Diversity Oriented Approach to Triazole Based Peptidomimetics by Click Chemistry as Mammalian Sterile 20 Kinase Inhibitors
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General Experimental:

All the reactions were monitored by employing TLC technique using appropriate solvent system for development. Reactions involving air/oxygen sensitive reagents or catalysts were performed in degassed solvents. Transfer of moisture sensitive materials were carried out in a glove box, using standard syringe-septum techniques and the reactions were maintained under nitrogen atmosphere until the work up. Yields reported are isolated yields of the materials. All the commercial reagents were used as such without further purification. Infrared (IR) spectra were recorded on Nicolet Impact-400 FT IR spectrometer in KBr. Proton Nuclear Magnetic Resonance (400 MHz, ¹H NMR) spectra and Carbon Nuclear Magnetic Resonance (100 MHz, ¹³C NMR) spectra were recorded on Bruker/ Varian spectrometers. The high-resolution mass measurements were carried out using Micromass Q-Tof spectrometer. Melting points were recorded on Buchi B-545.

Preparation of compound (2)

According to the general procedure, alkyne 1a (50 mg, 0.16 mmol), phenylazide (18.2 mg, 0.16 mmol), Cu(OAc)₂ (3.2 mg, 0.02 mmol) and sodium ascorbate (6.26 mg, 0.03 mmol) in tBuOH/H₂O (3:3 mL) was stirred at rt for 23 h. The crude mixture was purified by column
chromatography (100% ethyl acetate) to give the desired compound 2 (66 mg, 97%) as a white solid.

**R_f**: 0.20 (80% ethyl acetate/petroleum ether).

**Mp**: 176-178 °C.

**1H NMR (400 MHz, CDCl_3)**: δ = 2.01 (s, 3H), 3.01-3.29 (m, 3H), 3.31-3.60 (m, 1H), 3.63 (s, 3H), 4.73-4.86 (m, 2H), 7.02 (d, J = 7.5 Hz, 1H), 7.06-7.10 (m, 2H), 7.16 (d, J = 8.1 Hz, 1H), 7.18-7.29 (m, 3H), 7.41-7.43 (m, 1H), 7.55-7.64 (m, 2H), 7.67-7.70 (m, 2H), 7.77 (s, 1H) ppm.

**13C NMR (100 MHz, CDCl_3)**: δ = 23.4, 27.5, 37.8, 52.4, 52.8, 53.3, 120.6, 121.1, 127.3, 128.7, 128.9, 129.4, 129.9, 135.9, 137.1, 144.2, 170.6, 170.9, 171.7 ppm.

**I.R. (KBr)**: 1542.4, 1648.2, 1735.4, 2926.5, 3306.2 cm⁻¹.

**HRMS (Q-Tof) m/z**: Calcd. C_{23}H_{26}N_{5}O_{4} [M+H]^+ 436.1985, found: 436.1976.

**[α]_D^{25}**: - 10.0 (c = 0.15, CHCl_3).

**Preparation of compound (3)**

According to the general procedure, alkyne 1a (20 mg, 0.06 mmol), o-nitrophenylazide (9.8 mg, 0.06 mmol), Cu(OAc)$_2$ (1.2 mg, 0.006 mmol) and sodium ascorbate (2.4 mg, 0.01 mmol) in tBuOH/H$_2$O (3:3 mL) was stirred at rt for 20 h. The crude mixture was purified by column chromatography (50% ethyl acetate/petroleum ether) to give the compound 3 (25.2 mg, 82%) as a white solid.

**R_f**: 0.65 (80% ethyl acetate/petroleum ether).

**Mp**: 197-199 °C.

**1H NMR (400 MHz, CDCl_3)**: δ = 2.02 (s, 3H), 3.02-3.15 (m, 3H), 3.32-3.37 (m, 1H), 3.67 (s, 3H), 4.74-4.79 (m, 1H), 4.81-4.85 (m, 1H), 6.81 (d, J = 7.6 Hz, 1H), 6.92 (d, J = 7.8 Hz, 1H), 7.09-7.19 (m, 2H), 7.20-7.28 (m, 3H), 7.62-7.64 (m, 2H), 7.67 (s, 1H), 7.70-7.81 (m, 1H), 8.07-8.09 (m, 1H) ppm.

**13C NMR (100 MHz, CDCl$_3$+CD$_3$OD)**: δ = 22.5, 27.7, 37.5, 52.4, 53.5, 124.3, 125.5, 127.1, 127.9, 128.7, 129.2, 130.0, 130.9, 133.9, 136.0, 143.6, 144.4, 170.7, 171.5, 171.9 ppm.

**I.R. (KBr)**: 1263.7, 1656.7, 1736.5, 2930.0, 3291.8 cm⁻¹.

**HRMS (Q-Tof) m/z**: Calcd. C_{23}H_{25}N_{5}O_{6} [M+H]^+ 481.1836, found: 481.1830.

**[α]_D^{25}**: -9.900 (c = 0.12, CH$_3$OH).
Preparation of compound (4)

According to the general procedure, alkyne 1a’ (20.0 mg, 0.06 mmol), o-nitrophenylazide (9.8 mg, 0.06 mmol), Cu(OAc)$_2$ (1.2 mg, 0.006 mmol) and sodium ascorbate (2.4 mg, 0.01 mmol) in $^t$BuOH/H$_2$O (3:3 mL) was stirred at rt for 20 h. The crude mixture was purified by column chromatography (50% ethyl acetate/ petroleum ether) to give the compound 4 (27.1 mg, 88%) as a white solid.

$R_f$: 0.50 (60% ethyl acetate/ petroleum ether).

$M_p$: 175-177 °C.

$^1$H NMR (400 MHz, CD$_3$OD): $\delta$ = 1.93 (s, 3H), 2.99-3.27 (m, 4H), 3.65 (s, 3H), 4.65-4.69 (m, 1H), 4.74-4.78 (m, 1H), 7.18-7.19 (m, 3H), 7.20-7.28 (m, 2H), 7.75-7.80 (m, 2H), 7.82-7.91 (m, 1H), 8.09 (s, 1H), 8.13-8.15 (m, 1H) ppm.

$^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ = 22.6, 28.9, 38.4, 52.8, 54.0, 55.4, 125.9, 126.7, 128.0, 128.9, 129.6, 130.4, 131.3, 132.4, 135.3, 138.0, 145.2, 146.1, 172.8, 173.3, 173.3 ppm.

I.R. (KBr): 1449.5, 1663.3, 1742.6, 2942.2, 3403.8 cm$^{-1}$.

HRMS (Q-Tof) $m/z$: Calcd. C$_{23}$H$_{25}$N$_6$O$_6$ [M+H]$^+$ 481.1836, found: 481.1826.

[a]$^D_{25}$: -4.043 (c = 0.14, CH$_3$OH).

Preparation of compound (5)

According to the general procedure, alkyne 1a’ (20 mg, 0.06 mmol), m-nitrophenylazide (9.8 mg, 0.06 mmol), Cu(OAc)$_2$ (1.2 mg, 0.006 mmol) and sodium ascorbate (2.4 mg, 0.01 mmol) in $^t$BuOH/H$_2$O (3:3 mL) was stirred at rt for 24 h. The crude mixture was purified by column chromatography (70% ethyl acetate/ petroleum ether) to give the compound 5 (22.3 mg, 72%) as a white solid.

$R_f$: 0.50 (80% ethyl acetate/ petroleum ether).

$M_p$: 193-195 °C.

$^1$H NMR (400 MHz, DMSO): $\delta$ = 1.81 (s, 3H), 2.90-3.02 (m, 3H), 3.03-3.13 (m, 1H), 3.51 (s, 3H), 4.42-4.48 (m, 1H), 4.63-4.68 (m, 1H), 7.18-7.26 (m, 5H), 7.89 (t, $J = 8.2$ Hz, 1H), 8.16-8.18 (m, 1H), 8.30-8.36 (m, 2H), 8.50-8.52 (m, 1H), 8.64-8.68 (m, 2H) ppm.

$^{13}$C NMR (100 MHz, DMSO): $\delta$ = 22.5, 28.2, 36.5, 51.8, 51.9, 53.7, 114.5, 121.7, 122.7, 125.9, 126.6, 128.2, 128.3, 19.1, 129.2, 131.7, 137.0, 137.3, 144.5, 148.6, 169.3, 170.8, 171.8 ppm.

I.R. (KBr): 1408.3, 1642.4, 2945.0, 3398.9 cm$^{-1}$. 
HRMS (Q-Tof) m/z:  Calcd. C_{23}H_{25}N_{6}O_{6} [M+H]^+ 481.1836, found: 481.1851.
[α]_D^{25}: 2.320 (c = 0.17, DMSO).

**Preparation of compound (6)**

According to the general procedure, alkyne 1a’ (11.2 mg, 0.03 mmol), p-nitrophenylazide (5.8 mg, 0.03 mmol), Cu(OAc)\(_2\) (0.7 mg, 0.003 mmol) and sodium ascorbate (1.4 mg, 0.006 mmol) in \(^t\)BuOH/H\(_2\)O (3:3 mL) was stirred at rt for 22 h. The crude mixture was purified by column chromatography (60% ethyl acetate/ petroleum ether) to give compound 6 (12.3 mg, 70%) as a white solid.

\(R_f\) : 0.32 (80% ethyl acetate/ petroleum ether).

Mp: 254-256 °C.

\(^1\)H NMR (400 MHz, DMSO): \(\delta = 1.85\) (s, 3H), 2.93-3.08 (m, 3H), 3.15-3.20 (m, 1H), 3.57 (s, 3H), 4.51-4.56 (m, 1H), 4.70-4.73 (m, 1H), 7.18-7.27 (m, 5H), 8.10-8.17 (m, 4H), 8.43 (d, \(J = 8.9\) Hz, 2H), 8.58 (s, 1H) ppm.

\(^{13}\)C NMR (100 MHz, DMSO): \(\delta = 22.4, 28.0, 36.7, 51.7, 53.4, 53.5, 120.1, 121.3, 125.3, 126.4, 128.1, 128.9, 136.8, 141.0, 144.7, 146.5, 169.5, 170.7, 171.6\) ppm.

I.R. (KBr): 1408.1, 1652.6, 1742.1, 2950.5, 3393.0 cm\(^{-1}\).

HRMS (Q-Tof) m/z:  Calcd. C_{23}H_{25}N_{6}O_{6} [M+H]^+ 481.1836, found: 481.1856.
[α]_D^{25}: -35.444 (c = 0.09, DMSO).

**Preparation of compound (7)**

According to the general procedure, alkyne 1b (40 mg, 0.09 mmol), p-chlorophenylazide (14.3 mg, 0.09 mmol), Cu(OAc)\(_2\) (1.8 mg, 0.009 mmol) and sodium ascorbate (3.7 mg, 0.02 mmol) in \(^t\)BuOH/H\(_2\)O (3:3 mL) was stirred at rt for 10 h. The crude mixture was purified by column chromatography (100% ethyl acetate) to give the compound 7 (53.5 mg, 100%) as a white solid.

\(R_f\) : 0.29 (80% ethyl acetate/ petroleum ether).

Mp: 238-240 °C.

\(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta = 2.03\) (s, 3H), 2.94-3.15 (m, 3H), 3.32-3.33 (m, 1H), 3.70 (s, 3H), 4.69-4.71 (m, 1H), 4.78-4.79 (m, 1H), 6.78 (d, \(J = 8.0\) Hz, 2H), 6.97 (d, \(J = 7.6\) Hz, 1H), 7.28 (s, 1H), 7.51 (d, \(J = 8.8\) Hz, 2H), 7.56 (d, \(J = 7.6\) Hz, 2H), 7.67 (d, \(J = 8.4\) Hz, 2H), 7.88 (s, 1H) ppm.
$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ = 22.8, 27.7, 37.1, 48.7, 49.2, 49.4, 49.6, 49.8, 50.0, 52.5, 52.5, 53.4, 92.6, 120.9, 121.7, 130.0, 131.3, 134.7, 135.5, 135.7, 137.7, 144.3, 170.9, 171.3, 171.6 ppm.

I.R. (KBr): 1540.6, 1650.2, 1740.5, 2930.6, 3300.6 cm$^{-1}$.

HRMS (Q-Tof) m/z: Calcd. C$_{23}$H$_{24}$N$_5$O$_4$ClI [M+H]$^+$ 596.0562, found: 596.0566.

$[\alpha]_D^{25}$: 35.489 (c = 0.145, CHCl$_3$).

**Preparation of compound (8)**

According to the general procedure, alkyne 1b (20 mg, 0.05 mmol), p-nitrophenylazide (7.6 mg, 0.05 mmol), Cu(OAc)$_2$ (1 mg, 0.005 mmol) and sodium ascorbate (2 mg, 0.01 mmol) in $^t$BuOH/H$_2$O (3:3 mL) was stirred at rt for 22 h. The crude mixture was purified by column chromatography (80% ethyl acetate/ petroleum ether) to give the dipeptide 8 (22 mg, 80%) as a white solid.

$R_f$: 0.40 (100% ethyl acetate)

**Mp:** 277-279 °C

$^1$H NMR (400 MHz, DMSO): $\delta$ = 1.75 (s, 3H), 2.78-2.94 (m, 4H), 3.46 (s, 3H), 4.37-4.42 (m, 1H), 4.56-4.62 (m, 1H), 6.96 (d, $J$ = 8.2 Hz, 2H), 7.35 (d, $J$ = 8.2 Hz, 2H), 8.10-8.13 (m, 3H), 8.40-8.45 (m, 3H), 8.60 (s, 1H) ppm.

$^{13}$C NMR (100 MHz, DMSO): $\delta$ = 22.4, 28.1, 35.9, 51.8, 51.9, 53.2, 92.5, 120.3, 121.6, 125.6, 131.6, 136.9, 140.9, 144.6, 146.6, 169.2, 170.7, 171.4 ppm.

I.R. (KBr): 1437.7, 1652.6, 2824.1, 3429.0 cm$^{-1}$.

HRMS (Q-Tof) m/z: Calcd. C$_{23}$H$_{24}$N$_6$O$_6$I [M+H]$^+$ 607.0802, found 607.0787.

$[\alpha]_D^{25}$: 1.733 (c = 0.06, DMSO).

**Preparation of compound (9)**

According to the general procedure, alkyne 1b (20 mg, 0.05 mmol), m-nitrophenylazide (7.6 mg, 0.05 mmol), Cu(OAc)$_2$ (1 mg, 0.005 mmol) and sodium ascorbate (2 mg, 0.01 mmol) in $^t$BuOH/H$_2$O (3:3 mL) was stirred at rt for 9 h. The crude mixture was purified by column chromatography (50% ethyl acetate/ petroleum ether) to give the compound 9 (21 mg, 76%) as a white solid.

$R_f$: 0.48 (60% ethyl acetate/ petroleum ether).

**Mp:** 148-149 °C.
**1H NMR (400 MHz, DMSO):** \( \delta = 1.81 \) (s, 3H), 2.89-2.98 (m, 3H), 3.07-3.12 (m, 1H), 3.52 (s, 3H), 4.42-4.48 (m, 1H), 4.62-4.67 (m, 1H), 7.01 (d, \( J = 8.1 \) Hz, 2H), 7.58 (d, \( J = 8.1 \) Hz, 2H), 7.90 (t, \( J = 8.2 \) Hz, 1H), 8.15 (d, \( J = 8.2 \) Hz, 1H), 8.31-8.37 (m, 2H), 8.48 (d, \( J = 7.5 \) Hz, 1H), 8.67-8.68 (m, 2H) ppm.

**13C NMR (100 MHz, DMSO):** \( \delta = 22.7, 28.3, 36.2, 52.2, 52.3, 53.6, 92.8, 114.8, 122.0, 123.3, 126.2, 131.9, 132.0, 137.1, 137.3, 137.5, 144.7, 148.8, 169.9, 171.1, 171.8 \) ppm.

**I.R. (KBr):** 1437.6, 1660.1, 3422.1 cm\(^{-1}\).

**HRMS (Q-Tof) m/z:** Calcd. C\(_{23}\)H\(_{24}\)N\(_6\)O\(_6\)I [M+H]\(^+\) 607.0802, found 607.0789.

**[\(\alpha\)]\(^D\)\(_{25}\):** 2.672 (c = 0.11, DMSO).

### Preparation of compound (11)

According to the general procedure, alkyne 10 (30 mg, 0.09 mmol), \( p \)-methoxyphenyl azide (27.9 mg, 0.19 mmol), Cu(OAc)\(_2\) (3.7 mg, 0.02 mmol) and sodium ascorbate (7.4 mg, 0.04 mmol) in \(^t\)BuOH/H\(_2\)O (3:3 mL) was stirred at rt for 24 h. The crude mixture was purified by column chromatography (100% ethyl acetate) to give the compound 11 (57 mg, 99%) as a white solid.

**R\(_f\):** 0.16 (100% ethyl acetate).

**M.p:** 210-213 °C.

**1H NMR (400 MHz, CDCl\(_3\)):** \( \delta = 0.88-0.92 \) (m, 6H), 1.57-1.64 (m, 2H), 2.07 (bs, 1H), 2.08 (s, 3H), 3.40-3.68 (m, 4H), 3.69 (s, 3H), 3.87 (s, 6H), 4.41-4.43 (m, 1H), 7.00-7.02 (m, 4H), 7.35 (bs, 1H), 7.64-7.70 (m, 4H), 8.04 (s, 1H), 8.08 (s, 1H), 8.19 (d, \( J = 6.8 \) Hz, 1H) ppm.

**13C NMR (100 MHz, CDCl\(_3\)):** \( \delta = 20.8, 21.9, 22.9, 24.6, 25.1, 30.6, 31.1, 40.9, 51.8, 52.3, 55.8, 64.0, 114.8, 114.9, 122.1, 122.1, 122.5, 122.7, 130.6, 130.7, 142.9, 142.4, 159.9, 159.9, 172.3, 172.4, 173.6 \) ppm.

**I.R. (KBr):** 1685.1, 1736.3, 2928.7, 3054.7 cm\(^{-1}\).

**HRMS (Q-Tof) m/z:** Calcd. C\(_{31}\)H\(_{39}\)N\(_8\)O\(_6\) [M+H]\(^+\) 619.2993, found: 619.2994.

**[\(\alpha\)]\(^D\)\(_{25}\):** - 7.494 (c = 0.17, CHCl\(_3\)).

### Preparation of compound (12)

According to the general procedure, alkyne 10 (40 mg, 0.12 mmol), \( p \)-chlorophenyl azide (38.5 mg, 0.25 mmol), Cu(OAc)\(_2\) (3.7 mg, 0.02 mmol) and sodium ascorbate (7.4 mg, 0.04 mmol) in \(^t\)BuOH/H\(_2\)O (3:3 mL) was stirred at rt for 24 h. The crude mixture was purified by
column chromatography (80% ethyl acetate/petroleum ether) to give the compound 12 (72 mg, 92%) as a white solid.

R_f: 0.45 (100% ethyl acetate).

Mp: 243-245 °C.

^1^H NMR (400 MHz, CDCl_3): δ = 0.85-0.94 (m, 6H), 1.25 (bs, 3H), 2.08 (s, 3H), 3.36-3.42 (m, 2H), 3.53 (d, J = 15.2 Hz, 1H), 3.71 (s, 3H), 3.84 (d, J = 15.2 Hz, 1H), 4.38-4.39 (m, 1H), 7.29 (s, 1H), 7.48-7.52 (m, 4H), 7.72 (d, J = 8.8 Hz, 2H), 7.78 (d, J = 8.8 Hz, 2H), 8.14 (s, 1H), 8.25 (s, 1H), 8.30 (d, J = 6.8 Hz, 1H) ppm.

^13^C NMR (100 MHz, CDCl_3): δ = 21.9, 22.9, 24.6, 25.1, 30.5, 31.1, 40.8, 51.8, 52.4, 63.9, 121.6, 121.7, 122.5, 122.7, 130.0, 130.1, 134.5, 134.7, 135.6, 135.8, 143.2, 143.9, 172.3, 172.4, 173.8 ppm.

I.R. (KBr): 1409.5, 1654.3, 2951.5, 3389.3 cm^{-1}.

HRMS (Q-Tof) m/z: Calcd. C_{29}H_{33}N_8O_4Cl_2 [M+H]^+ 627.200, found: 627.201.

[α]_D^{25}: -3.05 (c = 0.67, CHCl_3).

### Preparation of compound (13)

According to the general procedure, alkyne 10 (20 mg, 0.06 mmol), o-nitronitrophenyl azide (19.7 mg, 0.12 mmol), Cu(OAc)_2 (1.8 mg, 0.01 mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in 'BuOH/H_2O (3:3 mL) was stirred at rt for 24 h. The crude mixture was purified by column chromatography (5% methanol/chloroform) to give the compound 13 (30.2 mg, 74%) as a white solid.

R_f: 0.64 (10% methanol/chloroform).

Mp: 165-167 °C.

^1^H NMR (400 MHz, CD_3OD): δ = 0.89 (d, J = 6.2 Hz, 3H), 0.93 (d, J = 6.2 Hz, 3H), 1.57-1.68 (m, 1H), 1.71-1.94 (m, 2H), 2.02 (s, 3H), 3.48-3.60 (m, 3H), 3.67 (s, 3H), 3.69-3.72 (m, 1H), 4.42-4.46 (m, 1H), 7.78-7.89 (m, 4H), 7.90-7.92 (m, 2H), 8.12-8.15 (m, 2H), 8.26 (s, 1H), 8.32 (s, 1H) ppm.

^13^C NMR (100 MHz, CD_3OD): δ = 21.8, 23.4, 25.8, 30.8, 31.9, 41.3, 52.7, 52.8, 63.8, 126.8, 127.2, 128.9, 131.2, 131.3, 132.4, 135.2, 135.3, 143.8, 144.5, 146.1, 173.4, 173.9, 175.3 ppm.

I.R. (KBr): 1537.7, 1667.1, 1743.1, 2955.5, 3365.6 cm^{-1}.

HRMS (Q-Tof) m/z: Calcd. C_{29}H_{33}N_8O_8 [M+H]^+ 649.2483, found: 649.2489.

[α]_D^{25}: -29.194 (c = 0.37, CHCl_3).
Preparation of compound (14)

According to the general procedure, alkyne 10 (30 mg, 0.09 mmol), p-nitrophenyl azide (31.2 mg, 0.19 mmol), Cu(OAc)$_2$ (3.7 mg, 0.02 mmol) and sodium ascorbate (7.4 mg, 0.04 mmol) in tBuOH/H$_2$O (3:3 mL) was stirred at rt for 22 h. The crude mixture was purified by column chromatography (5% methanol/ chloroform) to give the compound 14 (40 mg, 66%) as a white solid.

R$_f$: 0.74 (10% methanol/ chloroform).

Mp: 172-174 °C.

$^1$H NMR (400 MHz, DMSO+CD$_3$OD): δ = 0.72 (d, $J = 6.4$ Hz, 3H), 0.81 (d, $J = 6.4$ Hz, 3H), 1.37-1.65 (m, 3H), 1.89 (s, 3H), 3.40-3.52 (m, 4H), 3.58 (s, 3H), 4.19-4.22 (m, 2H), 8.15-8.21 (m, 4H), 8.31 (d, $J = 7.1$ Hz, 1H), 8.43-8.45 (m, 4H), 8.62 (s, 1H), 88.69, (s, 1H) ppm.

$^{13}$C NMR (100 MHz, DMSO+CD$_3$OD): δ = 22.3, 24.2, 24.7, 25.2, 30.3, 31.7, 34.7, 52.3, 53.3, 63.1, 111.1, 120.3, 121.3, 123.7, 126.3, 127.0, 128.9, 142.2, 142.3, 144.8, 145.2, 147.9, 148.0, 171.5, 172.8, 174.9 ppm.

IR (KBr): 1663.1, 1736.3, 2917.7, 3422.7 cm$^{-1}$.

HRMS (Q-Tof) m/z: Calcd. C$_{29}$H$_{33}$N$_{10}$O$_8$ [M+H]$^+$ 649.2483, found: 649.2476.

$[\alpha]_D^{25}$: 9.422 (c = 0.22, DMSO).

Preparation of compound (15)

According to the general procedure, alkyne 10 (20 mg, 0.06 mmol), 2-methoxy-4-nitrophenyl azide (23.7 mg, 0.12 mmol), Cu(OAc)$_2$ (1.8 mg, 0.01 mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in tBuOH/H$_2$O (3:3 mL) was stirred at rt for 24 h. The crude mixture was purified by column chromatography (70% ethyl acetate/ petroleum ether) to give the compound 15 (32.1 mg, 85%) as a white solid.

R$_f$: 0.36 (60% ethyl acetate/ petroleum ether).

Mp: 205-207 °C.

$^1$H NMR (400 MHz, CDCl$_3$): δ = 0.86-0.91 (m, 6H), 1.61-1.74 (m, 3H), 2.09 (s, 3H), 3.51-3.71 (m, 4H), 3.64 (s, 3H), 4.07 (s, 6H), 4.44-4.48 (m, 1H), 7.29 (bs, 1H), 7.79 (s, 2H), 8.01-8.08 (m, 3H), 8.13 (d, $J = 8.7$ Hz, 2H), 8.32 (d, $J = 4.7$ Hz, 2H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$): δ = 21.9, 22.9, 24.6, 25.1, 30.8, 31.3, 41.1, 51.5, 52.3, 56.9, 57.0, 64.1, 107.9, 108.1, 116.8, 116.9, 125.2, 125.3, 126.2, 126.3, 131.1, 131.2, 142.7, 143.1, 148.2, 150.8, 151.9, 171.9, 172.2, 173.3 ppm.
I.R. (KBr): 1457.7, 1525.1, 1650.6, 2925.1, 3399.1 cm\(^{-1}\).

HRMS (Q-Tof) m/z: Calcd. C\(_{31}\)H\(_{37}\)N\(_{10}\)O\(_{10}\) [M+H]\(^+\) 709.269, found: 709.272.

\([\alpha]_D^{25}\): -5.22 (c = 0.09, CHCl\(_3\)).

**Preparation of compound (16)**

To a solution of dipeptide 10 (267 mg, 0.83 mmol) in methanol (10 mL) was added 2N NaOH (0.31 mL) and the reaction mixture was stirred at rt for 24 h. Then the reaction mixture was concentrated, diluted with water (6 mL), then acidified with 1N HCl and extracted with ethyl acetate. Evaporation of the solvent gave 16 (250 mg, 98%) as a white solid, which was directly used in the subsequent reaction.

R\(_f\): 0.32 (20% methanol/ chloroform).

Mp: 213-215 °C

\(^1\)H NMR (400 MHz, CD\(_3\)OD): \(\delta = 0.89-0.94\) (m, 6H), 1.57-1.76 (m, 3H), 1.99 (s, 3H), 2.36-2.40 (m, 2H), 2.86-3.06 (m, 4H), 4.47-4.90 (m, 1H) ppm.

\(^{13}\)C NMR (100 MHz, CD\(_3\)OD): \(\delta = 22.0, 22.8, 22.9, 23.6, 25.5, 25.7, 42.3, 52.3, 61.9, 73.3, 73.3, 79.4, 79.5\) ppm.

I.R. (KBr): 1665.3, 2104.1, 3356.7 cm\(^{-1}\).

HRMS (Q-Tof) m/z: Calcd. C\(_{16}\)H\(_{23}\)N\(_2\)O\(_4\) [M+H]\(^+\) 307.1658, found: 307.1652.

\([\alpha]_D^{25}\): -26.91 (c = 0.13, CH\(_3\)OH).

**Preparation of compound (17)**

To a solution of acid 16 (130 mg, 0.42 mmol) and HOBt (114.6 mg, 0.84 mmol) in dry THF (10 mL) was added DCC (103.6 mg, 0.50 mmol) at 0 °C. Then, H-Leu-OMe.HCl (70.3 mg, 0.50 mmol) and NMM (33.9 mg, 0.33 mmol, reaction mixture should have around pH 9) in THF (10 mL) solution was added. The reaction mixture was stirred at rt for 24 h. The solvent was evaporated and the residue was diluted with water. The aqueous layer was extracted with ethyl acetate (3 × 10 mL). The combined organic layer was washed with water, brine and dried over Na\(_2\)SO\(_4\). Evaporation of the solvent gave the crude product, which was purified by column chromatography (1% methanol/ chloroform) to give the tripeptide 17 (120.5 mg, 70%) as a white solid.

R\(_f\): 0.38 (5% methanol/ chloroform).

Mp: 104-106 °C.
$^1$H NMR (400 MHz, CDCl$_3$): \( \delta = 0.92-0.95 \) (m, 6H), 1.42 (d, \( J = 7.2 \) Hz, 3H), 1.52-1.61 (m, 1H), 1.69-1.78 (m, 2H), 2.09 (s, 3H), 2.11 (t, \( J = 2.6 \) Hz, 1H), 2.16 (t, \( J = 2.6 \) Hz, 1H), 2.94-3.22 (m, 4H), 3.73 (s, 3H), 4.47-4.55 (m, 2H), 6.45 (s, 1H), 6.75 (d, \( J = 8.1 \) Hz, 1H), 6.99 (d, \( J = 7.1 \) Hz, 1H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$): \( \delta = 17.9, 21.6, 23.3, 23.9, 24.8, 24.9, 25.6, 40.6, 48.3, 52.4, 52.5, 60.9, 72.7, 73.2, 78.7, 79.1, 170.3, 171.3, 171.5, 173.2 \) ppm.

I.R. (KBr): 1542.0, 1650.9, 1743.5, 2279.1, 2950.0, 3285.3 cm$^{-1}$.

HRMS (Q-Tof) m/z: Calcd. for C$_{20}$H$_{30}$N$_3$O$_5$ [M+H]$^+$ 392.2185, found at 392.2167.

\([\alpha]_D^{25}\) : -15.541 (c = 0.76, CHCl$_3$).

**Preparation of compound (18)**

According to the general procedure, alkyne 17 (20 mg, 0.05 mmol), 2-methoxy-4-nitrophenyl azide (18.6 mg, 0.10 mmol), Cu(OAc)$_2$ (1.8 mg, 0.01 mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in tBuOH/H$_2$O (3:3 mL) was stirred at rt for 10 h. The crude mixture was purified by column chromatography (1% methanol/chloroform) to give the compound 18 (32 mg, 84%) as a white solid.

R$_f$: 0.22 (5% methanol/chloroform).

Mp: 135-137 °C.

$^1$H NMR (400 MHz, CD$_3$OD): \( \delta = 0.86 \) (d, \( J = 6.3 \) Hz, 3H), 0.91 (d, \( J = 6.4 \) Hz, 3H), 1.39 (d, \( J = 7.4 \) Hz, 3H), 1.62-1.66 (m, 3H), 2.08 (s, 3H), 3.41-3.64 (m, 4H), 3.69 (s, 3H), 4.12 (s, 3H), 4.13 (s, 3H), 4.27-4.32 (m, 1H), 4.41-4.47 (m, 1H), 8.07-8.08 (m, 4H), 8.15 (bs, 2H), 8.45 (s, 1H), 8.51 (s, 1H) ppm.

$^{13}$C NMR (100 MHz, CD$_3$OD): \( \delta = 15.6, 20.3, 22.1, 22.2, 24.1, 28.9, 29.3, 30.1, 39.9, 51.3, 51.9, 56.2, 62.5, 107.8, 107.9, 115.9, 116.0, 125.1, 125.2, 126.1, 130.7, 130.8, 141.9, 142.3, 148.5, 151.4, 151.5, 172.3, 173.2, 173.5 \) ppm.

I.R. (KBr): 1531.2, 1651.8, 2924.3, 3389.5 cm$^{-1}$.

HRMS (Q-Tof) m/z: Calcd. C$_{34}$H$_{42}$N$_{11}$O$_{11}$ [M+H]$^+$ 780.3065, found: 780.3046.

\([\alpha]_D^{25}\) : -22.05 (c = 0.08, CHCl$_3$).

**Preparation of compound (19)**

According to the general procedure, alkyne 17 (20 mg, 0.05 mmol), p-chloronitrophenyl azide (15.3 mg, 0.10 mmol), Cu(OAc)$_2$ (1.8 mg, 0.01 mmol) and sodium ascorbate (3.6 mg, 0.02
mmol) in 'BuOH/H2O (3:3 mL) was stirred at rt for 18 h. The crude mixture was purified by column chromatography (1% methanol/ chloroform) to give the compound 19 (28.8 mg, 84%) as a white solid.

\( R_f \): 0.22 (80% ethyl acetate/ petroleum ether).

\textbf{Mp:} 172-174 °C.

\textbf{H NMR (400 MHz, CDCl}_3\textbf{):} \( \delta = 0.78-0.89 \) (m, 6H), 1.36 (d, \( J = 7.2 \) Hz, 3H), 1.37-1.72 (m, 3H), 2.08 (s, 3H), 3.49-3.79 (m, 4H), 3.71 (s, 3H), 4.30-4.32 (m, 1H), 4.33-4.48 (m, 1H), 7.29 (d, \( J = 7.1 \) Hz, 1H), 7.33 (s, 1H), 7.48-7.52 (m, 4H), 7.69-7.71 (m, 5H), 8.10 (s, 1H), 8.14 (s, 1H) ppm.

\textbf{C NMR (100 MHz, CDCl}_3\textbf{):} \( \delta = 17.7, 21.6, 23.1, 24.6, 24.9, 30.8, 30.9, 40.6, 48.5, 52.5, 52.9, 63.6, 121.5, 121.6, 122.2, 122.3, 130.1, 130.2, 134.6, 134.8, 135.4, 135.6, 143.4, 143.6, 172.0, 172.1, 173.3 \) ppm.

\textbf{I.R. (KBr)):} 1501.8, 1647.2, 1662.5, 1739.3, 2945.0 cm\(^{-1}\).

\textbf{HRMS (Q-Tof) m/z:} Calcd. C\(_{32}\)H\(_{38}\)N\(_9\)O\(_5\)Cl\(_2\) [M+H]\(^+\) 698.2373, found: 698.2380.

\( \left[\alpha\right]_D^{25} \): 3.814 (c = 0.14, CH\(_3\)OH).

\textbf{Preparation of compound (20)}

According to the general procedure, alkyne 17 (20 mg, 0.05 mmol), \( p \)-methoxyphenylazide (14.6 mg, 0.10 mmol), Cu(OAc)\(_2\) (1.8 mg, 0.01 mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in 'BuOH/H2O (3:3 mL) was stirred at rt for 20 h. The crude mixture was purified by column chromatography (5% methanol/ chloroform) to give the compound 20 (29.5 mg, 85%) as a white solid.

\( R_f \): 0.45 (10% methanol/ chloroform).

\textbf{Mp:} 130-132 °C.

\textbf{H NMR (400 MHz, CDCl}_3\textbf{):} \( \delta = 0.78-0.83 \) (m, 6H), 1.37 (d, \( J = 7.2 \) Hz, 3H), 1.49-1.58 (m, 2H), 1.71-1.79 (m, 1H), 2.08 (s, 3H), 3.51-3.66 (m, 2H), 3.71-3.74 (m, 2H), 3.74 (s, 3H), 3.87 (s, 6H), 4.34-4.46 (m, 1H), 4.48-4.53 (m, 1H), 7.02 (d, \( J = 9.0 \) Hz, 4H), 7.36-7.39 (m, 2H), 7.51 (d, \( J = 7.4 \) Hz, 1H), 7.60-7.68(m, 4H), 7.92(s, 1H), 7.95 (s, 1H) ppm.

\textbf{C NMR (100 MHz, CDCl}_3\textbf{):} \( \delta = 17.9, 21.6, 22.9, 23.2, 24.7, 24.9, 30.7, 31.2, 40.5, 48.4, 52.5, 52.8, 55.8, 63.8, 114.9, 115.0, 122.0, 122.2, 122.4, 130.5, 130.7, 143.2, 159.9, 160.1, 171.9, 171.9, 172.2, 173.3 \) ppm.

\textbf{I.R. (KBr)):} 1519.1, 1647.2, 1662.5, 1739.3, 2945.0 cm\(^{-1}\).
**HRMS (Q-Tof) m/z:** Calcd. C_{34}H_{44}N_{9}O_{7} [M+H]^+ 690.3364, found: 690.3385.

[α]_{D}^{25}: -10.66 (c = 0.14, CHCl₃).

**Table S1:** List of various triazole based peptides synthesized

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<th>Azide</th>
<th>Mono-triazole based peptide</th>
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**Figure S1.** Screening of different inhibitors against MST1 kinase. A) with compound 7 B) with compound 8 C) with compound 9 D) with compound 12
$^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) and HRMS of compound 2
$^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$+CD$_3$OD) and HRMS of compound 3
Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM /  DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0  Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
169 formula(s) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:  Mass  Calc. Mass  mDa  PPM  DBE  Score  Formula
Maximum:  200.0  10.0  50.0

481.1830  481.1836  -0.6  -1.2  14.5  1  C23H25N6O6
$^1$H NMR (400 MHz, CD$_3$OD) and $^{13}$C NMR (100 MHz, CD$_3$OD) and HRMS of compound 4
**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

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**1H NMR (400 MHz, DMSO)** and **13C NMR (100 MHz, DMSO)** and HRMS of compound 5

![NMR and HRMS spectra of compound 5]
Elemental Composition Report

Single Mass Analysis
Tolerance = 60.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0, Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

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Maximum:
Mass Calc. Mass mDa PPM DBE Score Formula
481.1851 481.1836 1.5 3.2 14.5 1 C23 H25 N5 O6
$^1$H NMR (400 MHz, DMSO) and $^{13}$C NMR (100 MHz, DMSO) and HRMS of compound 6
**Elemental Composition Report**

**Single Mass Analysis (displaying only valid results)**

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Monoisotopic Mass, Odd and Even Electron Ions

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**1H NMR (400 MHz, CDCl3) and 13C NMR (100 MHz, CDCl3) and HRMS of compound 7**
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0  Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
442 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)


C2H2O2ClN5004I
SRK-00-52-323 50 (0.493) AM (Cen,5, 80.00, Ht,500,0,555.28,1.00): Sb (5,40.00 ); Cm (50.79)
596.0566

Minimum: 200.0  10.0  -1.5
Maximum: 50.0

Mass  Calc. Mass  mDa  PPM  DBE  Score  Formula
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$^{1}$H NMR (400 MHz, DMSO) and $^{13}$C NMR (100 MHz, DMSO) and HRMS of compound 8
Elemental Composition Report

Single Mass Analysis
Tolerance = 60.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 \& Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
93 formula(s) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-ToF micro (YA-105)  Dept. Of Chemistry U.T.(B)  27-Sep-201114:03:52
C22H42N6O6  SRF-08-02-386 38 (0.380) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cen (7,52)  TOF MS ES+
85.0617

H NMR (400 MHz, DMSO) and C NMR (100 MHz, DMSO) and HRMS of compound

\[ \text{AcHN} \quad \text{COOMe} \]

Electronic Supplementary Material (ESI) for RSC Advances
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Elemental Composition Report

Single Mass Analysis
Tolerance = 60.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
93 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass: Q-Tof micro (YA-105)
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SNK-D8-52-390 4 (0.040) AM (Can.5, 80.00, H15890.0,555.28,1.00); Sm (Mn, 2x4.00); Sb (5.40.00); Cm (1:49) 27-Sep-201114:21:29

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Mass Calc. Mass mDa PPM DBE Score Formula
607.0789 607.0802 -1.3 -2.1 14.5 1 C23 H24 N6 O6 I
$^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) and HRMS of compound 11
Elemental Composition Report

**Single Mass Analysis (displaying only valid results)**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0  Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105)
Dept. Of Chemistry I.I.T.(B)
18-Mar-2011 18:50:45

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\(^1\)H NMR (400 MHz, CDCl\(_3\)) and \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) and HRMS of compound 12
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
253 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass: Q-Tof micro (YA-105)
Dept. Of Chemistry I.I.T.,(B)

C23H17C5N8O4
SRK-DB-52-325.7 (0.058) AM (Top, Ar,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (1:33)

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$^1$H NMR (400 MHz, CD$_3$OD) and $^{13}$C NMR (100 MHz, CD$_3$OD) and HRMS of compound 13
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
91 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass: Q-Tof micro (VA-135) Dept. Of Chemistry I.T.(B)
C25H32N10O8
SRIC: 52-335 33 (0.327) AM (Cas, 5.00, HI, 5600.0, 556.28, 1.00); Sm (Mn, 2x4.00); Cm (136)

1H NMR (400 MHz, DMSO) and 13C NMR (100 MHz, DMSO) and HRMS of compound 14
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
273 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Inorganic Mass: Q-Tof micro (YA-105) 17-Nov-2011 10:14
C29H33N10O8 347
SRK-D8-52-397 29 (0.246) AM (Cen, 5, 80.00, Ht, 5562, 5,56, 26, 1.00); Sm (Sg, 2, 00); Sb (S, 4, 00); Cm (1,38)

Max. Mass: 801.1798 1952 287.4161

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Score</th>
<th>Formula</th>
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<tbody>
<tr>
<td>649.2476</td>
<td>649.2483</td>
<td>-0.7</td>
<td>-1.0</td>
<td>18.5</td>
<td>1</td>
<td>C29 H33 N10 O8</td>
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</tbody>
</table>
$^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) and HRMS of compound 15
$^1$H NMR (400 MHz, CD$_2$OD) and $^{13}$C NMR (100 MHz, CD$_3$OD) and HRMS of compound 16
**Elemental Composition Report**

**Single Mass Analysis** (displaying only valid results)
Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
13 formula(s) evaluated with 1 results within limits (up to 50 closest results for each mass)

<table>
<thead>
<tr>
<th>Micromass: Q-ToF micro (YA-105)</th>
<th>Dept. Of Chemistry I.I.T.(B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C16H22N2O4</td>
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<tr>
<td>SRK-D9-S2-338 7 (0.070) AM</td>
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<td>330.1516 420.2503</td>
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<tr>
<td>557.2795 635.3073</td>
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<td>712.3713 748.3933</td>
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<td>866.4443 930.8534</td>
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</table>

**Minimum: -1.5**
**Maximum: 1.0 50.0**

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<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Score</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>307.1652</td>
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<td>-0.6</td>
<td>-1.8</td>
<td>5.5</td>
<td>1</td>
<td>C16 H23 N2 O4</td>
</tr>
</tbody>
</table>
$^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) and HRMS of compound 17
Elemental Composition Report

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>FPM</th>
<th>DBE</th>
<th>Score</th>
<th>Formula</th>
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</thead>
<tbody>
<tr>
<td>392.2167</td>
<td>392.2185</td>
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<td>-4.6</td>
<td>7.5</td>
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</table>

$^1$H NMR (400 MHz, CD$_3$OD) and $^{13}$C NMR (100 MHz, CD$_3$OD) and HRMS of compound 18
### Elemental Composition Report

#### Single Mass Analysis (displaying only valid results)
- Tolerance = 200.0 mDa
- DBE: min = -1.5, max = 50.0
- Isotope cluster parameters: Separation = 1.0, Abundance = 1.0%

#### Monoisotopic Mass, Odd and Even Electron Ions
- 135 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

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<th>Molecular Mass: C34H41N1O11</th>
<th>Ions Found: C34H42N1O11</th>
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<tbody>
<tr>
<td>Micromass: Q-ToF micro (YA-105)</td>
<td>Dept. Of Chemistry U.T.B</td>
</tr>
<tr>
<td>SRK-09-52-344 7 (0.070) AM (Tcρ, Hτ, 5000.0, 556.28, 1.00); Sb (5.40.00); Cm (1:32)</td>
<td>TOF MS ES+</td>
</tr>
<tr>
<td>Minimum: 780.3046</td>
<td>Maximum: 804.2947</td>
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<tr>
<td>Mass (mDa)</td>
<td>PPM</td>
</tr>
<tr>
<td>780.3046</td>
<td>-2.0</td>
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</tbody>
</table>
$^1$H NMR (400 MHz, CDCl$_3$) and $^{13}$C NMR (100 MHz, CDCl$_3$) and HRMS of compound 19
 Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
663 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B)
26-May-2011 10:28:46

C16H17O3N5S2
SRK-DB-53-348 22 (0.216) AM (Cen,5, 80.00, Ht,5000,0.556,28.1,0.0); Sb (5,40.00); Cm (1:36)

698.2380
557.2186
514.0888
358.1609
308.0865

TOF MS ES+ 2.11e3

Minimum: 200.0 0.7 1.1 17.5 1
Maximum: 698.2380 698.2373
Mass Calc. Mass mDa PPM DBE Score Formula

1H NMR (400 MHz, CDCl3) and 13C NMR (100 MHz, CDCl3) and HRMS of compound 20

Electronic Supplementary Material (ESI) for RSC Advances
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Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0  Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
74 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

SRK-GD-52-350 2 (0.020) AM (Mw,5, Ht,5000,0,556.28,1,00); Sm (Mw, 4,00); Sb (5,40.00); Cm (1:39)  TOF MS ES+
7.03e3

Minimum:  Mass    Calc. Mass  mDa  PPM  DBE  Score  Formula
-1.5
200.0
10.0
50.0

690.3383  690.3364  2.1  3.1  17.5  1  C34 H44 N9 O7