

LCMS CHROMATOGRAM RESULT, SAMPLE ID: ISOLAT EKSTRAK DIKLOROMETANA KULIT BATANG  
SYZYGIUM SAMARANGENSE

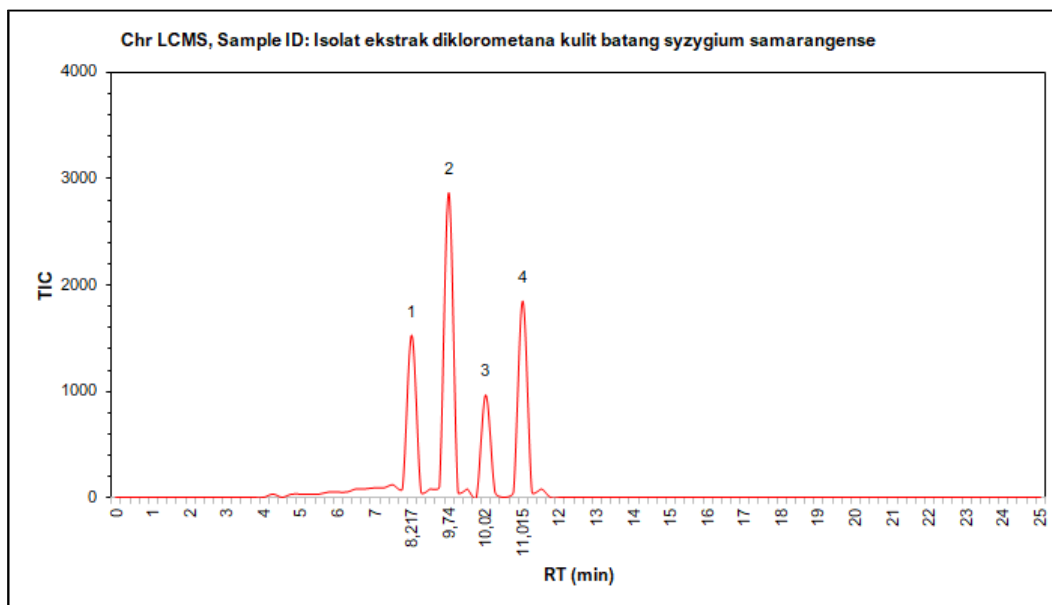
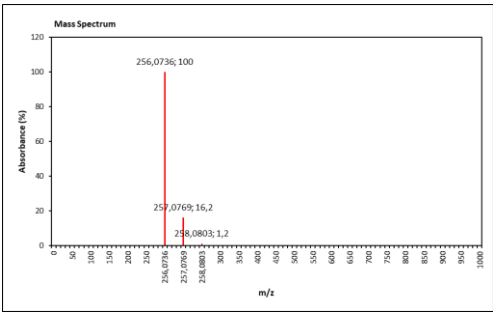
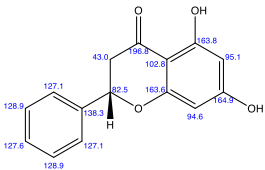
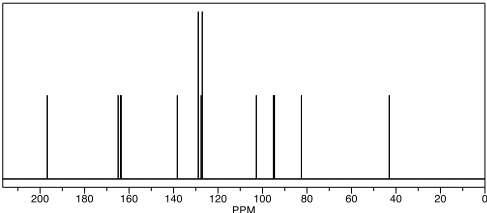
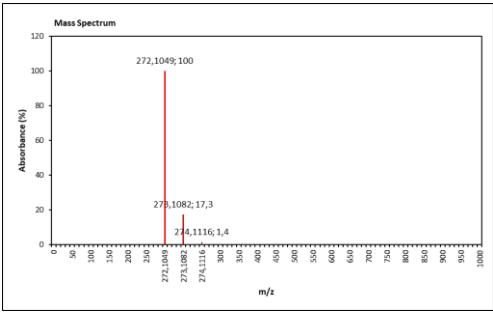
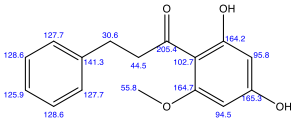
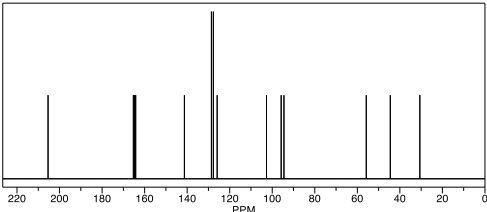
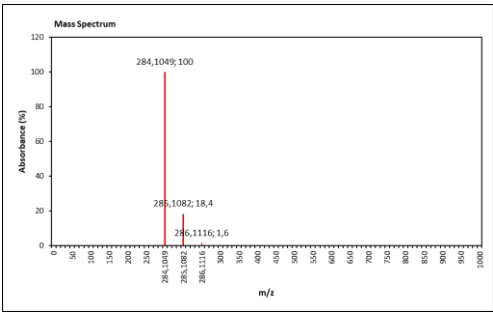
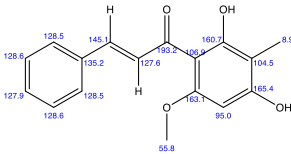
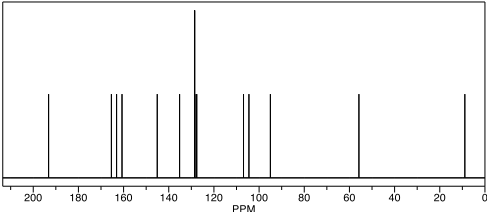


Table 1 Chromatogram Result

| Peak number | RT (min) | Similarity index (%) | Curve area | Composition (%) | Analysis                                                                                                                                                                                                   | Compound Result |
|-------------|----------|----------------------|------------|-----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|
|             |          |                      |            |                 |                                                                                                                                                                                                            | Structure       |
| 1           | 8,217    | 92                   | 1527,89182 | 21,19382        | <b>Pinocembrin</b><br>Chemical Formula: C <sub>15</sub> H <sub>12</sub> O <sub>4</sub><br>Exact Mass: 256,0736<br>Molecular Weight: 256,2570<br>m/z: 256.0736 (100.0%), 257.0769 (16.2%), 258.0803 (1.2%)  |                 |
| 2           | 9,74     | 92                   | 2869,10296 | 39,79814        | <b>Uvangoletin</b><br>Chemical Formula: C <sub>16</sub> H <sub>16</sub> O <sub>4</sub><br>Exact Mass: 272,1049<br>Molecular Weight: 272,3000<br>m/z: 272.1049 (100.0%), 273.1082 (17.3%), 274.1116 (1.4%)  |                 |
| 3           | 10,02    | 92                   | 964,57134  | 13,37984        | <b>Stercurensin</b><br>Chemical Formula: C <sub>17</sub> H <sub>16</sub> O <sub>4</sub><br>Exact Mass: 284,1049<br>Molecular Weight: 284,3110<br>m/z: 284.1049 (100.0%), 285.1082 (18.4%), 286.1116 (1.6%) |                 |
| 4           | 11,015   | 92                   | 1847,57282 | 25,62820        | <b>Aurentiacin</b><br>Chemical Formula: C <sub>18</sub> H <sub>18</sub> O <sub>4</sub><br>Exact Mass: 298,1205<br>Molecular Weight: 298,3380<br>m/z: 298.1205 (100.0%), 299.1239 (19.5%), 300.1272 (1.8%)  |                 |

Table 2 Chromatogram Mass Spectrum and NMR  $^{13}\text{C}$  Estimation Report

| Peak number | Compound name | Mass spectrum                                                                       | NMR $^{13}\text{C}$ estimation                                                                                                                                                                                                                                                                                                               |
|-------------|---------------|-------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1           | Pinocembrin   |    | <p>ChemNMR <math>^{13}\text{C}</math> Estimation</p>  <p>Estimation quality is indicated by color: <span>good</span>, <span>medium</span>, <span>rough</span></p>      |
| 2           | Uvangoletin   |   | <p>ChemNMR <math>^{13}\text{C}</math> Estimation</p>  <p>Estimation quality is indicated by color: <span>good</span>, <span>medium</span>, <span>rough</span></p>     |
| 3           | Stercurensin  |  | <p>ChemNMR <math>^{13}\text{C}</math> Estimation</p>  <p>Estimation quality is indicated by color: <span>good</span>, <span>medium</span>, <span>rough</span></p>  |

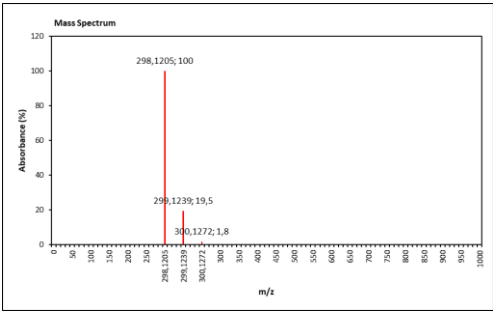
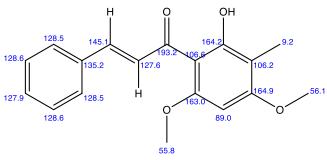
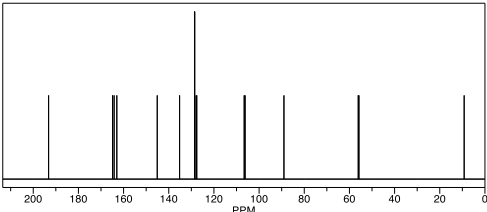
| Peak number | Compound name | Mass spectrum                                                                                                                                                                                                               | NMR <sup>13</sup> C estimation                                                                                                                                                                                                                                                                                                                                                                           |
|-------------|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 4           | Aurentiacin   |  <p>Mass Spectrum</p> <p>Abundance (%)</p> <p>m/z</p> <p>298.1205; 100</p> <p>299.1239; 19.5</p> <p>300.1272; 1.8</p> <p>301.1272; 1.8</p> | <p>ChemNMR <sup>13</sup>C Estimation</p>  <p>Estimation quality is indicated by color: <span style="color: green;">good</span>, <span style="color: yellow;">medium</span>, <span style="color: red;">rough</span></p>  <p>PPM</p> |

Table 3 LCMS Properties

|                         |                                                                 |
|-------------------------|-----------------------------------------------------------------|
| LCMS apparatus model    | Shimadzu LCMS – 8040 LC/MS                                      |
| Column                  | Shimadzu Shim Pack FC-ODS (2 mm x 150 mm, 3 µm)                 |
| Injection volume        | 1 µ                                                             |
| Capillary voltage       | 3,0 kV                                                          |
| Column temperature      | 35 °C                                                           |
| Mobile phase mode       | Isocratic                                                       |
| Flow rate               | 0,5 ml/min                                                      |
| Sampling cone           | 23,0 V                                                          |
| Solvent                 | Dichloromethane                                                 |
| MS focused ion mode     | Io type [M]⁺                                                    |
| Collision energy        | 5,0 V                                                           |
| Desolvation gas flow    | 60 ml/hr                                                        |
| Desolvation temperature | 350 °C                                                          |
| Fragmentation method    | Low energy CID                                                  |
| Ionization              | ESI                                                             |
| Scanning                | 0,6 sec/scan (mz: 10-1000)                                      |
| Source temperature      | 100 °C                                                          |
| Run time                | 25 minutes                                                      |
| LCMS method             | LCMS method                                                     |
| User name               | Frisca Nadya S, Univ Negeri Surabaya                            |
| Sample ID               | Isolat ekstrak diklorometana kulit batang syzygium samarangense |
| Injection date          | 10/19/2019                                                      |