SUPPLEMENTARY MATERIAL

NEW PRENYLATED BIBENZYLS FROM BORNEAN LIVERWORT *ACROBOLBUS SACCATUS*

Liverworts are the most primitive terrestrial plant which known to produce unique and wide variety of compounds. Ethyl acetate crude extract was subjected to several chromatographic techniques for purification. Three new compounds, saccatenes A-C (**1**-**3**) were isolated together with two known prenyl bibenzyl derivative, 2,2-dimethyl-5-hydroxy-6-carboxy-7-(2-phenylethyl) chromene (**4**) and radulanin A-5-one (**5**) from the Bornean liverwort *Acrobolbus saccatus* (Hook.) Trevis collected from Mountain Trus Madi, Sabah, Malaysia. The structures of the three new metabolites were established by analyses of the spectroscopic data (1D NMR, 2D NMR, HRESIMS and IR), and the antibacterial activity against eight selected human pathogenic species of bacteria were tested.

Keywords: prenyl bibenzyl derivatives; *Acrobolbus saccatus*; liverwort; Borneo Island

Supplementary Information

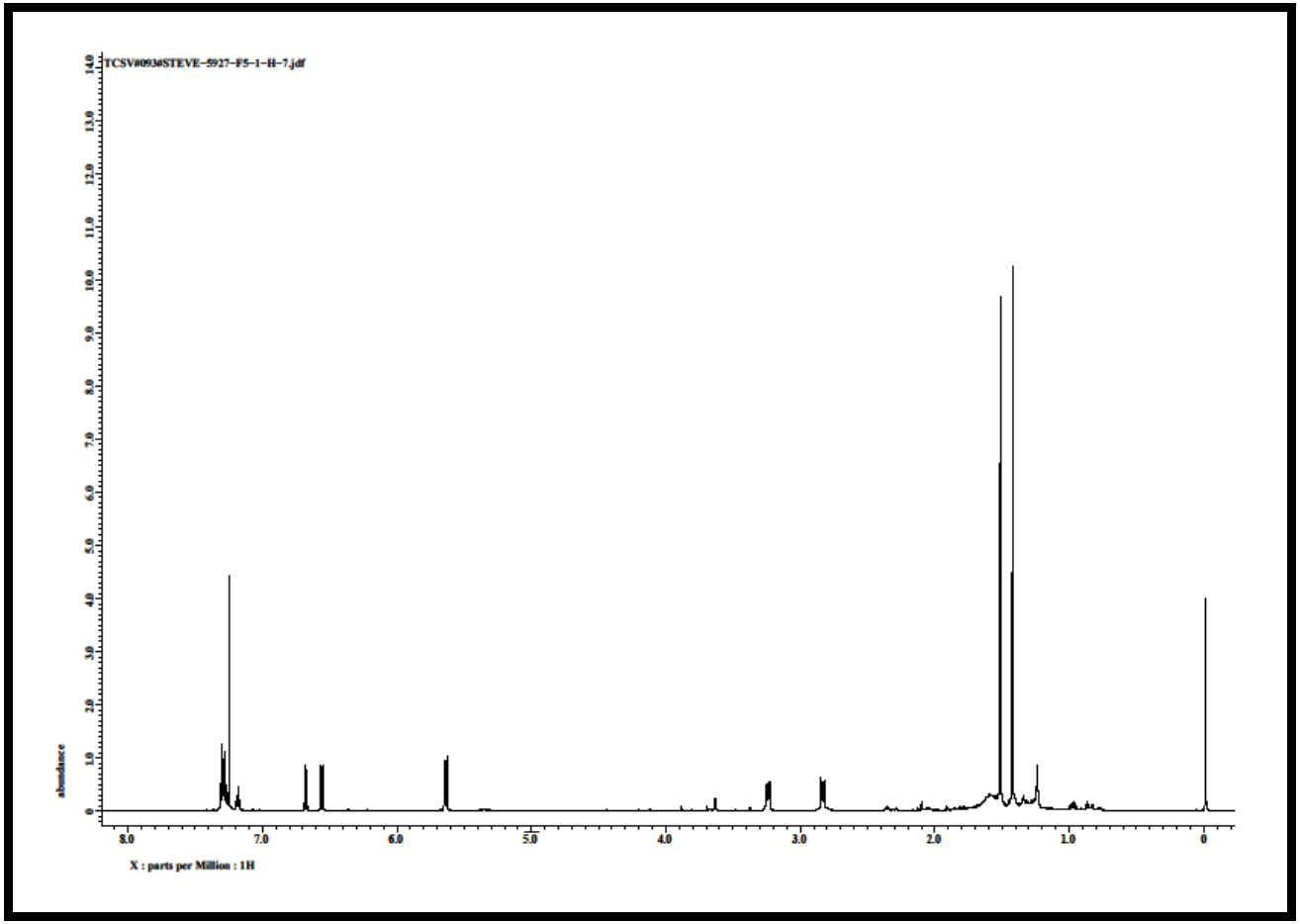


Figure S1. ^{1}H-NMR spectrum of **1** in $CDCl_3$ (600 MHz).

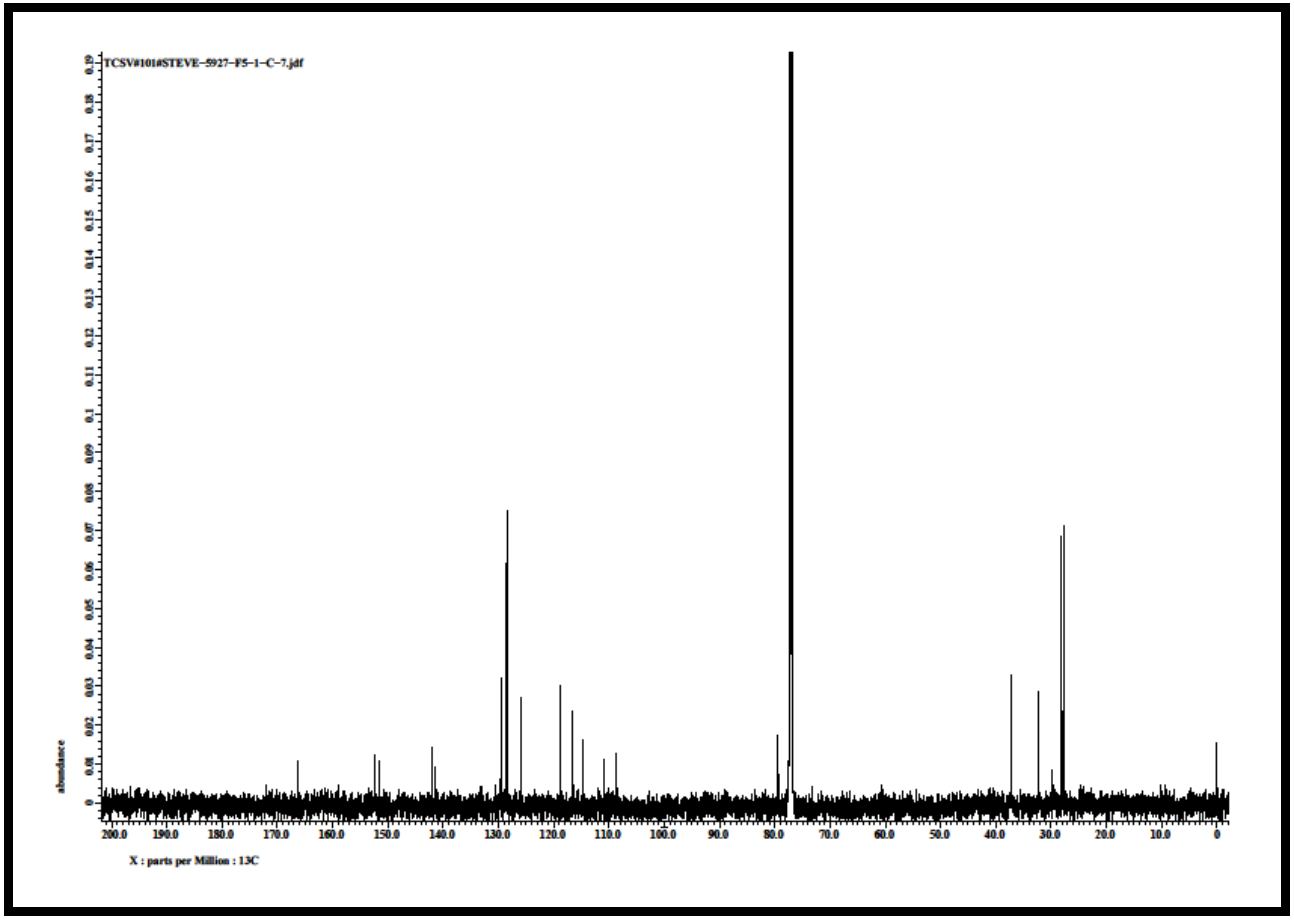


Figure S2. ^{13}C-NMR spectrum of **1** in $CDCl_3$ (150 MHz).

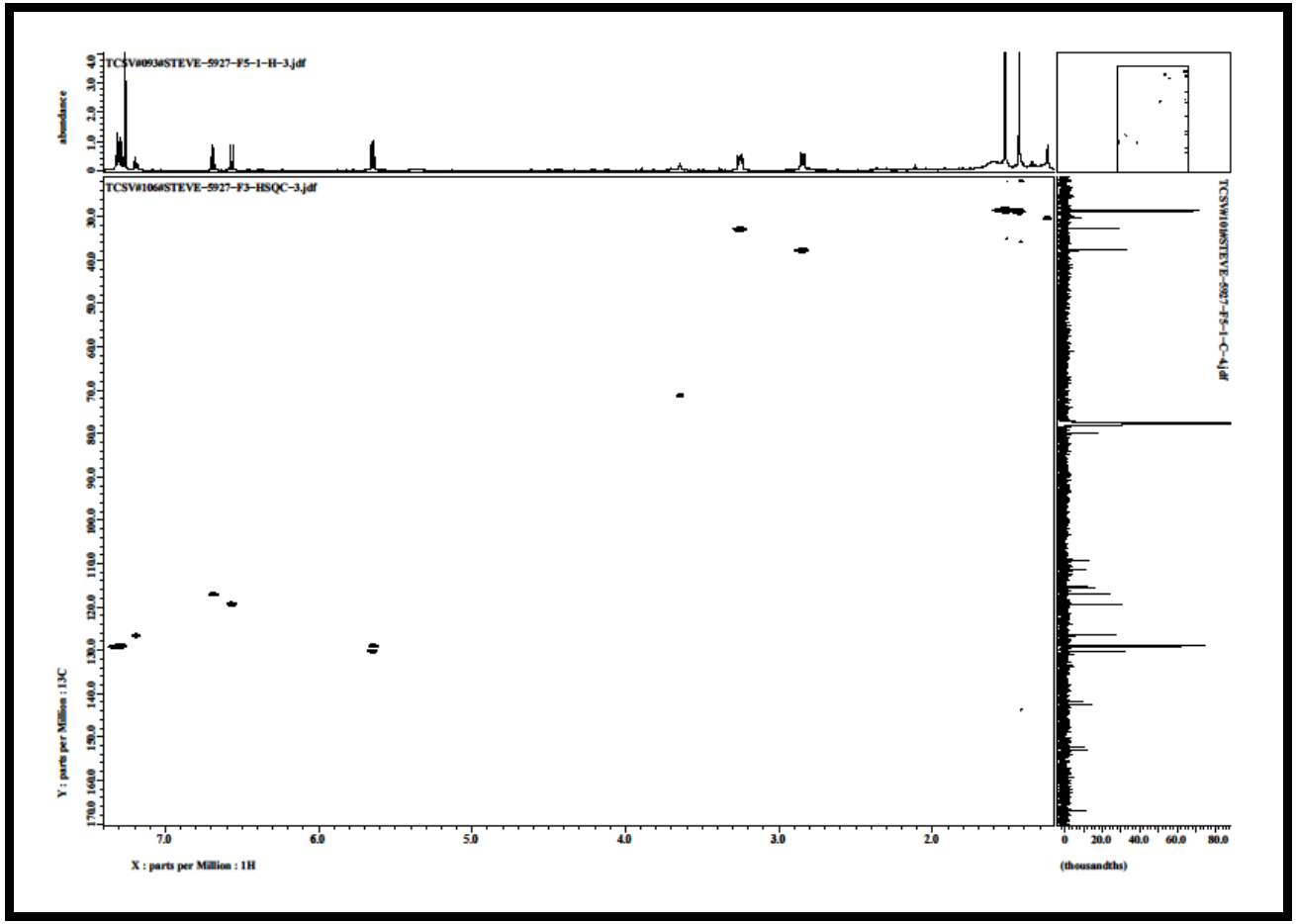


Figure S3. HSQC spectrum of **1** in $CDCl_3$.

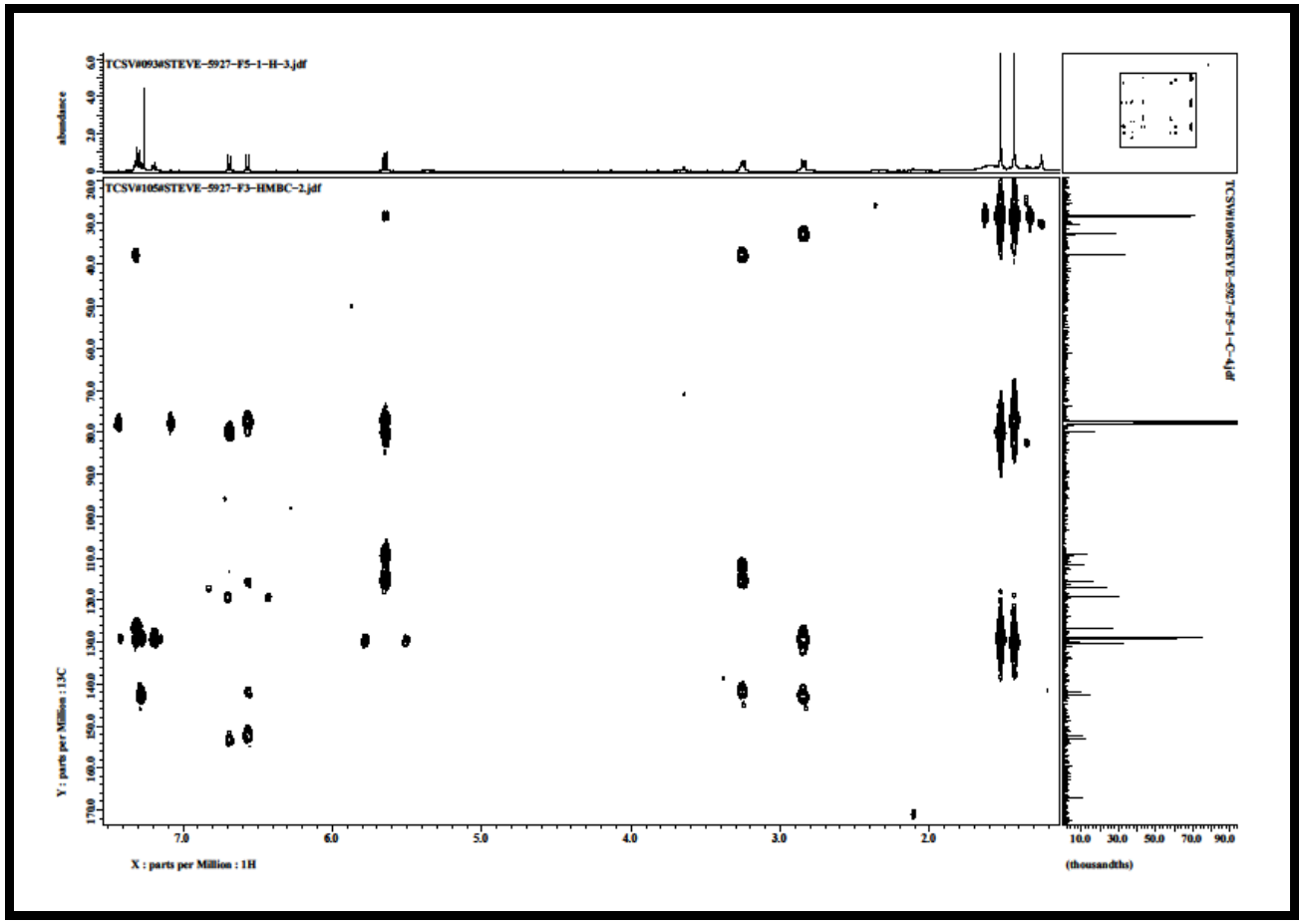


Figure S4. HMBC spectrum of **1** in $CDCl_3$.

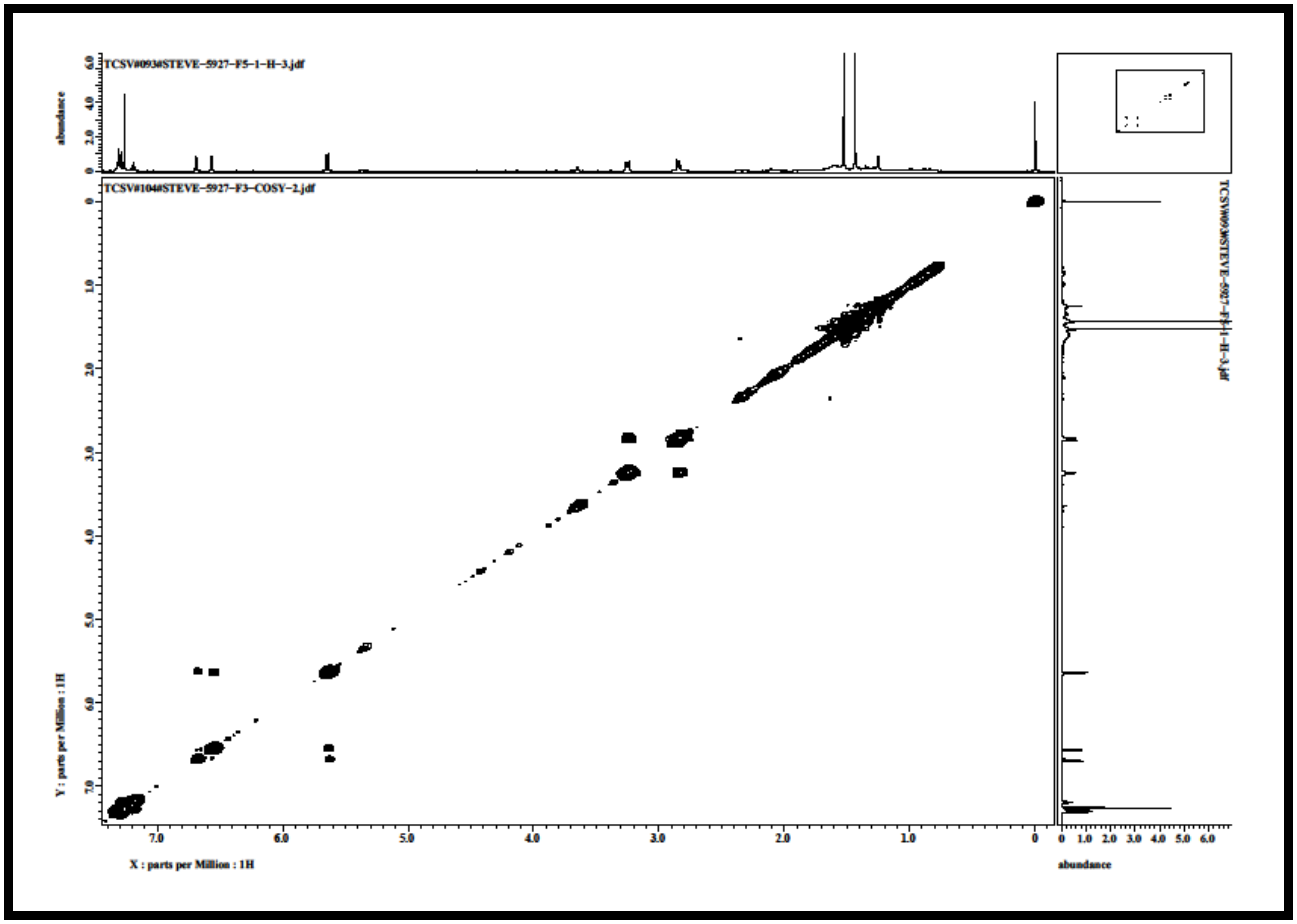


Figure S5. ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_3$.

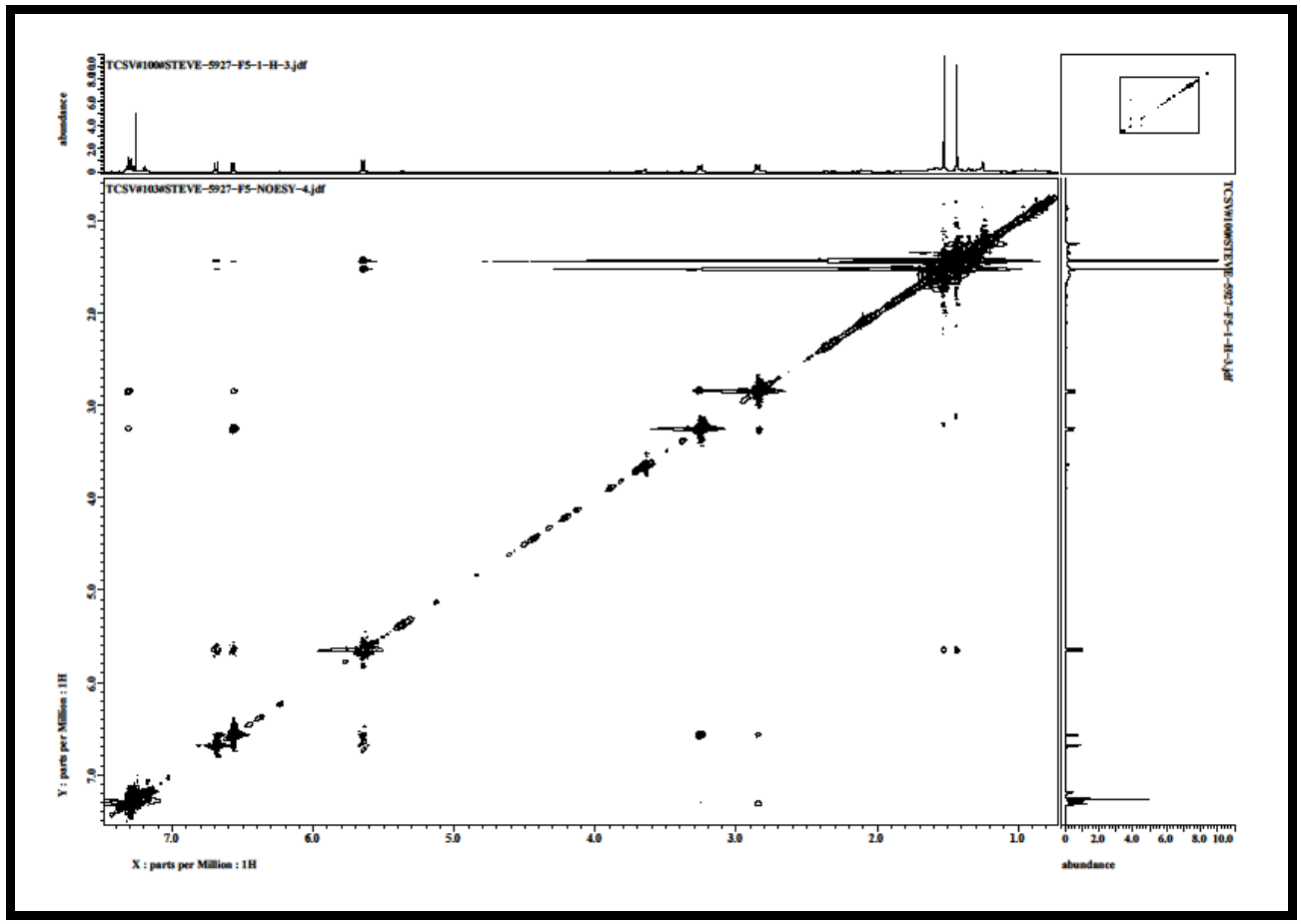
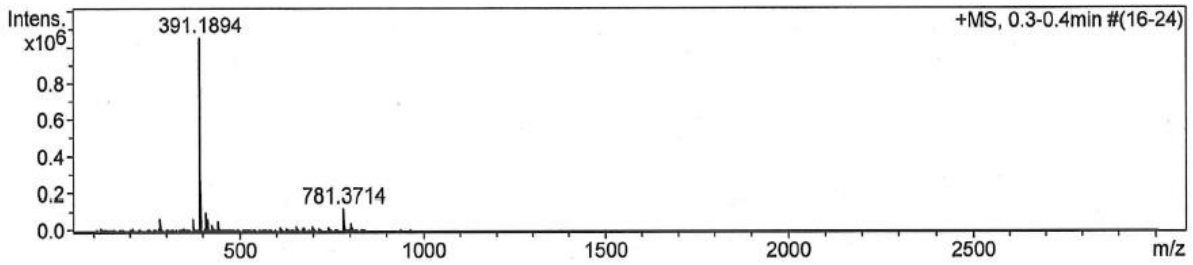


Figure S6. NOESY spectrum of **1** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
391.1894	1	C 22 H 23 N 4 O 3	0.00	391.1765	-12.9	-33.0	3.1	13.5	even	ok
	2	C 24 H 27 N 2 O 3	0.00	391.2016	12.3	31.3	5.4	12.5	even	ok
	3	C 21 H 23 N 6 O 2	69.34	391.1877	-1.7	-4.3	5.5	13.5	even	ok
	4	C 25 H 27 O 4	100.00	391.1904	1.0	2.6	7.8	12.5	even	ok
	5	C 20 H 23 N 8 O	0.00	391.1989	9.6	24.5	8.8	13.5	even	ok
	6	C 18 H 19 N 10 O	0.00	391.1738	-15.6	-39.8	16.9	14.5	even	ok
	7	C 21 H 27 O 7	0.00	391.1751	-14.2	-36.4	17.8	8.5	even	ok
	8	C 17 H 19 N 12	3.92	391.1850	-4.3	-11.1	18.9	14.5	even	ok
	9	C 20 H 27 N 2 O 6	17.32	391.1864	-3.0	-7.7	19.8	8.5	even	ok
	10	C 27 H 23 N 2 O	0.00	391.1805	-8.9	-22.7	20.9	17.5	even	ok
	11	C 19 H 27 N 4 O 5	0.00	391.1976	8.2	21.0	21.9	8.5	even	ok
	12	C 26 H 23 N 4	29.41	391.1917	2.4	6.0	22.1	17.5	even	ok
	13	C 18 H 27 N 6 O 4	0.00	391.2088	19.5	49.8	24.1	8.5	even	ok
	14	C 29 H 27 O	0.00	391.2056	16.3	41.6	28.3	16.5	even	ok
	15	C 18 H 31 O 9	0.06	391.1963	6.9	17.6	29.9	3.5	even	ok
	16	C 17 H 23 N 6 O 5	0.00	391.1724	-16.9	-43.3	30.3	9.5	even	ok
	17	C 17 H 31 N 2 O 8	0.00	391.2075	18.1	46.3	36.5	3.5	even	ok

Figure S7. HRESIMS data of **1**.

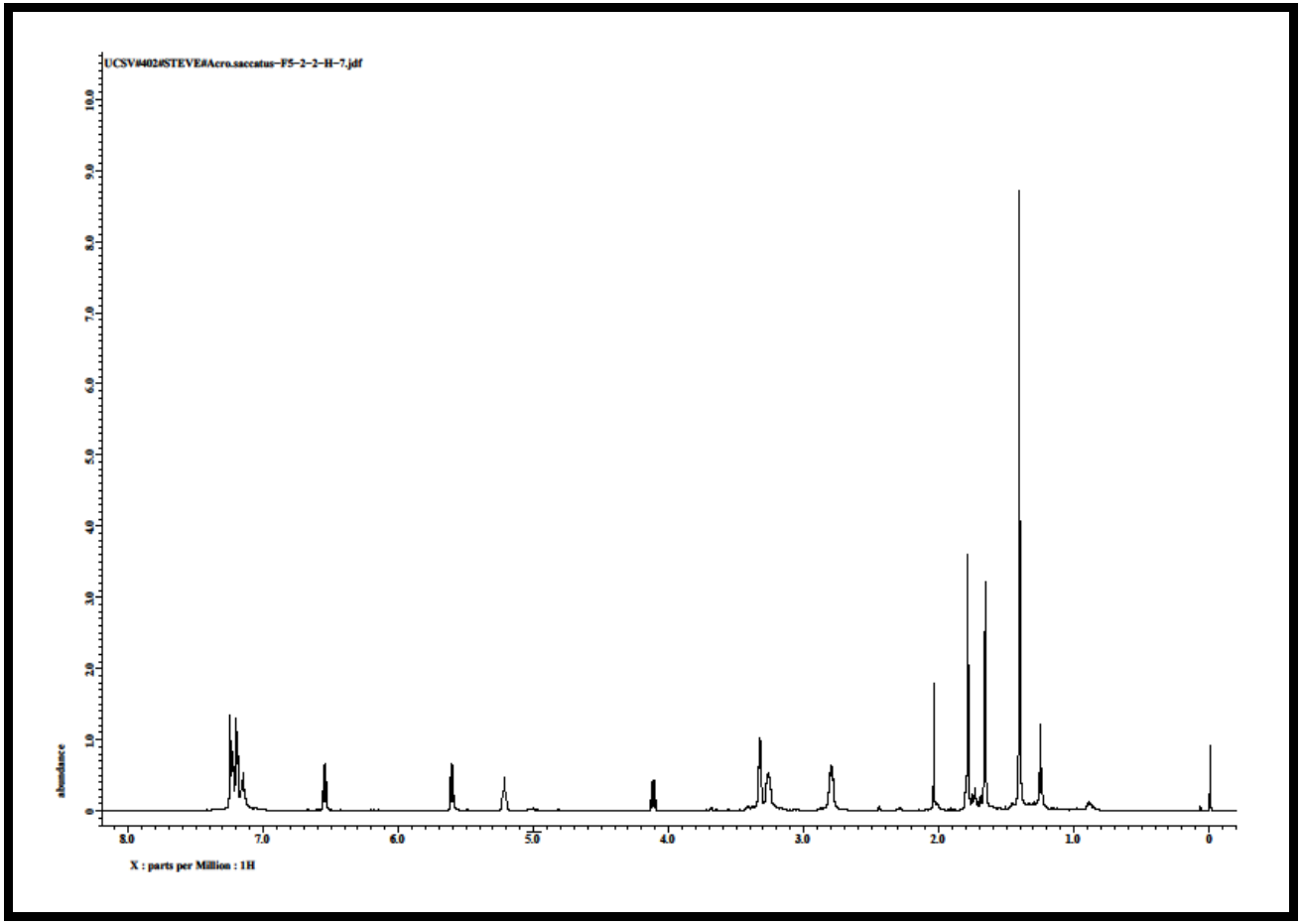


Figure S8. ^{1}H-NMR spectrum of **2** in $CDCl_3$ (600 MHz).

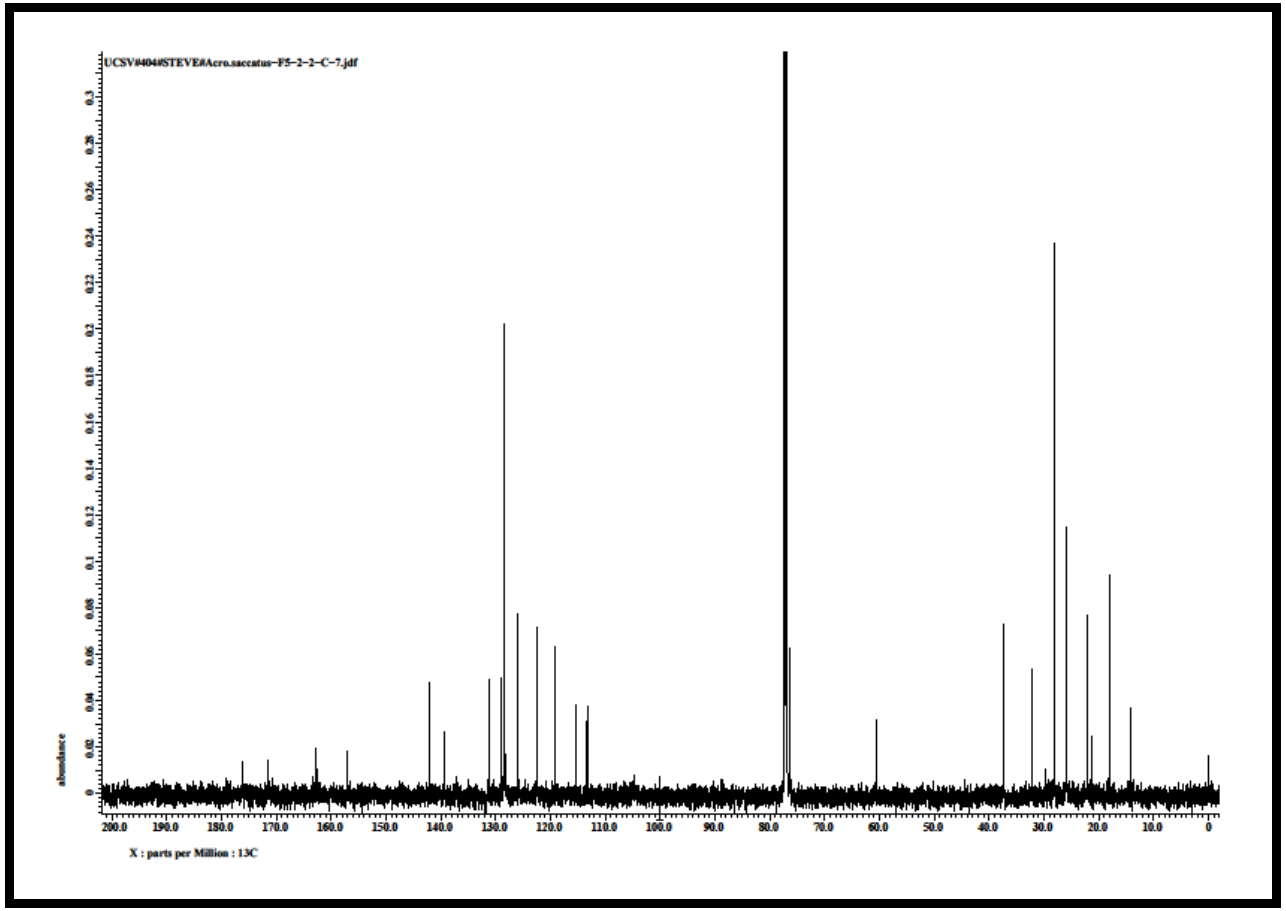


Figure S9. ^{13}C-NMR spectrum of **2** in $CDCl_3$ (150 MHz).

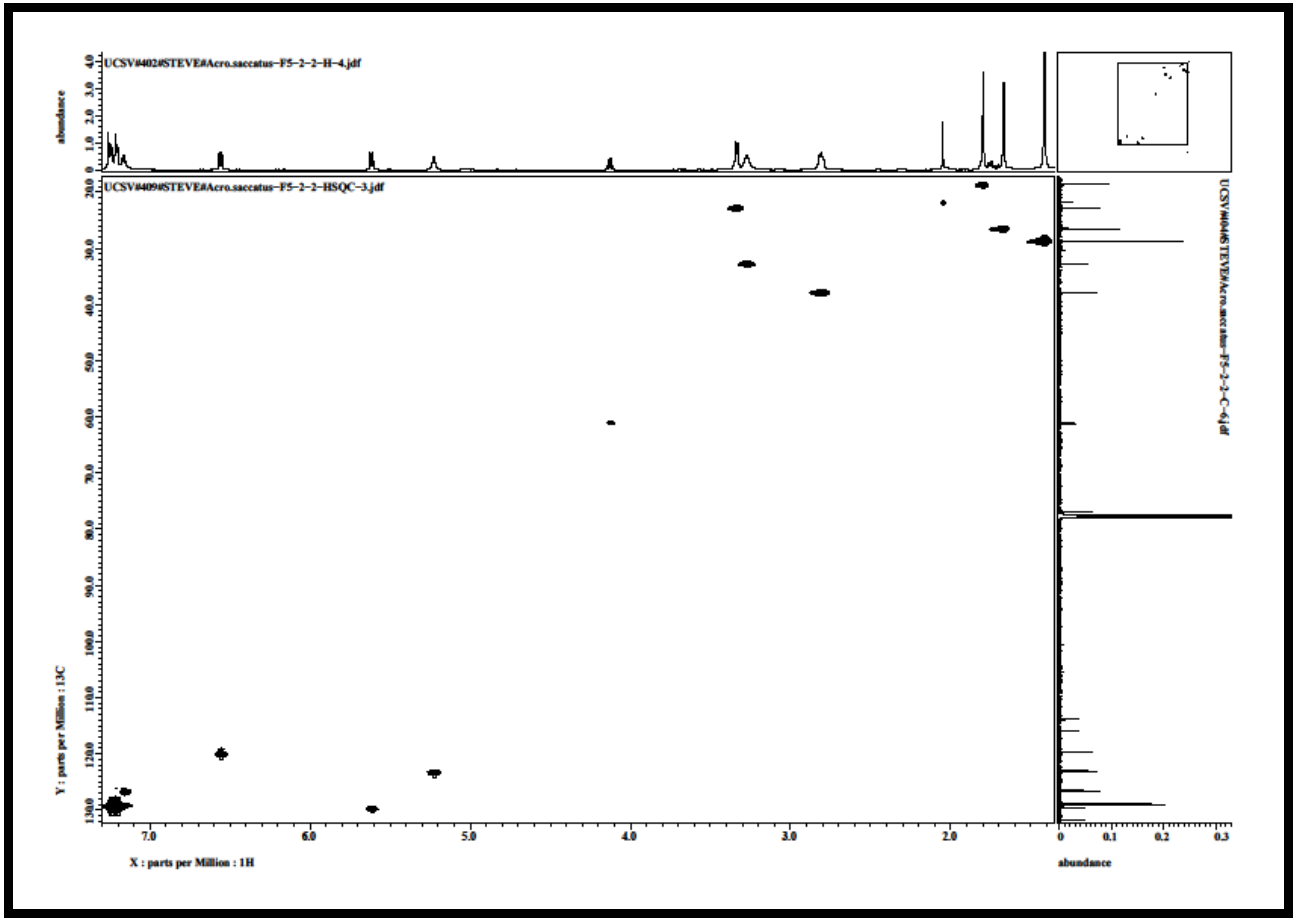


Figure S10. HSQC spectrum of **2** in $CDCl_3$.

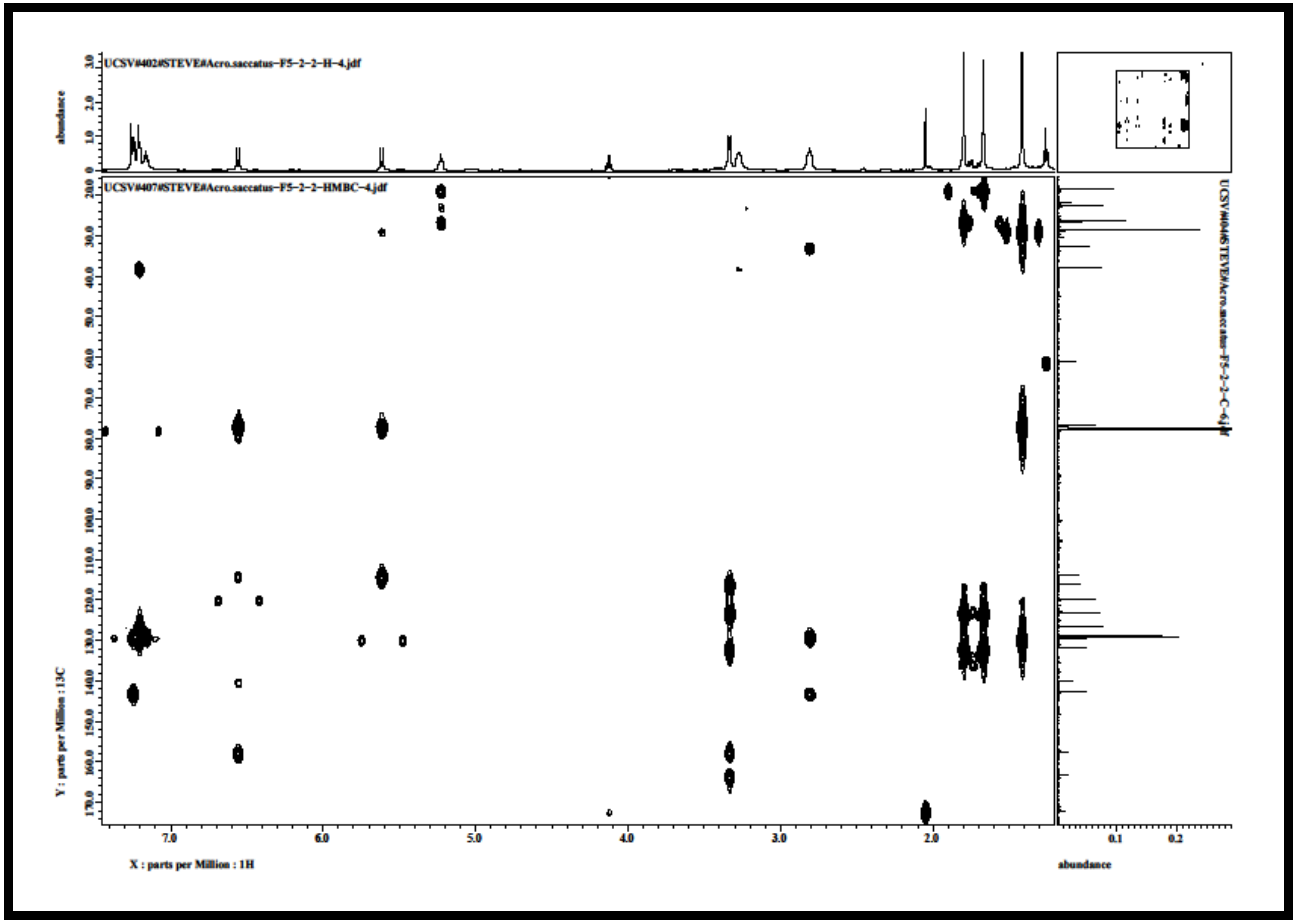


Figure S11. HMBC spectrum of **2** in $CDCl_3$.

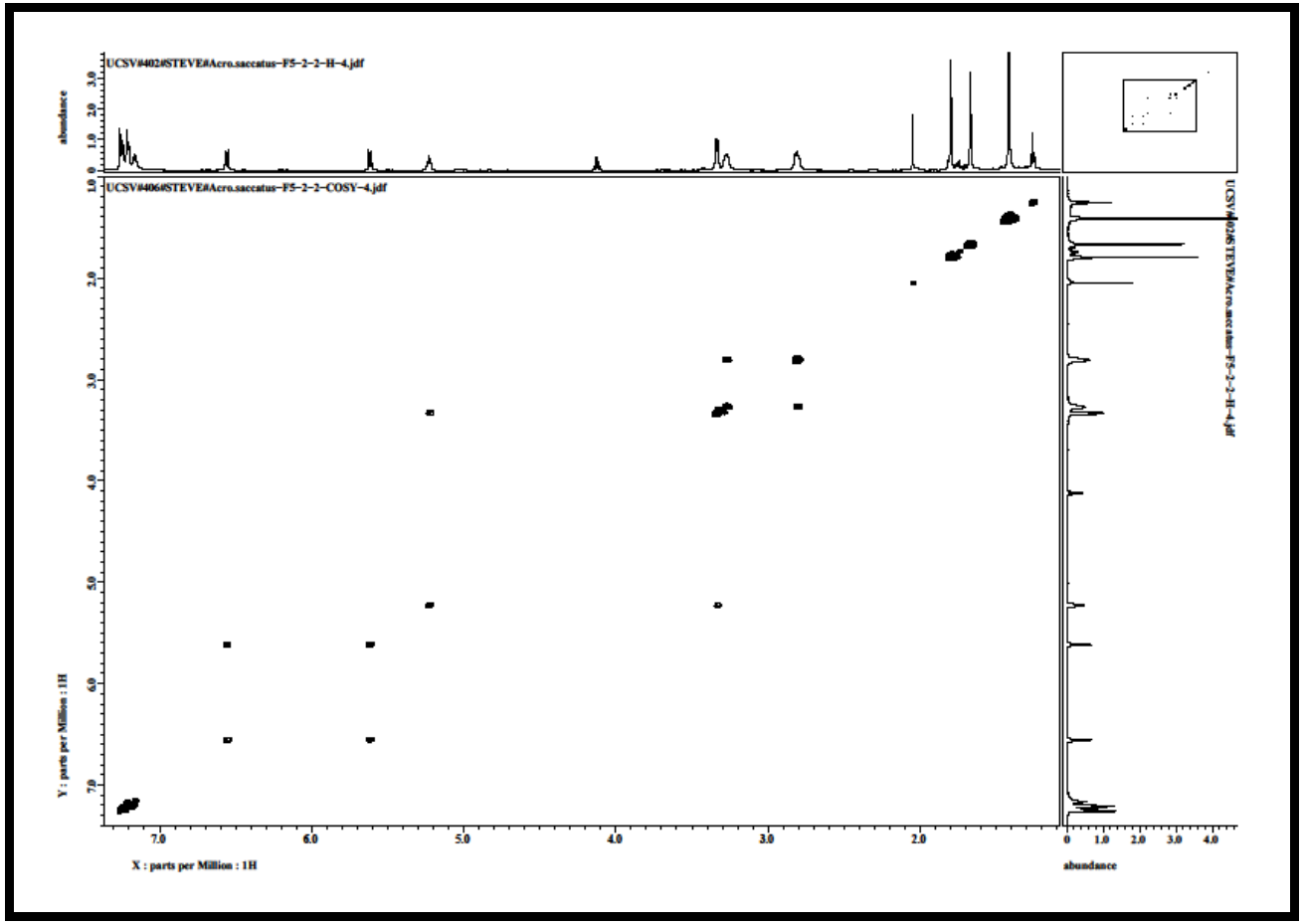


Figure S12. ^{1}H-^{1}H COSY spectrum of **2** in $CDCl_3$.

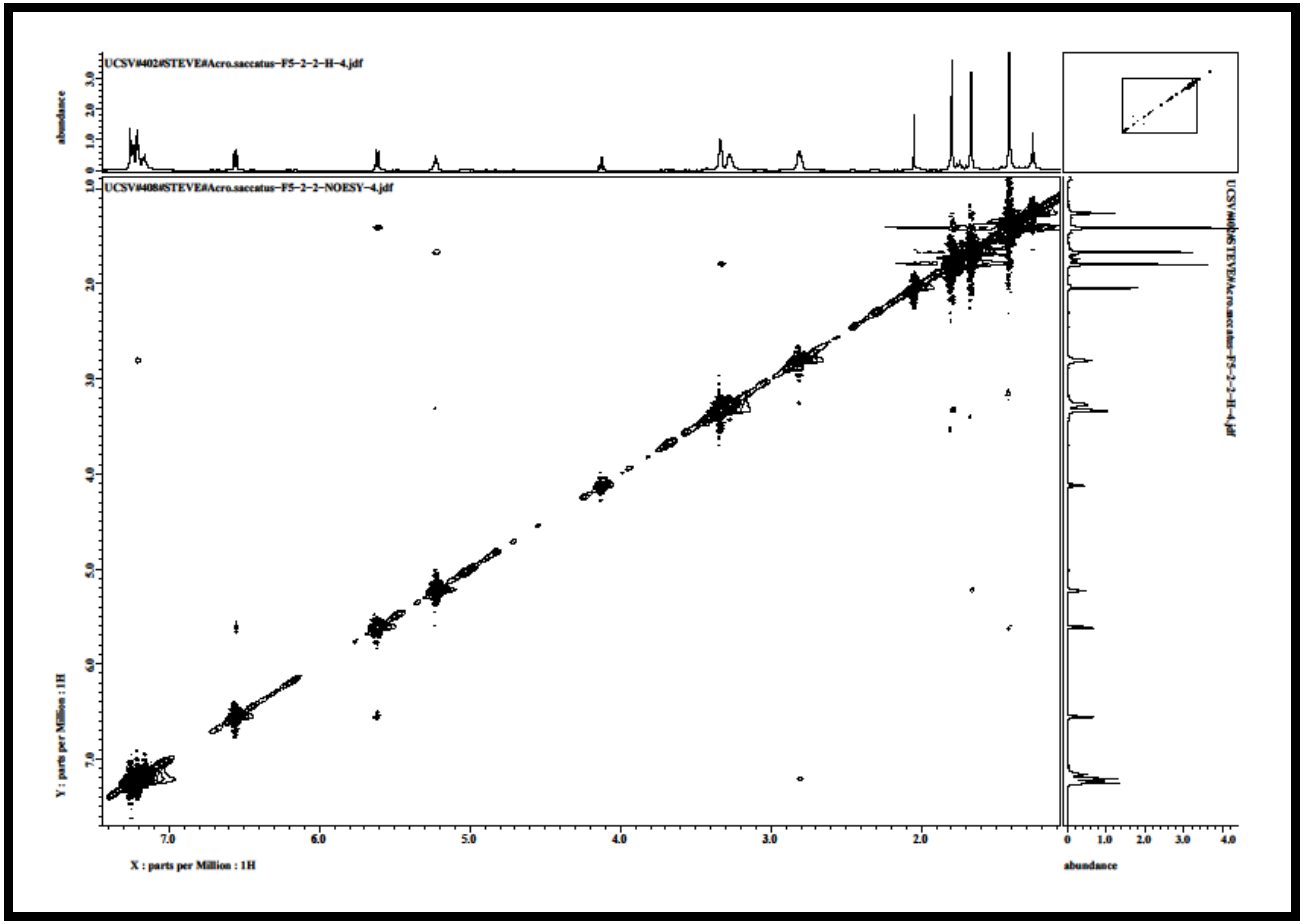
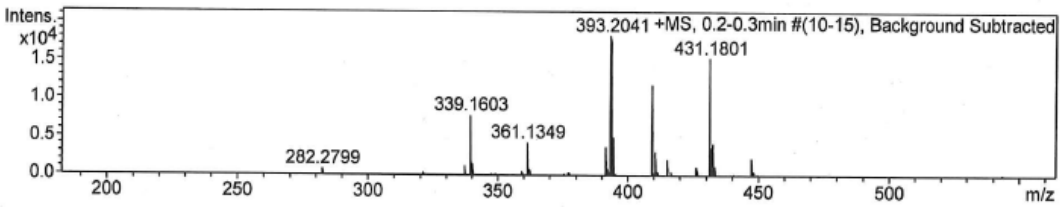


Figure S13. NOESY spectrum of **2** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
391.1830	1	C 27 H 23 N 2 O	100.00	391.1805	-2.5	-6.5	648.6	17.5	even	ok
	2	C 15 H 27 N 4 O 8	0.00	391.1823	-0.7	-1.7	727.3	4.5	even	ok
	3	C 21 H 27 O 7	0.00	391.1751	-7.9	-20.2	727.4	8.5	even	ok
	4	C 20 H 27 N 2 O 6	0.00	391.1864	3.3	8.6	728.3	8.5	even	ok
	5	C 18 H 28 N 2 Na O 6	0.00	391.1840	0.9	2.4	728.7	5.5	even	ok
	6	C 25 H 27 O 4	0.00	391.1904	7.4	18.8	729.4	12.5	even	ok
	7	C 23 H 28 Na O 4	0.00	391.1880	5.0	12.7	729.8	9.5	even	ok
	8	C 22 H 23 N 4 O 3	0.00	391.1765	-6.5	-16.7	730.6	13.5	even	ok
	9	C 16 H 23 N 8 O 4	0.00	391.1837	0.7	1.7	730.6	9.5	even	ok
	10	C 20 H 24 N 4 Na O 3	0.00	391.1741	-9.0	-22.9	731.0	10.5	even	ok
	11	C 21 H 23 N 6 O 2	0.00	391.1877	4.7	12.0	731.6	13.5	even	ok
	12	C 19 H 24 N 6 Na O 2	0.00	391.1853	2.3	5.8	732.0	10.5	even	ok
	13	C 26 H 23 N 4	0.00	391.1917	8.7	22.3	732.7	17.5	even	ok
	14	C 25 H 24 N 2 Na O	0.00	391.1781	-4.9	-12.6	732.9	14.5	even	ok
	15	C 24 H 24 N 4 Na	0.00	391.1893	6.3	16.1	733.0	14.5	even	ok
	16	C 18 H 19 N 10 O	0.00	391.1738	-9.2	-23.6	733.9	14.5	even	ok
	17	C 17 H 19 N 12	0.00	391.1850	2.0	5.1	734.0	14.5	even	ok
	18	C 15 H 20 N 12 Na	0.00	391.1826	-0.4	-1.0	734.4	11.5	even	ok
393.2041	1	C 24 H 26 N 4 Na	93.41	393.2050	0.9	2.2	14.0	13.5	even	ok
	2	C 25 H 29 O 4	42.99	393.2060	1.9	4.9	18.2	11.5	even	ok
	3	C 21 H 25 N 6 O 2	90.46	393.2034	-0.7	-1.9	18.7	12.5	even	ok
	4	C 23 H 30 Na O 4	100.00	393.2036	-0.5	-1.2	20.6	8.5	even	ok
	5	C 26 H 25 N 4	12.15	393.2074	3.3	8.3	21.8	16.5	even	ok
	6	C 19 H 26 N 6 Na O 2	11.05	393.2009	-3.2	-8.0	31.1	9.5	even	ok
	7	C 20 H 29 N 2 O 6	25.62	393.2020	-2.1	-5.3	35.4	7.5	even	ok

Figure S14. HRESIMS data of **2**.

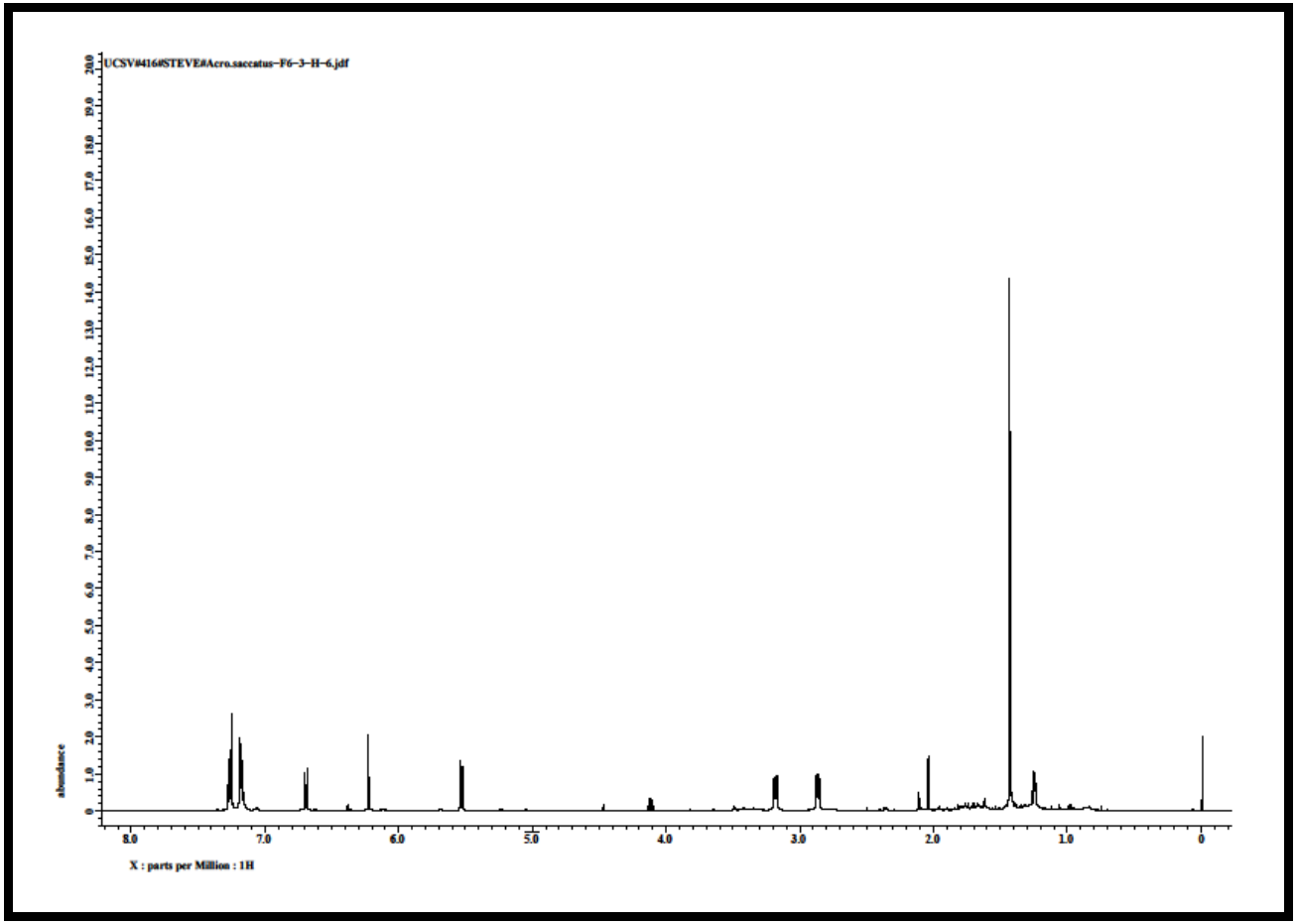


Figure S15. ^{1}H-NMR spectrum of **3** in $CDCl_3$ (600 MHz).

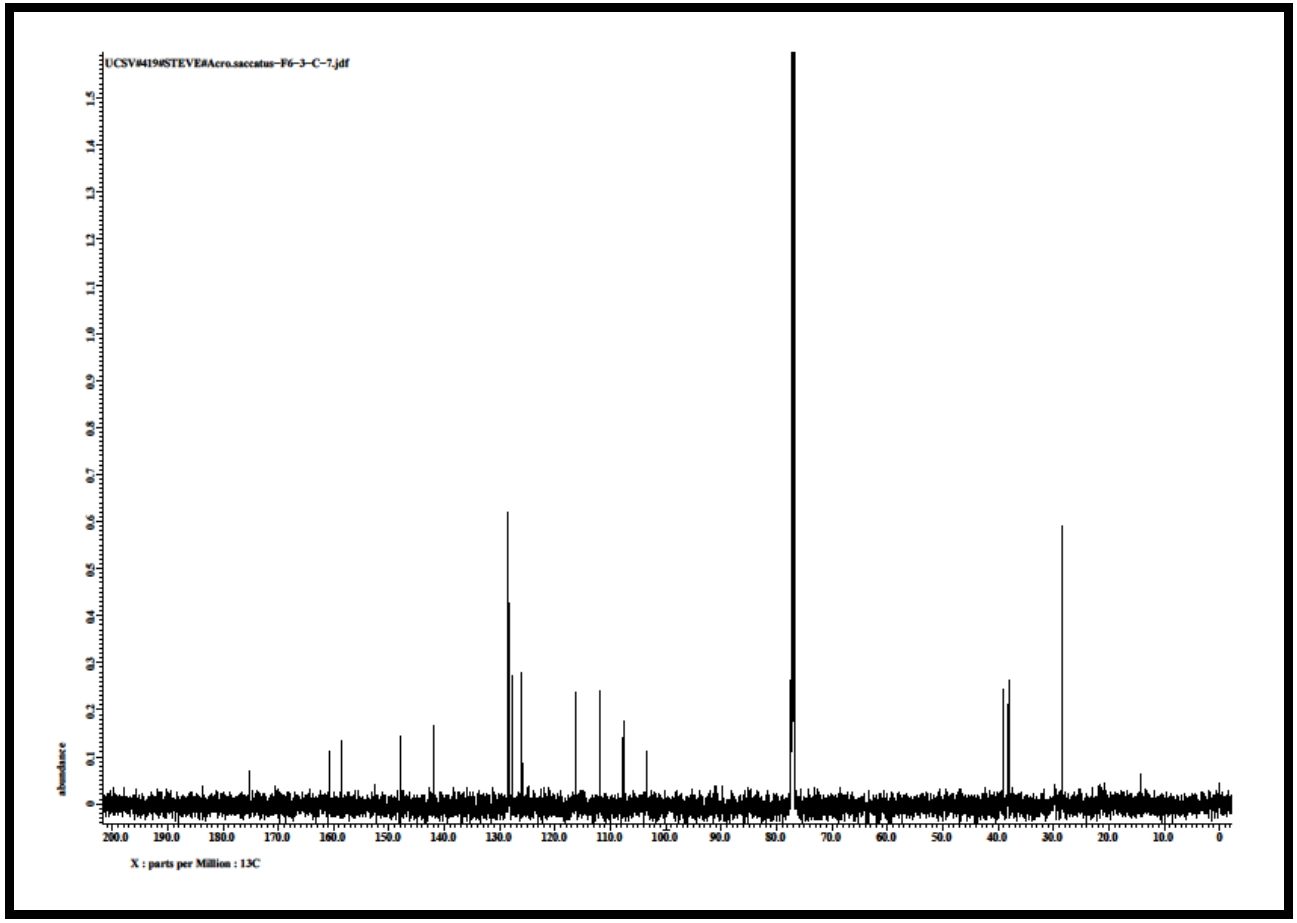


Figure S16. ^{13}C-NMR spectrum of **3** in $CDCl_3$ (150 MHz).

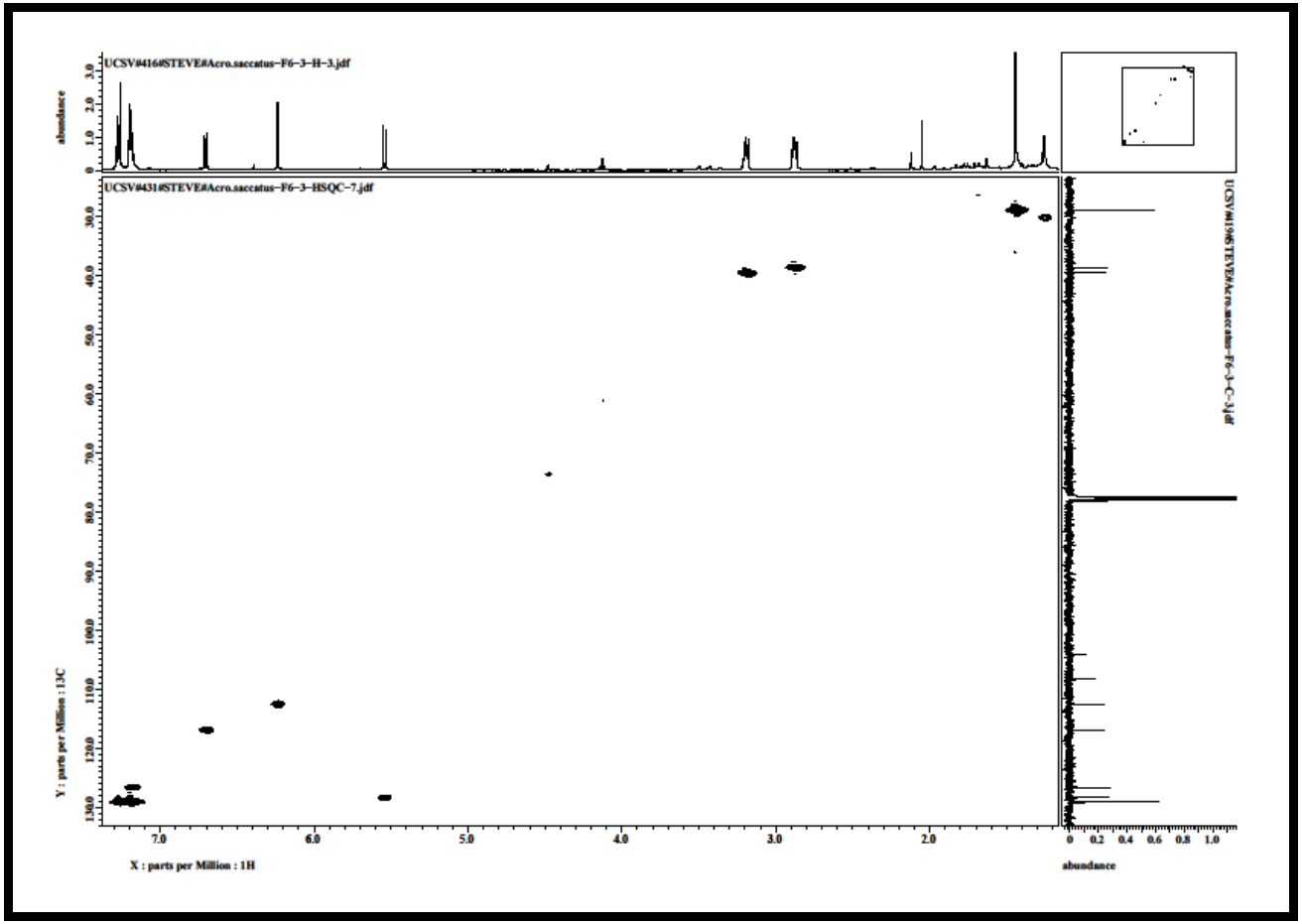


Figure S17. HSQC spectrum of **3** in $CDCl_3$.

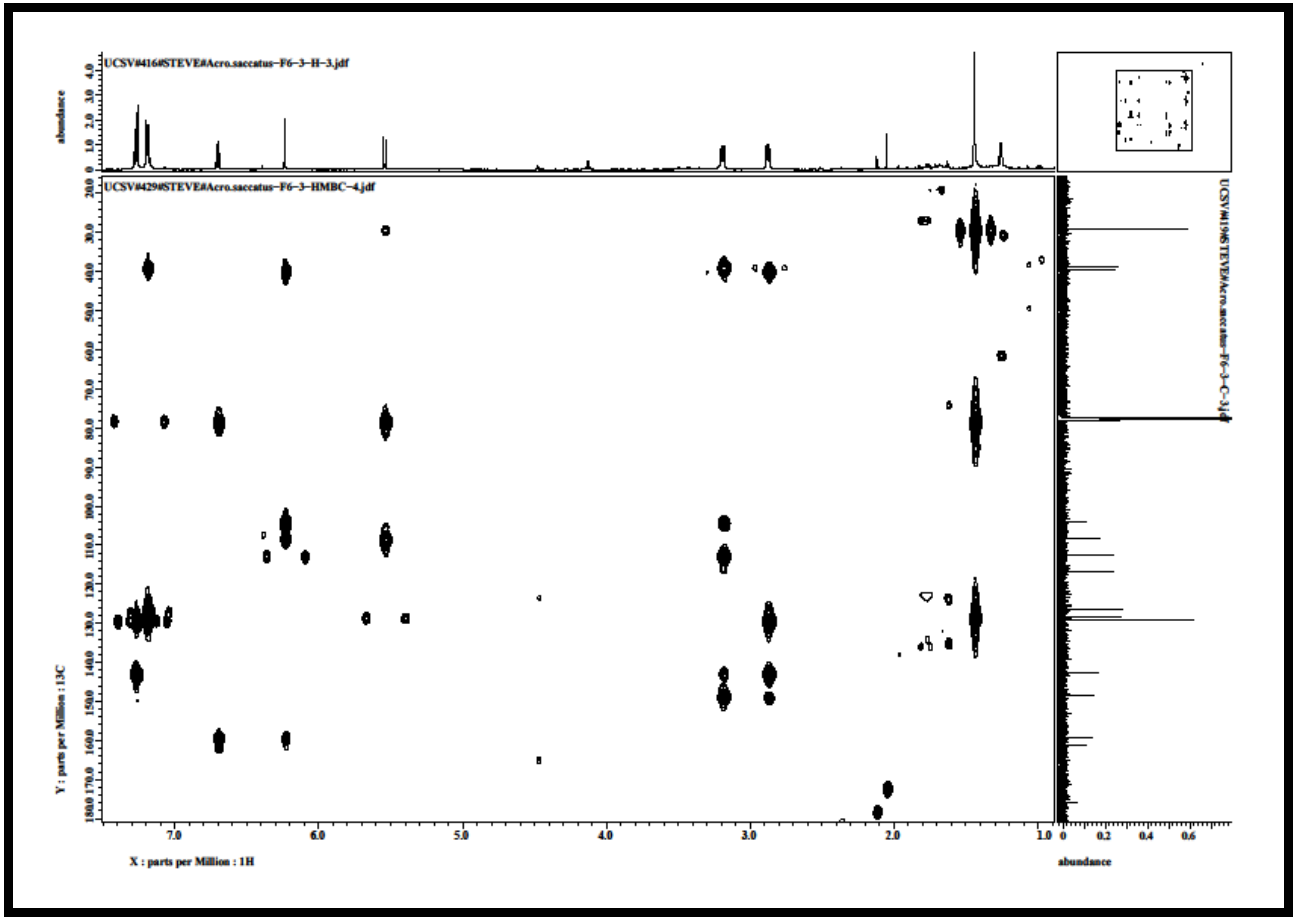


Figure S18. HMBC spectrum of **3** in $CDCl_3$.

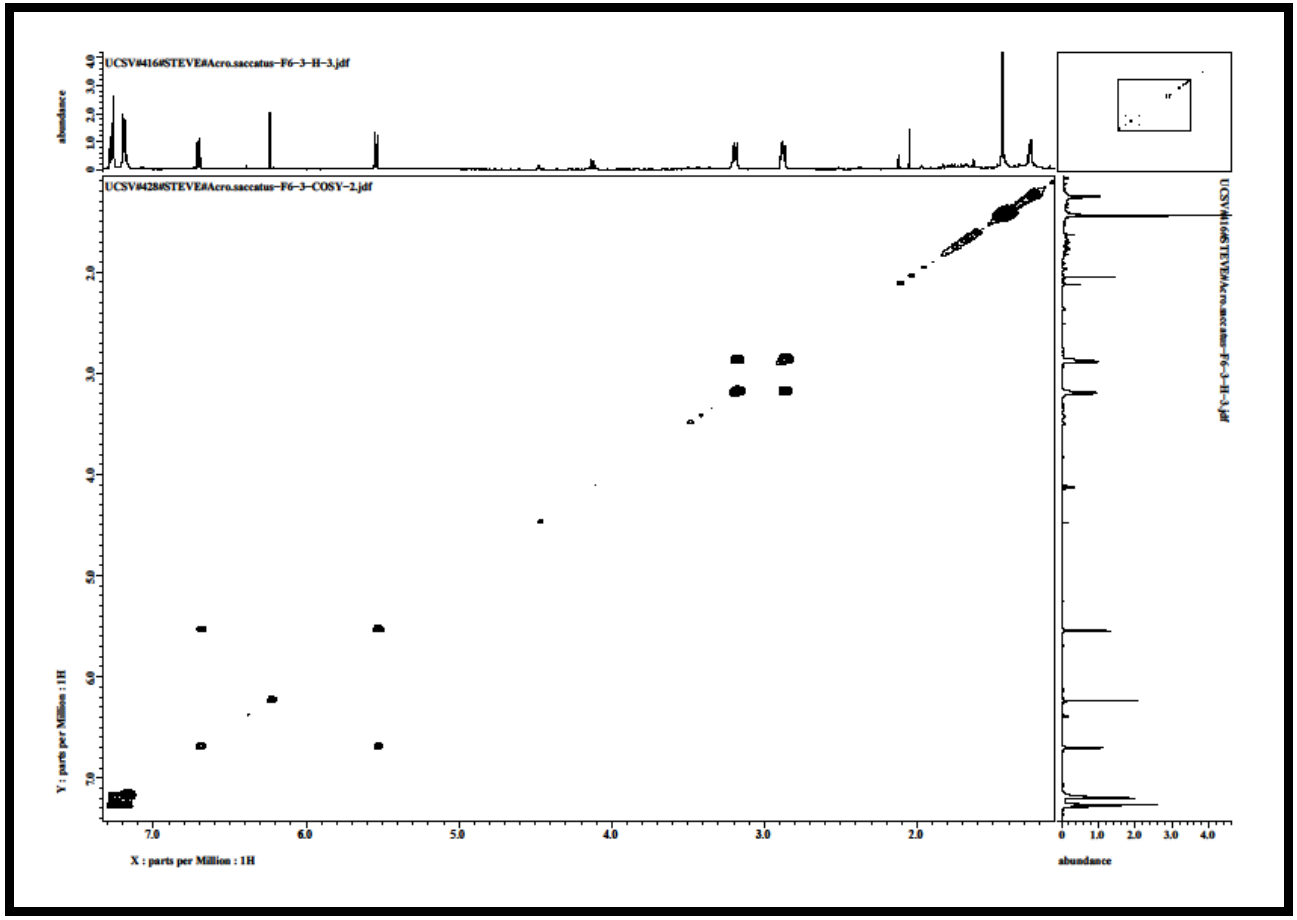


Figure S19. ^{1}H-^{1}H COSY spectrum of **3** in $CDCl_3$.

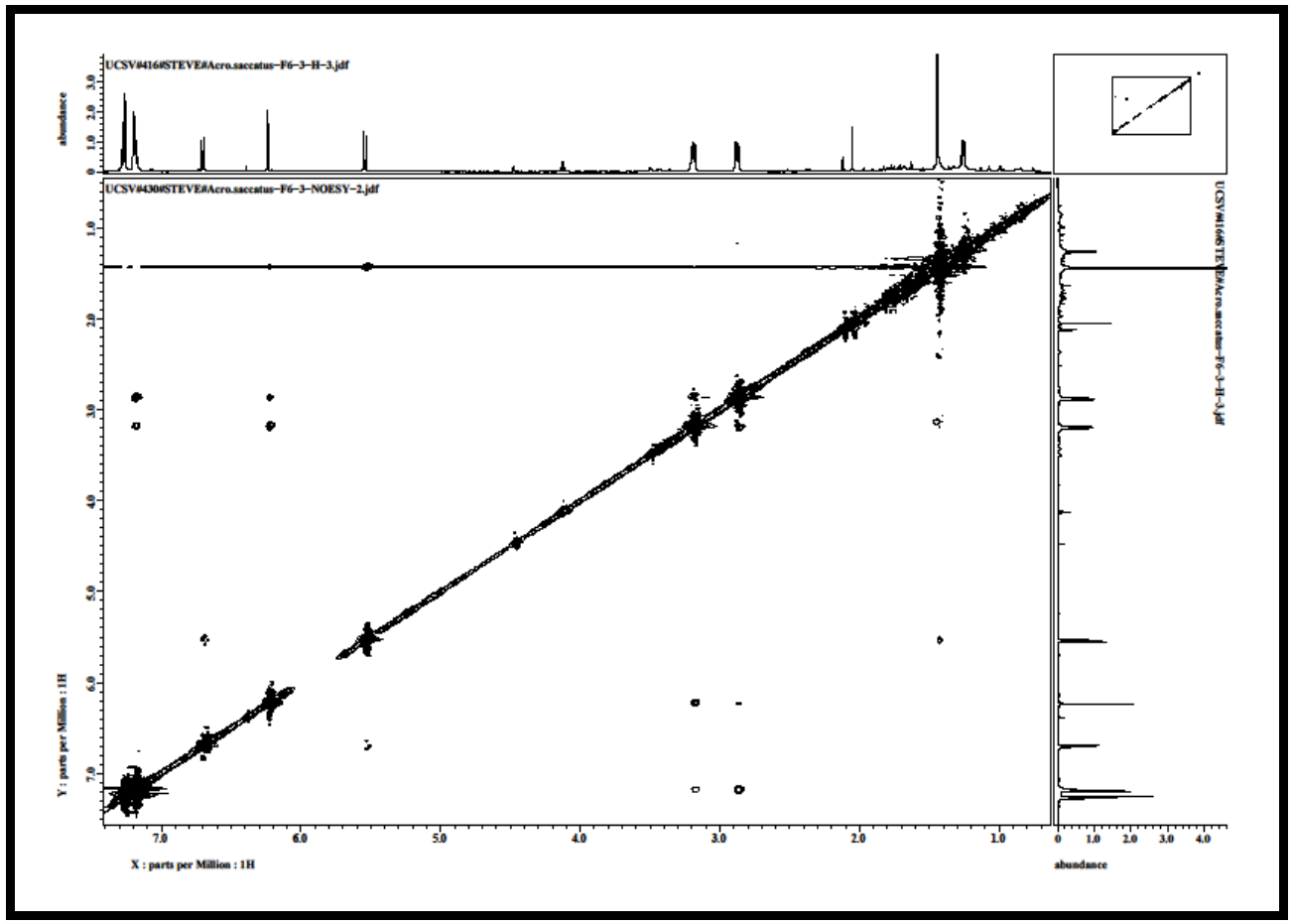
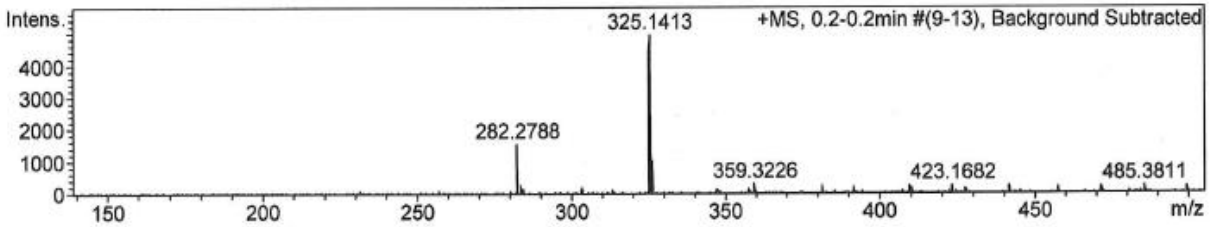


Figure S20. NOESY spectrum of **3** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
325.1413	1	C 19 H 18 N 4 Na	74.95	325.1424	1.0	3.2	13.9	12.5	even	ok
	2	C 16 H 17 N 6 O 2	91.50	325.1408	-0.6	-1.8	16.5	11.5	even	ok
	3	C 20 H 21 O 4	33.58	325.1434	2.1	6.5	17.7	10.5	even	ok
	4	C 18 H 22 Na O 4	100.00	325.1410	-0.3	-0.9	18.6	7.5	even	ok
	5	C 21 H 17 N 4	8.70	325.1448	3.4	10.6	23.0	15.5	even	ok
	6	C 14 H 18 N 6 Na O 2	13.32	325.1383	-3.0	-9.2	25.3	8.5	even	ok
	7	C 15 H 21 N 2 O 6	30.12	325.1394	-1.9	-5.9	29.4	6.5	even	ok

Figure S21. HRESIMS data of **3**.