

**Dataset 1H-NMR**

|    | '9.87 ppm' | '8.57 ppm' | '8.36 ppm' | '7.83 ppm' | '7.82 ppm' | '7.81 ppm' | '7.57 ppm' | '7.59 ppm' | '7.50 ppm' | '7.40 ppm' | '7.22 ppm' | '7.19 ppm' | '6.79 ppm' |
|----|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| A1 | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          |
| A2 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| A3 | 1          | 1          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          |
| A4 | 1          | 1          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          |
| B1 | 1          | 1          | 0          | 1          | 1          | 1          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| A5 | 1          | 1          | 0          | 0          | 1          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| C1 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| D1 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          |
| A6 | 1          | 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 1          | 1          | 1          | 0          |
| A7 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| E1 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| A8 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| A9 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 0          | 0          |
| F1 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 0          | 1          |
| G1 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 0          | 1          |
| B2 | 1          | 1          | 0          | 0          | 0          | 0          | 0          | 1          | 1          | 1          | 1          | 0          | 1          |



| '3.60 ppm' | '3.58 ppm' | '3.56 ppm' | '3.50 ppm' | '3.10 ppm' | '2.78 ppm' | '2.76 ppm' | '2.75 ppm' | '2.73 ppm' | '2.24 ppm' | '2.35 ppm' | '2.18 ppm' | '1.99 ppm' | '1.81-1.83 |
|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 1          | 1          | 1          | 1          |
| 1          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 1          | 1          | 1          | 1          | 1          |
| 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 1          | 1          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 1          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 1          | 1          | 1          |
| 1          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 0          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 0          | 0          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 0          | 1          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 0          | 1          | 0          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 1          | 0          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |
| 0          | 1          | 1          | 1          | 1          | 1          | 1          | 1          | 0          | 0          | 0          | 1          | 1          | 1          |

