Table S1. The mass spectrum parameters of 33 enrolled drugs.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Test compound | Mass | | | | | |
| Q1 | Q3 | Dwell time | DP | CE | CXP |
| (amu) | (amu) | (msec) | (v) | (v) | (v) |
| Apixaban | 460.3 | 443.2 | 50 | 140 | 35 | 10 |
| Apremilast | 461.3 | 257.2 | 50 | 100 | 15 | 10 |
| Axitinib | 386.9 | 356.1 | 50 | 131 | 28 | 12 |
| Baricitinib | 372.1 | 251.2 | 50 | 140 | 39 | 10 |
| Bosutinib | 530.2 | 141.3 | 50 | 100 | 32 | 10 |
| Crizotinib | 452 | 177.1 | 50 | 111 | 52 | 12 |
| Edoxaban | 548.1 | 349.3 | 50 | 120 | 35 | 10 |
| Elagollx | 632.1 | 529.2 | 50 | 105 | 40 | 10 |
| Fedratinib | 525.3 | 98.2 | 50 | 120 | 43 | 10 |
| Flibanserin | 391.3 | 161 | 50 | 140 | 39 | 10 |
| Fostamatinib | 581.1 | 483 | 50 | 113 | 23 | 12 |
| Ibrutinib | 441.1 | 304.1 | 50 | 147 | 39 | 12 |
| Istradefylline | 385.2 | 357.2 | 50 | 120 | 34 | 10 |
| Lenvatinib | 427.2 | 370.1 | 50 | 97 | 38 | 10 |
| Macitentan | 589 | 203.1 | 50 | 60 | 29 | 10 |
| Nintedanib | 540.2 | 113.2 | 50 | 96 | 35 | 10 |
| Ospemifene | 372.9 | 205.2 | 50 | 90 | 25 | 10 |
| Panobinostat | 350.3 | 158.2 | 50 | 74 | 23 | 10 |
| Pomalidomide | 274.3 | 256.5 | 50 | 100 | 29 | 10 |
| Ponatinib | 533.2 | 260.1 | 50 | 120 | 40 | 12 |
| Rivaroxaban | 436.2 | 145.2 | 50 | 100 | 36 | 10 |
| Roflumilast | 403.3 | 187.2 | 50 | 110 | 36 | 10 |
| Rolapltant | 501.3 | 198.3 | 50 | 88 | 39 | 10 |
| Ruxolitinib | 307.1 | 186 | 50 | 70 | 38 | 10 |
| Safinamide | 303.4 | 215.1 | 50 | 25 | 13 | 10 |
| Sonidegib | 486.2 | 427.9 | 50 | 153 | 38 | 12 |
| Suvorexant | 451.2 | 186.2 | 50 | 81 | 29 | 10 |
| Tasimelteon | 246.1 | 173.1 | 50 | 70 | 22 | 10 |
| Telaprevir | 680.4 | 322.3 | 50 | 100 | 26 | 10 |
| Tofacitinib | 313.2 | 149.2 | 50 | 100 | 39 | 10 |
| Venetoclax | 868.4 | 636.4 | 50 | 208 | 35 | 12 |
| Vilazodone | 442.3 | 425.4 | 50 | 22 | 31 | 10 |
| Vorapaxar | 493.3 | 447.3 | 50 | 100 | 34 | 10 |