

## Supporting Information

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### Thymol Derivatives from *Eupatorium fortunei*

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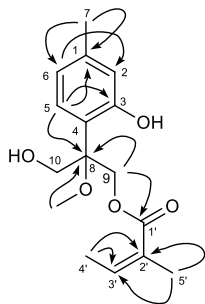
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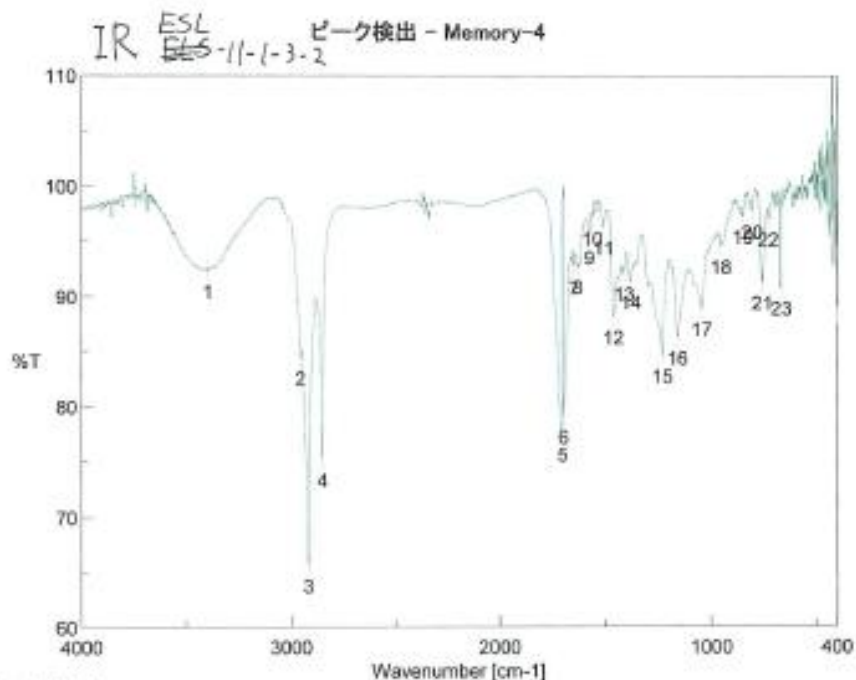
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**Figure S1:** HMBC correlations of compound **1**



[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]

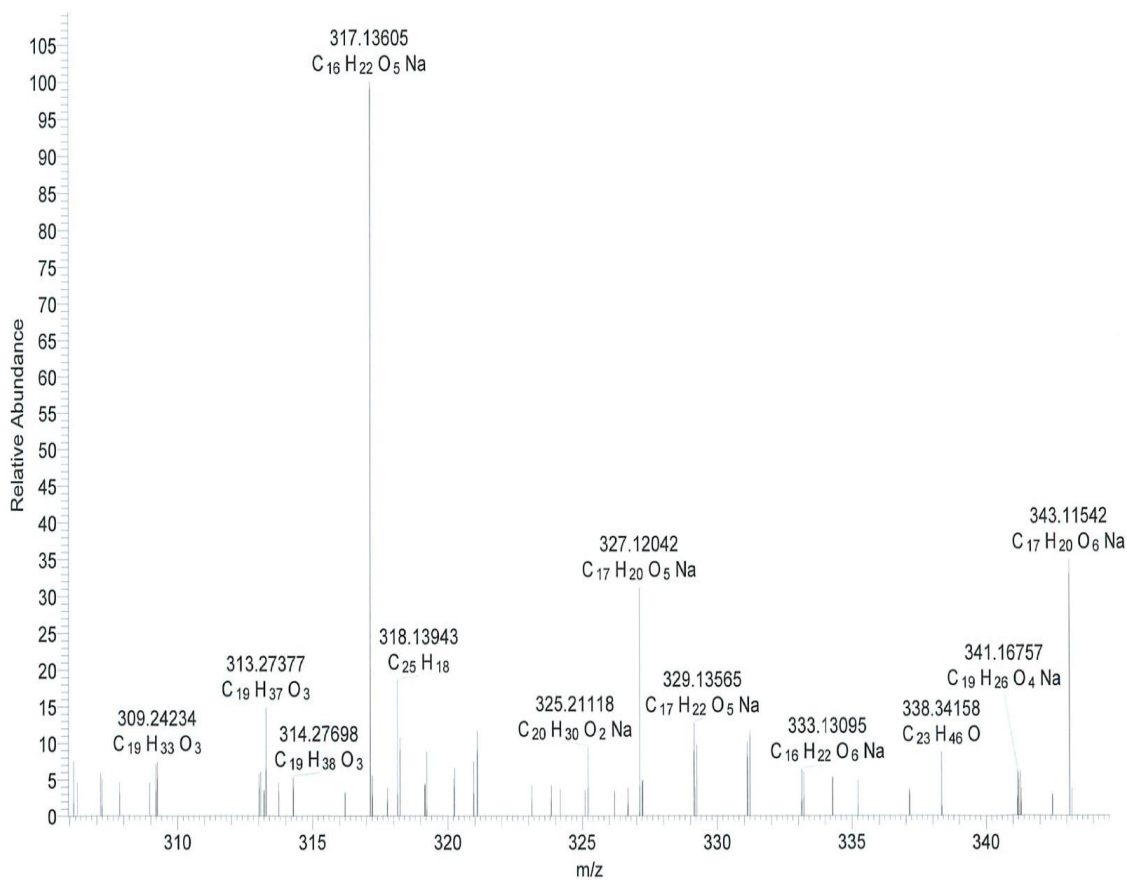
機種名 FT/IR-6100typeA  
シリアル番号 A024251020  
光源 標準光源  
検出器 TGS  
積算回数 10  
分解 1 cm-1  
ゼロフィリング On  
アポダイゼーション Cosine  
ゲイン Auto (8)  
アバーチャー Auto (3.5 mm)  
スキャンスピード Auto (2 mm/sec)  
フィルタ Auto (10000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度
①	3306.27	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	84.56101	⑯	1159.49	86.21875
⑰	1045.23	88.86149	⑱	952.904	94.54465

Figure S2: IR spectrum of compound 1

170622\_31 #7 RT: 0.07 AV: 1 NL: 1.37E5  
T: FTMS + p ESI Full ms [100.00-2000.00]

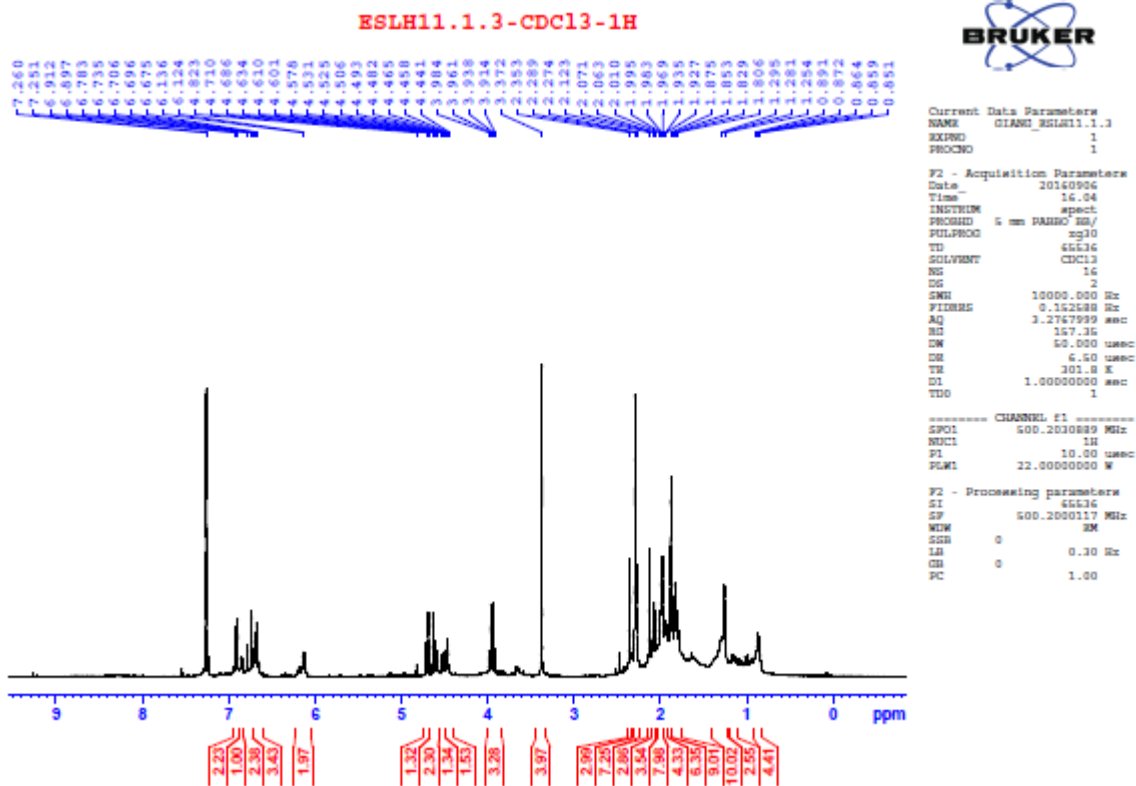


Elemental composition search on mass 317.14

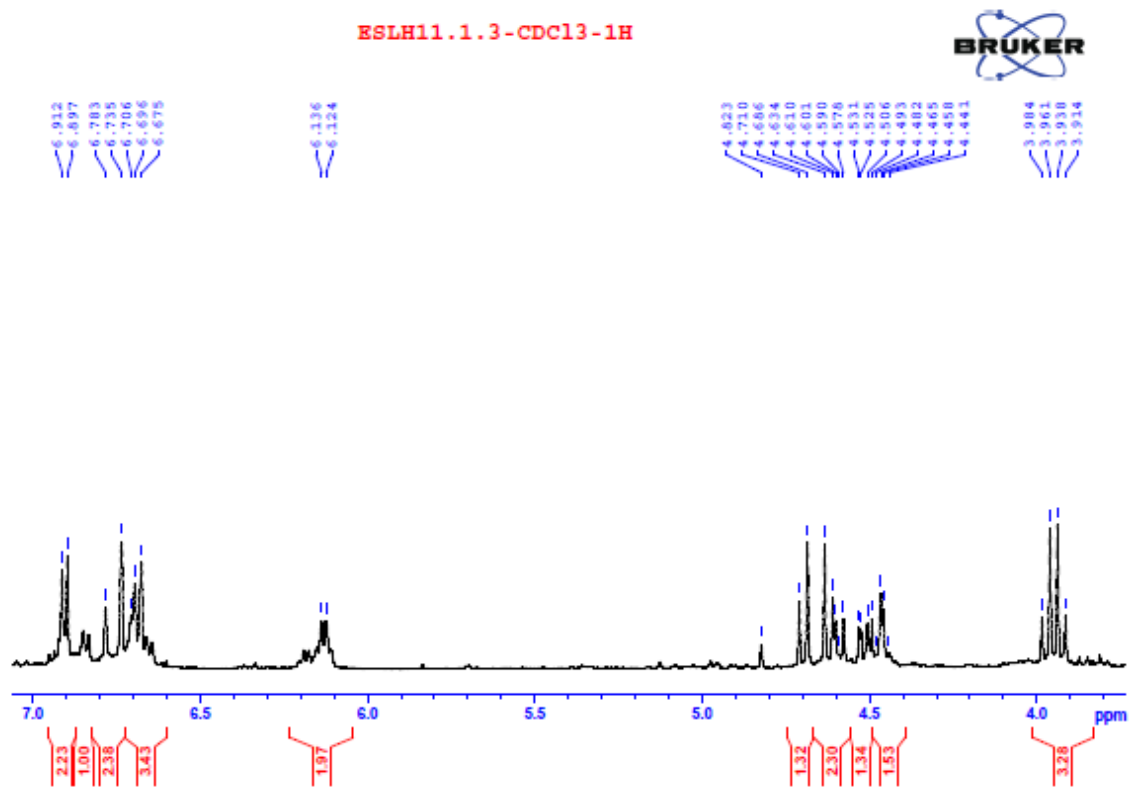
m/z= 312.14-322.14

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

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



**Figure S4:**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ ) of compound **1**



**Figure S5:** Expanded  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ ) of compound **1**

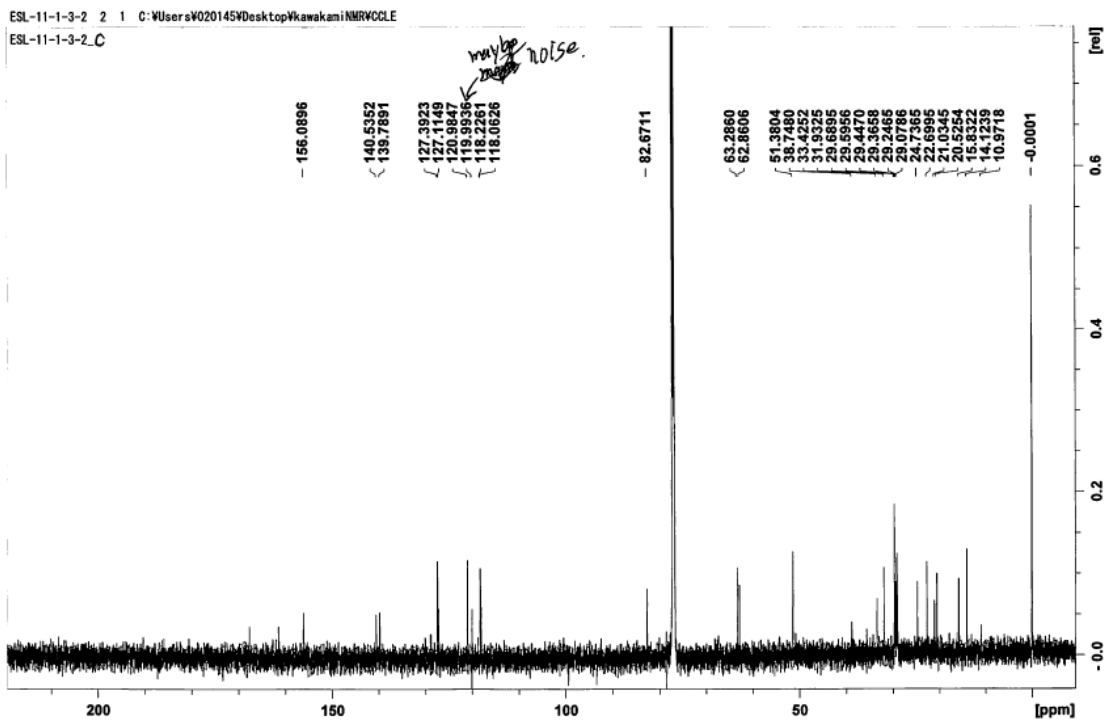
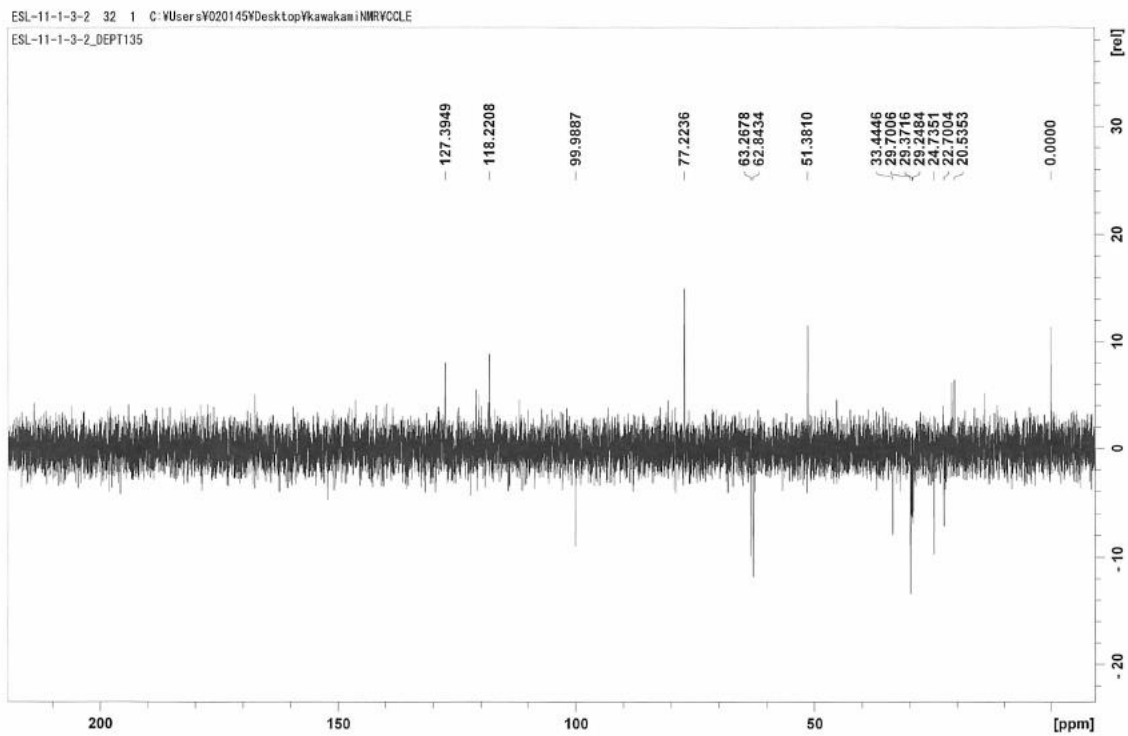
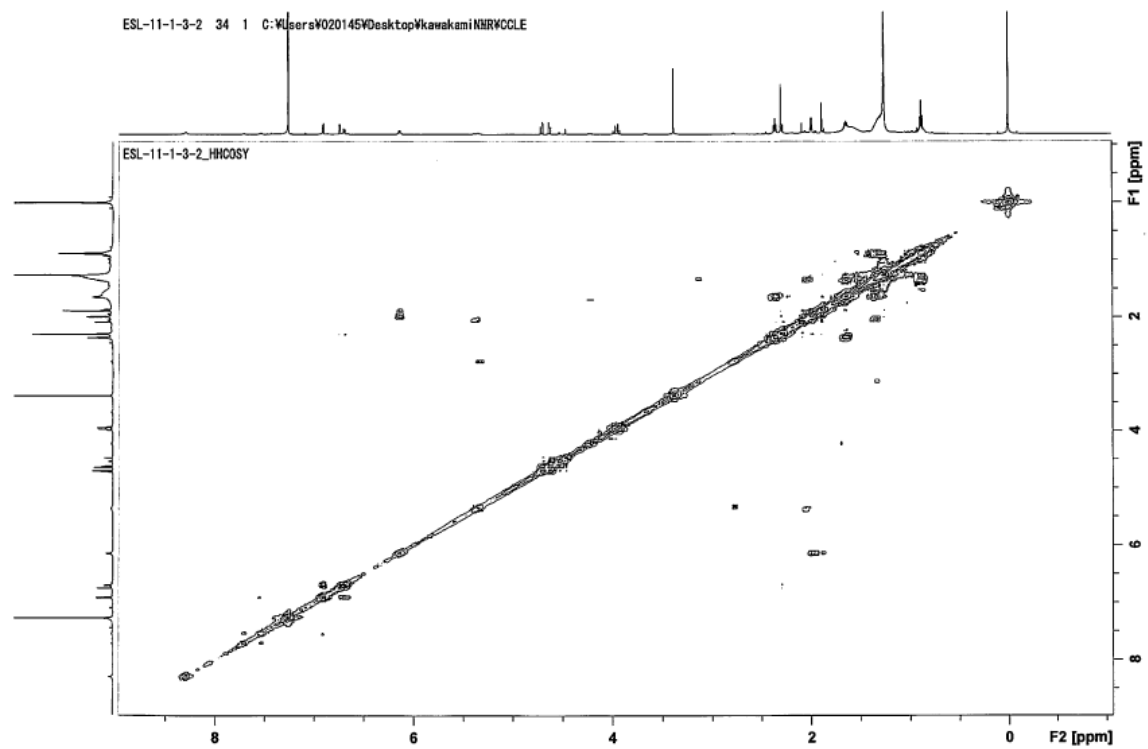


Figure S6:  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ ) of compound **1**

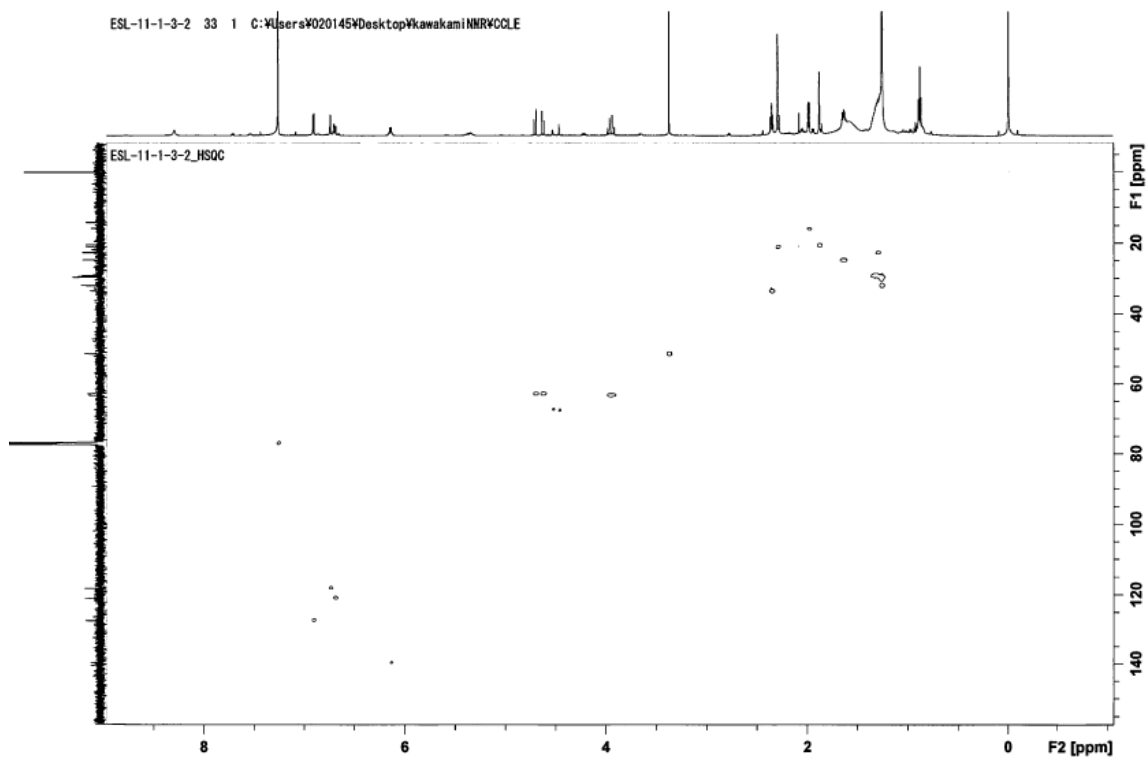


**Figure S7:** DEPT 135 spectrum of compound **1**





**Figure S8:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**



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

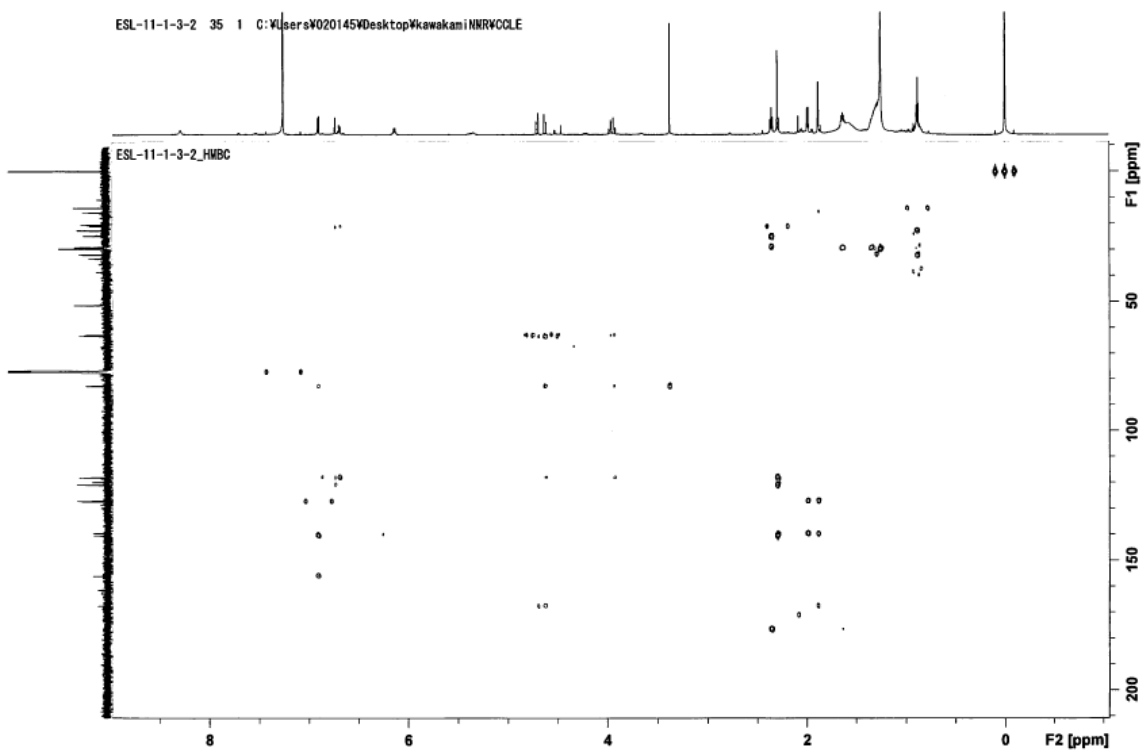


Figure S10: HMBC spectrum of compound 1