# ME9_3+:[GWGR(Me2)EENLFSWK+3H]3+

Fragmentation Diagram for: GWGREENLFSWK

b-line

y-line

| | 1 G | 2 GW | 3 GWG | 4 GWGR | 5 GWGRE | 6 GWGREE | 7 GWGREEN | 8 GWGREENL | 9 GWGREENLF | 10 GWGREENLFS | 11 GWGREENLFSW | 12 GWGREENLFSWK |

b-line values: 2 GW: 6, 8, 28, 34, 48; 3 GWG: 25; 5 GWGRE: 24, 31, 49; 6 GWGREE: 1, 2, 4, 14, 26; 7 GWGREEN: 3, 7, 9, 17; 8 GWGREENL: 5, 11, 15, 22, 27; 9 GWGREENLF: 10, 37; 10 GWGREENLFS: 18, 33, 46

y-line underlines: 21; 47, 12, 19; 20; 38; 35
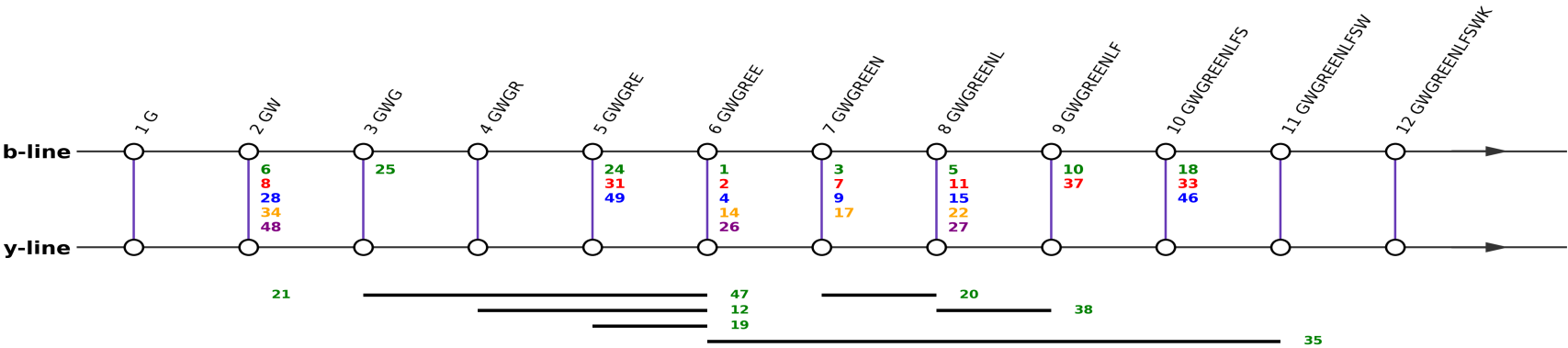
| | b1y11 | b2y10 | b3y9 | b4y8 | b5y7 | b6y6 | b7y5 | b8y4 | b9y3 | b10y2 | b11y1 | Row_Count | Unexplained Count | Abs Average Mass Difference | Unexplained Pairs |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Parent | -- | (b2,y10) (1+ , 2+) (-0.33, 0.31) 8 | (b3,y9) (1+ , 2+) (-0.11, 0.24) 25 | -- | (b5,y7) (2+ , 1+) (-0.13, 0.4) 24 | (b6,y6) (1+ , 2+) (0.03, 0.05) 4 | (b7,y5) (1+ , 2+) (0.04, 0.04) 7 | (b8,y4) (1+ , 2+) (-0.07, 0.23) 22 | -- | (b10,y2) (2+ , 1+) (-0.2, 0.21) 33 | -- | 7 | 0 | 0.27 | |
| (NH3) | -- | (b2,(NH3)) (1+ , 2+) (-0.31, 0.12) 28 | | -- | (b5,(NH3)) (1+ , 2+) (-0.1, -0.14) 49 | (b6,(NH3)) (1+ , 2+) (0.1, -0.19) 26 | ((NH3),y5) (2+ , 1+) (0.03, 0.11) 17 | ((NH3),y4) (1+ , 2+) (-0.16, -0.05) 11 | ((NH3),y3) (1+ , 2+) (-0.11, 0.18) 10 | ((NH3),y2) (2+ , 1+) (-0.16, 0.04) 18 | -- | 7 | 0 | 0.24 | |
| (H2O) | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | 0 | 0 | 0.0 | |
| (NH3)-(H2O) | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | 0 | 0 | 0.0 | |
| a | -- | (a2,y10) (1+ , 2+) (-0.38, 0.14) 6 | | -- | (a5,y7) (2+ , 1+) (-0.1, 0.19) 31 | (a6,y6) (2+ , 1+) (-0.02, 0.08) 2 | -- | -- | -- | -- | -- | 3 | 0 | 0.3 | |
| 2(H2O) | -- | -- | | -- | -- | -- | -- | (2(H2O),y4) (2+ , 1+) (0.24, -0.25) 27 | -- | -- | -- | 1 | 0 | 0.49 | |
| 2(NH3) | -- | -- | -- | -- | -- | -- | (2(NH3),y5) (2+ , 1+) (-0.49, 0.06) 9 | -- | -- | -- | -- | 1 | 0 | 0.56 | |
| Col_Count | 0 | 3 | 1 | 0 | 3 | 3 | 3 | 3 | 1 | 2 | 0 | 19 | 0 | 0.27 | nan |
| Ion Mass | (58.03, 1479.74) | (244.11, 1293.66) | (301.13, 1236.64) | (485.26, 1052.5) | (614.3, 923.46) | (743.35, 794.42) | (857.39, 680.38) | (970.47, 567.29) | (1117.54, 420.22) | (1204.57, 333.19) | (1390.65, 147.11) | 0 | 0 | 0.0 | 0 |

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50
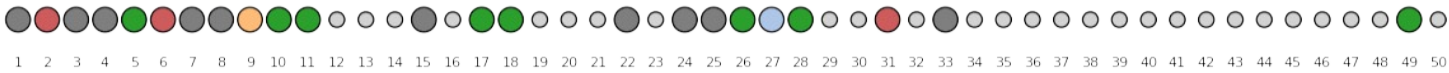
Not Highlighted   (H2O)   (H2O)-(NH3)   (NH3)   (NH3)-(H2O)   2(H2O)   2(NH3)   CH3-NH2   Parent   a

# Table ME9_3+

| n | classification | ion1 | loss1 | mass1 | correct_mass1 | mass_difference1 | ion2 | loss2 | mass2 | correct_mass2 | mass_difference2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | b6 | nan | 372.13 | 372.18 | -0.05 | y6 | nan | 794.48 | 794.42 | 0.06 | 1538.74 |
| 2 | usable | a6 | nan | 358.15 | 358.17 | -0.02 | y6 | nan | 794.5 | 794.42 | 0.08 | 1510.8 |
| 3 | usable | b7 | nan | 429.31 | 429.2 | 0.11 | y5 | nan | 680.44 | 680.38 | 0.06 | 1539.06 |
| 4 | usable | y6 | nan | 397.74 | 397.71 | 0.03 | b6 | nan | 743.4 | 743.35 | 0.05 | 1538.88 |
| 5 | usable | b8 | (NH3) | 477.27 | 477.23 | 0.04 | y4 | nan | 567.19 | 567.29 | -0.1 | 1521.73 |
| 6 | usable | a2 | nan | 215.72 | 216.1 | -0.38 | y10 | nan | 647.47 | 647.33 | 0.14 | 1510.66 |
| 7 | usable | y5 | nan | 340.73 | 340.69 | 0.04 | b7 | nan | 857.43 | 857.39 | 0.04 | 1538.89 |
| 8 | usable | b2 | nan | 243.78 | 244.11 | -0.33 | y10 | nan | 647.64 | 647.33 | 0.31 | 1539.06 |
| 9 | usable | b7 | 2(NH3) | 411.68 | 412.17 | -0.49 | y5 | nan | 680.44 | 680.38 | 0.06 | 1503.8 |
| 10 | usable | y3 | nan | 420.11 | 420.22 | -0.11 | b9 | (NH3) | 550.94 | 550.76 | 0.18 | 1521.99 |
| 11 | usable | y4 | nan | 283.99 | 284.15 | -0.16 | b8 | (NH3) | 953.4 | 953.45 | -0.05 | 1521.38 |
| 12 | internal_acid | bi(4-6) | (H2O)-(CH3NHCH3) | 380.45 | 379.15 | 1.3 | y6 | 2(NH3) | 760.33 | 760.37 | -0.04 | 1521.23 |
| 13 | rare_mode | y2 | (NH3) | 158.49 | 158.59 | -0.1 | a7 | (CH3NHCH3) | 784.36 | 784.32 | 0.04 | 1727.21 |
| 14 | usable | a6 | (H2O) | 349.07 | 349.17 | -0.1 | y6 | nan | 794.91 | 794.42 | 0.49 | 1493.05 |
| 15 | usable | b8 | nan | 485.73 | 485.74 | -0.01 | y4 | nan | 567.34 | 567.29 | 0.05 | 1538.8 |
| 16 | internal_acid | y4 | nan | 567.37 | 567.29 | 0.08 | ai(2-8) | (CH3NHCH3) | 840.47 | 839.38 | 1.09 | 1407.84 |
| 17 | usable | b7 | (NH3) | 420.72 | 420.69 | 0.03 | y5 | nan | 680.49 | 680.38 | 0.11 | 1521.93 |
| 18 | usable | y2 | nan | 333.03 | 333.19 | -0.16 | b10 | (NH3) | 594.32 | 594.28 | 0.04 | 1521.67 |
| 19 | non_complementary | b5 | (H2O) | 596.32 | 596.29 | 0.03 | y6 | nan | 794.51 | 794.42 | 0.09 | 1390.83 |
| 20 | internal_acid | bi(7-8) | nan | 227.68 | 227.13 | 0.55 | b6 | nan | 743.35 | 743.35 | 0.0 | 1714.38 |
| 21 | internal_acid | bi(2-2) | (H2O) | 169.35 | 168.07 | 1.28 | y10 | nan | 647.73 | 647.33 | 0.4 | 1464.81 |
| 22 | usable | y4 | nan | 284.08 | 284.15 | -0.07 | b8 | nan | 970.7 | 970.47 | 0.23 | 1538.86 |
| 23 | internal_acid | b4 | 2(NH3)-(CH3NH2) | 420.11 | 420.17 | -0.06 | ai(5-9) | (HCOOH) | 559.55 | 558.26 | 1.29 | 1539.21 |
| 24 | usable | b5 | nan | 307.53 | 307.66 | -0.13 | y7 | nan | 923.86 | 923.46 | 0.4 | 1538.92 |
| 25 | usable | b3 | nan | 301.02 | 301.13 | -0.11 | y9 | nan | 619.06 | 618.82 | 0.24 | 1539.14 |

| 26 | usable | y6 | (NH3) | 389.3 | 389.2 | 0.1 | b6 | nan | 743.16 | 743.35 | -0.19 | 1521.76 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 27 | usable | b8 | 2(H2O) | 467.97 | 467.73 | 0.24 | y4 | nan | 567.04 | 567.29 | -0.25 | 1502.98 |
| 28 | usable | b2 | nan | 243.8 | 244.11 | -0.31 | y10 | (NH3) | 638.94 | 638.82 | 0.12 | 1521.68 |
| 29 | internal_acid | ai(7-10) | 2(H2O) | 199.71 | 199.1 | 0.61 | b6 | nan | 743.49 | 743.35 | 0.14 | 1686.69 |
| 30 | internal_acid | ai(2-5) | 2(NH3)-(CH3NH2) | 232.69 | 232.09 | 0.6 | y7 | 2(H2O)-(HCOH) | 857.42 | 857.43 | -0.01 | 1322.8 |
| 31 | usable | a5 | nan | 293.55 | 293.65 | -0.1 | y7 | nan | 923.65 | 923.46 | 0.19 | 1510.75 |
| 32 | rare_mode | y4 | nan | 567.35 | 567.29 | 0.06 | a7 | (CH3NHCH3) | 784.36 | 784.32 | 0.04 | 1351.71 |
| 33 | usable | y2 | nan | 332.99 | 333.19 | -0.2 | b10 | nan | 603.0 | 602.79 | 0.21 | 1538.99 |
| 34 | usable | a2 | (H2O) | 198.41 | 198.09 | 0.32 | y10 | nan | 647.43 | 647.33 | 0.1 | 1493.27 |
| 35 | internal_acid | bi(6-11) | 2(H2O) | 371.1 | 370.67 | 0.43 | b5 | (CH3NH2) | 582.47 | 583.26 | -0.79 | 1536.04 |
| 36 | unclear | ??? | nan | 241.79 | nan | nan | ??? | nan | 581.32 | nan | nan | 1404.43 |
| 37 | usable | y3 | nan | 420.13 | 420.22 | -0.09 | a9 | (NH3) | 536.83 | 536.76 | 0.07 | 1493.79 |
| 38 | non_complementary | y3 | nan | 420.2 | 420.22 | -0.02 | b8 | (NH3) | 953.42 | 953.45 | -0.03 | 1373.62 |
| 39 | unclear | ??? | nan | 241.95 | nan | nan | ??? | nan | 483.97 | nan | nan | 1209.89 |
| 40 | unclear | ??? | nan | 557.35 | nan | nan | ??? | nan | 794.41 | nan | nan | 1351.76 |
| 41 | rare_mode | y2 | (NH3) | 158.65 | 158.59 | 0.06 | a7 | (NH3)-(CH3NHCH3) | 767.46 | 767.3 | 0.16 | 1693.57 |
| 42 | rare_mode | y4 | (NH3)-(HCOH) | 260.84 | 260.63 | 0.21 | b7 | nan | 857.43 | 857.39 | 0.04 | 1379.11 |
| 43 | unclear | ??? | nan | 228.71 | nan | nan | ??? | nan | 647.46 | nan | nan | 1523.63 |
| 44 | unclear | ??? | nan | 183.73 | nan | nan | ??? | nan | 619.13 | nan | nan | 1421.99 |
| 45 | internal_acid | ai(4-7) | 2(H2O)-(CH3NH2) | 462.33 | 461.19 | 1.14 | y5 | 2(H2O)-(HCOH) | 614.47 | 614.34 | 0.13 | 1539.13 |
| 46 | usable | y2 | nan | 333.2 | 333.19 | 0.01 | a10 | (NH3) | 580.36 | 580.27 | 0.09 | 1493.92 |
| 47 | internal_acid | bi(3-6) | (H2O) | 241.69 | 241.12 | 0.57 | y6 | nan | 794.36 | 794.42 | -0.06 | 1277.74 |
| 48 | usable | a2 | nan | 215.84 | 216.1 | -0.26 | y10 | (NH3) | 638.76 | 638.82 | -0.06 | 1493.36 |
| 49 | usable | y7 | (NH3) | 453.62 | 453.72 | -0.1 | b5 | nan | 614.16 | 614.3 | -0.14 | 1521.4 |
| 50 | internal_acid | ai(2-6) | (CH3NH2) | 313.84 | 313.64 | 0.2 | y6 | nan | 794.64 | 794.42 | 0.22 | 1422.32 |