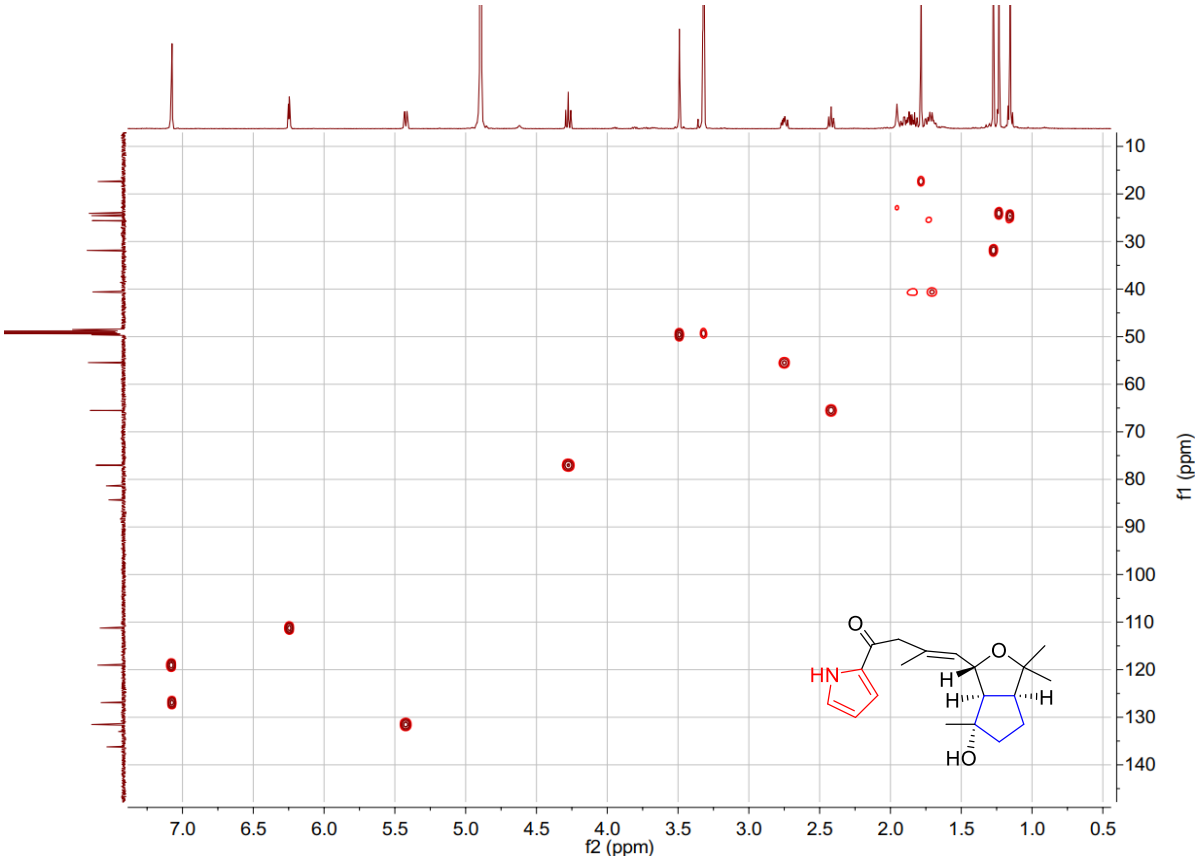


Figure S36. HSQC (500 MHz) spectrum of **1** in CD_3OD.

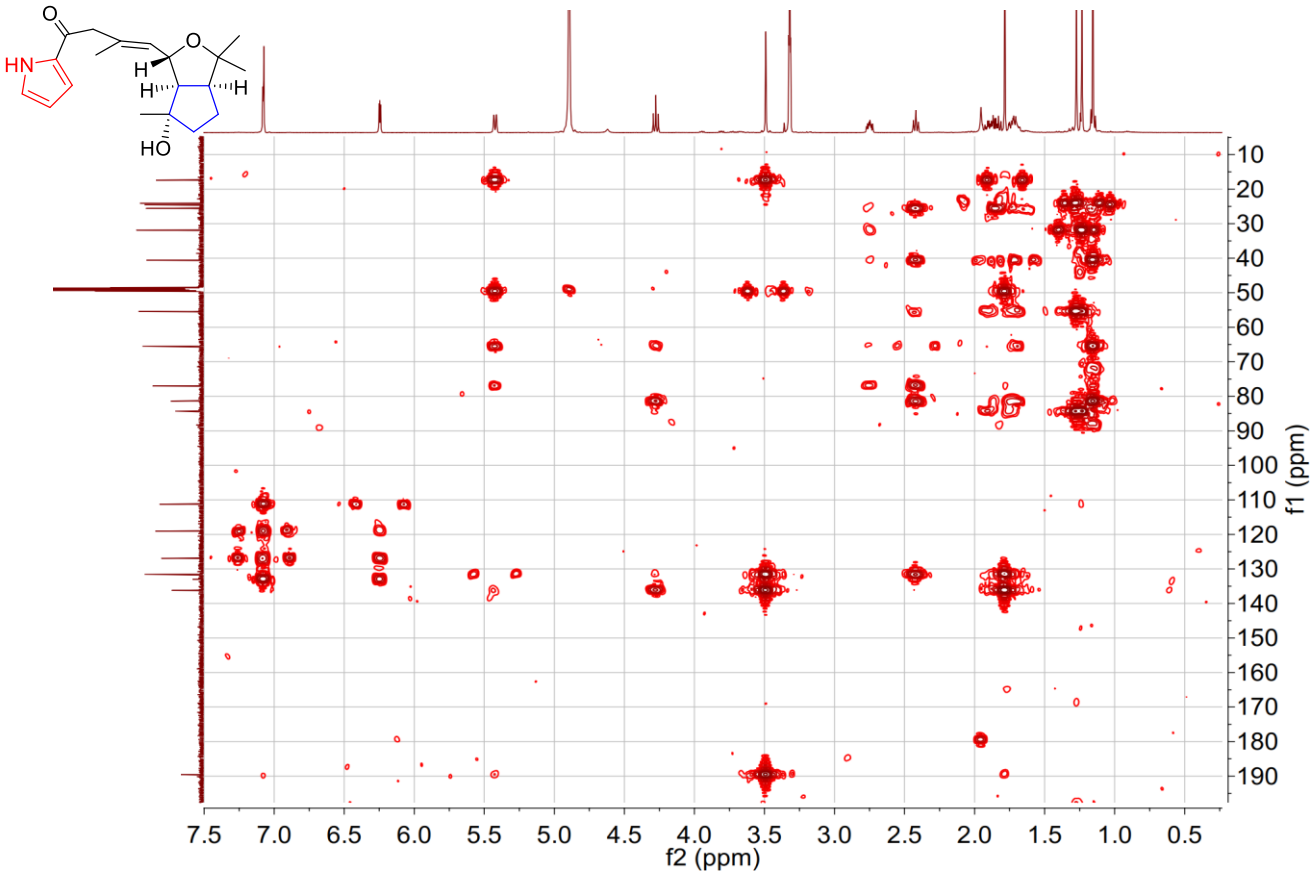


Figure S37. HMBC (500 MHz) spectrum of **1** in CD_3OD.

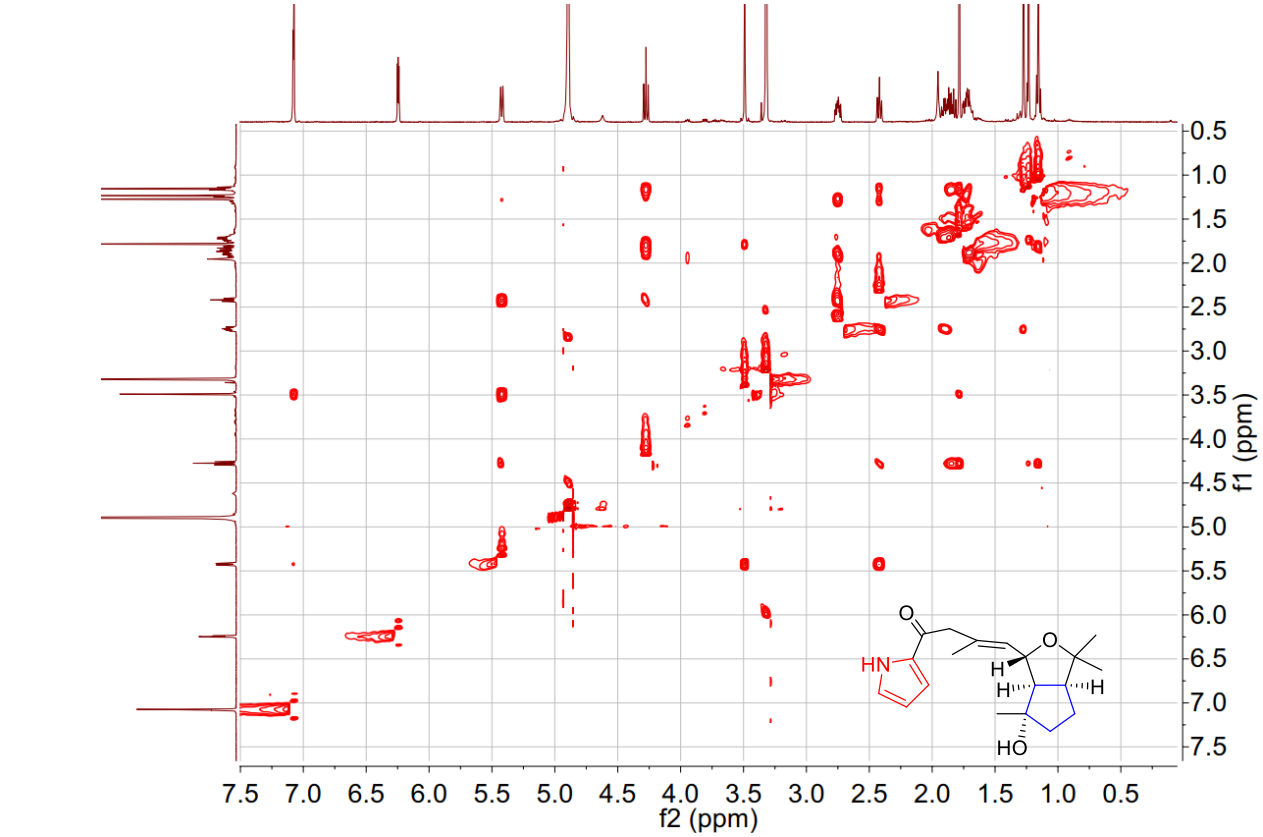
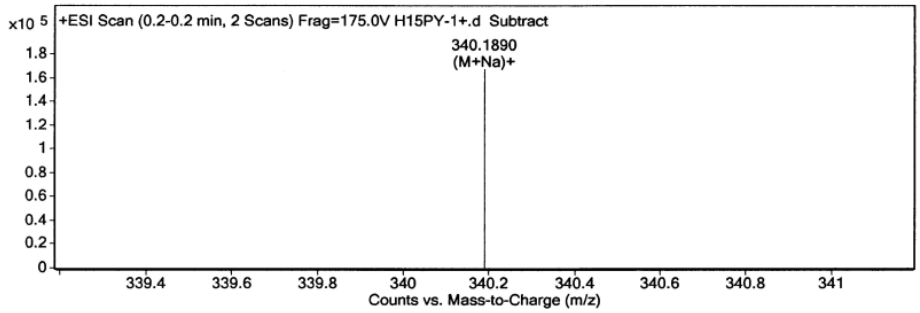


Figure S38. ROESY (500 MHz) spectrum of **1** in CD_3OD.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

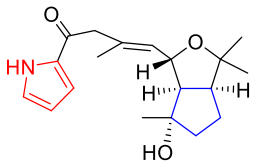


Peak List

m/z	z	Abund	Formula	Ion
191.1428	1	17893.69		
295.1881	1	16002.43		
300.1959	1	78487.69		
318.2068	1	17811.21		
340.189	1	168001.72	C19 H27 N O3	(M+Na)+
341.1921	1	34842.73	C19 H27 N O3	(M+Na)+
356.1628	1	84831.28		
657.3885	1	33420.38		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	10



Chemical Formula: $C_{19}H_{27}NO_3$
Exact Mass: 317.1991

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C19 H27 N O3	317.1991	340.1883	340.1890	-0.6	-1.9	7.0000

--- End Of Report ---

Figure S39. HR-ESI-MS spectrum of **1**.

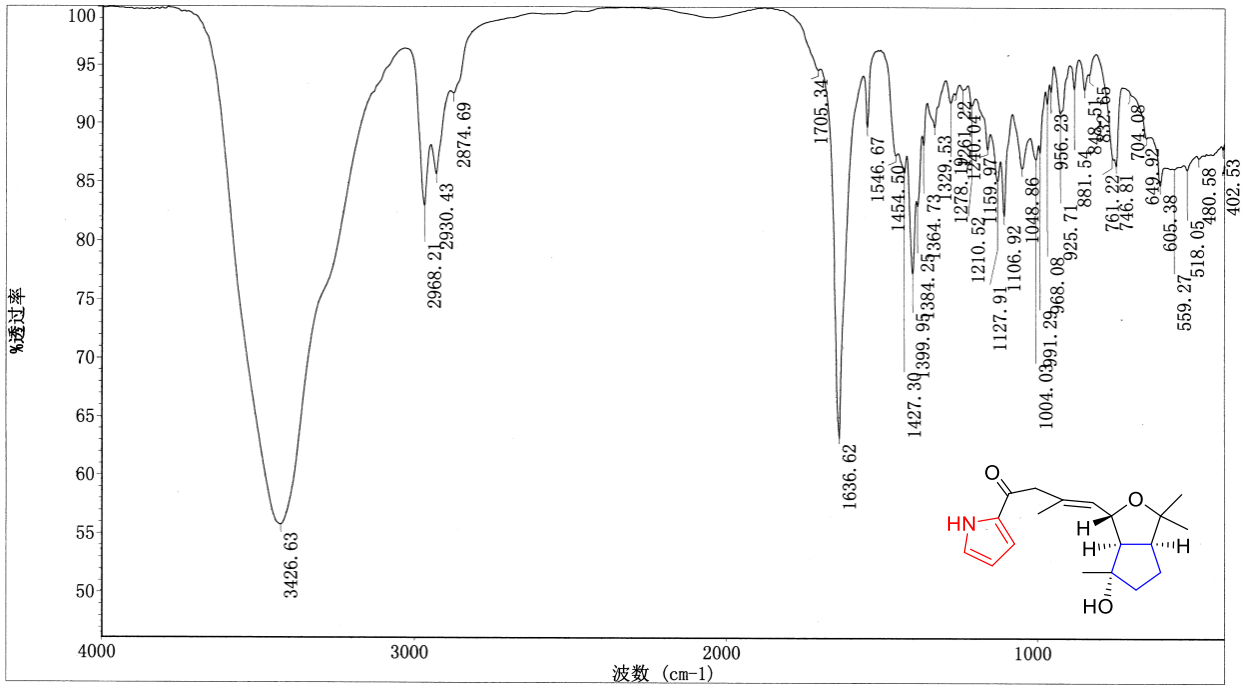


Figure S40. IR spectrum of **1**.

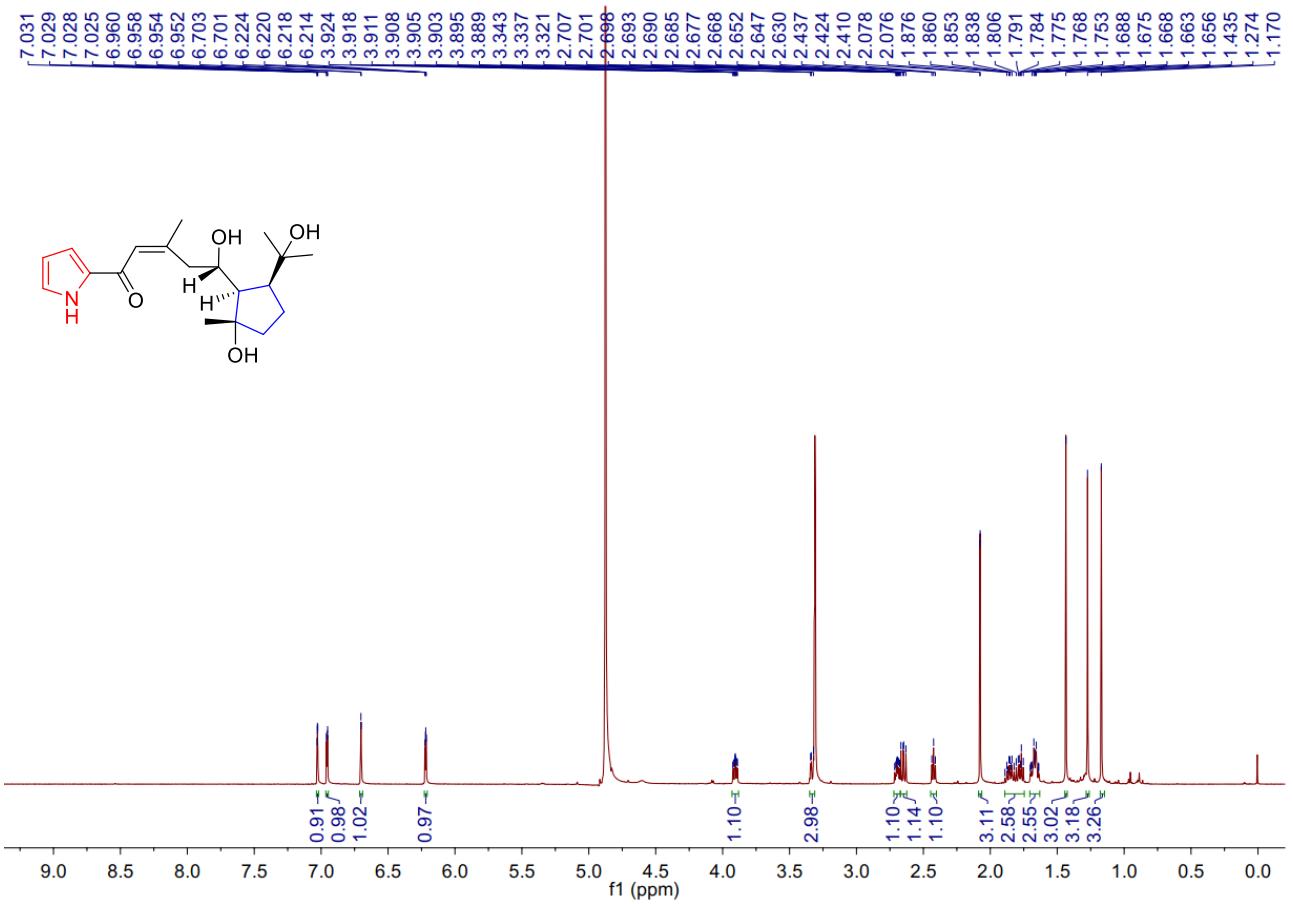


Figure S41. ^{1}H NMR (600 MHz) spectrum of **2** in CD_3OD.

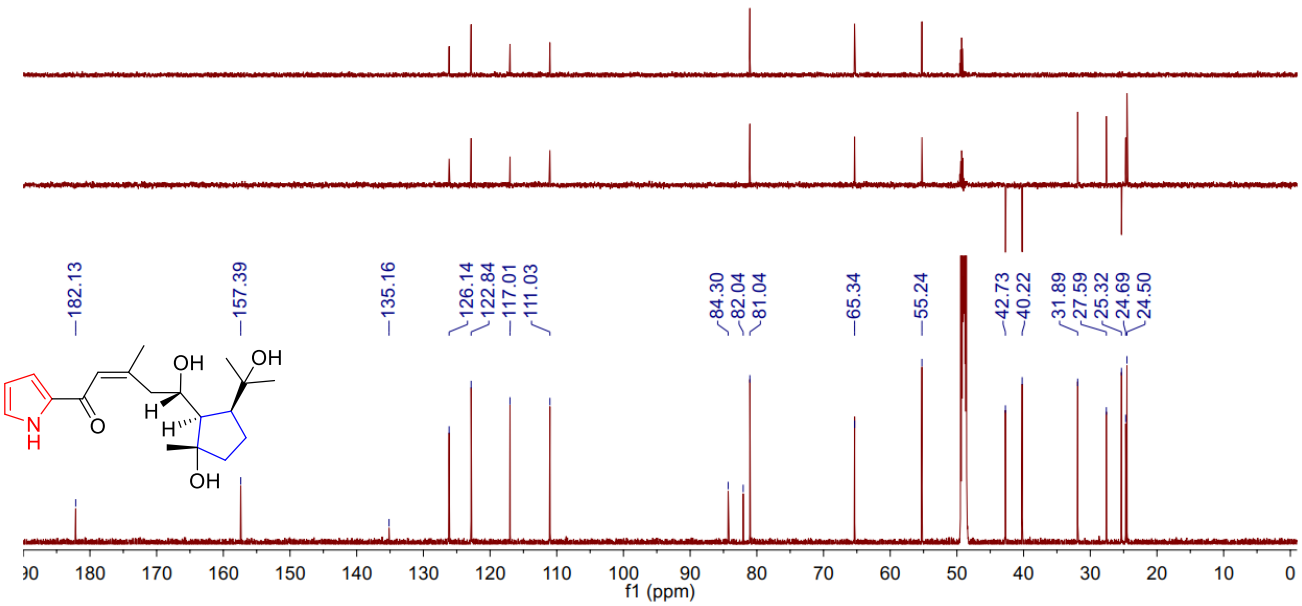


Figure S42. ^{13}C NMR (150 MHz) spectrum of **2** in CD_3OD.

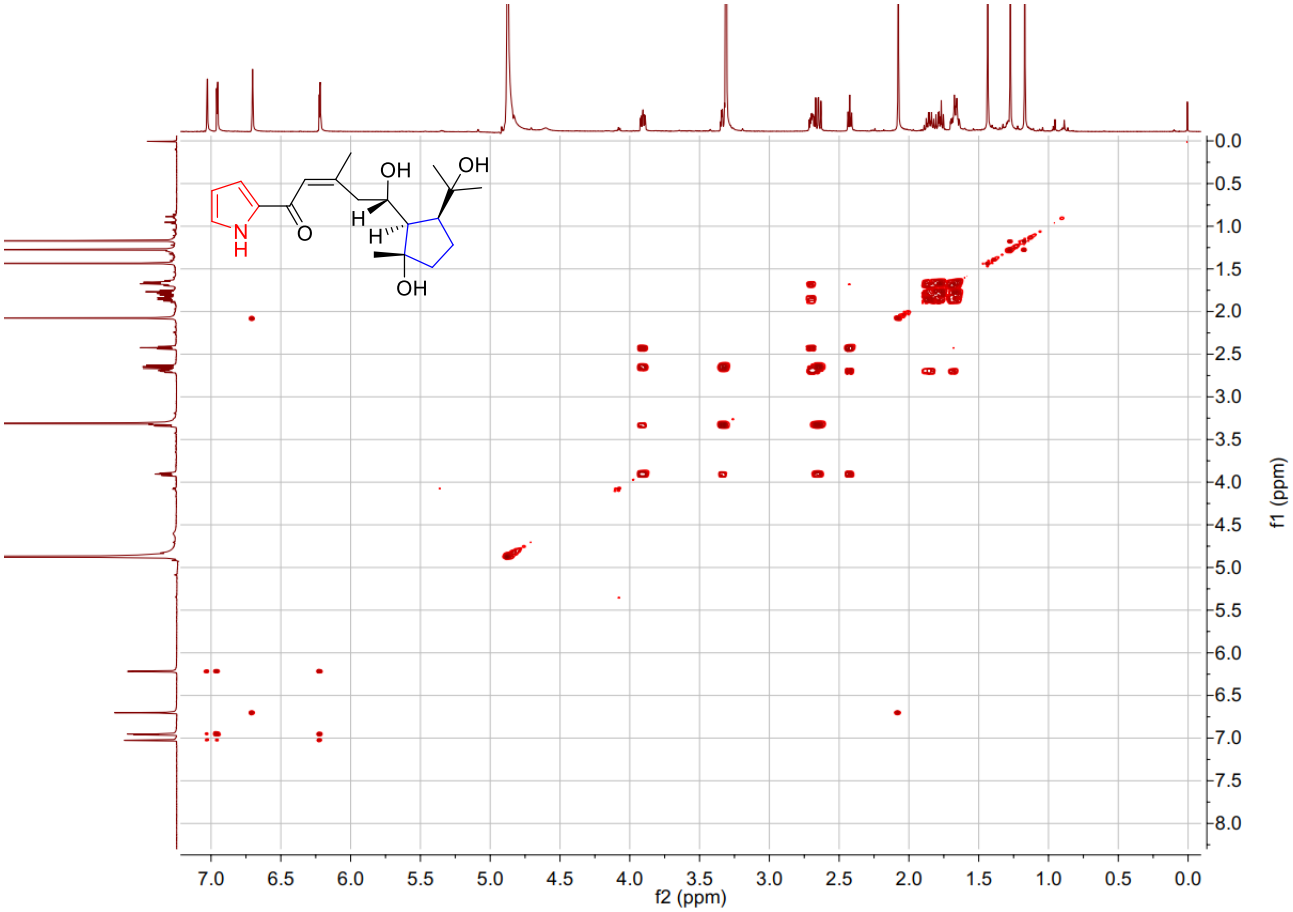


Figure S43. ^{1}H-^{1}H COSY (600 MHz) spectrum of **2** in CD_3OD.

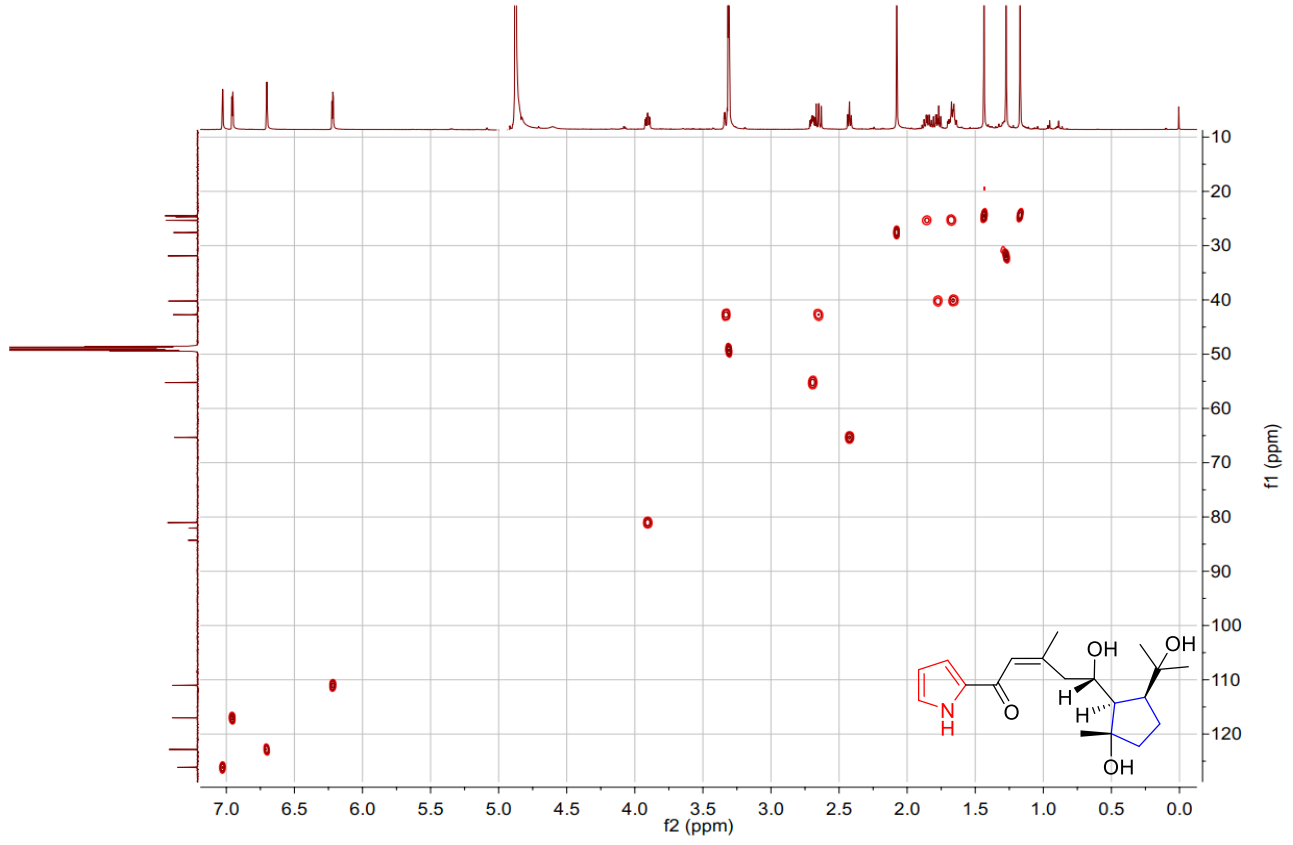


Figure S44. HSQC (600 MHz) spectrum of **2** in CD_3OD.

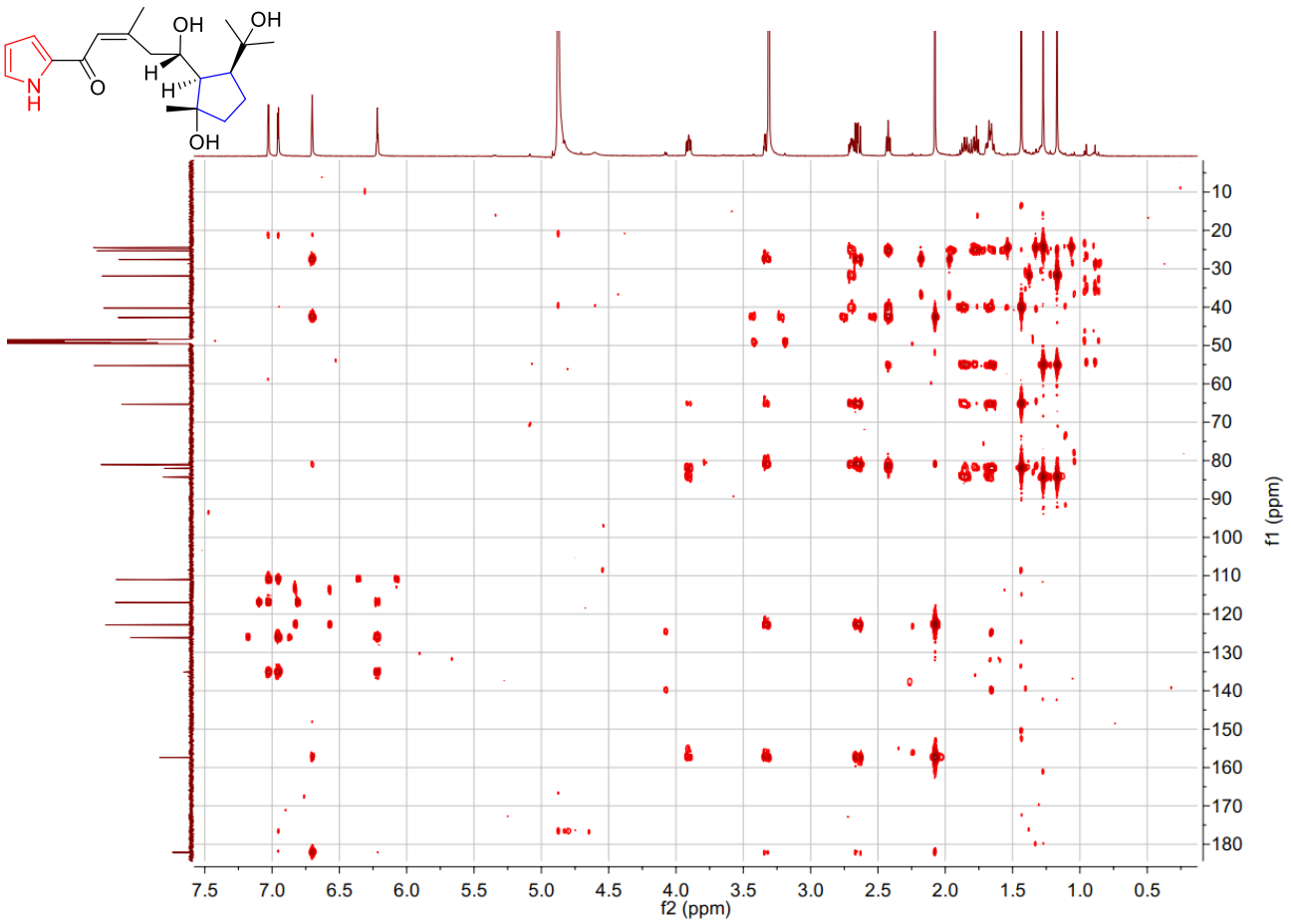


Figure S45. HMBC (600 MHz) spectrum of **2** in CD_3OD.

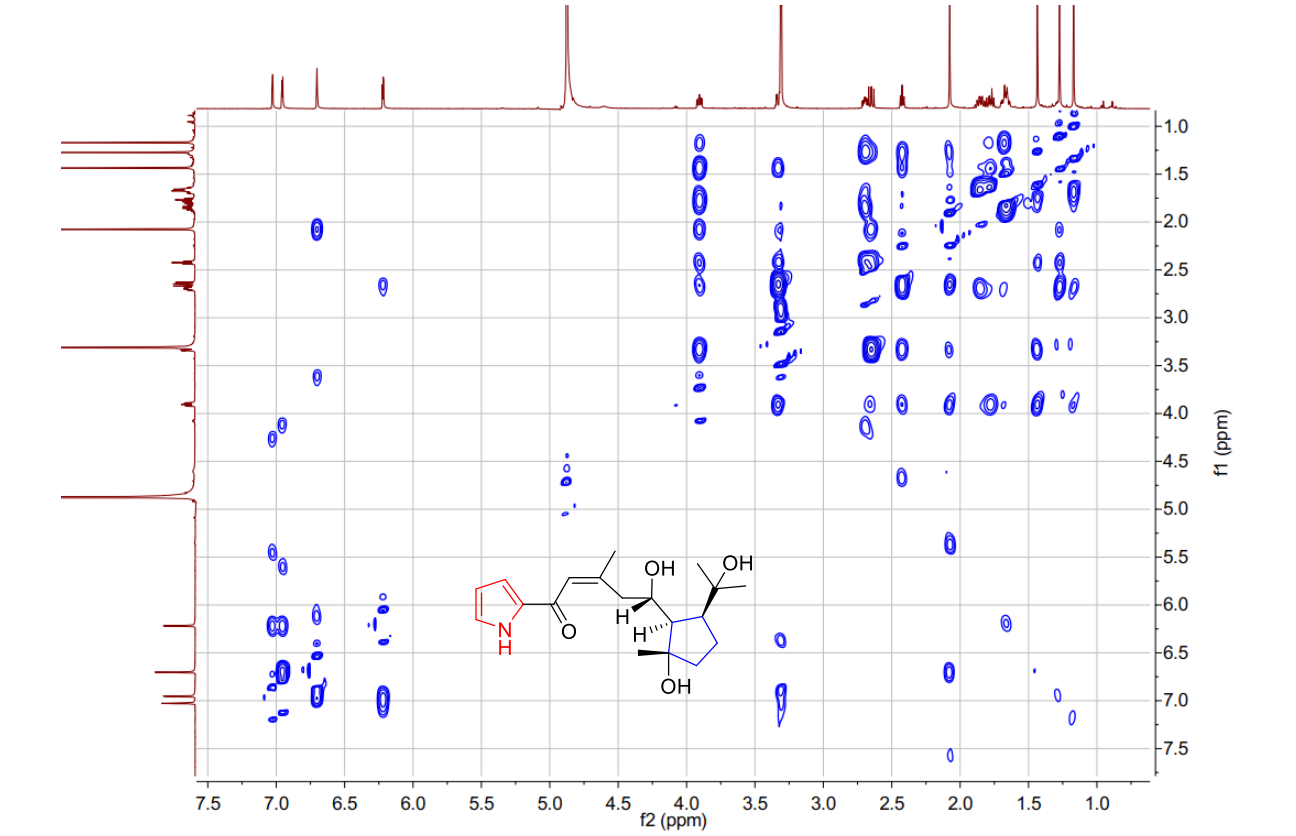
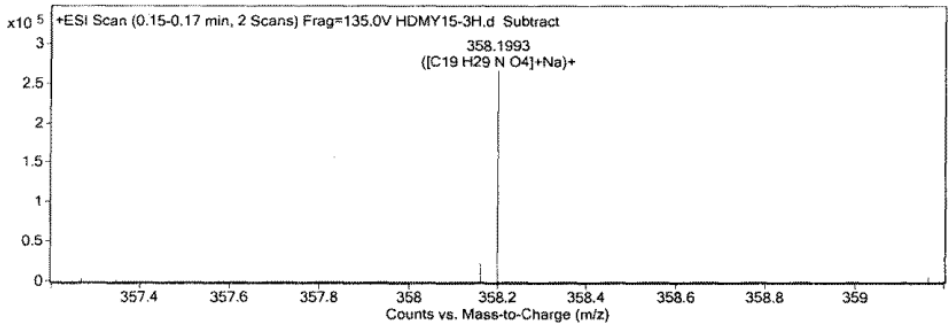


Figure S46. ROESY (600 MHz) spectrum of **2** in CD_3OD.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

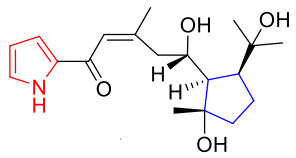


Peak List

m/z	z	Abund
318.2071	1	425683
340.1883	1	650800.88
625.3714	1	1349778.13
626.3751	1	493261.75
641.3384	1	3314152
642.3414	1	1296844
647.3541	1	340833.34
657.3881	1	681894.25
1265.7023	1	445890.81
1266.7057	1	350531.94

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3



Chemical Formula: $C_{19}H_{29}NO_4$
Exact Mass: 335.2097

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C19 H29 N O4	335.2097	358.1989	358.1993	-0.40	-1.12	6.0000

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Figure S47. HR-ESI-MS spectrum of **2**.

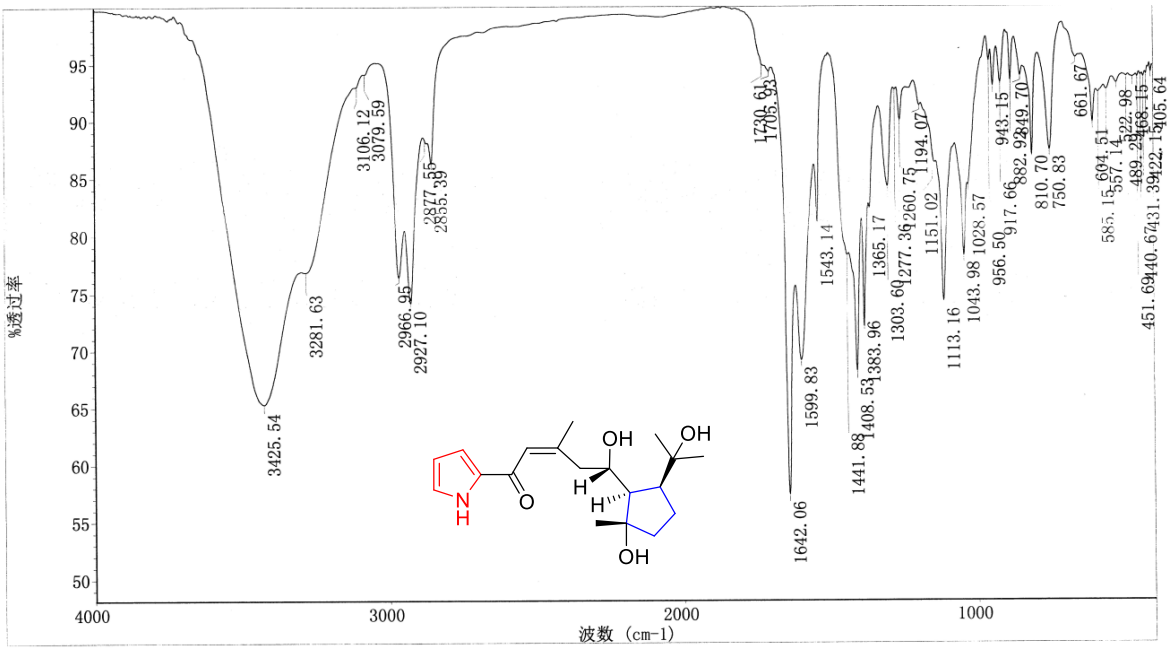


Figure S48. IR spectrum of **2**.

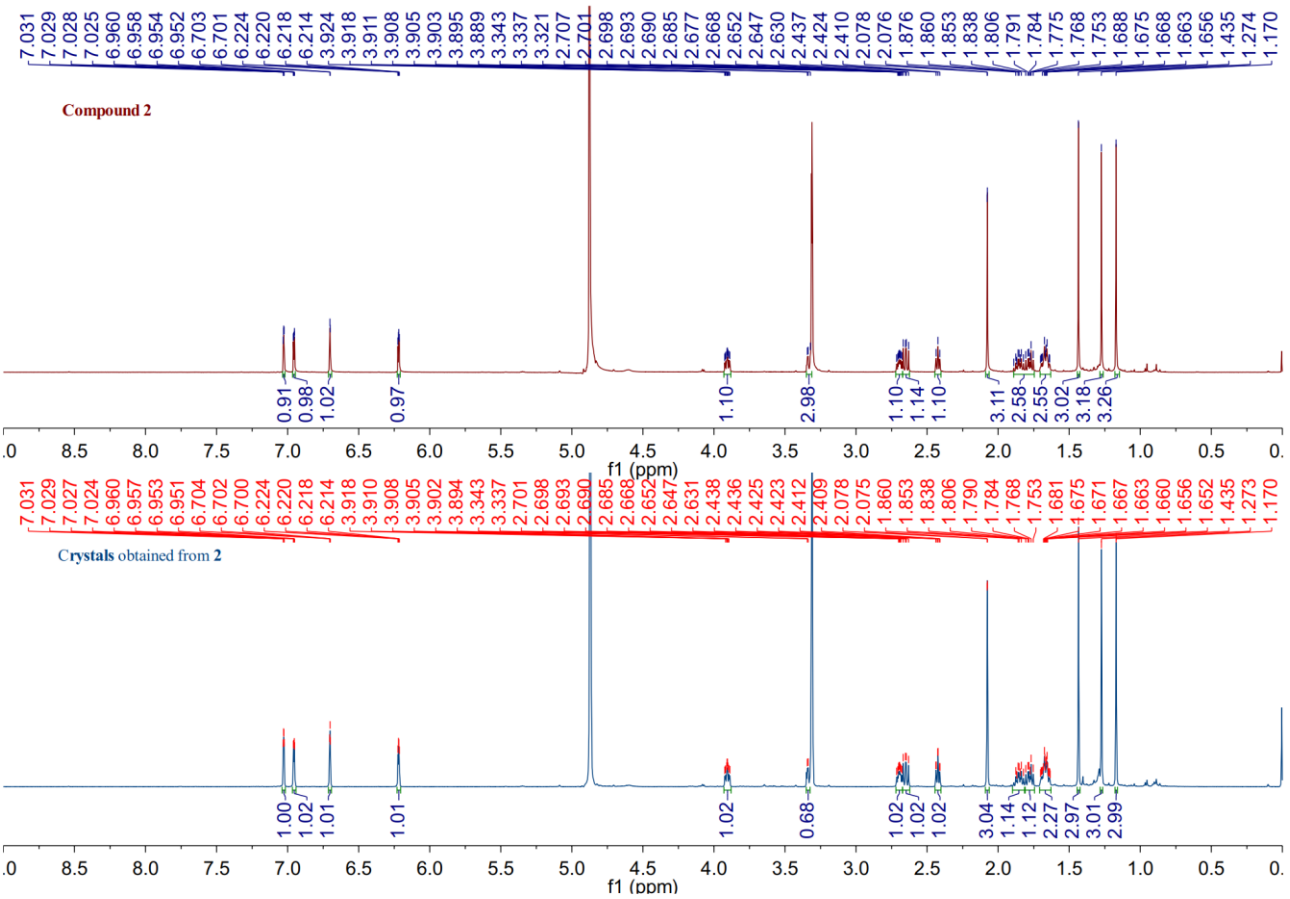


Figure S49. ^{1}H NMR (600 MHz) spectrum of crystals obtained from **2**.

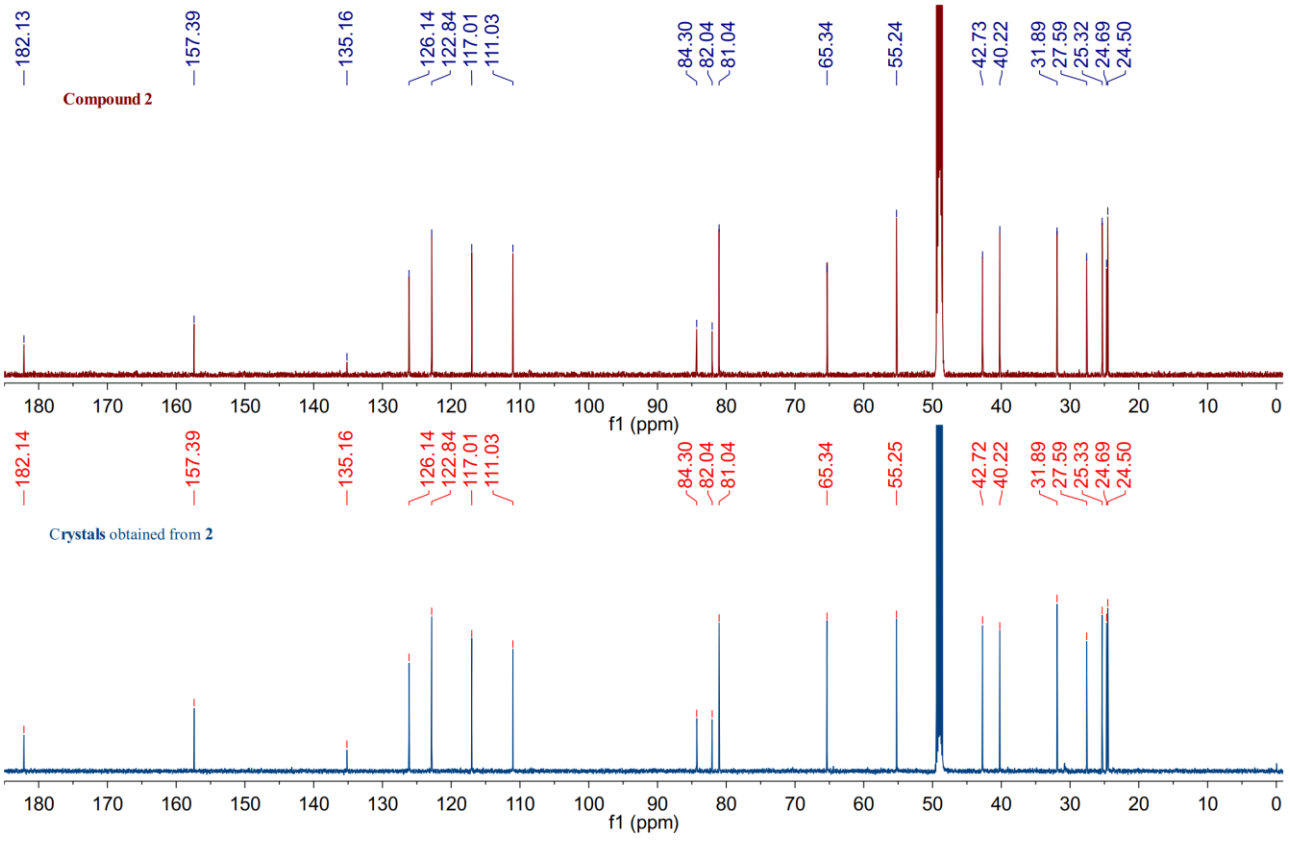


Figure S50. ^{13}C NMR (150 MHz) spectrum of crystals obtained from **2**.

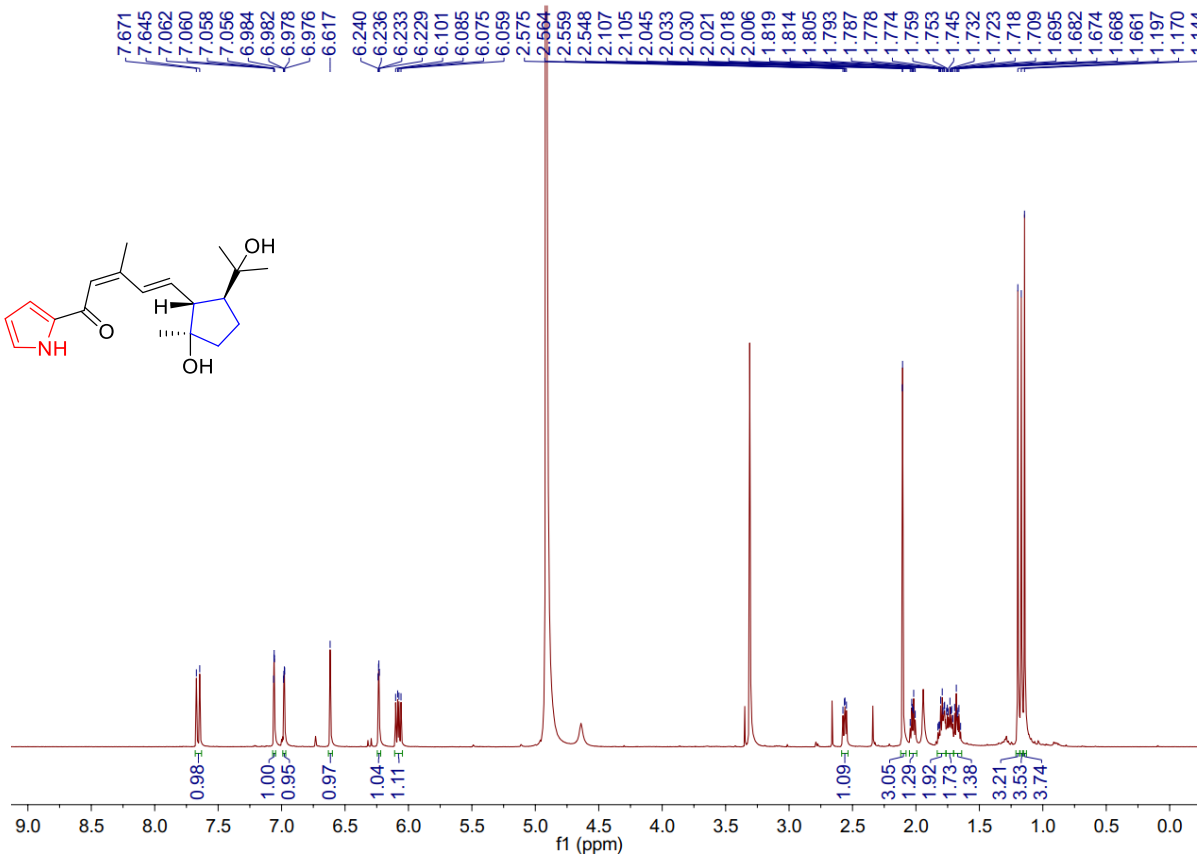


Figure S51. ^{1}H NMR (600 MHz) spectrum of **3** in CD_3OD.

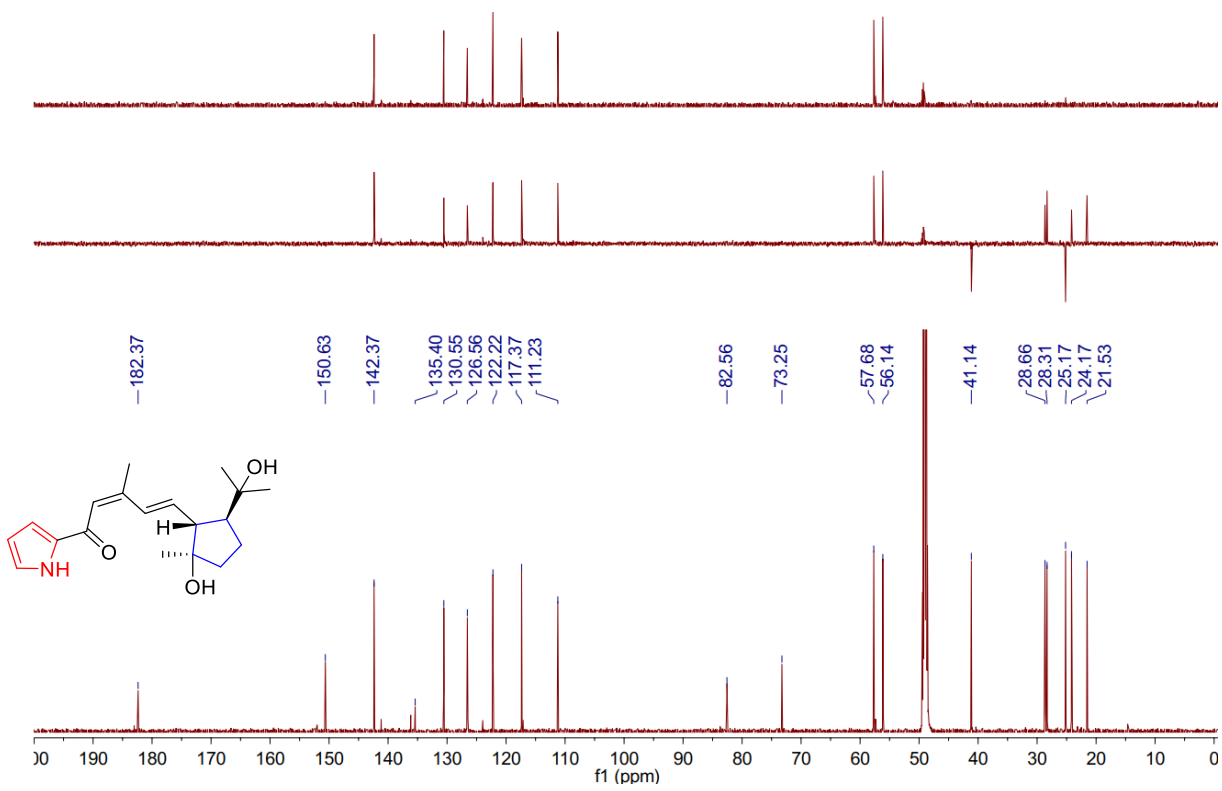


Figure S52. ^{13}C NMR (150 MHz) spectrum of **3** in CD_3OD.

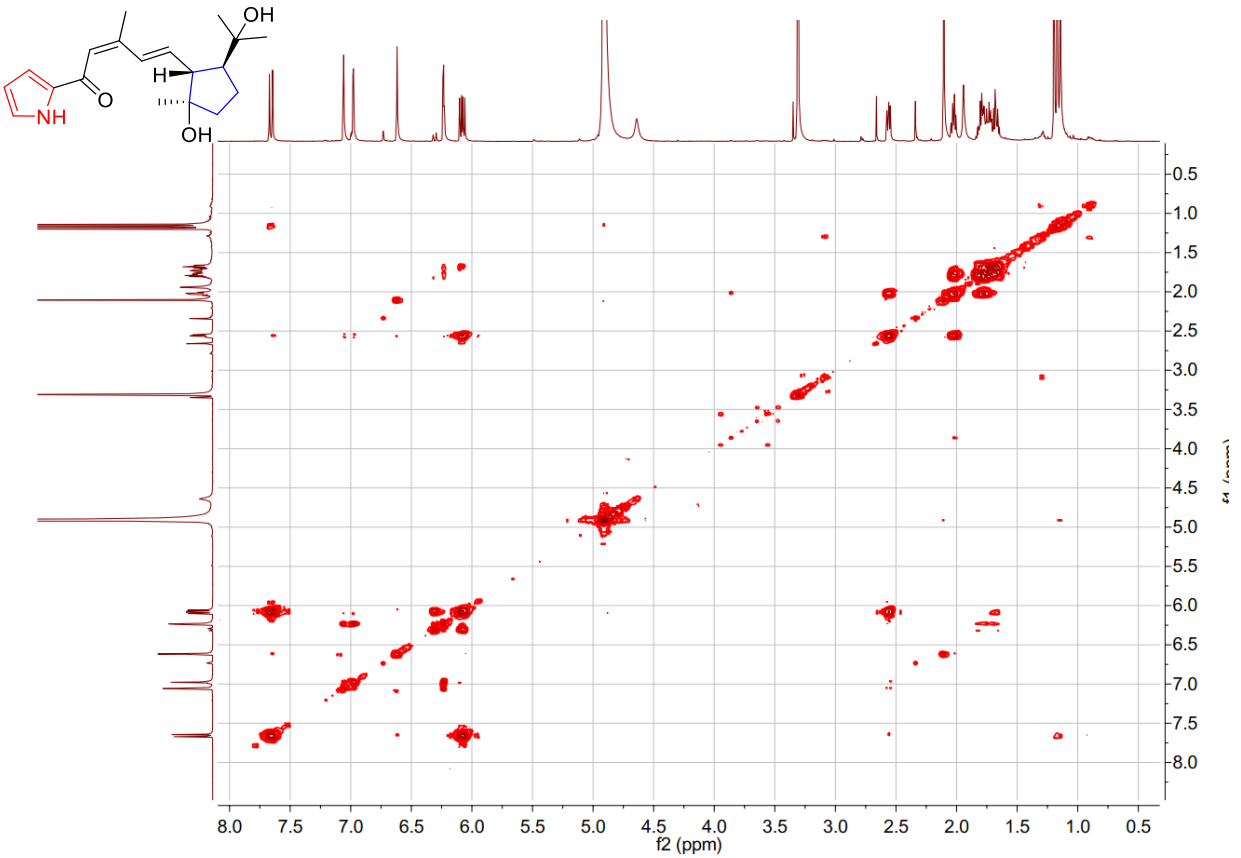


Figure S53. ^{1}H-^{1}H COSY (600 MHz) spectrum of **3** in CD_3OD.

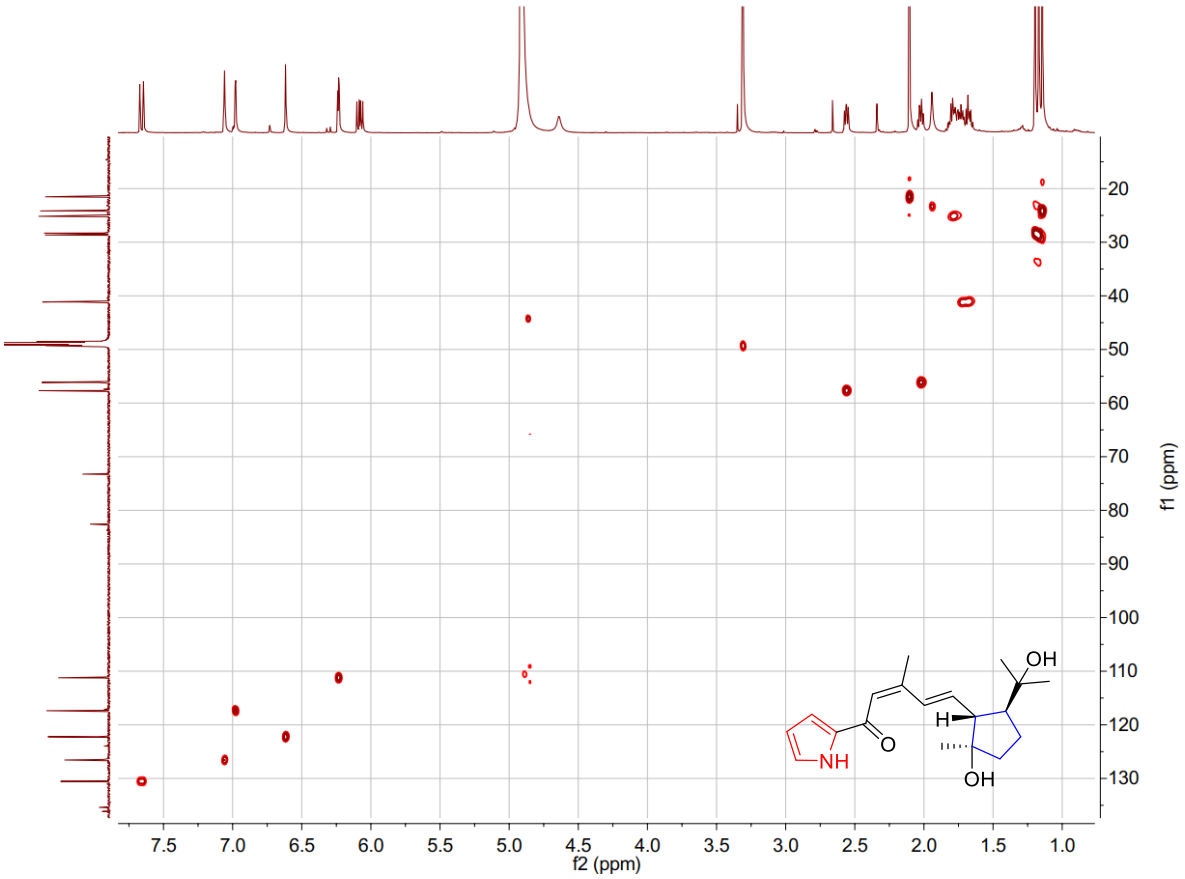


Figure S54. HSQC (600 MHz) spectrum of **3** in CD_3OD.

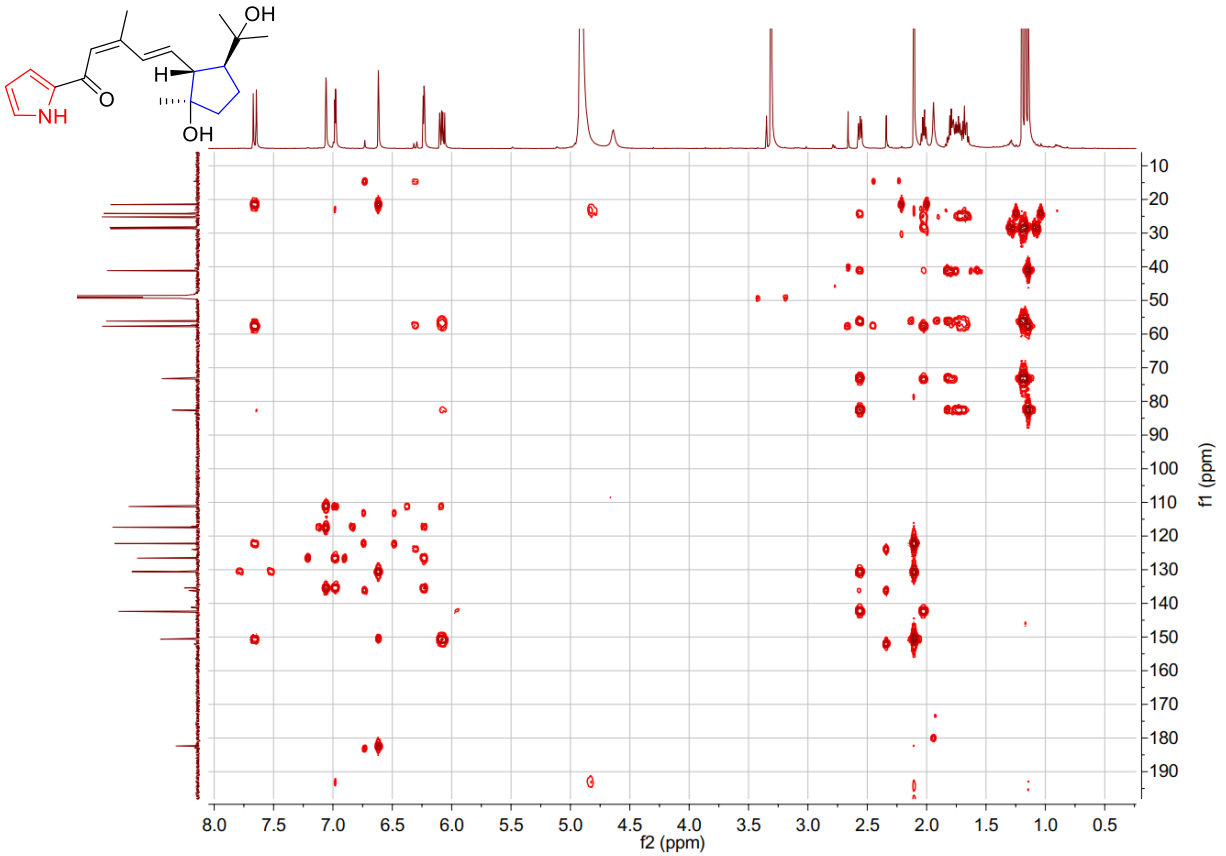


Figure S55. HMBC (600 MHz) spectrum of **3** in CD_3OD.

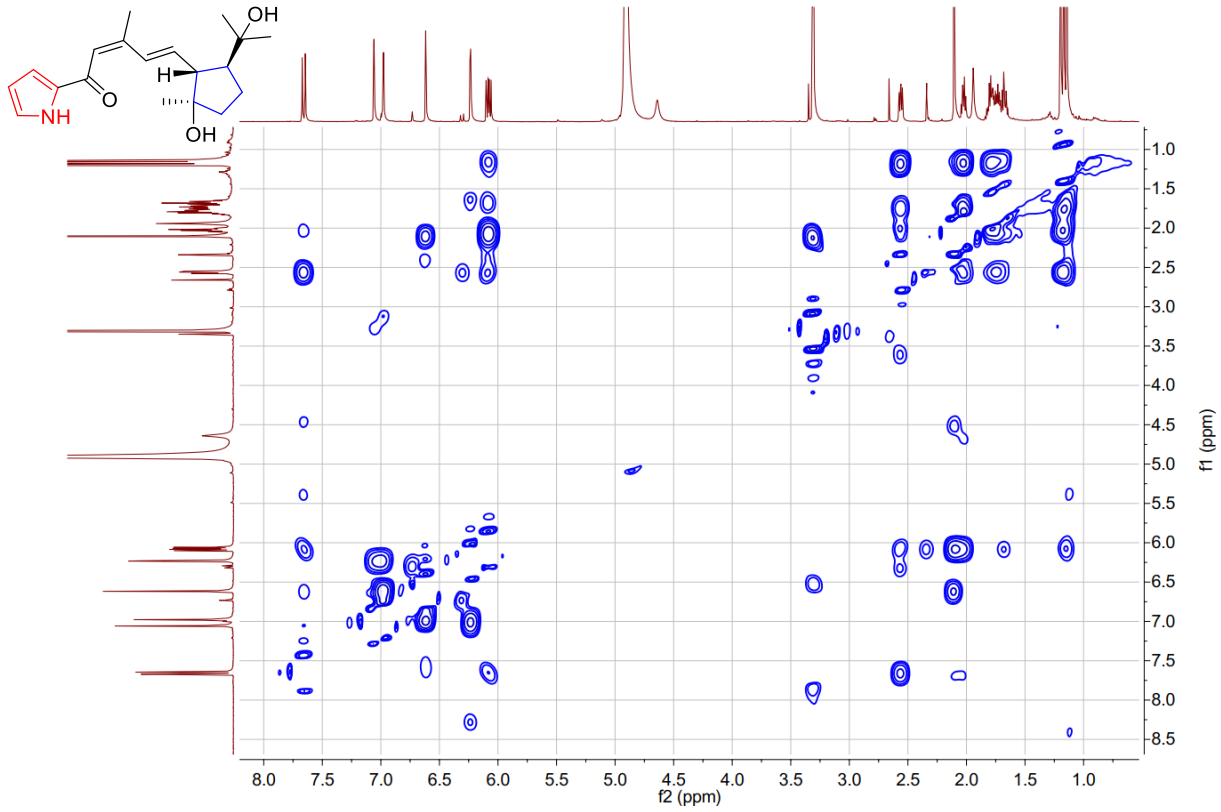
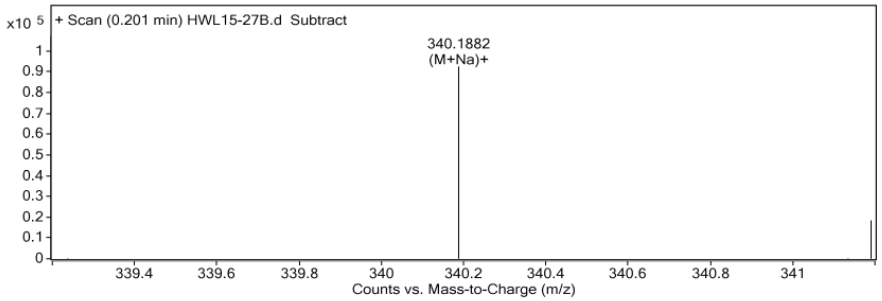


Figure S56. ROESY (600 MHz) spectrum of **3** in CD_3OD.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

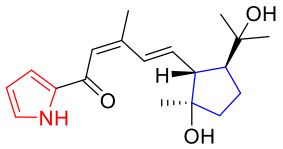


Peak List

m/z	z	Abund	Formula	Ion
282.1855	1	22982.51		
300.1958	1	60907.53		
318.2062	1	15909.82		
340.1882	1	92585.27	C19 H27 N O3	(M+Na)+
341.1918	1	18216.99	C19 H27 N O3	(M+Na)+
356.1625	1	27524.51		
657.3877	1	128837.84		
658.3909	1	51622.02		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30



Chemical Formula: $C_{19}H_{27}NO_3$
Exact Mass: 317.1991

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C19 H27 N O3	317.1991	340.1883	340.1882	0.1	0.2	7.0000

--- End Of Report ---

Figure S57. HR-ESI-MS spectrum of **3**.

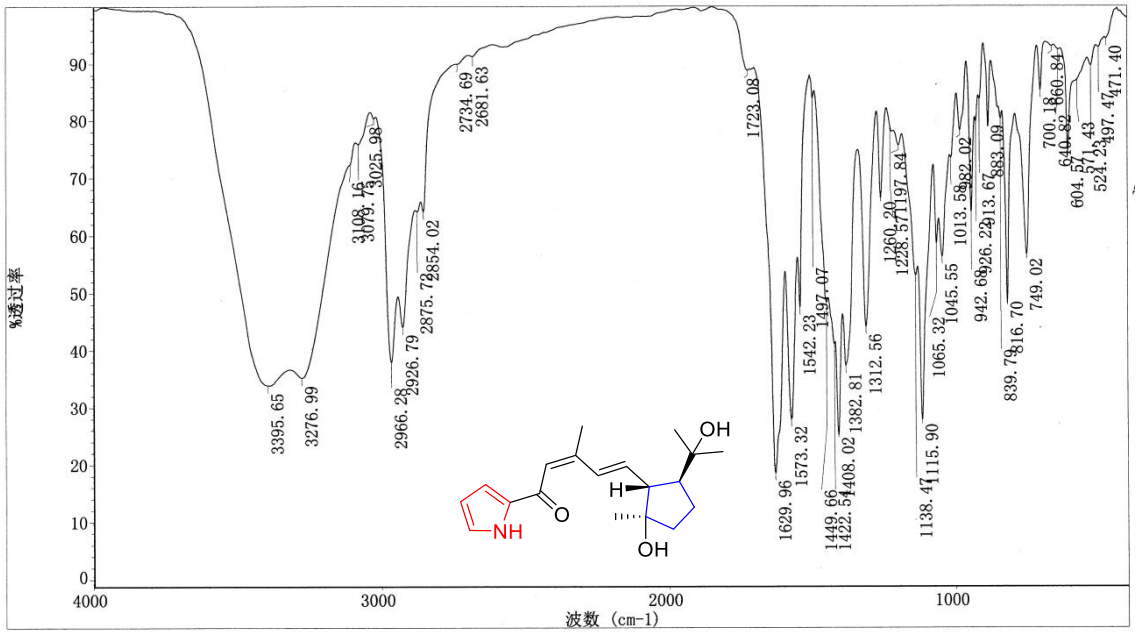


Figure S58. IR spectrum of **3**.

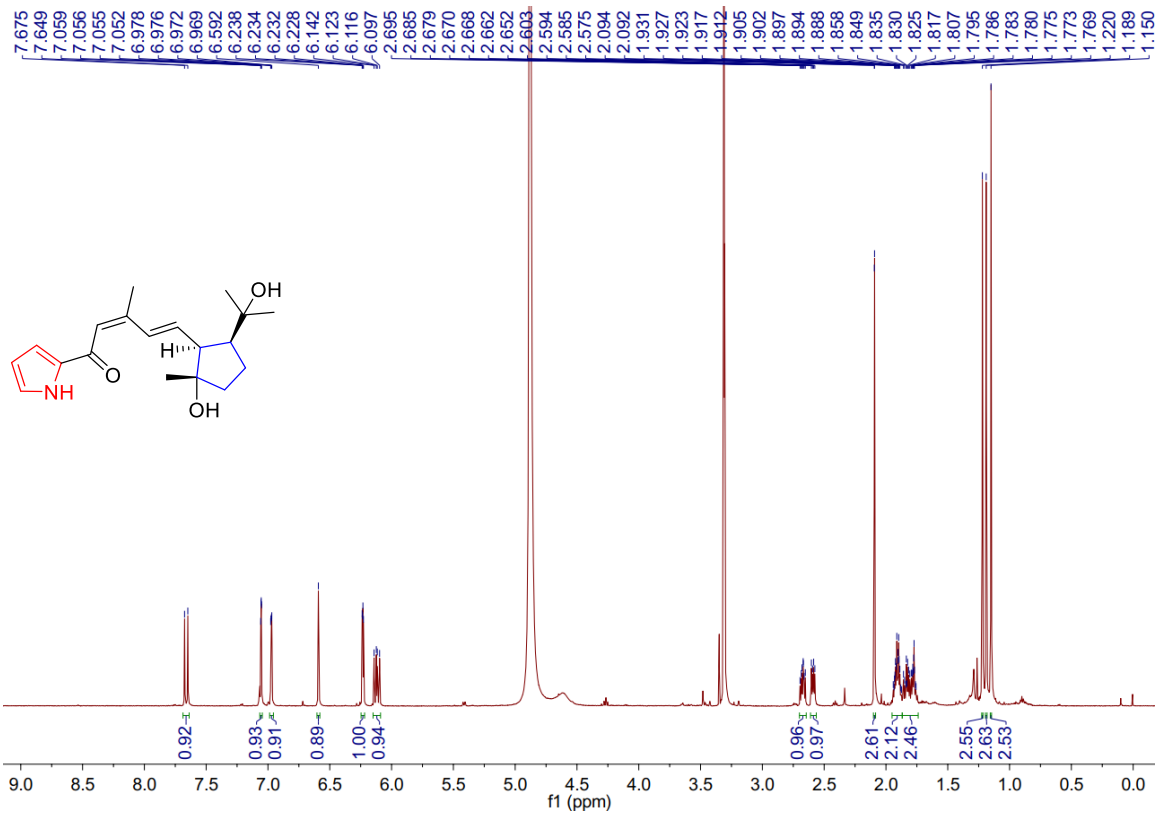


Figure S59. ^{1}H NMR (600 MHz) spectrum of **4** in CD_3OD.

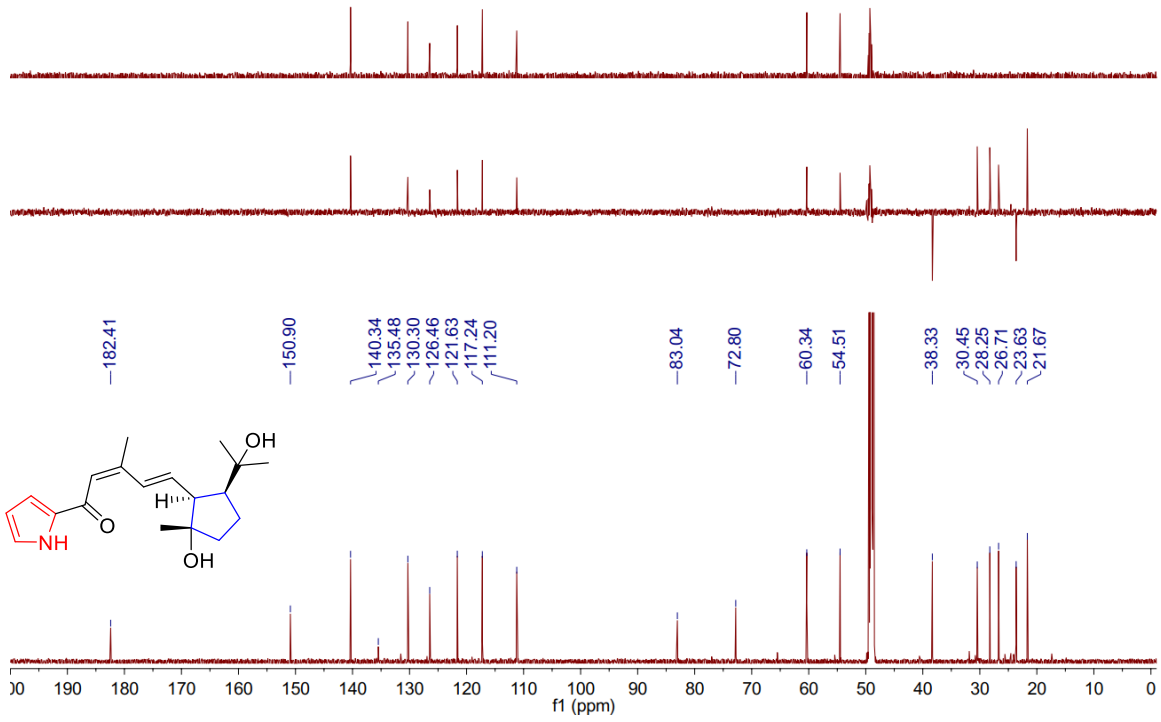


Figure S60. ^{13}C NMR (150 MHz) spectrum of **4** in CD_3OD.

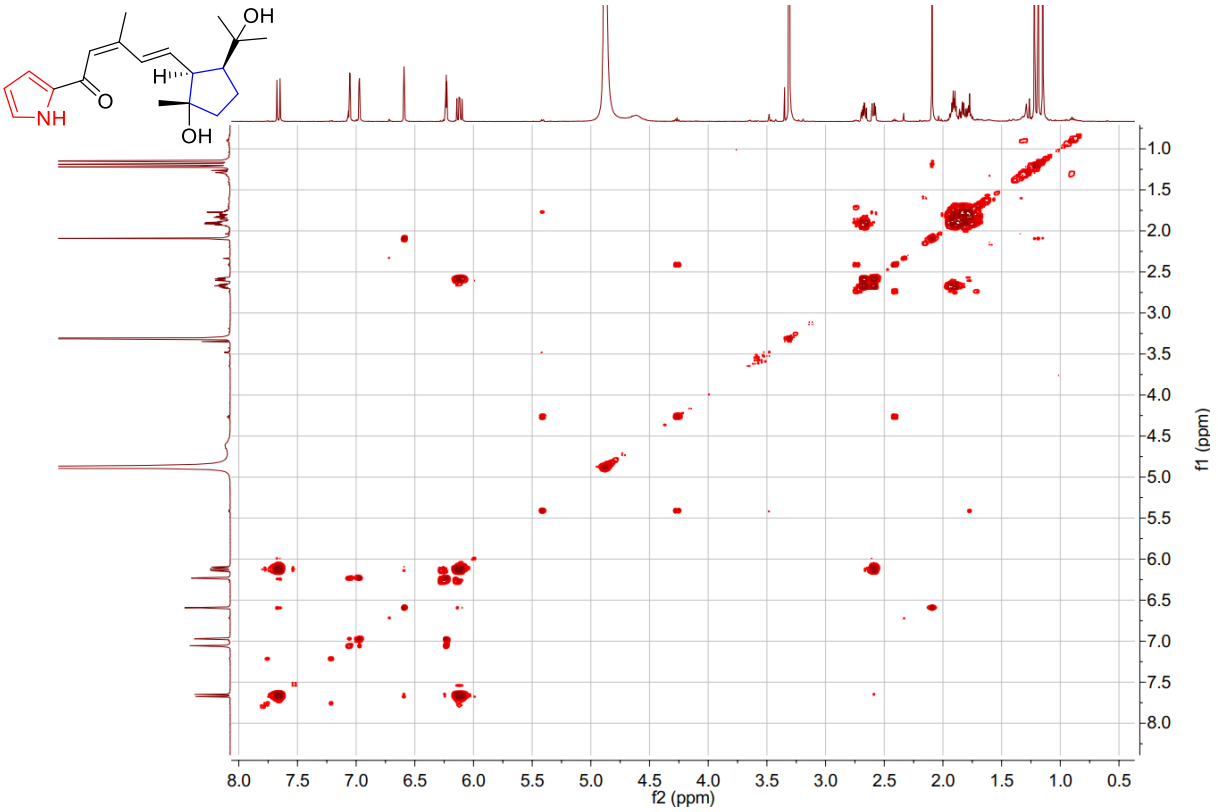


Figure S61. ^{1}H-^{1}H COSY (600 MHz) spectrum of **4** in CD_3OD.

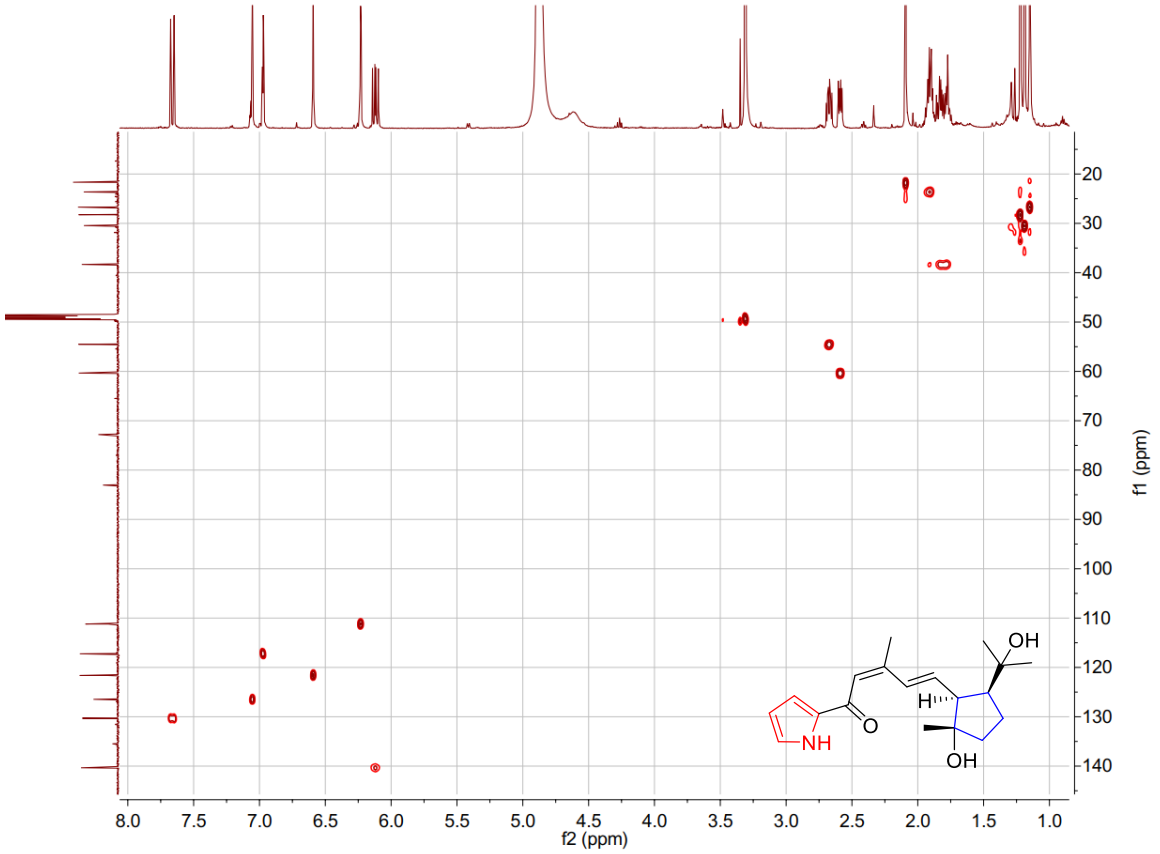


Figure S62. HSQC (600 MHz) spectrum of **4** in CD_3OD.

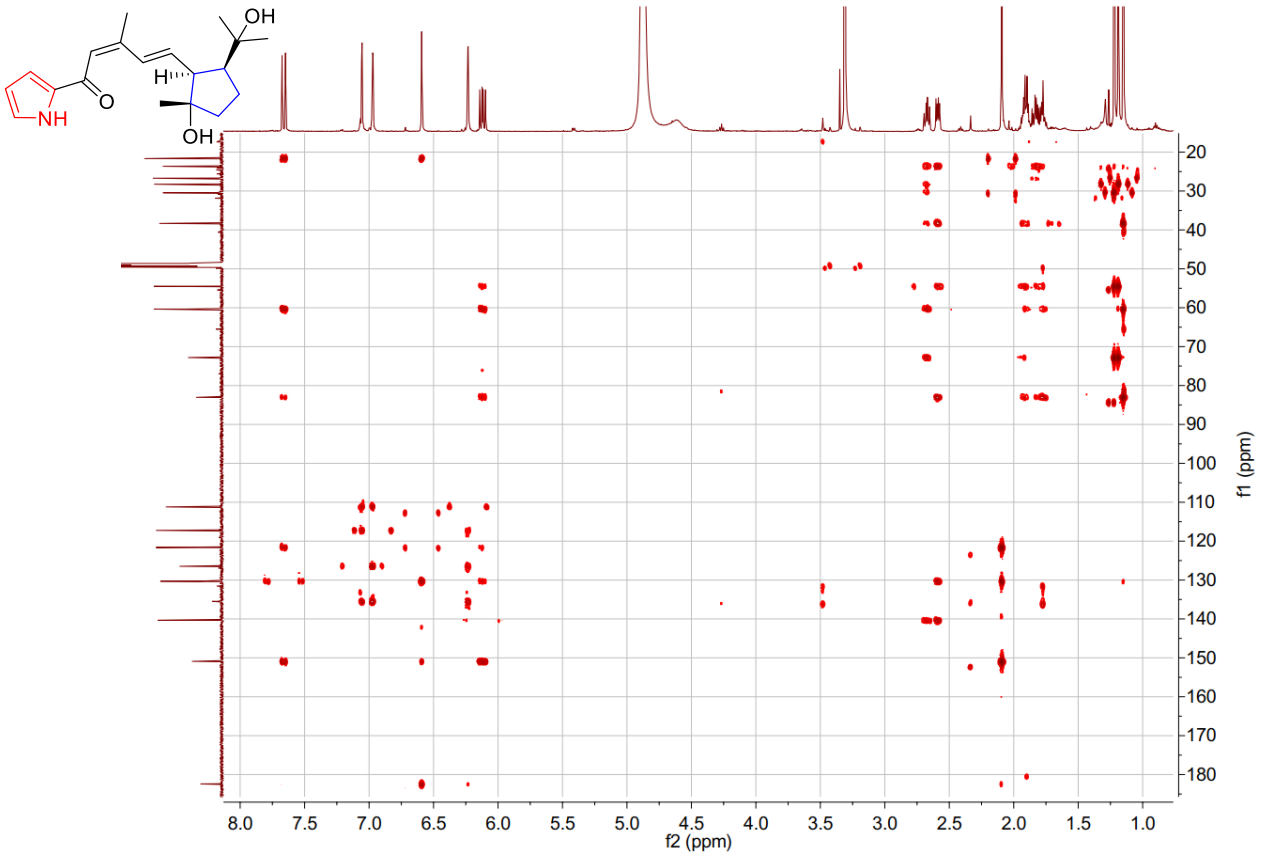


Figure S63. HMBC (600 MHz) spectrum of **4** in CD_3OD.

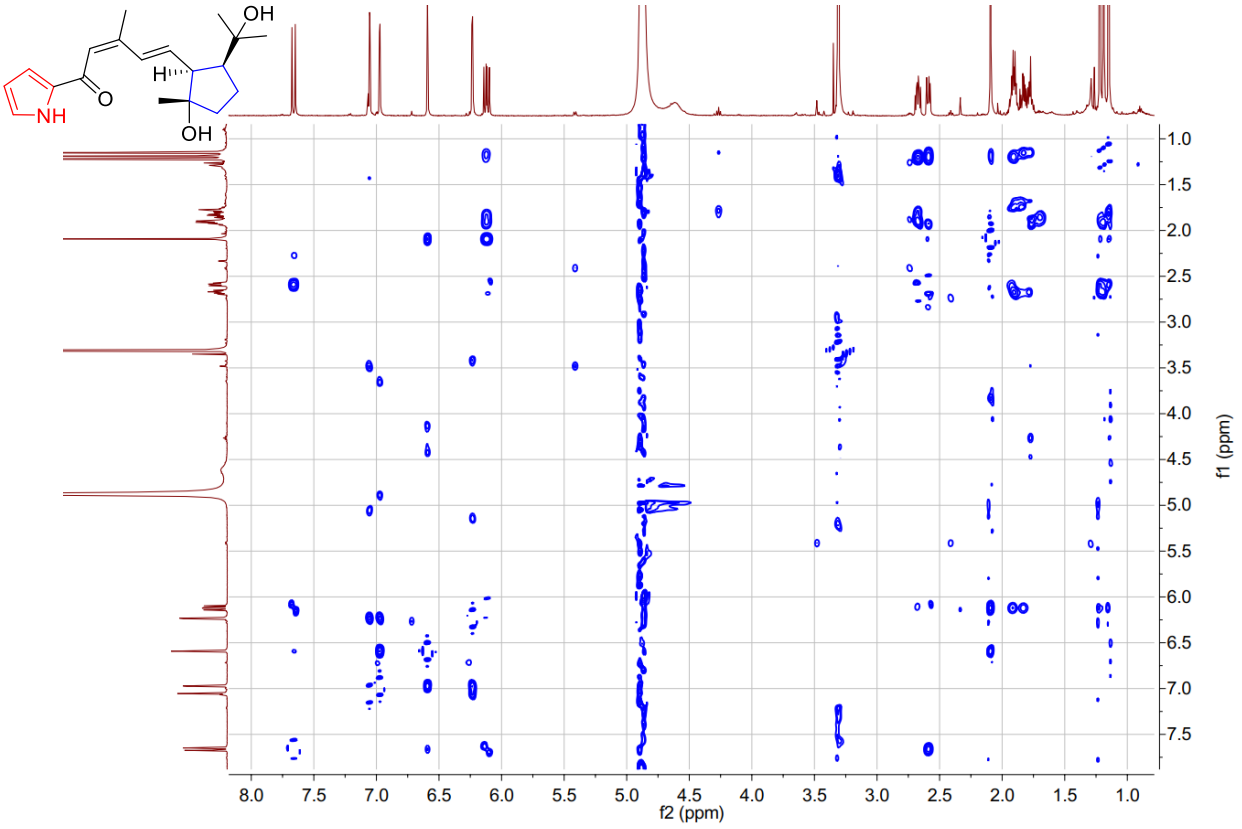
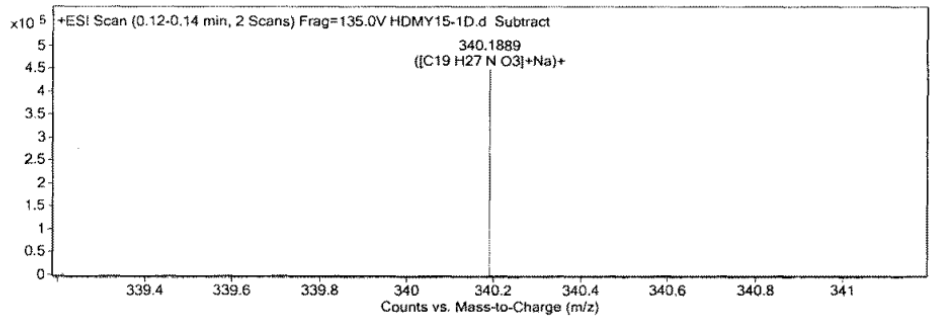


Figure S64. ROESY (600 MHz) spectrum of **4** in CD_3OD.

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

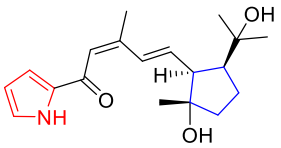


Peak List

m/z	z	Abund	Formula	Ion
300.1961	1	158351.17		
340.1889	1	448012.09	C19 H27 N O3	(M+Na)+
341.1923	1	100011.6	C19 H27 N O3	(M+Na)+
356.1711	1	170174.75		
625.3715	1	253442.86		
626.3744	1	101078.79		
641.3374	1	875264.19		
642.3411	1	321911.31		
657.3883	1	267952.41		
658.3915	1	117745.26		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	240
O	0	30
N	0	8



Chemical Formula: $C_{19}H_{27}NO_3$
Exact Mass: 317.1991

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C19 H27 N O3	317.1991	340.1883	340.1889	-0.60	-1.76	7.0000

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Figure S65. HR-ESI-MS spectrum of **4**.

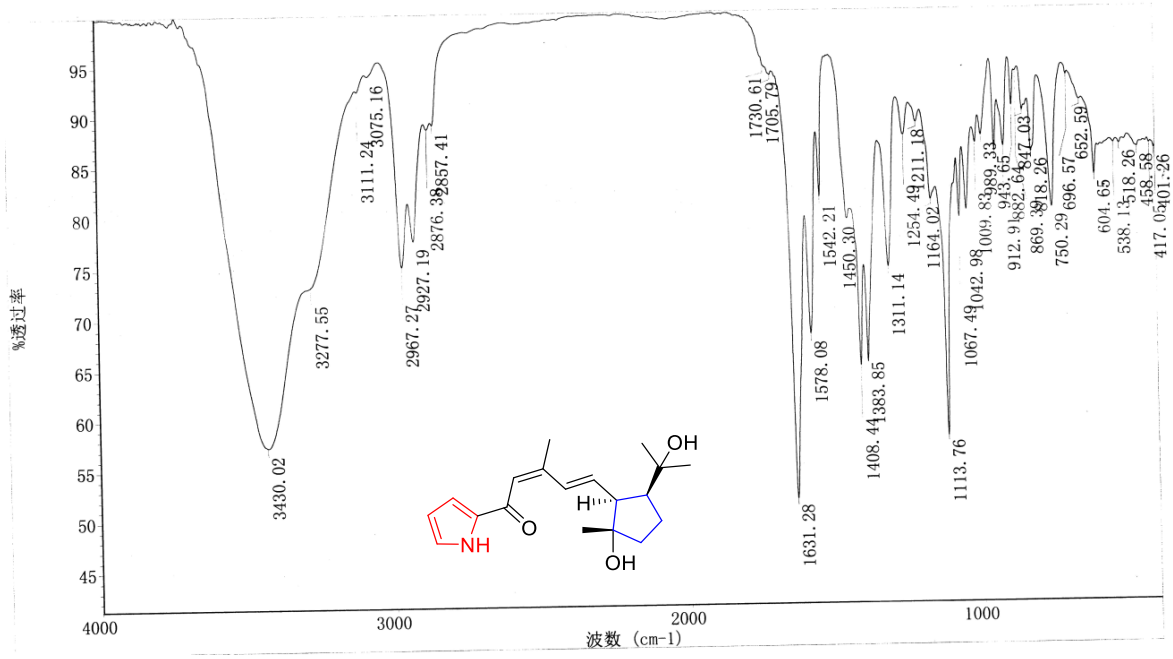

Figure S66. IR spectrum of **4**.

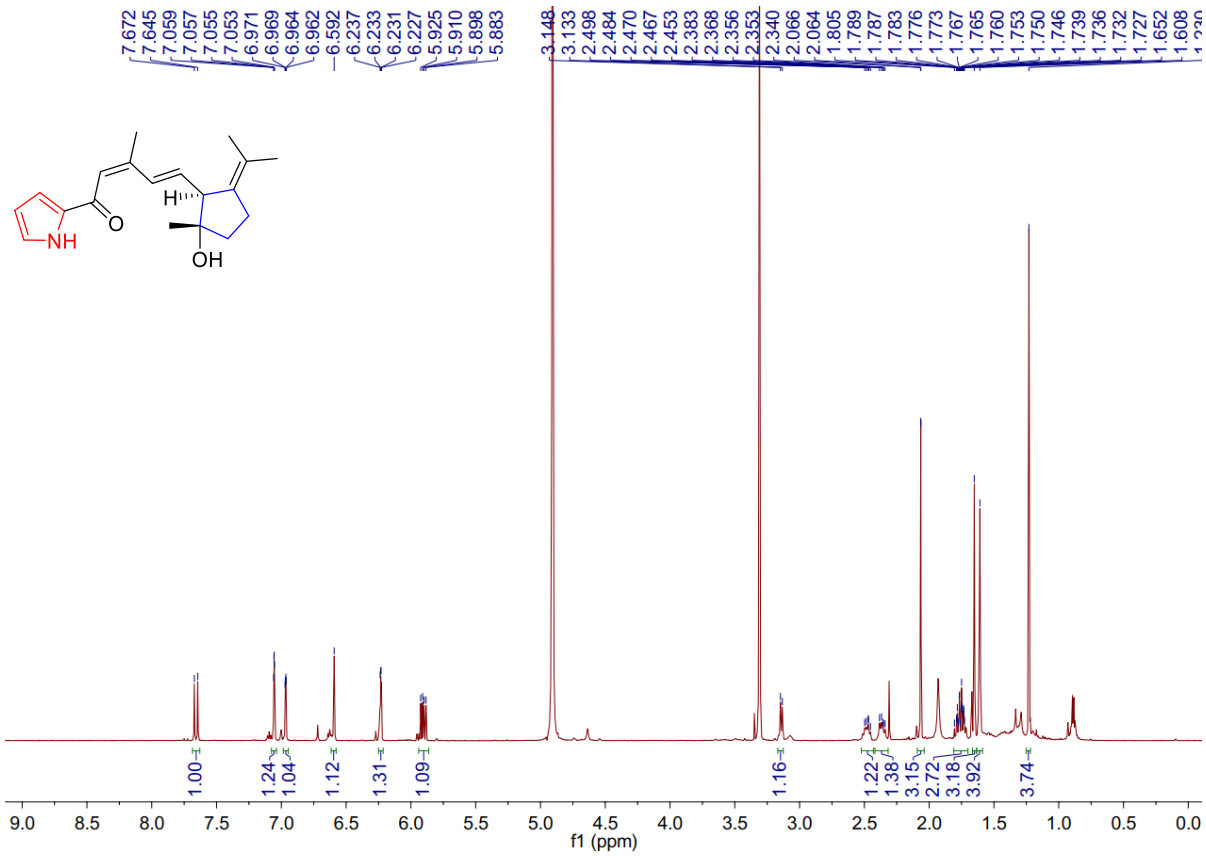

Figure S67. ^{1}H NMR (600 MHz) spectrum of **5** in CD_3OD.

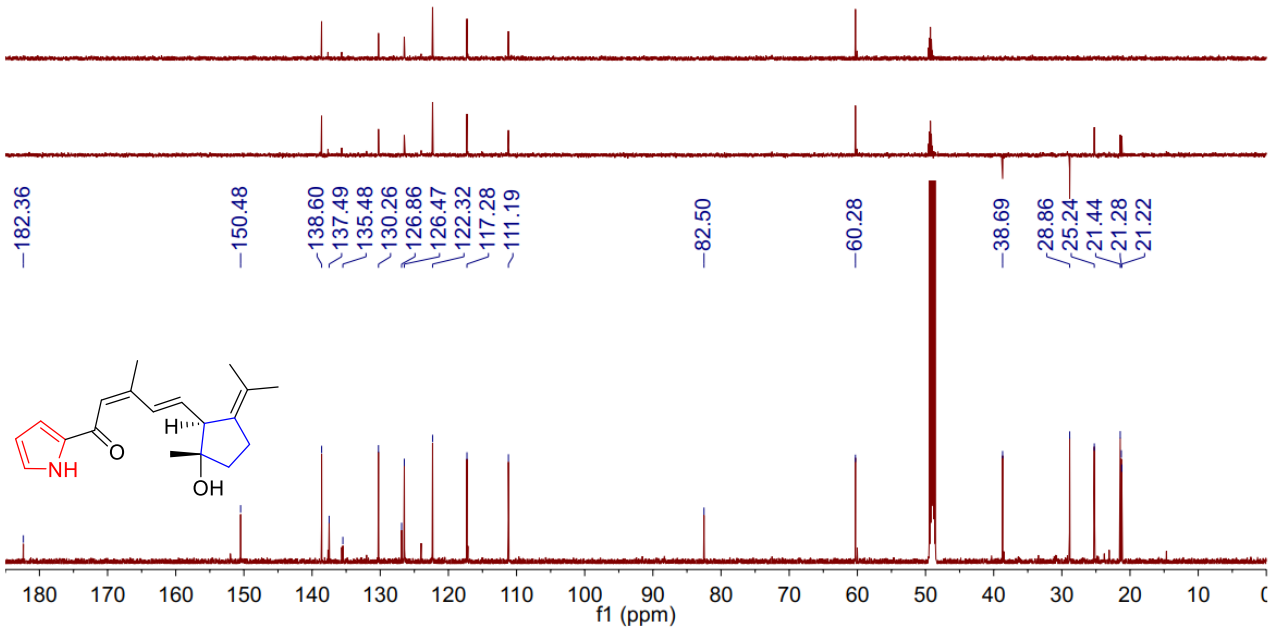

Figure S68. ^{13}C NMR (150 MHz) spectrum of **5** in CD_3OD.

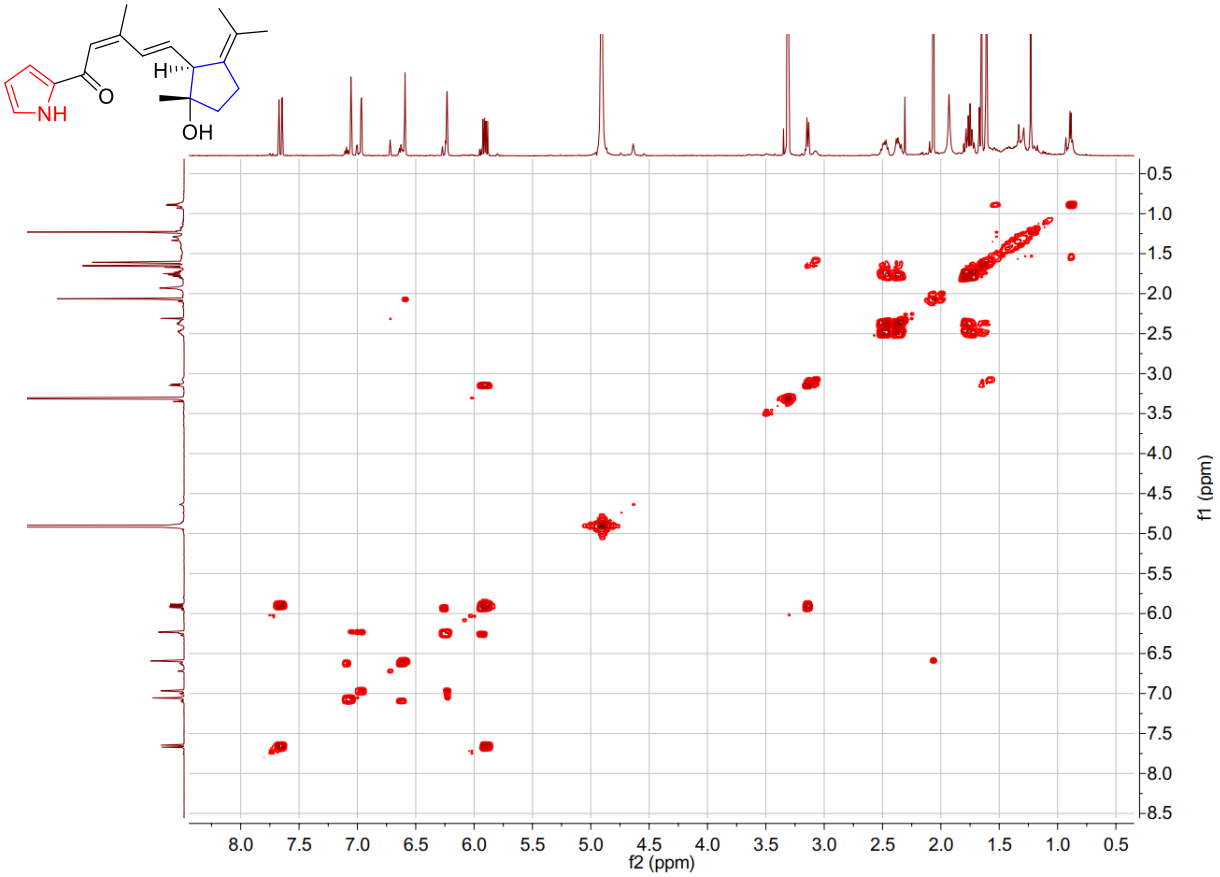

Figure S69. ^{1}H-^{1}H COSY (600 MHz) spectrum of **5** in CD_3OD.

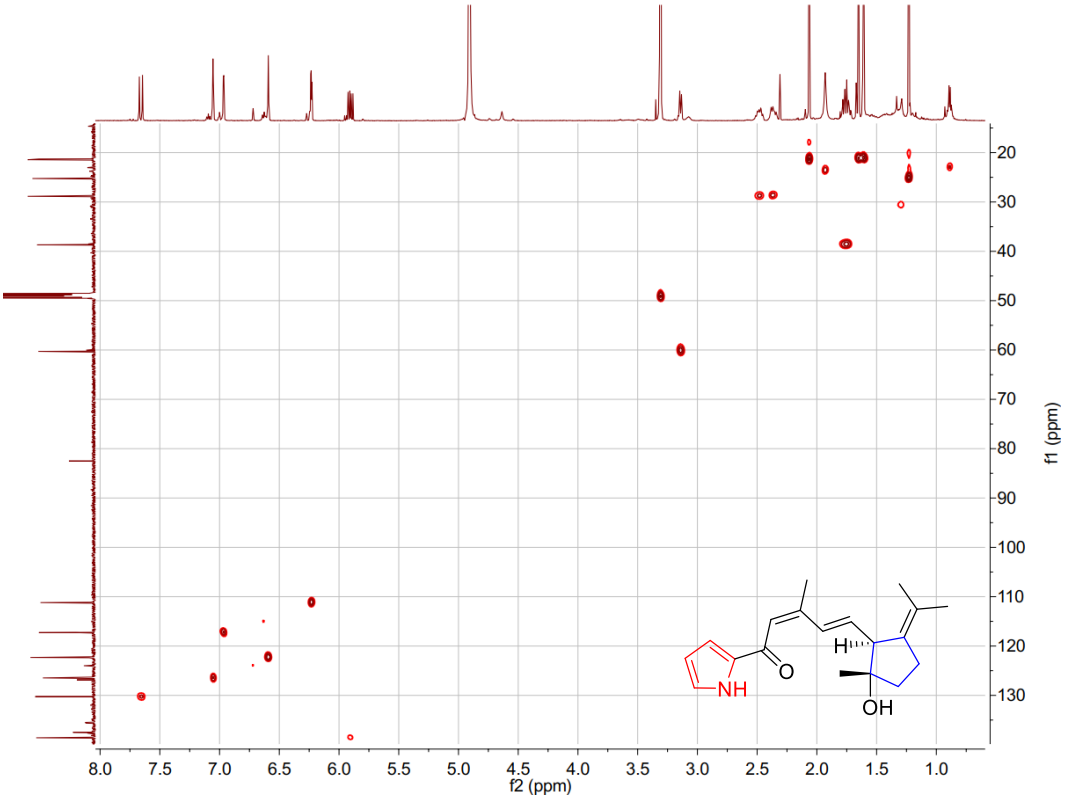

Figure S70. HSQC (600 MHz) spectrum of **5** in CD_3OD.

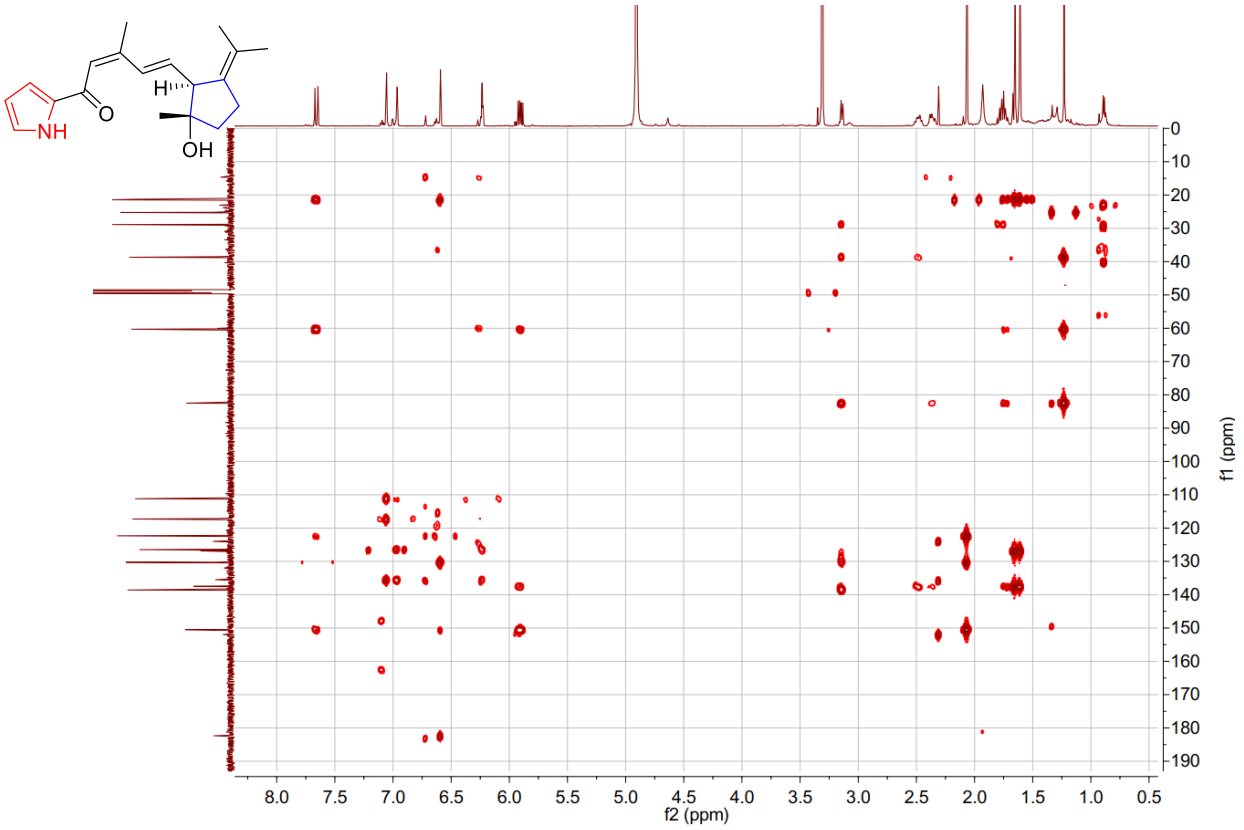

Figure S71. HMBC (600 MHz) spectrum of **5** in CD_3OD.

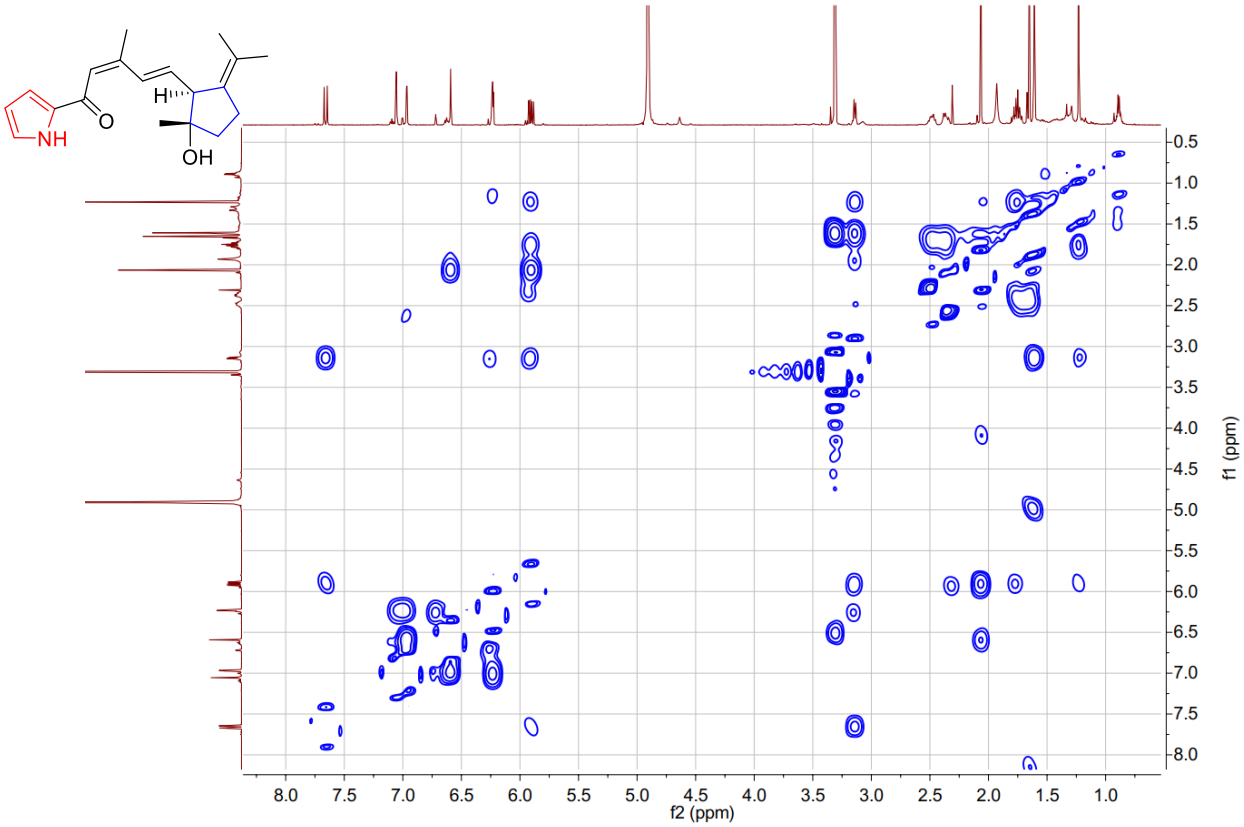

Figure S72. ROESY (600 MHz) spectrum of **5** in CD_3OD.

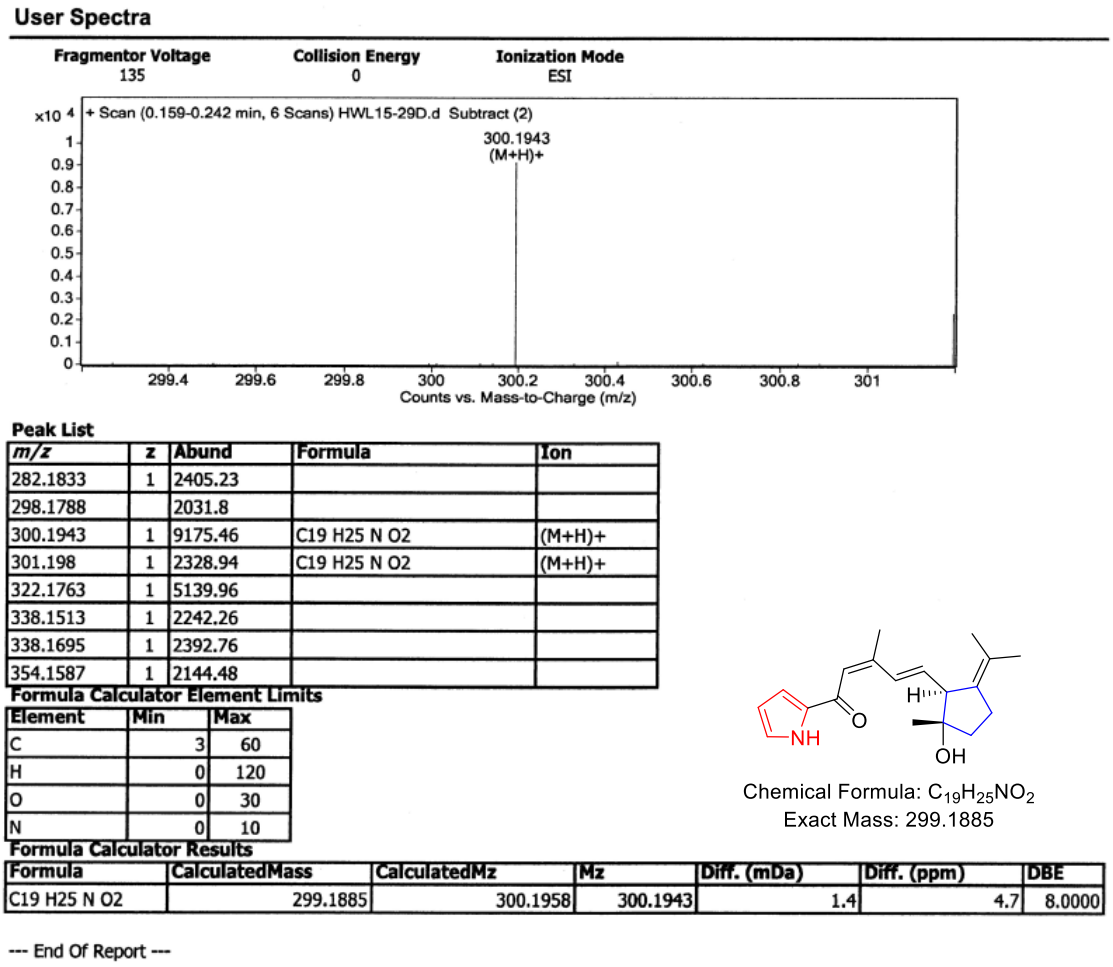

Figure S73. HR-ESI-MS spectrum of **5**.

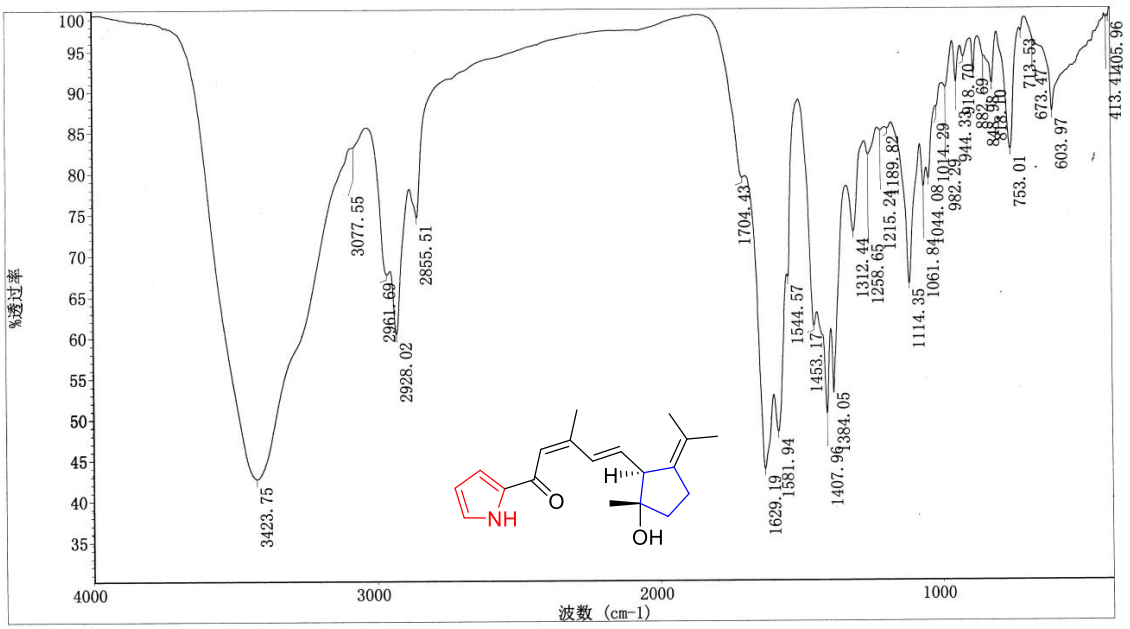

Figure S74. IR spectrum of **5**.