Supplementary Information

PMA-SiO₂ mediated MCR in PEG-400: A greener aza-Friedel-Crafts reaction leading to 3-arylmethyl/diarylmethyl indoles

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General methods: Unless stated otherwise, solvents and chemicals were obtained from commercial sources and were used without further purification. Reactions were monitored by thin layer chromatography (TLC) on silica gel plates (60 F254), visualizing with ultraviolet light or iodine spray. Flash chromatography was performed on silica gel (230-400 mesh) using hexane and ethyl acetate. ^1H and ^{13}C NMR spectra were determined in DMSO- d_6 solution by using 400 or 100 MHz spectrometers, respectively. Proton chemical shifts (δ) are relative to tetramethylsilane (TMS, $\delta = 0.00$) as internal standard and expressed in ppm. Spin multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) as well as b (broad). Coupling constants (J) are given in hertz. Infrared spectra were recorded on a FT-IR spectrometer. Melting points were determined using melting point B-540 apparatus and are uncorrected. HRMS was determined using waters LCT premier XETOF ARE-047 apparatus.

Preparation of PMA-SiO₂:

To a solution of $\text{H}_3\text{PMo}_{12}\text{O}_{40}$ (1.0 g, 0.1 equiv by wt) in Methanol (50 mL) was added silica gel (9.0 g, 0.9 equiv by wt, 60-120 mesh), and the mixture was stirred at room temperature for 4-5 hr. Evaporation of methanol under reduced pressure gave a dry yellowish powder which contained 10% w/w of PMA.

Ref: Murugan, K.; Srimurugan, S.; Chen, C. *Chem. Commun.* **2010**, 46, 1127 (see the ESI)

General procedure for the preparation of 3-arylmethyl/diarylmethyl indoles (4):

A mixture of indole (**1**) (1.0 equiv), aldehyde (**2**) (1.2 equiv), *N,N*-dimethyl aniline (**3**) (1.3 equiv) and PMA-SiO₂ (15 mol%) in PEG-400 (4 mL) was stirred at 90-95 °C for time indicated in Table 2. After completion of the reaction, the mixture was cooled to room temperature, diluted with EtOAc (5 mL) and filtered. The filtrate was washed with water (10 mL) and the aqueous layer was extracted with EtOAc (2 x 5 mL). The organic layers were collected, combined, dried over anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using ethyl acetate-hexane to give the desired product.

Recovery and reuse of catalyst:

The filtered catalyst was washed with EtOAc (2 x 3 mL) and dried under vacuum at 60-65 °C for 4-5 h. This recovered catalyst was reused as mentioned in the main text.

4-((1*H*-Indol-3-yl) (phenyl) methyl)-*N*, *N*-dimethylaniline (1a)

White solid, mp: 161 – 162 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.92 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.28 - 7.07 (m, 9H), 6.97 (t, *J* = 8.0 Hz, 1H), 6.67- 6.58 (m, 3H), 5.58 (s, 1H), 2.91 (s, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 149.0, 144.6, 136.7, 132.1, 129.5 (2C), 128.9 (2C), 128.1 (2C), 127.1, 125.9, 123.9, 121.9 (2C), 120.0, 119.2, 112.5 (2C), 110.9, 47.8, 40.7 (2C); HRMS (ESI) ([*M*]⁺) calcd for C₂₃H₂₃N₂: 327.1861, found: 327.1861; IR (KBr): 3394, 3047, 2877, 1613, 1519, 1491, 1457, 799, 741, 697 cm⁻¹.

4-((4-Chlorophenyl) (1*H*-indol-3-yl) methyl)-*N*, *N*-dimethylaniline (4b)

Off white solid, mp: 130 – 132 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.94 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.23 - 7.21 (m, 3H), 7.18 - 7.14 (m, 3H), 7.05 (d, *J* = 8.4 Hz, 2H), 7.00 - 6.96 (m, 1H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.57 (s, 1H), 5.54 (s, 1H), 2.91 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 149.1, 143.2, 136.7, 131.6, 130.2 (2C), 129.4 (2C), 128.2 (2C), 126.9, 123.9, 122.0, 120.1 (2C), 119.9, 119.3, 112.5 (2C), 111.0, 47.2, 40.6 (2C); HRMS (ESI) ([*M*]⁺) calcd for C₂₃H₂₂N₂Cl: 361.1472, found: 361.1455; IR (KBr): 3413, 3054, 2962, 1612, 1517, 1486, 800, 740 cm⁻¹.

4-((4-Chlorophenyl) (1*H*-indol-3-yl) methyl)-*N*, *N*-diethyl aniline (4c)

Red solid, mp: 118 – 120 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (s, 1H), 7.35 - 7.33 (m, 1H), 7.25 - 7.13 (m, 6H), 7.02 - 6.98 (m, 3H), 6.60 - 6.58 (m, 3H), 5.52 (s, 1H), 3.31 (q, J = 8.0 Hz, 4H), 1.13 (t, J = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.4, 143.4, 136.7, 131.6, 130.2 (2C), 129.6 (2C), 128.2 (2C), 123.9 (2C), 122.0 (2C), 119.9, 119.3 (2C), 111.7 (2C), 110.9, 47.1, 44.2 (2C), 12.6 (2C) ; HRMS (ESI) ($[\text{M}]^+$) calcd for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{Cl}$: 389.1785, found: 389.1796; IR (KBr): 3433, 3052, 2928, 2863, 1608, 1559, 1457, 838, 802, 741, 695 cm^{-1} .

4-((1*H*-Indol-3-yl) (4-nitrophenyl) methyl)-*N*, *N*-dimethylaniline (4d)

Pale yellow solid, mp: 107–109 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.12 - 8.02 (m, 3H), 7.40 - 7.36 (m, 3H), 7.19 - 7.16 (m, 2H), 7.04 - 6.98 (m, 3H), 6.66 - 6.59 (m, 3H), 5.66 (s, 1H), 2.93 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 152.5, 149.3, 146.3, 136.7, 130.2, 129.6 (2C), 129.4 (2C), 126.6, 124.0, 123.4 (2C), 122.2, 119.6, 119.5, 119.0, 112.5 (2C), 111.1, 47.7, 40.5 (2C); HRMS (ESI) ($[\text{M}]^+$) calcd for $\text{C}_{23}\text{H}_{22}\text{N}_3\text{O}_2$: 372.1712, found: 372.1706; IR (KBr): 3411, 2852, 1612, 1517, 1455, 1417, 1343, 800, 742, 694 cm^{-1} .

4-((1*H*-Indol-3-yl) (4-methoxyphenyl) methyl)-*N*, *N*-dimethylaniline (4e)

White solid, mp: 162–164 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.92 (s, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.26 - 7.23 (m, 1H), 7.16 - 7.12 (m, 3H), 7.07 (d, J = 8.4 Hz, 2H), 6.98 (t, J = 8.0 Hz, 1H), 6.80 (d, J = 8.8 Hz, 2H), 6.67 (d, J = 8.4 Hz, 2H), 6.58 (s, 1H), 5.53 (s, 1H), 3.77 (s, 3H), 2.91 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.7, 148.9, 136.9, 136.7, 129.7 (2C), 129.4 (2C), 127.0, 123.8, 121.9, 121.0, 120.1 (2C), 119.2 (2C), 113.5 (2C), 112.6, 110.9, 55.1, 46.9, 40.7 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{24}\text{H}_{25}\text{N}_2\text{O}$: 357.1967, found: 357.1965; IR (KBr): 3410, 3163, 2962, 2851, 1608, 1508, 1459, 1218, 1169, 1098, 802, 762, 739, 629 cm^{-1} .

4-((2-Chlorophenyl)(1H-indol-3-yl)methyl)-N,N-dimethylaniline (4f)

Off-white solid, mp 152 - 154 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.96 (s, 1H), 7.39 - 7.34 (m, 3H), 7.22 - 7.10 (m, 6H), 7.00 - 6.98 (m, 1H), 6.7 - 6.56 (m, 3H), 6.02 (s, 1H), 2.94 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.0, 141.7, 136.7, 134.1, 130.5 (2C), 129.8 (2C), 129.4 (2C), 127.4, 126.9, 126.5, 124.1, 122.0, 119.8, 119.3, 113.2 (2C), 110.9, 44.2, 41.1 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{Cl}$: 361.1472, found: 361.1467; IR (KBr): 3411, 2816, 2720, 1593, 1383, 1349, 800, 766 cm^{-1} .

4-((4-(Dimethylamino) phenyl)(1H-indol-3-yl)methyl) benzonitrile (4g)

Brown solid, mp: 109 - 113 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.00 (s, 1H), 7.55 (d, J = 8.4 Hz, 2H), 7.37-7.34 (m, 3H), 7.19 - 7.16 (m, 2H), 7.05 - 6.99 (m, 3H), 6.67 (d, J = 8.8 Hz, 2H), 6.58 (s, 1H), 5.61 (s, 1H), 2.92 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 150.3, 149.2, 136.7, 132.0 (2C), 129.6 (2C), 129.4 (2C), 126.6, 124.0, 122.2 (2C), 119.6, 119.5, 119.2, 119.1, 112.6 (2C), 111.1, 109.7, 47.9, 40.6 (2C) ; HRMS (ESI) ($[\text{M}]^+ + 1$) calcd for $\text{C}_{24}\text{H}_{22}\text{N}_3$: 352.1814, found: 352.1801; IR (KBr): 3408, 2962, 2923, 2227, 1612, 1520, 1455, 860, 799, 743 cm^{-1} .

4-((4-Bromophenyl)(1H-indol-3-yl)methyl)-N,N-diethyl aniline (4h)

Pink solid, mp: 124-126 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (s, 1H), 7.37-7.33 (m, 3H), 7.24 - 7.10 (m, 4H), 7.01 - 6.96 (m, 3H), 6.59 (d, J = 8.0 Hz, 3H), 5.50 (s, 1H), 3.30 (q, J = 8.0 Hz, 4H), 1.13 (t, J = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.4, 143.9, 136.7, 131.1 (2C), 130.7 (2C), 130.1, 129.6 (2C), 126.9, 123.9, 122.0, 120.2, 119.9, 119.7, 119.3, 111.7 (2C), 110.9, 47.2, 44.2 (2C), 12.6 (2C); HRMS (ESI) ($[\text{M}]^+ + 1$) calcd for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{Br}$: 433.1279, found: 433.1293; IR (KBr): 3433, 3051, 2965, 2862, 1607, 1559, 1483, 838, 789, 741 cm^{-1} .

4-((1H-Indol-3-yl)(thiophen-2-yl)methyl)-N,N-dimethylaniline (4i)

Green solid, mp: 119 – 121 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.97 (s, 1H), 7.54 (d, J = 7.6 Hz, 1H), 7.34 (d, J = 8.4 Hz, 2H), 7.16 - 7.02 (m, 5H), 6.90 (d, J = 8.4 Hz, 1H), 6.79 (s, 1H), 6.68 (t, J = 8.0 Hz, 2H), 5.79 (s, 1H), 2.91 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.2, 136.5, 133.0, 129.2 (2C), 126.3 (2C), 125.4, 124.4, 123.8, 122.1, 121.5, 121.2, 113.0, 112.4 (2C), 108.9 (2C), 43.0, 40.9 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{S}$: 333.1425, found: 333.1409; IR (KBr): 3408, 2963, 2852, 1613, 1518, 1456, 806, 745 cm^{-1} .

4-(Furan-2-yl (1*H*-indol-3-yl) methyl)-*N,N*-dimethylaniline (4j)

Brown solid, mp: 138 - 142 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.97 (s, 1H), 7.35 (t, J = 8.0 Hz, 3H), 7.17 - 7.14 (m, 3H), 7.03 - 7.00 (m, 1H), 6.79 (s, 1H), 6.68 (d, J = 8.0 Hz, 2H), 6.29 - 6.27 (m, 1H), 5.97 (d, J = 4.0 Hz, 1H), 5.57 (s, 1H), 2.91 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.7, 149.3, 141.3, 136.4, 129.9, 128.9 (2C), 126.7, 123.1, 121.9, 119.6, 119.3, 118.1, 112.6 (2C), 110.9, 109.9, 106.8, 41.6, 40.7 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}$: 317.1654, found: 317.1643; IR (KBr): 3391, 2962, 2919, 1611, 1522, 1456, 800, $761, 741\text{ cm}^{-1}$.

4-((1*H*-Indol-3-yl) methyl)-*N,N*-dimethylaniline (4k)

White solid, mp: 144 - 146 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.92, (s, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.18 - 7.14 (m, 3H), 7.07 (t, J = 8.0 Hz, 1H), 6.89 (s, 1H), 6.69 (d, J = 8.8 Hz, 2H), 4.02 (s, 2H), 2.90 (s, 6H); ^{13}C NMR (400 MHz, CDCl_3) δ 149.0, 136.4, 129.4, 129.2 (2C), 127.5, 122.1, 121.8, 119.2 (2C), 116.7, 113.0 (2C), 110.9, 40.9 (2C), 30.4; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{17}\text{H}_{19}\text{N}_2$: 251.1548, found: 251.1552; IR (KBr): 3395, 2902, 2836, 1613, 1518, 1477, 808, $769, 743\text{ cm}^{-1}$.

4-((5-Bromo-1*H*-indol-3-yl)(phenyl)methyl)-*N,N*-dimethylaniline (4l)

Off White solid, mp: 132 - 134 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.97 (s, 1H), 7.38 (s, 1H), 7.26 - 7.11 (m, 7H), 7.05 (d, J = 8.8 Hz, 2H), 6.70 - 6.60 (m, 3H), 5.51 (s, 1H), 2.91 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.7, 144.2, 135.3, 133.0, 129.4 (2C), 129.1, 128.8 (2C), 128.2 (2C), 126.1, 125.1, 124.8, 122.4, 120.4, 113.0, 112.6 (2C), 112.4, 47.5, 40.7 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{Br}$: 405.0966, found: 405.0970; IR (KBr): 3412, 2962, 2925, 1613, 1517, 1453, 802, 760, 698 cm^{-1} .

4-((5-Bromo-1*H*-indol-3-yl) (4-(dimethylamino) phenyl) methyl) benzonitrile (4m)

Brown solid, mp: 148-150 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.04 (s, 1H), 7.56 (d, J = 8.0 Hz, 2H), 7.32 - 7.22 (m, 4H), 7.01 - 6.96 (m, 3H), 6.67 (d, J = 8.4 Hz, 2H), 6.58 (s, 1H), 5.55 (s, 1H), 2.93 (s, 6H); ^{13}C NMR (400 MHz, CDCl_3) δ 149.9, 149.4, 135.3, 132.1 (2C), 129.8, 129.5 (2C), 129.4 (2C), 125.2, 125.1, 124.8, 123.3, 122.1, 121.7, 118.9, 112.9, 112.6 (2C), 110.0, 47.6, 40.5 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{24}\text{H}_{21}\text{N}_3\text{Br}$: 430.0919, found: 430.0905; IR (KBr): 3402, 2962, 2923, 2227, 1606, 1520, 1456, 864, 799 cm^{-1} .

4-((5-Bromo-1*H*-indol-3-yl) (4-nitrophenyl) methyl)-*N,N*-dimethylaniline (4n)

Red solid, mp: 161 - 163 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.13 (d, J = 8.8 Hz, 2H), 8.06 (s, 1H), 7.37 - 7.33 (m, 3H), 7.26 - 7.23 (m, 2H), 7.01 (d, J = 8.0 Hz, 2H), 6.67 (d, J = 8.4 Hz, 2H), 6.60 (s, 1H), 5.60 (s, 1H), 2.93 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 152.0, 149.4, 146.4, 135.3, 129.7, 129.6 (2C), 129.4 (2C), 128.4, 125.3, 125.1, 123.6 (2C), 122.0 (2C), 118.8, 112.9, 112.6 (2C), 47.4, 40.5 (2C); HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{23}\text{H}_{21}\text{N}_3\text{O}_2\text{Br}$: 450.0817, found: 450.0800; IR (KBr): 3418, 2816, 2721, 1594, 1384, 1351, 768 cm^{-1} .

4-((5-Bromo-1H-indol-3-yl)methyl)-N,N-dimethylaniline (4o)

Off white solid, mp: 184 - 186 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.96 (s, 1H), 7.66 (s, 1H), 7.23 - 7.20 (m, 2H), 7.12 (d, J = 8.4 Hz, 2H), 6.90 (s, 1H), 6.69 (d, J = 8.8 Hz, 2H), 3.96 (s, 2H), 2.91 (s, 6H); ^{13}C NMR (400 MHz, CDCl_3) δ 149.1, 135.0, 129.2, 129.1 (2C), 128.8, 124.7, 123.3, 121.7, 116.4, 113.0 (2C), 112.5, 112.4, 40.9 (2C), 30.2; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{17}\text{H}_{18}\text{N}_2\text{Br}$: 329.0653, found: 329.0659; IR (KBr): 3228, 2962, 2851, 1610, 1516, 1448, 838, 797, 742 cm^{-1} .

N,N-Dimethyl-4-((1-methyl-1H-indol-3-yl)(phenyl)methyl)aniline (4p)

Off white solid, mp: 139-141 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.54 (d, J = 8.4 Hz, 1H), 7.28-7.14 (m, 6H), 7.09 - 6.96 (m, 3H), 6.72 - 6.66 (m, 3H), 6.42 (s, 1H), 5.57 (s, 1H), 3.69 (s, 3H), 2.90 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.9, 144.6, 137.4, 129.5, 128.9 (2C), 128.6, 128.5, 128.1 (2C), 127.4 (2C), 125.8, 121.4, 120.1, 119.0, 118.6, 112.6 (2C), 109.0, 47.8, 40.7 (2C), 32.5; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{24}\text{H}_{25}\text{N}_2$: 341.2018, found: 341.2007; IR (KBr): 3024, 2921, 2850, 1614, 1566, 1472, 800, 739 cm^{-1} .

4-((4-Bromophenyl) (1-methyl-1H-indol-3-yl) methyl)-N, N-dimethylaniline (4q)

Brown gum; ^1H NMR (400 MHz, CDCl_3): δ 7.55-7.53 (m, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.33-6.97 (m, 6H), 6.95-6.65 (m, 3H), 6.40 (s, 1H), 5.52 (s, 1H), 3.69 (s, 3H), 2.90 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.7, 143.5, 137.4, 137.2, 131.2 (2C), 130.4 (2C), 128.2, 127.2, 126.9, 121.5 (2C), 119.8 (2C), 118.7 (2C), 118.5, 117.6, 109.1, 47.8, 39.5 (2C), 32.6 ; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{24}\text{H}_{24}\text{N}_2\text{Br}$: 419.1123, found: 419.1117; IR (KBr): 3028, 2920, 1607, 1559, 1456, 803, 789, 741 cm^{-1} .

4-((2-Chlorophenyl) (4-methyl-1H-indol-3-yl) methyl)-N, N-diethyl aniline (4r)

Pale yellow gum; ^1H NMR (400 MHz, CDCl_3): δ 7.92 (s, 1H), 7.35 (d, $J = 8.0$ Hz, 1H), 7.14 (m, 3H), 7.09 - 6.94 (m, 4H), 6.75 (d, $J = 8.0$ Hz, 1H), 6.59 (d, $J = 8.0$ Hz, 2H), 6.45 (s, 1H), 6.20 (s, 1H), 3.30 (q, $J = 6.8$ Hz, 4H), 2.35 (s, 3H), 1.13 (t, $J = 6.8$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.3, 143.4, 137.2, 133.9, 131.3, 130.7, 130.0 (2C), 129.4, 127.2, 126.4, 125.6, 124.8, 122.1, 122.0, 121.0, 120.4, 111.7 (2C), 108.8, 45.5, 44.2 (2C), 19.7, 12.6 (2C) ; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{26}\text{H}_{28}\text{N}_2\text{Cl}$: 403.1941, found: 403.1923; IR (KBr): 3408, 3051, 2966, 2868, 1611, 1567, 1463, 805, 772, 748, 701, 671 cm^{-1} .

***N,N*-Dimethyl-4-((4-methyl-1*H*-indol-3-yl) (thiophen-2-yl) methyl) aniline (4s)**

White solid, mp: 111 - 113 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ 7.94 (s, 1H), 7.20 - 7.14 (m, 2H), 7.09 - 6.99 (m, 3H), 6.89 - 6.62 (m, 6H), 6.08 (s, 1H), 2.92 (s, 6H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 150.6, 149.2, 136.9, 133.0, 131.1, 129.2 (2C), 126.3, 125.4, 124.2, 123.8, 122.1, 121.5, 121.2, 113.0, 112.4 (2C), 108.9, 43.7, 40.6 (2C), 20.2 ; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{22}\text{H}_{23}\text{N}_2\text{S}$: 347.1582, found: 347.1574; IR (KBr): 3411, 3052, 2916, 1612, 1518, 1436, 813, 766, 743, 715 cm^{-1} .

***N,N*-Dimethyl-4-(3-methyl-1-(4-methyl-1*H*-indol-3-yl) butyl) aniline (4t)**

Pale yellow oil; ^1H NMR (400 MHz, CDCl_3): δ 7.98 (s, 1H), 7.17 (d, $J = 7.6$ Hz, 1H), 7.08 - 6.98 (m, 4H), 6.74 (d, $J = 7.2$ Hz, 1H), 6.65 (d, $J = 8.8$ Hz, 2H), 4.53 (t, $J = 8.0$ Hz, 1H), 2.88 (s, 6H), 2.59 (s, 3H), 2.24-2.18 (m, 2H), 1.93-1.88 (m, 1H), 1.01 - 0.86 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.7, 136.7, 135.0, 131.0, 128.5 (2C), 125.8, 121.7, 121.5, 121.4, 121.0, 112.8 (2C), 108.8, 47.9, 40.8 (2C), 39.8, 25.6, 22.9, 22.5, 20.9; HRMS (ESI) ($[\text{M}]^+1$) calcd for $\text{C}_{22}\text{H}_{29}\text{N}_2$: 321.2331, found: 321.2318; IR (KBr): 3413, 2962, 2920, 1614, 1525, 801, 743 cm^{-1} .

Copies of spectra

TDC-119 0035/IND01/005/1 in CDCl₃
¹³C NMR

NMR-400MHz
 AR.No: ME1213/1831
 Analyst: Haribabu
 Date: 20th Dec.2013

NUCLEUS : C13
 FREQ (MHz): 100.625
 PULP : zgpg30

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-30 N: 0-2 Cl: 0-1

B035/INDO1/005

14016002 13 (0.365) Cm (9:14-21:28)

1: TOF MS ES+
7.43e+003

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
327.1861	327.1861	0.0	0.0	13.5	1.6	C23 H23 N2

TDC-119 B035/IND01/006 in CDCl₃

NMR-400MHz

AN.No: ME0114/1610

Analyst: Haribabu

Date: 23rd Jan.2014

NUCLEUS : H1
FREQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-006 in CDC13

NMR-400MHz

AR.No: ME0114/1728

Analyst: Haribabu

Date: 23rd Jan.2014

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-1 Br: 0-1

B035/INDO1/006(114020403)

140211002 4 (0.121) Cm (4-3)

1: TOF MS ES+
3.50e+002

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
405.0970	405.0966	0.4	1.0	13.5	3.8	C23 H22 N2 Br

TDC-119 B035-IN001-007 in CDC13

NMR-400MHz

AR.No: ME1213/1664

Analyst: Ganesh

Date: 19th Dec.2013

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

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TDC-119 B035/IND01/007 in CDCl₃
13C NMR

NMR-400MHZ
AR.No: ME1213/1830
Analyst: Haribabu
Date: 20th Dec.2013

NUCLEUS : C13
PRQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 Cl: 0-2 I: 0-1

B035/IND01/007

140102031 28 (0.747) Cm (28-44)

1: TOF MS ES+
2.04e+004

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
361.1455	361.1472	-1.7	-4.7	13.5	1.8	C23 H22 N2 Cl

TDC-119 B035/IND01/009 in CDCl3

NMR-400MHz

AR.No: ME1213/2128

Analyst: Haribabu

Date: 26th Dec.2013

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035/IND01/009 in CDCl₃
13C NMR

NMR-400MHz

AR.No: ME0114/788

Analyst: Haribabu

Date: 09th Jan.2014

NUCLEUS : C13
PULPROG : zgpg30
FREQ (MHz): 100.625
EXP : s2pul

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-30 N: 0-2 Cl: 0-1

B035/INDO1/009

14016001 7 (0.191) Cm (6:8-22:30)

1: TOF MS ES+
3.70e+004

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
389.1796	389.1785	1.1	2.8	13.5	2.5	C25 H26 N2 Cl

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TDC-119 B035-IND01-011A in CDCl3

DMR-400MHz
AR.No: ME1213/2410
Analyst: Ganesh
Date: 30th Dec.2013

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-011A 1n CDC13

NMR-400MHz

AR.No: ME0114/265

Analyst: Haribabu

Date: 03rd Jan.2014

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

51 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-30 N: 0-4 O: 0-2 Cl: 0-1

B035/INDO1/011A

14016003 7 (0.192) Cm (7:12-18:26)

1: TOF MS ES+
4.50e+004

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1706	372.1712	-0.6	-1.6	14.5	3.4	C ₂₃ H ₂₂ N ₃ O ₂

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TDC-119 B035/IND01/012A in CDCl₃

NMR-400MHz

AR.No: ME0114/18

Analyst: Haribabu

Date:02nd Jan.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-012A in CDC13

NMR-400MHz

AR.No: ME0114/259

Analyst: Ganesh

Date: 03rd Jan. 2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

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Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-2

B035/INDO1/012A

14016007 14 (0.385) Cm (9:14:21:40)

1: TOF MS ES+
7.13e+003

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
357.1965	357.1967	-0.2	-0.6	13.5	0.1	C24 H25 N2 O

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TDC-119 B035-IND01-012B 1a CDCl3

NMR-400MHz
AR.No: ME1213/2508
Analyst:Haribabu
Date: 30th Dec.2013

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035/IND01/012B in CDCl₃
13C NMR

NMR-400MHz
AR.No: ME0114/787
Analyst: Haribabu
Date: 09th Jan.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

142 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-2 Cl: 0-2 I: 0-1

1: TOF MS ES+
1.98e+004

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
361.1467	361.1472	-0.5	-1.4	13.5	1.4	C23 H22 N2 Cl

TDC-119 B035-IND01-012C in CDCl3

NMR-400MHz

AR.No: ME1213/2409

Analyst: Ganesh

Date: 30th Dec.2013

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-012C in CDCl₃

NMR-400MHz

AR.No: ME0114/264

Analyst: Haribabu

Date: 03rd Jan.2014

NUCLEUS : C13

FRQ (MHz): 100.63

EXP : s2pul

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

178 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-2 79Br: 0-3 I: 0-1

B035/INDO1/012C

140102034 18 (0.492) Cm (18:21-41:42)

1: TOF MS ES+
1.21e+005

Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
450.0800	450.0817	-1.7	-3.8	14.5	12.1	C23 H21 N3 O2 79Br

TDC-119 B035-IND01-014A in CDCl3

NMR-400MHz

AR.No: ME1213/2507

Analyst: Haribabu

Date: 30th Dec. 2013

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-014A 1n CDC13

NMR-400MHz
AR.No: ME0114/263
Analyst: Haribabu
Date: 03rd Jan.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3

B035/IND01/014A

140102035 21 (0.580) Cm (21-29:31)

1: TOF MS ES+
4.19e+004

Minimum:						
Maximum:		5.0	5.0	-5.0		
				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
352.1801	352.1814	-1.3	-3.7	15.5	26.5	C ₂₄ H ₂₂ N ₃

TDC-119 B035/IND01/014B in CDCl₃

NMR-400MHz

AR.No: ME0214/631

Analyst: Haribabu

Date: 07th Feb. 2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-014B in CDCl₃
13C NMR

NMR-400MHz
AR.No: ME0214/749
Analyst: Haribabu
Date: 07th Feb.2014

NUCLEUS : C13
PQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 S: 0-1

B035/INDO1/014B(114020404)

140211003 21 (0.670) Cm (19:21-25:28)

1: TOF MS ES+
1.24e+003

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
333.1409	333.1425	-1.6	-4.8	12.5	3.2	C21 H21 N2 S

TDC-119 B035/IND01/014C in CDCl₃

NMR-400MHz

AR.No: ME0114/951

Analyst: Haribabu

Date: 13th Jan.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-014C 1n CDC13

NMR-400MHz

AR.No: ME0114/1242

Analyst: Ganesh

Date: 19th Jan.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

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Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-1

B035/INDO1/014C(114020405)

140211004 19 (0.593) Cm (19:20-25:30)

1: TOF MS ES+
1.52e+003

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
317.1643	317.1654	-1.1	-3.5	12.5	1.0	C21 H21 N2 O

TDC-119 B035/IND01/015A in CDCl₃

NMR-400MHz

AR.No: ME0114/17

Analyst: Haribabu

Date:02nd Jan.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-015-A in CDCl₃

NMR-400MHZ

AR.No: ME0514/1317

:Analyst Haribabu

Date:14th May.2014

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-30 N: 0-4

B035/INDO1/015A

14016006 12 (0.319) Cm (9:13-24:33)

1: TOF MS ES+
3.70e+003

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
251.1552	251.1548	0.4	1.6	9.5	0.6	C17 H19 N2

TDC-119 B035-IND01-015B 1n CDC13

NMR-400MHz

AR.No: ME0114/173

Analyst: Ganesh

Date: 03rd Jan.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035/IND01/015B in CDCl₃
13C NMR

NMR-400MHz

AR.No: ME0114/786

Analyst: Haribabu

Date: 09th Jan.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-30 N: 0-4 Br: 0-1

B035/MND01/015B

14016005 7 (0.191) Cm (6:9-19:24)

1: TOF MS ES+
3.41e+004

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
433.1293	433.1279	1.4	3.2	13.5	1.3	C ₂₅ H ₂₆ N ₂ Br

TDC-119 B035/IND01/016A 1n CDCl3

NMR-400MHz

AR.No: ME0114/283

Analyst: Haribabu

Date: 06th Jan.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-016A in CDCl₃

NMR-400MHz

AR.No: ME0514/1460

Analyst: Haribabu

Date:15th May.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-30 N: 0-4 Br: 0-1

B035/IND01/016A

14016004 7 (0.191) Cm (5.8-21.44)

1: TOF MS ES+
3.26e+003

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
329.0659	329.0653	0.6	1.8	9.5	24.2	C17 H18 N2 Br

TDC-119 B035/IND01/016B in CDCl3

NMR-400MHz

AR.No: ME0114/1894

Analyst: Haribabu

Date: 27th Jan.2014

NUCLEUS : H1
FREQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-016B in CDCl₃
13C NMR

NMR-400MHz

AR.No: ME0214/754

Analyst: Haribabu

Date: 07th Feb.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-3 O: 0-1 Br: 0-1

B035/IND01/018B(114020408)

140211011 5 (0.173) Cm (5:8)

1: TOF MS ES+
1.30e+003

Minimum:

Maximum: 5.0 5.0 -5.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
430.0905	430.0919	-1.4	-3.3	15.5	5.5	C24 H21 N3 Br

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TDC-119 B035/IND01/018 in CDCl₃

NMR-400MHz

AR.No: ME0214/633

Analyst: Haribabu

Date: 07th Feb.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-INDOL-018 in CDCl₃
13C NMR

NMR-400MHz
AR.No: ME0214/751
Analyst: Haribabu
Date: 07th Feb.2014

NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2

B035/IND01/018

140218001 14 (0.445) Cm (14:18-24:29)

1: TOF MS ES+
3.81e+005

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
341.2007	341.2018	-1.1	3.2	12.5	73.7	C24 H25 N2

TDC-119 B035/IND01/020B/Pure in CDCl3

NMR-400MHz

AR.No: ME0114/2115

Analyst: Haribabu

Date: 29th Jan.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-020B-1 in CDCl3

NMR-400MHz

AR.No: ME0114/1842

Analyst: Saribabu

Date: 24th Jan.2014

NUCLEUS : C13
FREQ (MHz): 100.63
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-2 Br: 0-1

B035/INDO1/020(B)

140218005 20 (0.617) Cm (20:22-27:37)

1: TOF MS ES+
3.64e+002

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
419.1117	419.1123	-0.6	-1.4	13.5	8.4	C ₂₄ H ₂₄ N ₂ Br

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TDC-119 B035/IND01/021 in CDCl3

NMR-400MHz
AR.No: ME0214/1969
Analyst: Haribabu
Date:24th Feb.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-021 in CDCl₃

NMR-400MHz

AR.No: ME0314/697

Analyst: Ganesh

Date:07th March.2014

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-2

B035/INDO1/021

140219002 12 (0.369) Cm (9:12-(26:35+1:2))

1: TOF MS ES+
6.05e+003

Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
321.2318	321.2331	-1.3	-4.0	9.5	16.7	C22 H29 N2

TDC-119 B035-IND01-026A

in

CDCl₃

NMR-400MHz

AR.No: ME0214/155

Analyst: Haribabu

Date: 03rd Feb.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-026A 1n CDCl3

NMR-400MHz

AR.No: ME0214/732

Analyst: Haribabu

Date: 07th Feb. 2014

NUCLEUS : C13
PQQ (MHz): 100.65
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

26 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-1 Cl: 0-1

B035/INDO1/026A(114020406)

140211008 19 (0.593) Cm (17:19-33:43)

1: TOF MS ES+
4.95e+002

Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
403.1923	403.1941	-1.8	-4.5	13.5	4.1	C26 H28 N2 Cl

TDC-119 B035-IND01-026B in CDCl₃

NMR-400MHz
AR.No: ME0214/410
Analyst: Ganesh
Date: 05th Feb.2014

NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul

TDC-119 B035-IND01-026B in CDCl₃
¹³C NMR

NMR-400MHz
 AR.No: ME0214/753
 Analyst: Haribabu
 Date: 07th Feb.2014

NUCLEUS : C13
 FRQ (MHz) : 100.63
 EXP : s2pul

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-2 O: 0-1 S: 0-1

B035/INDO1/026B(114020407)

140211009 20 (0.617) Cm (19.20-29.35)

1: TOF MS ES+
8.22e+002

Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
347.1574	347.1582	-0.8	-2.3	12.5	n/a	C22 H23 N2 S