Supplemental Material

**Table S1.** The hydrogen bonds summary

**LASW1976**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Acceptor** | **Donor** | **Occupancy (%)** | **Distance** | **Angle** |
| LIG@O4 | LYS\_779@HZ1: LYS\_779@NZ | 19.38 | 2.8321 | 154.2841 |
| LIG@O11 | TYR\_813@HH: TYR\_813@OH | 19.00 | 2.8056 | 151.4145 |
| LIG@O4 | LYS\_779@HZ2: LYS\_779@NZ | 18.96 | 2.8288 | 154.4780 |
| LIG@O4 | LYS\_779@HZ3: LYS\_779@NZ | 17.17 | 2.8309 | 154.1194 |
| ASP\_787@OD1 | LIG@H22: LIG@O11 | 12.75 | 2.7040 | 163.9481 |
| LIG@O11 | ASP\_911@H: ASP\_911@N | 10.98 | 2.9121 | 147.4844 |
| TYR\_813@OH | LIG@H22: LIG@O11 | 10.77 | 2.8217 | 158.2042 |
| ASP\_787@OD2 | LIG@H22: LIG@O11 | 9.10 | 2.7047 | 164.5774 |

**Lig25/ZINC253496376**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Acceptor** | **Donor** | **Occupancy****(%)** | **Distance (Å)** | **Angle** |
| ASN\_836@OD1 | LIG@H10: LIG@N1 | 18.17 | 2.8508 | 161.7049 |
| LIG@O2 | ASN\_836@HD21: ASN\_836@ND2 | 12.58 | 2.8665 | 161.3705 |
| ASP\_897@OD1 | LIG@H11: LIG@O1 | 6.14 | 2.705 | 157.9328 |
| LIG@O4 | LYS\_779@HZ1: LYS\_779@NZ | 6.08 | 2.834 | 153.6269 |
| LIG@O4 | LYS\_779@HZ3: LYS\_779@NZ | 4.59 | 2.8385 | 153.1854 |
| LIG@O4 | LYS\_779@HZ2: LYS\_779@NZ | 4.29 | 2.8376 | 152.9561 |
| LIG@O4 | SER\_754@HG: SER\_754@OG | 4.1 | 2.7551 | 160.871 |
| ASP\_897@OD2 | LIG@H11: LIG@O1 | 2.55 | 2.6948 | 157.8535 |
| ASP\_753@O | LIG@H11: LIG@O1 | 1.21 | 2.7306 | 155.9408 |

**Lig199/ZINC12638303**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Acceptor** | **Donor** | **Occupancy****(%)** | **Distance (Å)** | **Angle** |
| LIG@O3 | ASP\_911@H: ASP\_911@N | 29.37 | 2.8572 | 155.433 |
| LIG@O | LYS\_779@HZ2: LYS\_779@NZ | 17.73 | 2.8494 | 158.0609 |
| LIG@O | LYS\_779@HZ3: LYS\_779@NZ | 17.27 | 2.8509 | 158.3119 |
| LIG@O | LYS\_779@HZ1: LYS\_779@NZ | 17.03 | 2.8488 | 158.1917 |
| LIG@O3 | PHE\_912@H: PHE\_912@N | 8.48 | 2.9122 | 161.5461 |
| LIG@O3 | TYR\_813@HH: TYR\_813@OH | 0.56 | 2.8 | 157.2852 |

**Lig449/ZINC85878047**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Acceptor** | **Donor** | **Occupancy (%)** | **Distance (Å)** | **Angle** |
| LIG@N | SER\_754@HG: SER\_754@OG | 12.56 | 2.8348 | 161.0314 |
| LIG@O2 | ASP\_911@H: ASP\_911@N | 3.98 | 2.8956 | 149.7736 |
| LIG@O5 | ASN\_836@HD21: ASN\_836@ND2 | 3.61 | 2.8949 | 155.151 |
| LIG@O2 | TYR\_813@HH: TYR\_813@OH | 0.94 | 2.7947 | 151.3205 |

**Lig554/ZINC253389510**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Acceptor** | **Donor** | **Occupancy (%)** | **Distance (Å)** | **Angle** |
| GLU\_826@O | LIG@H49: LIG@O2 | 17.43 | 2.7683 | 149.2093 |
| ASP\_832@OD2 | LIG@H49:LIG@O2 | 15.99 | 2.6771 | 164.9243 |
| ASP\_911@OD1 | LIG@H54: LIG@O4 | 15.4 | 2.6663 | 163.5248 |
| ASP\_911@OD1 | LIG@H73: LIG@O14 | 12.8 | 2.6889 | 160.5992 |
| ASP\_753@O | LIG@H75: LIG@O15 | 12.5 | 2.7488 | 152.2243 |
| LIG@O2 | VAL\_828@H: VAL\_828@N | 11.6 | 2.9046 | 154.3873 |
| ASP\_911@OD2 | LIG@H54: LIG@O4 | 8.32 | 2.6839 | 162.1231 |
| ASP\_911@OD2 | LIG@H52: LIG@O3 | 7.74 | 2.7059 | 162.2474 |
| ASP\_911@OD1 | LIG@H71: LIG@O13 | 7.47 | 2.7205 | 162.0516 |
| ASP\_832@OD1 | LIG@H49: LIG@O2 | 5.3 | 2.6716 | 164.6396 |
| LIG@O15 | SER\_754@HG: SER\_754@OG | 5.07 | 2.7794 | 162.2276 |
| ASP\_911@OD1 | LIG@H52: LIG@O3 | 4.66 | 2.7094 | 162.4811 |
| VAL\_828@O | LIG@H49: LIG@O2 | 4.1 | 2.7805 | 158.1816 |
| SER\_749@O | LIG@H49: LIG@O2 | 4.02 | 2.7497 | 158.3409 |
| ASP\_753@O | LIG@H65: LIG@O11 | 3.98 | 2.729 | 158.5985 |
| LIG@O6 | LYS\_779@HZ2: LYS\_779@NZ | 3.85 | 2.8663 | 155.1535 |
| LIG@O11 | ASP\_753@H: ASP\_753@N | 3.84 | 2.9079 | 161.8676 |
| LIG@O6 | LYS\_779@HZ3: LYS\_779@NZ | 3.73 | 2.8534 | 154.9095 |
| ASP\_753@OD2 | LIG@H65: LIG@O11 | 3.05 | 2.7129 | 155.0601 |
| ASP\_753@OD2 | LIG@H63: LIG@O10 | 2.93 | 2.6682 | 163.9365 |
| ASP\_911@OD2 | LIG@H73: LIG@O14 | 2.8 | 2.7502 | 159.7989 |
| LIG@O13 | LYS\_779@HZ1: LYS\_779@NZ | 2.57 | 2.8804 | 156.8394 |
| LIG@O6 | LYS\_779@HZ1: LYS\_779@NZ | 2.46 | 2.8665 | 155.2725 |
| ASP\_897@OD1 | LIG@H54: LIG@O4 | 1.74 | 2.6572 | 163.4485 |
| ASP\_753@OD1 | LIG@H63: LIG@O10 | 1.58 | 2.6847 | 164.1326 |
| ASP\_753@OD1 | LIG@H65: LIG@O11 | 1.46 | 2.7115 | 152.5103 |
| ASP\_753@O | LIG@H63: LIG@O10 | 1.41 | 2.7781 | 158.6556 |
| ASP\_897@OD2 | LIG@H54: LIG@O4 | 1.11 | 2.6637 | 162.7398 |
| LIG@O13 | LYS\_779@HZ3: LYS\_779@NZ | 1.05 | 2.8727 | 156.1291 |
| ASP\_911@OD2 | LIG@H71: LIG@O13 | 1.03 | 2.6941 | 161.9972 |

**Lig682/ZINC98047241**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Acceptor** | **Donor** | **Occupancy (%)** | **Distance (Å)** | **Angle** |
| ASP\_832@OD1 | LIG@H1: LIG@O1 | 96.26 | 2.5762 | 160.8423 |
| LIG@O | THR\_751@HG1: THR\_751@OG1 | 52.23 | 2.8151 | 160.591 |
| ASP\_832@OD2 | LIG@H1: LIG@O1 | 2.89 | 2.5814 | 161.5876 |
| LIG@O | THR\_751@H: THR\_751@N | 2.22 | 2.9229 | 146.8994 |
| LIG@O | ASN\_836@HD22: ASN\_836@ND2 | 1.35 | 2.8636 | 151.0019 |
| LIG@F | TRP\_760@HE1: TRP\_760@NE1 | 1.35 | 2.8948 | 143.8625 |
| LIG@O3 | ASP\_753@H: ASP\_753@N | 0.24 | 2.9288 | 157.3903 |