**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** | **7139** |