

Supporting Information

Rec. Nat. Prod. X:X (2019) XX-XX

Thymol Derivatives from *Eupatorium fortunei*

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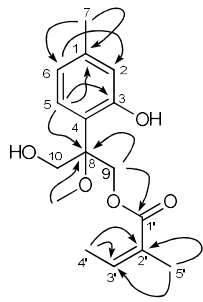
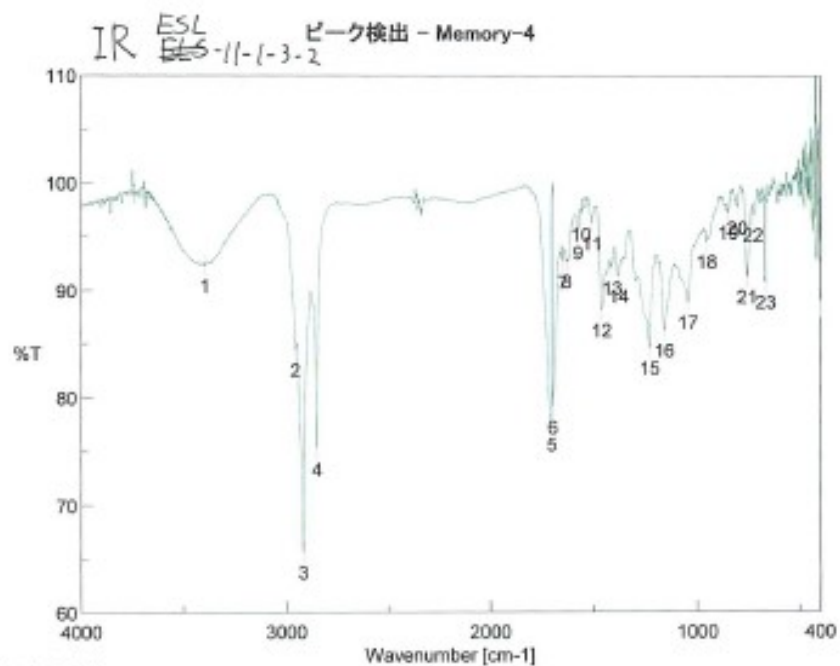


Figure S1. HMBC correlations of compound **1**



[コメント情報]

試料名
コメント
測定者
所属
会社
安田女子大学 薬学部

[データ情報]

作成日時 2017/06/24 10:03
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.916 cm-1
エンド 4000.12 cm-1
データ間隔 0.241058 cm-1
データ数 14936

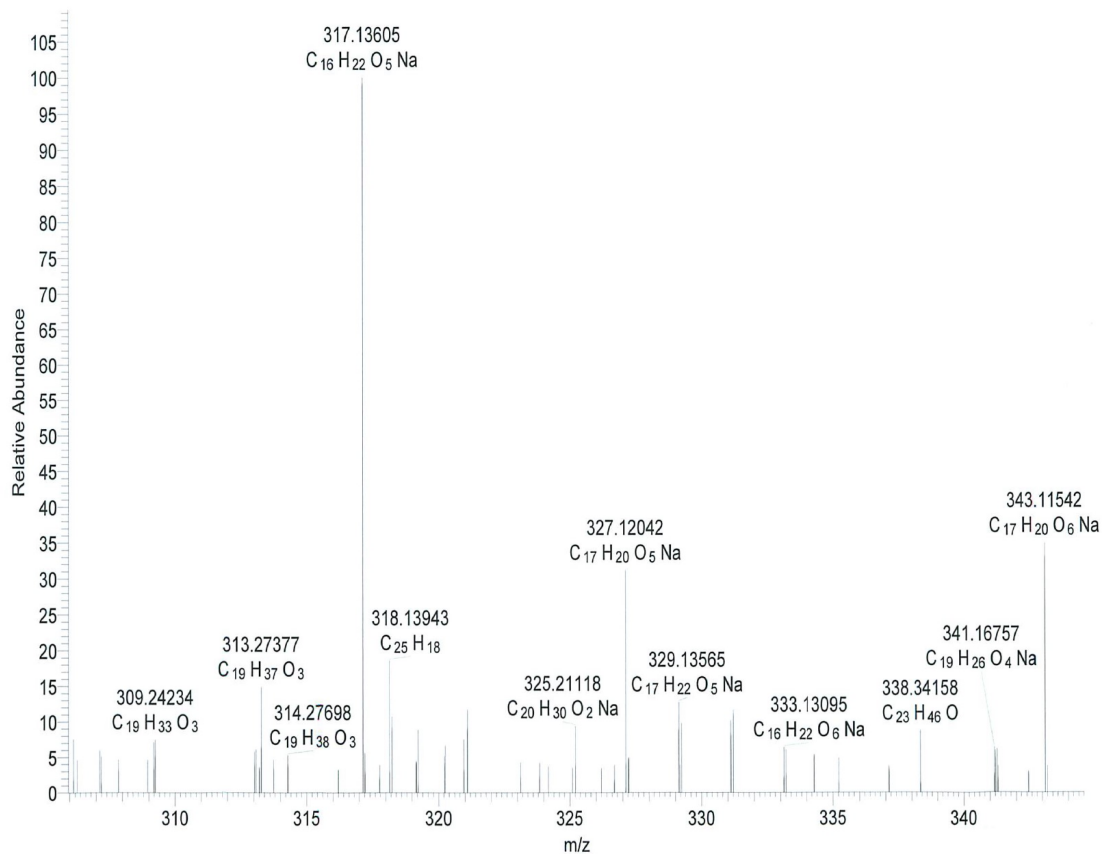
[測定情報]

機種名 FT/IR-6100typeA
シリアル番号 A024251020
光源 標準光源
検出器 TGS
積算回数 10
分解 1 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (3.5 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (10000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度
①	3396.27	92.32475	②	2953.45	84.41346
③	2917.77	65.60741	④	2849.55	75.22690
5	1703.32	77.49766	⑥	1697.05	79.07168
7	1649.56	92.65968	⑧	1629.8	92.71458
9	1575.32	95.36937	10	1561.58	97.07725
11	1507.58	96.24892	⑫	1462.02	88.11804
13	1412.12	92.09080	14	1379.82	91.32291
⑮	1231.33	84.58101	⑰	1159.49	86.21875
⑱	1045.23	88.86149	18	952.904	94.54465

Figure S2. IR spectrum of compound 1



Elemental composition search on mass 317.14

m/z= 312.14-322.14

m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
317.13605	317.13594	0.11	5.5	C ₁₆ H ₂₂ O ₅ Na
	317.13835	-2.30	8.5	C ₁₈ H ₂₁ O ₅
	317.13248	3.57	17.5	C ₂₅ H ₁₇
	317.13007	5.98	14.5	C ₂₃ H ₁₈ Na
	317.14422	-8.17	-0.5	C ₁₁ H ₂₅ O ₁₀
	317.12309	12.96	4.5	C ₁₄ H ₂₁ O ₈
	317.15120	-15.15	9.5	C ₂₀ H ₂₂ O ₂ Na
	317.12069	15.36	1.5	C ₁₂ H ₂₂ O ₈ Na
	317.15361	-17.56	12.5	C ₂₂ H ₂₁ O ₂
	317.11722	18.83	13.5	C ₂₁ H ₁₇ O ₃

Figure S3. Positive-ion HR-ESI-MS spectrum of compound **1**

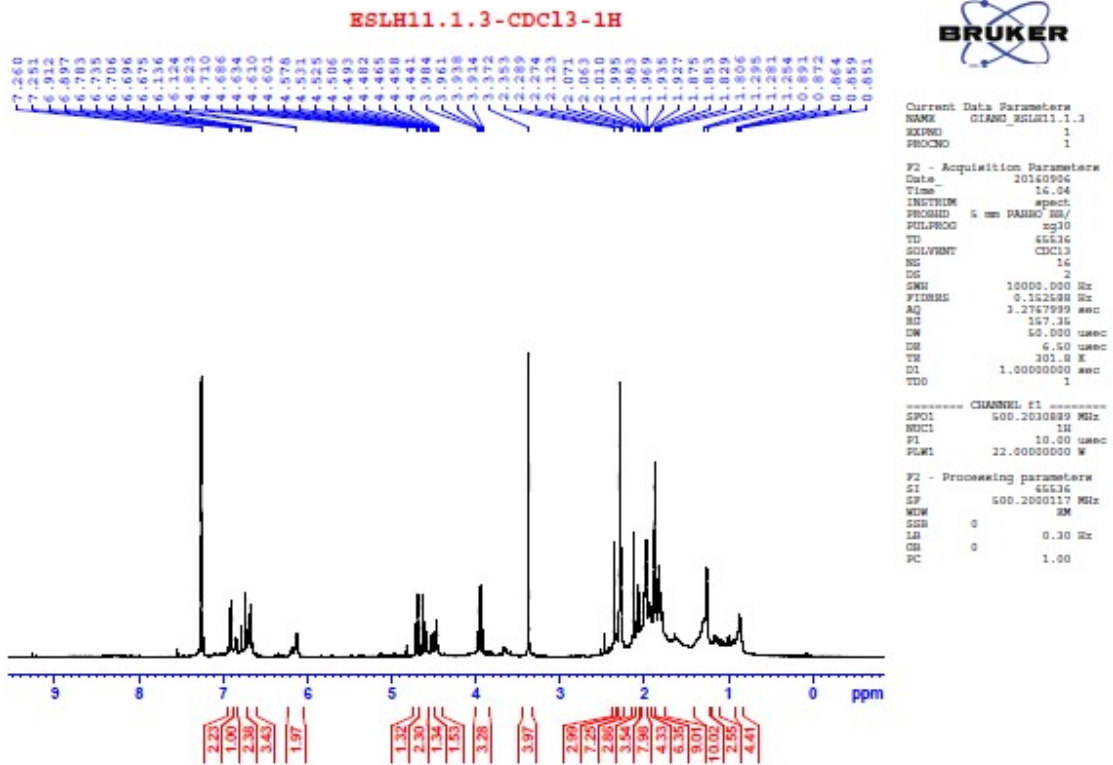


Figure S4. ¹H NMR spectrum (CDCl₃) of compound 1

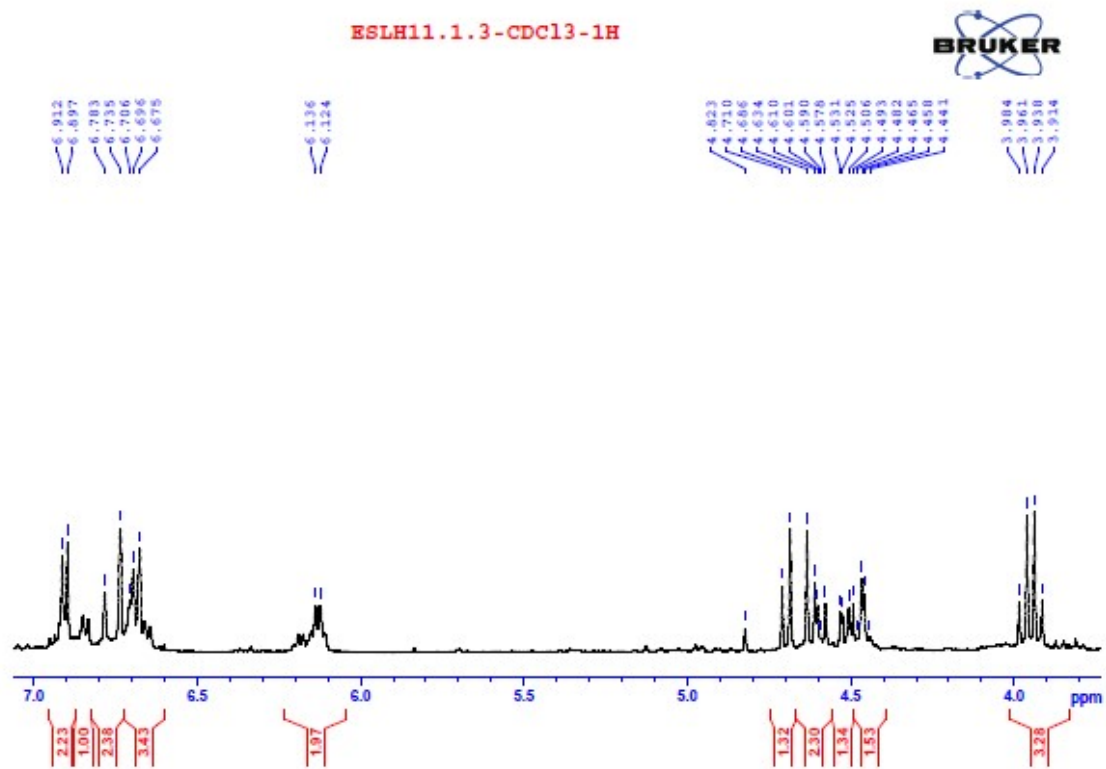


Figure S5. Expanded ^1H NMR spectrum (CDCl_3) of compound **1**

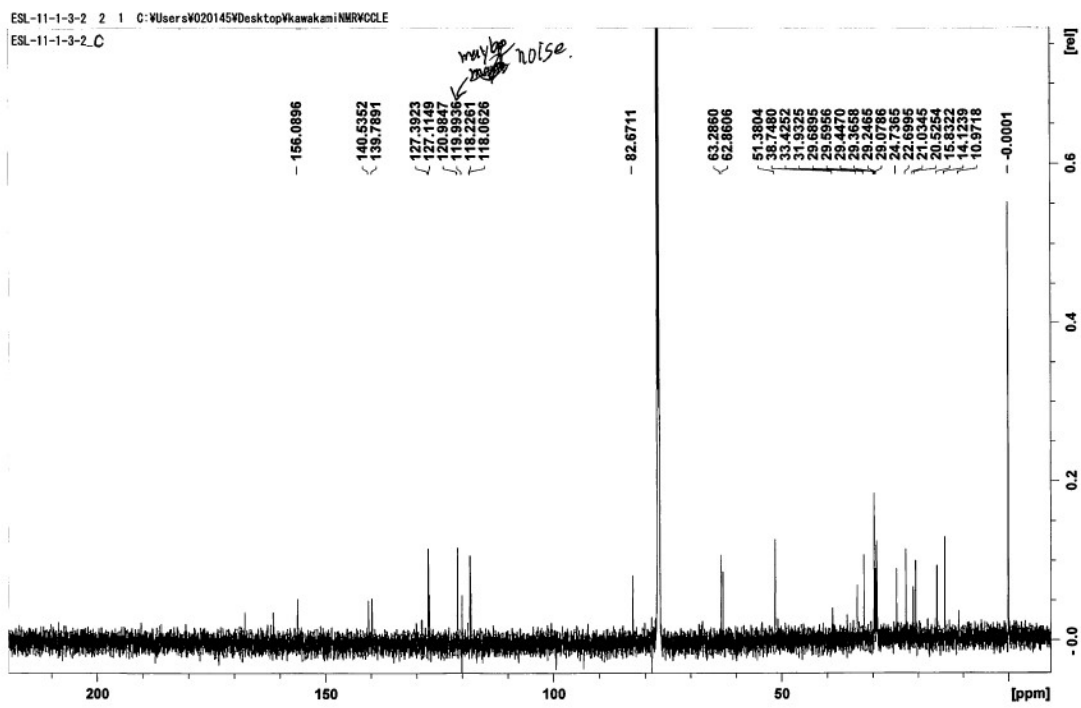


Figure S6. ^{13}C NMR spectrum (CDCl_3) of compound 1

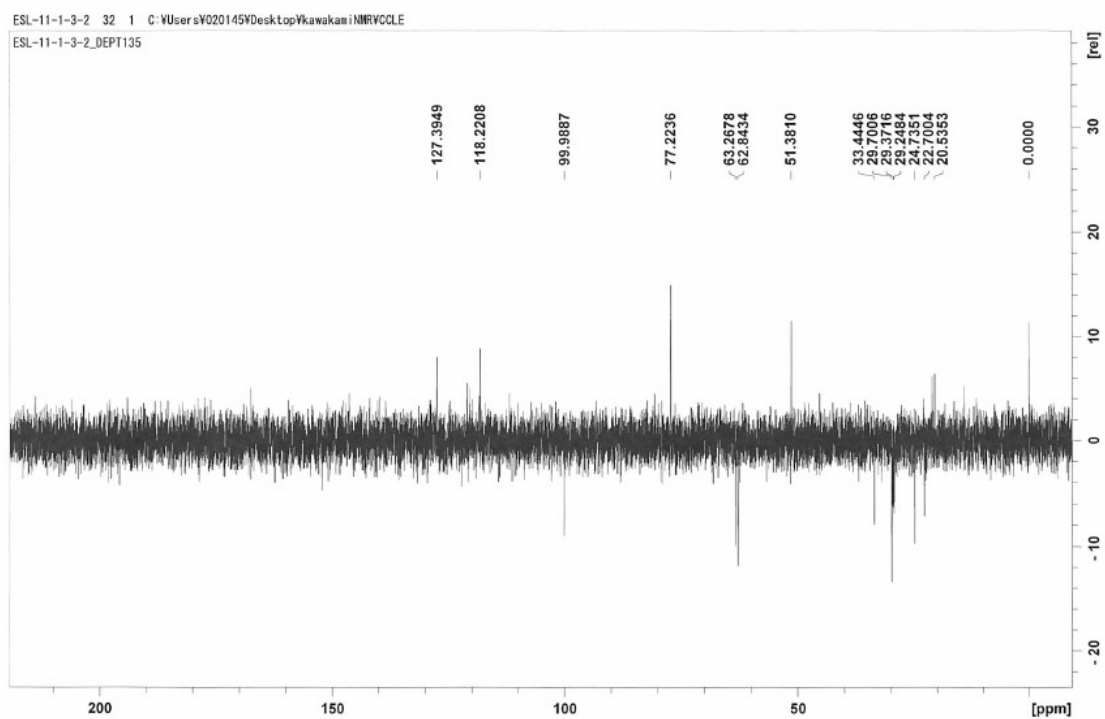


Figure S7. DEPT 135 spectrum of compound **1**

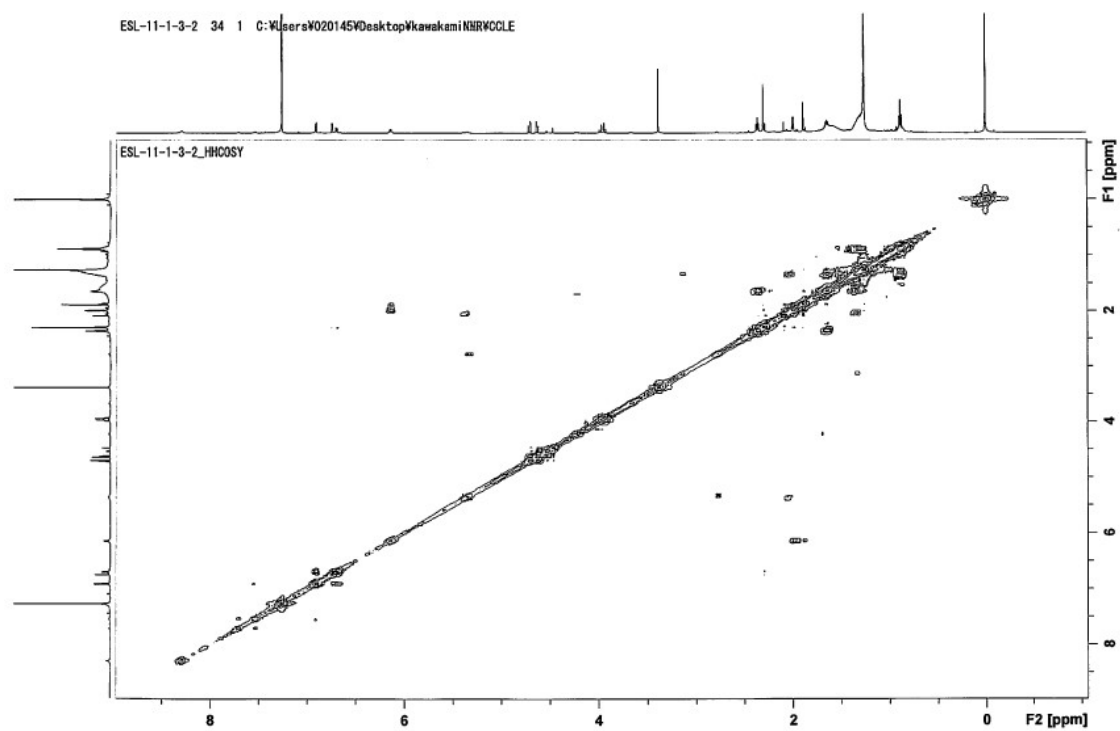


Figure S8. ^1H - ^1H COSY spectrum of compound **1**

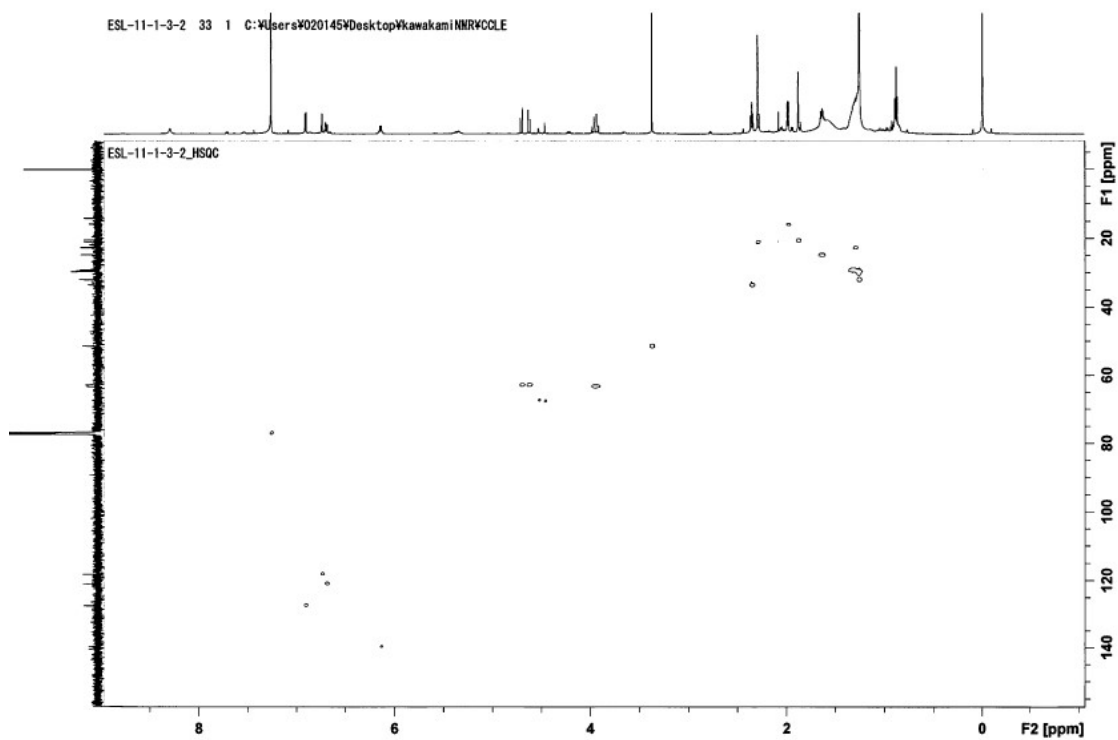


Figure S9. HSQC spectrum of compound **1**

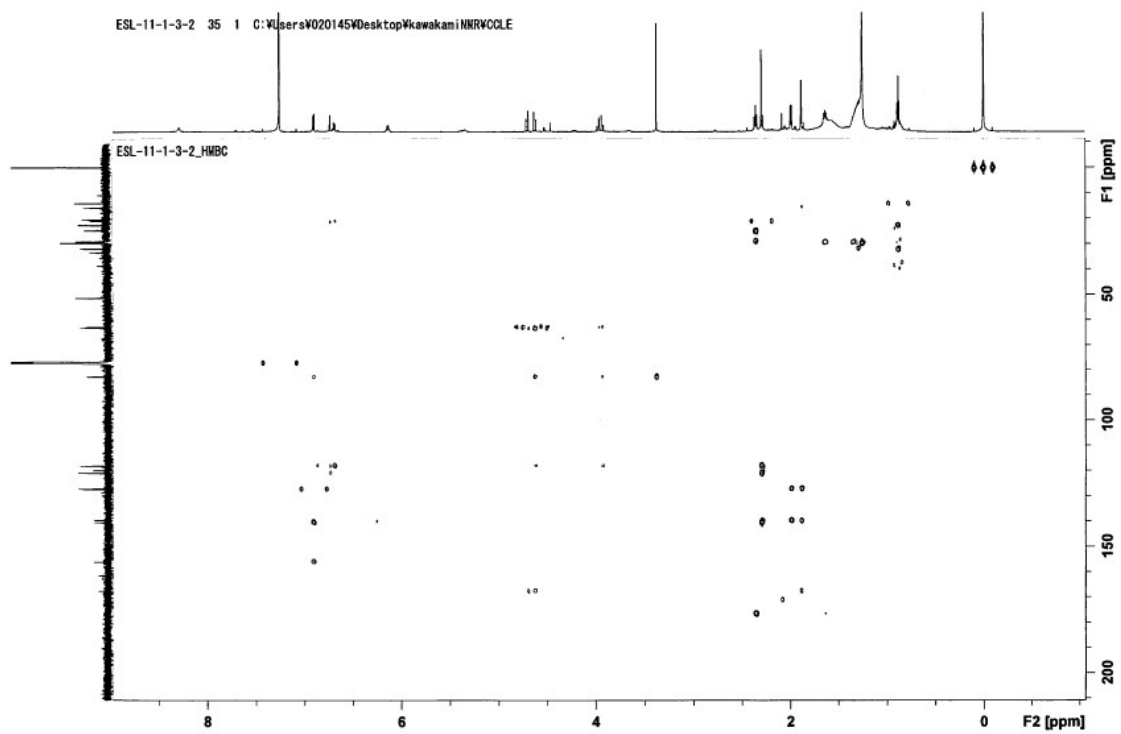


Figure S10. HMBC spectrum of compound 1