**Table S3.** Database hits for different adducts of the exact mass of 363.25047.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **adduct** | **no. of hits in Chemspider** | **empirical formula of the parent (mass defect)** | **no. of unique chemical structures** | **no. of structures with matching *in silico* and experimental fragmentation** |
| [M+H]+ | 78 | 1 x C20H35NaO4 (0.0001)  1 x C20H33F3O2 (0.0001)  76 x C18H30N6O2 (-0.0002) | 69 | 0 |
| [M+K]+ | 0 | - | - | - |
| [M+Na]+ | 254 | 254 x C20H36O4 (-0.0002) | 166 | 8 |
| [M+NH4]+ | 275 | 1 x C18H35KNaO2 (0.0000)  274 x C18H27N5O2 (-0.0001) | 248 | 0 |