

Supporting Information

Antitumor Agents 280. Multidrug Resistance-Selective Desmosdumotin B Analogous

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Physical data of 6–19, 21–26, 28, 30–34, 36–48, and 50–55

4'-*iso*-Propyl-6,8,8-triethyldesmosdumotin B (6). Pale yellow prisms, mp 186–187 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.13 (s, 1H, 5-OH), 7.73 (d, 2H, J = 8.2 Hz, Ar-H), 7.42 (d, 2H, J = 8.2 Hz, Ar-H), 6.87 (s, 1H, 3-H), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.32–2.19 (m, 2H, 8- CH_2CH_3), 2.06–1.92 (m, 2H, 8- CH_2CH_3), 1.57 [s, 1H, 4'-CH(CH_3)₂], 1.31 and 1.29 [s, 3H each, 4'-CH(CH_3)₂], 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 381 (M^++1). Anal. ($\text{C}_{24}\text{H}_{28}\text{O}_4$) C, H, O.

4'-Butyl-6,8,8-triethyldesmosdumotin B (7). Pale yellow prisms, mp 165–166 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.14 (s, 1H, 5-OH), 7.71 (d, 2H, J = 8.2 Hz, Ar-H), 7.37 (d, 2H, J = 8.2 Hz, Ar-H), 6.87 (s, 1H, 3-H), 2.71 [t, 2H, J = 7.8 Hz, 4'- $\text{CH}_2(\text{CH}_2)_2\text{CH}_3$], 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.33–2.18 (m, 2H, 8- CH_2CH_3), 2.08–1.92 (m, 2H, 8- CH_2CH_3), 1.71–1.58 (m, 2H, 4'- $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$), 1.46–1.30 [m, 2H, 4'-(CH_2)₂ CH_2CH_3], 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.95 [t, 3H, J = 7.8 Hz, 4'-(CH_2)₃ CH_3], 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 395 (M^++1). Anal. ($\text{C}_{25}\text{H}_{30}\text{O}_4$) C, H, O.

4'-*tert*-Butyl-6,8,8-triethyldesmosdumotin B (8). Pale yellow prisms, mp 222–223 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.13 (s, 1H, 5-OH), 7.75 (d, 2H, J = 8.7 Hz, Ar-H), 7.58 (d, 2H, J = 8.7 Hz, Ar-H), 6.88 (s, 1H, 3-H), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.32–1.98 (m, 2H, 8- CH_2CH_3), 2.06–1.92 (m, 2H, 8- CH_2CH_3), 1.37 [s, 9H, 4'-CH(CH_3)₃], 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 395 (M^++1). Anal. ($\text{C}_{25}\text{H}_{30}\text{O}_4 \cdot 1/8\text{H}_2\text{O}$) C, H, O.

6,8,8-Triethyl-4'-trifluoromethyl-desmosdumotin B (9). Pale yellow prisms, mp 168–169 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.82 (s, 1H, 5-OH), 7.93 (d, 2H, J = 8.2 Hz, Ar-H), 7.84 (d, 2H, J = 8.2 Hz, Ar-H), 6.97 (s, 1H, 3-H), 2.46 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.26–2.21 (m, 2H, 8- CH_2CH_3), 2.04–1.92 (m, 2H, 8- CH_2CH_3), 1.05 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.68 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 407 (M^++1). Anal. ($\text{C}_{22}\text{H}_{21}\text{F}_3\text{O}_4$) C, H, O.

4'-Hydroxy-6,8,8-triethyldesmosdumotin B (10). Pale yellow prisms, mp 213–214 °C (EtOAc-hexane). ^1H NMR (300 MHz, DMSO-d_6): δ 13.80 (br s, 1H, 5-OH), 10.50 (br s, 1H, 4'-OH), 7.93 (d, 2H, J = 9.0 Hz, Ar-H), 7.25 (s, 1H, 3-H), 2.30 (q, 2H, J = 7.4 Hz, 6- CH_2CH_3), 2.10–1.97 (m, 4H, 8- CH_2CH_3), 0.93 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.58 (t, 6H, J = 7.4 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 355 (M^++1). Anal. ($\text{C}_{21}\text{H}_{22}\text{O}_5$) C, H, O.

4'-Methoxy-6,8,8-triethyldesmosdumotin B (11). Pale yellow prisms, mp 139–140 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.21 (s, 1H, 5-OH), 7.79–7.72 (m, 2H, Ar-H), 7.10–7.02 (m, 2H, Ar-H), 6.80 (s, 1H, 3-H), 3.91 (s, 3H, 4'-OCH₃), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.34–2.18

(m, 2H, 8-CH₂CH₃), 2.05-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.3 Hz, 6-CH₂CH₃), 0.67 (t, 3H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 369 (M⁺+1). Anal. (C₂₂H₂₄O₅) C, H, O.

4'-Ethoxy-6,8,8-triethyldesmosdumotin B (12). Pale yellow prisms, mp 161-162 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.22 (s, 1H, 5-OH), 7.74 (dt, 2H, *J* = 8.7 and 1.8 Hz, Ar-H), 7.03 (dt, 2H, *J* = 8.7 and 1.8 Hz, Ar-H), 6.79 (s, 1H, 3-H), 4.13 (q, 2H, *J* = 6.9 Hz, 4'-OCH₂CH₃), 2.45 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.32-2.18 (m, 2H, 8-CH₂CH₃), 2.06-1.91 (m, 2H, 8-CH₂CH₃), 1.48 (t, 3H, *J* = 6.9 Hz, 4'-OCH₂CH₃), 1.04 (t, 3H, *J* = 7.3 Hz, 6-CH₂CH₃), 0.67 (t, 3H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 383 (M⁺+1). Anal. (C₂₃H₂₆O₅·1/8H₂O) C, H, O.

4'-Propoxy-6,8,8-triethyldesmosdumotin B (13). Pale yellow prisms, mp 162-163 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.22 (s, 1H, 5-OH), 7.73 (d, 2H, *J* = 9.2 Hz, Ar-H), 7.03 (d, 2H, *J* = 9.2 Hz, Ar-H), 6.79 (s, 1H, 3-H), 4.01 (t, 2H, *J* = 6.4 Hz, 4'-OCH₂CH₂CH₃), 2.45 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.12-2.18 (m, 2H, 8-CH₂CH₃), 2.06-1.79 (m, 4H, 8-CH₂CH₃ and 4'-OCH₂CH₂CH₃), 1.07 (t, 3H, *J* = 7.3 Hz, 4'-OCH₂CH₂CH₃), 1.04 (t, 3H, *J* = 7.3 Hz, 6-CH₂CH₃), 0.67 (t, 3H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 397 (M⁺+1). Anal. (C₂₄H₂₈O₅) C, H, O.

4'-Trifluoromethoxy-6,8,8-triethyldesmosdumotin B (14). Pale yellow prisms, mp 157-158 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.91 (s, 1H, 5-OH), 7.88-7.81 (m, 2H, Ar-H), 7.42 (br d, 2H, *J* = 8.7 Hz, Ar-H), 6.89 (s, 1H, 3-H), 2.46 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.04-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.68 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 445 (M⁺+Na). Anal. (C₂₂H₂₁F₃O₅) C, H, O.

4'-Methylthio-6,8,8-triethyldesmosdumotin B (15). Yellow prisms, mp 190-191 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.11 (s, 1H, 5-OH), 7.70 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.37 (d, 2H, *J* = 8.7 Hz, Ar-H), 6.85 (s, 1H, 3-H), 2.56 (s, 3H, 4'-SCH₃), 2.45 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.34-2.19 (m, 2H, 8-CH₂CH₃), 2.05-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.3 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 385 (M⁺+1). Anal. (C₂₂H₂₄O₄S·1/8H₂O) C, H, O.

4'-Bromo-6,8,8-triethyldesmosdumotin B (16). Yellow prisms, mp 244-245 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.93 (s, 1H, 5-OH), 7.74-7.64 (m, 4H, Ar-H), 6.89 (s, 1H, 3-H), 2.45 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.04-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 433 and 431 (1:1, M⁺+1). Anal. (C₂₁H₂₁BrO₄) C, H, O.

4'-Fluoro-6,8,8-triethyldesmosdumotin B (17). Pale yellow prisms, mp 196-197 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.99 (s, 1H, 5-OH), 7.84-7.76 (m, 2H, Ar-H), 7.31-7.22 (m, 2H, Ar-H), 6.85 (s, 1H, 3-H), 2.46 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.05-

1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.68 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 357 (M⁺+1). Anal. (C₂₁H₂₁FO₄) C, H, O.

4'-Bromomethyl-6,8,8-triethyldesmosdumotin B (18). Yellow prisms, mp 154-155 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.99 (s, 1H, 5-OH), 7.79 (d, 2H, *J* = 8.5 Hz, 2' and 6'-H), 7.59 (d, 2H, *J* = 8.5 Hz, 3' and 5'-H), 6.91 (s, 1H, 3-H), 4.54 (s, 2H, 4'-CH₂Br), 2.45 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.06-1.92 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 433 and 431 (1:1, M⁺+1). Anal. (C₂₂H₂₃BrO₄) C, H, O.

4'-Methoxymethyl-6,8,8-triethyldesmosdumotin B (19). Pale yellow prisms, mp 174-175 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.07 (s, 1H, 5-OH), 7.78 (d, 2H, *J* = 8.5 Hz, 2' and 6'-H), 7.53 (d, 2H, *J* = 8.5 Hz, 3' and 5'-H), 6.90 (s, 1H, 3-H), 3.45 (s, 2H, 4'-CH₂OCH₃), 2.45 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.06-1.92 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 383 (M⁺+1). Anal. (C₂₃H₂₆O₅) C, H, O.

3'-Trifluoromethyl-6,8,8-triethyldesmosdumotin B (21). Pale yellow prisms, mp 161-162 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.84 (s, 1H, 5-OH), 8.03-7.95 (m, 2H, Ar-H), 7.90-7.84 (m, 1H, Ar-H), 7.74 (t, 1H, *J* = 7.8 Hz, Ar-H), 6.96 (s, 1H, 3-H), 2.46 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.34-2.21 (m, 2H, 8-CH₂CH₃), 2.04-1.91 (m, 2H, 8-CH₂CH₃), 1.05 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.69 (t, 6H, *J* = 7.4 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 407 (M⁺+1). Anal. (C₂₂H₂₁F₃O₄) C, H, O.

3'-Methoxy-6,8,8-triethyldesmosdumotin B (22). Pale yellow prisms, mp 129-130 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.03 (s, 1H, 5-OH), 7.48 (dd, 1H, *J* = 8.0, 8.5 Hz, 5'-H), 7.38 (br d, 1H, *J* = 8.0 Hz, 6'-H), 7.29 (t, 1H, *J* = 2.4 Hz, 2'-H), 7.13 (dd, 1H, *J* = 2.4, 8.5 Hz, 4'-H), 6.89 (s, 1H, 3-H), 3.90 (s, 3H, 4'-OCH₃), 2.46 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.33-2.19 (m, 2H, 8-CH₂CH₃), 2.08-1.92 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.4 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 369 (M⁺+1). Anal. (C₂₂H₂₄O₅) C, H, O.

3'-Trifluoromethoxy-6,8,8-triethyldesmosdumotin B (23). Pale yellow prisms, mp 158-159 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 12.85 (s, 1H, 5-OH), 7.76-7.71 (m, 1H, Ar-H), 7.67-7.59 (m, 2H, Ar-H), 7.50-7.44 (m, 1H, Ar-H), 6.92 (s, 1H, 3-H), 2.45 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.04-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.68 (t, 6H, *J* = 7.4 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 445 (M⁺+Na). Anal. (C₂₂H₂₁F₃O₅) C, H, O.

3'-Fluoro-6,8,8-triethyldesmosdumotin B (24). Pale yellow prisms, mp 191-192 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.90 (s, 1H, 5-OH), 7.62-7.51 (2H, m, Ar-H), 7.50-7.44 (1H, m, Ar-H), 7.36-7.26 (m, 1H, Ar-H), 6.90 (s, 1H, 3-H), 2.46 (q, 2H, $J = 7.4$ Hz, 6- CH_2CH_3), 2.37-2.20 (m, 2H, 8- CH_2CH_3), 2.06-1.91 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, $J = 7.4$ Hz, 6- CH_2CH_3), 0.68 (t, 6H, $J = 7.4$ Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 379 ($\text{M}^+ + \text{Na}$). Anal. ($\text{C}_{21}\text{H}_{21}\text{FO}_4$) C, H, O.

2'-Trifluoromethyl-6,8,8-triethyldesmosdumotin B (26). Pale yellow prisms, mp 152-154 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.89 (s, 1H, 5-OH), 7.90-7.84 (m, 1H, Ar-H), 7.78-7.72 (m, 2H, Ar-H), 7.58-7.54 (m, 1H, Ar-H), 6.62 (s, 1H, 3-H), 2.46 (q, 2H, $J = 7.3$ Hz, 6- CH_2CH_3), 2.21-2.08 (m, 2H, 8- CH_2CH_3), 1.98-1.82 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, $J = 7.4$ Hz, 6- CH_2CH_3), 0.64 (t, 6H, $J = 7.3$ Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 407 ($\text{M}^+ + 1$). Anal. ($\text{C}_{22}\text{H}_{21}\text{F}_3\text{O}_4$) C, H, O.

2'-Fluoro-6,8,8-triethyldesmosdumotin B (28). Yellow prisms, mp 140-141 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.96 (s, 1H, 5-OH), 7.74 (dt, 1H, $J = 8.0, 1.6$ Hz, Ar-H), 7.64-7.55 (m, 1H, Ar-H), 7.36 (ddd, 1H, $J = 8.6, 7.4, 1.1$ Hz, Ar-H), 7.28 (ddd, 1H, $J = 9.3, 8.6, 1.1$ Hz, Ar-H), 7.04 (s, 1H, 3-H), 2.46 (q, 2H, $J = 7.4$ Hz, 6- CH_2CH_3), 2.31-2.18 (m, 2H, 8- CH_2CH_3), 2.05-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, $J = 7.4$ Hz, 6- CH_2CH_3), 0.67 (t, 6H, $J = 7.4$ Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 379 ($\text{M}^+ + \text{Na}$). Anal. ($\text{C}_{21}\text{H}_{21}\text{FO}_4$) C, H, O.

3',4'-Dimethyl-6,8,8-triethyldesmosdumotin B (30). Orange prisms, mp 160-161 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.16 (s, 1H, 5-OH), 7.56-7.50 (m, 2H, Ar-H), 7.34-7.29 (m, 1H, Ar-H), 6.86 (s, 1H, 3-H), 2.46 (q, 2H, $J = 7.4$ Hz, 6- CH_2CH_3), 2.37 (s, 6H, 3'- and 4'- CH_3), 2.35-2.18 (m, 2H, 8- CH_2CH_3), 2.06-1.82 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, $J = 7.4$ Hz, 6- CH_2CH_3), 0.67 (t, 6H, $J = 7.3$ Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 367 ($\text{M}^+ + 1$). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_4$) C, H, O.

3'-Chloro-4'-methyl-6,8,8-triethyldesmosdumotin B (31). Pale yellow prisms, mp 167-168 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.98 (s, 1H, 5-OH), 7.76-7.72 (m, 1H, 2'-H), 7.58 (d, 1H, $J = 8.0$ Hz, 5'- or 6'-H), 7.42 (d, 1H, $J = 8.0$ Hz, 5'- or 6'-H), 6.86 (s, 1H, 3-H), 2.48 (s, 3H, 4'- CH_3), 2.51-2.39 (m, 2H, 6- CH_2CH_3), 2.34-2.19 (m, 2H, 8- CH_2CH_3), 2.06-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, $J = 7.0$ Hz, 6- CH_2CH_3), 0.67 (t, 6H, $J = 7.0$ Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 409 ($\text{M}^+ + \text{Na}$). Anal. ($\text{C}_{22}\text{H}_{23}\text{ClO}_4$) C, H, O.

3'-Fluoro-4'-methyl-6,8,8-triethyldesmosdumotin B (32). Pale yellow prisms, mp 189-190 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.98 (s, 1H, 5-OH), 7.52-7.34 (m, 3H, Ar-H), 6.85 (s, 1H, 3-H), 2.45 (q, 2H, $J = 7.4$ Hz, 6- CH_2CH_3), 2.38 (d, 3H, $J = 1.9$ Hz, 4'- CH_3), 2.34-2.20 (m, 2H, 8- CH_2CH_3), 2.03-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, $J = 7.4$ Hz, 6- CH_2CH_3), 0.67 (t, 6H, $J = 7.4$ Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 371 ($\text{M}^+ + 1$). Anal. ($\text{C}_{22}\text{H}_{23}\text{FO}_4 \cdot 1/16\text{H}_2\text{O}$) C, H, O.

6,8,8-Triethyl-2',4',5'-trimethyldesmosdumotin B (33). Pale yellow prisms, mp 129-130 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.18 (s, 1H, 5-OH), 7.21 (s, 1H, Ar-H), 7.13 (s, 1H, Ar-H), 6.59 (s, 1H, 3-H), 2.46 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.39, 2.32, and 2.30 (s, 3H each, 2', 4', and 5'- CH_3), 2.26-2.12 (m, 2H, 8- CH_2CH_3), 1.97-1.82 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.65 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS m/z 381 (M^+ +1). Anal. ($\text{C}_{24}\text{H}_{28}\text{O}_4$) C, H, O

4'-Methoxy-2'-methyl-6,8,8-triethyldesmosdumotin B (34). Pale yellow prisms, mp 142-143 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.19 (s, 1H, 5-OH), 7.44-7.38 (dd, 1H, 6'-H), 6.90-6.84 (m, 2H, 3', and 5'-H), 6.57 (s, 1H, 3-H), 3.88 (s, 3H, 4'- OCH_3), 2.46 (q, 2H, J = 7.4 Hz, 6- CH_2CH_3), 2.46 (s, 3H, 2'- CH_3), 2.25-2.12 (m, 2H, 8- CH_2CH_3), 1.97-1.83 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.65 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS m/z 383 (M^+ +1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_5$) C, H, O.

3',4'-Dimethoxy-6,8,8-triethyldesmosdumotin B (36). Yellow prisms, mp 148-149 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.17 (s, 1H, 5-OH), 7.65 (dd, 1H, J = 8.2, 2.3 Hz, 6'-H), 7.23 (d, 1H, J = 2.3 Hz, 2'-H), 7.01 (d, 1H, J = 8.2 Hz, 5'-H), 6.81 (s, 1H, 3-H), 3.9 and 3.97 (s, 3H each, 3' and 4'- OCH_3), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.33-2.21 (m, 2H, 6- or 8- CH_2CH_3), 2.04-1.91 (m, 2H, 6- or 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.68 (t, 3H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 399 (M^+ +1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_6$) C, H, O.

3'-Fluoro-4'-methoxy-6,8,8-triethyldesmosdumotin B (37). Yellow prisms, mp 175-176 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.04 (s, 1H, 5-OH), 7.60-7.54 (m, 1H, 6'-H), 7.54-7.46 (m, 1H, 2'-H), 7.11 (dd, 1H, J = 8.2, 8.5 Hz, 5'-H), 6.79 (s, 1H, 3-H), 4.00 (s, 3H, 4'- OCH_3), 2.45 (q, 2H, J = 7.5 Hz, 4'- CH_2CH_3), 2.33-2.18 (m, 2H, 6- or 8- CH_2CH_3), 2.04-1.90 (m, 2H, 6- or 8- CH_2CH_3), 1.04 (t, 3H, J = 7.5 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.5 Hz, 4'- CH_2CH_3). MS (ESI $^+$) m/z : 387 (M^+ +1). Anal. ($\text{C}_{22}\text{H}_{23}\text{FO}_5$) C, H, O.

3'-Chloro-4'-methoxy-6,8,8-triethyldesmosdumotin B (38). Pale yellow prisms, mp 175-176 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.04 (s, 1H, 5-OH), 7.78 (d, 1H, J = 2.1 Hz, 2'-H), 7.69 (dd, 1H, J = 8.8, 2.1 Hz, 6'-H), 7.08 (dd, 1H, J = 8.8 Hz, 5'-H), 6.79 (s, 1H, 3-H), 4.01 (s, 3H, 4'- OCH_3), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.34-2.19 (m, 2H, 8- CH_2CH_3), 2.04-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 403 (M^+ +1). Anal. ($\text{C}_{22}\text{H}_{23}\text{ClO}_5$) C, H, O.

4'-Methoxy-2',3'-dimethyl-6,8,8-triethyldesmosdumotin B (39). Pale yellow prisms, mp 127-128 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.21 (s, 1H, 5-OH), 7.26 (d, 1H, J = 8.5 Hz, 6'-H), 6.84 (d, 1H, J = 8.5 Hz, 5'-H), 6.54 (s, 1H, 3-H), 2.46 (q, 2H, J = 7.4 Hz, 6- CH_2CH_3), 2.31 (s, 3H, 2'or 3'- CH_3), 2.23 (s, 3H, 2'or 3'- CH_3), 2.24-2.10 (m, 2H, 8- CH_2CH_3), 1.96-1.82 (m, 2H, 8- CH_2CH_3),

1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.65 (t, 6H, J = 7.4 Hz, 8- CH_2CH_3). MS m/z 397 (M^++1). Anal. ($\text{C}_{24}\text{H}_{28}\text{O}_5$) C, H, O.

4'-Methoxy-2',5'-dimethyl-6,8,8-triethyldesmosdumotin B (40). Pale yellow prisms, mp 159-160 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.25 (s, 1H, 5-OH), 7.22 (s, 1H, 6'-H), 6.75 (s, 1H, 3'-H), 6.56 (s, 1H, 3-H), 2.46 (q, 2H, J = 7.4 Hz, 6- CH_2CH_3), 2.45 (s, 3H, 2'- CH_3), 2.27-2.12 (m, 2H, 8- CH_2CH_3), 2.23 (s, 3H, 2'- CH_3), 1.98-1.83 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.65 (t, 6H, J = 7.4 Hz, 8- CH_2CH_3). MS m/z 397 (M^++1). Anal. ($\text{C}_{24}\text{H}_{28}\text{O}_5$) C, H, O.

6,8,8-Triethyl-2',3',4'-trimethoxydesmosdumotin B (41). Pale yellow prisms, mp 115-116 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.28 (s, 1H, 5-OH), 7.42 (d, 1H, J = 9.0 Hz, 5' or 6'-H), 7.15 (s, 1H, 3-H), 6.82 (d, 1H, J = 9.0 Hz, 5' or 6'-H), 3.98, 3.95, and 3.91 (s, 3H each, 3', 4', and 5'- OCH_3), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.30-2.16 (m, 2H, 8- CH_2CH_3), 2.04-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 429 (M^++1). Anal. ($\text{C}_{24}\text{H}_{28}\text{O}_7$) C, H, O.

6,8,8-Triethyl-3',4',5'-trimethoxydesmosdumotin B (42). Pale yellow prisms, mp 156-157 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.05 (s, 1H, 5-OH), 7.00 (s, 2H, 2' and 6'-H), 6.84 (s, 1H, 3-H), 3.95 (s, 6H, 3' and 5'- OCH_3), 3.94 (s, 3H, 4'- OCH_3), 2.46 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.34-2.20 (m, 2H, 8- CH_2CH_3), 2.02-1.88 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.69 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 429 (M^++1). Anal. ($\text{C}_{24}\text{H}_{28}\text{O}_7$) C, H, O.

3'-Chloro-4',5'-dimethoxy-6,8,8-triethyldesmosdumotin B (43). Pale yellow prisms, mp 147-148 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 12.94 (s, 1H, 5-OH), 7.43 (d, 1H, J = 2.3 Hz, 2'-H), 7.17 (d, 1H, J = 2.5 Hz, 6'-H), 6.83 (s, 1H, 3-H), 3.97 (s, 6H, 4' and 5'- OCH_3), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.38-2.20 (m, 2H, 8- CH_2CH_3), 2.04-1.89 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.68 (t, 3H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 433 and 435 (3:1, M^++1). Anal. ($\text{C}_{23}\text{H}_{25}\text{ClO}_6$) C, H, O.

3',4'-Dihydoroxy-6,8,8-triethyldesmosdumotin B (44). Pale yellow prisms, mp 200-201 °C (EtOAc-hexane). ^1H NMR (300 MHz, 10% CD_3OD in CDCl_3): δ 7.31-7.25 (m, 2H, Ar-H), 7.00-6.95 (m, 1H, Ar-H), 6.76 (s, 1H, 3-H), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.30-2.16 (m, 2H, 8- CH_2CH_3), 2.07-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.66 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 393 (M^++Na). Anal. ($\text{C}_{21}\text{H}_{22}\text{O}_6$) C, H, O.

2',3'-Dimethyl-4'-hydroxy-6,8,8-triethyldesmosdumotin B (45). Pale yellow prisms, mp 254-256 °C (EtOAc-hexane). ^1H NMR (300 MHz, 10% CD_3OD in CDCl_3): δ 7.12 (d, 1H, J = 8.5 Hz, 6'-H), 6.78 (d, 1H, J = 8.5 Hz, 5'-H), 6.53 (s, 1H, 3-H), 2.45 (q, 2H, J = 7.4 Hz, 6- CH_2CH_3), 2.30 (s, 3H, 2' or 3'- CH_3), 2.23 (s, 3H, 2' or 3'- CH_3), 2.24-2.10 (m, 2H, 8- CH_2CH_3), 1.99-1.84 (m, 2H, 8- CH_2CH_3), 1.04

(t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.65 (t, 6H, J = 7.4 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 383 (M^++1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_5 \cdot 1/8\text{H}_2\text{O}$) C, H, O.

3',5'-Dimethyl-4'-hydroxy-6,8,8-triethyldesmosdumotin B (46). Pale yellow prisms, mp 204-205 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.27 (s, 1H, 5-OH), 7.42 (s, 2H, 2' and 6'-H), 6.7 (s, 1H, 3-H), 5.31 (s, 1H, 4'-OH), 2.46 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.35 (s, 3H, 3' and 5'- CH_3), 2.31-2.20 (m, 2H, 8- CH_2CH_3), 2.06-1.94 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.3 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 383 (M^++1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_3$) C, H, O.

2',3'-Dimethyl-6,8,8-triethyldesmosdumotin B (47). Pale yellow prisms, mp 133-134 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.10 (s, 1H, 5-OH), 7.41-7.34 (m, 1H, Ar-H), 7.30-7.24 (m, 2H, Ar-H), 6.57 (s, 1H, 3-H), 2.46 (q, 2H, J = 7.4 Hz, 6- CH_2CH_3), 2.38 (s, 3H, 2' or 3'- CH_3), 2.29 (s, 3H, 2' or 3'- CH_3), 2.26-2.10 (m, 2H, 8- CH_2CH_3), 1.94-1.82 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.66 (t, 6H, J = 7.4 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 367 (M^++1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_4$) C, H, O.

2',5'-Dimethyl-6,8,8-triethyldesmosdumotin B (48). Pale yellow prisms, mp 110-111 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.12 (s, 1H, 5-OH), 7.32-7.21 (m, 3H, Ar-H), 6.60 (s, 1H, 3-H), 3.95 and 3.89 (s, 3H each, 2' and 3'- OCH_3), 2.46 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.40 (s, 6H, 2' and 5'- CH_3), 2.62-2.12 (m, 2H, 8- CH_2CH_3), 1.98-1.84 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.66 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 399 (M^++Na). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_4$) C, H, O.

2',3'-Dimethoxy-6,8,8-triethyldesmosdumotin B (50). Pale yellow prisms, mp 145-146 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.16 (s, 1H, 5-OH), 7.25-7.10 (m, 3H, Ar-H), 7.15 (s, 1H, 3-H), 3.95 and 3.89 (s, 3H each, 2' and 3'- OCH_3), 2.46 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.29-2.14 (m, 2H, 8- CH_2CH_3), 2.04-1.91 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 399 (M^++1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_6$) C, H, O.

2',5'-Dimethoxy-6,8,8-triethyldesmosdumotin B (51). Pale yellow prisms, mp 95-96 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.21 (s, 1H, 5-OH), 7.26 (s, 1H, 3-H), 7.23 (d, 1H, J = 3.0 Hz, 6'-H), 7.09 (dd, 1H, J = 9.2 and 3.0 Hz, 4'-H), 7.01 (d, 1H, J = 9.2 Hz, 3'-H), 3.92 and 3.84 (s, 3H each, 2' and 5'- OCH_3), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.30-2.16 (m, 2H, 8- CH_2CH_3), 2.04-1.90 (m, 2H, 8- CH_2CH_3), 1.04 (t, 3H, J = 7.4 Hz, 6- CH_2CH_3), 0.67 (t, 6H, J = 7.3 Hz, 8- CH_2CH_3). MS (ESI $^+$) m/z : 399 (M^++1). Anal. ($\text{C}_{23}\text{H}_{26}\text{O}_6$) C, H, O.

3',5'-Dimethoxy-6,8,8-triethyldesmosdumotin B (52). Pale yellow prisms, mp 133-134 °C (EtOAc-hexane). ^1H NMR (300 MHz, CDCl_3): δ 13.2 (s, 1H, 5-OH), 6.90 (d, 2H, J = 2.4 Hz, 2' and 6'-H), 6.87 (s, 1H, 3-H), 6.66 (t, 1H, J = 2.4 Hz, 4'-H), 3.88 (s, 6H, 2' and 5'- OCH_3), 3.92 and 3.84 (s, 3H each, 2' and 5'- OCH_3), 2.45 (q, 2H, J = 7.3 Hz, 6- CH_2CH_3), 2.32-2.17 (m, 2H, 8- CH_2CH_3), 2.05-1.91

(m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS (ESI⁺) *m/z*: 399 (M⁺+1). Anal. (C₂₃H₂₆O₆) C, H, O.

2',3'-Diethoxy-6,8,8-triethyldesmosdumotin B (53). Pale orange prisms, mp 115-116 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.21 (s, 1H, 5-OH), 7.24-7.07 (m, 4H, Ar-*H* and 3-*H*), 4.14 and 4.12 (q, 2H each, *J* = 6.9 Hz, 2' and 3'-OCH₂CH₃), 2.46 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.29-2.14 (m, 2H, 8-CH₂CH₃), 2.04-1.90 (m, 2H, 8-CH₂CH₃), 1.51 and 1.35 (t, 3H each, *J* = 6.9 Hz, 2' and 3'-OCH₂CH₃), 1.04 (t, 3H, *J* = 7.3 Hz, 6-CH₂CH₃), 0.66 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS *m/z* 459 (M⁺+Na). Anal. (C₂₅H₃₀O₆) C, H, O.

2'-Fluoro-5'-methyl-6,8,8-triethyldesmosdumotin B (54). Pale yellow prisms, mp 118-119 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.00 (s, 1H, 5-OH), 7.50-7.42 (m, 1H, Ar-*H*), 7.40-7.33 (m, 1H, Ar-*H*), 7.15 (dd, 1H, *J* = 11.0 and 8.5 Hz, Ar-*H*), 7.00 (s, 1H, 3-*H*), 2.46 (q, 2H, *J* = 7.4 Hz, 6-CH₂CH₃), 2.44 (s, 3H, 5'-CH₃), 2.31-2.18 (m, 2H, 8-CH₂CH₃), 2.04-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS *m/z* 403 (M⁺+Na). Anal. (C₂₂H₂₃FO₄) C, H, O.

4'-Fluoro-3'-methyl-6,8,8-triethyldesmosdumotin B (55). Pale yellow prisms, mp 178-179 °C (EtOAc-hexane). ¹H NMR (300 MHz, CDCl₃): δ 13.04 (s, 1H, 5-OH), 7.65-7.58 (m, 2H, Ar-*H*), 7.23-7.15 (m, 1H, Ar-*H*), 6.83 (s, 1H, 3-*H*), 2.45 (q, 2H, *J* = 7.3 Hz, 6-CH₂CH₃), 2.39 (d, 3H, *J* = 1.8 Hz, 3'-CH₃), 2.34-2.20 (m, 2H, 8-CH₂CH₃), 2.05-1.90 (m, 2H, 8-CH₂CH₃), 1.04 (t, 3H, *J* = 7.4 Hz, 6-CH₂CH₃), 0.67 (t, 6H, *J* = 7.3 Hz, 8-CH₂CH₃). MS *m/z* 403 (M⁺+Na). Anal. (C₂₂H₂₃FO₄) C, H, O.

Table S1. Elemental Analyses of Synthesized Compounds 5-55

| Comp. | Formula | C% | | H% | | O% | |
|-----------|---|--------|-------|--------|-------|--------|-------|
| | | Calcd. | Found | Calcd. | Found | Calcd. | Found |
| 5 | C ₂₄ H ₂₈ O ₄ ·1/8H ₂ O | 75.32 | 75.06 | 7.44 | 7.41 | 17.24 | 16.93 |
| 6 | C ₂₄ H ₂₈ O ₄ | 75.76 | 75.65 | 7.42 | 7.41 | 16.82 | 16.98 |
| 7 | C ₂₅ H ₃₀ O ₄ | 76.00 | 76.11 | 7.66 | 7.61 | 16.22 | 16.34 |
| 8 | C ₂₅ H ₃₀ O ₄ ·1/8H ₂ O | 75.68 | 75.57 | 7.68 | 7.71 | - | - |
| 9 | C ₂₂ H ₂₁ F ₃ O ₄ | 65.02 | 64.94 | 5.21 | 5.06 | 15.75 | 15.85 |
| 10 | C ₂₁ H ₂₂ O ₅ | 71.17 | 71.14 | 6.26 | 6.26 | 22.57 | 22.44 |
| 11 | C ₂₂ H ₂₄ O ₅ ·1/8H ₂ O | 71.28 | 71.14 | 6.59 | 6.54 | - | - |
| 12 | C ₂₃ H ₂₆ O ₅ ·1/8H ₂ O | 71.81 | 71.65 | 6.88 | 6.77 | 21.31 | 21.01 |
| 13 | C ₂₄ H ₂₈ O ₅ | 72.70 | 72.49 | 7.12 | 7.18 | - | - |
| 14 | C ₂₂ H ₂₁ F ₃ O ₅ | 62.56 | 62.56 | 5.01 | 4.86 | 18.94 | 19.04 |
| 15 | C ₂₂ H ₂₄ O ₄ S·1/8H ₂ O | 68.32 | 68.09 | 6.32 | 6.11 | - | - |
| 16 | C ₂₁ H ₂₁ BrO ₄ | 60.44 | 60.57 | 5.07 | 5.13 | 15.34 | 15.08 |
| 17 | C ₂₁ H ₂₁ FO ₄ | 70.77 | 70.61 | 5.94 | 5.82 | 17.96 | 17.74 |
| 18 | C ₂₂ H ₂₃ BrO ₄ | 61.26 | 61.17 | 5.37 | 5.28 | 14.84 | 14.99 |
| 19 | C ₂₃ H ₂₆ O ₅ | 72.23 | 72.03 | 6.85 | 6.83 | 20.92 | 20.75 |
| 20 | C ₂₂ H ₂₄ O ₄ | 74.98 | 74.90 | 6.86 | 6.89 | 18.16 | 18.27 |
| 21 | C ₂₂ H ₂₁ F ₃ O ₄ | 65.02 | 64.84 | 5.21 | 5.02 | 15.75 | 15.93 |
| 22 | C ₂₂ H ₂₄ O | 71.72 | 71.60 | 6.57 | 6.65 | - | - |
| 23 | C ₂₂ H ₂₁ F ₃ O ₅ | 62.56 | 62.64 | 5.01 | 4.91 | 18.94 | 19.13 |
| 24 | C ₂₁ H ₂₁ FO ₄ | 70.77 | 70.59 | 5.94 | 5.98 | - | - |
| 26 | C ₂₂ H ₂₁ F ₃ O ₄ | 65.02 | 64.73 | 5.21 | 4.96 | 15.75 | 16.04 |
| 27 | C ₂₂ H ₂₄ O ₅ | 71.72 | 71.69 | 6.57 | 6.51 | 21.71 | 21.72 |
| 28 | C ₂₁ H ₂₁ FO ₄ | 70.77 | 70.67 | 5.94 | 5.96 | 17.96 | 17.91 |
| 29 | C ₂₃ H ₂₆ O ₄ | 75.38 | 75.54 | 7.15 | 6.99 | 17.46 | 17.71 |
| 30 | C ₂₃ H ₂₆ O ₄ | 75.38 | 75.10 | 7.15 | 7.13 | 17.86 | 17.31 |
| 31 | C ₂₂ H ₂₃ ClO ₄ | 68.30 | 68.03 | 5.99 | 5.89 | 16.54 | 16.54 |
| 32 | C ₂₂ H ₂₃ FO ₄ ·1/16H ₂ O | 71.12 | 70.91 | 6.27 | 6.16 | 17.49 | 17.10 |
| 33 | C ₂₄ H ₂₈ O ₄ | 75.76 | 75.62 | 7.42 | 7.41 | 16.82 | 16.95 |
| 34 | C ₂₃ H ₂₆ O ₅ | 72.23 | 72.29 | 6.85 | 6.89 | 20.92 | 20.75 |
| 35 | C ₂₃ H ₂₆ O ₅ | 72.23 | 72.29 | 6.85 | 6.82 | 20.92 | 20.90 |

| | | | | | | | |
|-----------|---|-------|-------|------|------|-------|-------|
| 36 | C ₂₃ H ₂₆ O ₆ | 69.33 | 69.33 | 6.58 | 6.54 | 24.09 | 23.95 |
| 37 | C ₂₂ H ₂₃ FO ₅ | 68.38 | 68.28 | 6.00 | 5.97 | 20.70 | 20.60 |
| 38 | C ₂₂ H ₂₃ ClO ₅ | 65.59 | 65.65 | 5.75 | 5.72 | 19.86 | 19.92 |
| 39 | C ₂₄ H ₂₈ O ₅ | 72.70 | 72.49 | 7.12 | 7.21 | 20.18 | 19.96 |
| 40 | C ₂₄ H ₂₈ O ₅ | 72.70 | 72.41 | 7.12 | 7.14 | 20.18 | 20.00 |
| 41 | C ₂₄ H ₂₈ O ₇ | 67.28 | 67.17 | 6.59 | 6.44 | - | - |
| 42 | C ₂₄ H ₂₈ O ₇ | 67.28 | 67.30 | 6.59 | 6.74 | 26.14 | 25.93 |
| 43 | C ₂₃ H ₂₅ ClO ₆ ·1/2H ₂ O | 61.51 | 61.32 | 5.93 | 5.58 | - | - |
| 44 | C ₂₁ H ₂₂ O ₆ | 68.10 | 67.56 | 5.99 | 5.94 | - | - |
| 45 | C ₂₃ H ₂₆ O ₅ ·1/8H ₂ O | 71.81 | 71.61 | 6.88 | 6.97 | - | - |
| 46 | C ₂₃ H ₂₆ O ₅ | 72.23 | 72.53 | 6.85 | 6.94 | 20.92 | 20.74 |
| 47 | C ₂₃ H ₂₆ O ₄ | 75.38 | 75.48 | 7.15 | 7.18 | 17.46 | 17.30 |
| 48 | C ₂₃ H ₂₆ O ₄ | 75.38 | 75.10 | 7.15 | 7.16 | 17.46 | 17.40 |
| 49 | C ₂₃ H ₂₆ O ₄ | 75.38 | 75.59 | 7.15 | 7.16 | 17.46 | 17.54 |
| 50 | C ₂₃ H ₂₆ O ₆ | 69.33 | 69.34 | 6.58 | 6.74 | 24.09 | 24.08 |
| 51 | C ₂₃ H ₂₆ O ₆ | 69.33 | 68.81 | 6.58 | 6.49 | 24.09 | 24.18 |
| 52 | C ₂₃ H ₂₆ O ₆ | 69.33 | 69.13 | 6.58 | 6.44 | 24.09 | 24.20 |
| 53 | C ₂₅ H ₃₀ O ₆ | 70.40 | 70.70 | 7.09 | 7.25 | - | - |
| 54 | C ₂₂ H ₂₃ FO ₄ | 71.34 | 71.52 | 6.26 | 6.26 | 17.28 | 17.00 |
| 55 | C ₂₂ H ₂₃ FO ₄ | 71.34 | 71.42 | 6.26 | 6.17 | 17.28 | 17.34 |