Electronic Supplementary Material (ESI) for RSC Advances.


# Incensfuran: Isolation, X-Ray Crystal Structure and Absolute Configuration by Means of Chiroptical Studies in Solution and Solid State

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**Table S1**. Conformers of (1*S*,4*R*,5*R*)-incensfuran (**1**) calculated *in vacuo* at B3LYP/6-311G+(d,p) level with their relative energy ($\Delta E$) and populations (at 298 K).

| **Conformer** | $\Delta E$ / kcal mol$^{-1}$ | Population / % |
|---|---|---|
| **#1** | 0.00 | 74.31 |
| **#2** | 1.00 | 13.78 |
| **#3** | 1.54 | 5.48 |
| **#4** | 1.91 | 2.97 |
| **#5** | 2.10 | 2.14 |
| **#6** | 2.39 | 1.32 |

**Table S2**. Conformers of (1*S*,4*R*,5*R*)-incensfuran (**1**) calculated at B3LYP/6-311G+(d,p) using PCM solvent model for $CHCl_3$ with their relative energy ($\Delta E$) and populations (at 298 K).

| **Conformer** | $\Delta E$ / kcal mol$^{-1}$ | Population / % |
|---|---|---|
| **#1** | 0.00 | 79.51 |
| **#2** | 1.38 | 7.72 |
| **#3** | 1.42 | 7.23 |
| **#4** | 2.06 | 2.46 |
| **#6** | 2.26 | 1.73 |
| **#5** | 2.41 | 1.35 |

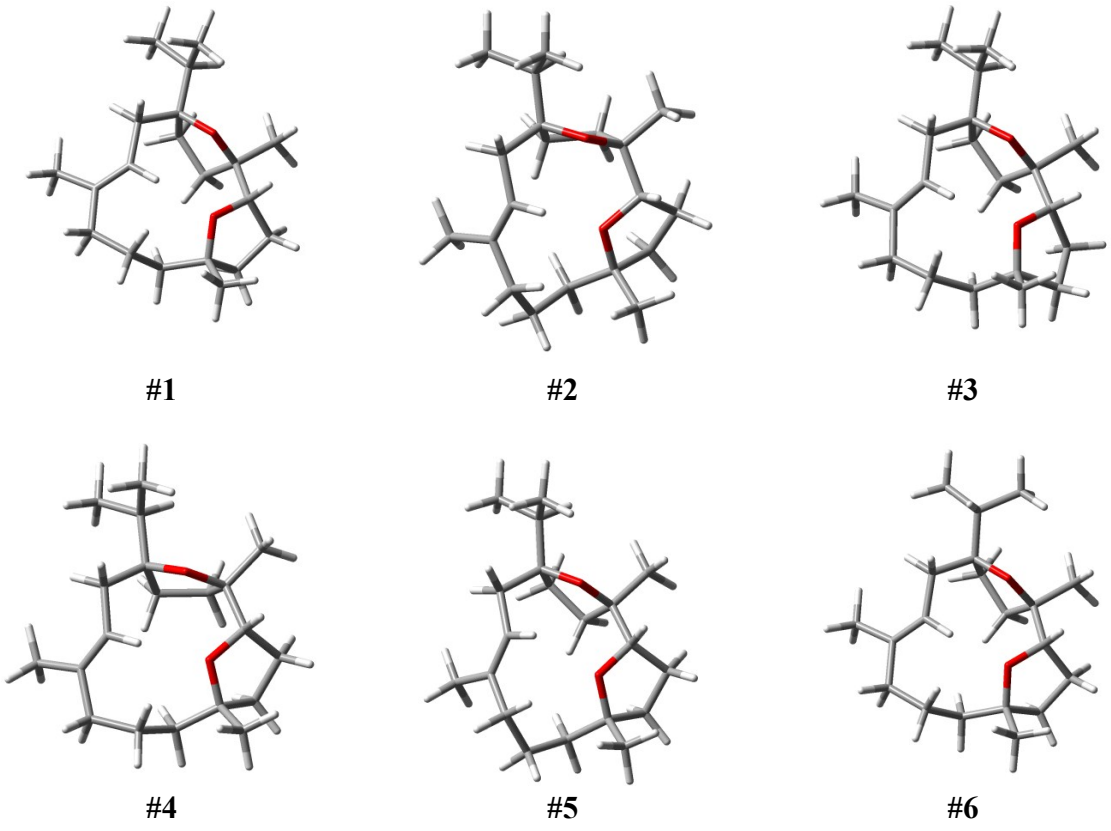


**Figure S1**. Conformers of (1*S*,4*R*,5*R*)-incensfuran (**1**) calculated *in vacuo* at B3LYP/6-311G+(d,p) level of theory.

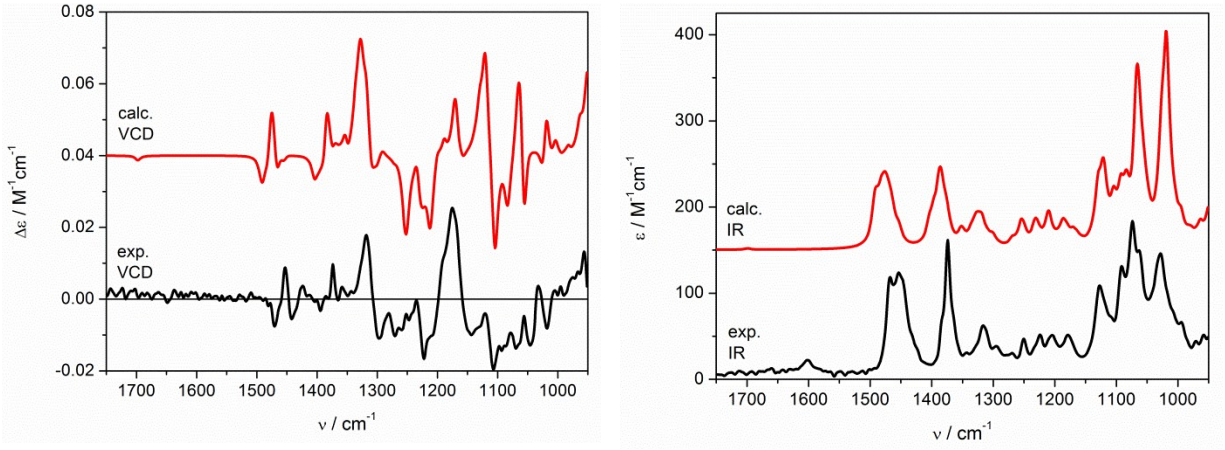


**Figure S2.** Calculated (red lines) and experimental (black lines) VCD (left) and IR (right) spectra for (1*S*,4*R*,5*R*)-incensfuran (**1**). Calculated spectra are shown with a vertical offset for clarity. Calculations run *in vacuo* at B3LYP/6-311+G(d,p) level as Boltzmann average over 6 conformers; for better comparison the calculated VCD spectrum was multiplied by 2; frequencies scaled by a factor 0.985; band-width $\sigma = 6$ cm$^{-1}$.

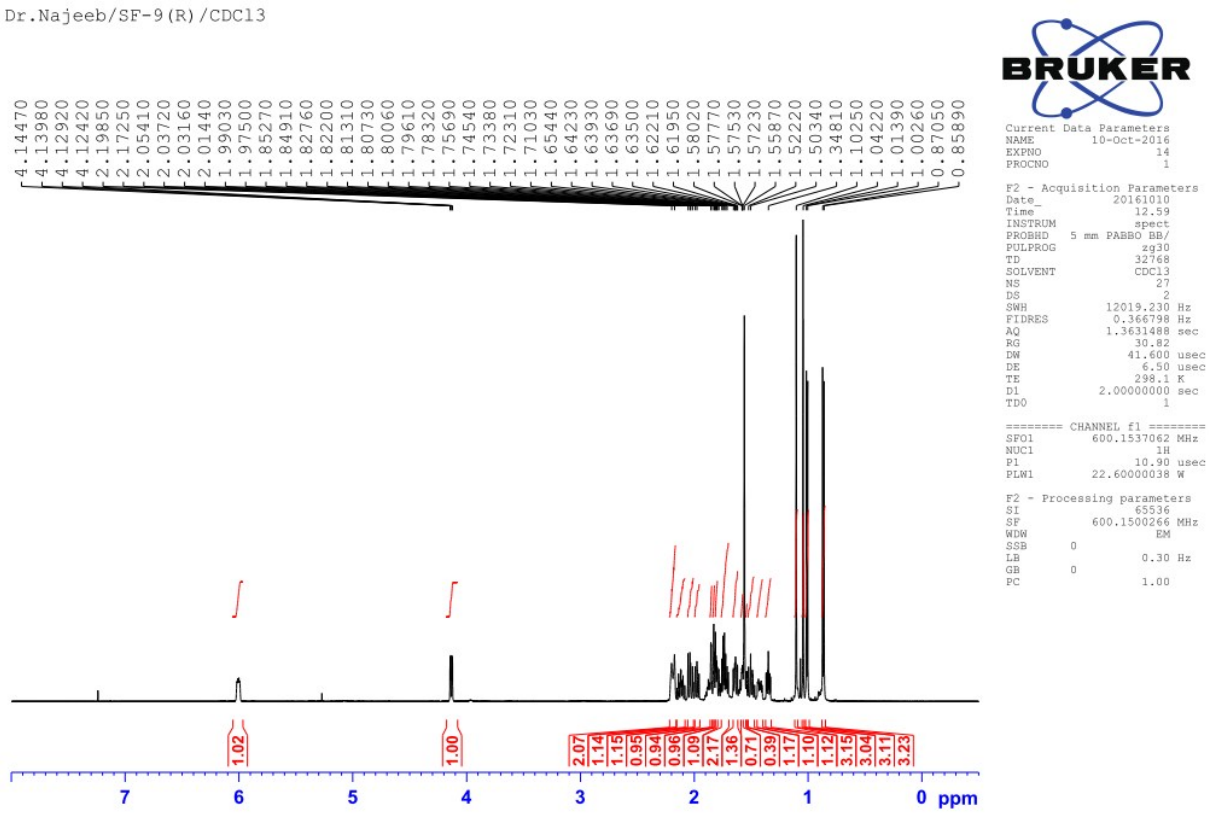


**Figure S3**: $^{1}$H-NMR spectrum ($CDCl_3$) of incensfuran (**1**).

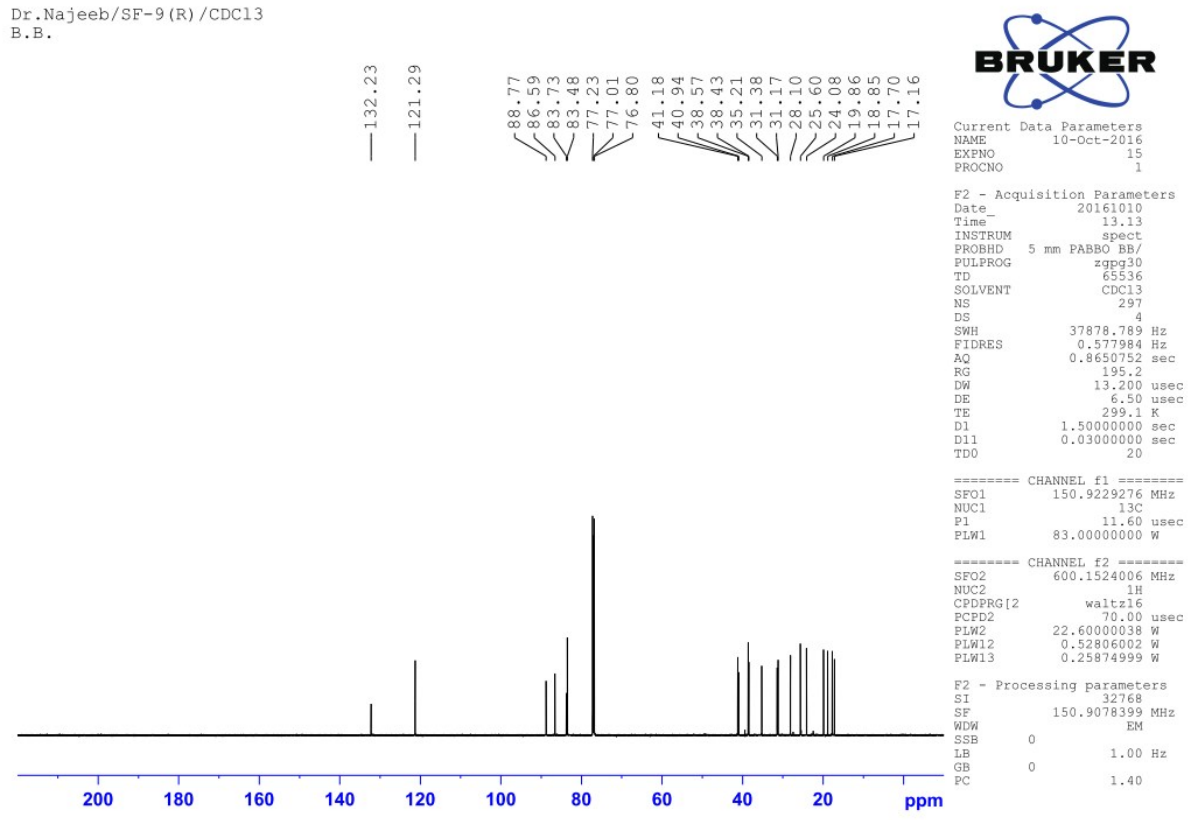


**Figure S4**: $^{13}$C-NMR spectrum ($CDCl_3$) of incensfuran (**1**).

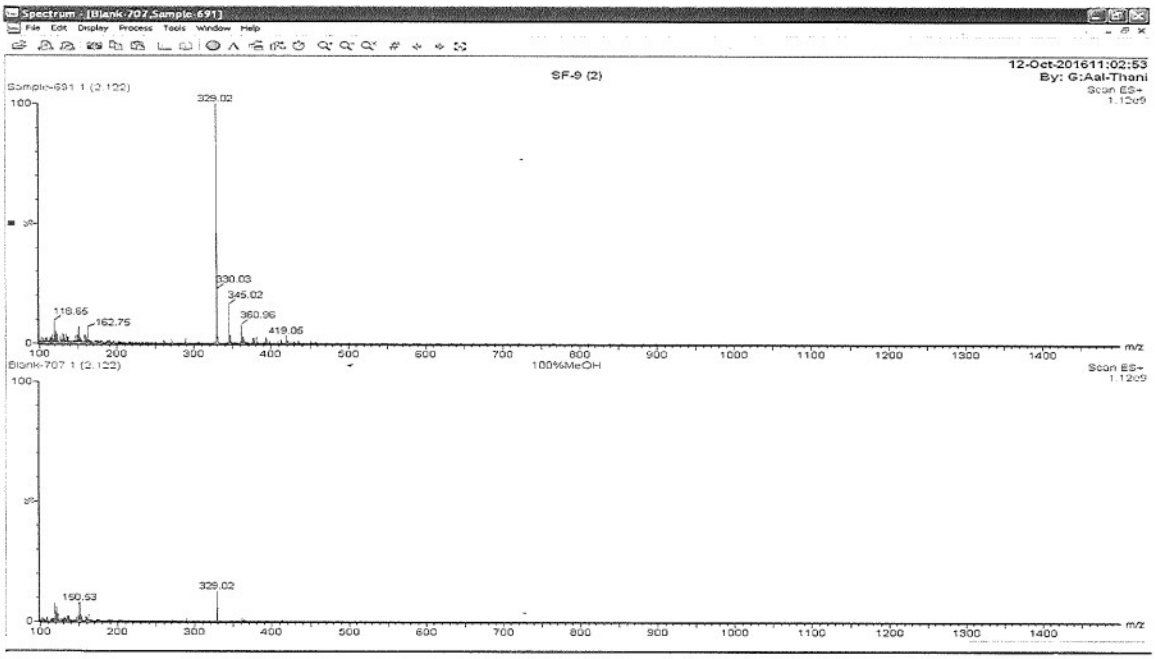


**Figure S5**: ESI-MS spectrum of incensfuran (**1**).

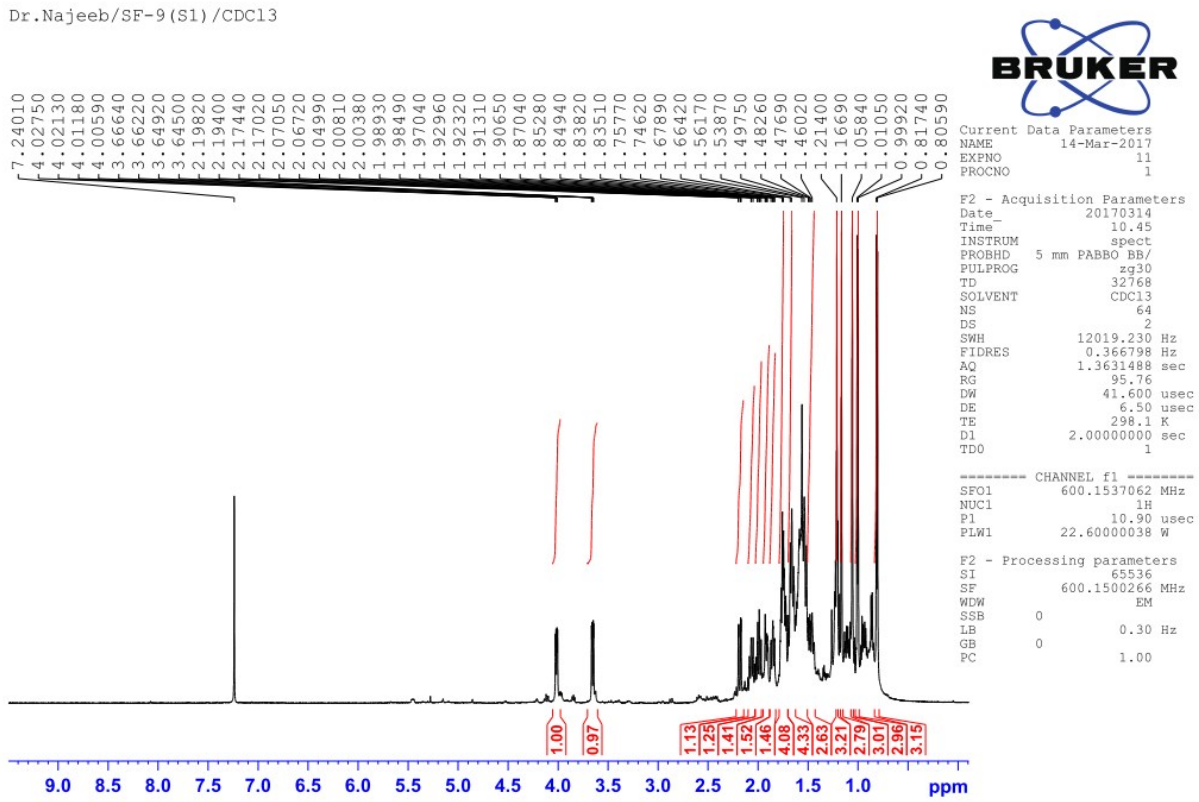


**Figure S6**: $^{1}$H-NMR spectrum ($CDCl_3$) of compound **3**.

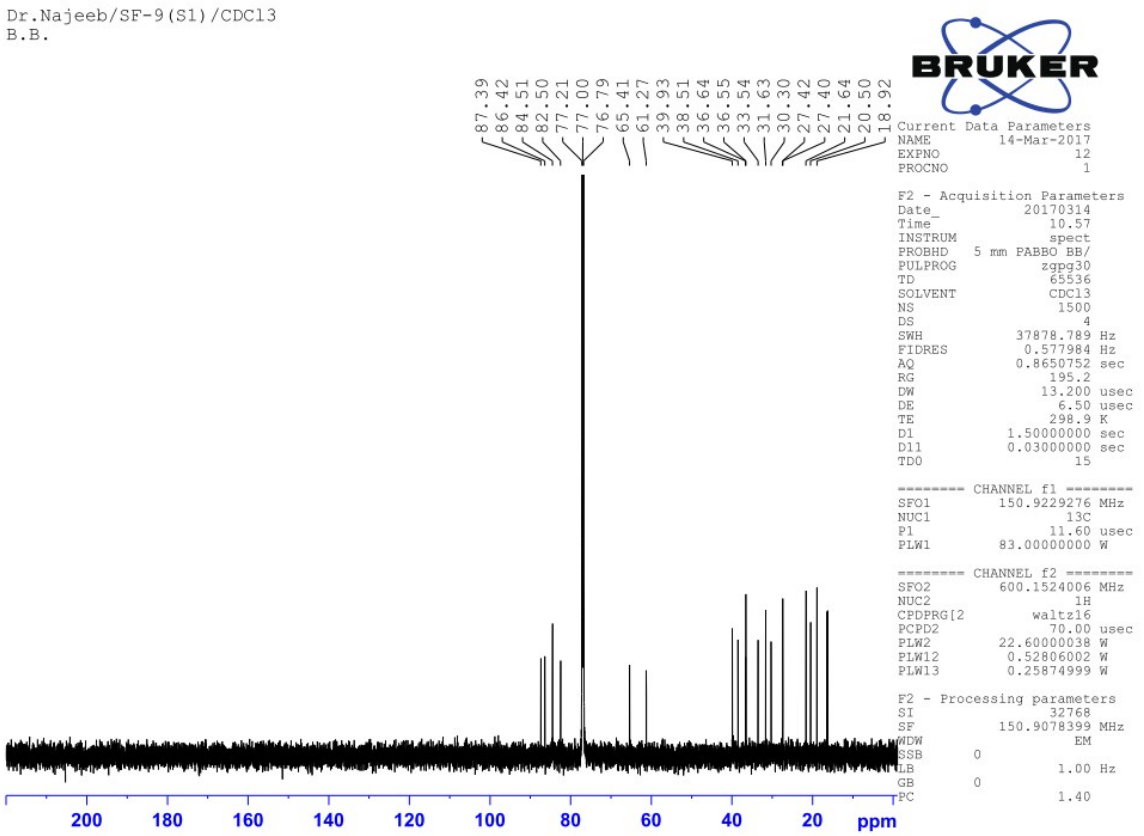


**Figure S7**: $^{13}$C-NMR spectrum ($CDCl_3$) of compound **3**.

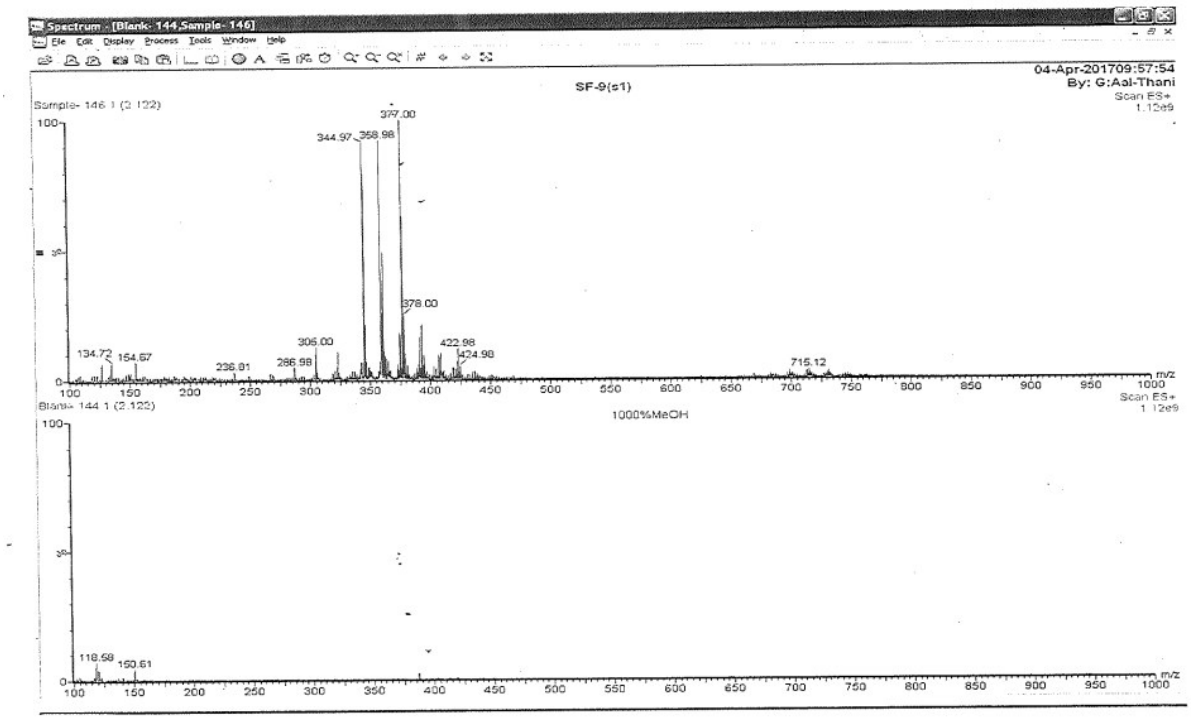


**Figure S8**: ESI-MS spectrum of compound **3**.