# Supplementary Materials:

# Current Research on the Bioprospection of Linear Diterpenes from *Bifurcaria bifurcata*: from Extraction Methodologies to Possible Applications

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**Table S1** – MS data of linear diterpenes identified in *B. bifurcata*.

| Compound | MS data | Ref. |
|---|---|---|
| **1** | EIMS (70 eV) *m/z*: 288, 189, 153, 135, 121, 85 and 69. | [1] |
| **2** | EIMS (70 eV) *m/z* (rel. Int.): 320 (1);<br>HRMS (peak matching): *m/z* 320.2362 calc. for $C_{20}H_{32}O_3$, 320.2351. | [2] |
| **3** | HRMS: 334.2506 $[M]^+$ (calc. for $C_{21}H_{34}O_3$, 334.2508);<br>EIMS (70 eV) *m/z* (rel. int.): 334 $[M]^+$ (0.1), 316 $[M-H_2O]^+$ (0.2), 265(20), 233(100), 215(0.4), 187(0.7), 137(21), 123(60), 107(19), 93(65), 81(40), 69(58), 55(53). | [3] |
| **4** | HRMS: 304.2408 $[M]^+$ (calc. for $C_{20}H_{32}O_2$, 304.2402);<br>EIMS (70 eV) *m/z* (rel. Int.): 304 $[M]^+$ (0.02), 286 $[M-H_2O]^+$ (0.90), 235 (6), 217(7), 199(6), 189(3), 159(14), 149(7), 147(9), 135(18), 133(16), 123(20), 109(24), 107(30), 95(100), 93(71), 81(86), 69(68), 55(83). | [3] |

| | | |
|---|---|---|
| **5** | HRMS: 304.2410 [M]$^+$ (calc. for $C_{20}H_{32}O_2$, 304.2402);<br>EIMS (70 eV) *m/z* (rel. Int.): 304 [M]$^+$ (0.05), 286 [M-$H_2O$]$^+$ (0.16), 235 (34), 217(4), 199(4), 189(3), 159(11), 149(10), 147(8), 135(9), 133(14), 123(20), 109(24), 107(23), 95(55), 93(91), 81(87), 69(72), 55(100). | [3] |
| **6** | HRMS: 304.2407 [M-$H_2O$]$^+$ (calc. for $C_{20}H_{32}O_2$, 304.2402);<br>EIMS (70 eV) *m/z* (rel. Int.): 304 [M-$H_2O$]$^+$ (0.3), 286 [M-2$H_2O$]$^+$ (0.3), 253(0.5), 137(9), 136(9), 95(1), 81(53), 69(100), 55(9). | [4] |
| **7** | HRMS: 306.2565 [M-$H_2O$]$^+$ (calc. for $C_{20}H_{34}O_2$, 306.2559);<br>EIMS (70 eV) *m/z* (rel. Int.): 306 [M-$H_2O$]$^+$ (0.1), 288 [M-2$H_2O$]$^+$ (0.5), 237(2), 219(2), 201(4), 135(11), 121(8), 109(11), 95(16), 85(2), 81(100), 71(10), 69(25), 67(9), 55(23), 53(6). | [4] |
| **8** | HRMS: $C_{20}H_{34}O_3$ | [5] |
| **9** | [M]$^+$ 306 $C_{20}H_{34}O_2$; [M-$H_2O$]$^+$ 288 | [6] |
| **10** | EIMS (70 eV) *m/z* (rel. int.): 284 [M-$H_2O$]$^+$ (9), 218 (10), 203 (8), 175 (10), 135 (21), 107 (15), 93 (23), 85 (100), 81 (58), 69 (37), 43 (99). | [7] |
| **11** | HRMS: 316.2042 [M-$H_2O$]$^+$ (calc. for $C_{20}H_{28}O_3$, 316.2038);<br>EIMS (70 eV) *m/z* (rel. Int.): 334 [M]$^+$ (0.2), 316 [M-$H_2O$]$^+$ (0.4), 218 (15), 203 (14), 175 (12), 136 (12), 123 (9), 94 (13), 85 (100), 81 (51), 69 (27). | [7] |
| **12** | HRMS: 316.2044 [M-$H_2O$]$^+$ (calc. for $C_{20}H_{28}O_3$, 316.2038);<br>EIMS (70 eV) *m/z* (rel. int,): 316 [M-$H_2O$]$^+$ (0.4), 207 (4), 135 (6), 123 (5), 109 (7), 107 (7), 93 (12), 85 (100), 69 (19), 68 (27), 67 (15), 55 (14). | [8] |
| **13** | HRMS: *m/z* 322.2505 [M]$^+$ (calc. for $C_{20}H_{34}O_3$, *m/z* 322.2508);<br>EIMS (70 eV) *m/z* (rel. int.): 322 [M]$^+$ (0.1), 304 [M-$H_2O$]$^+$ (0.1), 286 [M-2$H_2O$]$^+$ (0.1), 219 (5), 186 (7),168 (13), 119 (22), 107 (18), 93 (38), 85 (96), 69 (15), 57 (100). | [9] |
| **14** | HRMS (ESI-TOF) *m/z* 347.2559 [M+Na]$^+$ (calc. for $C_{20}H_{36}O_3Na$, 347.2557). | [10] |

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|---|---|---|
| **15** | HREIMS $[M+Na]^+$ *m/z* 327.23193 (calc. for $C_{20}H_{32}O_2Na$, 327.22945). | [11] |
| **16** | $[M]^+$ 320 ($C_{20}H_{32}O_3$) (*m/z* calculated for 320.23511, found 320.2353) | [6] |
| **17** | MS *m/z*: 300 $[M-18]^+$, 83.0497 | [12] |
| **21** | HRMS: 306.2558 $[M]^+$ (calc. for $C_{20}H_{34}O_2$, 306.2559);<br>EIMS (70 eV) *m/z* (rel. int.): 306 $[M]^+$ (0.4), 288 $[M-H_2O]^+$ (0.9), 211 (3), 188 (6), 135 (12),121 (24), 107 (12), 93 (15), 85 (100), 81 (11), 68 (29), 57 (60), 41 (19). | [8] |
| **22** | (Acetylated): HRMS: 360.2297 $[M]^+$ (calc. for $C_{22}H_{32}O_4$, 360.2300);<br>EIMS (70 eV) *m/z* (rel. Int.): 360 $[M]^+$ (0.1), 300 $[M-HOAc]^+$ (0.5), 277 (2.9), 217 (4.3), 207 (3.4), 199 (1.5), 151 (20.4), 149 (6.7), 134 (4.6), 123 (3.8), 119(3.2), 107(2.7) 95(5.1), 83(100), 77(2.1), 60(1.0), 55(19.3). | [8] |
| **26** | HRMS: *m/z* 322.2511 $[M]^+$ (calc. for $C_{20}H_{34}O_3$, *m/z* 322.2508);<br>EIMS (70 eV) *m/z* (rel. int.): 322 $[M]^+$ (0.3), 286 $[M-2H_2O]^+$ (0.3), 253 (0.5), 137 (9), 136 (9), 95 (1), 83 (53), 69 (100), 55 (9). | [9] |
| **27** | HRMS: *m/z* 320.2353 $[M]^+$ (calc. for $C_{20}H_{32}O_3$, *m/z* 320.2352);<br>EIMS (70 eV) *m/z* (rel. int.): 320 $[M]^+$ (0.4), 302 $[M-H_2O]^+$ (0.1), 289 (0.1), 201 (0.1), 151 (2), 138 (2), 99 (10), 95 (6), 93 (3), 83 (100), 81 (6), 73 (5), 71 (6), 69 (6), 55 (19),43 (34). | [9] |
| **28** | HRMS: *m/z* 322.2501 $[M]^+$ (calc. for $C_{20}H_{34}O_3$, *m/z* 322.2508);<br>EIMS (70 eV) *m/z* (rel. int.): 322 $[M]^+$ (0.2), 286 $[M-2H_2O]^+$ (0.1), 211 (4), 188 (7), 121 (25), 107 (15), 93 (13), 85 (100), 81 (12), 68 (28), 57 (59). | [9] |
| **31** | HR(+)ESI-MS: *m/z* calc. for $C_{20}H_{30}O_3Na$, $[M + Na]^+$ 341.2093, found: 341.2092 | [13] |
| **32** | HR(+)ESI-MS: *m/z* calc. for $C_{20}H_{28}O_3Na$, $[M + Na]^+$ 339.1936, found: 339.1933 | [13] |

| | | |
|---|---|---|
| **33** | HR(+)ESI-MS: *m*/*z* calc. for $C_{20}H_{32}O_3Na$, $[M + Na]^+$ 343.2249, found: 343.2264 | [13] |
| **34** | HR(+)ESI-MS: *m*/*z* calc. for $C_{20}H_{32}O_2Na$, $[M + Na]^+$ 327.2300, found: 327.2298 | [13] |
| **35** | HRESI(+)MS: *m*/*z* calc. for $C_{21}H_{32}O_3K$, $[M + K]^+$ 371.1983, found: 371.2131 | [14] |
| **36** | HREI(+)MS: *m*/*z* calc. for $C_{20}H_{26}O_2$, $[M]^+$ 298.1932, found: 298.1928 | [14] |
| **39** | $[M]^+$ *m*/*z* 290, 69 $[C_5H_9]^+$, 81 $[C_6H_9]^+$, 121 $[C_{11}H_{19}]^+$, 272 $[M\text{-}H_2O]^+$ | [15] |
| **40** | EIMS (70 eV) *m*/*z* (rel. Int.): 288 (2);<br>HRMS (peak matching) *m*/*z* 288.2465 calc. for $C_{20}H_{32}O$, 288.2453. | [2] |
| **41** | HRMS of the TMSi ether: $[M\text{-}TMSiOH]^+$ 360.2855 (calc. for $C_{23}H_{40}SiO$, 360.2848);<br>EIMS (70 eV) *m*/*z* (rel. Int.): 288 (1) $[M\text{-}H_2O]^+$, 257 (1), 147 (11), 135 (31), 109 (36), 93 (57), 81 (100), 43 (77). | [16] |
| **42** | HRMS: 288.2450 $[M]^+$ (calc. for $C_{20}H_{32}O$, 288,2453);<br>EIMS (70 eV) *m*/*z* (rel. int.): 288 $[M]^+$ (0.1), 270 $[M\text{-}H_2O]^+$ (0.4), 255 (0.2), 201(10), 187 (4), 175 (9), 159 (12), 148 (19), 135 (55), 119 (32), 107 (60), 93 (100), 81 (35), 69 (70), 55 (41). | [3] |
| **44** | HRESI(+)MS *m*/*z* calc. for $C_{20}H_{34}O_2Na$, $[M + Na]^+$ 329.2457, found: 329.2478. | [14] |
| **46** | $[M]^+$ *m*/*z* 278, *m*/*z* 43 $[C_3H_7]^+$, 57 $[C_4H_9]^+$, 68, 82, 95 $[C_7H_{11}]^+$, 109 and 123 $[C_9H_{15}]^+$ | [15] |

Calc. – calculated; rel. int – relative intensity;

**Table S2** – $^1$H NMR spectral data for linear diterpenes identified in *B. bifurcata*.$^a$

| | **1 (360 MHz)** | **2 (360 MHz)** | **3 (200 MHz)** | **4 (200 MHz)** | **5 (200 MHz)** | **6 (400 MHz)** | **7 (400 MHz)** | **8 (200 MHz)** | **9 (360 MHz)** | **9 (200 MHz)** |
|---|---|---|---|---|---|---|---|---|---|---|
| **H** | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | CDCl$_3$ $^b$ | C$_6$D$_6$ $^b$ |
| **1** | 4.09 *d* (6.8) | | | 9.88 *d* (8.0) | 9.82 *d* (8.0) | 4.10 *d* (7.0) | 4.12 *d* (6.9) | 4.19 *d* (6.8) | 4.10 *d* (6.7) | 4.11 *d* (6.6) |
| **2** | 5.35 *t* (6.8) | 5.66 *s* | 5.66 *s* | 5.78 *d* (8.0) | 5.82 *d* (8.0) | 5.39 *t* (7.0) | 5.38 *t* (7.0) | 5.46 *t* (6.8) | 5.42 *t* (6.7) | 5.50 *t* (6.6) |
| **3** | | | | | | | | | | |
| **4** | 1.99 *m* | 2.17 *m* | 2.15 *m* | 2.15 *m* | 2.55 *t* (7.3) | 1.95 – 2.15 *m* | 1.99 *t* (7.0) | 2.77 *d* (5.0) | 2.00 *m* | 2.04 *m* |
| **5** | 2.07 *m* | 2.16 *d* (4.5) | 2.12 *m* | 2.15 *m* | 2.11 *m* | 1.55 – 1.75 *m* | 1.40-1.48 *m* | 5.65 *dt* (15.0; 5.0) | 2.08 *m* | 2.12 *m* |
| **6** | 5.07 *t* (6.8) | 5.06 *t* (4.5) | 5.09 *t* (7.0) | 4.99 *t* (4.0) | 5.05 *t* (7.3) | 4.01 *t* (7.0) | 1.38-1.44 *m* | 5.57 *d* (15.0) | 5.12 *t* (6.7) | 5.22 *t* (6.7) |
| **7** | | | | | | | | | | |
| **8** | 1.99 *m* | 2.00 *m* | 2.00 *m* | 1.95 *m* | 1.98 *m* | 1.95-2.15 *m* | 1.45-1.50 *m* | 1.58 *m* | 2.00 *m* | 2.04 *m* |
| **9** | 2.07 *m* | 2.10 *m* | 2.10 *m* | 1.95 *m* | 2.07 *m* | 2.10-2.30 *m* | 2.05 *m* | 2.08 *m* | 2.08 *m* | 2.18 *m* |
| **10** | 5.32 *t* (6.8) | 5.34 *t* (6.8) | 5.36 *t* (7.0) | 5.26 *t* (6.3) | 5.28 *t* (6.8) | 5.36 *t* (7.0) | 5.37 *t* (7.0) | 5.43 *t* (6.6) | 5.18 *t* (6.7) | 5.25 *t* (6.7) |
| **11** | | | | | | | | | | |
| **12** | 3.92 *t* (6.7) | 3.96 *dd* (6,7) | 3.97 *t* (7.0) | 3.87 *t* (6.6) | 3.90 *t* (6.8) | 3.94 *t* (6.7) | 3.94 *t* (6.7) | 4.00 *t* (7.0) | 2.09 *m* | 2.21-2.29 *m* |
| **13** | 2.20 *dd* (6.7,7) | 2.2 *ddd* (6,7,7) | 2.20 *m* | 2.19 *m* | 2.18 *m* | 2.10-2.30 *m* | 2.20-2.28 *m* | 2.21 *m* | 4.37 *ddd* (8.2; 8.2; 5.3) | 4.48 *ddd* (8.2; 8.2; 5.1) |
| **14** | 5.04 *t* (7) | 5.06 *t* (7) | 5.09 *t* (7.0) | 4.99 *t* (6.9) | 5.05 *t* (7.0) | 5.04 *t* (7.0) | 5.05 *t* (7.2) | 5.11 *t* (7.0) | 5.16 *d* (8.2) | 5.32 *d* (8.3) |
| **15** | | | | | | | | | | |
| **16** | 1.68 *s* | 1.70 *s* | 1.71 *s* | 1.61 *s* | 1.65 *s* | 1.67 *s* | 1.69 *s* | 1.75 *s* | 1.69 *s* | 1.63 *s* |
| **17** | 1.60 *s* | 1.59 *s* | 1.60 *s* | 1.52 *s* | 1.55 *s* | 1.59 *s* | 1.60 *s* | 1.66 *s* | 1.66 *s* | 1.58 *s* |
| **18** | 1.57 *s* | 1.60 *s* | 1.61 *s* | 1.52 *s* | 1.55 *s* | 1.59 *s* | 1.60 *s* | 1.64 *s* | 1.62 *s* | 1.60 *s* |
| **19** | 1.56 *s* | 1.62 *s* | 1.63 *s* | 1.53 *s* | 1.57 *s* | 4.83-5.01 *s* | 1.14 *s* | 1.32 *s* | 1.57 *s* | 1.56 *s* |
| **20** | 1.63 *s* | 2.14 *s* | 2.16 *s* | 2.08 *s* | 1.93 *s* | 1.64 *s* | 1.64 *s* | 1.70 *s* | 1.64 *s* | 1.54 *s* |
| **21** | | | 3.68 *s* | | | | | | | |
| **Ref.** | [1] | [2] | [3] | [3] | [3] | [4] | [4] | [5] | [7] | |

$^a$ Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; $^b$ TMS as internal standard.

**Table S2** – Cont. [a]

| | 10 (200 MHz) | 11 (200 MHz) | | 12 (400 MHz) | | 13 (400 MHz) | 14 (500 MHz) | 15 (400 MHz) | 15 (600 MHz) | 15 (250 MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| **H** | $\mathrm{CDCl_3}$ [b] | $\mathrm{CDCl_3}$ [b] | $\mathrm{C_6D_6}$ [b] | $\mathrm{CDCl_3}$ [b] | $\mathrm{C_6D_6}$ [b] | $\mathrm{CDCl_3}$ [b] | $\mathrm{CDCl_3}$ | $\mathrm{CDCl_3}$ | $\mathrm{CDCl_3}$ * | $\mathrm{CDCl_3}$ [b] |
| **1** | 7.34 *m* | 5.58 *d* (2.4) | 4.70 *d* (2.5) | - | - | 4.16 *d* (6.8) | 4.13 *d* (6.8) | 4.11 *d* (6.8) | 4.13 *d* (6.5) | 4.15 *d* (6.5) |
| **2** | 6.28 *m* | 3.80 *t* (2.5)<br>2.82 *ddd* (10.0; 5.0; 2.5) | 2.86 *m*<br>2.07 *m* | 2.64 *d* (19)<br>2.75 *d* (19) | 1.87 *d* (19)<br>2.24 *d* (19) | 5.44 *t* (6.8) | 5.39 *t* (6.8) | 5.36 *t* (6.8) | 5.39 *t* (6.5) | 5.40 *t* (6.5) |
| **3** | | | | | | | | | | |
| **4** | 2.47 *t* (7.3) | 1.90-1.78 *m* | 1.82-1.69 *m* | 1.75-1.90 *m* | 1.18-1.33 *m* | 2.74 *d* (4.8) | 2.00 *t* (7.0) | 2.04 *t* (8.0) | 2.02 *m* | 2.04 *m* |
| **5** | 2.24 *m* | 2.28 *m* | 2.02 *m* | 2.09 *m* | 1.77 *m* | 5.57 *dt* (15.5; 4.8) | 1.45 *m* | 1.97 *dt* (8.0) | 2.09 *m* | 2.04 *m* |
| **6** | 5.17 *t* (7.0) | 5.16 *t* (6.8) | 5.01 *t* (7.0) | 5.01 *t* (6.8) | 4.93 *m* | 5.61 *d* (15.5) | 1.40 *m* | 5.08 *t* (6.4) | 5.10 *t* (6.5) | 5.10 *t* (6.5) |
| **7** | | | | | | | | | | |
| **8** | 2.03 *m* | 2.03 *m* | 2.02 *m* | 2.00 *m* | 1.97 *m* | 1.60 *m* | 1.49 *t* (7.8) | 2.04 *t* (8.0) | 2.02 *m* | 2.04 *m* |
| **9** | 2.12 *m* | 2.14 *m* | 2.12 *m* | 2.09 *m* | 2.09 *m* | 2.15 *m* | 2.07 *dt* (7.0; 7.8) | 1.97 *dt* (8.0) | 2.09 *m* | 2.04 *m* |
| **10** | 5.21 *t* (7.0) | 5.21 *t* (6.8) | 5.22 *t* (6.7) | 5.12 *t* (6.8) | 5.21 *t* (6.8) | 5.27 *t* (7.0) | 5.25 *t* (7.0) | 5.20 *t* (6.4) | 5.22 *t* (6.5) | 5.21 *t* (6.5) |
| **11** | | | | | | | | | | |
| **12** | 2.13 *m* | 2.10 *m* | 2.24 *m* | 2.07 *m* | 2.21 *m* | 2.12 *m* | 2.11 *d* (6.9) | 2.99 *br,s* | 3.01 *s* | 3.03 *s* |
| **13** | 4.41 *ddd* (8.3; 8.3; 5.0) | 4.40 *ddd* (8.2; 8.2; 8.2; 5.3) | 4.45 *ddd* (8.3; 8.3; 5.5) | 4.33 *ddd* (8.3; 8.3; 5.2) | 4.46 *ddd* (8.3; 8.3; 5.5) | 4.43 *ddd* (8.2; 8.2; 5.3) | 4.41 *dt* (8.2; 6.9) | | | |
| **14** | 5.16 *d* (8.3) | 5.15 *d* (8.2) | 5.29 *d* (8.3) | 5.07 *d* (8.3) | 5.31 *d* (8.3) | 5.15 *d* (8.2) | 5.13 *d* (8.2) | | 6.10 *s* | 6.10 *s* |
| **15** | | | | | | | | | | |
| **16** | 1.72 *s* | 1.72 *s* | 1.61 *s* | 1.65 *s* | 1.61 *s* | 1.72 *s* | 1.69 *br.s* | 1.55 *br,s* | 1.86 *s* | 1.87 *s* |
| **17** | 1.69 *s* | 1.69 *s* | 1.56 *s* | 1.62 *s* | 1.56 *s* | 1.69 *s* | 1.66 *br.s* | 1.82 *br,s* | 2.12 *s* | 2.12 *s* |
| **18** | 1.66 *s* | 1.66 *s* | 1.59 *s* | 1.59 *s* | 1.59 *s* | 1.67 *s* | 1.65 *br.s* | 1.62 *br,s* | 1.59 *s* | 1.60 *s* |
| **19** | 1.59 *s* | 1.65 *s* | 1.47 *s* | 1.55 *s* | 1.43 *s* | 1.28 *s* | 1.14 *s* | 1.55 *br,s* | 1.59 *s* | 1.60 *s* |
| **20** | 7.21 *s* | | | 5.36 *s* | 4.69 *s* | 1.65 *s* | 1.65 *br.s* | 1.55 *br,s* | 1.66 *s* | 1.66 *s* |
| **21** | | | | | | | | | | |
| **Ref.** | [7] | [7] | | [8] | | [9] | [10] | [11] | [13] | [8] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard.

**Table S2** – Cont. [a]

| | 15 (400 MHz) | | 17 | 18 (250 MHz) | 19 (500 MHz) | 20 (500 MHz) | 21 (400 MHz) | | 22 (400 MHz) | | 23 (400 MHz) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **H** | $CDCl_3$ [b] | $CDCl_3$ | | $CD_3OD$ | $CDCl_3$ | $CDCl_3$ | $CDCl_3$ [b] | $C_6D_6$ [b] | $CDCl_3$ [b] | $C_6D_6$ [b] | $CDCl_3$ |
| **1** | 4.13 *d* (6.5) | 4.09 *d* (6.8) | 4.08 *d* (6.7) | 7.32 *t* (1.7) | | 5.57 *d* (2.2) | 4.15 *d* (6.5) | 4.02 *d* (6.5) | 4.58 *d* (6.5) | 4.59 *d* (6.5) | 9.92 *d* (8.0) |
| **2** | 5.39 *t* (6.5) | 5.35 *t* (6.8) | 5.42 *t* (6.7) | 6.24 *d* (1.1) | 5.96 *s* | 3.78 *t* (2.4) | 5.41 *t* (6.5) | 5.40 *t* (6.5) | 5.34 *t* (6.5) | 5.39 *t* (6.5) | 5.87 *d* (8.0) |
| **3** | | | 1.62 | | | 2.80 *ddd* (2.5; 4.8; 10.1) | | | | | |
| **4** | 2.02 *m* | 1.99 *m* | 2.72 *d* | 2.40 *t* (7.4) | 2.42, 2.53 *m* | 1.76, 1.88 *m* | 1.98 *m* | 2.00 *m* | 2.05 *m* | 1.91 *t* (8.0) | 2.22 *m* |
| **5** | 2.09 *m* | 2.06 *m* | 5.17 *m* | 2.20 *q* (7.4) | 2.32 *m* | 2.26 *m* | 2.10 *m* | 2.12 *m* | 2.10 *m* | 2.00 *m* | 2.21 *m* |
| **6** | 5.10 *t* (6.5) | 5.06 *t* (6.7) | 5.44 *d* (15.6) | 5.14 *dt* (1.2; 7.1) | 5.10 *t* (7) | 5.15 *t* (7) | 5.11 *t* (6.5) | 5.21 *t* (6.5) | 5.12 *t* (7.5) | 5.06 *t* (8.0) | 5.09 *t* (6.2) |
| **7** | | | 1.27 *s* | | | | | | | | |
| **8** | 2.02 *m* | 1.98 *m* | 3.55 *dd* (6.7, 12) | 2.09 *t* (6.5) | 2.14 *t* (7) | 2.15 *t* (8) | 1.98 *m* | 2.03 *m* | 2.29 *t* (7.5) | 2.35 *t* (7.5) | 2.02 *m* |
| **9** | 2.09 *m* | 2.08 *m* | 2.11 | 2.01 *q* (6.5) | 2.04 *q* (7.5) | 2.03 *q* (8) | 2.10 *m* | 2.11 *m* | 2.82 *t* (7.5) | 2.62 *t* (7.5) | 2.12 *m* |
| **10** | 5.22 *t* (6.5) | 5.19 *t* (6.8) | | 5.22 *dt* (1.2; 6.9) | 5.12 *t* (7) | 5.20 *t* (7) | 5.23 *t* (6.5) | 5.21 *t* (6.5) | | | 5.22 *t* (6.2) |
| **11** | | | 1.62 | | | | | | | | |
| **12** | 3.01 *s* | 2.97 *s* | 2.98 *s* | 2.99 *s* | 3.03 *s* | 3.02 *s* | 3.01 *s* | 2.81 *s* | 3.40 *s* | 3.27 *s* | 3.03 *s* |
| **13** | | | | | | | | | | | |
| **14** | 6.10 *s* | 6.06 *s* | 6.09 *s* | 6.14 *t* (1.3) | 6.09 *s* | 6.09 *s* | 2.26 *d* (6.5) | 2.01 *d* (6.5) | 6.12 *s* | 5.88 *s* | 6.10 *s* |
| **15** | - | | 2.11 | | | | 2.07 *m* | 2.11 *m* | | | |
| **16** | 1.86 *s* | 1.82 *s* | 1.87 *s* | 1.85 *d* (1.2) | 1.86 *s* | 1.86 *s* | 0.87 *d* (7.0) | 0.82 *d* (7.0) | 1.89 *s* | 1.43 *s* | 1.88 *s* |
| **17** | 2.12 *s* | 2.11 *s* | | 2.08 *d* (1.1) | 2.12 *s* | 2.12 *s* | 0.87 *d* (7.0) | 0.82 *d* (7.0) | 2.12 *s* | 2.04 *s* | 2.14 *s* |
| **18** | 1.59 *s* | 1.56 *s* | | 1.65 *s* | 1.61 *s* | 1.61 *s* | 1.60 *s* | 1.60 *s* | 5.84 *s*<br>6.18 *s* | 5.39 *s*<br>5.70 *s* | 1.61 *s* |
| **19** | 1.59 *s* | 1.55 *s* | | 1.65 *s* | 1.61 *s* | 1.61 *s* | 1.60 *s* | 1.54 *s* | 1.62 *s* | 1.43 *s* | 1.61 *s* |
| **20** | 1.66 *s* | 1.61 *s* | | 7.19 *t* (1.7) | 5.81 *s* | | 1.65 *s* | 1.49 *s* | 1.70 *s* | 1.49 *s* | 2.17 *s* |
| **22** | | | | | | | | | 2.07 *s* | 1.70 *s* | |
| **Ref.** | [8] | [17] | [12] | [18] | | | [8] | | [8] | | [17] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard.

**Table S2** – Cont. [a]

|  | **25 (270 MHz)** | **25 (400 MHz)** | **26 (400 MHz)** | **27 (400 MHz)** | **28 (400 MHz)** | **29 (400 MHz)** | **30 (400 MHz)** | **31 (600 MHz)** | **32 (600 MHz)** | **33 (600 MHz)** |
|---|---|---|---|---|---|---|---|---|---|---|
| **H** | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ | $CDCl_3$ | $CDCl_3$ |
| **1** | 4.12 *d* (6.5) | 4.15 *d* (6.8) | 4.15 *d* (6.8) | a: 3.69 *dd* (11.2; 2.7)<br>b: 3.53 *dd* (11.2; 2.7) | 4.14 *d* (6.8) | 4.11 *d* (6.7) | 4.15 *d* (6.8) |  |  |  |
| **2** | 5.36 *t* (6.5) | 5.40 *t* (6.8) | 5.41 *t* (6.8) | 4.20 *dd* (7.3; 2.7) | 5.43 *t* (6.8) | 5.40 *t* (6.7) | 5.43 *t* (6.8) | 5.71 *s* | 5.86 *quintet* (1.6) | 5.70 *s* |
| **3** |  |  |  |  |  |  |  |  |  |  |
| **4** | 2.29 *t* (7.0) | 2.33 *t* (7.0) | 2.04 *m* | 2.01 *m* | 2.05-2.11 *m* | 2.08-2.11 *m* | 2.73 *d* (5.2) | 2.19 *m* | 2.48 *t* (7.3) | 2.20 *m* |
| **5** | 2.84 *t* (7.0) | 2.81 *t* (7.0) | 2.12 *m* | 2.17 *m* | 1.66 *m* | 1.61-1.63 *m* | 5.57 *dt* (15.4; 5.2) | 2.19 *m* | 2.32 *m* | 2.20 *m* |
| **6** |  |  | 5.11 *t* (6.8) | 5.12 *t* (7.0) | 4.06 *t* (6.4) | 4.03 *t* (6.3) | 5.62 *d* (15.4) | 5.11 *t* (6.0) | 5.10 *dt* (1.2; 6.8) | 5.10 *t* (6.1) |
| **7** |  |  |  |  |  |  |  |  |  |  |
| **8** | 2.24 *m* | 2.31 *t* (7.0) | 2.02 *m* | 2.02 *m* | 2.06-2.18 *m* | 2.11-2.14 *m* | 1.61 *m* | 2.04 *t* (7.8) | 2.05 *t* (7.1) | 2.04 *t* (7.0) |
| **9** | 2.15 *m* | 2.17 *m* | 2.14 *m* | 2.13 *m* | 2.21 *m* | 2.24 *m* | 2.16 *m* | 2.15 *m* | 2.16 *d* (0.9) | 2.14 *m* |
| **10** | 5.18 *t* (6.5) | 5.22 *t* (6.8) | 5.26 *t* (7.0) | 5.22 *t* (7.0) | 5.24 *t* (6.5) | 5.22 *t* (6.3) | 5.25 *t* (6.8) | 5.24 *t* (6.8) | 5.22 *dt* (0.9; 7.1) | 5.24 *t* (6.3) |
| **11** |  |  |  |  |  |  |  |  |  |  |
| **12** | 3.01 *s* | 3.03 *s* | 3.03 *s* | 3.02 *s* | 3.02 *s* | 3.01 *s* | 3.03 *s* | 3.05 *s* | 3.06 *s* | 3.03 *s* |
| **13** |  |  |  |  |  |  |  |  |  |  |
| **14** | 6.30 *s* | 6.10 *s* | 2.61 *s* | 6.10 *s* | 2.27 *d* (6.7) | 6.07 *s* | 6.09 *s* | 6.12 *s* | 6.12 *m* | 2.30 *d* (6.9) |
| **15** |  |  |  |  | 2.11 *m* |  |  |  |  | 2.13 *m* |
| **16** | 1.88 *s* | 1.88 *s* | 1.23 *s* | 1.87 *s* | 0.89 *d* (6.5) | 1.84 *s* | 2.13 *s* | 1.89 *s* | 1.89 *d* (0.9) | 0.91 *d* (6.7) |
| **17** | 2.12 *s* | 2.14 *s* | 1.23 *s* | 2.13 *s* | 0.89 *d* (6.5) | 2.10 *s* | 1.87 *s* | 2.16 *s* | 2.16 *d* (0.8) | 0.91 *d* (6.7) |
| **18** | 1.59 *s* | 1.60 *s* | 1.62 *s* | 1.61 *s* | 1.60 *s* | 1.59 *s* | 1.60 *s* | 1.63 *s* | 1.64 *s* | 1.62 *s* |
| **19** | 5.70 *s*<br>5.96 *s* | a: 6.00 *s*<br>b: 5.74 *s* | 1.60 *s* | 1.61 *s* | a: 5.05 *s*<br>b: 4.87 *s* | a: 5.02 *s*<br>b: 4.84 *s* | 1.28 *s* | 1.63 *s* | 1.63 *s* | 1.62 *s* |
| **20** | 1.67 *s* | 1.69 *s* | 1.68 *s* | a: 5.14 *s*<br>b: 4.97 *s* | 1.67 *s* | 1.65 *s* | 1.66 *s* | 2.18 *s* | 4.75 *d* (1.6) | 2.18 *s* |
| **21** |  |  |  |  |  |  |  |  |  |  |
| **Ref.** | [8] | [9] | [9] | [9] | [9] | [9] | [9] | [13] | [13] | [13] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard.

**Table S2** – Cont. [a]

| | **34 (600 MHz)** | **35 (600 MHz)** | **36 (600 MHz)** | **40 (360 MHz)** | **40 (400 MHz)** | **41 (400 MHz)** | **42 (200 MHz)** | **43 (400 MHz)** | **44 (600 MHz)** |
|---|---|---|---|---|---|---|---|---|---|
| **H** | $CDCl_3$ | $CDCl_3$ | $CDCl_3$ | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ |
| **1** | 4.18 *s* (6.5) | 4.70 *d* (7.2) | 7.36 *t* (1.5) | 4.10 *d* (6.8) | 4.10 *d* (6.8) | 4.15 *d* (6.8) | 4.15 *d* (7.0) | 4.15 *d* (6.8) | 4.17 *d* (6.8) |
| **2** | 5.44 *t* (6.5) | 5.38 *t* (7.2) | 6.30 *s* | 5.37 *t* (6.8) | 5.37 *t* (6.8) | 5.42 *t* (6.8) | 5.42 *t* (7.0) | 5.41 *t* (7.0) | 5.44 *t* (6.8) |
| **3** | | | | | | | | | |
| **4** | 2.05 *m* | 2.07 *m* | 2.47 *t* (7.6) | 2.00 *m* | 2.0 *m* | 2.00 *m* | 2.00-2.20 *m* | 2.02 *d* (6.5) | 2.07 *m* |
| **5** | 2.14 *m* | 2.13 *m* | 2.26 *q* (7.5) | 2.07 *m* | 2.07 *m* | 2.07 *m* | 2.00-2.20 *m* | 1.45-1.50 *m* | 2.14 *m* |
| **6** | 5.14 *t* (6.3) | 5.12 *t* (6.8) | 5.19 *t* (7.0) | 5.09 *t* (6.8) | 5.09 *t* (6.8) | 5.11 *t* (6.8) | 5.15 *t* (7.0) | 1.45-1.50 *m* | 5.13 *t* (6.8) |
| **7** | | | | | | | | | |
| **8** | 2.04 *m* | 2.3 *t* (7.2) | 2.04 *t* (7.6) | 2.00 *m* | 2.0 *m* | 2.00 *m* | 2.75 *d* (7.0) | 1.68 *m*<br>1.80 *m* | 2.05 *s* |
| **9** | 1.59 *m* | 2.13 *m* | 2.13 *q* (7.6) | 2.07 *m* | 2.07 *m* | 2.07 *m* | 5.51 *dt* (15.0; 70) | 1.78 *m*<br>1.91 *m* | 2.14 *m* |
| **10** | 2.20 *m* | 5.26 *t* (6.8) | 5.23 *t* (6.8) | 5.13 *t* (6.8) | 5.13 *t* (6.8) | 5.13 *t* (6.8) | 6.05 *d* (15.0) | 4.25 *t* (7.0) | 5.13 *t* (6.8) |
| **11** | | | | | | | | | |
| **12** | 6.04 *s* | 3.05 *s* | 3.25 *s* | 2.72 *d* (7.2) | 2.72 *d* (7.2) | 2.67 *d* (5.6) | 5.35 *t* (7.0) | 5.41 *t* (7.0) | 2.04 *s* |
| **13** | | | | 5.58 *dt* (7.2; 15.6) | 5.58 *dt* (15.6; 7.2) | 5.57 *dt* (15.6; 5.6) | 2.81 *t* (7.0) | 2.71 *t* (7.0) | 2.14 *m* |
| **14** | 6.09 *s* | 6.13 *s* | 5.89 *s* | 6.10 *d* (15.6) | 6.10 *d* (15.6) | 5.63 *d* (15.6) | 5.11 *t* (7.0) | 5.10 *t* (7.0) | 5.41 *t* (6.9) |
| **15** | | | | | | | | | |
| **16** | 1.89 *s* | 1.89 *s* | 7.09 *s* | 4.84 *s* | 1.81 *s* | 1.32 *s* | 1.68 *s* | 1.68 *s* | 4.01 *s* |
| **17** | 2.16 *s* | 2.16 *s* | 2.00 *s* | 1.81 *s* | 4.84 *s* | 1.32 *s* | 1.64 *s* | 1.62 *s* | 1.68 *s* |
| **18** | 2.19 *s* | 1.63 *s* | 1.61 *s* | 1.57 *s* | 1.57 *s* | 1.57 *s* | 1.75 *s* | 1.62 *s* | 1.62 *s* |
| **19** | 1.62 *s* | 1.62 *s* | 1.62 *s* | 1.58 *s* | 1.58 *s* | 1.60 *s* | 1.59 *s* | 1.22 *s* | 1.62 *s* |
| **20** | 1.62 *s* | 1.74 *s* | 7.23 *s* | 1.65 *s* | 1.65 *s* | 1.68 *s* | 1.68 *s* | 1.67 *s* | 1.70 *s* |
| **21** | | 8.09 *s* | | | | | | | |
| **Ref.** | [13] | [14] | [14] | [2] | [16] | [16] | [3] | [5] | [14] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard.

**Table S3** – $^{13}$C NMR spectral data of linear diterpenes identified in *B. bifurcata*. [a, b, c]

| | **1 (90.5 MHz)** | **2 (50 MHz)** | **3 (50 MHz)** | **4 (50 MHz)** | **5 (50 MHz)** | **6 (100 MHz)** | **7 (100 MHz)** | **8 (62.5 MHz)** | **9** | **9 (90 MHz)** |
|---|---|---|---|---|---|---|---|---|---|---|
| **C** | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | | $CDCl_3$ [b] |
| **1** | 59.21 *t* (106) | 171.3 *s* | 167.2 - C | 191.3 – CH | 190.9 – CH | 59.2 – $CH_2$ | 59.2 – $CH_2$ | 59.4 *t* | 59.3 | 59.3 – $CH_2$ |
| **2** | 123.53 *d* (153) | 115.2 *d* | 115.3 – CH | 127.4 – CH | 128.6 – CH | 123.7 – CH | 123.6 – CH | 124.2 *d* | 123.6 | 124.3 – CH |
| **3** | 139.09 *s* | 162.4 *s* | 159.9 – C | 163.9 – C | 164.0 – C | 139.1 – C | 139.4 – C | 138.4 *s* | 135.0 | 139.4 – C |
| **4** | 39.40 *t* (94) | 41.1 *t* | 40.8 – $CH_2$ | 40.5 – $CH_2$ | 34.1 – $CH_2$ | 35.5 – $CH_2$ | 39.8 – $CH_2$ | 42.3 *t* | 39.5 | 39.5 – $CH_2$ |
| **5** | 26.71 *t* (92) | 26.1 *t* (4.5) | 26.1 – $CH_2$ | 26.0 – $CH_2$ | 26.8 – $CH_2$ | 33.3 – $CH_2$ | 21.9 – $CH_2$ | 125.3 *d* | 25.7 | 25.8 – $CH_2$ |
| **6** | 123.98 *d* (150) | 122.9 *d* (4.5) | 123.0 - CH | 122.6 – CH | 122.2 – CH | 74.9 – CH | 41.4 – $CH_2$ | 138.8 *d* | 124.3 | 123.6 – CH |
| **7** | 134.89 *s* | 136.0 *s* | 135.9 – C | 136.3 – C | 137.0 – C | 151.3 – C | 72.8 – C | 72.9 *s* | 134.7 | 134.8 – C |
| **8** | 39.18 *t* (94) | 39.2 *t* | 39.2 – $CH_2$ | 39.2 – $CH_2$ | 39.1 – $CH_2$ | 30.9 – $CH_2$ | 41.2 – $CH_2$ | 42.2 *t* | 39.4 | 39.4 – $CH_2$ |
| **9** | 26.00 *t* (94) | 25.9 *t* | 25.9 – $CH_2$ | 25.8 – $CH_2$ | 25.8 – $CH_2$ | 26.1 – CH | 22.1 – $CH_2$ | 22.5 *t* | 26.2 | 26.2 – $CH_2$ |
| **10** | 125.80 *d* (151) | 125.9 *d* (6.8) | 125.8 – CH | 125.6 – CH | 125.5 – CH | 125.6 – CH | 126.1 – CH | 126.1 *d* | 127.5 | 127.4 – CH |
| **11** | 136.71 *s* | 136.7 *s* | 136.9 – C | 136.9 – C | 137.0 – C | 137.1 – C | 136.9 – C | 137.0 *s* | 131.6 | 131.6 – C |
| **12** | 77.14 *d* (109) | 77.3 *d* (6.7) | 77.2 – CH | 77.1 – CH | 77.1 – CH | 77.1 – CH | 77.1 – CH | 77.1 *t* | 48.2 | 48.2 – $CH_2$ |
| **13** | 34.17 *t* (96) | 34.2 *t* (6.7; 7) | 34.2 – $CH_2$ | 34.2 – $CH_2$ | 32.3 – $CH_2$ | 34.1 – $CH_2$ | 34.2 – $CH_2$ | 34.2 *t* | 65.8 | 65.6 – CH |
| **14** | 120.23 *d* (151) | 120.2 *d* (7) | 120.3 – CH | 120.3 – CH | 120.4 – CH | 120.1 – CH | 120.1 – CH | 120.1 *d* | 128.4 | 128.5 – CH |
| **15** | 134.20 *s* | 134.4 *s* | 134.1 – C | 134.3 – C | 134.1 – C | 134.6 – C | 134.7 – C | 134.9 *s* | 139.3 | 135.0 – C |
| **16** | 25.76 *q* (70) | 25.8 *q* | 25.8 – $CH_3$ | 25.6 – $CH_3$ | 25.0 – $CH_3$ | 25.8 – $CH_3$ | 25.9 – $CH_3$ | 25.9 *q* | 26.4 | 26.4 – $CH_3$ |
| **17** | 17.89 *q* (95) | 17.9 *q* | 17.9 – $CH_3$ | 17.5 – $CH_3$ | 17.9 – $CH_3$ | 17.9 – $CH_3$ | 18.0 – $CH_3$ | 18.0 *q* | 15.9 | 18.2 – $CH_3$ |
| **18** | 11.63 *q* (92) | 19.1 *q* | 11.5 – $CH_3$ | 11.6 – $CH_3$ | 11.6 – $CH_3$ | 11.7 – $CH_3$ | 11.7 – $CH_3$ | 11.7 *q* | 16.2 | 16.3 – $CH_3$ |
| **19** | 15.92 *q* (96) | 16.0 *q* | 15.9 – $CH_3$ | 16.0 – $CH_3$ | 16.0 – $CH_3$ | 109.9 – $CH_3$ | 26.7 – $CH_3$ | 28.2 *q* | 16.3 | 15.9 – $CH_3$ |
| **20** | 16.17 *q* (96) | 11.6 *q* | 18.7 – $CH_3$ | 17.9 – $CH_3$ | 25.8 – $CH_3$ | 16.2 – $CH_3$ | 16.1 – $CH_3$ | 16.4 *q* | 18.2 | 16.2 – $CH_3$ |
| **21** | | | 50.7 – $CH_3$ | | | | | | | |
| **22** | | | | | | | | | | |
| **Ref.** | [1] | [2] | [3] | [3] | [3] | [4] | [4] | [5] | [6] | [7] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard; [c] Multiplicities were obtained with DEPT sequences.

**Table S3** – Cont. [a, b, c]

|  | **9 (50 MHz)** | **10 (50 MHz)** | **11 (50 MHz)** |  | **12 (100 MHz)** |  | **13 (100 MHz)** | **14 (500 MHz)** | **15 (100, 25, 18 MHz)** |
|---|---|---|---|---|---|---|---|---|---|
| **C** | $C_6D_6$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $C_6D_6$ [b] | $CDCl_3$ [b] | $C_6D_6$ [b] | $CDCl_3$ [b] | $CDCl_3$ | $CDCl_3$ |
| **1** | 59.3 – CH$_2$ | 142.5 – CH | 77.6 – CH | 78.2 – CH | 173.5 – C | 173.0 – C | 59.4 *t* | 59.3 – CH$_2$ | 58.8 |
| **2** | 125.3 – CH | 111.1 – CH | 53.7 – CH | 54.3 – CH | 36.1 – CH$_2$ | 35.7 – CH$_2$ | 124.3 *d* | 123.6 – CH | 124.5 |
| **3** | 137.6 – C | 125.0 – C | 43.1 - CH | 43.8 - CH | 62.3 – C | 61.8 – C | 138.3 *s* | 139.5 – C | 137.6 |
| **4** | 39.9 – CH$_2$ | 25.0 – CH$_2$ | 26.8 – CH$_2$ | 27.9 – CH$_2$ | 29.5 – CH$_2$ | 29.3 – CH$_2$ | 42.3 *t* | 39.9 – CH$_2$ | 39.6 |
| **5** | 26.7 – CH$_2$ | 28.4 – CH$_2$ | 25.8 – CH$_2$ | 26.7 – CH$_2$ | 23.1 – CH$_2$ | 23.1 – CH$_2$ | 125.2 *d* | 22.0 – CH$_2$ | 26.5 |
| **6** | 124.9 – CH | 124.2 – CH | 123.0 – CH | 124.5– CH | 122.5 – CH | 123.4 – CH | 138.9 *d* | 41.7 – CH$_2$ | 124.4 |
| **7** | 134.9 – C | 134.9 – C | 134.9 – C | 134.5 – C | 136.9 – C | 136.4 – C | 73.0 *s* | 72.7 – C | 134.6 |
| **8** | 39.8 – CH$_2$ | 39.5 – CH$_2$ | 39.5 – CH$_2$ | 40.6 – CH$_2$ | 39.4 – CH$_2$ | 39.7 – CH$_2$ | 42.4 *t* | 41.3 – CH$_2$ | 39.4 |
| **9** | 26.5 – CH$_2$ | 26.4 – CH$_2$ | 26.4 – CH$_2$ | 27.5 – CH$_2$ | 26.2 – CH$_2$ | 26.4 – CH$_2$ | 23.1 *t* | 22.8 – CH$_2$ | 26.8 |
| **10** | 128.2 – CH | 127.5 – CH | 128.2 – CH | 129.1 – CH | 127.5 – CH | 128.6 – CH | 127.5 *d* | 128.6 – CH | 122.9 |
| **11** | 132.1 – C | 131.7 – C | 131.9 – C | 133.3 – C | 131.9 – C | 132.5 – C | 131.7 *s* | 131.6 – C | 129.5 |
| **12** | 48.7 – CH$_2$ | 48.2 – CH$_2$ | 48.2 – CH$_2$ | 49.5 – CH$_2$ | 48.2 – CH$_2$ | 48.7 – CH$_2$ | 48.1 *t* | 48.1 – CH$_2$ | 55.3 |
| **13** | 66.5 – CH | 65.6 – CH | 65.7 – CH | 67.2 – CH | 65.5 – CH | 66.2 – CH | 65.9 *d* | 65.9 – CH | 198.8 |
| **14** | 129.1 – CH | 128.5 – CH | 127.5 – CH | 129.9 – CH | 129.2 – CH | 129.1 – CH | 128.6 *d* | 127.5 – CH | 129.1 |
| **15** | 133.5 – C | 135.5 – C | 137.0 – C | 137.4 – C | 135.0 – C | 133.7 – C | 134.6 *s* | 134.8 – C | 155.1 |
| **16** | 25.8 – CH$_3$ | 25.8 – CH$_3$ | 25.8 – CH$_3$ | 26.6 – CH$_3$ | 25.8 – CH$_3$ | 25.7 – CH$_3$ | 25.8 *q* | 25.7 – CH$_3$ | 27.5 |
| **17** | 18.2 – CH$_3$ | 18.2 – CH$_3$ | 18.2– CH$_3$ | 19.0– CH$_3$ | 18.2 – CH$_3$ | 18.1 – CH$_3$ | 18.2 *q* | 18.2 – CH$_3$ | 20.5 |
| **18** | 16.4 – CH$_3$ | 16.2 – CH$_3$ | 16.2 – CH$_3$ | 17.2 – CH$_3$ | 16.1 – CH$_3$ | 16.3 – CH$_3$ | 16.4 *q* | 16.1 – CH$_3$ | 15.9 |
| **19** | 15.9 – CH$_3$ | 15.9 – CH$_3$ | 16.0 – CH$_3$ | 16.7 – CH$_3$ | 15.9 – CH$_3$ | 15.7 – CH$_3$ | 28.5 *q* | 26.7 – CH$_3$ | 16.2 |
| **20** | 16.2 – CH$_3$ | 138.9 - CH | 175.6 – C | 175.3 – C | 82.9 – CH | 82.6 – CH | 16.2 *q* | 16.2 – CH$_3$ | 17.6 |
| **21** |  |  |  |  |  |  |  |  |  |
| **22** |  |  |  |  |  |  |  |  |  |
| **Ref.** | [7] | [7] | [7] |  | [8] |  | [9] | [10] | [19] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard; [c] Multiplicities were obtained with DEPT sequences.

**Table S3** – Cont. [a, b, c]

| | **15 (100 MHz)** | **15 (150 MHz)** | **15 (62.5 MHz)** | **15 (100 MHz)** | **15 (100 MHz)** | **16** | **18 (62.85 MHz)** | **19 (62.85 MHz)** | **20 (62.85 MHz)** |
|---|---|---|---|---|---|---|---|---|---|
| **C** | $CDCl_3$ | $CDCl_3$ * | $CDCl_3$ [b] | | $CDCl_3$ | | $CD_3OD$ | $CDCl_3$ | $CDCl_3$ |
| **1** | 59.0 – $CH_2$ | 59.2 | 59.4 – $CH_2$ | 59.2 – $CH_2$ | 59.33 | 62.2 | 138.12 - CH | 173.09 | 77.16 |
| **2** | 123.0 – CH | 123.4 | 124.4 – CH | 123.4 – CH | 123.34 | 60.8 | 110.09 – CH | 117.31 | 53.01 |
| **3** | 139.8 – C | 139.4 | 139.4 – C | 139.4 – C | 139.58 | 60.5 | 124.22 – C | 169.51 | 42.39 |
| **4** | 39.8 – $CH_2$ | 39.4 | 39.7 – $CH_2$ | 39.4 – $CH_2$ | 39.46 | 37.9 | 24.04 – $CH_2$ | 24.62 | 24.85 |
| **5** | 26.7 – $CH_2$ | 26.2 | 26.4 – $CH_2$ | 26.2 – $CH_2$ | 26.21 | 29.0 | 27.64 – $CH_2$ | 27.52 | 26.20 |
| **6** | 122.7 – CH | 124.0 | 124.1 – CH | 124.0 – CH | 123.92 | 122.8 | 122.0 – CH | 122.45 | 122.02 |
| **7** | 138.8 – C | 135.0 | 135.3 – C | 135.0 – C | 135.02 | 134.9 | 134.36 – C | 136.56 | 135.64 |
| **8** | 39.8 – $CH_2$ | 39.3 | 39.4 – $CH_2$ | 39.3 – $CH_2$ | 39.29 | 38.7 | 38.46 – $CH_2$ | 39.02 | 38.44 |
| **9** | 26.4 – $CH_2$ | 26.7 | 26.9 – $CH_2$ | 26.7 – $CH_2$ | 26.70 | 26.1 | 25.74 – $CH_2$ | 26.24 | 25.65 |
| **10** | 123.5 – CH | 129.1 | 123.2 – CH | 129.1 – CH | 129.10 | 122.3 | 123.52 – CH | 123.02 | 122.62 |
| **11** | 130.9 – C | 129.5 | 129.8 – C | 129.5 – C | 129.52 | 128.4 | 128.66 – CH | 128.37 | 128.86 |
| **12** | 55.3 – $CH_2$ | 55.3 | 55.5 – $CH_2$ | 55.3 – $CH_2$ | 55.35 | 54.7 | 54.17 – $CH_2$ | 54.86 | 54.09 |
| **13** | 199.5 - C | 199.5 | 199.9 – C | 199.5 – C | 199.55 | 198.9 | 199.71 – C | | 199.72 |
| **14** | 124.7 – CH | 122.8 | 129.7 – CH | 122.8 – CH | 122.80 | 129.1 | 128.46 – CH | 128.58 | 128.32 |
| **15** | 155.8 – C | 155.6 | 155.8 – C | 155.6 – C | 155.68 | 155.1 | 155.63 – C | 156.05 | 155.74 |
| **16** | 25.1 – $CH_3$ | 27.7 | 27.7 – $CH_3$ | 27.7 – $CH_3$ | 27.71 | 27.1 | 18.99 – $CH_3$ | 18.05 | 18.98 |
| **17** | 17.5 – $CH_3$ | 20.6 | 20.7 – $CH_3$ | 20.6 – $CH_3$ | 20.66 | 15.4 | 25.86 – $CH_3$ | 25.13 | 25.87 |
| **18** | 17.2 – $CH_3$ | 16.3 | 16.4 – $CH_3$ | 16.3 – $CH_3$ | 16.36 | 15.9 | 14.64 –$CH_3$ | 15.99 | 14.66 |
| **19** | 16.9 – $CH_3$ | 15.9 | 16.0 – $CH_3$ | 15.9 – $CH_3$ | 15.92 | 16.2 | 14.28 – $CH_3$ | 13.95 | 14.28 |
| **20** | 19.9 – $CH_3$ | 16.2 | 16.0 – $CH_3$ | 16.2 – $CH_3$ | 16.24 | 20.1 | 141.83 - CH | 99.47 | 175.95 |
| **21** | | | | | | | | | |
| **22** | | | | | | | | | |
| **Ref.** | [11] | [13] | [8] | | [17] | [6] | [18] | | |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard; [c] Multiplicities were obtained with DEPT sequences.

**Table S3 –** Cont. [a, b, c]

|  | **21 (100 MHz)** |  | **22 (100 MHz)** |  | **23 (100 MHz)** | **25 (20.1 MHz)** | **25 (100 MHz)** | **26 (100 MHz)** | **27 (100 MHz)** | **28 (100 MHz)** |
|---|---|---|---|---|---|---|---|---|---|---|
| **C** | $CDCl_3$ [b] | $C_6D_6$ [b] | $CDCl_3$ [b] | $C_6D_6$ [b] | $CDCl_3$ | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] | $CDCl_3$ [b] |
| **1** | 59.3 – $CH_2$ | 59.3 – $CH_2$ | 61.4 – $CH_2$ | 61.2 – $CH_2$ | 191.32 | 59.5 – $CH_2$ | 59.2 *t* | 59.3 *t* | 65.6 *t* | 59.3 *t* |
| **2** | 123.3 – CH | 125.0 – CH | 118.3 – CH | 119.4 – CH | 127.40 | 124.3 – CH | 124.1 *d* | 123.4 *d* | 75.0 *d* | 123.6 *d* |
| **3** | 139.6 – C | 137.9 – C | 142.1 – C | 141.5 – C | 163.87 | 138.7 – C | 138.5 *s* | 139.5 *s* | 148.2 *s* | 139.3 *s* |
| **4** | 39.5 – $CH_2$ | 39.8 – $CH_2$ | 39.4 – $CH_2$ | 39.6 – $CH_2$ | 40.56 | 34.1 – $CH_2$ | 33.9 *t* | 39.5 *t* | 32.4 *t* | 35.6 *t* |
| **5** | 26.2 – $CH_2$ | 26.6 – $CH_2$ | 26.1 – $CH_2$ | 26.4 – $CH_2$ | 25.62 | 36.3 – $CH_2$ | 36.3 *t* | 26.2 *t* | 26.3 *t* | 33.3 *t* |
| **6** | 124.0 – CH | 124.7 – CH | 124.2 – CH | 124.3 – CH | 122.64 | 201.6 – C | 201.1 *s* | 124.2 *d* | 123.8 *d* | 74.9 *d* |
| **7** | 135.0 – C | 134.9 – C | 134.3 – C | 134.7 – C | 136.30 | 148.8 – C | 148.0 *s* | 134.8 *s* | 135.3 *s* | 151.3 *s* |
| **8** | 39.2 – $CH_2$ | 39.7 – $CH_2$ | 34.0 – $CH_2$ | 34.3 – $CH_2$ | 39.28 | 31.0 – $CH_2$ | 30.8 *t* | 39.2 *t* | 39.2 *t* | 30.8 *t* |
| **9** | 26.6 – $CH_2$ | 26.9 – $CH_2$ | 36.1 – $CH_2$ | 36.3 – $CH_2$ | 26.68 | 27.2 – $CH_2$ | 27.0 *t* | 26.6 *t* | 26.6 *t* | 26.6 *t* |
| **10** | 129.4 – CH | 129.2 – CH | 200.7 – C | 199.8 – C | 128.90 | 123.3 – CH | 128.4 *d* | 130.2 *d* | 129.0 *d* | 129.1 *d* |
| **11** | 129.4 – C | 129.6 – C | 143.3 – C | 144.1 – C | 129.75 | 130.8 – C | 130.6 *s* | 128.2 *s* | 129.5 *s* | 129.6 *s* |
| **12** | 54.4 – $CH_2$ | 54.4 – $CH_2$ | 46.4 – $CH_2$ | 46.7 – $CH_2$ | 55.34 | 55.4 – $CH_2$ | 55.2 *t* | 55.4 *t* | 55.3 *t* | 54.2 *t* |
| **13** | 209.7 – C | 207.3 – C | 197.1 – C | 196.0 – C | 199.49 | 199.6 – C | 199.4 *s* | 212.0 *s* | 199.7 *s* | 209.7 *s* |
| **14** | 50.5 – $CH_2$ | 50.4 – $CH_2$ | 123.3 – CH | 123.7 – CH | 122.86 | 128.6 – CH | 122.9 *d* | 51.5 *t* | 122.8 *d* | 50.8 *t* |
| **15** | 24.4 – CH | 24.4 – CH | 156.4 – C | 154.9 – C | 155.66 | 155.8 – C | 155.6 *s* | 69.6 *s* | 155.8 *s* | 24.4 *s* |
| **16** | 22.5 – $CH_3$ | 22.6 – $CH_3$ | 27.7 – $CH_3$ | 27.2 – $CH_3$ | 27.73 | 20.8 – $CH_3$ | 27.7 *q* | 29.2 *q* | 27.7 *q* | 22.5 *q* |
| **17** | 22.5 – $CH_3$ | 22.6 – $CH_3$ | 20.8 – $CH_2$ | 20.6 – $CH_2$ | 20.68 | 27.7 – $CH_3$ | 20.7 *q* | 29.2 *q* | 20.7 *q* | 22.5 *q* |
| **18** | 16.4 – $CH_3$ | 16.5 – $CH_3$ | 126.9 – $CH_2$ | 125.7 – $CH_2$ | 16.40 | 16.5 – $CH_3$ | 16.5 *q* | 16.4 *q* | 16.4 *q* | 16.5 *q* |
| **19** | 15.9 – $CH_3$ | 16.0 – $CH_3$ | 16.1 – $CH_3$ | 16.1 – $CH_3$ | 16.05 | 124.3 – $CH_2$ | 124.1 *q* | 15.9 *q* | 16.0 *q* | 110.1 *q* |
| **20** | 16.2 – $CH_3$ | 16.2 – $CH_3$ | 16.5 – $CH_3$ | 16.3 – $CH_3$ | 17.60 | 16.5 – $CH_3$ | 16.2 *q* | 16.3 *q* | 110.8 *t* | 16.3 *q* |
| **21** |  |  | 171.2 – C | 170.2 – C |  |  |  |  |  |  |
| **22** |  |  | 21.1 – $CH_3$ | 20.6 – $CH_3$ |  |  |  |  |  |  |
| **Ref.** | [8] |  | [8] |  | [17] | [8] | [9] | [9] | [9] | [9] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard; [c] Multiplicities were obtained with DEPT sequences.

**Table S3** – Cont. [a, b, c]

| | **29 (100 MHz)** | **30 (100 MHz)** | **31 (150 MHz)** | **32 (150 MHz)** | **33 (150 MHz)** | **34 (150 MHz)** | **35 (600 MHz)** | **36 (600 MHz)** |
|---|---|---|---|---|---|---|---|---|
| **C** | CDCl$_3$ [b] | CDCl$_3$ [b] | CDCl$_3$ | CDCl$_3$ | CDCl$_3$ | CDCl$_3$ | CDCl$_3$ | CDCl$_3$ |
| **1** | 59.2 *t* | 59.3 *t* | 171.8 | 174.2 | 171.9 | 59.4 | 60.7 | 142.6 |
| **2** | 123.6 *d* | 124.2 *d* | 115.2 | 115.6 | 115.2 | 123.3 | 117.6 | 111.1 |
| **3** | 139.3 *s* | 138.2 *s* | 163.0 | 170.3 | 162.9 | 139.8 | 143.2 | 125.0 |
| **4** | 35.6 *t* | 42.1 *t* | 41.2 | 28.7 | 41.2 | 39.5 | 39.5 | 25.0 |
| **5** | 33.4 *t* | 125.2 *d* | 25.9 | 25.6 | 25.9 | 26.3 | 26.2 | 28.5 |
| **6** | 74.8 *d* | 138.7 *d* | 122.9 | 122.1 | 123.0 | 124.0 | 123.7 | 123.9 |
| **7** | 151.3 *s* | 72.9 *s* | 136.1 | 137.3 | 135.9 | 135.8 | 135.3 | 135.6 |
| **8** | 30.9 *t* | 42.3 *t* | 39.3 | 39.3 | 39.3 | 39.4 | 39.4 | 39.5 |
| **9** | 26.7 *t* | 23.1 *t* | 26.7 | 26.6 | 26.6 | 25.7 | 26.8 | 26.6 |
| **10** | 128.8 *d* | 129.3 *d* | 129.0 | 128.7 | 129.0 | 40.8 | 129.2 | 126.6 |
| **11** | 130.0 *s* | 129.8 *s* | 129.7 | 130.0 | 129.4 | 158.1 | 129.6 | 131.8 |
| **12** | 55.1 *t* | 55.1 *t* | 55.4 | 55.3 | 54.5 | 125.7 | 55.5 | 38.5 |
| **13** | 199.8 *s* | 199.3 *s* | 199.7 | 199.4 | 209.9 | 191.8 | 199.5 | 154.5 |
| **14** | 122.9 *d* | 122.9 *d* | 122.8 | 122.9 | 50.5 | 126.3 | 122.8 | 108.8 |
| **15** | 156.0 *s* | 155.9 *s* | 155.9 | 155.8 | 24.4 | 154.5 | 155.7 | 120.5 |
| **16** | 27.7 *q* | 27.7 *q* | 27.8 | 27.8 | 22.6 | 27.7 | 27.8 | 137.7 |
| **17** | 20.7 *q* | 20.7 *q* | 20.7 | 20.7 | 22.6 | 20.7 | 20.7 | 9.9 |
| **18** | 16.5 *q* | 16.4 *q* | 16.4 | 16.5 | 16.4 | 19.2 | 16.4 | 15.9 |
| **19** | 110.0 *t* | 28.2 *q* | 16.0 | 16.2 | 16.0 | 16.3 | 16.0 | 16.1 |
| **20** | 16.3 *q* | 16.3 *q* | 19.2 | 73.2 | 19.2 | 16.4 | 16.5 | 138.8 |
| **21** | | | | | | | 161.2 | |
| **22** | | | | | | | | |
| **Ref.** | [9] | [9] | [13] | [13] | [13] | [13] | [14] | [14] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard; [c] Multiplicities were obtained with DEPT sequences.

**Table S3** – Cont. [a, b, c]

| | **40 (50 MHz)** | **40 (100.5 MHz)** | **41 (100.5 MHz)** | **42 (50 MHz)** | **43 (100 MHz)** | **44 (600 MHz)** |
|---|---|---|---|---|---|---|
| **C** | CDCl$_3$ [b] | CDCl$_3$ [b] | CDCl$_3$ [b] | CDCl$_3$ [b] | CDCl$_3$ [b] | CDCl$_3$ |
| **1** | 59.0 *t* (6.8) | 59.0 | 59.4 | 59.4 – CH$_2$ | 59.4 *t* | 59.4 |
| **2** | 123.4 *d* (6.8) | 123.3 | 123.4 | 123.4 – CH | 123.3 *d* | 123.3 |
| **3** | 139.1 *s* | 139.1 | 139.7 | 139.6 – C | 139.9 *s* | 139.8 |
| **4** | 39.4 *t* | 39.4 | 39.6 | 39.5 – CH$_2$ | 39.9 *t* | 39.3 |
| **5** | 26.5 *t* | 26.5 | 26.3 | 26.4 – CH$_2$ | 22.6 *t* | 26.3 |
| **6** | 123.8 *d* (6.8) | 123.8 | 123.9 | 124.5 – CH | 41.0 *t* | 123.9 |
| **7** | 135.0 *s* | 135.0 | 135.3 | 134.6 – C | 82.8 *s* | 134.6 |
| **8** | 39.4 *t* | 39.4 | 39.6 | 43.1 – CH$_2$ | 37.2 *t* | 39.7 |
| **9** | 26.2 *t* | 26.2 | 26.7 | 125.6 – CH | 30.8 *t* | 26.6 |
| **10** | 125.1 *d* (6.8) | 125.1 | 125.2 | 135.9 – CH | 84.5 *d* | 124.5 |
| **11** | 133.5 *s* | 133.5 | 133.7 | 131.8 – C | 134.9 *s* | 135.3 |
| **12** | 42.7 *t* (7.2) | 42.7 | 42.4 | 129.4 – CH | 125.4 *d* | 39.6 |
| **13** | 128.7 *d* (7.2; 15.6) | 128.7 | 125.4 | 27.2 – CH$_2$ | 26.8 *t* | 26.2 |
| **14** | 133.7 *d* (15.6) | 133.7 | 139.2 | 122.5 – CH | 122.8 *d* | 126.2 |
| **15** | 141.9 *s* | 141.9 | 70.7 | 133.3 – C | 131.5 *s* | 134.7 |
| **16** | 114.3 *t* | 18.5 | 29.8 | 25.7 – CH$_3$ | 25.6 *q* | 69.1 |
| **17** | 18.5 *q* | 114.3 | 29.8 | 17.7 – CH$_3$ | 17.7 *q* | 13.7 |
| **18** | 15.9 *q* | 15.9 | 16.0 | 12.5 – CH$_3$ | 11.4 *q* | 16.0 |
| **19** | 15.8 *q* | 15.8 | 16.0 | 16.1 – CH$_3$ | 26.7 *q* | 16.0 |
| **20** | 16.1 *q* | 16.1 | 16.3 | 16.2– CH$_3$ | 16.1 *q* | 16.3 |
| **21** | | | | | | |
| **22** | | | | | | |
| **Ref.** | [2] | [16] | [16] | [3] | [5] | [14] |

[a] Chemical shits are given in ppm and coupling constants (*J* in parentheses) in Hz; [b] TMS as internal standard; [c] Multiplicities were obtained with DEPT sequences

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