

**7-methoxycoumarin**

Supplementary data 1

Supplementary data 2

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Tr | m/z | EC | ppm | DBE | Fragments (m/z, EC, DBE) |
| 2.16 | 463.1452  927.2968 [2M-H]- | C19H27O13  C38H55O26 | -0.6 | 8.5 |  |
| 2.32 | 233.1022 | C10H17O6 | -1.3 | 2.5 |  |
| 2.41 | 241.0707 | C11H13O6 | -2.1 | 5.5 |  |
| 2.52 | 447.1500  493.1559 [M-H+HCOOH]- | C19H27O12  C20H29O14 | -0.7  0.4 | 6.5  6.5 |  |
| 2.91 | 477.1604  523.1663 [M-H+HCOOH]- | C20H29O13  C21H31O15 | -0.8  0 | 6.5  6.5 |  |
| 3.07 | 461.1653  507.1708 [M-H+HCOOH]- | C20H29O12  C21H31O14 | 1.3  -1.2 | 6.5  6.5 | 329.1219, C15H21O8, 5.5  271.0808, C12H15O7, 5.5  161.0444, C6H9O5, 2.5 |
| 3.50 | 517.2291  563.2346 [M-H+HCOOH]- | C24H37O12  C25H39O14 | 1.1  1.2 | 6.5  6.5 | 387.2017, C19H31O8, 4.5 |
| 3.34 | 491.1759  537.1820 [M-H+HCOOH]- | C21H31O13  C22H33O15 | -1.2  0.2 | 6.5  6.5 | 359.1330, C16H23O9, 5.5 |
| 3.46 | 549.2914  595.2975 [M-H+HCOOH]- | C26H45O12  C27H47O14 | 1.2  1.5 | 4.5  4.5 | 417.2460, C21H37O8, 3.5 |
| 3.55 | 211.0607 | C10H11O5 | 0.5 | 5.5 | 193.0496, C10H9O4, 6.5  165.0552, C9H9O3, 5.5  149.0600, C9H9O2, 5.5 |
| 3.75 | 713.1927 | C31H37O19 | -0.3 | 13.5 | 567.1350, C25H27O15, 12.5  545.2609, C22H41O15, 2.5  399.0917, C17H19O11, 8.5 |
| 4.34 | 263.0919 | C14H15O5 | 0 | 7.5 | 175.0394, C10H7O3, 7.5  147.0447, C9H7O2, 6.5 |
| 4.57 | 265.1074 | C14H17O5 | -0.2 | 6.5 | 221.1174, C13H17O3, 5.5  163.0753, C10H11O2, 4.5 |
| 4.73 | 269.1024 | C13H17O6 | -0.4 | 5.5 | 195.0650, C10H11O4, 5.5  151.0753, C9H11O2, 4.5 |
| 4.88 | 387.1076  775.2242 [2M-H]- | C20H19O8  C40H39O16 | -0.4  -3.1 | 11.5  12.5 | 369.0969, C20H17O7, 12.5  325.1072, C19H15O5, 11.5 |
| 5.75 | 531.2808  577.2866 [M-H+HCOOH]- | C26H43O11 C27H45O13 | 0.8  1 | 5.5  5.5 | 399.2375, C21H35O7, 4.5  167.0341, C8H7O4, 5.5 |
| 6.66 | 369.0970  739.2011 [2M-H]- | C20H17O7  C40H35O14 | -1.1 | 12.5 | 325.1076, C19H17O5, 11.5  271.0964, C16H15O4, 9.5  189.0549, C11H9O3, 7.5  149.0602, C9H9O2, 5.5 |
| 6.78 | 401.1238 | C21H21O8 | 0.5 | 11.5 | 369.0971, C20H17O7, 12.5  189.0549, C11H9O3, 7.5  149.0602, C9H9O2, 5.5 |
| 8.28 | 383.1130  207.0654 (maj) | C21H19O7  C11H11O4 | -0.3  -1.4 | 12.5  6.5 | 175.0387, C10H7O3, 7.5  161.0238, C9H5O3, 7.5  147.0439, C9H7O2, 6.5 |
| 8.50 | 611.3797 | C33H55O10 | 0 | 6.5 | 453.2492, C24H37O8, 6.5  391.2491, C23H35O5, 6.5  329.2332, C18H33O5, 2.5  303.1965, C19H27O3, 6.5 |
| 17.74 | 281.2848  327.2900 [M-H+HCOOH]- | C19H37O C20H39O3 | 0.3  0.2 | 1.5  1.5 |  |
| 18.29 | 295.2996  341.3052 [M-H+HCOOH]- | C20H39O  C21H41O3 | 0.2  -0.9 | 1.5  1.5 |  |