Enamine Acids Selection for Synthesising Tom Docked Compounds Targeting SARS-COV2-Nsp13.

Please note, some docking results are based on the structure of one enantiomers, whille the compounds we are going to make are mixture of two stereoisomers.

I didn’t find any motif containing fluorine in the top scoring compounds with binding energy < -8 kcal/mol. There are a few in the compounds with higher binding energy, but I think since the idea is that compounds with higher binding energy won’t bind well to the target, so I didn’t try to buy them.

The highlighted yellow ones are the ones I ordered. The other two are candidates which are not very expensive but can be used to synthesise compounds with lower binding energy.

We have acetic acid, propiolic acid, etc, in the department.

Number 1-3 are acids that can be used to make compounds with lower binding energy. Number 4 is an acid to make compounds with higher binding energy.

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| --- | --- | --- | --- | --- | --- |
| NO. | Enamine Code | Acids | Website  Price | Target Compounds | Average Binding Energy (kcal/mol) |
| 1 | EN300-06233 |  | 50 mg/135$ |  | -8.79 |
|  |  |  |  |  | -8.73 |
|  |  |  |  |  | -8.17 |
| 2 | EN300-10273  Ordered 250 mg.  135 euro |  | 50 mg/66$;  250 mg/142$ |  | -8.62 |
|  |  |  |  |  | -8.1 |
|  |  |  |  |  | -8.03 |
| 3 | EN300-30836 |  | 50 mg/88$; 250 mg/188$ |  | -8.07 |
| 4 | EN300-91129  Ordered 1 gram  24 euro |  | 1 g/ 25$ |  | -5.83 |
|  |  |  |  |  | -6.05 |
|  |  |  |  |  | -5.86 |