

Supplementary Material

Six New Phenylpropanoid Derivatives from Chemically Converted Extract of *Alpinia galanga* (L.) and their anti-parasitic activities

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Figure S1 HPLC chromatogram for the isolation of 1, 7 and 8

20% aq. acetone

Peak 1 = Cpd 7 (t_R = 10.7 min)

Peak 2 = Cpd 8 (t_R = 36.5 min)

Peak 3 = Cpd 1 (t_R = 45.3 min)

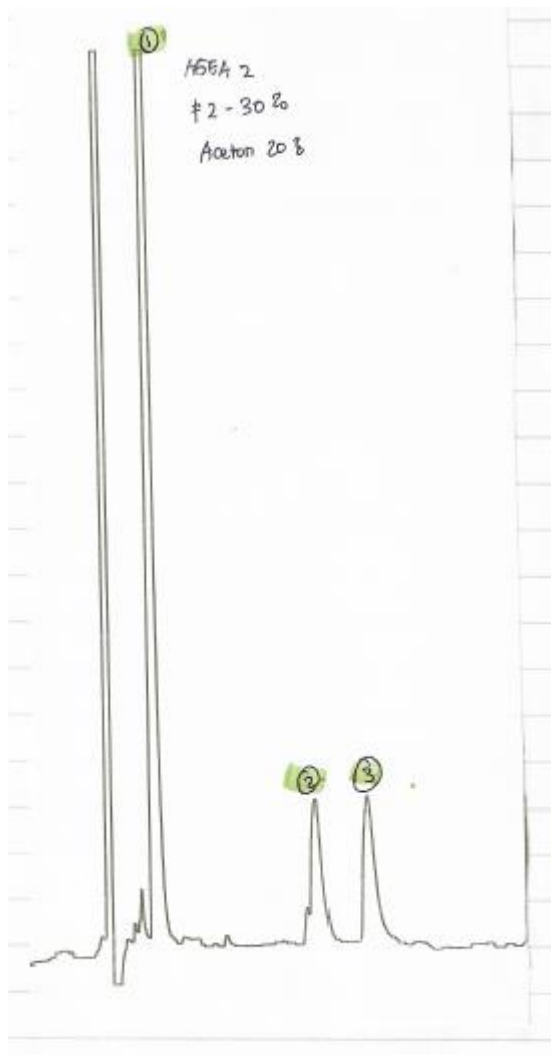


Figure S2 HPLC chromatogram for the isolation of 1, 2, 6, 9 and 10

30% aq. MeOH

Peak 1 = Cpd **1** (t_R = 18.7 min)

Peak 2 = Cpd **9** (t_R = 26.5 min)

Peak 3 = Cpd **2** (t_R = 30.2 min)

Peak 4 = Cpd **6** (t_R = 38.4 min)

Peak 5 = Cpd **10** (t_R = 46.3 min)

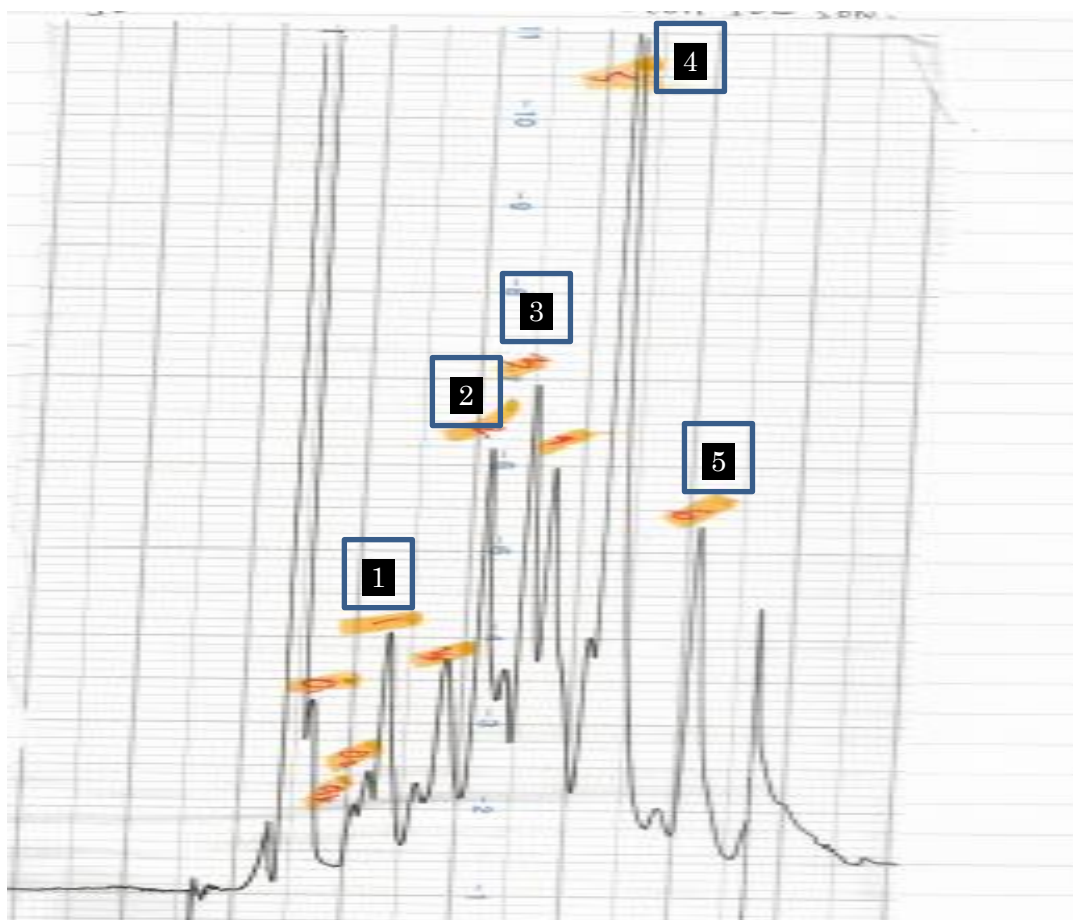


Figure S3 HPLC chromatogram for the isolation of 3, 4, 5 and 7

20% aq. acetone

Peak 1 = Cpd **3** (t_R = 9.5 min)

Peak 2 = Cpd **7** (t_R = 12.7 min)

Peak 3 = Cpd **4** (t_R = 16.3 min)

Peak 4 = Cpd **5** (t_R = 22.8 min)

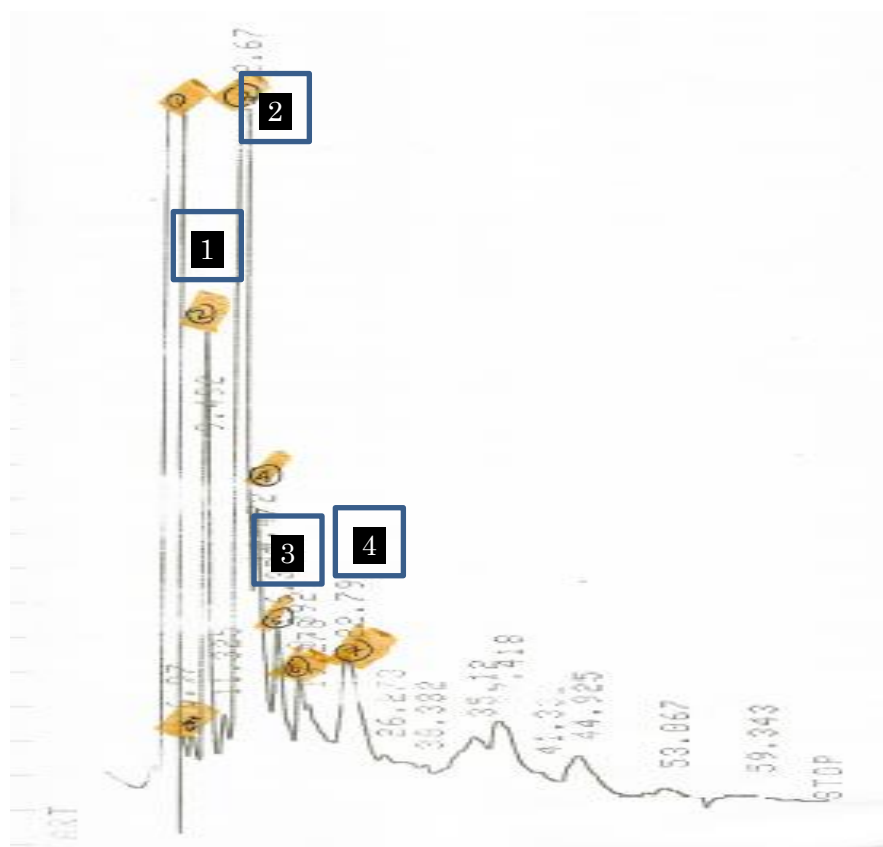
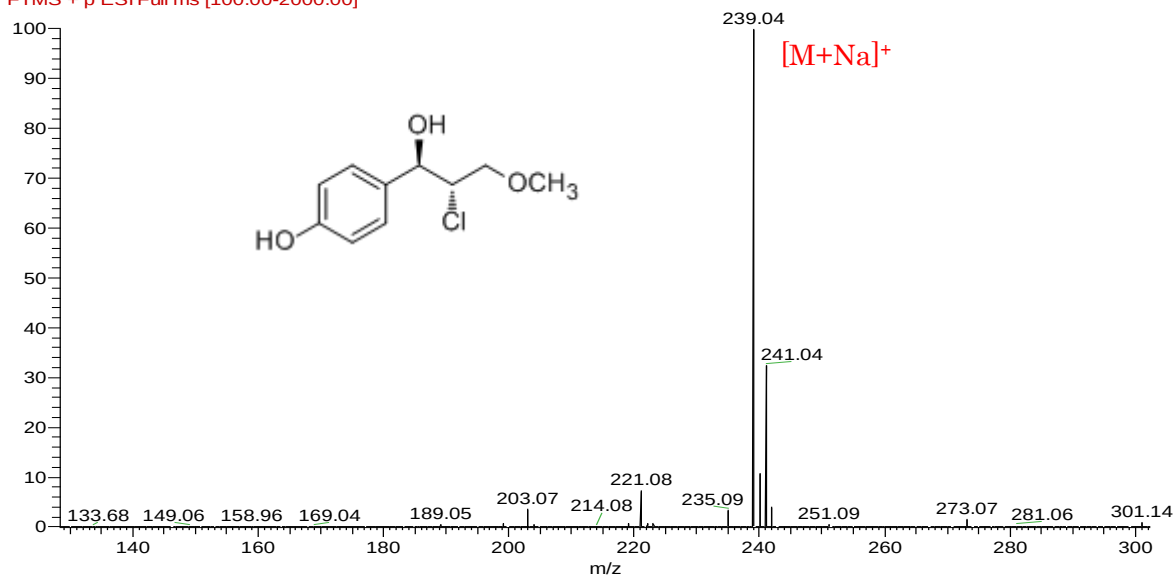


Figure S4 **HR-ESI-MS of 1**

180130_35 #7 RT: 0.07 AV: 1 NL: 3.16E7
F: FTMS + p ESI Full ms [100.00-2000.00]



Elemental composition search on mass 239.04

m/z = 234.04-244.04

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
239.0446	239.0445	0.36	3.5	C ₁₀ H ₁₃ O ₃ Cl Na

Figure S5 ^1H NMR spectrum of **1**

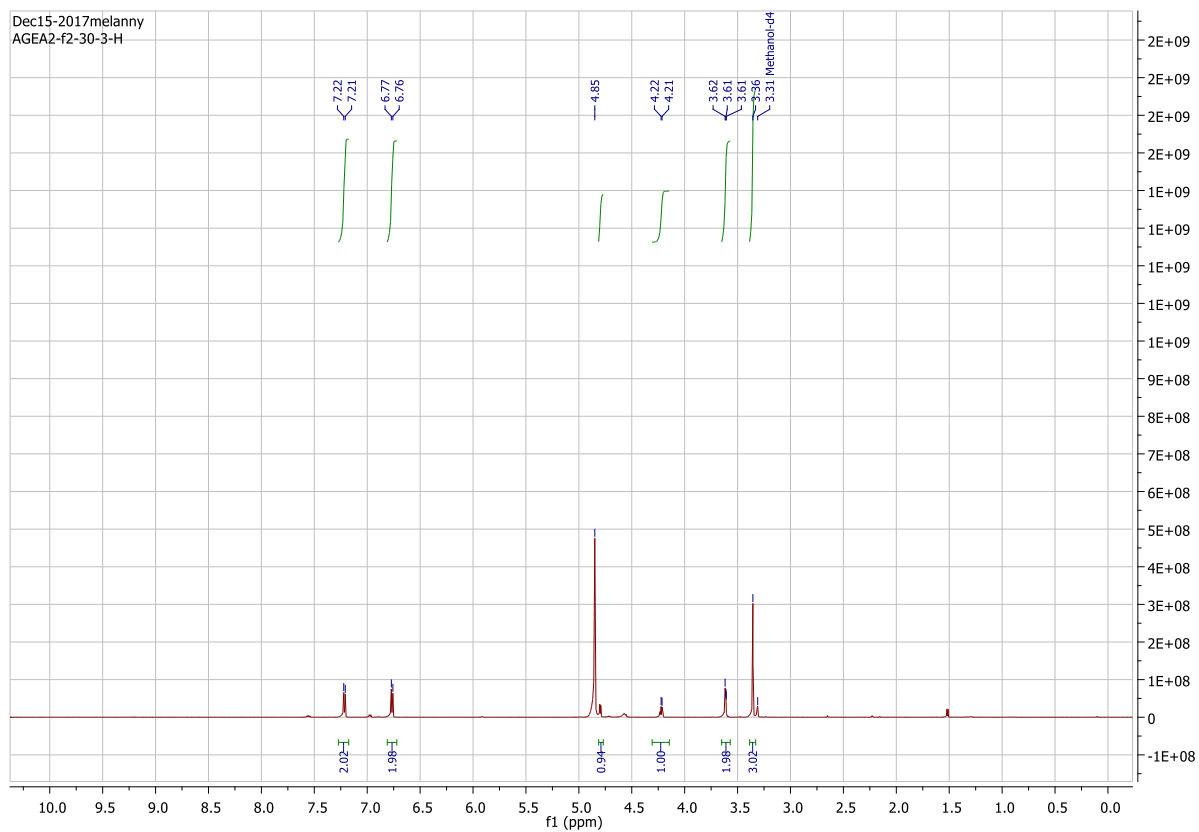


Figure S6 ^{13}C NMR spectrum of **1**

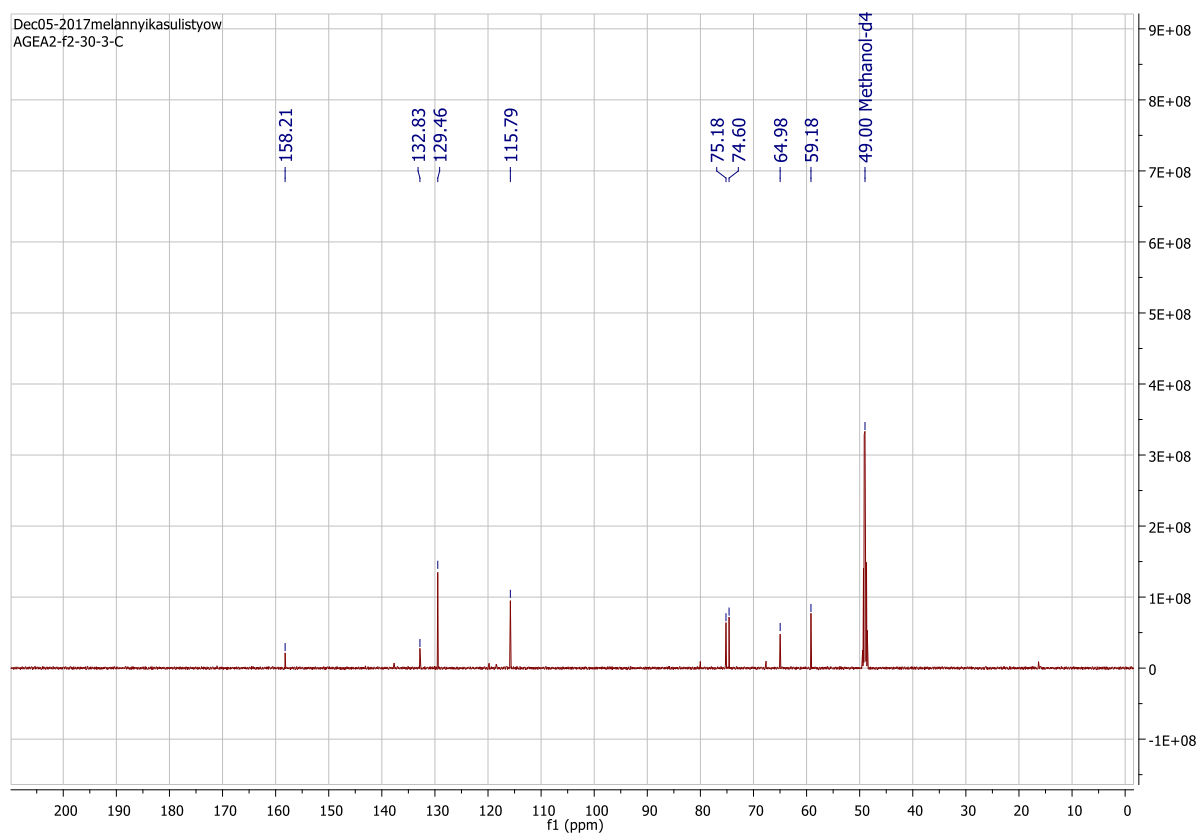


Figure S7 **DEPT 135 spectrum of 1**

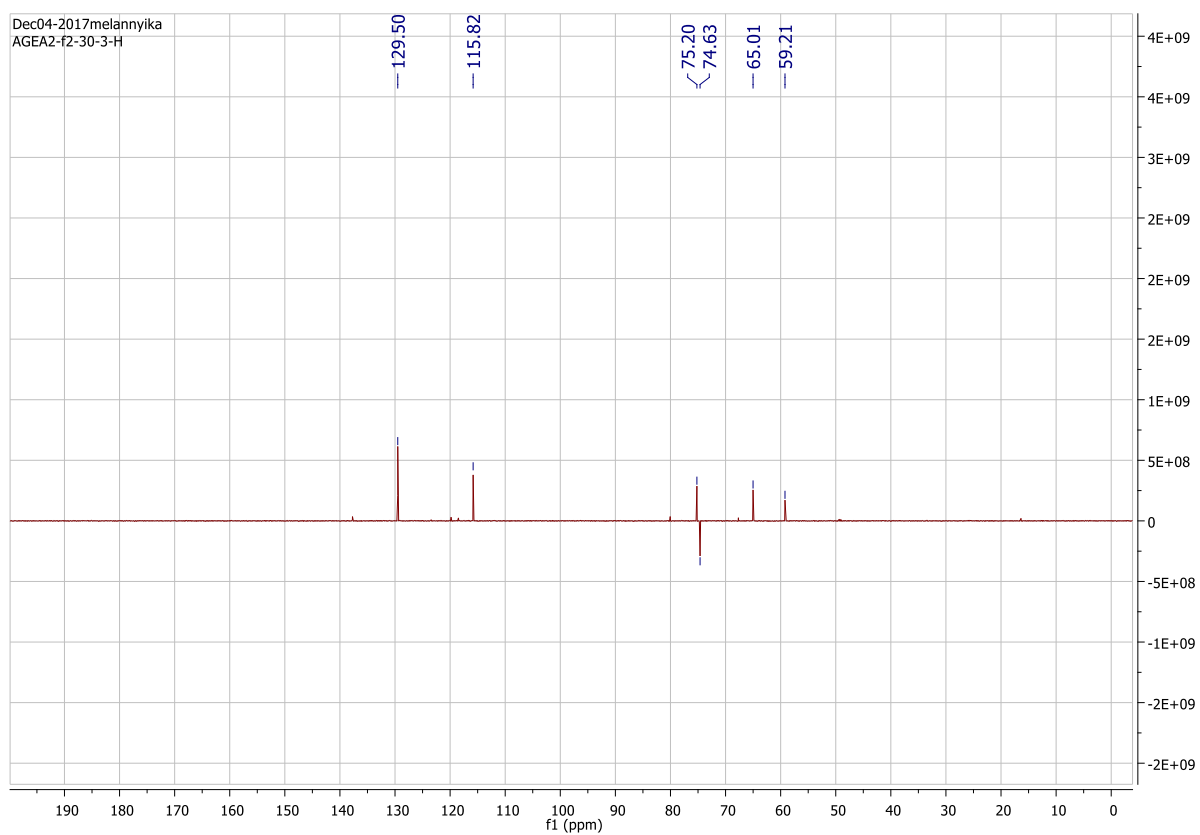


Figure S8 COSY spectrum of 1

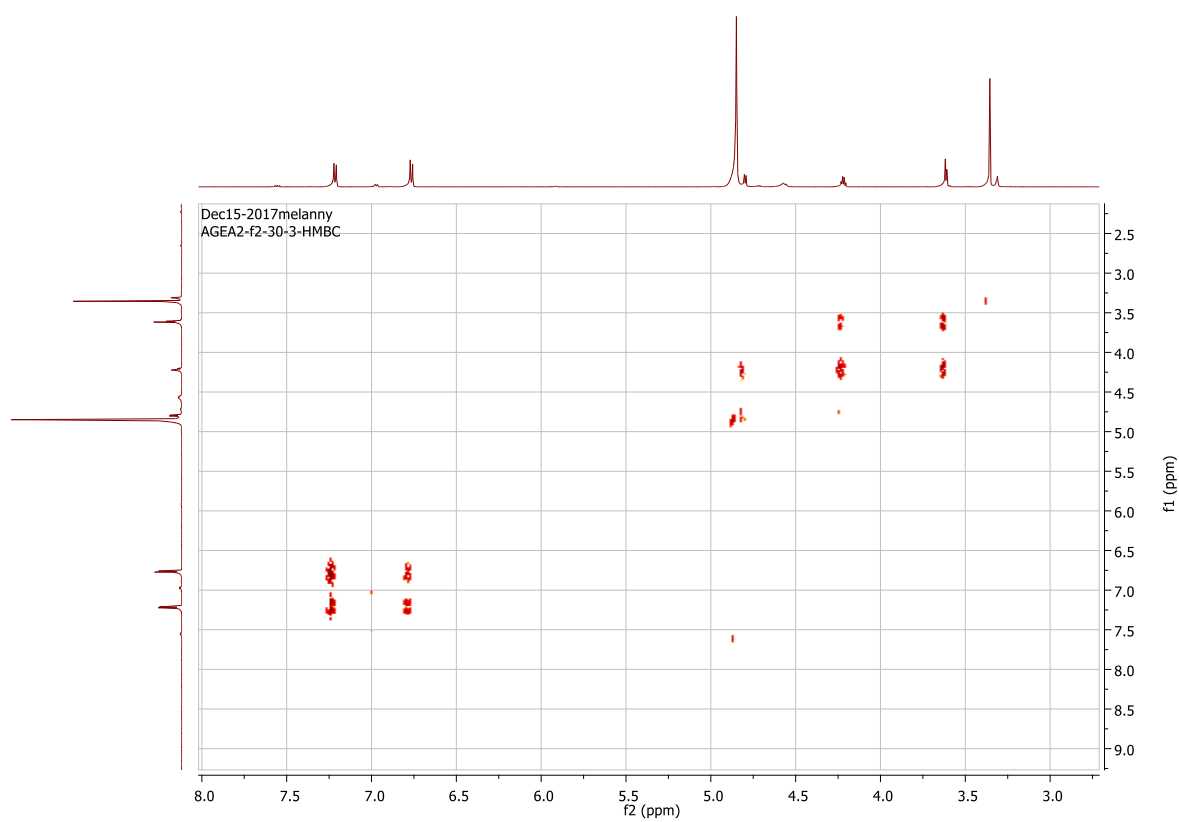


Figure S9 HSQC spectrum of 1

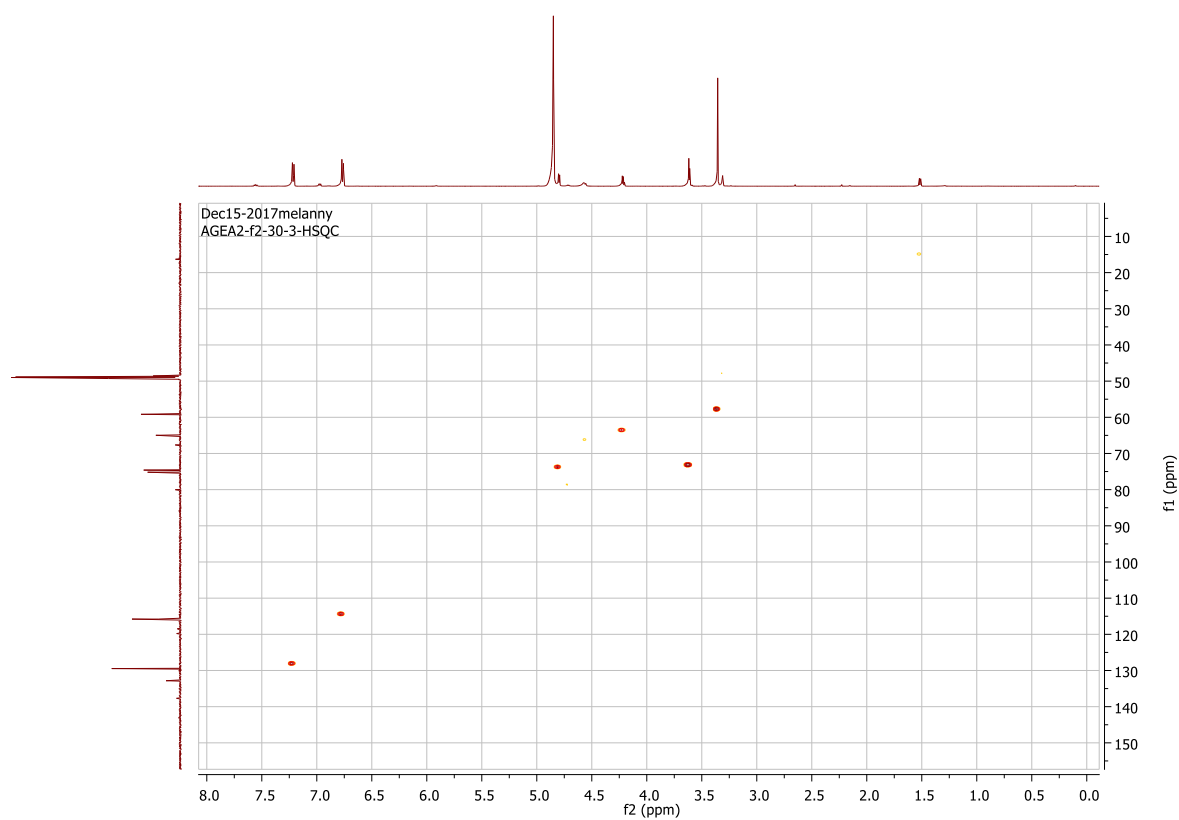


Figure S10 HMBC spectrum of 1

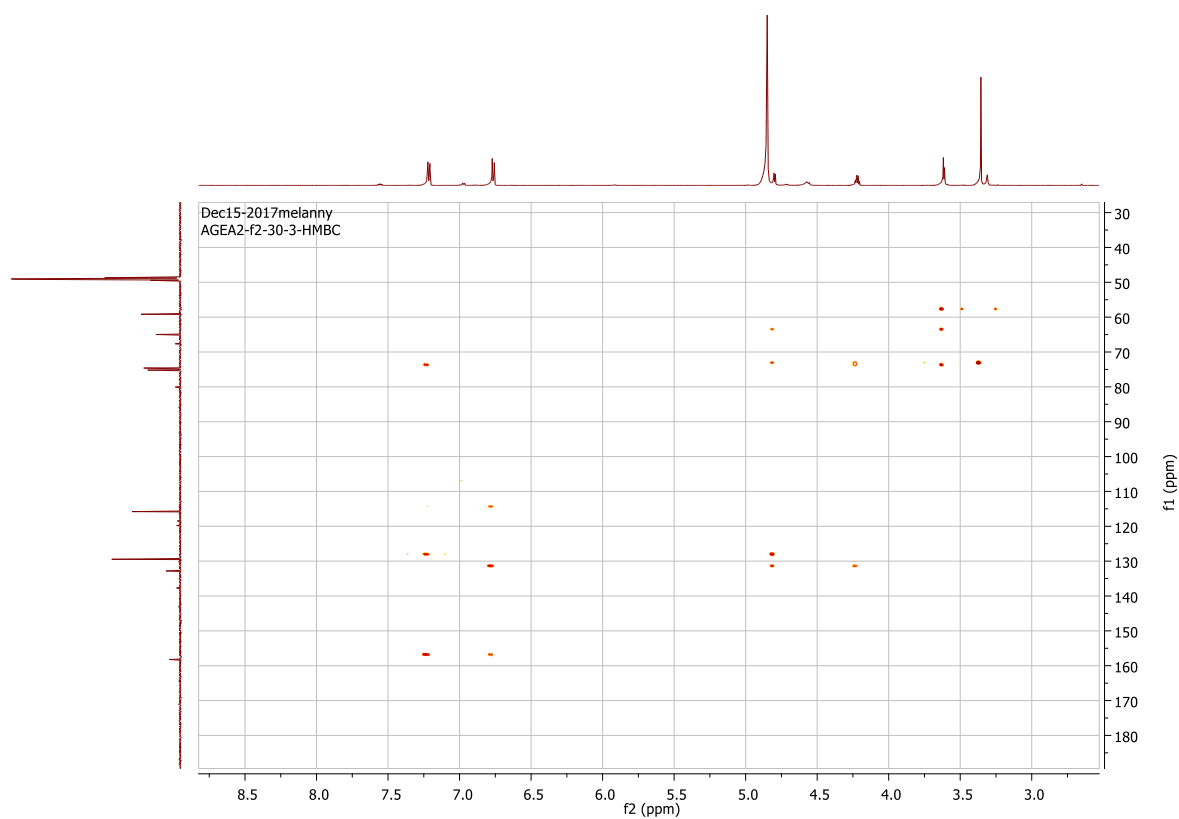
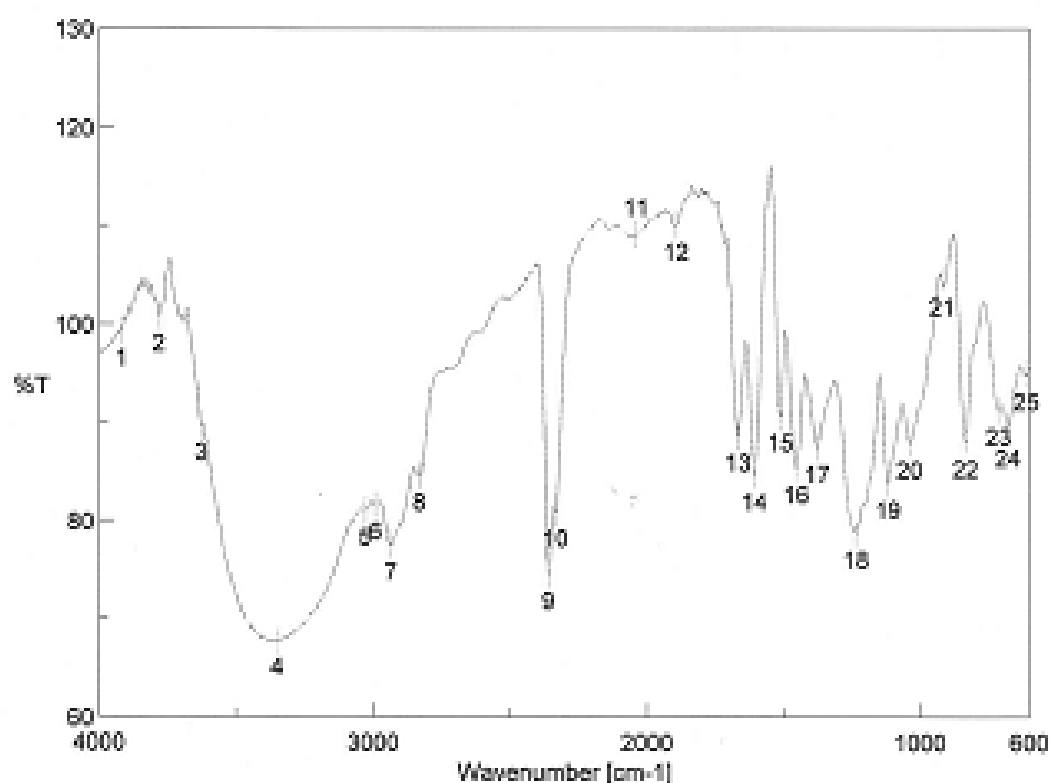


Figure S11 IR spectrum of 1



【コメント情報】

試料名
コメント
測定者
所属
会社

【データ情報】

作成日時 2018/08/20 13:05
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 599.753 cm-1
エンド 7800.65 cm-1
データ間隔 0.564233 cm-1
データ数 7469

【測定情報】

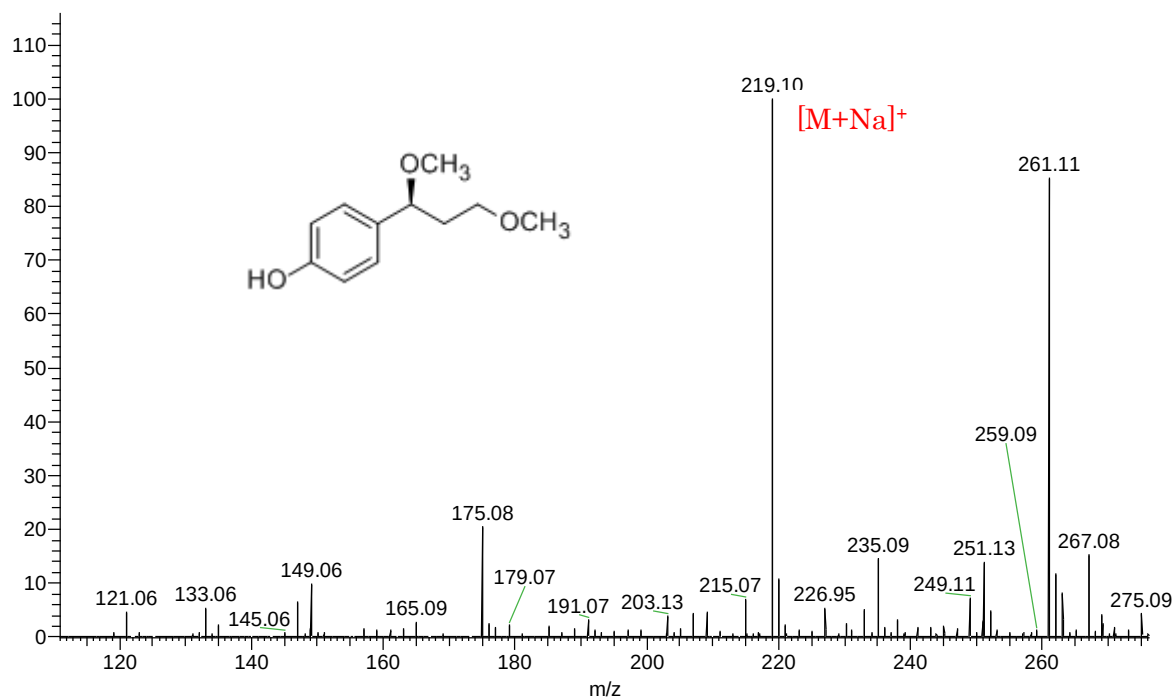
機種名 FT/IR-4600typeA
シリアル番号 D015461768
測定日時 2018/08/20 12:59
光源 標準光源
検出器 TGS
積算回数 10
分解 4 cm-1
ゼロフィリング On
アボダイゼーション Cosine
ゲイン Auto (2)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

【ピーク検出結果】

No.	位置	強度	No.	位置	強度
1	3518.64	99.2509	2	3761.72	100.787
3	3628.41	89.708	4	3350.71	67.8306
5	3030.59	81.0018	6	2992.02	81.6134
7	2835.13	77.4889	8	2831.95	84.5991
9	2360.44	74.5306	10	2335.37	80.9006
11	2040.32	109.045	12	1893.75	110.019
13	1668.12	88.6298	14	1607.38	84.8285

Figure S12 **HR-ESI-MS of 2**

180130 31 #7 RT: 0.07 AV: 1 NL: 2.62E6
F: FTMS + p ESI Full ms [100.00-2000.00]



Elemental composition search on mass 219.10

m/z = 214.10-224.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
219.0991	219.0992	-0.21	3.5	C ₁₁ H ₁₆ O ₃ Na

Figure S13 ^1H NMR spectrum of 2

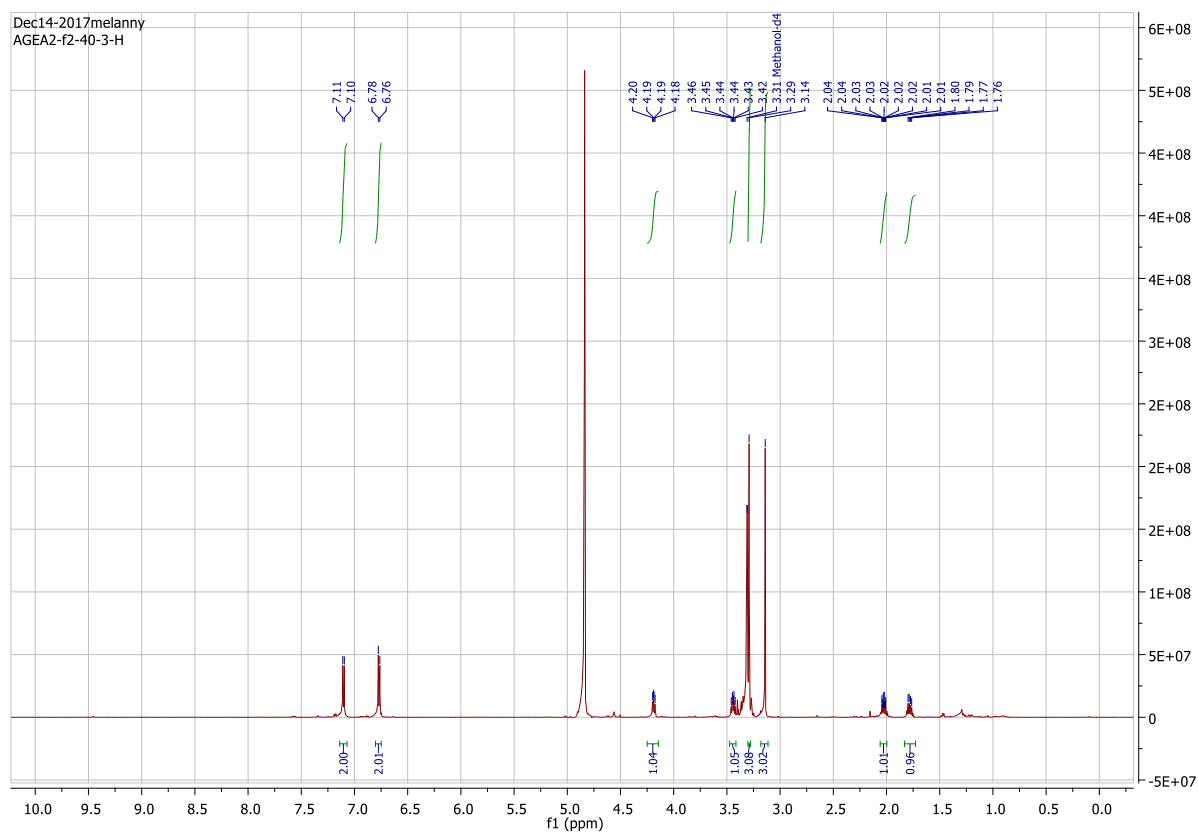


Figure S14 ^{13}C NMR spectrum of 2

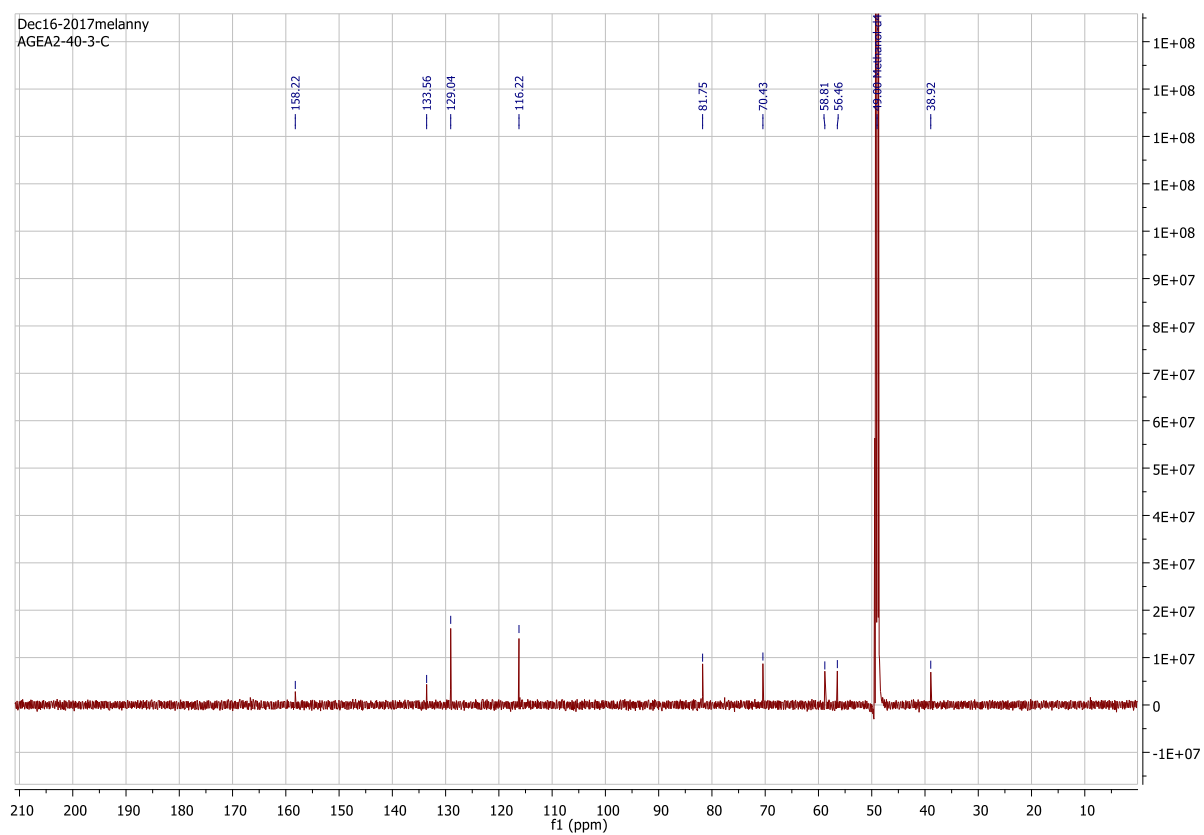


Figure S15 DEPT 135 spectrum of 2

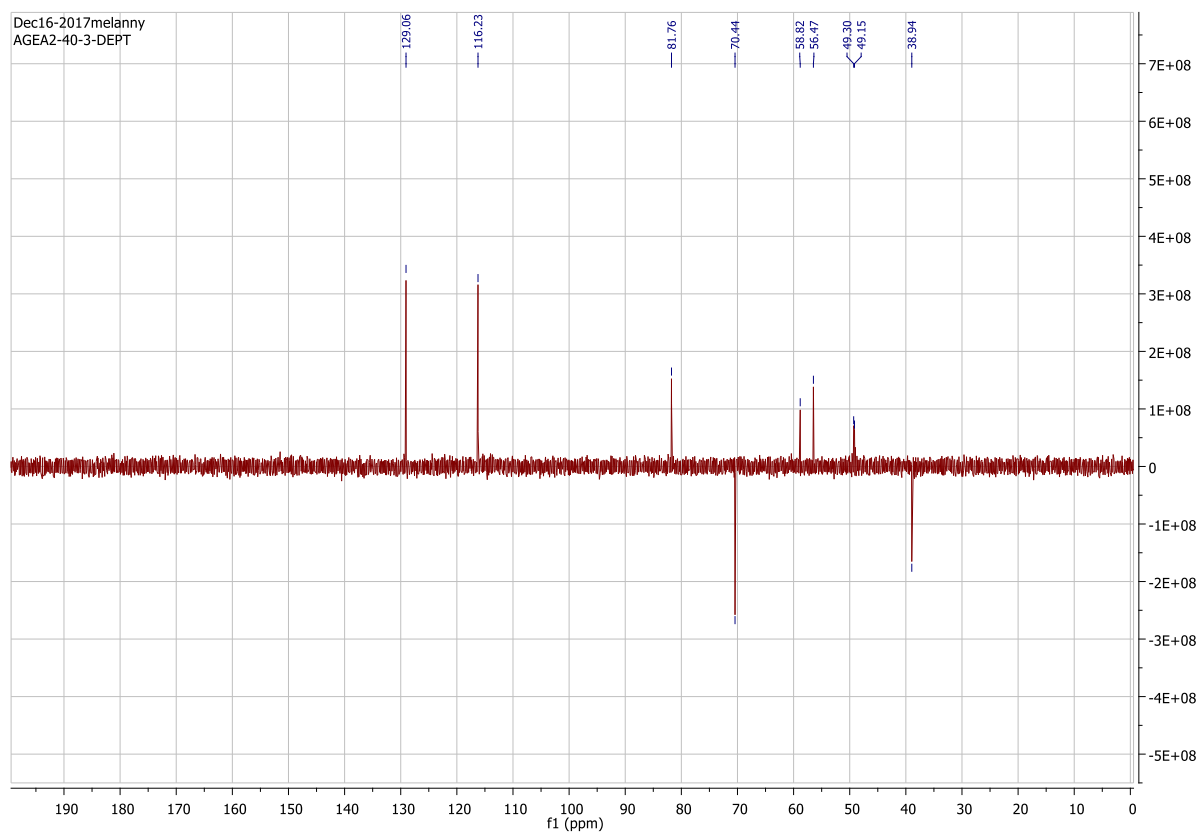


Figure S16 COSY spectrum of 2

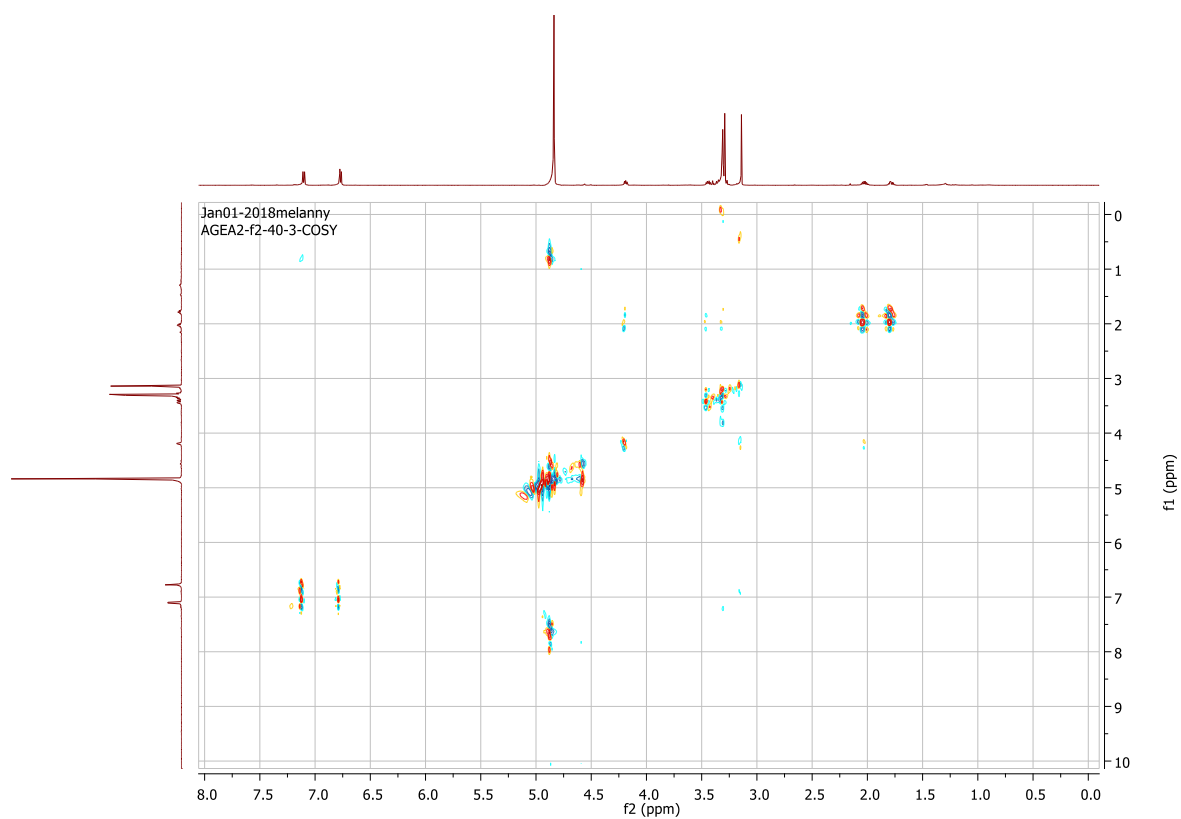


Figure S17 HSQC spectrum of 2

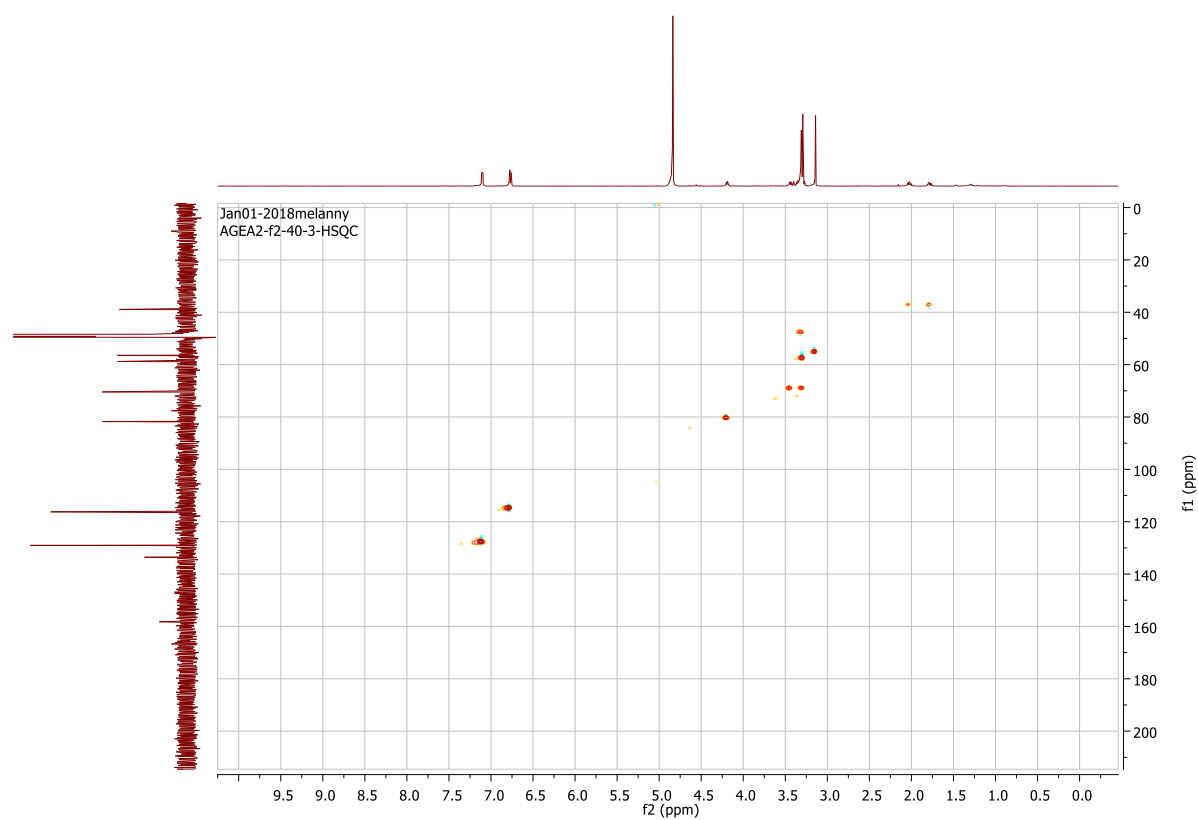


Figure S18 HMBC spectrum of 2

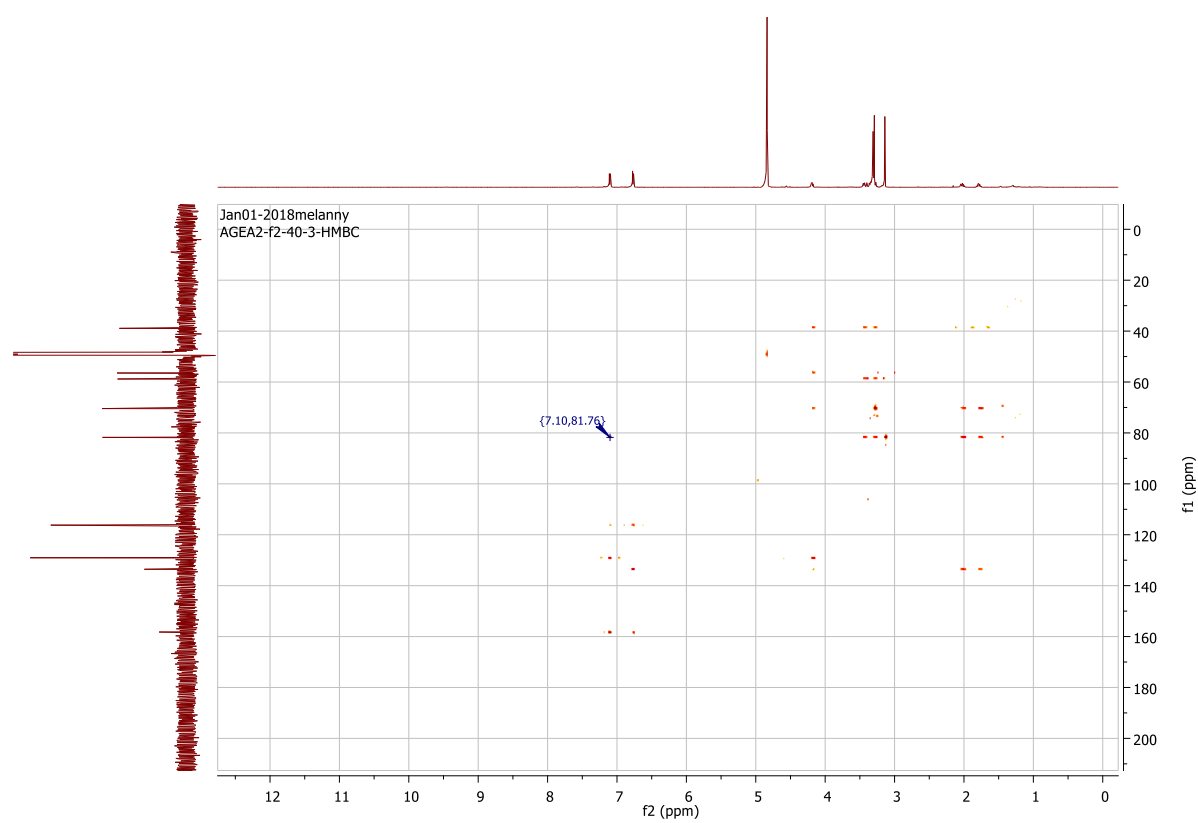
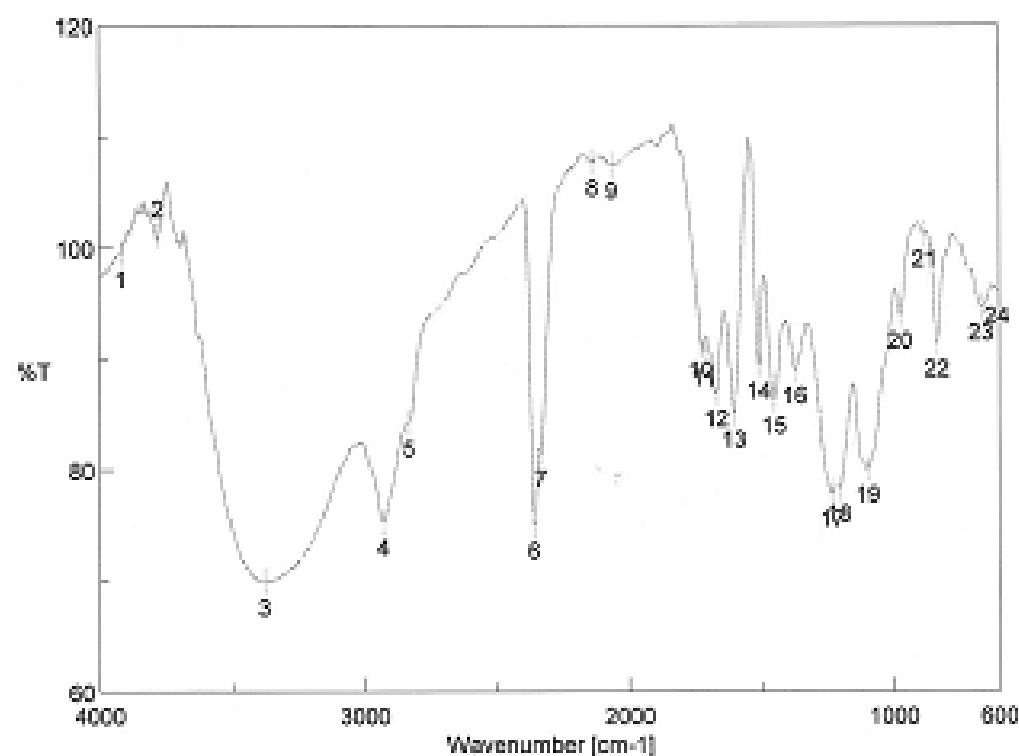


Figure S19 IR spectrum of 2



【コメント情報】

試料名
コメント
測定者
所属
会社

【データ情報】

作成日時 2018/08/20 13:20
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 599.753 cm-1
エンド 7800.65 cm-1
データ間隔 0.864233 cm-1
データ数 7469

【測定情報】

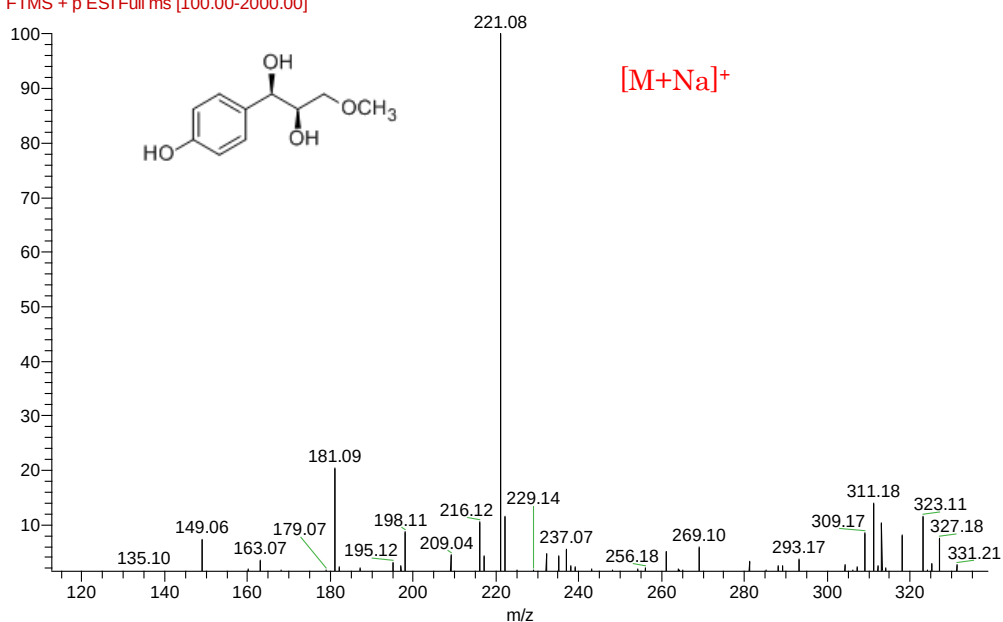
機種名 FT/IR-4600typeA
シリアル番号 0015481786
測定日時 2018/08/20 12:41
光源 標準光源
検出器 TGS
積算回数 10
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (2)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

【ピーク検出結果】

No.	位置	強度	No.	位置	強度
1	3518.64	99.4911	2	3777.87	101.081
3	3378.67	89.9189	4	2930.31	75.3527
5	2833.88	84.2422	6	2360.44	75.0184
7	2335.37	81.525	8	2138.87	107.858
9	2086.35	107.594	10	1729.83	91.3333
11	1718.26	90.6165	12	1671.02	86.9529
13	1604.48	85.0544	14	1509.99	89.4425

Figure S20 **HR-ESI-MS of 3**

181116_02_#7 RT: 0.06 AV: 1 NL: 2.31E7
F: FTMS + p ESI Full ms [100.00-2000.00]



Elemental composition search on mass 221.08

m/z = 216.08-226.08

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
221.0781	221.0784	-1.58	3.5	C ₁₀ H ₁₄ O ₄ Na

Figure S21 ^1H NMR spectrum of 3

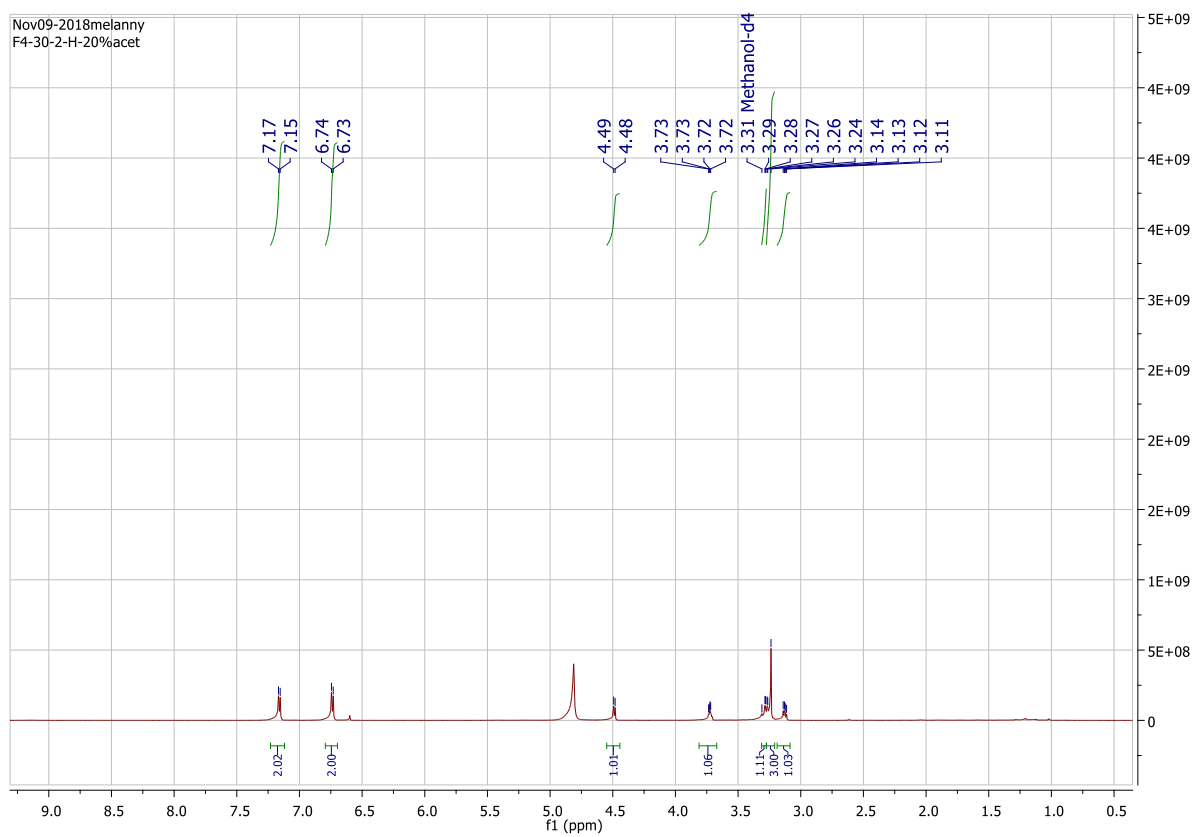


Figure S22 ^{13}C NMR spectrum of 3

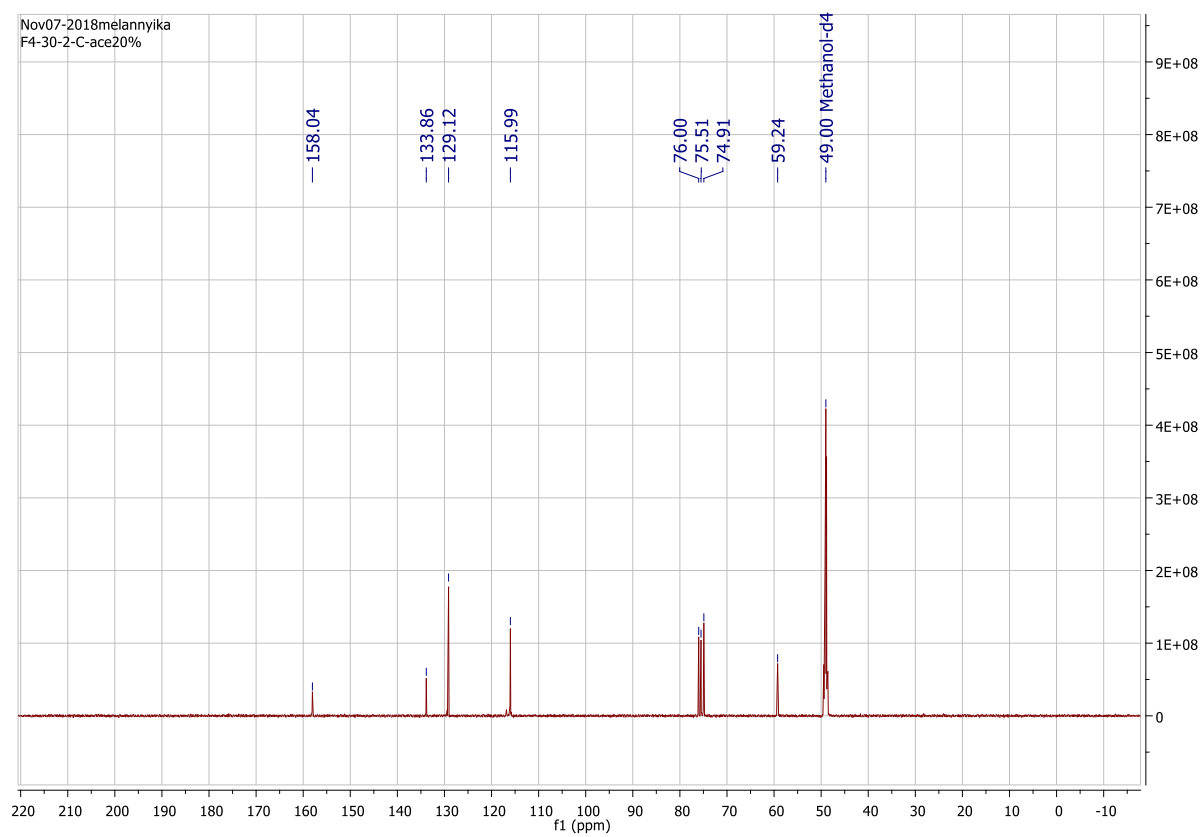


Figure S23 DEPT 135 spectrum of 3

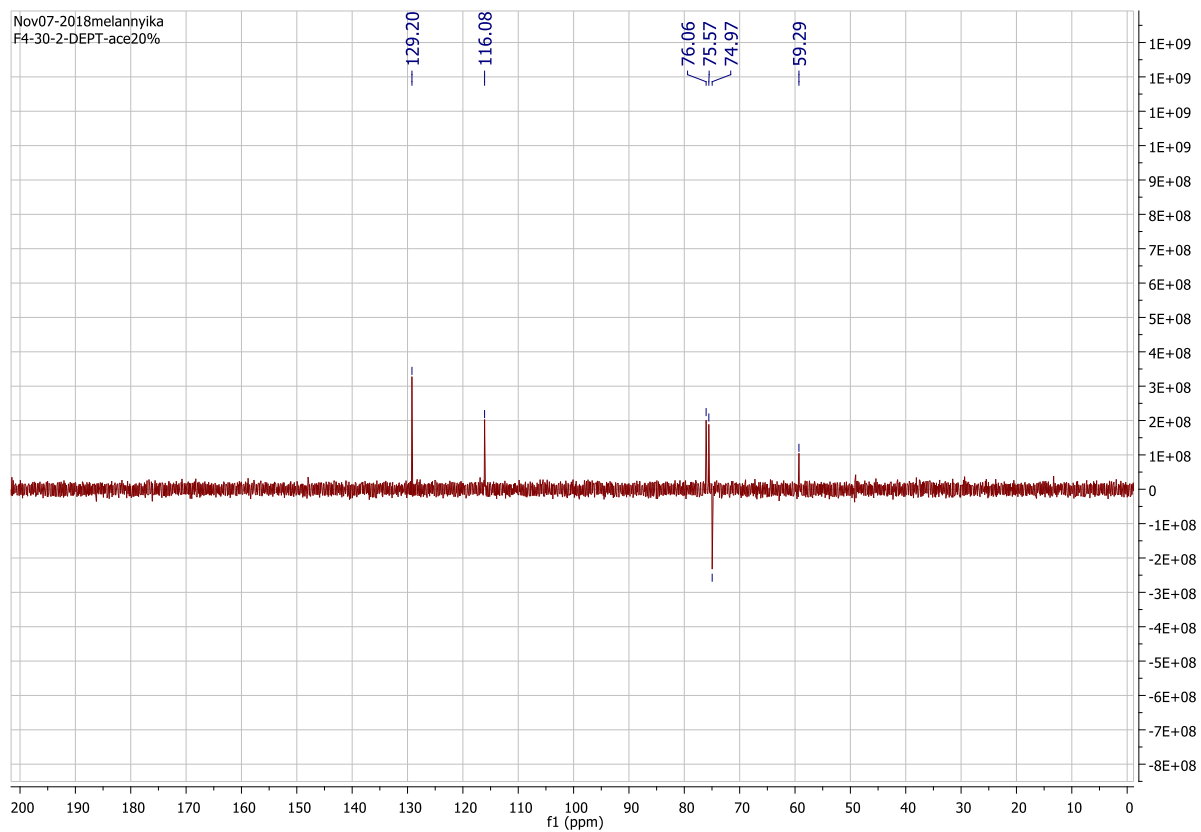


Figure S24 COSY spectrum of 3

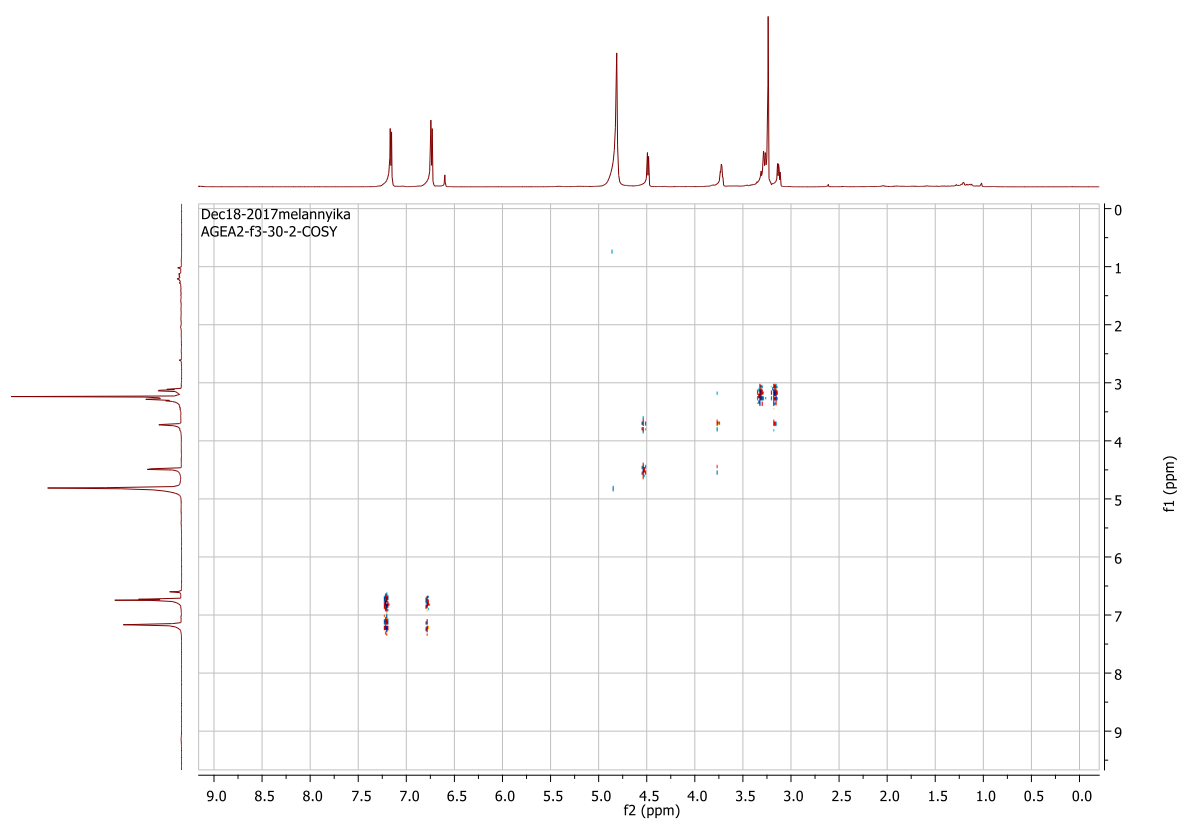


Figure S25 HSQC spectrum of 3

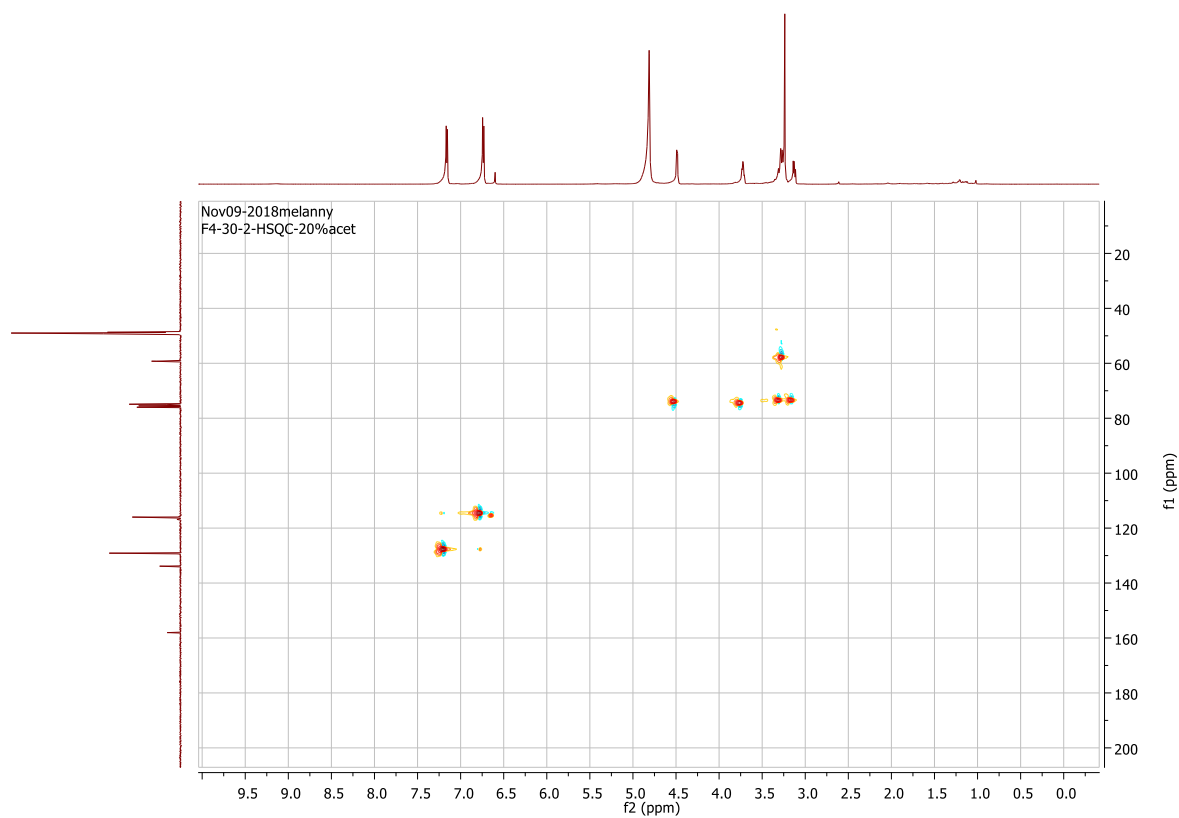


Figure S26 HMBC spectrum of 3

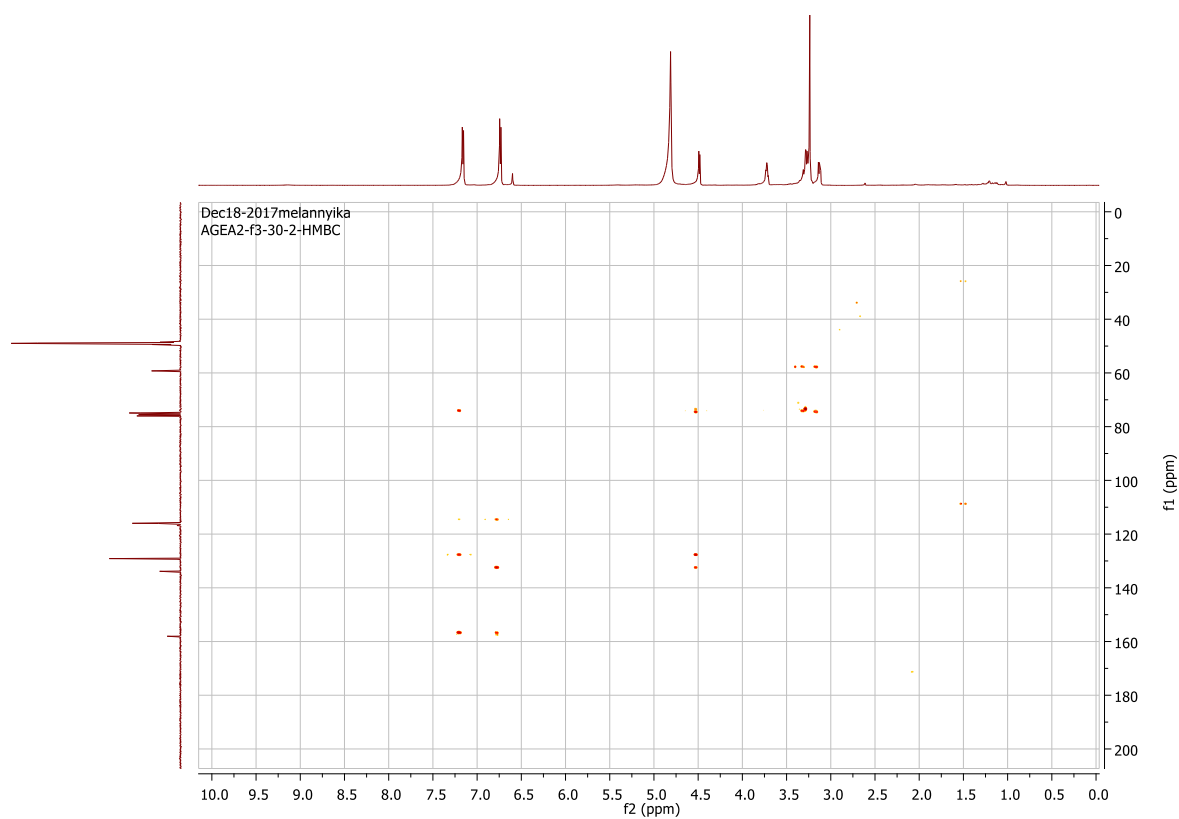
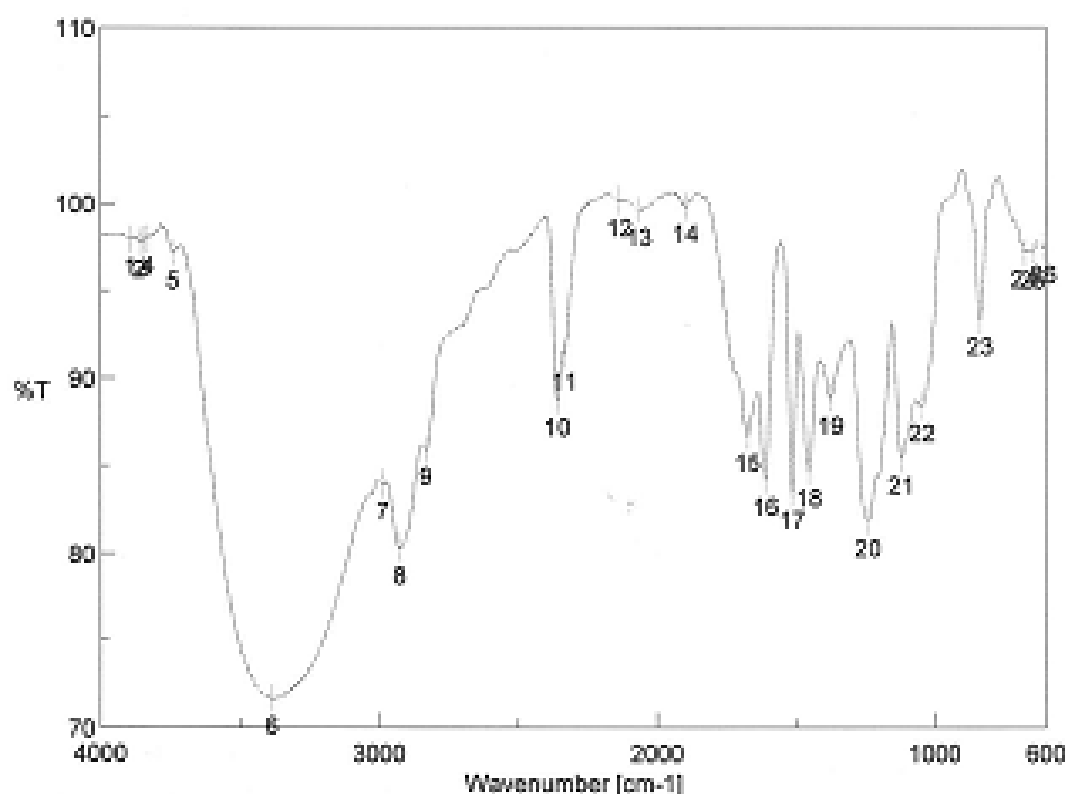


Figure S27 IR spectrum of 3



【コメント情報】

試料名
コメント
測定者
所属
会社

HU

【データ情報】

作成日時 2018/08/20 13:16
データタイプ 時間隔データ
横軸 Wavenumber [cm⁻¹]
縦軸 %T
スタート 558.753 cm⁻¹
エンド 7800.65 cm⁻¹
データ間隔 0.964233 cm⁻¹
データ数 7469

【測定情報】

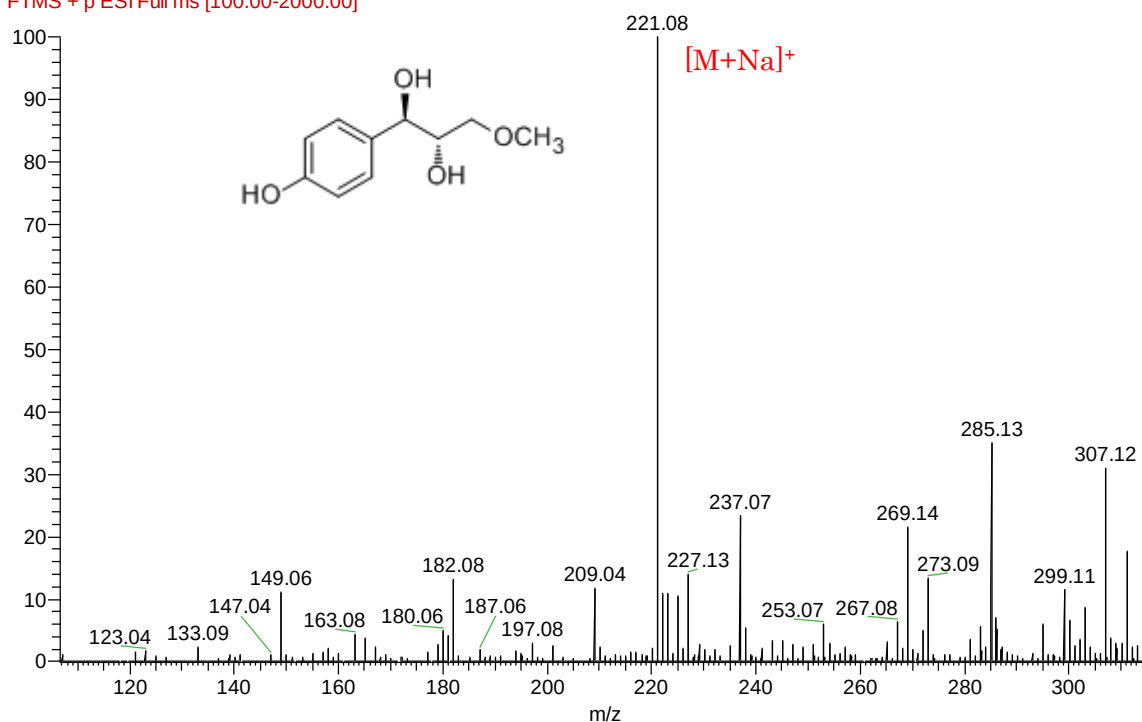
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シリアル番号 D015461706
測定日時 2018/08/20 11:37
光源 標準光源
検出器 TGS
積算回数 10
分解 4 cm⁻¹
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (2)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

【ピーク検出結果】

No.	位置	強度	No.	位置	強度
1	3892.61	97.8906	2	3861.76	97.76
3	3844.4	97.8238	4	3828.64	97.9445
5	3740.28	97.1194	6	3383.5	71.6524
7	2887.2	83.9784	8	2828.45	80.2416
9	2830.99	83.9292	10	2360.44	88.7435
11	2334.41	91.3363	12	2134.81	100.125
13	2064.42	89.5811	14	1897.61	89.5014

Figure S28 **HR-ESI-MS of 4**

180222_36 #7 RT: 0.07 AV: 1 NL: 2.61E6
F: FTMS + p ESI Full ms [100.00-2000.00]



Elemental composition search on mass 221.08

m/z = 216.08-226.08

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
221.0781	221.0784	-1.58	3.5	C ₁₀ H ₁₄ O ₄ Na

Figure S29 ^1H NMR spectrum of 4

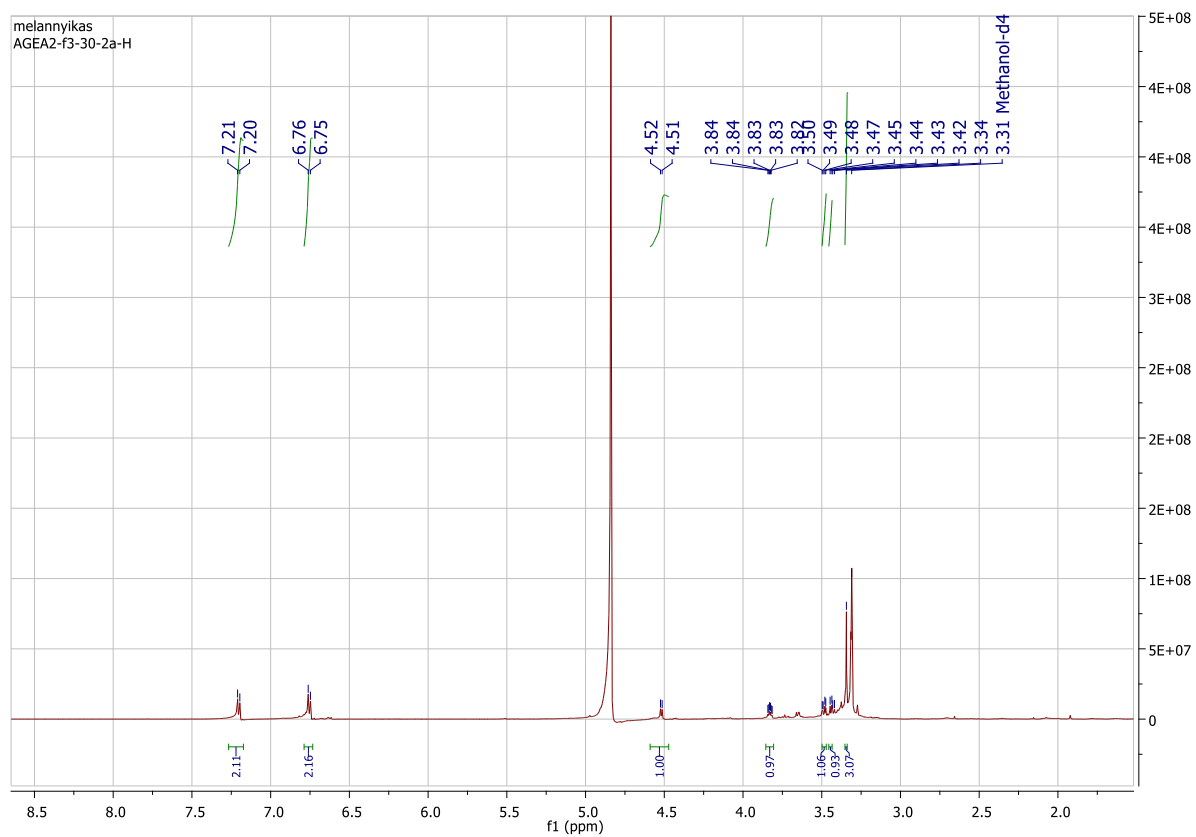


Figure S30 ^{13}C NMR spectrum of 4

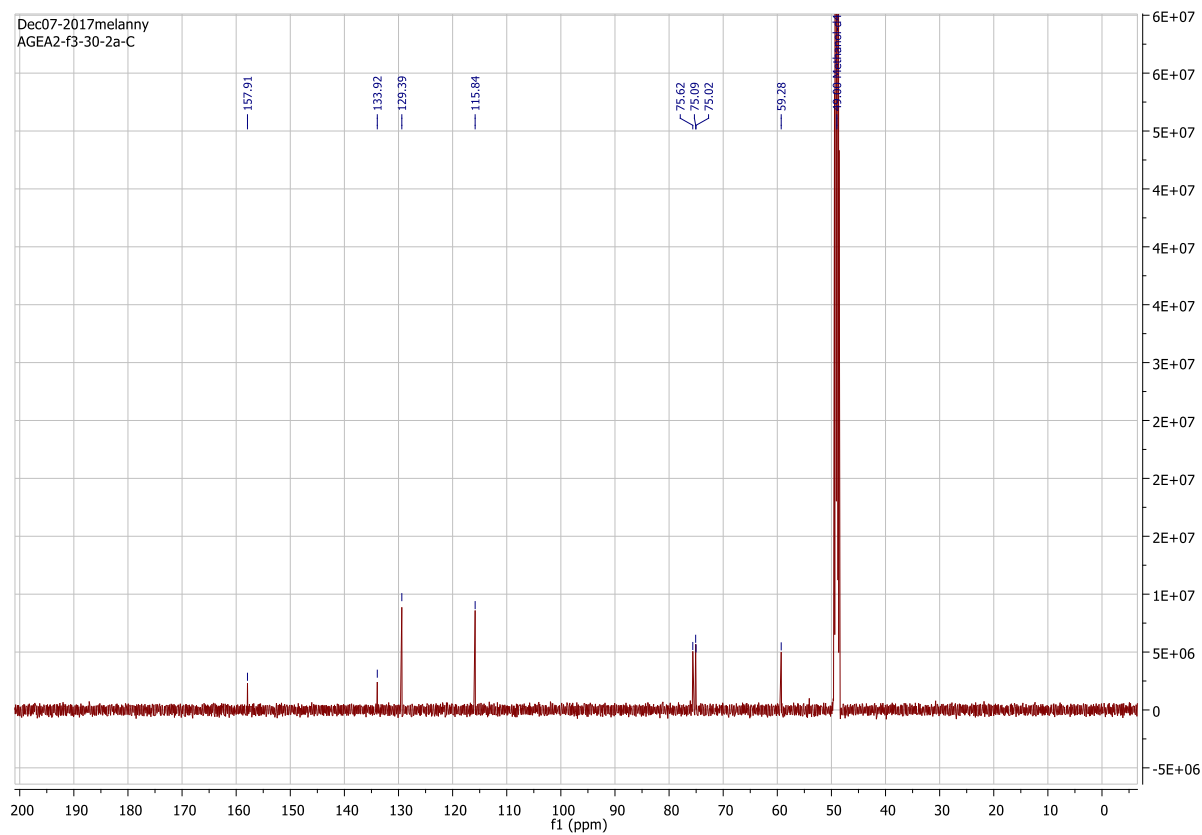


Figure S31 DEPT 135 spectrum of 4

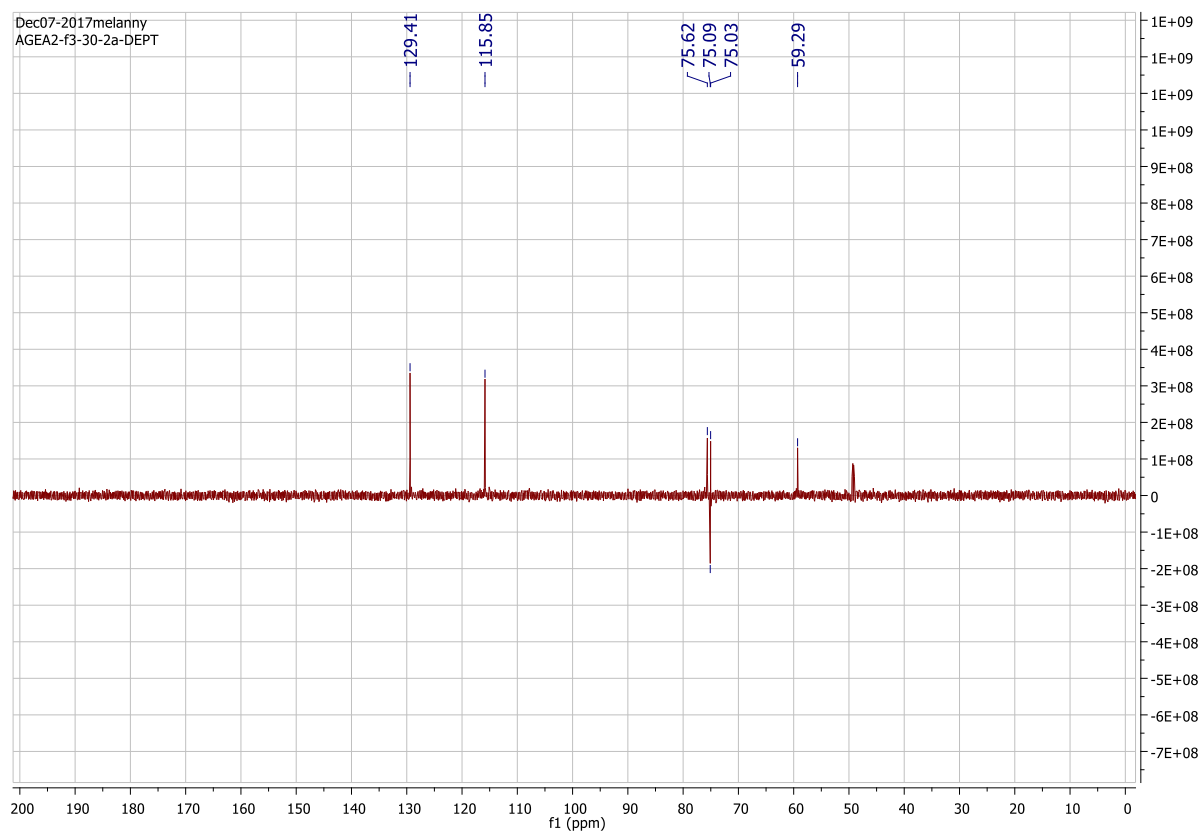


Figure S32 COSY spectrum of 4

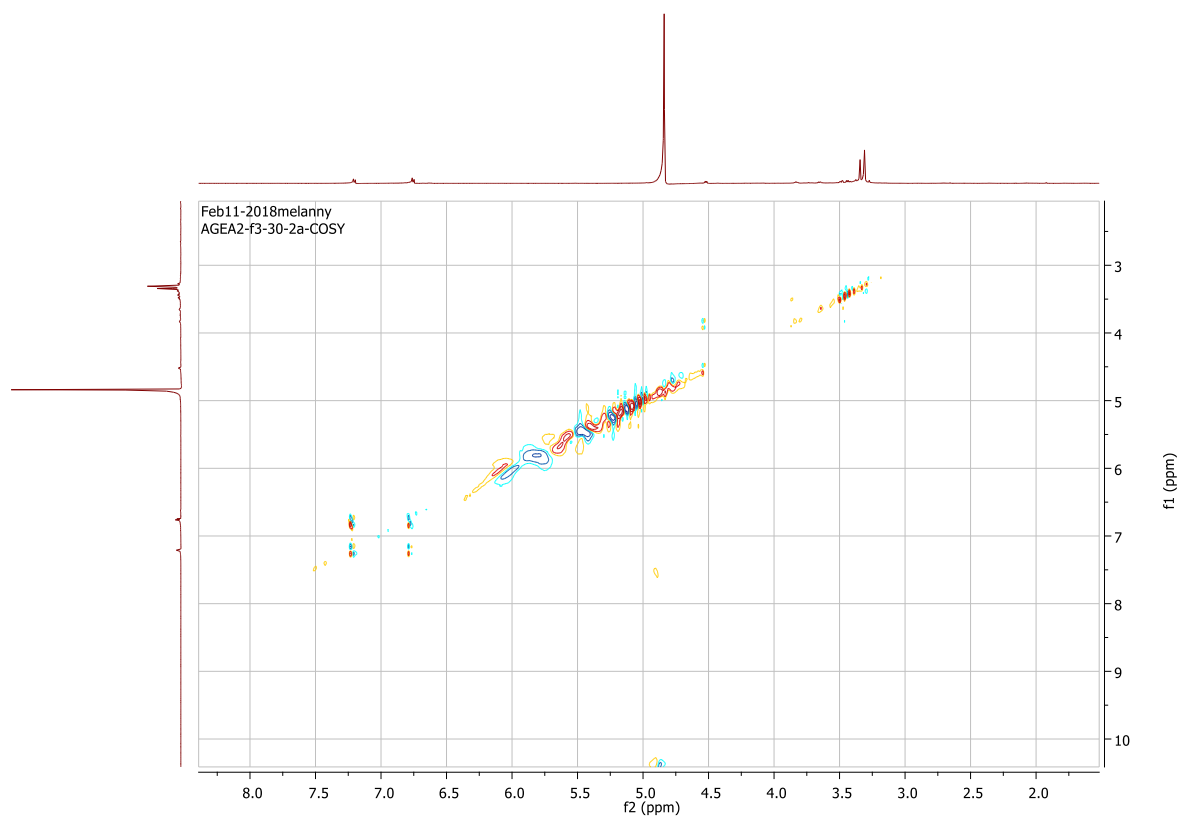


Figure S33 HSQC spectrum of 4

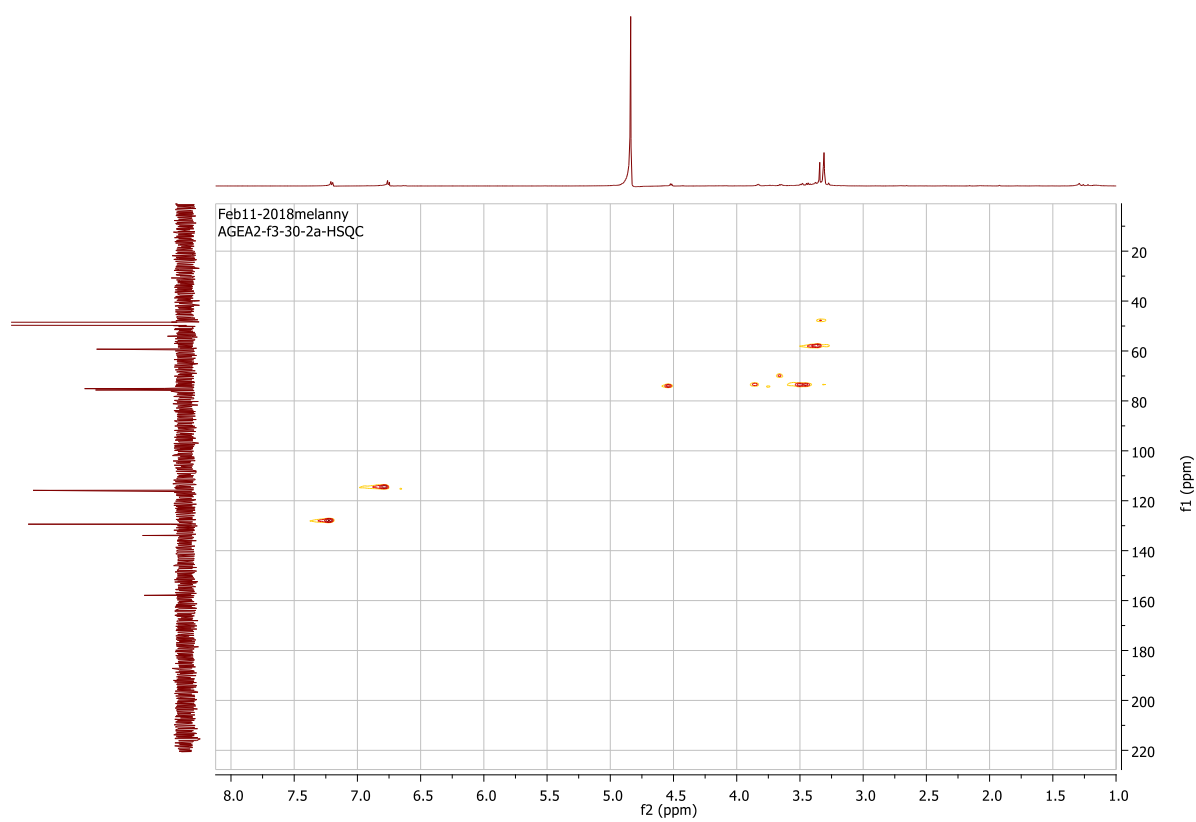


Figure S34 HMBC spectrum of 4

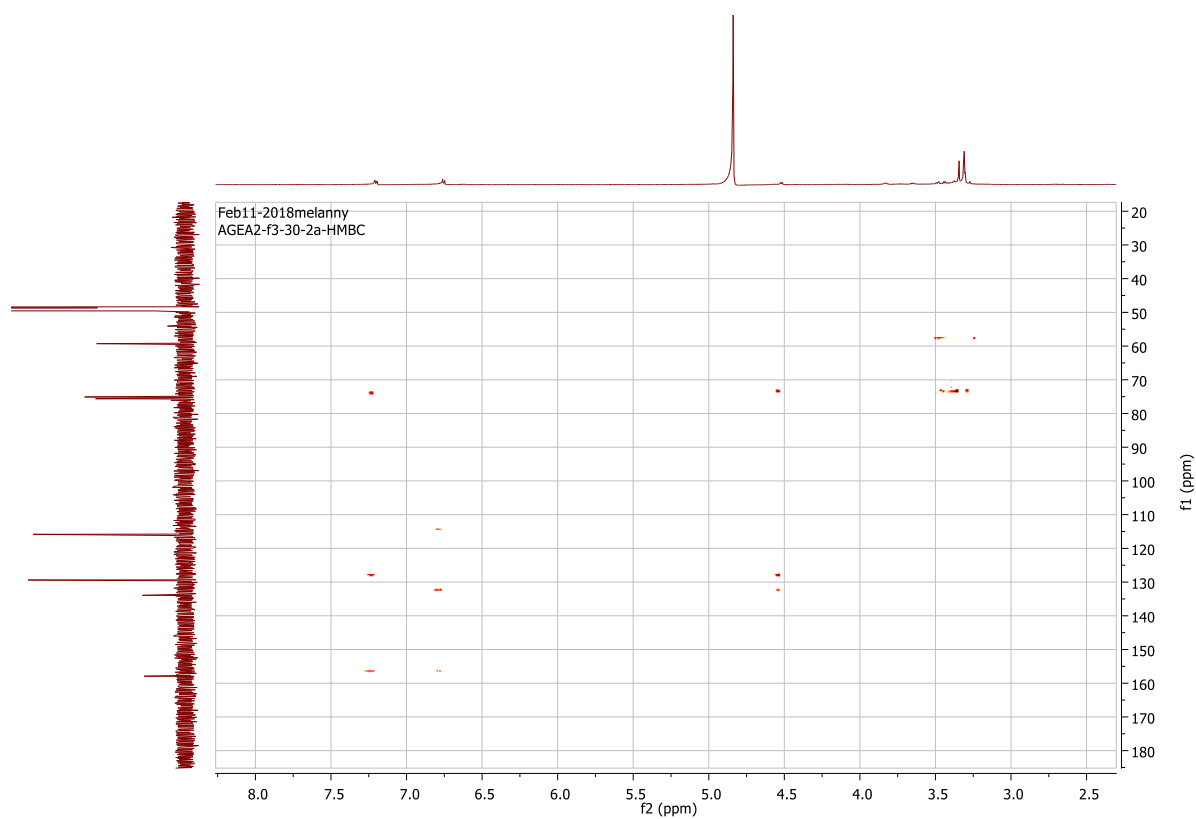
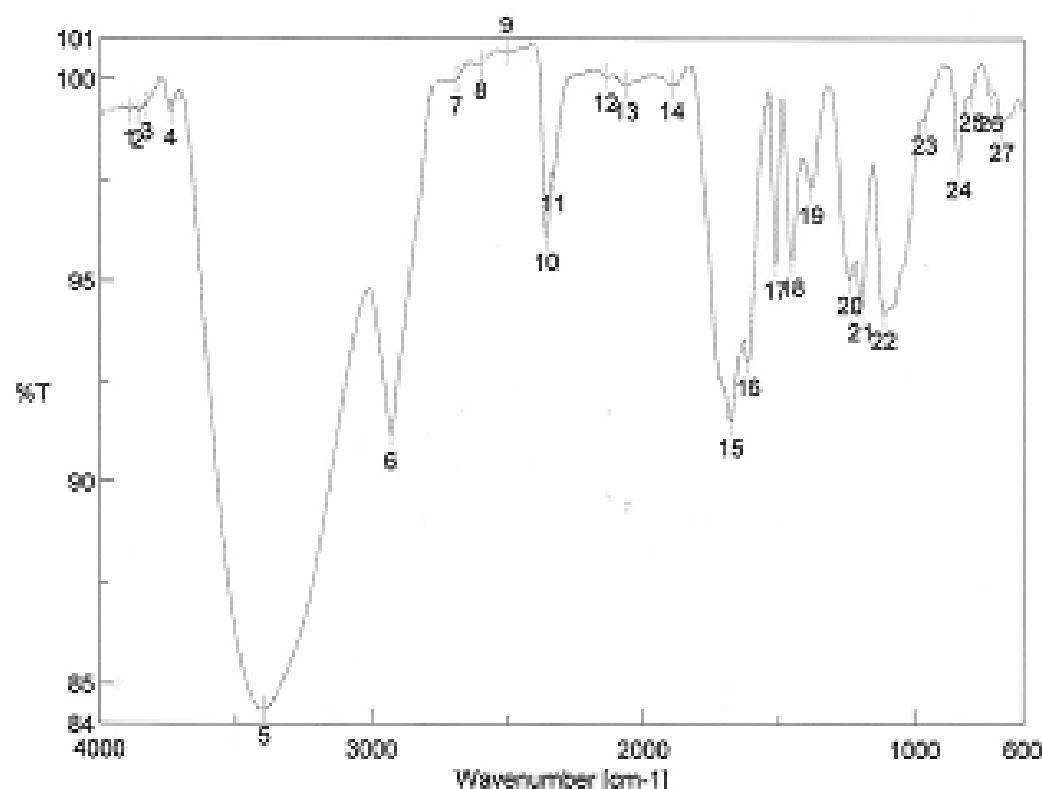


Figure S35 IR spectrum of 4



【コメント情報】

試料名
コメント
測定者
所属
会社

HU

【データ情報】

作成日時 2018/08/20 13:25
データタイプ 等間隔データ
横軸 Wavenumber [cm⁻¹]
縦軸 %T
スタート 3593.53 cm⁻¹
エンド 7000.65 cm⁻¹
データ間隔 0.964233 cm⁻¹
データ数 7469

【測定情報】

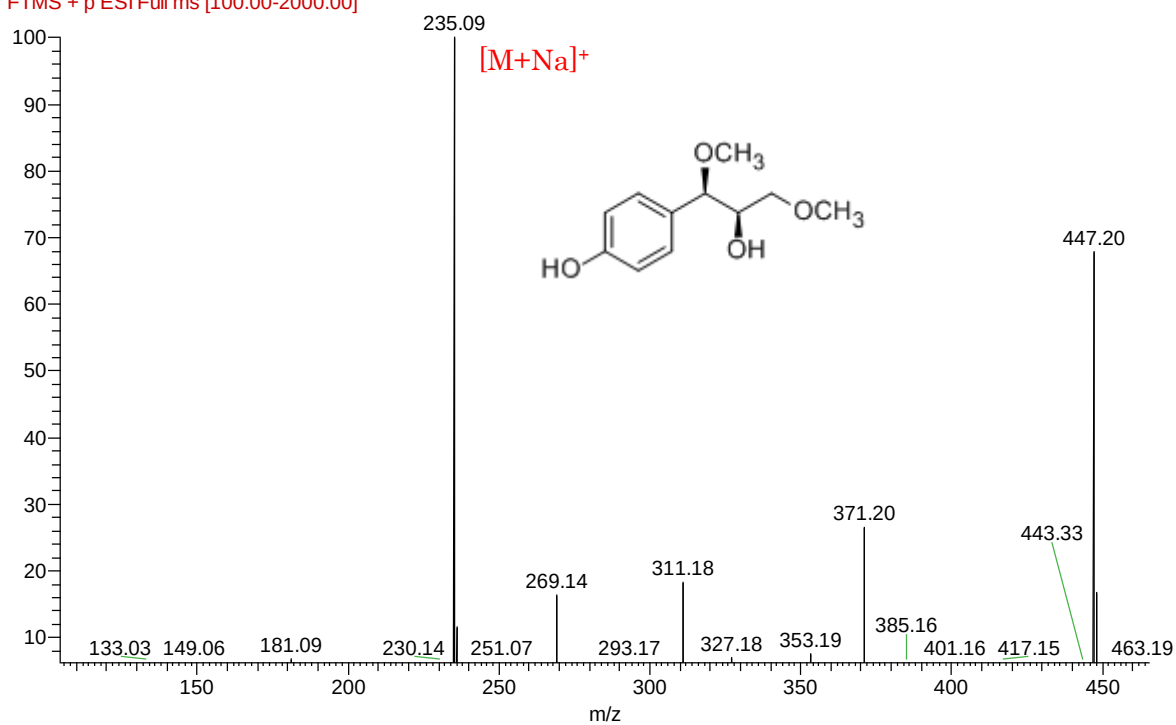
機種名 FT/IR-4600typeA
シリアル番号 D015451786
測定日時 2018/08/20 11:21
光源 標準光源
検出器 TGS
積算回数 10
分解 4 cm⁻¹
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (2)
アパーチャ Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

【ピーク検出結果】

No.	位置	強度	No.	位置	強度
1	3382.61	99.1829	2	3361.76	99.146
3	3029.94	99.3463	4	3742.19	99.196
5	3094.1	94.3637	6	2930.31	91.1735
7	2891.18	100.008	8	2600.54	100.387
9	2507.01	100.673	10	2380.44	98.1302
11	2333.43	97.5762	12	2142.53	100.076
13	2067.32	99.8592	14	1897.61	99.8663

Figure S36 HR-ESI-MS of 5

181129 42 #7 RT: 0.07 AV: 1 NL: 2.59E7
F: FTMS + p ESI Full ms [100.00-2000.00]



Elemental composition search on mass 235.09

m/z = 230.09-240.09

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
235.0939	235.0941	-0.89	3.5	C ₁₁ H ₁₆ O ₄ Na

Figure S37 ^1H NMR spectrum of 5

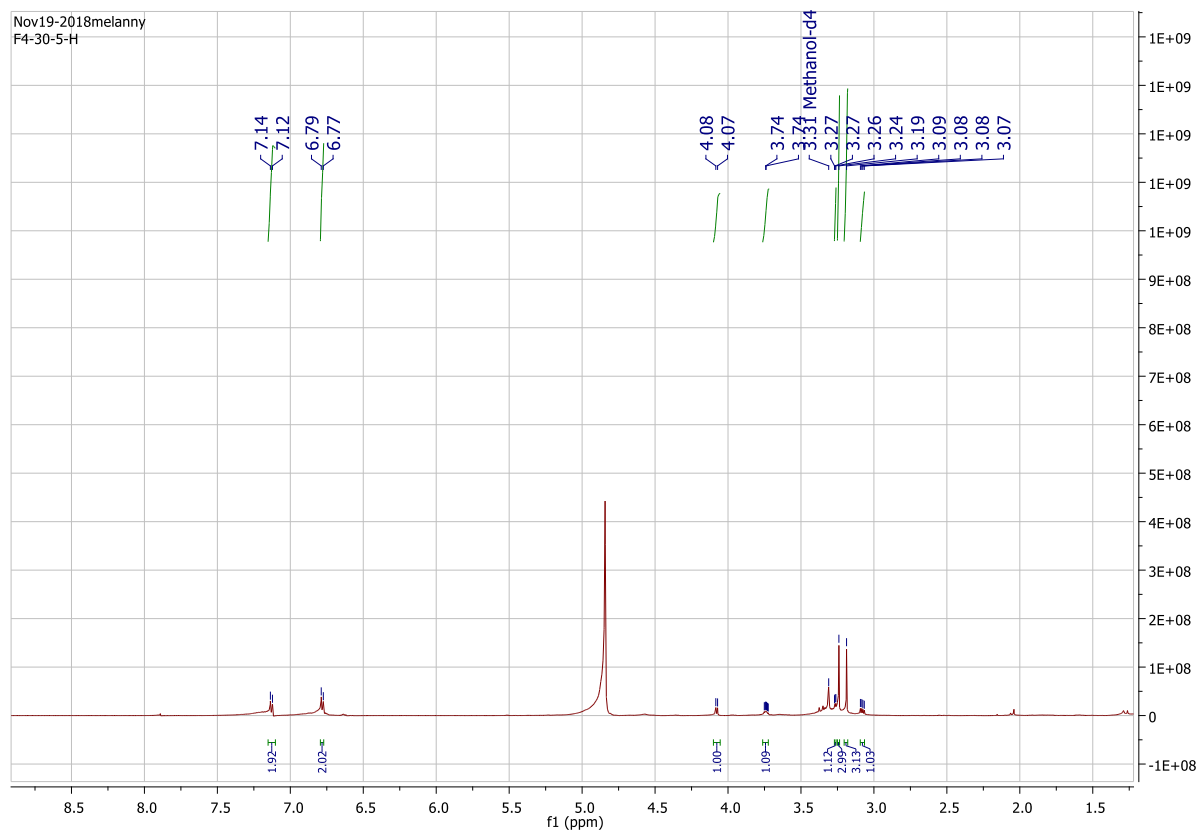


Figure S38 ^{13}C NMR spectrum of 5

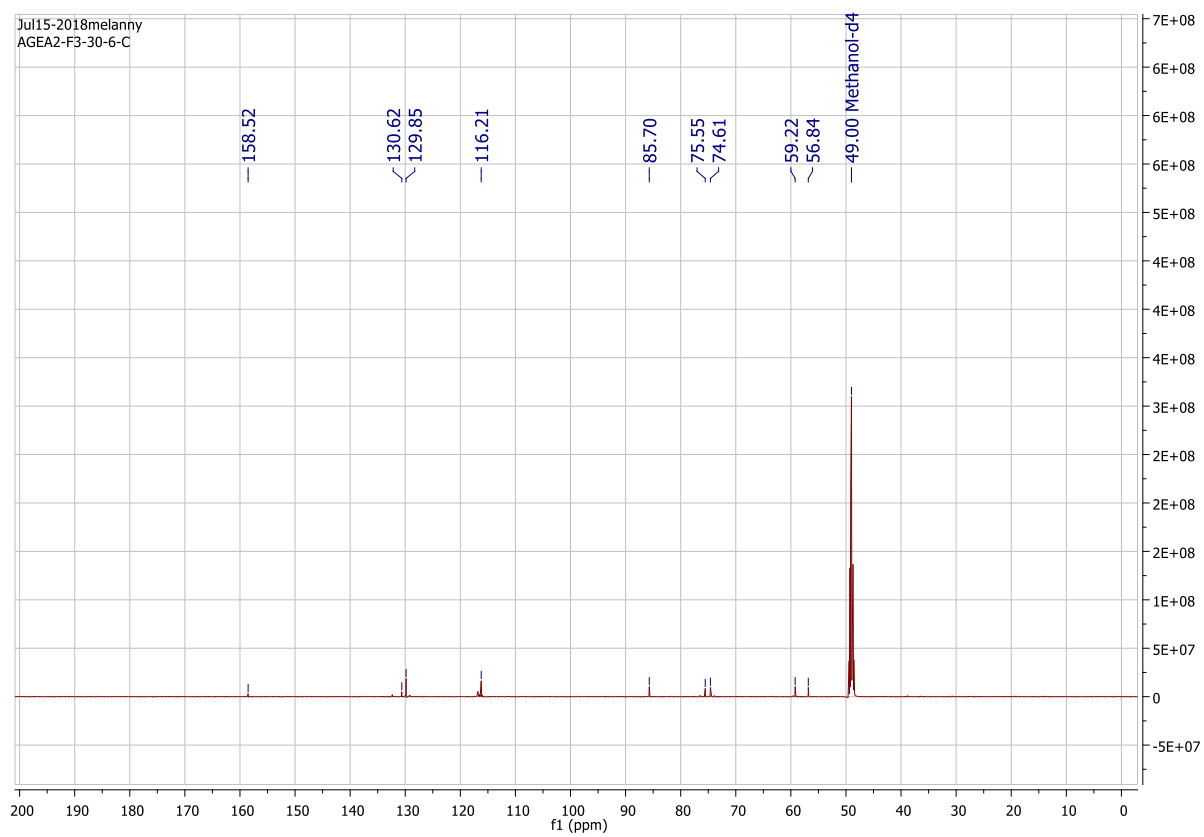


Figure S39 DEPT 135 spectrum of 5

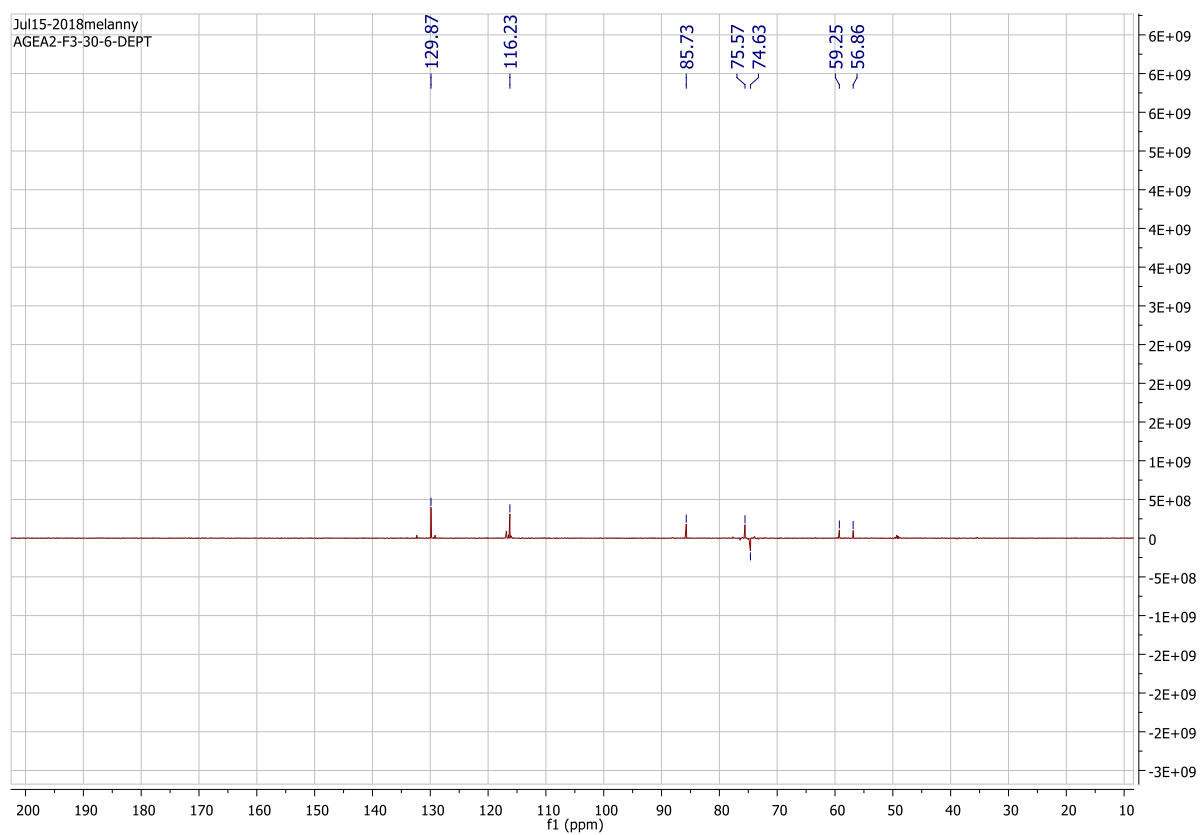


Figure S40 COSY spectrum of 5

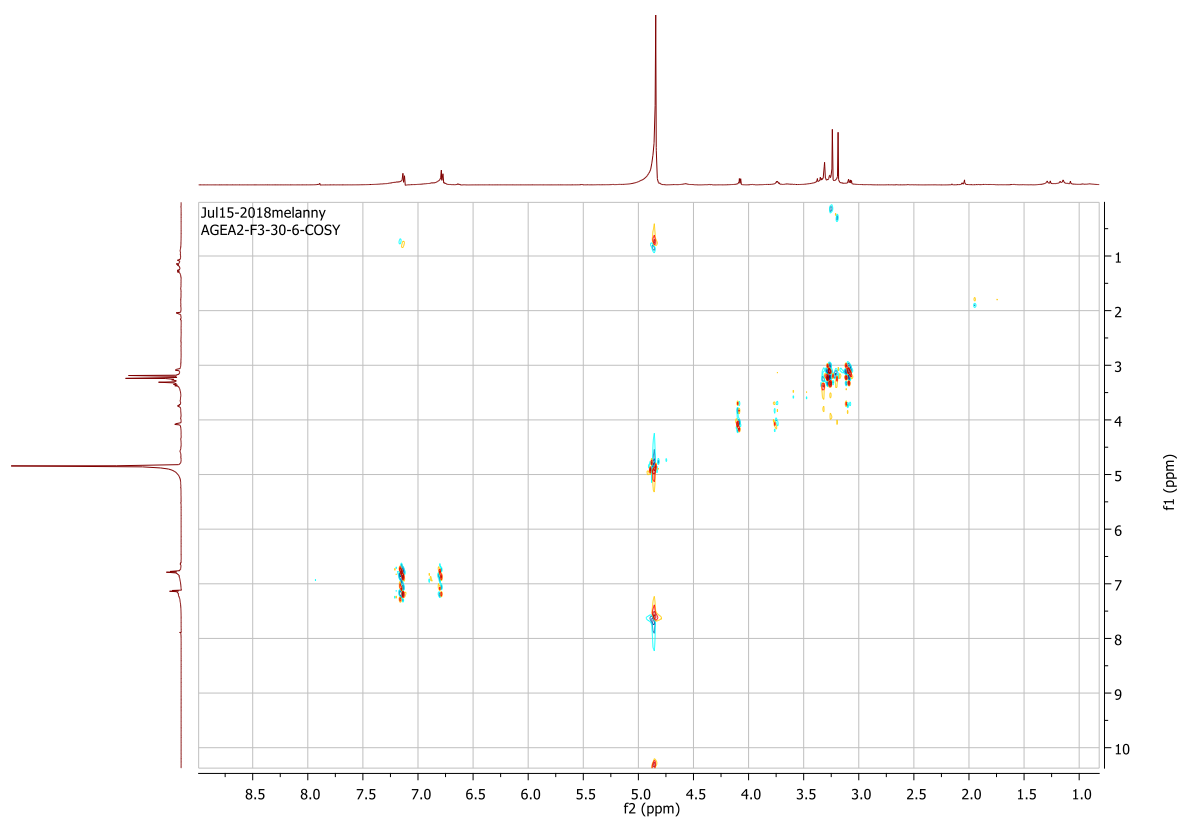


Figure S41 HSQC spectrum of 5

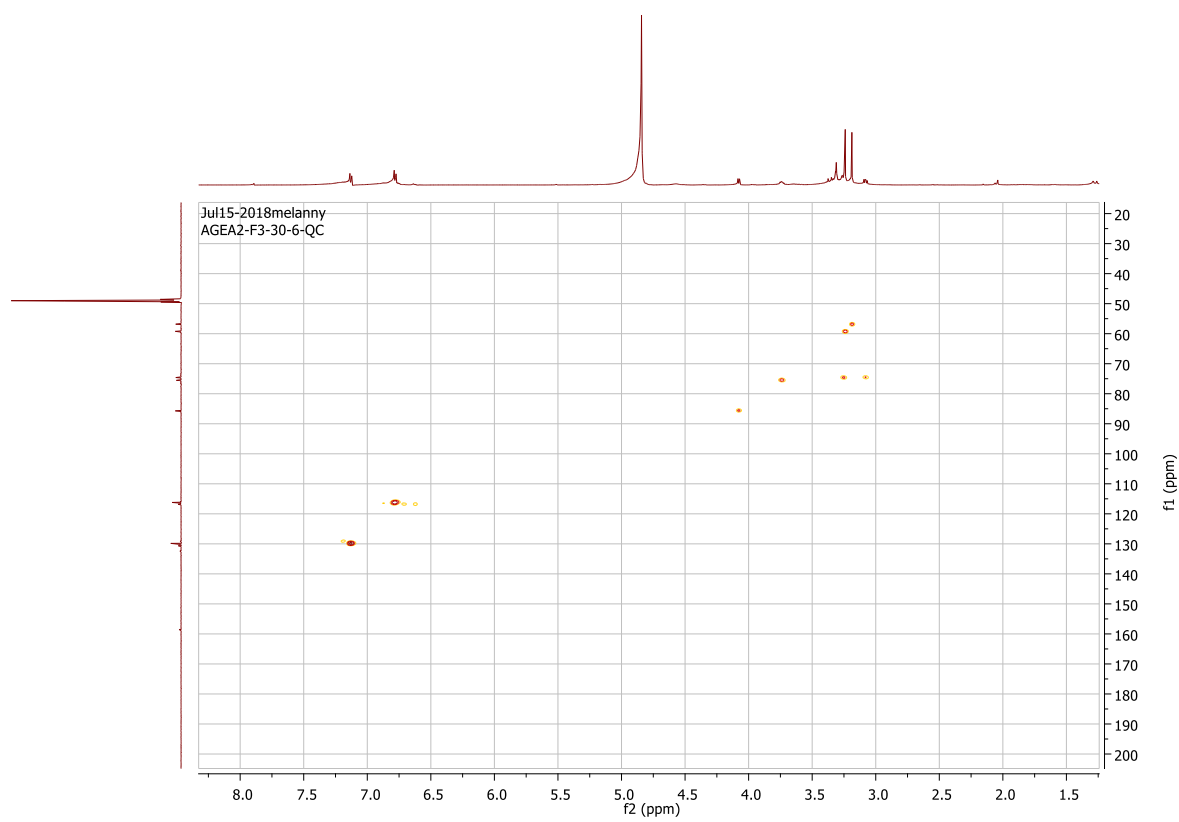


Figure S42 **HMBC spectrum of 5**

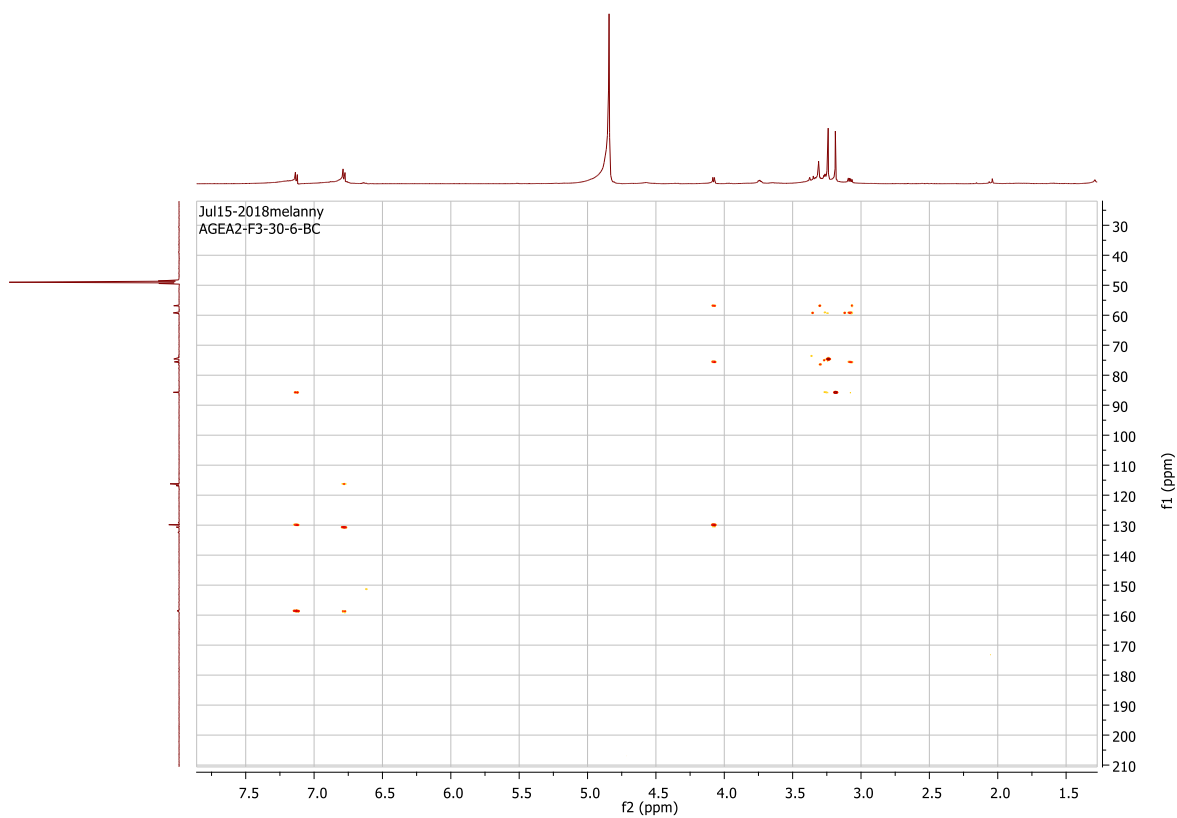
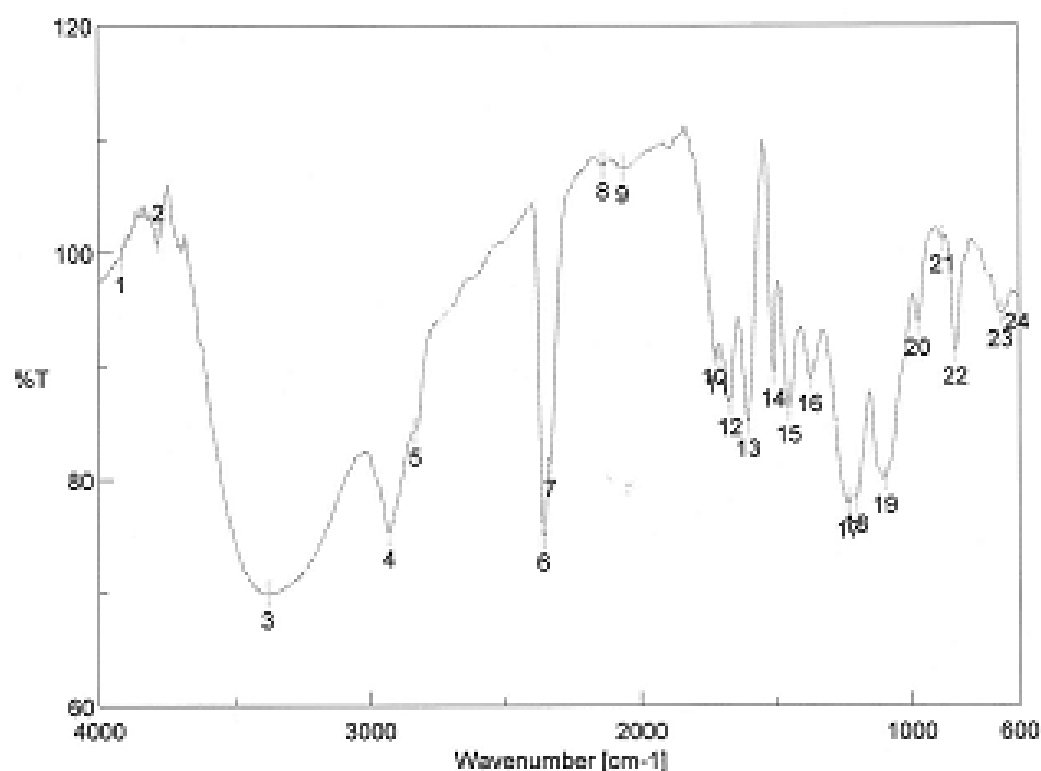


Figure S43 IR spectrum of 5



【コメント情報】

試料名
コメント
測定者
所属
会社

HU

【データ情報】

作成日時 2018/08/20 13:20
データタイプ 等間隔データ
横軸 Wavenumber [cm⁻¹]
縦軸 %T
スタート 599.753 cm⁻¹
エンド 7800.65 cm⁻¹
データ間隔 0.864233 cm⁻¹
データ数 7469

【測定情報】

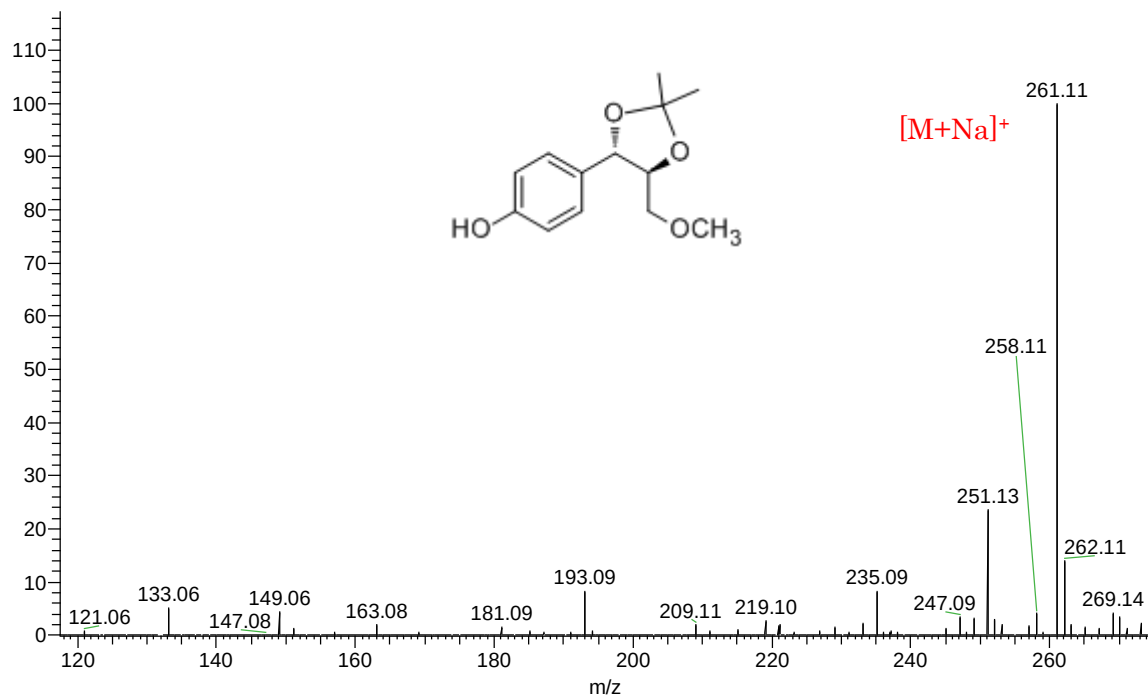
機種名 FT/IR-4600typeA
シリアル番号 D015461786
測定日時 2018/08/20 12:41
光源 標準光源
検出器 TGS
積算回数 10
分解 4 cm⁻¹
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (2)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

【ピーク検出結果】

No.	位置	強度	No.	位置	強度
1	3518.64	99.4911	2	3777.87	101.081
3	3378.67	69.9199	4	2930.31	75.3527
5	2933.08	84.2422	6	2360.44	75.0184
7	2335.37	81.525	8	2138.67	107.658
9	2058.35	107.394	10	1725.83	91.3333
11	1718.26	90.6165	12	1671.02	86.9629
13	1604.48	85.0544	14	1509.99	89.4423

Figure S44 **HR-ESI-MS of 6**

180130_32 #7 RT: 0.07 AV: 1 NL: 9.49E6
F: FTMS + p ESI Full ms [100.00-2000.00]



Elemental composition search on mass 261.11

m/z = 256.11-266.11

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
261.1099	261.1097	0.50	4.5	C ₁₃ H ₁₈ O ₄ Na

Figure S45 ^1H NMR spectrum of 6

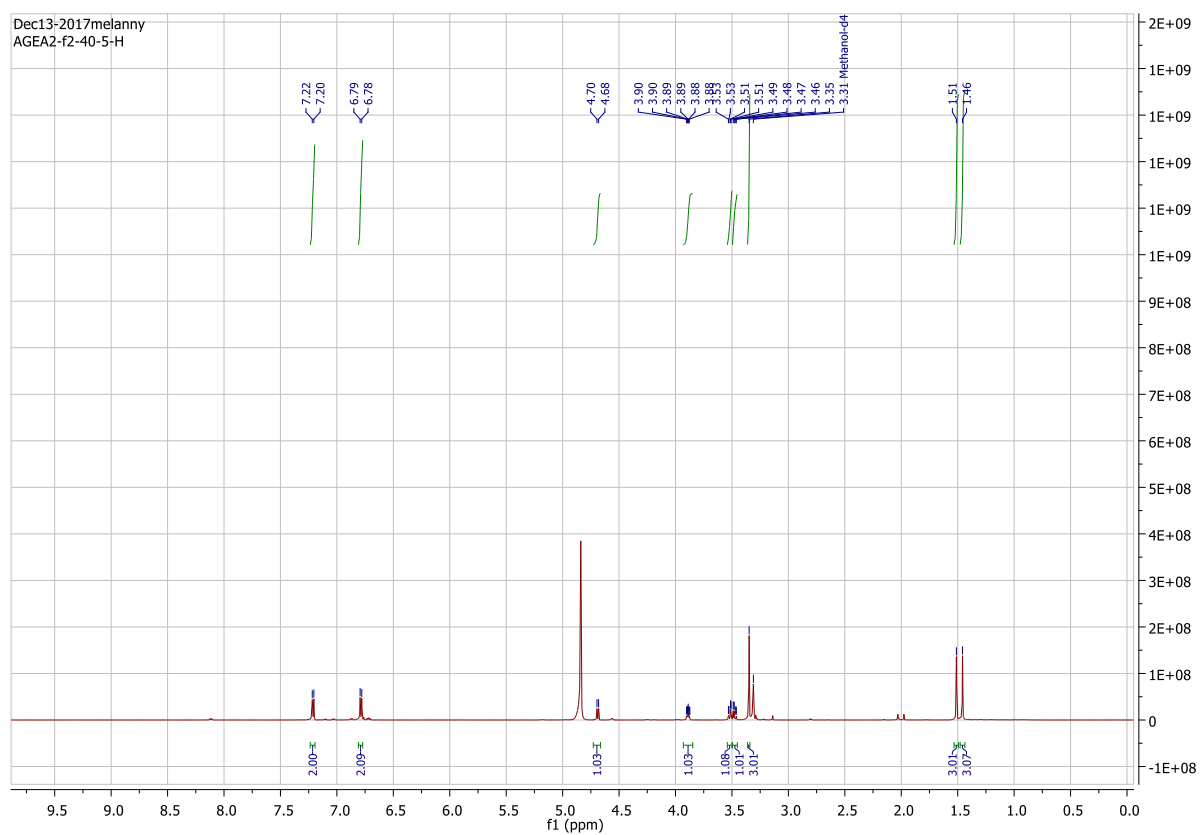


Figure S46 ^{13}C NMR spectrum of 6

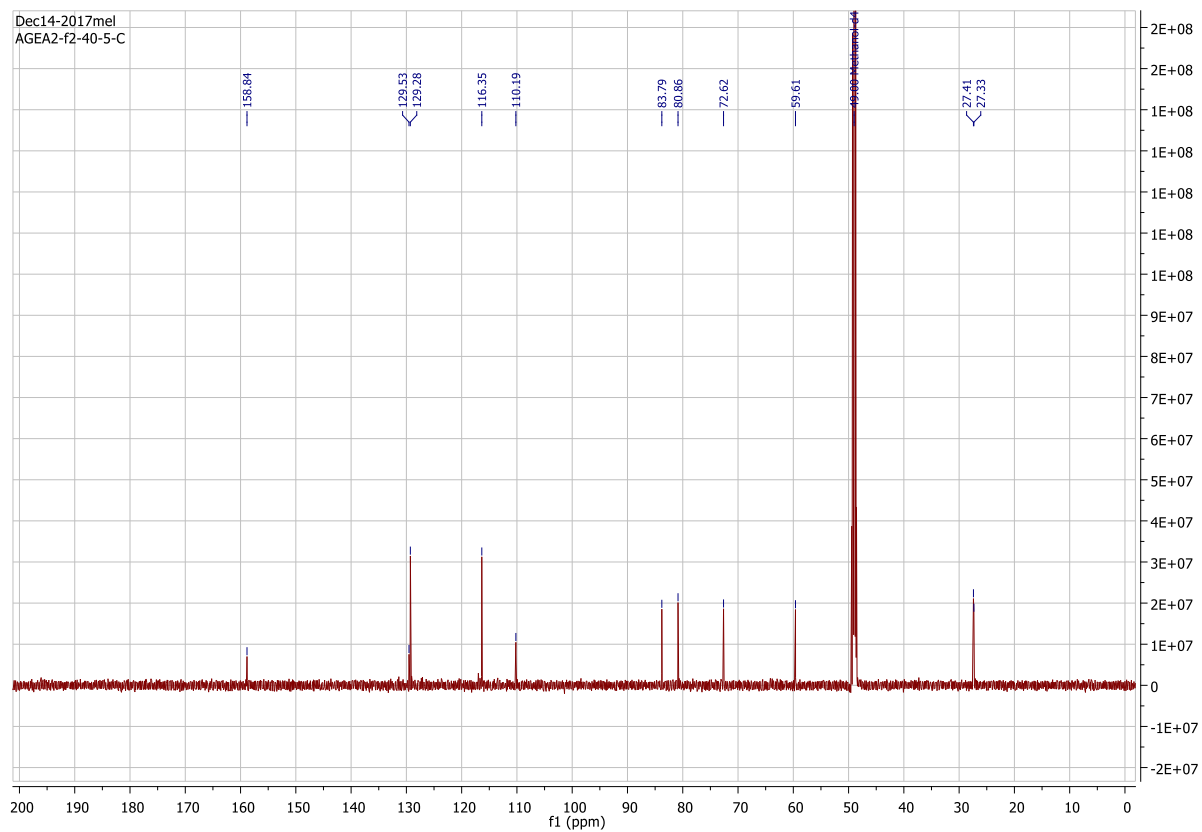


Figure S47 DEPT 135 spectrum of 6

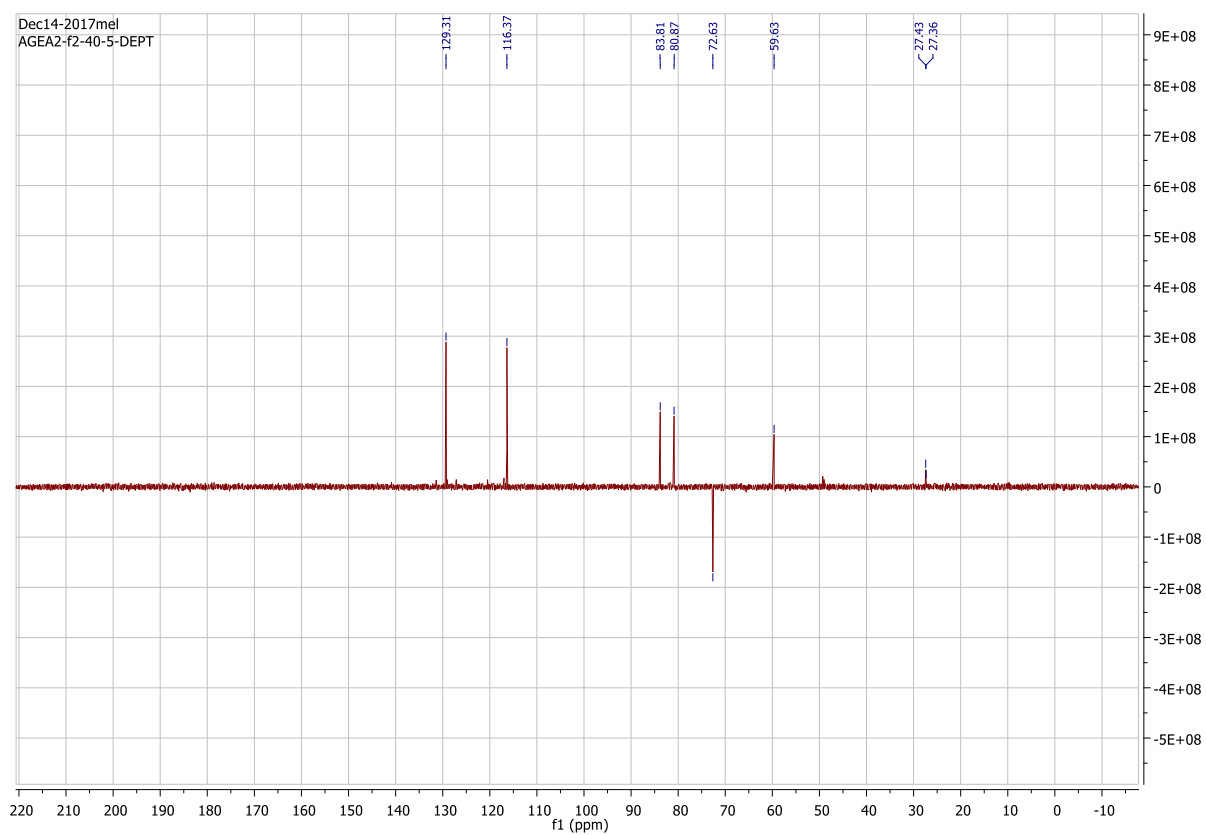


Figure S48 COSY spectrum of 6

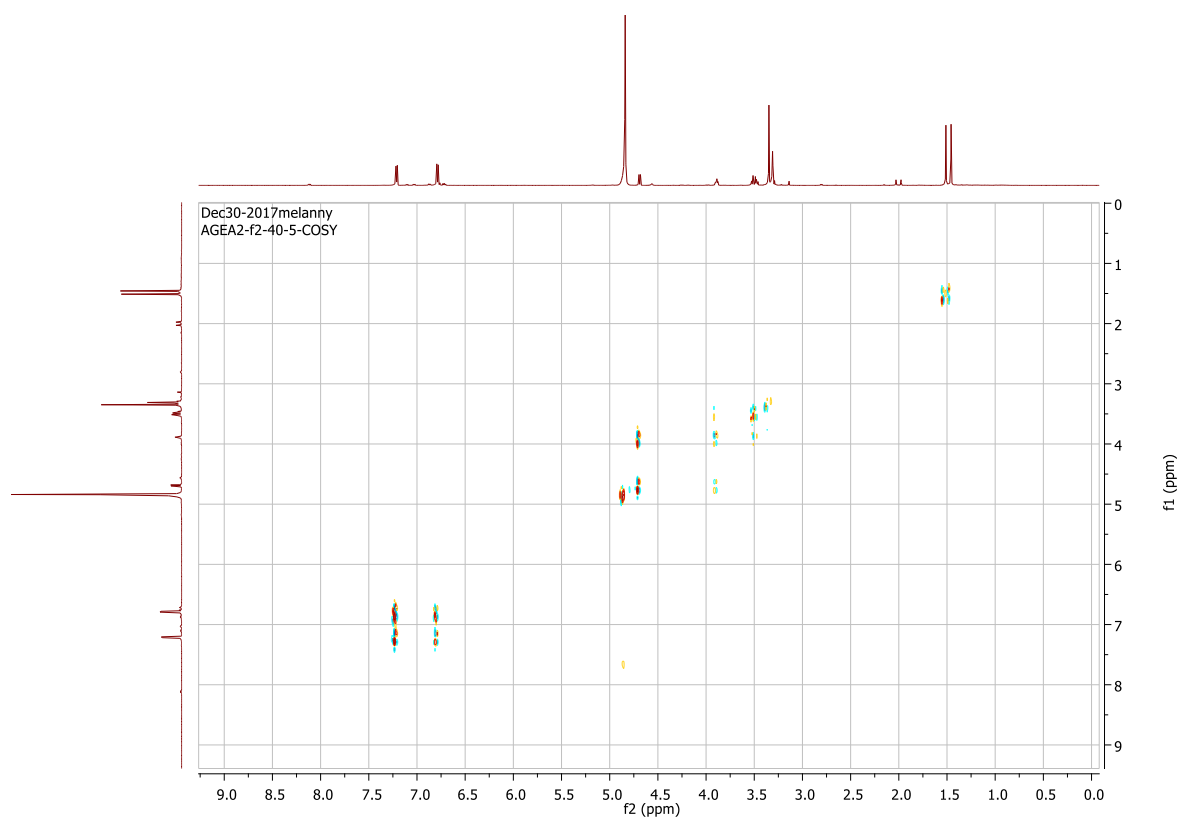


Figure S49 HSQC spectrum of 6

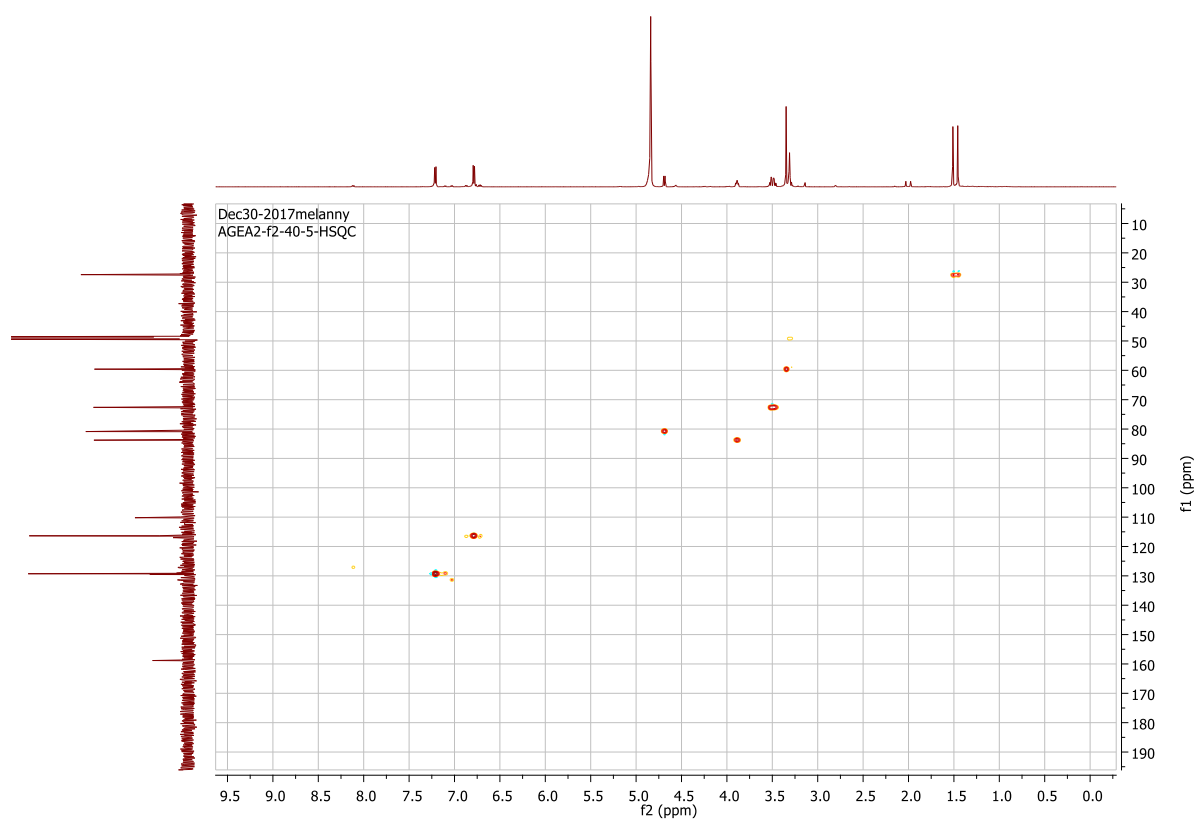


Figure S50 HMBC spectrum of 6

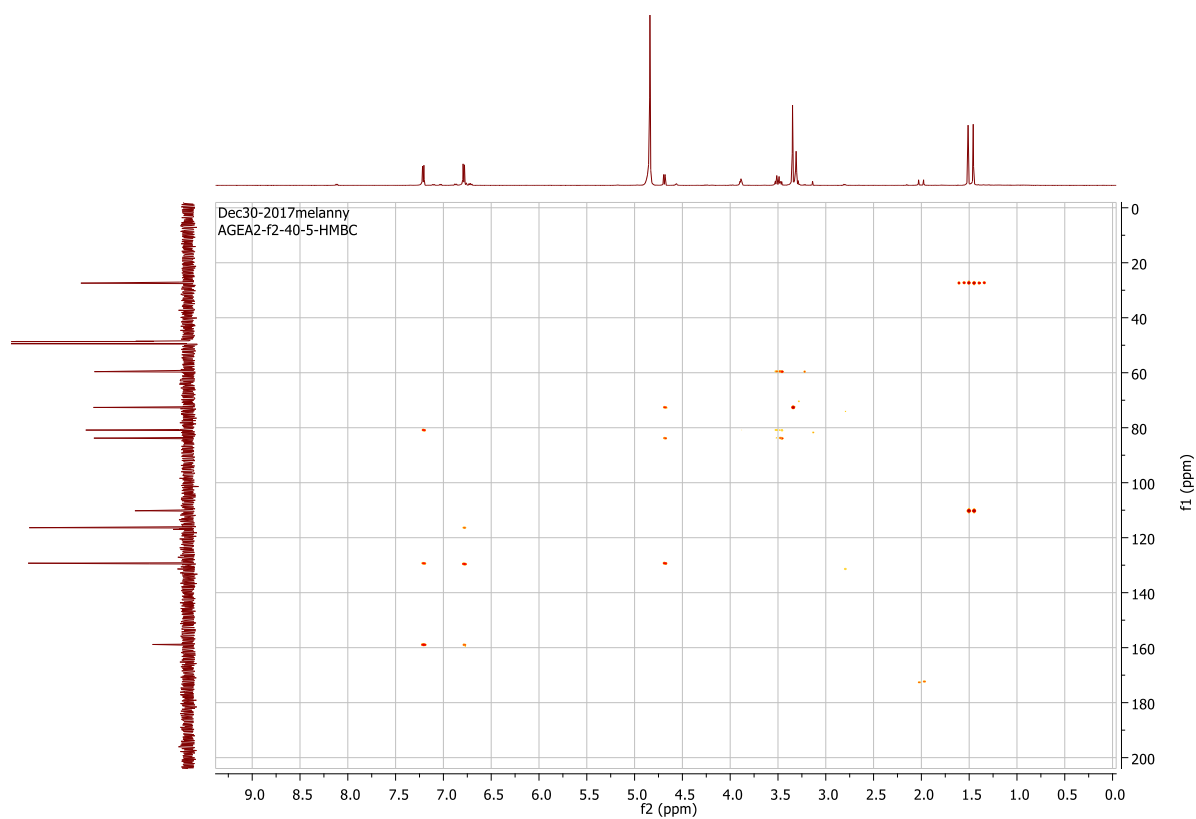
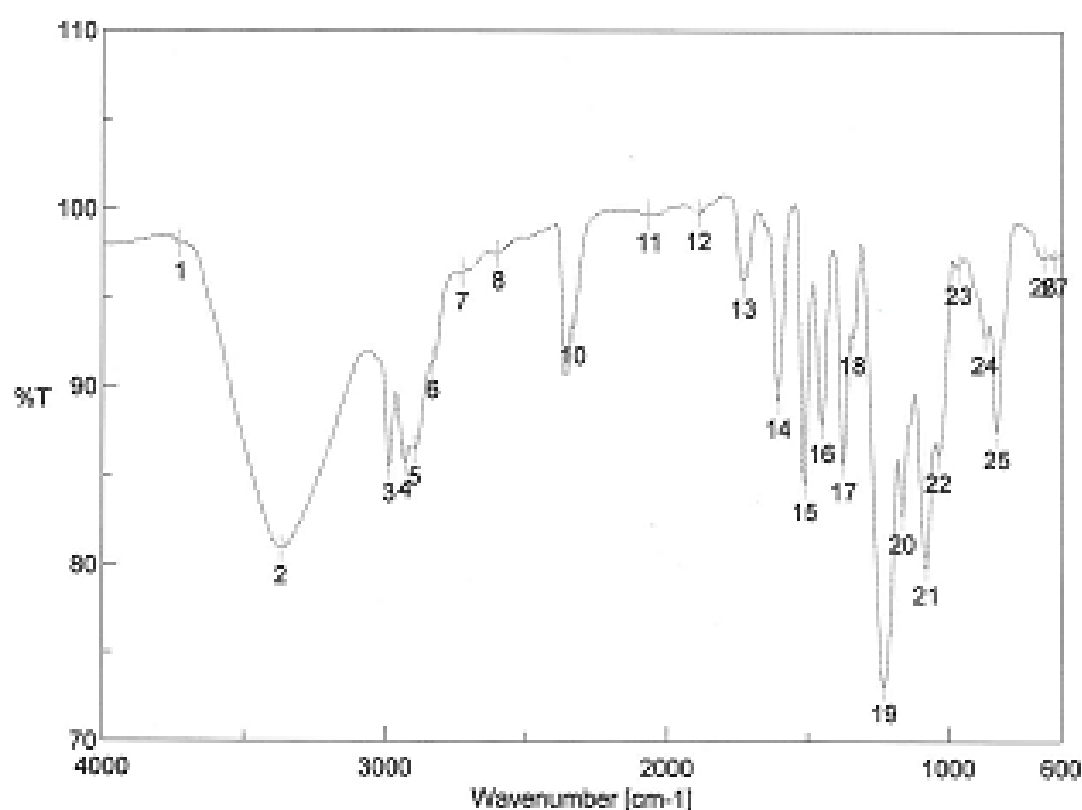


Figure S51 IR spectrum of 6



【コメント情報】

試料名
コメント
測定者
所属
会社

HU

【データ情報】

作成日時 2018/08/20 14:25
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 599.753 cm-1
エンド 7800.65 cm-1
データ間隔 0.964233 cm-1
データ数 7469

【測定情報】

機種名 FT/IR-4600typeA
シリアル番号 D015461738
測定日時 2018/08/20 14:24
光源 標準光源
検出器 TGS
積算回数 10
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (2)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

【ピーク検出結果】

No.	位置	強度	No.	位置	強度
1	3725.8	97.9921	2	3368.07	90.9102
3	2906.23	85.5728	4	2929.34	85.7724
5	2895.59	95.4058	6	2830.03	91.3661
7	2728.78	98.3808	8	2600.54	97.5193
9	2360.44	90.2334	10	2335.37	93.3024
11	2067.32	99.8626	12	1891.63	99.7419
13	1732.73	95.9512	14	1607.38	89.204

Figure S52 ^1H NMR spectrum of 7

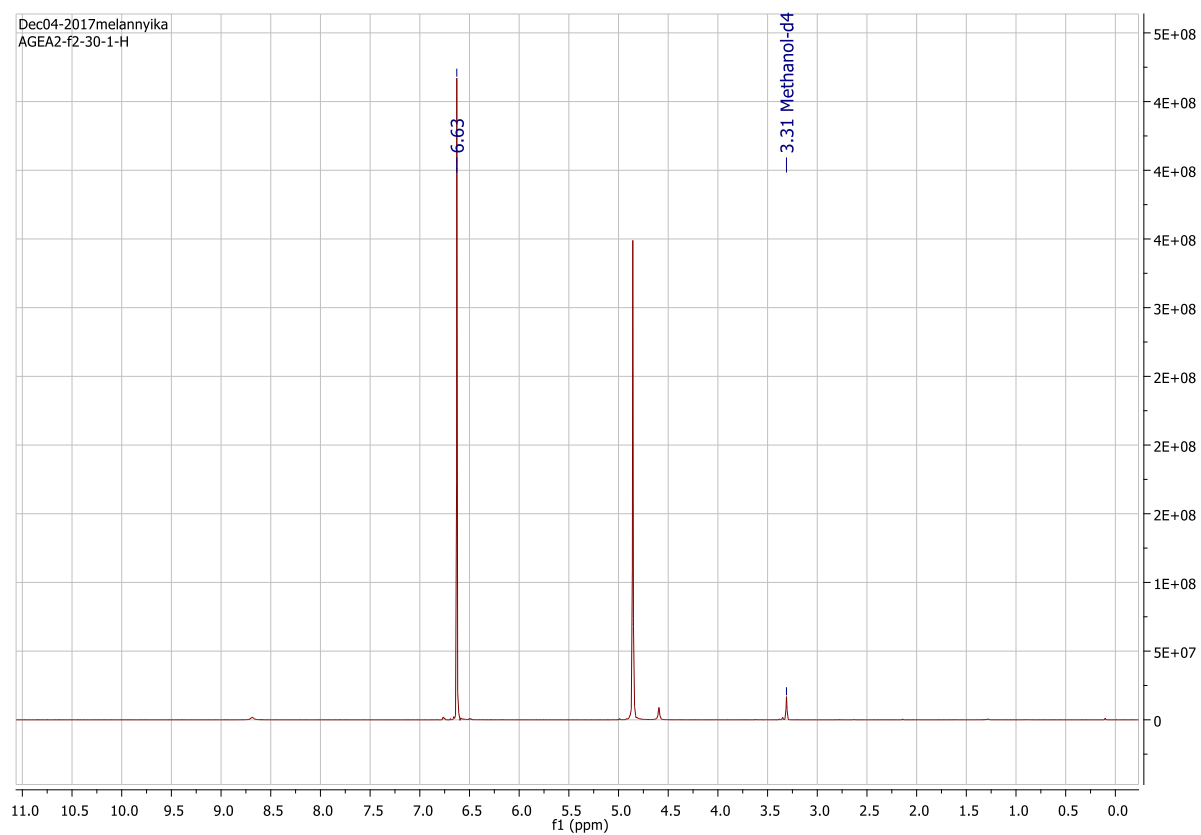


Figure S53 ^{13}C NMR spectrum of 7

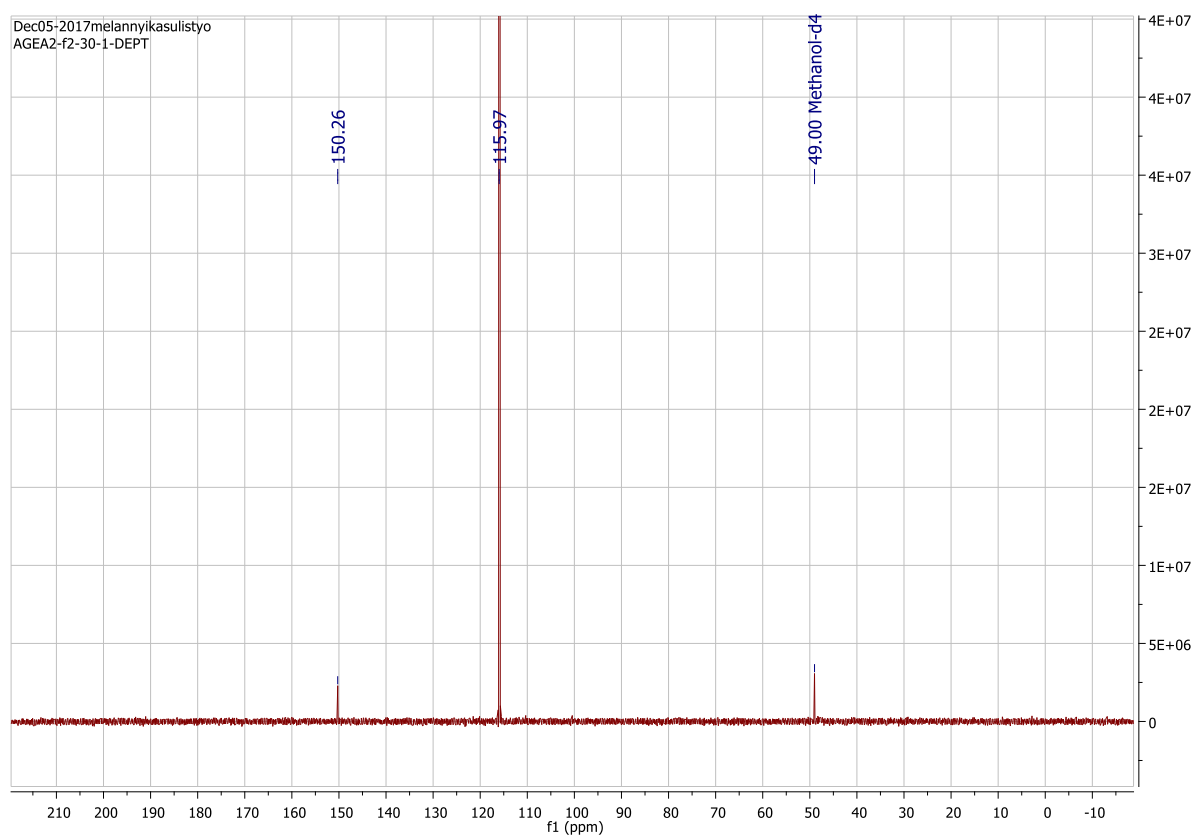


Figure S54 ^1H NMR spectrum of 8

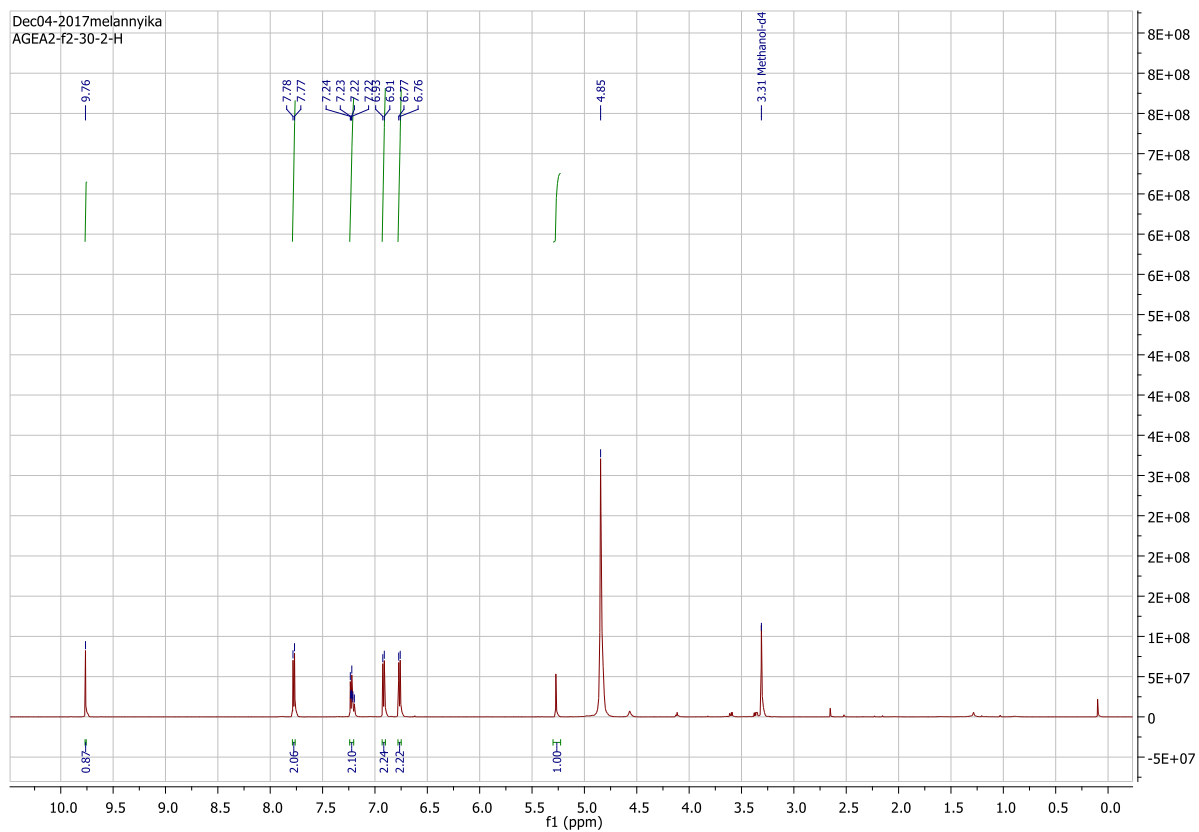


Figure S55 ^{13}C NMR spectrum of 8

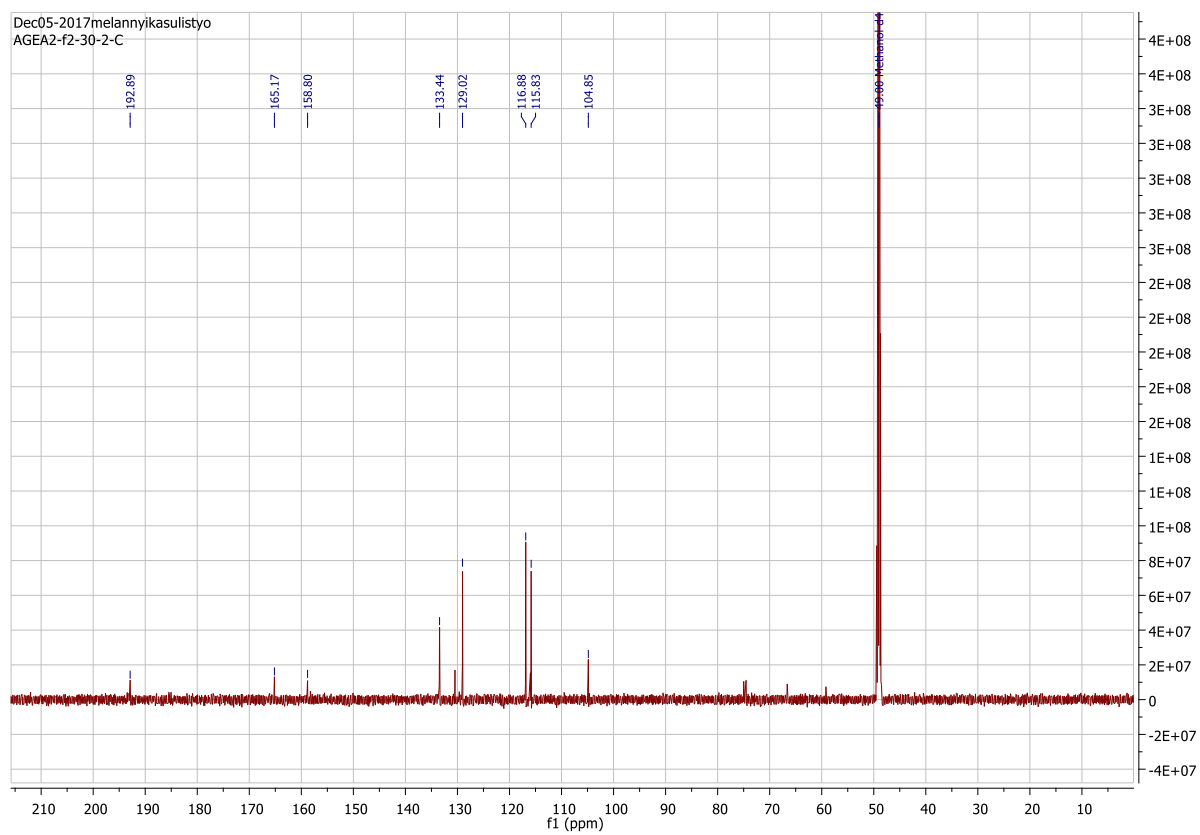


Figure S56 ^1H NMR spectrum of 9

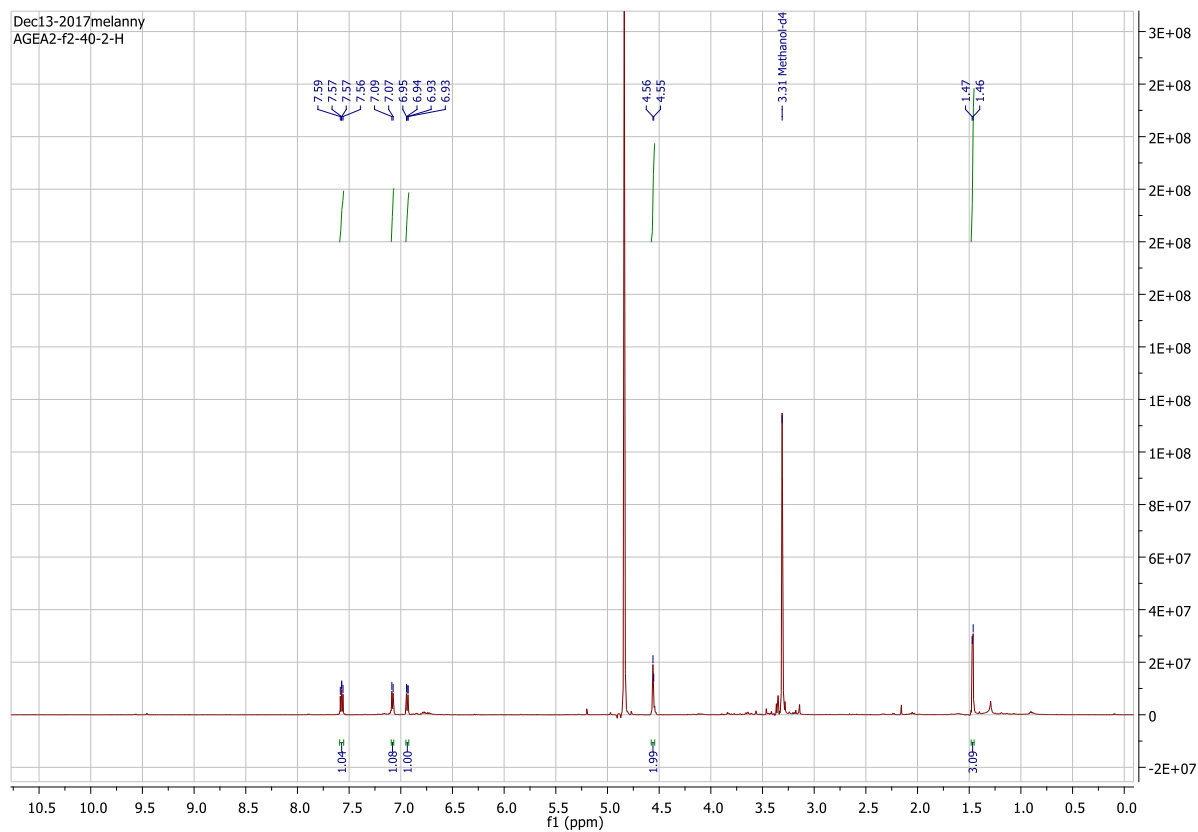


Figure S57 ^{13}C NMR spectrum of 9

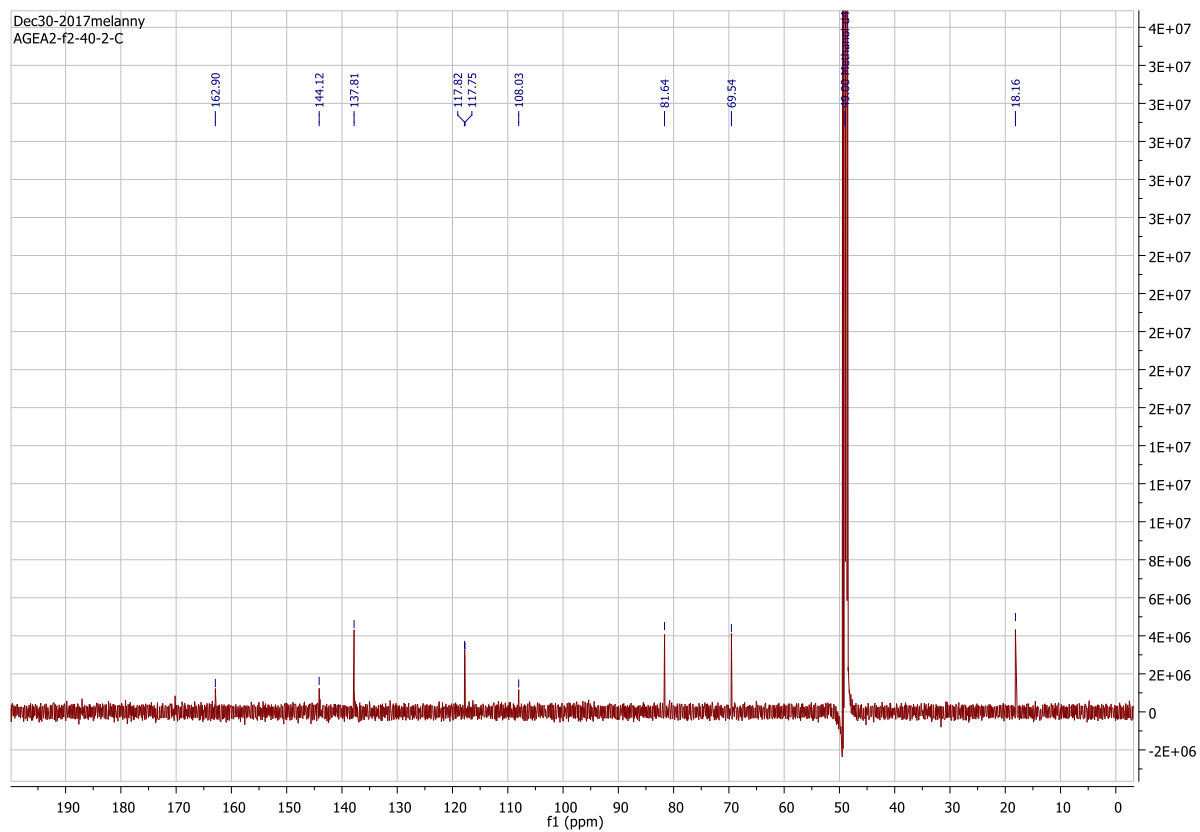


Figure S58 ^1H NMR spectrum of 10

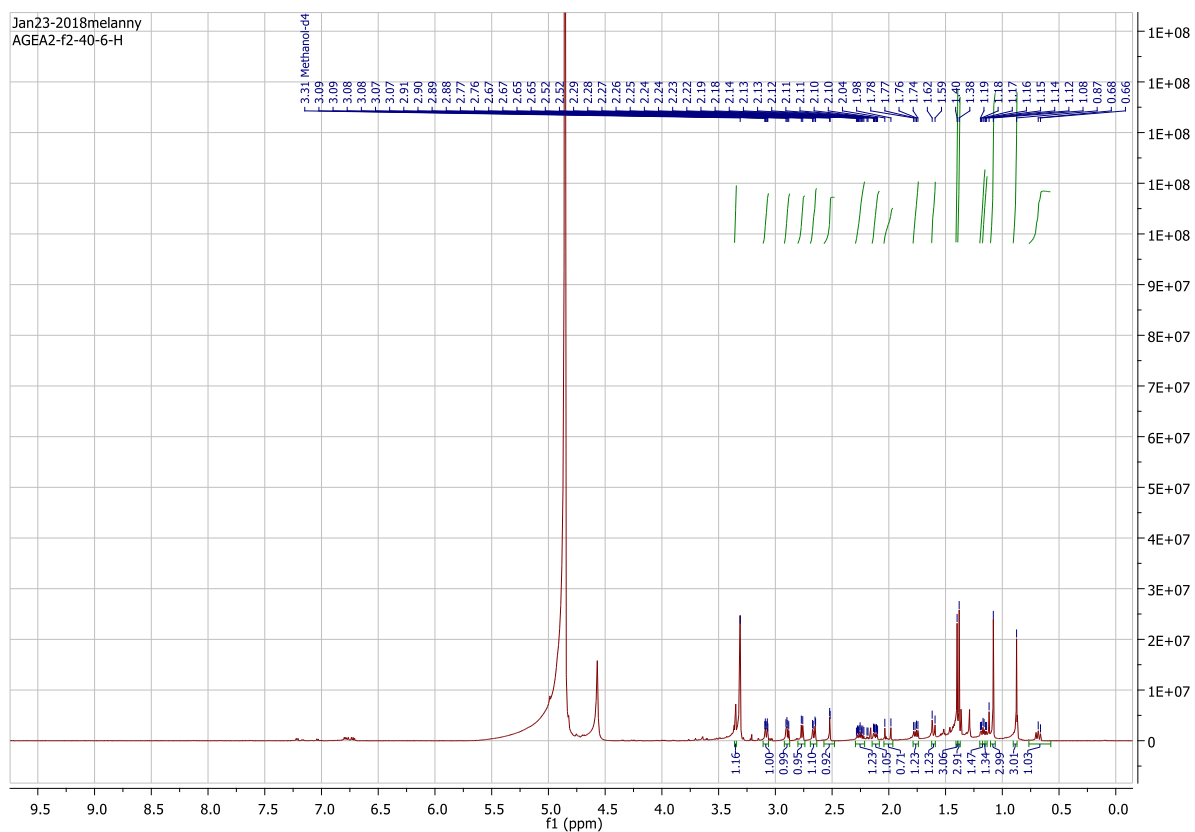


Figure S59 ^{13}C NMR spectrum of 10

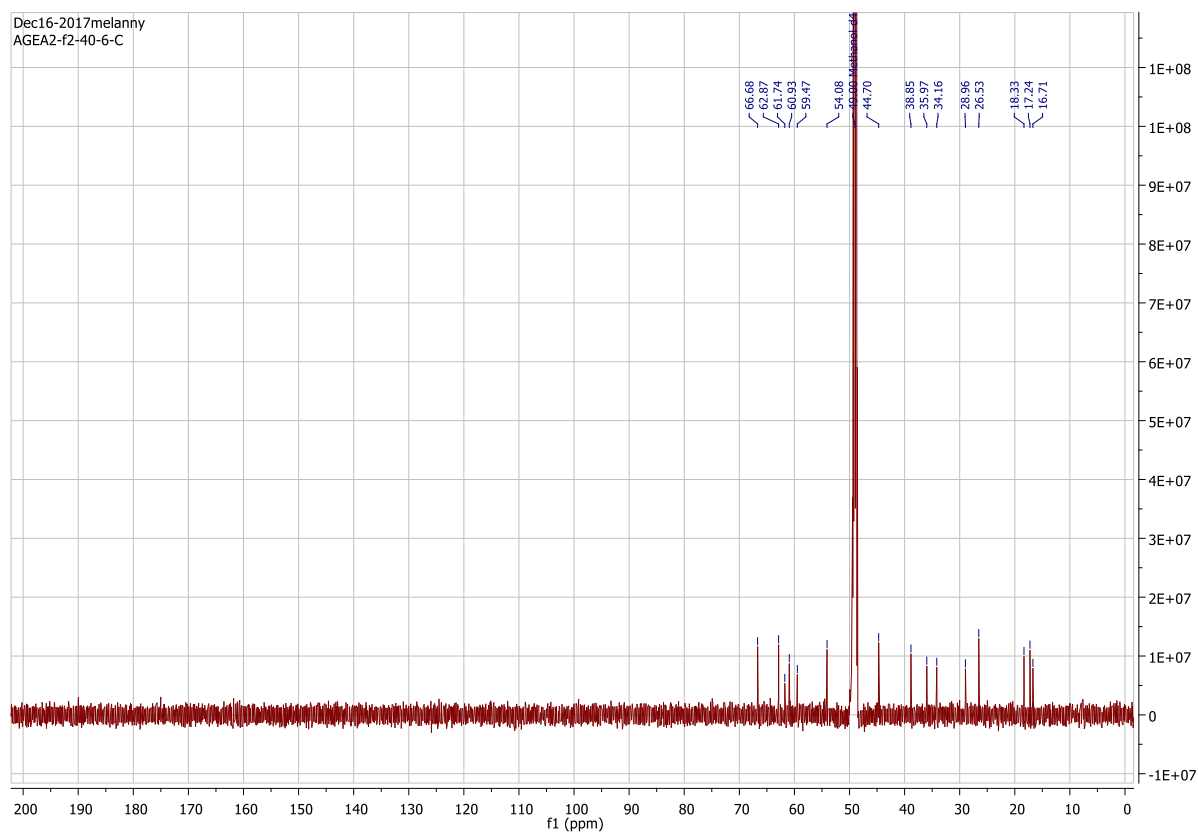
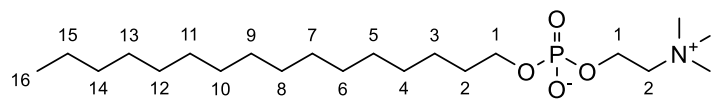
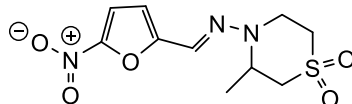


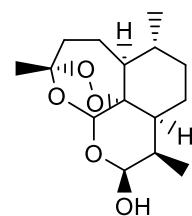
Figure S60 **Structures of positive control for the bioassay**



miltefosine



niflutimox



dihydroartemisinin

Table S1 **COSY correlations of compounds 1-6**

Position	Compound 1	2	3	4	5	6
H-2, 6	H-3, 5	H-3, 5	H-3, 5	H-3, 5	H-3, 5	H-3, 5
H-3, 5	H-2, 6	H-2, 6	H-2, 6	H-2, 6	H-2, 6	H-2, 6
H-1'	H-2'	H-2'	H-2'	H-2'	H-2'	H-2'
H-1'-OCH ₃	-	-	-	-	-	-
H-2'	H-1', 3'	H-1', 3'	H-1', 3'	H-1', 3'	H-1', 3'	H-1', 3'
H-3'	H-2'	H-2'	H-2'	H-2'	H-2'	H-2'

Table S2 **HMBC correlations of compounds 1-6**

Position	Compound 1	2	3
H-2, 6	C-4, 6(2)	C-4, 6(2), 3(5), 1'	C-4, 6(2), 3(5), 1'
H-3, 5	C-1, 5(3), 4	C-1, 5(3), 4	C-1, 5(3), 4
H-1'	C-1, 2(6), 2'	C-1, 2(6), 2', 3', 1'-OCH ₃	C-1, 2(6), 2', 3'
H-1'-OCH ₃	-	C-1'	-
H-2'	C-1, 1'	C-1, 1', 3'	C-1, 1', 3'
H-3'	C-1', 2', 3'-OCH ₃	C-1', 2', 3'-OCH ₃	C-1', 2', 3'-OCH ₃
H-3'-OCH ₃	C-3'	C-3'	C-3'

Position	Compound 4	5	6
H-2, 6	C-4, 6(2), 3(5), 1'	C-4, 6(2), 3(5), 1'	C-4, 6(2), 3(5)
H-3, 5	C-1, 5(3), 4	C-1, 5(3), 4	C-1, 5(3), 4
H-1'	C-1, 2(6), 2', 3'	C-1, 2(6), 2', 1'-OCH ₃	C-1, 2', 3'
H-1'-OCH ₃	-	C-1'	-
H-2'	C-1', 3'	C-1	C-1, 1'
H-3'	C-1', 2', 3'-OCH ₃	C-1', 2', 3'-OCH ₃	C-1', 3'-OCH ₃
H-3'-OCH ₃	C-3'	C-3'	C-3'
H-2''	-	-	C-1''
H-3''	-	-	C-1''

