

Supplementary file

Table 1: Chemical constituents present in the methanolic plant extract of *Bougainvillea*

| PEAK | AREA % | RTN. TIME | NAME OF THE COMPOUNDS  |
|------|--------|-----------|--|
| 1    | 3.47   | 13.92     | 2,3,4,4-TRETRAPROPYL-1-(TRIMETHYLSILYL)-1-(TRIMETHYLSILOXY)-1,3-DIAZA-2,4-DIBORABUTANE |
| 2    | 2.24   | 25.702    | Furo[2,3-c]pyridine,2,3-dihydro-2,7-dimethyl-  |
| 3    | 14.84  | 26.498    | Furo[2,3-c]pyridine,2,3-dihydro-2,7-dimethyl-  |
| 4    | 8.24   | 26.793    | Furo[2,3-c]pyridine,2,3-dihydro-2,7-dimethyl-  |
| 5    | 4.25   | 28.025    | Furo[2,3-c]pyridine,2,3-dihydro-2,7-dimethyl-  |
| 6    | 18.41  | 37.239    | (2,3,3-TRI-TERT-BUTYLCYCLOPROPEN-1-YL) PHOSPHINE                                       |
| 7    | 18.18  | 37.462    | 2-PROPENOIC ACID, 2-ETHYLHEXYL ESTER   |
| 8    | 2.18   | 39.312    | 3,4-DIHYDRO-4-(1,3-DIOXOLAN-2-YL)-5,7-DIMETHOXY-1(2H)-BENZOPYRAN-2-ONE                 |
| 9    | 2.7    | 39.62     | 3,4-DIHYDRO-4-(1,3-DIOXOLAN-2-YL)-5,7-DIMETHOXY-1(2H)-BENZOPYRAN-2-ONE                 |
| 10   | 3.31   | 39.71     | 3,4-DIHYDRO-4-(1,3-DIOXOLAN-2-YL)-5,7-DIMETHOXY-1(2H)-BENZOPYRAN-2-ONE                 |
| 11   | 5.39   | 39.823    | 3,4-DIHYDRO-4-(1,3-DIOXOLAN-2-YL)-5,7-DIMETHOXY-1(2H)-BENZOPYRAN-2-ONE                 |
| 12   | 6.78   | 39.9      | (SS)- or (RR)-2,3-hexanediol   |

|    |      |        |  |
|----|------|--------|--|
| 13 | 3.31 | 40.011 | (SS)- or (RR)-2,3-hexanediol   |
| 14 | 3.28 | 40.106 | 3,4-DIHYDRO-4-(1,3-DIOXOLAN-2-YL)-5,7-DIMETHOXY-1(2H)-BENZOPYRAN-2-ONE |
| 15 | 3.43 | 40.234 | (SS)- or (RR)-2,3-hexanediol   |

**Table 2: Antioxidant activity of *Bougainvillea* by DPPH Assay**

| <b>VALUE OF PLANT SAMPLE EA</b> | <b>STANDARD (ASCORBIC ACID)</b> | <b>SAMPLE % RSA</b> |
|---------------------------------|---------------------------------|---------------------|
| 10µL                            | 95.97                           | 63.9                |
| 20µL                            | 96.98                           | 67.45               |
| 30µL                            | 97.48                           | 71.59               |
| 40µL                            | 98.49                           | 76.33               |
| 50µL                            | 98.99                           | 77.57               |



## DRUGLIKENES

**TABLE 4:** Drug likeness of *Bougainvillea glabra*

| <b>COMPONENTS</b>  | Lipinski<br>#violations | Ghose<br>#violations | Veber<br>#violations | Egan<br>#violations | Muegge<br>#violations | Bioavailability<br>Score | PAINS<br>#alerts |
|--|-------------------------|----------------------|----------------------|---------------------|-----------------------|--------------------------|------------------|
| 3-Diaza-2,4-Diborabutane   | 1                       | 3                    | 0                    | 1                   | 1                     | 0.55                     | 0                |
| Furo[2,3-c]pyridine,<br>2,3-dihydro-2,7-dimethyl-                      | 0                       | 1                    | 0                    | 0                   | 1                     | 0.55                     | 0                |
| 2-Propenoic acid,<br>2-ethylhexyl ester                                | 0                       | 0                    | 0                    | 0                   | 1                     | 0.55                     | 0                |
| 3,4-Dihydro-4-(1,3-Dioxolan-2-yl)-5,7-dimethoxy-1(2H)-Benzopyran-2-ONE | 0                       | 0                    | 0                    | 0                   | 0                     | 0.55                     | 0                |
| (SS)- or (RR)-2,3-hexanediol   | 0                       | 2                    | 0                    | 0                   | 1                     | 0.55                     | 0                |

**TOXICITY**

**TABLE 5:** Toxicity of *Bougainvillea glabra*

| COMPONENTS                                     | AMES TOXICITY | MAX.TOLERATED DOSE (HUMAN) | hERG I inhibitor | hERG II inhibitor | ORAL RAT ACUTE TOXICITY (LD 50) | ORAL RAT ACUTE TOXICITY (LOAEL) | HEPTATOTOXICITY | SKIN SENSITIZATION | T.Pyrifor mis TOXICITY | MINNOW TOXICITY |
|--|---------------|----------------------------|------------------|-------------------|---------------------------------|---------------------------------|-----------------|--------------------|------------------------|-----------------|
| 3-Diaza-2,4-Diborabutane                       | No            | -0.966                     | No               | Yes               | 2.917                           | -0.925                          | No              | No                 | 0.5                    | -1.998          |
| Furo[2,3-c]pyridine, 2,3-dihydro-2,7-dimethyl- | No            | 0.958                      | No               | No                | 2.151                           | 2.389                           | Yes             | No                 | -0.19                  | 1.457           |
| 2-Propenoic acid, 2-ethylhexyl ester           | No            | 0.607                      | No               | No                | 1.679                           | 2.314                           | No              | Yes                | 1.116                  | 0.609           |

|  |     |       |    |    |       |       |    |     |        |       |
|--|-----|-------|----|----|-------|-------|----|-----|--------|-------|
| 3,4-Dihydro-4-(1,3-Dioxolan-2-yl)-5,7-dimethoxy-1(2H)-Benzopyran-2-ONE | Yes | 0.699 | No | NO | 2.468 | 2.099 | NO | NO  | 0.467  | 2.376 |
| (SS)- or (RR)-2,3-hexanediol   | No  | 1.325 | No | No | 1.534 | 2.73  | No | Yes | -1.588 | 2.364 |