

ELECTRONIC SUPPORTING INFORMATION (ESI)

An efficient transformation of furano-hydroxychalcones to furanoflavones via base mediated intramolecular tandem *O*-arylation and C-O bond cleavage: A new approach for synthesis of furanoflavones

Rajni Sharma,^{a,b} Ram A. Vishwakarma,^{a,b} and Sandip B. Bharate^{a,b,*}

^aNatural Products Chemistry Division, CSIR-Indian Institute of Integrative Medicine (CSIR), Canal Road, Jammu-180001, India

^bAcademy of Scientific & Innovative Research (AcSIR), CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu-180001, India

^cMedicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu-180001, India

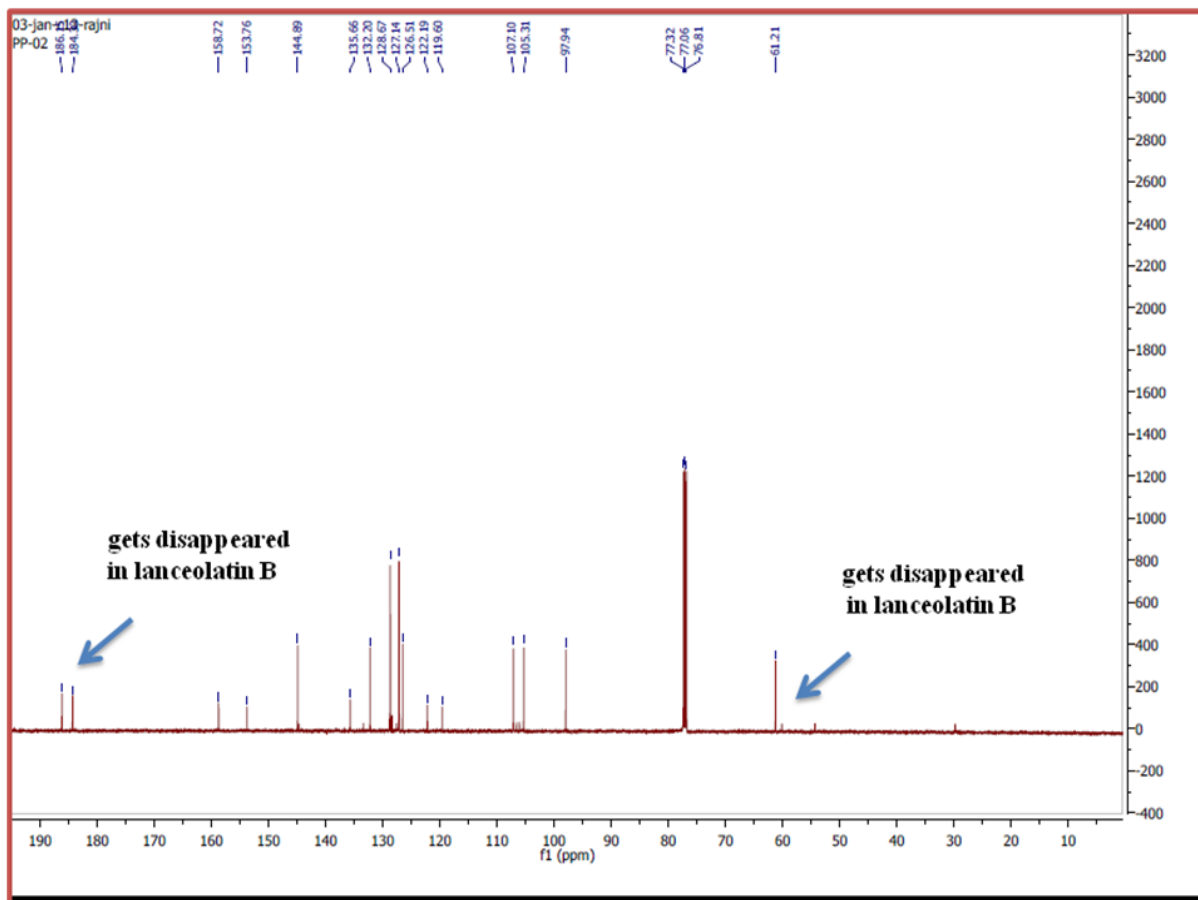
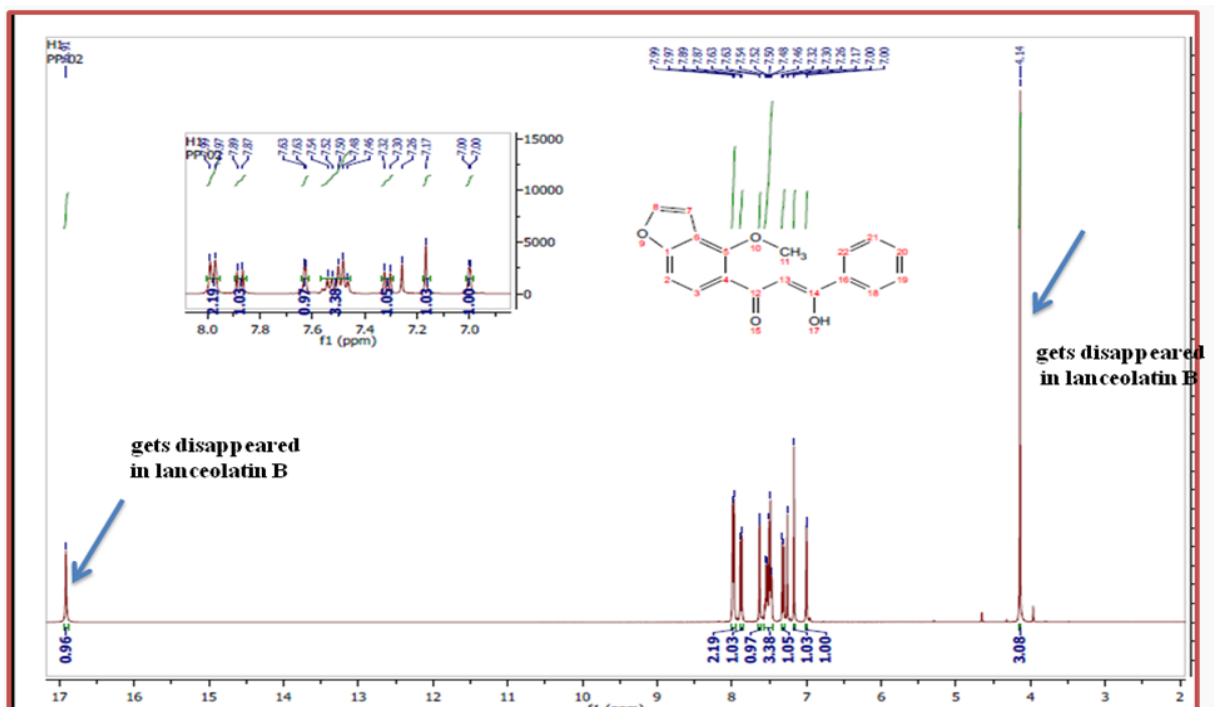
*E-mail: sbharate@iiim.ac.in (SBB)

Fax: +91-191-2585333; Tel: +91-191-2585006

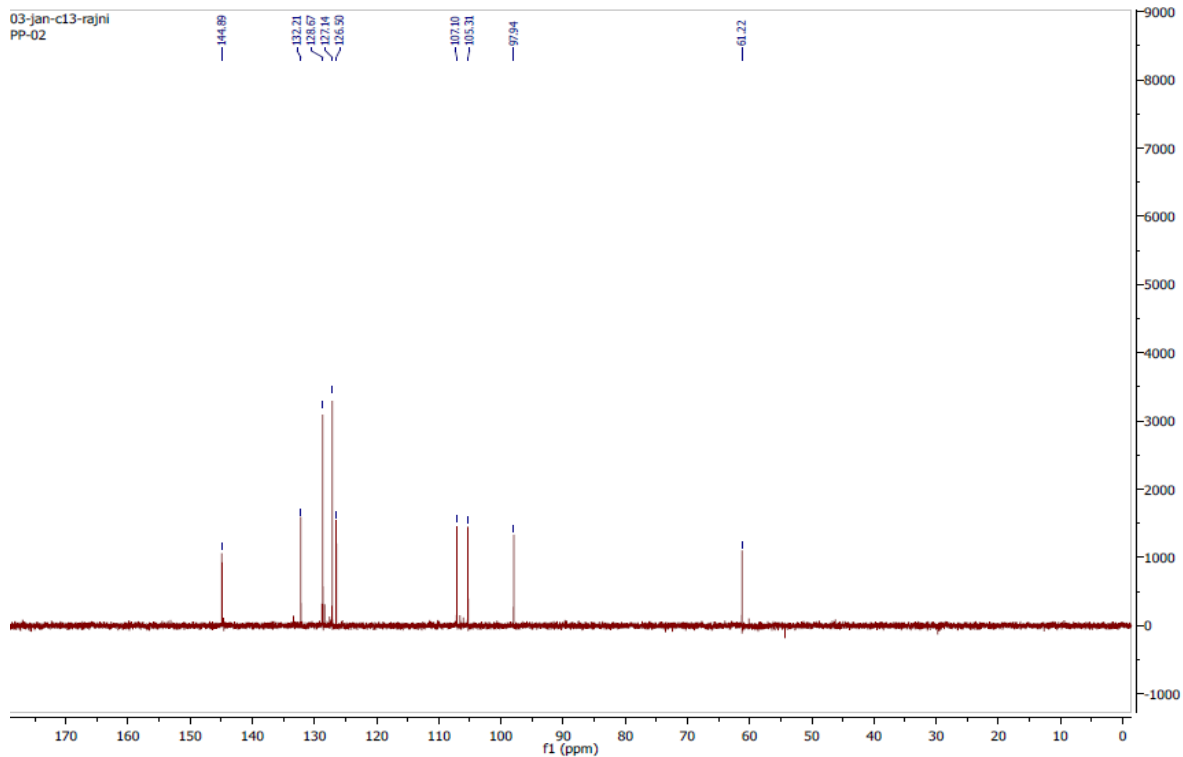
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S1. Scan copies of ^1H , ^{13}C , DEPT-135 NMR (in CDCl_3) and HRMS of pongamol (1a)

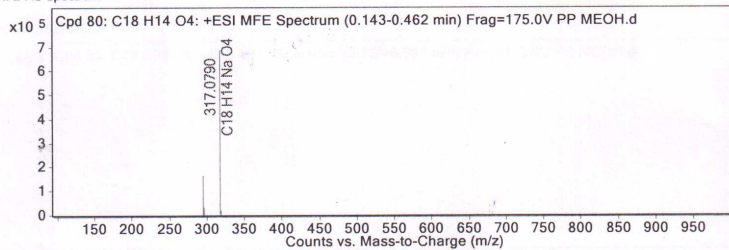


03-jan-c13-rajni
PP-02



| Compound Label | m/z | RT | Algorithm | Mass |
|--------------------|---------|-------|---------------------------|----------|
| Cpd 80: C18 H14 O4 | 317.079 | 0.197 | Find by Molecular Feature | 294.0897 |

MFE MS Spectrum



MS Spectrum Peak List

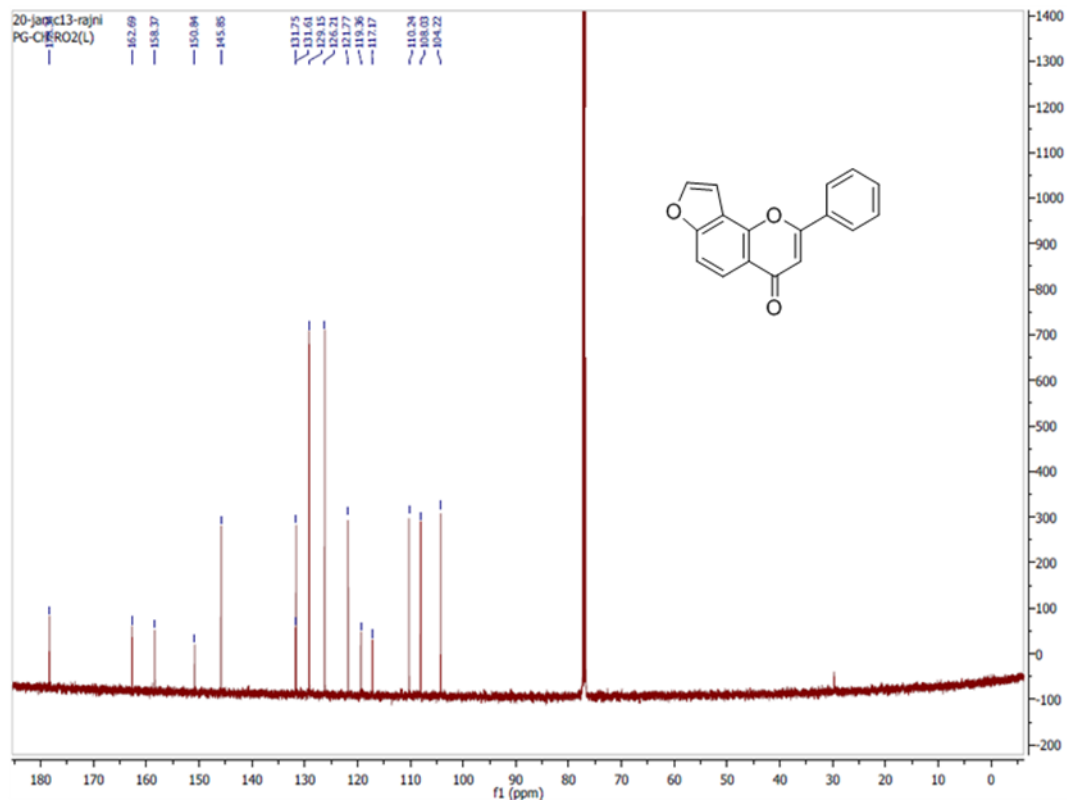
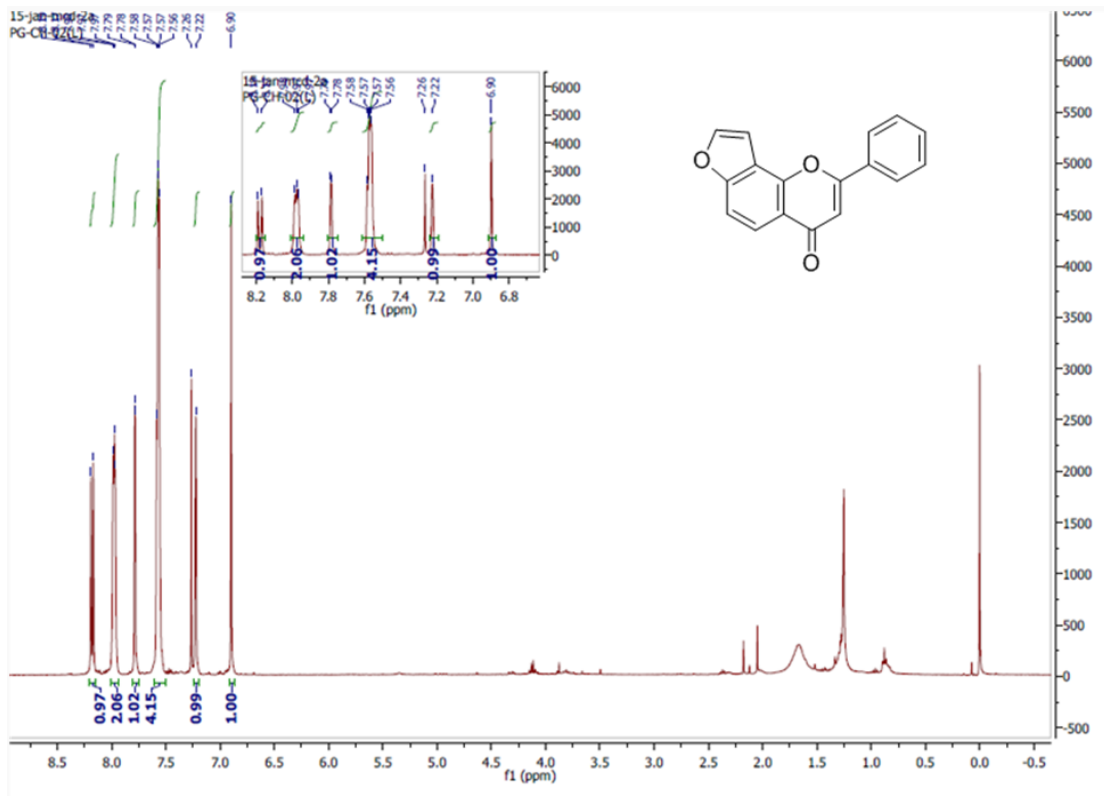
| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|---------------|---------|
| 295.0955 | 1 | 162812.47 | C18 H15 O4 | (M+H)+ |
| 296.0994 | 1 | 31289.7 | C18 H15 O4 | (M+H)+ |
| 317.079 | 1 | 687940.25 | C18 H14 Na O4 | (M+Na)+ |
| 318.0818 | 1 | 124403.03 | C18 H14 Na O4 | (M+Na)+ |
| 319.0862 | 1 | 19246.07 | C18 H14 Na O4 | (M+Na)+ |

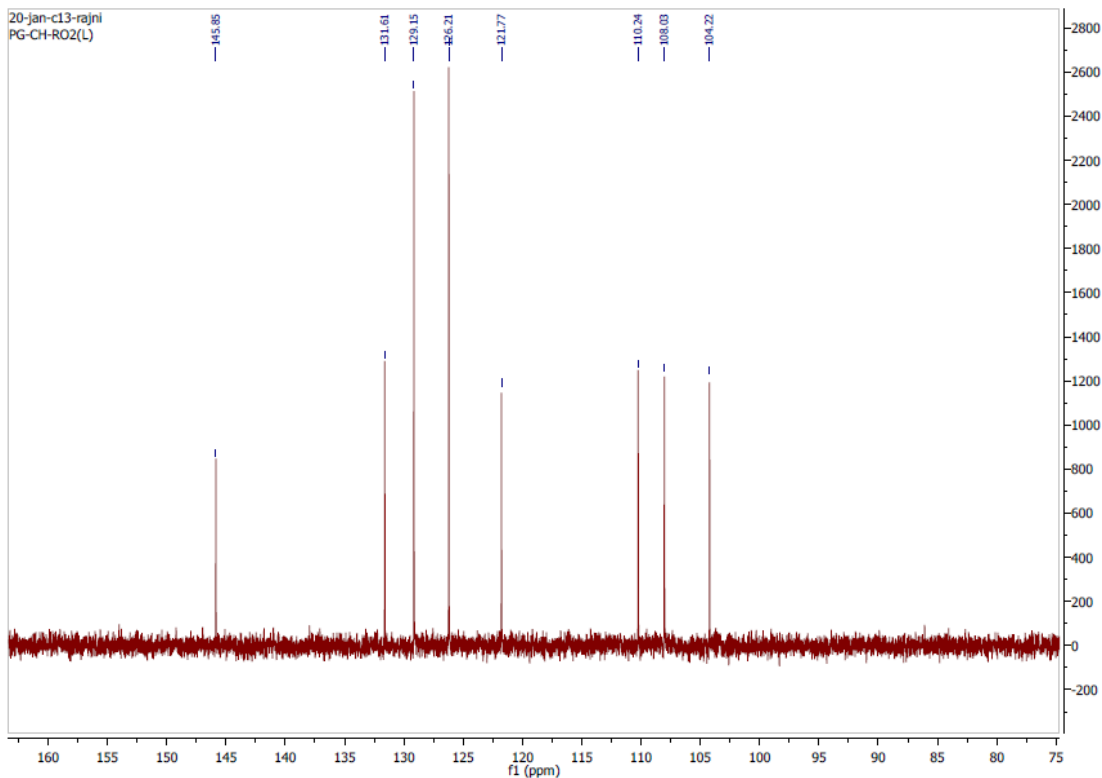
Predicted Isotope Match Table

| Isotope | m/z | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---------|----------|----------|------------|---------|--------------|-------------|------------------|
| 1 | 295.0955 | 295.0965 | 3.36 | 100 | 100 | 83.88 | 83.48 |
| 2 | 296.0994 | 296.0999 | 1.64 | 19.22 | 19.79 | 16.12 | 16.52 |

--- End Of Report ---

S2. Scan copies of ^1H , ^{13}C , DEPT-135 NMR (in CDCl_3) and HRMS of lanceolatin B (**3ab**)



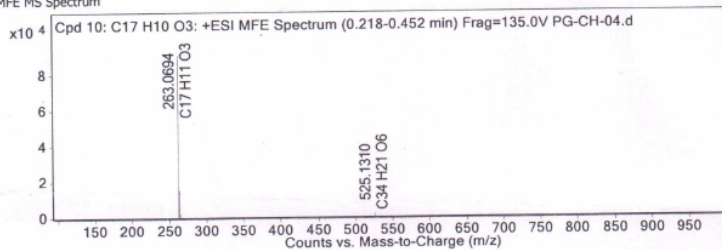


Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|--------------------|-------|----------|------------|-------------|----------------|------------|
| Cpd 10: C17 H10 O3 | 0.285 | 262.0622 | C17 H10 O3 | C17 H10 O3 | 3.17 | C17 H10 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|--------------------|----------|-------|---------------------------|----------|
| Cpd 10: C17 H10 O3 | 263.0694 | 0.285 | Find by Molecular Feature | 262.0622 |

MFE MS Spectrum



263.0702
263.0694
26

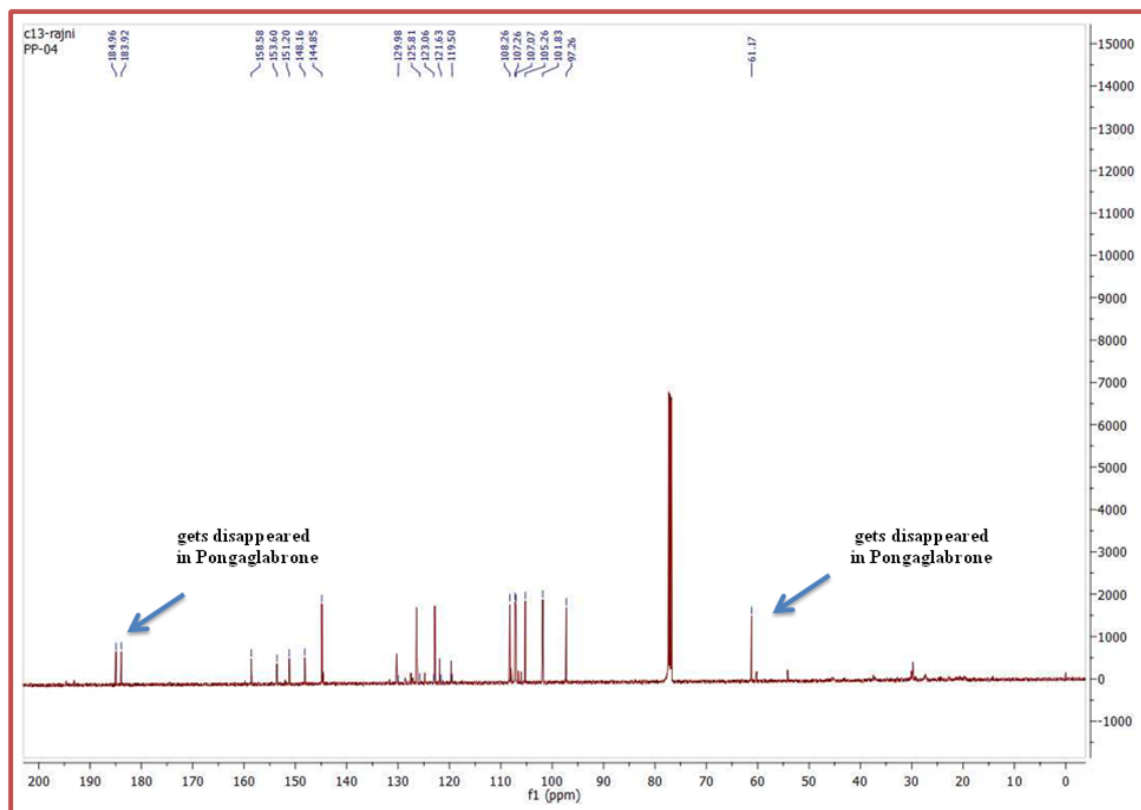
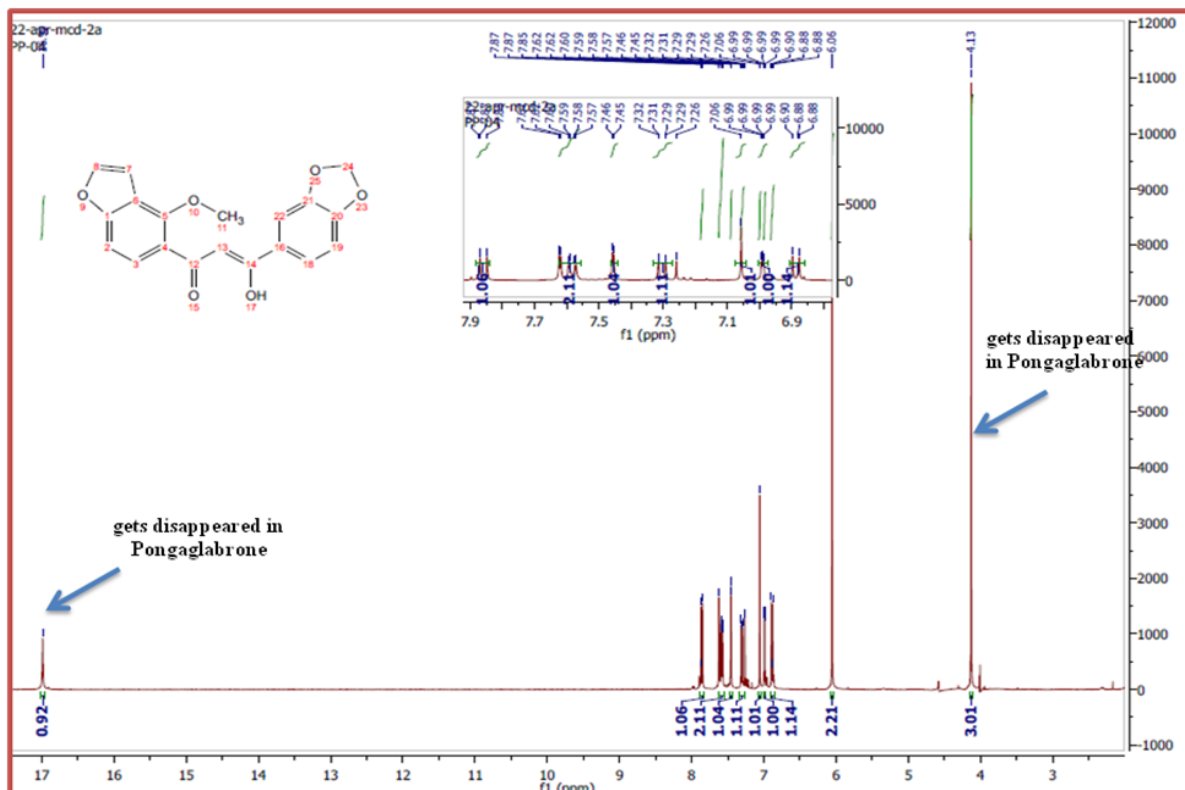
MS Spectrum Peak List

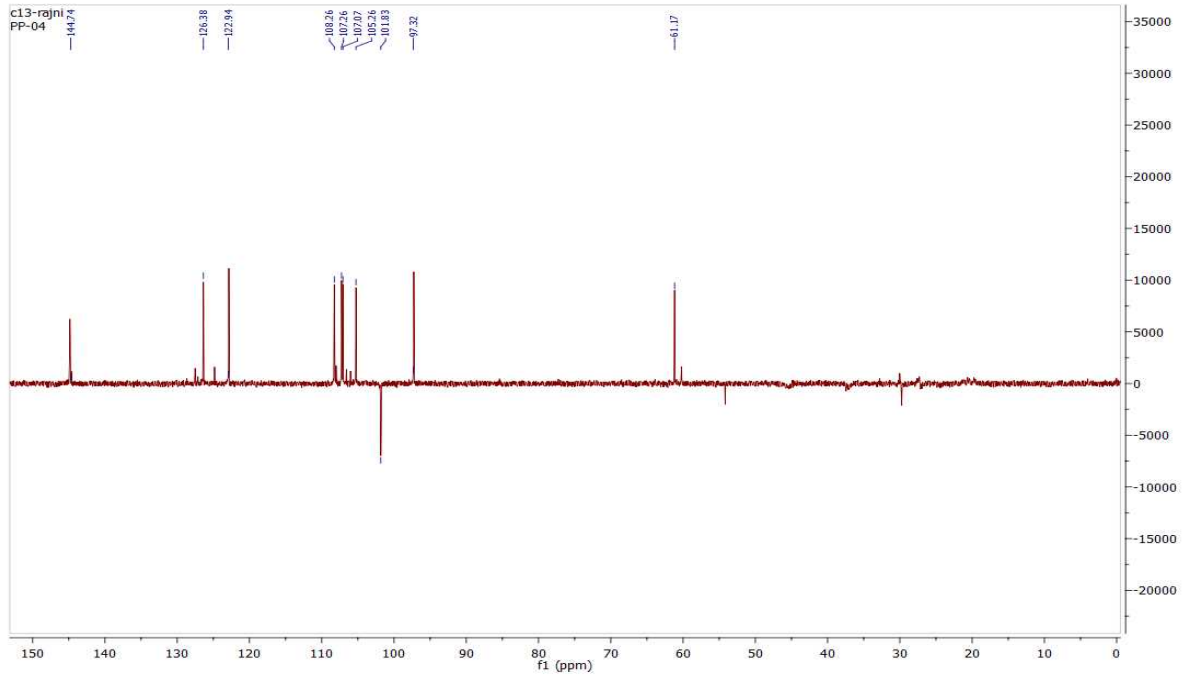
| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|---------|
| 263.0694 | 1 | 90452.87 | C17 H11 O3 | (M+H)+ |
| 264.073 | 1 | 15573.41 | C17 H11 O3 | (M+H)+ |
| 265.0751 | 1 | 2236.65 | C17 H11 O3 | (M+H)+ |
| 266.0756 | 1 | 309.43 | C17 H11 O3 | (M+H)+ |
| 525.131 | 1 | 1565.03 | C34 H21 O6 | (2M+H)+ |
| 526.1338 | 1 | 518.08 | C34 H21 O6 | (2M+H)+ |

Predicted Isotope Match Table

| Isotope | m/z | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---------|----------|----------|------------|---------|--------------|-------------|------------------|
| 1 | 263.0694 | 263.0703 | 3.21 | 100 | 100 | 83.31 | 82.59 |
| 2 | 264.073 | 264.0737 | 2.39 | 17.22 | 18.63 | 14.34 | 15.38 |
| 3 | 265.0751 | 265.0763 | 4.72 | 2.47 | 2.25 | 2.06 | 1.86 |
| 4 | 266.0756 | 266.079 | 12.9 | 0.34 | 0.2 | 0.28 | 0.17 |

S3. Scan copies of ^1H , ^{13}C , DEPT-135 NMR (in CDCl_3) and HRMS of ovalitenone (2a)



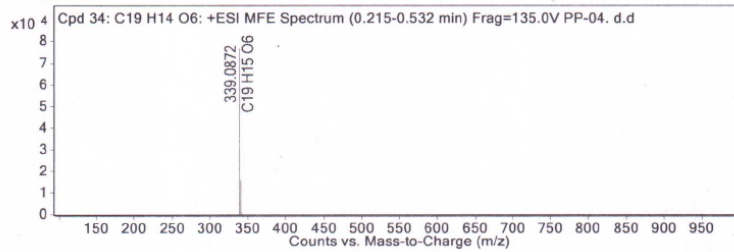


Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|--------------------|-------|----------|------------|-------------|----------------|------------|
| Cpd 34: C19 H14 O6 | 0.283 | 338.0798 | C19 H14 O6 | C19 H14 O6 | -2.35 | C19 H14 O6 |

| Compound Label | m/z | RT | Algorithm | Mass |
|--------------------|----------|-------|---------------------------|----------|
| Cpd 34: C19 H14 O6 | 339.0872 | 0.283 | Find by Molecular Feature | 338.0798 |

MFE MS Spectrum



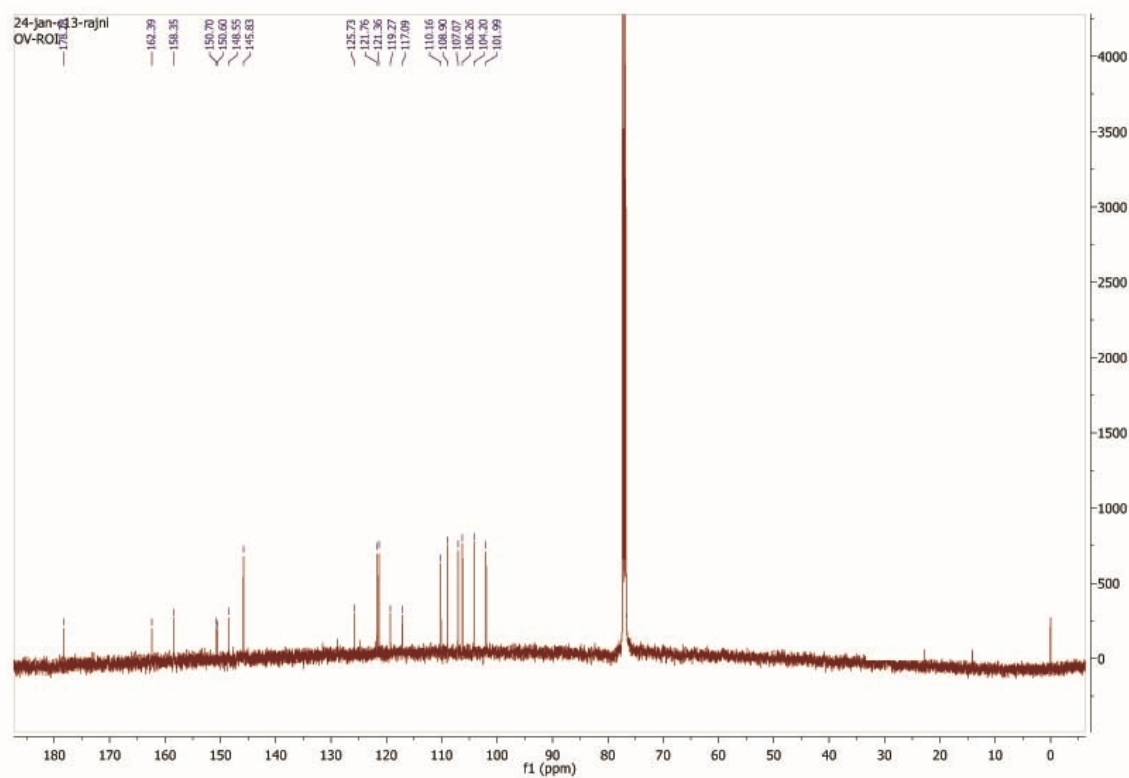
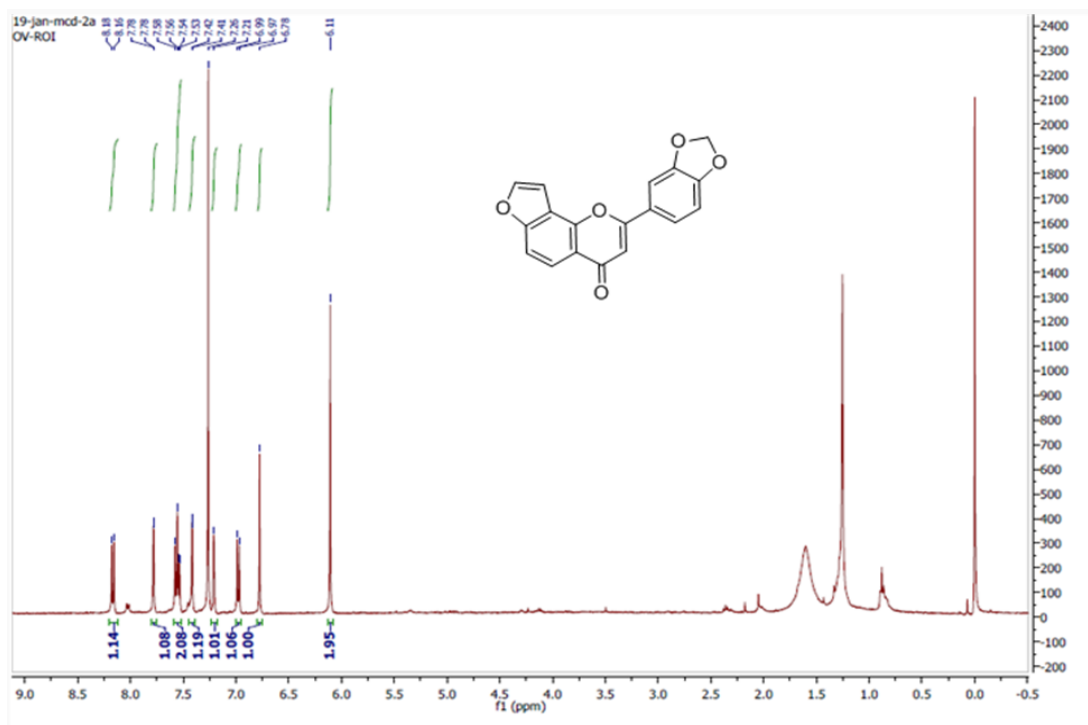
MS Spectrum Peak List

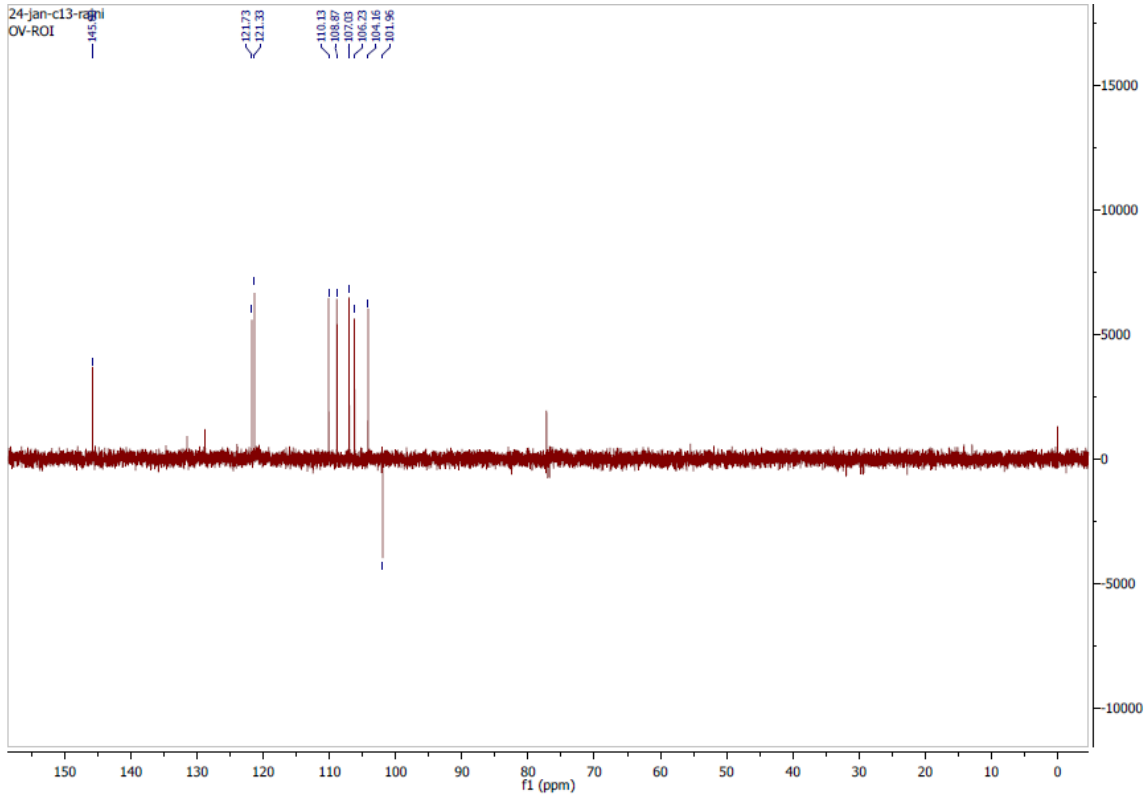
| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|--------|
| 339.0872 | 1 | 76727.1 | C19 H15 O6 | (M+H)+ |
| 340.0903 | 1 | 15908.79 | C19 H15 O6 | (M+H)+ |
| 341.092 | 1 | 3410.74 | C19 H15 O6 | (M+H)+ |
| 342.0964 | 1 | 747.22 | C19 H15 O6 | (M+H)+ |

Predicted Isotope Match Table

| Isotope | m/z | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---------|----------|----------|------------|---------|--------------|-------------|------------------|
| 1 | 339.0872 | 339.0863 | -2.58 | 100 | 100 | 79.27 | 80.22 |
| 2 | 340.0903 | 340.0897 | -1.7 | 20.73 | 20.95 | 16.44 | 16.81 |
| 3 | 341.092 | 341.0922 | 0.45 | 4.45 | 3.32 | 3.52 | 2.66 |
| 4 | 342.0964 | 342.0948 | -4.61 | 0.97 | 0.39 | 0.77 | 0.31 |

S4. Scan copies of ^1H , ^{13}C , DEPT-135 NMR (in CDCl_3) and HRMS of pongaglabrone (**4ab**)



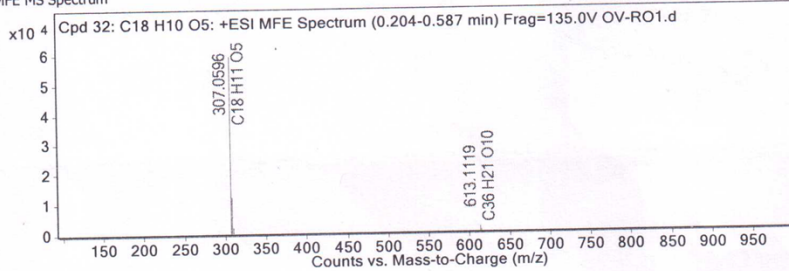


Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|--------------------|-------|----------|------------|-------------|----------------|------------|
| Cpd 32: C18 H10 O5 | 0.279 | 306.0524 | C18 H10 O5 | C18 H10 O5 | 1.29 | C18 H10 O5 |

| Compound Label | m/z | RT | Algorithm | Mass |
|--------------------|----------|-------|---------------------------|----------|
| Cpd 32: C18 H10 O5 | 307.0596 | 0.279 | Find by Molecular Feature | 306.0524 |

MFE MS Spectrum



307.06010

MS Spectrum Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|-------------|---------|
| 307.0596 | 1 | 59277.93 | C18 H11 O5 | (M+H)+ |
| 308.0633 | 1 | 11938.3 | C18 H11 O5 | (M+H)+ |
| 309.0674 | 1 | 2093.85 | C18 H11 O5 | (M+H)+ |
| 310.0655 | 1 | 287.5 | C18 H11 O5 | (M+H)+ |
| 613.1119 | 1 | 1631.01 | C36 H21 O10 | (2M+H)+ |
| 614.1119 | 1 | 809.91 | C36 H21 O10 | (2M+H)+ |
| 615.1076 | 1 | 128.85 | C36 H21 O10 | (2M+H)+ |

Predicted Isotope Match Table

| Isotope | m/z | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---------|----------|----------|------------|---------|--------------|-------------|------------------|
| 1 | 307.0596 | 307.0601 | 1.58 | 100 | 100 | 80.54 | 81.32 |
| 2 | 308.0633 | 308.0635 | 0.67 | 20.14 | 19.79 | 16.22 | 16.09 |
| 3 | 309.0674 | 309.066 | -4.64 | 3.53 | 2.88 | 2.85 | 2.34 |
| 4 | 310.0655 | 310.0686 | 10.07 | 0.48 | 0.31 | 0.39 | 0.25 |