

## Supplementary Information

### Synthesis, *in vitro* antibacterial, antifungal biological activities along with *in silico* molecular docking studies of substituted 2-[4-(3-oxo-[1,2,4] triazolo [4,3-a]pyridin-2-ylmethyl)-[1,2,3]triazol-1-yl]-N-(4-phenyl-thiazol-2-yl)-acetamide

K Joshi<sup>a</sup>, S Maheta<sup>a</sup>, A Mahida<sup>a</sup> & G G Dubal<sup>\*b</sup>

<sup>a</sup>Department of Chemistry, D K V Arts and Science College, Jamnagar 361 008, Gujarat, India

<sup>b</sup>Department of Chemistry, School of Science, R K University, Rajkot 360 020, Gujarat, India

E-mail: [dr.gaurangdubal@gmail.com](mailto:dr.gaurangdubal@gmail.com)

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**2-(4-((3-oxo-[1,2,4]triazolo[4,3-a]pyridin-2(3H)-yl)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-*p*-tolylthiazol-2-yl)acetamide (8a):** White Solid; Yield: 85%; mp: 165-167°C; Mol. Formula: C<sub>21</sub>H<sub>18</sub>N<sub>8</sub>O<sub>2</sub>S; Mol. Mass: 447 g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 646; <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.78 (brs, 1H, N-H), 8.16 (s, 1H), 7.89-7.88 (d,  $j=6.6$ , 1H), 7.79-7.77 (d,  $j=6.6$ , 2H), 7.57 (s, 1H), 7.22 (s, 4H), 6.63 (s, 1H), 5.45 (s, 2H, -CH<sub>2</sub>), 5.22 (s, 2H, -CH<sub>2</sub>), 2.32 (s, 3H, -CH<sub>3</sub>); EI MS:  $m/z$  447 [ $M^+$ ]; Elemental analysis: C (56.49%), H (4.06%), N (25.10%), S (7.18%).

**N-(4-(4-chlorophenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-a]pyridin-2(3H)-yl)methyl)-1H-1,2,3-triazol-1-yl)acetamide (8b):** White Solid; Yield: 82%; mp: 180-182°C; Mol. Formula: C<sub>20</sub>H<sub>15</sub>ClN<sub>8</sub>O<sub>2</sub>S; Mol. Mass: 466 g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 646. <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.78 (brs, 1H, N-H), 8.15 (s, 1H), 7.92-7.87 (m, 3H), 7.67 (s, 1H), 7.49-7.47 (d,  $j=8.4$ , 2H), 7.22 (s, 2H), 6.64-6.61 (m, 1H), 5.43 (s, 2H, -CH<sub>2</sub>), 5.21 (s, 2H, -

CH<sub>2</sub>); EI MS:  $m/z$  466 [ $M^+$ ]; Elemental analysis: C (51.45%), H (3.24%), N (24.00%), S (6.87%).

***N*-(4-(4-bromophenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-*a*]pyridin-2(3*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (8c)**: White Solid; Yield: 79%; mp: 145-147°C; Mol. Formula: C<sub>20</sub>H<sub>15</sub>BrN<sub>8</sub>O<sub>2</sub>S; Mol. Mass: 510 g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 652; <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.77 (brs, 1H, N-H), 8.16 (s, 1H), 7.94-7.88 (m, 3H), 7.66 (s, 1H), 7.49-7.46 (d,  $j=8.3$ , 2H), 7.22 (s, 2H), 6.65-6.62 (m, 1H), 5.43 (s, 2H, -CH<sub>2</sub>), 5.21 (s, 2H, -CH<sub>2</sub>); EI MS:  $m/z$  510 [ $M^+$ ]; Elemental analysis: C (46.98%), H (2.96%), N (21.91%), S (6.27%).

***N*-(4-(4-methoxyphenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-*a*]pyridin-2(3*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (8d)**: White Solid; Yield: 87%; mp: 162-166°C; Mol. Formula: C<sub>21</sub>H<sub>18</sub>N<sub>8</sub>O<sub>3</sub>S; Mol. Mass: 462 g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 648; <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.81 (brs, 1H, N-H), 8.15 (s, 1H), 8.05-7.99 (m, 3H), 7.69 (s, 1H), 7.53-7.50 (d,  $j=8.3$ , 2H), 7.25 (s, 2H), 6.68-6.65 (m, 1H), 5.41 (s, 2H, -CH<sub>2</sub>), 5.22 (s, 2H, -CH<sub>2</sub>), 3.81 (s, 3H, -OCH<sub>3</sub>); EI MS:  $m/z$  462 [ $M^+$ ]; Elemental analysis: C (54.54%), H (3.92%), N (24.23%), S (6.93%).

**2-(4-((3-oxo-[1,2,4]triazolo[4,3-*a*]pyridin-2(3*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-phenylthiazol-2-yl)acetamide (8e)**: White Solid; Yield: 81%; mp: 178-182°C; Mol. Formula: C<sub>20</sub>H<sub>16</sub>N<sub>8</sub>O<sub>3</sub>S; Mol. Mass: 432 g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 648. <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.80 (brs, 1H, N-H), 8.20 (s, 1H), 7.87-7.83 (d,  $j=6.6$ , 1H), 7.77-7.75 (d,

$j=6.6$ , 2H), 7.57 (s, 1H), 7.22 (s, 5H), 6.63 (s, 1H), 5.45 (s, 2H, -CH<sub>2</sub>), 5.22 (s, 2H, -CH<sub>2</sub>); EI MS:  $m/z$  432 [ $M^+$ ]; Elemental analysis C (55.55%), H (3.73%), N (25.91%), S (7.41%).

**2-(4-((3-oxo-[1,2,4]triazolo[4,3-a]pyridin-2(3H)-yl)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-*o*-tolylthiazol-2-yl)acetamide (8f):** White Solid; Yield: 78%; mp: 170-173°C; Mol. Formula: C<sub>21</sub>H<sub>18</sub>N<sub>8</sub>O<sub>2</sub>S; Mol. Mass: 447g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 646. <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.78 (brs, 1H, N-H), 8.16 (s, 1H), 7.87-7.86 (d,  $j=6.6$ , 1H), 7.78-7.77 (d,  $j=6.6$ , 2H), 7.59 (s, 1H), 7.24 (s, 4H), 6.60 (s, 1H), 5.47 (s, 2H, -CH<sub>2</sub>), 5.23 (s, 2H, -CH<sub>2</sub>), 2.34 (s, 3H, -CH<sub>3</sub>); EI MS:  $m/z$  447 [ $M^+$ ]; Elemental analysis: C (56.49%), H (4.06%), N (25.10%), S (7.18%).

**N-(4-(2-chlorophenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-a]pyridin-2(3H)-yl)methyl)-1H-1,2,3-triazol-1-yl)acetamide (8g):** White Solid; Yield: 62%; mp: 149-153°C; Mol. Formula: C<sub>20</sub>H<sub>15</sub>ClN<sub>8</sub>O<sub>2</sub>S; Mol. Mass: 466g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 646. <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.81 (brs, 1H, N-H), 8.16 (s, 1H), 7.95-7.89 (m, 3H), 7.69 (s, 1H), 7.49-7.47 (d,  $j=8.4$ , 2H), 7.21 (s, 2H), 6.64-6.61 (m, 1H), 5.70 (s, 2H, -CH<sub>2</sub>), 5.65 (s, 2H, -CH<sub>2</sub>); EI MS:  $m/z$  466 [ $M^+$ ]; Elemental analysis: C (51.45%), H (3.24%), N (24.00%), S (6.87%).

**N-(4-(2-bromophenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-a]pyridin-2(3H)-yl)methyl)-1H-1,2,3-triazol-1-yl)acetamide (8h):** White Solid; Yield: 49%; mp: 154-157°C; Mol. Formula: C<sub>20</sub>H<sub>15</sub>BrN<sub>8</sub>O<sub>2</sub>S; Mol. Mass: 510g mol<sup>-1</sup>; IR (KBr,  $\nu_{\max}$ , cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 652; <sup>1</sup>H NMR (400 MHz, DMSO) in  $\delta$  ppm: 12.79 (brs, 1H, N-H), 8.24 (s, 1H), 7.94-7.87 (m, 3H), 7.65 (s, 1H), 7.51-7.47 (d,  $j=8.4$ , 2H), 7.21 (s, 2H), 6.54-6.51 (m, 1H), 5.22 (s, 2H, -CH<sub>2</sub>), 5.09 (s, 2H, -CH<sub>2</sub>); EI MS:  $m/z$  510 [ $M^+$ ]; Elemental analysis: C (46.98%), H (2.96%), N (21.91%), S (6.27%).

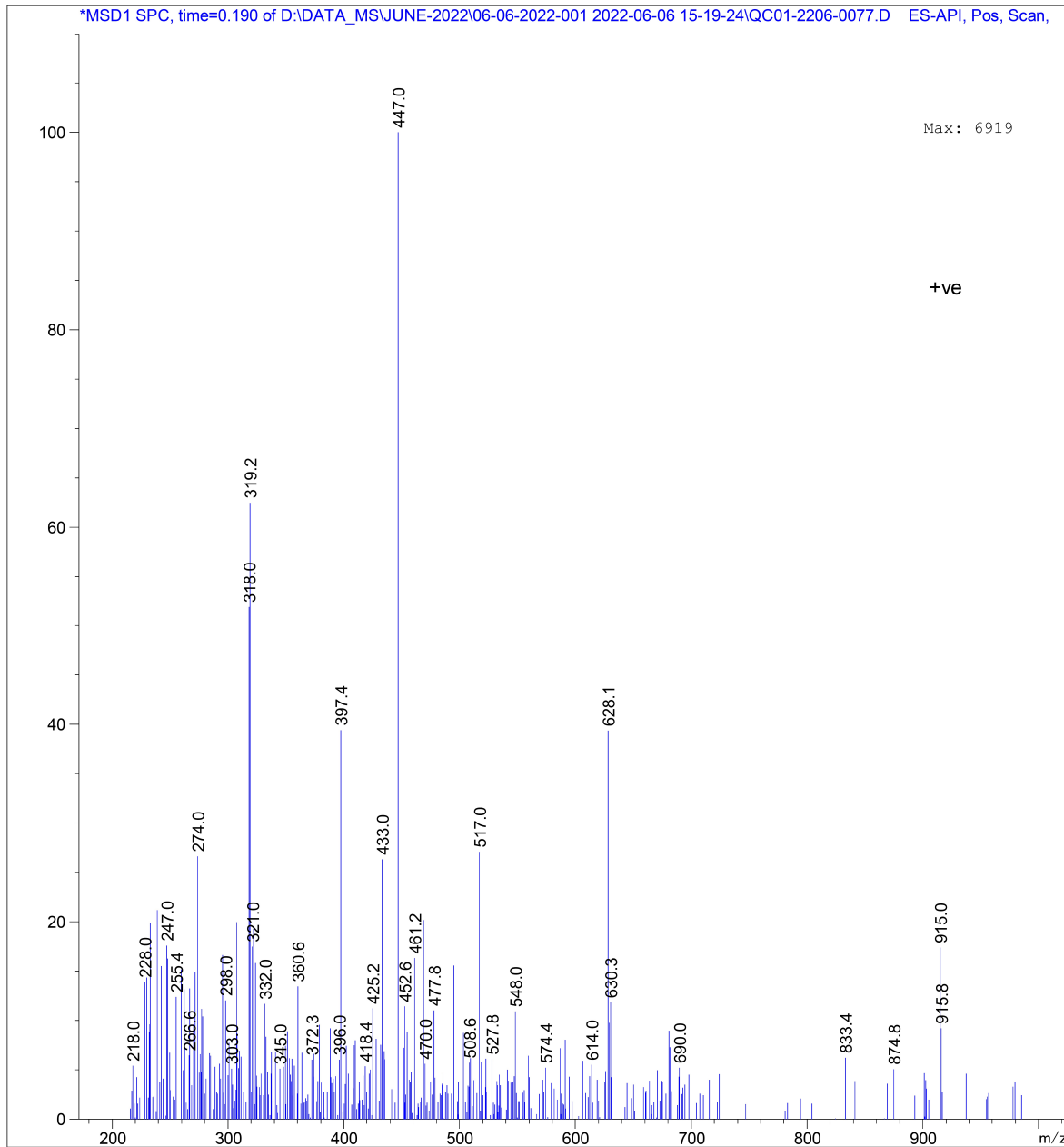
***N*-(4-(2-methoxyphenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-*a*]pyridin-2(3*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (8i):** White Solid; Yield: 87%; mp: 138-141°C; Mol. Formula: C<sub>21</sub>H<sub>18</sub>N<sub>8</sub>O<sub>3</sub>S; Mol. Mass: 462 g mol<sup>-1</sup>; IR (KBr, ν<sub>max</sub>, cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 648; <sup>1</sup>H NMR (400 MHz, DMSO) in δ ppm: 12.81 (brs, 1H, N-H), 8.15 (s, 1H), 8.05-7.99 (m, 3H), 7.65 (s, 1H), 7.51-7.46 (d, *j*=8.3, 2H), 7.25 (s, 2H), 6.61-6.65 (m, 1H), 5.63 (s, 2H, -CH<sub>2</sub>), 4.89 (s, 2H, -CH<sub>2</sub>), 3.83 (s, 3H, -OCH<sub>3</sub>); EI MS: *m/z* 462 [*M*<sup>+</sup>]; Elemental analysis: C (54.54%), H (3.92%), N (24.23%), S (6.93%).

***N*-(4-(2-nitrophenyl)thiazol-2-yl)-2-(4-((3-oxo-[1,2,4]triazolo[4,3-*a*]pyridin-2(3*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (8j):** White Solid; Yield: 77%; mp: 159-162°C; Mol. Formula: C<sub>20</sub>H<sub>15</sub>N<sub>9</sub>O<sub>4</sub>S; Mol. Mass: 477 g mol<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, DMSO) in δ ppm: 12.81 (brs, 1H, N-H), 8.54 (s, 1H), 7.87-7.83 (d, *j*=6.6, 1H), 7.75-7.71 (d, *j*=6.6, 2H), 7.53 (s, 1H), 7.21 (s, 5H), 6.28 (s, 1H), 5.51 (s, 2H, -CH<sub>2</sub>), 4.93 (s, 2H, -CH<sub>2</sub>); IR (KBr, ν<sub>max</sub>, cm<sup>-1</sup>): 3934, 3888, 3801, 3767, 3730, 3635, 3108, 3040, 2980, 2890, 2813, 2214, 1738, 1608, 1569, 1536, 1486, 1449, 1416, 1368, 1327, 1287, 1173, 1144, 1056, 992, 964, 926, 819, 778, 749, 686 and 648; EI MS: *m/z* 477 [*M*<sup>+</sup>]; Elemental analysis: C (50.31%), H (3.17%), N (26.40%), S (6.72%).

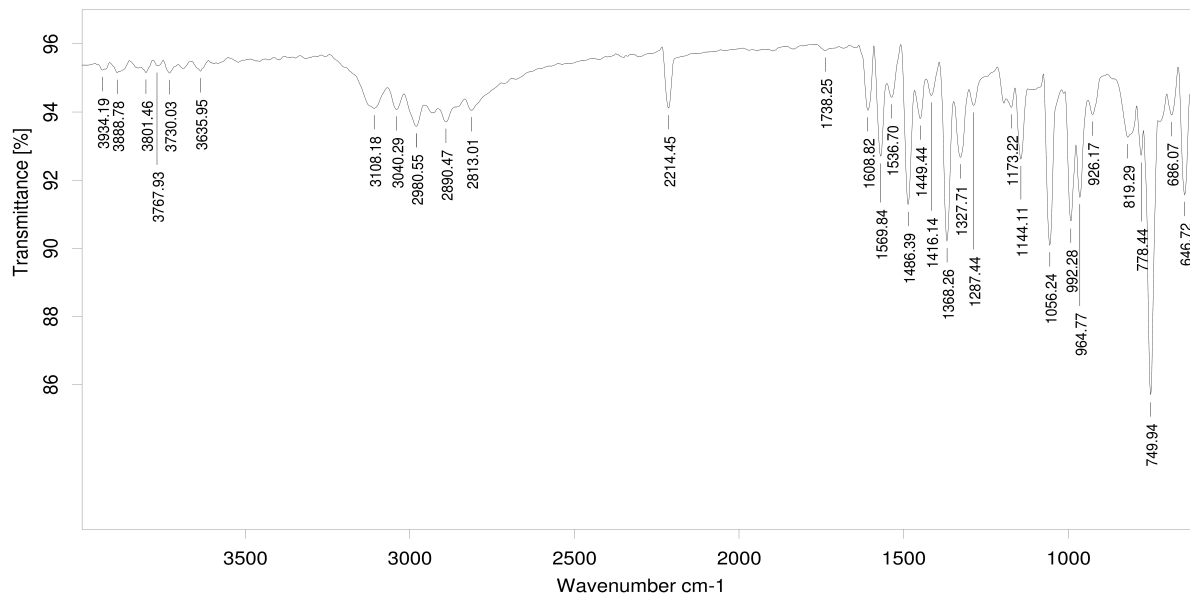
8a:

Mass

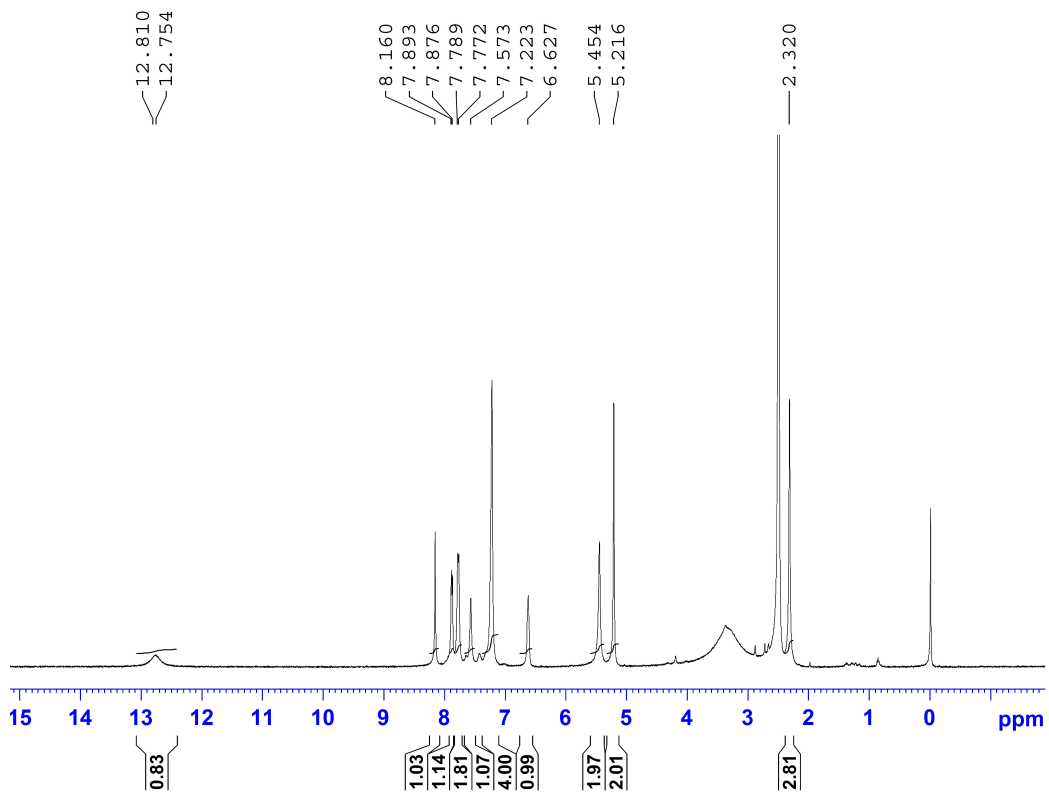
MS Spectrum



# IR

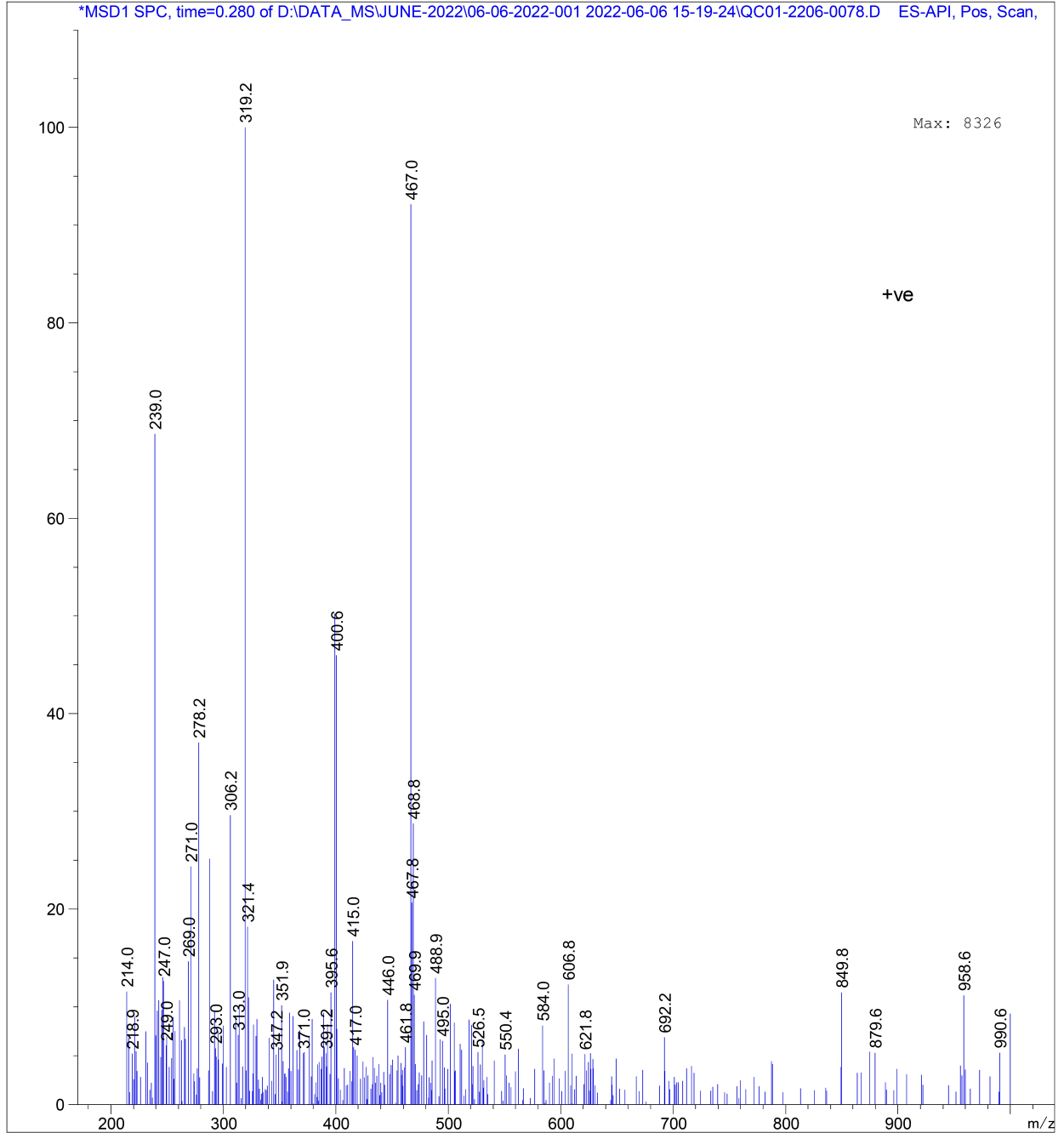


# <sup>1</sup>H NMR

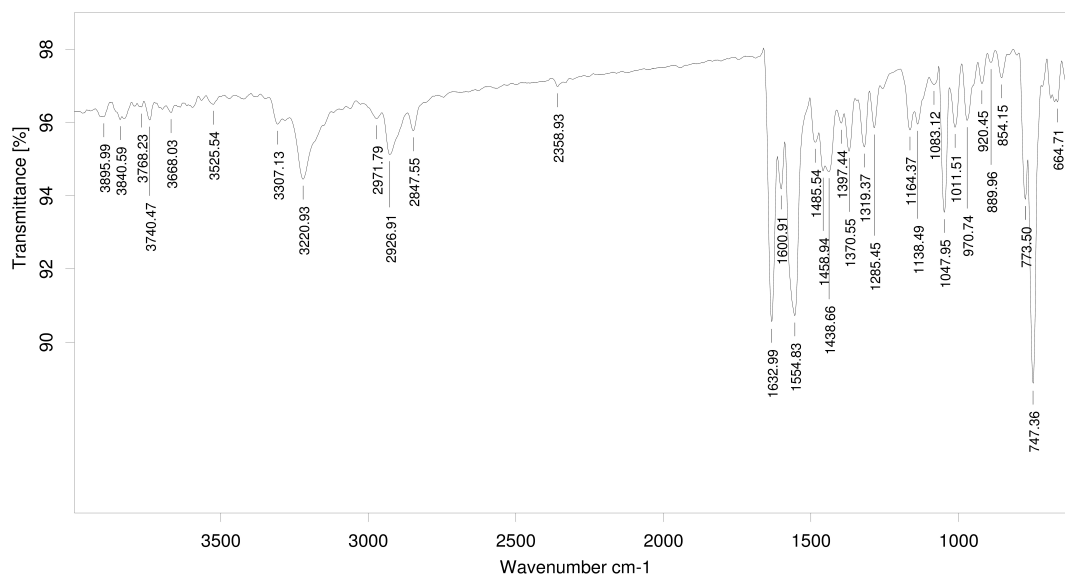


**8b:**  
**Mass**

MS Spectrum



# IR



# <sup>1</sup>H NMR

