Supporting Information

One-pot Total Synthesis of Streptindole, Arsindoline B and Their Congeners Through Tandem Decarboxylicative Deaminative Dual-Coupling Reaction of Amino Acids with Indoles

Jiachen Xiang, Jungang Wang, Miao Wang, Xianggao Meng, Anxin Wu*

Key Laboratory of Pesticide & Chemical Biology, Ministry of Education, Central China Normal University, Wuhan 430079, P. R. China

E-mail: chwuax@mail.ccnu.edu.cn

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1. General
All substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). IR spectra were recorded on a Perkin-Elmer PE-983 infrared spectrometer as KBr pellets with absorption in cm⁻¹. ¹H spectra were recorded in CDCl₃ or DMSO-d₆ or CD₂COCD₃ on 400/600 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet q = quadruple), coupling constants (Hz) and integration. ¹³C spectra were recorded in CDCl₃ or DMSO-d₆ or CD₂COCD₃ on 100/150 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source. The X-ray crystal-structure determinations of 3b and 3g were obtained on a Bruker SMART APEX CCD system. Melting points were determined using XT-4 apparatus and not corrected. Optical rotation were measured with polarimeter: Atopol IV (an average value of 10 times parallel tests).

2. General procedure for the synthesis of 3 and 4 (3a and 4a as an example)
A mixture of 2-amino-2-phenylacetic acid 1a (0.5 mmol), 1H-indole 2a (1.0 mmol), alloxan monohydrate (1.0 mmol), phosphotungstic acid 44-hydrate (0.125 mmol) in DMF (1.0 mL) was stirred at 110 °C for 6 hours. Then added 50 mL water and 30 mL saturated brine solution to the mixture, extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% NaHCO₃ solution, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc=5/1) to afford the product 3a as yellow solid.

A mixture of 3-acetoxy-2-aminopropanoic acid hydrochloride 1’a (0.5 mmol), 1H-indole 2a (1.0 mmol), alloxan monohydrate (1.0 mmol), phosphotungstic acid 44-hydrate (0.125 mmol) in DMF (1.0 mL) was stirred at 110 °C for 6 hours. Then added 50 mL water and 30 mL saturated brine solution to the mixture, extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% NaHCO₃ solution, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc=2/1) to afford the product 4a as yellow oil.

3. The side reaction of benzyl group amino acid in present of I₂ (phenylalanine as an example)

Probable Reaction Pathway:

\[
\text{HOOC-CH₂-NH₂} \xrightarrow{I₂, DMSO, 110°C} \text{PTA} \xrightarrow{DMSO, 110°C} \text{major product} + \text{trace} \]

\[
\text{HOOC-CH₂-NH₂} \xrightarrow{I₂, DMSO, 110°C} \text{I₂} \xrightarrow{\text{Oxidation}} \text{OAc} \]

\[
\text{H₂O, H₂O} \xrightarrow{-\text{CO₂}, -\text{NH}_{33}} \text{OAc} \xrightarrow{-\text{CO₂}} \text{H₂N} \]

\[
\text{O} \xrightarrow{-\text{H₂N}} \text{N} \]

2
### 4. Optimization details

![Chemical diagram]

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AM = Alloxan Monohydrate; PTA = phosphotungstic acid 44-hydrate; †Reaction conditions: 1a (0.5 mmol), 2a (1.0 mmol), Additive (1.0 mmol, If no otherwise specified), solvent (1.0 mL). ‡AM (0.2 eq.). §AM (0.4 eq.). ¶AM (2.0 eq.). †I₂ (1.0 eq.). ‡I₂ (0.2 eq.), for aliphatic amino acid. §§I₂ (0.2 eq.), for amino acid hydrochloride. ¶¶I₂ (0.2 eq.), for aromatic amino acids. ††isolated yields.
5. Characterization data for compound 3, 4 and 6

3,3’-(phenylmethylene)bis(1H-indole) (3a)

Yellow solid; mp = 86-87 °C. 1H NMR (600 MHz, dmsod6)  δ 10.84 (br, 2H), 7.37 (m, 4H), 7.31 – 7.24 (m, 4H), 7.16 (t, J = 7.2 Hz, 1H), 7.04 (t, J = 7.2 Hz, 2H), 6.90 – 6.82 (m, 4H), 5.85 (s, 1H). 13C NMR (100 MHz, CDCl3) IR (KBr): 1620.79, 1490.42, 1454.28, 1416.13, 1337.45, 1216.99, 1091.94, 1009.68. HRMS (ESI): m/z [M+Na]+ calcd for C23H18N2Na: 345.1362; found: 345.1365.

3,3’-(phenylmethylene)bis(6-bromo-1H-indole) (3b)

Red solid; mp = 140-142 °C. 1H NMR (600 MHz, dmsod6)  δ 11.03 (br, 1H), 7.57 (s, 2H), 7.34 (m, 2H), 7.27 (m, 2H), 7.19 (m, 3H), 7.01 (d, J = 7.8 Hz, 2H), 6.87 (s, 2H), 5.83 (s, 1H). 13C NMR (100 MHz, dmsod6) δ 144.34, 137.50, 137.34, 128.25, 126.05, 125.60, 124.52, 121.18, 120.84, 118.16, 114.10, 113.86. IR (KBr): 1687.23, 1610.42, 1451.65, 1404.27, 1332.34, 1284.79, 1221.54, 1133.97, 1094.93, 1047.51. HRMS (ESI): m/z [M+Na]+ calcd for C23H16Br2N2Na: 500.9572; found: 500.9573.

3,3’-(phenylmethylene)bis(5-bromo-1H-indole) (3c)

Yellow solid; mp = 230-232 °C. 1H NMR (600 MHz, dmsod6)  δ 11.09 (br, 2H), 7.43 (s, 2H), 7.34 (d, J = 8.4 Hz, 4H), 7.29 (m, 2H), 7.24 – 7.11 (m, 3H), 6.89 (s, 2H), 5.86 (s, 1H). 13C NMR (100 MHz, dmsod6) δ 144.32, 135.31, 128.42, 128.26, 126.11, 125.30, 121.26, 117.70, 113.65, 111.00. IR (KBr): 1598.14, 1558.08, 1455.91, 1416.74, 1333.07, 1216.33, 1098.23. HRMS (ESI): m/z [M+Na]+ calcd for C23H16Br2N2Na: 500.9572; found: 500.9581.

Dimethyl 3,3’-(phenylmethylene)bis(1H-indole-4-carboxylate) (3d)

White solid; mp = 251-253 °C. 1H NMR (600 MHz, dmsod6)  δ 11.12 (br, 2H), 7.59 (d, J = 7.8Hz, 2H), 7.23 (m, 4H), 7.16 (m, 1H), 7.12 (m, 2H), 6.99 (d, J = 7.2 Hz, 2H), 6.39 (s, 1H), 5.62 (s, 2H), 5.94 (s, 1H). 13C NMR (100 MHz, dmsod6) δ 168.56, 145.57, 137.90, 129.02, 127.62, 127.24, 125.53, 124.85, 122.84, 120.73, 119.88, 119.02, 115.33, 51.47, 40.98. IR (KBr): 2948.80, 1704.03, 1613.51, 1495.85, 1433.76, 1344.88, 1280.51, 1243.23, 1198.55, 1143.32, 1036.28. HRMS (ESI): m/z [M+Na]+ calcd for C27H22N2NaO4: 461.1472; found: 461.1475.

Dimethyl 3,3’-(phenylmethylene)bis(1H-indole-6-carboxylate) (3e)
White solid; mp = 258-261 °C: ¹H NMR (600 MHz, dmso-d₆) δ 11.31 (br, 2H), 8.05 (s, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 4H), 7.29 (t, J = 7.8 Hz, 2H), 7.20 (t, J = 7.2 Hz, 1H), 7.11 (d, J = 2.4 Hz, 2H), 5.93 (s, 1H), 3.83 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 167.28, 144.29, 135.87, 129.98, 128.80 – 128.39 (m), 127.67, 122.07, 119.03, 118.85, 118.46, 113.64, 51.7. IR (KBr): 1696.87, 1623.33, 1567.29, 1500.36, 1438.20, 1410.83, 1359.07, 1303.66, 1273.72, 1088.27. HRMS (ESI): m/z [M+Na]+ calcd for C₂₇H₂₂N₂NaO₄ : 461.1472; found: 461.1475.

3,3’-(phenylmethylene)bis(5-methoxy-1H-indole)

Pale red solid; mp = 215-216 °C: ¹H NMR (600 MHz, dmso-d₆) δ 10.74 (s, 2H), 7.44 (d, J = 7.8 Hz, 2H), 7.36 – 7.26 (m, 4H), 7.19 (t, J = 7.2 Hz, 1H), 6.91 (s, 2H), 6.84 (s, 2H), 6.77 (d, J = 8.4 Hz, 2H), 5.84 (s, 1H), 3.62 (s, 6H). ¹³C NMR (100 MHz, dmso-d₆) δ 152.81, 145.11, 131.95, 128.45, 128.11, 127.17, 125.84, 124.44, 117.85, 112.16, 110.70, 101.58, 55.30, 39.83. IR (KBr): 2937.48, 2829.91, 1622.11, 1584.33, 1485.20, 1450.00, 1331.96, 1291.41, 1258.69, 1208.51, 1171.40, 1127.40, 1095.04, 1024.07. HRMS (ESI): m/z [M+Na]+ calcd for C₂₅H₂₂N₂NaO₂ : 405.1573; found: 405.1578.

3,3’-(phenylmethylene)bis(6-nitro-1H-indole)

Yellow solid; mp = 268-270 °C: ¹H NMR (400 MHz, dmso-d₆) δ 11.69 (br, 2H), 8.33 (s, 2H), 7.78 (d, J = 8.8 Hz, 2H), 7.43 (d, J = 8.8 Hz, 2H), 7.35 (s, 2H), 7.21 (s, 1H), 6.02 (s, 1H). ¹³C NMR (100 MHz, dmso-d₆) δ 141.93, 134.99, 131.04, 130.7, 128.48, 128.21, 119.17, 118.93, 113.67, 109.36, 108.51. IR (KBr): 1737.65, 1619.40, 1587.25, 1501.51, 1456.64, 1416.07, 1373.16, 1333.60, 1105.12, 1057.28. HRMS (ESI): m/z [M+Na]+ calcd for C₂₃H₁₆N₄NaO₄ : 435.1064; found: 435.1070.

3,3’-(phenylmethylene)bis(2-methyl-1H-indole)

Yellow solid; mp = 257-258 °C: ¹H NMR (600 MHz, dmso-d₆) δ 10.75 (s, 2H), 7.27 – 7.22 (m, 2H), 7.22 (m, 1H), 7.20 (m, 4H), 6.88 (t, J = 7.8 Hz, 2H), 6.80 (d, J = 7.8 Hz, 2H), 6.67 (t, J = 7.2 Hz, 2H), 5.92 (s, 1H), 2.06 (s, 6H). ¹³C NMR (100 MHz, dmso-d₆) δ 143.93, 134.79, 131.04, 130.7, 128.48, 128.21, 119.17, 118.93, 113.67, 109.36, 108.51. IR (KBr): 1737.65, 1619.40, 1587.25, 1501.51, 1456.64, 1416.07, 1373.16, 1333.60, 1105.12, 1057.28. HRMS (ESI): m/z [M+Na]+ calcd for C₂₅H₂₂N₂ : 373.1675; found: 373.1676.

3,3’-(phenylmethylene)bis(1-methyl-1H-indole)

Pale yellow solid; mp = 200-201 °C: ¹H NMR (600 MHz, CDCl₃) δ 7.40 (d, J = 7.8 Hz, 2H), 7.36 (m, 2H), 7.33 – 7.27 (m, 4H), 7.22 (m, 3H), 7.01 (t, J = 7.2 Hz, 2H), 6.54 (s, 2H), 5.90 (s, 1H), 3.69 (s, 6H). ¹³C NMR (100 MHz, dmso-d₆) δ 144.38, 137.32, 128.64, 128.23, 128.16, 127.37, 125.97, 121.35,
119.98, 118.57, 118.16, 109.02, 40.01, 32.66. IR (KBr): 2933.88, 1615.96, 1549.16, 1474.03, 1424.27, 1368.49, 1328.04, 1227.01, 1200.36, 1152.02, 1119.60, 1055.18, 1010.97. HRMS (ESI): m/z [M+Na]+ calcd for C25H22N2Na : 373.1675; found: 373.1677.

3,3’-(4-fluorophenyl)methylene)bis(1-methyl-1H-indole)

Pale yellow solid; mp = 202-204 °C; 1H NMR (600 MHz, CDCl3) δ 7.35 (d, J = 7.8 Hz, 2H), 7.28 (m, 4H), 7.20 (m, 3H), 6.97 (m, 4H), 6.50 (s, 2H), 5.86 (s, 1H), 3.66 (s, 6H). 13C NMR (100 MHz, CDCl3) δ 161.27 (d, J = 242 Hz), 140.06, 137.34, 129.96 (d, J = 7.4 Hz), 128.17, 127.22, 121.47, 119.90, 118.66, 118.01, 114.88 (d, J = 21 Hz), 109.09, 39.28, 32.65. IR (KBr): 2935.40, 2845.35, 1894.64, 1599.08, 1550.48, 1501.82, 1472.47, 1424.37, 1368.57, 1328.47, 1218.25, 1153.02, 1119.65, 1091.86, 1056.89, 1010.97. HRMS (ESI): m/z [M+Na]+ calcd for C25H21F2N2Na : 391.1581; found: 391.1581.

4-(bis(1-methyl-1H-indol-3-yl)methyl)phenol

Red solid; mp = 248-249 °C; 1H NMR (400 MHz, dmso-d6) δ 9.21 (s, 1H), 7.34 (m, 4H), 7.14 (m, 4H), 6.92 (m, 2H), 6.78 (s, 2H), 6.70 (m, 2H), 5.74 (s, 6H), 1H NMR (100 MHz, CDCl3) δ 155.40, 136.98, 135.00, 129.13, 127.77, 126.95, 121.00, 119.35, 118.26, 117.99, 114.88, 109.54, 32.21. IR (KBr): 3457.56, 3107.37, 3050.25, 2933.36, 1669.94, 1604.61, 1545.20, 1508.17, 1474.58, 1422.66, 1370.30, 1300.18, 1289.21, 1254.72, 1231.94, 1196.96, 1159.19, 1129.67, 1053.64, 1011.37. HRMS (ESI): m/z [M+Na]+ calcd for C25H21F2N2NaO : 389.1624; found: 389.1623.

3,3’-(p-tolylmethylene)bis(1-methyl-1H-indole)

Red solid; mp = 202-203 °C; 1H NMR (600 MHz, CDCl3) δ 7.38 (d, J = 7.8 Hz, 2H), 7.26 (m, 2H), 7.22 (m, 2H), 7.19 - 7.15 (m, 2H), 7.06 (d, J = 7.8 Hz, 2H), 6.97 (t, J = 7.2 Hz, 2H), 6.51 (s, 2H), 5.84 (s, 1H), 3.62 (s, 6H), 2.30 (s, 3H). 13C NMR (100 MHz, CDCl3) δ 141.35, 137.29, 135.29, 128.83, 128.45, 128.13, 127.38, 121.29, 119.99, 118.51, 118.34, 108.97, 39.58, 32.59, 21.08. IR (KBr): 2915.01, 2825.11, 1909.76, 1614.31, 1550.34, 1507.85, 1472.65, 1422.66, 1370.30, 1328.83, 1224.78, 1151.72, 1118.45, 1057.13, 1011.48. HRMS (ESI): m/z [M+Na]+ calcd for C26H24N2NaO : 387.1832; found: 387.1831.

3,3’-(4-chlorophenyl)methylene)bis(1-methyl-1H-indole)
Red solid; mp = 209-212 °C; 1H NMR (600 MHz, CDCl3) δ 7.34 (d, J = 7.8 Hz, 2H), 7.31 – 7.23 (m, 4H), 7.20 (m, 2H), 6.99 (m, 2H), 6.49 (s, 2H), 5.84 (s, 1H), 3.64 (s, 6H). 13C NMR (100 MHz, CDCl3) δ 142.94, 137.32, 131.57, 129.98 (s), 128.27, 128.20, 127.17, 121.50, 119.85, 118.70, 117.62, 109.11, 39.43, 32.64. IR (KBr): 2930.46, 2862.45, 2818.70, 1902.16, 1614.17, 1586.11, 1547.31, 1480.63, 1329.67, 1253.08, 1224.12, 1200.90, 1152.55, 1127.68, 1085.48, 1058.98, 1011.98. HRMS (ESI): m/z [M+Na]+ calcd for C25H21ClIN2Na : 407.1285; found: 407.1287.

White solid; mp = 264-265 °C; 1H NMR (600 MHz, CDCl3) δ 7.39 (m, 3H), 7.28 (m, 2H), 7.228 (m, 4H), 7.138 (m, 2H), 6.50 (s, 2H), 6.34 (s, 1H), 3.66 (s, 6H). 13C NMR (100 MHz, CDCl3) δ 141.69, 137.40, 133.83, 130.30, 129.43, 128.38, 127.35, 126.56, 121.47, 119.92, 118.68, 116.83, 109.06, 36.45, 32.68. IR (KBr): 2929.96, 2821.48, 1922.60, 1613.35, 1548.40, 1475.43, 1424.53, 1371.06, 1331.02, 1245.64, 1222.74, 1202.59, 1156.04, 1127.08, 1035.23, 1010.70. HRMS (ESI): m/z [M+Na]+ calcd for C25H21ClIN2Na : 407.1285; found: 407.1287.

3,3’-(2-chlorophenyl)methylene)bis(1-methyl-1H-indole)

Pale red solid; mp = 171-174 °C; 1H NMR (600 MHz, CDCl3) δ 7.90 (s, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.21 – 7.14 (m, 3H), 7.04 (M, 2H), 6.92 (M, 2H), 6.83 (s, 2H), 6.17 (s, 1H). 13C NMR (100 MHz, CDCl3) δ 148.60, 136.55, 126.73, 126.39, 125.11, 123.58, 123.14, 122.00, 119.74, 119.70, 119.35, 111.08, 77.32, 77.00, 76.68, 35.30. IR (KBr): 1619.36, 1456.24, 1418.50, 1336.37, 1217.33, 1091.23, 1009.90. HRMS (ESI): m/z [M+Na]+ calcd for C21H16N2S : 351.0926; found: 351.0929.

Tri(1H-indol-3-yl)methane

Pale yellow oil; 1H NMR (400 MHz, CDCl3) δ 10.73 (br, 3H), 7.41 (d, J = 6.8 Hz, 3H), 7.35 (d, J = 6.8 Hz, 3H), 7.02 (m, 3H), 6.95 (s, 3H), 6.86 (m, 3H), 6.07 (s, 1H). 13C NMR (100 MHz, CDCl3) δ 136.54, 126.73, 123.16, 120.57, 119.25, 118.24, 117.89, 111.33. IR (KBr): 3258.22, 3052.04, 2922.32, 2588.32, 1618.05, 1485.57, 1455.06, 1338.65, 1240.95, 1216.52, 1225.91, 1093.99, 1022.28, 1003.19. MS: m/z [M]+ calcd for C29H19N3 : 361.16; found: 361.36.

3,3’-(propane-1,1-diyl)bis(1-methyl-1H-indole)
White solid; mp = 88-90 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.77 (m, 2H), 7.42 – 7.36 (m, 2H), 7.33 (s, 2H), 7.18 (m, 2H), 6.97 (s, 2H), 4.52 (m, 1H), 3.78 (s, 6H), 2.37 (m, 2H), 1.21 – 1.06 (m, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 137.14, 127.52, 126.13, 121.14, 119.68, 118.88, 118.29, 109.01, 35.68, 32.48, 29.16, 13.17. IR (KBr): 2957.08, 2924.95, 2866.10, 1915.48, 1879.76, 1761.55, 1612.09, 1585.35, 1549.25, 1476.09, 1423.20, 1371.17, 1327.82, 1250.41, 1228.94, 1195.25, 1156.49, 1132.64, 1085.11, 1052.96, 1011.39. HRMS (ESI): m/z [M+Na]+ calced for C\(_{21}\)H\(_{22}\)N\(_2\)Na : 325.1675; found: 325.1672.

![3r](image)

3,3'-[(2-methylpropane-1,1-diyl)bis(1-methyl-1H-indole)]

White solid; mp = 102-103 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.64 (d, \(J = 7.8\) Hz, 2H), 7.24 – 7.18 (m, 2H), 7.15 (t, \(J = 8.4\) Hz, 2H), 7.03 (t, \(J = 6.6\) Hz, 2H), 6.92 (s, 2H), 4.21 (d, \(J = 9.0\) Hz, 1H), 3.67 (m, 6H), 2.69 – 2.51 (m, 1H), 0.97 (d, \(J = 6.6\) Hz, 6H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 136.83, 127.93, 128.07, 127.78, 126.37, 121.06, 119.96, 119.7, 118.30, 109.94, 40.94, 33.24, 32.62, 21.90. IR (KBr): 2956.41, 2867.47, 1612.97, 1541.31, 1472.37, 1423.39, 1371.34, 1327.24, 1228.66, 1157.33, 1127.79, 1055.32, 1011.63. HRMS (ESI): m/z [M+Na]+ calced for C\(_{22}\)H\(_{24}\)N\(_2\)Na : 339.1832; found: 339.1832.

![3s](image)

3,3'-[3-(methylthio)propane-1,1-diyl]bis(1-methyl-1H-indole)

Yellow oil; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.62 (d, \(J = 7.8\) Hz, 2H), 7.24 (d, \(J = 8.4\) Hz, 2H), 7.17 (d, \(J = 8.4\) Hz, 2H), 7.03 (t, \(J = 7.2\) Hz, 2H), 6.85 (s, 2H), 4.65 (s, 1H), 3.66 (s, 6H), 2.55 (t, \(J = 7.2\) Hz, 2H), 2.47 (t, \(J = 7.2\) Hz, 2H), 2.07 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 137.13, 127.25, 126.20, 121.28, 119.56, 118.46, 118.02, 109.06, 35.30, 32.81, 32.75, 32.52, 15.46. IR (KBr): 2921.08, 1613.80, 1546.10, 1471.08, 1423.00, 1371.83, 1326.62, 1237.90, 1153.88, 1125.06, 1064.22, 1012.40. HRMS (ESI): m/z [M+Na]+ calced for C\(_{22}\)H\(_{24}\)N\(_2\)Na : 371.1552; found: 371.1553.

![3t](image)

(S)-3,3'-[2-methylbutane-1,1-diyl]bis(5-methoxy-1H-indole)

Red oil; [\(\alpha\)]\(_D\) +1.83 (c 10mg/ml, MeOH). \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.69 (d, \(J = 8.4\) Hz, 2H), 7.06 (m, 4H), 6.89 (s, 2H), 6.77 (d, \(J = 8.4\) Hz, 2H), 4.23 (d, \(J = 7.8\) Hz, 1H), 3.77 (m, 6H), 2.31 (m, 1H), 1.64 – 1.55 (m, 1H), 1.17 – 1.08 (m, 1H), 0.95 (d, \(J = 6.6\) Hz, 3H), 0.90 (t, \(J = 7.2\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 153.41, 131.53, 131.40, 128.18, 127.98, 122.78, 122.56, 119.19, 118.64, 111.60, 111.16, 102.02, 55.90, 39.35, 39.14, 27.89, 17.68, 11.97. IR (KBr): 2958.22, 2872.27, 2830.29, 1623.79, 1580.76, 1482.81, 1454.38, 1376.77, 1347.05, 1291.58, 1248.39, 1209.91, 1171.95, 1095.93, 1027.95. MS: m/z [M]+ calced for C\(_{23}\)H\(_{26}\)NO\(_2\) : 362.20; found: 362.37.

![3u](image)

3,3'-[(3-methylbutane-1,1-diyl)bis(1H-indole)]
Yellow oil; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.59 (d, \(J = 8.0\) Hz, 2H), 7.43 (s, 2H), 7.09 (s, 1H), 7.08 (s, 1H), 7.02 (m, 2H), 6.65 (d, \(J = 2.0\) Hz, 2H), 4.53 (t, \(J = 7.6\) Hz, 1H), 2.02 (t, \(J = 7.2\) Hz, 2H), 1.65 – 1.49 (m, 1H), 0.93 (d, \(J = 6.8\) Hz, 6H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 136.34, 126.88, 121.50, 121.46, 120.09, 119.40, 118.82, 111.14, 77.32, 77.00, 76.68, 45.11, 31.46, 25.80, 22.77. IR (KBr): 2953.91, 2865.73, 1618.06, 1456.93, 1419.00, 1338.93, 1220.38, 1094.36, 1010.92. HRMS (ESI): m/z [M+Na]^+ calcd for C21H22N2Na : 325.1675; found: 325.1675.

[Diagram 3v]

3,3’-(pentane-1,1-diyl)bis(1H-indole)

Red oil; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.57 (d, \(J = 7.8\) Hz, 2H), 7.50 (s, 2H), 7.15 (d, \(J = 7.8\) Hz, 2H), 7.10 (t, \(J = 7.8\) Hz, 2H), 7.01 (t, \(J = 7.2\) Hz, 2H), 6.75 (s, 2H), 4.41 (t, \(J = 7.2\) Hz, 1H), 2.16 (d, \(J = 6.6\) Hz, 2H), 1.35 (s, 4H), 0.84 (d, \(J = 6.6\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 136.43, 127.05, 121.57, 121.42, 120.34, 119.55, 118.88, 111.08, 35.57, 33.86, 30.47, 22.77, 14.08. IR (KBr): 2954.67, 2926.62, 2857.79, 1617.55, 1521.63, 1486.14, 1455.68, 1418.68, 1337.90, 1219.63, 1151.37, 1093.40, 1010.27. MS: m/z [M+Na]^+ calcd for C21H22N2 : 302.18; found: 302.34.

[Diagram 3w]

3,3’-(ethane-1,1-diyl)bis(1H-indole) (vibrindole A)

White solid; mp = 153-155°C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.75 (br, 2H), 7.63 (d, \(J = 7.8\) Hz, 2H), 7.34 (d, \(J = 8.4\) Hz, 2H), 7.22 (t, \(J = 7.8\) Hz, 2H), 7.10 (t, \(J = 7.2\) Hz, 2H), 6.86 (s, 2H), 4.71 (d, \(J = 6.6\) Hz, 1H), 1.84 (d, \(J = 7.2\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 136.56, 126.83, 121.69, 121.53, 121.19, 119.66, 118.94, 111.05, 28.11, 21.69. IR (KBr): 2958.13, 2866.18, 2836.91, 1624.23, 1548.86, 1484.13, 1454.83, 1421.09, 1337.75, 1291.37, 1220.61, 1124.66, 1095.80, 1013.70. HRMS (ESI): m/z [M+Na]^+ calcd for C18H16N2Na : 283.1206; found: 283.1209.

[Diagram 4a]

2,2-di(1H-indol-3-yl)ethyl acetate

Yellow oil; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.80 (br, 2H), 7.57 (d, \(J = 7.8\) Hz, 2H), 7.18 (d, \(J = 7.8\) Hz, 2H), 7.11 (t, \(J = 7.8\) Hz, 2H), 7.01 (t, \(J = 7.2\) Hz, 2H), 6.70 (s, 2H), 4.88 (t, \(J = 7.2\) Hz, 1H), 4.67 (d, \(J = 6.6\) Hz, 2H), 1.89 (s, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 171.41, 136.34, 126.90, 122.14, 121.93, 119.40, 116.07, 111.16, 67.42, 33.45, 21.03. IR (KBr): 2924.62, 2853.71, 1721.32, 1631.42, 1457.13, 1422.17, 1384.17, 1263.84, 1097.32, 1038.64. HRMS (ESI): m/z [M+Na]^+ calcd for C20H18N2NaO : 341.1260; found: 341.1261.

[Diagram 4b]

2,2-di(1H-indol-3-yl)ethyl butyrate

Yellow oil; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.84 (br, 2H), 7.59 (d, \(J = 7.8\) Hz, 2H), 7.22 (m, 2H), 7.13 (m, 2H), 7.03 (m, 2H), 6.76 (s, 2H), 4.90 (t, \(J = 7.2\) Hz, 1H), 4.70 (d, \(J = 7.2\) Hz, 2H), 2.17 (t, \(J = 7.2\) Hz, 2H), 1.51 (m, 2H), 0.79 (t, \(J = 7.2\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 174.00, 136.35, 126.93,
IR (KBr): 2962.23, 2928.69, 2872.81, 1714.79, 1456.92, 1421.18, 1385.17, 1341.43, 1266.21, 1184.96, 1096.08, 1008.02. HRMS (ESI): m/z [M+Na]+ calcd for C22H22N2Na: 369.1573; found: 369.1577.

![di(1H-indol-3-yl)methane]

Yellow oil; $^1$H NMR (600 MHz, dmso-$d_6$) δ 10.83 (br, 2H), 7.63 (d, $J = 7.8$ Hz, 2H), 7.43 (d, $J = 8.4$ Hz, 2H), 7.22 (s, 2H), 7.12 (m, 2H), 7.01 (m, 2H). $^{13}$C NMR (150 MHz, dmso-$d_6$) δ 136.54, 136.38, 127.34, 122.87, 122.71, 120.91, 118.83, 118.20, 114.37, 114.33, 111.45, 21.10. IR (KBr): 2921.85, 1620.61, 1488.27, 1455.74, 1422.61, 1341.12, 1221.66, 1091.03, 1006.56. HRMS (ESI): m/z [M+Na]+ calcd for C17H14N2Na: 269.1047; found: 269.1047.

![3,3’-(2-phenylethane-1,1-diyl)bis(1H-indole)]

White solid; mp = 76-78°C; $^1$H NMR (600 MHz, CDCl$_3$) δ 7.58 (d, $J = 7.8$ Hz, 2H), 7.15 – 7.08 (m, 10H), 7.05 (m, 3H), 6.61 (m, 2H), 4.76 (t, $J = 7.8$ Hz, 2H), 3.50 (d, $J = 7.2$ Hz, 2H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 141.17, 136.26, 128.85, 127.89, 126.68, 125.63, 121.99, 121.54, 119.46, 118.91, 118.88, 111.11, 41.57, 36.02. IR (KBr): 3413.36, 2933.77, 2831.05, 1619.97, 1582.11, 1513.25, 1482.86, 1446.52, 1350.50, 1290.68, 1170.18, 1097.02, 1058.26, 1025.49. HRMS (ESI): m/z [M+Na]+ calcd for C24H20N2: 336.22; found: 336.22.

![4-(2,2-bis(5-methoxy-1H-indol-3-yl)ethyl)phenol]

Yellow oil; $^1$H NMR (600 MHz, acetone-$d_6$) δ 9.75 (br, 1H), 7.65 (d, $J = 7.8$ Hz, 2H), 7.63 (d, $J = 8.4$ Hz, 2H), 7.31 (d, $J = 7.8$ Hz, 1H), 7.28 (d, $J = 8.4$ Hz, 2H), 7.10 (m, 3H), 7.09 – 7.04 (m, 2H), 6.94 (m, 2H), 6.90 (s, 1H), 5.00 (t, $J = 7.2$ Hz, 1H), 3.85 – 3.55 (m, 8H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 153.60, 153.46, 133.47, 131.78, 130.12, 127.43, 122.79, 119.15, 114.80, 111.64, 111.55, 101.99, 55.90, 40.71, 36.53. IR (KBr): 3413.36, 2933.77, 2831.05, 1619.97, 1582.11, 1513.25, 1482.86, 1446.52, 1350.50, 1290.68, 1170.18, 1097.02, 1058.26, 1025.49. HRMS (ESI): m/z [M+Na]+ calcd for C26H24N2O3Na: 435.1679; found: 435.1687.

![3,3’-(2-(1H-indol-3-yl)ethane-1,1-diyl)bis(1-methyl-1H-indole)]

$^1$H NMR (600 MHz, acetone-$d_6$) δ 9.75 (br, 1H), 7.65 (d, $J = 7.8$ Hz, 1H), 7.63 (d, $J = 8.4$ Hz, 2H), 7.31 (d, $J = 7.8$ Hz, 1H), 7.28 (d, $J = 8.4$ Hz, 2H), 7.10 (m, 3H), 7.09 – 7.04 (m, 2H), 7.01 (m, 1H), 6.94 (m, 2H), 6.90 (s, 1H), 5.00 (t, $J = 7.2$ Hz, 1H), 3.85 – 3.55 (m, 8H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 137.23, 135.88, 127.88, 127.50, 126.62, 122.14, 121.60, 121.22, 121.21, 119.76, 119.03, 118.88,
IR (KBr): 3050.19, 2927.13, 1616.00, 1547.46, 1475.55, 1421.04, 1372.09, 1328.48, 1244.95, 1154.10, 1125.57, 1012.44. HRMS (ESI): m/z [M+Na]+ calcd for C28H25N2Na: 426.1941; found: 426.1952.

3-((1H-indol-3-yl)(phenyl)methyl)-1-methyl-1H-indole

Red oil; $^1$H NMR (600 MHz, CDCl$_3$) δ 7.63 (br, 1H), 7.36 (m, 2H), 7.31 (m, 2H), 7.27 – 7.08 (m, 7H), 6.96 (m, 2H), 6.51 (s, 1H), 6.45 (s, 1H), 5.85 (s, 1H), 3.55 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 144.15, 137.24, 136.36, 128.55, 128.08, 127.31, 126.81, 125.96, 123.50, 121.64, 121.34, 119.89, 119.66, 119.25, 119.00, 118.57, 117.90, 110.99, 109.05, 40.00, 32.19. IR (KBr): 2929.97, 1609.63, 1546.59, 1455.04, 1418.74, 1369.65, 1330.07, 1221.13, 1153.63, 1123.54, 1091.74, 1048.21, 1010.29. HRMS (ESI): m/z [M+Na]+ calcd for C24H20N2Na: 359.1519; found: 359.1518.

ethyl 4-(4-(bis(1-methyl-1H-indol-3-yl)methyl)phenoxy)butanoate

Red oil; $^1$H NMR (600 MHz, CDCl$_3$) δ 7.37 (d, $J = 7.8$ Hz, 2H), 7.28 (d, $J = 8.4$ Hz, 2H), 7.22 (m, 2H), 7.19 (t, $J = 7.2$ Hz, 2H), 6.98 (t, $J = 7.2$ Hz, 2H), 6.79 (d, $J = 8.4$ Hz, 2H), 6.51 (s, 2H), 5.82 (s, 1H), 4.13 (m, 2H), 3.96 (t, $J = 6.6$ Hz, 2H), 3.66 (s, 6H), 2.50 (t, $J = 7.2$ Hz, 2H), 2.083 (m, 2H), 1.25 (t, $J = 7.2$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 173.16, 157.02, 137.32, 136.64, 124.44, 128.07, 127.35, 121.28, 119.96, 118.48, 114.00, 108.94, 100.76, 39.15, 32.50, 30.80, 24.67, 14.16. IR (KBr): 2933.26, 1731.78, 1609.57, 1507.87, 1470.47, 1422.45, 1371.27, 1327.34, 1244.44, 1175.10, 1121.39, 1046.63. HRMS (ESI): m/z [M+Na]+ calcd for C31H32N2NaO: 503.2305; found: 503.2308.
4. 3,3’-(phenylmethylene)bis(1-methyl-1H-indole)

X-ray structure determination was obtained via slow evaporation of compound 3i in CHCl₃/MeOH (10:1) at room temperature.

Figure S1 X-ray crystal structure of 3i; ellipsoids depicted at the 30% probability level.

Table S1. Crystal data and structure refinement for compound 3i (CCDC: 1030461)

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<td>F(000)</td>
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<tr>
<td>Temperature</td>
<td>298(2)</td>
<td>Crystal size</td>
<td>0.15 x 0.12 x 0.10 mm³</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073</td>
<td>Reflections collected</td>
<td>12169</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Monoclinic</td>
<td>Independent reflections</td>
<td>3388 [R(int) = 0.0446]</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/c</td>
<td>Max. and min. transmission</td>
<td>0.992 and 0.993</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Goodness-of-fit on F²</td>
<td>1.014</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Final R indices</td>
<td>R1 =0.0476, wR2 = 0.1148</td>
</tr>
<tr>
<td></td>
<td></td>
<td>R indices (all data)</td>
<td>R1 = 0.0871, wR2 = 0.1367</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Largest diff. peak and hole</td>
<td>0.180 and -0.162e⁻³</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Density (calculated)</td>
<td>1.204 Mg/m³</td>
</tr>
</tbody>
</table>

Z = 4
5. Copies of $^1$H NMR, $^{13}$C NMR and HRMS/MS Spectra
tris(3-indolyl)methane

3p

400 NMR
DMSO-\(d_2\)
arsindoline B

600 MHz NMR
CDCl₃

arsindoline B

100 MHz NMR
CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-1\JC\c513_000002.d
Method: Student_L_Cms-140618
Sample Name: Student_4-8
Comment:

Acquisition Date: 2014-7-2 17:04:27
Operator: apex-Ultra

Acquisition Parameter
Potency: Positive
Averaged Scans: 2
Broadband Low Mass: 100.3 m/z
Broadband High Mass: 1200.0 m/z
Acquisition Mode: Single MS
Source Accumulation: 0.0 sec
Ion Accumulation Time: 0.1 sec
Flight Time to Acq. Cell: 0.0 sec

Intensity (x10^6)

![Chemical Structure](image)

3b

Calibration Date: Wed Jun 18 07:18:23
Data Acquisition Size: 321072
Apodization: Sine-Bell Multiplication

### Mass Spectral Data

<table>
<thead>
<tr>
<th>m/z</th>
<th>Formula</th>
<th>Error [ppm]</th>
<th>Mean Error [ppm]</th>
<th>N-Rule</th>
<th>e-Conf</th>
<th>mSig</th>
<th>StdI</th>
<th>Std Mean m/z</th>
<th>Std Mean VarNorm</th>
<th>Std Dev ComDev</th>
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</thead>
<tbody>
<tr>
<td>500.9</td>
<td>C13 H16 Br2 N2</td>
<td>-0.2</td>
<td>15.5</td>
<td>18.27</td>
<td>0.017</td>
<td>0.001</td>
<td>0.005</td>
<td>0.001</td>
<td>0.842</td>
<td></td>
</tr>
</tbody>
</table>

46
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\2014\0702-1\JC\c555_000002.d
Method: Student_LCMS-140516
Sample Name: Student_4-6
Comment

Acquisition Info
Acquisition Date: 2014-7-2 17:06:27
Operator: apex-Ultra
Instrument: MALDI-TOF

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
Laser Power: 51.0 %
MALDI Plate: 300.0 V
Imaging Spot Diameter: 200.0 μm
Calibration Date: Wed Jun 18 07:10:23
Data Acquisition Size: 231072
Apodization: Sine-Bell Multiplication

Chemical Structure:

461.1475
475.3282

Meas. m/z
461.1
475

Form
C27H22N2O4

m/z
461.1
472

err
0.7
0.6

Mean
17.5

Std
0.004
0.003

Var
7
3

Conf
3
7

Diff
0.001
0.000

Dev
0.642
7

Com
1

R = COOME

3e
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-1\JCyc664_000002.d
Method: Student_L_Cms-140618
Sample Name: Student_4-6
Comment:
Acquisition Date: 2014-7-2 17:09:15
Operator:
Instrument: apex-Ultra

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
Laser Power: 51.0 %
MALDI Plate: 380.0 V
Imaging Spot Diameter: 2000.0 µm
ACQ Start Time: 2014-7-2 17:09:15

Broadband Low Mass: 100.3 m/z
End Plate: 3500.0 V
Broadband High Mass: 1200.0 m/z
Capillary Entrance: 4000.0 V
Acquisition Mode: Single MS
Skimmer 1: 20.0 V
Drying Gas Temperature: 180.0 °C
Pulse Program: basic
Drying Gas Flow Rate: 4.0 L/min
Source Accumulation: 0.0 sec
Neutrlzer Gas Flow Rate: 1.0 L/min
Ion Accumulation Time: 0.1 sec
Calibration Date: Wed Jun 18 07:18:23
Flight Time to Acq. Cell: 0.0 sec
Data Acquisition Size: 281472
Addition: None-Cell Multiplication

Chemical Structure:

![Chemical Structure Image]

Mass Spectral Data:

| m/z  | Formula | Error [ppm] | Mean Error [ppm] | N-Rule | ePik | mSig | lMean [m/z] | Std Dev [m/z] | Std Dev [m/z] | Std Dev [m/z] | Std Dev [m/z] | Std Dev [m/z] |
|------|---------|-------------|------------------|--------|------|------|-------------|---------------|---------------|---------------|---------------|---------------|---------------|
| 405.1| C25      | -1.1        | -1.0             | 15.5   | ok   | even| 2.45        | 0.003         | 0.000         | 0.001         | 0.000         | 0.642         |
| 578  | H22      |             |                  |        |      |     |              |               |               |               |               |               |               |
| 573  | N2       |             |                  |        |      |     |              |               |               |               |               |               |
| 2    | NaO      |             |                  |        |      |     |              |               |               |               |               |               |               |

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Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-1\UC\jc6522_000002.d
Method: Student_L.Cms-140518
Sample Name: Student_4-6
Comment:

Acquisition Parameter
Polarity: Positive
Averaged Scans: 2
Broadband Low Mass: 100.3 m/z
Broadband High Mass: 1200.0 m/z
Acquisition Mode: Single MS
Source Accumulation: 0.0 sec
Ion Accumulation Time: 0.1 sec
Flight Time to Acq. Cell: 0.0 sec
No. of Cell Fills: 1
End Plate: 3500.0 V
Capillary Entrance: 4000.0 V
Skimmer: 20.0 V
Drying Gas Temperature: 180.0 °C
Nebulizer Gas Flow Rate: 1.0 L/min
Calibration Date: Wed Jun 18 07:18:23
Data Acquisition Size: 281872
Apodization: Sine-Bell Multiplication

Instrument: apex-Ultra

Acquisition Date: 2014-7-2 17:12:45
Operator:

Interpreting the data...
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-1UCjic526_000002.d
Method: Student_LCms-140518
Sample Name: Student_4-6
Comment:

Acquisition Info
Acquisition Date: 2014-7-2 17:15:08
Operator: apex-Ultra
Instrument:

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
Laser Power: 51.0 %
MALDI Plate: 300.0 V
Imaging Spot Diameter: 200.0 µm

Broadband Low Mass: 100.3 m/z
Capillary Entrance: 3500.0 V
Drying Gas Temperature: 180.0 °C
Data Acquisition Size: 381872

Broadband High Mass: 1200.0 m/z
Skimmer 1: 4000.0 V
Drying Gas Flow Rate: 4.0 L/min
Calibration Date: Wed Jun 18 07:18:23

Acquisition Mode: Single MS
Capillary Voltage: 20.0 V
Nebulizer Gas Flow Rate: 1.0 L/min
Apodization: Sine-Bell Multiplication

Flight Time to Acq. Cell: 0.0 sec

Intensity: 6

Formula: C_{26}H_{24}N_{2}Na

m/z: 387.1

Error (ppm): 0.2

Significance: ok

Boundary Dev: 7
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: Hi20140702-1UCjg526_000002.d
Method: Student_LCMS-140818
Sample Name: Student_4-5
Comment:

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
Laser Power: 51.0 %
Mass of MALDI Plate: 300.0 V
Imaging Spot Diameter: 2000.0 μm

Broadband Low Mass: 100.3 m/z
End Plate: 3900.0 V
Capillary Entrance: 4000.0 V
Skimmer 1: 20.0 V

Calibration Date: Wed Jun 10 07:16:23
Data Acquisition Size: 251972
Apocitation: She-Bell Multiplication

Flight Time to Acc. Cell: 0.0 sec

RS = 1

<table>
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<tr>
<th>m/z</th>
<th>Form ula</th>
<th>err [ppm]</th>
<th>Mean err [ppm]</th>
<th>N-Rule Conf</th>
<th>mSig</th>
<th>Std I Mean m/z</th>
<th>Std I VanN crm</th>
<th>Std I m/z Diff</th>
<th>Std I b Dev</th>
</tr>
</thead>
<tbody>
<tr>
<td>407.1</td>
<td>C25 H21 Cl2 N2</td>
<td>-0.4</td>
<td>-0.8</td>
<td>15.5</td>
<td>ok even</td>
<td>12.34</td>
<td>0.015</td>
<td>0.000</td>
<td>0.905</td>
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<tr>
<td>285</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Mass Spectrum SmartFormula Report**

**Analysis Info**
- **Analysis Name**: H:\20140702-1\UC\jc524_000002.d
- **Sample Name**: Student_L.Cms-140618
- **Comment**: Student_4-6
- **Acquisition Date**: 2014-7-2 17:05:57
- **Operator**: apex-Ultra
- **Instrument**: apex-Ultra

**Acquisition Parameter**
- **Polarity**: Positive
- **Averaged Scans**: 2
- **Broadband Low Mass**: 100.3 m/z
- **Broadband High Mass**: 1200.0 m/z
- **Acquisition Mode**: Single MS
- **Source**: End Plate
- **ESI**: 3500.0 V
- **No. of Laser Shots**: 20
- **Capillary Entrance**: 4000.0 V
- **Skimmer 1**: 20.0 V
- **Laser Power**: 51.0 %
- **Imaging Spot Diameter**: 2000.0 µm
- **Drying Gas Temperature**: 150.0 °C
- **Nebulizer Gas Flow Rate**: 1.0 L/min
- **Calibration Date**: Wed Jun 18 07:18:23
- **Data Acquisition Size**: Sine-Bell Multiplication

**Formula Table**

<table>
<thead>
<tr>
<th>m/z</th>
<th>C</th>
<th>H</th>
<th>N</th>
<th>Na</th>
<th>351.0</th>
<th>920</th>
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<tr>
<td>351.0</td>
<td>21</td>
<td>16</td>
<td>2</td>
<td>1</td>
<td>14.5</td>
<td>0.842</td>
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<tr>
<td>362.2418</td>
<td>0.014</td>
<td>0.000</td>
<td>0.038</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
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</table>

**Diagram**

![Graphical representation of the molecule](image)
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-1\JC\j0689_000002.d
Method: Student_1Cms-140618
Sample Name: Student_1-6
Comment: 

Acquisition Date: 2014-7-2 17:45:35
Operator: 
Instrument: apex-Ultra

Acquisition Parameter
Polarity: Positive
Averaged Scans: 2
Broadband Low Mass: 100.3 m/z
Broadband High Mass: 1200.0 m/z
Acquisition Mode: Single MS
Pulse Program: basic
Source Accumulation: 0.0 sec
Ion Accumulation Time: 0.1 sec
Rt Time to Acq. Cell: 0.0 sec

ESI No. of Laser Shots: 20
End Plate: 1
Capillary Entrance: 4000.0 V
Skimmer 1: 20.0 V
Drying Gas Temperature: 150.0 °C
Drying Gas Flow Rate: 4.0 L/min
Nebulizer Gas Flow Rate: 1.0 L/min
Calibration Date: Wed Jun 18 07:18:23
Data Acquisition Size: 20197/2
Apodization: Sine-Bell Multiplication

Chemical Compound: 3q

![Chemical Structure](image)

Mass spectrum data with peak at m/z 325.1672 and 318.2083.
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-134514\140501_000002.d
Method: Student_L_Cms-140518
Sample Name: Student_4-6
Comment:

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20

Averaged Scans: 2
No. of Cell Fills: 1
Laser Power: 81.0 %

Broadband Low Mass: 100 m/z
End Plate: 3500 V
MALDI Plate: 3000 V

Broadband High Mass: 1200 m/z
Capillary Entrance: 4000 V
Imaging Spot Diameter: 2000.0 μm

Acquisition Mode: Single MS
Skimmer 1: 20.6 V
Calibration Date: Wed Jun 18 07:18:23

Pulse Program: Basic
Drying Gas Temperature: 160.0 °C
Data Acquisition Size: 2B1772

Source Accumulation: 0.0 sec
Drying Gas Flow Rate: 4.0 L/min
Apodization: Sinh-Bell Multiplication

Ion Accumulation Time: 0.1 sec
Nebulizer Gas Flow Rate: 1.0 L/min

Flight Time to Acq. Cell: 0.0 sec

---

Chemical Structure:

3r

Mass Table:

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<tr>
<th>m/z</th>
<th>Error</th>
<th>Mean</th>
<th>Std</th>
<th>Confi</th>
<th>m/z</th>
<th>Form</th>
<th>std</th>
<th>Dev</th>
</tr>
</thead>
<tbody>
<tr>
<td>330.1</td>
<td>0.1</td>
<td>-11.5</td>
<td>4.22</td>
<td>2.0</td>
<td>0.006</td>
<td>C22</td>
<td>0.002</td>
<td>0.000</td>
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<tr>
<td>334.3</td>
<td>0.1</td>
<td>-11.5</td>
<td>4.22</td>
<td>2.0</td>
<td>0.006</td>
<td>H24</td>
<td>0.002</td>
<td>0.000</td>
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<tr>
<td>340.1</td>
<td>0.1</td>
<td>-11.5</td>
<td>4.22</td>
<td>2.0</td>
<td>0.006</td>
<td>N2</td>
<td>0.002</td>
<td>0.000</td>
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</tbody>
</table>

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**Mass Spectrum SmartFormula Report**

**Analysis Info**
- Analysis Name: H:\20140702-1UClc041_000002.d
- Method: Student_L_Cms-140618
- Sample Name: Student_4-6
- Acquisition Date: 2014-7-2 17:47:25
- Operator: apex-Ultra

**Acquisition Parameter**
- Polarity: Positive
- Averaged Scans: 2
- Broadband Low Mass: 100.0 m/z
- Broadband High Mass: 1200.0 m/z
- Acquisition Mode: Single MS
- Pulse Program: Basic
- Source Accumulation: 0.0 sec
- Ion Accumulation Time: 0.1 sec
- Flight Time to Acq. Cell: 0.0 sec

**Instrument Settings**
- End Plate: 3500.0 V
- Capillary Entrance: 4000.0 V
- Skimmer I: 20.0 V
- Nebulizer Gas Flow Rate: 4.0 L/min
- Nebulizer Gas Flow Rate: 1.0 L/min
- MALDI Plate: 302.0 V
- Imaging Spot Diameter: 2000.0 μm
- Laser Power: 61.0 %
- Calibration Date: Wed Jan 18 07:18:23
- Data Acquisition Size: 384872
- Apodization: Sine-Bell Multiplication

**Mass Spectrum**

![Mass Spectrum Image]

**Formula Table**

<table>
<thead>
<tr>
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<th>#</th>
<th>Formula</th>
<th>err ppm</th>
<th>Mean err [ppm]</th>
<th>N-Rule</th>
<th>N-Rule Conf</th>
<th>mSig ma</th>
<th>Std I</th>
<th>Std Mean m/z</th>
<th>Std VarN orm</th>
<th>Std m/z</th>
<th>Std Com b</th>
<th>Std Dev</th>
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<tbody>
<tr>
<td>371.1</td>
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<td>-0.2</td>
<td>11.5</td>
<td>ok even</td>
<td>17.03</td>
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<td>0.013</td>
<td>0.001</td>
<td>0.042</td>
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63
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H1-20140702-1WCj0650_000002.d
Method: Student_L_Cms-140618
Sample Name: Student_4-6
Comment
Acquisition Date: 2014-7-2 17:51:30
Operator: apex-Ultra
Instrument: apex-Ultra

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
Laser Power: 51.0 %
MALDI Plate: 300.0 V
Imaging Spot Diameter: 2000.0 µm

Broadband Low Mass: 100.3 m/z
End Plate: 3500.0 V

Broadband High Mass: 1200.0 m/z
Capillary Entrance: 4000.0 V

Acquisition Mode: Single MS
Skimmer 1: 20.0 V

Source Accumulation: 0.0 sec
Drying Gas Temperature: 190.0 °C
Calibration Date: Wed Jun 18 07:18:23
Data Acquisition Size: 31972

Ion Accumulation Time: 0.1 sec
Drying Gas Flow Rate: 4.0 L/min
Apodization: Sinh-Bell Multiplication

Flight Time to Acq. Cell: 0.0 sec
Nebulizer Gas Flow Rate: 1.0 L/min

Chemical Structure:

Intens. x10^5

313.1334
317.0826
321.1569
325.1675
335.1537

m/z

325.1

N
2
H 22
675

O
21

C
21
675

Meas. m/z

Form. m/z

err (ppm)

Mean err (ppm)

N-Rule

eConf

mSig

ma

Std l

Mean

m/z

VarN

corr

Std

m/z

Diff

Com

D ev

1

20.1

1.1

11.5

dk
even

9.15

0.016

0.003

0.000

0.000

0.642

9

6

1

8

7
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H_20140702_1JUc6502_000002.d
Method: Student_LCms-140618
Sample Name: Student_4-6
Comment:

Acquisition Date: 2014-7-2 17:53:02
Operator: apex-Ultra
Instrument: apex-Ultra

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
Laser Power: 51.0 %
MALDI Plate: 360.0 V
Imaging Spot Diameter: 2000.0 µm

Broadband Low Mass: 100.0 m/z
End Plate: 3500.0 V
Capillary Entrance: 4000.0 V

 Acquisition Mode: Single MS
Skimmer 1: 20.0 V
Drying Gas Temperature: 180.0 °C

Pulse Program: basic
Drying Gas Flow Rate: 4.0 L/min
Nebulizer Gas Flow Rate: 1.0 L/min

Ion Accumulation Time: 0.1 sec
Flight Time to Acq. Cell: 0.0 sec

Calibration Date: Wed Jun 18 07:18:23
Data Acquisition Size: 261872
Apodization: Sine-Bell Multiplication

![Mass Spectrum Graph]

Table:

<table>
<thead>
<tr>
<th>m/z</th>
<th>Intensity</th>
<th>m/z err</th>
<th>Intensity err</th>
<th>m/z</th>
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<th>Intensity</th>
<th>m/z err</th>
<th>Intensity err</th>
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<tbody>
<tr>
<td>283.1</td>
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<td>1.5</td>
<td>1.1</td>
<td>283.1</td>
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<td>1.1</td>
<td>283.1</td>
<td>2.1</td>
<td>1.5</td>
<td>1.1</td>
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<tr>
<td>288.6</td>
<td>2.1</td>
<td>1.5</td>
<td>1.1</td>
<td>288.6</td>
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<td>1.1</td>
<td>288.6</td>
<td>2.1</td>
<td>1.5</td>
<td>1.1</td>
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</table>

Formula: C_18 H_16 N_2 Na

N Reform: 4.50
N Error: 0.008
N Error: 0.003
N Error: 0.000
N Error: 0.842
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H20140702-1U0jy580_000002.d
Method: Student_LCms-140619
Sample Name: Student_4-6
Comment

Acquisition Date: 2014-7-2 17:54:43
Operator: apex-Ultra
Instrument: apex-Ultra

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Laser Shots: 20
No. of Cell Fills: 1
Laser Power: 51.0 %
Broadband Low Mass: 100.3 m/z
End Plate: 3500.0 V
MALDI Plate: 300.0 V
Broadband High Mass: 1200.0 m/z
Capillary Entrance: 4000.0 V
Imaging Spot Diameter: 2000.0 μm
Acquisition Mode: Single MS
Skimmer 1: 20.0 V
Data Acquisition Size: 391672
Pulse Program: basic
Drying Gas Temperature: 180.0 °C
Calibration Date: Wed Jun 18 07:18:23
Source Accumulation Time: 0.0 sec
Drying Gas Flow Rate: 4.0 L/min
Data Acquisition Size: 391672
Ion Accumulation Time: 0.1 sec
Nebulizer Gas Flow Rate: 1.0 L/min
Apodization: Sine-Bell Multiplication
Right Time to Acq. Cell: 0.0 sec

Chemical Structure:

Table:

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<tr>
<th>m/z</th>
<th>Intensity</th>
</tr>
</thead>
<tbody>
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<tr>
<td>366.1577</td>
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</tr>
<tr>
<td>370.1610</td>
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<td>371.1636</td>
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</table>

Formula:

C_{16}H_{24}N_2O

Mass Accuracy:

m/z 369.1

Isotopic Distribution:

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<tr>
<td>C</td>
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</tr>
<tr>
<td>H</td>
<td>1.0000</td>
</tr>
<tr>
<td>N</td>
<td>1.0000</td>
</tr>
<tr>
<td>O</td>
<td>1.0000</td>
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</tbody>
</table>

Charge State: 1
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: H:\20140702-1\JC\jc560_000003.d
Method: Student_LCMS-140618
Sample Name: Student_4-6
Comment:

Acquisition Info
Acquisition Date: 2014-7-2 17:59:08
Operator: apex-Ultra
Instrument:

Acquisition Parameter
Polarity: Positive
Source: ESI
No. of Cell Fills: 1
Laser Power: 51.0 %
End Plate: 3500.0 V
Capillary Entrance: 4000.0 V
IMAGING Spot Diameter: 200.0 µm
Acquisition Mode: Single MS
Skimmer 1: 20.0 V
Drying Gas Temperature: 180.0 °C
Drying Gas Flow Rate: 4.0 L/min
Nebulizer Gas Flow Rate: 1.0 L/min
Calibration Date: Wed Jun 18 07:16:23
Data Acquisition Size: 351072
Apodization: Sine-Bell Multiplication

![Mass Spectrum Image]

<table>
<thead>
<tr>
<th>m/z</th>
<th>Formula</th>
<th>m/z [ppm]</th>
<th>err [ppm]</th>
<th>Mean err [ppm]</th>
<th>N-Rule</th>
<th>eV</th>
<th>Conf</th>
<th>mSiga</th>
<th>Std I</th>
<th>Std Mean m/z</th>
<th>Std VarN</th>
<th>Std Dev</th>
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<tbody>
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