

Electronic Supporting Information

Systematic Virtual Screening in Search of SARS CoV-2 Inhibitors against Spike Glycoprotein: Pharmacophore Screening, Molecular Docking, ADMET Analysis and MD Simulations

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1. Site Map Analysis

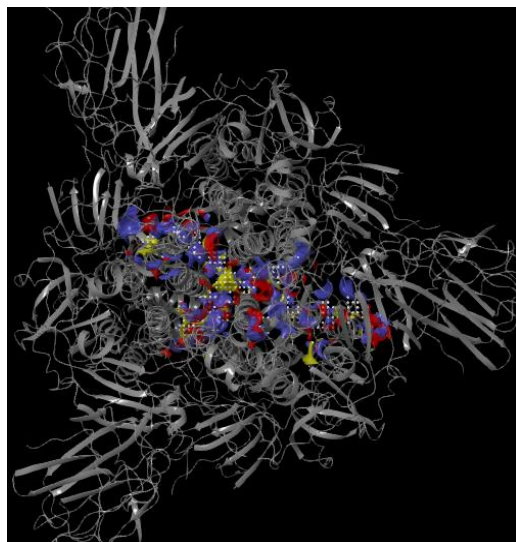


Figure S1. Residues of identified top five sites from site map analysis.

2. Pharmacophore Hypothesis Model

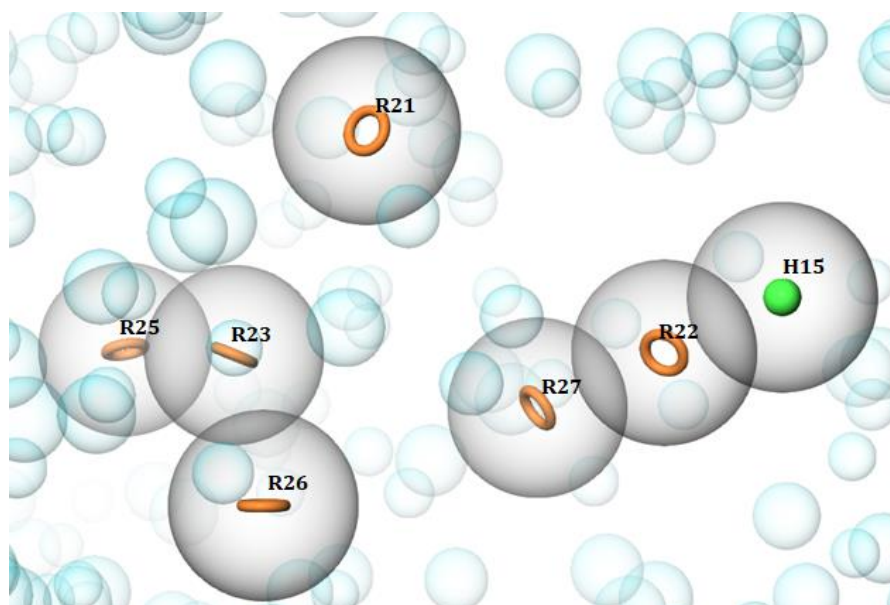
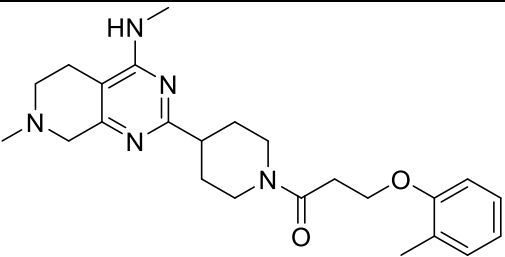
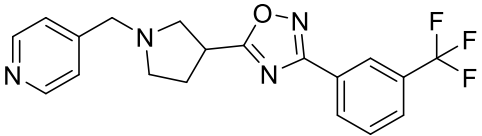
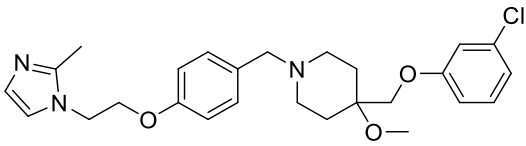
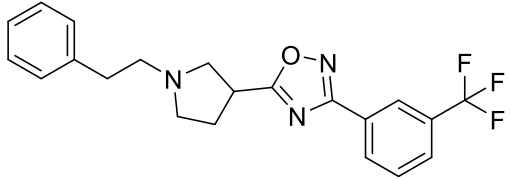
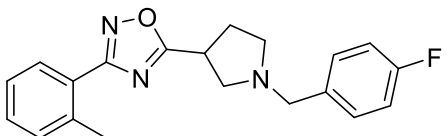
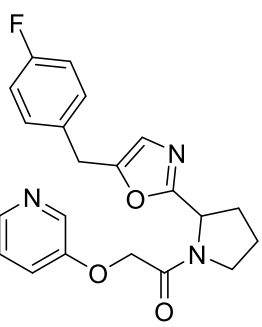
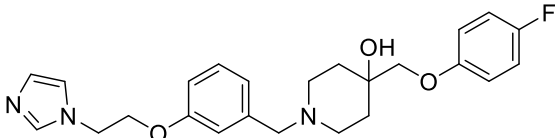


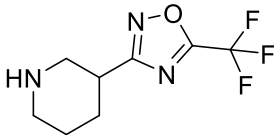
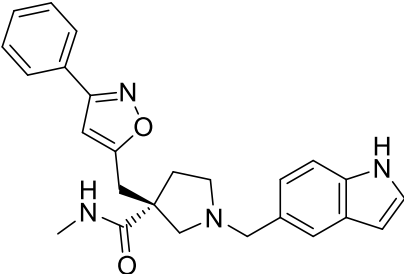
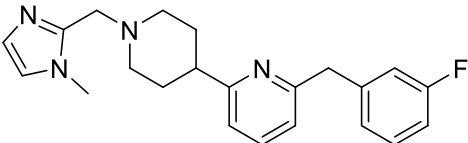
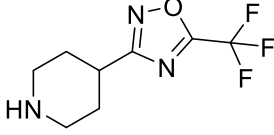
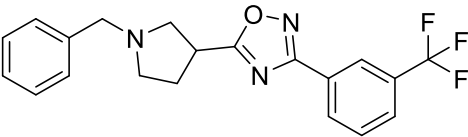
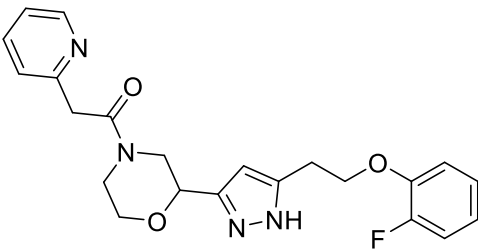
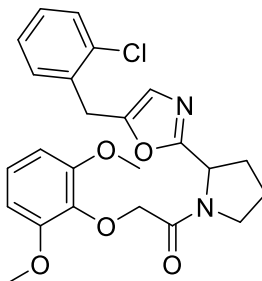
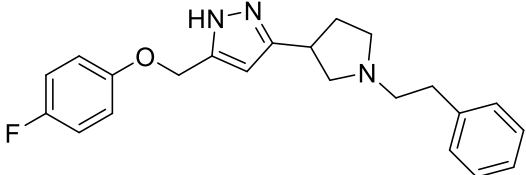
Figure S2. Pharmacophore hypothesis model with Identified seven features of pharmacophore hypothesis (RRRRRRH). The key features aromatic rings (R21, R22, R23, R25, R26, and R27) and hydrophobic features (H15) have been presented in brown colored rings and light green colored spheres, respectively.

3. Molecular Docking

Table S1. Docking scores of top 29 compounds having docking score of ≤ -6.9 using HTVS module against spike glycoprotein (PDB ID: 6VXX)

| Entry | Dataset ID | Compounds | Docking score | G Score |
|-------|--------------|--|---------------|---------|
| 1 | BDE 25380824 |  | -8.07 | -8.11 |
| 2 | BDE 19706316 |  | -8.00 | -8.03 |
| 3 | LAS 52154116 |  | -7.90 | -8.03 |
| 4 | BDE 19706304 |  | -7.89 | -7.89 |
| 5 | BDE 19705849 |  | -7.87 | -7.88 |
| 6 | BDE 33513330 |  | -7.70 | -7.70 |
| 7 | LAS 52170321 |  | -7.68 | -8.12 |

| | | | | |
|----|--------------|--|-------|-------|
| 8 | BDE 19703726 | | -7.67 | -7.68 |
| 9 | LAS 52165134 | | -7.65 | -7.95 |
| 10 | BBB 30061285 | | -7.58 | -7.68 |
| 11 | BBE 27288594 | | -7.44 | -7.45 |
| 12 | BBF 32237938 | | -7.44 | -7.44 |
| 13 | LAS 52463628 | | -7.44 | -7.54 |
| 14 | BDE 19706384 | | -7.41 | -7.46 |
| 15 | BDE 19704741 | | -7.41 | -7.42 |
| 16 | BBF 30702477 | | -7.40 | -7.41 |
| 17 | BBD 30699213 | | -7.36 | -7.36 |

| | | | | |
|----|--------------|--|-------|-------|
| 18 | BBC 27288400 |  | -7.30 | -7.31 |
| 19 | BDF 26908734 |  | -7.27 | -7.28 |
| 20 | BDC 27860794 |  | -7.23 | -7.29 |
| 21 | BBD 27288215 |  | -7.20 | -7.20 |
| 22 | BDE 19706291 |  | -7.12 | -7.13 |
| 23 | BDF 25425575 |  | -7.11 | -7.52 |
| 24 | BDE 33513945 |  | -7.09 | -7.09 |
| 25 | BDF 24967434 |  | -7.08 | -7.46 |

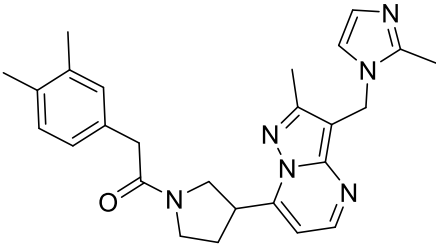
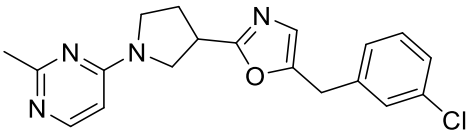
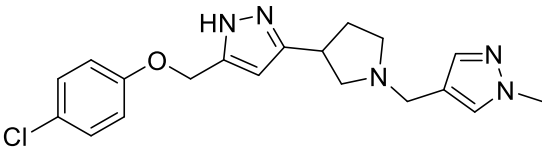
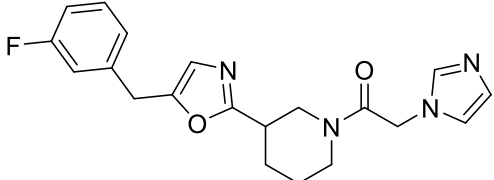
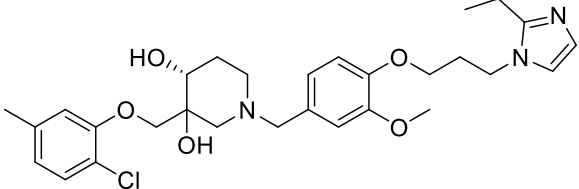
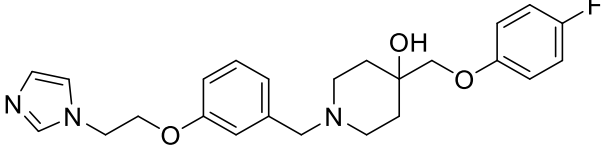
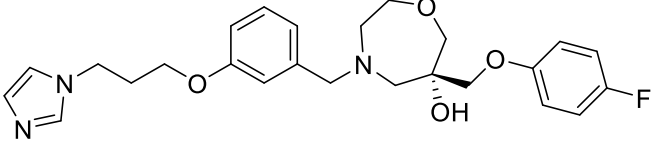
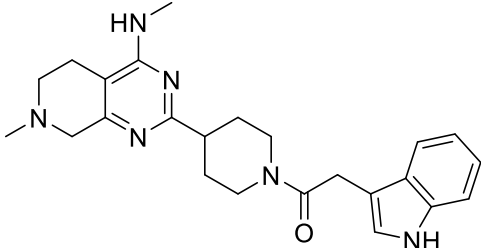
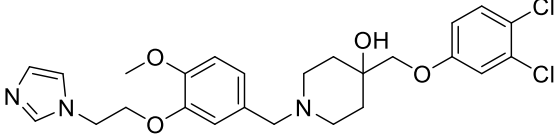
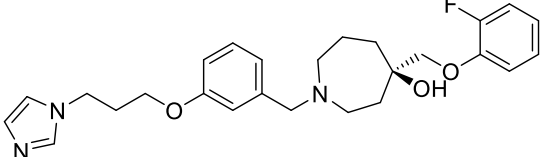
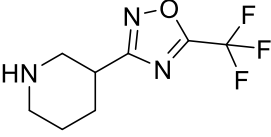
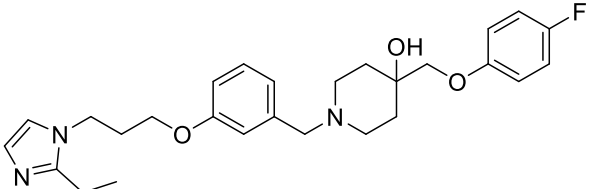
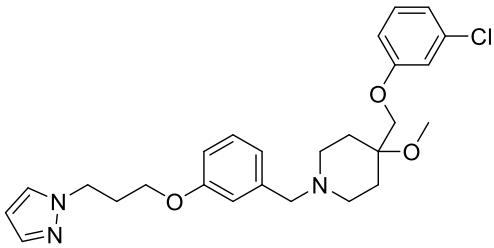
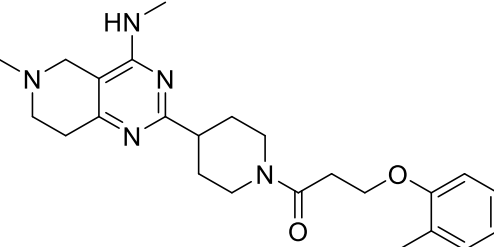
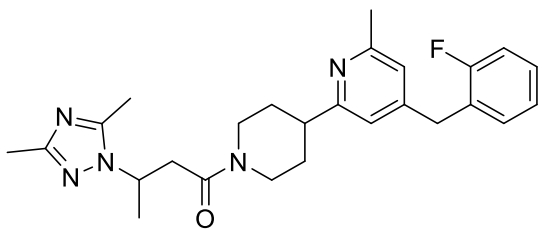
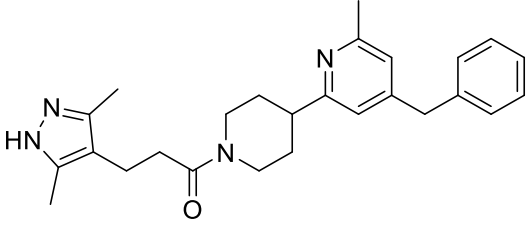
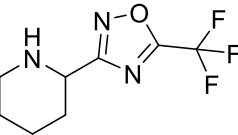
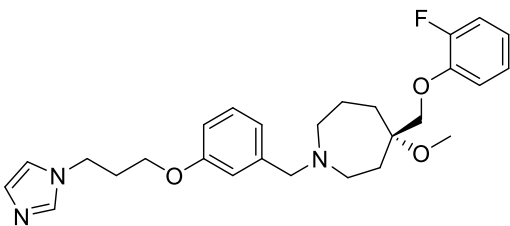
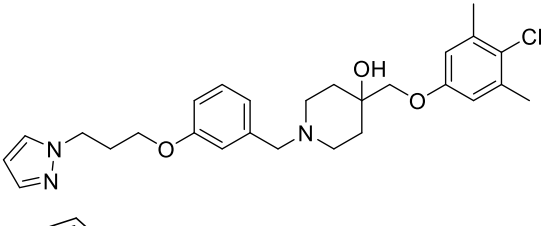
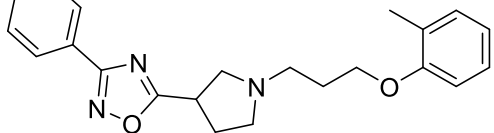
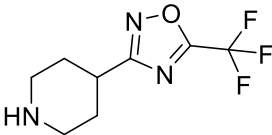
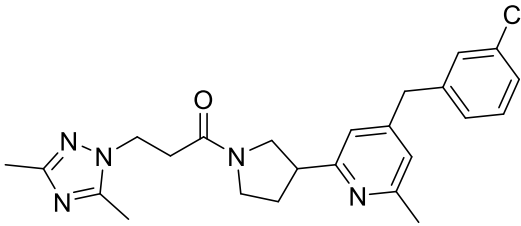
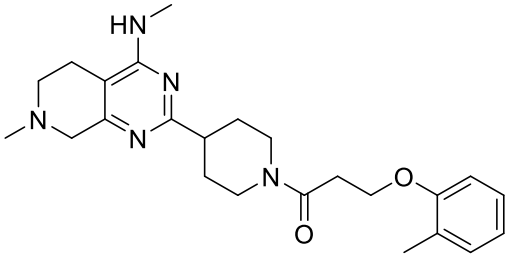
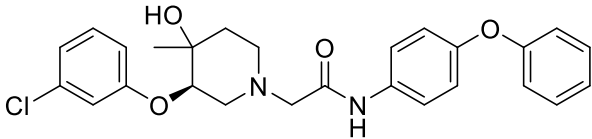
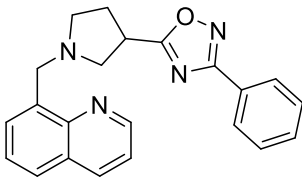
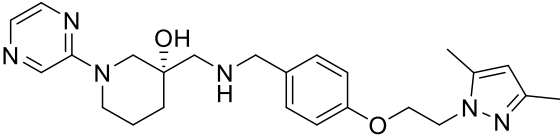
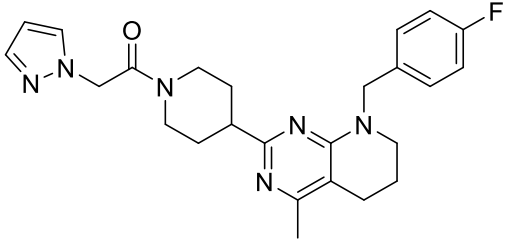
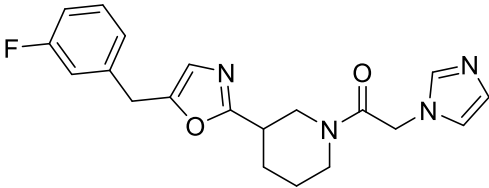
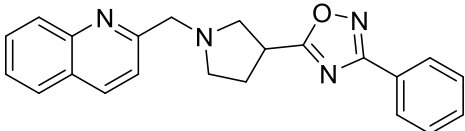
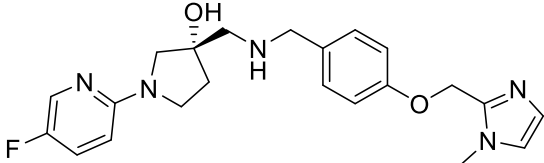
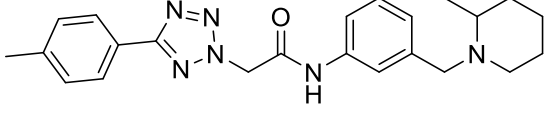
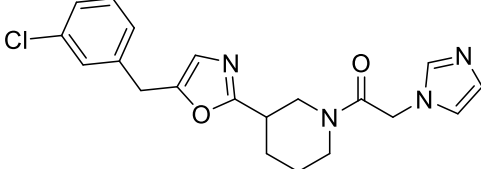
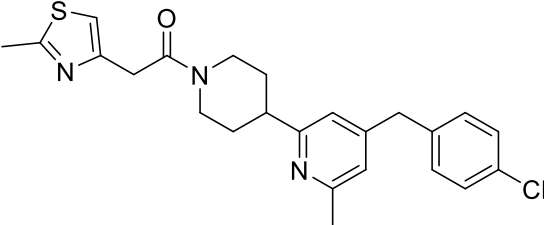
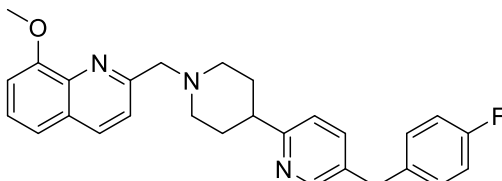
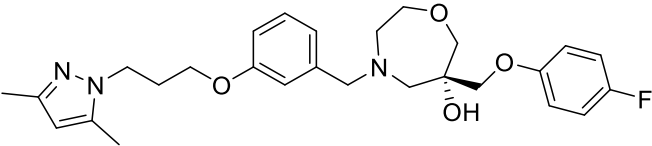
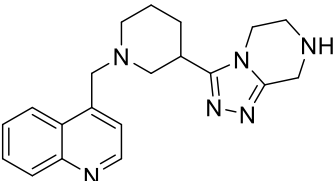
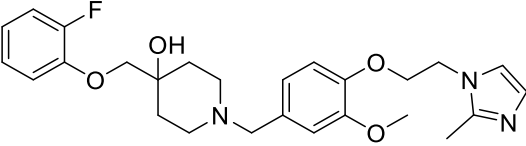
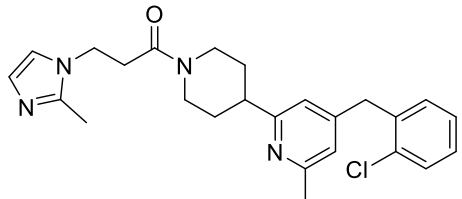
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|----|--------------|--|-------|-------|
| 26 | BDF 25210950 |  | -7.05 | -7.15 |
| 27 | BDE 31971839 |  | -7.01 | -7.37 |
| 28 | BDF 24970256 |  | -7.00 | -7.41 |
| 29 | BDE 33507948 |  | -7.00 | -7.26 |

Table S2. Docking scores of top 35 compounds having docking score of ≤ -6.9 using SP module against spike glycoprotein (PDB ID: 6VXX)

| Entry | Dataset ID | Compounds | Docking score | G Score |
|-------|-----------------|--|---------------|---------|
| 1 | LAS 52463628 |  | -8.88 | -8.99 |
| 2 | LAS 52170321 |  | -8.68 | -9.12 |
| 3 | LAS 52202853 |  | -8.67 | -9.03 |
| 4 | BDE 25381797 |  | -8.67 | -8.71 |
| 5 | LAS 52167198 |  | -8.58 | -9.01 |
| 6 | LAS 52167276 |  | -8.22 | -8.53 |
| 7 | BBC 27288400 |  | -8.04 | -8.04 |
| 8 | LAS 52160889 |  | -7.98 | -8.07 |

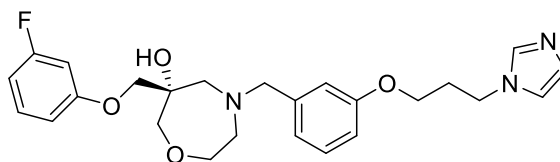
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|----|-----------------|--|-------|-------|
| 9 | LAS 52160945 |  | -7.81 | -7.83 |
| 10 | BDE 25357489 |  | -7.63 | -7.78 |
| 11 | BDE 25462094 |  | -7.61 | -8.17 |
| 12 | BDE 25461784 |  | -7.60 | -8.17 |
| 13 | BBE 27288594 |  | -7.58 | -7.59 |
| 14 | LAS 52167278 |  | -7.52 | -7.84 |
| 15 | LAS 52160955 |  | -7.49 | -7.51 |
| 16 | BDE 19703753 |  | -7.46 | -7.47 |

| | | | | |
|----|-----------------|--|-------|-------|
| 17 | BBD 27288215 |  | -7.40 | -7.41 |
| 18 | BDE 26188290 |  | -7.33 | -7.63 |
| 19 | BDE 25380824 |  | -7.28 | -7.32 |
| 20 | LAS 51217062 |  | -7.27 | -7.33 |
| 21 | BDE 19703721 |  | -7.23 | -7.25 |
| 22 | LAS 52129262 |  | -7.22 | -7.22 |
| 23 | BDE 25439571 |  | -7.20 | -7.23 |
| 24 | BDE 33507948 |  | -7.18 | -7.44 |
| 25 | BDE 19703717 |  | -7.18 | -7.20 |

| | | | | |
|----|-----------------|--|-------|-------|
| 26 | LAS 52126405 |  | -7.16 | -7.48 |
| 27 | BDD 22956907 |  | -7.16 | -7.17 |
| 28 | BDE 33507961 |  | -7.13 | -7.39 |
| 29 | BDE 25462490 |  | -7.13 | -7.71 |
| 30 | BDE 25664675 |  | -7.10 | -7.13 |
| 31 | LAS 52205117 |  | -7.09 | -7.16 |
| 32 | BDE 25327002 |  | -7.05 | -7.11 |
| 33 | LAS 52164733 |  | -7.05 | -7.18 |
| 34 | BDE 25462007 |  | -7.03 | -7.69 |

35

LAS
52202837



-7.02

-7.39
