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Supporting information for article:

A concise, efficient and versatile synthesis of amino-substituted benzo[*b*]pyrimido[5,4-*f*]azepines: synthesis and spectroscopic characterization, together with the molecular and supramolecular structures of three products and one intermediate

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Spectroscopic data for compounds (II), (III), (IVa,b), (Va,b), (VIIa,b,c), (VIIIa,b,c)

5-Allyl-*N*⁴,*N*⁶,2-trimethyl-*N*⁴,*N*⁶-diphenylpyrimidine-4,6-diamine, (II).

IR (ATR, cm⁻¹) 1550 (C=N), 1523 [C=C (arom)],

1252 (C-N), 963 [=C-H (allyl)]; NMR (CDCl₃) δ(¹H) 2.18

(dt, J = 6.2, 1.6 Hz, 2H, -CH₂-), 2.59 (s, 3H, 2-CH₃), 3.48

(s, 6H, 4-N-CH₃, 6-N-CH₃), 4.42

(dq, J = 17.2, 1.6 Hz, 1H, =CH₂ (H-trans)), 4.73

(dq, J = 10.2, 1.6 Hz, 1H, =CH₂ (H-cis)), 5.38

(ddt, J = 17.2, 10.2, 6.2 Hz, 1H, -CH=), 6.82-6.85

(m, 4H, 2'-H, 2''-H, 6'-H, 6''-H), 6.92-6.96 (m, 2H, 4'-H, 4''-H),

7.20-7.25 (m, 4H, 3'-H, 3''-H, 5'-H, 5''-H), δ(¹³C) 25.8 (2-CH₃),

31.9 (-CH₂-), 39.6 (4-N-CH₃, 6-N-CH₃), 109.2 (5-C),

114.5 (=CH₂), 120.5 (2'-C, 2''-C, 6'-C, 6''-C), 122.3 (4'-C, 4''-C),

129.0 (3'-C, 3''-C, 5'-C, 5''-C), 136.4 (-CH=), 147.5 (1'-C, 1''-C),

164.2 (4-C, 6-C), 164.9 (2-C); GC-MS (70 eV) m/z (%) 344 (M⁺, 82),

343 (88), 329 (100), 238 (55).

N,2,6,11-Tetramethyl-*N*-phenyl-6,11-dihydro-5*H*-benzo[*b*]pyrimido[5,4-*f*]azepin-4-amine, (III).

IR (ATR, cm⁻¹) 1538 (C=N), 1483 [C=C (arom)], 1368 (C-HMe), 1272 (C-N);

NMR (CDCl₃) δ(¹H) 1.24 (d, J = 6.8 Hz, 3H, 6-CH₃), 1.99

(dd, J = 16.4, 1.6 Hz, 1H, 5-H_B), 2.52

(dd, J = 16.4, 10.6 Hz, 1H, 5-H_A), 2.56 (s, 3H, 2-CH₃),

3.33-3.37 (m, 1H, 6-H), 3.56 (s, 3H, 11-CH₃), 6.78-6.80

(m, 2H, 2'-H, 6-H), 6.84-6.88 (m, 1H, 4'-H), 7.02

(dd, J = 7.6, 1.6 Hz, 1H, 10-H), 7.05 (td, J = 7.6, 1.6 Hz, 1H, 9-H),

7.11-7.15 (m, 2H, 3'-H, 5'-H), 7.17-7.22 (m, 2H, 7-H, 8-H),

δ(¹³C) 18.2 (6-CH₃), 25.9 (2-CH₃), 33.3 (6-C), 40.2 (6-N-CH₃),

40.4 (5-C), 40.8 (11-CH₃), 105.0 (4a-C), 120.0 (2'-C, 6'-C),

121.5 (4'-C), 122.7 (7-C), 123.8 (10-C), 124.5 (9-C), 126.4 (8-C),

129.1 (3'-C, 5'-C), 141.4 (10a-C), 145.6 (6a-C), 148.1 (1'-C),

161.0 (11a-C), 163.4 (2-C), 164.0 (4-C); GC-MS (70 eV) m/z (%)

344 (M⁺ 26), 329 (39), 315 (63), 239 (100), 77 (26), HRMS

(EI-MS) m/z found 344.2006, $C_{22}H_{24}N_4$ requires 344.2001.

N^1 -(5-Allyl-6-chloropyrimidin-4-yl)benzene-1,2-diamine, (IVa).

IR (ATR, cm^{-1}) 3284 (N-H/ NH_2), 1620 [C=C (allyl)], 1550 [C=N/C=C (arom)], 1500 [C=C (arom)], 1453, 1407, 1374 (C-N), 930 [=C-H (allyl)]; NMR ($CDCl_3$) $\delta(^1H)$ 3.59 (dt, $J = 5.9$, 1.6 Hz, 2H, $-CH_2-$), 3.68 (br s, 2H, 2- NH_2), 5.23-5.32 (m, 2H, = CH_2), 5.95 (ddt, $J = 16.0, 10.2, 5.9$ Hz, 1H, $-CH=$), 6.47 (br s, 1H, 1-NH), 6.83 (dd, $J = 7.8, 1.4$ Hz, 1H, 6-H), 6.85 (td, $J = 8.0, 1.4$ Hz, 1H, 4-H), 7.10 (td, $J = 7.6, 1.2$ Hz, 1H, 5-H), 7.26 (dd, $J = 8.2, 1.2$ Hz, 1H, 3-H), 8.35 (s, 1H, 2'-H), $\delta(^{13}C)$ 31.7 ($-CH_2-$), 112.7 (5'-C), 117.6 (6-C), 117.9 (=CH₂), 119.6 (4-C), 124.7 (2-C), 126.2 (3-C), 127.6 (5-C), 132.3 ($-CH=$), 141.4 (1-C), 156.5 (2'-C), 158.9 (6'-C), 160.7 (4'-C); GC-MS (70 eV) m/z (%) 260 (M^+ , ^{35}Cl , 69), 259 (42), 245 (100), 225 (29), 196 (45), 93 (28), HRMS (EI-MS, 30 eV) m/z found 260.0830, $C_{13}H_{13}ClN_4$ requires 260.0829.

N^1 -(5-Allyl-6-chloropyrimidin-4-yl)-4-methylbenzene-1,2-diamine, (IVb).

IR (ATR, cm^{-1}) 3279 (N-H/ NH_2), 1633 [C=C (allyl)], 1550 [C=N/C=C (arom)], 1511, 1470, 1407 [C=C (arom)], 1369 (C-N), 923 [=C-H (allyl)]; NMR ($CDCl_3$) $\delta(^1H)$ 2.27 (s, 3H, 4- CH_3), 3.58 (dt, $J = 6.4, 1.4$ Hz, 2H, $-CH_2-$), 3.64 (br s, 2H, 2- NH_2), 5.24 (dq, $J = 17.2, 1.4$ Hz, 1H, =CH₂ (H-trans)), 5.29 (dq, $J = 10.2, 1.4$ Hz, 1H, =CH₂ (H-cis)), 5.95 (ddt, $J = 17.2, 10.2, 6.4$ Hz, 1H, $-CH=$), 6.36 (br s, 1H, 1-NH), 6.63 (dd, $J = 7.8, 1.2$ Hz, 1H, 5-H), 6.65 (s, 1H, 3-H), 7.05 (d, $J = 7.8$ Hz, 1H, 6-H), 8.34 (s, 1H, 2'-H), $\delta(^{13}C)$ 21.2 (4- CH_3), 31.6 ($-CH_2-$), 112.5 (5'-C), 117.9 (=CH₂), 118.0 (3-C), 120.3 (5-C), 121.8 (1-C), 126.6 (6-C), 132.4 ($-CH=$), 137.9 (4-C), 141.7 (2-C), 156.6 (2'-C), 158.8 (6'-C), 161.0 (4'-C); GC-MS (70 eV) m/z (%) 274 (M^+ , ^{35}Cl , 82), 273 (36), 259 (100), 239 (23), 210 (47), 107 (60), 77 (45), HRMS (Q-TOF-ESI) m/z found 275.1059, $C_{14}H_{15}^{35}ClN_4$, [$M + H$]⁺, requires 275.1058.

1-(5-Allyl-6-chloropyrimidin-4-yl)-1H-benzo[*d*]imidazole, (Va).

IR (ATR, cm^{-1}) 1632 [C=C (allyl)], 1534 [C=N/C=C (arom)], 1451, 1432 [C=C (arom)], 910 [=C-H (allyl)]; NMR (CDCl_3) $\delta(^1\text{H})$ 3.58-3.60 (m, 2H, $-\text{CH}_2-$), 4.95 (br d, $J = 17.3$ Hz, 1H, $=\text{CH}_2$ (H-trans)), 5.28 (br d, $J = 10.3$ Hz, 1H, $=\text{CH}_2$ (H-cis)), 6.01 (ddt, $J = 17.3, 10.3, 5.2$ Hz, 1H, $-\text{CH}=\text{}$), 7.36-7.41 (m, 2H, 5-H, 6-H), 7.68-7.72 (m, 1H, 4-H), 7.84-7.89 (m, 1H, 7-H), 8.28 (s, 1H, 2-H), 8.95 (s, 1H, 2'-H), $\delta(^{13}\text{C})$ 32.7 ($-\text{CH}_2-$), 112.6 (4-C), 118.5 ($=\text{CH}_2$), 120.8 (7-C), 124.1 (6-C), 124.5 (5'-C), 124.8 (5-C), 132.5 ($-\text{CH}=\text{}$), 132.8 (3a-C), 141.6 (2-C), 143.7 (7a-C), 156.7 (6'-C), 156.8 (2'-C), 164.9 (4'-C); GC-MS (70 eV) m/z (%) 270 (M^+ , ^{35}Cl , 100), 269 (81), 255 (90), 235 (26), HRMS (EI-MS, 20 eV) m/z found 270.0675, $\text{C}_{14}\text{H}_{11}^{35}\text{ClN}_4$ requires 270.0672.

1-(5-Allyl-6-chloropyrimidin-4-yl)-5-methyl-1*H*-benzo[*d*]imidazole, (Vb).

IR (ATR, cm^{-1}) 1639 [C=C (allyl)], 1531 [C=N/C=C (arom)], 1433 [C=C (arom)], 933 [=C-H (allyl)]; NMR (CHCl_3) $\delta(^1\text{H})$ 2.50 (s, 3H, 5- CH_3), 3.59 (br d, $J = 5.2$ Hz, 2H, $-\text{CH}_2-$), 4.96 (br d, $J = 17.2$ Hz, 1H, $=\text{CH}_2$ (H-trans)), 5.28 (br d, $J = 10.3$ Hz, 1H, $=\text{CH}_2$ (H-cis)), 6.02 (ddt, $J = 17.2, 10.3, 5.2$ Hz, 1H, $-\text{CH}=\text{}$), 7.21 (d, $J = 8.4$ Hz, 1H, 6-H), 7.60 (d, $J = 8.4$ Hz, 1H, 7-H), 7.64 (br s, 1H, 4-H), 8.25 (s, 1H, 2-H), 8.93 (s, 1H, 2'-H), $\delta(^{13}\text{C})$ 21.5 (5- CH_3), 32.7 ($-\text{CH}_2-$), 112.2 (7-C), 118.5 ($=\text{CH}_2$), 120.5 (4-C), 124.2 (5-C), 126.2 (6-C), 130.8 (7a-C), 132.5 ($-\text{CH}=\text{}$), 134.0 (5-C), 141.6 (2-C), 144.0 (3a-C), 156.7 (2'-C, 4'-C), 164.9 (6'-C); GC-MS (70 eV) m/z (%) 284 (M^+ , ^{35}Cl , 100), 283 (70), 269 (85), 249 (18), HRMS (Q-TOF-ESI) m/z found 285.0900, $\text{C}_{15}\text{H}_{13}^{35}\text{ClN}_4$, $[\text{M} + \text{H}]^+$, requires 285.0902.

5-Allyl-6-(1*H*-benzo[*d*]imidazol-1-yl)-*N*-methyl-*N*-phenylpyrimidin-4-amine,

(VIIa). IR (ATR, cm^{-1}) 1638 [C=C (allyl)], 1561 [C=N/C=C (arom)], 1526, 1453 [C=C (arom)], 914 [=C-H (allyl)]; NMR (CDCl_3) $\delta(^1\text{H})$ 2.59 (dt, $J = 6.0, 1.5$ Hz, 2H, $-\text{CH}_2-$), 3.59 (s, 3H, $-\text{N}-\text{CH}_3$), 4.30 (dq, $J = 17.1, 1.6$ Hz, 1H, $=\text{CH}_2$ (H-trans)), 4.65 (dq, $J = 10.2, 1.5$ Hz, 1H, $=\text{CH}_2$ (H-cis)), 5.22 (ddt, $J = 17.1, 10.2, 6.0$ Hz, 1H, $-\text{CH}=\text{}$), 7.15-7.17 (m, 1H, 7''-H), 7.19-7.21 (m, 2H, 2'-H, 6'-H), 7.25-7.28 (m, 1H, 4'-H), 7.29-7.31

(m, 2H, 5''-H, 6''-H), 7.41-7.46 (m, 2H, 3'-H, 5'-H), 7.80-7.84
(m, 1H, 4''-H), 8.16 (s, 1H, 2''-H), 8.73 (s, 1H, 2-H), $\delta(^{13}\text{C})$
31.7 (-CH₂-), 41.9 (-N-CH₃), 111.1 (7''-C), 113.7 (5-C),
116.2 (=CH₂), 120.8 (4''-C), 123.1 (5''-C), 123.9 (6''-C),
124.4 (2'-C, 6'-C), 126.2 (4'-C), 129.9 (3'-C, 5'-C), 132.9 (7a''-C),
133.3 (-CH=), 142.4 (2''-C), 143.7 (3a''-C), 147.0 (1'-C), 154.7 (6-C),
156.3 (2-C), 165.3 (4-C); GC-MS (70 eV) m/z (%) 341 (M⁺, 80),
340 (100), 326 (69), 250 (20), 224 (30), 77 (31), HRMS (EI-MS)
m/z found 341.1634, C₂₁H₁₉N₅ requires 341.1640.

5-Allyl-6-(1*H*-benzo[*d*]imidazol-1-yl)-*N*-methyl-*N*-
(4-methylphenyl)pyrimidin-4-amine, (VIIb). IR (ATR, cm⁻¹)
1633 [C=C (allyl)], 1533 [C=N/C=C (arom)], 911 [=C-H (allyl)];
NMR (CDCl₃) $\delta(^1\text{H})$ 2.39 (s, 3H, 4'-CH₃), 2.59
(dt, J = 6.0, 1.6 Hz, 2H, -CH₂-), 3.56 (s, 3H, -N-CH~3~), 4.32
(dq, J = 17.2, 1.6 Hz, 1H, =CH₂ (H-trans)), 4.65
(dq, J = 10.1, 1.6 Hz, 1H, =CH₂ (H-cis)), 5.24
(ddt, J = 17.2, 10.1, 6.0 Hz, 1H, -CH=), 7.08-7.11 (m, 2H, 2'-H, 6'-H),
7.15-7.20 (m, 1H, 7''-H), 7.23 (br d, J = 8.2 Hz, 2H, 3'-H, 5'-H),
7.29-7.33 (m, 2H, 5''-H, 6''-H), 7.81-7.85 (m, 1H, 4''-H), 8.15
(s, 1H, 2''-H), 8.71 (s, 1H, 2-H), $\delta(^{13}\text{C})$
21.1 (4'-CH₃), 31.6 (-CH₂-), 42.0 (-N-CH~3~), 111.2 (7''-C),
113.4 (5-C), 116.1 (=CH₂), 120.7 (4''-C), 123.1 (5''-C),
123.9 (6''-C), 124.4 (2'-C, 6'-C), 130.5 (3'-C, 5'-C), 133.0 (7a''-C),
133.4 (-CH=), 136.2 (4'-C), 142.5 (2''-C), 143.7 (3a''-C),
144.4 (1'-C), 154.6 (6-C), 156.2 (2-C), 165.2 (4-C); GC-MS (70 eV)
m/z (%) 355 (M⁺, 100), 354 (96), 340 (80), 250 (24), 238 (24),
91 (32), HRMS (EI-MS, 20 eV) m/z found 355.1801, C₂₂H₂₁N₅
requires 355.1797.

5-Allyl-*N*-(3,5-dimethylphenyl)-*N*-methyl-6-(5-methyl-1*H*-
benzo[*d*]imidazol-1-yl)pyrimidin-4-amine, (VIIc). IR (ATR, cm⁻¹)
1638 [C=C (allyl)], 1561 [C=N/C=C (arom)], 1524, 1446 [C=C (arom)],
911 [=C-H (allyl)]; NMR (CDCl₃) $\delta(^1\text{H})$ 2.36
(s, 6H, 3'-CH₃, 5'-CH₃), 2.47 (s, 3H, 5''-CH₃), 2.58
(dt, J = 6.1, 1.5 Hz, 2H, -CH₂-), 3.56 (s, 3H, -N-CH₃), 4.27

(dq, $J = 17.1, 1.5$ Hz, 1H, =CH₂ (H-trans)), 4.63
(dq, $J = 10.1, 1.5$ Hz, 1H, =CH₂ (H-cis)), 5.21
(ddt, $J = 17.1, 10.1, 6.1$ Hz, 1H, -CH=), 6.81 (s, 2H, 2'-H, 6'-H),
6.90 (s, 1H, 4'-H), 6.94 (d, $J = 8.4$ Hz, 1H, 7''-H), 7.09
(dd, $J = 8.4, 1.0$ Hz, 1H, 6''-H), 7.61 (s, 1H, 4''-H), 8.17
(s, 1H, 2''-H), 8.68 (s, 1H, 2-H), $\delta(^{13}\text{C})$ 21.3
(3'-CH₃, 5'-CH₃), 21.5 (5''-CH₃), 31.9 (-CH₂-),
41.5 (N-CH₃), 110.4 (7''-C), 113.4 (5-C), 116.0 (=CH₂),
120.6 (4''-C), 121.9 (2'-C, 6'-C), 125.2 (6''-C), 127.8 (4'-C),
131.0 (7a''-C), 132.8 (5''-C), 133.6 (-CH=), 139.6 (3'-C, 5'-C),
142.3 (2''-C), 144.1 (3a''-C), 146.9 (1'-C), 154.4 (6-C),
156.1 (2-C), 165.2 (4-C); GC-MS (70 eV) m/z (%) 383 (M⁺, 93),
382 (100), 368 (77), 264 (21), 252 (22), 105 (10), HRMS (Q-TOF-ESI)
 m/z found 384.2181, C₂₄H₂₅N₅, [M + H]⁺, requires 384.2183.

4-(1*H*-Benzo[*d*]imidazol-1-yl)-6,11-dimethyl-6,11-dihydro-5*H*-
benzo[*b*]pyrimido[5,4-*f*]azepine, (VIIIa). IR (ATR, cm⁻¹)
1560 [C=N/C=C (arom)], 1532 [C=C (arom)], 1480, 1365 (C-HMe/C-N);
NMR (CDCl₃) $\delta(^1\text{H})$ 1.30 (d, $J = 7.0$ Hz, 3H, 6-CH₃), 2.63
(dd, $J = 16.5, 2.0$ Hz, 1H, 5-H_B), 2.75
(dd, $J = 16.5, 10.4$ Hz, 1H, 5-H_A), 3.46-3.54 (m, 1H, 6-H),
3.67 (s, 3H, 11-CH₃), 7.19 (dd, $J = 7.7, 2.0$ Hz, 1H, 7-H),
7.23 (dd, $J = 7.7, 1.6$ Hz, 1H, 10-H), 7.27-7.32 (m, 2H, 8-H, 9-H),
7.32-7.35 (m, 2H, 5'-H, 6'-H), 7.37-7.42 (m, 1H, 7'-H), 7.82-
7.88 (m, 1H, 4'-H), 8.08 (s, 1H, 2'-H), 8.64 (s, 1H, 2-H), $\delta(^{13}\text{C})$
17.9 (6-CH₃), 33.1 (6-C), 40.5 (5-C), 41.3 (11-CH~3~), 111.1 (4a-C),
112.1 (7'-C), 120.6 (4'-C), 123.2 (8-C, 5'-C), 124.0 (7-C),
124.1 (6'-C), 125.8 (10-C), 127.2 (9-C), 132.8 (7a'-C), 140.7 (6a-C),
142.3 (2'-C), 143.6 (3a'-C), 144.4 (10a-C), 154.4 (4-C), 155.3 (2-C),
162.0 (11a-C); GC-MS (70 eV) m/z (%) 341 (M⁺, 100), 340 (61),
326 (48), 312 (22), 285 (20); HRMS (EI-MS) m/z found 341.1628,
C₂₁H₁₉N₅ requires 341.1640.

4-(1*H*-Benzo[*d*]imidazol-1-yl)-6,8,11-trimethyl-6,11-dihydro-5*H*-
benzo[*b*]pyrimido[5,4-*f*]azepine, (VIIIb). IR (ATR, cm⁻¹)
1563 [C=N/C=C (arom)], 1528 [C=C (arom)], 1483, 1453,

1361 (C-HMe/C-N); NMR (CDCl₃) δ(¹H) 1.27

(d, J = 7.0 Hz, 3H, 6-CH~3~),

2.38 (s, 3H, 8-CH₃), 2.63 (dd, J = 16.5, 1.6 Hz, 1H, 5-H_B),

2.73 (dd, J = 16.5, 10.2 Hz, 1H, 5-H_A), 3.41-3.48 (m, 1H, 6-H),

3.65 (s, 3H, 11-CH₃), 6.98 (br s, 1H, 7-H), 7.12

(dd, J = 8.3, 1.5 Hz, 1H, 9-H), 7.15 (d, J = 8.3 Hz, 1H, 10-H),

7.29-7.35 (m, 2H, 5'-H, 6'-H), 7.37-7.42 (m, 1H, 7'-H), 7.82-7.87

(m, 1H, 4'-H), 8.08 (s, 1H, 2'-H), 8.63 (s, 1H, 2-H), δ(¹³C)

17.9 (6-CH₃), 21.1 (8-CH₃), 33.1 (6-C), 40.5 (5-C), 41.3 (11-CH~3~),

110.9 (4a-C), 112.2 (7'-C), 120.6 (4'-C), 123.0 (10-C), 123.2 (5'-C),

124.1 (6'-C), 124.6 (7-C), 127.7 (9-C), 132.8 (7a'-C), 135.5 (8-C),

140.4 (6a-C), 141.8 (10a-C), 142.4 (2'-C), 143.6 (3a'-C), 154.4 (4-C),

155.2 (2-C), 162.1 (11a-C); GC-MS (70 eV) m/z (%) 355 (M⁺, 100),

354 (65), 340 (56), 326 (19), 299 (18), 170 (24), HRMS (EI-MS) m/z

found 355.1808, C₂₂H₂₁N₅ requires 355.1797.

6,7,9,11-Tetramethyl-4-(5-methyl-1*H*-benzo[*d*]imidazol-1-yl)-

6,11-dihydro-5*H*-benzo[*b*]pyrimido[5,4-*f*]azepine, (VIIIc).

IR (ATR, cm⁻¹) 1559 [C=N/C=C (arom)], 1532 [C=C (arom)], 1441,

1400 [C-H (Me)], 1366 (C-HMe/C-N); NMR (CDCl₃) δ(¹H) 1.23

(d, J = 7.3 Hz, 3H, 6-CH₃), 2.27 (s, 3H, 7-CH₃), 2.32

(s, 3H, 9-CH₃), 2.49 (s, 3H, 5'-CH₃), 2.56

(dd, J = 16.7, 4.9 Hz, 1H, 5-H_B), 3.04

(dd, J = 16.7, 2.6 Hz, 1H, 5-H_A), 3.44-3.51 (m, 1H, 6-H),

3.66 (s, 3H, 11-CH₃), 6.86 (s, 1H, 8-H), 6.94 (s, 1H, 10-H),

7.12 (dd, J = 8.3, 1.2 Hz, 1H, 6'-H), 7.26 (d, J = 8.3 Hz, 1H, 7'-H),

7.63 (s, 1H, 4'-H), 8.06 (s, 1H, 2'-H), 8.65 (s, 1H, 2-H), δ(¹³C)

14.8 (6-CH₃), 20.2 (7-CH₃), 21.0 (9-CH₃), 21.5 (5'-CH₃),

31.0 (6-C), 36.9 (5-C), 42.2 (11-CH₃), 109.7 (4a-C), 111.5 (7'-C),

120.3 (4'-C), 123.3 (10-C), 125.4 (6'-C), 128.3 (8-C), 131.1 (7a'-C),

132.9 (5'-C), 134.7 (7-C), 135.9 (6a-C), 136.5 (9-C), 142.3 (2'-C),

143.9 (3a'-C), 144.7 (10a-C), 155.5 (2-C, 4-C), 161.5 (11a-C);

GC-MS (70 eV) m/z (%) 383 (M⁺, 100), 382 (33), 368 (61), 354 (51),

207 (27), HRMS (Q-TOF-ESI) m/z found 384.2181,

C₂₄H₂₅N₅, [M + H]⁺, requires 384.2183.