

SUPPLEMENTARY MATERIALS

Targeted Isolation of Tsitsikammamines from the Antarctic Deep-Sea Sponge *Latrunculia biformis* by Molecular Networking and Anticancer Activity

Fengjie Li ¹, Dorte Janussen ², Christian Peifer ³, Ignacio Pérez-Victoria ⁴ and Deniz Tasdemir ^{1,5,*}

¹ GEOMAR Centre for Marine Biotechnology (GEOMAR-Biotech), Marine Natural Products Research Unit Chemistry, GEOMAR Helmholtz Centre for Ocean Research Kiel, Am Kiel-Kanal 44, 24106 Kiel, Germany; fli@geomar.de

² Senckenberg Research Institute and Natural History Museum, Senckenberganlage 25, 60325 Frankfurt, Germany; dorte.janussen@senckenberg.de

³ Pharmaceutical Chemistry, Kiel University, Gutenbergstraße 76, 24118 Kiel, Germany; cpeifer@pharmazie.uni-kiel.de

⁴ Fundación MEDINA, Parque Tecnológico de la Salud, Av. Conocimiento 18016 Granada, Spain; ignacio.perez-victoria@medinaandalucia.es

⁵ Faculty of Mathematics and Natural Sciences, Kiel University, Christian-Albrechts-Platz 4, 24118 Kiel, Germany

* Correspondence: dtasdemir@geomar.de; Tel.: +49-431-600-4430

Figure No	Page No
Figure S1. ^1H NMR spectrum of compound 1 (free base, 600 MHz, DMSO- d_6).	3
Figure S2. ^{13}C NMR spectrum of compound 1 (free base, 150 MHz, DMSO- d_6).	3
Figure S3. HSQC NMR spectrum of compound 1 (free base, 600 MHz, DMSO- d_6).	4
Figure S4. HMBC spectrum of compound 1 (free base, 600 MHz, DMSO- d_6).	4
Figure S5. COSY spectrum of compound 1 (free base, 600 MHz, DMSO- d_6).	5
Figure S6. NOESY spectrum of compound 1 (free base, 600 MHz, DMSO- d_6).	5
Figure S7. ^1H NMR spectrum of compound 1 (free base, 600 MHz, MeOD).	6
Figure S8. ^1H NMR spectrum of compound 1 (TFA salt, 600 MHz, DMSO- d_6).	6
Figure S9. ^{13}C NMR spectrum of compound 1 (TFA salt, 150 MHz, DMSO- d_6).	7
Figure S10. HR-ESIMS spectrum of compound 1 .	7
Figure S11. ^1H NMR spectrum of compound 2 (600 MHz, MeOD).	8
Figure S12. HSQC spectrum of compound 2 (600 MHz, MeOD).	8
Figure S13. HMBC spectrum of compound 2 (600 MHz, MeOD).	9
Figure S14. HMBC spectrum of compound 2 (500 MHz, MeOD).	9
Figure S15. COSY spectrum of compound 2 (500 MHz, MeOD).	10
Figure S16. NOESY spectrum of compound 2 (500 MHz, MeOD).	10
Figure S17. HR-ESIMS spectrum of compound 2 .	11
Figure S18. In vitro activity of crude <i>Latrunculia</i> extract and its SPE fractions against cancer cell lines.	11

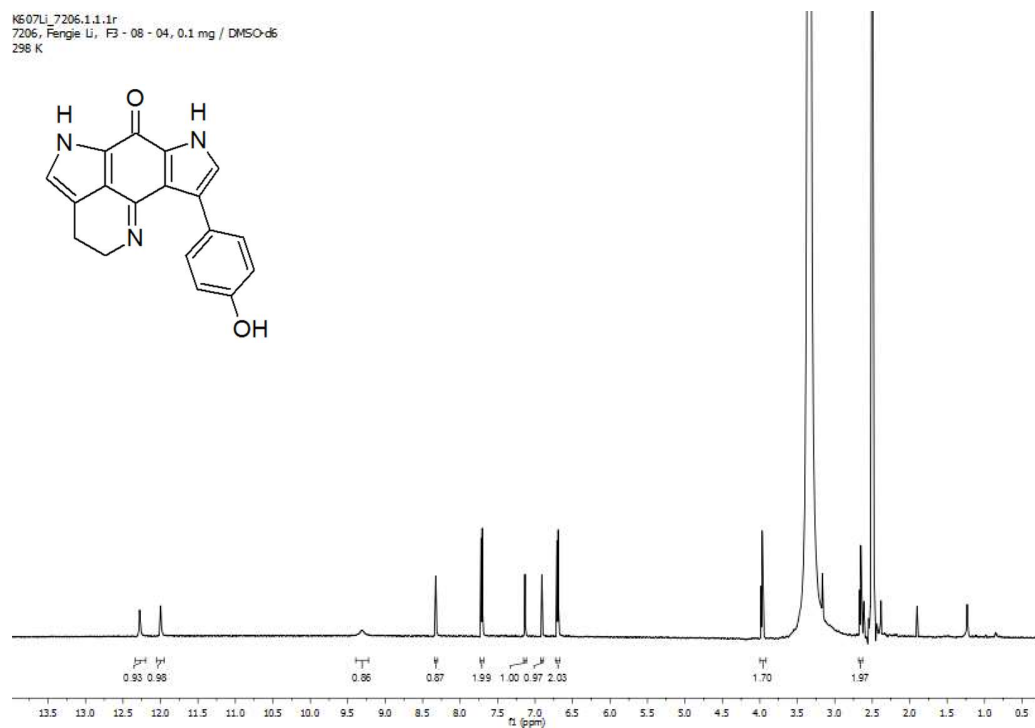


Figure S1. ¹H NMR spectrum of compound **1** (free base, 600 MHz, DMSO-*d*₆).

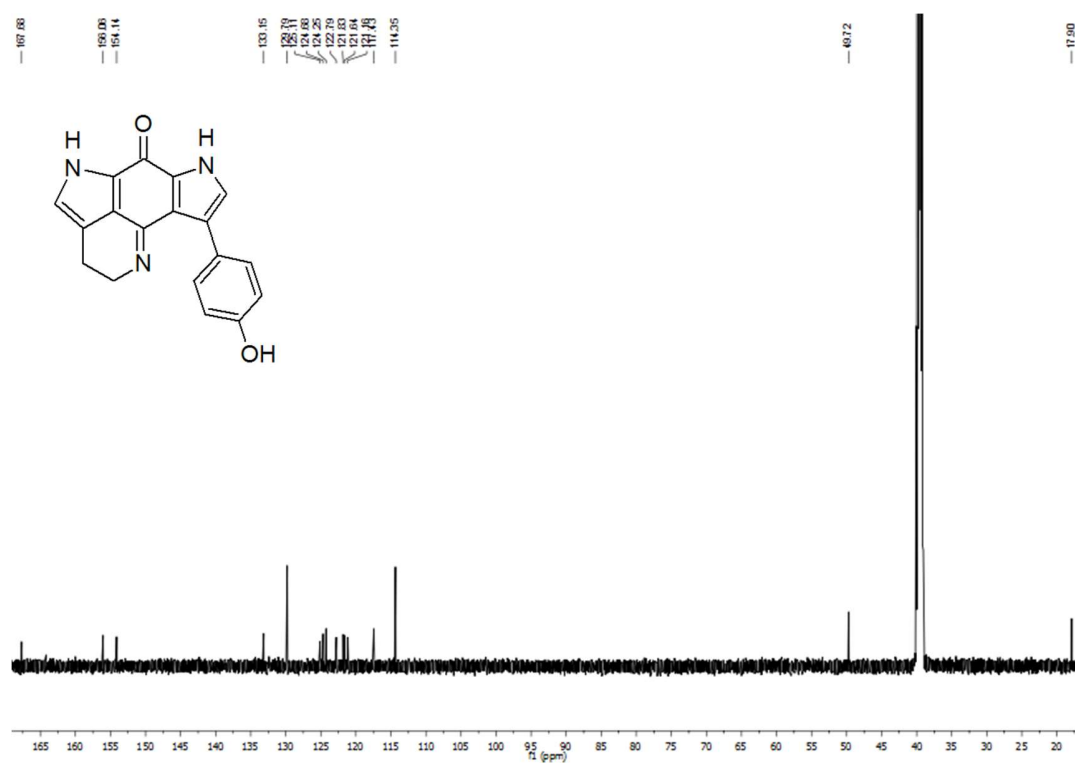


Figure S2. ¹³C NMR spectrum of compound **1** (free base, 150 MHz, DMSO-*d*₆).

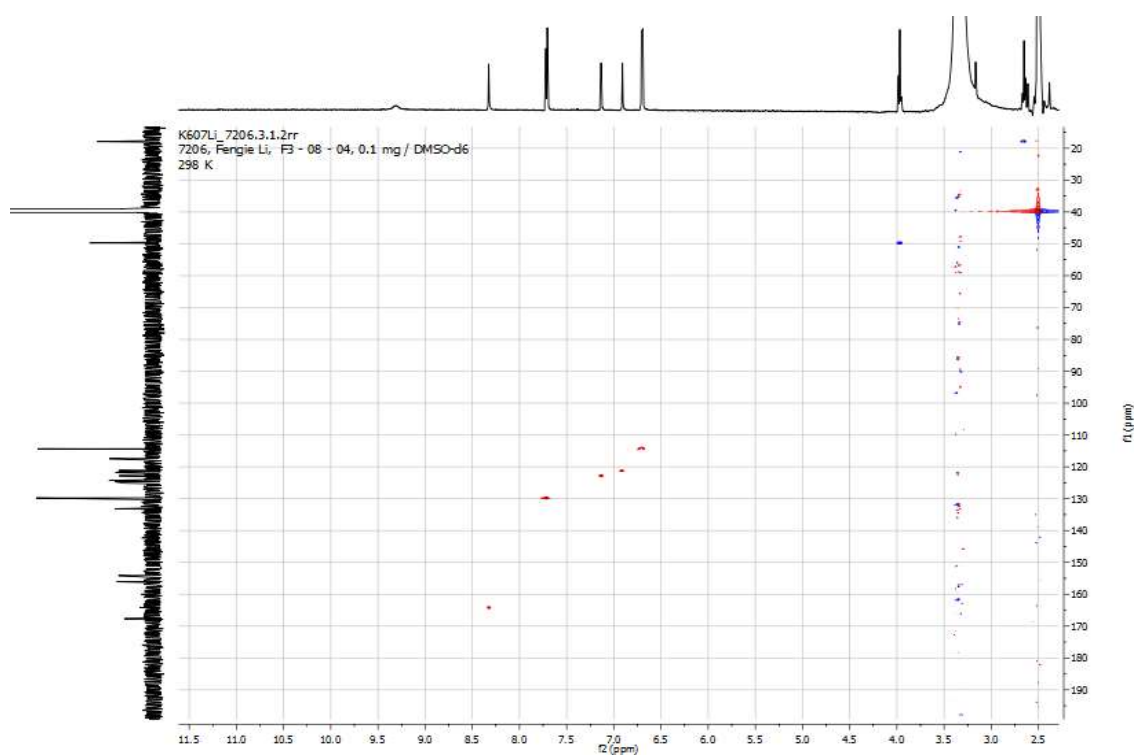


Figure S3. HSQC NMR spectrum of compound **1** (free base, 600 MHz, DMSO-*d*₆).

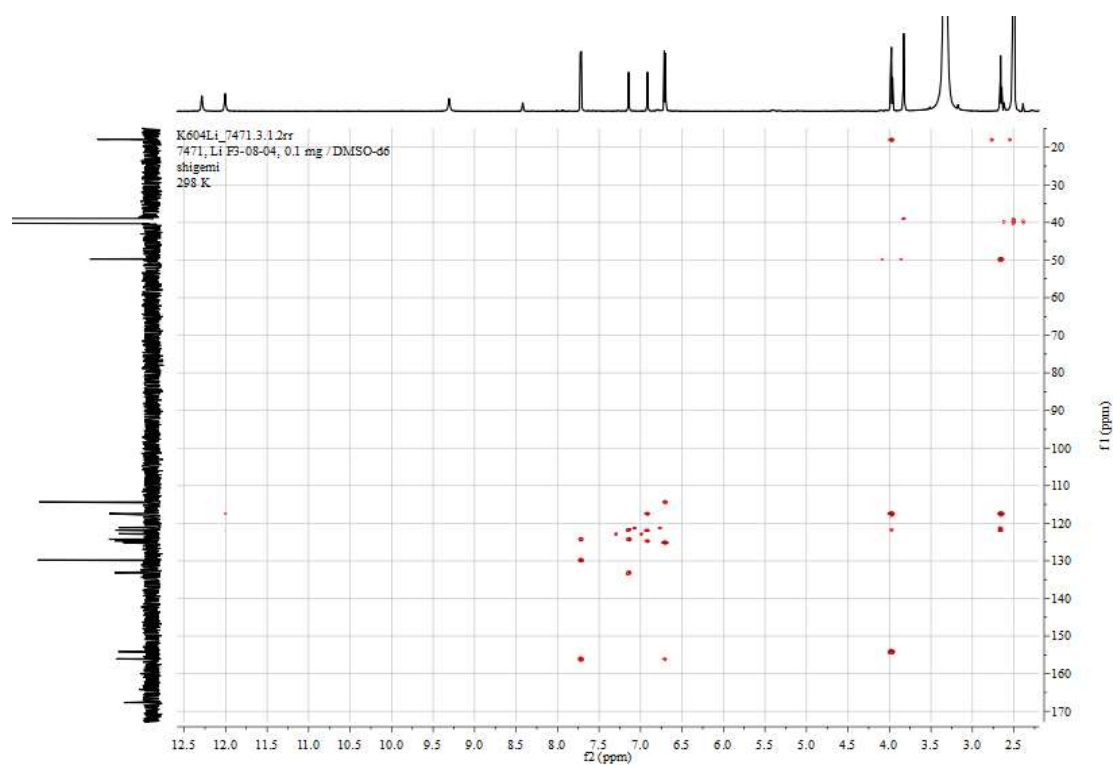


Figure S4. HMBC spectrum of compound **1** (free base, 600 MHz, DMSO-*d*₆).

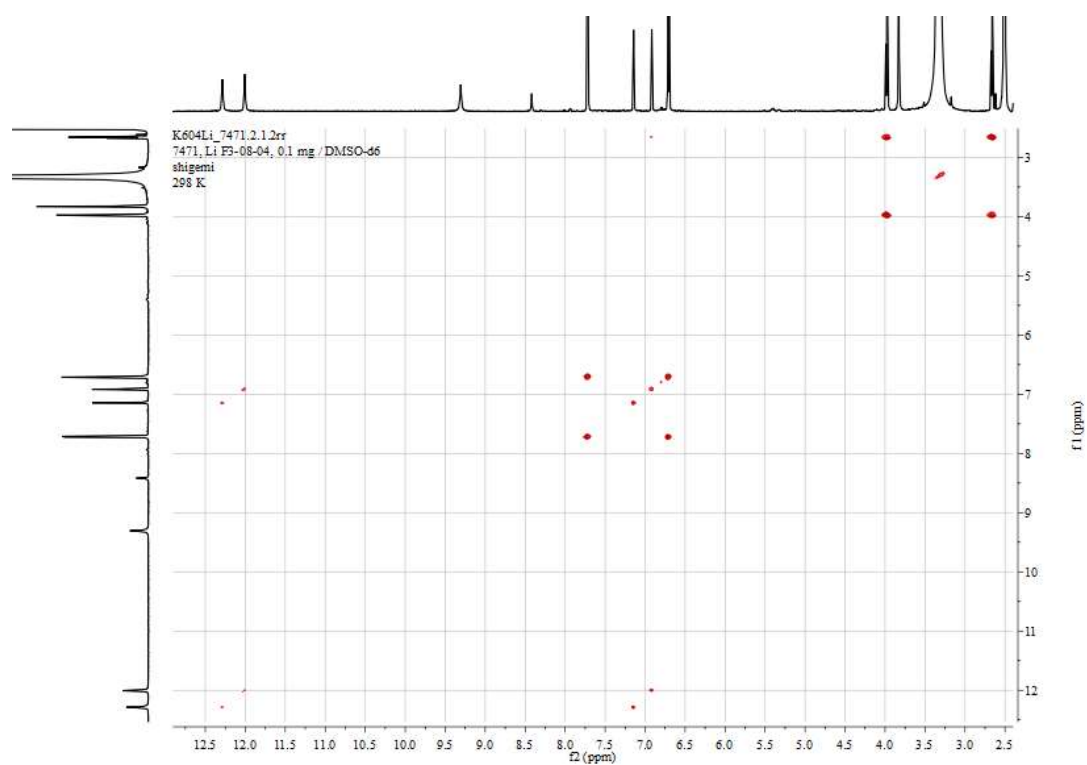


Figure S5. COSY spectrum of compound **1** (free base, 600 MHz, DMSO-*d*₆).

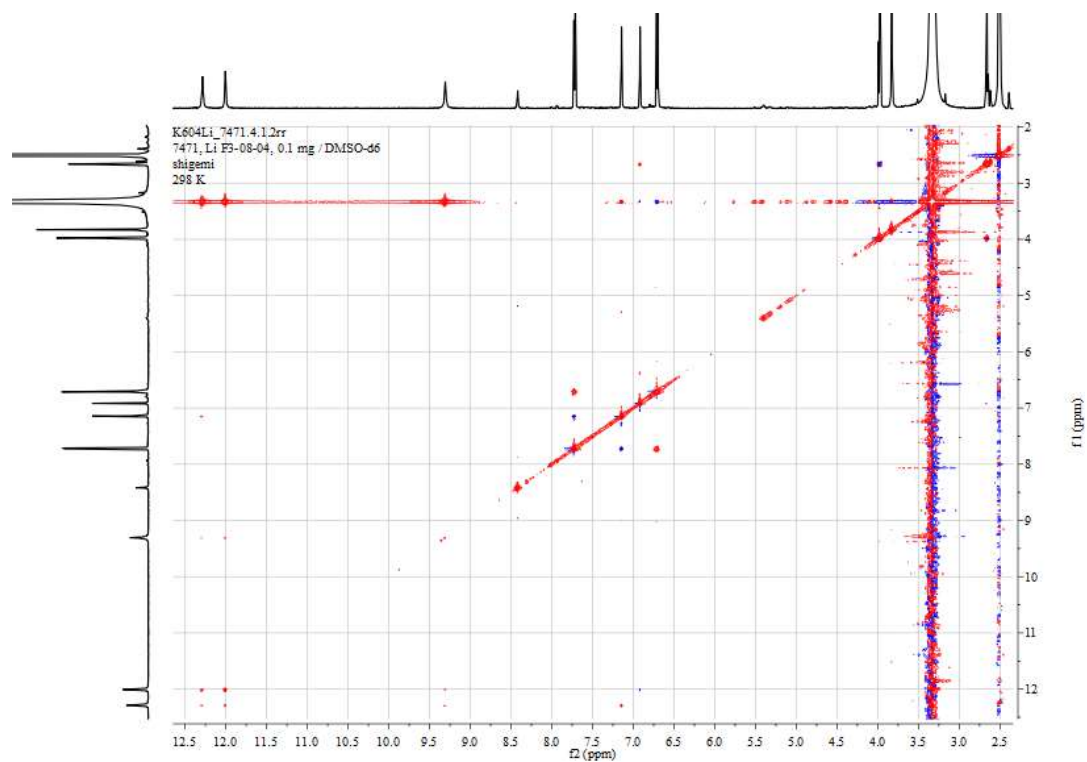


Figure S6. NOESY spectrum of compound **1** (free base, 600 MHz, DMSO-*d*₆).

K607Li_7204.1.1.1r
7204, Fengjie Li, F3 - 08 - 04, 0.1 mg/CD3OD
298 K

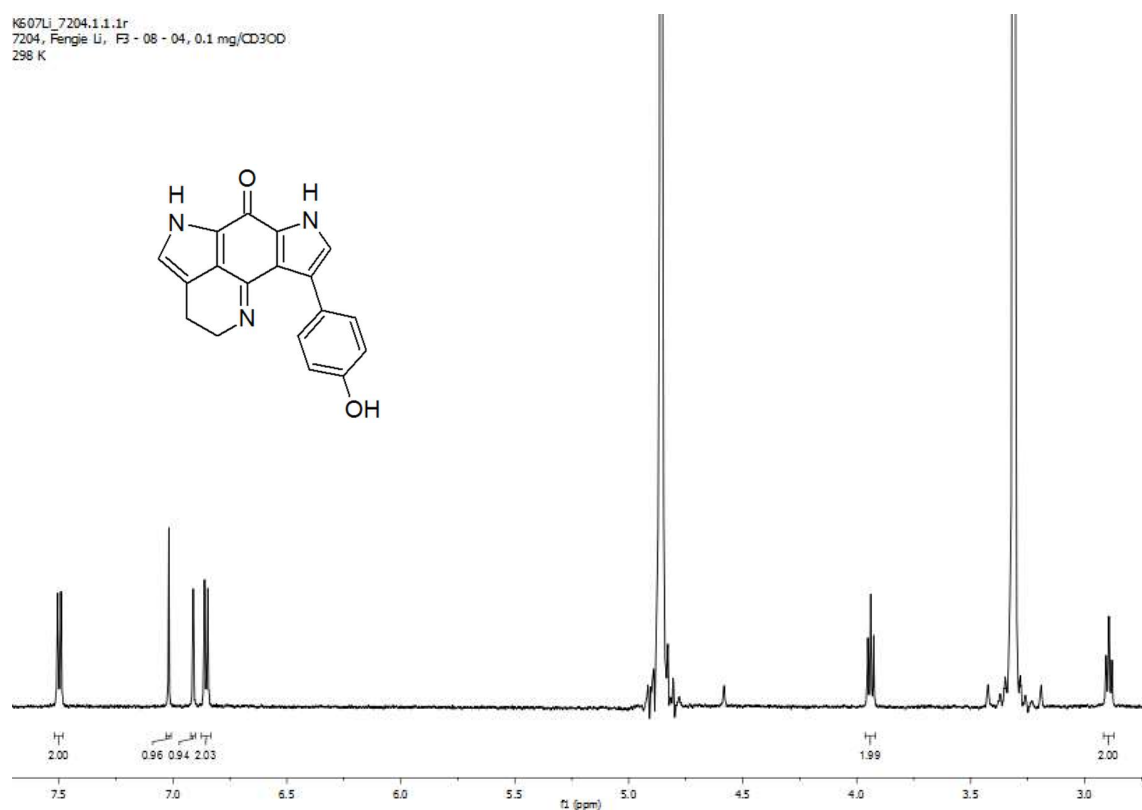


Figure S7. ¹H NMR spectrum of compound 1 (free base, 600 MHz, MeOD).

20180406-10-K504Li_6943.1.1.1r
Position 10, Mitarbeiter Fengjie Li, Sample F3-08-04, Menge 0.1 mg / DMSO-d6, Re kein

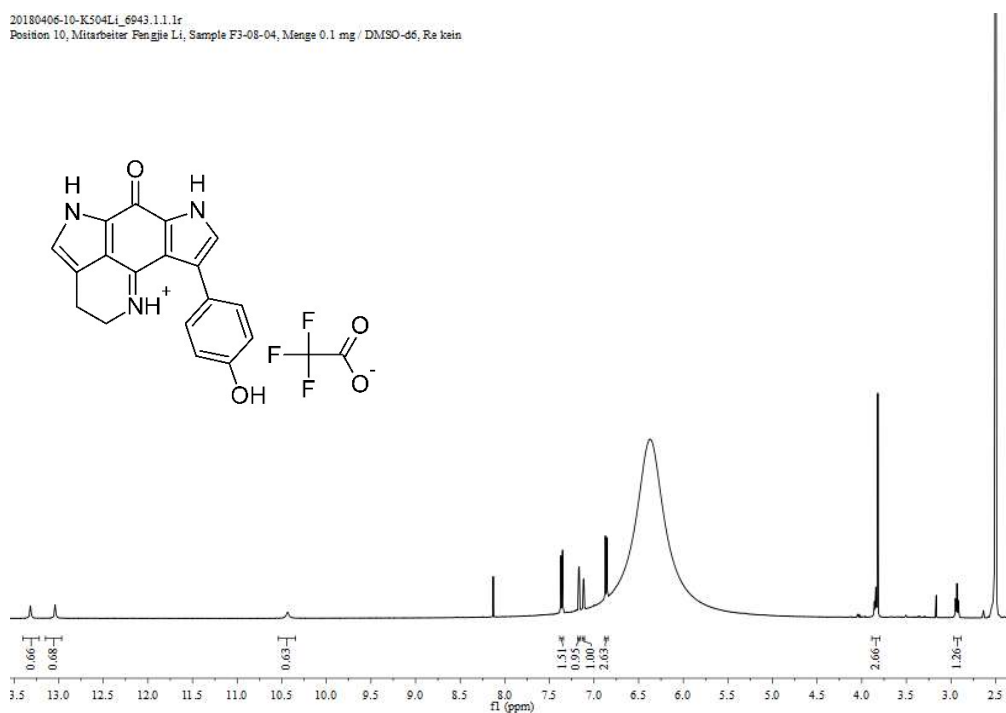


Figure S8. ¹H NMR spectrum of compound 1 (TFA salt, 600 MHz, DMSO-d₆).

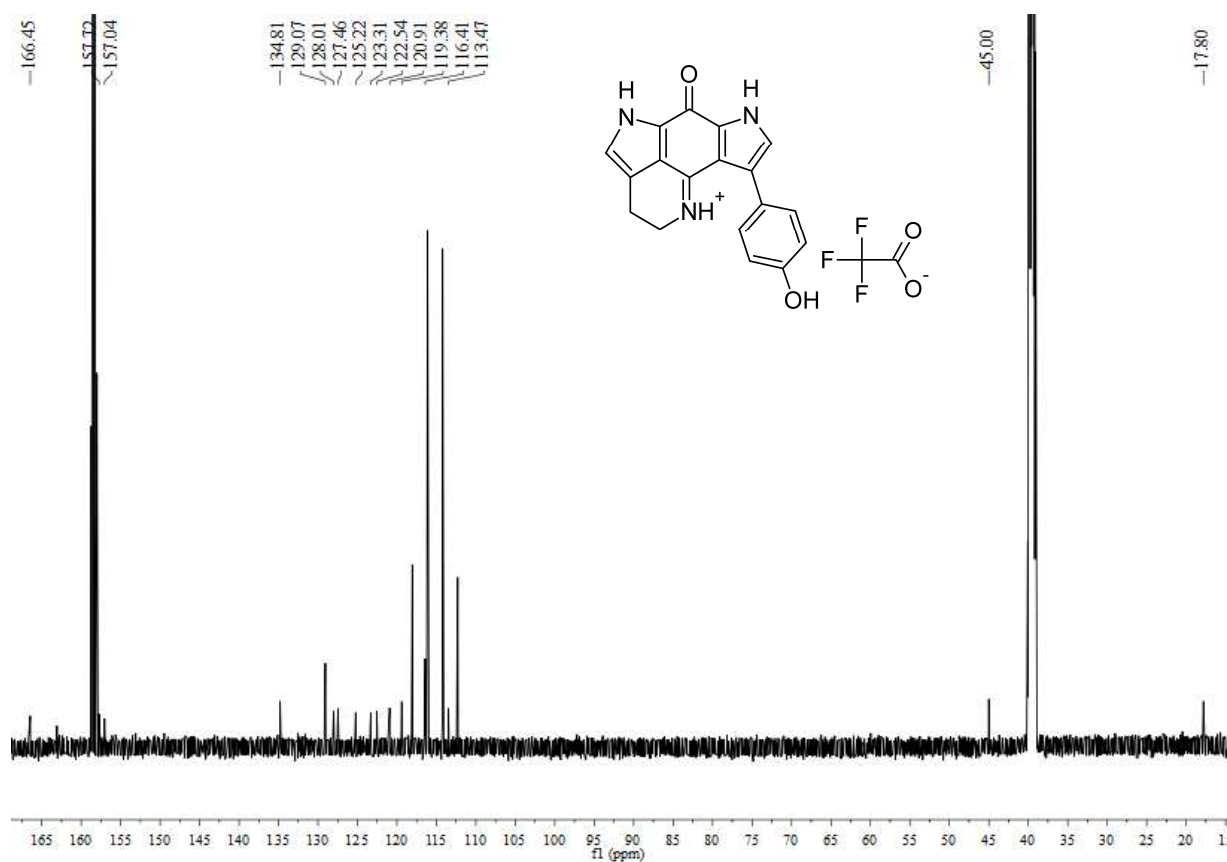


Figure S9. ¹³C NMR spectrum of compound **1** (TFA salt, 150 MHz, DMSO-*d*₆).

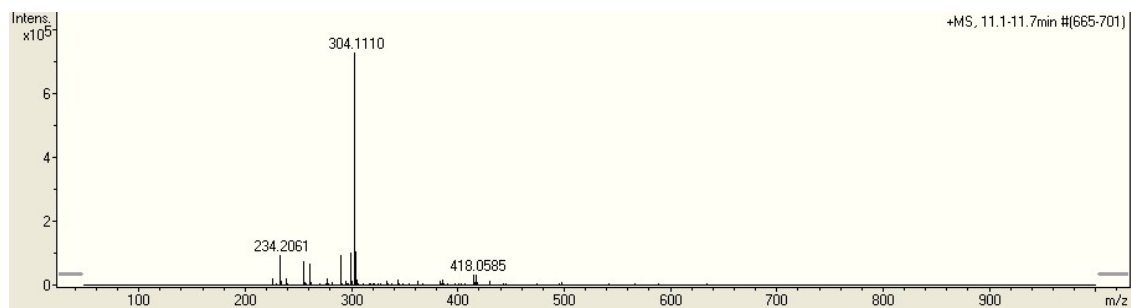


Figure S10. HR-ESIMS spectrum of compound **1**.

F3-08-03-CD3OD.1.1.1r
7222 Fengie Li F3-08-03, 0.1 mg / CD3OD, Shigemii-tube
298 K

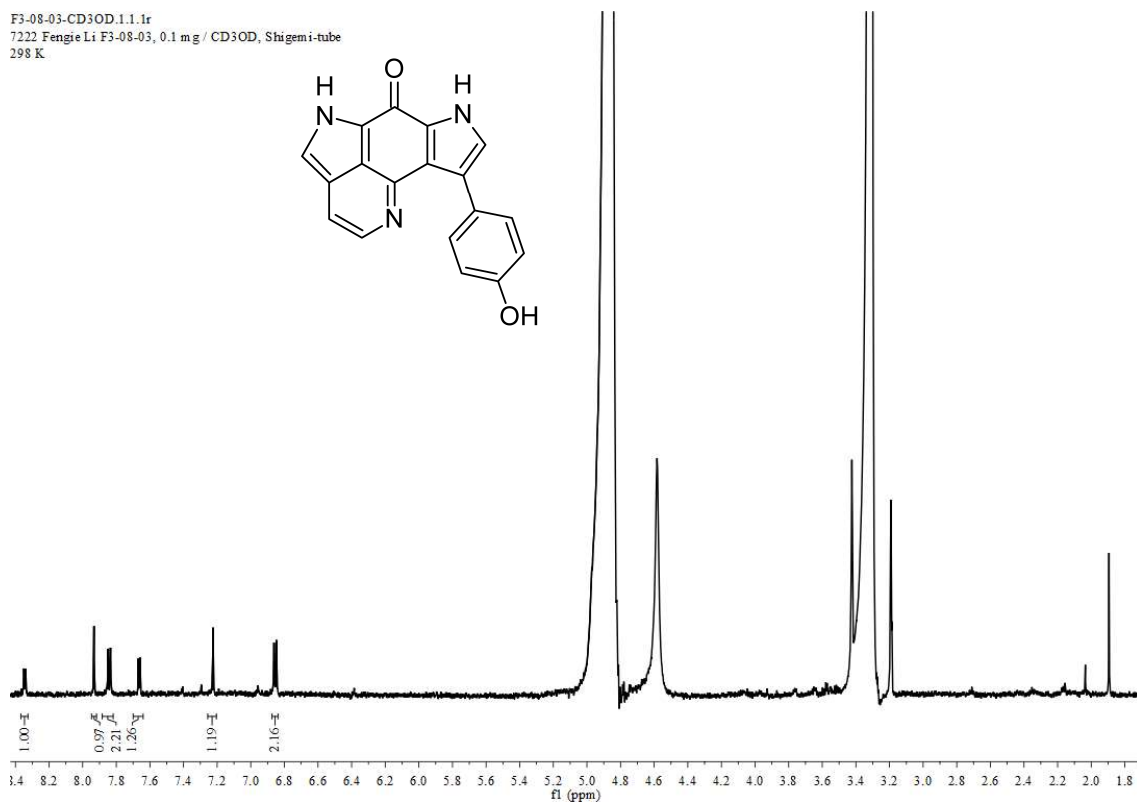


Figure S11. ^1H NMR spectrum of compound 2 (600 MHz, MeOD).

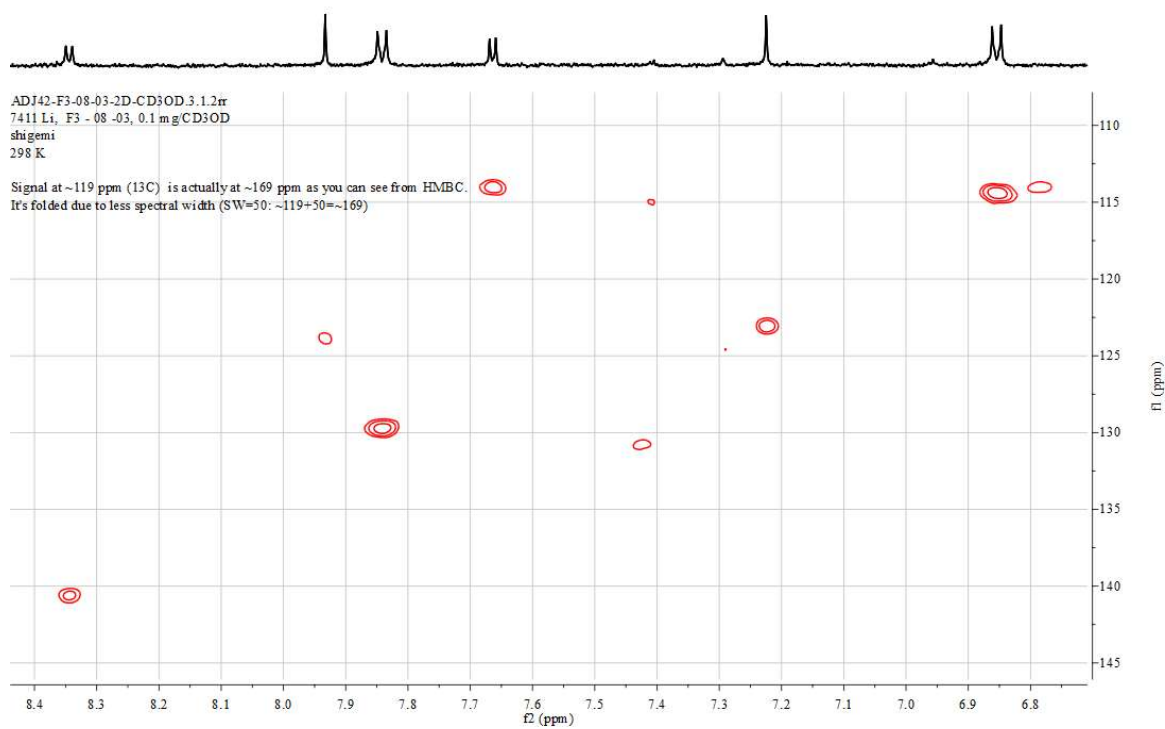


Figure S12. HSQC spectrum of compound 2 (600 MHz, MeOD).

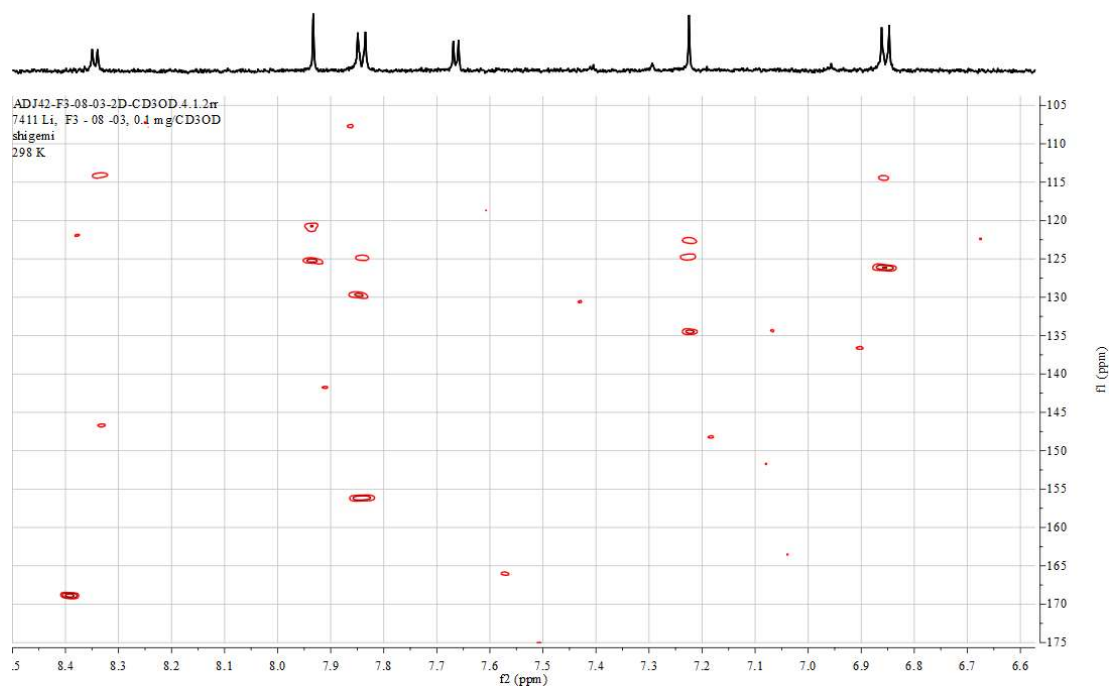


Figure S13. HMBC spectrum of compound **2** (600 MHz, MeOD).

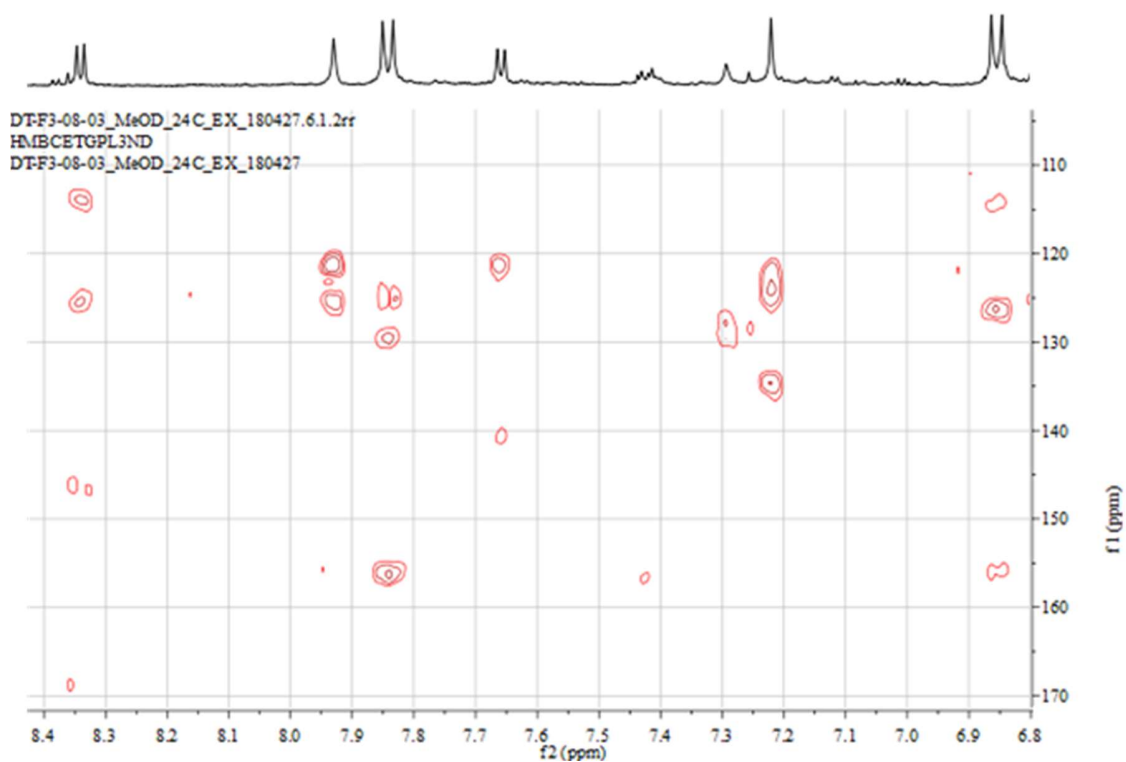


Figure S14. HMBC spectrum of compound **2** (500 MHz, MeOD).

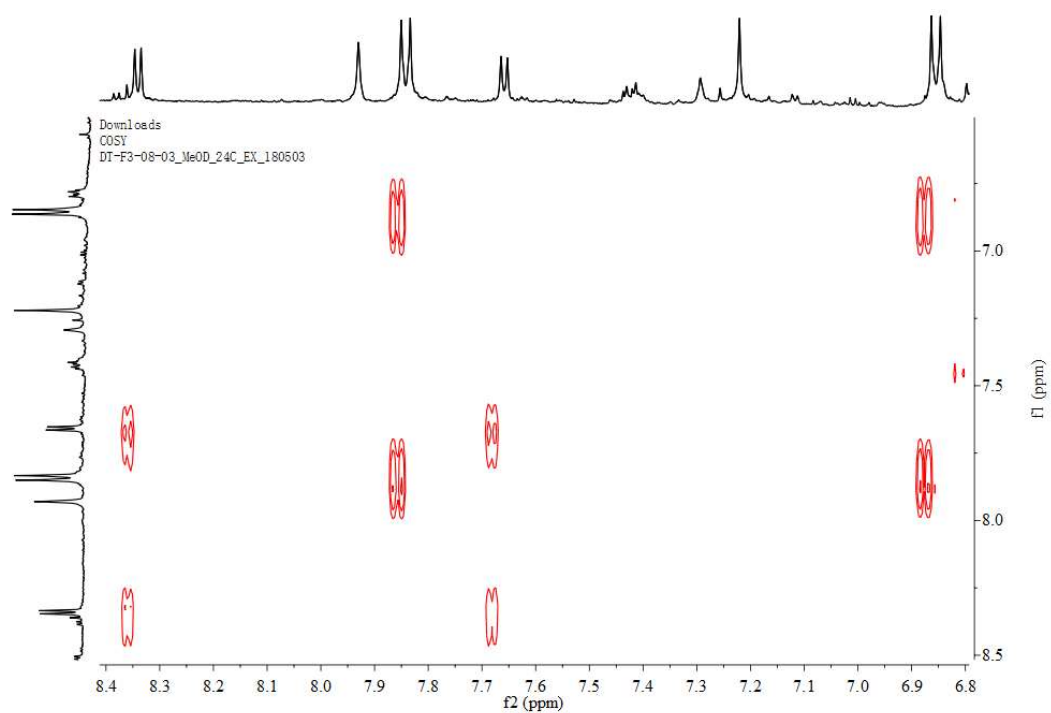


Figure S15. COSY spectrum of compound **2** (500 MHz, MeOD).

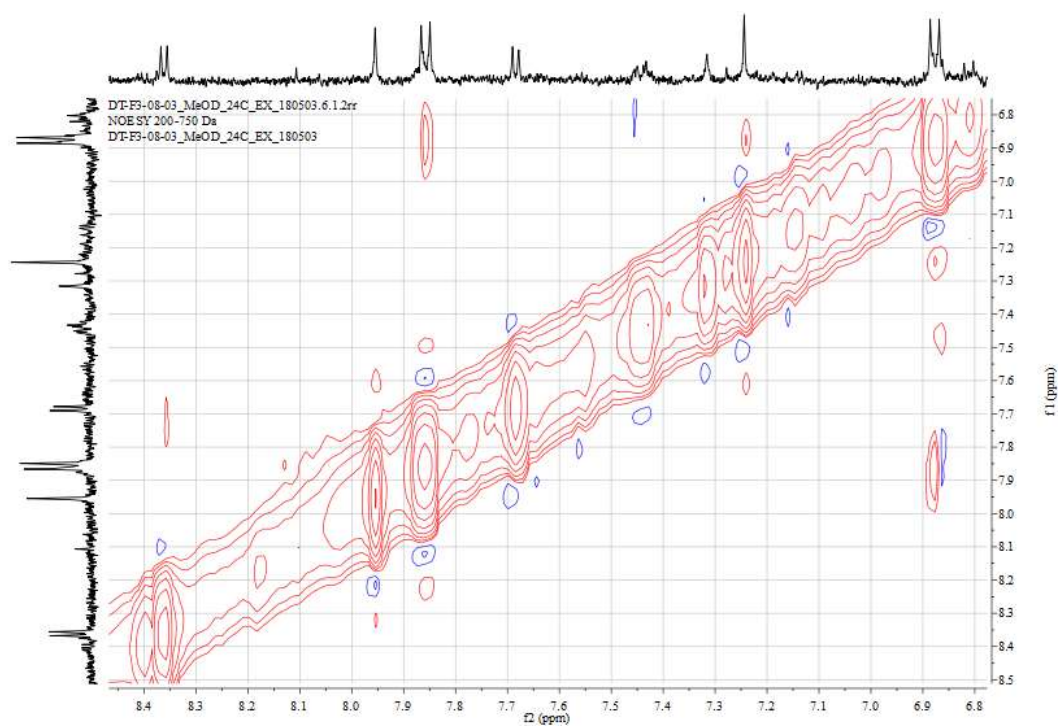


Figure S16. NOESY spectrum of compound **2** (500 MHz, MeOD).

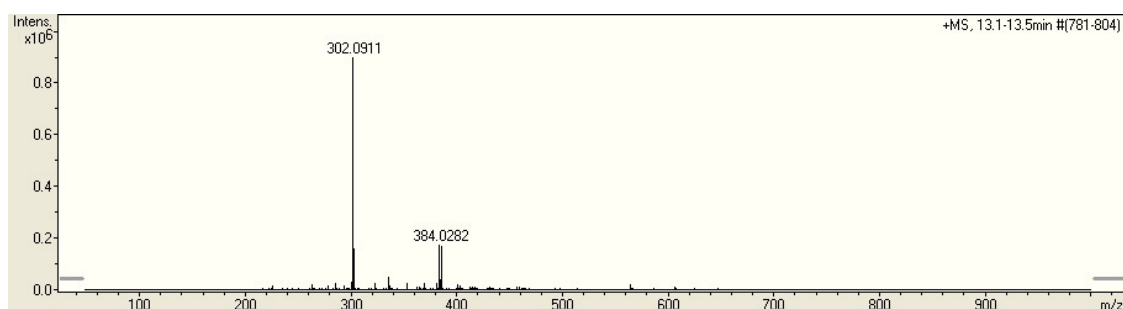


Figure S17. HR-ESIMS spectrum of compound 2.

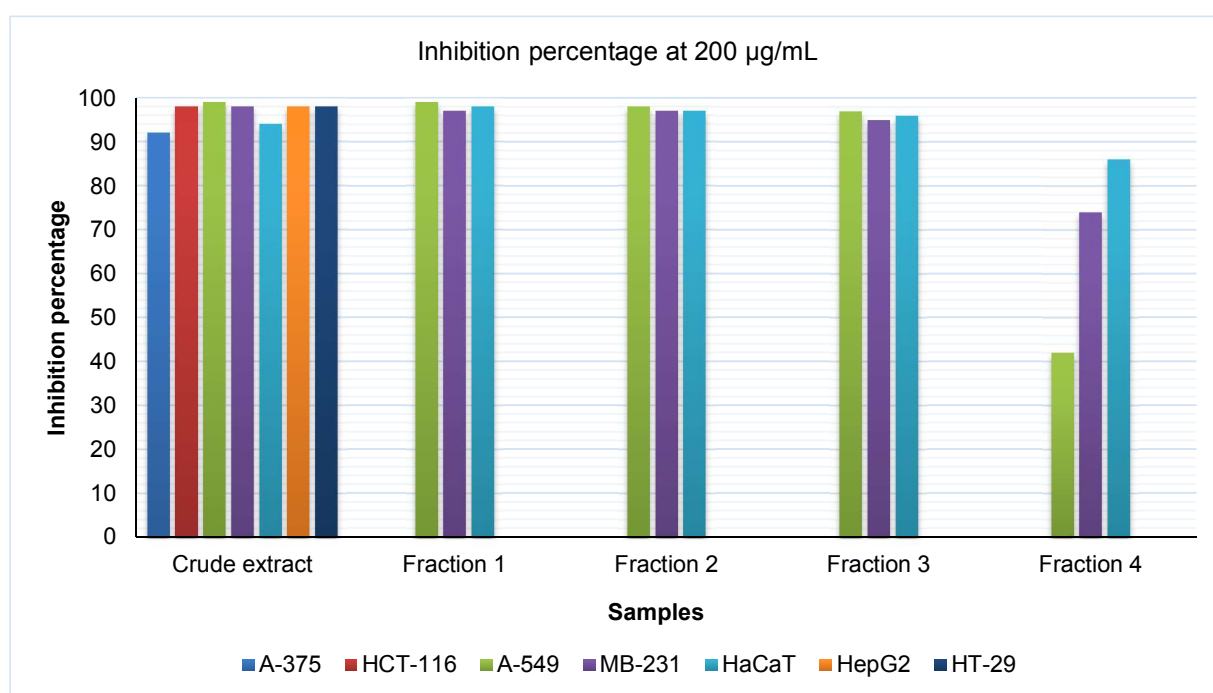


Figure S18. In vitro activity of crude *Latrunculia* extract and its SPE fractions against cancer cell lines. Test concentration: 200 µg/mL. Because of limited amounts available, fraction 5 was not tested against any cell lines while the other 4 fractions were tested only against three cancer cell lines.