**Characterization of metabolism feature and potential pharmacological changes of** morusin-a promising anti-tumor drug-by ultra high-performance liquid chromatography coupled time-of-flight mass spectrometry and network pharmacology

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**Captions**

**Table S1** Mass defect profile of metabolites of morusin

**Table S2** The peak area of morusin and its metabolites in rats.

**Table S1** Mass defect profile of metabolites of morusin

|  |  |  |  |
| --- | --- | --- | --- |
| Biotransformation reaction | Mass defect shift (mDa) | Mass shift (Da) | Molecular formula change |
| glycosylation |  |  |  |
| glucose | 52.8 mDa | ±162.0528 | ±C6H10O5 |
| rhamnose | 57.9 mDa | ±146.0579 | ±C6H10O4 |
| hydration/dehydration | 10.6 mDa | ±18.0106 | ±H2O4 |
| hydroxylation/dehydroxylation | 5.1 mDa | ±15.9949 | ±O |
| acetylation | 10.6 mDa | 42.0106 | +C2H2O |
| methylation/demethylation | 15.7 mDa | ±14.0517 | ±CH2 |
| desaturations/reduction | 15.7 mDa | ±2.0517 | ±H2 |
| two sequential desaturations | 31.3 mDa | ±4.0313 | ±H4 |
| 2×glucuronidation | 64.1mDa | 352.0641 | +C12H16O12 |
| glucuronidation | 32.1 mDa | 176.0321 | +C6H8O6 |
| sulfate conjugation | 43.2 mDa | 79.9568 | +SO3 |
| glycine conjugation | 21.5 mDa | 57.0215 | +C2H3NO3 |
| cysteine conjugation | 4.1 mDa | 119.0041 | +C3H5NO2S |
| taurine conjugation | 4.1 mDa | 107.0041 | +C2H5NO2S |
| GSH conjugation | 68.2 mDa | 305.682 | +C10H15N3O6S |
|  |  |  |  |

**Table S2** The peak area of morusin and its metabolites in rats.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | Plasma | Urine | Feces | Heart | Liver | Spleen | Lung | Kidney | Brain |
| **M0** | 35892 | 1880 | 183044 | 25336 | 30489 | 7954 | 19873 | 26956 | 2327 |
| **M1** | 50 | 729 | 200 | 141 | - | - | - | - | - |
| **M2** | - | - | 1351 | - | 72 | - | - | - | - |
| **M3** | - | - | 236 | - | - | - | - | - | - |
| **M4** | 948 | - | 5545 | - | 401 | - | 299 | - | - |
| **M5** | - | - | 1694 | - | 71 | - | - | - | - |
| **M6** | 4556 | 500 | 7715 | 155 | 1873 | - | 204 | 566 | 38 |
| **M7** | 87 | - | 852 | - | - | - | - | - | - |
| **M8** | 191 | - | 965 | - | 84 | - | - | - | - |
| **M9** | - | - | 881 | - | - | - | - | - | - |
| **M10** | 38 | - | 1121 | - | 28 | - | - | - | - |
| **M11** | 41 | - | 93 | - | - | - | - | - | - |
| **M12** | 311 | - | 473 | - | - | - | - | - | - |
| **M13** | - | - | 1813 | - | 154 | - | - | - | - |
| **M14** | 41 | - | 101 | - | 15 | - | - | - | - |
| **M15** | 593 | - | 2237 | - | 207 | - | - | - | - |
| **M16** | - | - | - | - | 48 | - | - | - | - |
| **M17** | - | - | 3061 | - | 242 | - | - | - | - |
| **M18** | 68128 | 815 | 7928 | 2082 | 5283 | 605 | 1930 | 6171 | 303 |
| **M19** | 1810 | 613 | 58691 | 1292 | - | 448 | 1070 | 1452 | 43 |
| **M20** | 3486 | 19 | 19911 | - | 949 | - | - | - | - |
| **M21** | 713 | - | 85 | - | - | - | - | - | - |
| **M22** | 159 | - | 1515 | - | 122 | - | - | - | - |
| **M23** | 22 | - | 673 | - | - | - | - | - | - |
| **M24** | 99 | - | 2101 | - | 68 | - | - | - | - |
| **M25** | - | - | 2975 | - | - | - | - | - | - |
| **M26** | - | - | 1318 | - | - | - | - | 58 | - |
| **M27** | - | - | 680 | - | - | - | - | - | - |
| **M28** | - | 249 | 9178 | - | - | - | - | - | - |
| **M29** | - | - | 6707 | - | - | - | - | - | - |
| **M30** | 57 | 63 | 7683 | 57 | 232 | 15 | 76 | 56 | - |
| **M31** | 99 | 58 | 2443 | 114 | 313 | 44 | 73 | 127 | - |

-No detected.