**Supplementary Data 2: Composition of custom-made library**

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| --- | --- |
| **Type of molecules** | **Number** |
| 1. Terpenes
 | 313 |
| 1. Terpenoids
 | 3254 |
| 1. Anti-tussive
 | 82 |
| 1. Synthetic antivirals
 | 75 |
| 1. Anti Influenza
 | 17 |
| 1. Flavanoids
 | 1288 |
| 1. Alkaloids
 | 1080 |
| 1. Predicted anti-COVID-19 molecules (from literature
 | 130 |
| **Total** | **7140** |