

Electronic Supplementary Information for

Dysohonin A, a Meroditerpenoid Incorporating a 6,15,6-Fused Heterotricyclic Ring System from *Dysoxylum hongkongense*

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Bioassays

PTP1B Inhibitory Activity Assay. The PTP1B inhibitory activity was measured according to the reported protocol.¹

Cytotoxicity Assay. The cytotoxicity activities were evaluated against HL-60 and A-549 cell lines by an MTT method² and the SRB protein staining method,³ respectively.

References

1. W. Zhang, D. Hong, Y. Zhou, Y. Zhang, Q. Shen, J. Y. Li, L. H. Hu and J. Li, *Biochim. Biophys. Acta*, 2006, **1760**, 1505–1512.
2. D. Xiao, S. P. Zhu and Z. L. Gu, *Acta Pharmacol. Sin.*, 1997, **18**, 280–283.
3. P. Skehan, R. Storeng, D. Scudiero, A. Monks, J. McMahon, D. Vistica, J. T. Warren, H. Bokesch, S. Kenney and M. R. Boyd, *J. Natl. Cancer Inst.*, 1990, **82**, 1107–1112.

Figure S1. Selected 2D NMR correlations for **3**

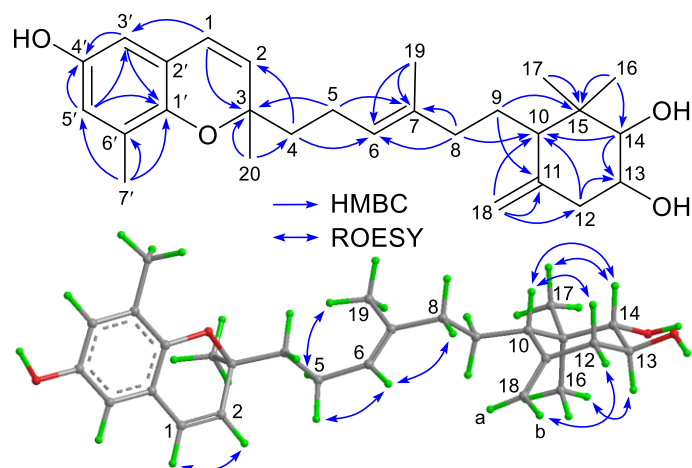


Figure S2. Selected 2D NMR correlations for **4**

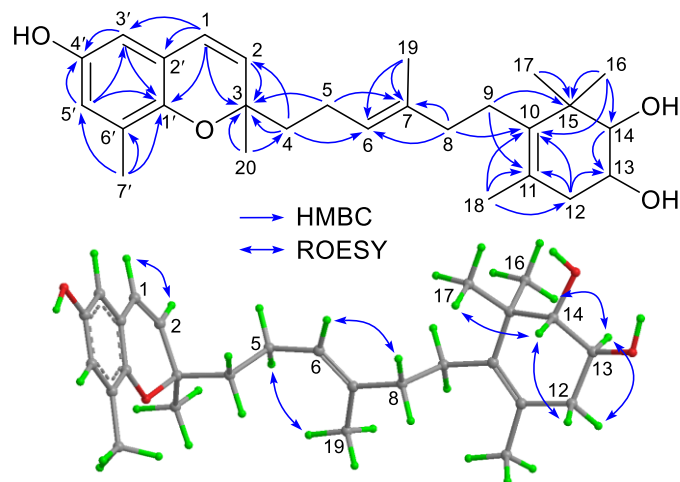


Figure S3. CD spectra of **4** and in situ formed Mo-complex of **4** recorded in DMSO (the *R* configuration of C-3 was determined by the negative Cotton effect at 278 nm)

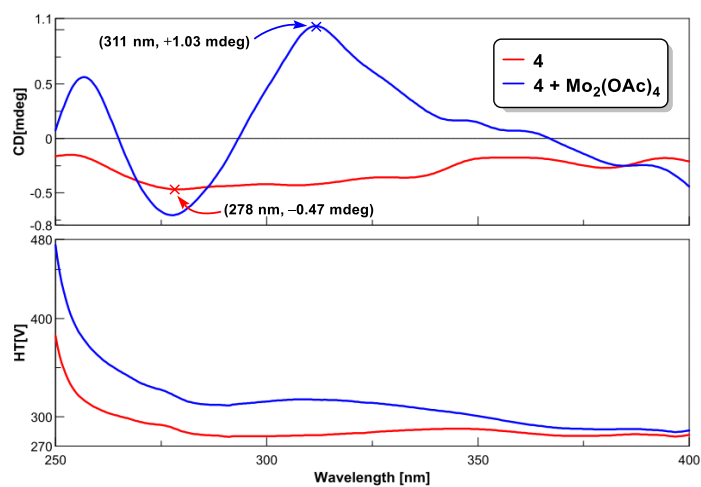


Figure S4. UV spectrum of **1**

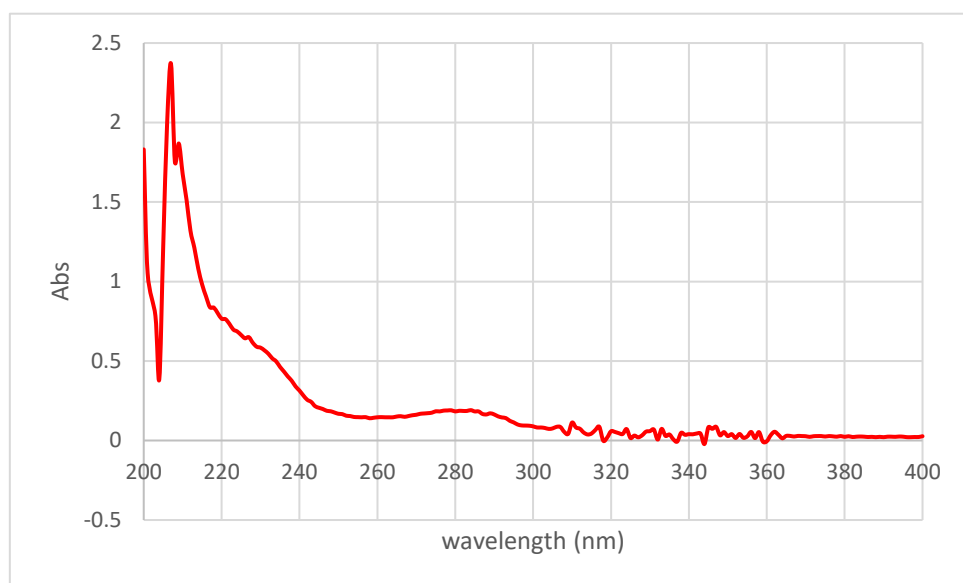


Figure S5. UV spectrum of **2**

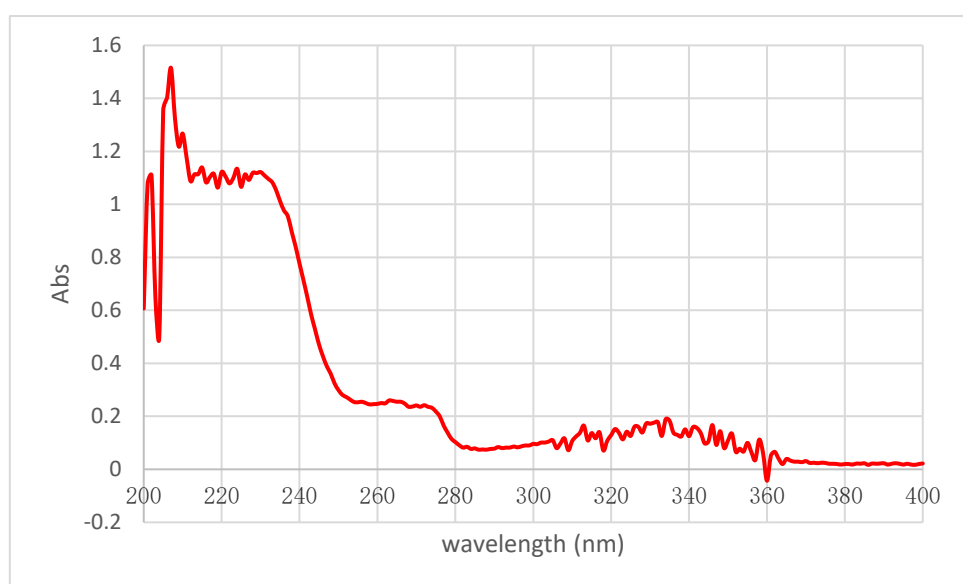


Figure S6. UV spectrum of **3**

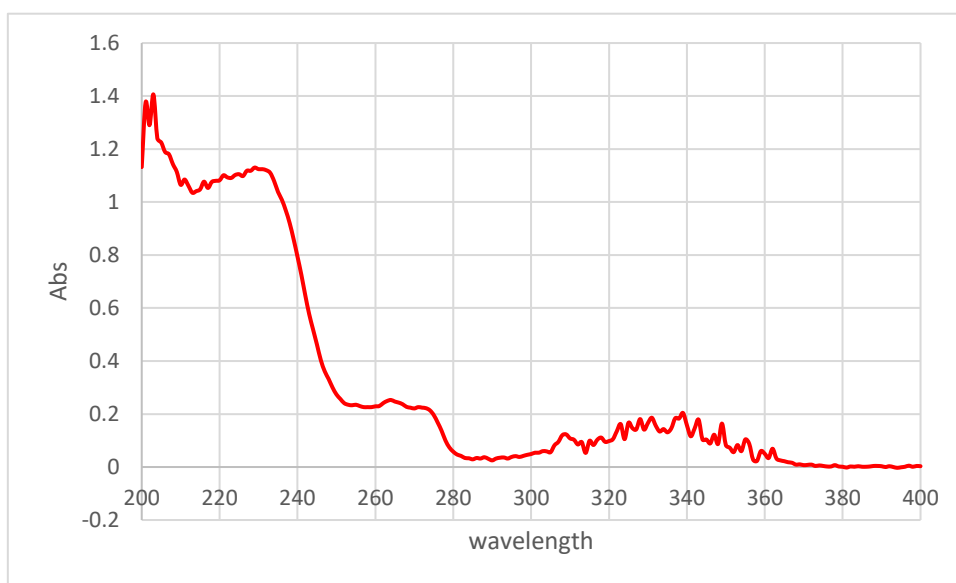


Figure S7. UV spectrum of **4**

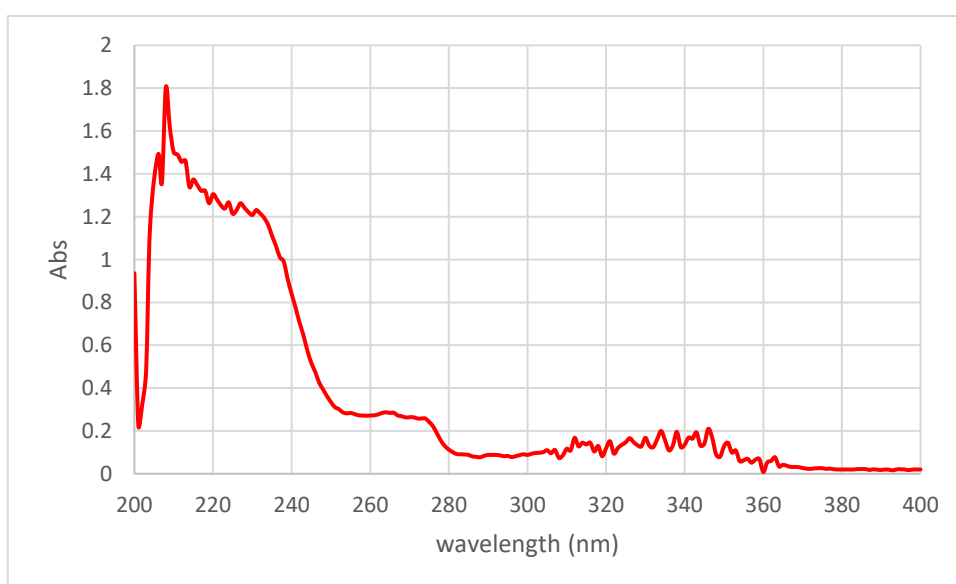


Figure S8. ^1H NMR spectra of **1**

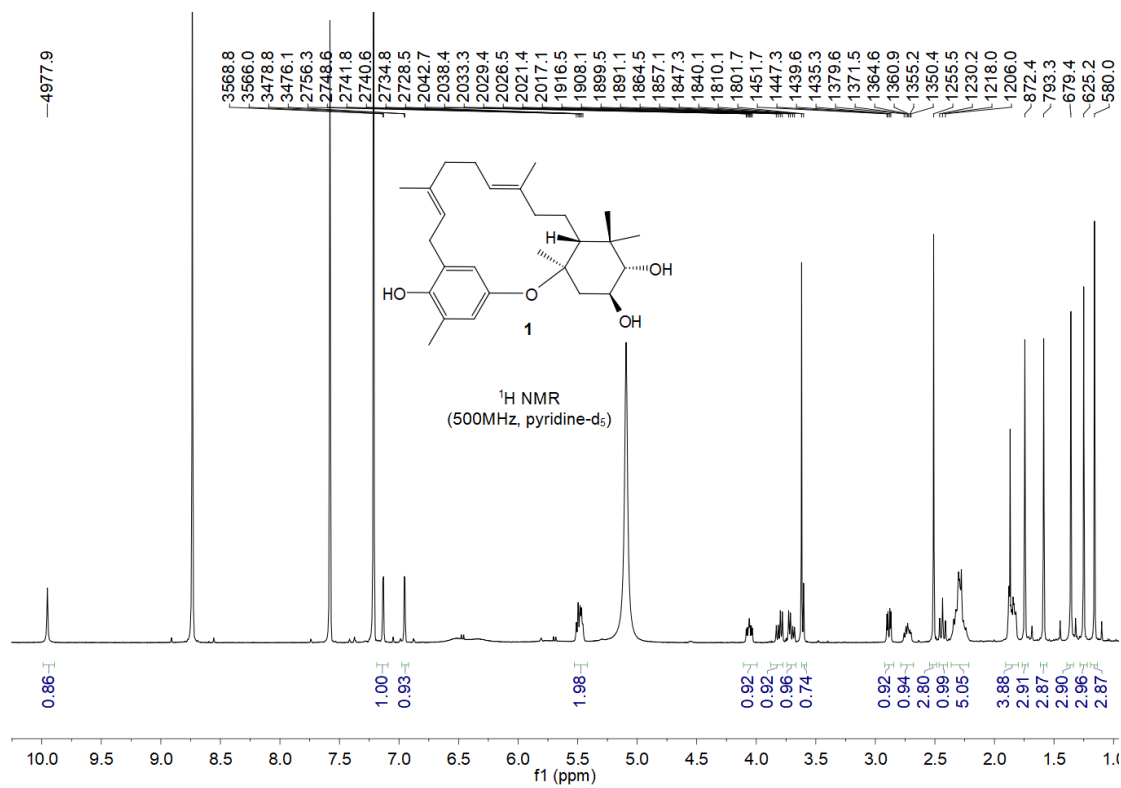
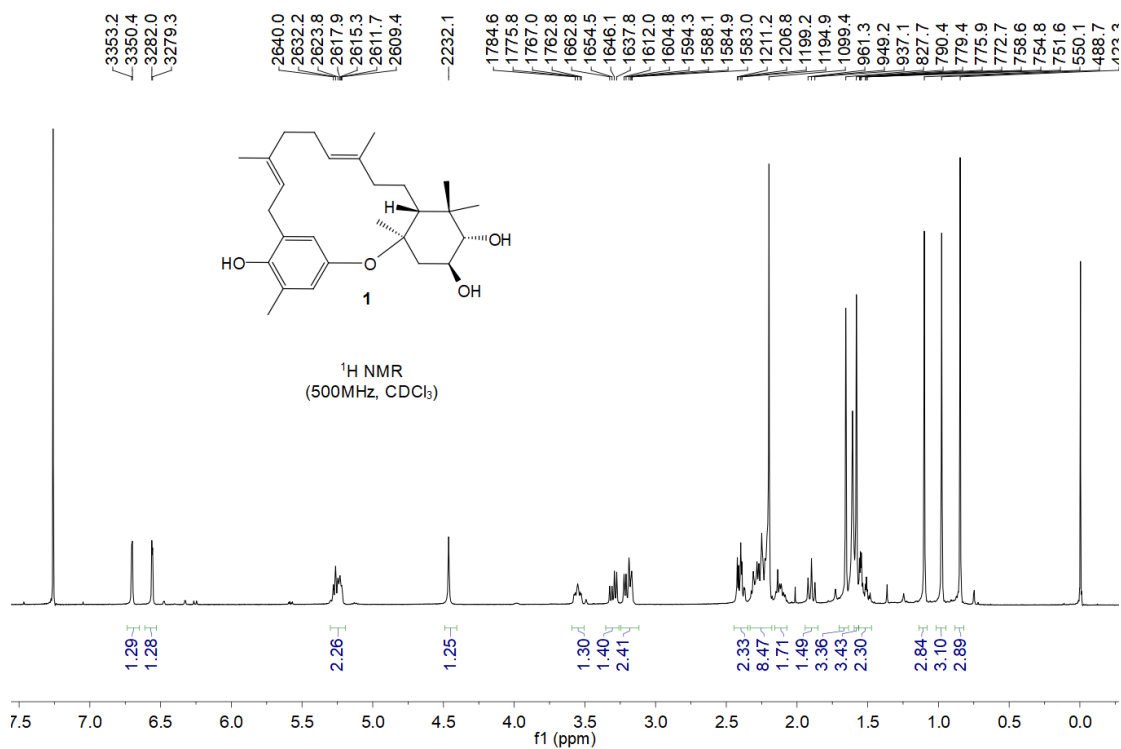


Figure S9. ^{13}C NMR spectra of **1**

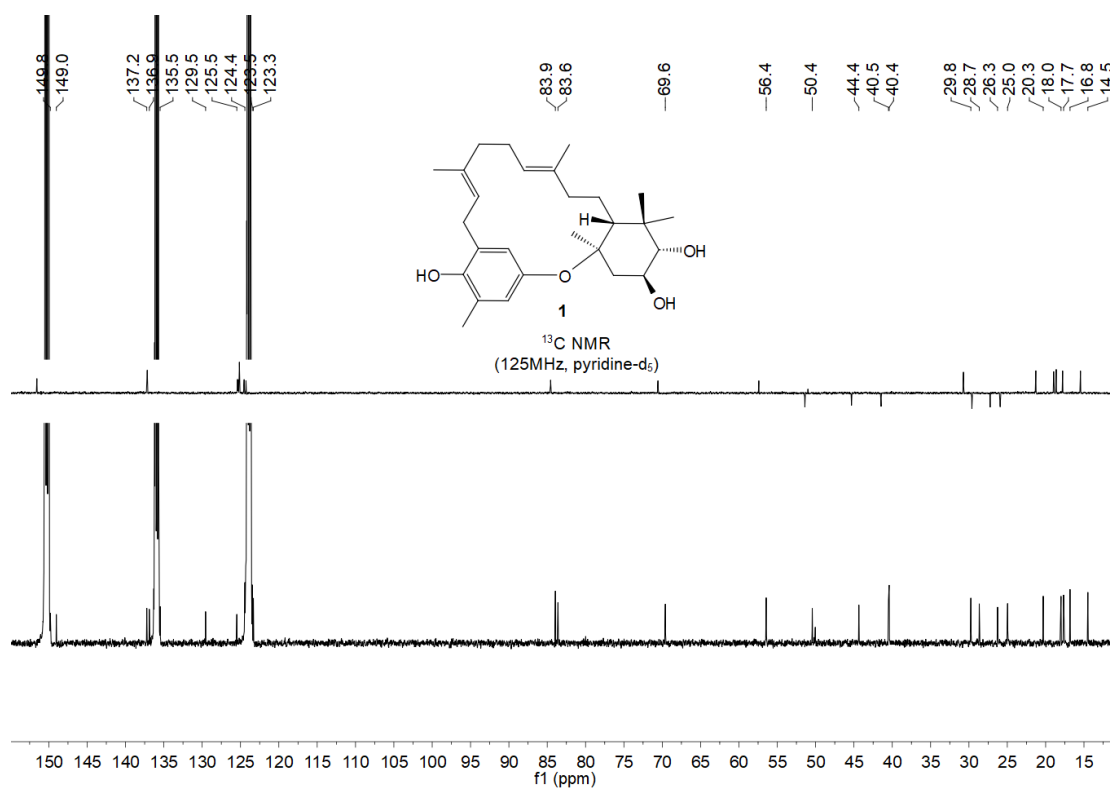
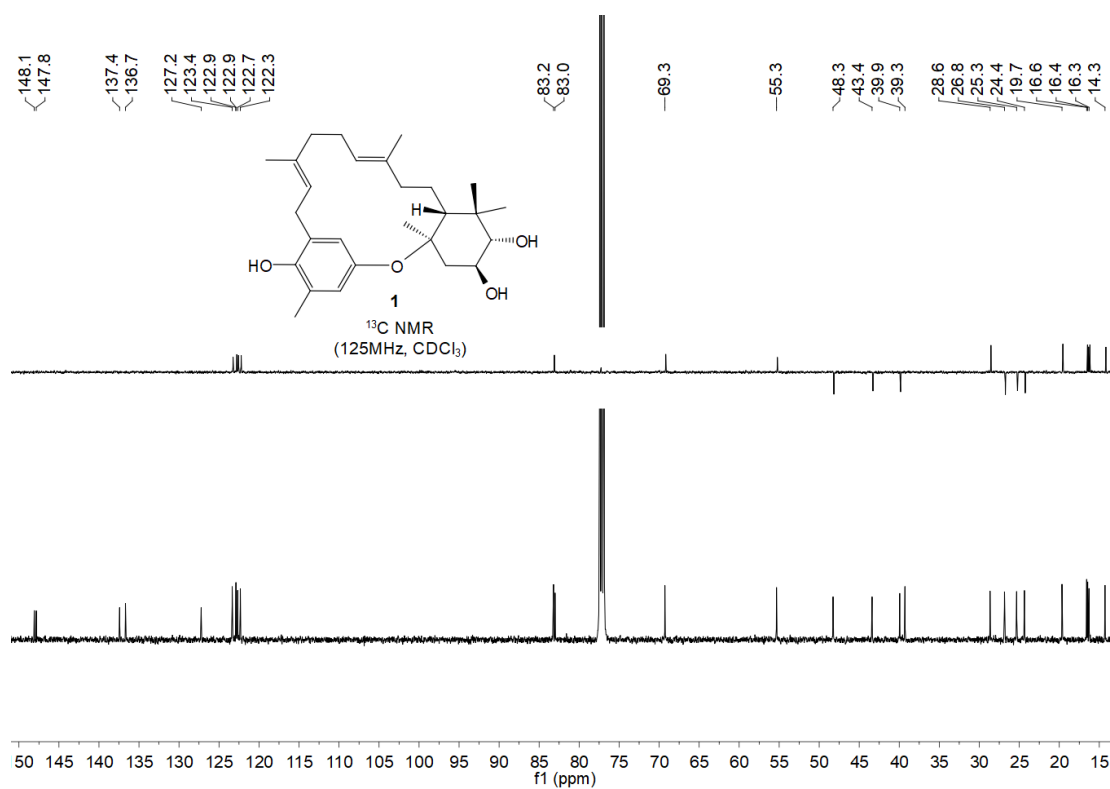


Figure S10. HSQC spectra of **1**

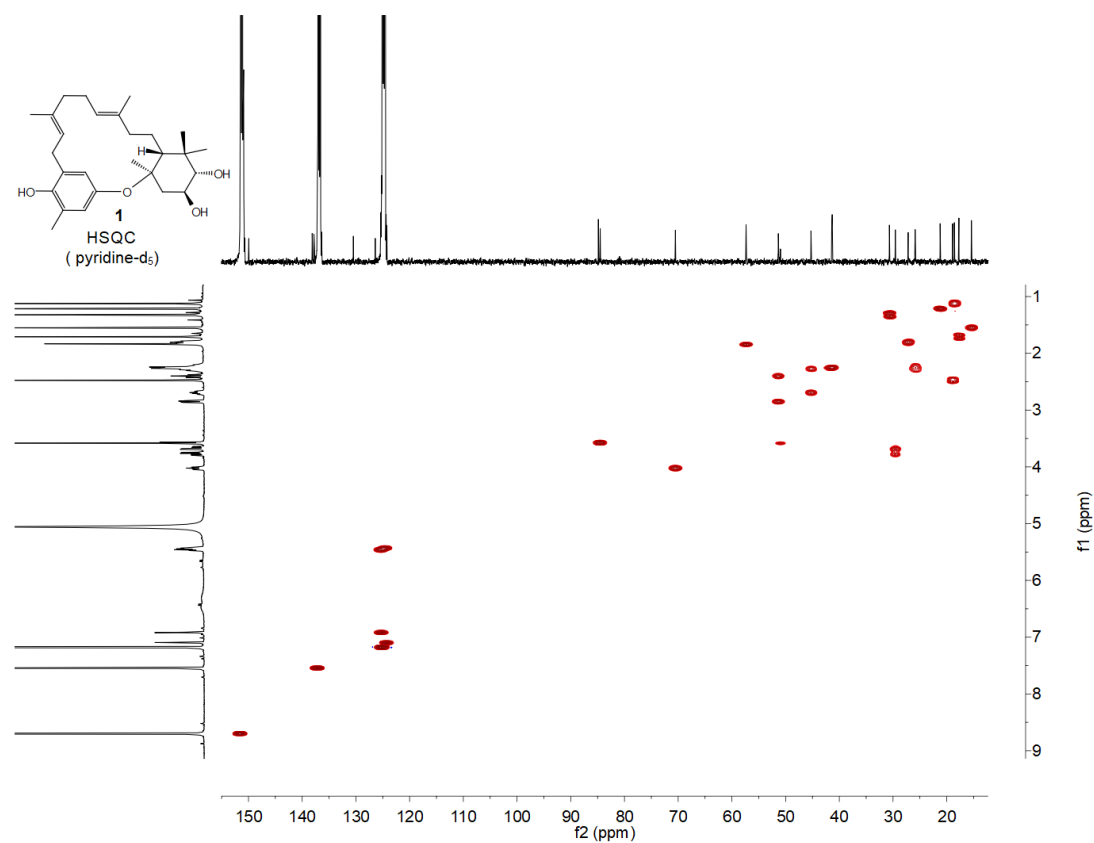
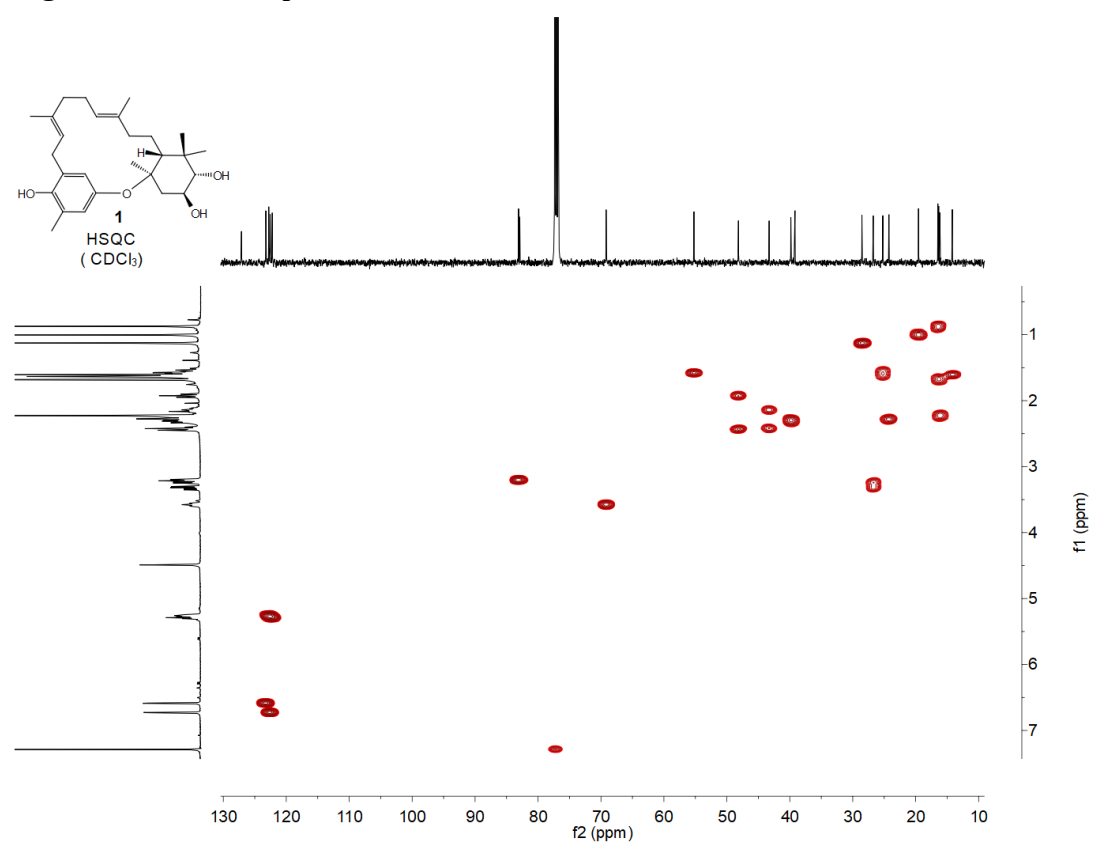


Figure S11. HMBC spectra of **1**

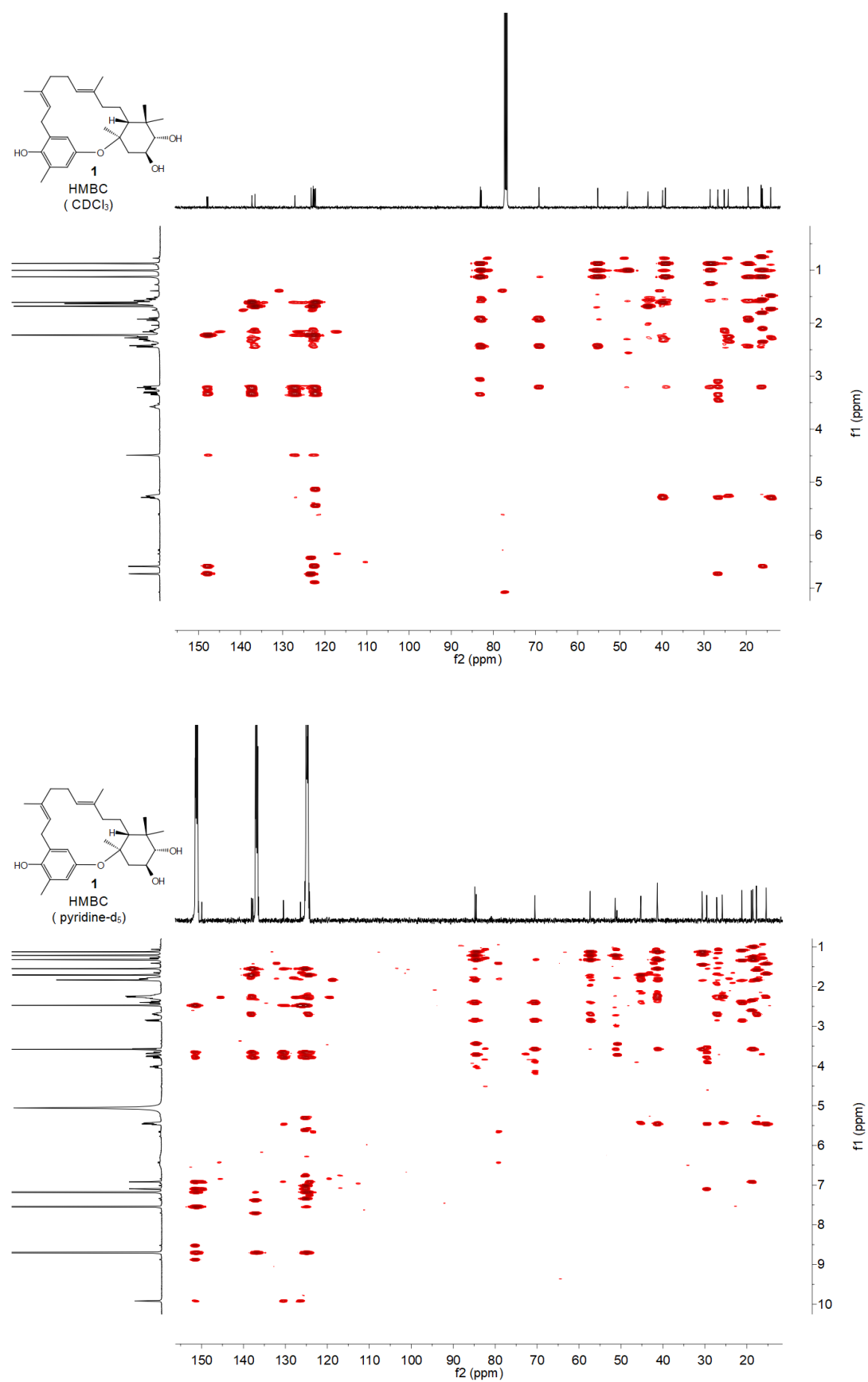


Figure S12. ^1H - ^1H COSY spectrum of **1**

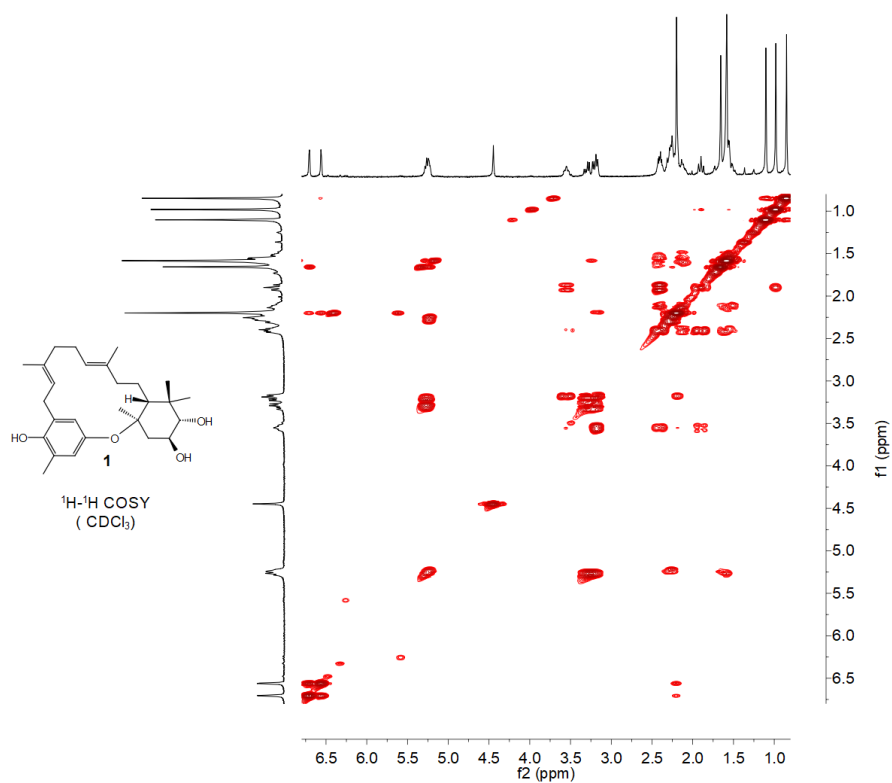


Figure S13. ROESY spectrum of **1**

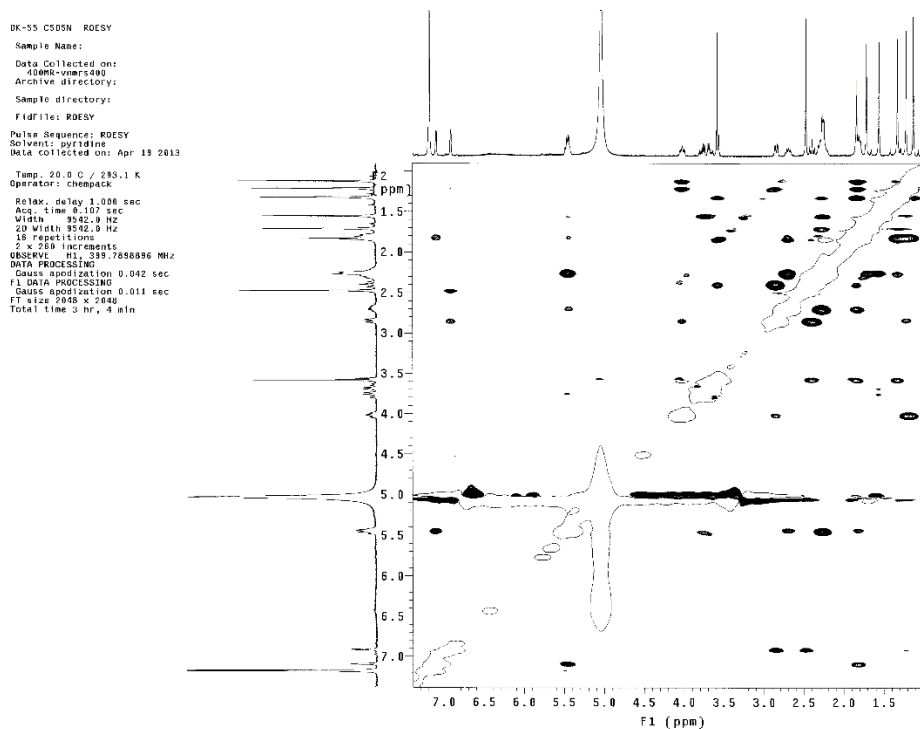


Figure S14. (+)-ESIMS spectrum of **1**

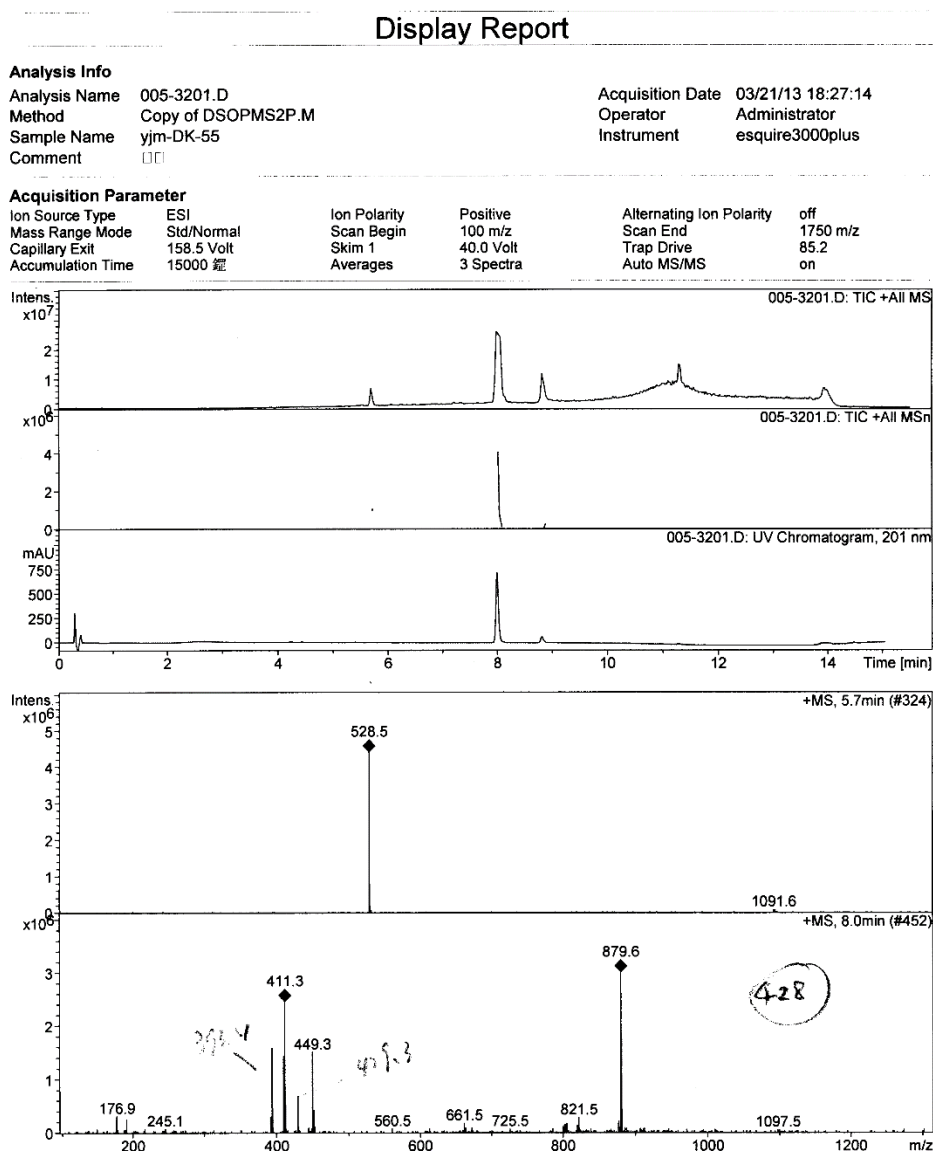


Figure S15. (-)-ESIMS spectrum of 1

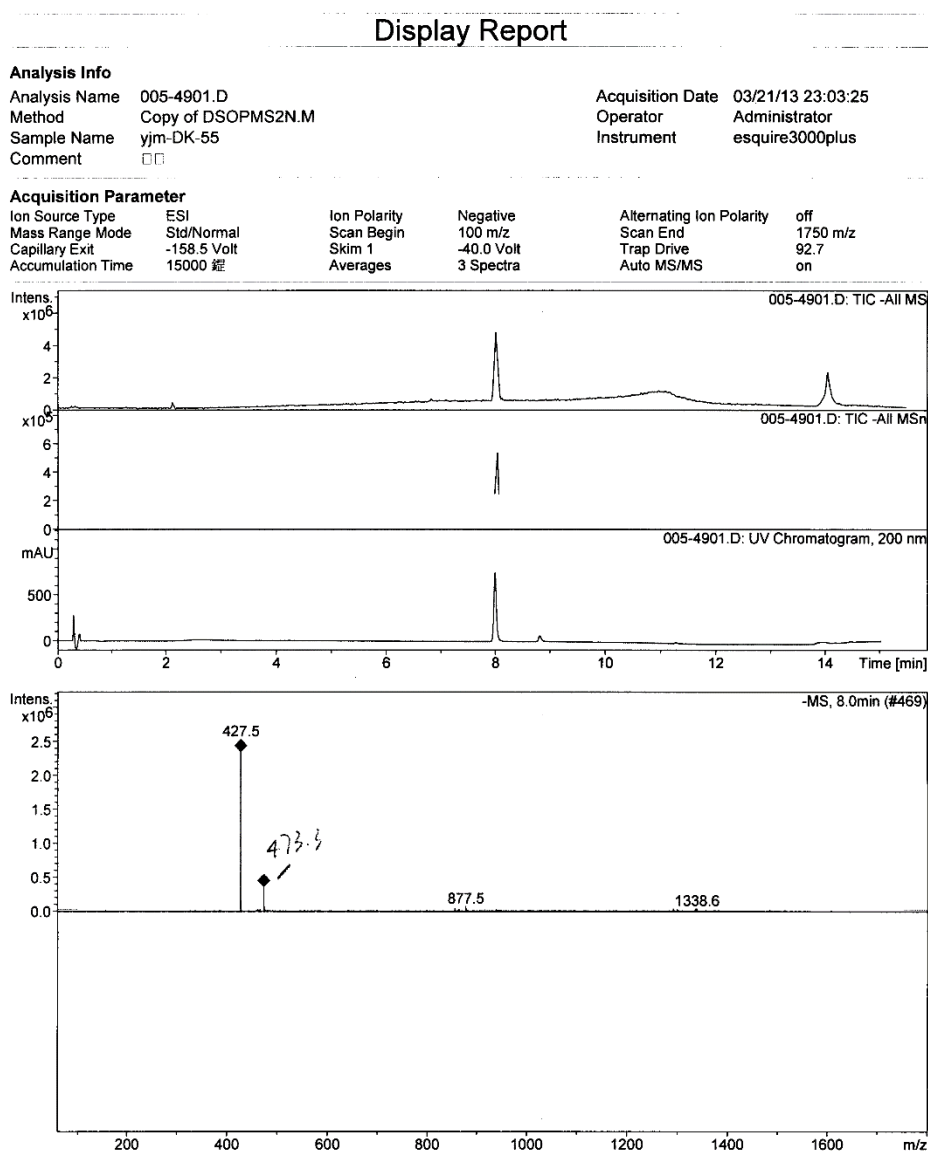


Figure S16. (-)-HRESIMS spectrum of 1

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

183 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 6-80 H: 2-120 N: 0-1 O: 0-20

DK-55

LCT PXE KE324

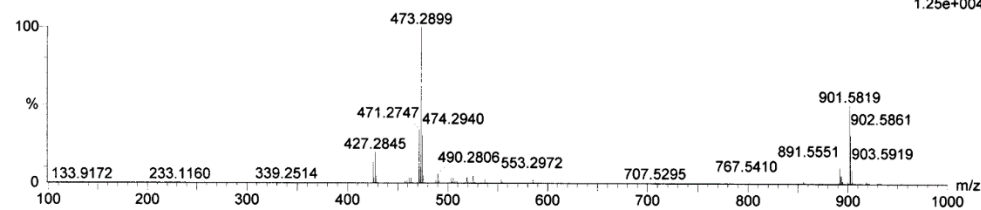
28-Mar-2013

10:16:57

1: TOF MS ES-

1.25e+004

DK-55_0328 13 (0.300) AM2 (Ar, 10000.0, 0.00, 1.00); ABS; Cm (13:28)



Minimum:

Maximum:

3.0

5.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

i-FIT (Norm)

Formula

473.2899

473.2903

-0.4

-0.8

8.5

69.0

0.0

C28 H41 O6

Figure S17. IR spectrum of 1

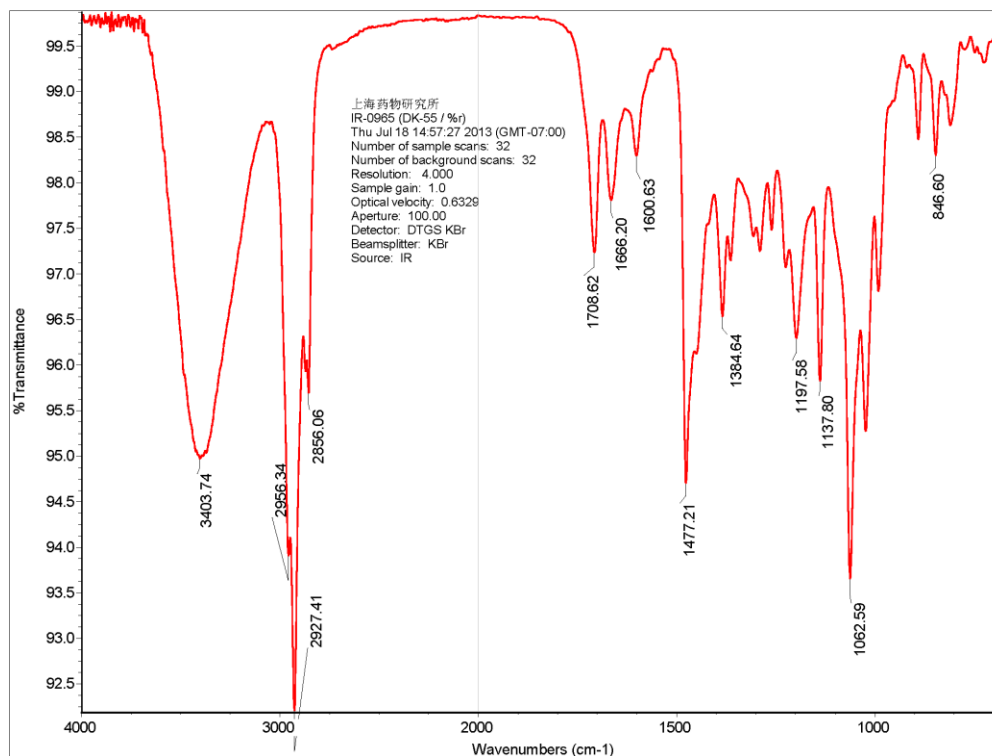


Figure S18. ^1H NMR spectrum of **2**

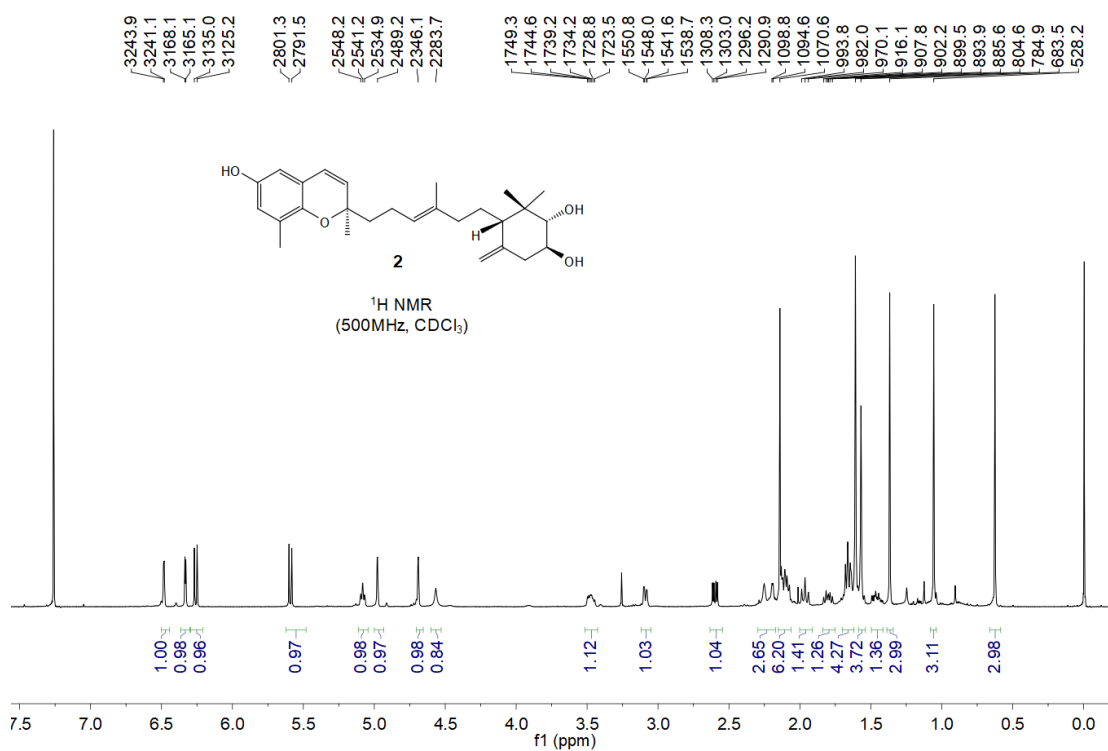


Figure S19. ^{13}C NMR spectrum of **2**

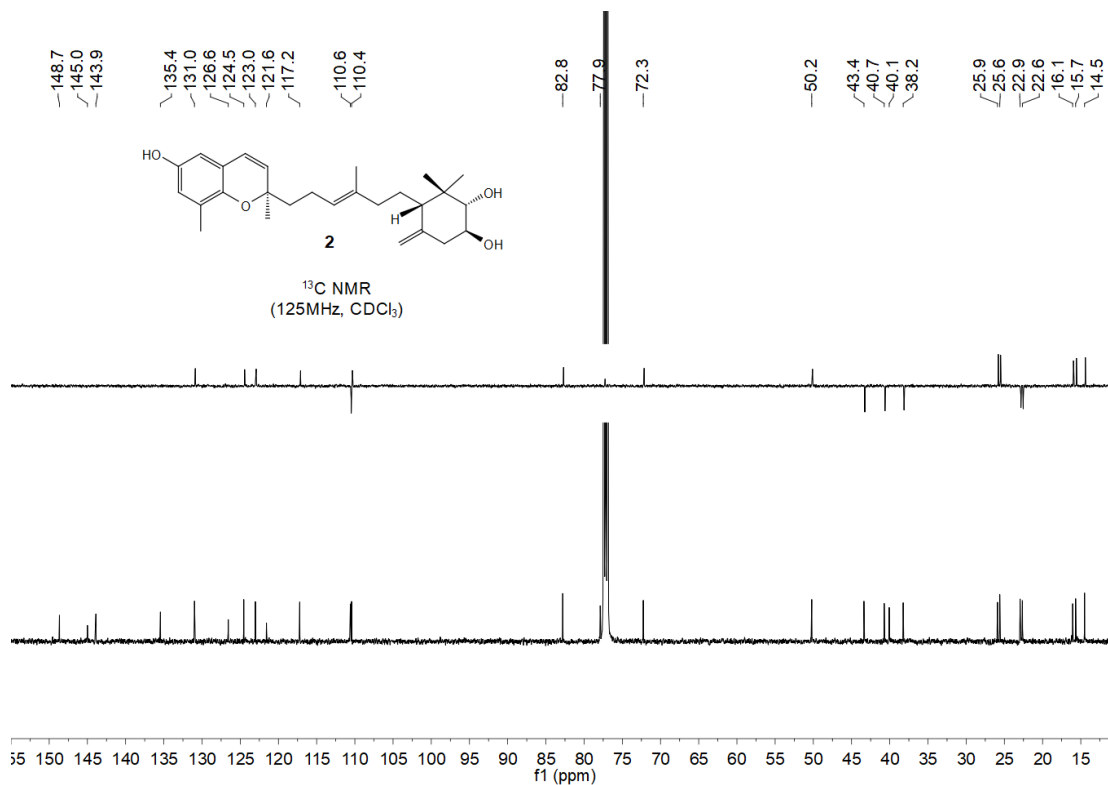


Figure S20. HSQC spectrum of **2**

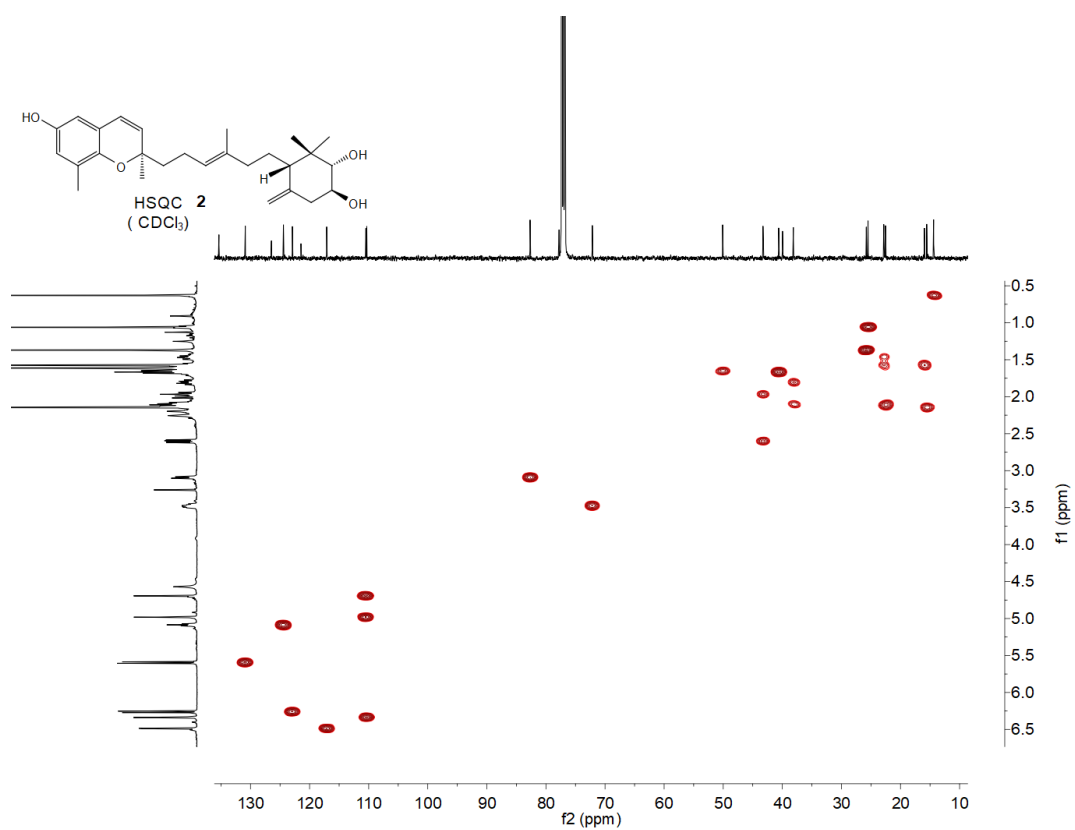


Figure S21. HMBC spectrum of **2**

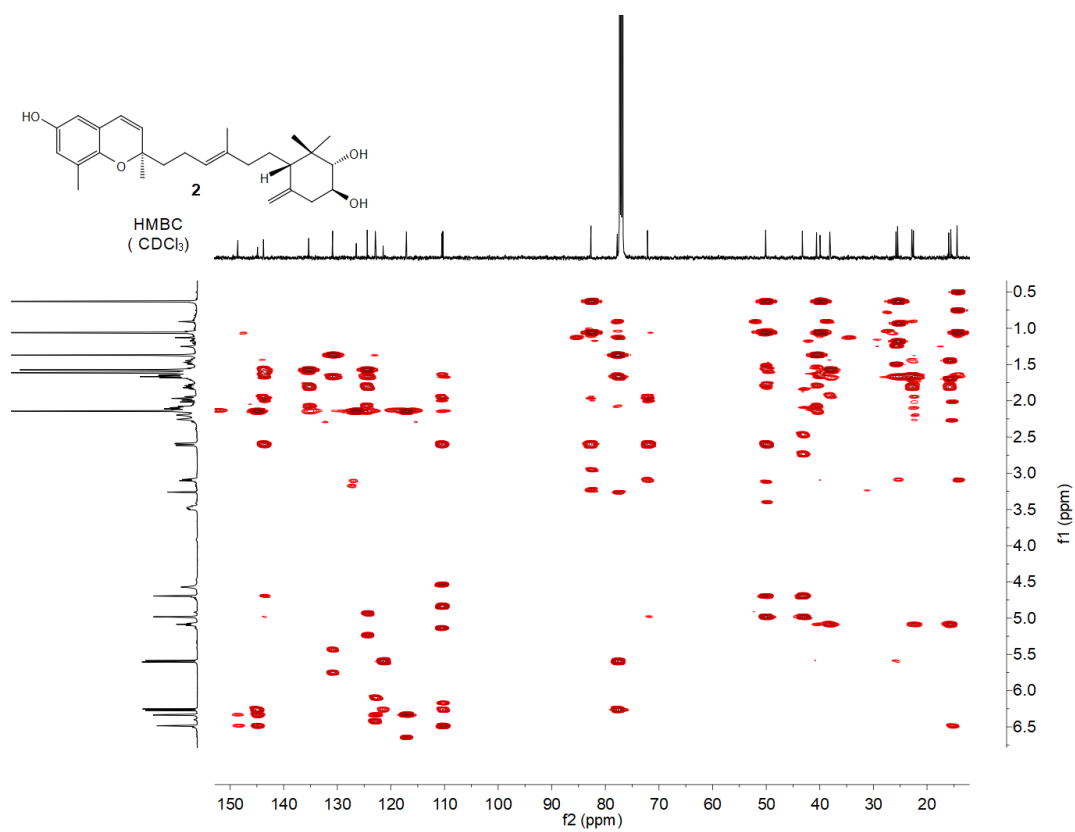


Figure S22. ROESY spectrum of **2**

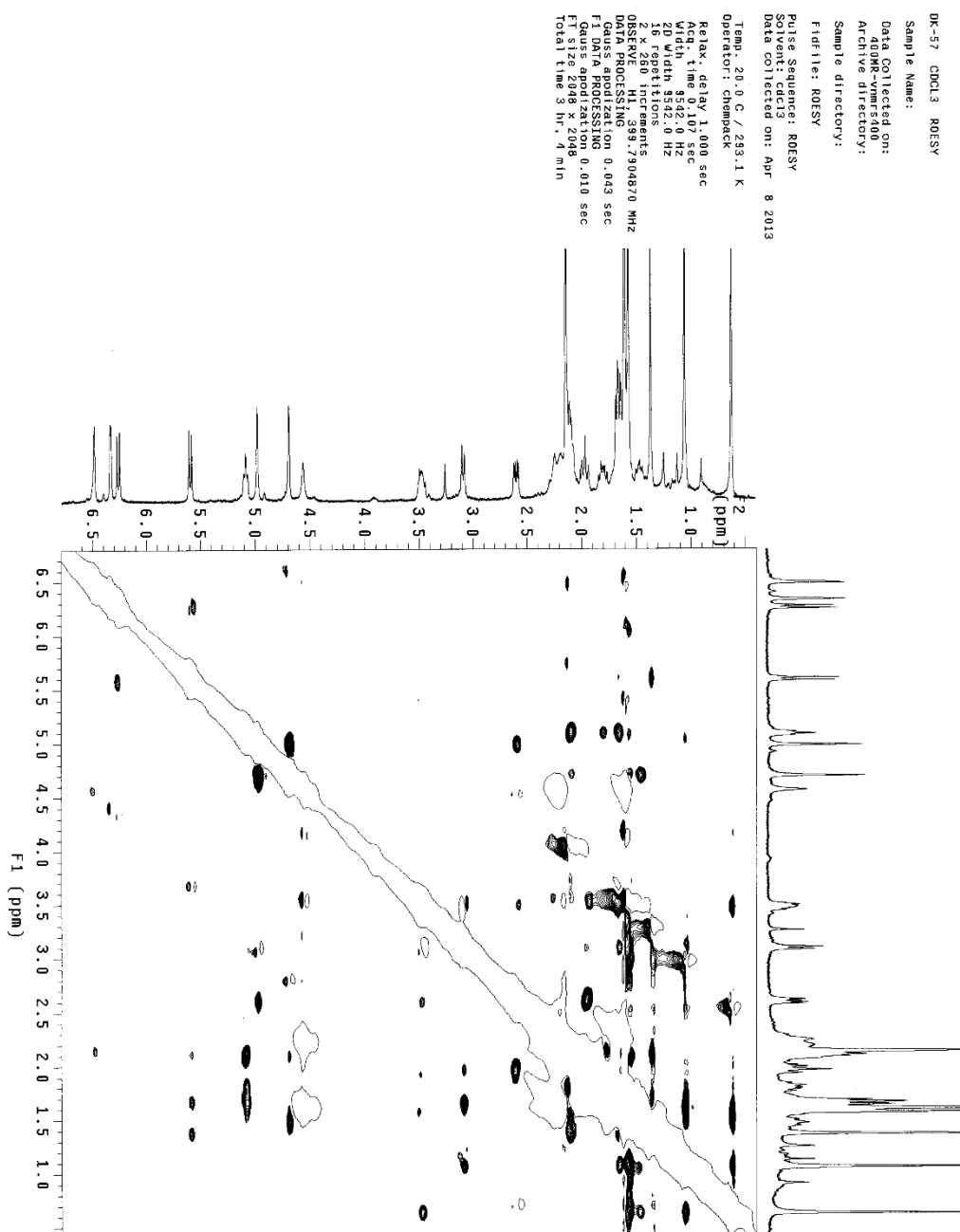


Figure S23. (+)-ESIMS spectrum of 2

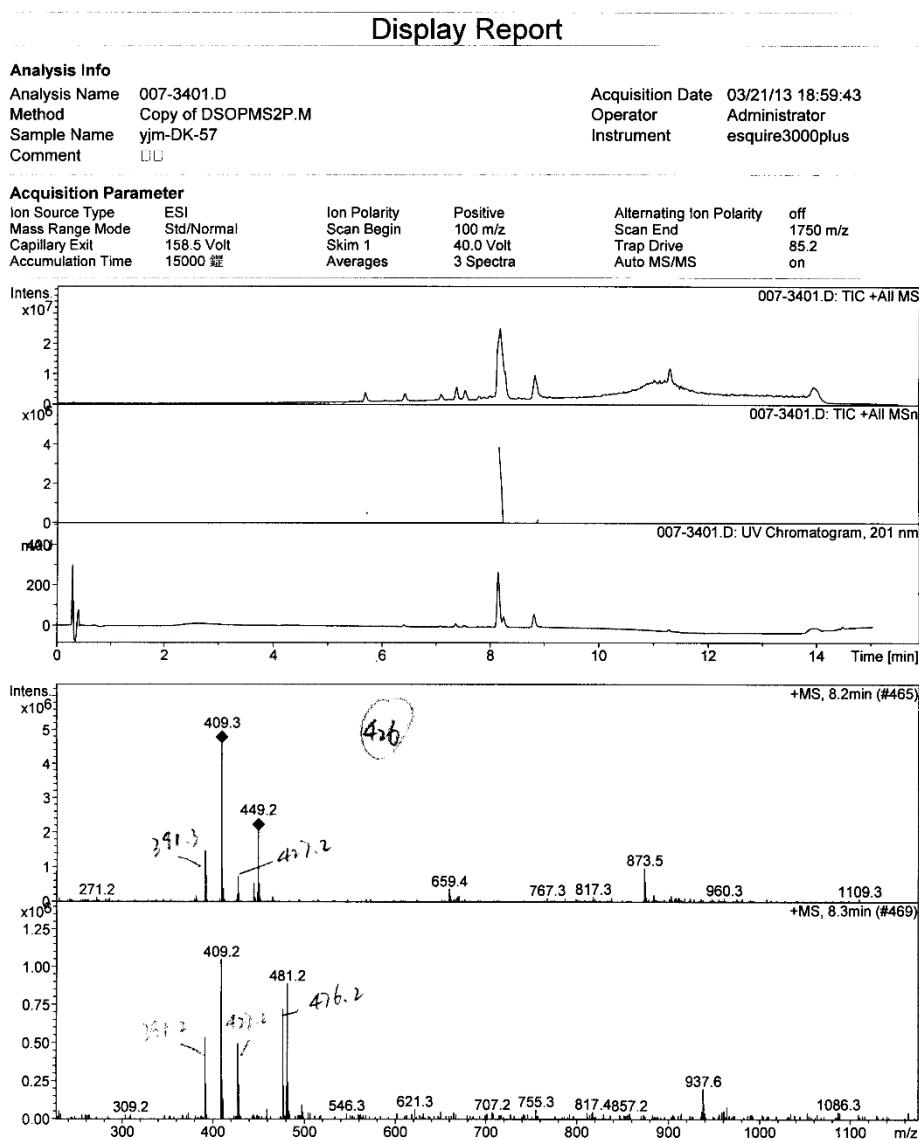


Figure S24. (-)-ESIMS spectrum of 2

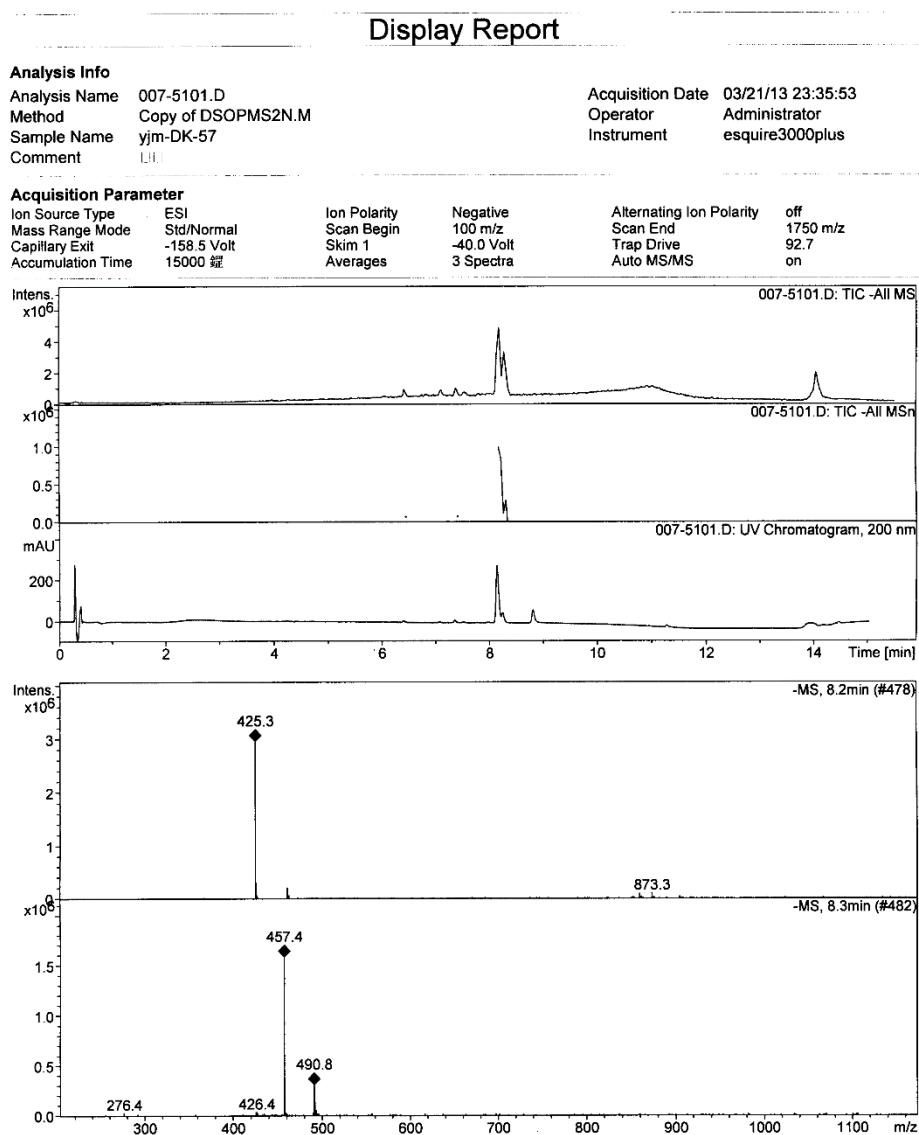


Figure S25. (-)-HRESIMS spectrum of 2

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

160 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 6-80 H: 2-120 N: 0-1 O: 0-20

DK-57

LCT PXE KE324

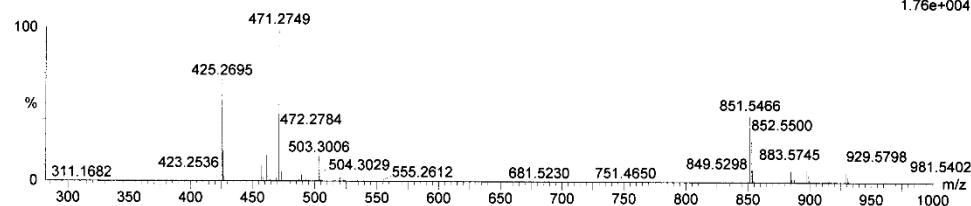
28-Mar-2013

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1: TOF MS ES-

1.76e+004



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
425.2695	425.2692	0.3	0.7	9.5	70.1	0.0	C27 H37 O4

Figure S26. IR spectrum of 2

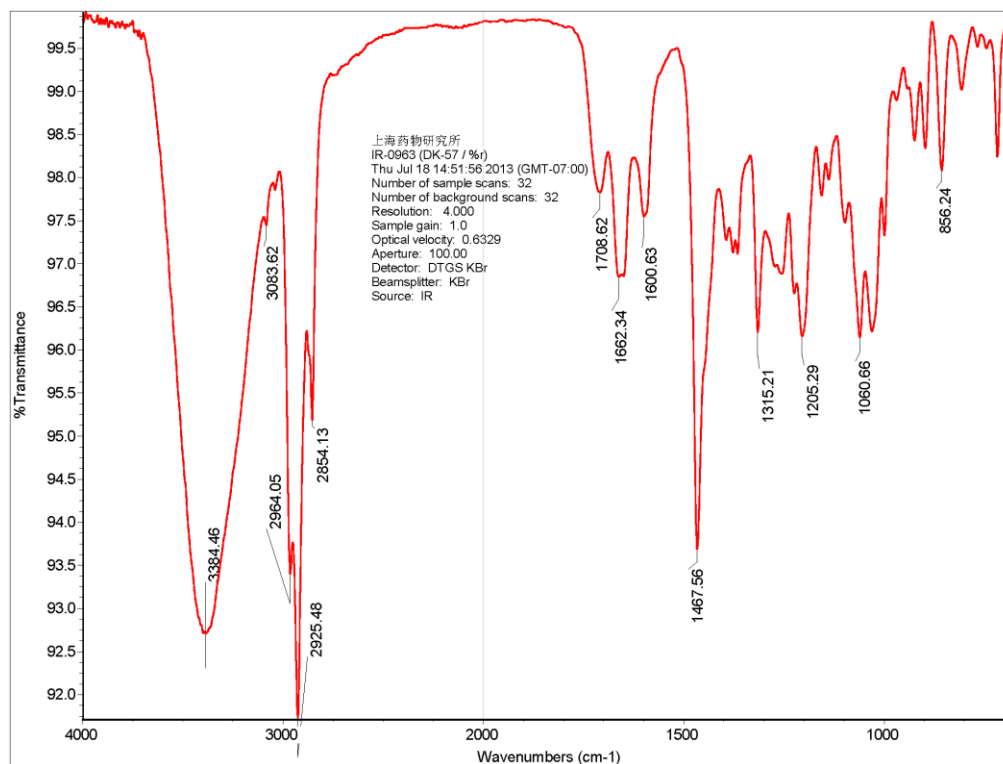


Figure S27. ^1H NMR spectrum of **3**

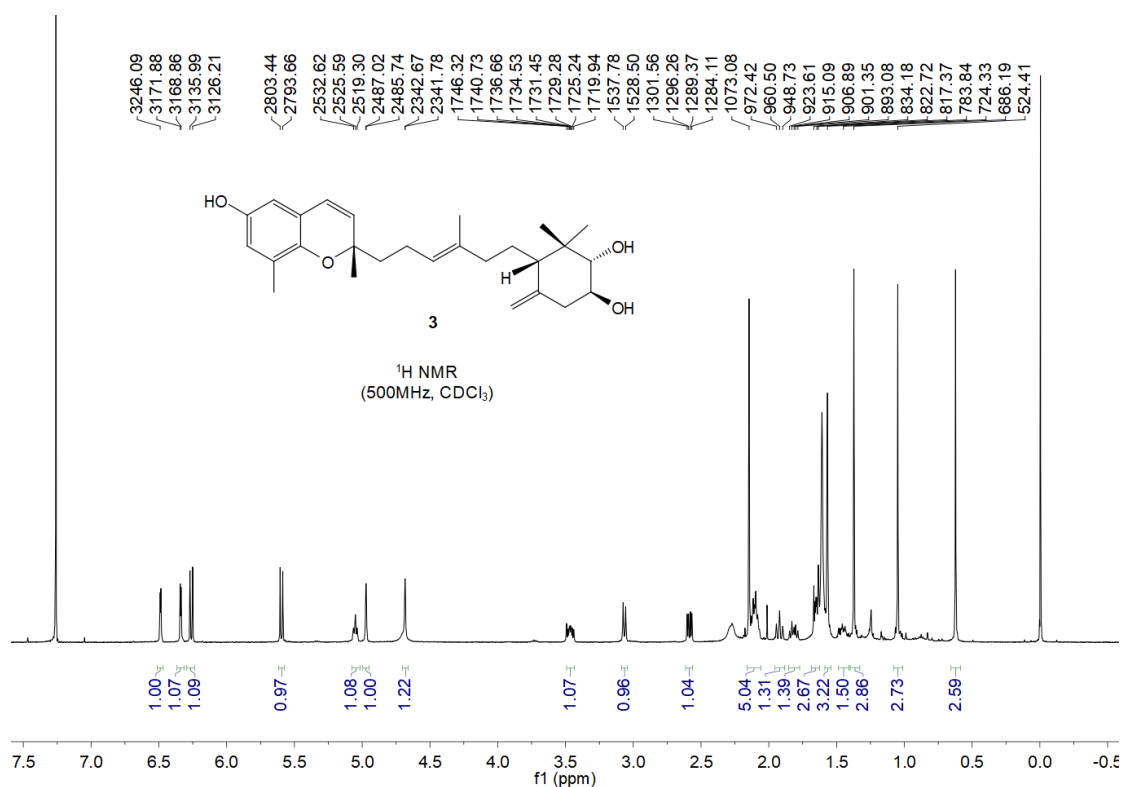
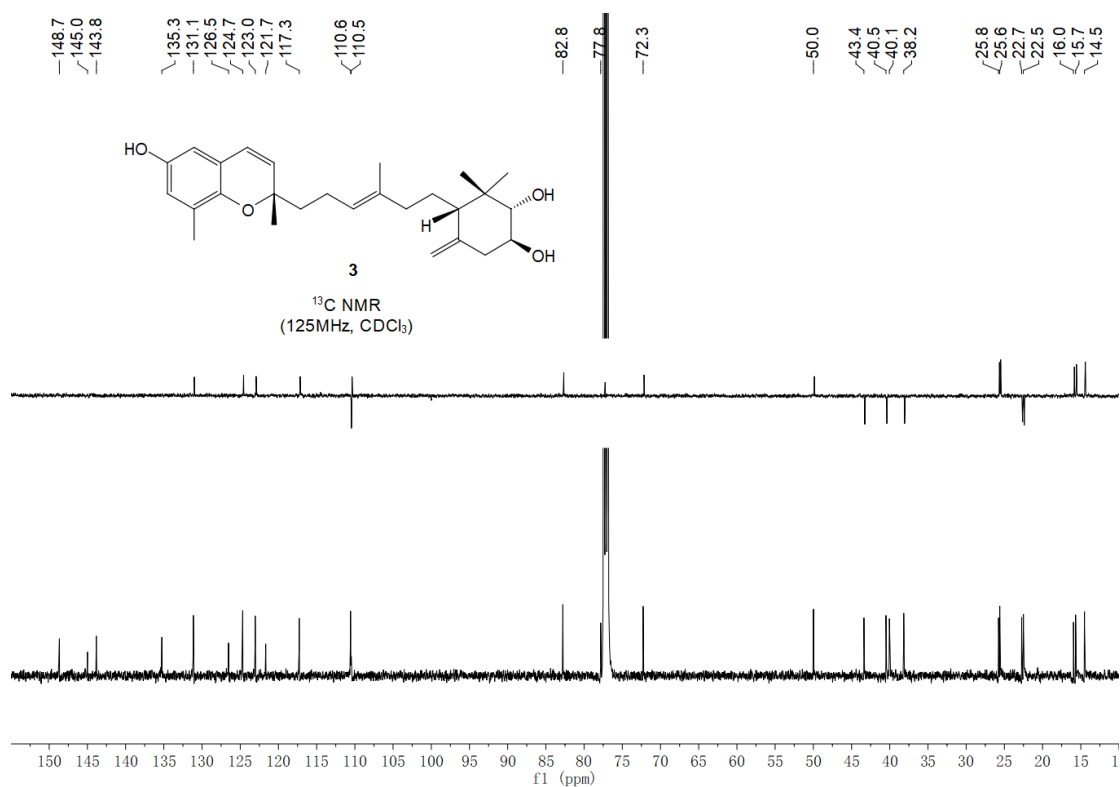


Figure S28. ^{13}C NMR spectrum of **3**



Chemical structure of compound **3** is shown above the NMR spectra. The structure is a complex molecule featuring a phenol ring, a furan ring, and a cyclohexene ring with multiple hydroxyl groups and a methyl group. The NMR spectra are recorded in CDCl₃.

The ¹H NMR spectrum (top) shows peaks in the aromatic region (6.5-7.5 ppm), a region with multiple peaks (3.5-5.5 ppm), and a region with multiple peaks (1.5-3.0 ppm). The ¹³C NMR spectrum (bottom) shows peaks in the aromatic region (110-155 ppm), a region with multiple peaks (35-55 ppm), and a region with multiple peaks (65-75 ppm).

The 2D HMBC spectrum (middle) shows correlations between the ¹H and ¹³C NMR spectra. The horizontal axis represents the ¹³C chemical shift (f2, ppm) and the vertical axis represents the ¹H chemical shift (f1, ppm). The correlations are indicated by red dots.

DL-65C CDCL3 ROESY

Sample Name:

Data Collected on: 409MR-vmr/s400

Archive directory:

Sample directory:

Fidfile: ROESY

Pulse Sequence: ROESY

Solvent: cdcl3

Date collected on: Apr 24 2013

Temp: 20.0 C / 289.1 K

Operator: chempack

Relax. delay 1.000 sec

Acq. time 0.107 sec

Width: 9542.0 Hz

2D Width 9542.0 Hz

20 repetitions

2 x 200 Increments

OBSERVE H1: 399.7804870 MHz

DATA PROCESSING

Gauss apodization 0.042 sec

F1 DATA PROCESSING

Gauss apodization 0.009 sec

F1 size 2048 x 2048

Total time 2 hr, 57 min

Figure S31. (+)-ESIMS spectrum of **3**

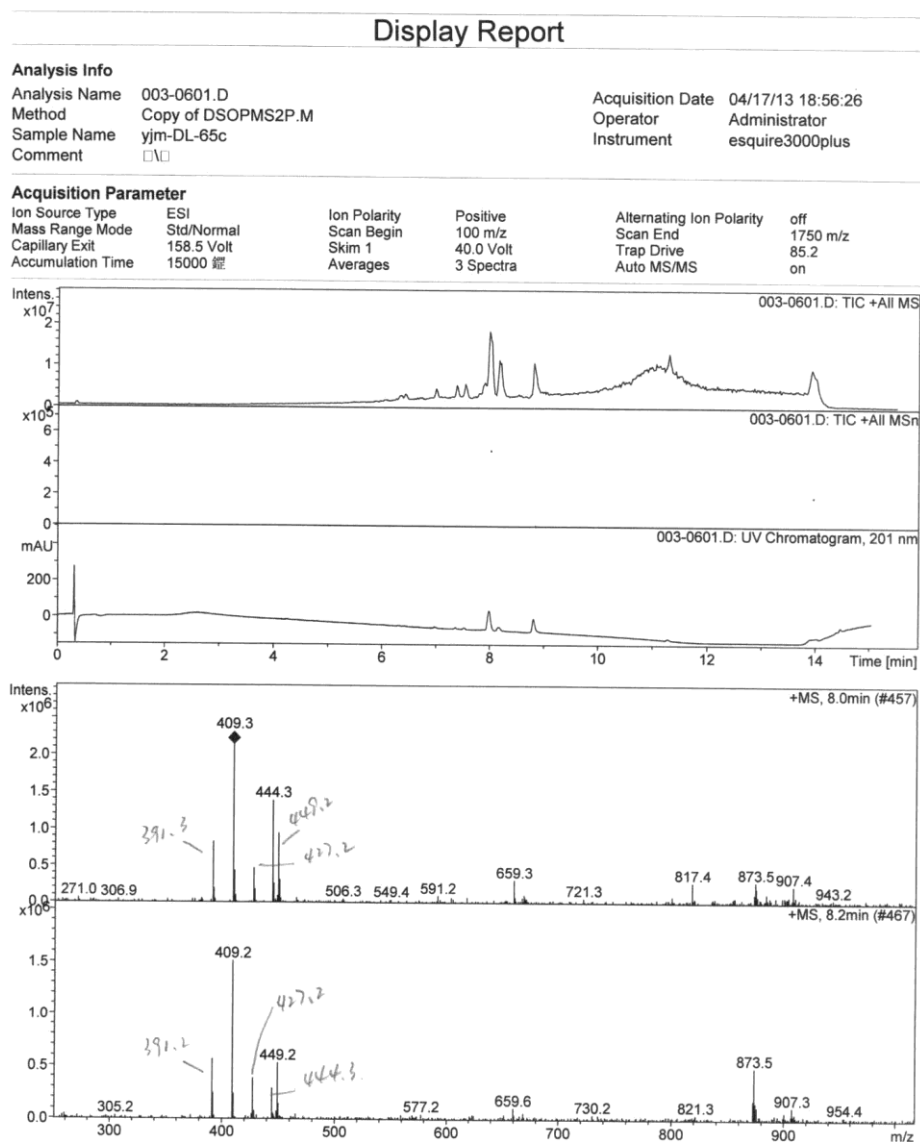


Figure S32. (-)-ESIMS spectrum of 3

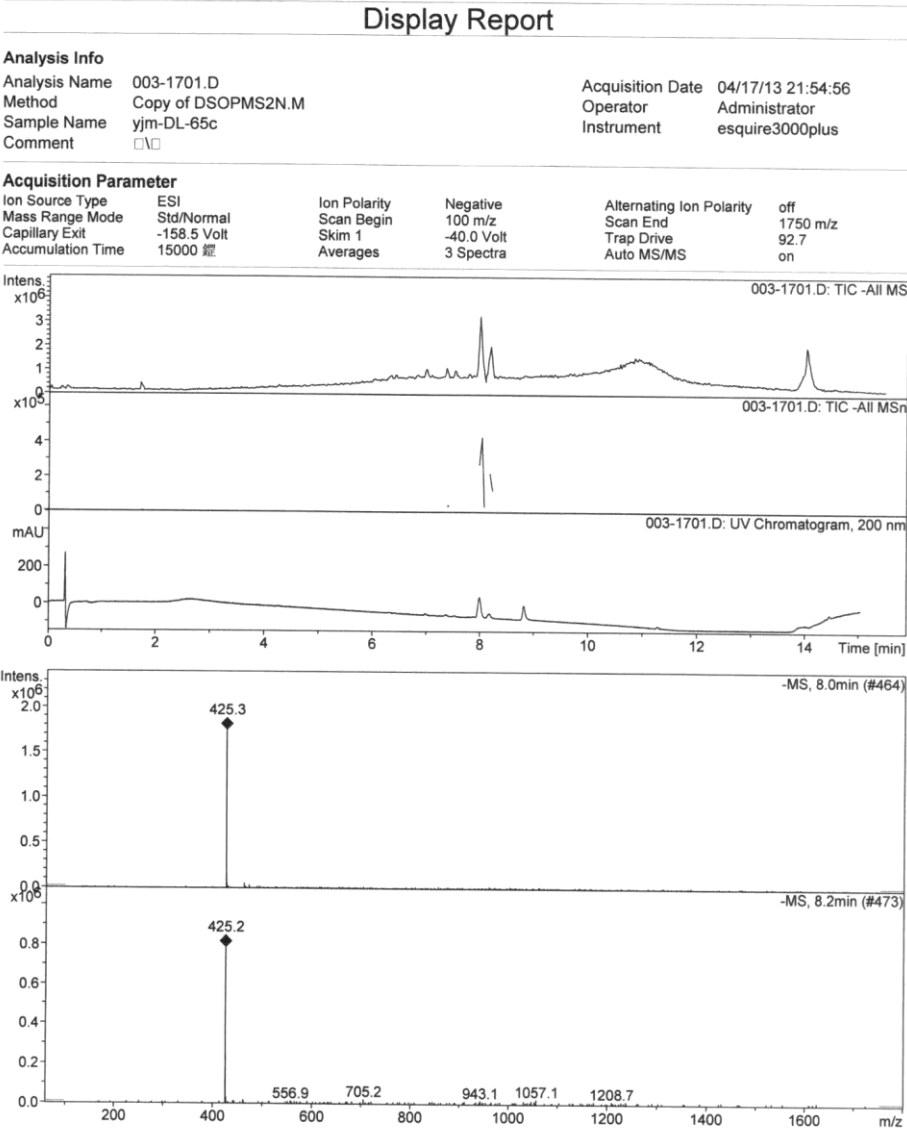


Figure S33. (+)-HRESIMS spectrum of 3

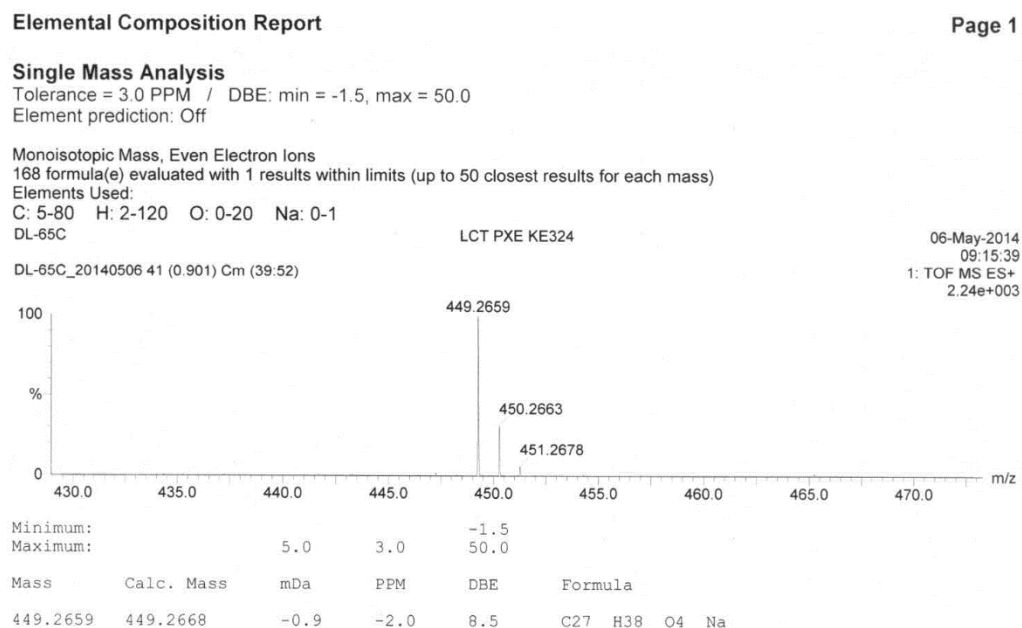


Figure S34. IR spectrum of 3

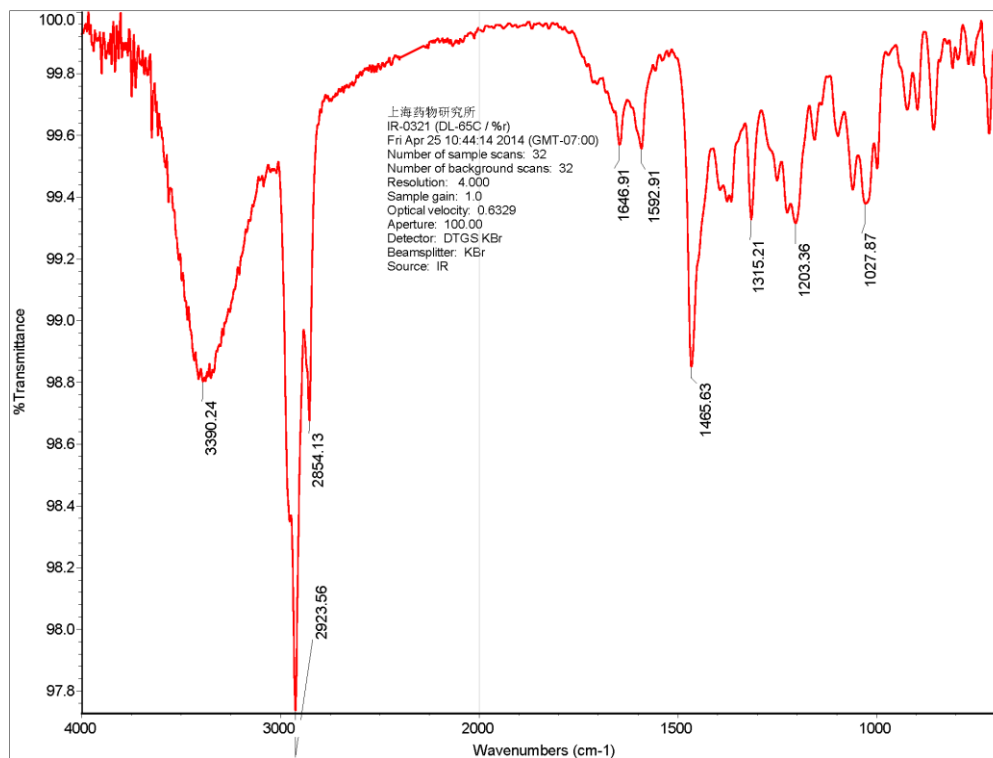


Figure S35. ^1H NMR spectrum of **4**

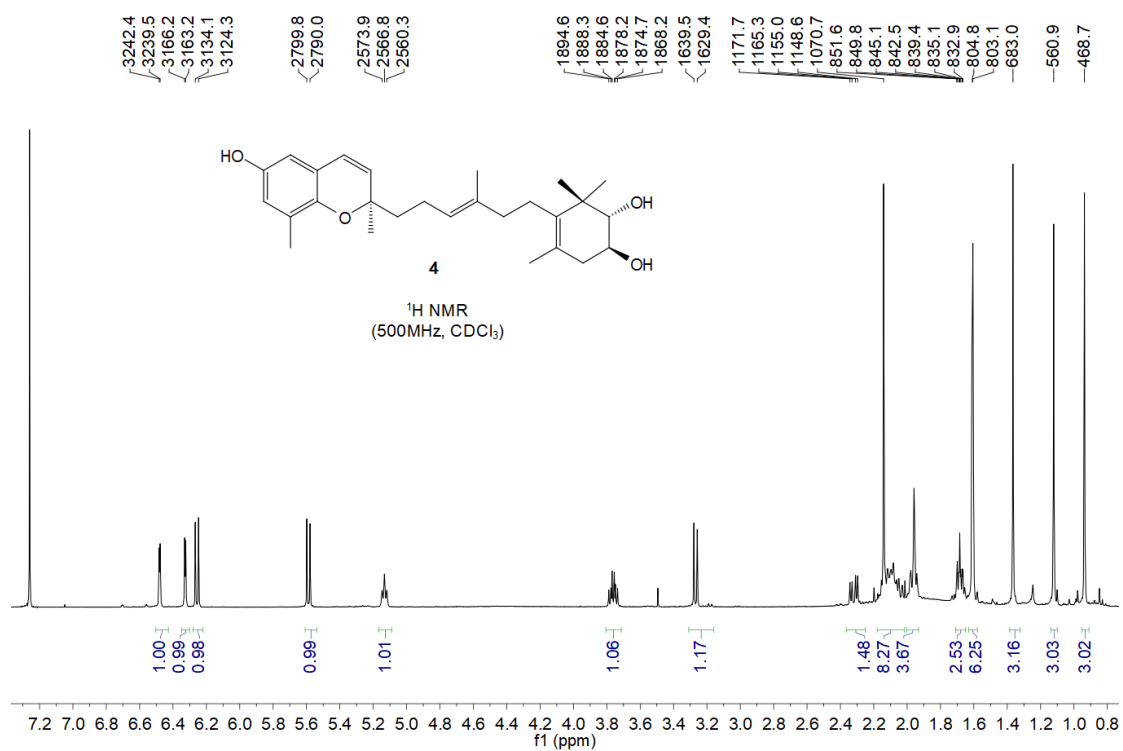


Figure S36. ^{13}C NMR spectrum of **4**

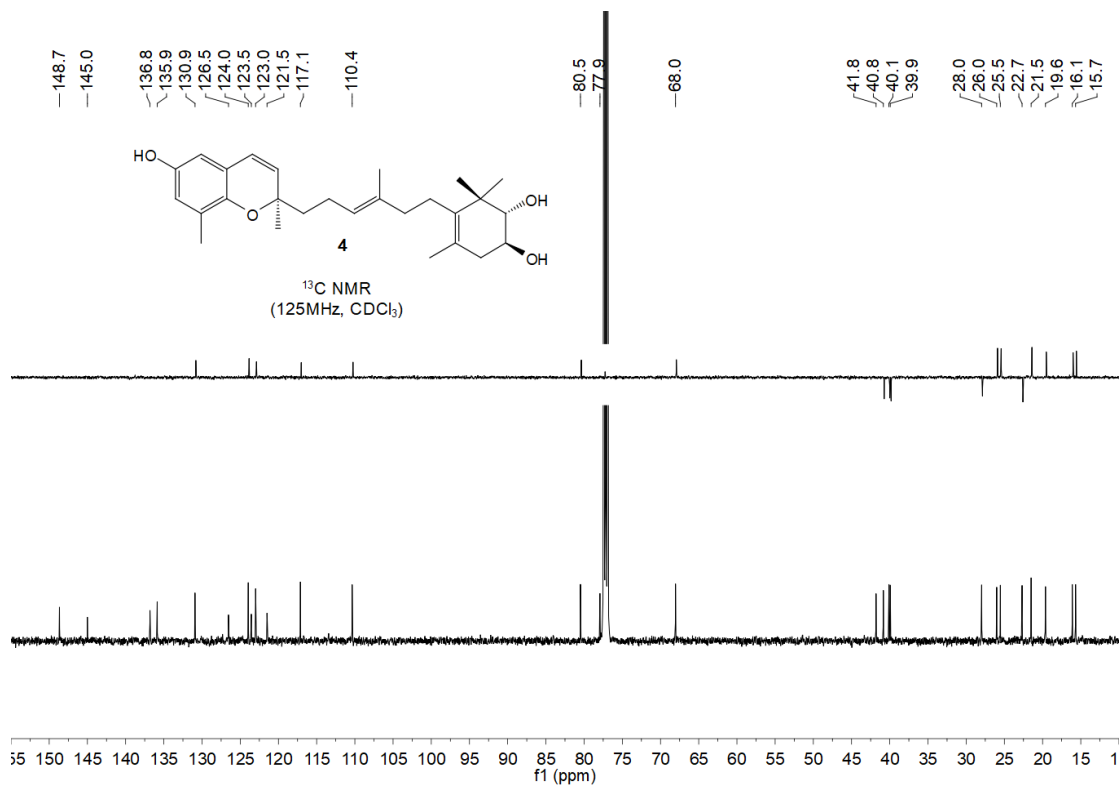


Figure S37. HSQC spectrum of **4**

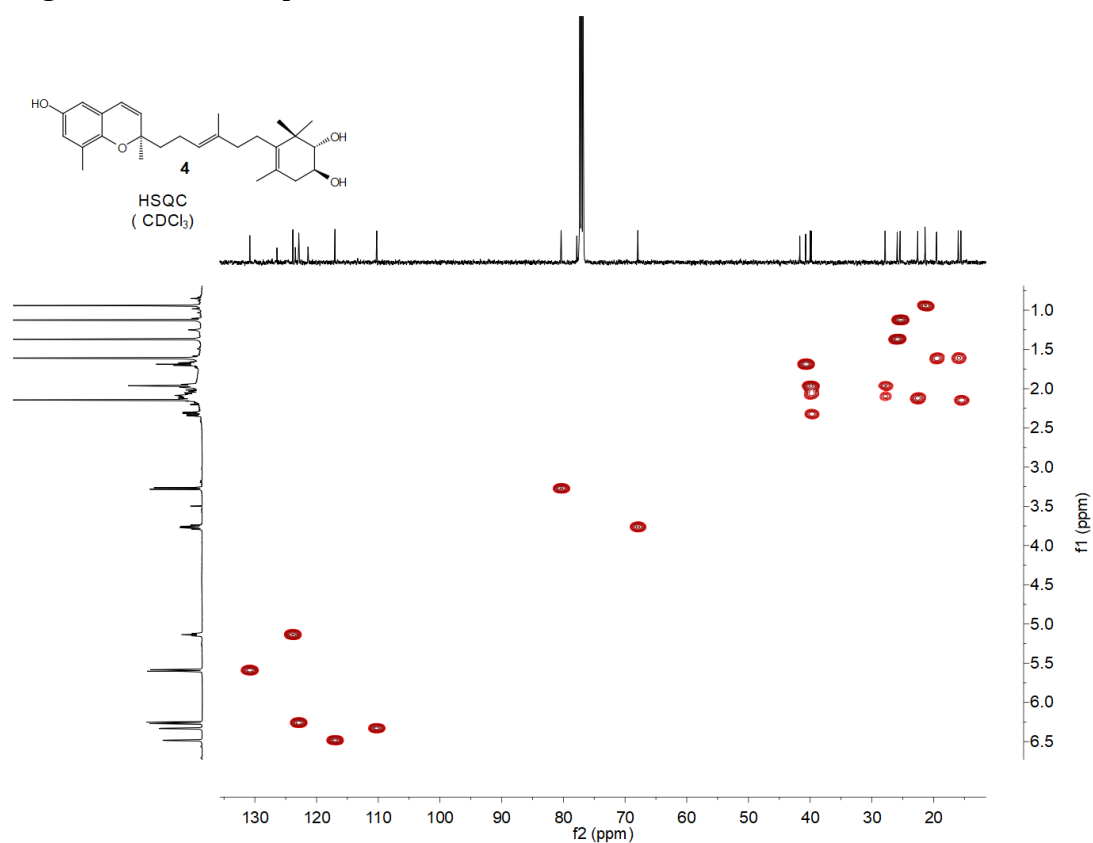


Figure S38. HMBC spectrum of **4**

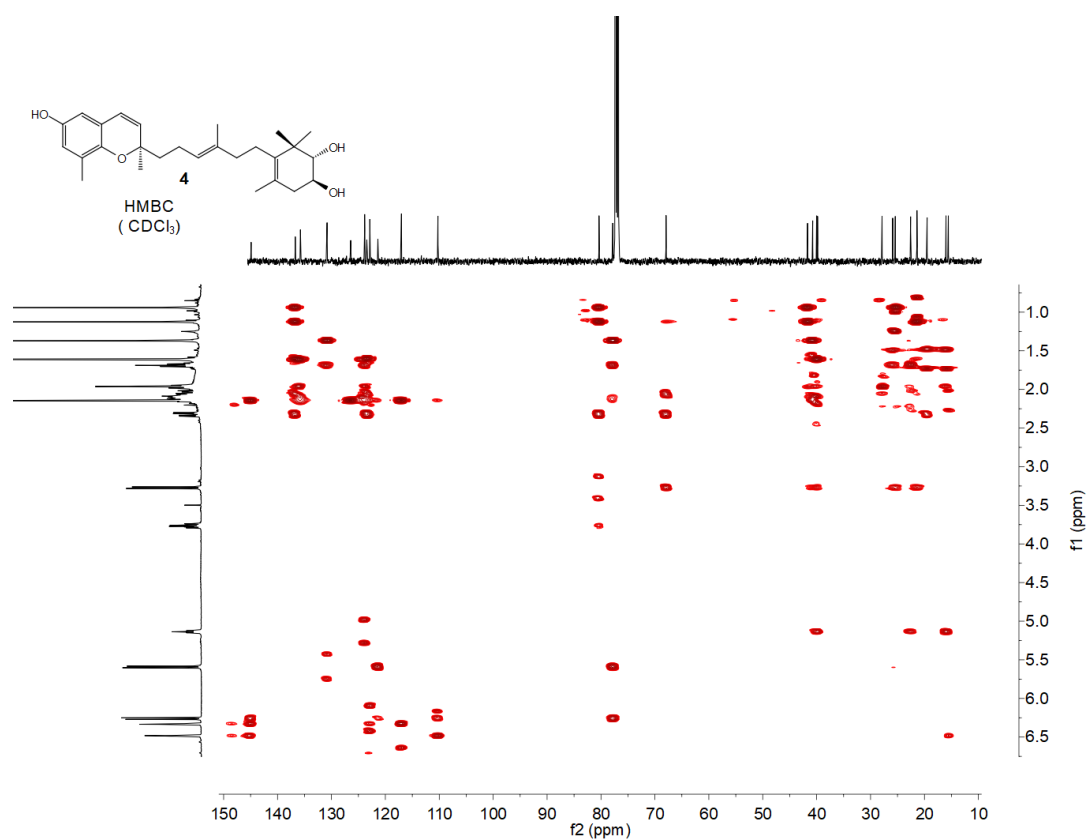


Figure S39. ROESY spectrum of **4**

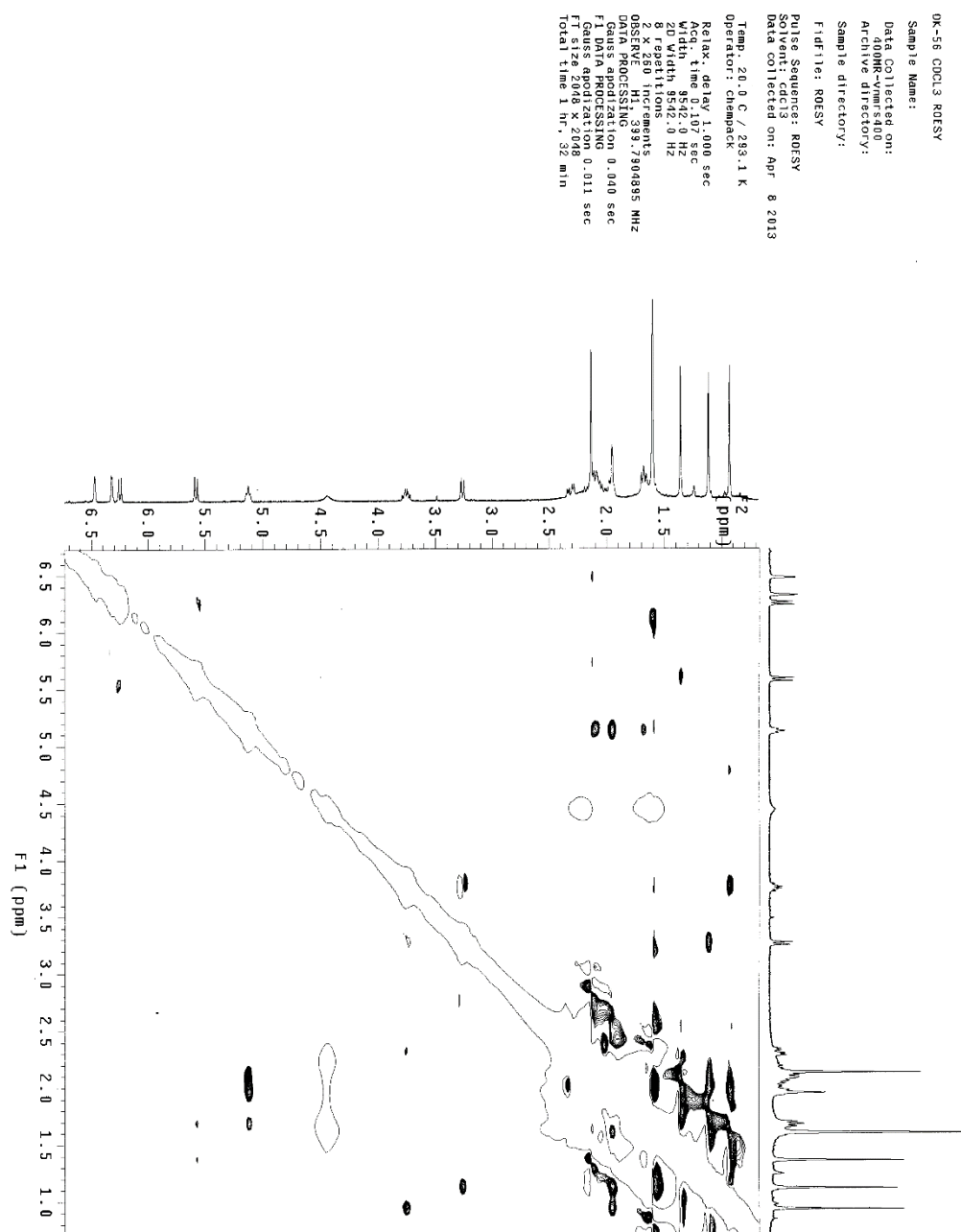


Figure S40. (+)-ESIMS spectrum of **4**

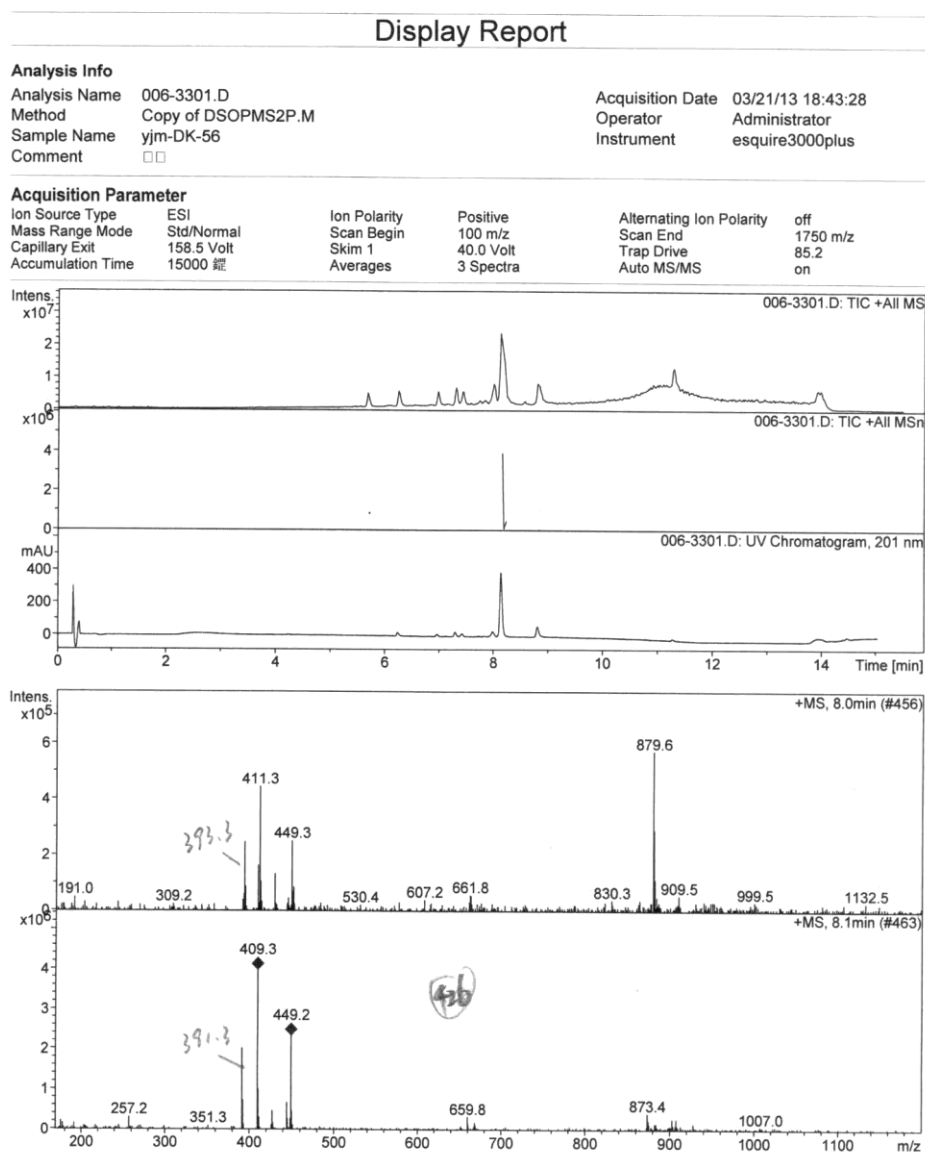


Figure S41. (-)-ESIMS spectrum of **4**

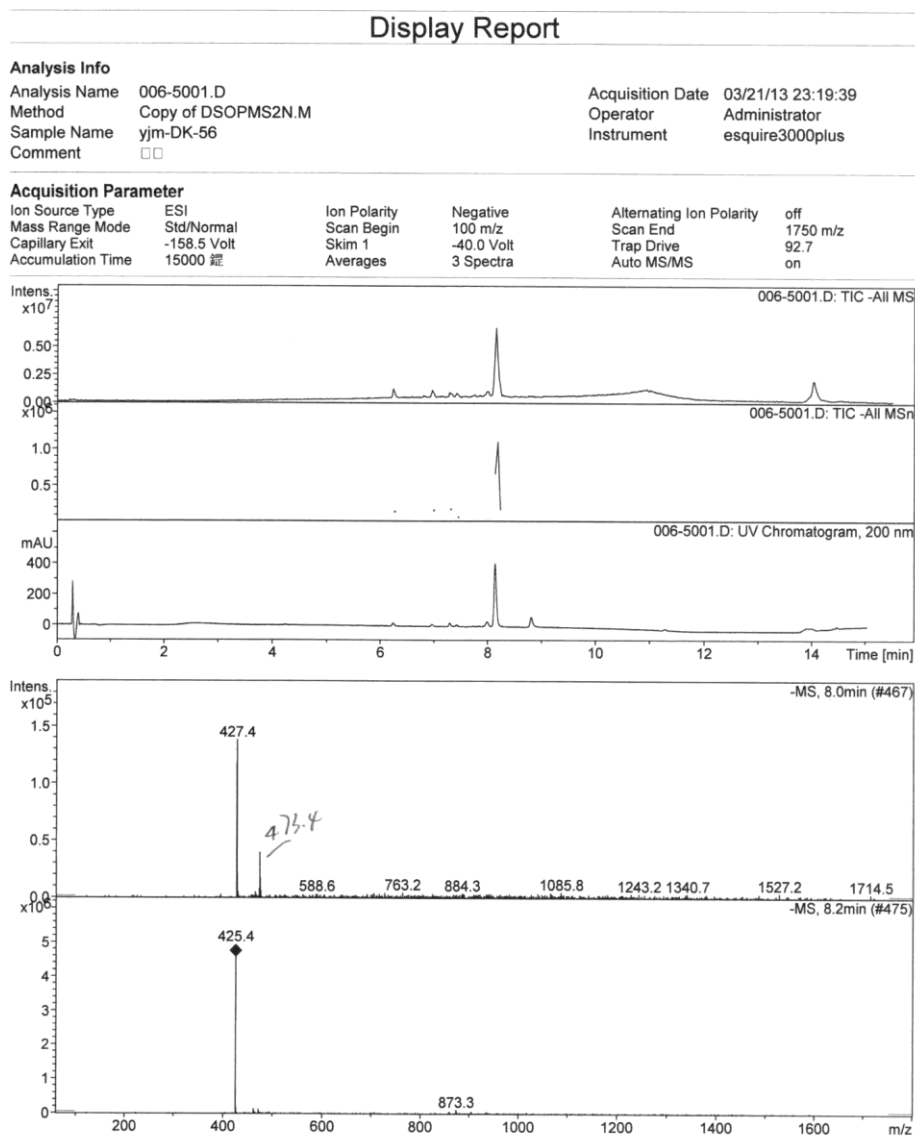


Figure S42. (-)-HRESIMS spectrum of 4

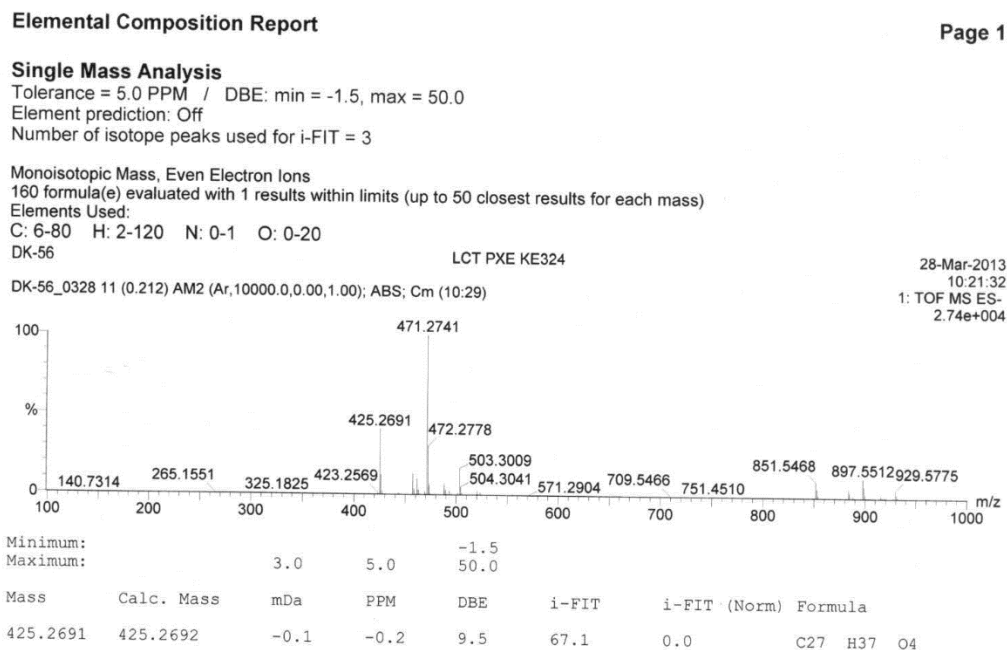


Figure S43. IR spectrum of 4

