

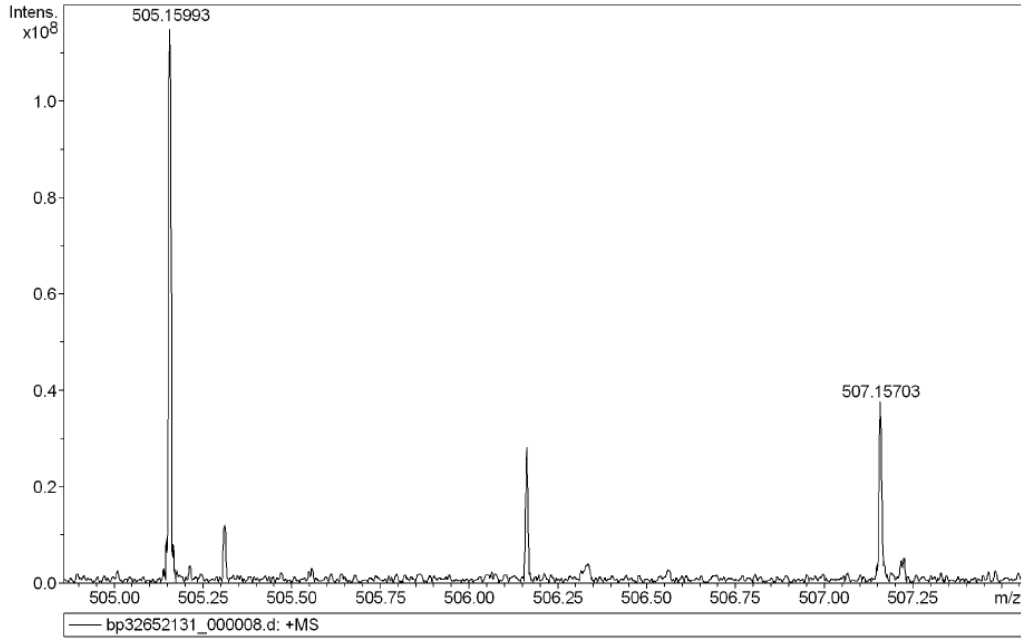
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Mass Spectrum SmartFormula Report

Analysis Info

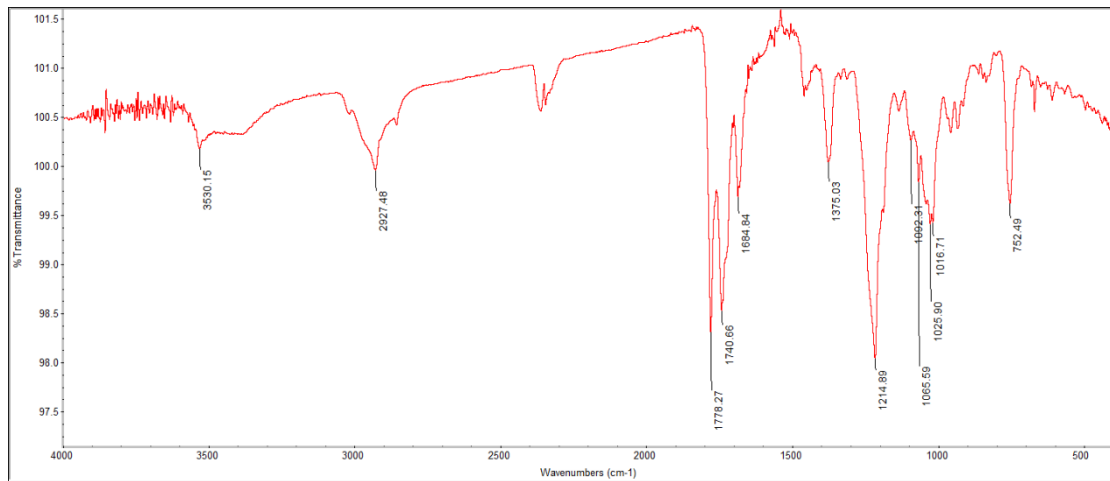
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Method broadband first signal
Sample Name bp3-2-6-5-2-1-3-1
Comment ESI Positive

2/17/2020 4:13:22 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix

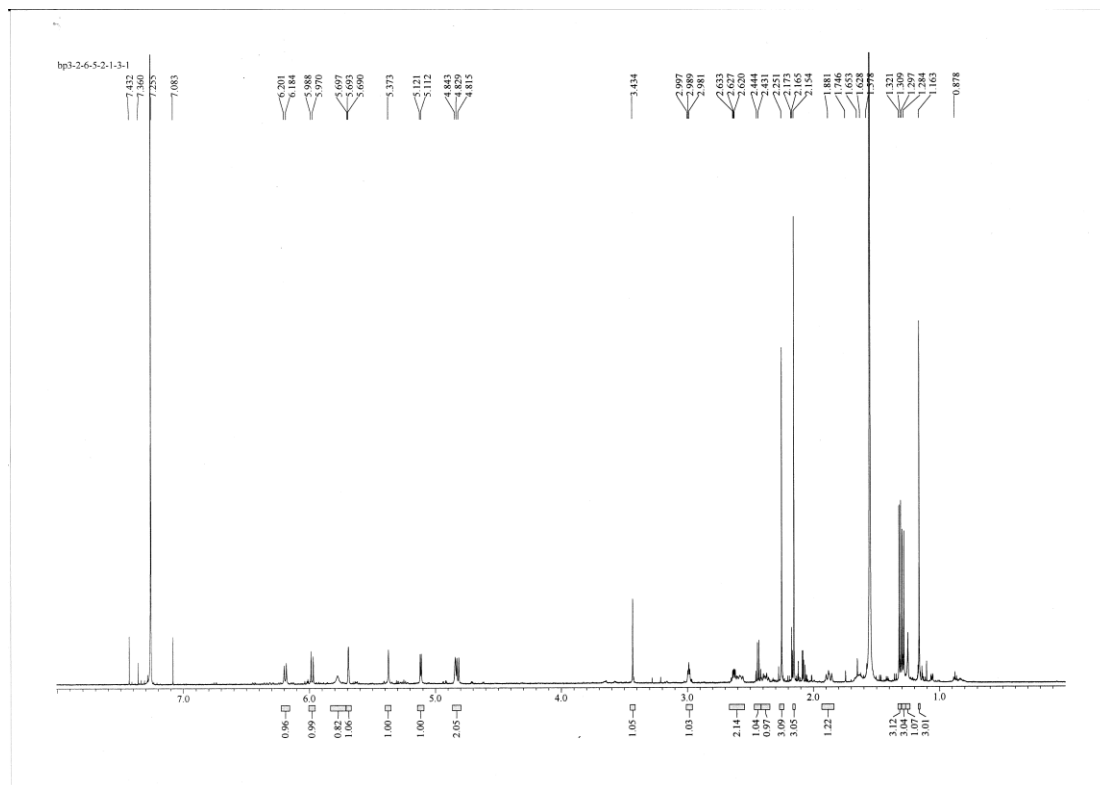


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
505.15993	1	C ₂₄ H ₃₁ ClNaO ₈	100.00	505.15997	0.04	0.07	22.6	8.5	even		ok

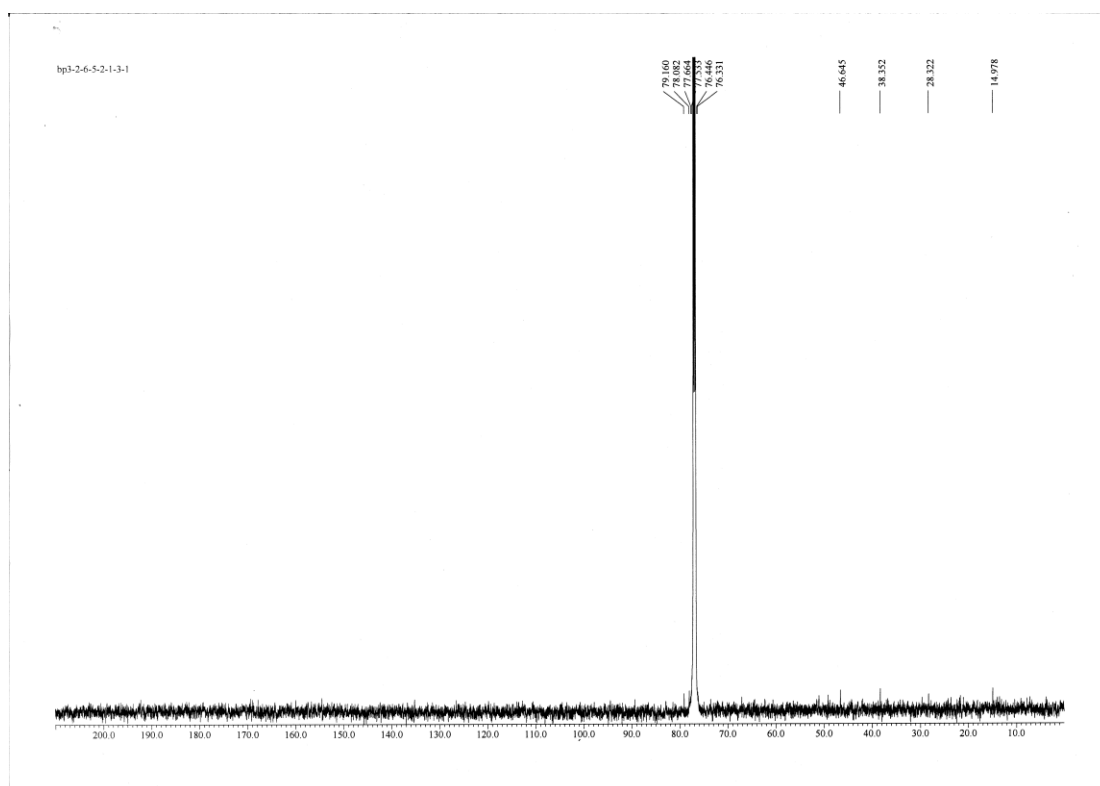
S1. HRESIMS spectrum of compound 1



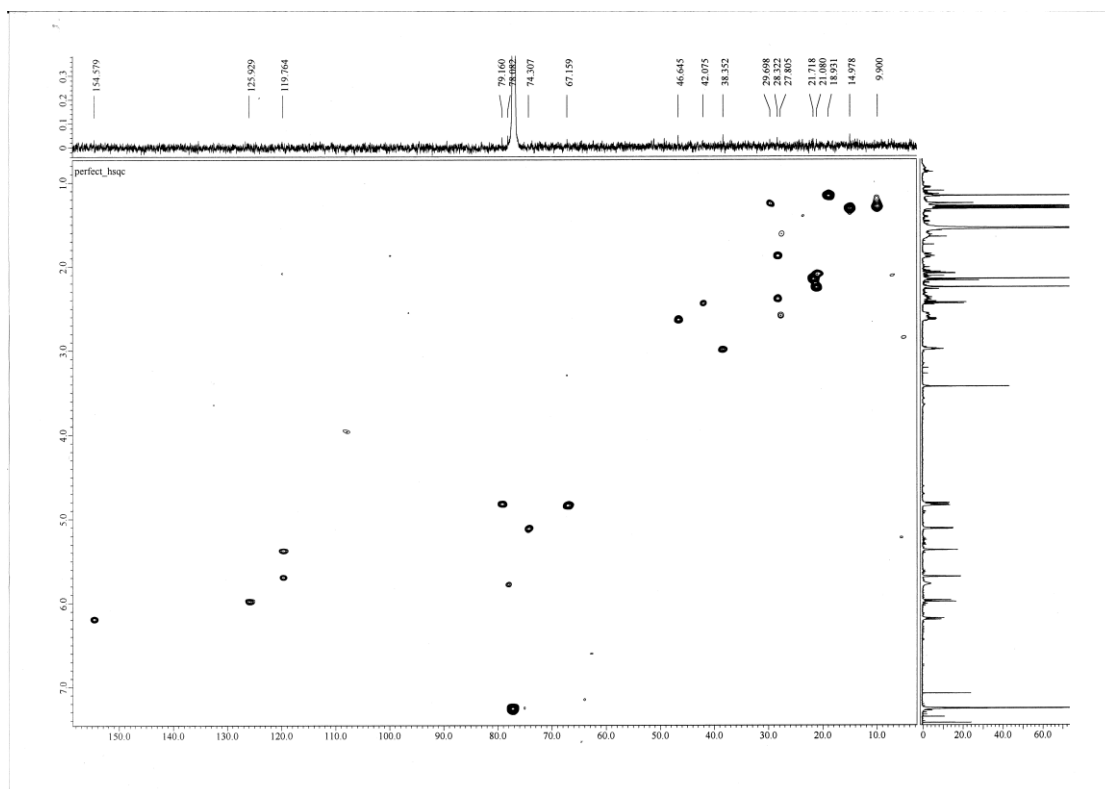
S2. IR spectrum of compound 1



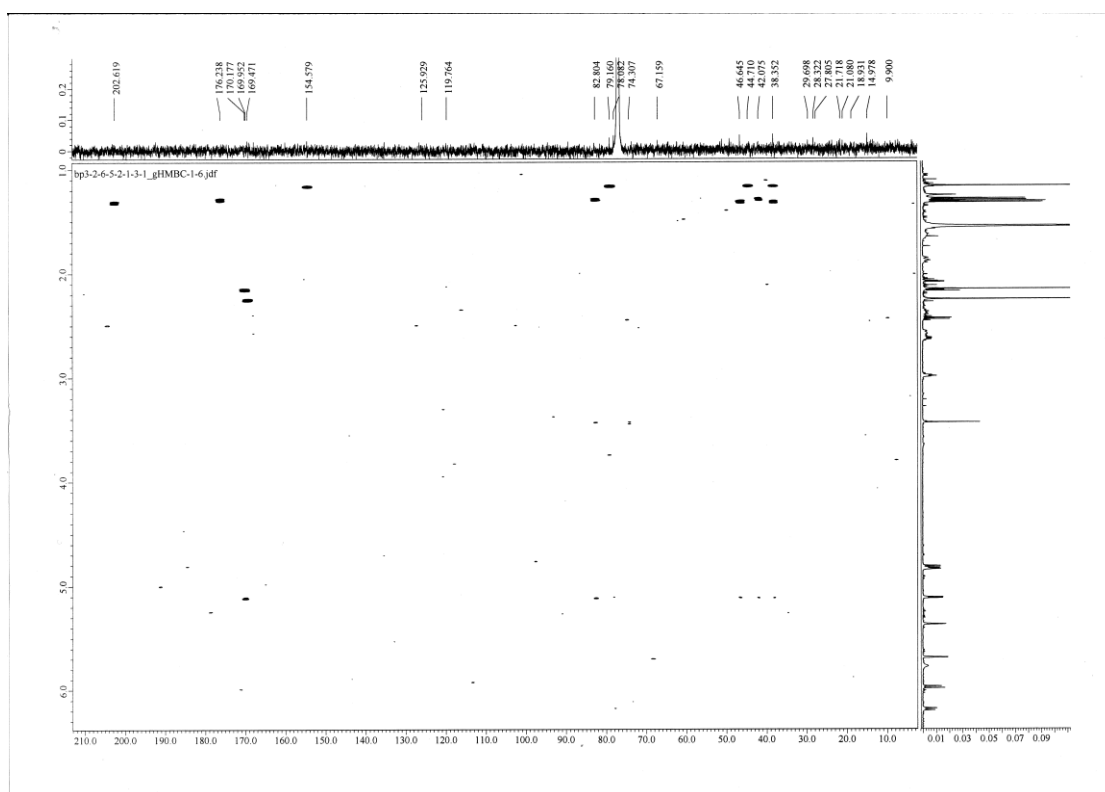
S3. ^1H NMR spectrum (600 MHz) of compound **1** in CDCl_3



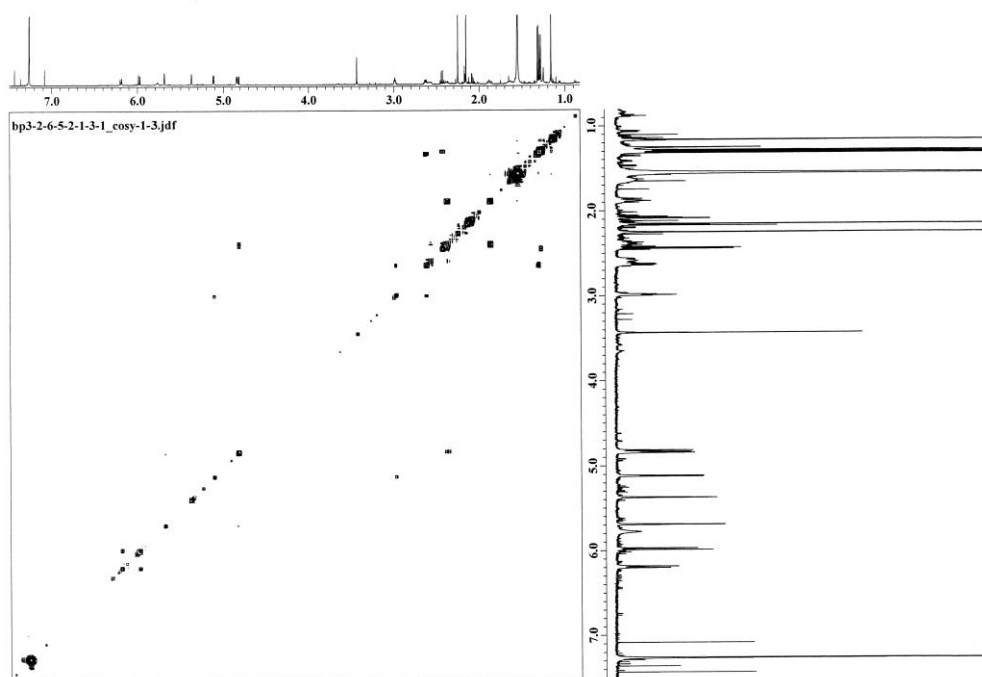
S4. ^{13}C NMR spectrum (150 MHz) of compound **1** in CDCl_3



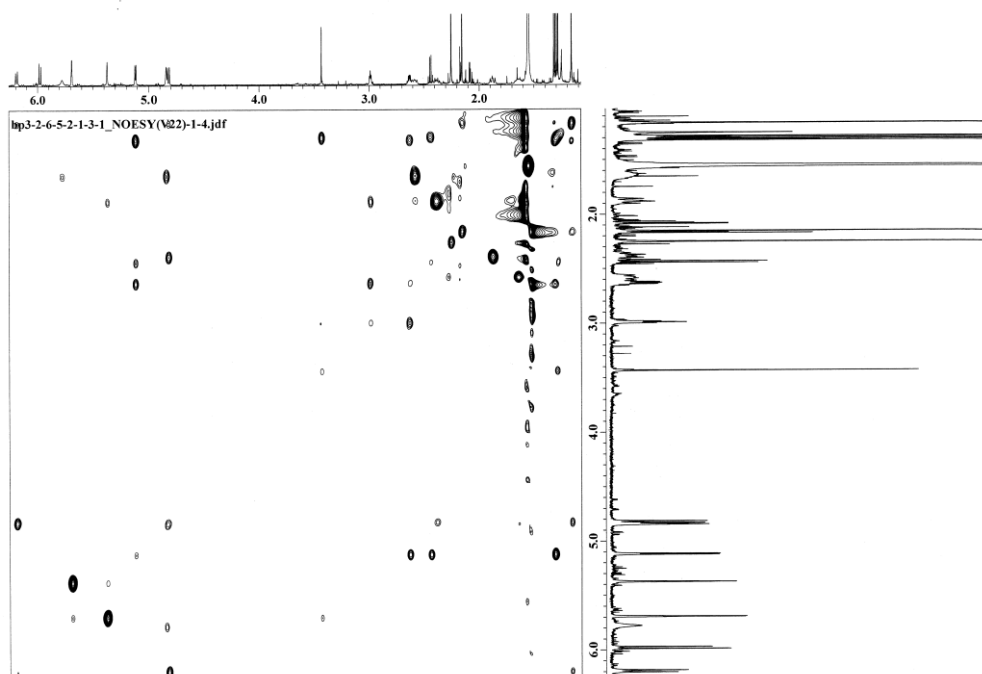
S5. HSQC spectrum of compound 1 in $CDCl_3$



S6. HMBC spectrum of compound 1 in $CDCl_3$



S7. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3



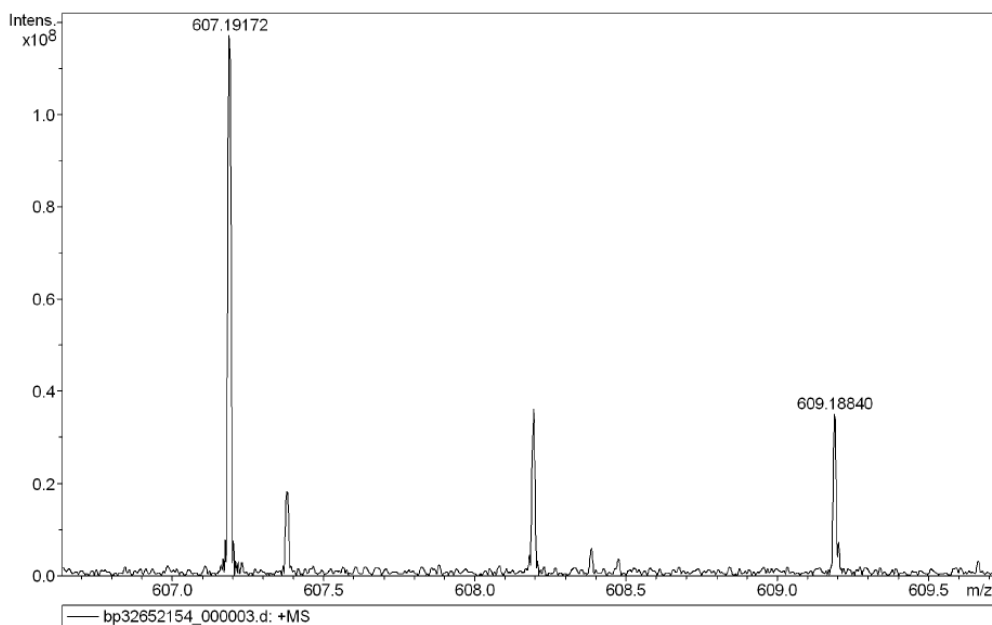
S8. NOESY spectrum of compound **1** in CDCl_3

Mass Spectrum SmartFormula Report

Analysis Info

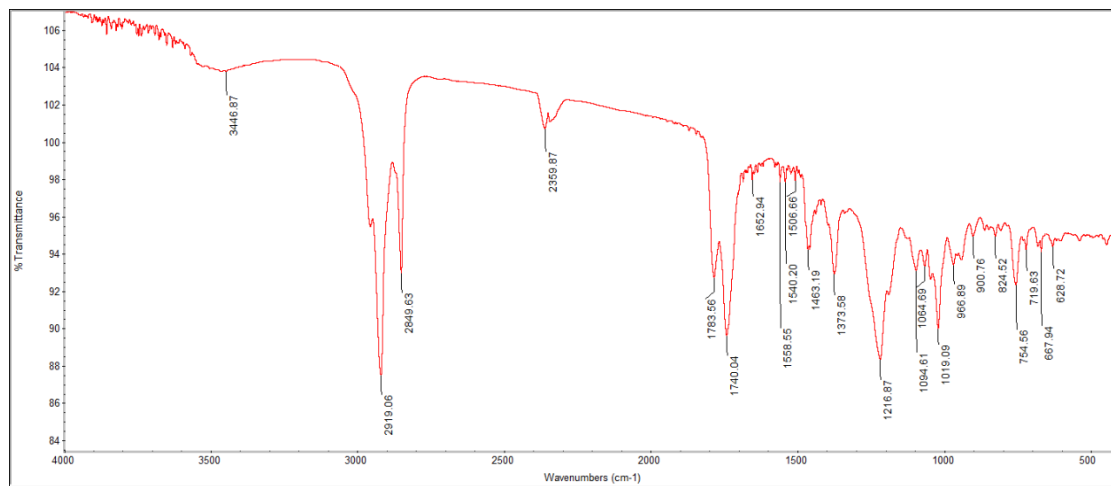
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Sample Name bp3-2-6-5-2-1-5-4
Comment ESI Positive

2/17/2020 4:22:33 PM
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Instrument: BRUKER FT-MS solariX

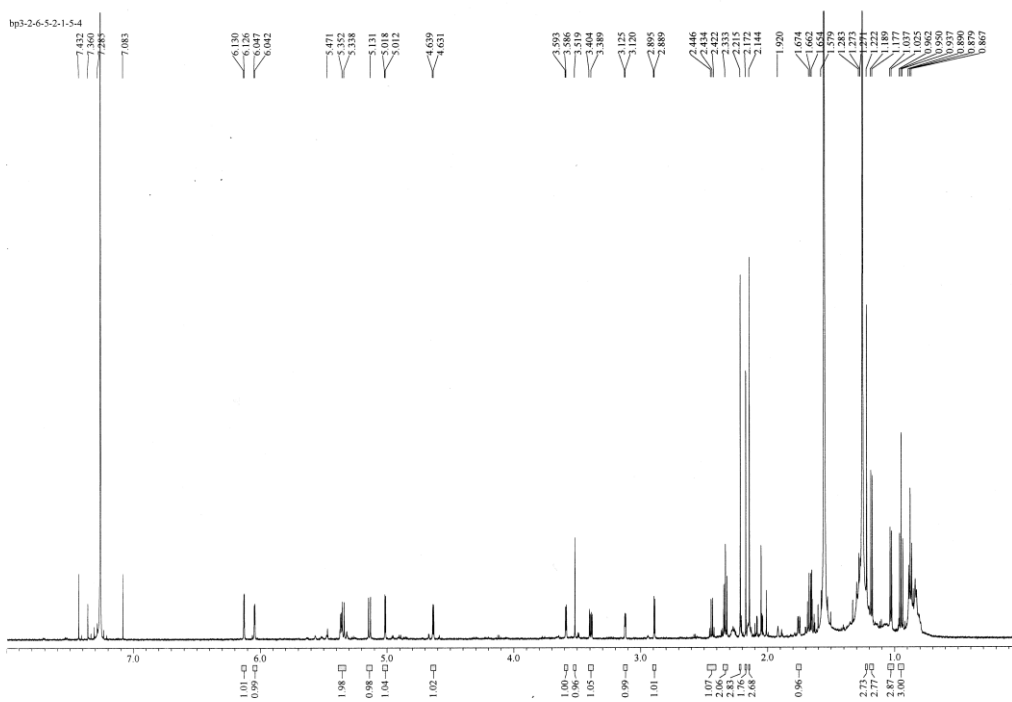


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
607.19172	1	C 28 H 37 Cl Na O 11	100.00	607.19166	-0.05	-0.09	41.0	9.5	even	ok

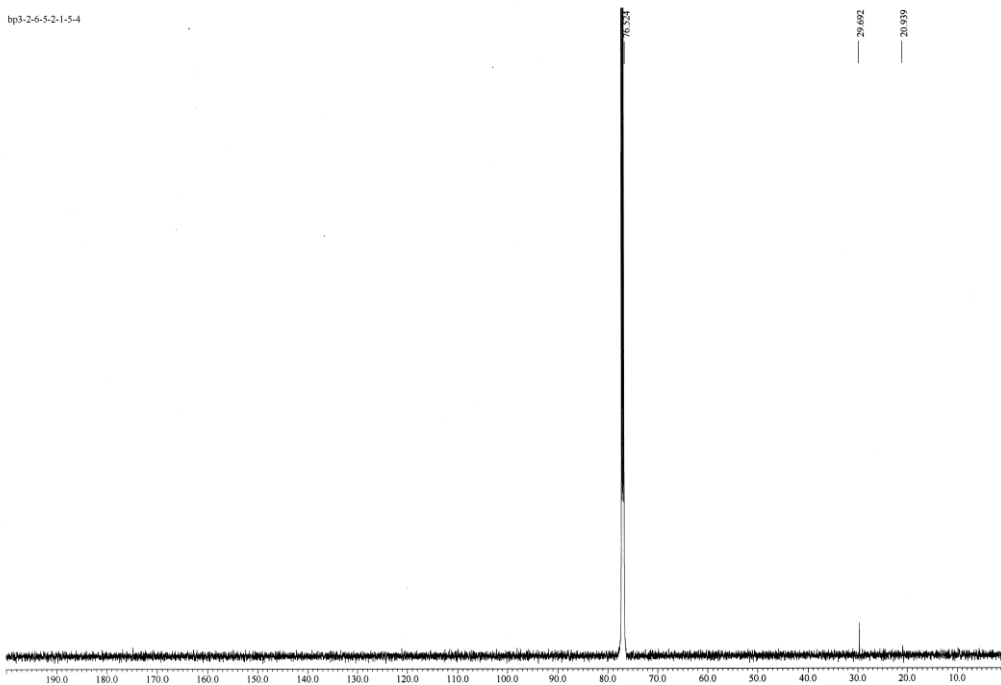
S9. HRESIMS spectrum of compound 2



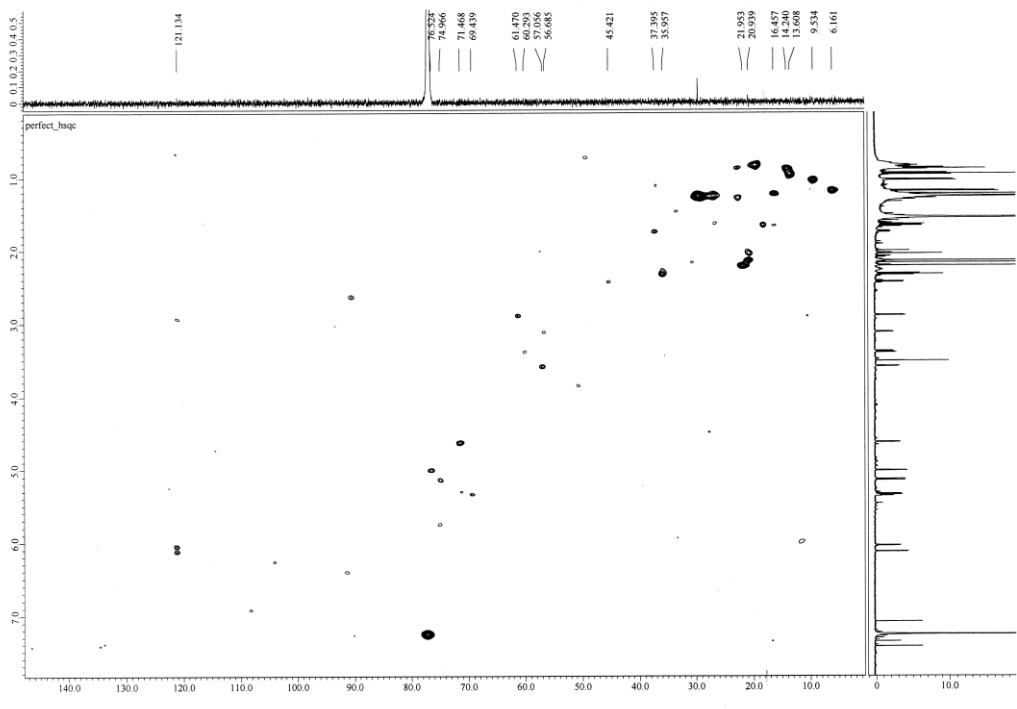
S10. IR spectrum of compound 2



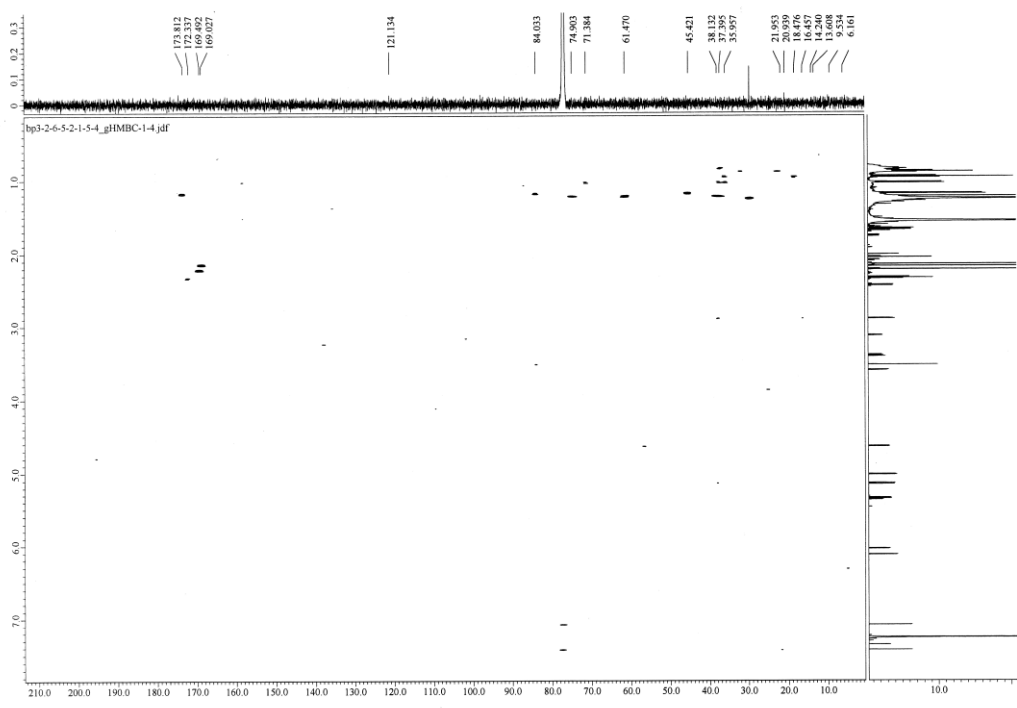
S11. ^1H NMR spectrum (600 MHz) of compound **2** in CDCl_3



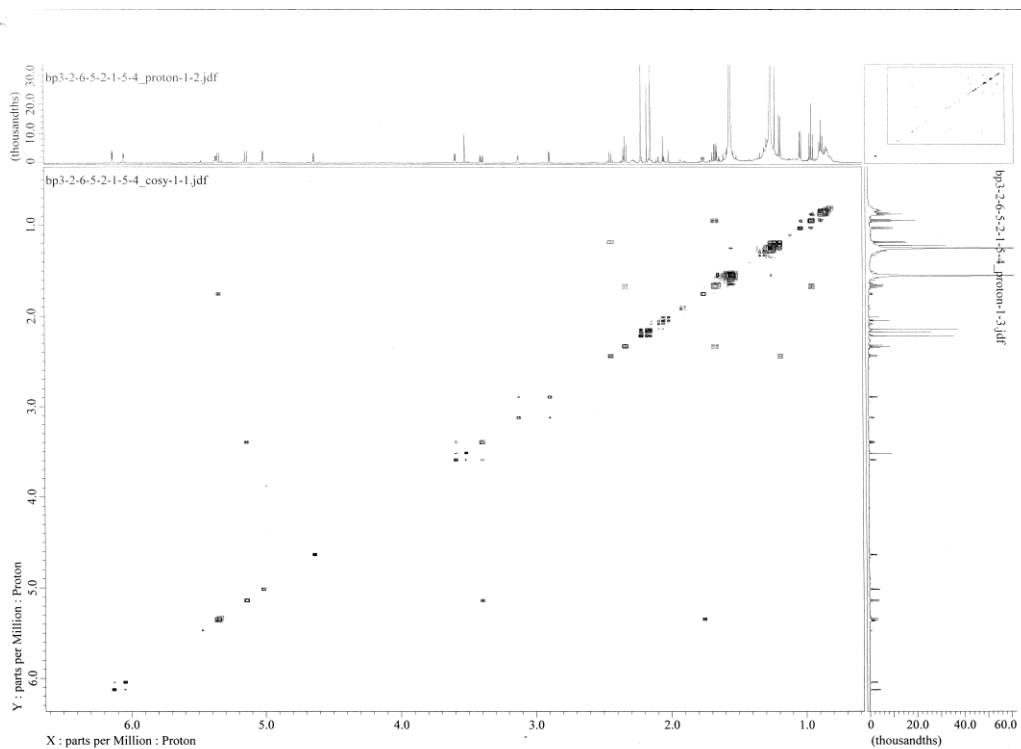
S12. ^{13}C NMR spectrum (150 MHz) of compound **2** in CDCl_3



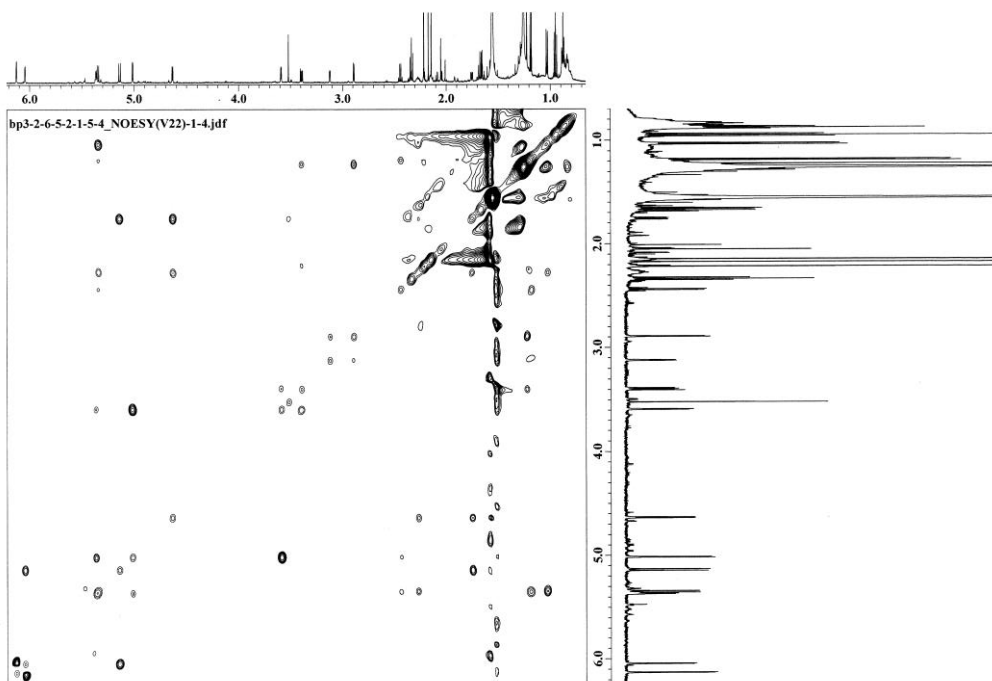
S13. HSQC spectrum of compound **2** in CDCl₃



S14. HMBC spectrum of compound **2** in CDCl₃



S15. ^1H - ^1H COSY spectrum of compound **2** in CDCl_3



S16. NOESY spectrum of compound **2** in CDCl_3