

Supporting Information:

Saquayamycins G-K, Cytotoxic Angucyclines from *Streptomyces* sp. Including Two Angucycline Derivatives Bearing Aminosugar Rednose

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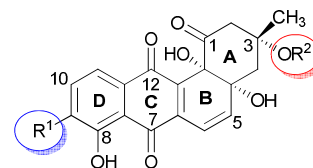
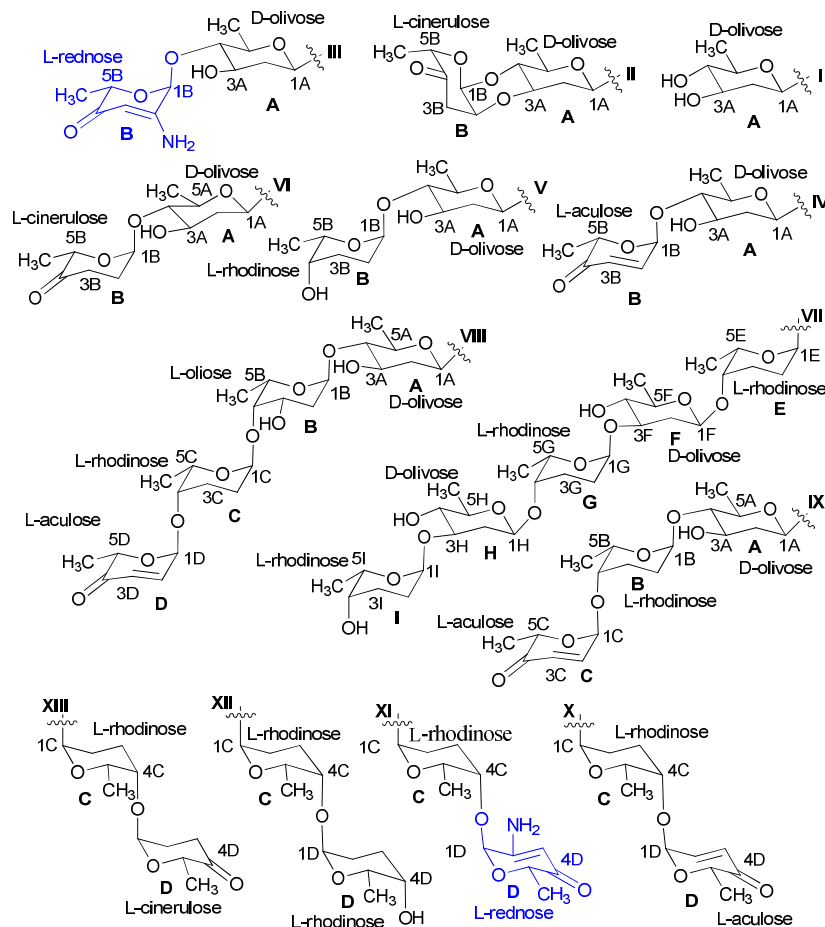
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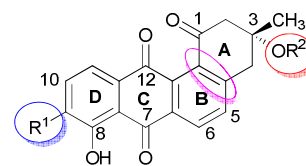
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Supporting Information

HPLC analysis of the crude extract obtained from the *Streptomyces* sp. KY40-1; work-up procedure scheme; NMR and mass spectra of isolated angucyclines (**1-8**).



- 1: R¹ = I, R² = X; Saquayamycin G
- 2: R¹ = II, R² = XI; Saquayamycin H
- 3: R¹ = III, R² = X; Saquayamycin I
- 4: R¹ = II, R² = XII; Saquayamycin J
- 5: R¹ = V, R² = X; Saquayamycin K
- 6: R¹ = II, R² = H; Saquayamycin B1
- 7: R¹ = IV, R² = X; Saquayamycin A
- 8: R¹ = II, R² = X; Saquayamycin B
- 9: R¹ = VI, R² = XIII; Saquayamycin C
- 10: R¹ = II, R² = XIII; Saquayamycin D
- 11: R¹ = IV, R² = H; Saquayamycin A1
- 12: R¹ = VI, R² = H; Saquayamycin C1
- 13: R¹ = IV, R² = XIII; Saquayamycin E
- 14: R¹ = VI, R² = X; Saquayamycin F
- 15: R¹ = VIII, R² = VII; Saquayamycin Z
- 16: R¹ = IX, R² = H; A-7884
- 17: R¹ = I, R² = H; Aquayamycin



- 18: R¹ = II, R² = X; Moromycin A
- 19: R¹ = II, R² = H; Moromycin B

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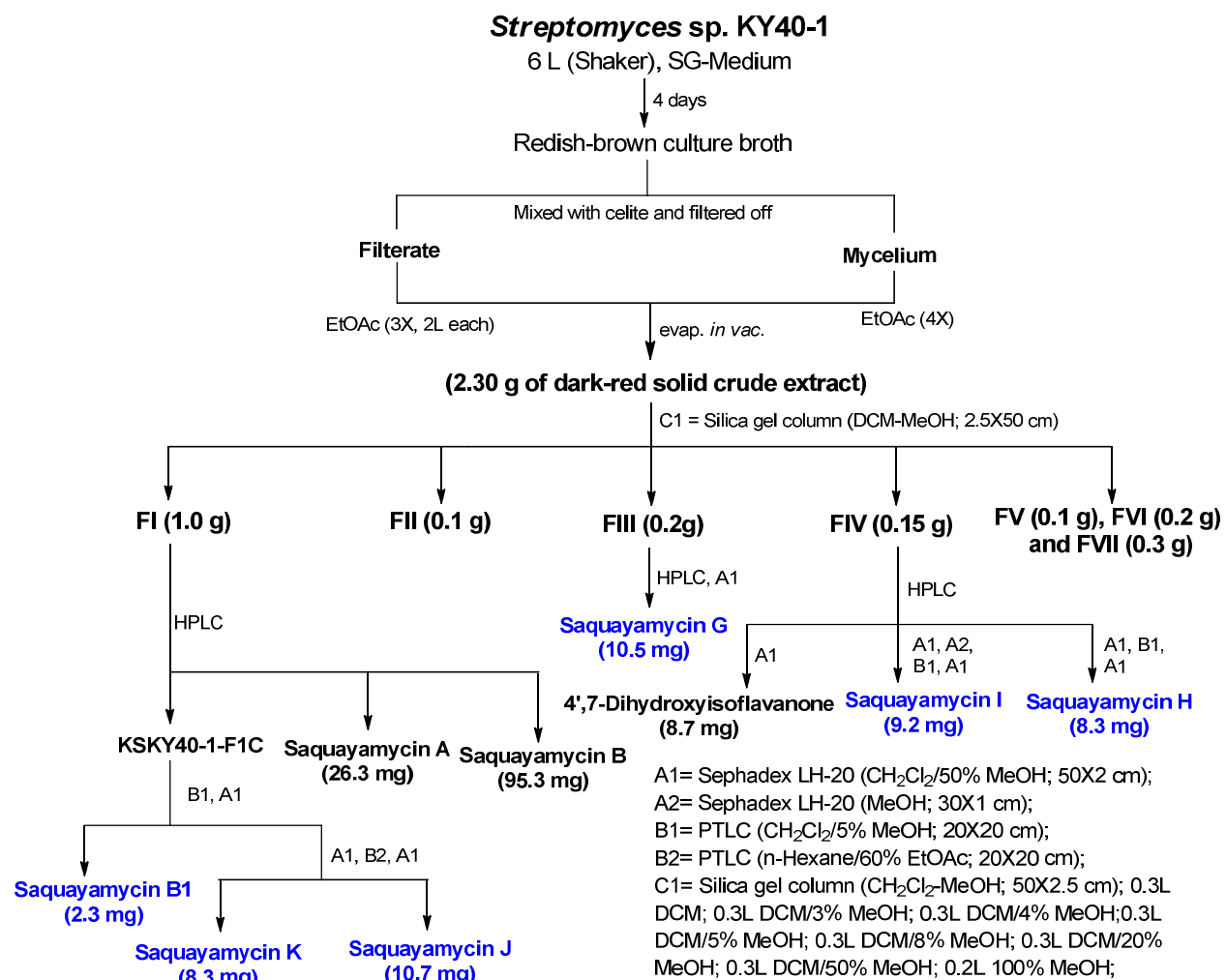


Figure S1: Work-up procedure of extracts from the *Streptomyces* sp. KY40-1

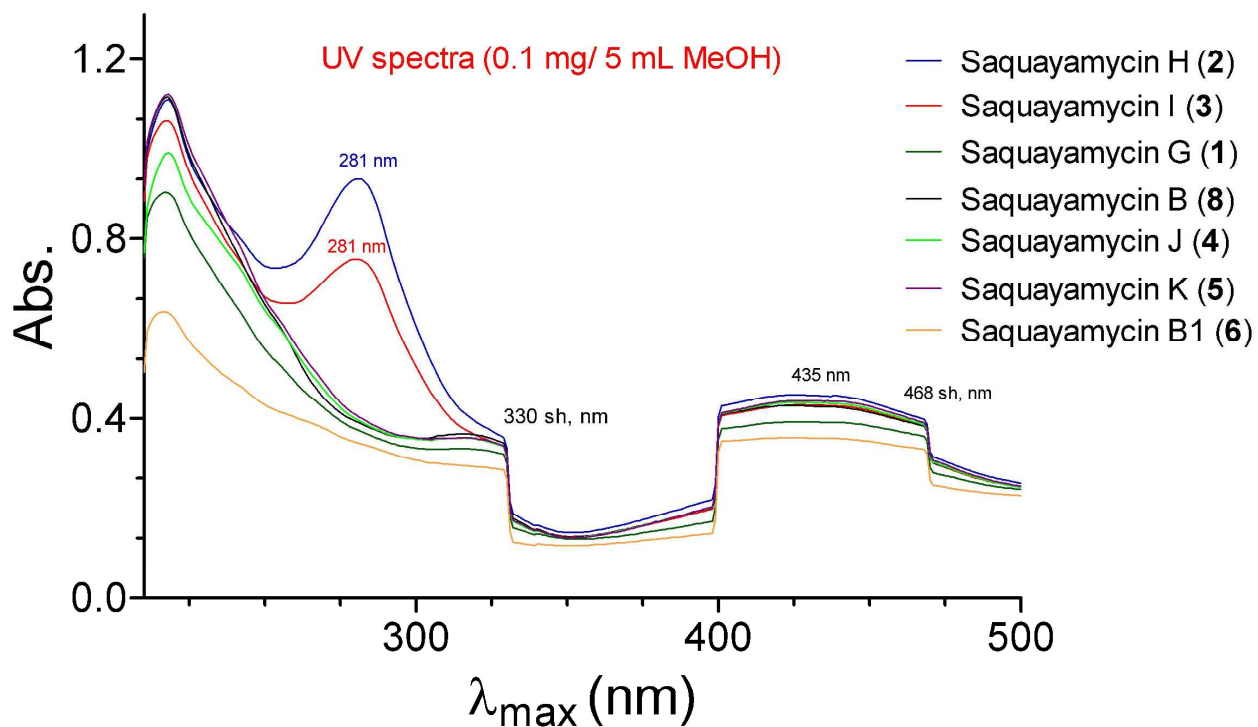


Figure S2: UV (MeOH) spectra of the new Saquayamycins G-K (**1-5**) and Saquayamycin B1 (**6**) in comparison with Saquayamycin B (**8**)

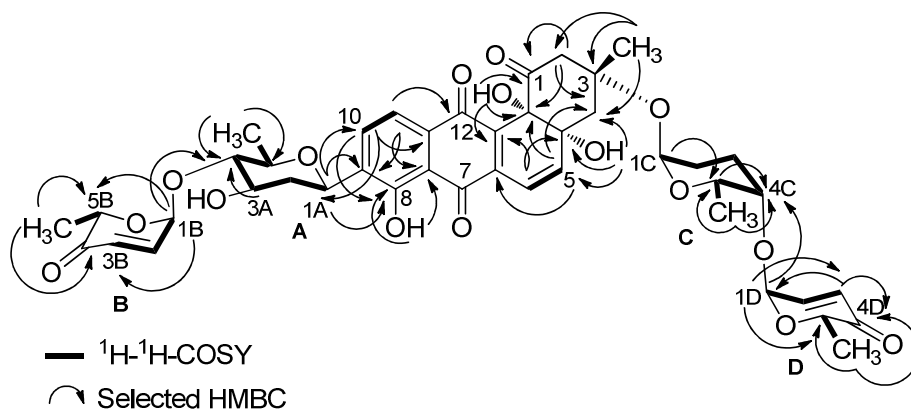


Figure S3: ^1H - ^1H -COSY (bold lines) and selected HMBC (\rightarrow) couplings in saquayamycin A (**7**)

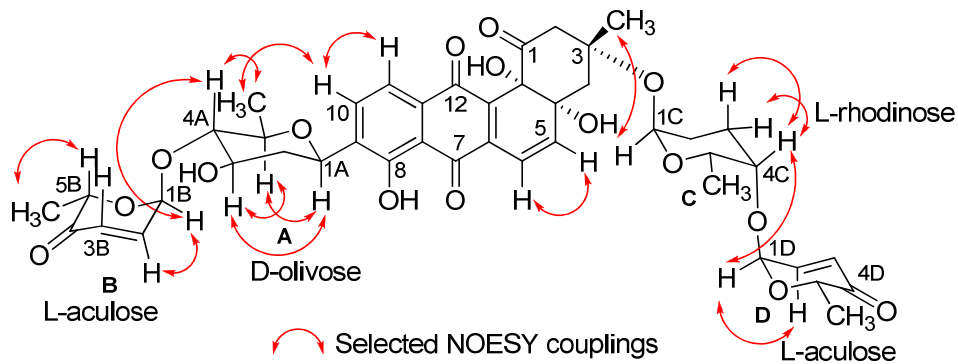


Figure S4: Selected NOESY correlations (\leftrightarrow) of saquayamycin A (7)

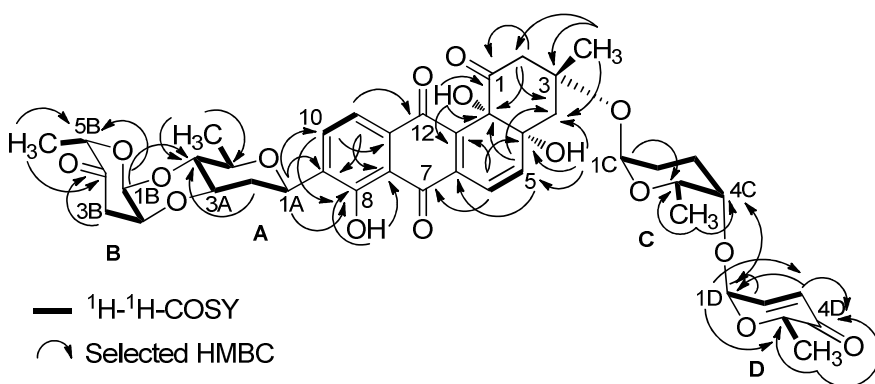


Figure S5: ^1H - ^1H -COSY (bold lines) and selected HMBC (\rightarrow) couplings in saquayamycin B (8)

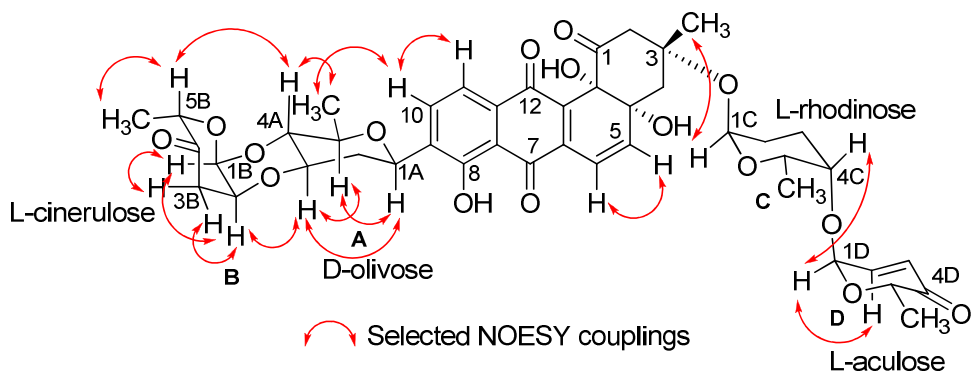


Figure S6: Selected NOESY correlations (\leftrightarrow) of saquayamycin B (8)

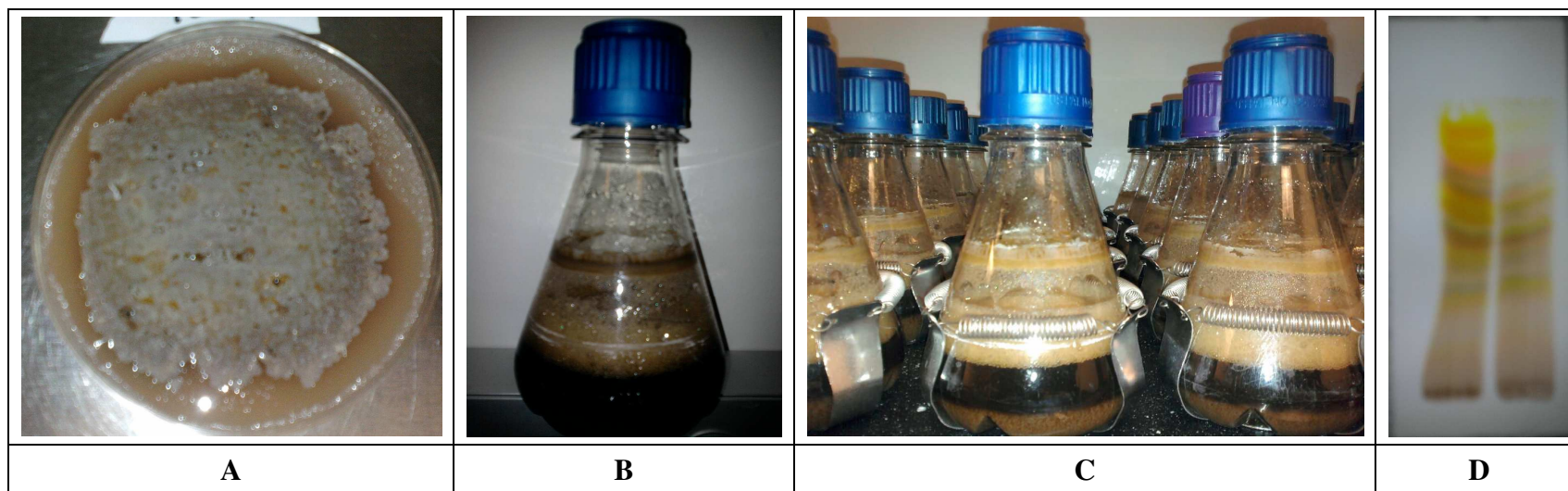
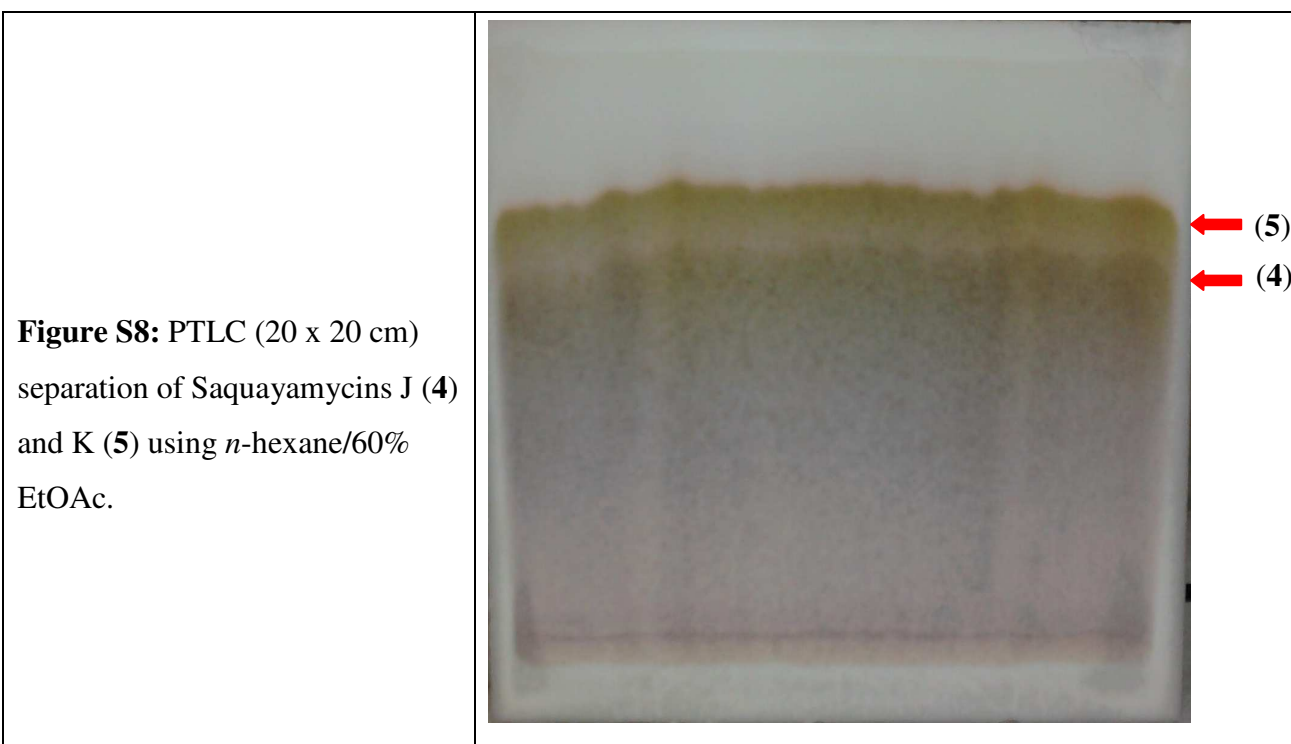


Figure S7: **A)** The *Streptomyces* sp. KY40-1 was cultivated on M2-agar plates at 28 °C for 3 days; **B)** A 100 ml of the reddish brown culture broth from *Streptomyces* sp. KY40-1 after inoculation and cultivation at 28 °C (250 rpm) for 48 hrs on SG-medium. **C)** Large scale cultivation (6 L) of *Streptomyces* sp. KY40-1 after inoculation using grown 100 mL preculture, at 28 °C (250 rpm) for 4 days on SG-medium. **D)** TLC (DCM/5% MeOH) of the water phase and mycelium extracts obtained from the 6 L cultivation of *Streptomyces* sp. KY40-1.



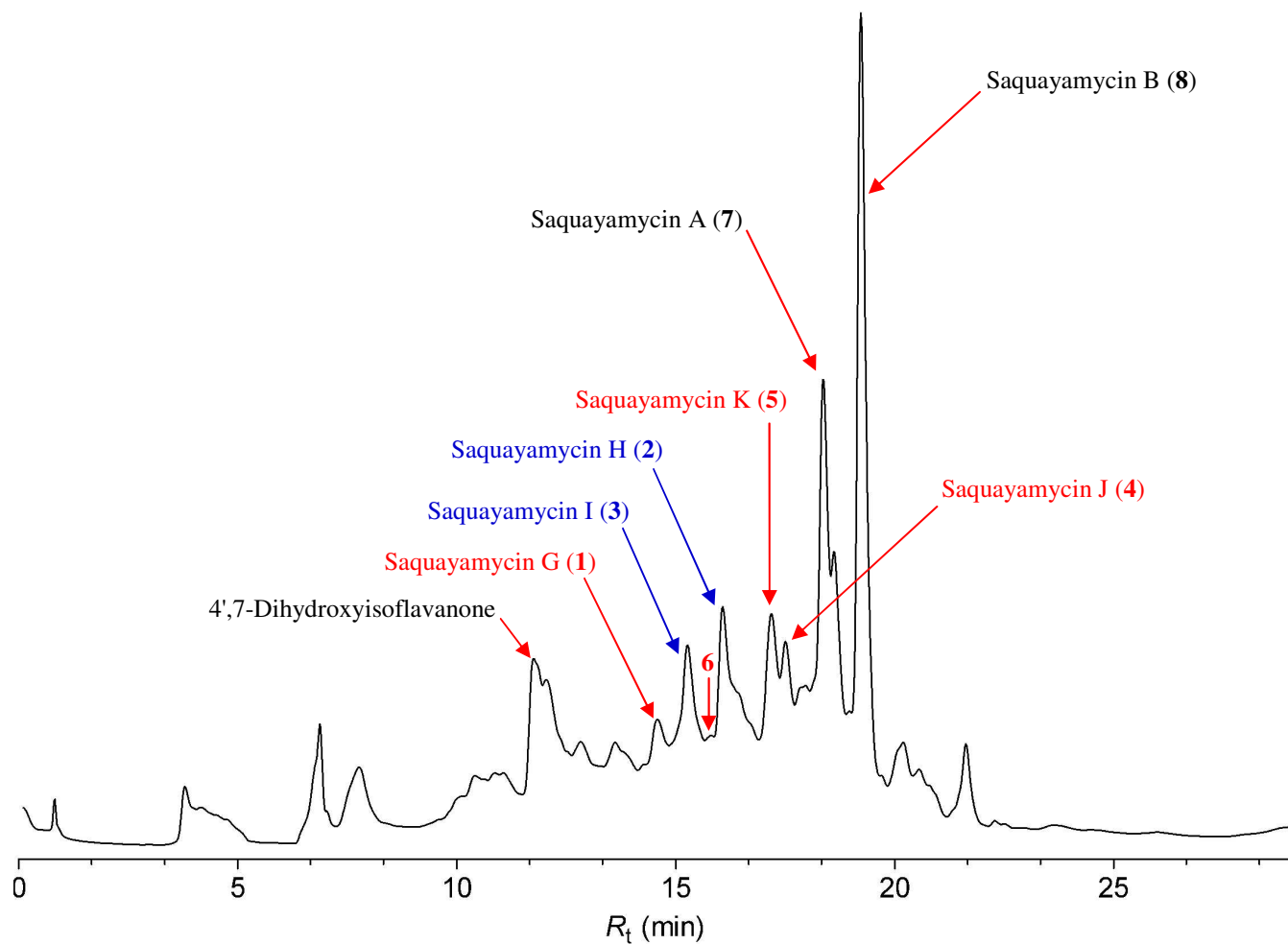


Figure S9: HPLC analysis of the crude extract obtained from the *Streptomyces* sp. KY40-1 strain, the detection wavelength was 300 nm. Solvent A: H₂O, solvent B: acetonitrile; flow rate: 0.5 mLmin⁻¹; 0–15 min, 75–0% A (linear gradient), 15–24 min 0% A and 100% B, 24–26 min 0–75% A (linear gradient), 26–29 min 75% A.

■ -TOF MS: 1.038 to 1.238 min from KSKY40-1-F3A.wiff Agilent

Max. 3.5e5 counts

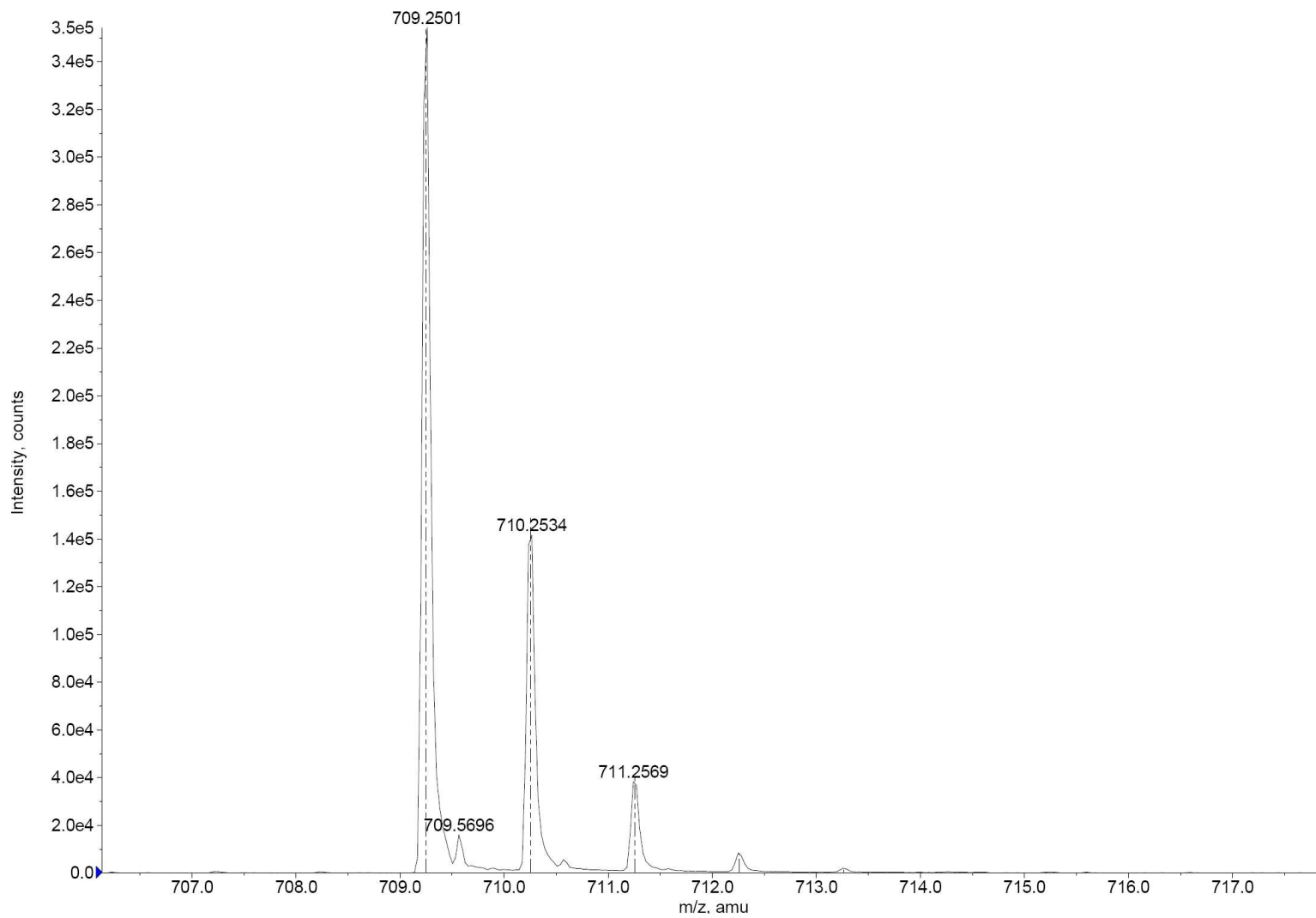


Figure S10: (-)-HRESI-MS spectrum of saquayamycin G (**1**)

■ -TOF MS: 1.038 to 1.238 min from KSKY40-1-F3A.wiff Agilent

Max. 3.5e5 counts

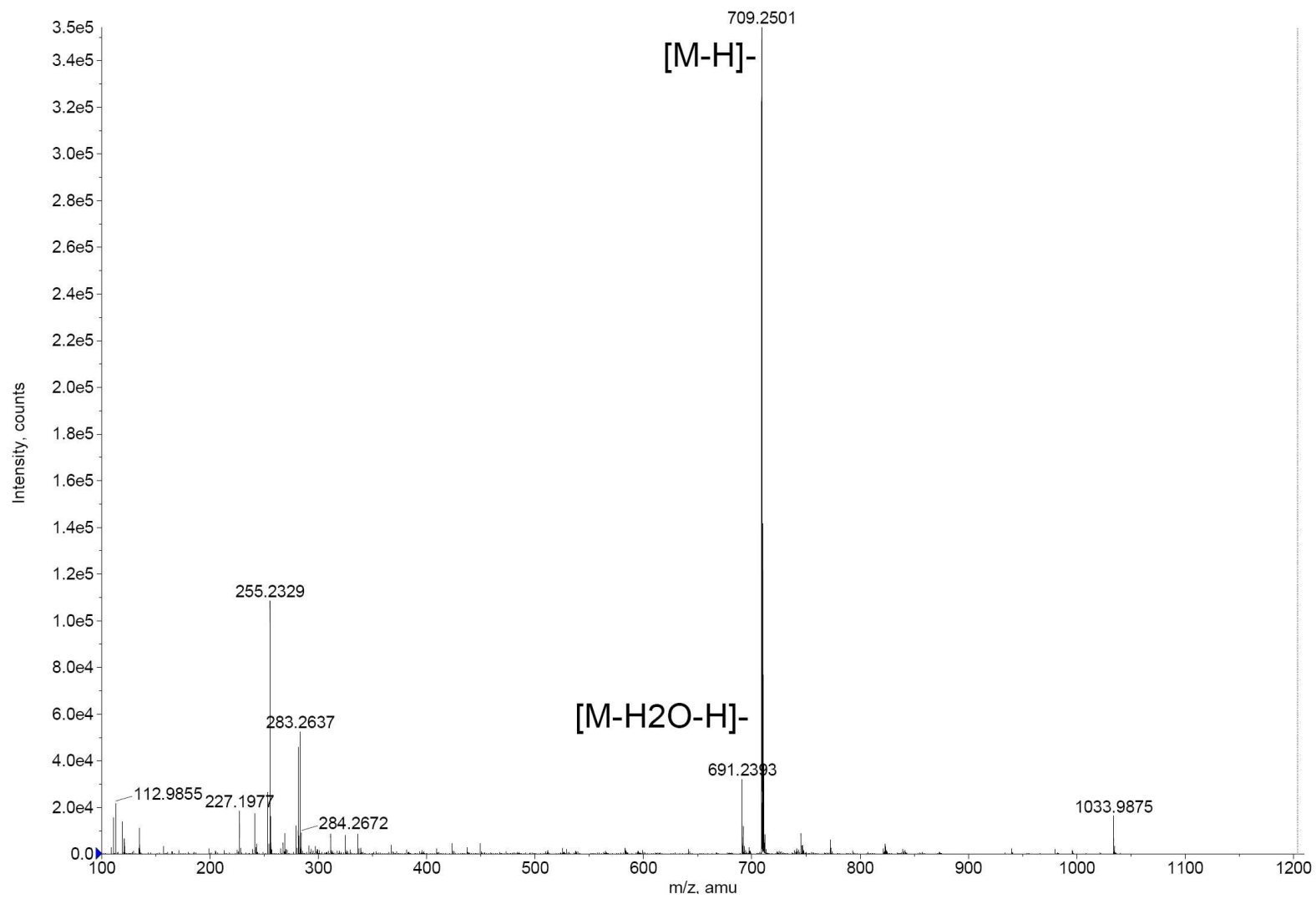


Figure S11: (-)-HRESI-MS spectrum of saquayamycin G (1)

KS_KY40-1_F3A_1HNMR_CDC13_11_18_2010
CDC13, 500 MHz, nt=16
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: s2pul

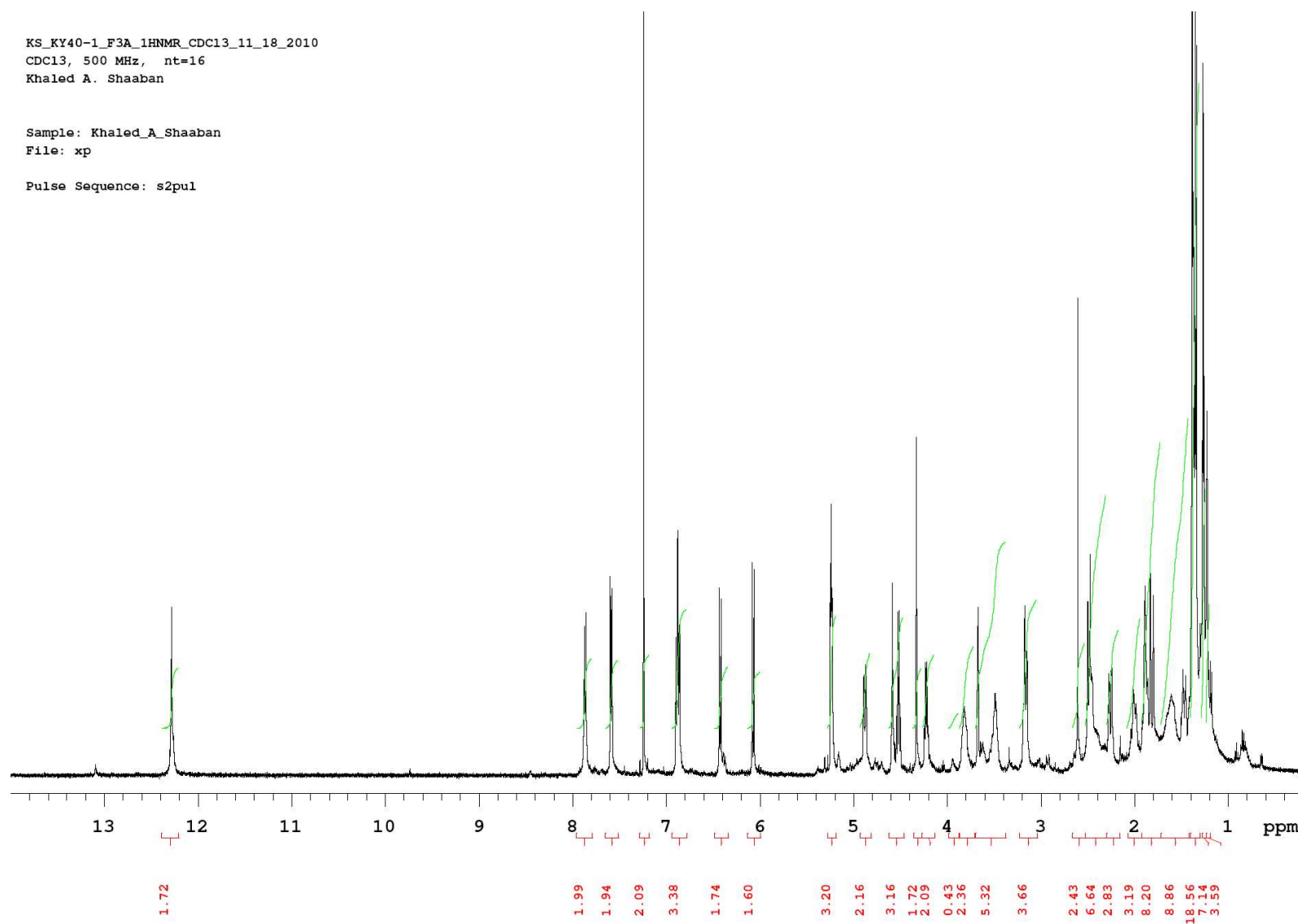


Figure S12: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin G (1)

KS_KY40-1_F3A_13CNMR_CDCl3_11_20_2010
 CDC13, 125 MHz, time=19 hrs
 Khaled A. Shaaban

exp2 Carbon

SAMPLE		SPECIAL	
date	Nov 19 2010	temp	not used
solvent	cdc13	gain	30
file	exp	spin	20
ACQUISITION		hst	0.008
sw	30487.8	pw90	11.900
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	64000	hs	nn
ct	29760	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	125.665	DISPLAY	
tof	1285.1	sp	-1120.4
tpwr	59	wp	29583.0
pw	5.950	rfl	11728.3
DECOUPLER		rfp	9704.1
dn	H1	rp	-66.4
dof	0	lp	-6.8
dm	yyy	PLOT	
dmm	w	wc	250
dpwr	35	sc	0
dmf	11448	vs	981015
		th	6
		ai	cdc ph

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	25772.8	205.113	10.2	40	1932.3	15.378	33.7
2	24765.1	197.094	12.5				
3	23672.8	188.401	12.7				
4	22924.8	182.448	13.2				
5	19876.7	158.190	16.7				
6	18308.5	145.709	15.4				
7	18006.1	143.302	18.3				
8	17464.6	138.993	16.5				
9	17416.3	138.608	12.3				
10	16823.6	133.891	14.9				
11	16410.0	130.600	11.2				
12	16022.0	127.512	21.4				
13	15069.3	119.929	14.7				
14	14789.7	117.704	16.1				
15	14338.4	114.113	12.7				
16	11998.9	95.494	26.8				
17	11638.8	92.628	21.8				
18	10396.3	82.739	19.2				
19	10073.0	80.166	19.8				
20	9823.1	78.178	9.1				
21	9754.8	77.634	22.8				
22	9736.1	77.485	342.1				
23	9704.1	77.230	345.6				
24	9672.4	76.978	335.4				
25	9595.2	76.364	25.4				
26	9563.1	76.108	11.6				
27	9190.5	73.143	8.8				
28	8967.2	71.365	16.7				
29	8898.3	70.818	24.9				
30	8437.3	67.148	22.9				
31	6330.8	50.384	11.0				
32	5620.5	44.731	12.7				
33	4967.3	39.533	11.4				
34	3757.8	29.906	7.8				
35	3221.4	25.638	20.3				
36	3130.7	24.916	18.7				
37	3108.3	24.738	15.4				
38	2297.0	18.281	20.4				
39	2182.1	17.366	29.8				

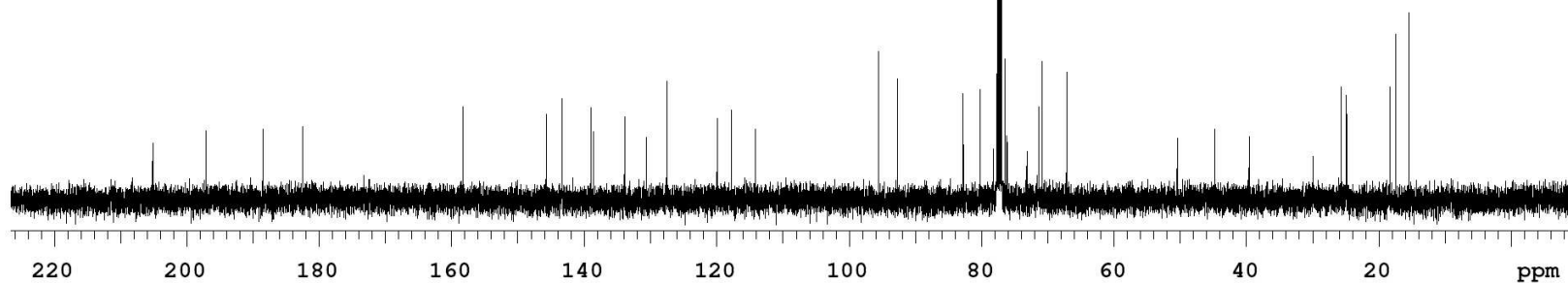


Figure S13: ¹³C NMR spectrum (CDCl₃, 125 MHz) of saquayamycin G (1)

KS_KY40-1_F3A_gCOSY_CDC13_11_21_2010
CDC13, 500 MHz, nt=4, time=1:20 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban

File: xp

Pulse Sequence: gCOSY

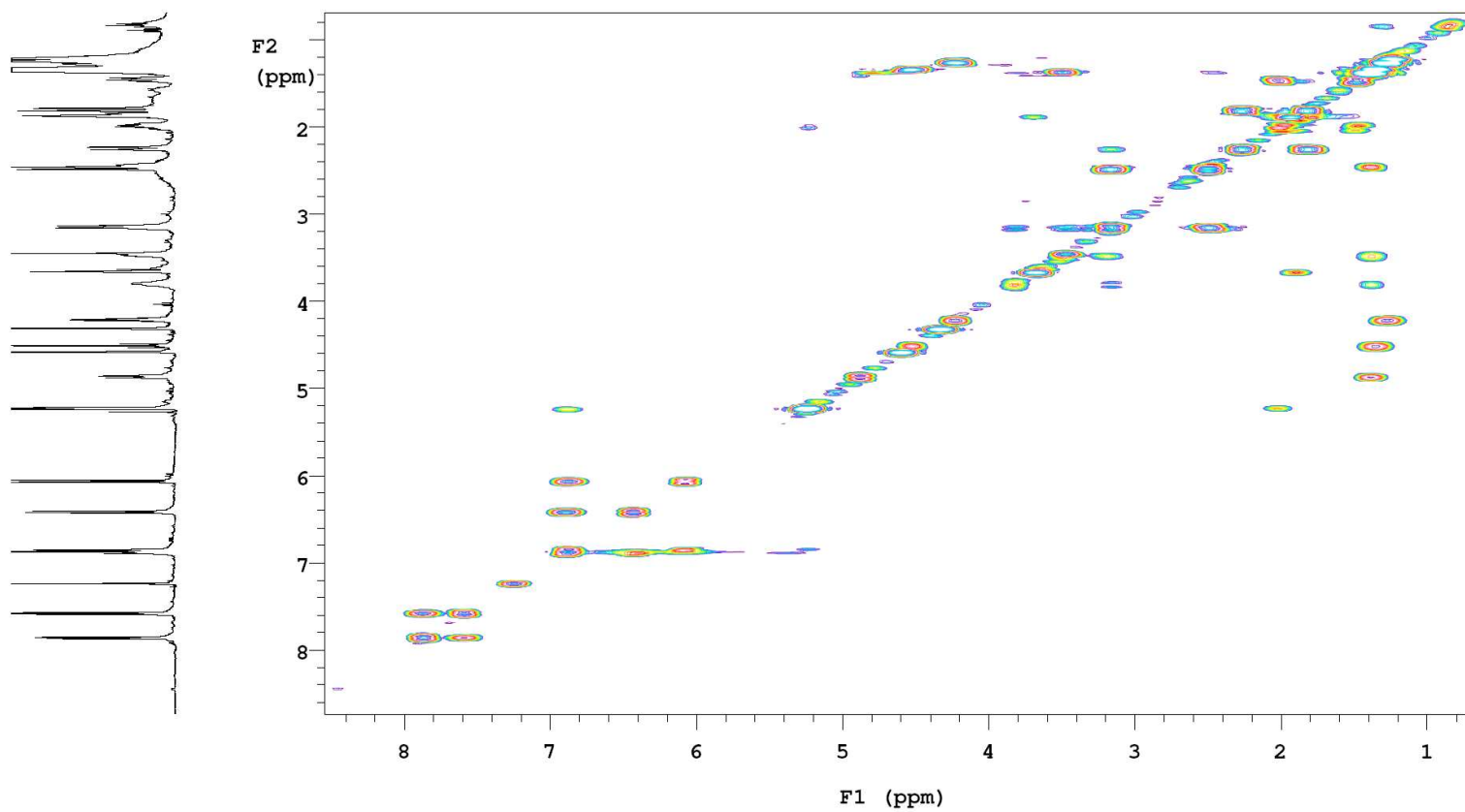
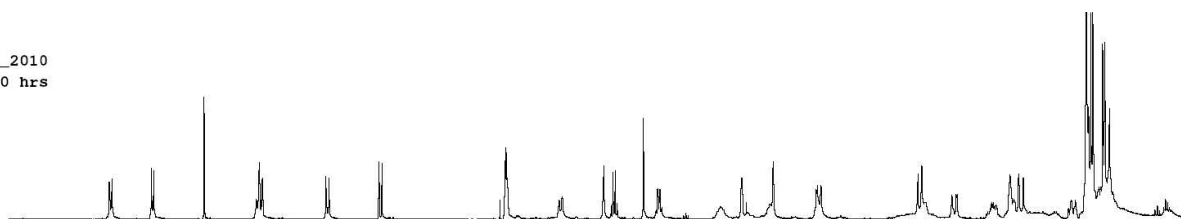


Figure S14: ¹H-¹H COSY spectrum (CDCl₃, 500 MHz) of saquayamycin G (**1**)

KS_KY40-1_F3A_gHSQC_CDCl3_11_20_2010
CDCl3, 500 MHz, nt=8, time=5 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

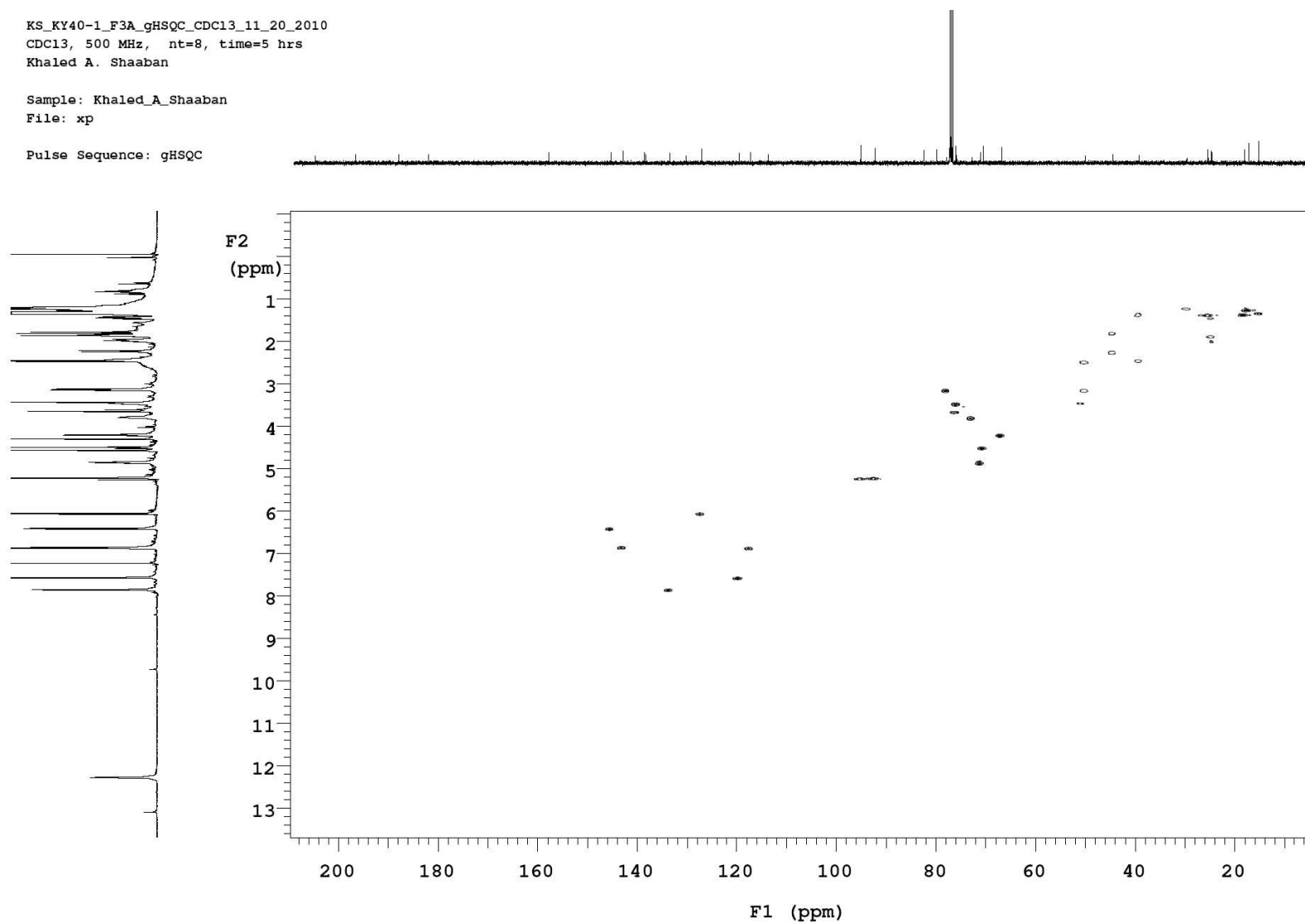


Figure S15: HSQC spectrum (CDCl₃, 500 MHz) of saquayamycin G (**1**)

KS_KY40-1_F3A_gHMBC_CDC13_11_21_2010
CDC13, 500 MHz, nt=32, time=11 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

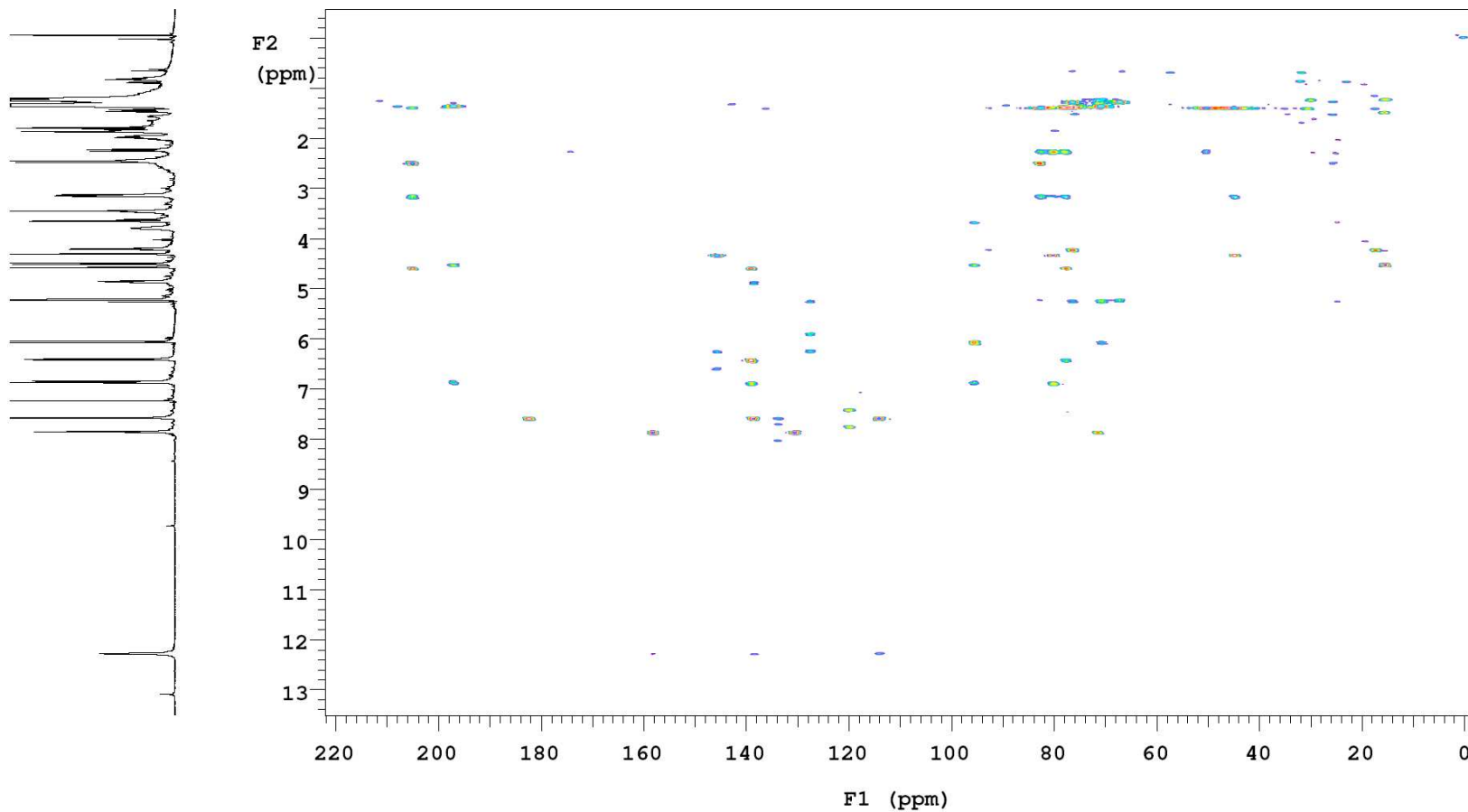


Figure S16: HMBC spectrum (CDCl₃, 500 MHz) of saquayamycin G (1)

KS_KY40-1_F3A_NOESY_CDCl3_11_21_2010
CDCl3, 500 MHz, nt=4, time=4:33 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: home/khaled/vnmrsys/data/KS_KY40-1_F3A_NOESY_CDCl3_11_21_2010.fid

Pulse Sequence: NOESY

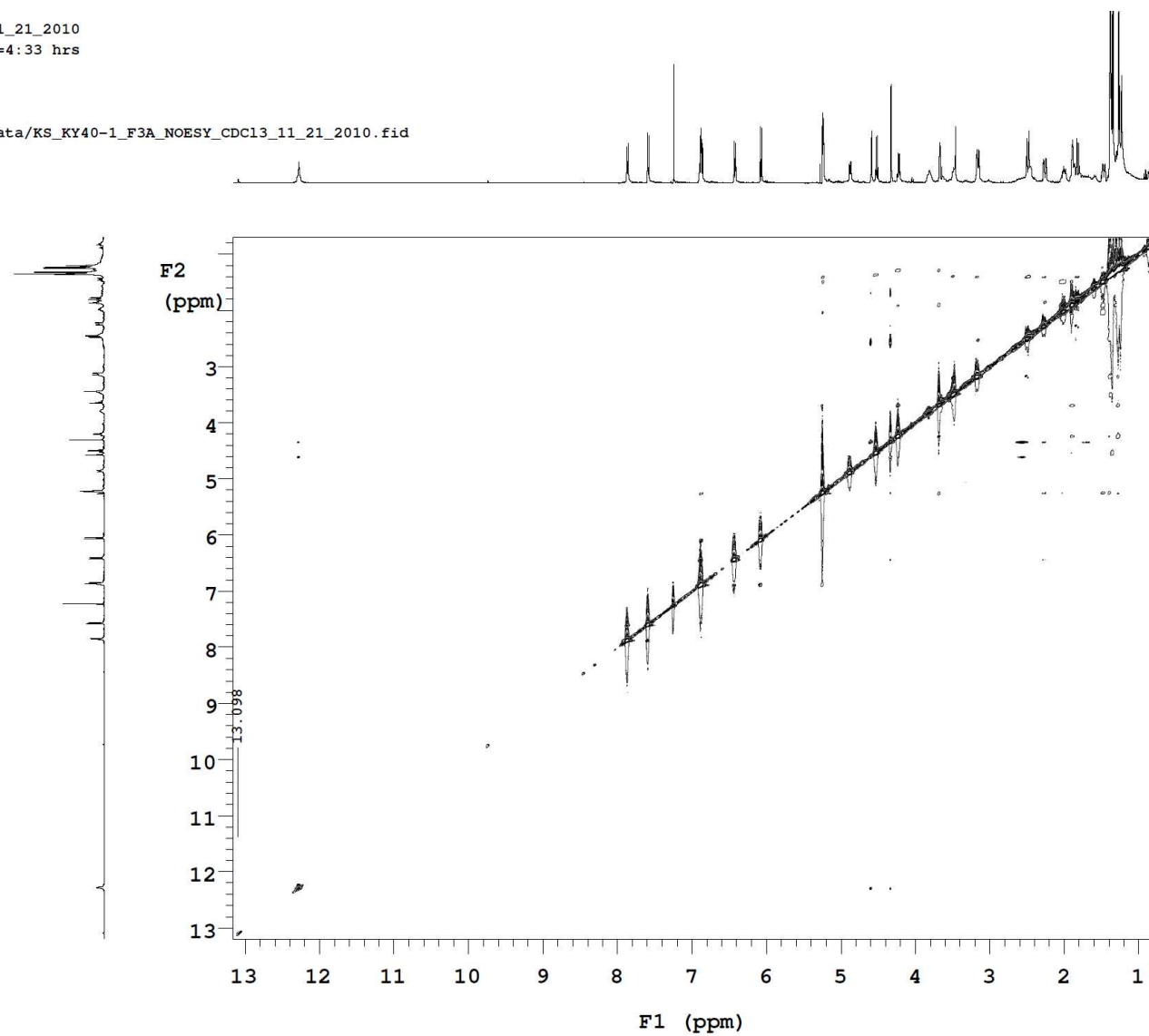


Figure S17: NOESY spectrum (CDCl₃, 500 MHz) of saquayamycin G (1)

■ -TOF MS: 2.508 to 2.617 min from KSKY40-1-F4D2.wiff Agilent

Max. 1.5e5 count

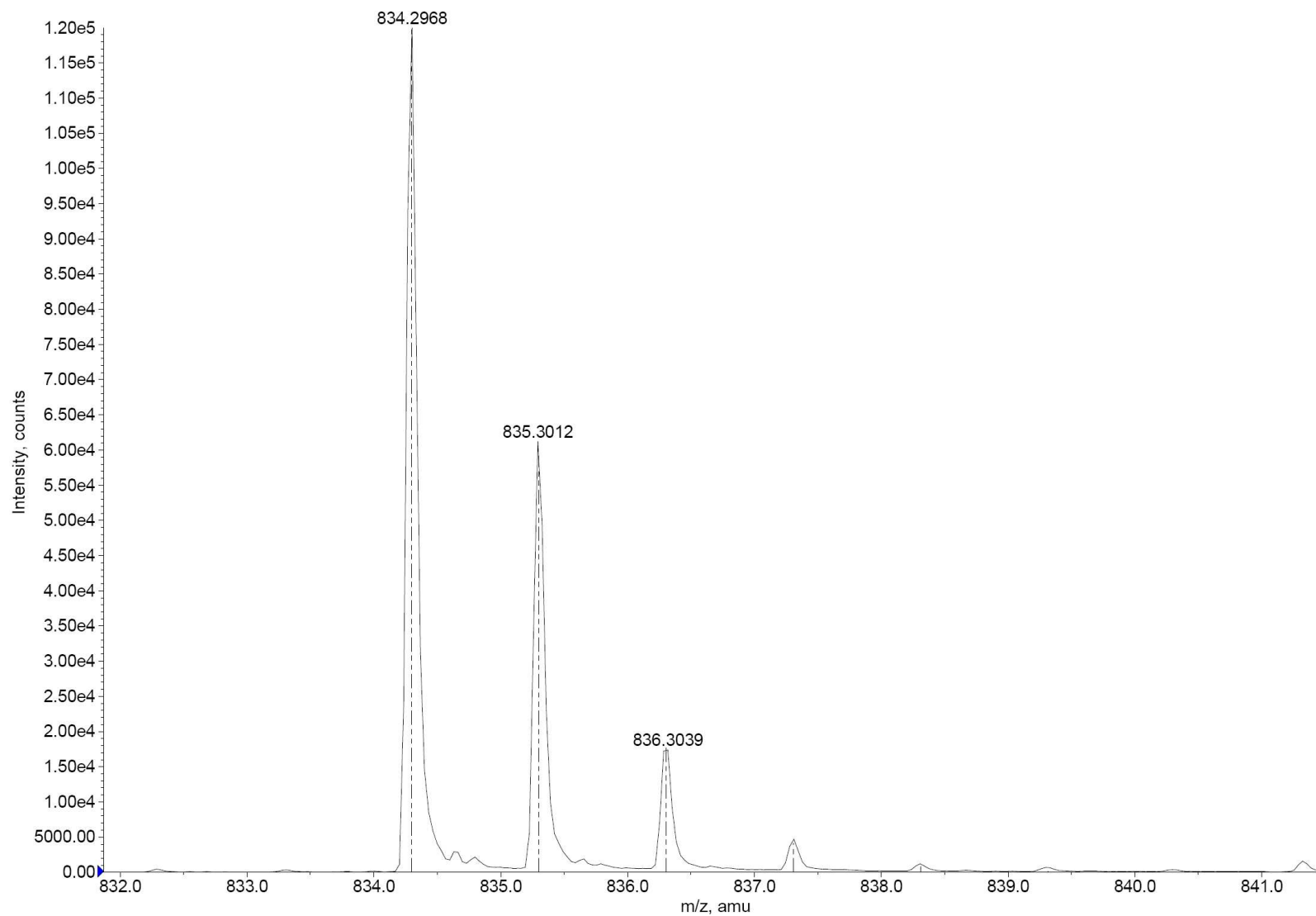


Figure S18: (-)-HRESI-MS spectrum of saquayamycin H (**2**)

■ -TOF MS: 2.508 to 2.617 min from KSKY40-1-F4D2.wiff Agilent

Max. 1.5e5 counts.

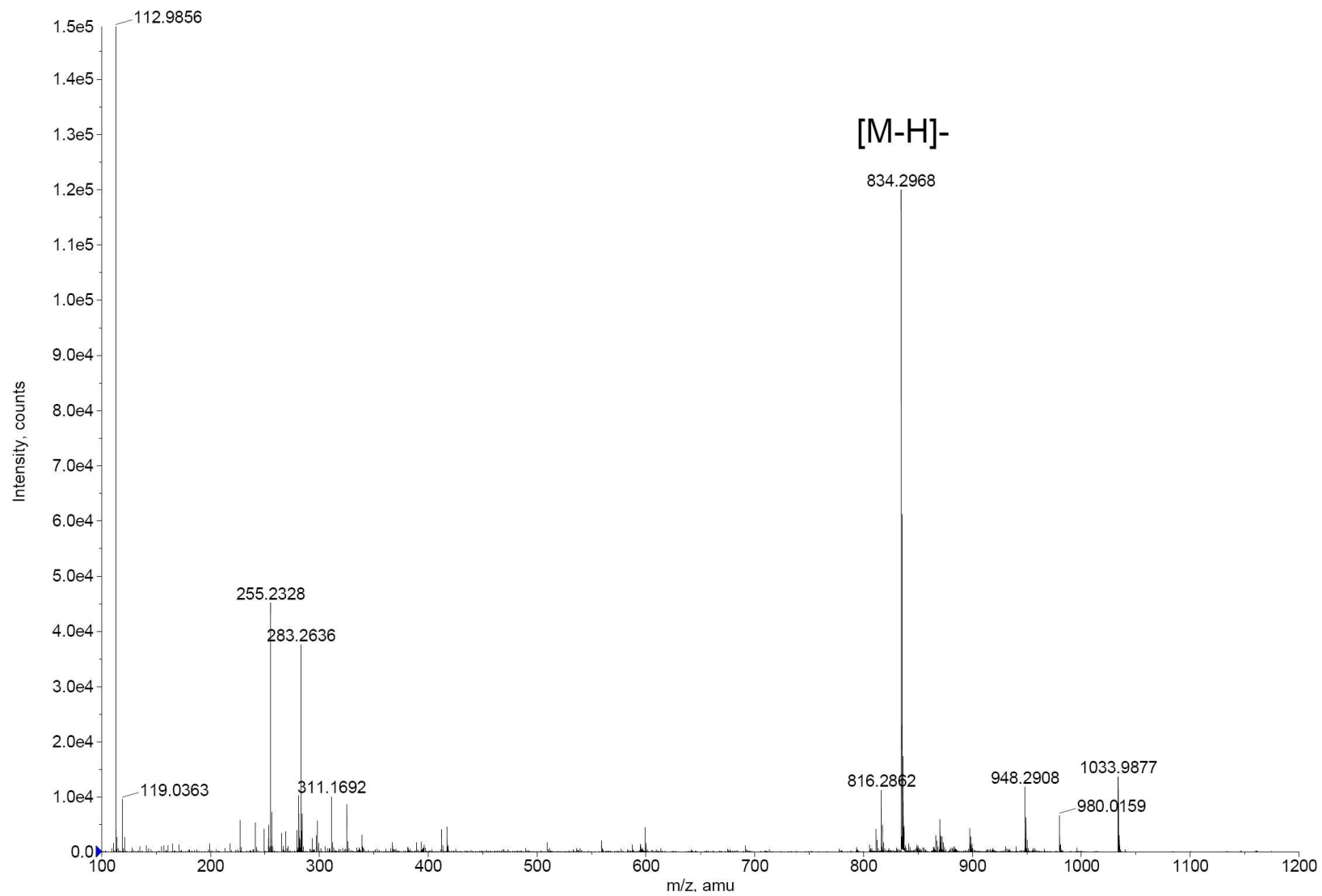


Figure S19: (-)-HRESI-MS spectrum of saquayamycin H (2)

KS_KY40-1_F4D2_1HNMR_CDCl3_11_24_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp
Pulse Sequence: s2pul

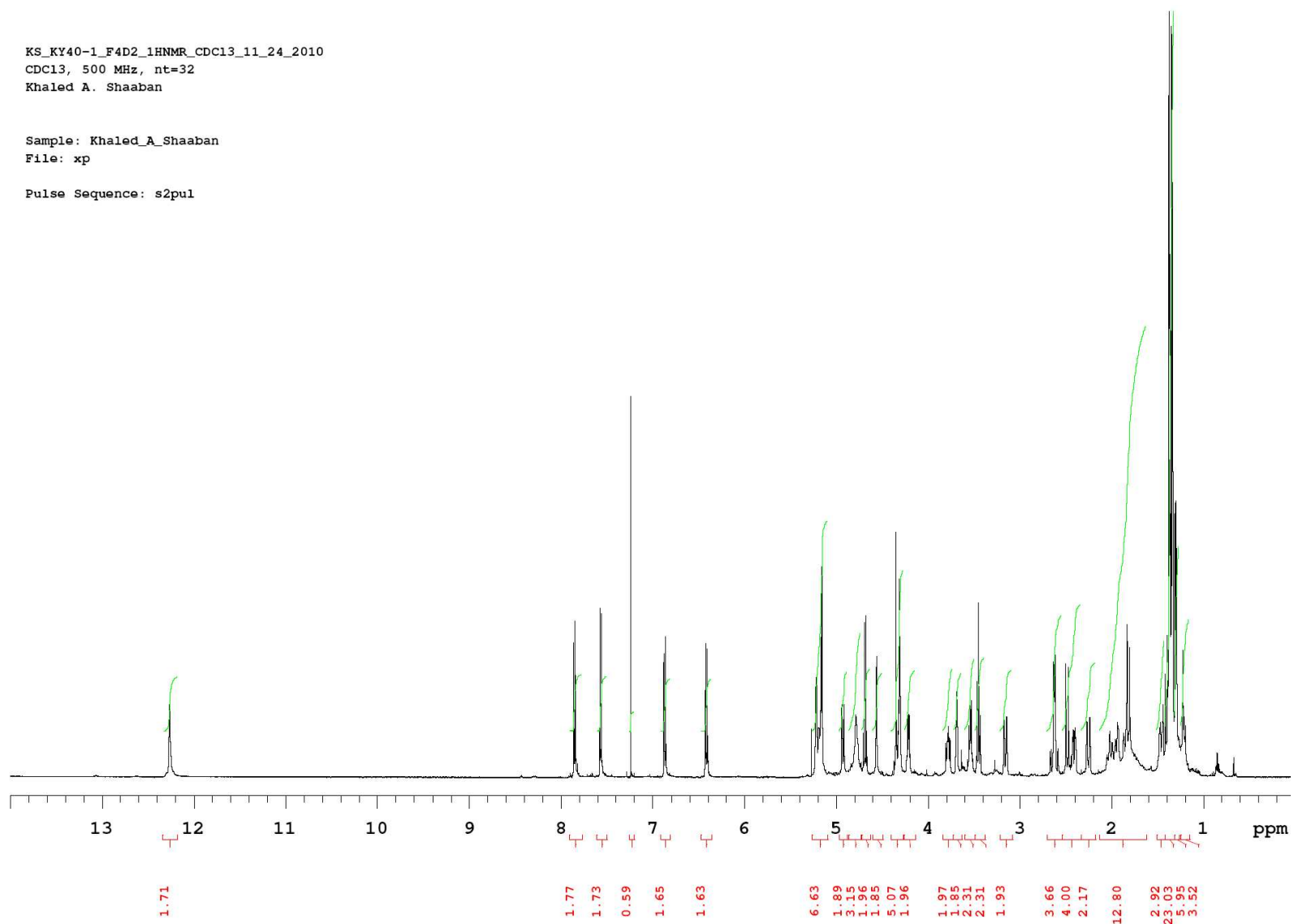


Figure S20: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin H (2)

KS_KY40-1_F4D2_13CNMR_CDCl3_11_25_2010
 CDC13, 125 MHz, time= 15 hrs
 Khaled A. Shaaban

exp2 Carbon

SAMPLE		SPECIAL	
date	Nov 24 2010	temp	not used
solvent	cdcl3	gain	30
file	exp	spin	20
ACQUISITION			
		hst	0.008
sw	30487.8	pw90	11.900
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	64000	hs	nn
ct	24256	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	125.665	DISPLAY	
tof	1285.1	sp	-1023.6
tpwr	59	wp	29483.9
pw	5.950	rfl	11730.7
DECOUPLER		rfp	9704.1
dn	H1	rp	-90.6
dof	0	lp	52.1
dm	YYY	PLOT	
dmm	w	wc	250
dpwr	35	sc	0
dmf	11448	vs	893299
		th	7
		ai	cdc ph

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	26144.9	208.075	10.1	40	3219.1	25.619	25.5
2	25787.2	205.228	10.1	41	3124.2	24.864	18.9
3	24523.2	195.169	12.0	42	3113.5	24.779	17.0
4	23668.2	188.364	22.7	43	2227.7	17.729	32.0
5	22922.4	182.429	17.7	44	2217.0	17.644	38.5
6	19988.8	159.082	10.2	45	2055.6	16.359	42.3
7	19863.2	158.082	31.3	46	2015.1	16.037	28.0
8	18320.6	145.805	23.2				
9	17464.6	138.993	22.9				
10	17460.0	138.956	14.0				
11	17349.3	138.075	22.4				
12	16817.5	133.843	23.3				
13	16420.2	130.681	18.2				
14	15059.0	119.848	18.6				
15	14783.2	117.652	19.1				
16	14341.7	114.139	19.2				
17	12238.0	97.397	13.1				
18	12146.4	96.667	22.5				
19	11638.4	92.624	27.6				
20	11501.6	91.536	20.6				
21	10405.6	82.813	22.6				
22	10073.9	80.173	25.2				
23	9793.4	77.941	21.6				
24	9756.2	77.645	39.9				
25	9735.7	77.482	380.8				
26	9704.1	77.230	386.5				
27	9672.0	76.975	386.2				
28	9656.1	76.849	26.1				
29	9634.7	76.678	24.9				
30	9387.7	74.712	30.6				
31	9379.3	74.646	29.2				
32	8998.3	71.614	28.4				
33	8959.7	71.306	23.3				
34	8862.5	70.532	16.7				
35	8448.0	67.234	26.4				
36	6313.2	50.243	14.3				
37	5629.3	44.801	14.7				
38	5045.0	40.151	17.7				
39	4633.8	36.878	21.2				

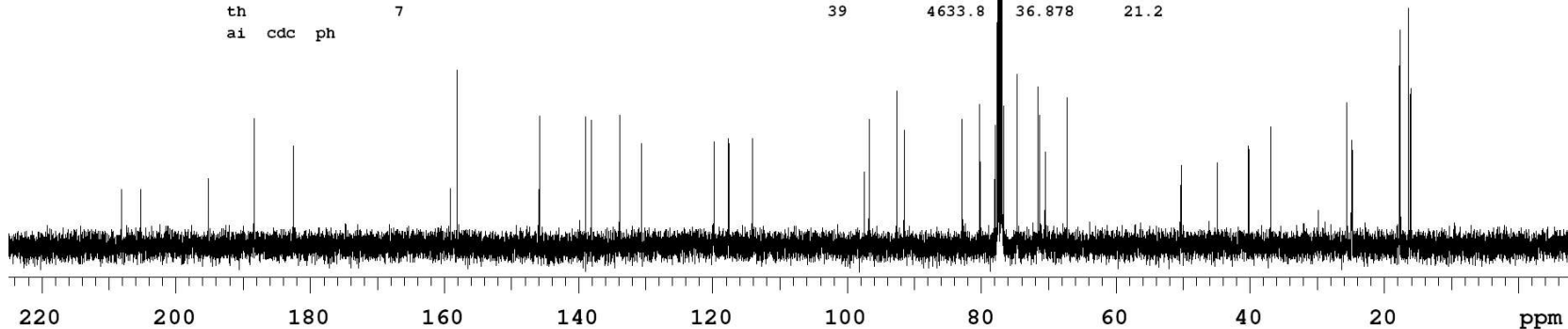


Figure S21: ^{13}C NMR spectrum (CDCl_3 , 125 MHz) of saquayamycin H (2)

KS_KY40-1_F4D2_gCOSY_CDC13_11_24_2010
CDC13, 500 MHz, nt=4, time=1:20 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban

File: xp

Pulse Sequence: gCOSY

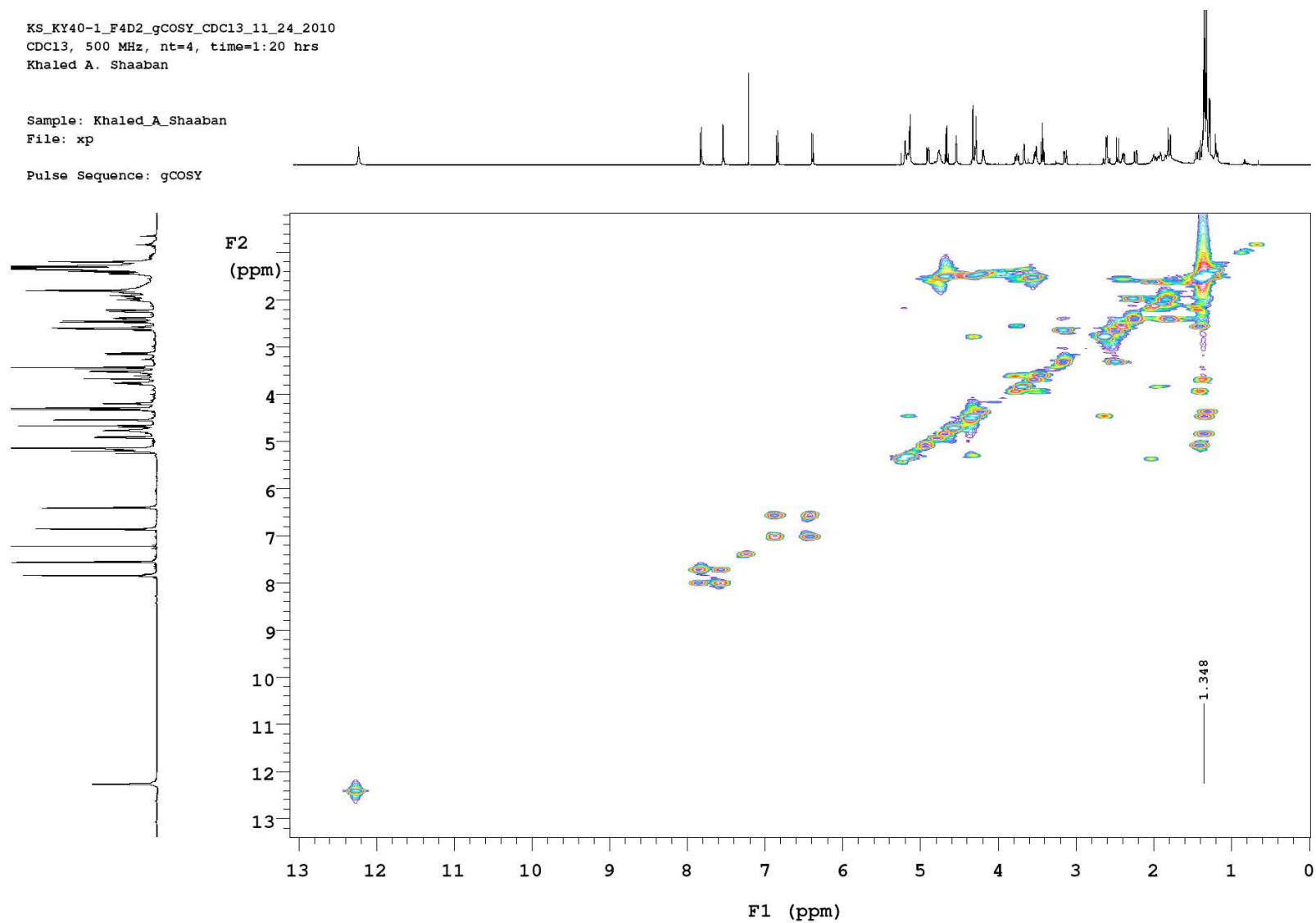


Figure S22: ^1H - ^1H COSY spectrum (CDCl_3 , 500 MHz) of saquayamycin H (**2**)

KS_KY40-1_F4D2_GHSQC_CDC13_11_25_2010
CDC13, 500 MHz, nt=8, time= 5:30 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

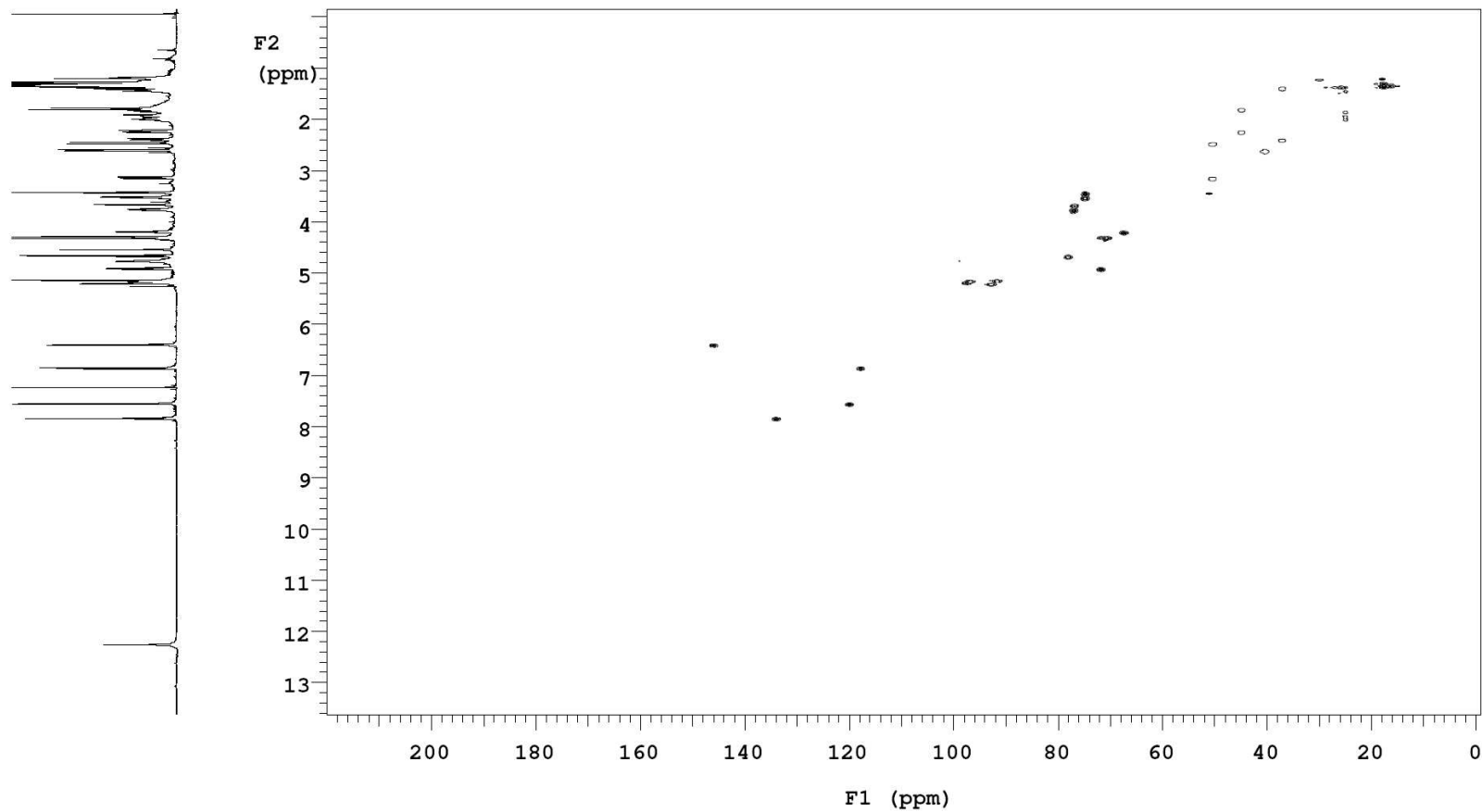


Figure S23: HSQC spectrum (CDCl₃, 500 MHz) of saquayamycin H (2)

KS_KY40-1_F4D2_GHMBC_CDCl3_11_26_2010
CDC13, 500 MHz, nt=32, time= 11:10 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban

File: xp

Pulse Sequence: gHMBC

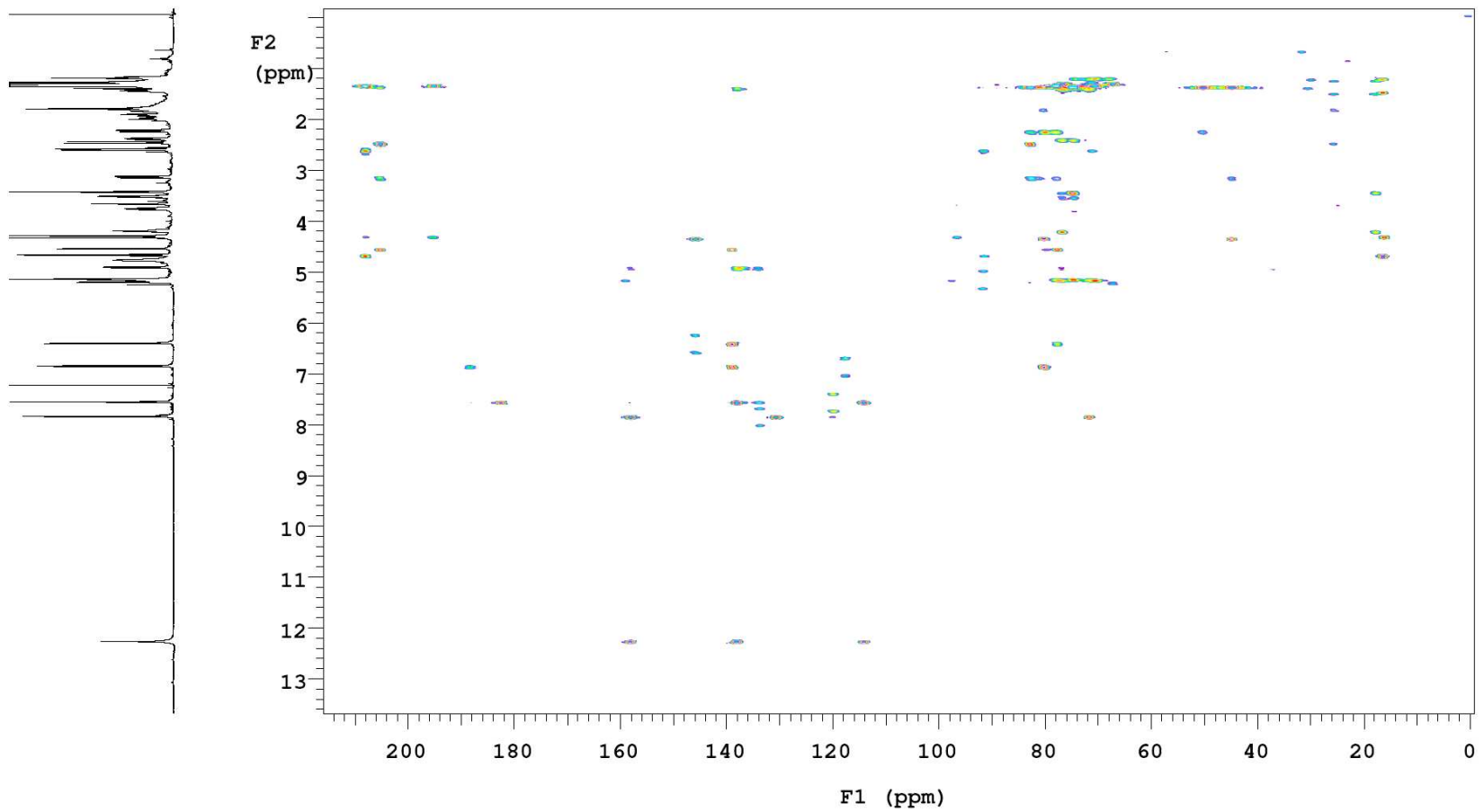


Figure S24: HMBC spectrum (CDCl₃, 500 MHz) of saquayamycin H (2)

KS_KY40-1_F4D2_NOESY_CDC13_11_26_2010
CDC13, 500 MHz, nt=4, time=4:34 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban

File: xp

Pulse Sequence: NOESY

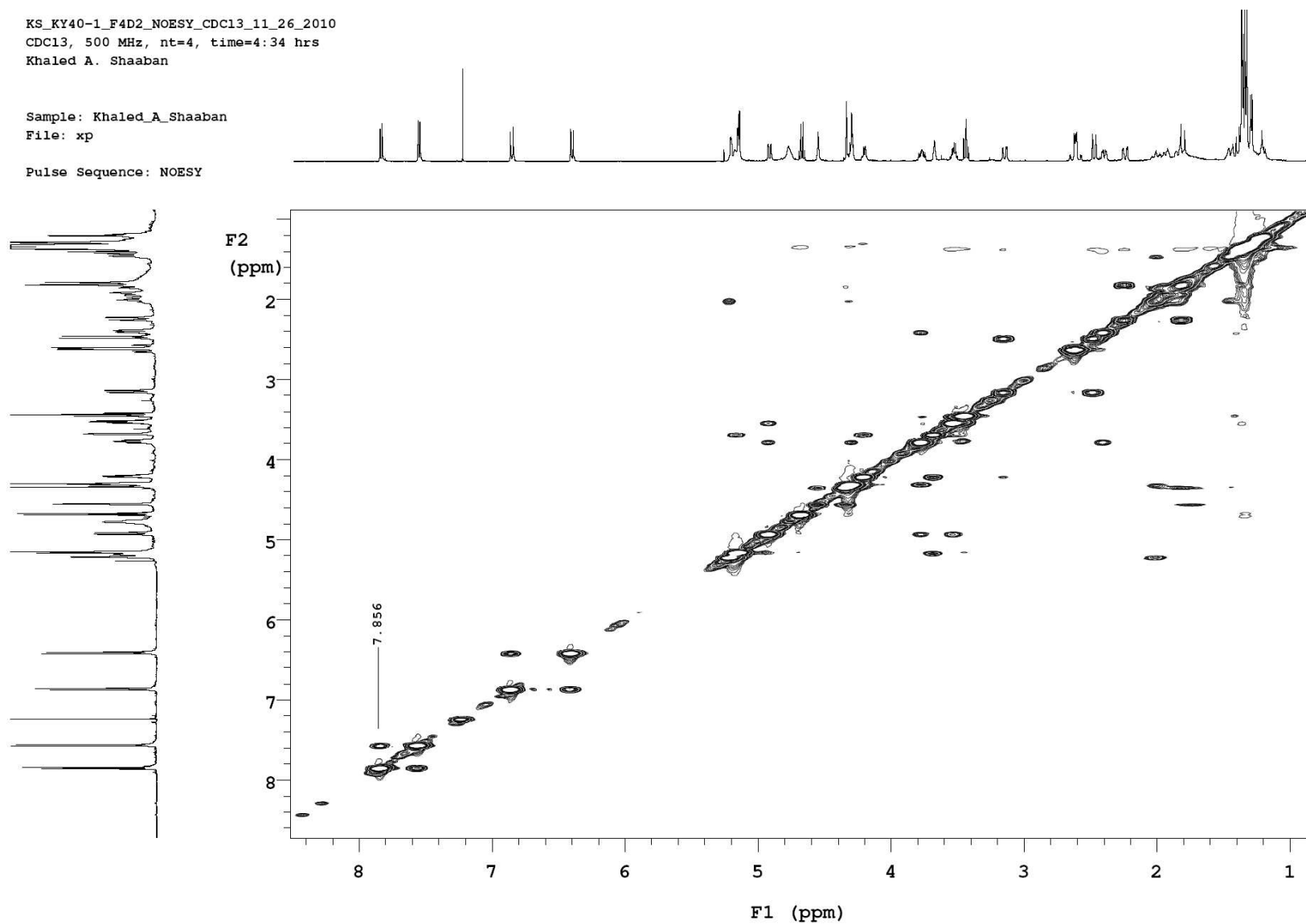


Figure S25: NOESY spectrum (CDCl₃, 500 MHz) of saquayamycin H (2)

KS_KY40-1_F4C2_1HNMR_Acetone_11_24_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: s2pul

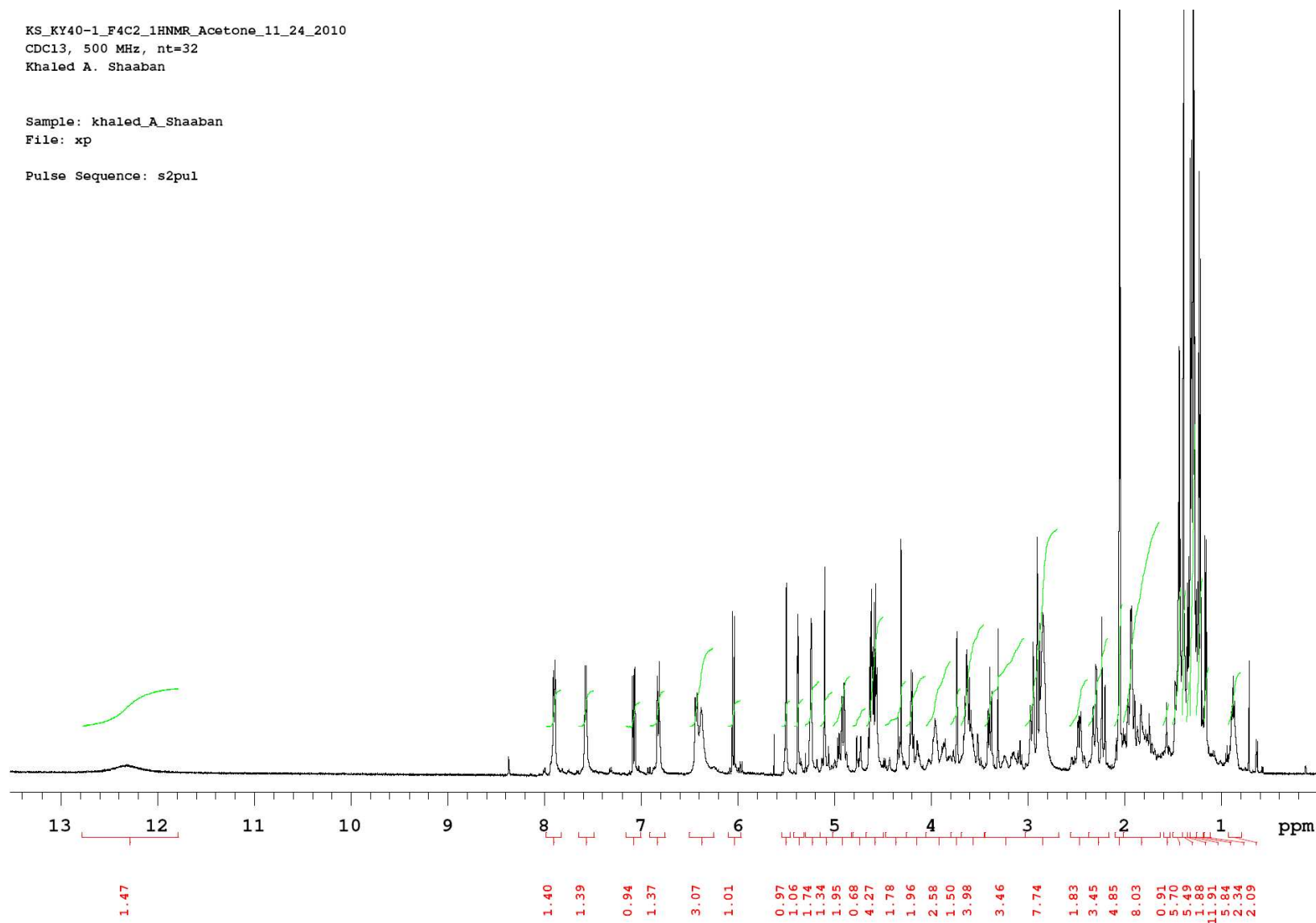


Figure S26: ^1H NMR spectrum (acetone- d_6 , 500 MHz) of saquayamycin I (**3**)

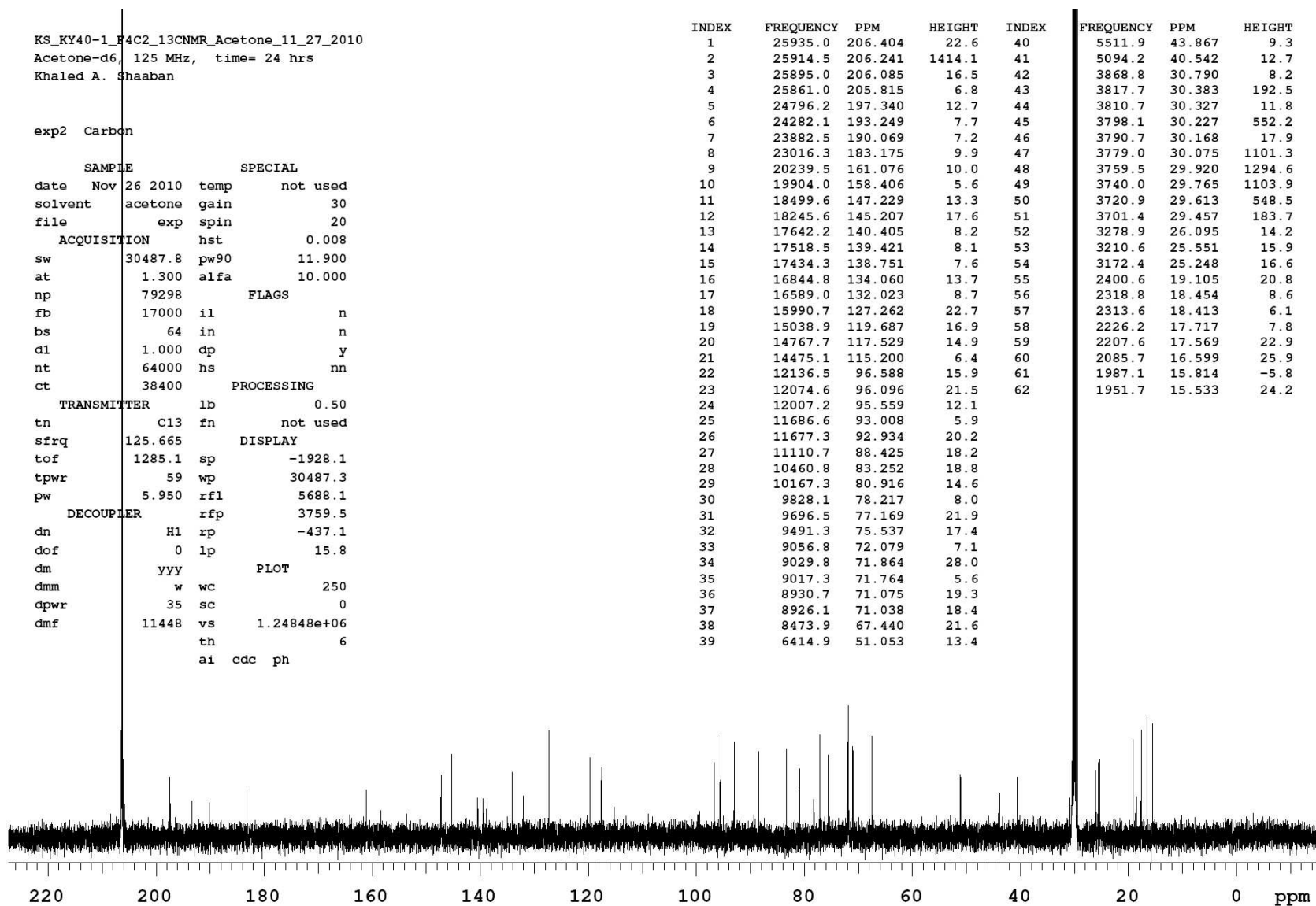


Figure S27: ¹³C NMR spectrum (acetone-d₆, 125 MHz) of saquayamycin I (3)

KS_KY40-1_F4C2_gCOSY_Acetone_11_29_2010
Acetone-d6, 500 MHz, nt=4, time=1:25 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gCOSY

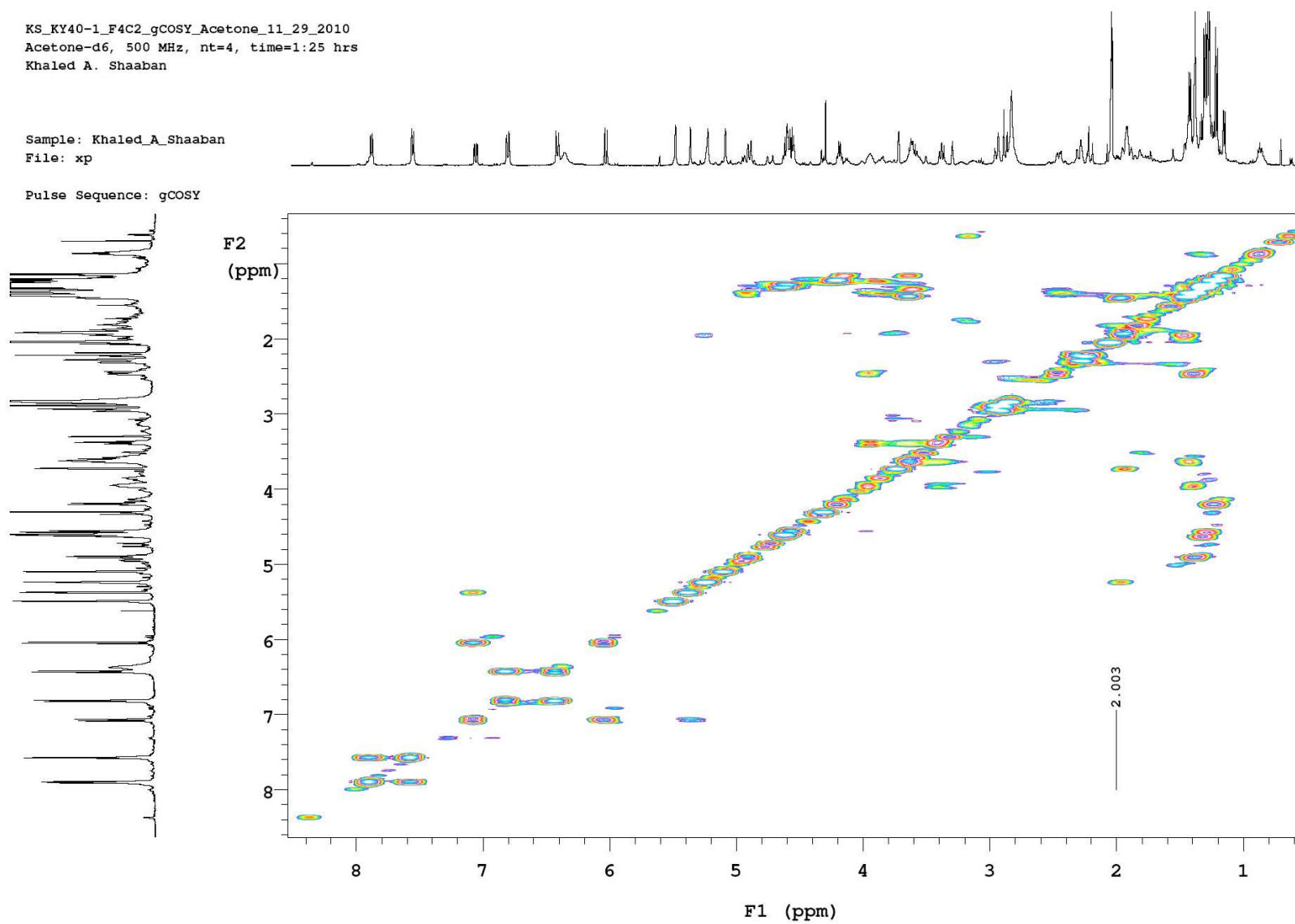


Figure S28: ^1H - ^1H COSY spectrum (acetone- d_6 , 500 MHz) of saquayamycin I (3)

KS_KY40-1_F4C2_GHSQC_Acetone_11_28_2010
Acetone-d₆, 500 MHz, nt=8, time=5:30 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

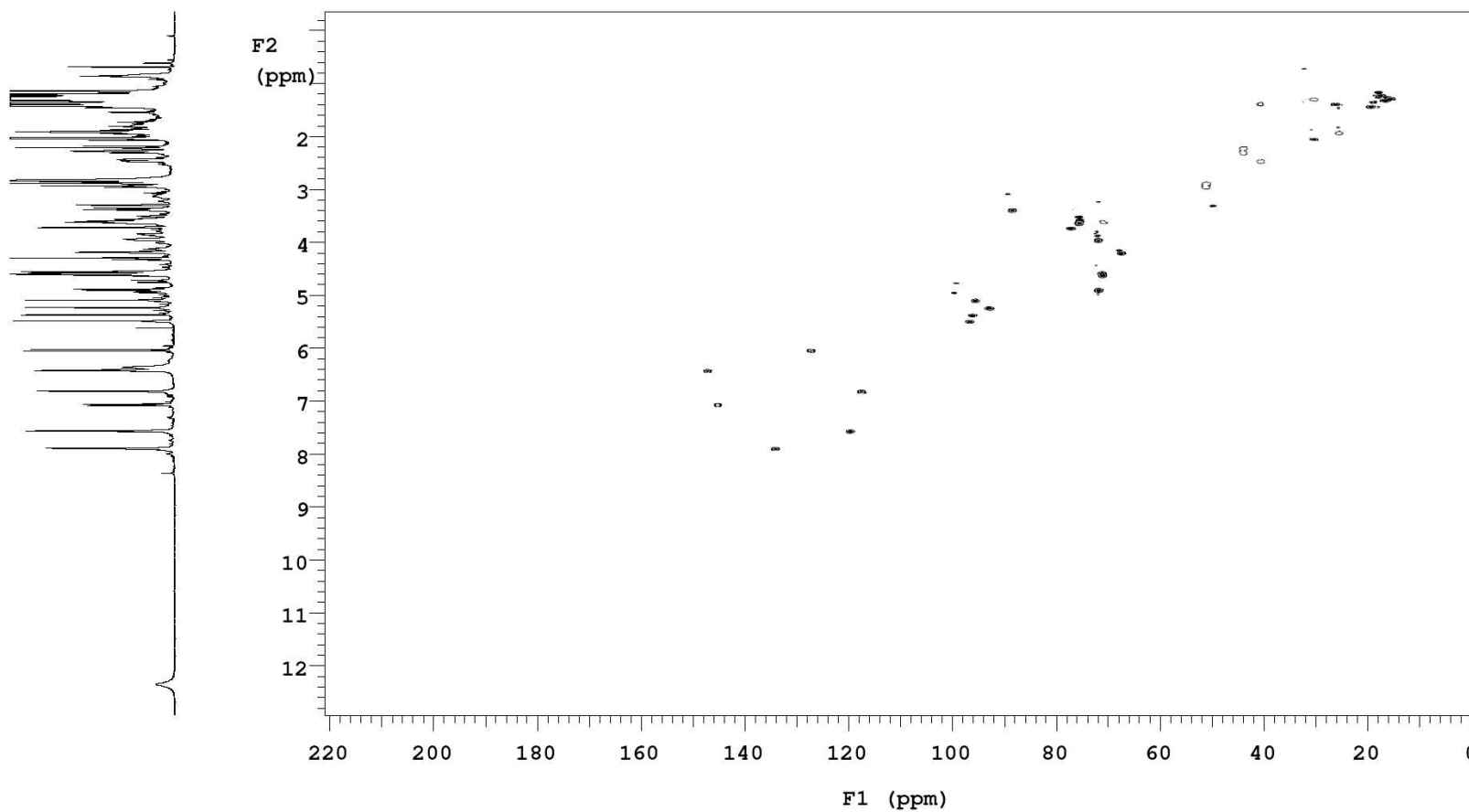


Figure S29: HSQC spectrum (acetone-*d*₆, 500 MHz) of saquayamycin I (**3**)

KS_KY40-1_F4C2_GHMBC_Acetone_11_28_2010
Acetone-d6, 500 MHz, nt=12, time=11:14 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

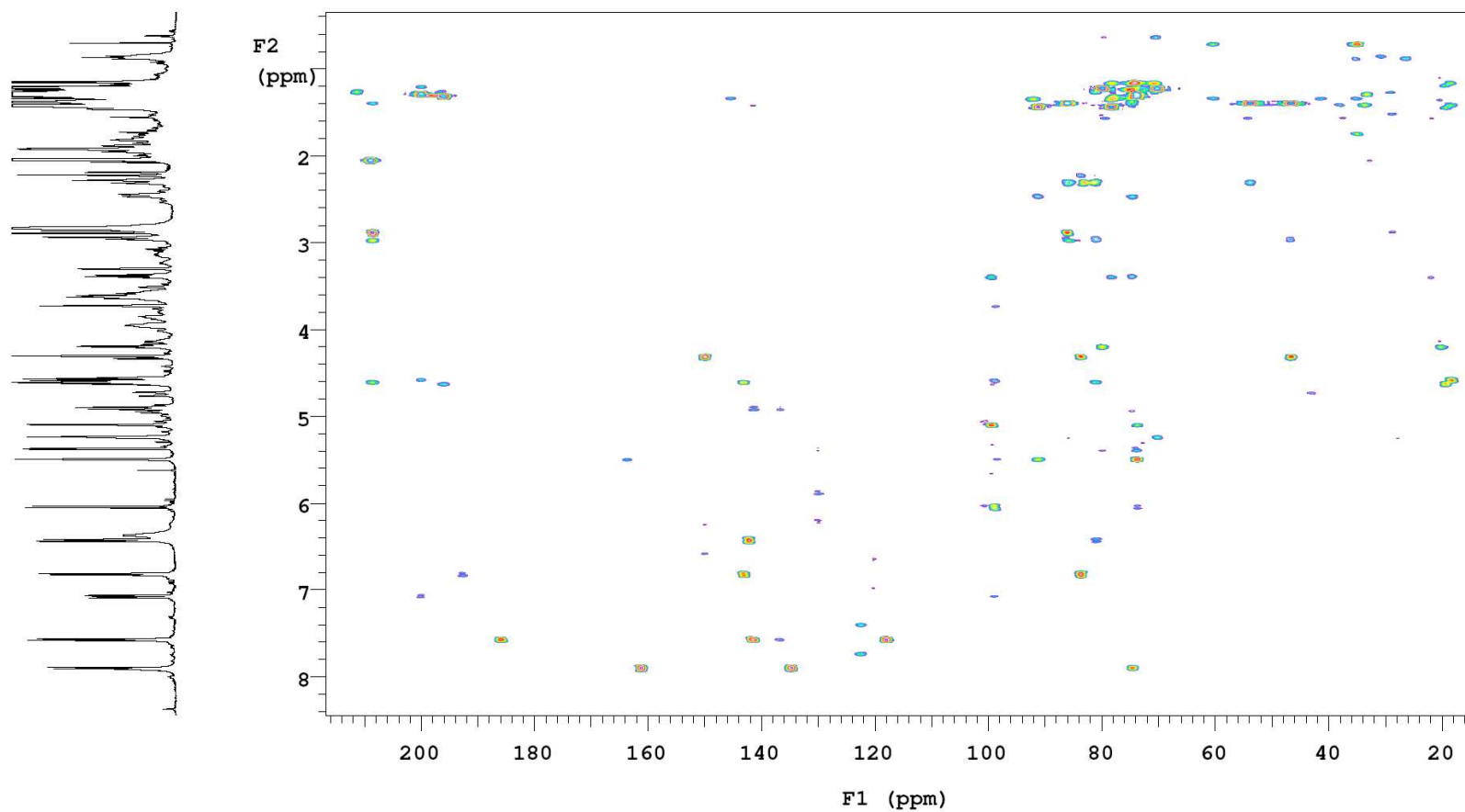


Figure S30: HMBC spectrum (acetone-*d*₆, 500 MHz) of saquayamycin I (**3**)

KS_KY40-1_F4C2_NOESY_Acetone_12_01_2010
Acetone-d₆, 500 MHz, nt=8, time=9:10 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: NOESY

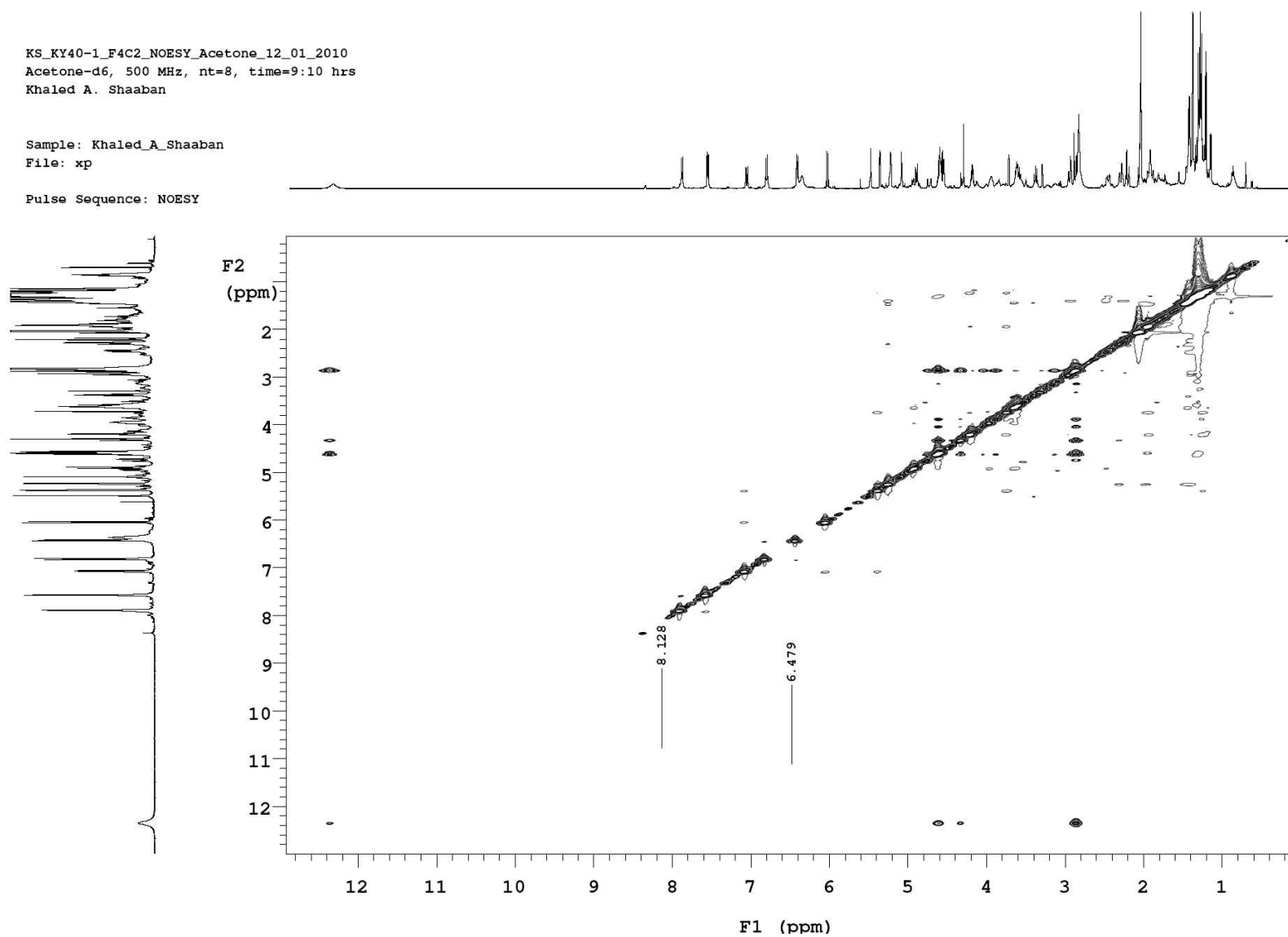


Figure S31: NOESY spectrum (acetone-*d*₆, 500 MHz) of saquayamycin I (**3**)

KS_KY40-1_F1C3B_1HNMR_CDC13_12_17_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: s2pul

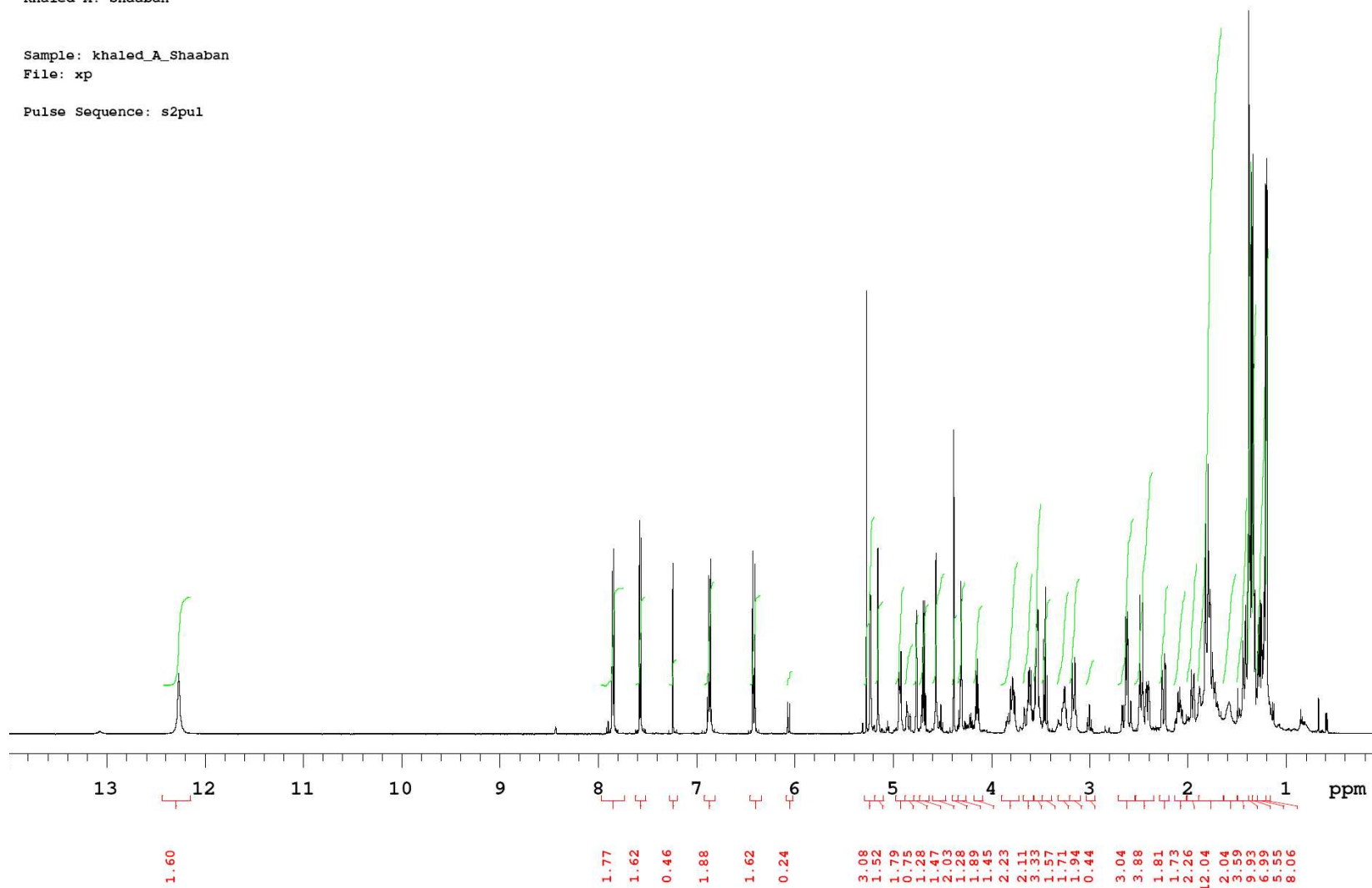


Figure S32: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin J (4)

KS_KY40-1_F1C3B_13CNMR_CDC13_12_26_2010
 CDC13, 125 MHz, time=10 hrs
 Khaled A. Shaaban

exp4 Carbon

SAMPLE		SPECIAL	
date	Dec 26 2010	temp	not used
solvent	cdcl3	gain	30
file	exp	spin	20
ACQUISITION		hst	0.008
sw	30487.8	pw90	11.900
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	il	n
bs	64	in	n
dl	1.000	dp	y
nt	100000	hs	nn
ct	14528	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	125.665	DISPLAY	
tof	1285.1	sp	-802.6
tpwr	59	wp	28964.3
pw	5.950	rf1	11730.7
DECOUPLER		rfp	9704.1
dn	H1	rp	118.8
dof	0	lp	2.8
dm	yyy	PLOT	
dmm	w	wc	250
dpwr	35	sc	0
dmf	11448	vs	434141
		th	7
		ai	cdc ph

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	26138.4	208.023	11.1	40	3219.1	25.619	16.0
2	25755.1	204.973	11.8	41	3153.5	25.097	12.1
3	23678.9	188.449	10.0	42	3098.1	24.656	10.2
4	22914.5	182.366	10.7	43	2256.1	17.955	22.5
5	19858.6	158.045	15.3	44	2216.5	17.640	25.2
6	18324.3	145.835	11.5	45	2187.2	17.407	20.8
7	17472.5	139.056	9.7	46	2054.2	16.348	24.1
8	17459.1	138.948	10.8				
9	17336.2	137.971	12.6				
10	16814.3	133.817	12.3				
11	16424.9	130.718	10.7				
12	15058.6	119.844	13.3				
13	14774.8	117.586	13.6				
14	14343.1	114.150	12.8				
15	12408.8	98.756	19.4				
16	11660.7	92.802	16.0				
17	11502.5	91.543	10.9				
18	10383.7	82.639	18.9				
19	10070.2	80.144	19.9				
20	9792.0	77.930	11.2				
21	9753.8	77.626	18.1				
22	9736.2	77.485	190.4				
23	9704.1	77.230	200.9				
24	9672.0	76.975	197.4				
25	9657.5	76.860	18.4				
26	9387.2	74.709	16.2				
27	9378.9	74.642	17.6				
28	9351.0	74.420	16.7				
29	9083.0	72.287	15.0				
30	8999.3	71.621	15.8				
31	8957.9	71.291	18.0				
32	8841.1	70.362	15.9				
33	8498.2	67.633	16.5				
34	6326.6	50.351	10.9				
35	5622.3	44.745	9.0				
36	5043.6	40.140	9.2				
37	4633.8	36.878	11.4				
38	3761.5	29.936	13.6				
39	3510.8	27.940	12.8				

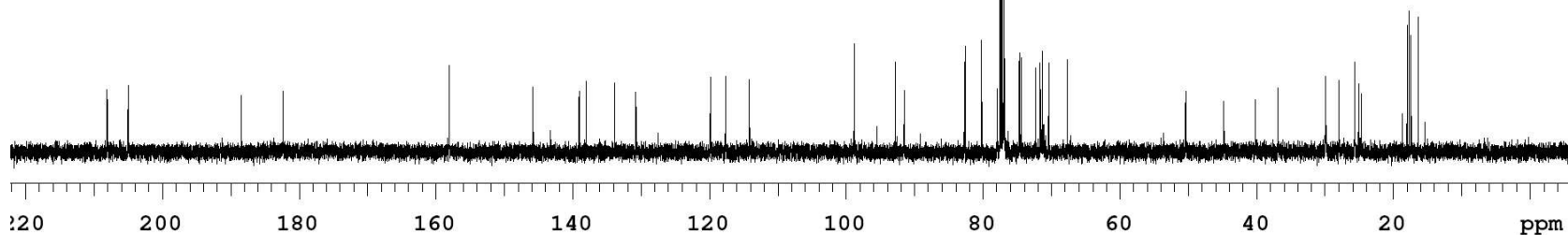


Figure S33: ¹³C NMR spectrum (CDCl₃, 125 MHz) of saquayamycin J (4)

KS_KY40-1_F1C3B_gCOSY_CDC13_12_20_2010
CDC13, 500 MHz, nt=4, time = 38 mins
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp
Pulse Sequence: gCOSY

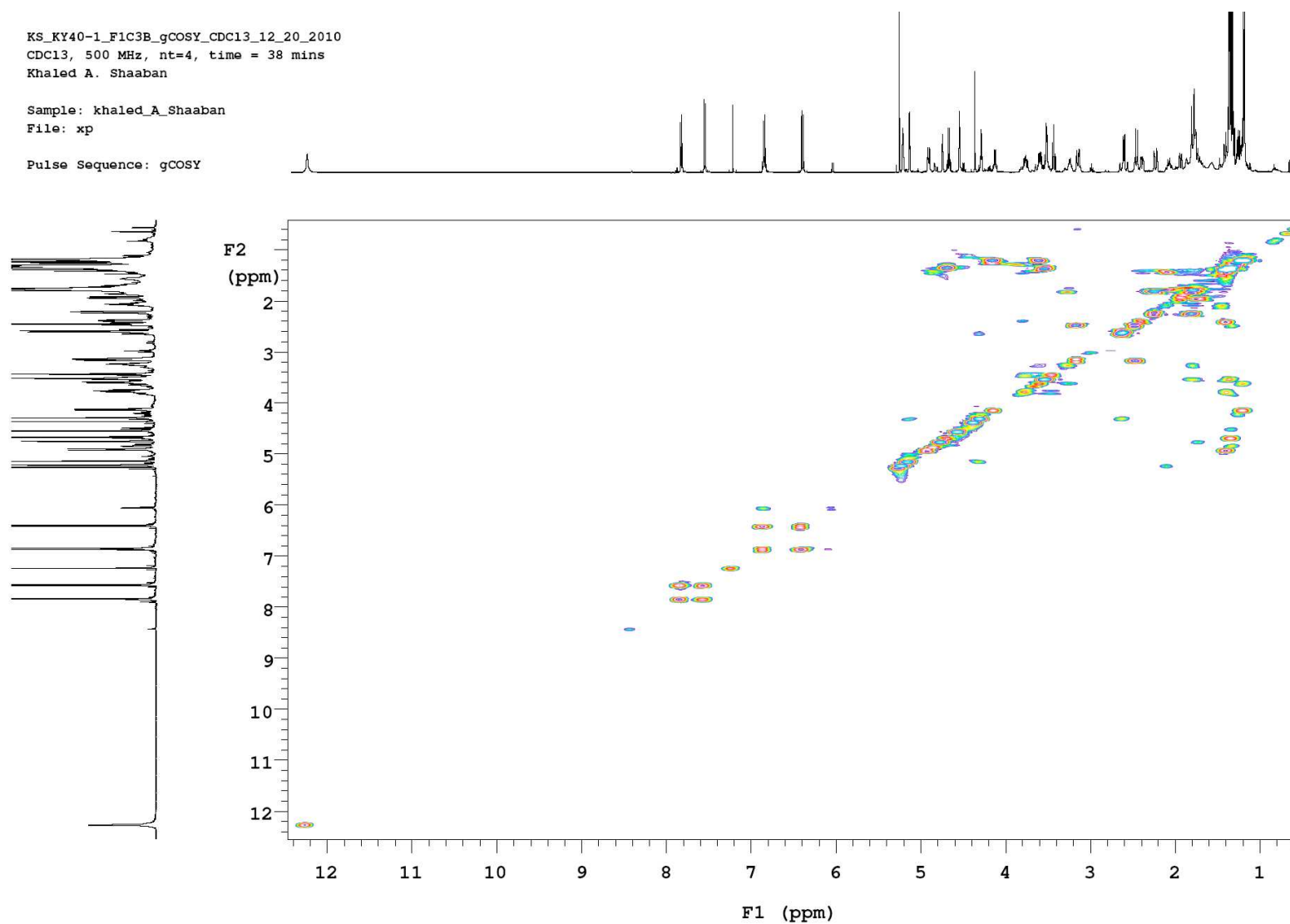


Figure S34: ^1H - ^1H COSY spectrum (CDCl_3 , 500 MHz) of saquayamycin J (**4**)

KS_KY40-1_F1C3B_GHSQC_CDC13_12_26_2010
CDC13, 500 MHz, time=1:17 hrs
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

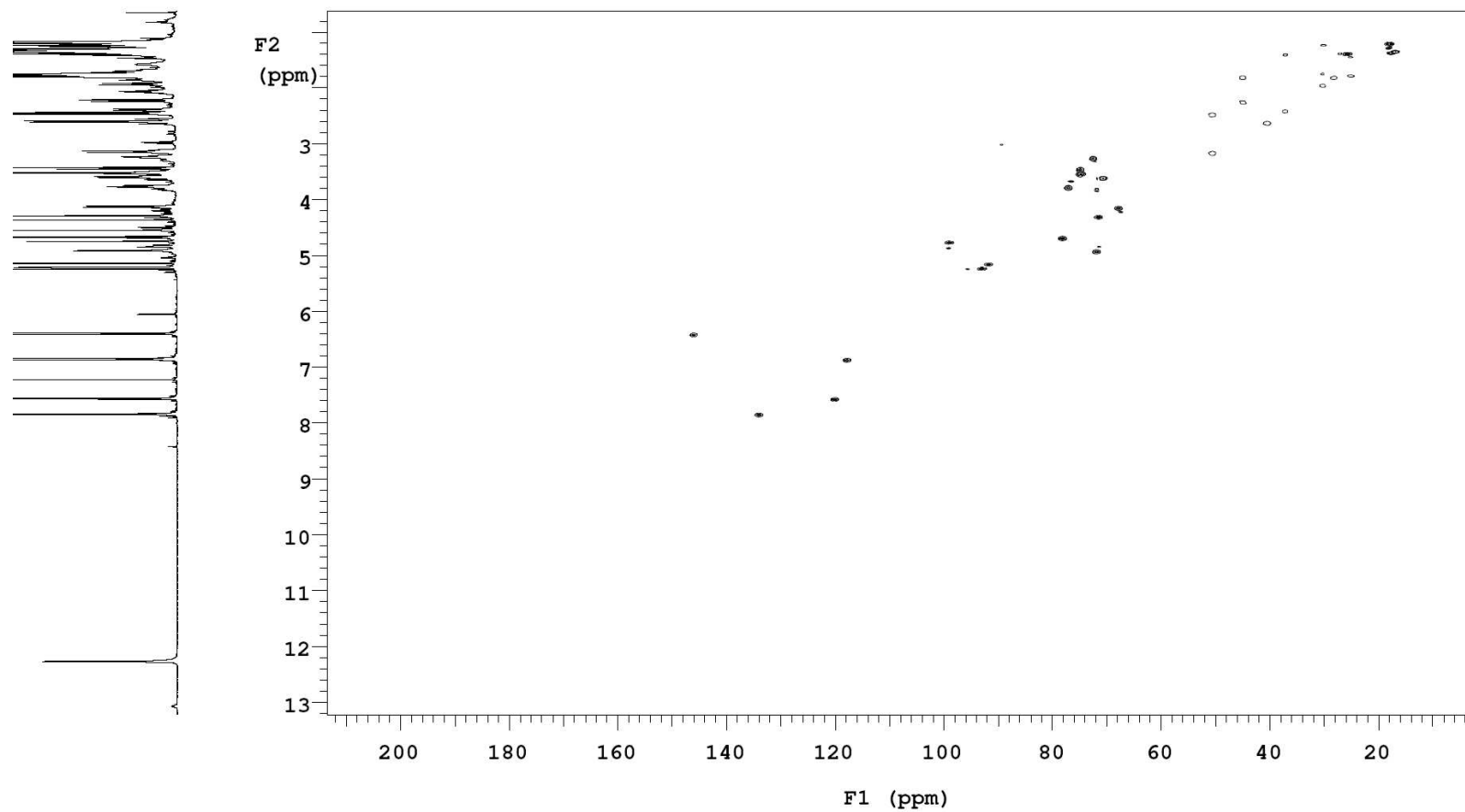


Figure S35: HSQC spectrum (CDCl₃, 500 MHz) of saquayamycin J (**4**)

KS_KY40-1_F1C3B_GHMBC_CDC13_12_27_2010
CDC13, 500 MHz, time=10:37 hrs
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

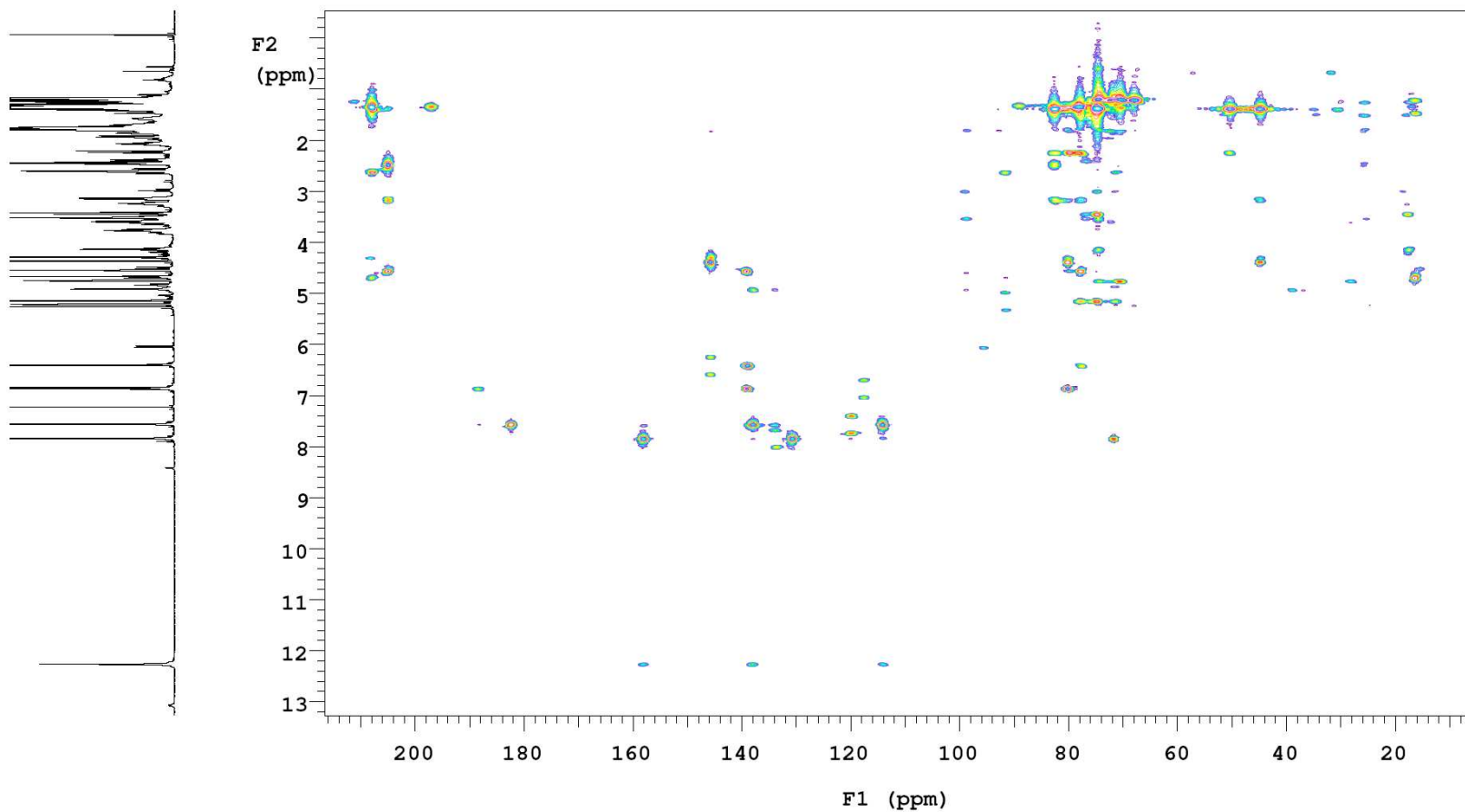
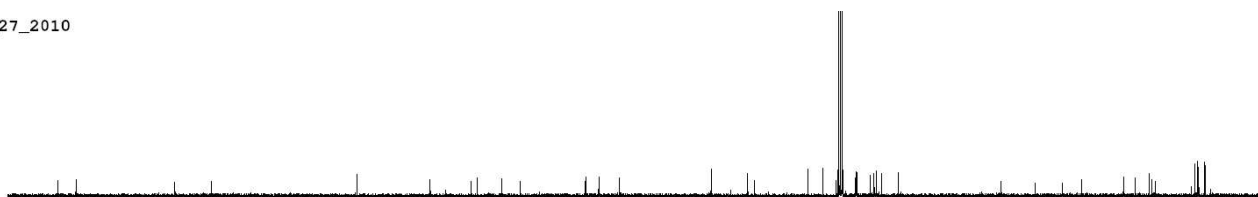


Figure S36: HMBC spectrum (CDCl_3 , 500 MHz) of saquayamycin J (**4**)

KS_KY40-1_F1C3B_NOESY_CDC13_12_27_2010
CDC13, 500 MHz, time=2:10 hrs
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: NOESY

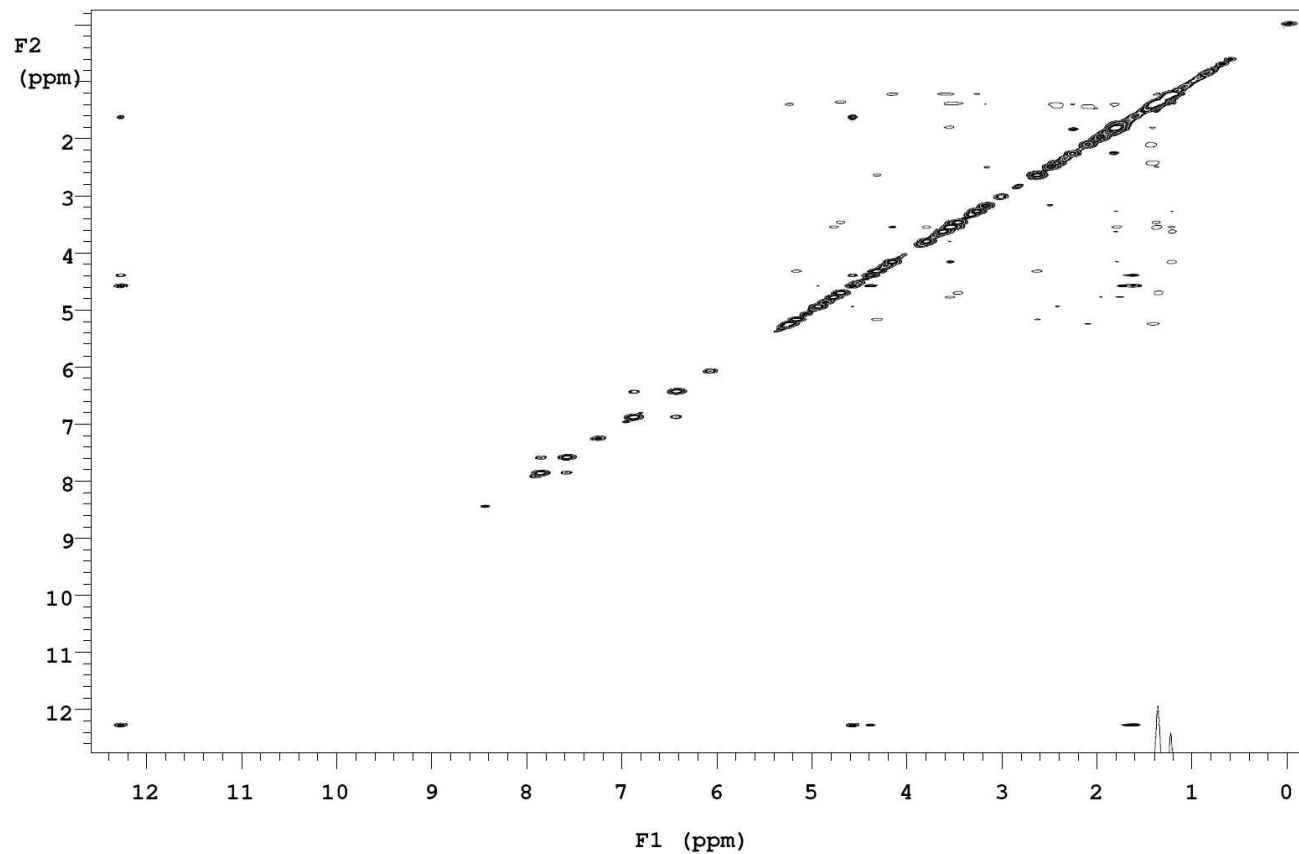
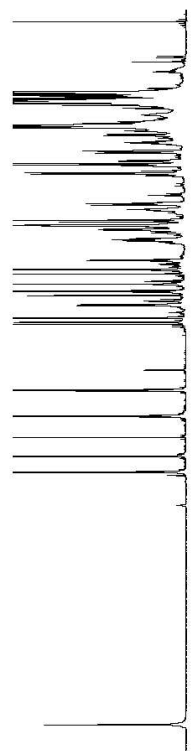
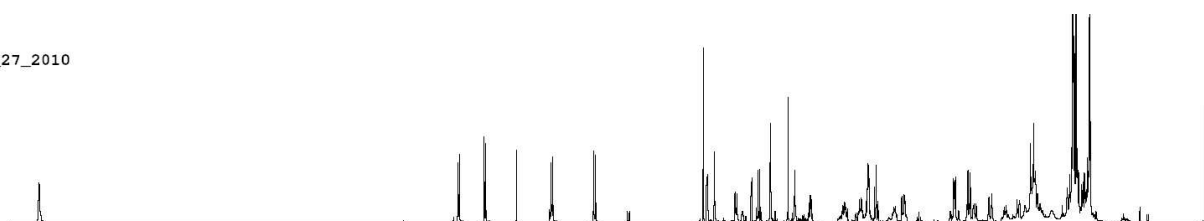


Figure S37: NOESY spectrum (CDCl_3 , 500 MHz) of saquayamycin J (**4**)

■ -TOF MS: 1.257 to 1.365 min from KSKY40-1-F1C3A.wiff Agilent

Max. 8.3e4 coun

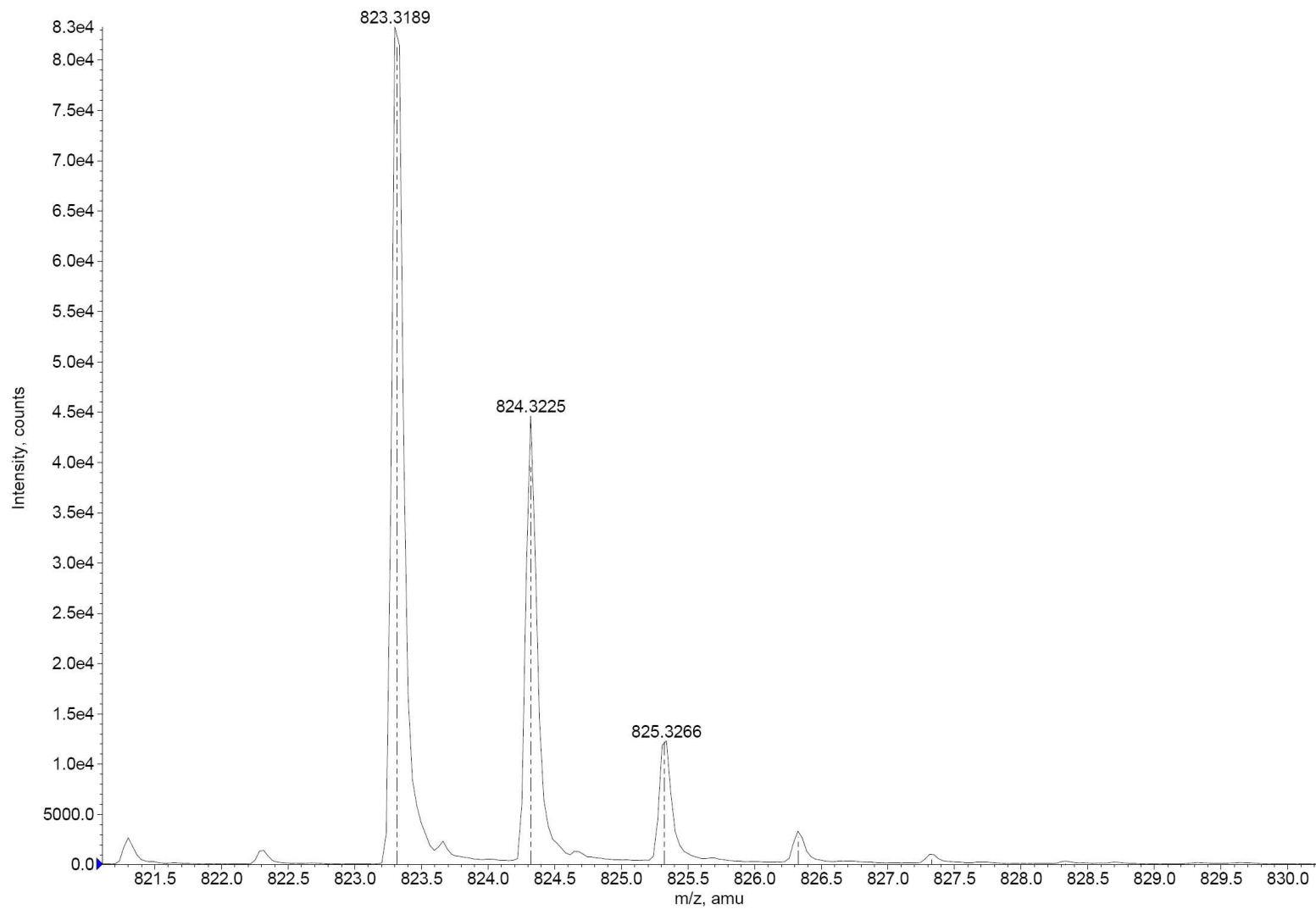


Figure S38: (-)-HRESI-MS spectrum of saquayamycin K (5)

■ -TOF MS: 1.257 to 1.365 min from KSKY40-1-F1C3A.wiff Agilent

Max. 8.3e4 counts

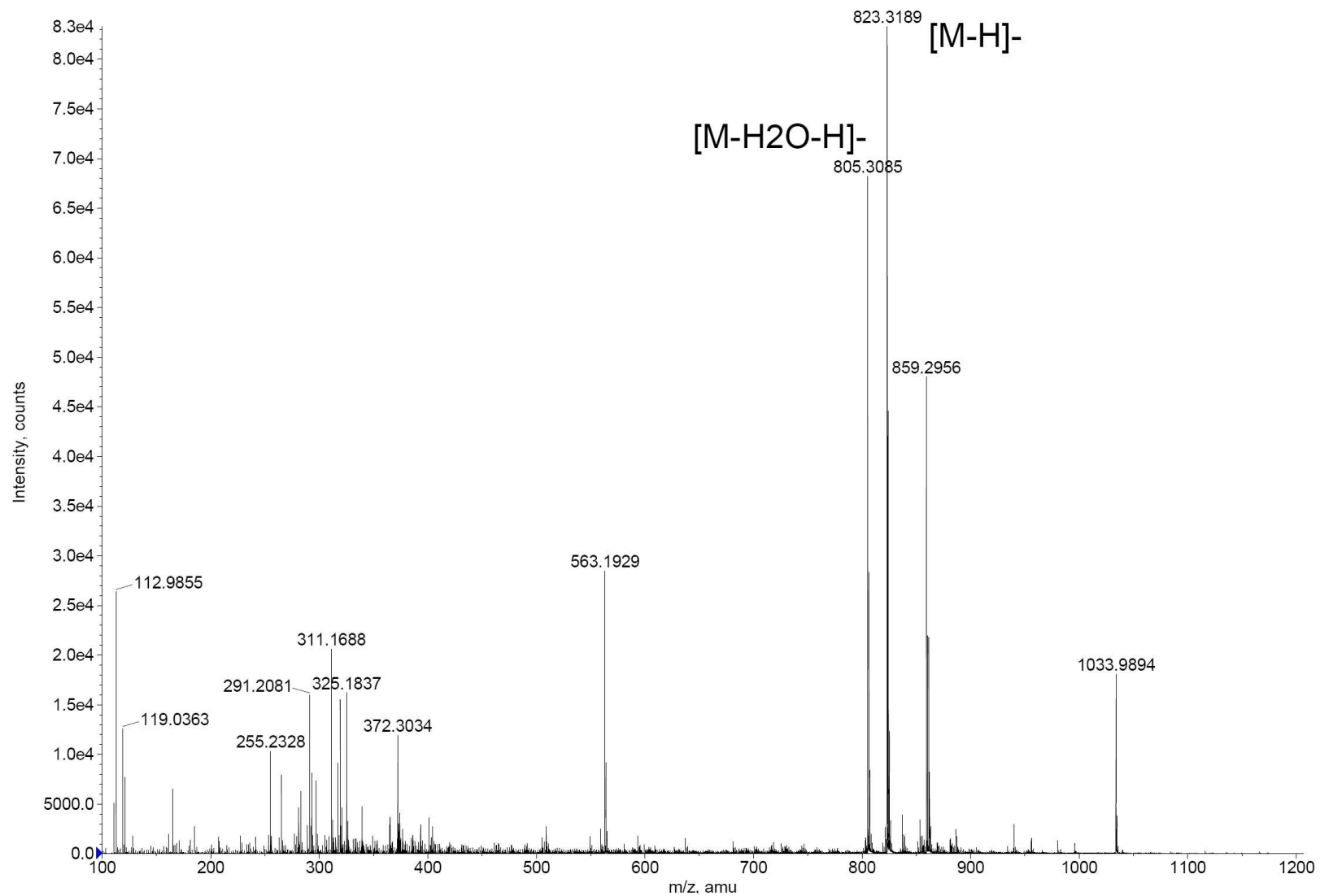


Figure S39: (-)-HRESI-MS spectrum of saquayamycin K (5)

KS_KY40-1_F1C3A_1HNMR_CDC13_12_17_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: s2pul

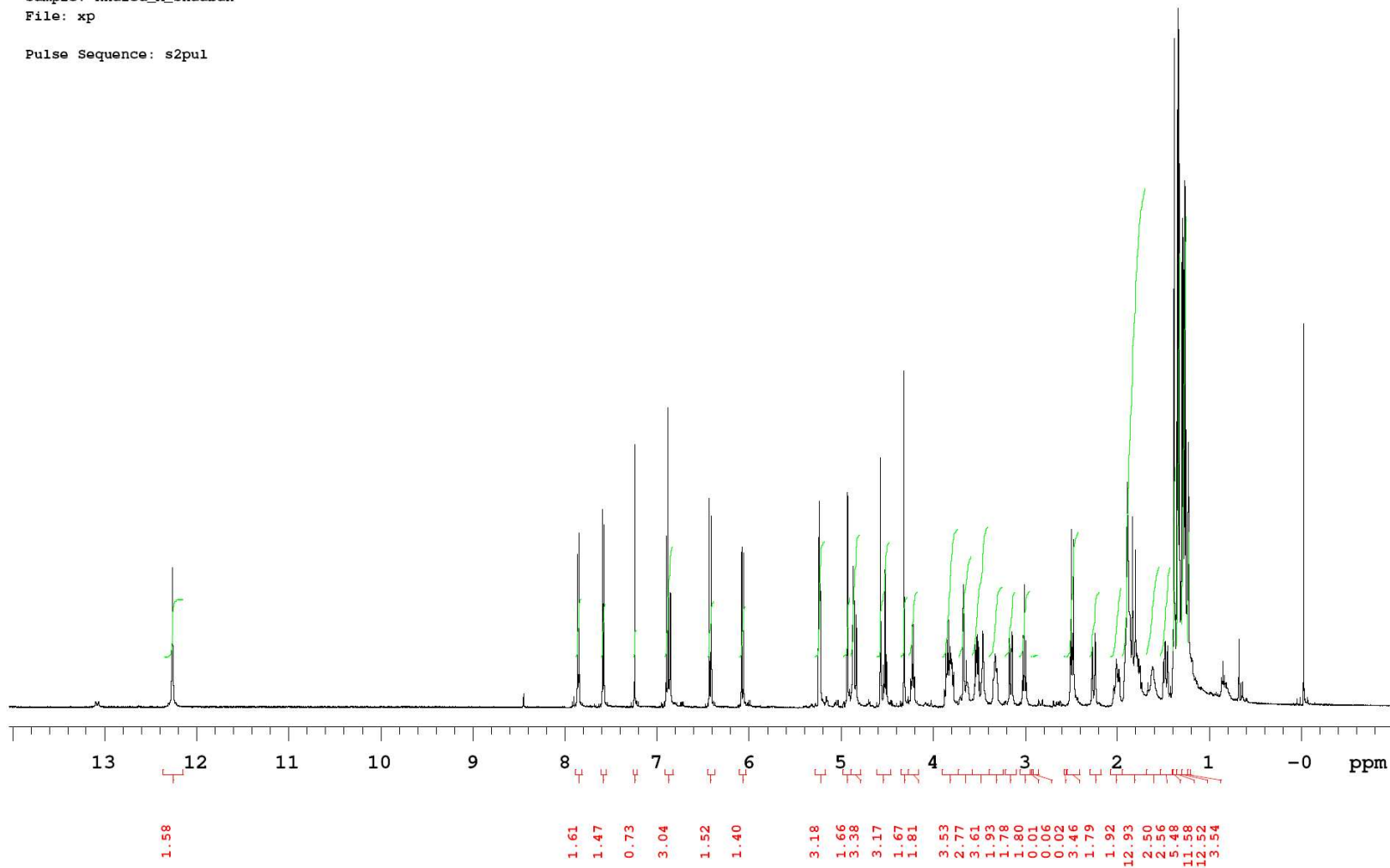


Figure S40: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin K (**5**)

KS_KY40-1_F1C3A_13CNMR_CDC13_12_21_2010
 CDC13, 125 MHz, time=16 hrs
 Khaled A. Shaaban

exp2 Carbon

SAMPLE		SPECIAL	
date	Dec 20 2010	temp	not used
solvent	cdc13	gain	30
file	exp	spin	20
ACQUISITION		hst	0.008
sw	30487.8	pw90	11.900
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	64000	hs	nn
ct	25600	PROCESSING	
TRANSMITTER	lb	0.50	
tn	C13	fn	not used
sfrq	125.665	DISPLAY	
tof	1285.1	sp	-995.2
tpwr	59	wp	29457.4
pw	5.950	rfl	11728.8
DECOUPLER	rfp	9704.1	
dn	H1	rp	133.5
dof	0	lp	-40.7
dm	YYY	PLOT	
dmm	w	wc	250
dpwr	35	sc	0
dmf	11448	vs	772995
		th	6
		ai	cdc ph

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	25774.2	205.124	14.4	40	3220.0	25.626	17.1
2	24760.9	197.061	16.2	41	3130.7	24.916	14.4
3	23667.7	188.360	10.7	42	3108.8	24.742	11.9
4	22926.6	182.462	11.8	43	2343.5	18.651	28.1
5	19889.3	158.290	15.9	44	2263.5	18.014	26.1
6	18304.8	145.679	14.6	45	2181.7	17.363	26.9
7	18004.3	143.288	18.3	46	1931.8	15.375	29.5
8	17464.2	138.989	18.4				
9	17442.8	138.819	14.2				
10	16811.0	133.791	14.8				
11	16407.7	130.581	12.2				
12	16021.1	127.504	19.4				
13	15065.1	119.896	14.7				
14	14792.0	117.723	15.3				
15	14336.6	114.098	12.0				
16	12431.1	98.933	18.9				
17	11998.9	95.494	23.5				
18	11637.0	92.613	19.7				
19	11209.0	89.207	20.7				
20	10398.1	82.754	23.4				
21	10073.0	80.166	23.2				
22	9753.8	77.626	20.0				
23	9735.7	77.482	242.0				
24	9704.1	77.230	252.4				
25	9672.0	76.975	250.3				
26	9595.7	76.367	21.2				
27	9376.5	74.624	16.5				
28	9012.3	71.725	20.3				
29	8990.9	71.554	18.5				
30	8979.7	71.465	21.4				
31	8943.4	71.177	20.3				
32	8897.4	70.810	21.9				
33	8435.0	67.130	19.8				
34	6329.9	50.377	10.6				
35	5620.9	44.734	11.1				
36	4884.5	38.874	15.1				
37	3780.1	30.084	15.2				
38	3757.3	29.903	8.2				
39	3431.7	27.311	13.0				

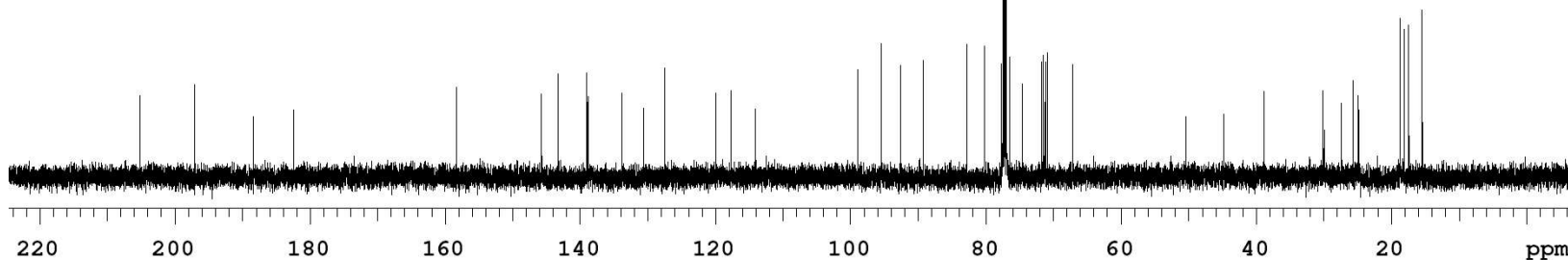


Figure S41: ¹³C NMR spectrum (CDCl₃, 125 MHz) of saquayamycin K (5)

KS_KY40-1_F1C3A_gCOSY_CDC13_12_20_2010
CDC13, 500 MHz, nt=4, time = 1:18 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gCOSY

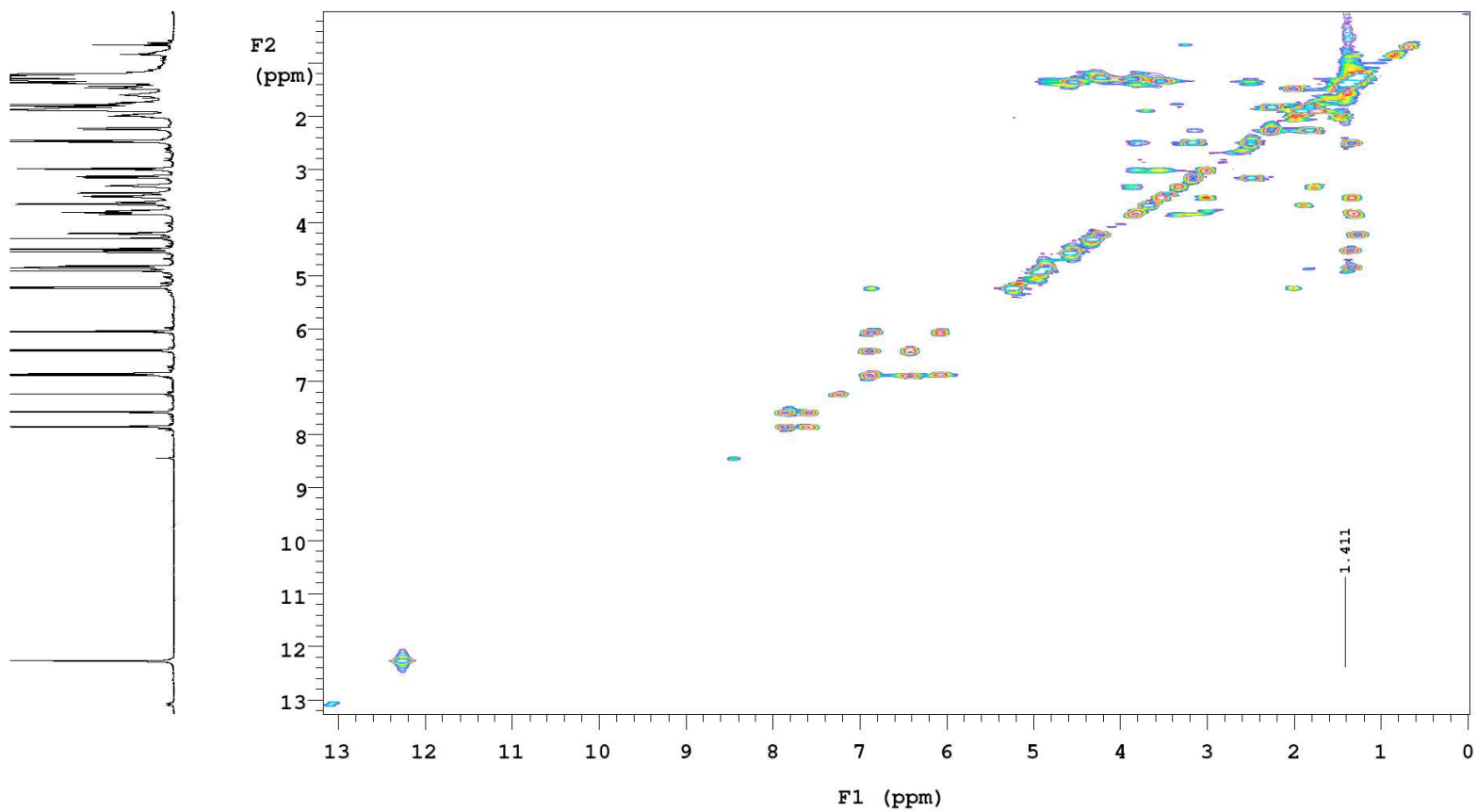
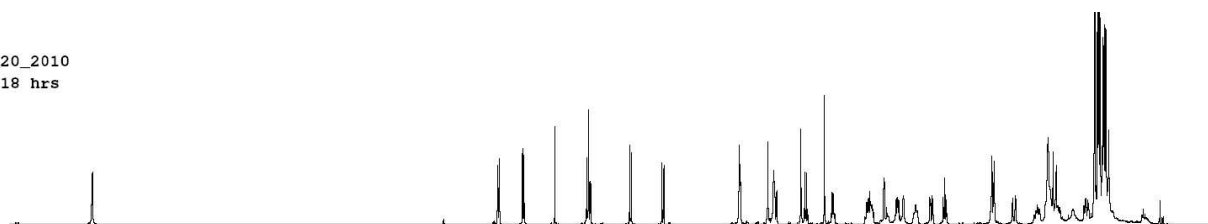


Figure S42: ^1H - ^1H COSY spectrum (CDCl_3 , 500 MHz) of saquayamycin K (**5**)

KS_KY40-1_F1C3A_GHSQC_CDC13_12_21_2010
CDC13, 500 MHz, nt=4, time = 1:16 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

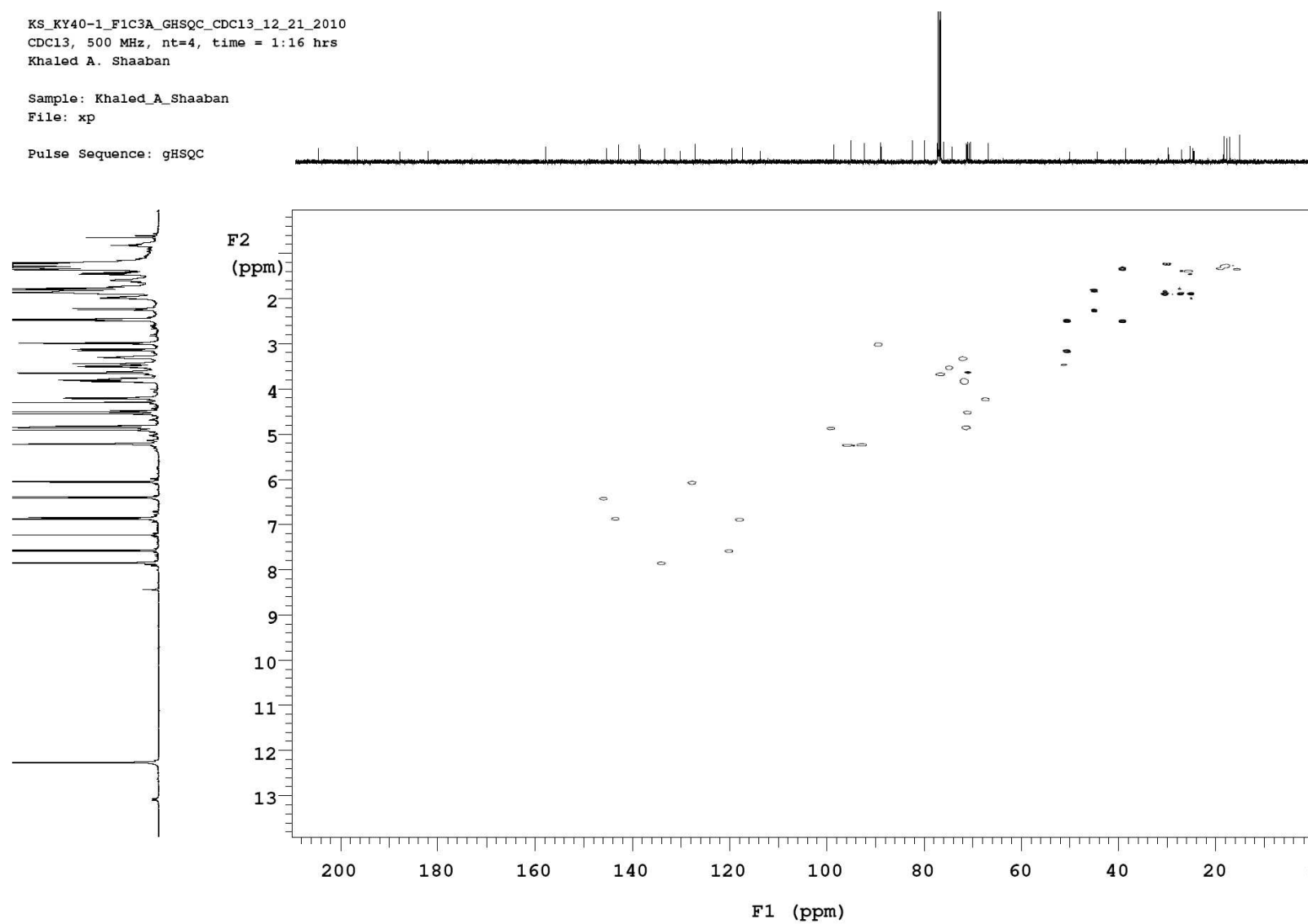


Figure S43: HSQC spectrum (CDCl₃, 500 MHz) of saquayamycin K (**5**)

CDCl₃, 500 MHz, nt=32, time = 10:36 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

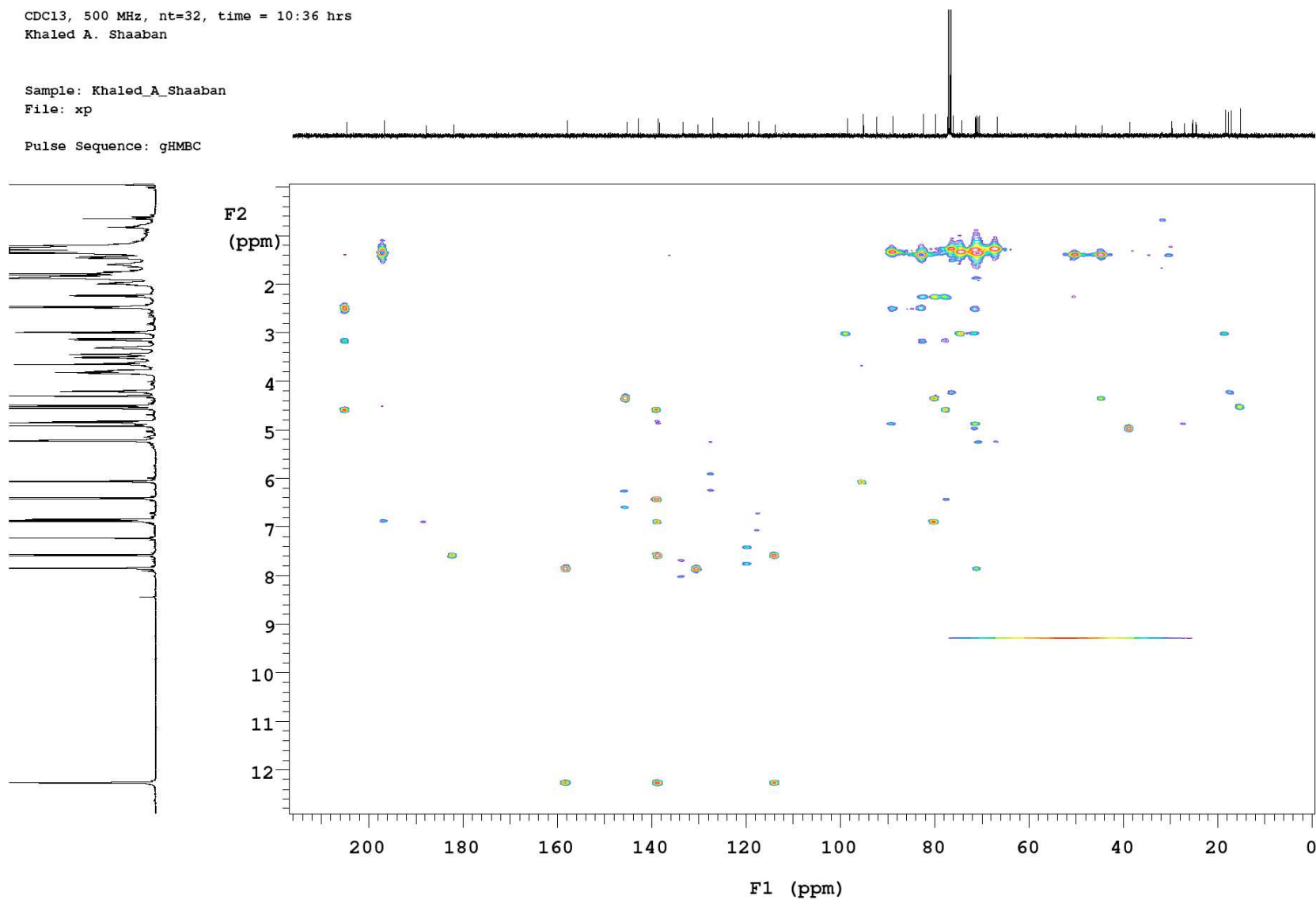


Figure S44: HMBC spectrum (CDCl₃, 500 MHz) of saquayamycin K (5)

KS_KY40-1_F1C3A_NOESY_CDC13_12_22_2010
CDC13, 500 MHz, nt=4, time = 1:45 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: NOESY

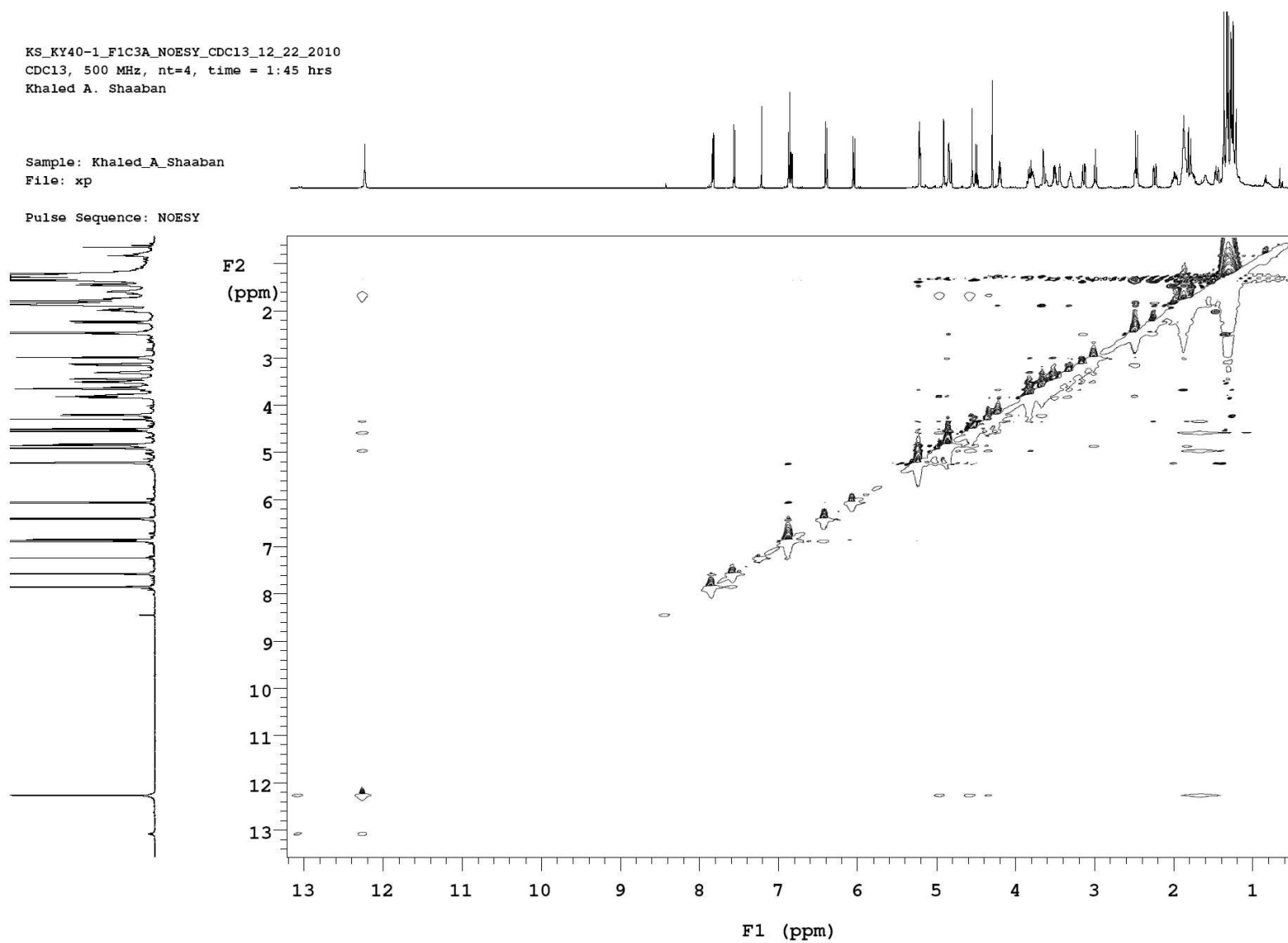


Figure S45: NOESY spectrum (CDCl₃, 500 MHz) of saquayamycin K (**5**)

■ -TOF MS: 1.020 to 1.128 min from KSKY40-1-F1C2B.wiff Agilent

Max. 3.3e5 coun

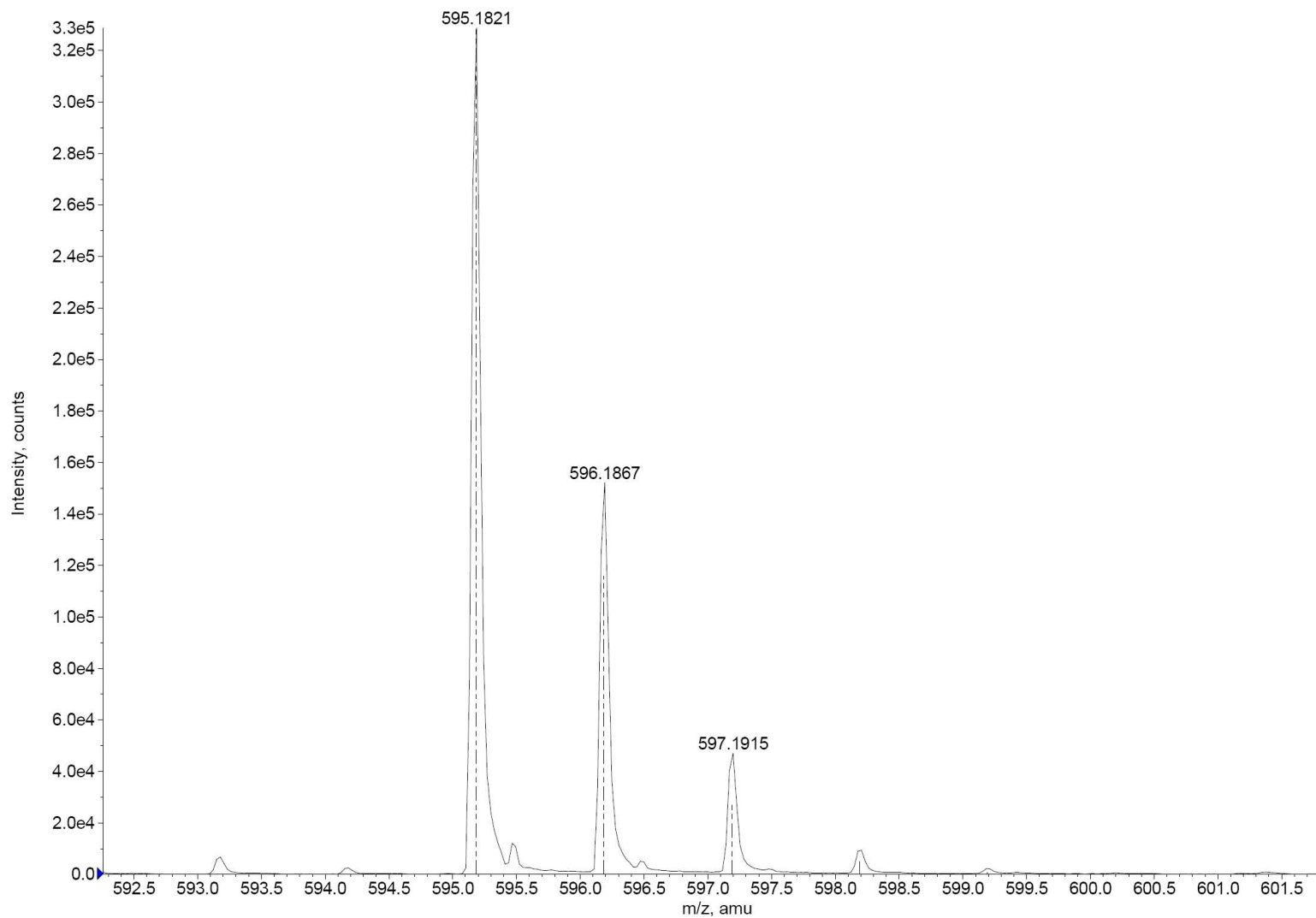


Figure S46: (-)-HRESI-MS spectrum of saquayamycin B1 (**6**)

■ -TOF MS: 1.020 to 1.128 min from KSKY40-1-F1C2B.wiff Agilent

Max. 3.3e5 counts

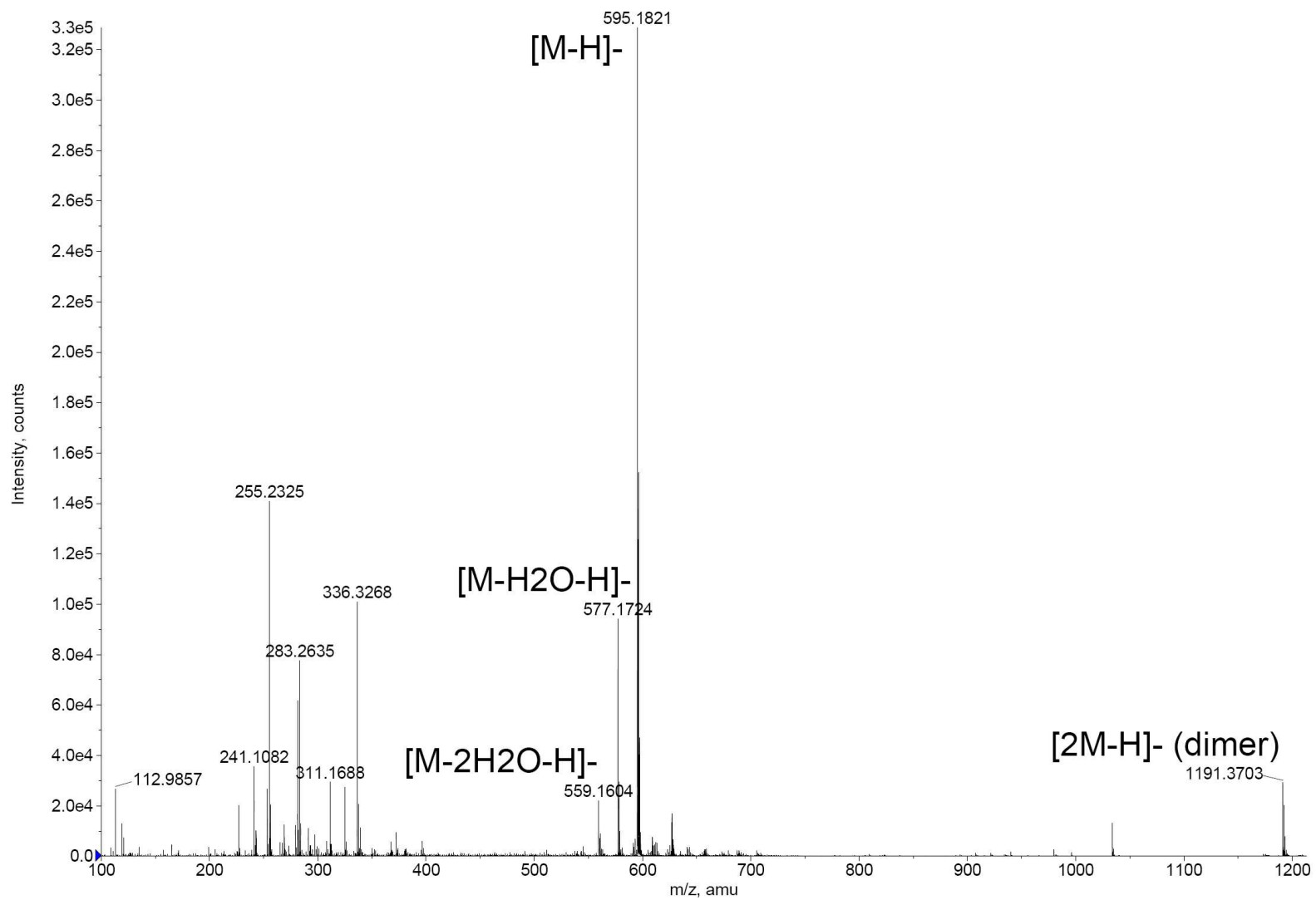


Figure S47: (-)-HRESI-MS spectrum of saquayamycin B1 (**6**)

KS_KY40-1_F1C2B_1HNMR_CDC13_12_17_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: s2pul

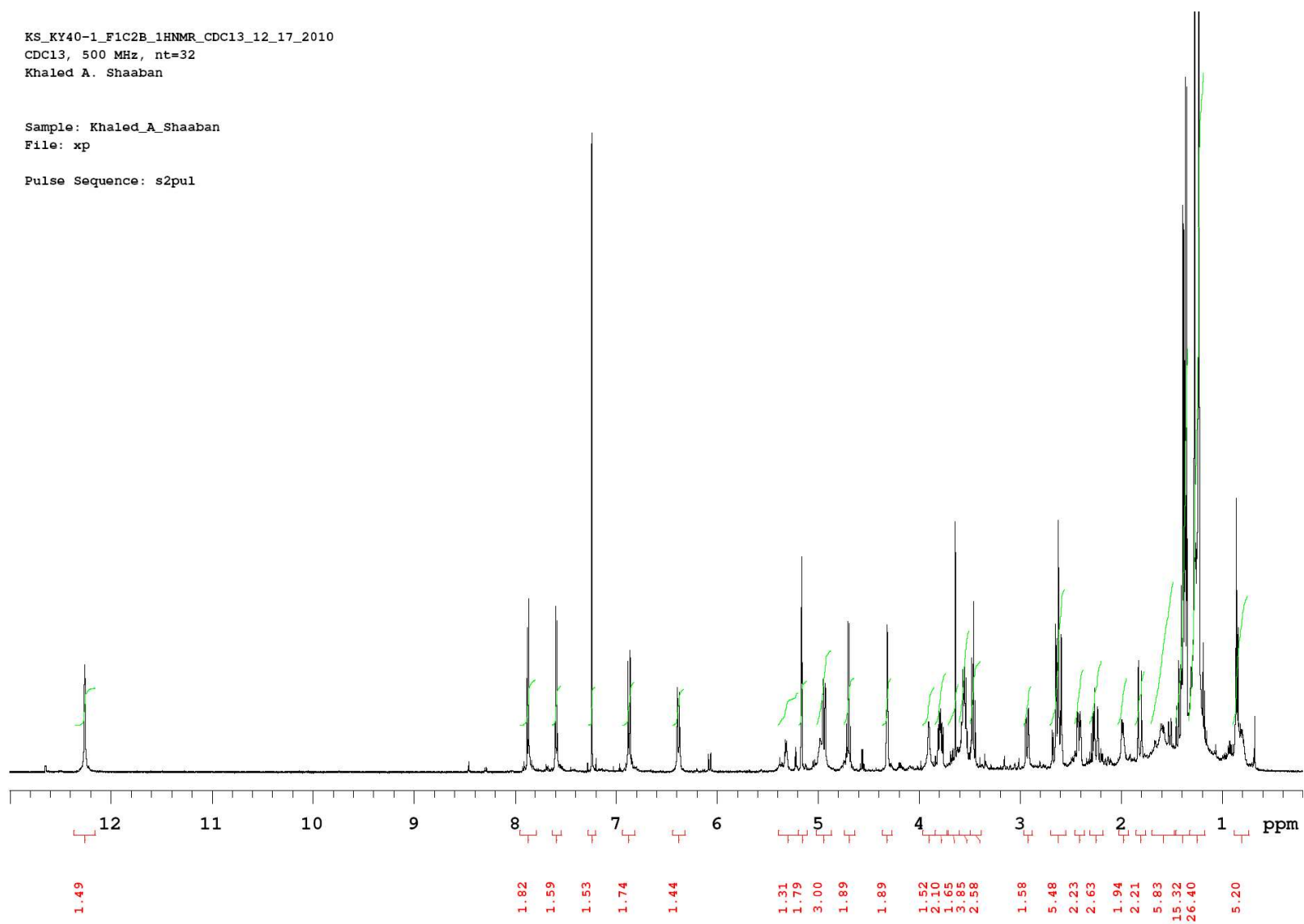


Figure S48: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin B1 (6)

KS_KY40-1_F1C2E_13CNMR_CDC13_12_28_2010
 CDC13, 125 MHz, time=24 hrs
 Khaled A. Shaaban

exp2 Carbon

SAMPLE		SPECIAL	
date	Dec 27 2010	temp	not used
solvent	cdcl3	gain	30
file	exp	spin	20
ACQUISITION		hst	0.008
sw	30487.8	pw90	11.900
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	64000	hs	nn
ct	37696	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	125.665	DISPLAY	
tof	1285.1	sp	-2022.9
tpwr	59	wp	30487.3
pw	5.950	rfl	11727.4
DECOUPLER		rfp	9704.1
dn	H1	rp	149.6
dof	0	lp	-64.6
dm	YYY	PLOT	
dmm	w	wc	250
dpwr	35	sc	0
dmf	11448	vs	1.19538e+06
		th	5
		ai	cdc ph

INDEX	FREQUENCY	PPM	HEIGHT
1	26135.6	208.001	9.2
2	25775.1	205.132	5.3
3	23644.0	188.171	8.4
4	19875.8	158.182	9.0
5	18162.4	144.546	10.5
6	17461.4	138.967	8.0
7	17381.8	138.334	7.7
8	17367.9	138.223	9.4
9	16833.8	133.972	13.2
10	16406.3	130.570	8.0
11	15077.2	119.992	13.5
12	14788.8	117.697	12.5
13	14344.0	114.157	6.8
14	11507.2	91.580	13.6
15	10145.5	80.744	9.7
16	9797.6	77.974	16.4
17	9736.1	77.485	330.4
18	9704.1	77.230	329.1
19	9672.4	76.978	326.4
20	9661.3	76.889	16.1
21	9582.2	76.260	12.3
22	9395.2	74.772	15.9
23	9380.7	74.657	17.1
24	9002.1	71.643	12.5
25	8964.4	71.343	14.9
26	6570.9	52.295	10.0
27	5452.1	43.390	10.6
28	5047.3	40.169	10.9
29	4635.2	36.889	12.9
30	4038.3	32.139	5.6
31	3828.0	30.465	12.6
32	3758.2	29.910	31.3
33	3710.8	29.532	6.6
34	2878.5	22.909	7.3
35	2220.7	17.674	16.9
36	2058.4	16.382	20.1
37	1803.0	14.349	7.8

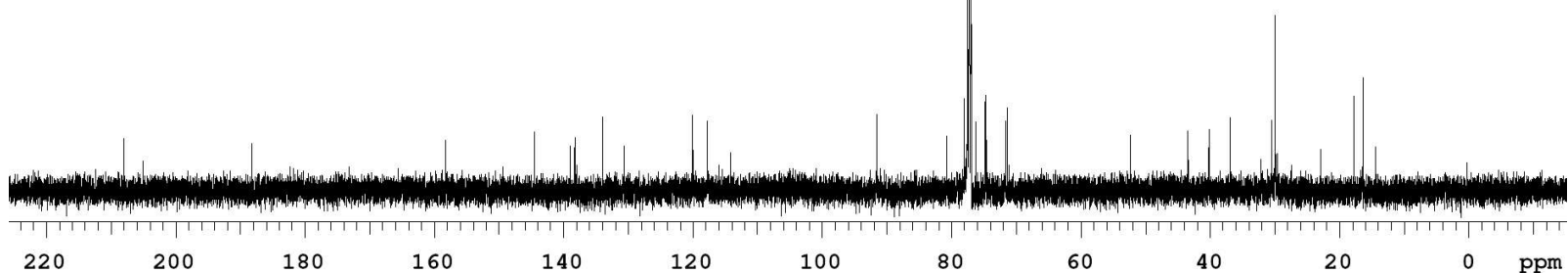


Figure S49: ^{13}C NMR spectrum (CDCl_3 , 125 MHz) of saquayamycin B1 (6)

KS_KY40-1_F1C2B_gCOSY_CDC13_12_17_2010
CDC13, 500 MHz, nt=4, time = 38 mins
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gCOSY

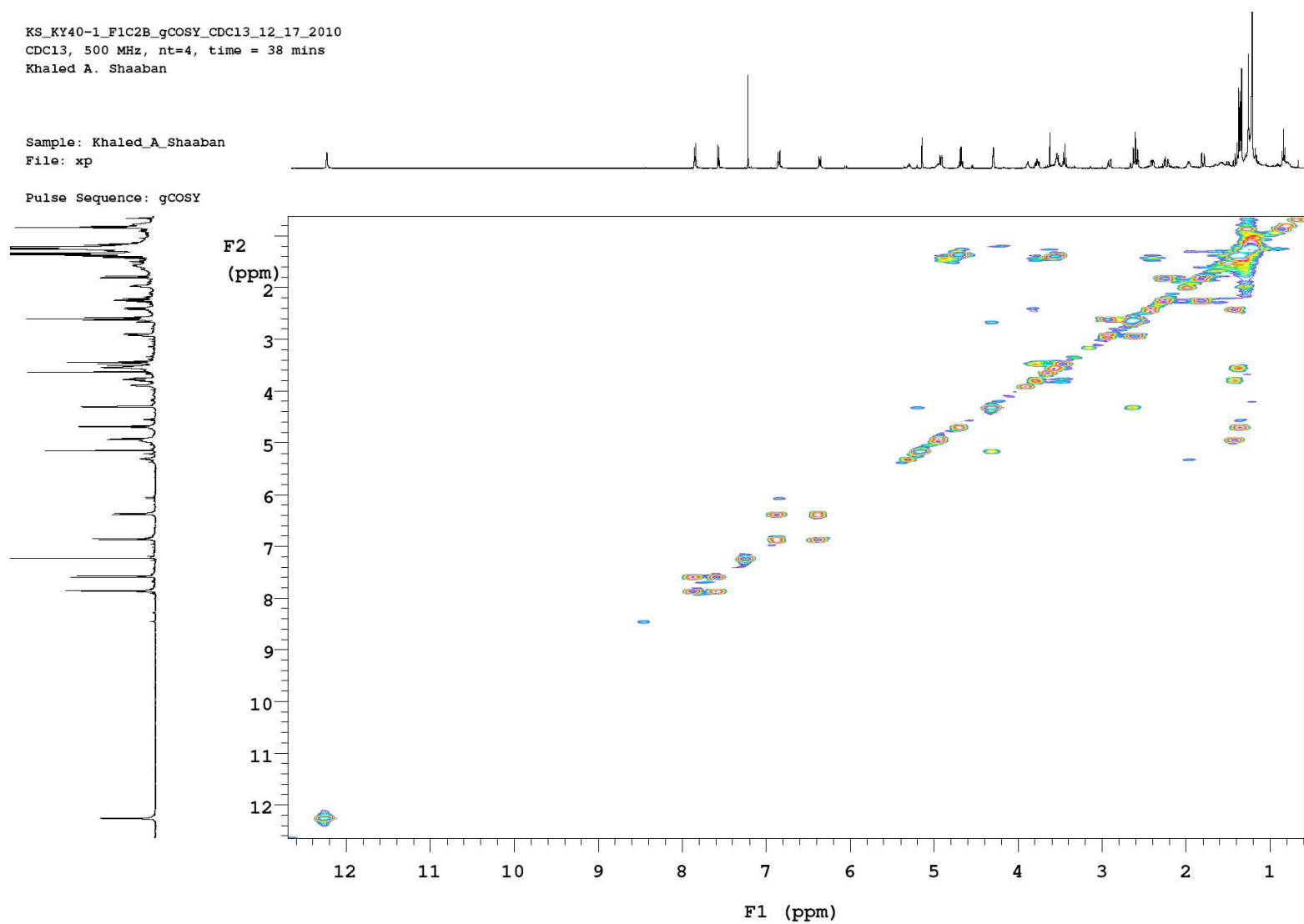


Figure S50: ^1H - ^1H COSY spectrum (CDCl_3 , 500 MHz) of saquayamycin B1 (**6**)

CDC13, 500 MHz, nt=8, time=5 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

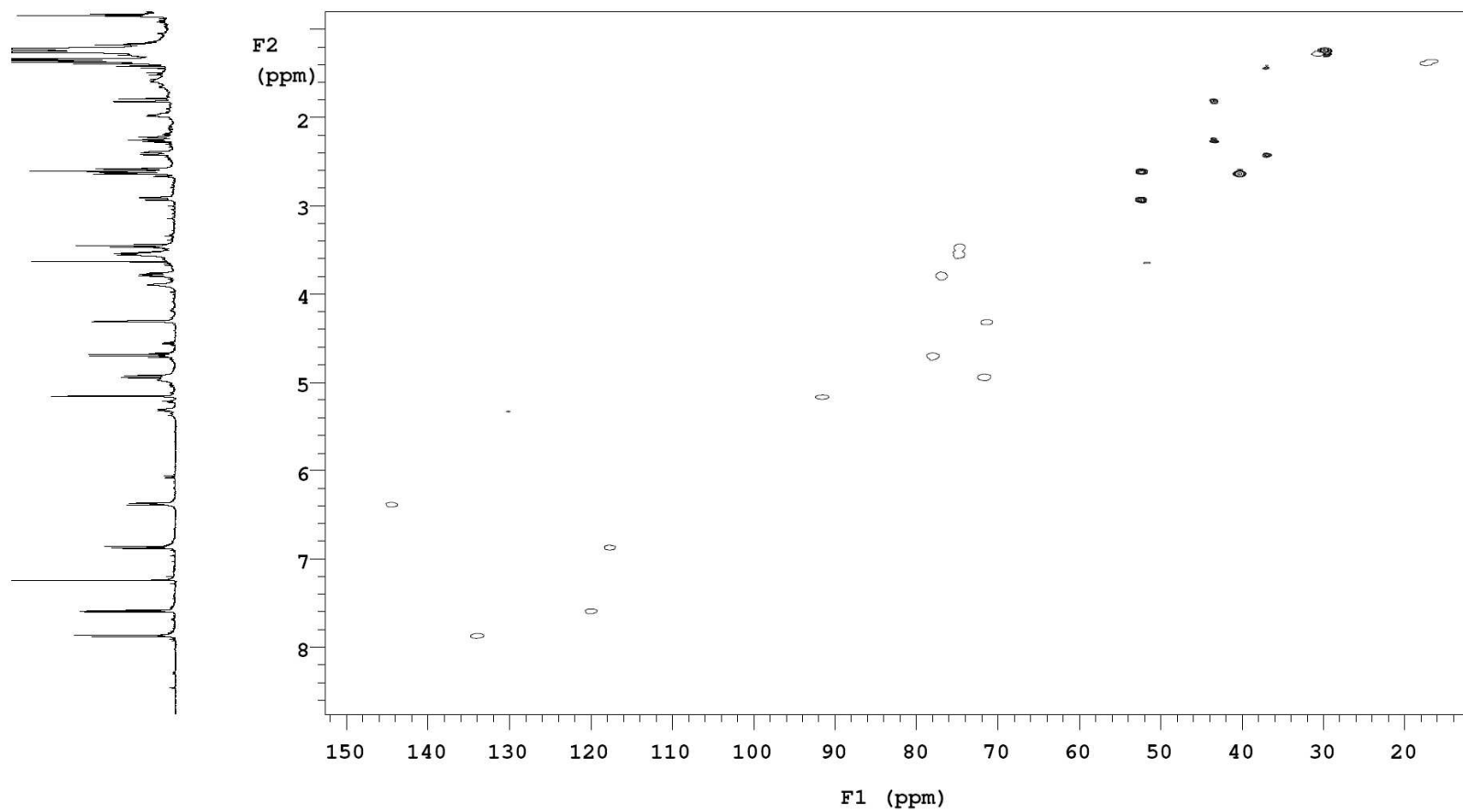
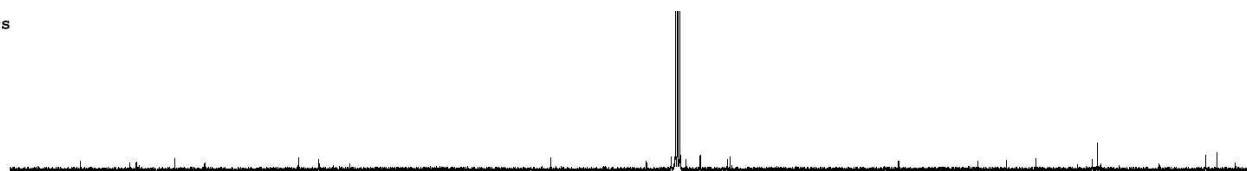


Figure S51: HSQC spectrum (CDCl_3 , 500 MHz) of saquayamycin B1 (**6**)

CDCl₃, 500 MHz, nt=32, time=10:37 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

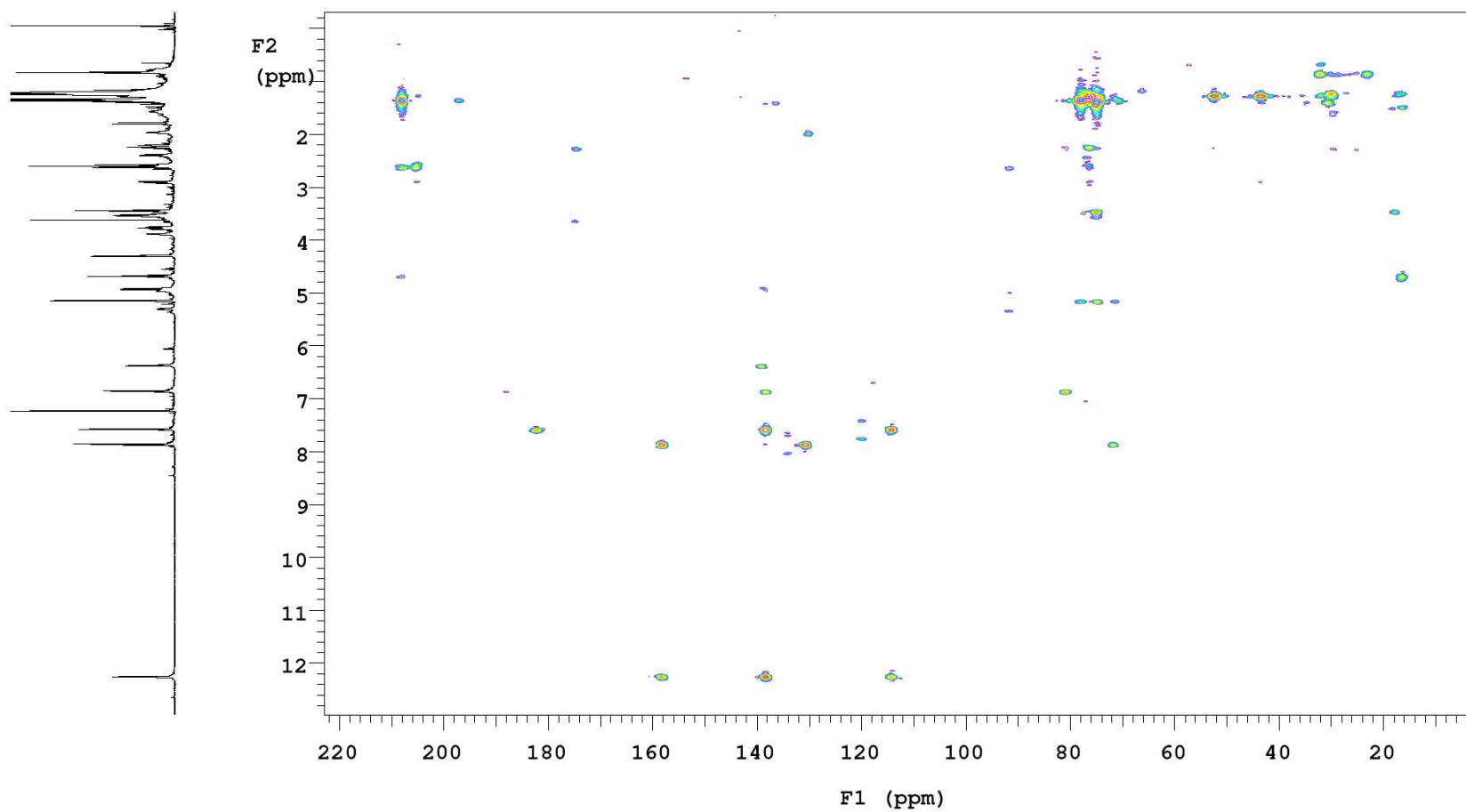


Figure S52: HMBC spectrum (CDCl₃, 500 MHz) of saquayamycin B1 (**6**)

CDCl₃, 500 MHz, nt=4, time=2 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: NOESY

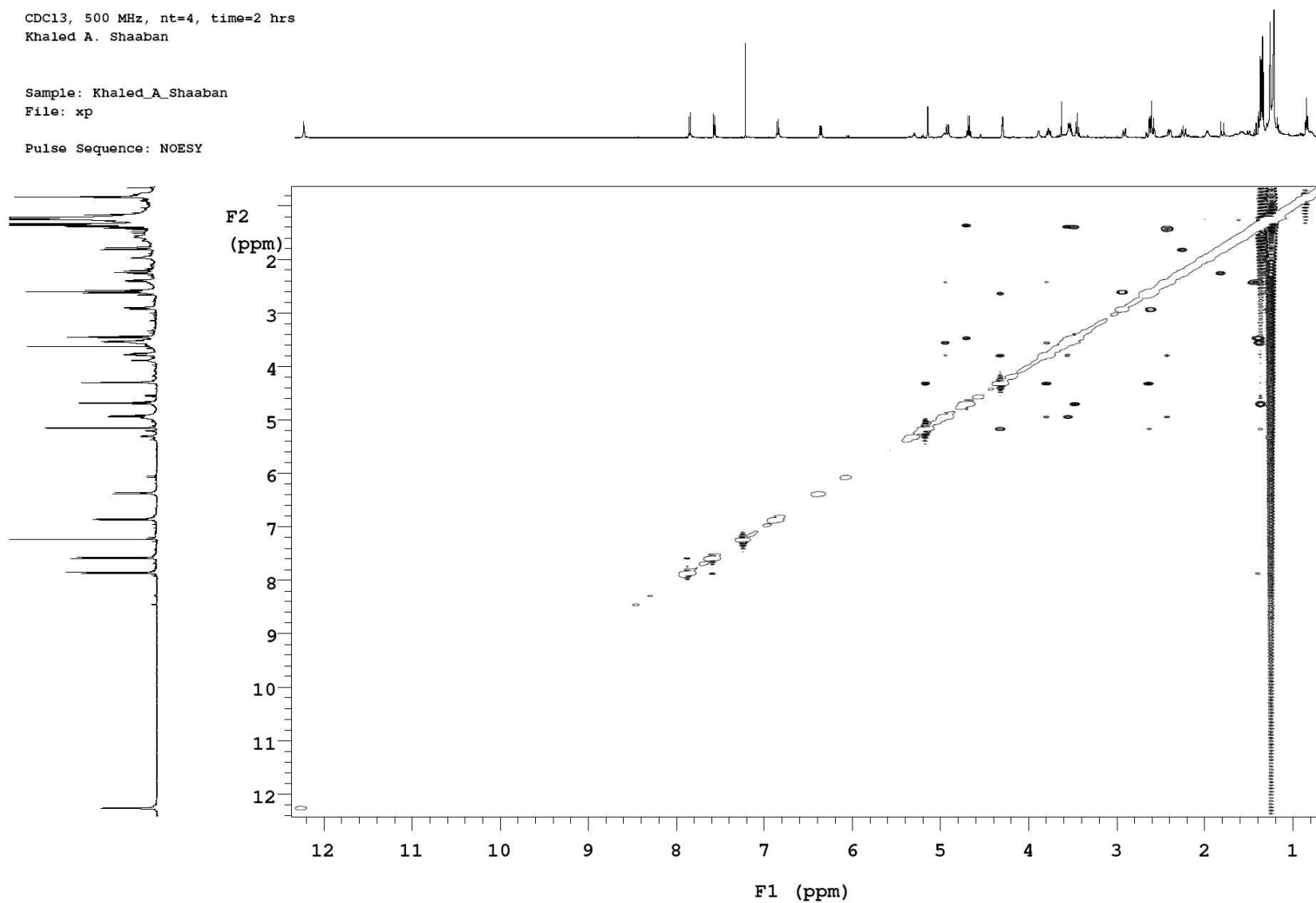


Figure S53: NOESY spectrum (CDCl₃, 500 MHz) of saquayamycin B1 (**6**)

KS_KY40-1_F1D_1HNMR_CDC13_12_01_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: s2pul

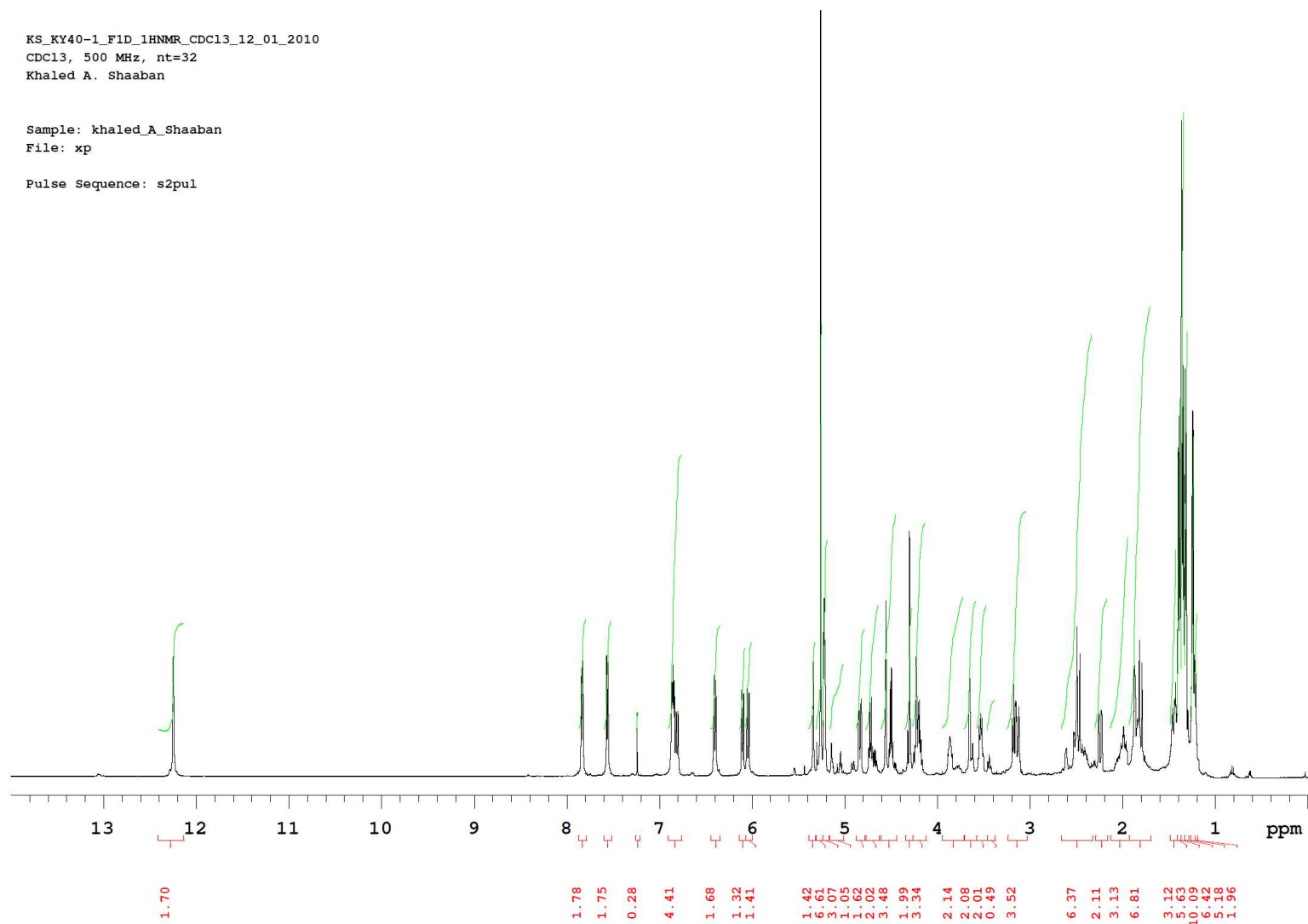


Figure S54: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin A (7)

KS_KY40-1_F1D_13CNMR_CDCl3_12_07_2010
 CDC13, 125 MHz, time= 10 hrs
 Khaled A. Shaaban

expl0 Carbon

SAMPLE		SPECIAL	
date	Dec 6 2010	temp	not used
solvent	cdcl3	gain	30
file	exp	spin	20
ACQUISITION		hst	0.008
sw	30487.8	pw90	11.900
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	100000	hs	nn
ct	15424	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	125.665	DISPLAY	
tof	1285.1	sp	-1028.7
tpwr	59	wp	29432.7
pw	5.950	rfl	11736.7
DECOUPLER		rfp	9704.1
dn	H1	rp	-76.1
dof	0	lp	19.6
dm	yyy	PLOT	
dmm	w	wc	250
dpwr	35	sc	0
dmf	11448	vs	377449
		th	9
		ai	cdc ph

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	25766.3	205.062	14.9	40	3120.9	24.838	19.4
2	24752.6	196.994	18.9	41	3098.6	24.660	16.2
3	24557.6	195.443	20.0	42	2325.9	18.510	34.5
4	23661.7	188.312	15.2	43	2172.8	17.292	39.0
5	22913.1	182.355	17.3	44	1924.9	15.319	38.5
6	19868.8	158.127	20.4	45	1922.5	15.301	40.3
7	18306.2	145.690	17.8				
8	18000.1	143.254	23.4				
9	17888.9	142.369	21.5				
10	17454.9	138.915	23.9				
11	17380.4	138.323	14.7				
12	16794.3	133.658	17.3				
13	16407.2	130.577	17.2				
14	16008.1	127.401	38.8				
15	15051.1	119.785	20.3				
16	14775.3	117.589	18.9				
17	14330.5	114.050	18.8				
18	11987.8	95.405	31.2				
19	11967.3	95.242	27.6				
20	11626.3	92.528	26.9				
21	11226.2	89.344	24.3				
22	10388.4	82.676	28.8				
23	10063.7	80.092	28.5				
24	9744.5	77.552	33.3				
25	9736.2	77.485	407.2				
26	9704.1	77.230	419.6				
27	9672.0	76.975	413.9				
28	9585.9	76.290	24.9				
29	9358.9	74.483	22.5				
30	8999.3	71.621	26.4				
31	8970.4	71.391	22.6				
32	8943.9	71.180	23.3				
33	8885.3	70.714	27.2				
34	8424.7	67.048	23.8				
35	6737.4	53.620	25.1				
36	6320.1	50.299	15.4				
37	5604.2	44.601	14.6				
38	4898.9	38.988	17.7				
39	3212.1	25.564	23.9				

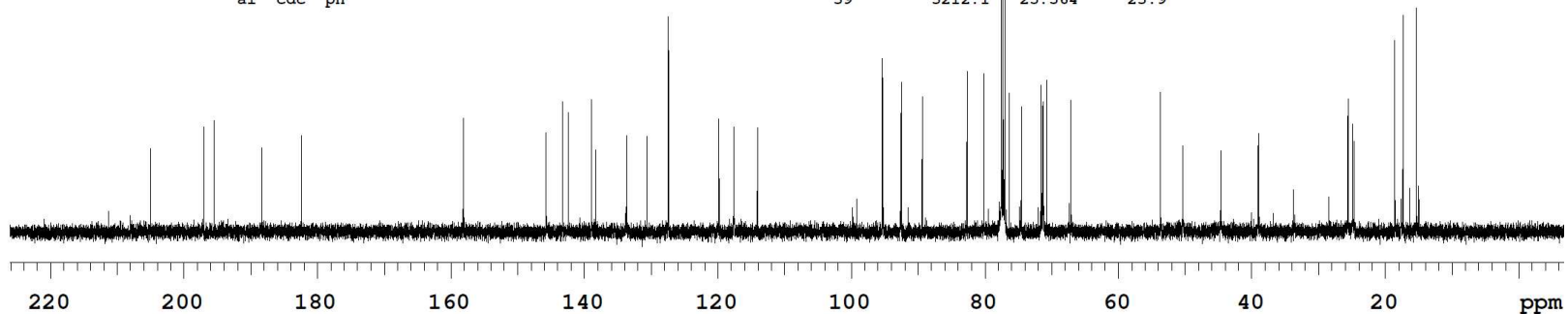


Figure S55: ¹³C NMR spectrum (CDCl₃, 125 MHz) of saquayamycin A (7)

KS_KY40-1_F1D_gCOSY_CDCl3_12_13_2010
CDCl3, 500 MHz, nt=4, time = 1:18 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gCOSY

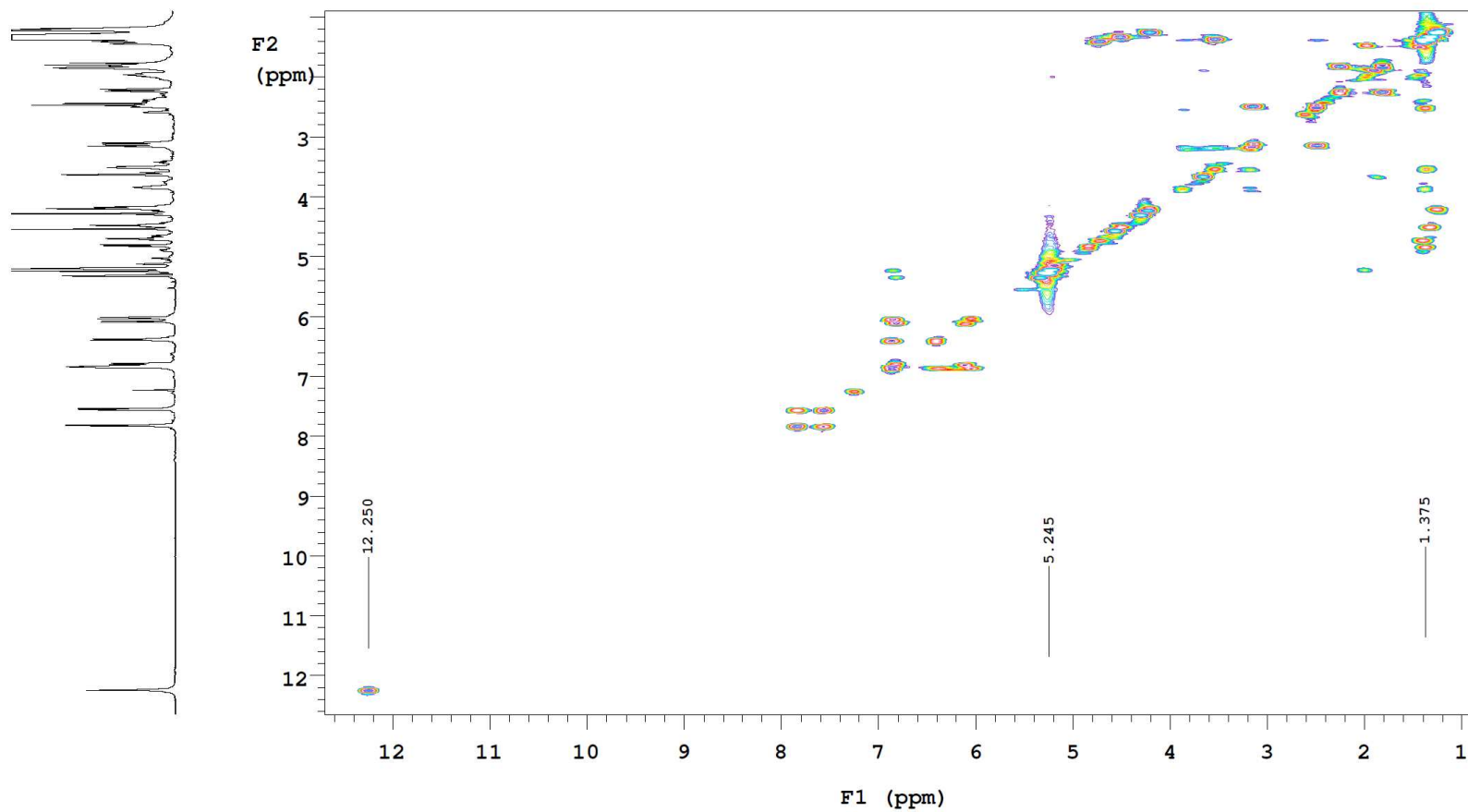


Figure S56: ¹H-¹H COSY spectrum (CDCl₃, 500 MHz) of saquayamycin A (7)

KS_KY40-1_F1D_gHSQC_CDCl3_12_14_2010
CDCl3, 500 MHz, nt=4, time = 1:17 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

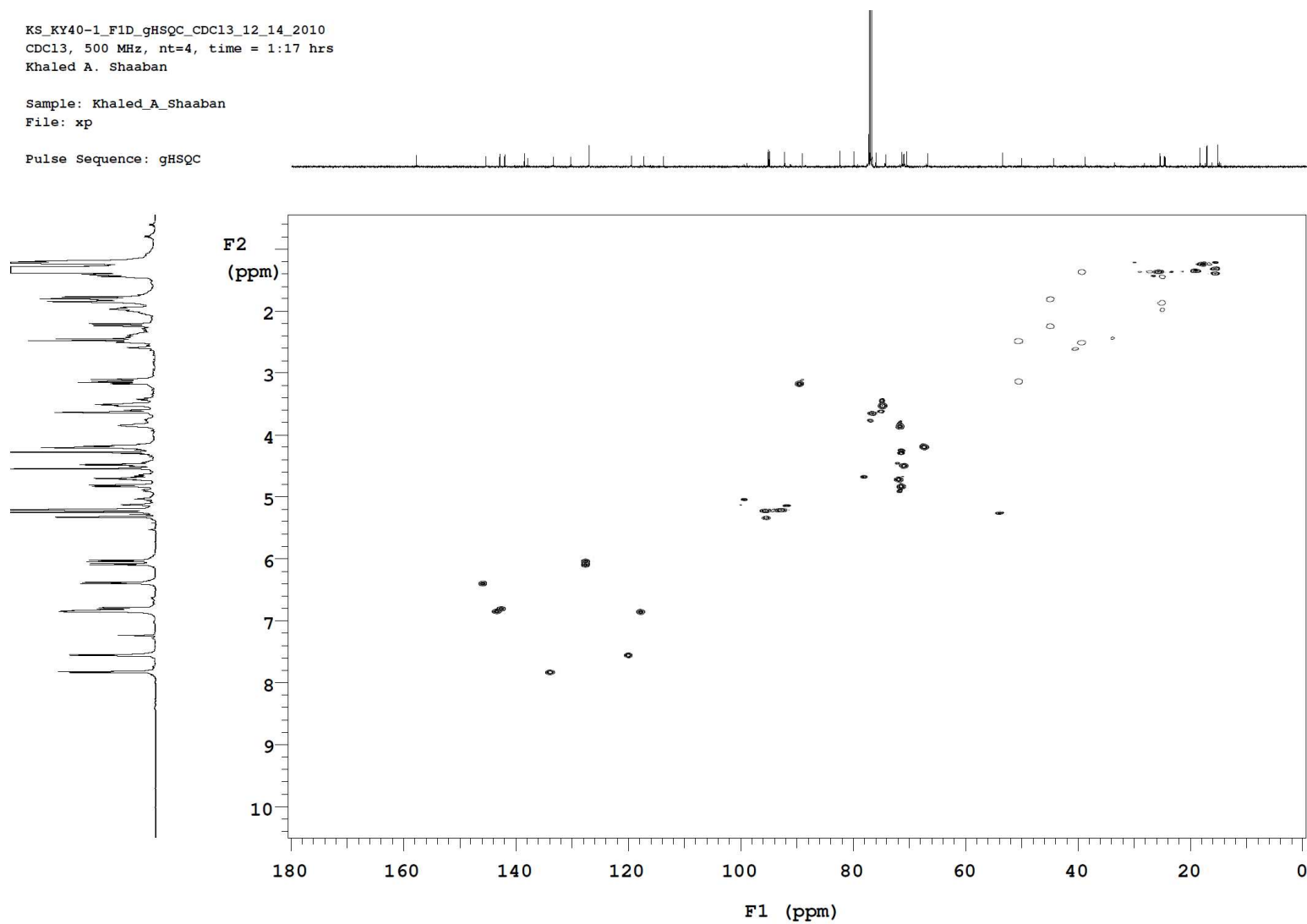


Figure S57: HSQC spectrum (CDCl₃, 500 MHz) of saquayamycin A (7)

KS_KY40-1_F1D_GHMBC_CDCl3_12_13_2010
CDCl3, 500 MHz, nt=32, time = 11:18 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

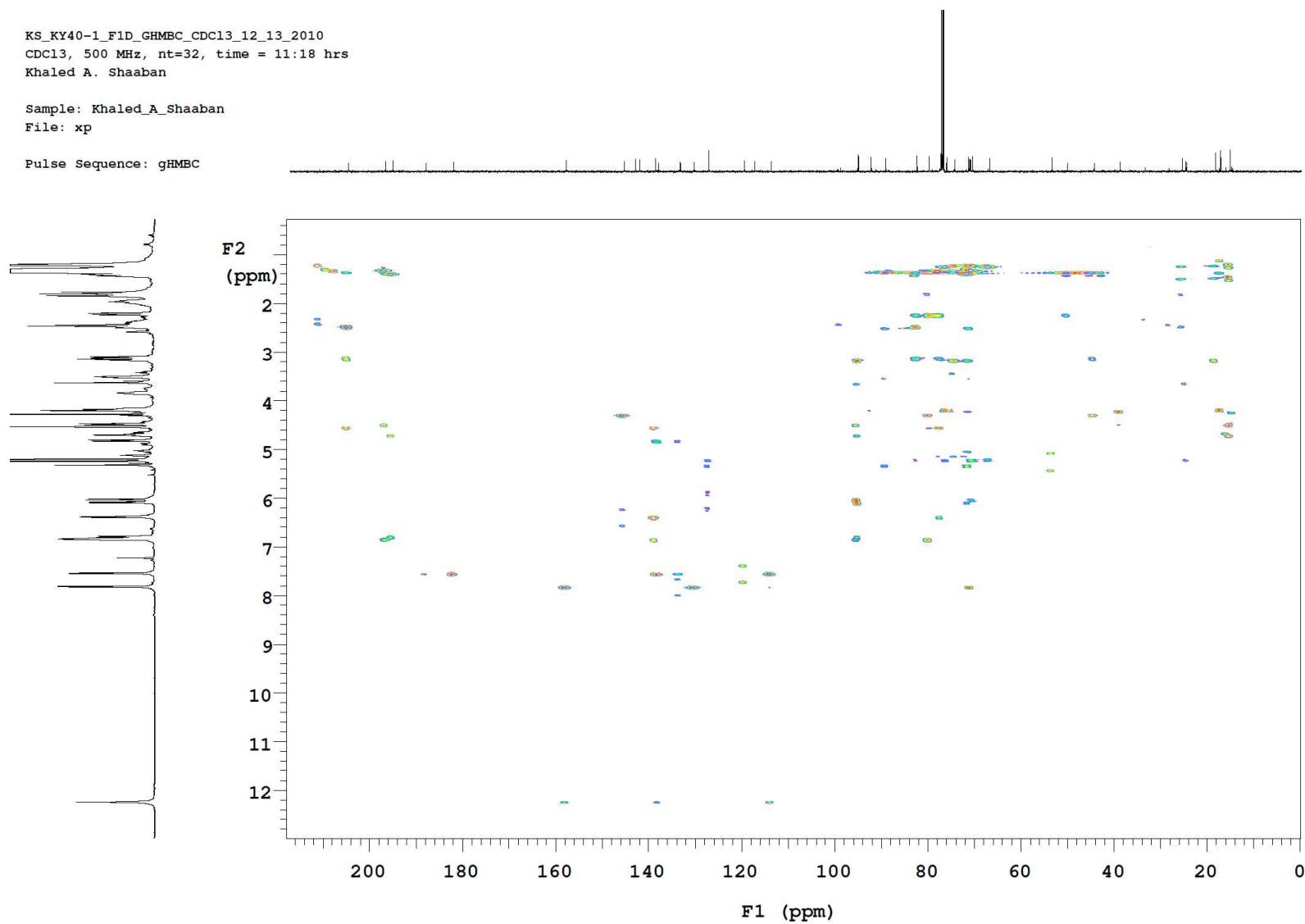


Figure S58: HMBC spectrum (CDCl₃, 500 MHz) of saquayamycin A (7)

KS_KY40-1_F1D_NOESY_CDC13_12_14_2010
CDC13, 500 MHz, nt=4, time = 2:07 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: NOESY

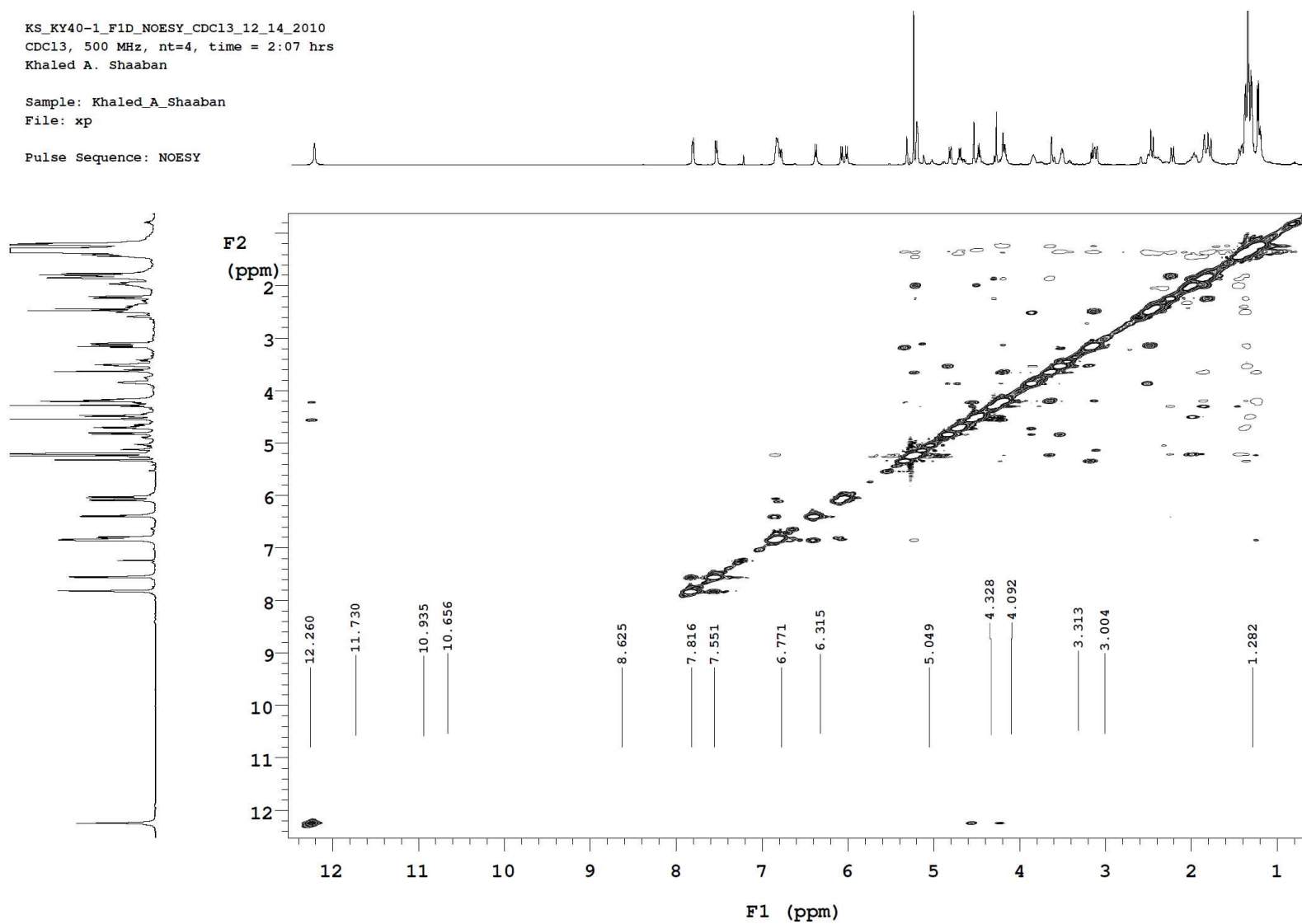


Figure S59: NOESY spectrum (CDCl₃, 500 MHz) of saquayamycin A (7)

KS_KY40-1_F1E_1HNMR_CDC13_12_01_2010
CDC13, 500 MHz, nt=32
Khaled A. Shaaban

Sample: khaled_A_Shaaban
File: xp

Pulse Sequence: s2pu1

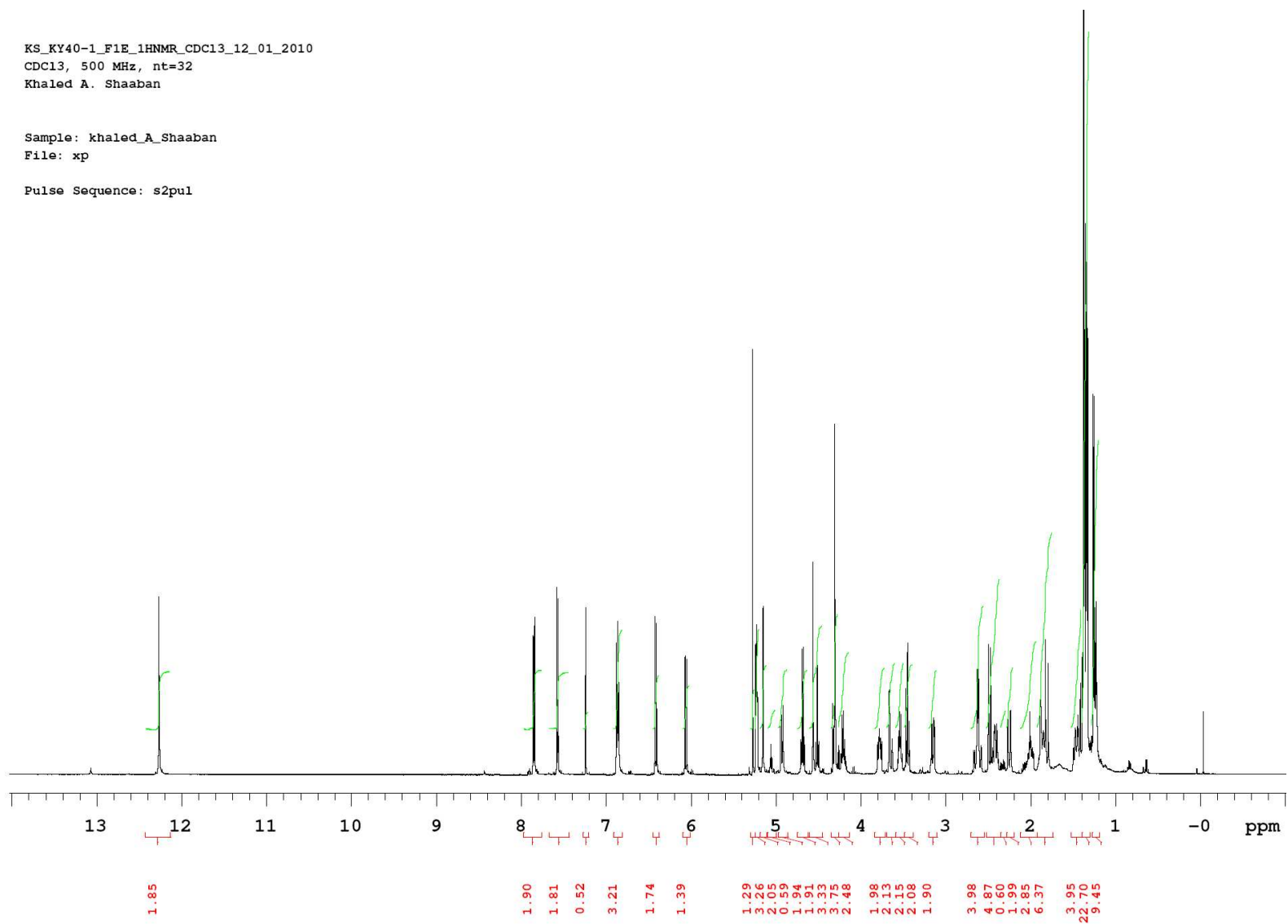


Figure S60: ¹H NMR spectrum (CDCl₃, 500 MHz) of saquayamycin B (8)

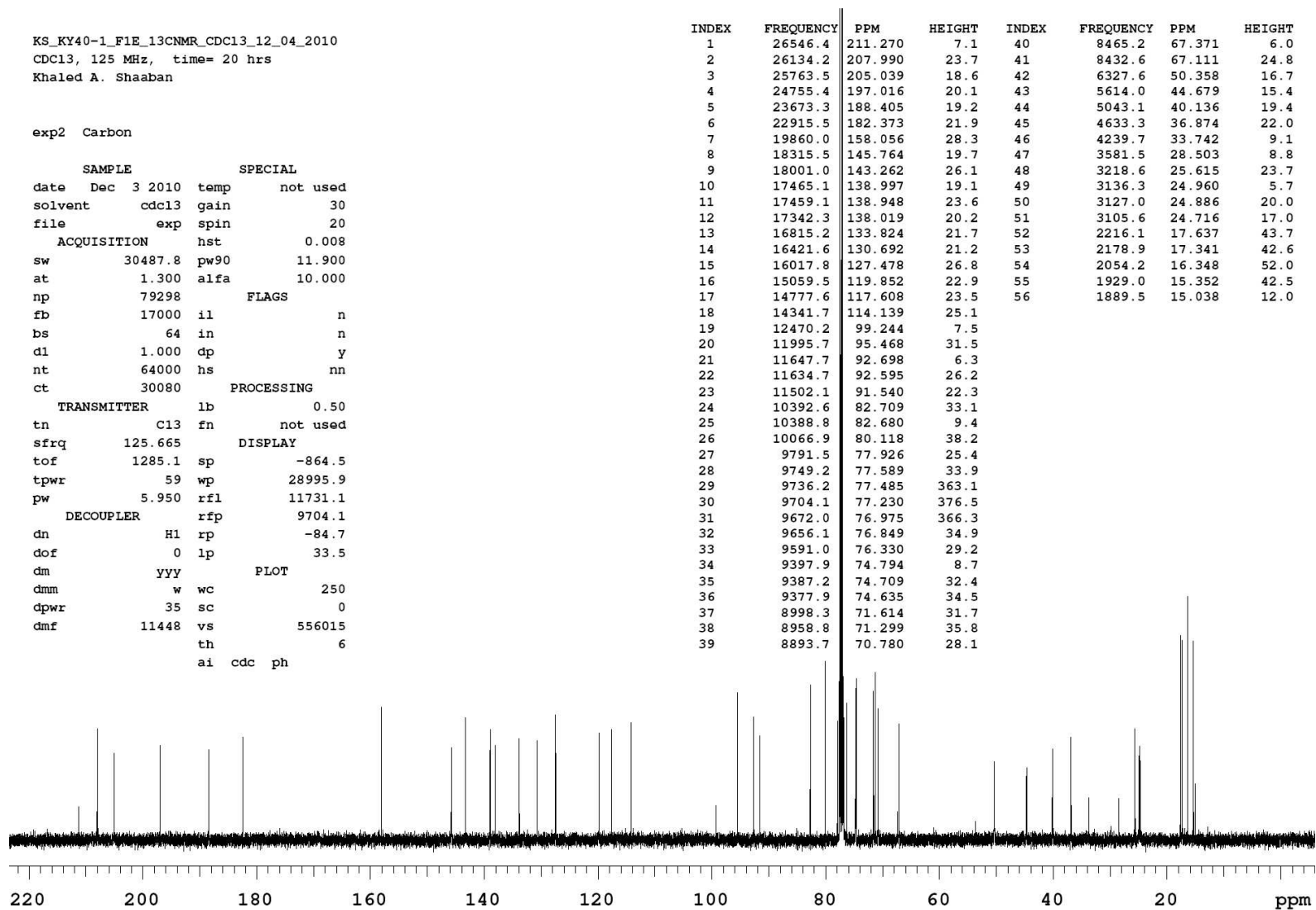


Figure S61: ^{13}C NMR spectrum (CDCl_3 , 125 MHz) of saquayamycin B (**8**)

KS_KY40-1_F1E_gCOSY_CDC13_12_01_2010
CDC13, 500 MHz, nt=8, time=2:36 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gCOSY

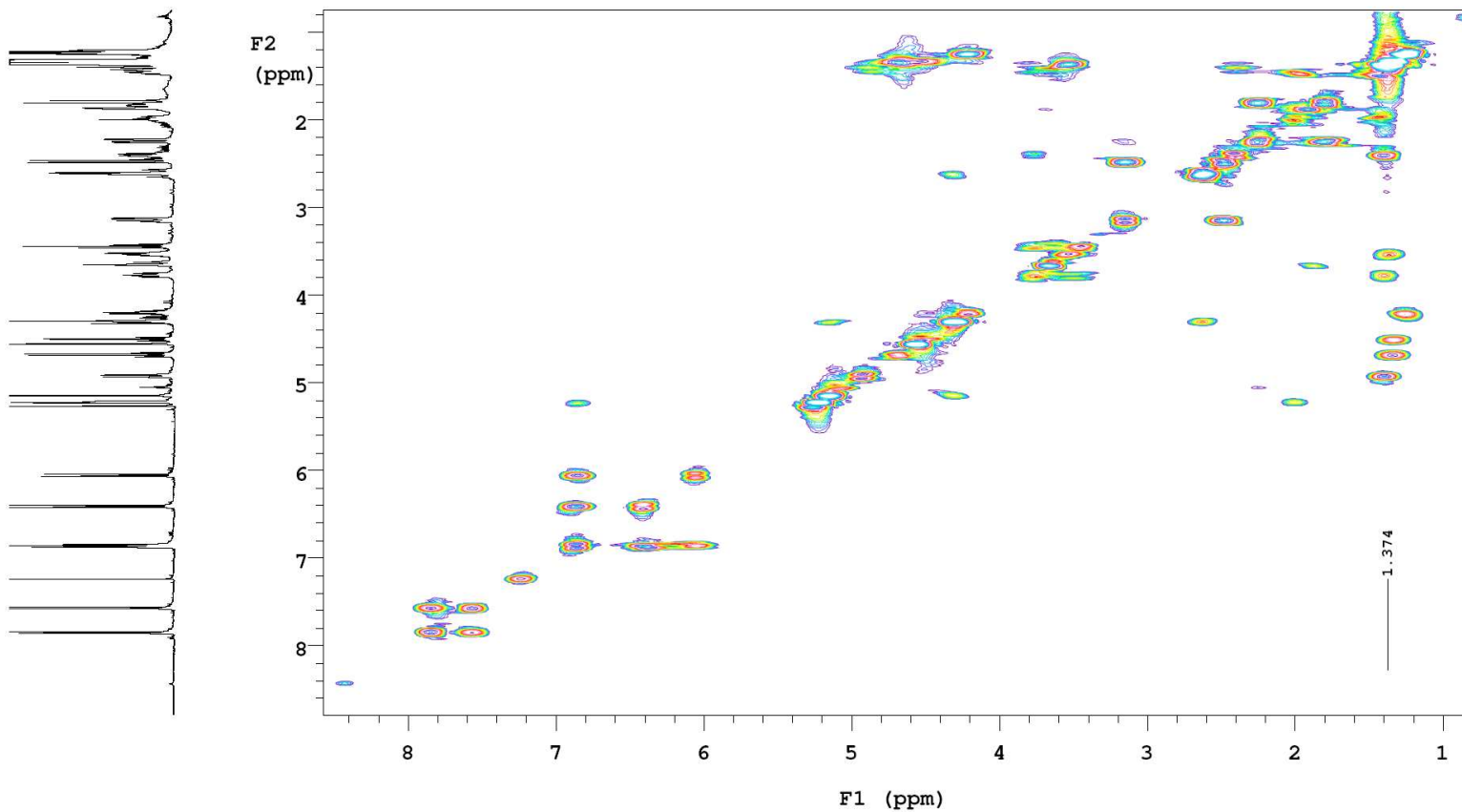
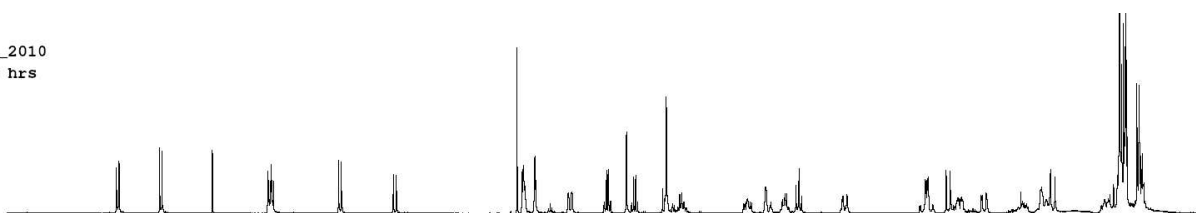


Figure S62: ^1H - ^1H COSY spectrum (CDCl_3 , 500 MHz) of saquayamycin B (**8**)

KS_KY40-1_F1E_GHSQC_CDC13_12_04_2010
CDC13, 500 MHz, nt=8, time=5:30 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHSQC

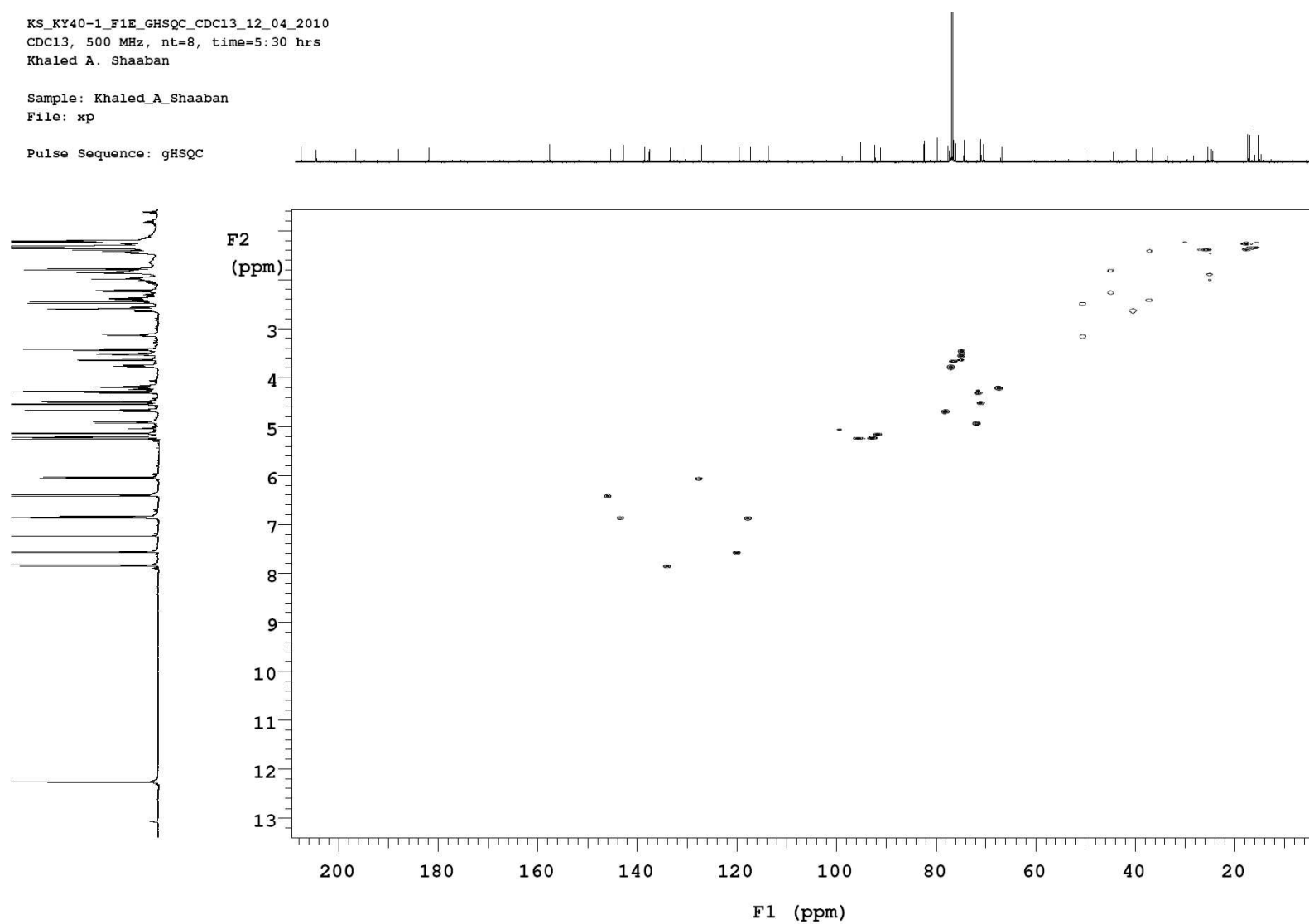


Figure S63: HSQC spectrum (CDCl₃, 500 MHz) of saquayamycin B (**8**)

KS_KY40-1_F1E_GHMB_CDC13_12_05_2010
CDC13, 500 MHz, nt=32, time=11:15 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: gHMBC

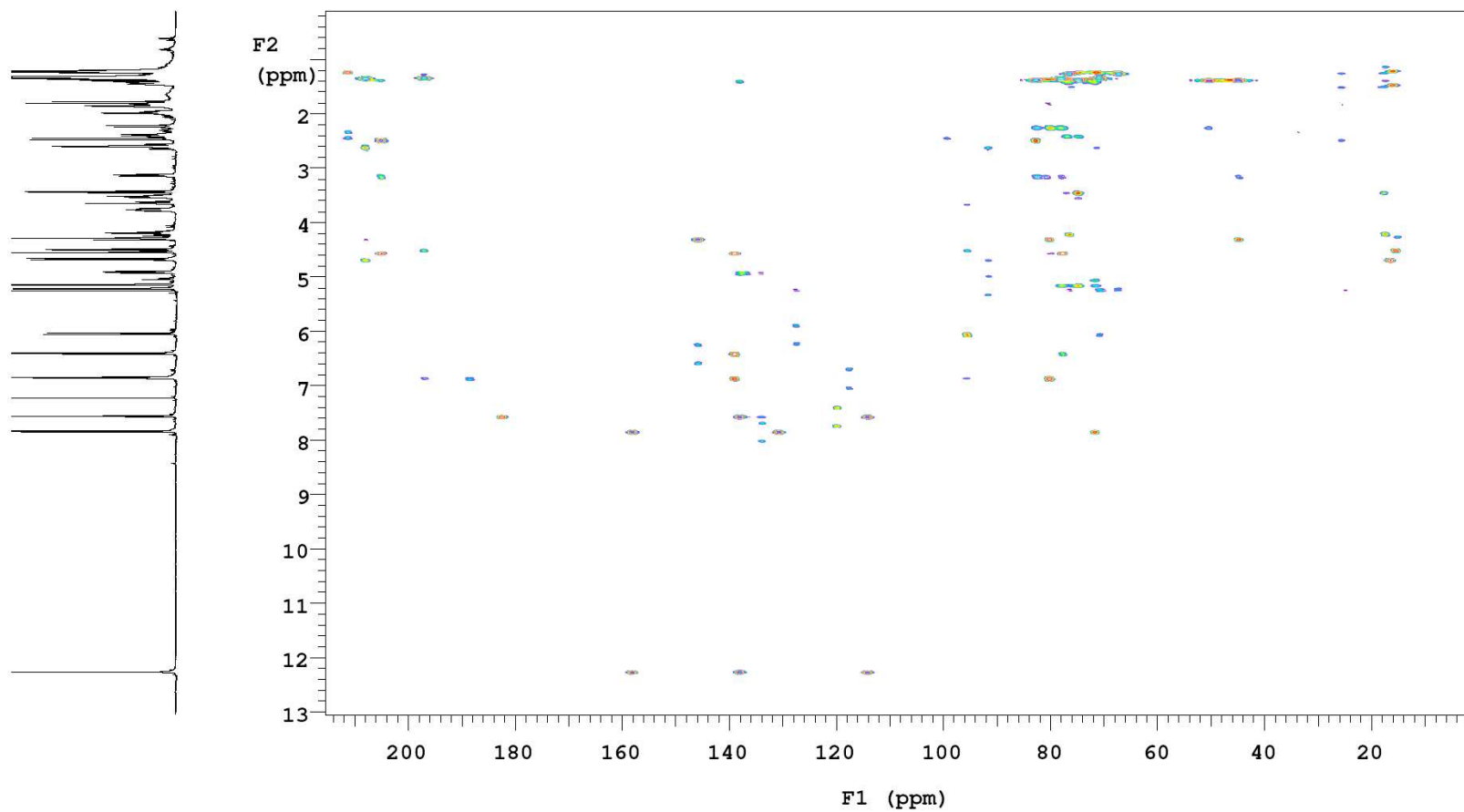
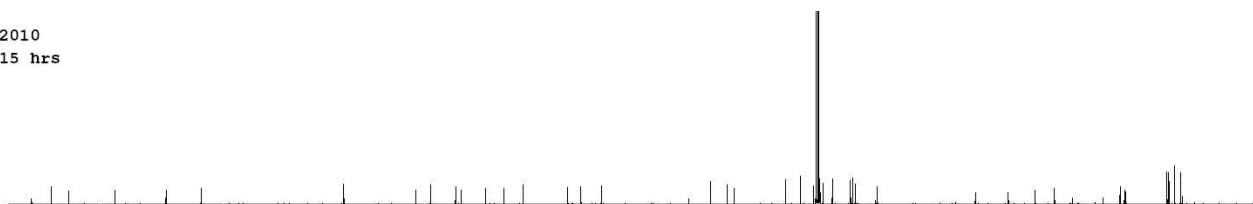


Figure S64: HMBC spectrum (CDCl_3 , 500 MHz) of saquayamycin B (**8**)

KS_KY40-1_F1E_NOESY_CDCl3_12_05_2010
CDCl3, 500 MHz, nt=4, time=4:30 hrs
Khaled A. Shaaban

Sample: Khaled_A_Shaaban
File: xp

Pulse Sequence: NOESY

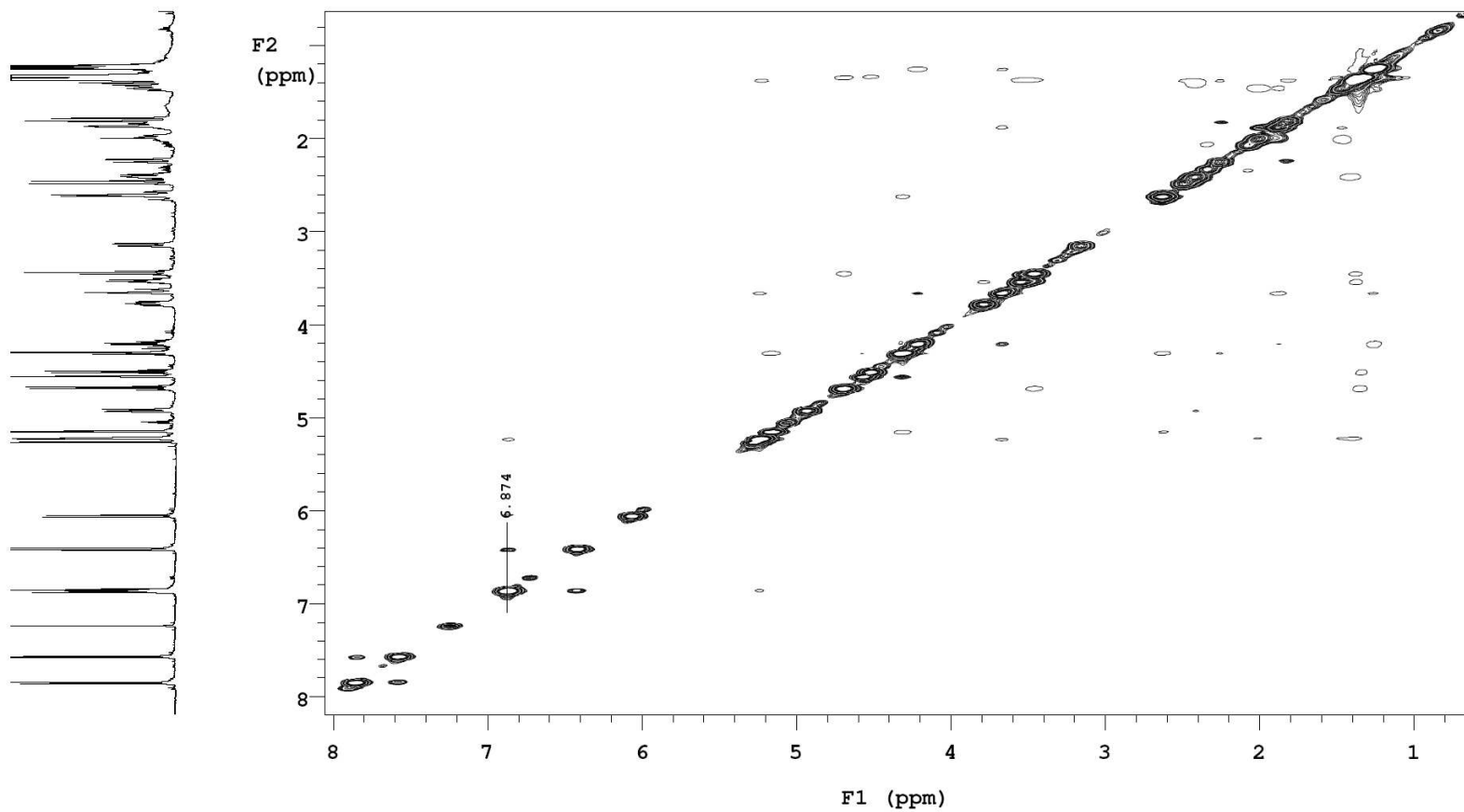
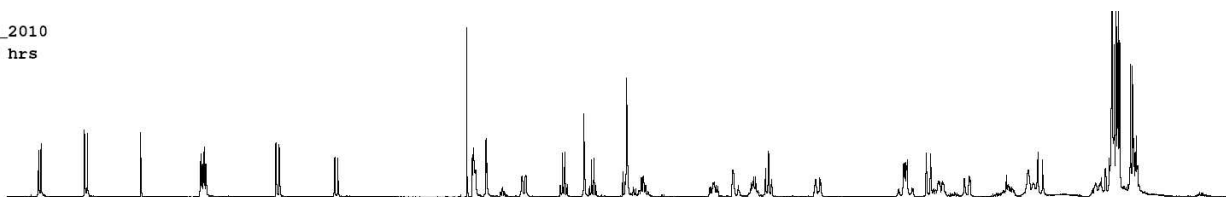


Figure S65: NOESY spectrum (CDCl₃, 500 MHz) of saquayamycin B (**8**)

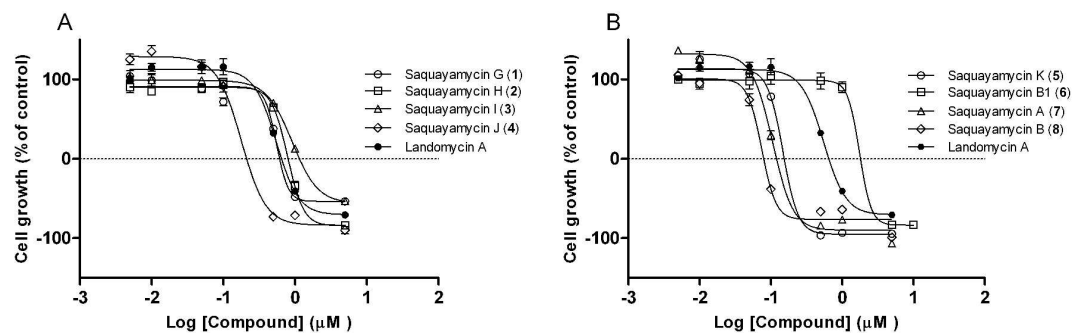


Figure S 66: Dose response curve of **A)** saquayamycins G-J (1-4), and **B)** saquayamycins K, B1, A and B (5-8); in comparison with landomycin A in a prostate cancer cell line (PC3) at 48 h.

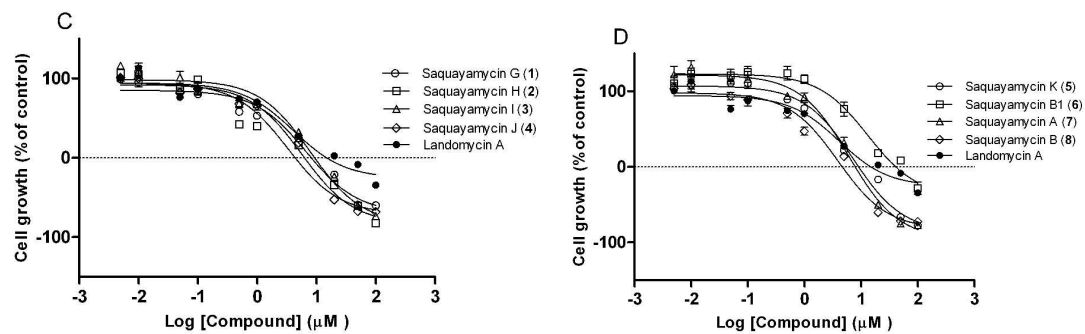


Figure S67: Dose response curve of **C)** saquayamycins G-J (1-4), and **D)** saquayamycins K, B1, A and B (5-8); in comparison with landomycin A in a non-small lung cancer cell line (H460) at 48 h.