Appendix A.   Supplementary data

Neo-5,22E-cholestadienol derivatives from *Buthus martensi* karsch and targeted bactericide action mechanisms

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NMR spectra of reported compounds, HR-ESIMS and their Circular Dichromism spectra.

Compound 1(QX75-5)**.**

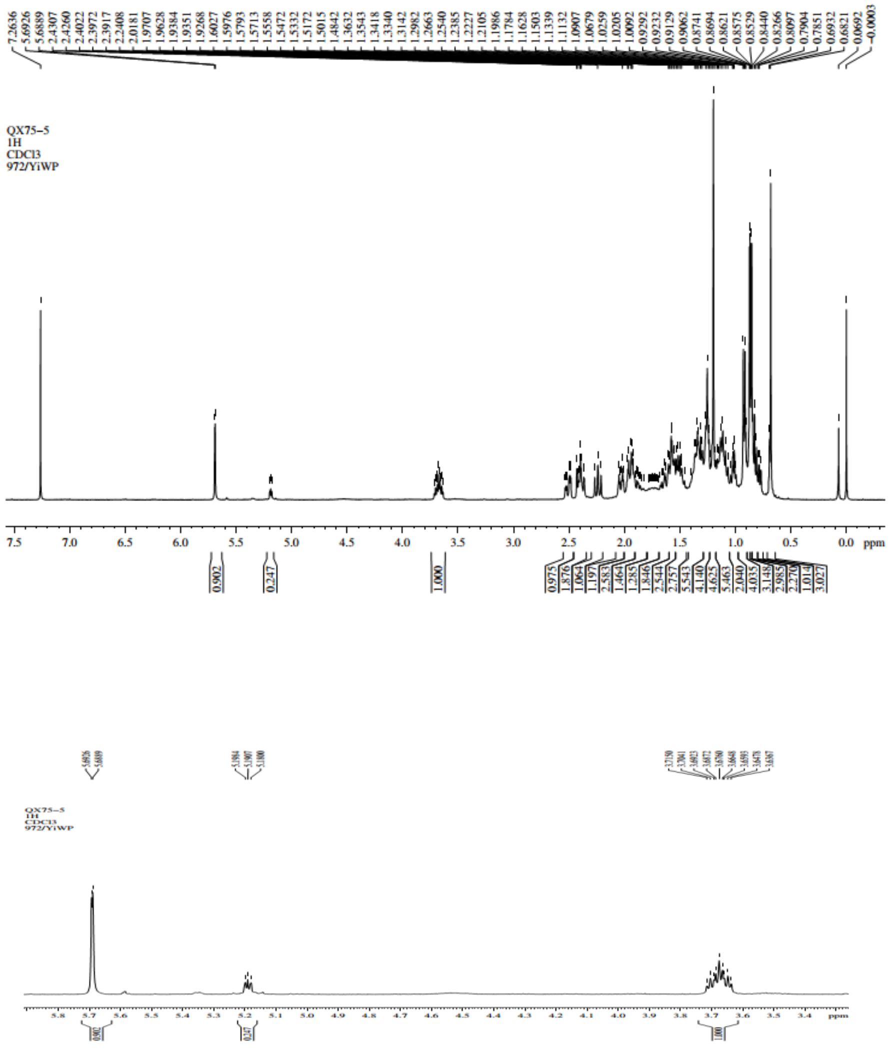


Figure S1.^{1}H NMR spectrum of Compound 1 in $CDCl_3$ (400 MHz).

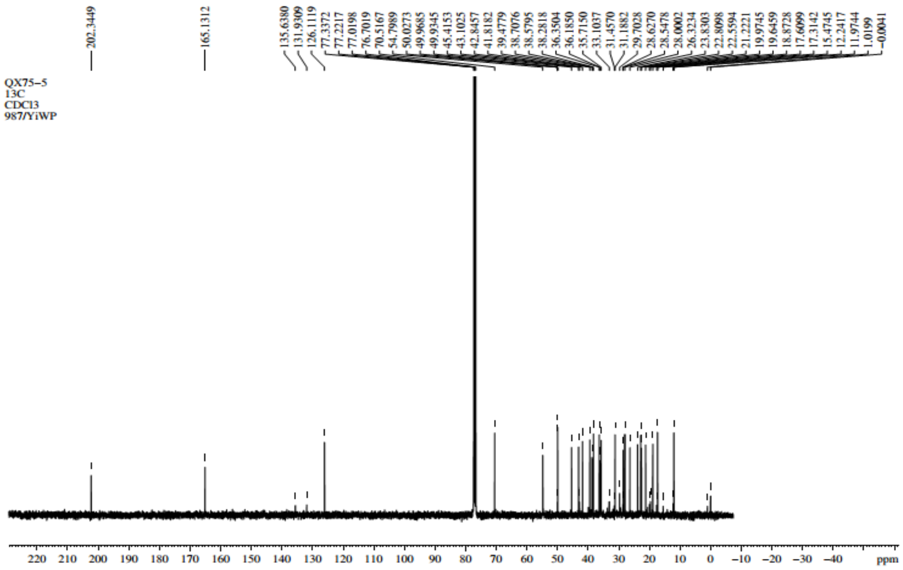


Figure S2. ^{13}C NMR spectrum of Compound 1 in $CDCl_3$ (400 MHz).

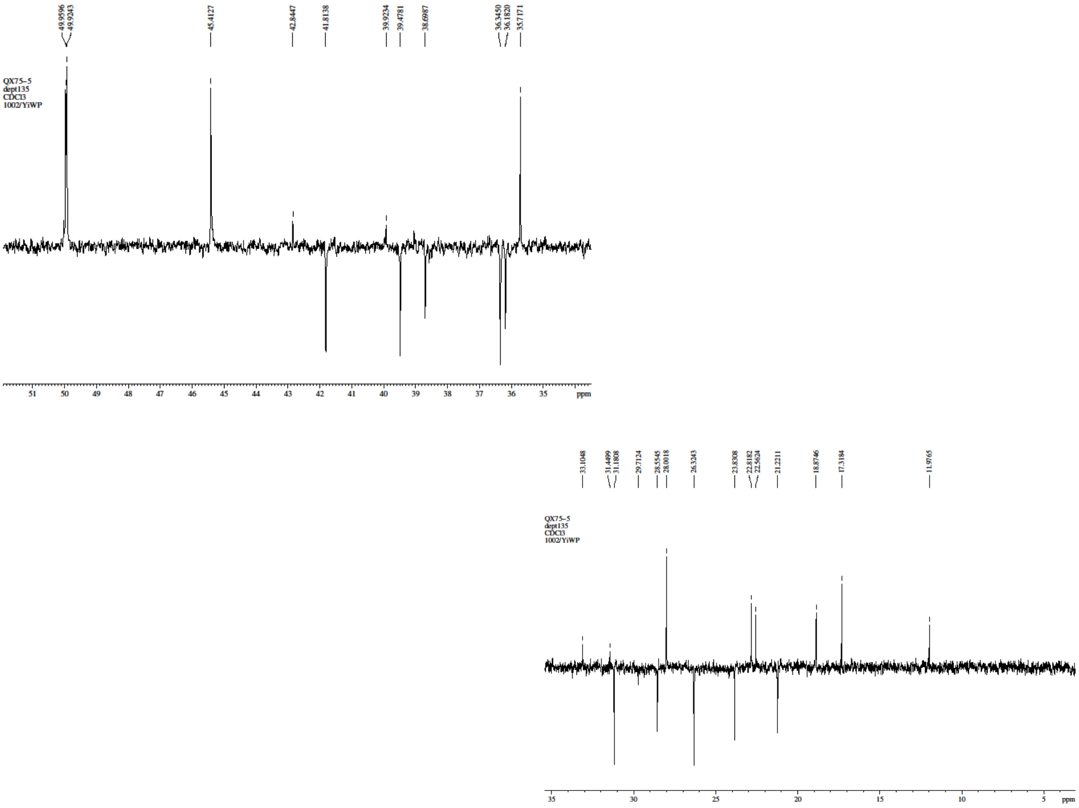


Figure S3. DEPT spectrum of Compound 1 in $CDCl_3$ (400 MHz).

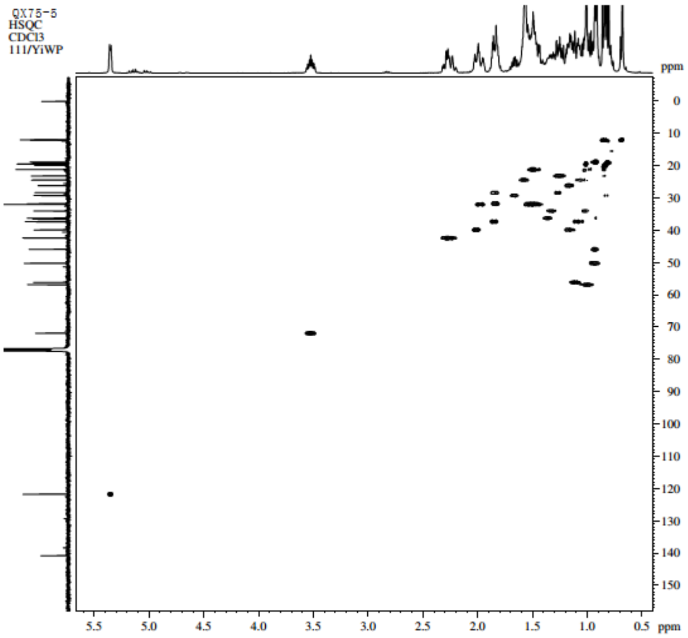


Figure S4. HSQC spectrum of Compound 1 in CDCl$_3$ (400 MHz).

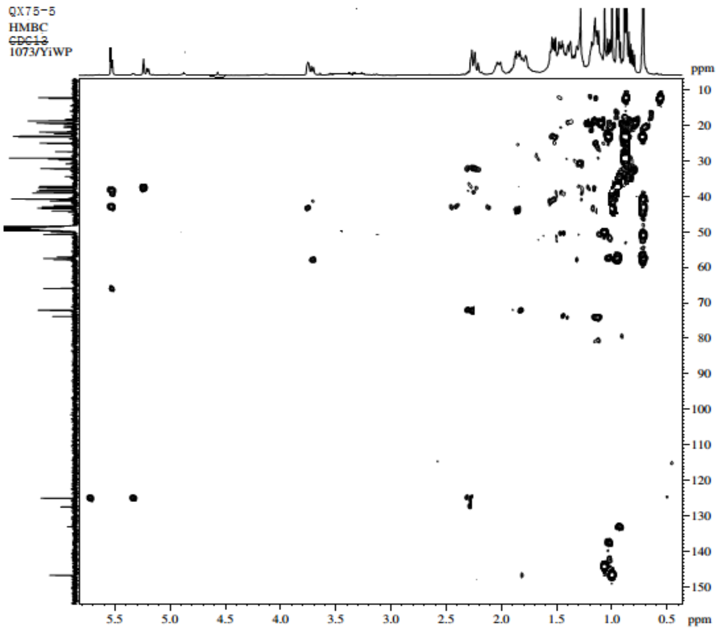
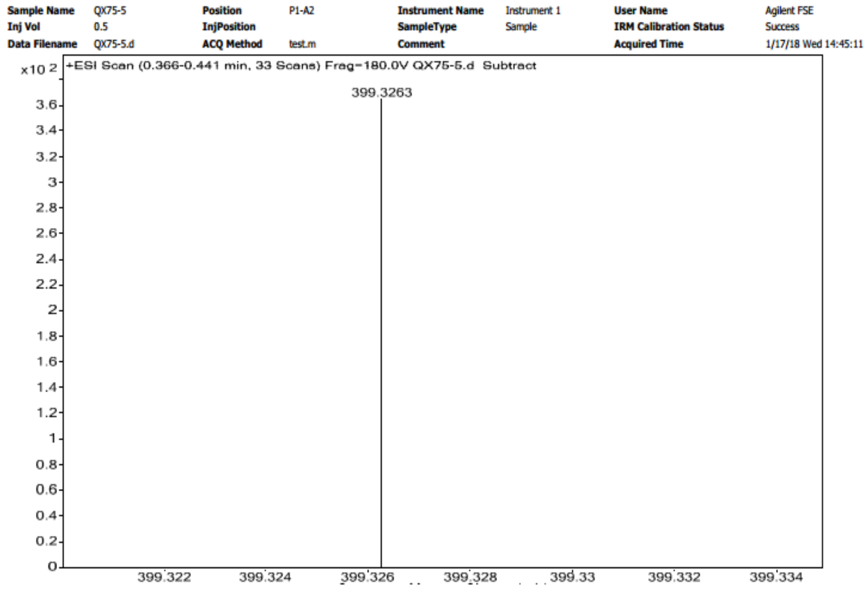


Figure S5. HMBC spectrum of Compound 1 in CDCl$_3$ (400 MHz)



Sample Name	QX75-5	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.5	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	QX75-5.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	1/17/18 Wed 14:45:11

Figure S6.HR-ESIMS spectrum of Compound 1

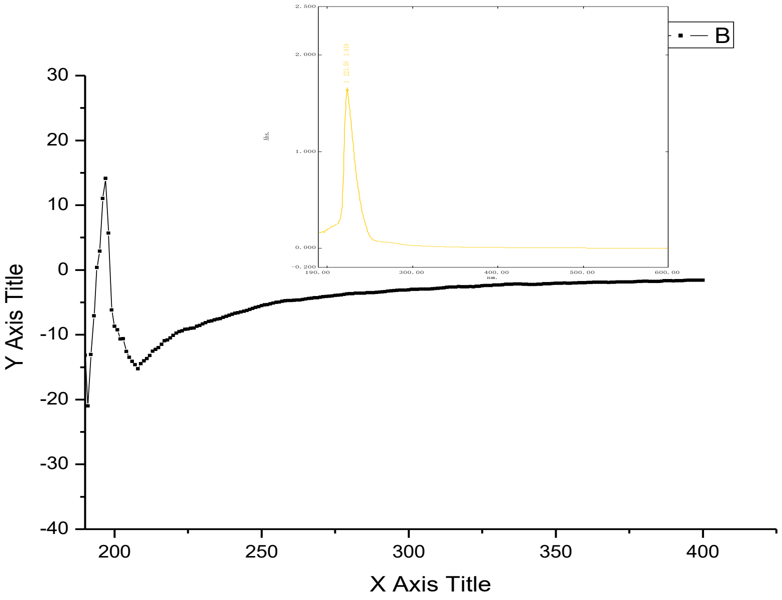


Figure S7 . Circular Dichromism spectra spectrum of Compound 1

Compound 2 (QX37-45-4)**.**

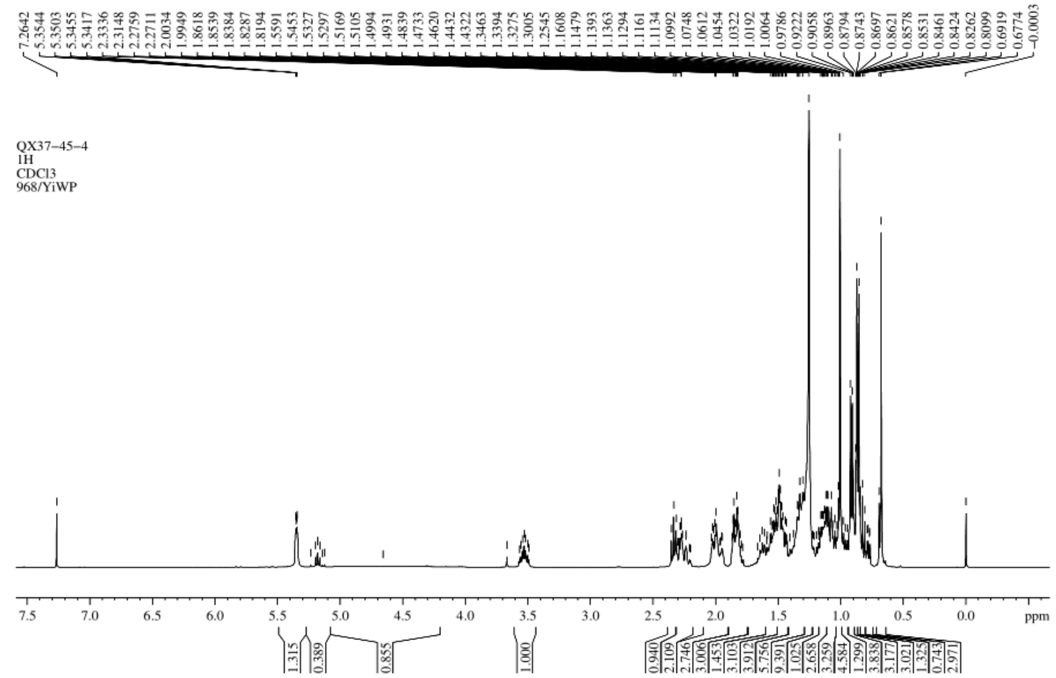


Figure S8. ^{1}H NMR spectrum of Compound 2 in $CDCl_3$ (400 MHz).

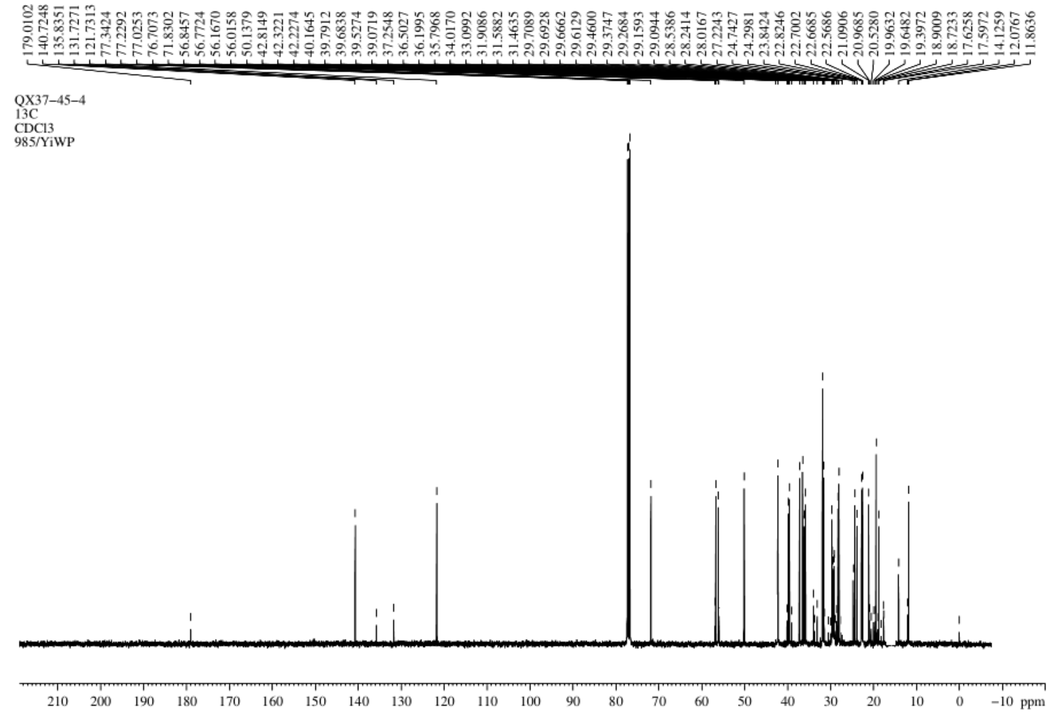


Figure S9. ^{13}C NMR spectrum of Compound 2 in $CDCl_3$ (400 MHz).

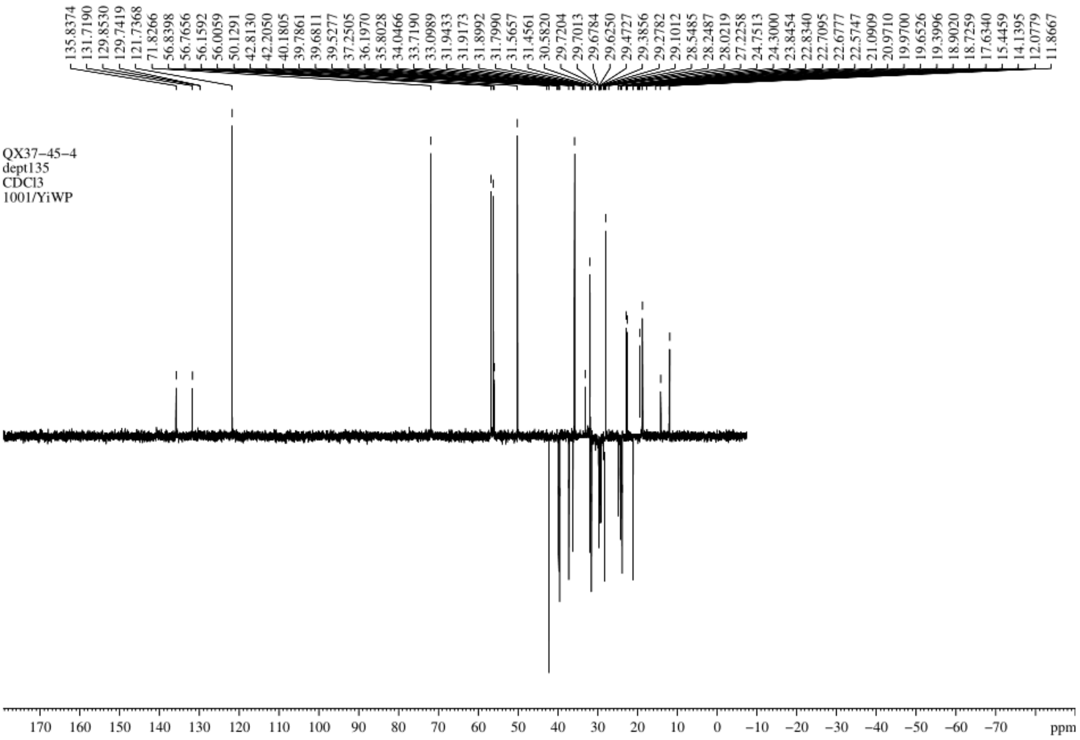


Figure S10. DEPT spectrum of Compound 2 in $CDCl_3$ (400 MHz).

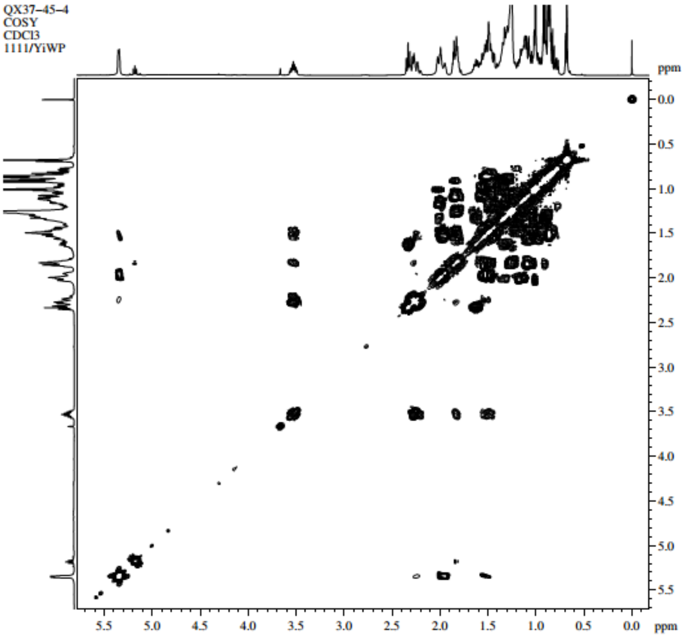


Figure S11. ^1H- ^1H COSY spectrum of Compound 2 in $CDCl_3$ (400 MHz).

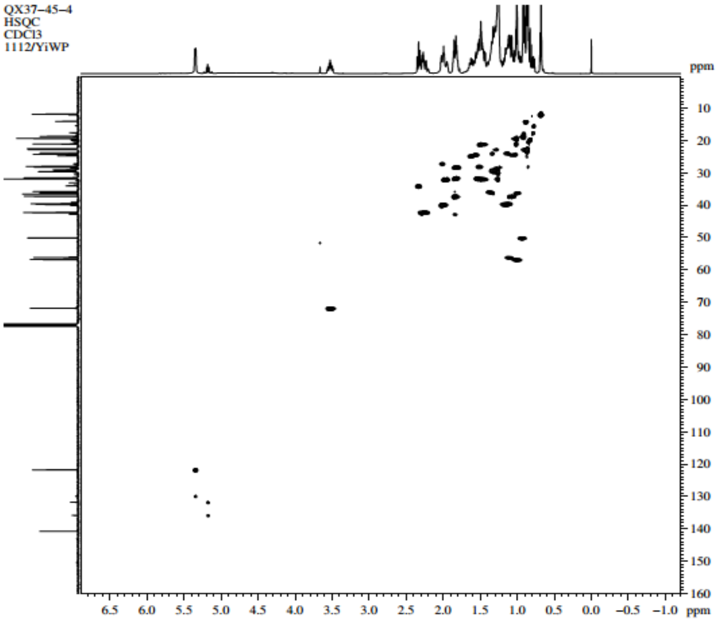


Figure S12. HSQC spectrum of Compound 2 in $CDCl_3$ (400 MHz).

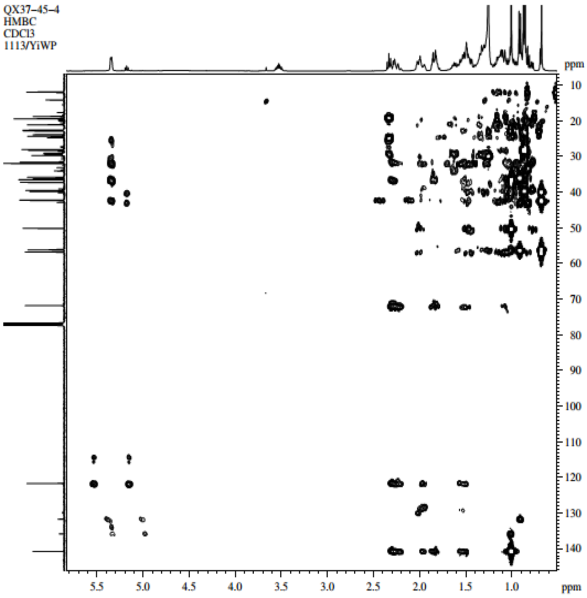
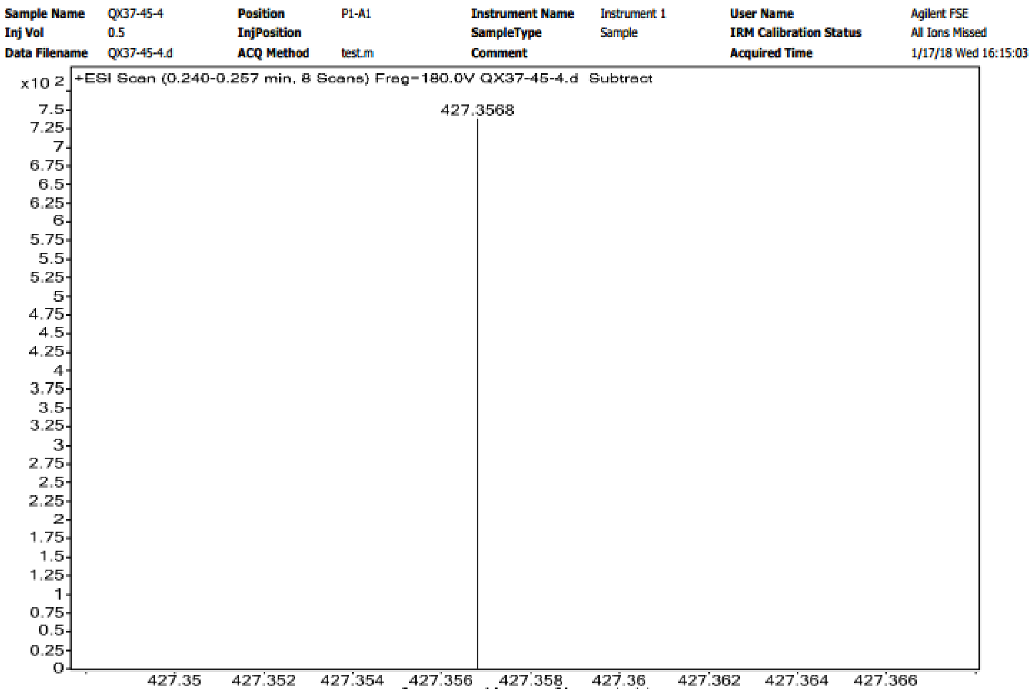


Figure S13. HMBC spectrum of Compound 2 in $CDCl_3$ (400 MHz).



Sample Name	QX37-45-4	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.5	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	QX37-45-4.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	1/17/18 Wed 16:15:03

+ESI Scan (0.240-0.257 min, 8 Scans) Frag=180.0V QX37-45-4.d Subtract

Figure S14.HR-ESIMS spectrum of Compound 2

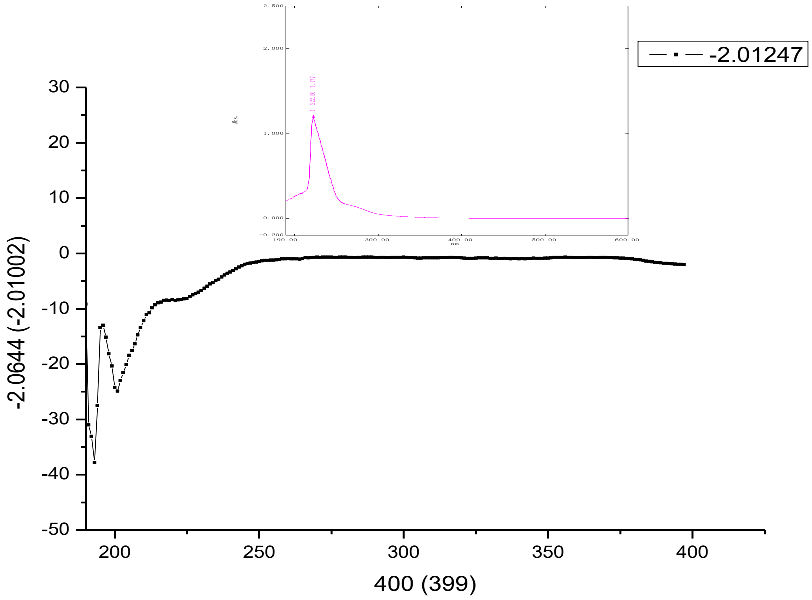


Figure S15 . Circular Dichromism spectra spectrum of Compound 2

Compound 3(QX3-2-7)**.**

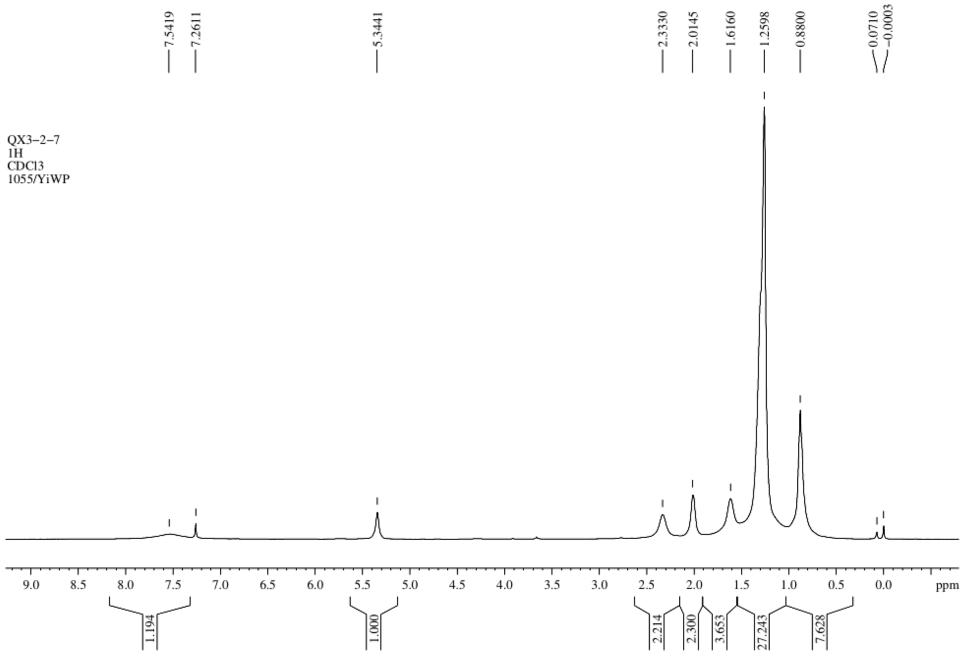


Figure S16. ^{1}H NMR spectrum of Compound 3 in $CDCl_3$ (400 MHz).

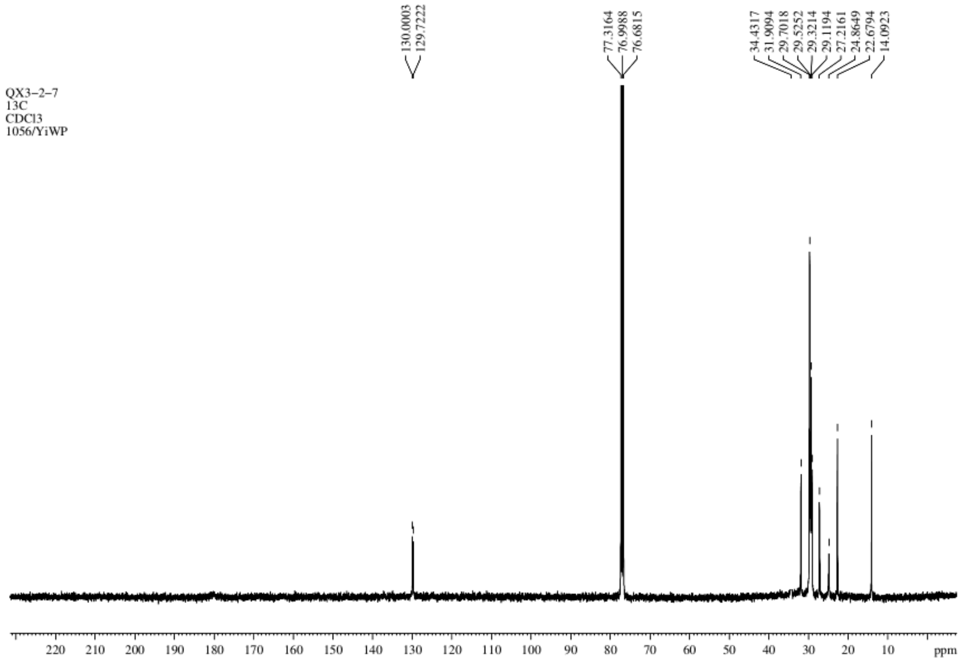


Figure S17. ^{13}C NMR spectrum of Compound 3 in $CDCl_3$ (400 MHz).

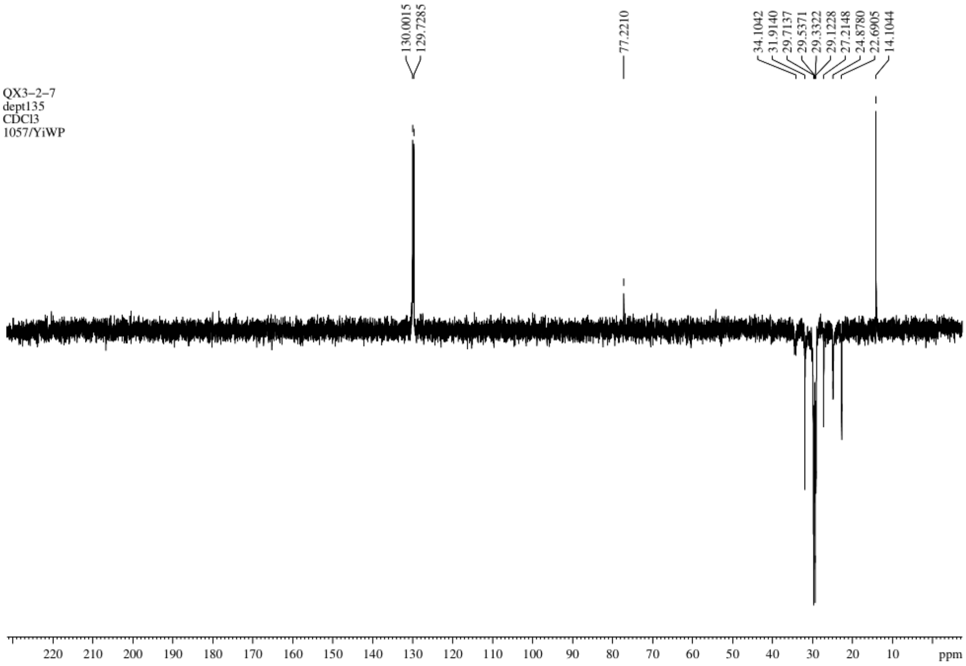


Figure S18. DEPT spectrum of Compound 3 in $CDCl_3$ (400 MHz).

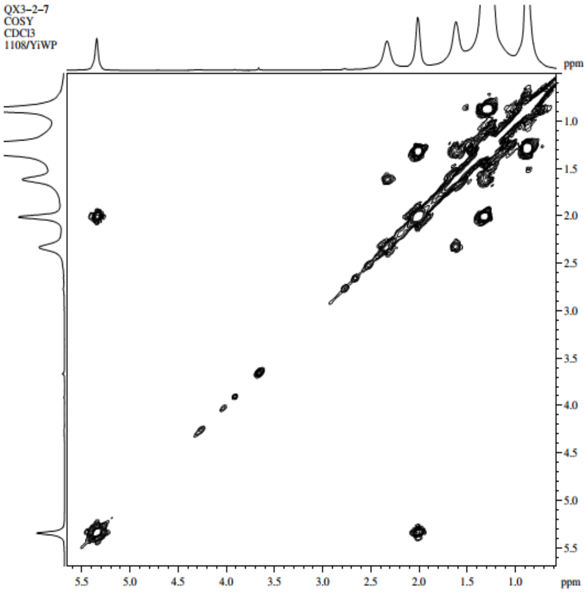


Figure S19. ^{1}H- ^{1}H COSY spectrum of Compound 3 in $CDCl_3$ (400 MHz)

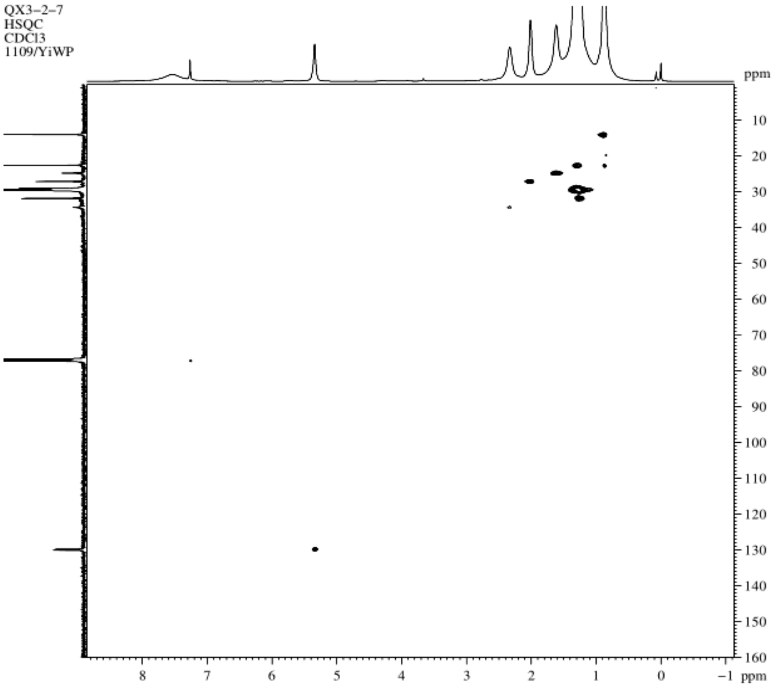


Figure S20. HSQC spectrum of Compound 3 in $CDCl_3$ (400 MHz).

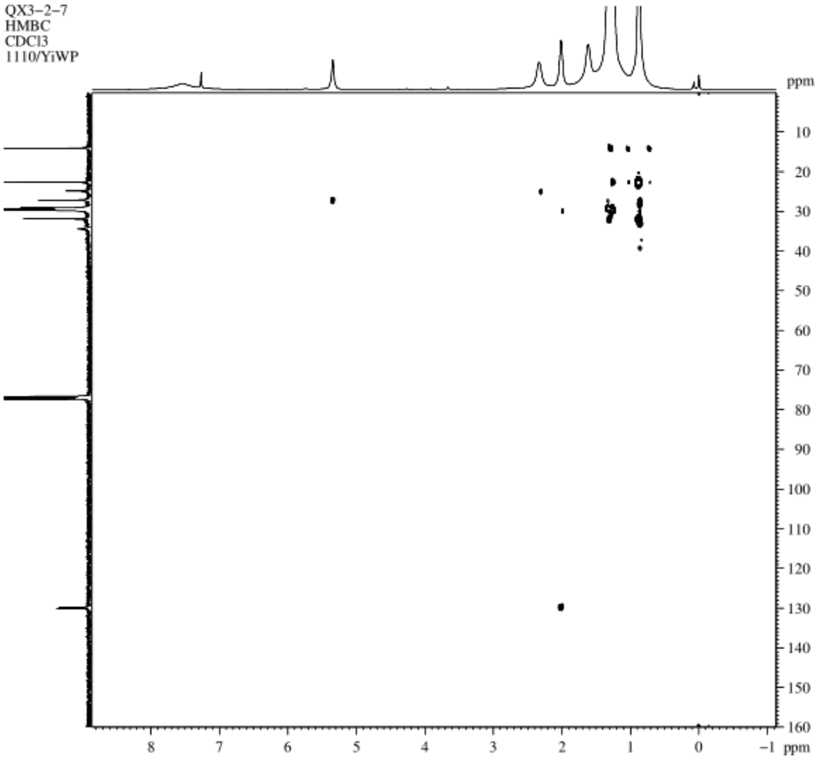
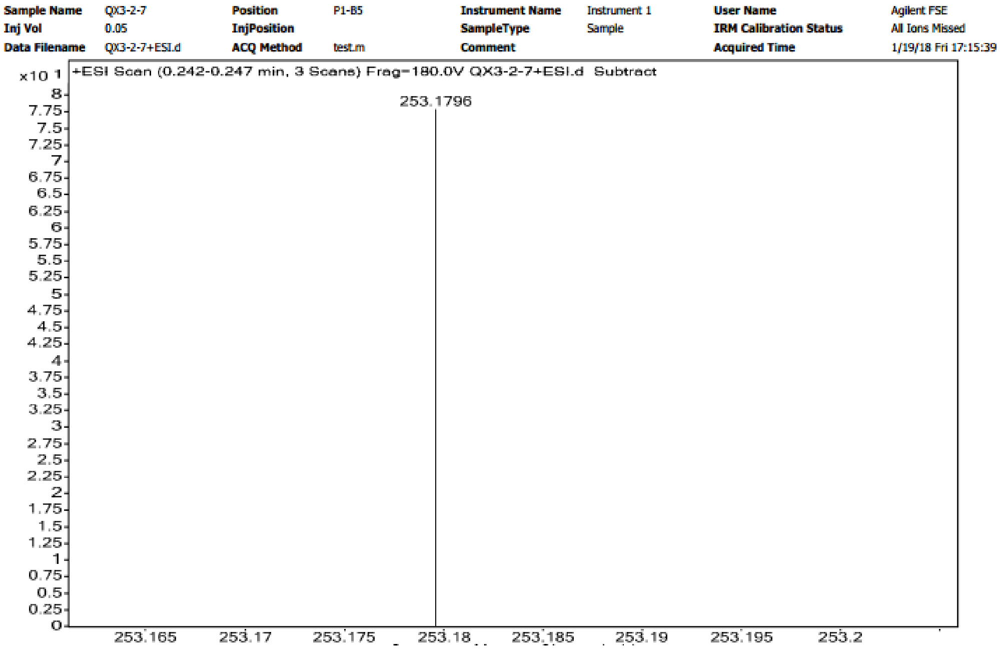


Figure S21. HMBC spectrum of Compound 3in $CDCl_3$ (400 MHz).



Sample Name	QX3-2-7	**Position**	P1-B5	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.05	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	QX3-2-7+ESI.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	1/19/18 Fri 17:15:39

Figure S22. HR-ESIMS spectrum of Compound 3

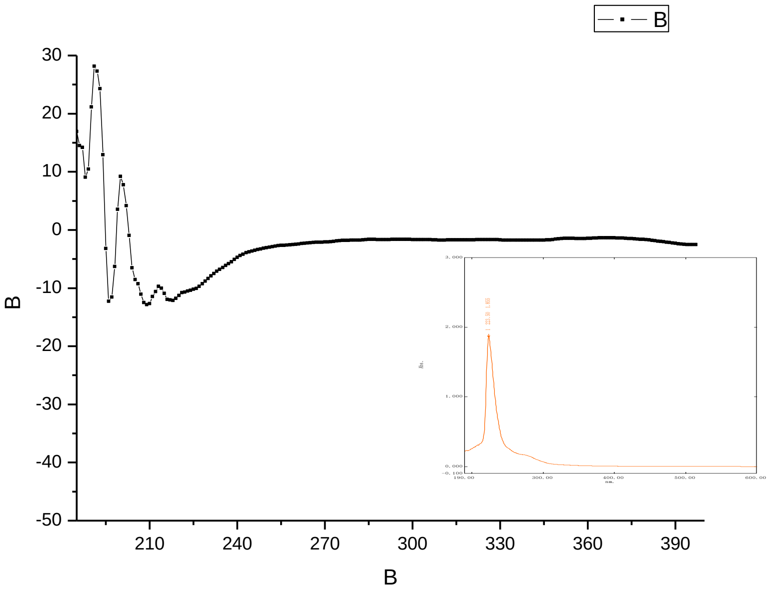


Figure S23 . Circular Dichromism spectra spectrum of Compound 3