Two novel oxetane containing lignans and a new megastigmane from Paronychia arabica and *in silico* analysis as prospective SARS-CoV-2 Inhibitors

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徳島文理大学

測定日時 2018/03/27 11:33

[測定情報]
検査名 FT/IR-4200typeA
シリアル番号 C094361018
付属品名 ATR PRO470-H
付属品シリアルNo. A012081293
入射角 45度
測定日時 2018/03/27 11:32

光源 標準光源
検出器 TGS
検査回数 04
分解 On
ゼロフィリング Cosine
アボダイゼーション Auto (16)
アプチャ Auto (7.1 mm)
S1: FT-IR of 1
S2: TOF-ESI-MS of 1
S3: $^1$H NMR of 1 (500 Hz, MeOD)
S4: $^{13}$C NMR of 1 (125 Hz, MeOD)
S5: DEPT-135 of 1
S6: HSQC of 1
S7: HMBC of 1
S8: $^1$H-$^1$H COSY of 1
S9: NOESY of 1

| [Measuring Information] |  | [Measurement Information] |  |
|-------------------------|---|---------------------------|---|
| Instrument Name         | FT/IR-4200 type A | Memory-3                   |  |
| Serial Number           | C0943811018       |                            |  |
| Sample Name             | ATR PRO470-H      |                            |  |
| Sample Serial Number    | A012061293        |                            |  |
| Angle                   | 45 degrees        |                            |  |
| Measurement Date        | 2019/03/27 11:33  |                            |  |
| Source                   | Standard Source   |                            |  |
| Detector                | TGS               |                            |  |
| Wavenumber [cm⁻¹]       | 499.473 cm⁻¹     |                            |  |
| Time                     | 4000.8 cm⁻¹      |                            |  |
| Spectra Width [cm⁻¹]    | 4994.233 cm⁻¹    |                            |  |
| Spectra Number          | 3632              |                            |  |
S10: FTIR of 2
S11: CIMS of 2

Data: Umeyama-CIHR.18-Mar-2019.004  Date: 18-Mar-2019 18:04
Instrument: MStation
Sample: PA-3-2
Note: MStation
Inlet: Direct  Ion Mode: CH+
RT: 2.65 min  Scan#: 70
Elements: C 150/0, H 250/0, O 50/0
Mass Tolerance: 5mmu
Unsaturation (U.S.): 0.0 - 20.0

| Observed m/z  | Int%  | Err [ppm / mmu]  | U.S. Composition |
|---------------|-------|------------------|------------------|
| 1 536.2030    | 3.05  | -3.0 / -1.6      | 15.0 C30 H32 O9  |

S12: HRCIMS of 2
S13: $^1$H NMR of 2 (500 Hz, MeOD)
S14: $^{13}$C NMR of 2 (125 Hz, MeOD)
S15: DEPT-135 of 2
S16: HSQC of 2
S17: HMBC of 2
S18: $^1\text{H} - ^1\text{H}$ COSY of 2
S19: NOESY of 2
[測定情報]
測定機種 FT/IR-4200TypeA
シリアル番号 C0946301018
付属ストリニング ATR PRO470-H
付属品シリアルNo. A032061293
入射角 45度
測定日時 2019/03/27 11:53
光源 標準光源
検出器 TGS
検出器目盛 84
分割 4 cm⁻¹
セレクタリング On
アロー設定 Auto (16)
スキャンスピード Auto (1.5 mm/sec)
スキャン時間 1000 sec
データ数 1
カウント 128
スキャン数 1
レンジ 0.0000001 cm⁻¹
スペクトル幅 1000 cm⁻¹
バッファー 鎌田文庫
S20: FT-IR of 3
S21: FAB-ESIMS of 3

Data: Umeyama-FABHR.26-Mar-2019.002 Date: 26-Mar-2019 08:46
Instrument: MS700D
Sample: PA-1-83-4
Note: MStation
Inlet: Direct Ion Mode: FAB+
RT: 11.83 min Scan#: 44
Elements: C 150/0, H 250/0, O 50/0, Na 1/0
Mass Tolerance: 5mmu
Unsaturation (U.S.): 0.0 - 15.0

| Observed m/z | Int % | Err[ppm / mmu] | U.S. Composition |
|--------------|-------|----------------|------------------|
| 1 559.2157   | 7.12  | -4.0 / -2.2    | C29 H35 O11     |
| 2            |       | +0.3 / +0.2    | C27 H36 O11 Na  |

S22: HRFAB-ESIMS of 3
S23: $^1$H NMR of 3 (500 Hz, MeOD)
S24: $^{13}\text{C}$ NMR of 3 (125 Hz, MeOD)
S25: DEPT-135 of 3
S27: HMBC of 3
S28: $^1$H-$^1$H COSY of 3
