

Supplementary Table 4. DeepSite prediction results

| PDB ID | Cavity | scores      | centers                 |
|--------|--------|-------------|-------------------------|
| 6LZG   | 1      | 0.996699    | [-11.4, -0.874, -24.16] |
|        | 2      | 0.932989    | [-27.4, 13.13, 5.84]    |
| 5R84   | 1      | 0.977018    | [15.5, 3.65, -4.35]     |
|        | 2      | 0.989906    | [9.5, -1.65, 23.65]     |
|        | 3      | 0.814471    | [1.5, -19.65, 9.65]     |
|        | 4      | 0.747475    | [19.5, 10.35, -0.35]    |
| 1A7C   | 1      | 0.998783872 | [19.63, 21.56, 9.28]    |
|        | 2      | 0.995458469 | [19.63, 21.56, 19.28]   |
|        | 3      | 0.819185138 | [19.63, -6.44, 23.28]   |