# Diversity Oriented Approach to Triazole Based Peptidiomimetics by Click Chemistry as Mammalian Sterile 20 Kinase Inhibitors

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## Supporting Information

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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, $^{1}$H NMR) spectra and Carbon Nuclear Magnetic Resonance (100 MHz, $^{13}$C 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 $^{t}BuOH/H_2O$ (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 $^{o}$C.

**$^{1}$H NMR (400 MHz, $CDCl_3$):** $\delta$ = 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.

**$^{13}$C NMR (100 MHz, $CDCl_3$):** $\delta$ = 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. $C_{23}H_{26}N_5O_4$ $[M+H]^+$ 436.1985, found: 436.1976.

**$[\alpha]_D^{25}$:** - 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 $^{t}$BuOH/$H_2O$ (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 $^{o}$C.

**$^{1}$H NMR (400 MHz, $CDCl_3$):** $\delta$ = 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.

**$^{13}$C NMR (100 MHz, $CDCl_3$+$CD_3OD$):** $\delta$ = 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. $C_{23}H_{25}N_6O_6$ $[M+H]^+$ 481.1836, found: 481.1830.

**$[\alpha]_D^{25}$:** -9.900 (c = 0.12, $CH_3OH$).

**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 $^tBuOH/H_2O$ (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).

**Mp:** 175-177 $^oC$.

**$^1$H NMR (400 MHz, $CD_3OD$):** $\delta$ = 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, $CD_3OD$):** $\delta$ = 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. $C_{23}H_{25}N_6O_6$ $[M+H]^+$ 481.1836, found: 481.1826.

**$[\alpha]_D^{25}$:** -4.043 (c = 0.14, $CH_3OH$).

**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 $^tBuOH/H_2O$ (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).

**Mp:** 193-195 $^oC$.

**$^1$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. $C_{23}H_{25}N_6O_6$ $[M+H]^+$ 481.1836, found: 481.1851.

**$[\alpha]_D^{25}$:** 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 $^tBuOH/H_2O$ (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 $^oC$.

**$^1$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. $C_{23}H_{25}N_6O_6$ $[M+H]^+$ 481.1836, found: 481.1856.

**$[\alpha]_D^{25}$:** -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 $^tBuOH/H_2O$ (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 $^oC$.

**$^1$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, 48.9, 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. $C_{23}H_{24}N_5O_4ClI$ $[M+H]^+$ 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/$H_2O$ (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 $^oC$

**$^1$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. $C_{23}H_{24}N_6O_6I$ $[M+H]^+$ 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/$H_2O$ (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 $^oC$.

**$^1$H 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.

**$^{13}$C 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. $C_{23}H_{24}N_6O_6I$ $[M+H]^+$ 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/$H_2O$ (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).

**Mp:** 210-213 $^o$C.

**$^1$H 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.

**$^{13}$C 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. $C_{31}H_{39}N_8O_6$ $[M+H]^+$ 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/$H_2O$ (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 $^{o}$C.

**$^{1}$H NMR (400 MHz, $CDCl_3$):** $\delta$ = 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, $CDCl_3$):** $\delta$ = 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.

**$[\alpha]_D^{25}$:** - 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, 0.01mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in $^{t}$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 $^{o}$C.

**$^{1}$H NMR (400 MHz, $CD_3OD$):** $\delta$ = 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, $CD_3OD$):** $\delta$ = 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. $C_{29}H_{33}N_{10}O_8$ $[M+H]^+$ 649.2483, found: 649.2489.

**$[\alpha]_D^{25}$:** - 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 $^tBuOH/H_2O$ (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 $^oC$.

**$^1$H NMR (400 MHz, DMSO+$CD_3OD$):** $\delta$ = 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+$CD_3OD$ ):** $\delta$ =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.

**I.R. (**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, 0.01mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in $^tBuOH/H_2O$ (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 $^oC$.

**$^1$H NMR (400 MHz, $CDCl_3$):** $\delta$ = 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, $CDCl_3$):** $\delta$ = 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 $^oC$

**$^1$H NMR (400 MHz, $CD_3OD$):** $\delta$ = 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, $CD_3OD$):** $\delta$ = 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. $C_{16}H_{23}N_2O_4$ $[M+H]^+$ 307.1658, found: 307.1652.

**$[\alpha]_D^{25}$:** - 26.91 (c = 0.13, $CH_3OH$).

**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 $^oC$. Then, H-Leu-OMe.HCl (70.3 mg, 0.50 mmol) and NMM (33.9 mg, 0.33 mmol, reaction mixture should have around *p*H 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 $Na_2SO_4$. 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 $^oC$.

**$^1$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 $C_{20}H_{30}N_3O_5$ $[M+H]^+$ 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, 0.01mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in $^t$BuOH/$H_2O$ (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 $^o$C.

**$^1$H NMR (400 MHz, $CD_3OD$):** $\delta$ = 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, $CD_3OD$):** $\delta$ = 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, 0.01mmol) and sodium ascorbate (3.6 mg, 0.02

mmol) in $^{t}$BuOH/$H_2O$ (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).

**Mp:** 172-174 $^{o}$C.

**$^{1}$H NMR (400 MHz, $CDCl_3$):** $\delta$ = 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.

**$^{13}$C NMR (100 MHz, $CDCl_3$):** $\delta$ = 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.

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

**HRMS (Q-Tof) *m/z*:** Calcd. $C_{32}H_{38}N_9O_5Cl_2$ $[M+H]^+$ 698.2373, found: 698.2380.

**$[\alpha]_D^{25}$:** 3.814 (c = 0.14, $CH_3OH$).

**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, 0.01mmol) and sodium ascorbate (3.6 mg, 0.02 mmol) in $^{t}$BuOH/$H_2O$ (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).

**Mp:** 130-132 $^{o}$C.

**$^{1}$H NMR (400 MHz, $CDCl_3$):** $\delta$ = 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.

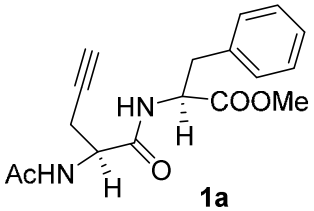
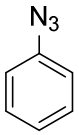
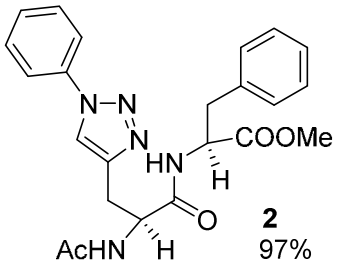
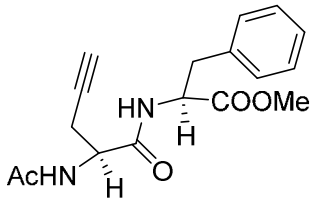
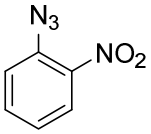
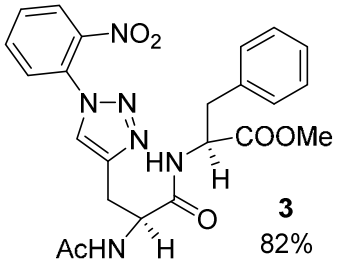
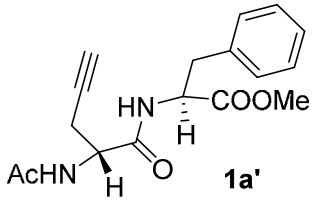
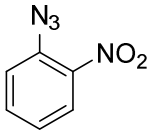
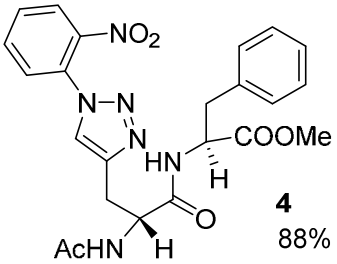
**$^{13}$C NMR (100 MHz, $CDCl_3$):** $\delta$ = 17.9, 21.6, 22.9, 23.2, 24.7, 24.9, 30.7, 31.2, 40.5, 48.4, 52.5, 52.8, 55.8, 63.8, 114.9, 115.0, 122.0, 122.2, 122.4, 130.5, 130.7, 143.2, 159.9, 160.1, 171.9, 171.9, 172.2, 173.3 ppm.

**I.R. (**KBr **):** 1519.1, 1657.1, 1743.4, 2836.6, 2929.4 $cm^{-1}$.

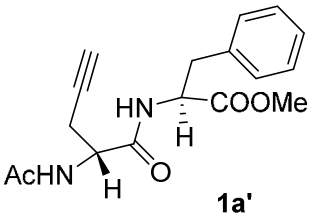
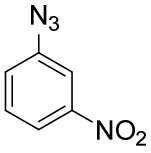
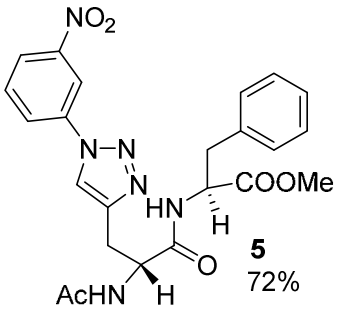
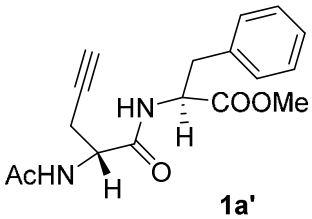
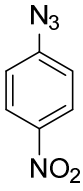
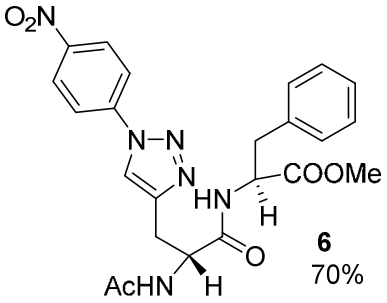
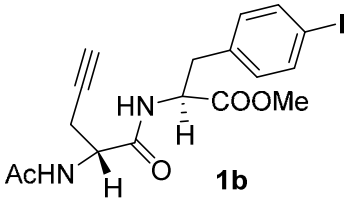
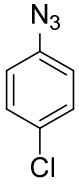
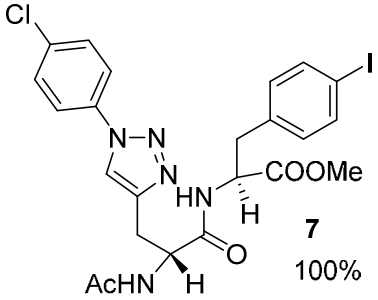
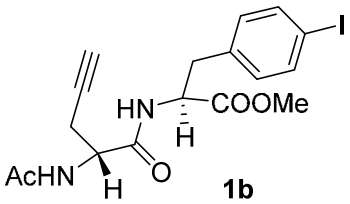
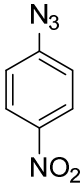
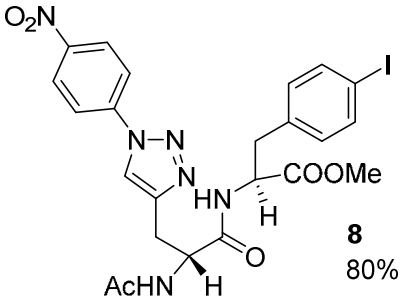
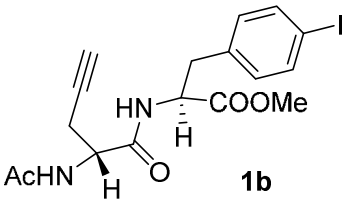
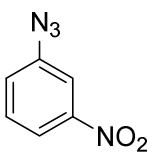
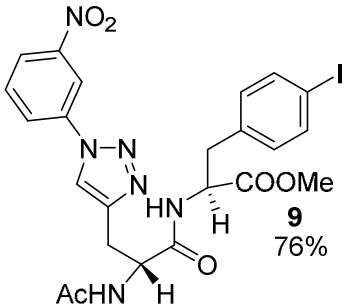
**HRMS (Q-Tof) *m/z*:** Calcd. $C_{34}H_{44}N_9O_7$ $[M+H]^+$ 690.3364, found: 690.3385.

**$[\alpha]_D^{25}$:** - 10.66 (c = 0.14, $CHCl_3$).

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

| Alkyne precussor | Azide | Mono-triazole based peptide |
|---|---|---|
|  **1a** |  |  **2** 97% |
|  **1a** |  |  **3** 82% |
|  **1a'** |  |  **4** 88% |

*contd…..*

| Alkyne precussor | Azide | Mono-triazole based peptide |
|---|---|---|
|  **1a'** |  |  **5** 72% |
|  **1a'** |  |  **6** 70% |
|  **1b** |  |  **7** 100% |
|  **1b** |  |  **8** 80% |
|  **1b** |  |  **9** 76% |

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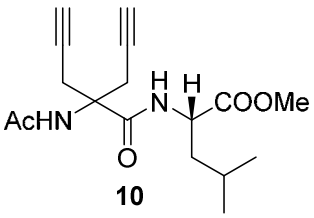
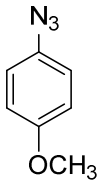
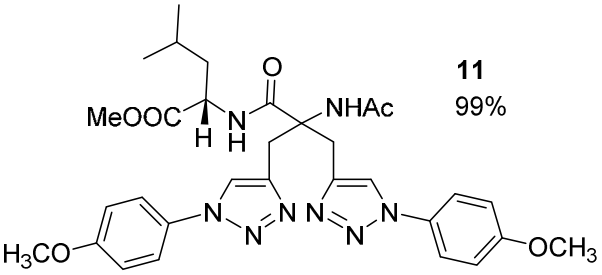
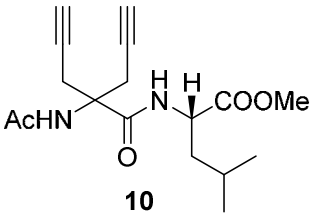
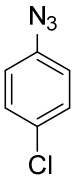
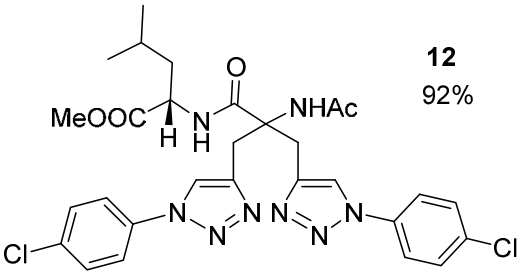
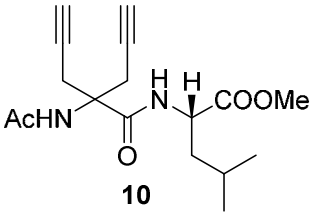
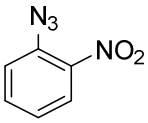
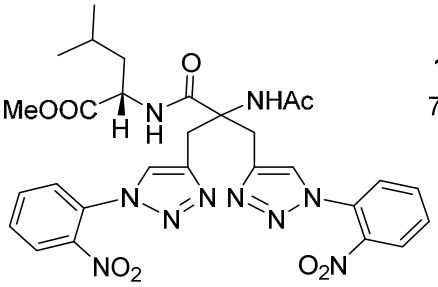
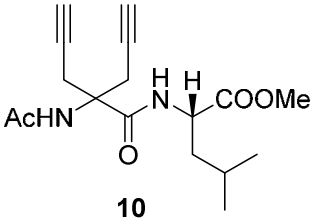
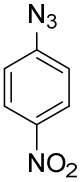
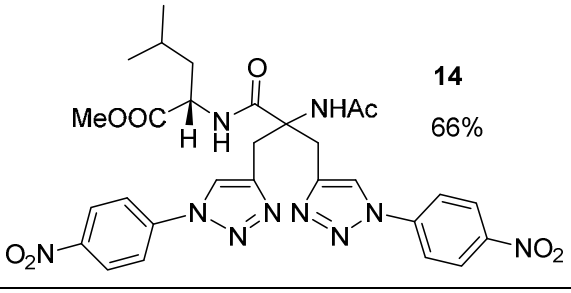
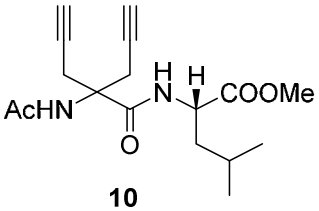
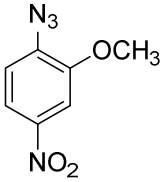
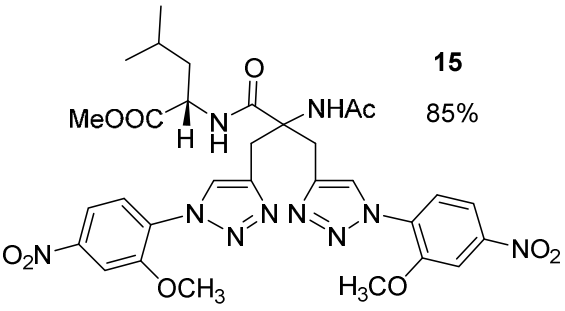
| Alkye precussor | Azide | Di-triazole based peptide |
|---|---|---|
|  **10** |  |  **11** 99% |
|  **10** |  |  **12** 92% |
|  **10** |  |  **13** 74% |
|  **10** |  |  **14** 66% |
|  **10** |  |  **15** 85% |

*contd*

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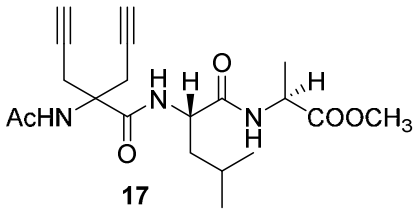
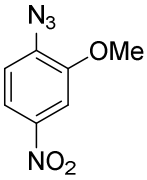
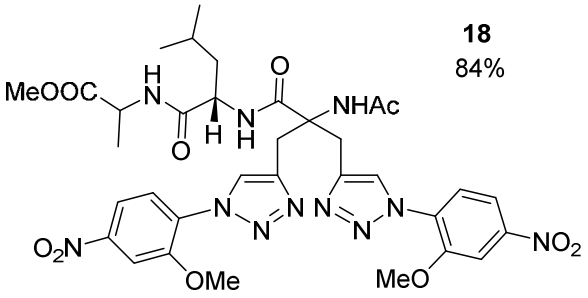
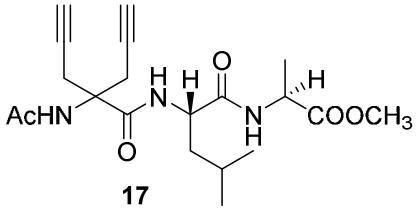
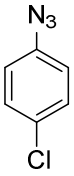
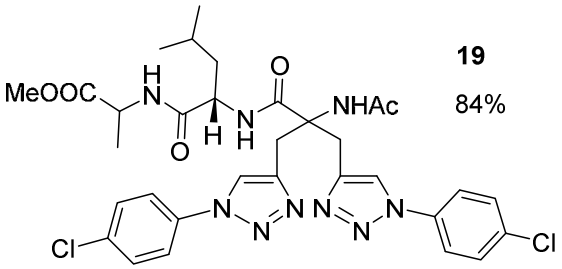
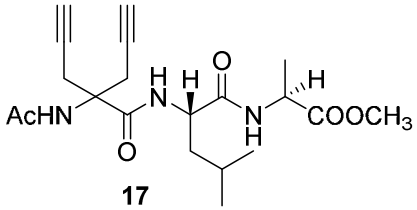
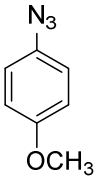
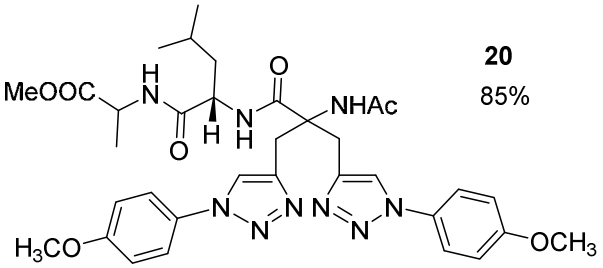
| Alkye Precussor | Azide | Di-triazole Based Tripeptide Yield(%) |
|---|---|---|
|  **17** |  |  **18** 84% |
|  **17** |  |  **19** 84% |
|  **17** |  |  **20** 85% |

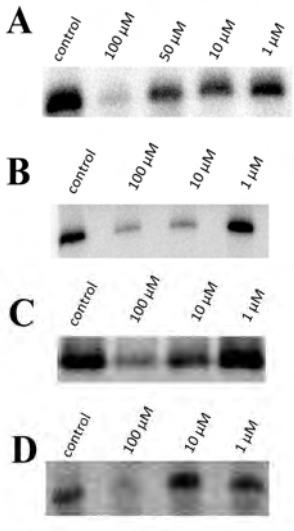
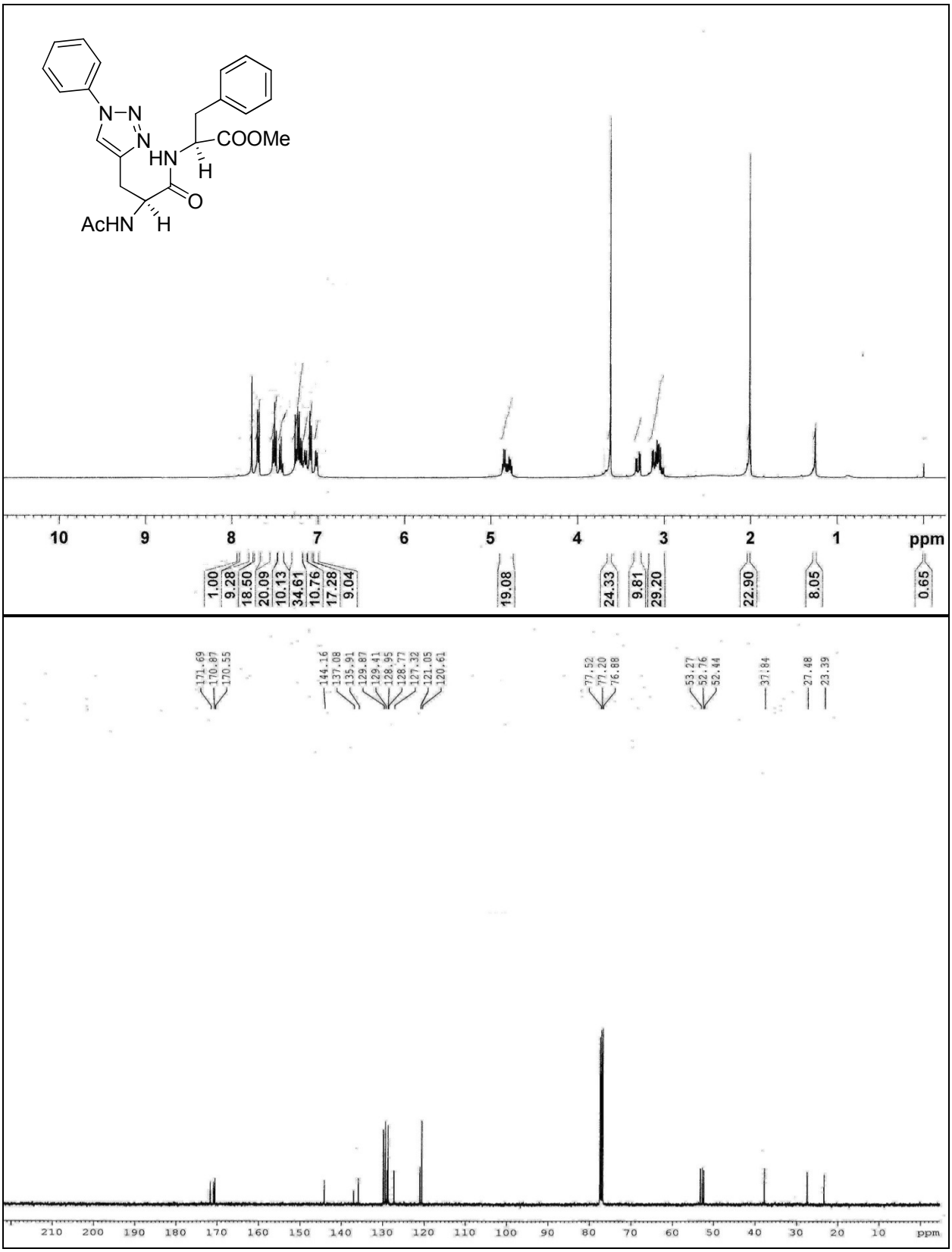
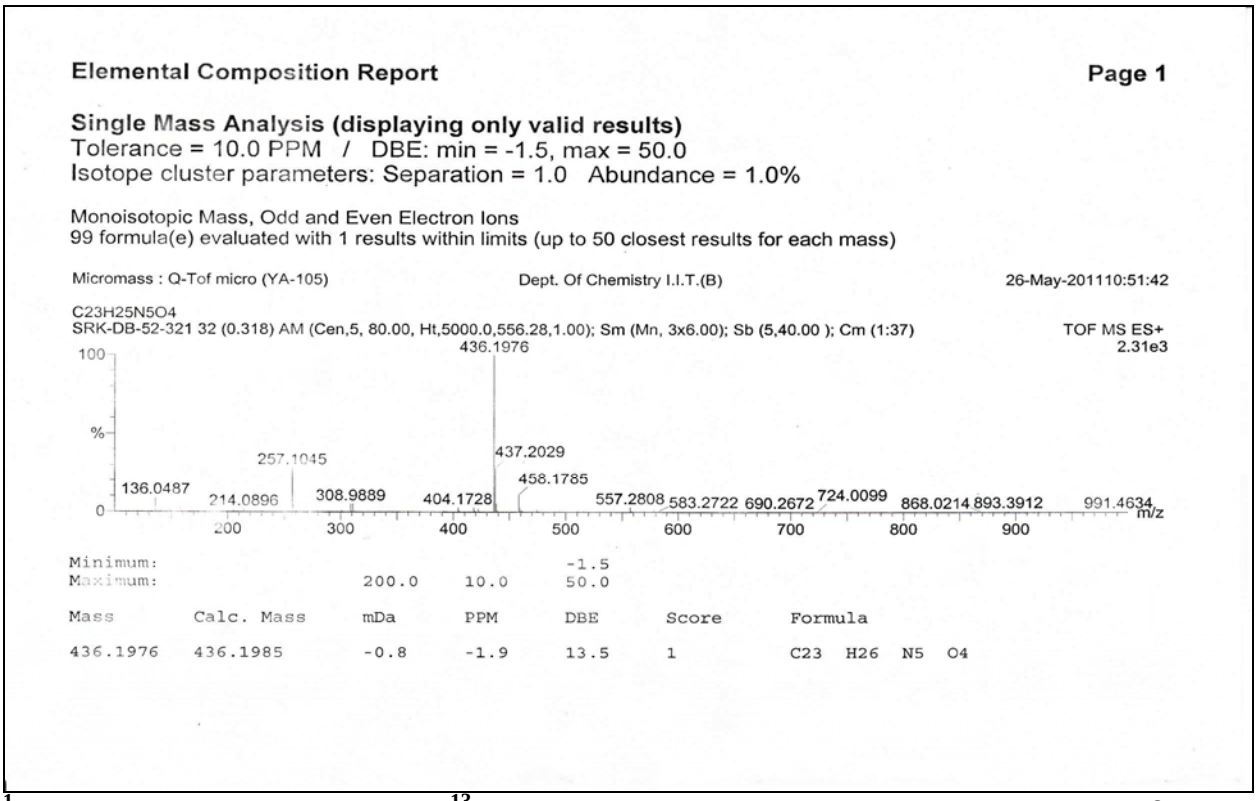



**Figure S1.** Screening of different inhibitors against MST1 kinase. A) with compound **7** B) with compound **8** C) with compound **9** D) with compound **12**

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 2**





**Elemental Composition Report** **Page 1**

**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
99 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

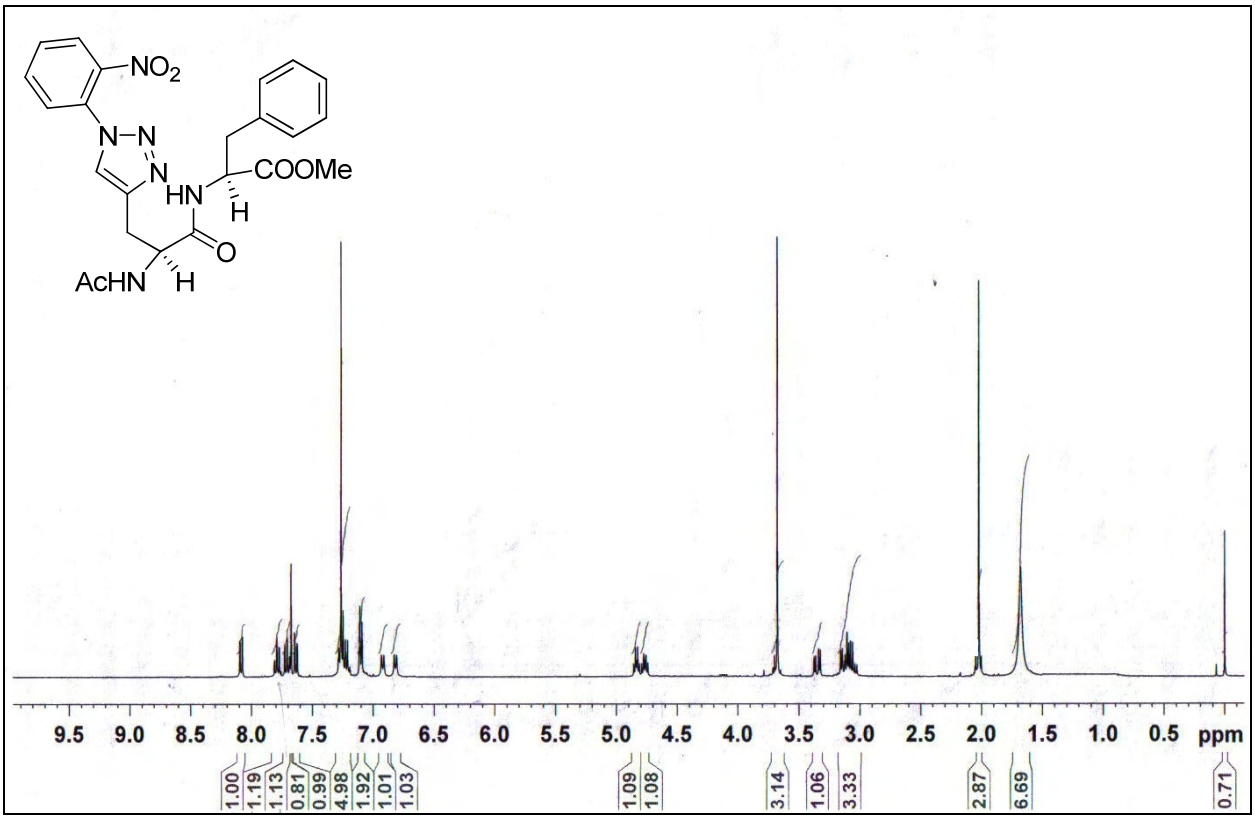
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 26-May-201110:51:42

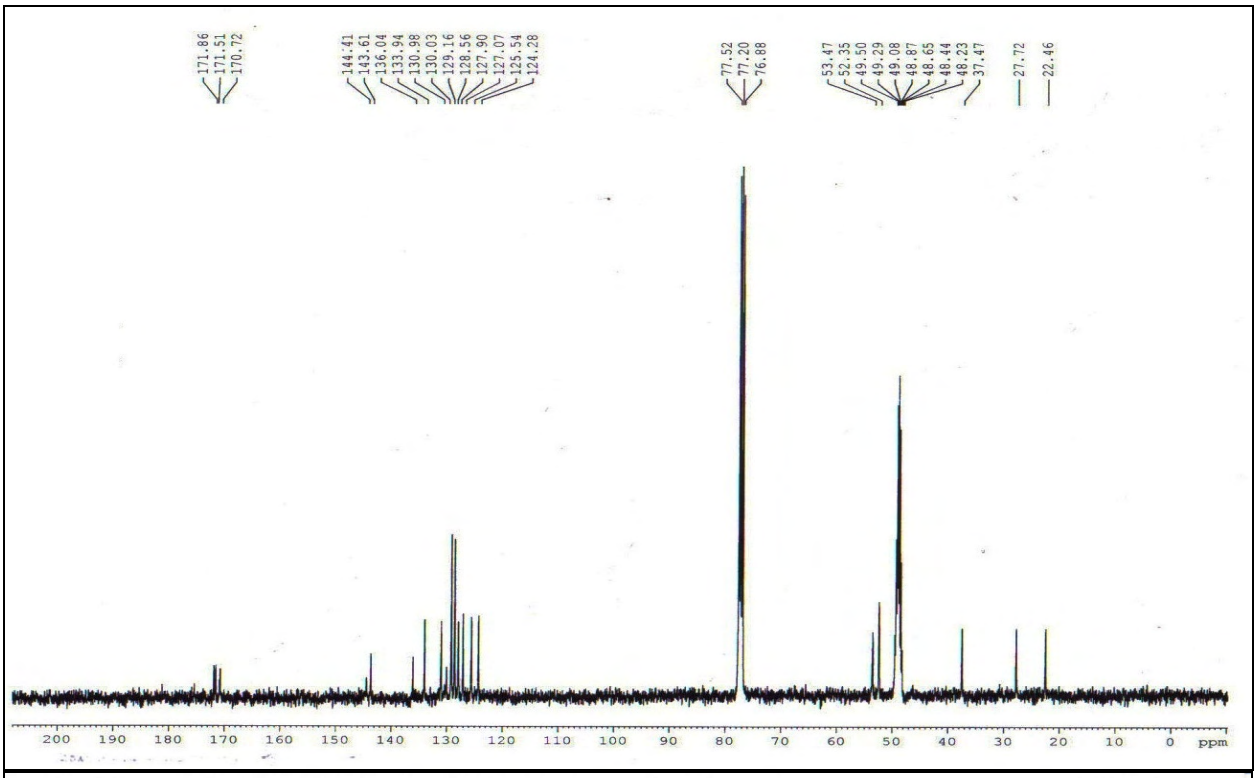
C23H25N5O4
SRK-DB-52-321 32 (0.318) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 3x6.00); Sb (5,40.00 ); Cm (1:37) TOF MS ES+
2.31e3



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 436.1976 | 436.1985 | -0.8 | -1.9 | 13.5 | 1 | C23 H26 N5 O4 |

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$+$CD_3OD$) and HRMS of compound 3**



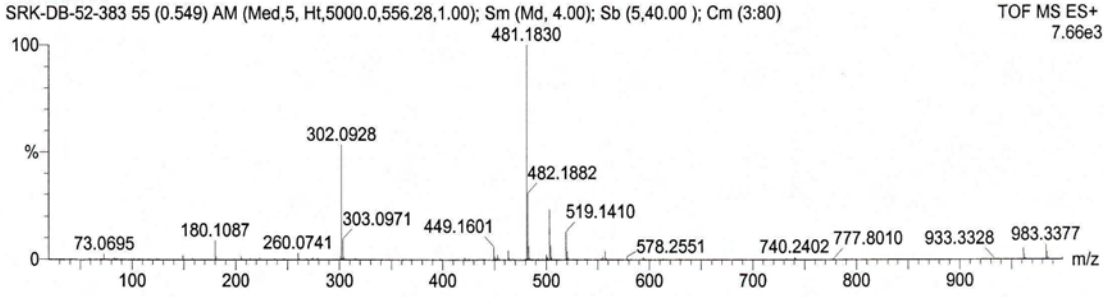



**Elemental Composition Report** **Page 1**

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

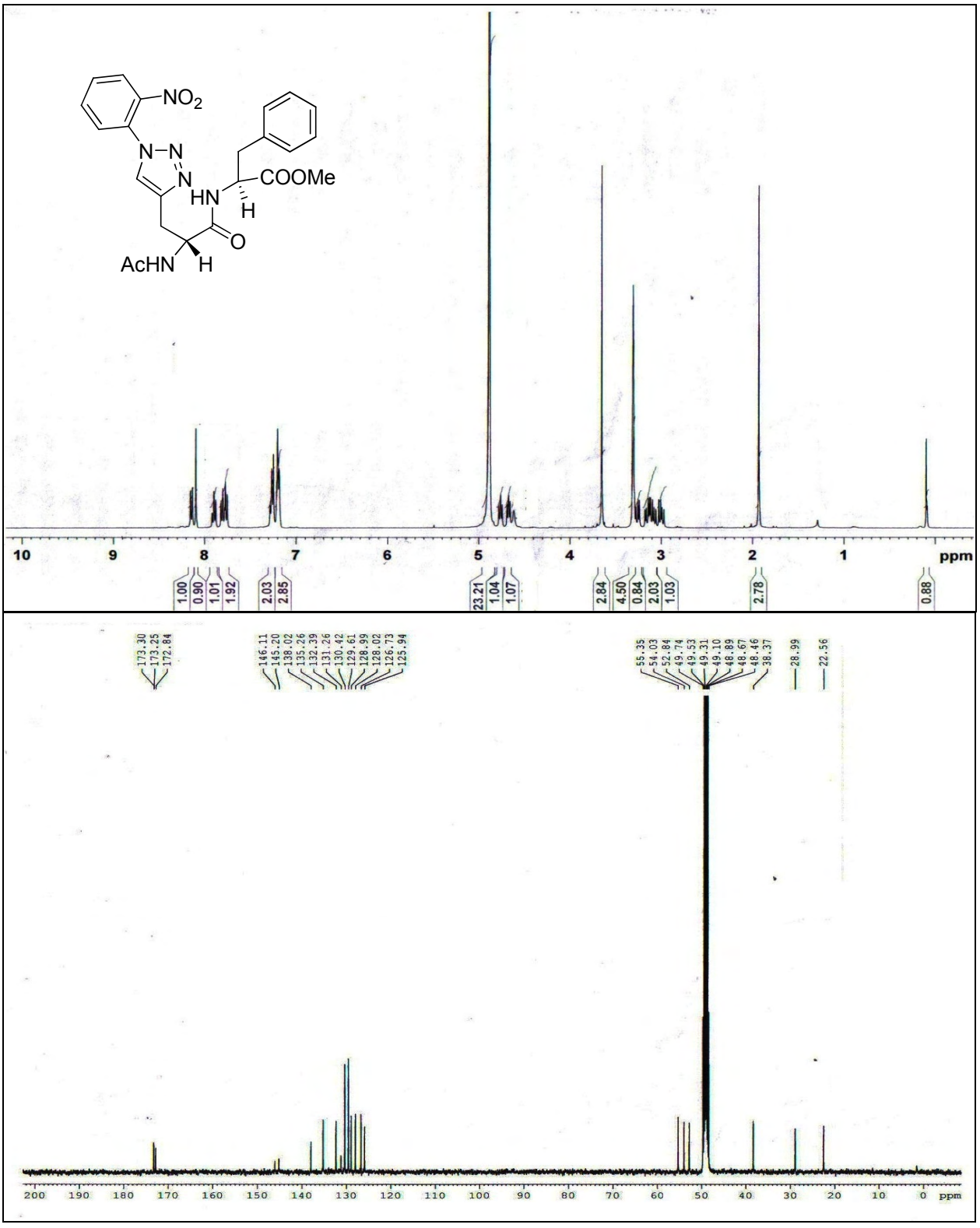
Monoisotopic Mass, Odd and Even Electron Ions
169 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

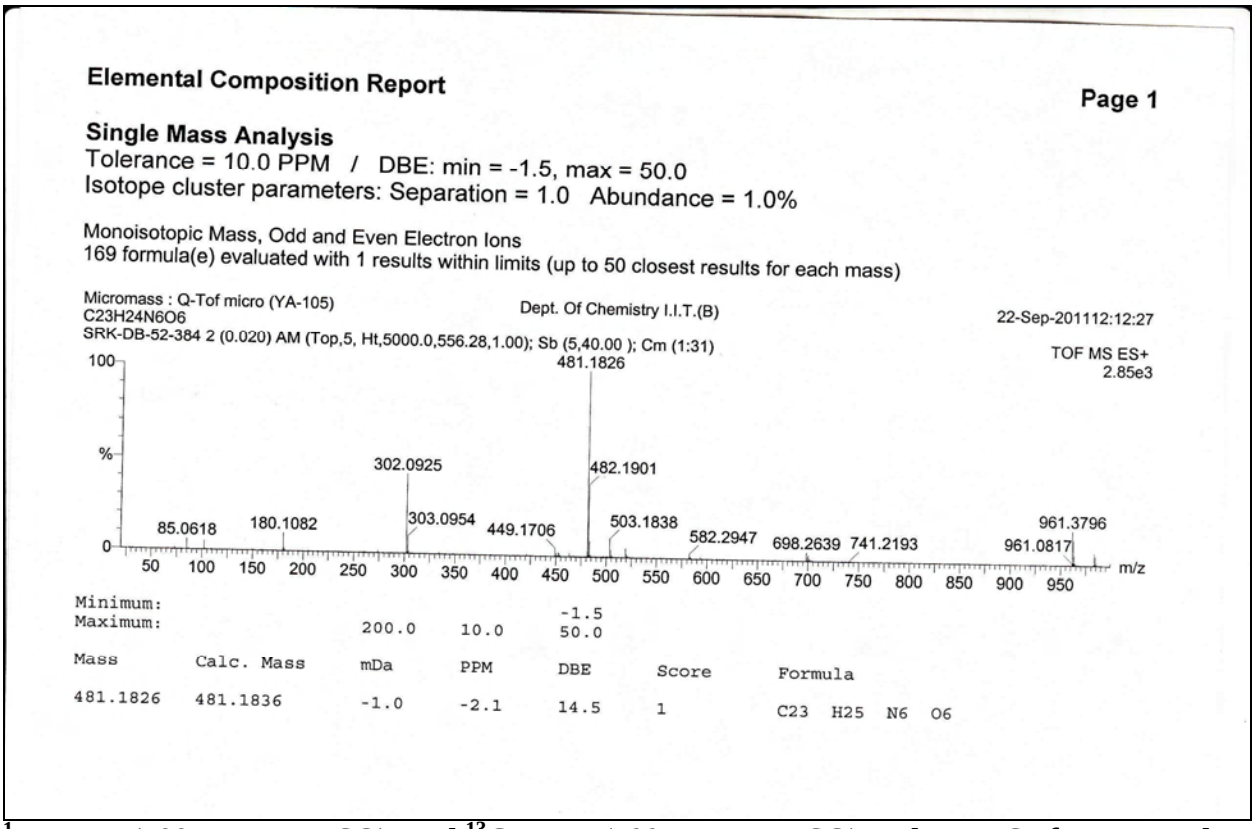
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 22-Sep-201113:11:53
C23H24N6O6
SRK-DB-52-383 55 (0.549) AM (Med,5, Ht,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (5,40.00 ); Cm (3:80) TOF MS ES+
7.66e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 481.1830 | 481.1836 | -0.6 | -1.2 | 14.5 | 1 | C23 H25 N6 O6 |

**$^{1}$H NMR (400 MHz, $CD_3OD$) and $^{13}$C NMR (100 MHz, $CD_3OD$) and HRMS of compound 4**





**Elemental Composition Report** Page 1

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

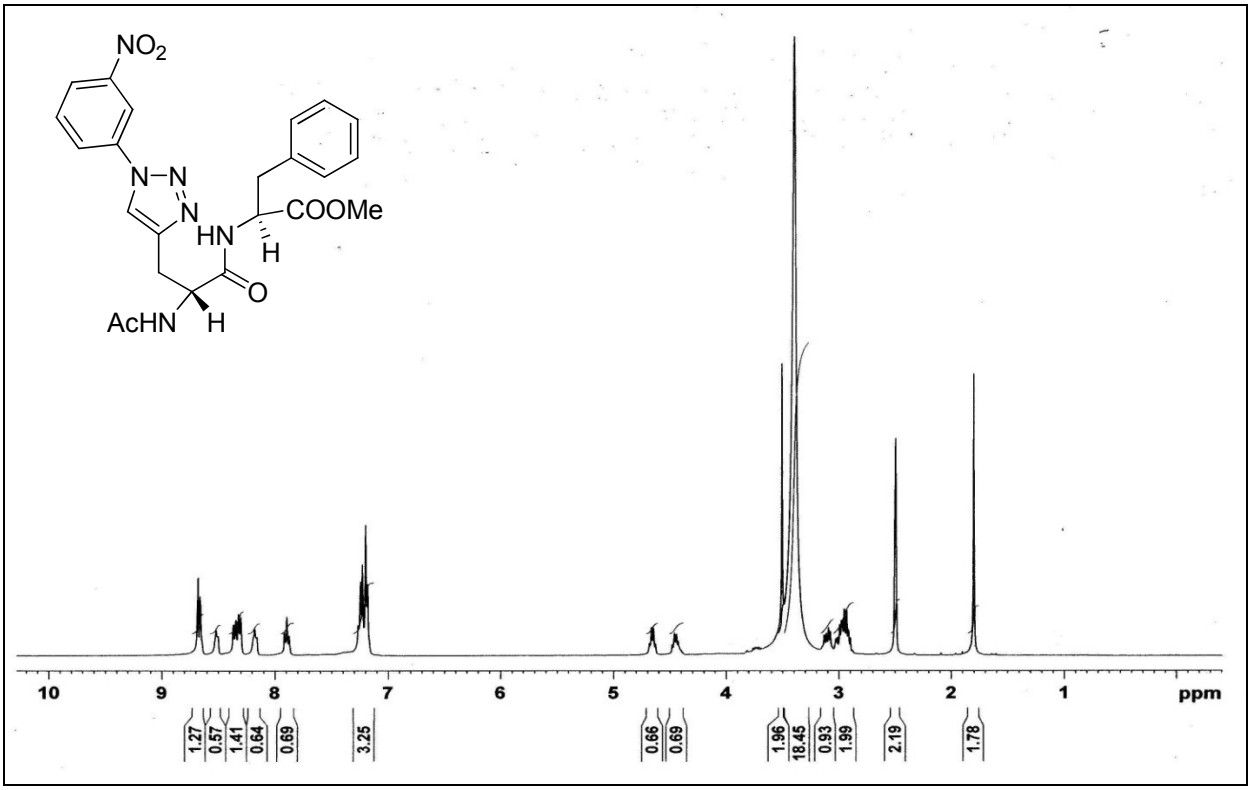
Monoisotopic Mass, Odd and Even Electron Ions
169 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

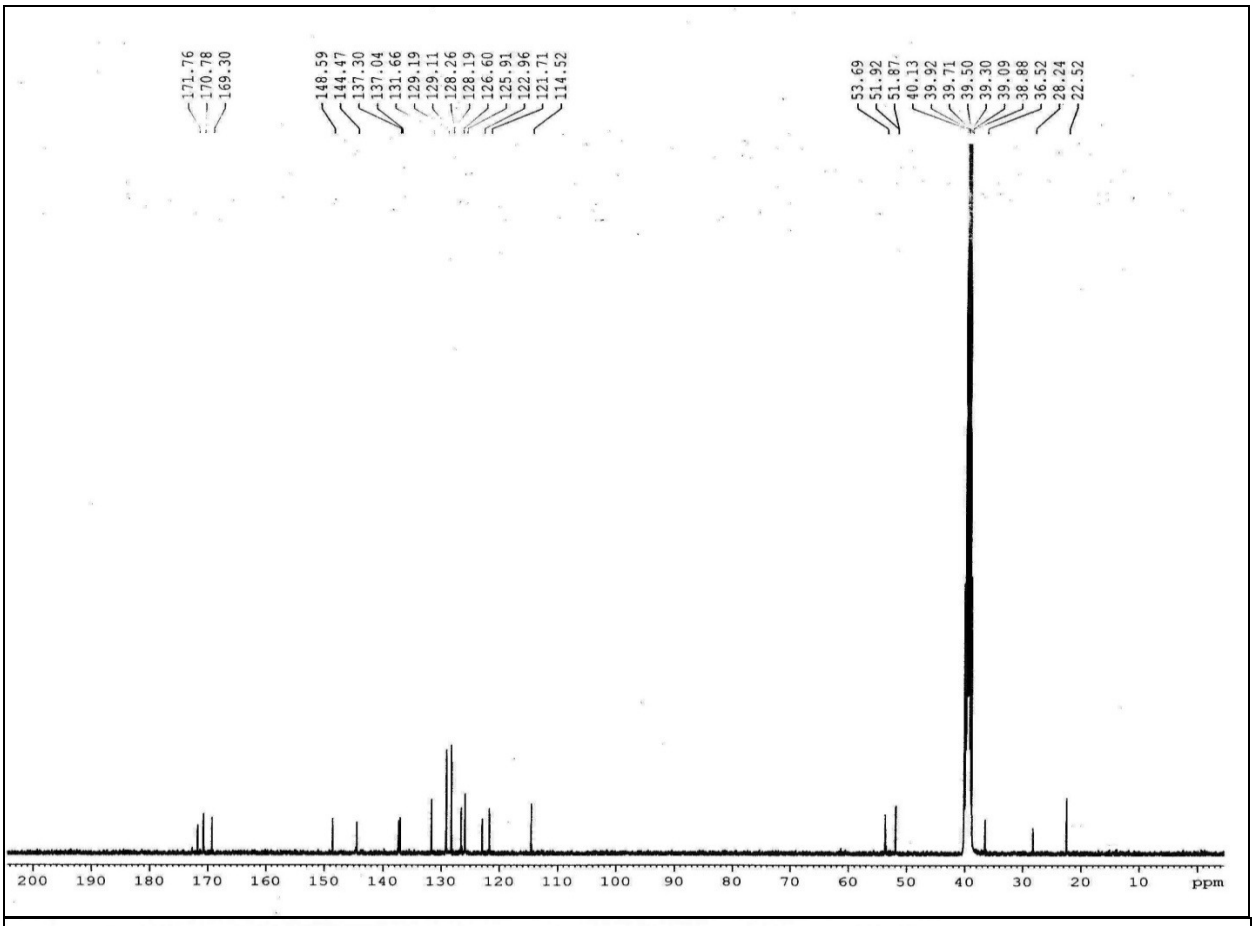
Micromass : Q-Tof micro (YA-105)
C23H24N6O6
Dept. Of Chemistry I.I.T.(B)
22-Sep-201112:12:27
SRK-DB-52-384 2 (0.020) AM (Top,5, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (1:31)
TOF MS ES+
2.85e3



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 481.1826 | 481.1836 | -1.0 | -2.1 | 14.5 | 1 | C23 H25 N6 O6 |

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






**Elemental Composition Report**

**Page 1**

**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

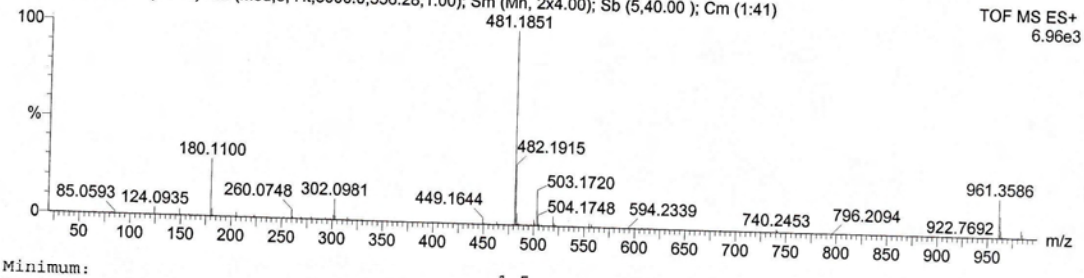
44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105)
C23H24N6O6
SRK-DB-52-392 7 (0.070) AM (Med,5, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00 ); Cm (1:41)

Dept. Of Chemistry I.I.T.(B)

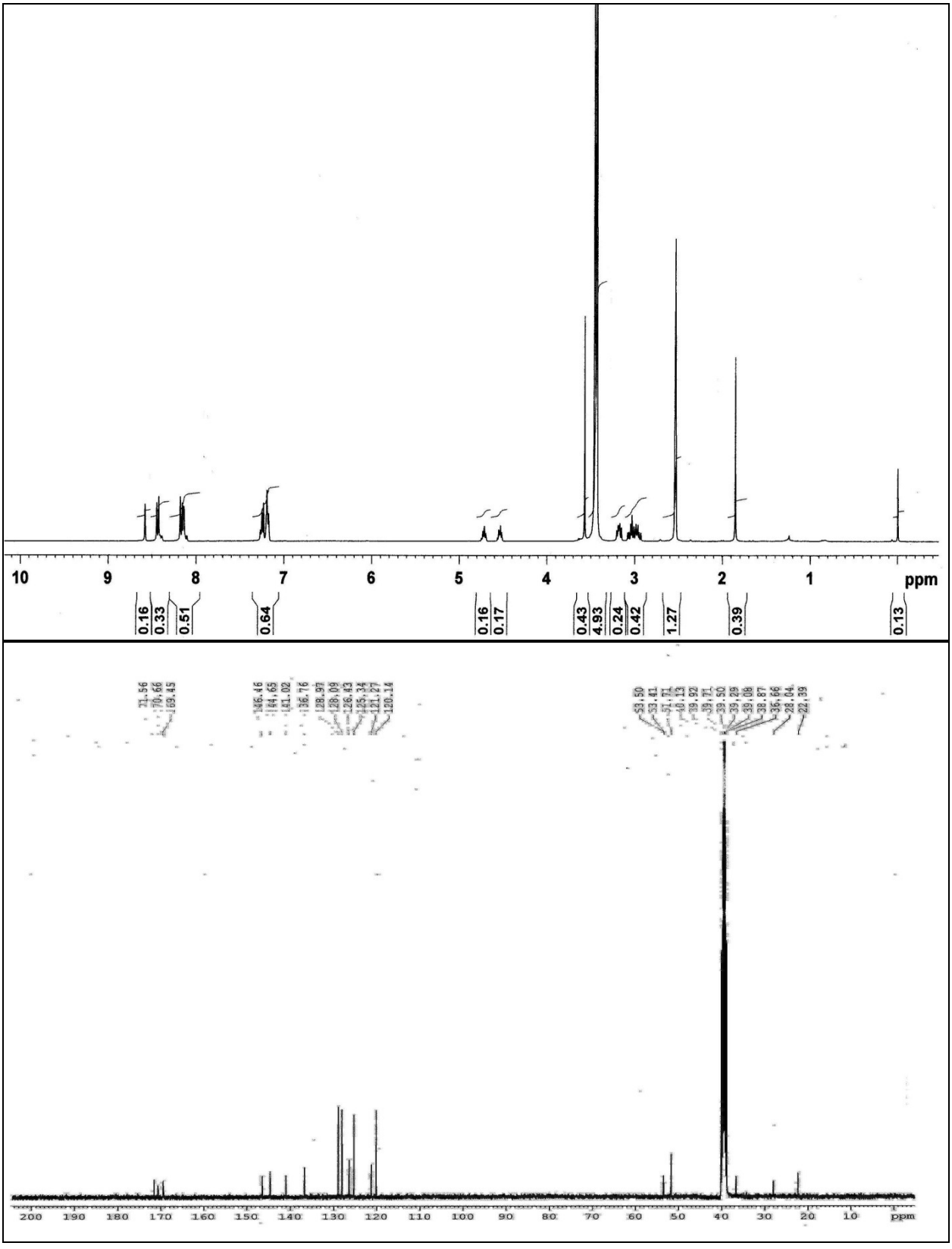
27-Sep-201114:14:23

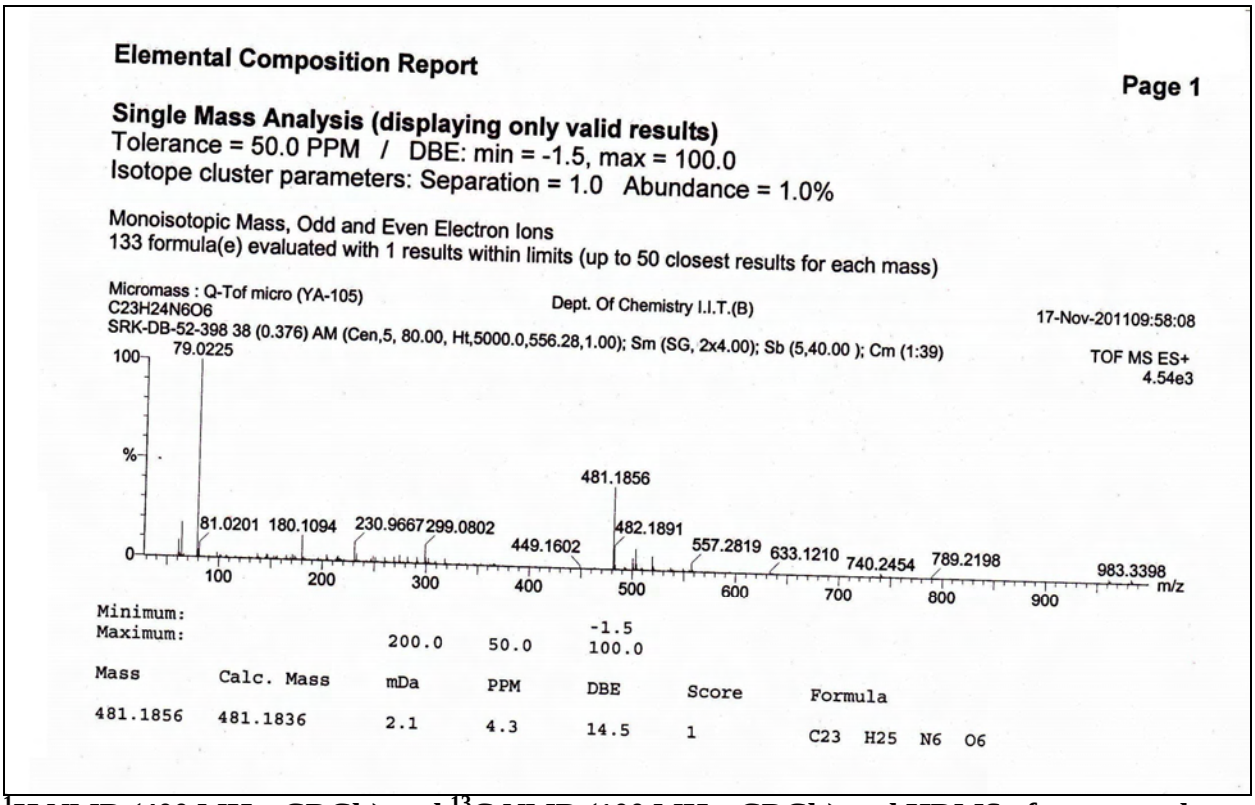
TOF MS ES+
6.96e3



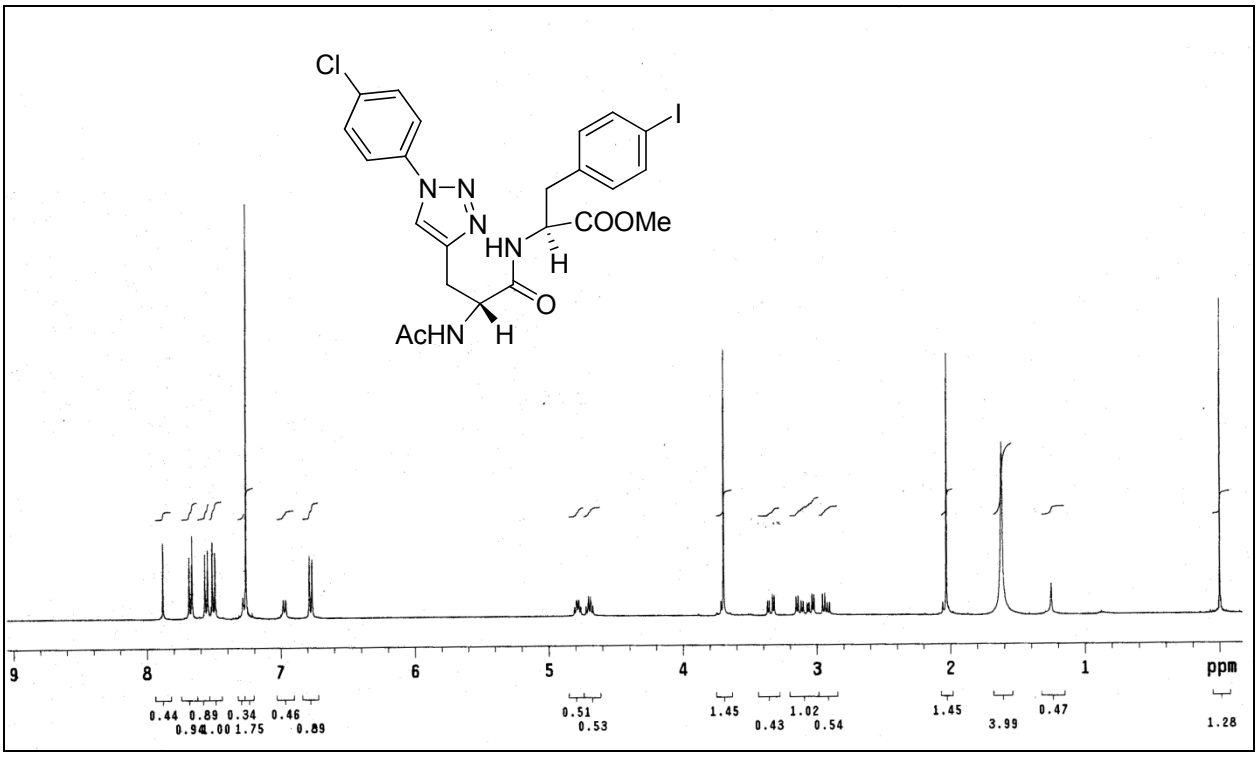

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 60.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 481.1851 | 481.1836 | 1.5 | 3.2 | 14.5 | 1 | C23 H25 N6 O6 |

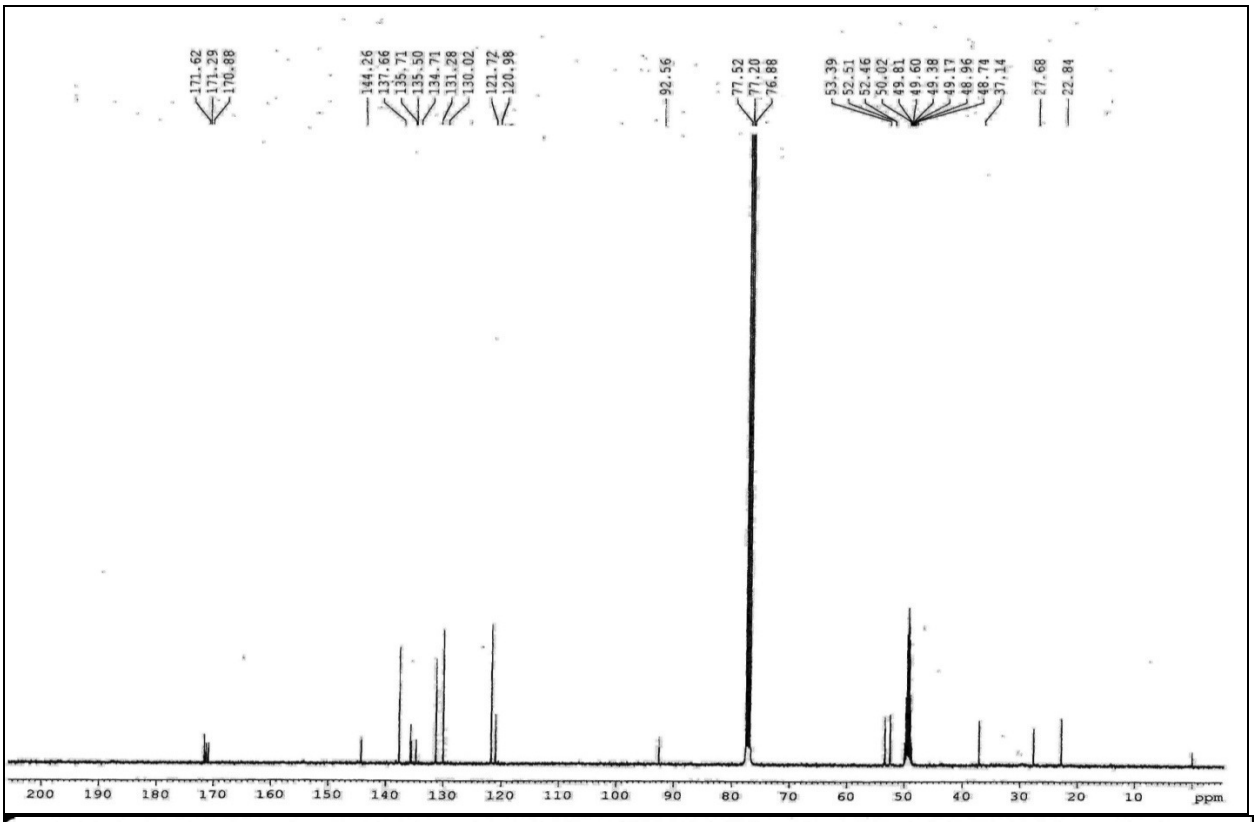
**$^{1}$H NMR (400 MHz, DMSO) and $^{13}$C NMR (100 MHz, DMSO) and HRMS of compound 6**






**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 7**





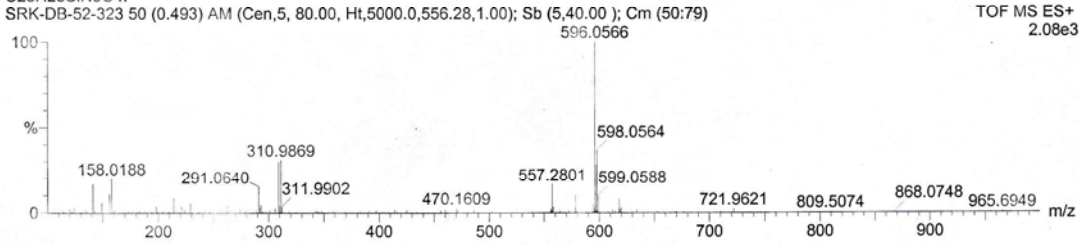

**Elemental Composition Report** **Page 1**

**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)

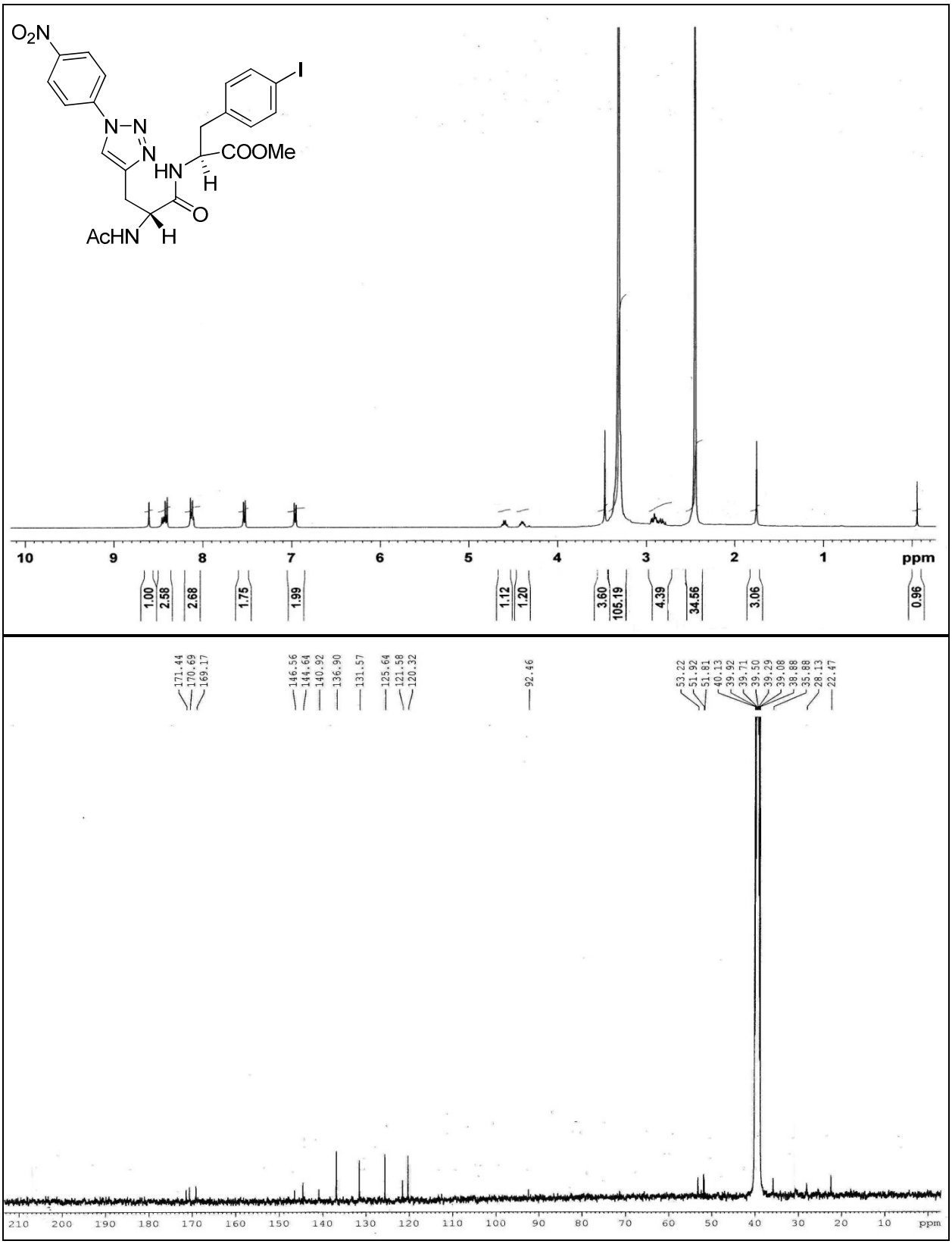
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 26-May-201111:17:45

C23H23ClN5O4I
SRK-DB-52-323 50 (0.493) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (50:79) TOF MS ES+
2.08e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 596.0566 | 596.0562 | 0.5 | 0.8 | 13.5 | 1 | C23 H24 N5 O4 Cl I |

**$^{1}$H NMR (400 MHz, DMSO) and $^{13}$C NMR (100 MHz, DMSO) and HRMS of compound 8**

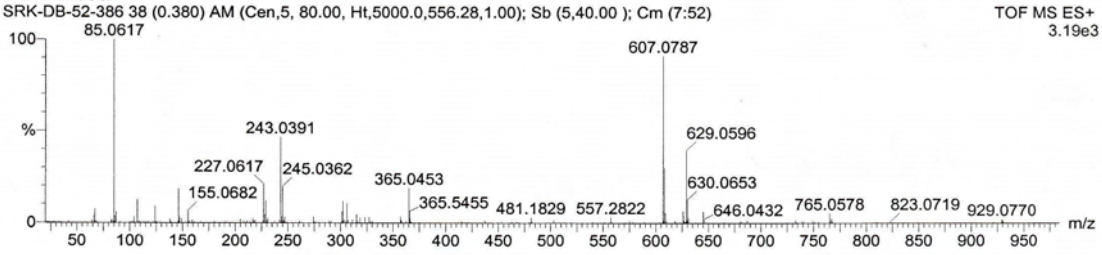


**Elemental Composition Report** **Page 1**

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

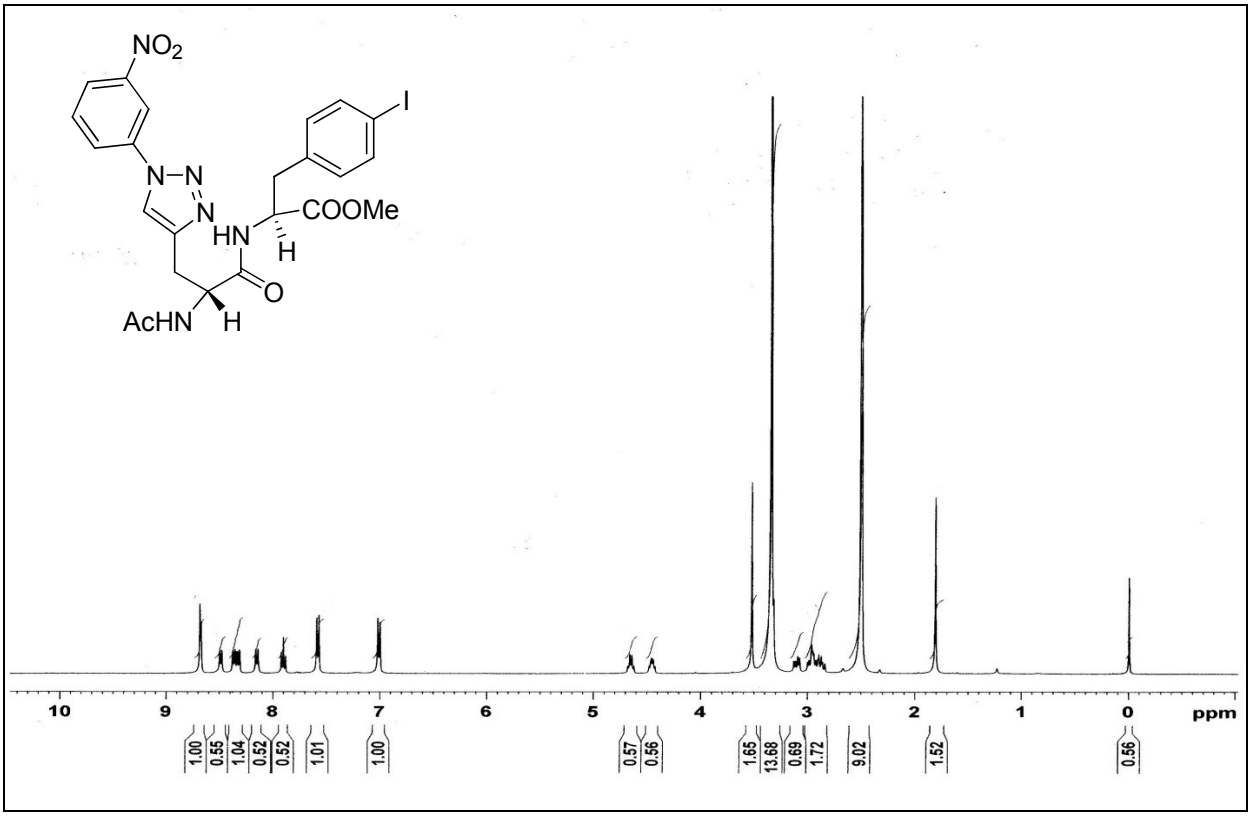
Monoisotopic Mass, Odd and Even Electron Ions
93 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

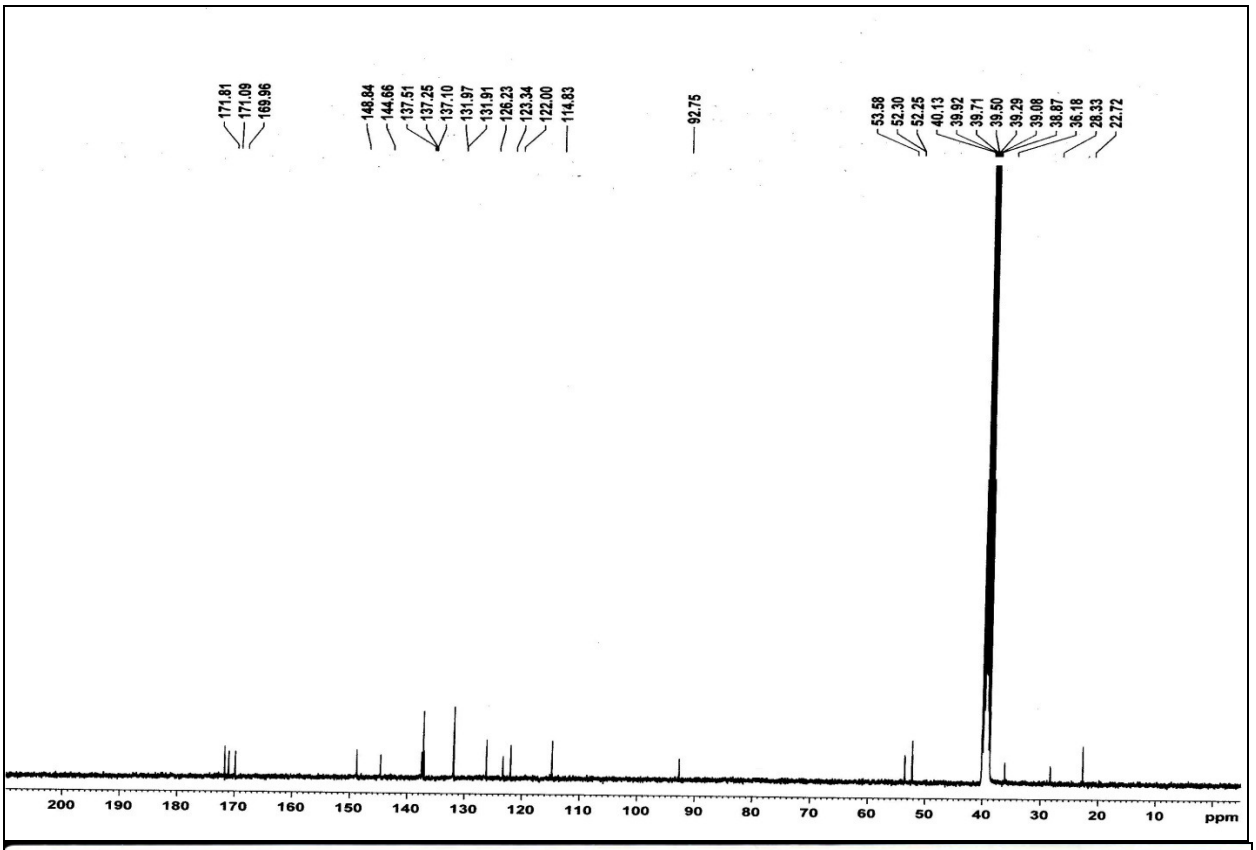
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 27-Sep-201114:03:52
C23H23N6O6I
SRK-DB-52-386 38 (0.380) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (7:52) TOF MS ES+
3.19e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 60.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 607.0787 | 607.0802 | -1.5 | -2.5 | 14.5 | 1 | C23 H24 N6 O6 I |

**$^{1}$H NMR (400 MHz, DMSO) and $^{13}$C NMR (100 MHz, DMSO) and HRMS of compound 9**



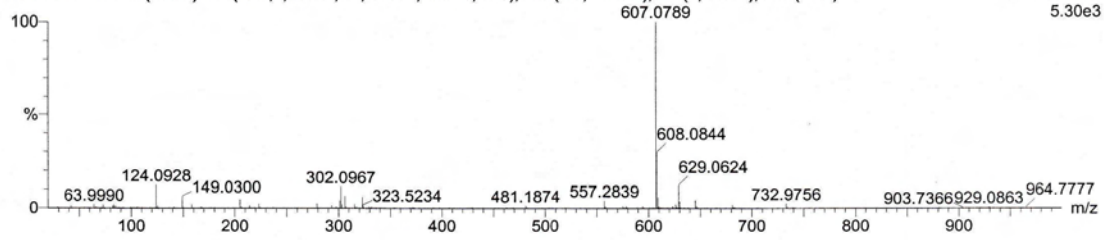



**Elemental Composition Report** **Page 1**

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

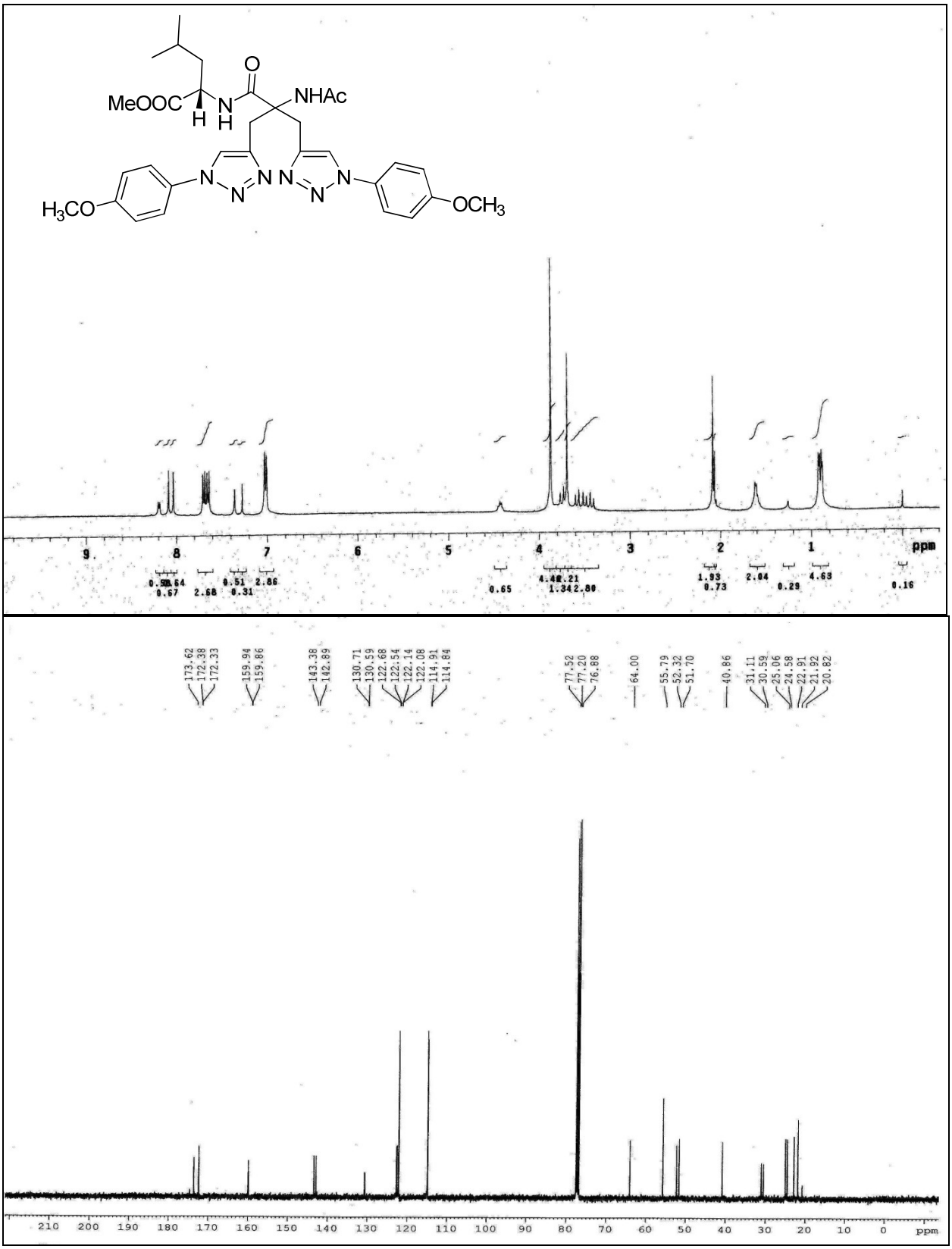
Monoisotopic Mass, Odd and Even Electron Ions
93 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

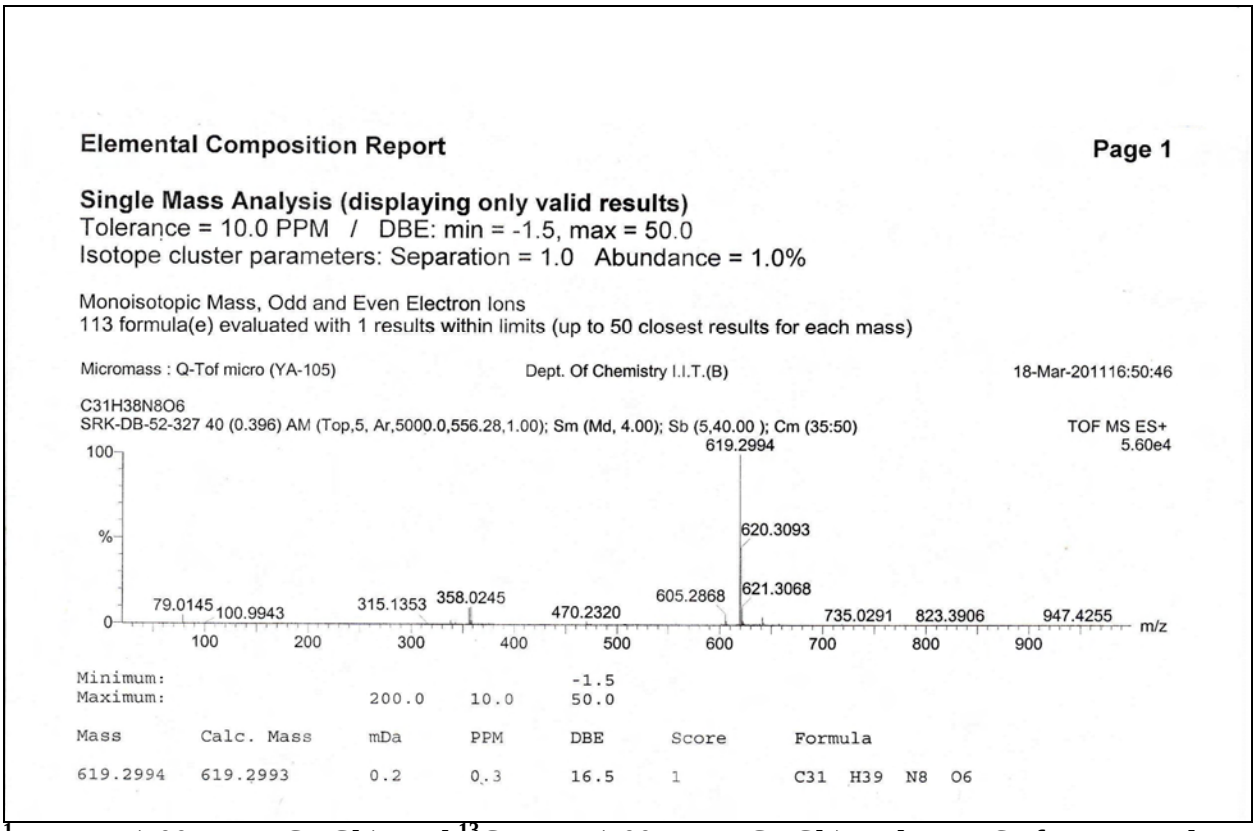
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 27-Sep-201114:21:29
C23H23N6O6I
SRK-DB-52-390 4 (0.040) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00 ); Cm (1:49) TOF MS ES+
5.30e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 60.0 | 50.0 | | |
| 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** **Page 1**

**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)

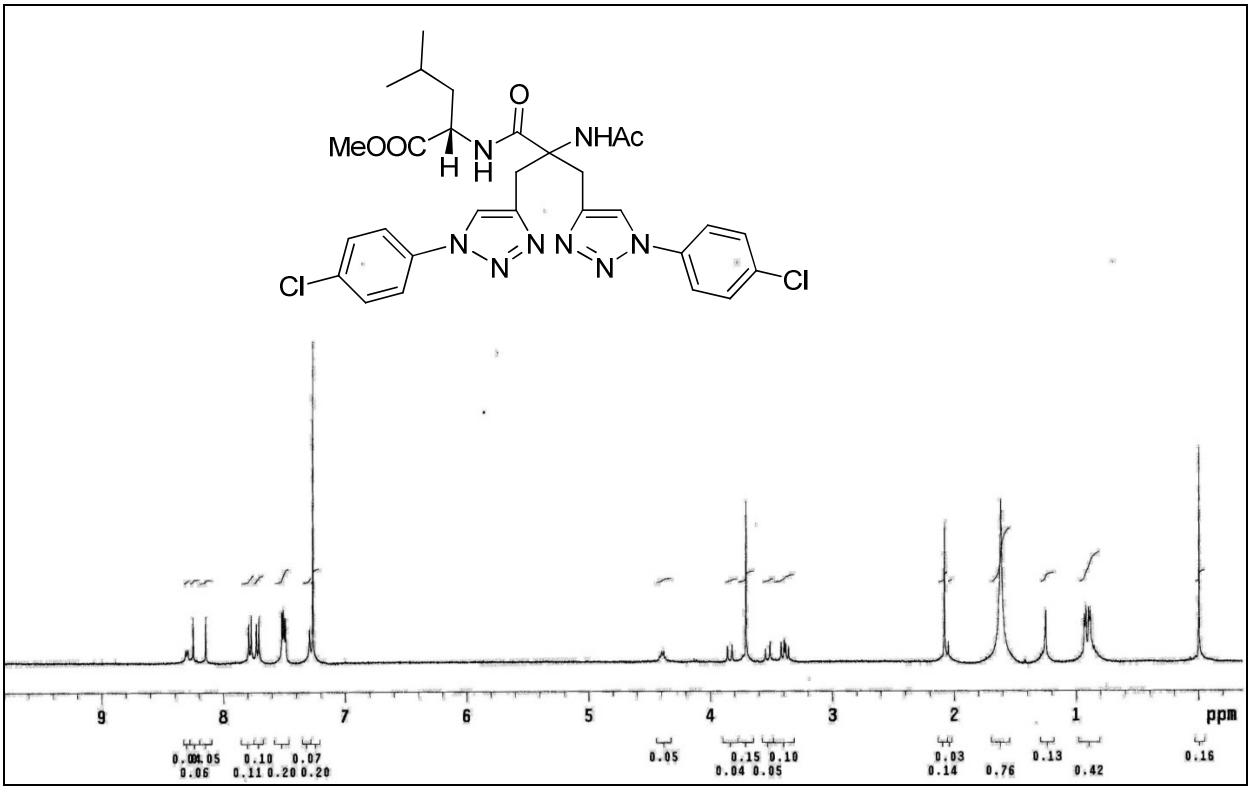
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 18-Mar-201116:50:46

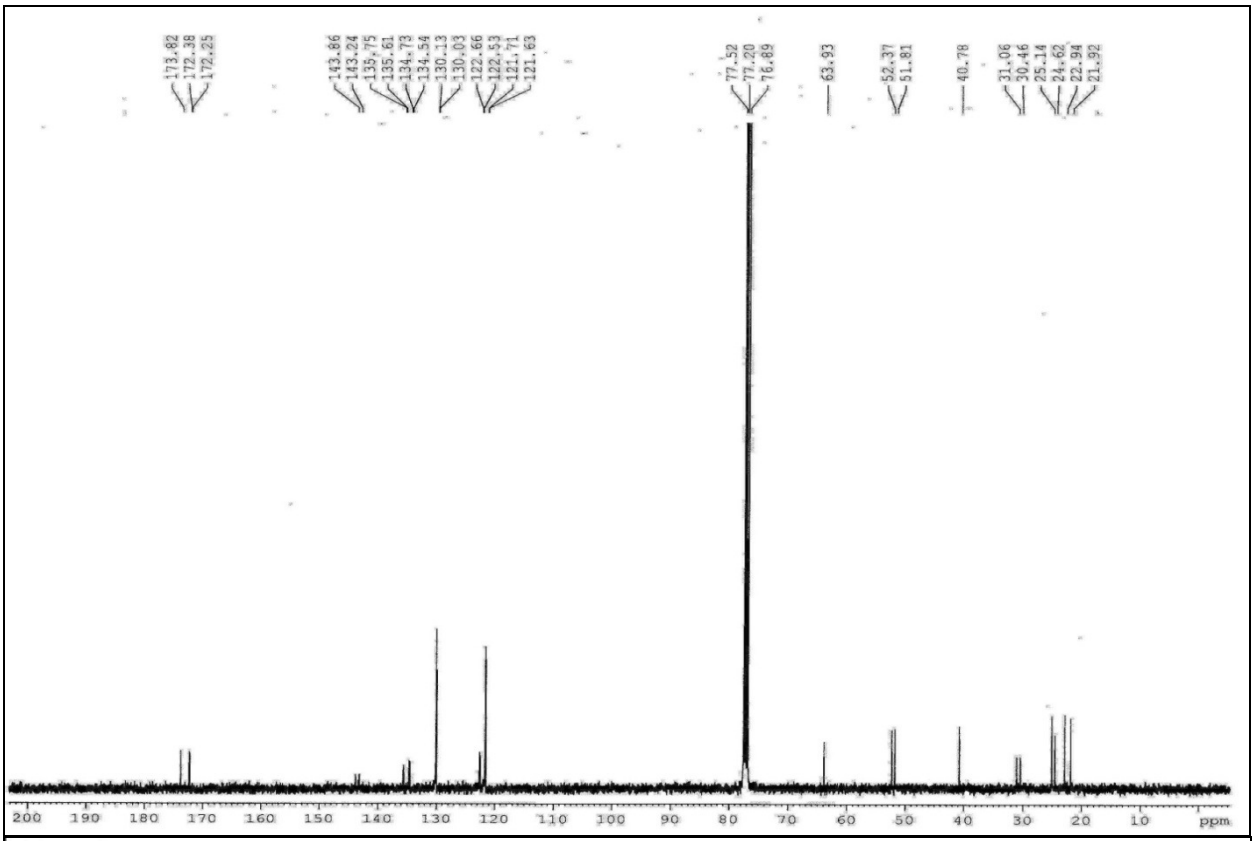
C31H38N8O6
SRK-DB-52-327 40 (0.396) AM (Top,5, Ar,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (5,40.00 ); Cm (35:50) TOF MS ES+ 5.60e4



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 619.2994 | 619.2993 | 0.2 | 0.3 | 16.5 | 1 | C31 H39 N8 O6 |

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 12**






**Elemental Composition Report**

**Page 1**

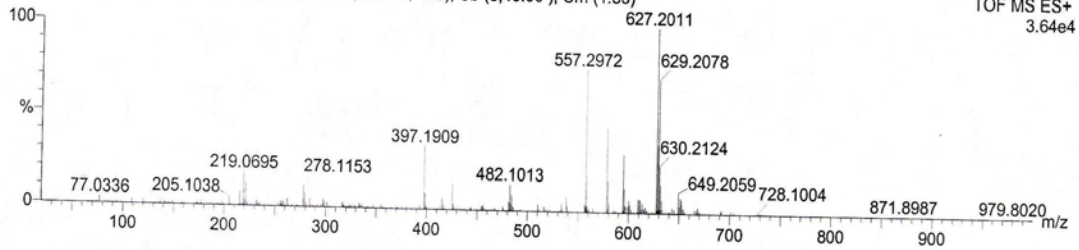
**Single Mass Analysis (displaying only valid results)**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

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) 17-Mar-201116:51:42

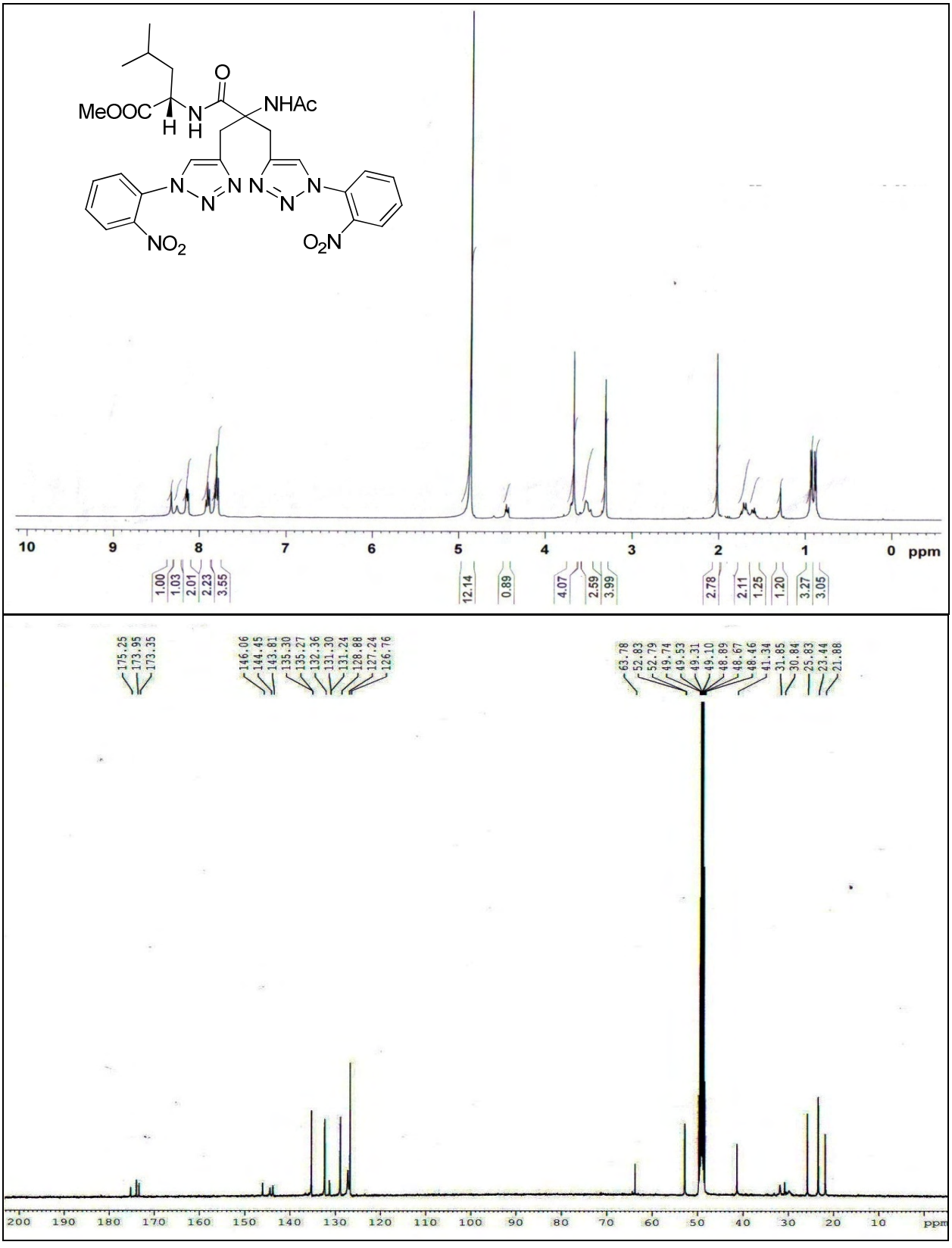
C29H32Cl2N8O4
SRK-DB-52-325 7 (0.058) AM (Top,5, Ar,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (1:33)

TOF MS ES+
3.64e4




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 627.2011 | 627.2002 | 0.9 | 1.5 | 16.5 | 1 | C29 H33 N8 O4 Cl2 |

**$^{1}$H NMR (400 MHz, $CD_3OD$) and $^{13}$C NMR (100 MHz, $CD_3OD$) and HRMS of compound 13**



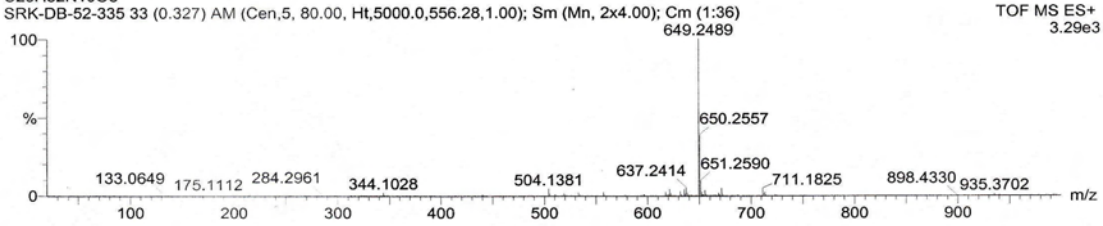
**Elemental Composition Report** **Page 1**

**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)

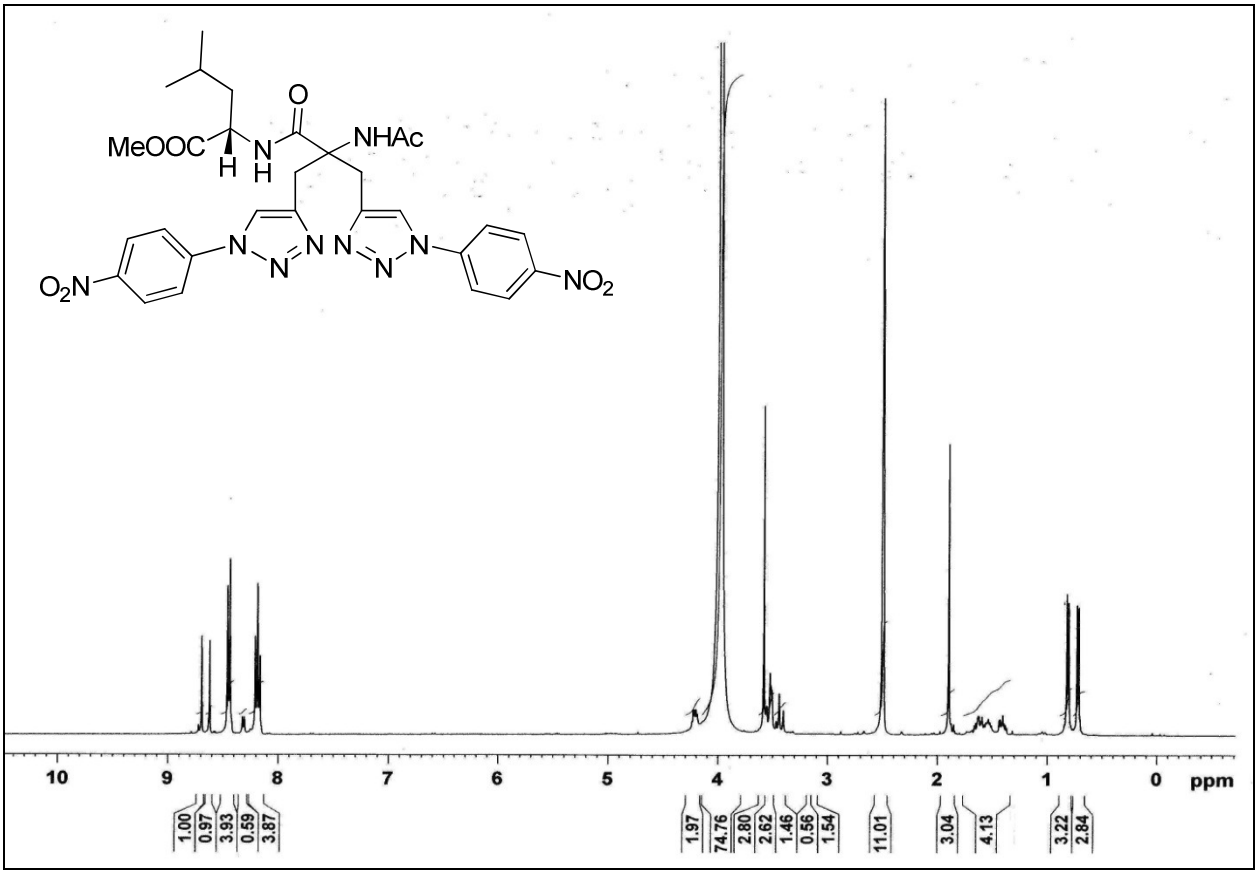
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 20-Apr-201116:20:58

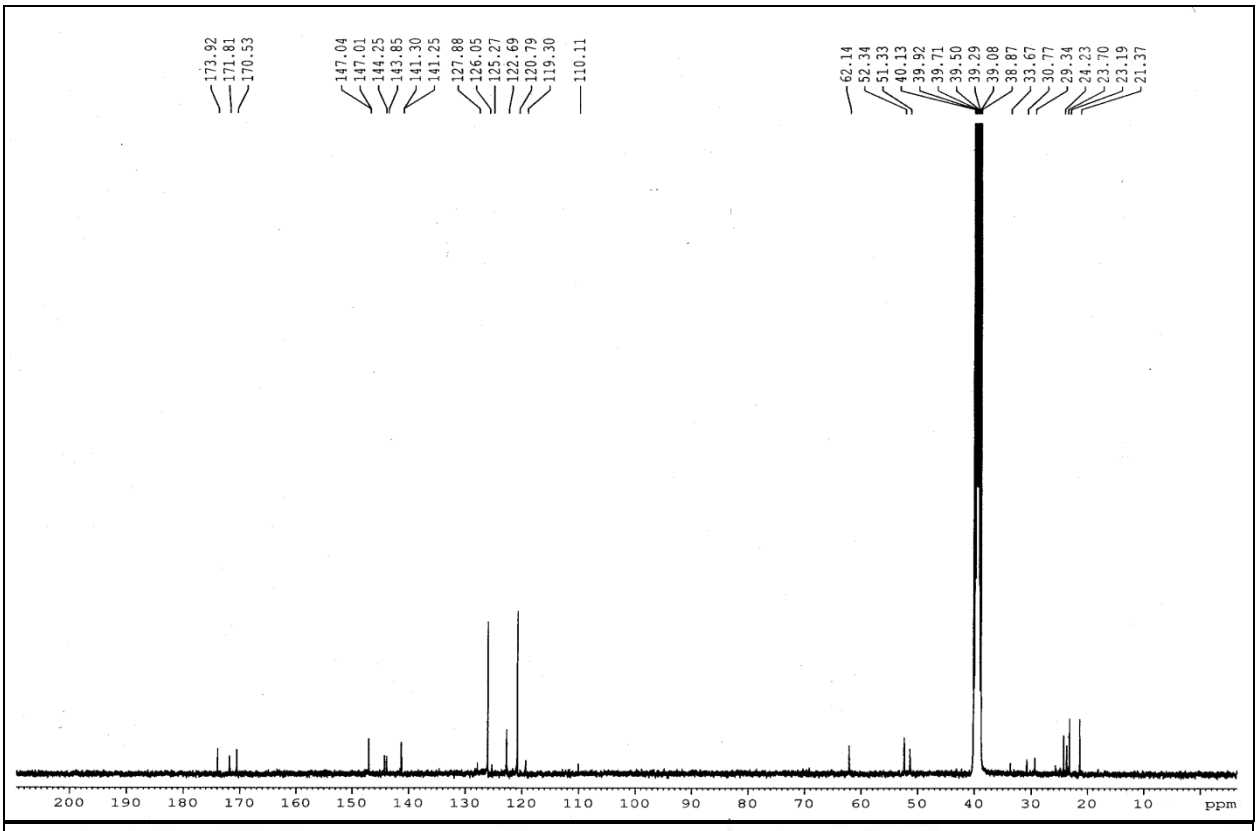
C29H32N10O8
SRK-DB-52-335 33 (0.327) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Cm (1:36) TOF MS ES+
3.29e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 649.2489 | 649.2483 | 0.6 | 1.0 | 18.5 | 1 | C29 H33 N10 O8 |

**$^{1}$H NMR (400 MHz, DMSO) and $^{13}$C NMR (100 MHz, DMSO) and HRMS of compound 14**



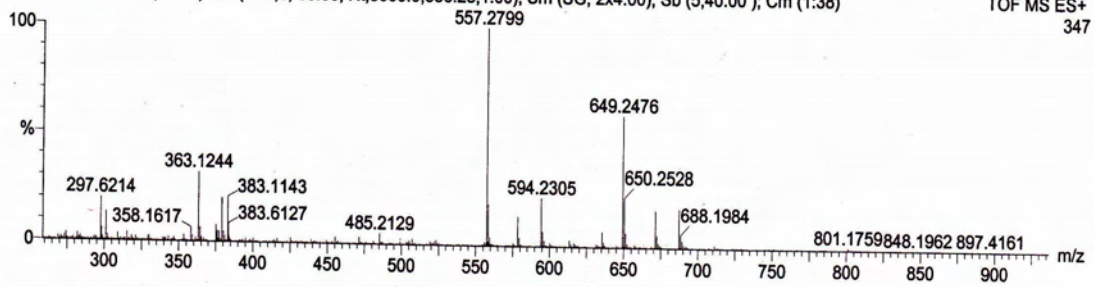



**Elemental Composition Report** **Page 1**

**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%

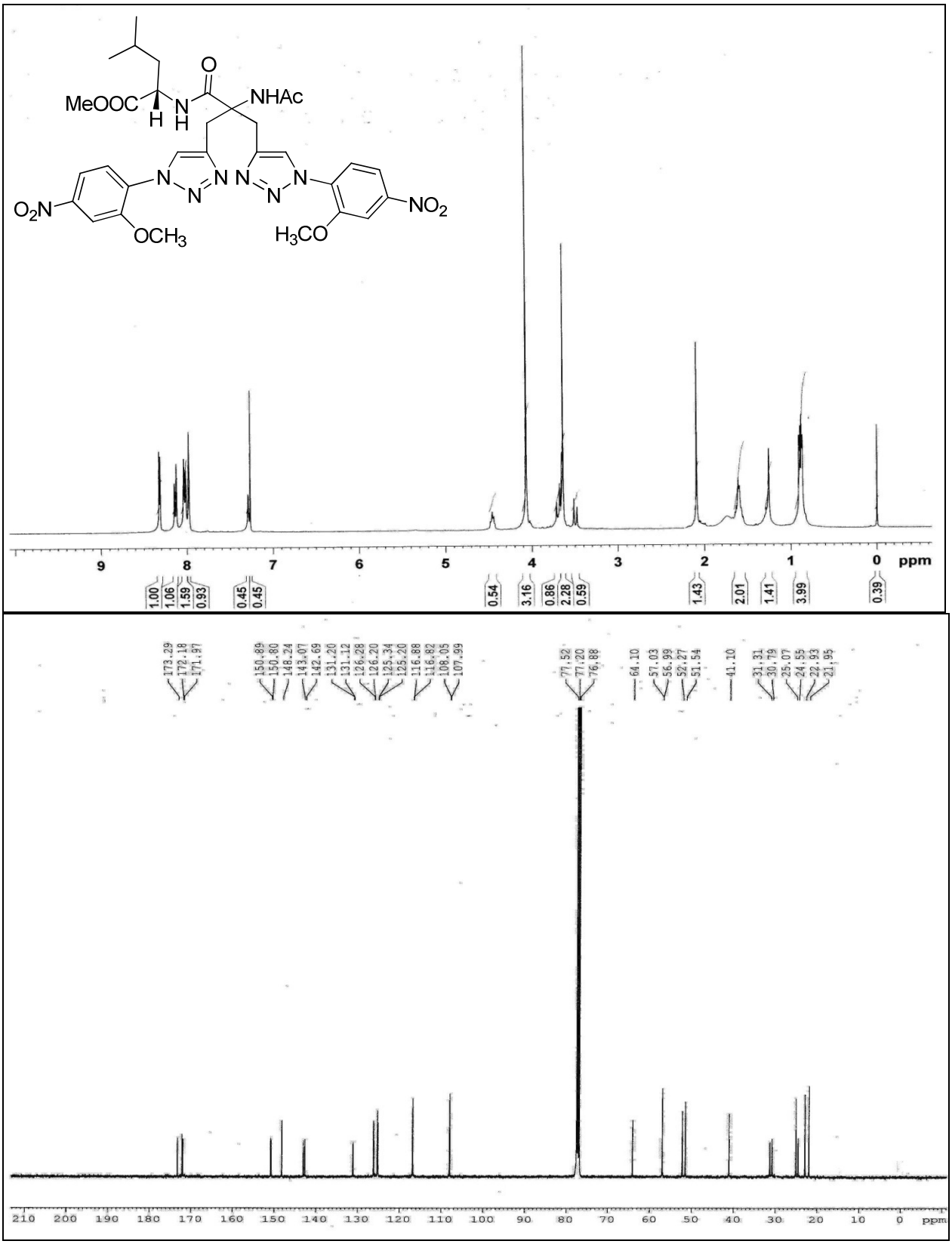
Monoisotopic Mass, Odd and Even Electron Ions
273 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

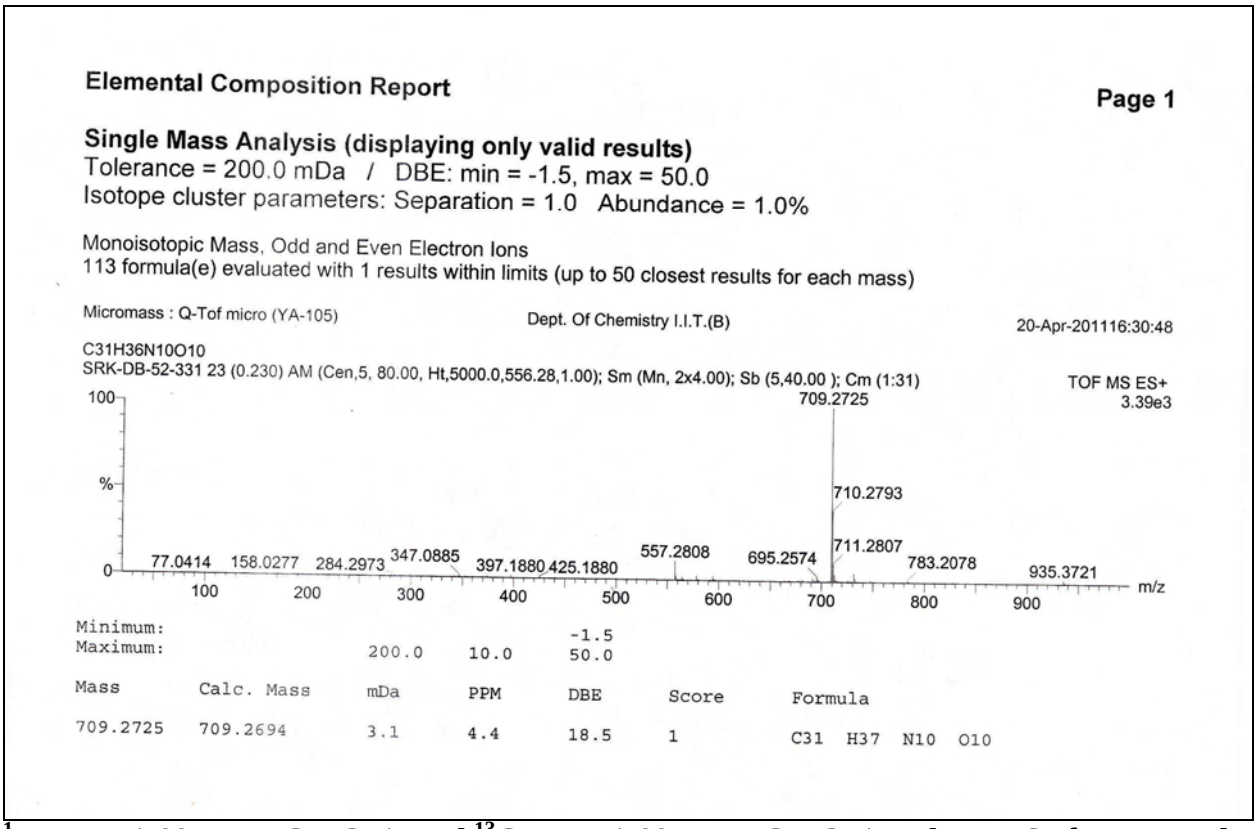
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 17-Nov-201110:10:14
C29H32N10O8
SRK-DB-52-397 25 (0.246) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (SG, 2x4.00); Sb (5,40.00 ); Cm (1:38) TOF MS ES+
347




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 5.0 | 100.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 649.2476 | 649.2483 | -0.7 | -1.0 | 18.5 | 1 | C29 H33 N10 O8 |

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 15**





**Elemental Composition Report** Page 1

**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
113 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

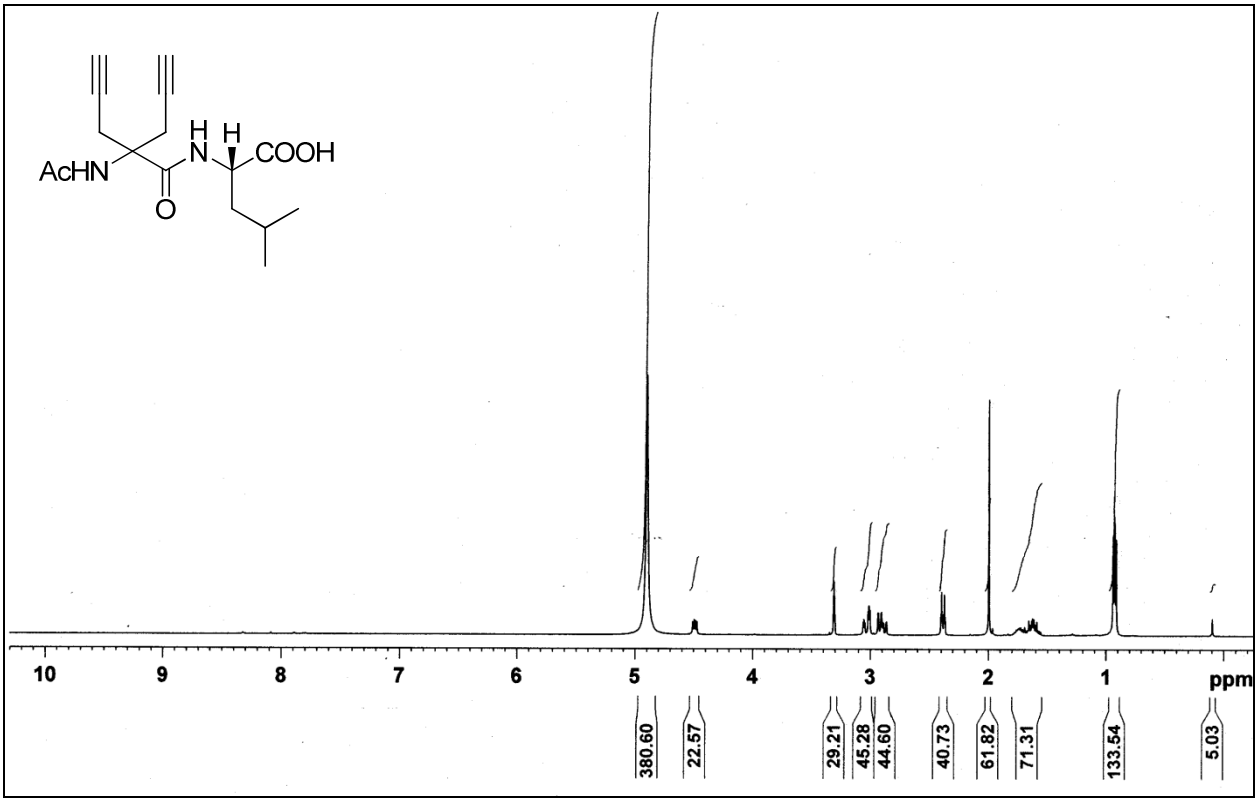
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 20-Apr-201116:30:48

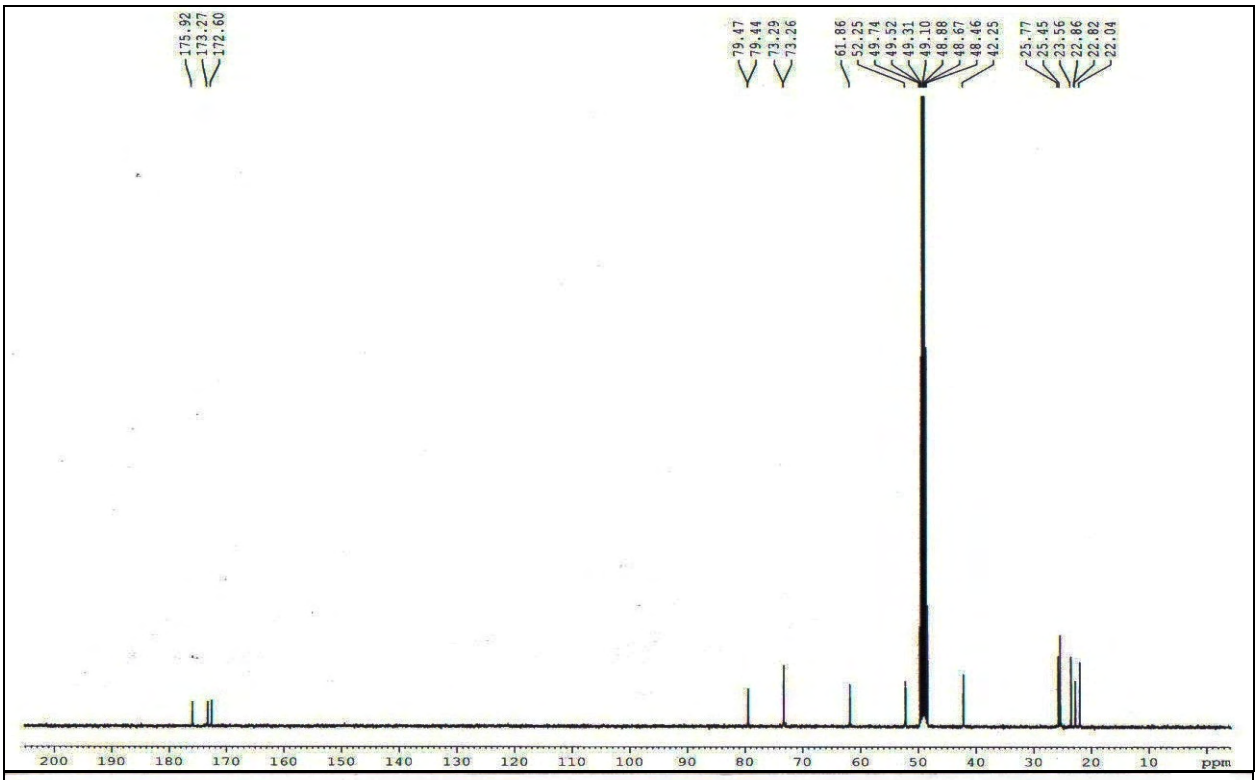
C31H36N10O10
SRK-DB-52-331 23 (0.230) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00 ); Cm (1:31) TOF MS ES+ 3.39e3



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 709.2725 | 709.2694 | 3.1 | 4.4 | 18.5 | 1 | C31 H37 N10 O10 |

**$^{1}$H NMR (400 MHz, $CD_3OD$) and $^{13}$C NMR (100 MHz, $CD_3OD$) and HRMS of compound 16**





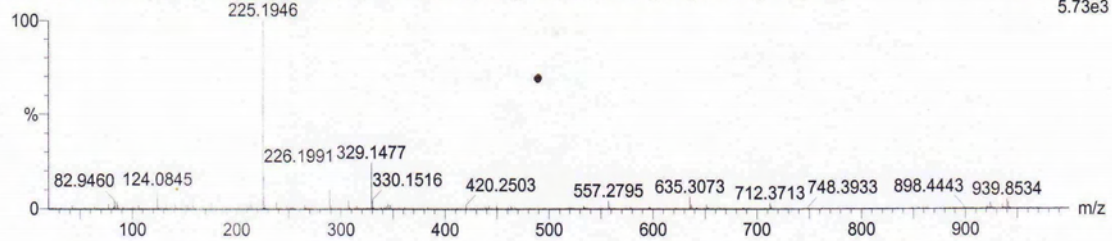

**Elemental Composition Report** **Page 1**

**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(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

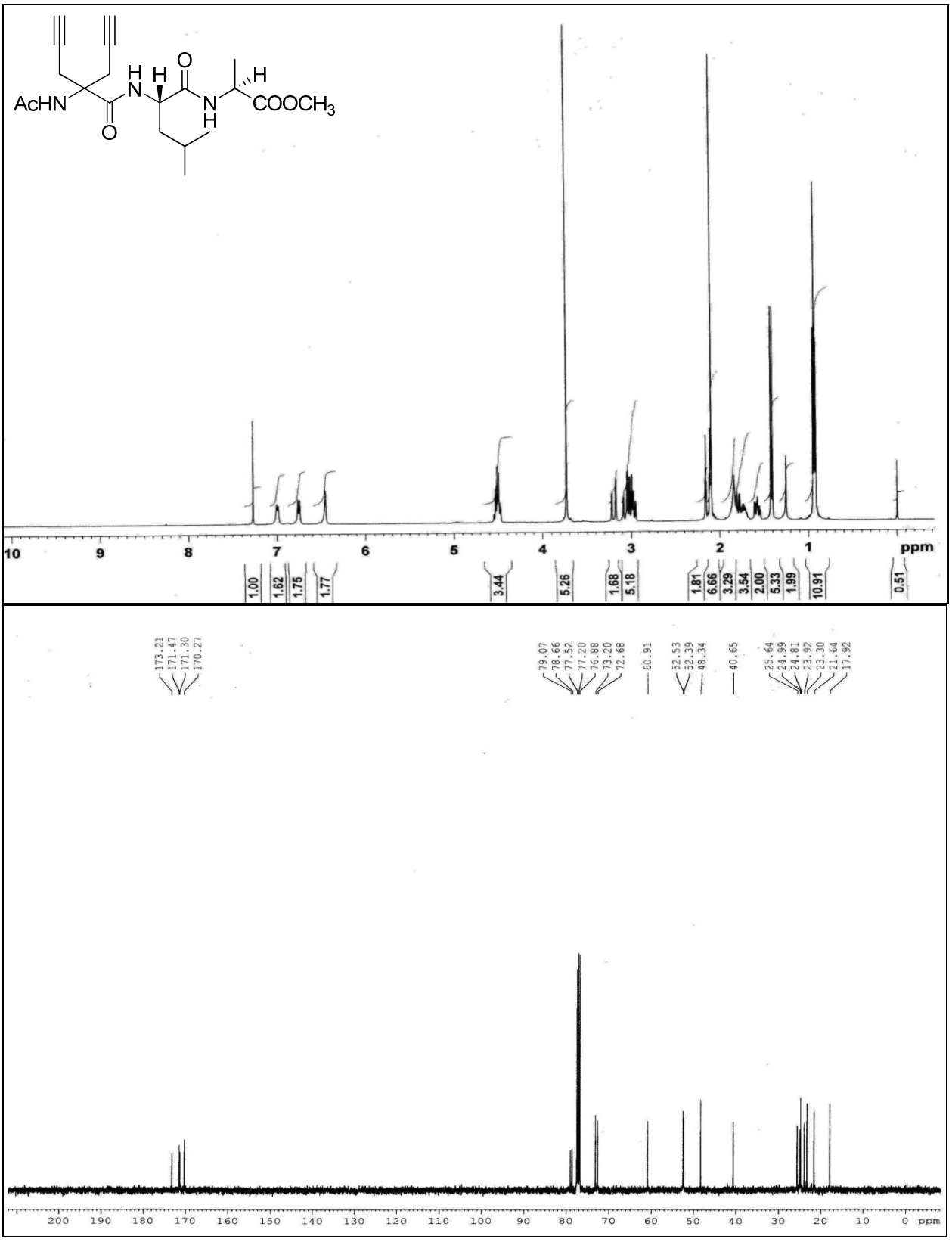
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 20-Apr-201116:57:32

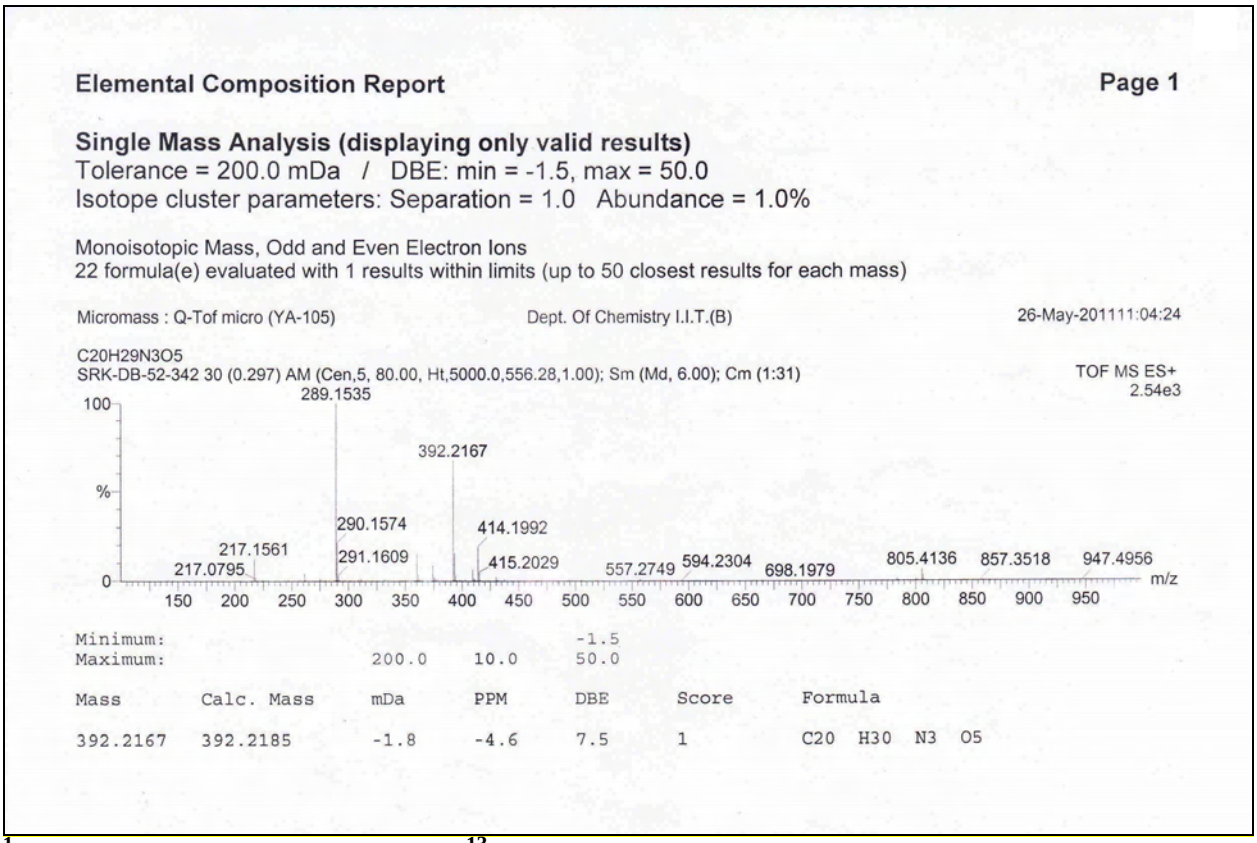
C16H22N2O4
SRK-DB-52-336 7 (0.070) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (SG, 2x4.00); Sb (5,40.00 ); Cm (1:34) TOF MS ES+
5.73e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 307.1652 | 307.1658 | -0.6 | -1.8 | 6.5 | 1 | C16 H23 N2 O4 |

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 17**





**Elemental Composition Report** Page 1

**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
22 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

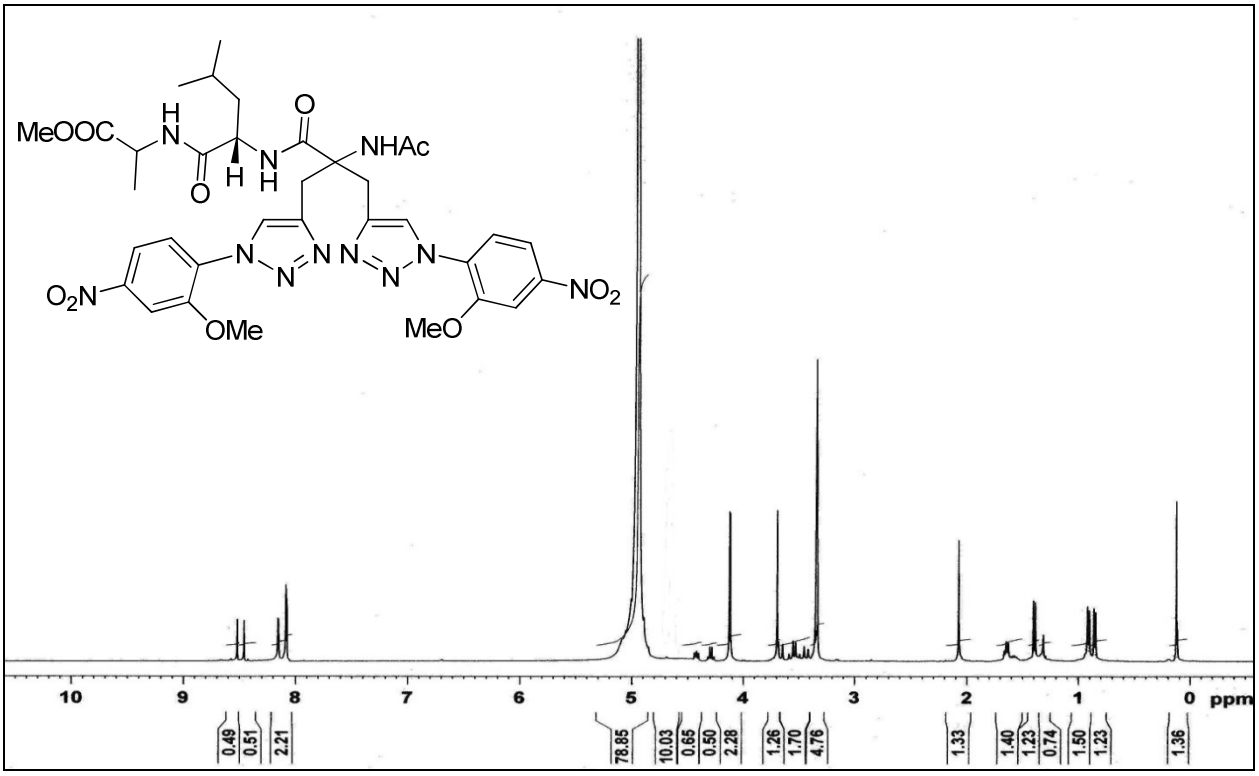
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 26-May-201111:04:24

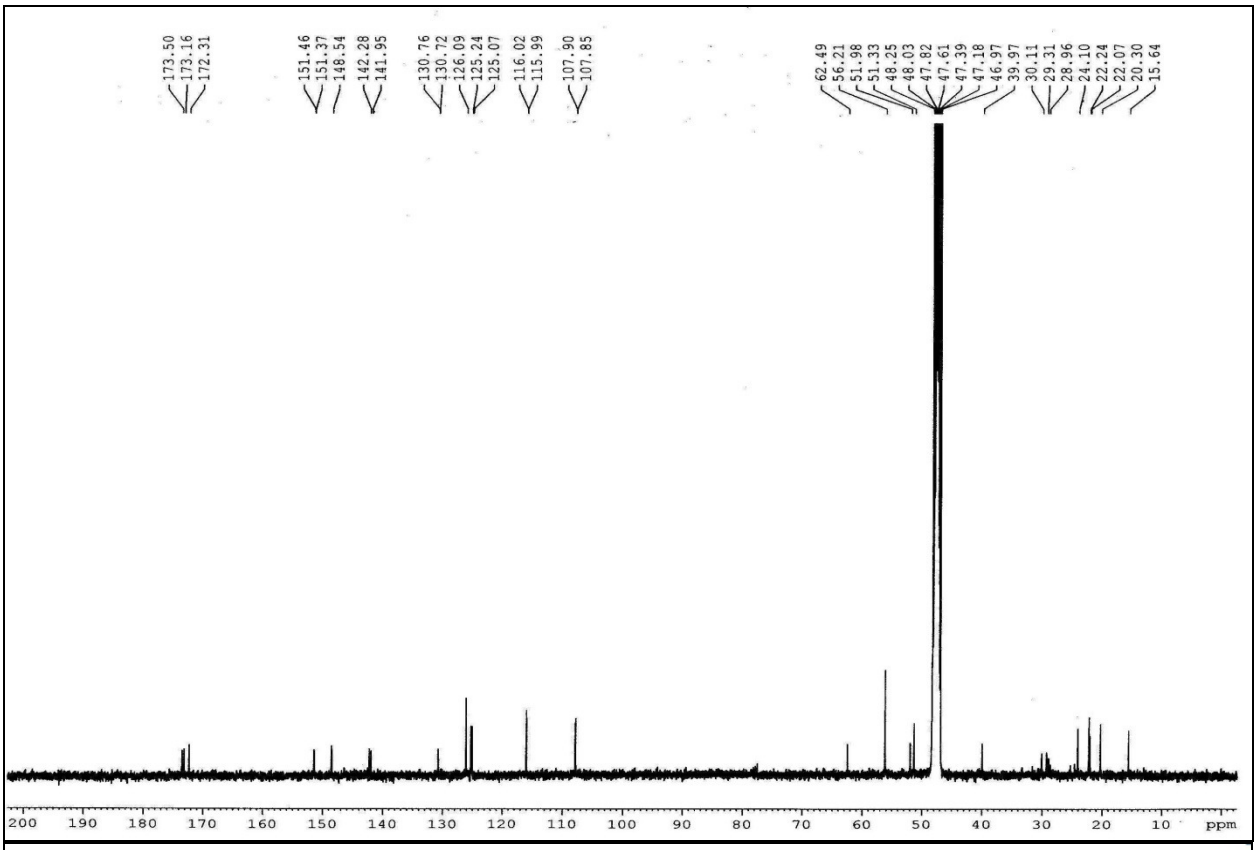
C20H29N3O5
SRK-DB-52-342 30 (0.297) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Md, 6.00); Cm (1:31)
TOF MS ES+
2.54e3



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 392.2167 | 392.2185 | -1.8 | -4.6 | 7.5 | 1 | C20 H30 N3 O5 |

**$^{1}$H NMR (400 MHz, $CD_3OD$) and $^{13}$C NMR (100 MHz, $CD_3OD$) and HRMS of compound 18**





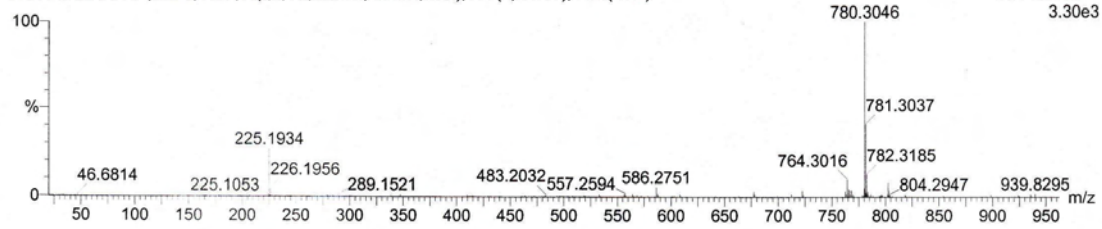

**Elemental Composition Report** **Page 1**

**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)

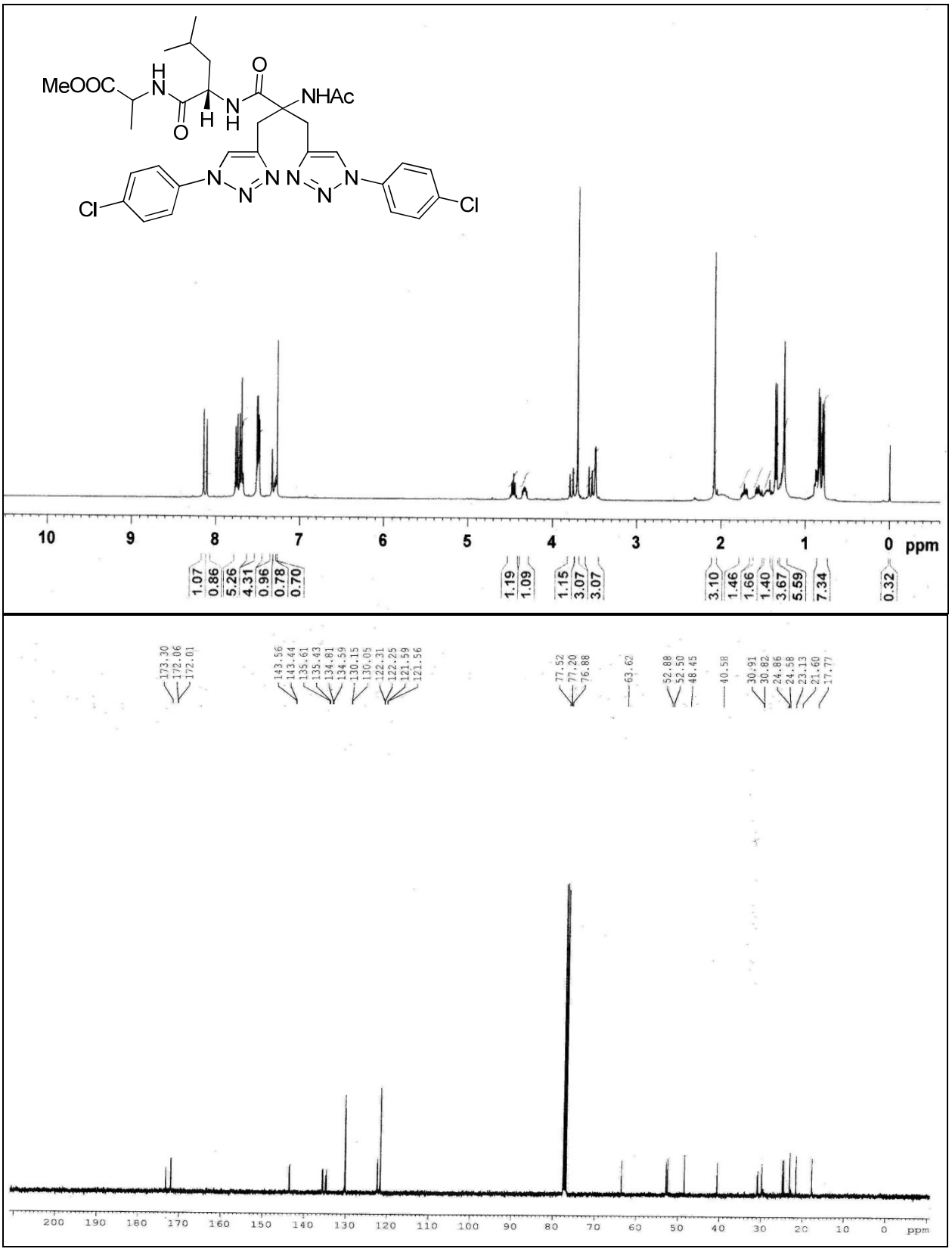
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 20-Apr-201117:15:00

C34H41N11O11
SRK-DB-52-344 7 (0.070) AM (Top,5, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (1:32) TOF MS ES+
3.30e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 780.3046 | 780.3065 | -2.0 | -2.5 | 19.5 | 1 | C34 H42 N11 O11 |

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 19**



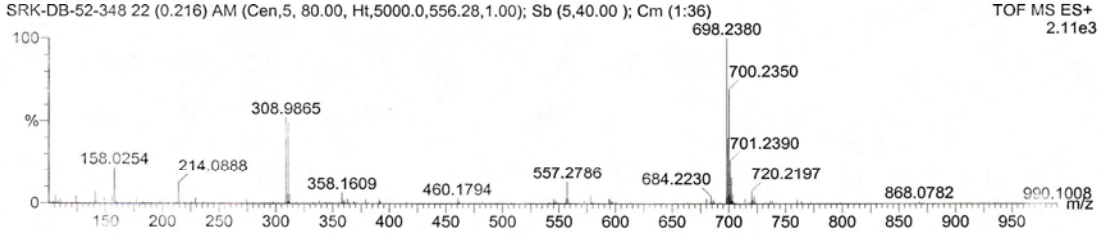
**Elemental Composition Report** **Page 1**

**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)

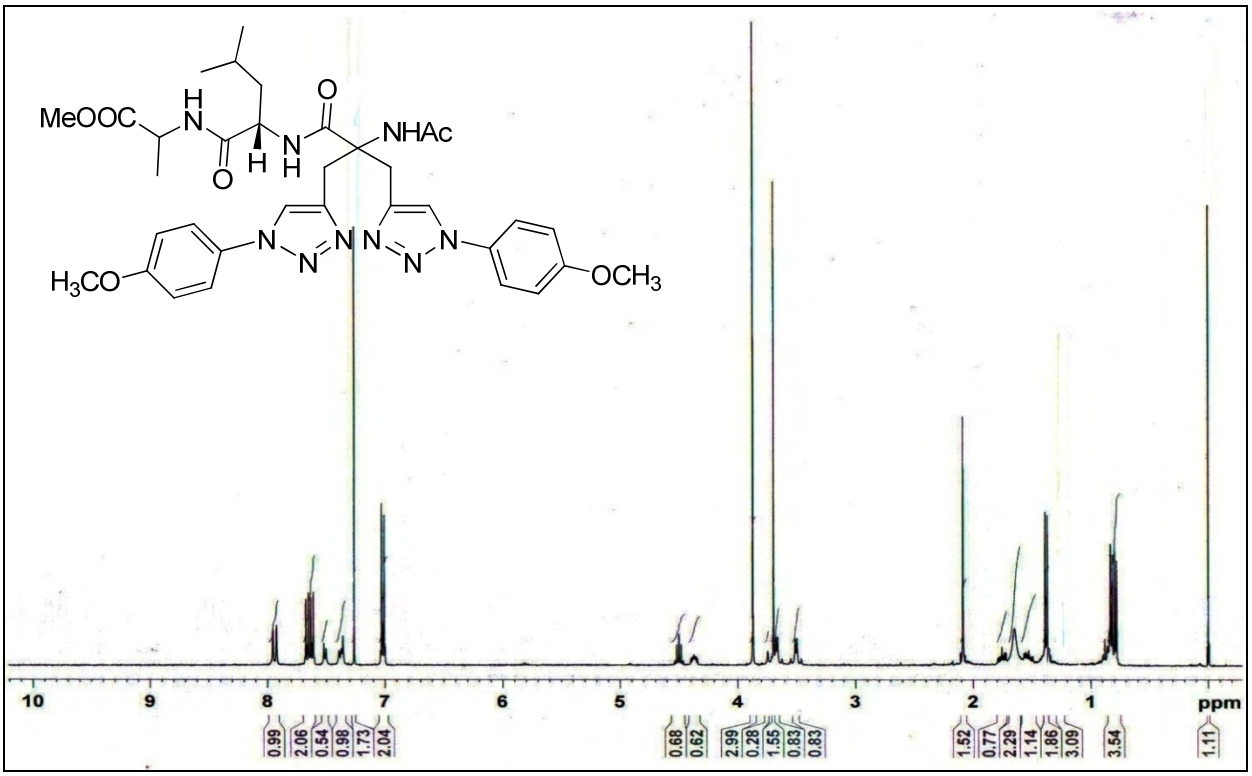
Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 26-May-201110:26:46

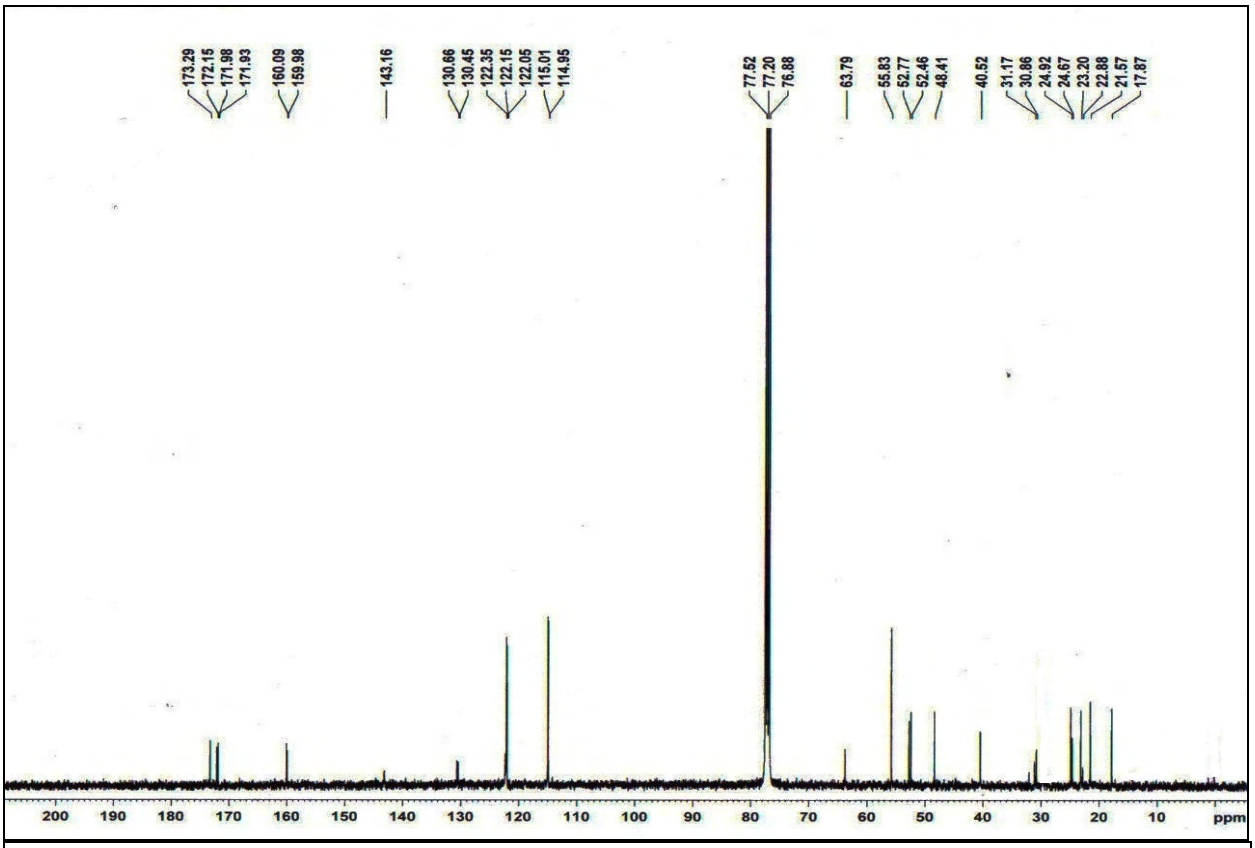
C32H37Cl2N9O5
SRK-DB-52-348 22 (0.216) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (1:36) TOF MS ES+ 2.11e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 698.2380 | 698.2373 | 0.7 | 1.1 | 17.5 | 1 | C32 H38 N9 O5 Cl2 |

**$^{1}$H NMR (400 MHz, $CDCl_3$) and $^{13}$C NMR (100 MHz, $CDCl_3$) and HRMS of compound 20**





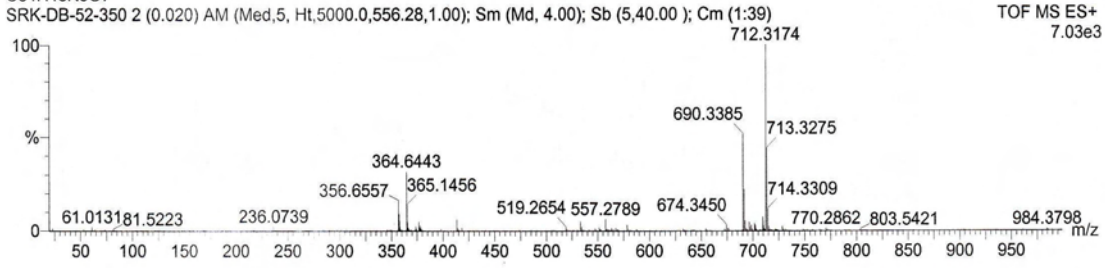

**Elemental Composition Report** **Page 1**

**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)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 20-Apr-201116:39:25

C34H43N9O7
SRK-DB-52-350 2 (0.020) AM (Med,5, Ht,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (5,40.00 ); Cm (1:39) TOF MS ES+
7.03e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 690.3385 | 690.3364 | 2.1 | 3.1 | 17.5 | 1 | C34 H44 N9 O7 |