Fermentation of *Illigera aromatica* with *Clonostachys rogersoniana* producing novel cytotoxic menthane-type monoterpenoid dimmers

Jian-Wei Dong, Le Cai,* Xue-Jiao Li, Rui-Feng Mei, Jia-Peng Wang, Ping Luo, Yan Shu, Zhong-Tao Ding*

Functional Molecules Analysis and Biotransformation key laboratory of Universities in Yunnan Province, School of Chemical Science and Technology, Yunnan University, Kunming 650091, P.R. China.

Supporting Information

* Corresponding authors.

E-mail addresses: ztding@ynu.edu.cn (Z.T. Ding); caile@ynu.edu.cn (L. Cai).

****

Table of Content

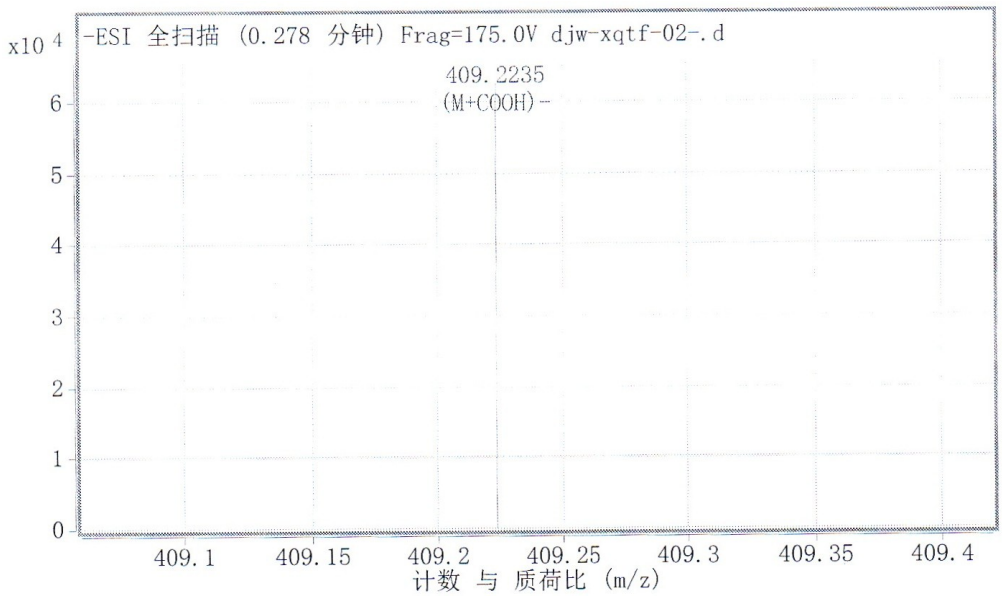


Figure S1 HRESIMS spetrum of dimericilligerate E (1)

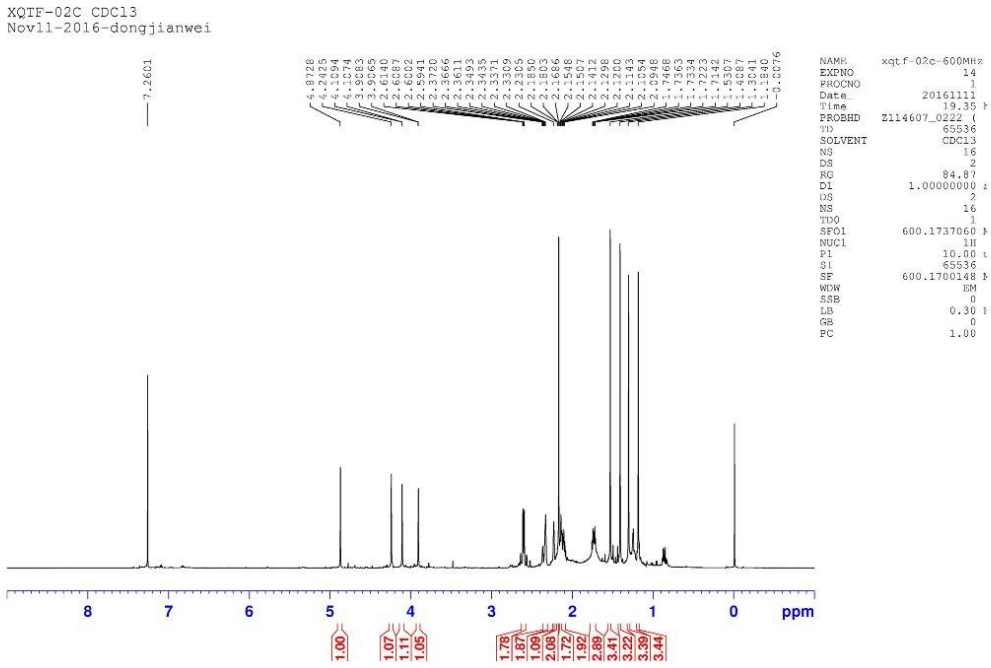


Figure S2 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of dimericilligerate E (1)

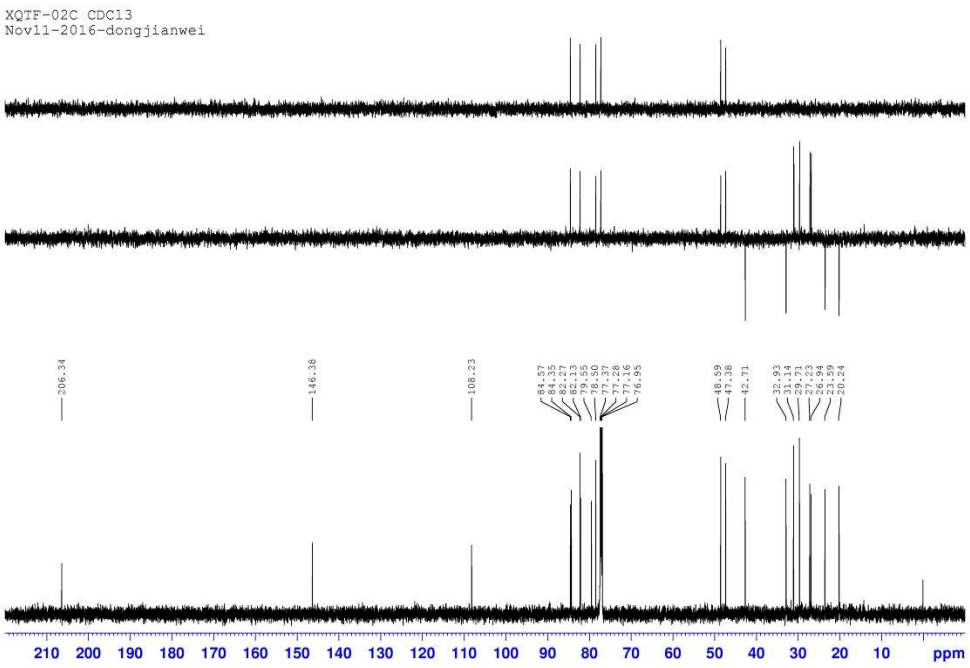


Figure S3 ^{13}C NMR and DEPT spectra ($CDCl_3$, 150 MHz) of dimericilligerate E (1)

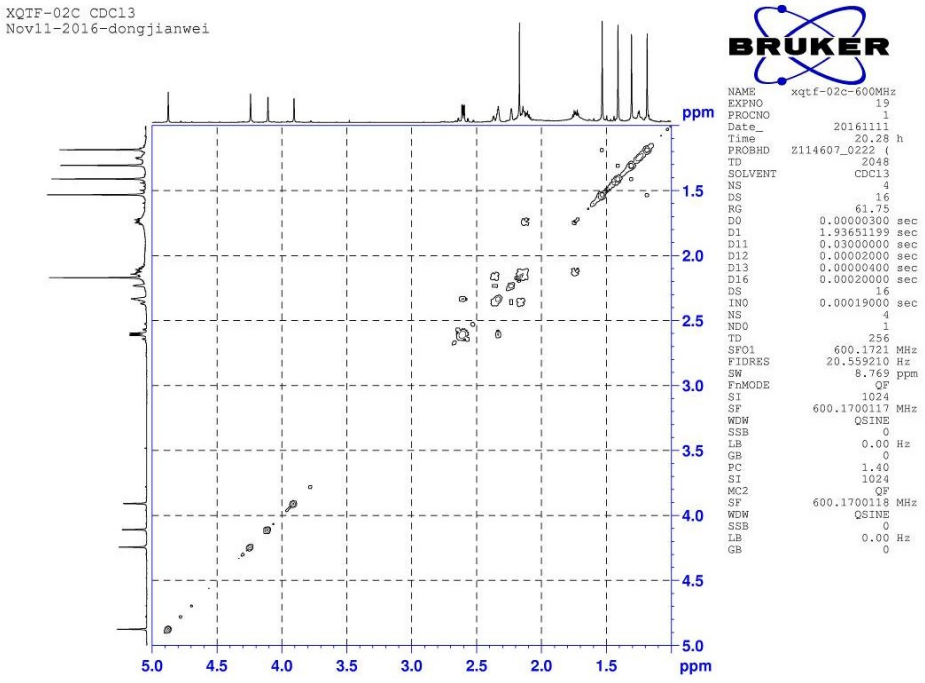


Figure S4 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate E (1)

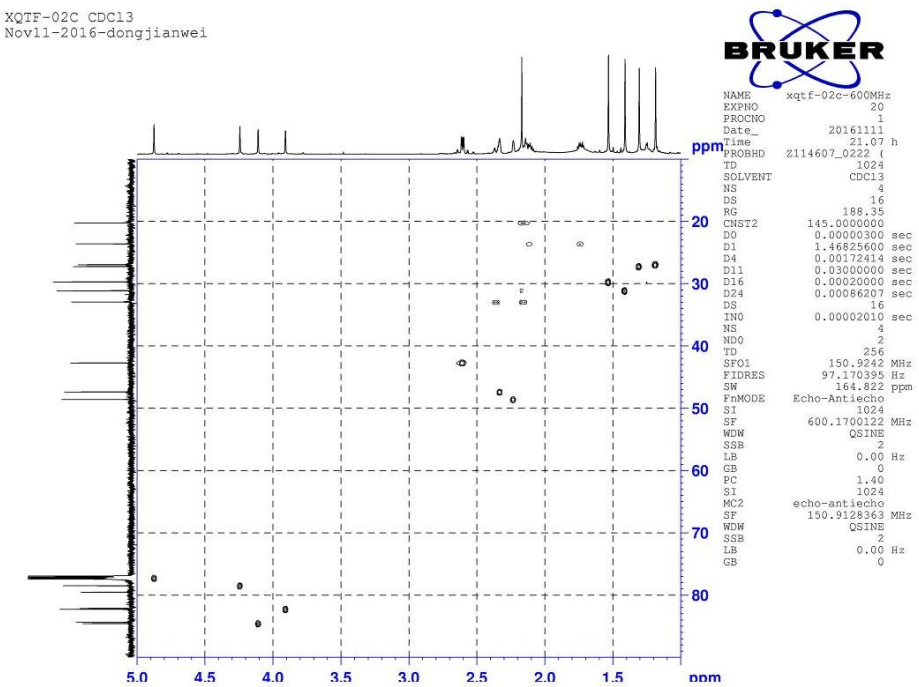


Figure S5 HSQCspectrum ($CDCl_3$, 600 MHz) of dimericilligerate E (1)

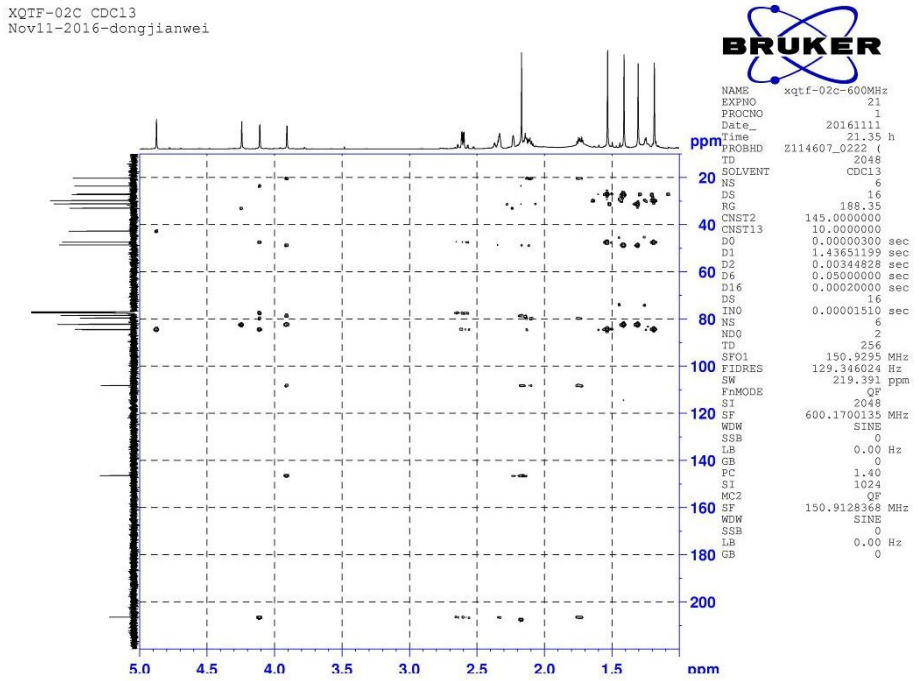


Figure S6 HMBC spectrum ($CDCl_3$, 600 MHz) of dimericilligerate E (1)

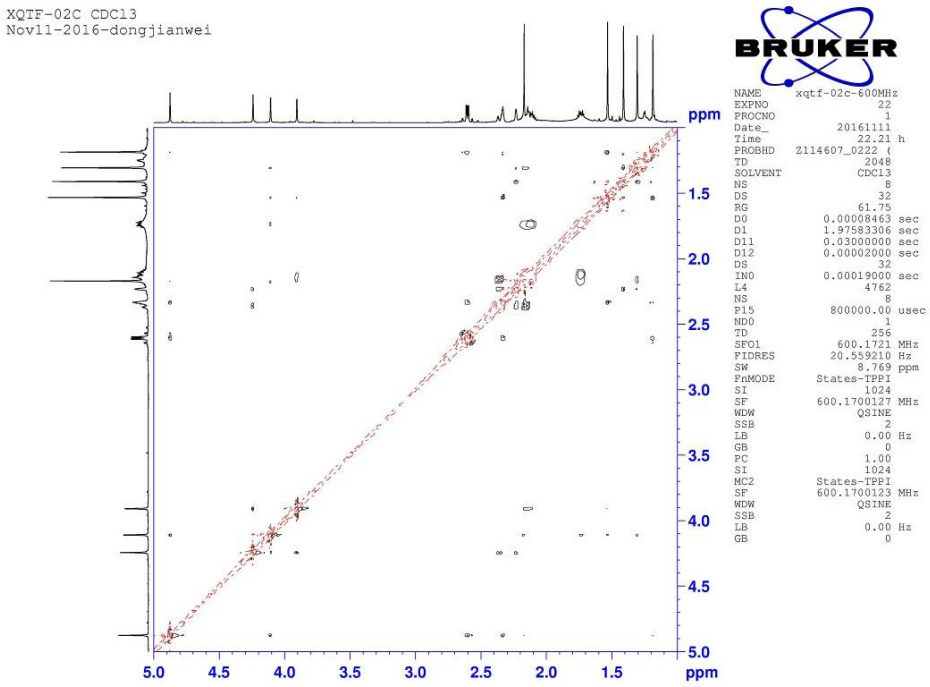


Figure S7 ROESY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate E (1)

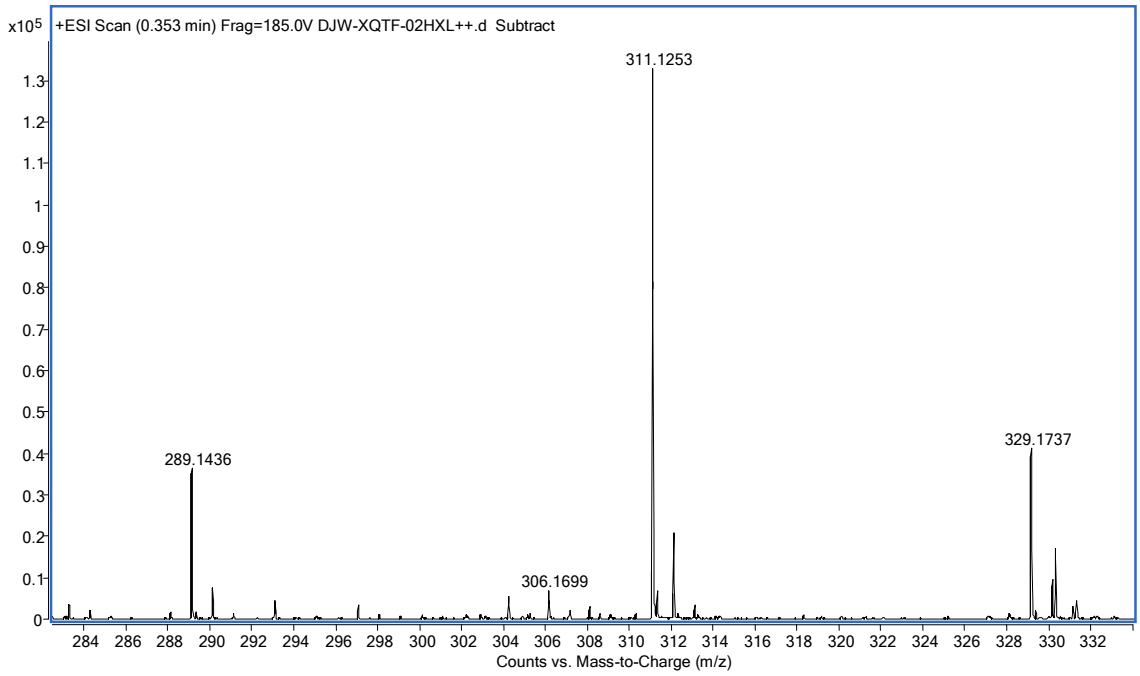


Figure S8 HRESIMS spetrum of 1a

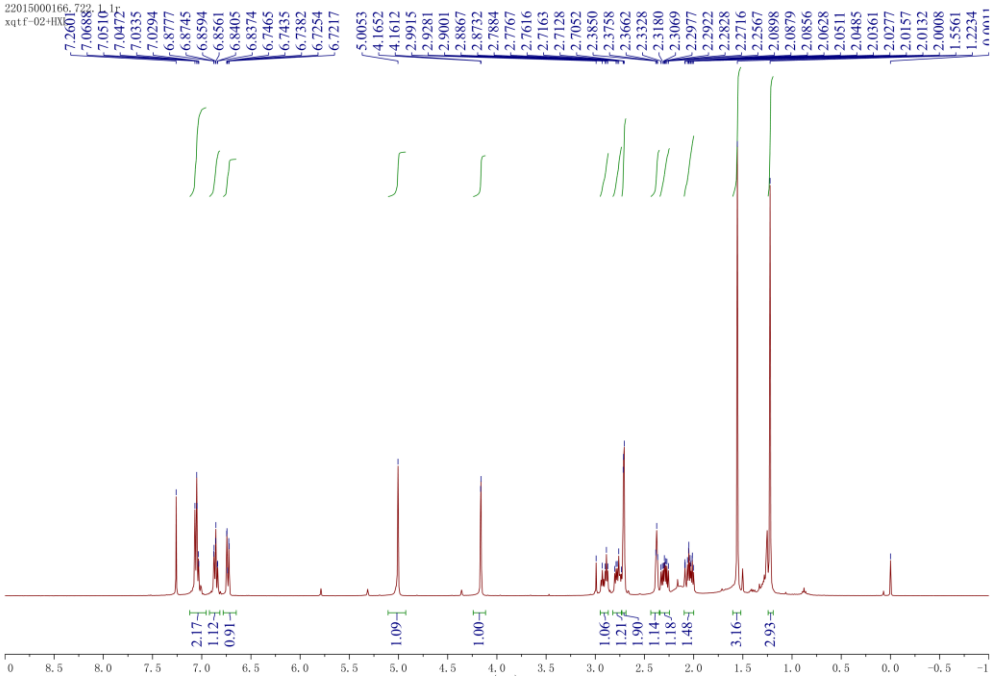


Figure S9 ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of 1a

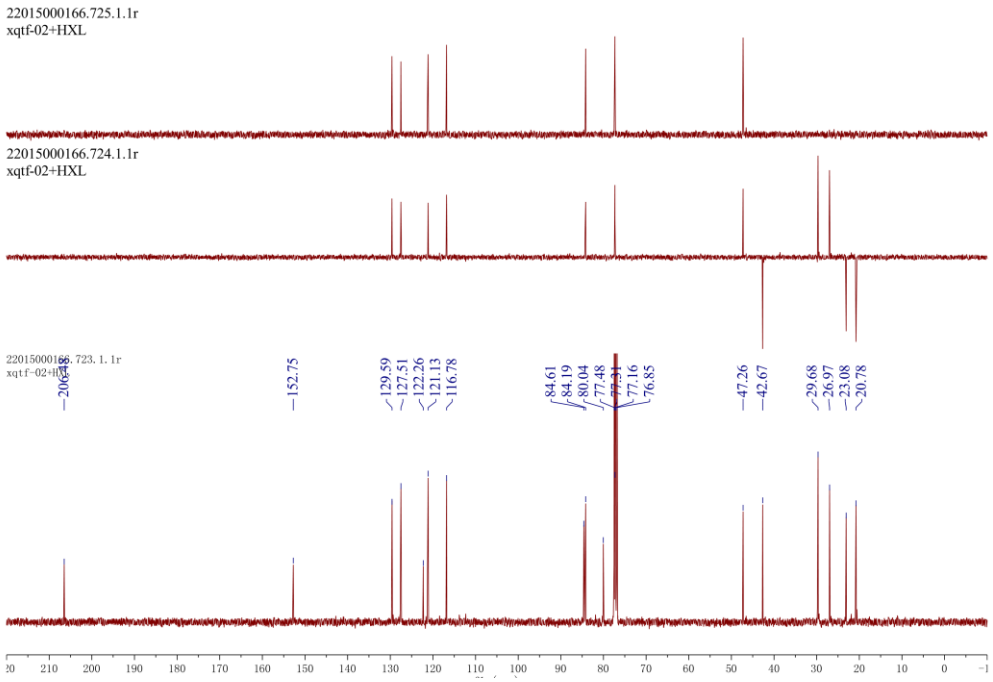


Figure S10 ^{13}C NMR and DEPT spectra ($CDCl_3$, 100 MHz) of 1a

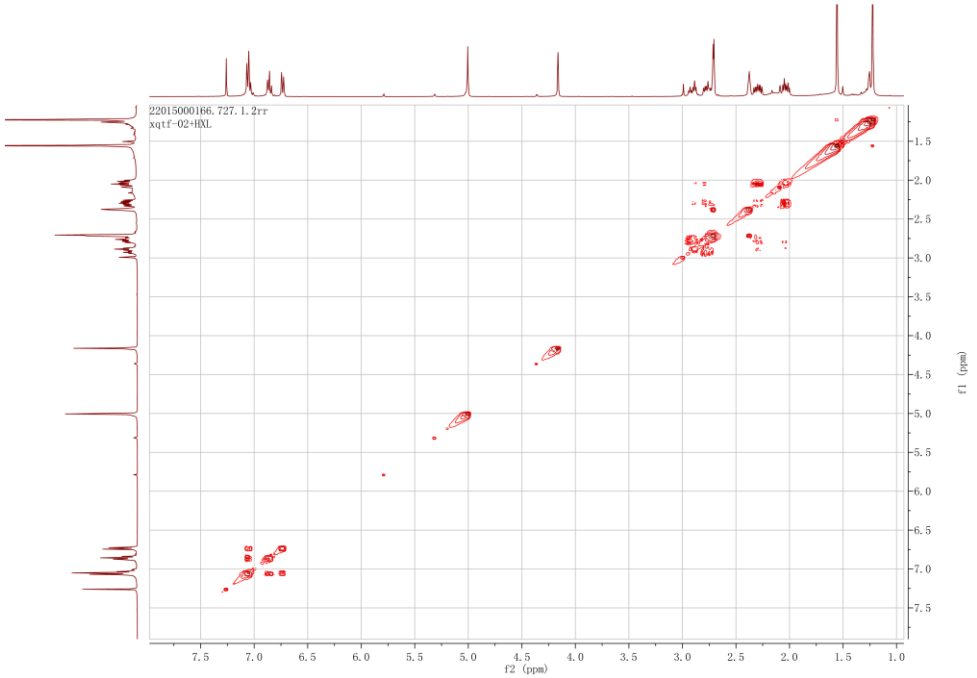


Figure S11 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 400 MHz) of 1a

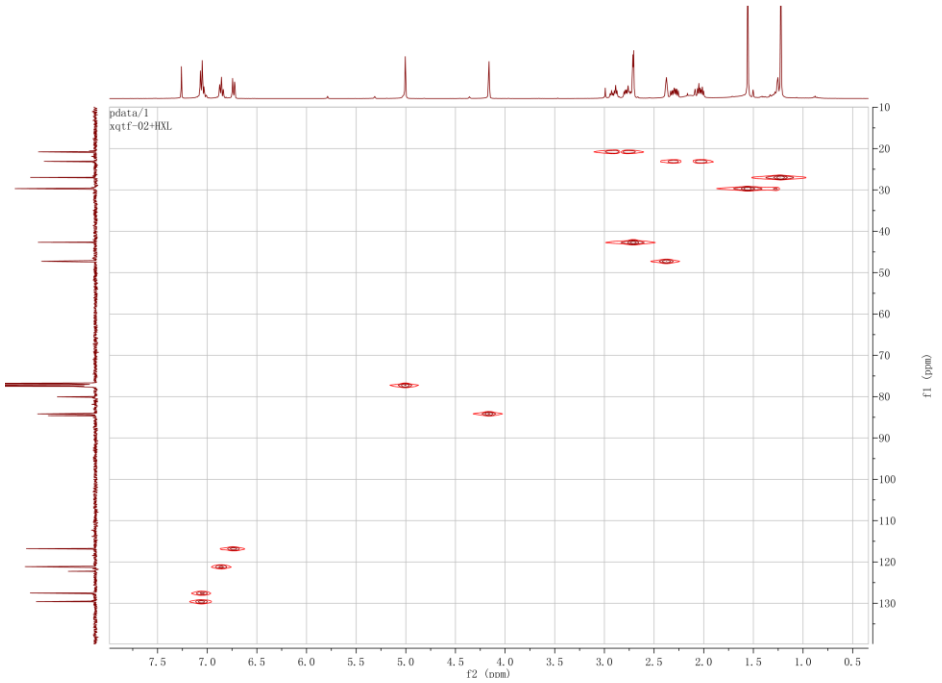


Figure S12 HSQCspectrum ($CDCl_3$, 400 MHz) of 1a

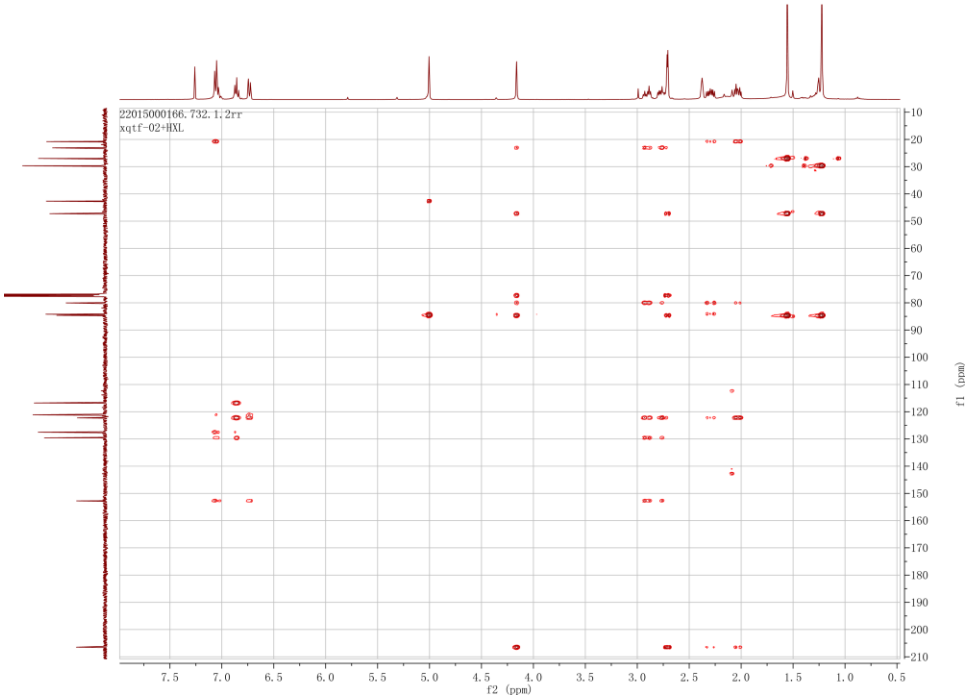


Figure S13 HMBC spectrum ($CDCl_3$, 400 MHz) of 1a

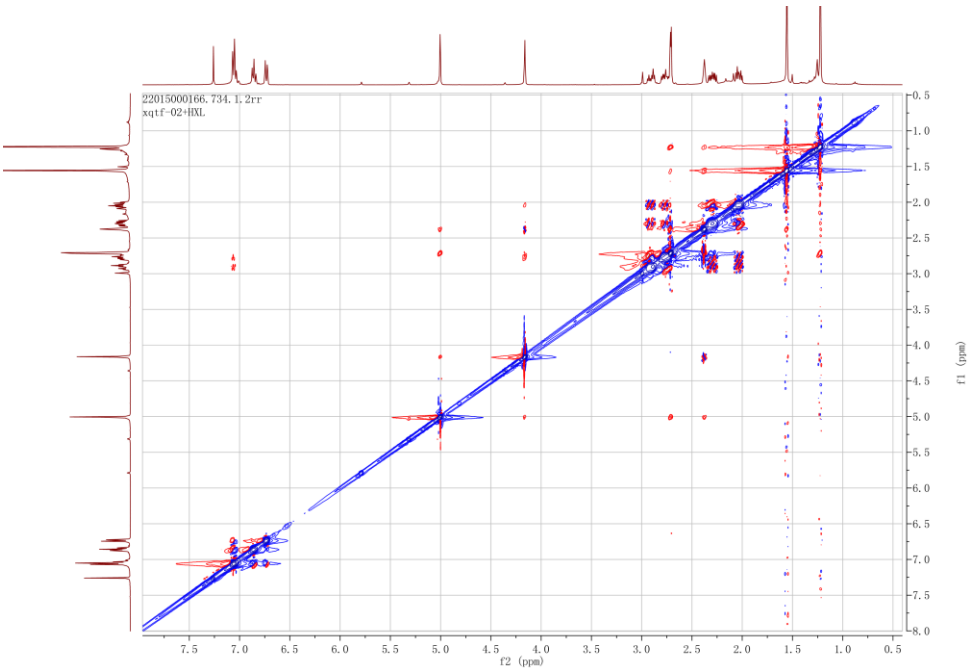


Figure S14 ROESY spectrum ($CDCl_3$, 400 MHz) of 1a

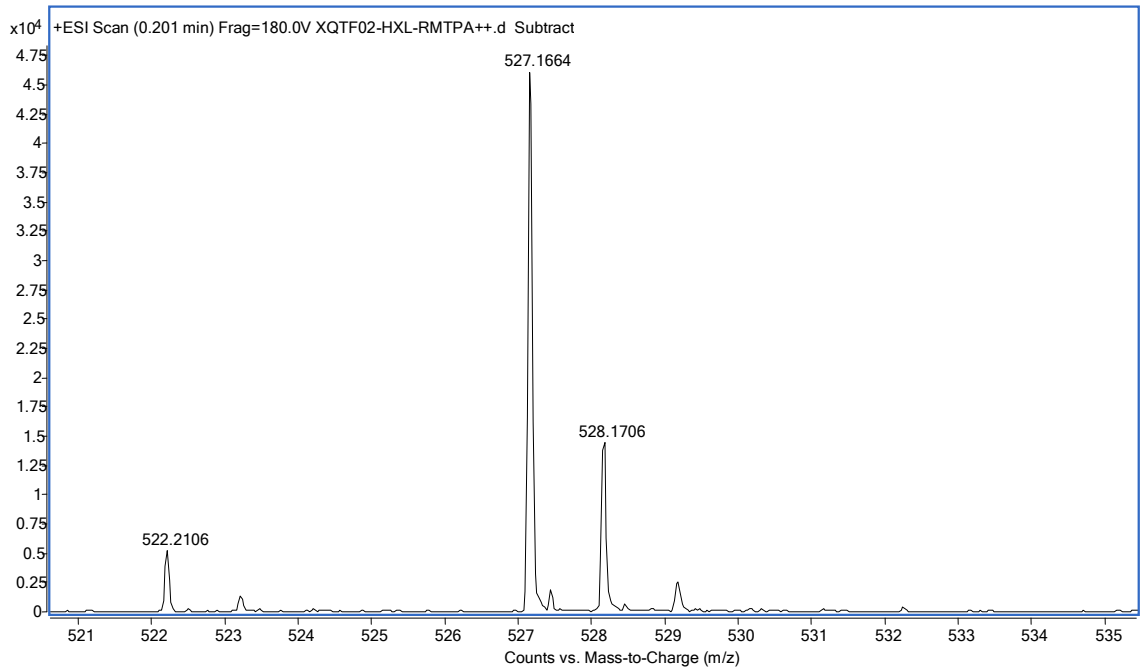


Figure S15 HRESIMS spetrum of (*R*)-MTPA ester of 1a

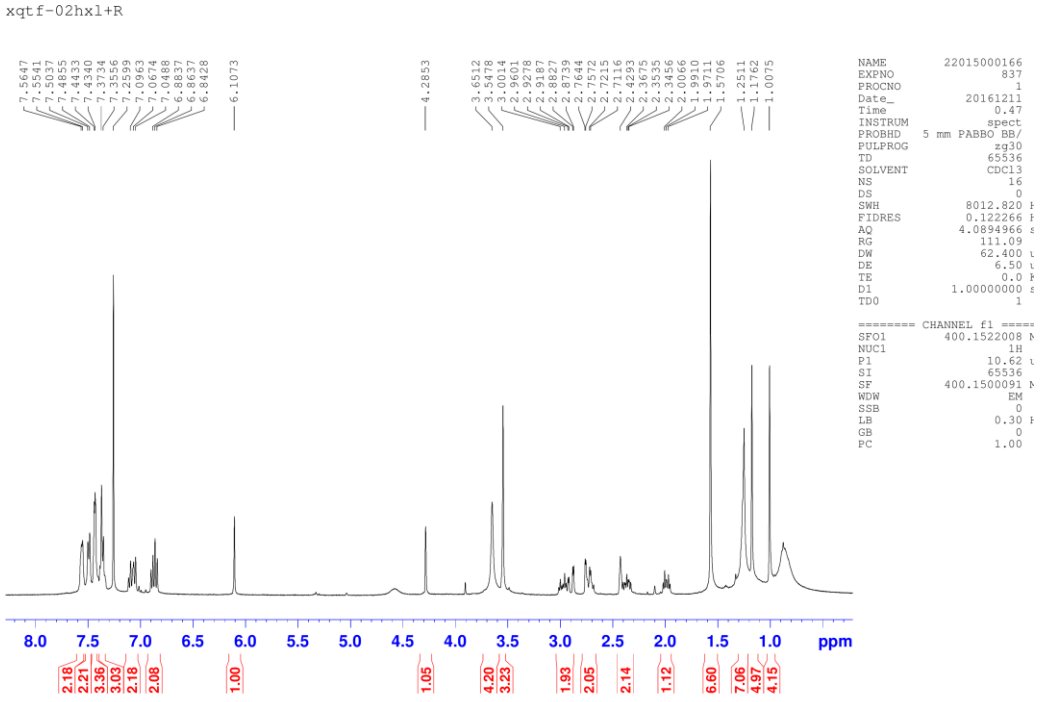


Figure S16 ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of (*R*)-MTPA ester of 1a

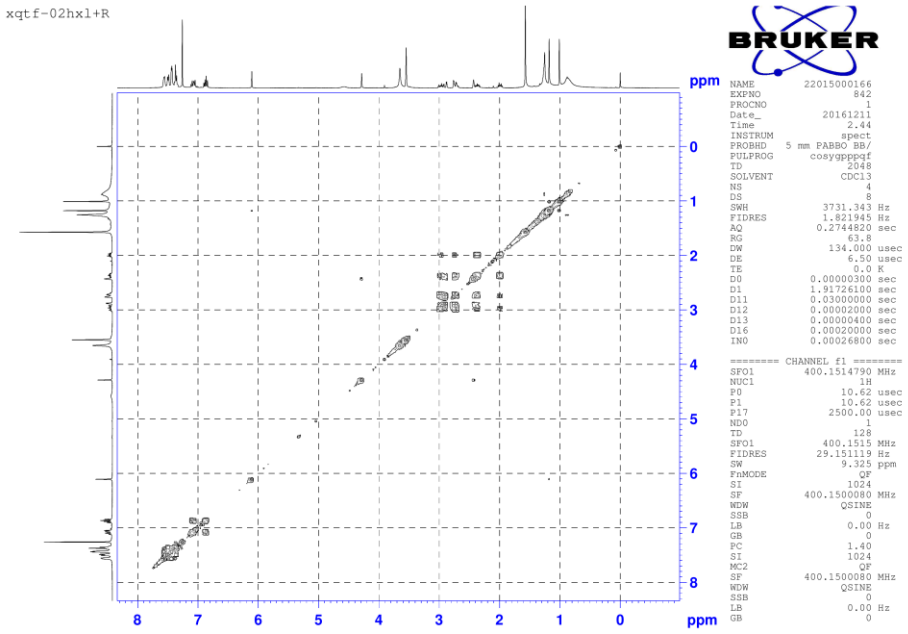


Figure S17 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 400 MHz) of (*R*)-MTPA ester of 1a

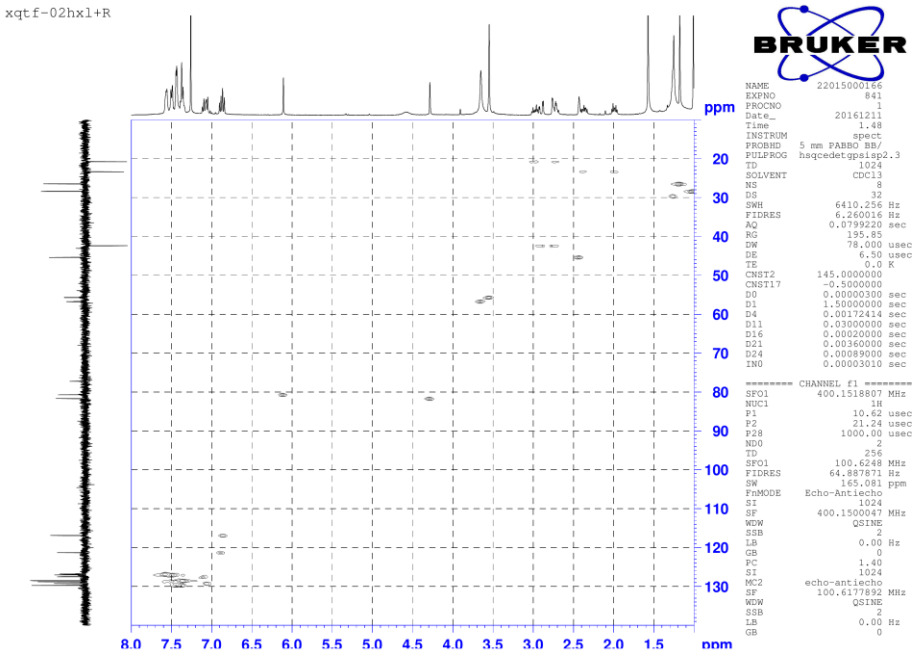


Figure S18 HSQC spectrum ($CDCl_3$, 400 MHz) of (*R*)-MTPA ester of 1a

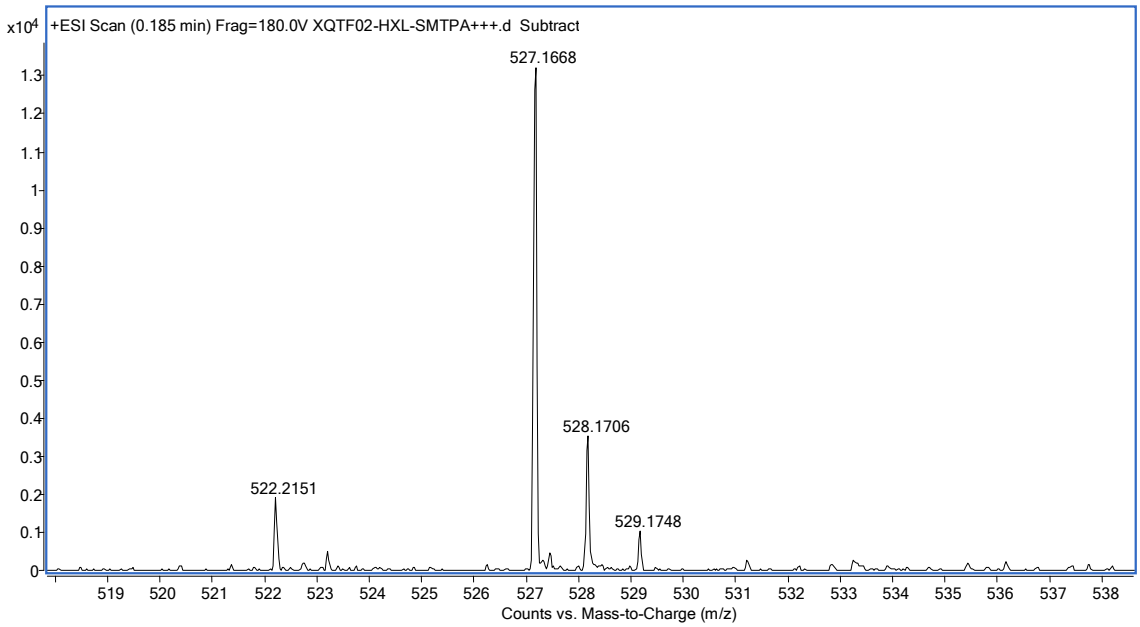


Figure S19 HRESIMS spetrum of (*S*)-MTPA ester of 1a

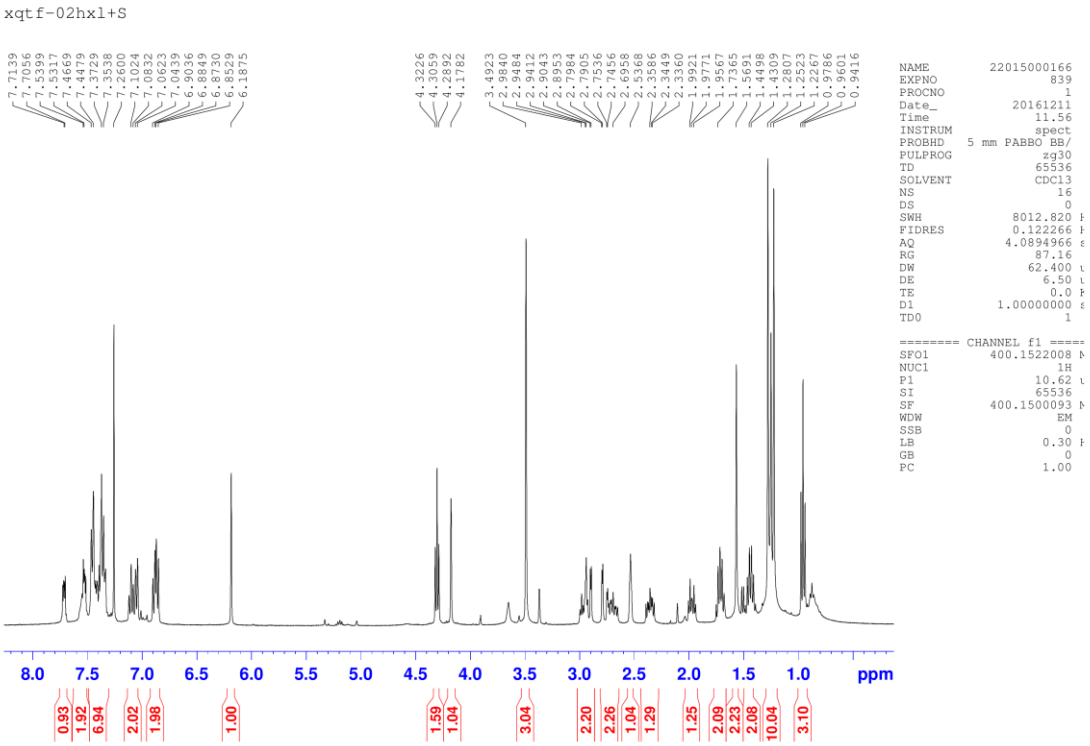


Figure S20 ^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of (*S*)-MTPA ester of 1a

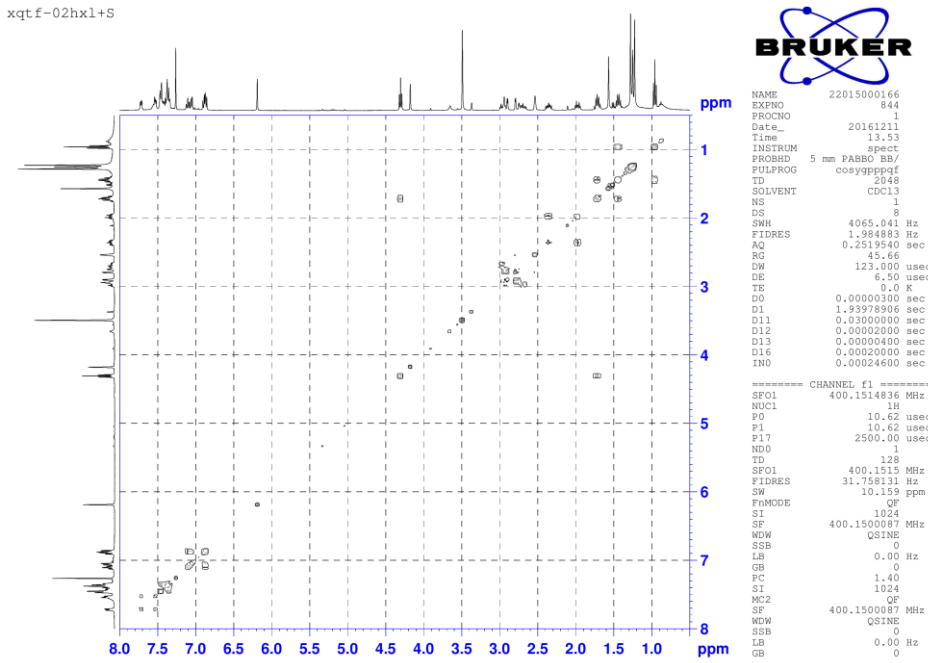


Figure S21 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 400 MHz) of (*S*)-MTPA ester of 1a

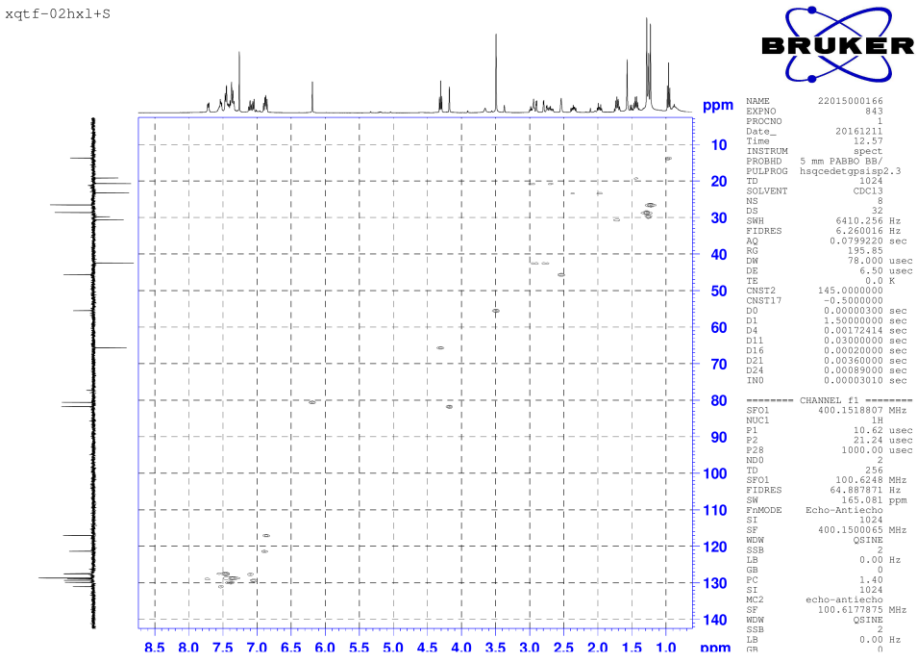
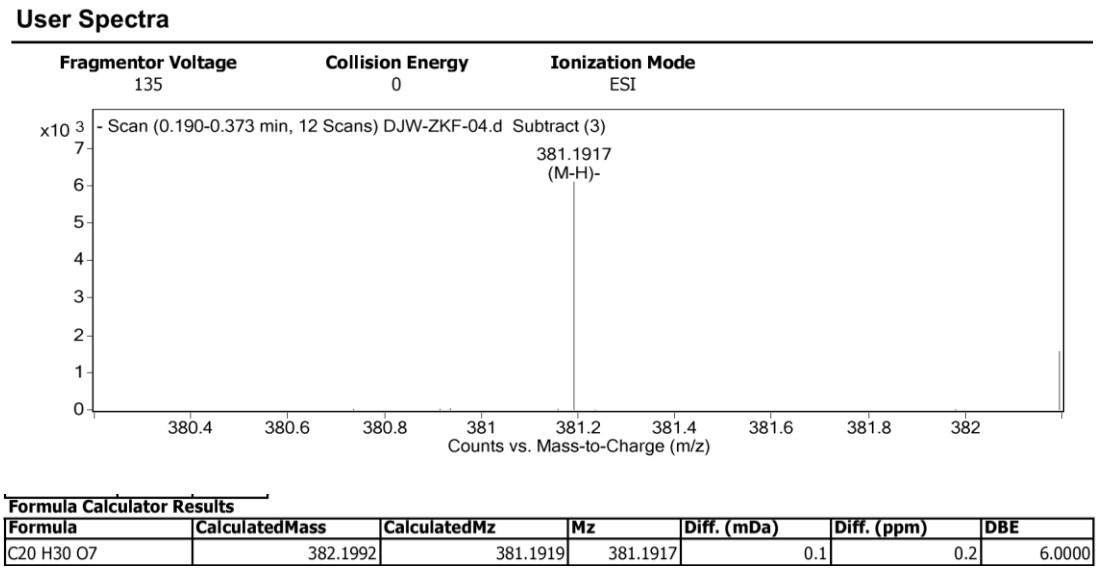


Figure S22 ROESY spectrum ($CDCl_3$, 400 MHz) of (*S*)-MTPA ester of 1a



Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H30 O7	382.1992	381.1919	381.1917	0.1	0.2	6.0000

Figure S23 HRESIMS spetrum of dimericilligerate F (2)

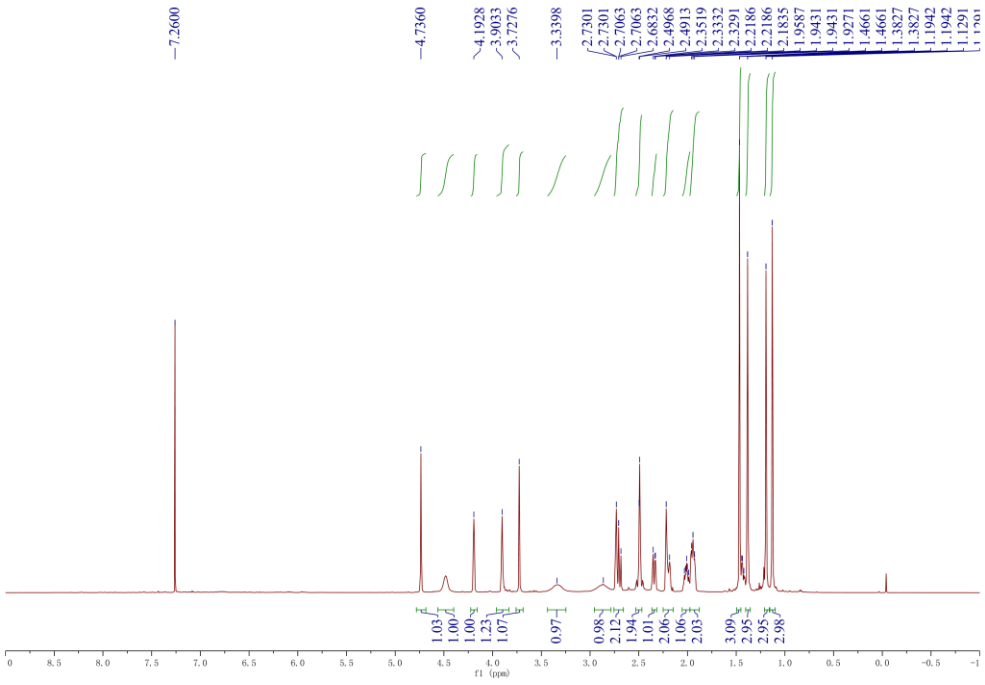


Figure S24 ^{1}H-NMR spectrum ($CDCl_3$, 600 MHz) of dimericilligerate F (2)

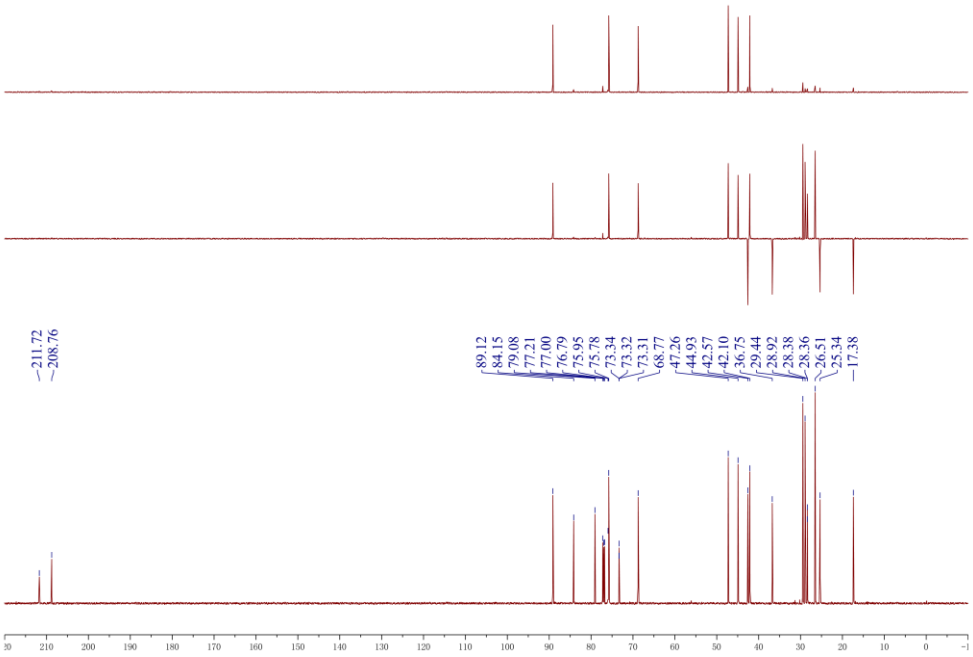


Figure S25 ^{13}C-NMR and DEPT spectra ($CDCl_3$, 150 MHz) of dimericilligerate F (2)

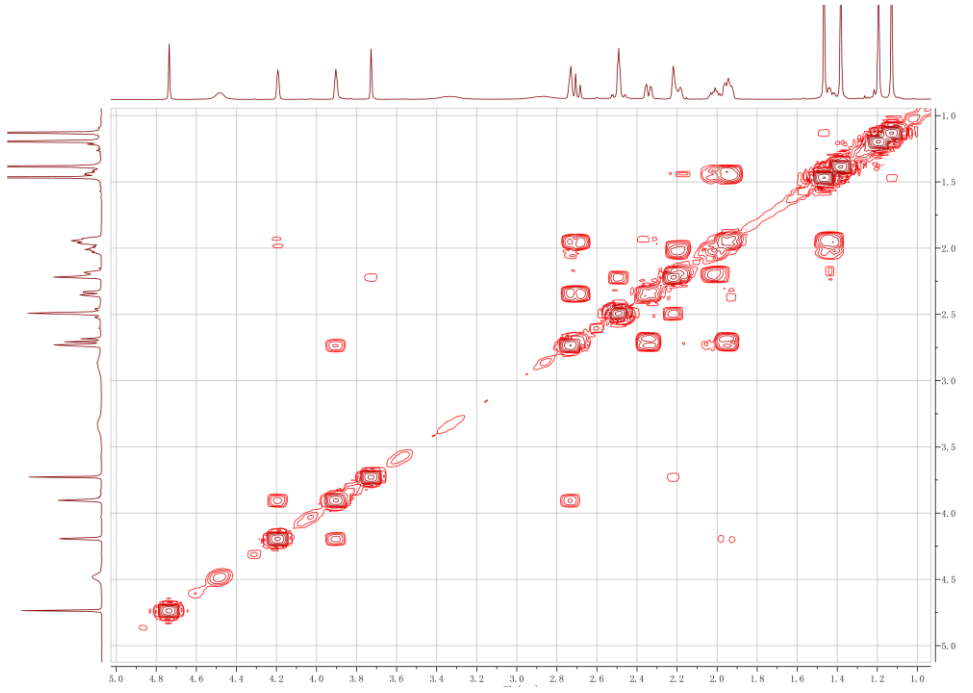


Figure S26 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate F (2)

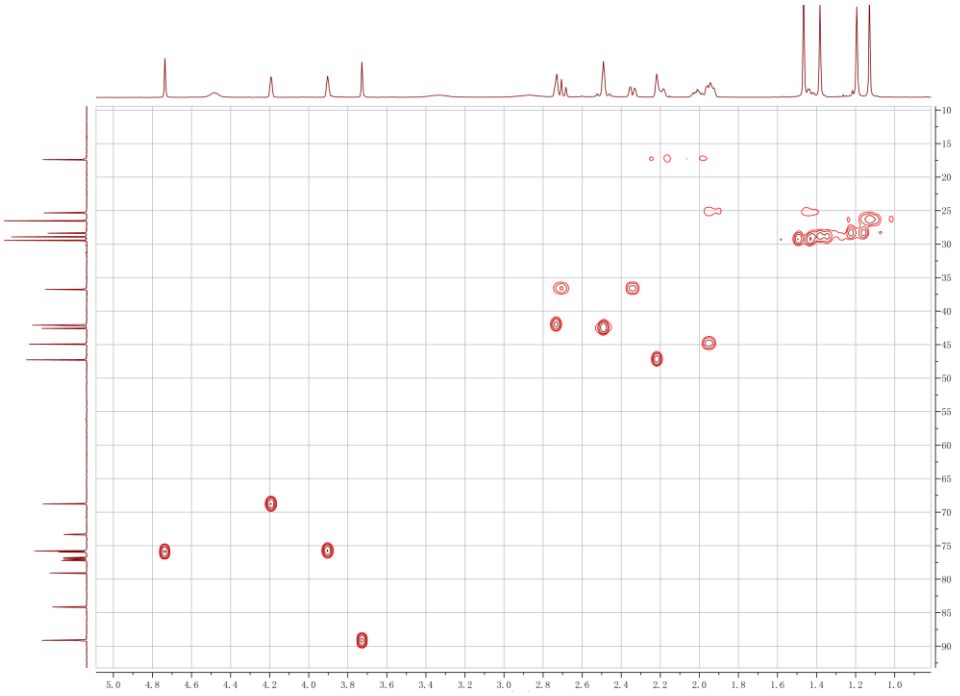


Figure S27 HSQCspectrum ($CDCl_3$, 600 MHz) of dimericilligerate F (2)

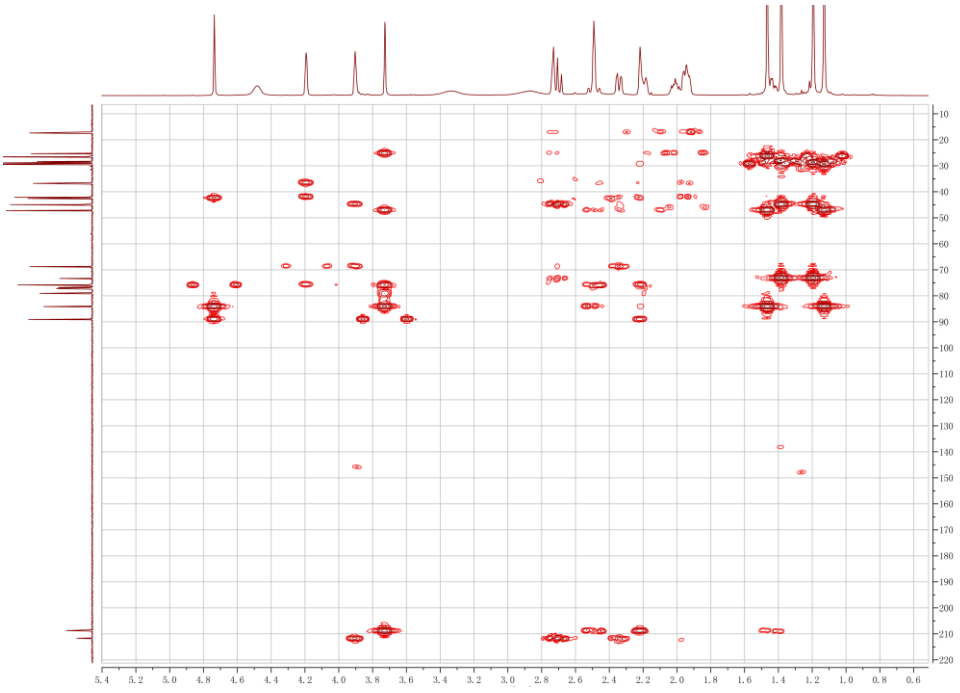


Figure S28 HMBC spectrum ($CDCl_3$, 600 MHz) of dimericilligerate F (2)

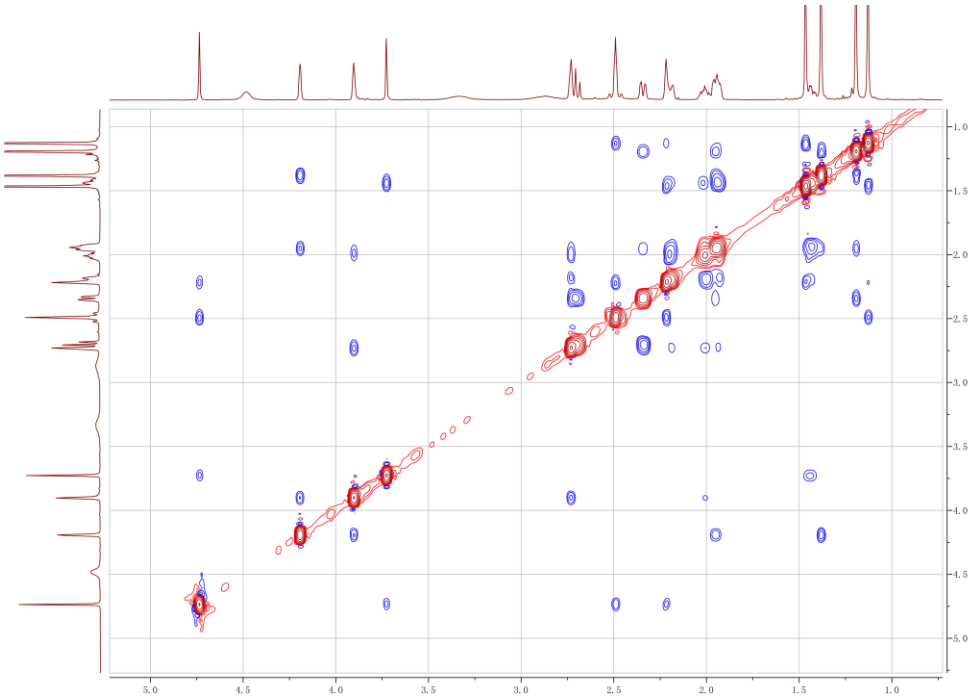


Figure S29 NOESY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate F (2)

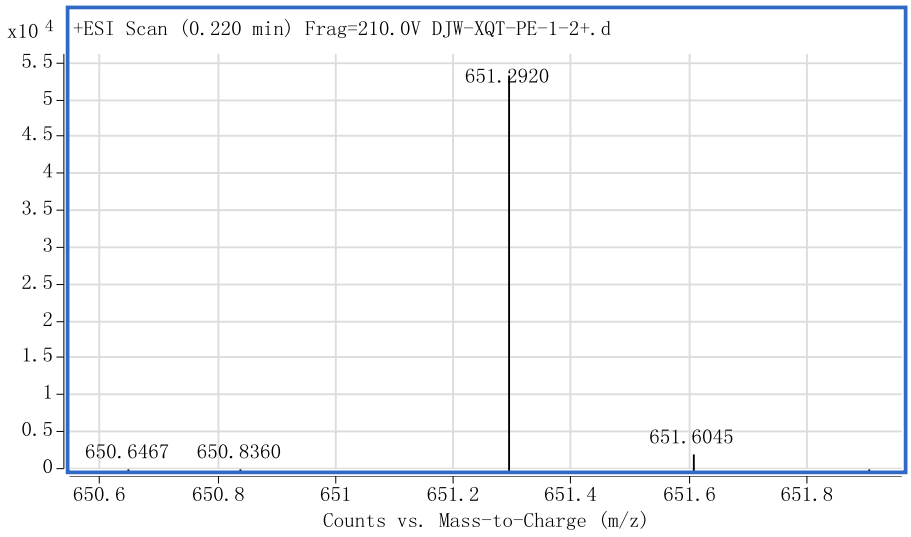


Figure S30 HRESIMS spetrum of dimericilligerate A (3)

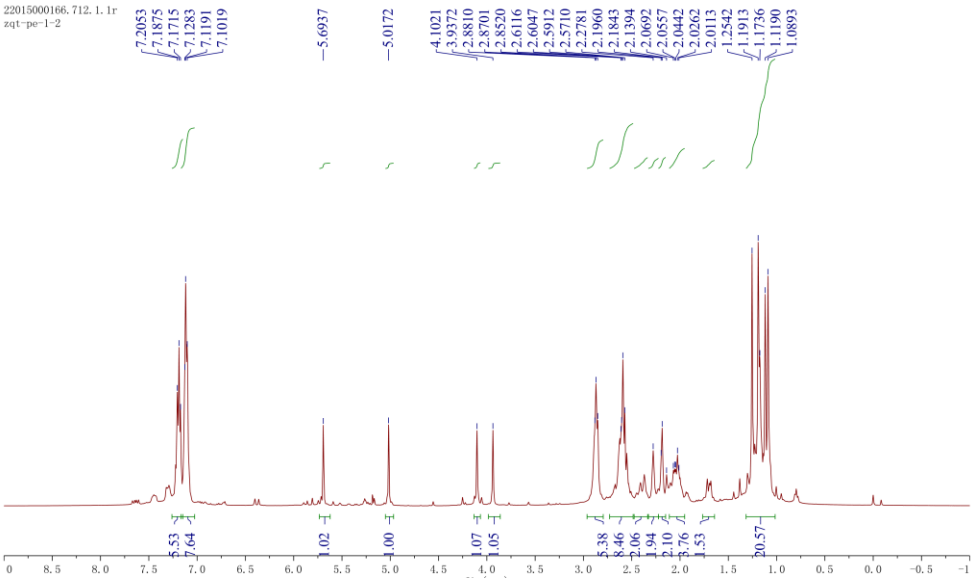


Figure S31 ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of dimericilligerate A (3)

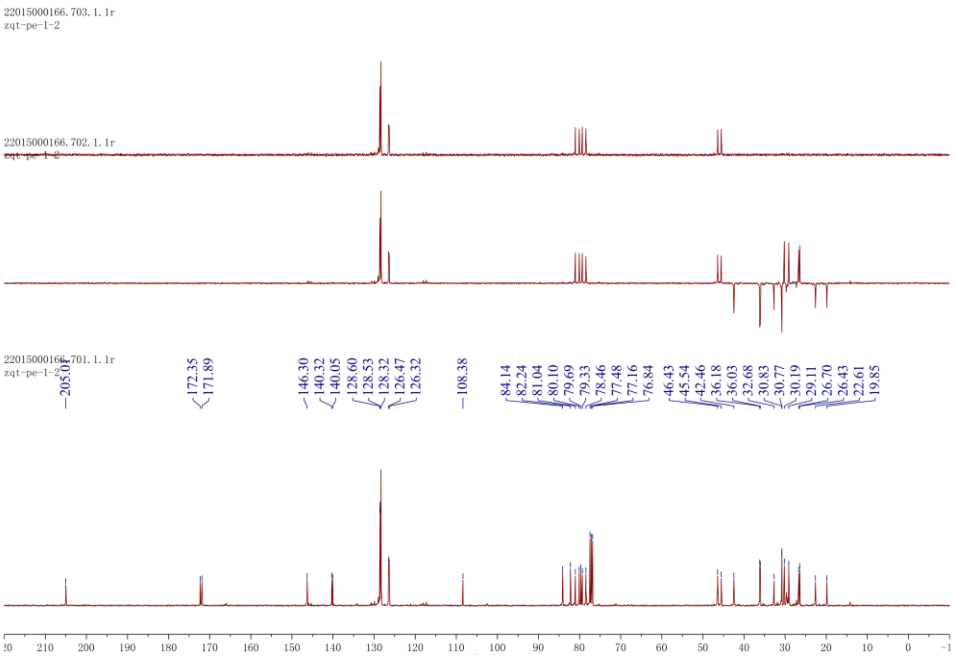


Figure S32 ^{13}C NMR and DEPT spectra ($CDCl_3$, 100 MHz) of dimericilligerate A (3)

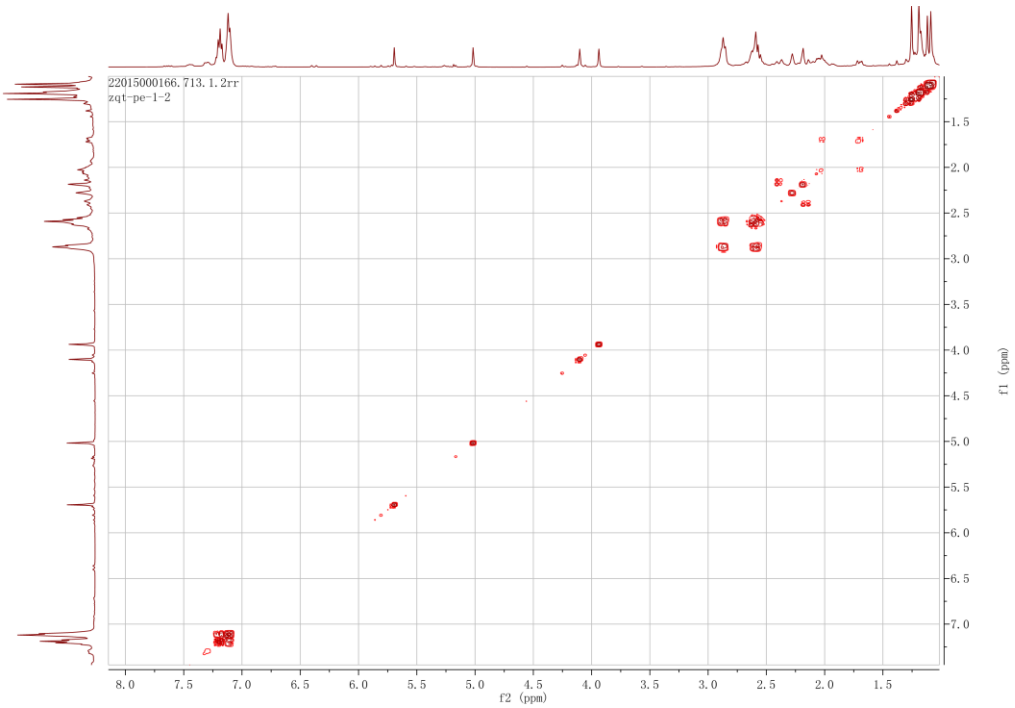


Figure S33 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 400 MHz) of dimericilligerate A (3)

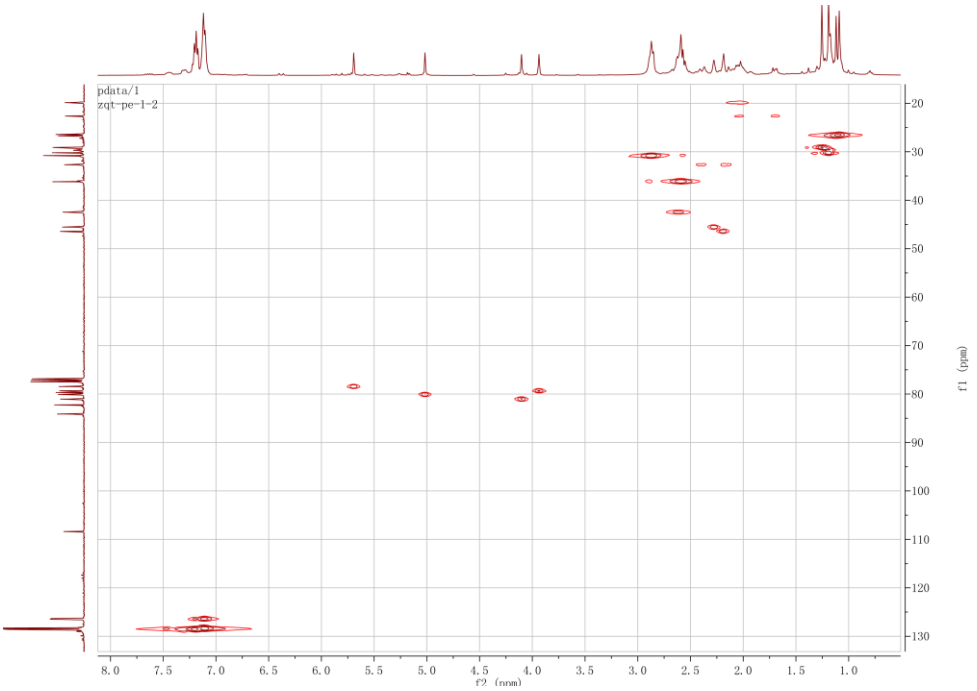


Figure S34 HSQCspectrum ($CDCl_3$, 400 MHz) of dimericilligerate A (3)

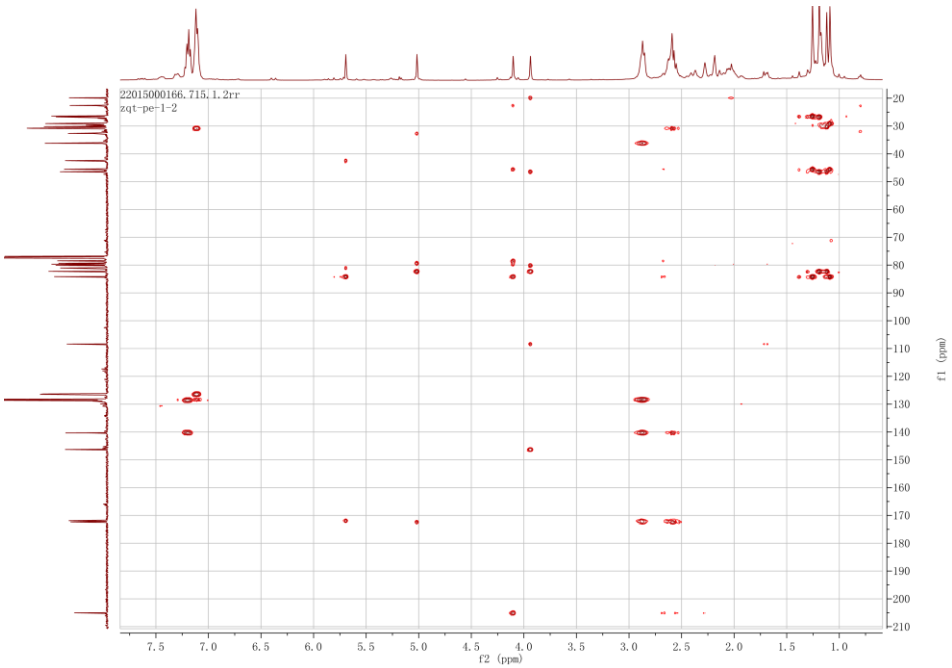


Figure S35 HMBC spectrum ($CDCl_3$, 400 MHz) of dimericilligerate A (3)

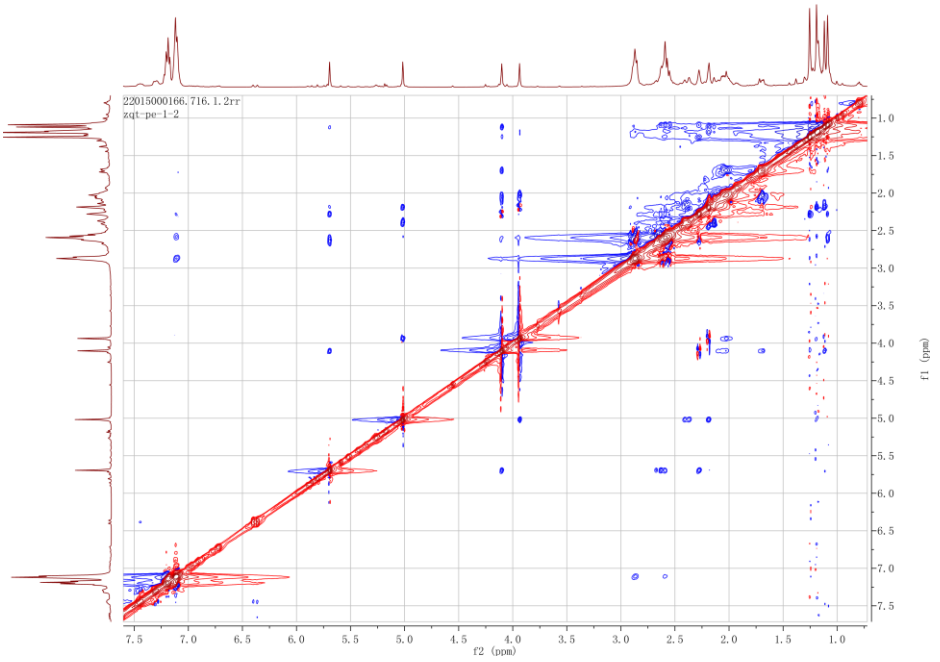


Figure S36 ROESY spectrum ($CDCl_3$, 400 MHz) of dimericilligerate A (3)

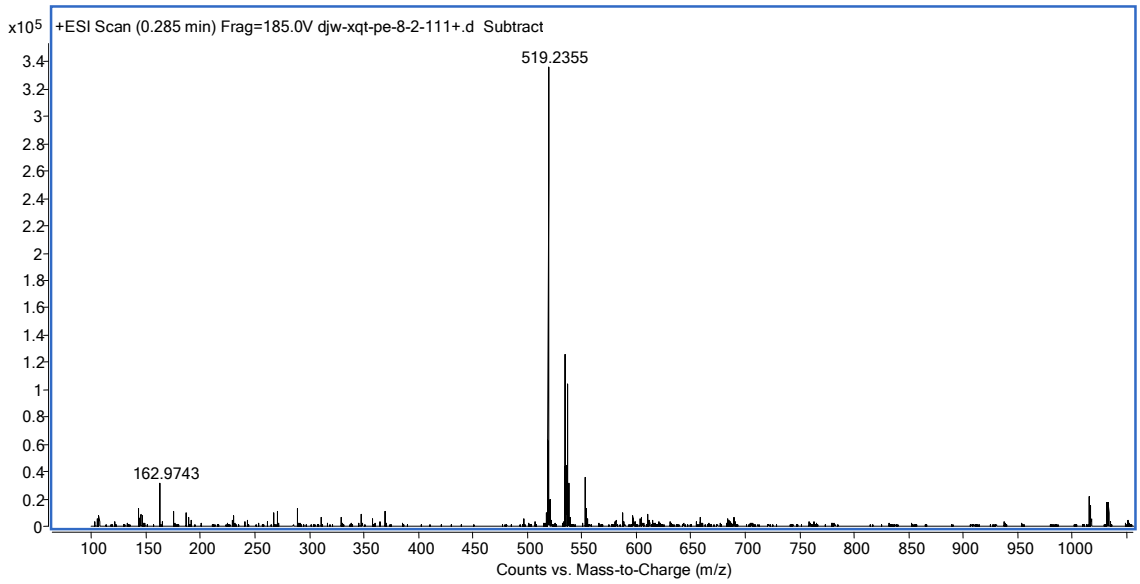


Figure S37 HRESIMS spetrum of dimericilligerate B (4)

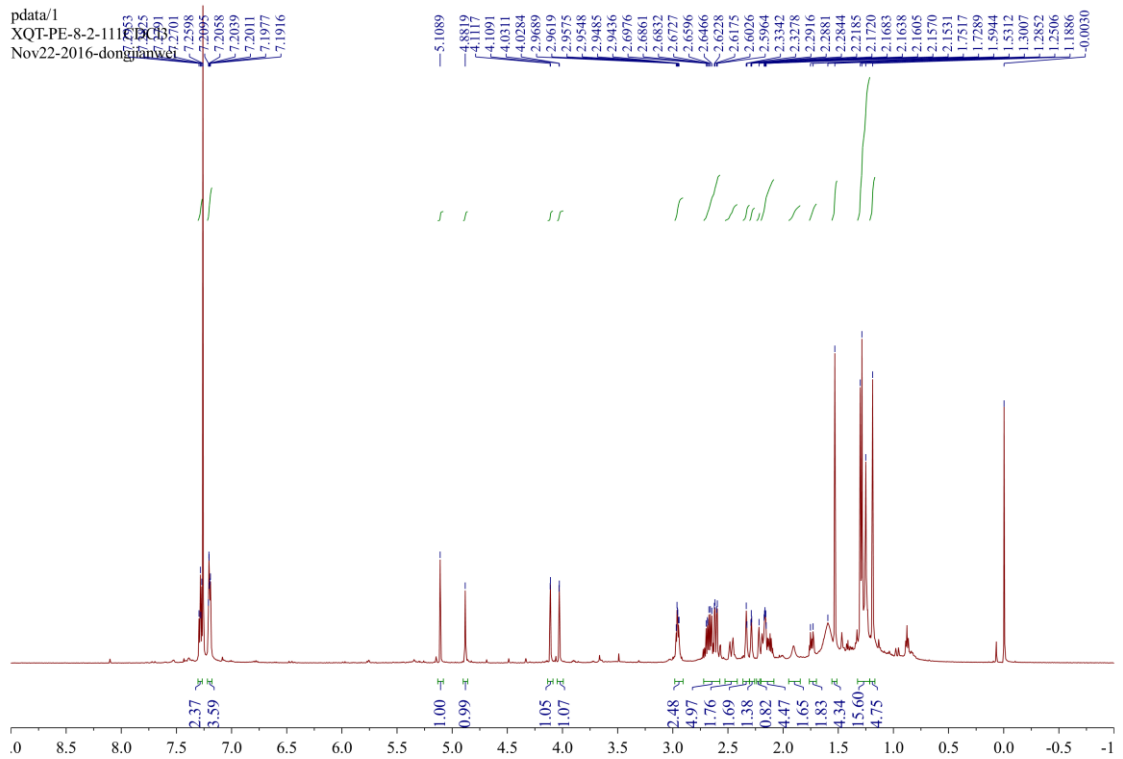


Figure S38 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of dimericilligerate B (4)

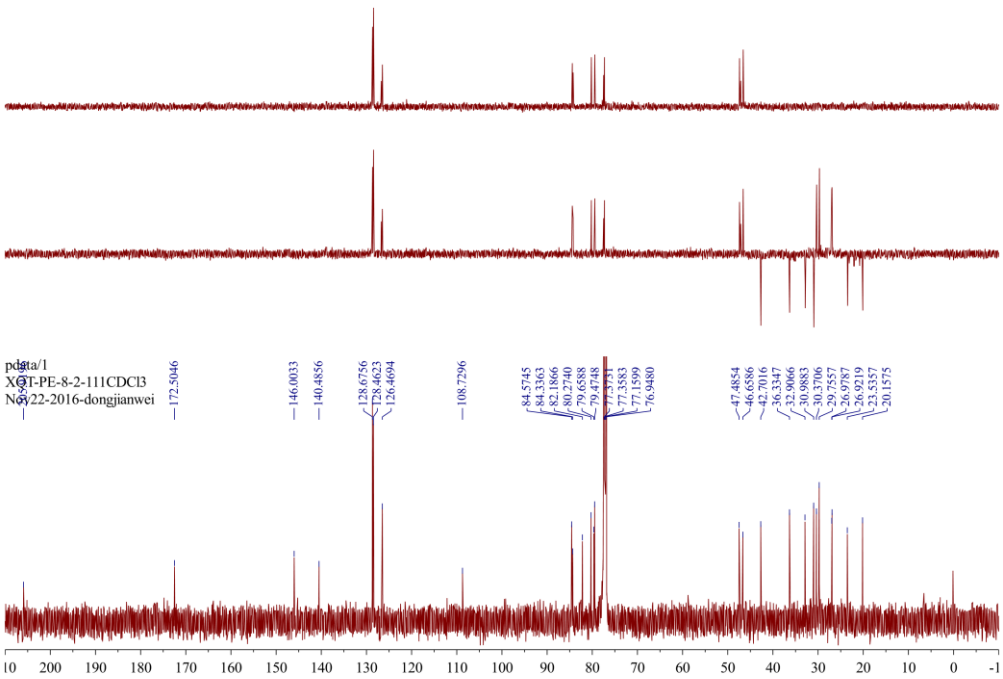


Figure S39 ^{13}C NMR and DEPT spectra ($CDCl_3$, 150 MHz) of dimericilligerate B (4)

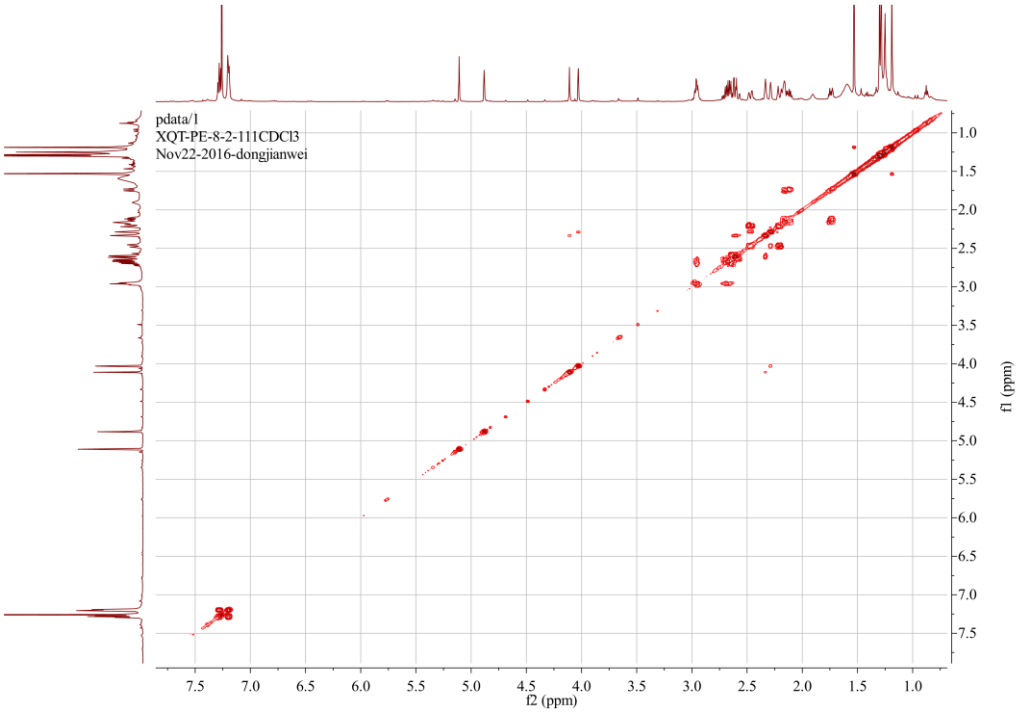


Figure S40 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate B (4)

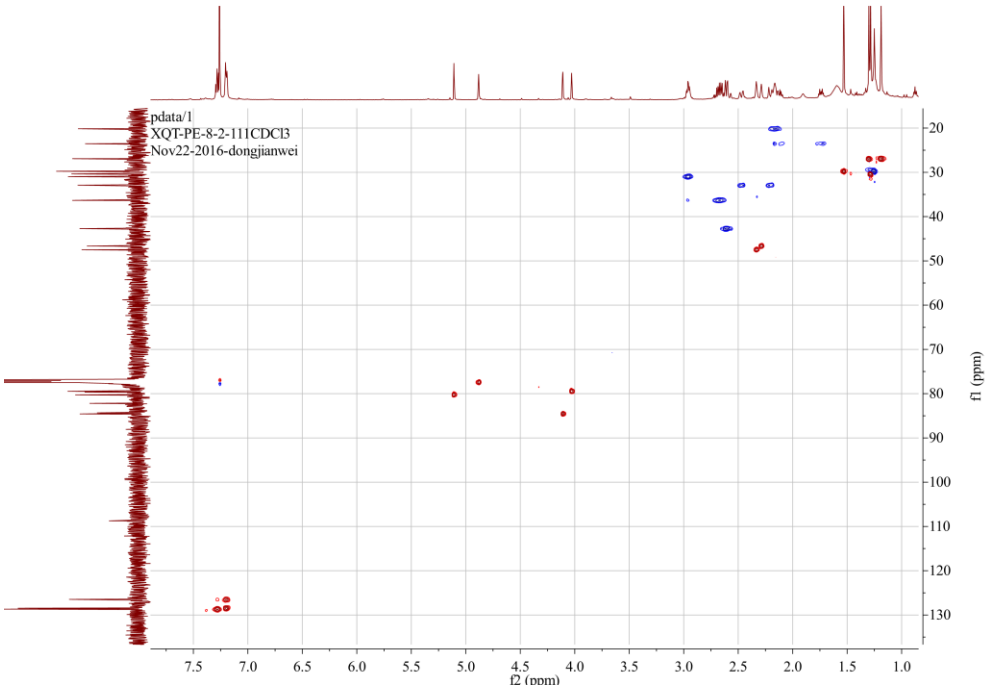


Figure S41 HSQCspectrum ($CDCl_3$, 600 MHz) of dimericilligerate B (4)

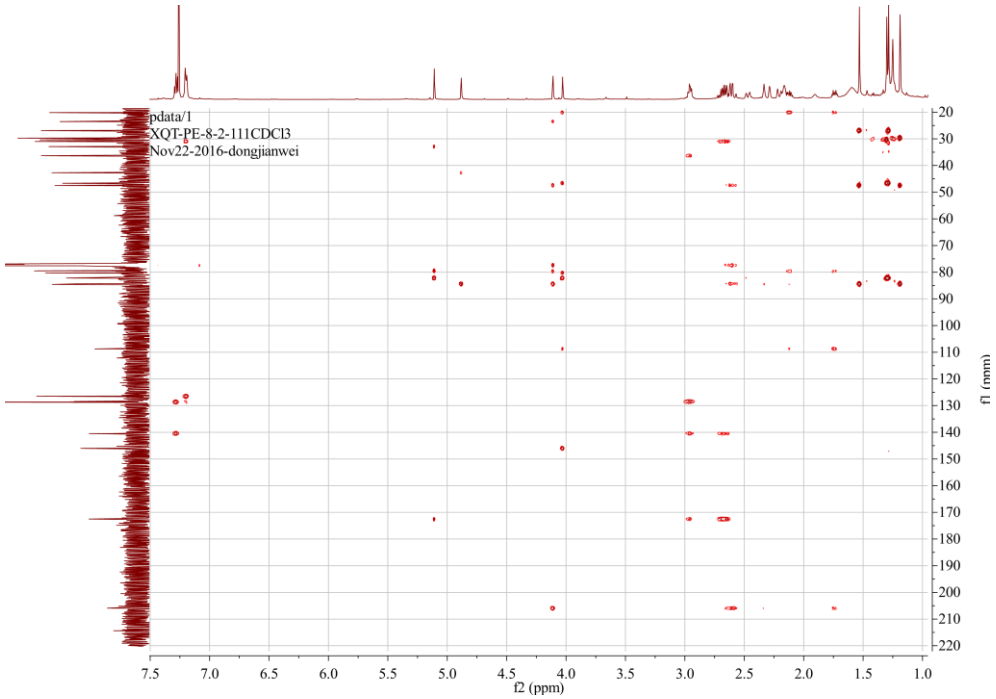


Figure S42 HMBC spectrum ($CDCl_3$, 600 MHz) of dimericilligerate B (4)

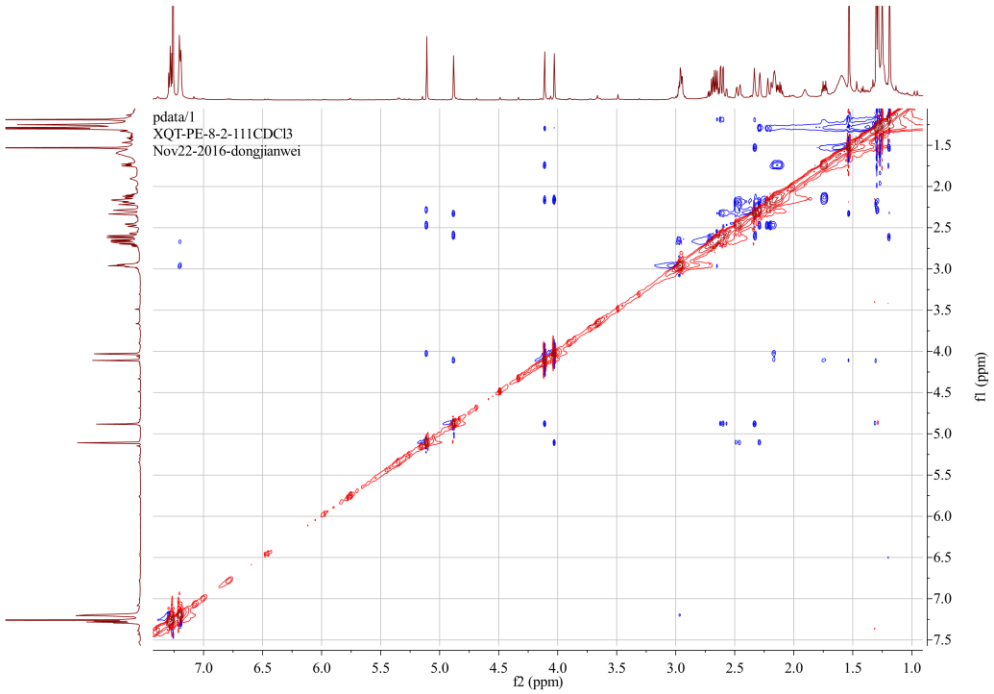


Figure S43 ROESY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate B (4)

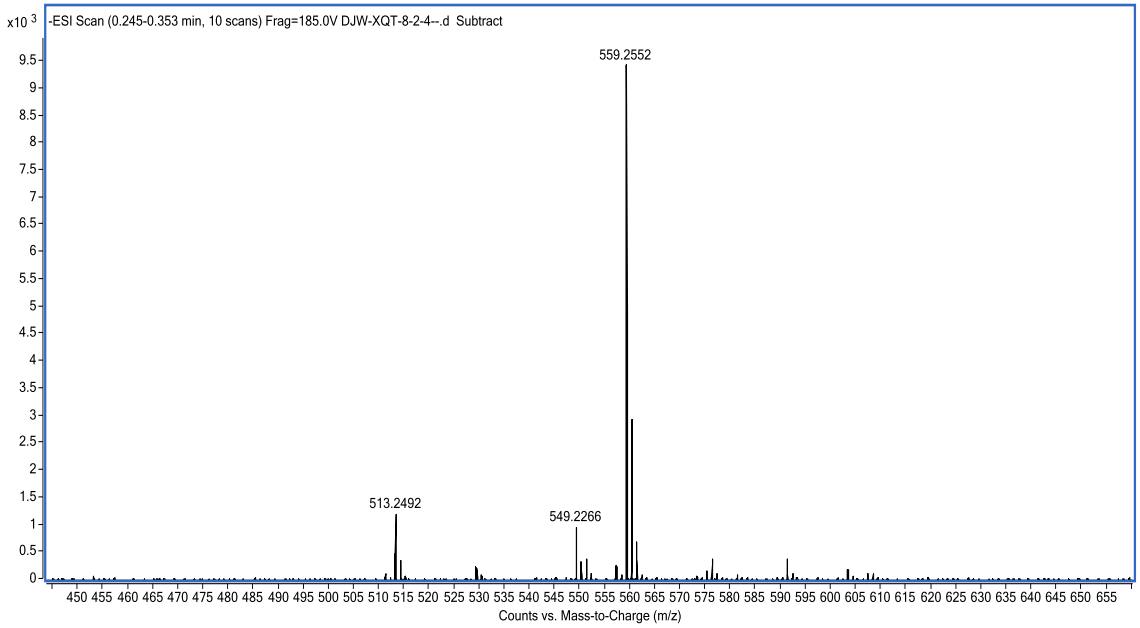


Figure S44 HRESIMS spetrum of dimericilligerate C (5)

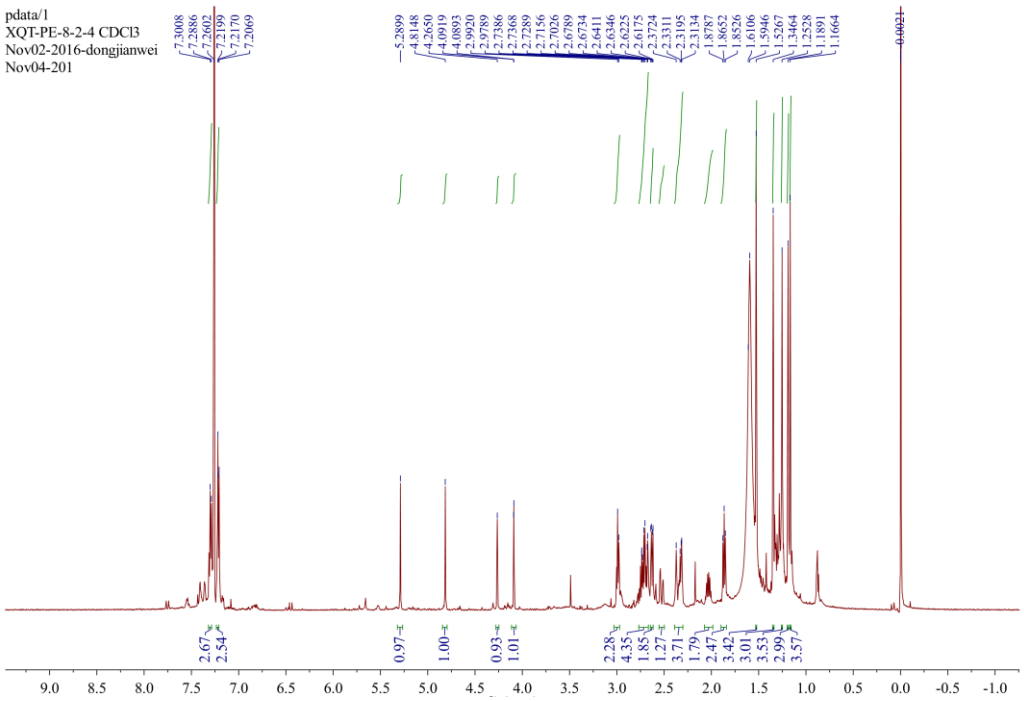


Figure S45 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of dimericilligerate C (5)

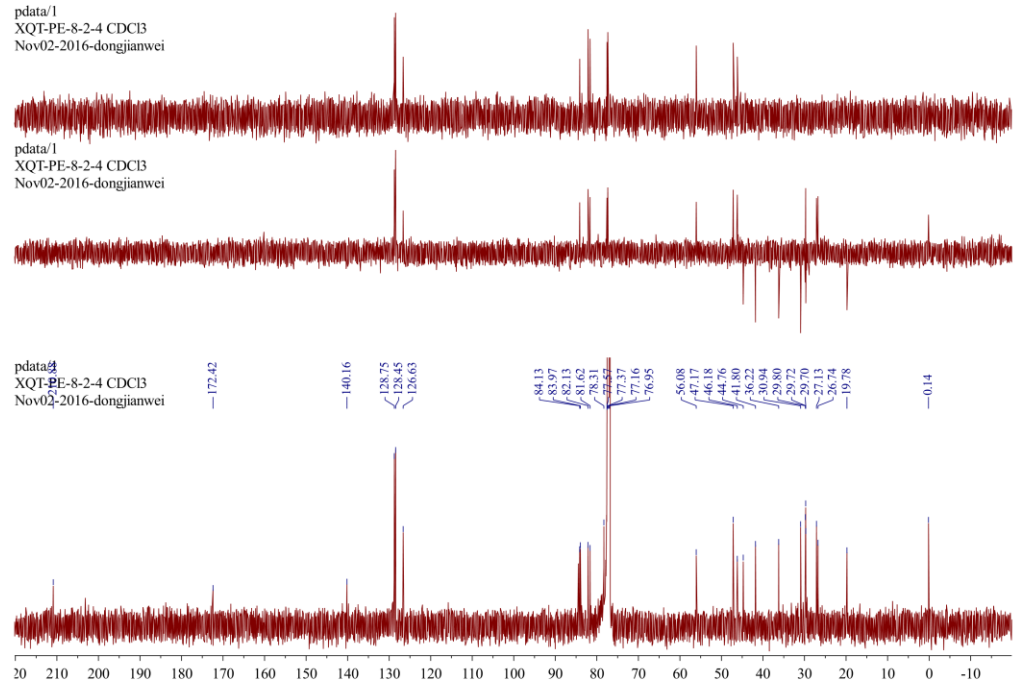


Figure S46 ^{13}C NMR and DEPT spectra ($CDCl_3$, 150 MHz) of dimericilligerate C (5)

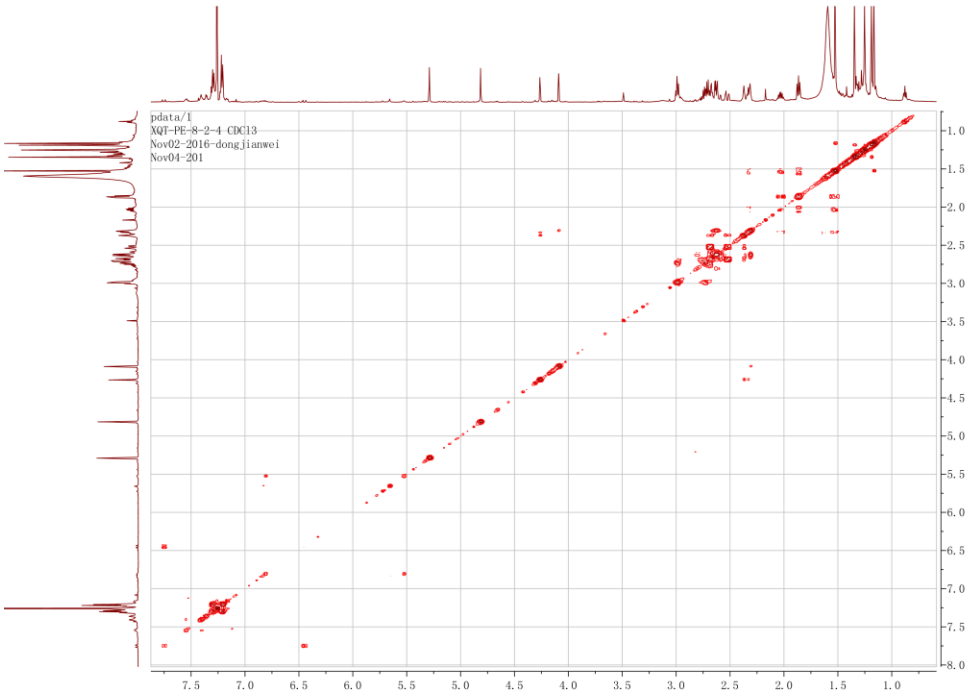


Figure S47 ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate C (5)

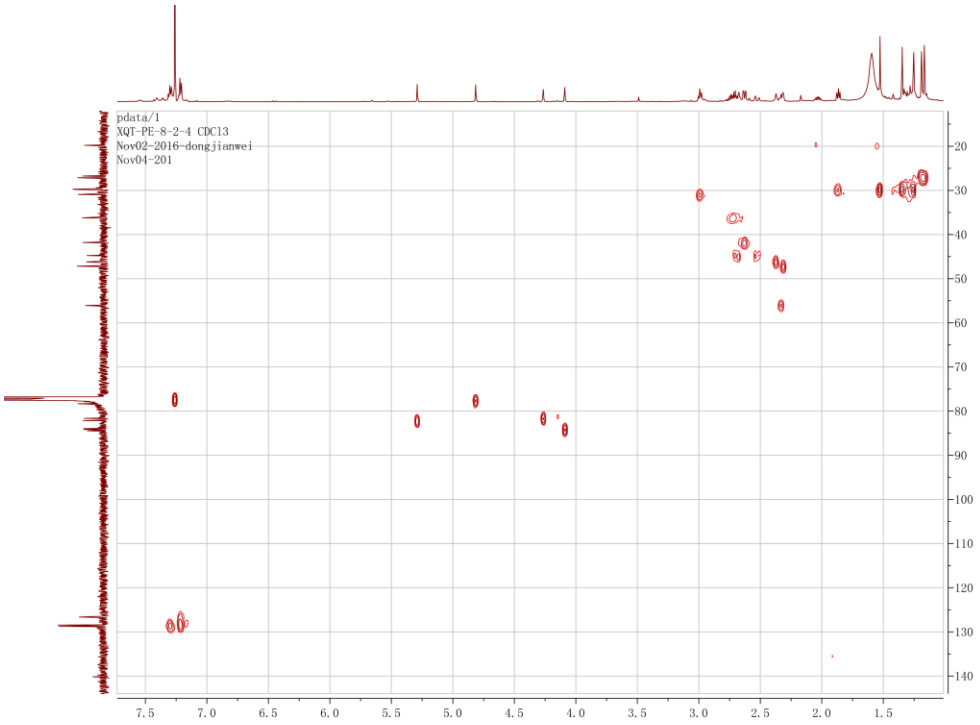


Figure S48 HSQCspectrum ($CDCl_3$, 600 MHz) of dimericilligerate C (5)

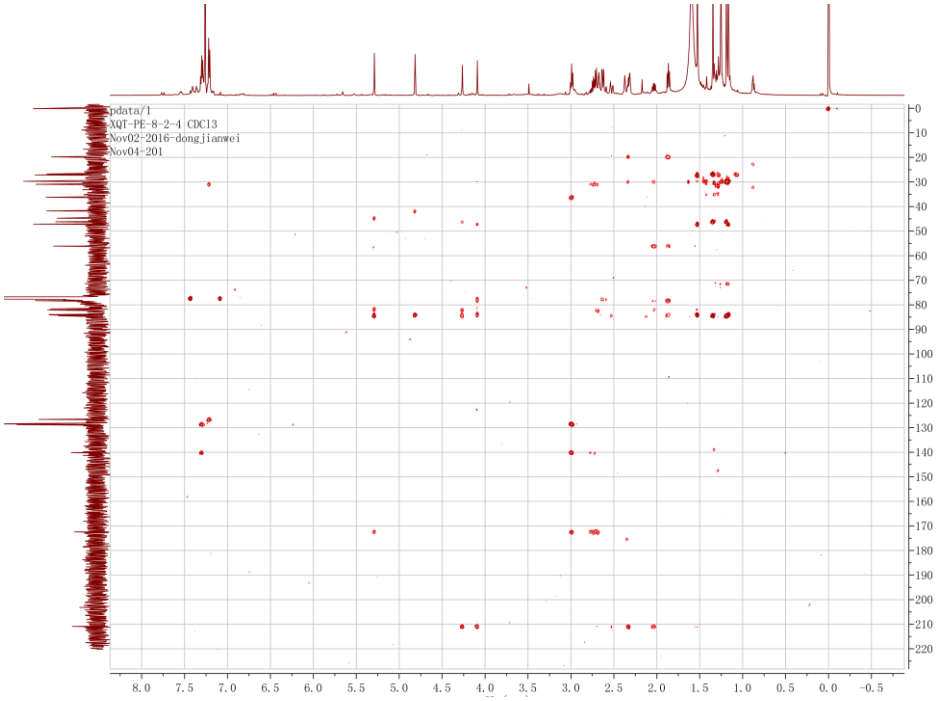


Figure S49 HMBC spectrum ($CDCl_3$, 600 MHz) of dimericilligerate C (5)

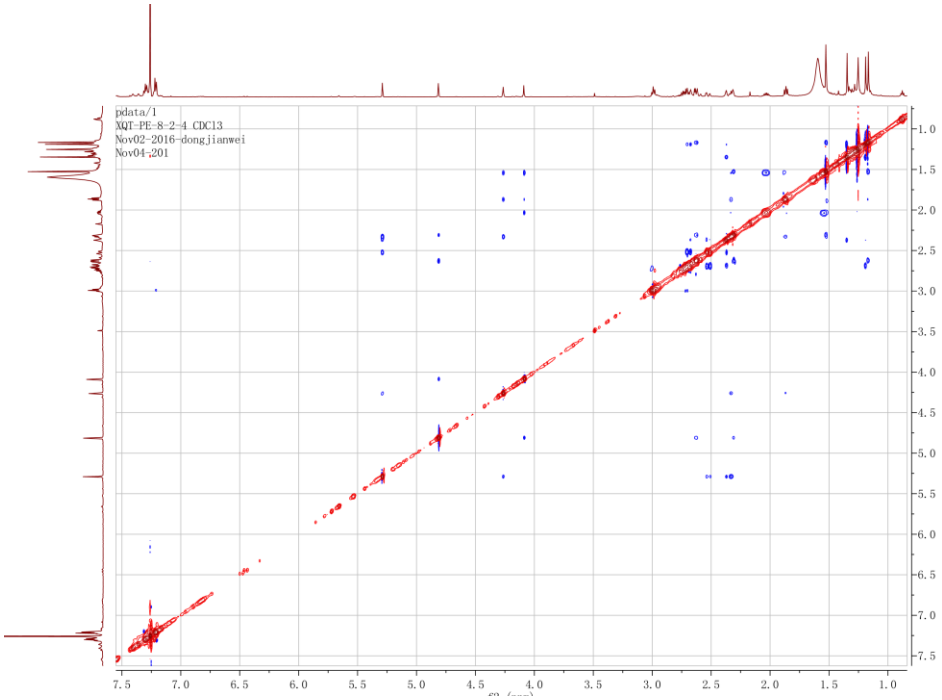


Figure S50 ROESY spectrum ($CDCl_3$, 600 MHz) of dimericilligerate C (5)

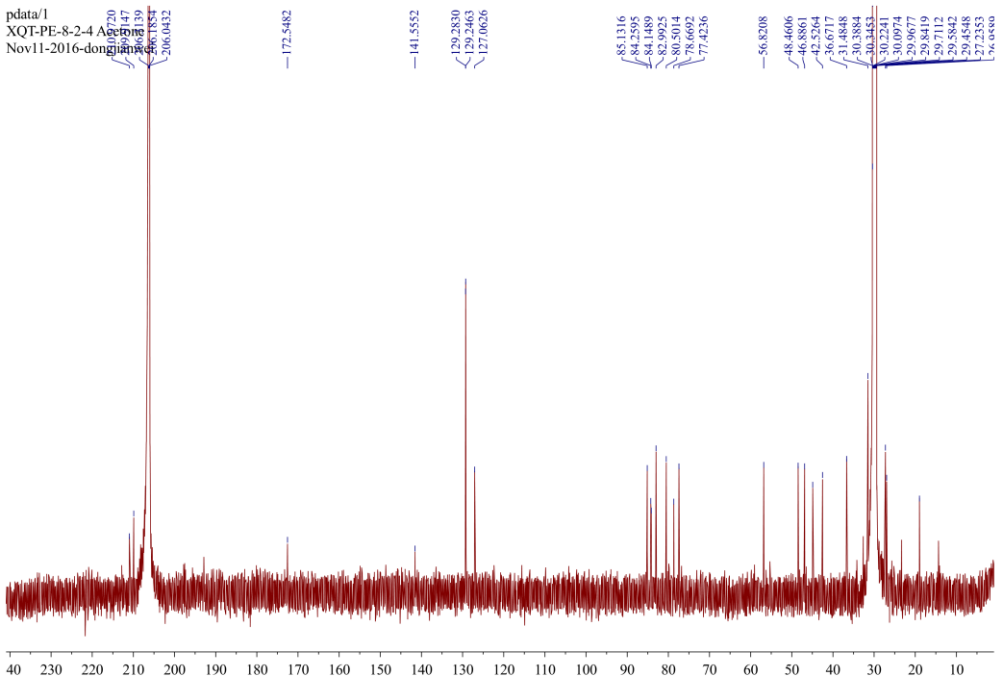


Figure S51 ^{13}C NMR spectrum (acetone-d_6, 150 MHz) of dimericilligerate C (5)

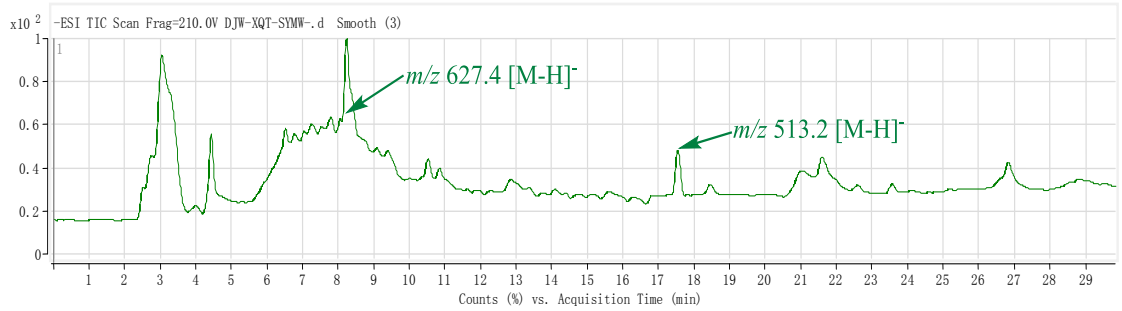


Figure S52 Total ion chromatogram (ESI-) of the petroleum ether extract.