* 1. Summary tables for MC1037

Table 14: ”Original”

Table 14: Summary table for MC1037 (1 of 2): Shifts, splitting, COSY, HSQC and HMBC

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Amino acid | Atom name | C | H | Multip. | COSY | HSQC | HSQC\_+/- | HMBC |
| Leu1 | 1 |  | - |  | - | - |  | - |
|  | 2 | 50.1 | 4.50 | dd (12.8) | 1.13, 1.80, 7.14 | 50.1 | + | - |
|  | 2-NH |  | 7.14 | br d (13.8) | 4.50 | - |  | - |
|  | 3 | 39.4 | 1.80 | dd (14.3) | 1.13, 1.44, 4.50 | 39.4 | - | - |
|  |  |  | 1.13 | br Weak s/m | 1.80, 4.50 | 39.4 |  | - |
|  | 4 | 24.5 | 1.44 | m | 0.78, 1.80 | 24.5 | + | - |
|  | 5a | 23.1 | 0.78 | d (7.2) | 1.44 | 23.1 | + | - |
|  | 5b | 21.0 | 0.78 | d (7.0) | 1.44 | 21.0 | + | - |
| Leu2 | 1 |  | - |  | - | - | 0 | - |
|  | 2 | 53.5 | 4.00 | m | 1.49, 1.74, 7.64 | 53.5 | + | - |
|  | 2-NH |  | 7.64 | d (6.2) | 4.00 | - |  | - |
|  | 3 | 39.2 | 1.74 | m | 1.49, 4.00 | 39.2 | - | - |
|  |  |  | 1.49 | m | 1.66, 1.74, 4.00 | 39.2 |  | - |
|  | 4 | 24.2 | 1.66 | m | 0.80, 0.86, 1.49 | 24.2 | + | - |
|  | 5a | 23.0 | 0.86 | d (6.8) | 1.66 | 23.0 | + | 21.0, 39.2 |
|  | 5b | 21.0 | 0.80 | d (6.8) | 1.66 | 21.0 | + | 39.2 |
| Me-Asp3 | 1 |  | - |  | - | - | 0 | - |
|  | 2 | 55.4 | 4.12 | m | 7.87 | - | ? | - |
|  | 2-NH |  | 7.87 | d (10.7) | 4.12 | - |  | - |
|  | 3 | 39.4 | 3.12 | m | 0.89 | 39.4 | ? | - |
|  | 3-Me | 15.1 | 0.89 | d (7.8) | 3.12 | 15.1 | + | 178.4, 39.4, 55.4 |
|  | 4 | 178.4 | - |  | - | - |  | - |
| Arg4 | 1 |  | - |  | - | - | 0 | - |
|  | 2 | 51.6 | 4.13 | td (10.1, 3.6) | 1.30, 1.97, 8.83 | 51.6 | + | - |
|  | 2-NH |  | 8.83 | d (10.5) | 4.13 | - |  | - |
|  | 3 | 28.4 | 1.97 |  | 1.30, 1.37, 4.13 | 28.4 | - | - |
|  |  |  | 1.30 |  | - | 28.4 |  | - |
|  | 4 | 25.9 | 1.37 |  | 1.97, 3.01 | 25.9 | - | - |
|  |  |  | 1.30 |  | 1.97, 3.01, 4.13 | 25.9 |  | - |
|  | 5 | 40.5 | 3.01 |  | 1.30, 1.37, 7.37 | 40.5 | - | - |
|  | 5-NH |  | 7.37 |  | 3.01 | - |  | 128.1 |
| Adda5 | 1 | 173.8 | - |  | - | - | 0 | - |
|  | 2 | 43.1 | 2.78 | br dd (?, ?) | 0.92, 4.35 | 43.1 | + | - |
|  | 2-Me | 16.0 | 0.92 | d (7.2) | 2.78 | 16.0 | + | 173.8, 43.1, 54.4 |
|  | 3 | 54.4 | 4.35 | ddd (?, ?, ?) | 2.78, 5.32, 7.75 | 54.4 | + | - |
|  | 3-NH |  | 7.75 | br d (?) | 4.35 | - |  | - |
|  | 4 | 126.3 | 5.32 | dd (16.4, 8.3) | 4.35, 6.09 | 126.3 | + | 132.0 |
|  | 5 | 135.4 | 6.09 | d (16.4) | 5.32 | 135.4 | + | 12.5, 135.3, 54.4 |
|  | 6 | 132.0 | - |  | - | - | 0 | - |
|  | 6-Me | 12.5 | 1.55 | d (1.0) | 5.45 | 12.5 | + | 132.0 |
|  | 7 | 135.3 | 5.45 | dd (10.8, 1.0) | 1.55, 2.56 | 135.3 | + | 12.5, 135.4 |
|  | 8 | 35.4 | 2.56 | ddd (10.8, 7.0, 5.4) | 0.98, 3.25, 5.45 | 35.4 | + | - |
|  | 8-Me | 15.8 | 0.98 | d (7.0) | 2.56 | 15.8 | + | 135.3, 35.4, 85.8 |
|  | 9 | 85.8 | 3.25 | ddd (7.2, 5.4, 5.4) | 2.56, 2.68, 2.74 | 85.8 | + | 139.2, 15.8, 57.4 |
|  | 9-OMe | 57.4 | - | s | - | - | + | - |
|  | 10 | 37.0 | 2.74 | dd (14.0, 5.4) | 3.25 | 37.0 | - | 129.3, 139.2, 35.4, 85.8 |
|  |  |  | 2.68 | dd (14.0, 7.2) | 3.25 | 37.0 |  | 129.3, 139.2, 35.4, 85.8 |
|  | 11 | 139.2 | - |  | - | - | 0 | - |
|  | 12 | 129.3 | 7.19 | dd (8.3, 1.2) | - | 129.3 | + | 125.9, 129.3, 37.0 |
|  | 13 | 128.1 | 7.27 | dd (8.3, 7.3) | - | 128.1 | + | 128.1, 139.2 |
|  | 14 | 125.9 | 7.18 | dt (7.3, 1.2) | - | 125.9 | + | - |
| Glu6 | 1 |  | - |  | - | - | 0 | - |
|  | 2 | 52.8 | 4.35 |  | 1.88, 9.28 | 52.8 | + | - |
|  | 2-NH |  | 9.28 |  | 4.35 | - |  | - |
|  | 3 |  | 1.88 |  | 2.21, 4.35 | - | - | - |
|  | 4 | 31.3 | 2.21 |  | 1.88 | 31.3 | - | - |
|  |  |  | 2.31 |  | - | 31.3 |  | - |
|  | 5 | 175.1 | - |  | - | - | 0 | - |
| Mdha7 | 1 | 163.0 | - |  | - | - | 0 | - |
|  | 2 | 144.8 | - |  | - | - | 0 | - |
|  | 2-N-Me | 37.3 | 3.12 | s | - | 37.3 | + | 144.8, 175.1 |
|  | 3 | 113.9 | 5.81 |  | - | 113.9 | - | 163.0 |
|  |  |  | 5.39 |  | - | 113.9 |  | 144.8, 163.0 |

Table 15: Summary table for MC1037 (2 of 2): TOCSY and ROESY

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Amino acid | Atom name | C | H | TOCSY | ROESY |
| Leu1 | 1 |  | - | - | - |
|  | 2 | 50.1 | 4.50 | 0.78, 1.13, 1.44, 1.80, 7.14 | 1.13, 1.44, 1.80, 7.14, 7.64 |
|  | 2-NH |  | 7.14 | 0.78, 1.13, 1.44, 1.80, 4.50 | 1.13, 1.44, 3.12, 4.13, 4.50, 7.64, 7.87 |
|  | 3 | 39.4 | 1.80 | 1.13, 1.44, 4.50, 7.14 | 1.13, 4.50 |
|  |  |  | 1.13 | 1.80, 4.50, 7.14 | 1.80, 4.50, 7.14 |
|  | 4 | 24.5 | 1.44 | 0.78, 1.80, 4.50, 7.14 | 4.50, 7.14 |
|  | 5a | 23.1 | 0.78 | 1.44, 4.50, 7.14 | - |
|  | 5b | 21.0 | 0.78 | 1.44, 4.50, 7.14 | - |
| Leu2 | 1 |  | - | - | - |
|  | 2 | 53.5 | 4.00 | 0.80, 0.86, 1.49, 1.66, 1.74, 7.64 | 0.80, 1.49, 7.64, 7.87 |
|  | 2-NH |  | 7.64 | 0.80, 0.86, 1.49, 1.66, 1.74, 4.00 | 1.66, 1.74, 4.00, 4.50, 7.14, 7.87 |
|  | 3 | 39.2 | 1.74 | 0.80, 0.86, 1.49, 4.00, 7.64 | 0.86, 1.49, 4.35, 7.64, 7.87 |
|  |  |  | 1.49 | 0.80, 0.86, 1.66, 1.74, 4.00, 7.64 | 1.74, 4.00, 7.87 |
|  | 4 | 24.2 | 1.66 | 0.80, 0.86, 1.49, 4.00, 7.64 | 7.64 |
|  | 5a | 23.0 | 0.86 | 1.49, 1.66, 1.74, 4.00, 7.64 | 1.74 |
|  | 5b | 21.0 | 0.80 | 1.49, 1.66, 1.74, 4.00, 7.64 | 4.00, 5.81 |
| Me-Asp3 | 1 |  | - | - | - |
|  | 2 | 55.4 | 4.12 | 0.89, 3.12, 7.87 | 0.89, 3.12, 7.87 |
|  | 2-NH |  | 7.87 | 0.89, 3.12, 4.12 | 0.89, 1.49, 1.74, 1.88, 4.00, 4.12, 7.14, 7.64 |
|  | 3 | 39.4 | 3.12 | 0.89, 4.12, 7.87 | 0.89, 4.12, 7.14, 7.37, 8.83 |
|  | 3-Me | 15.1 | 0.89 | 3.12, 4.12, 7.87 | 3.12, 4.12, 7.87, 8.83 |
|  | 4 | 178.4 | - | - | - |
| Arg4 | 1 |  | - | - | - |
|  | 2 | 51.6 | 4.13 | 1.30, 1.37, 1.97, 3.01, 7.37, 8.83 | 1.30, 1.37, 1.97, 2.31, 7.14, 7.75, 8.83 |
|  | 2-NH |  | 8.83 | 1.30, 1.37, 1.97, 3.01, 4.13 | 0.89, 1.30, 1.37, 3.12, 4.13, 6.09, 7.75 |
|  | 3 | 28.4 | 1.97 | 1.30, 1.37, 3.01, 4.13, 7.37, 8.83 | 3.01, 4.13, 7.37 |
|  |  |  | 1.30 | - | - |
|  | 4 | 25.9 | 1.37 | 1.97, 3.01, 4.13, 7.37, 8.83 | 3.01, 4.13, 8.83 |
|  |  |  | 1.30 | 1.97, 3.01, 4.13, 7.37, 8.83 | 3.01, 4.13, 8.83 |
|  | 5 | 40.5 | 3.01 | 1.30, 1.37, 1.97, 4.13, 7.37, 8.83 | 1.30, 1.37, 1.97, 7.19, 7.27, 7.37 |
|  | 5-NH |  | 7.37 | 1.30, 1.37, 1.97, 3.01, 4.13 | 1.97, 3.01, 3.12 |
| Adda5 | 1 | 173.8 | - | - | - |
|  | 2 | 43.1 | 2.78 | 0.92, 4.35, 5.32, 6.09, 7.75 | 0.92, 4.35, 5.32, 6.09, 7.75, 9.28 |
|  | 2-Me | 16.0 | 0.92 | 2.78, 4.35, 5.32, 6.09, 7.75 | 2.78, 4.35, 5.32, 6.09 |
|  | 3 | 54.4 | 4.35 | 0.92, 2.78, 5.32, 6.09, 7.75 | 0.92, 1.55, 2.78, 5.32, 5.45, 6.09, 7.75 |
|  | 3-NH |  | 7.75 | 0.92, 2.78, 4.35, 5.32, 6.09 | 2.78, 4.13, 4.35, 5.32, 6.09, 8.83 |
|  | 4 | 126.3 | 5.32 | 0.92, 2.78, 4.35, 6.09, 7.75 | 0.92, 1.55, 2.78, 4.35, 6.09, 7.75 |
|  | 5 | 135.4 | 6.09 | 0.92, 2.78, 4.35, 5.32, 7.75 | 0.92, 1.55, 2.78, 4.35, 5.32, 5.45, 7.75, 8.83 |
|  | 6 | 132.0 | - | - | - |
|  | 6-Me | 12.5 | 1.55 | 5.45 | 4.35, 5.32, 5.45, 6.09 |
|  | 7 | 135.3 | 5.45 | 1.55, 2.56, 2.68, 2.74, 3.25 | 0.98, 1.55, 2.56, 2.68, 2.74, 3.25, 4.35, 6.09 |
|  | 8 | 35.4 | 2.56 | 0.98, 2.68, 2.74, 3.25, 5.45 | 5.45, 7.19 |
|  | 8-Me | 15.8 | 0.98 | 2.56, 2.68, 2.74, 3.25 | 2.68, 2.74, 3.25, 5.45 |
|  | 9 | 85.8 | 3.25 | 0.98, 2.56, 2.68, 2.74, 5.45, 5.56 | 0.98, 5.45, 7.19 |
|  | 9-OMe | 57.4 | - | - | - |
|  | 10 | 37.0 | 2.74 | 0.98, 2.56, 2.68, 3.25, 5.45 | 0.98, 5.45, 7.19, 7.27 |
|  |  |  | 2.68 | 0.98, 2.56, 2.74, 3.25, 5.45 | 0.98, 5.45, 7.19 |
|  | 11 | 139.2 | - | - | - |
|  | 12 | 129.3 | 7.19 | - | 2.56, 2.68, 2.74, 3.01, 3.19, 3.25 |
|  | 13 | 128.1 | 7.27 | - | 2.74, 3.01, 3.19 |
|  | 14 | 125.9 | 7.18 | - | - |
| Glu6 | 1 |  | - | - | - |
|  | 2 | 52.8 | 4.35 | 1.88, 2.21, 2.31, 9.28 | 1.74, 1.88, 2.21, 2.31, 9.28 |
|  | 2-NH |  | 9.28 | 1.88, 2.21, 2.31, 4.35 | 2.78, 4.35 |
|  | 3 |  | 1.88 | 2.21, 2.31, 4.35, 9.28 | 4.35, 7.87 |
|  | 4 | 31.3 | 2.21 | 1.88, 4.35, 9.28 | 3.12, 4.35 |
|  |  |  | 2.31 | 1.88, 4.35, 9.28 | 3.12, 4.13, 4.35 |
|  | 5 | 175.1 | - | - | - |
| Mdha7 | 1 | 163.0 | - | - | - |
|  | 2 | 144.8 | - | - | - |
|  | 2-N-Me | 37.3 | 3.12 | - | 2.21, 2.31, 5.39, 5.81 |
|  | 3 | 113.9 | 5.81 | 5.39 | 0.80, 3.12, 5.39 |
|  |  |  | 5.39 | 5.81 | 3.12, 5.81 |