**Table S4.** Compounds with an exact mass of 363.25047 [M+Na]+ and consistent *in silico* and experimental fragmentation.

|  |  |  |
| --- | --- | --- |
| **structure** | **ChemSpider ID**  **CAS** | **systematic name and synonyms** |
| 363_M+Na_1.png | 4517207  142-16-5 | bis(2-ethylhexyl) (2Z)-but-2-enedioate  di(2-ethylhexyl) maleate  DEHM |
| 363_M+Na_2.png | 4938521  2915-53-9 | dioctyl (2Z)-but-2-enedioate  dioctyl maleate  DOM |
| 363_M+Na_4.png | 4940564  56970-73-1 | bis(1-methylheptyl) (2Z)-but-2-enedioate  bis(1-methylheptyl) maleate |
| 363_M+Na_6.png | 5288522  - | bis(1,1-dimethylhexyl) (2Z)-but-2-enedioate  bis(1,1-dimethylhexyl) maleate |
| 363_M+Na_3.png | 4940955  1330-75-2 | bis(6-methylheptyl) (2E)-but-2-enedioate  diisooctyl fumarate |
| 363_M+Na_5.png | 192221  - | bis(3-methylheptyl) (2E)-but-2-enedioate |
| 363_M+Na_7.png | 14638680  - | bis(1-tert-butylbutyl) (2E)-but-2-enedioate |
| 363_M+Na_9.png | 14638681  - | bis[2,2-dimethyl-1-(1-methylethyl)propyl] (2E)-but-2-enedioate |