**Table 1**
**Optimized geometrical parameters of 4-((4-acetylphenyl)amino)-2-methylene-4-oxobutanoic acid with XRD data**

| Bond lengths (Å) DFT/XRD | | | |
|---|---|---|---|
| C8-O1 | 1.2164/1.2222 | C13-O2 | 1.2043/1.2492 |
| O3-H4 | 0.9699/0.9750 | C13-O3 | 1.3720/1.2882 |
| C27-O5 | 1.2186/1.2162 | N6-H7 | 1.0120/0.8800 |
| C8-N6 | 1.3756/1.3542 | C17-N6 | 1.4056/1.4202 |
| C8-C9 | 1.5388 /1.5232 | C9-H10 | 1.0891/0.9900 |
| C9-H11 | 1.0923/0.9900 | C9-C12 | 1.5162/1.5042 |
| C12-C13 | 1.4922/1.4852 | C12-C14 | 1.3369/1.3282 |
| C14-H15 | 1.0843/0.9820 | C14-H16 | 1.0835/1.0030 |
| C17-C18 | 1.4068/1.3892 | C17-C25 | 1.4012 /1.3952 |
| C18-H19 | 1.0868 /0.9500 | C18-C20 | 1.3822 /1.3802 |
| C20-H21 | 1.0838/0.9500 | C20-C22 | 1.4033/1.3972 |
| C22-C23 | 1.3999/1.3922 | C22-C27 | 1.4944/1.4972 |
| C23-H24 | 1.0843/0.9500 | C23-C25 | 1.3914/1.3852 |
| C25-H26 | 1.0792/0.9500 | C27-C28 | 1.5182/1.5042 |
| C28-H29 | 1.0941/0.9800 | C28-H30 | 1.0941/0.9800 |
| C28-H31 | 1.0888/0.9800 | | |

| Bond angles (°) DFT/XRD | | | |
|---|---|---|---|
| H4-O3-C13 | 107.1/118.2 | H7-N6-C8 | 115.3/116.8 |
| H7-N6-C17 | 115.6/116.8 | C8-N6-C17 | 129.0/126.5 |
| O1-C8-N6 | 124.7/123.5 | O1-C8-C9 | 121.2/121.4 |
| N6-C8-C9 | 114.1/115.0 | C8-C9-H10 | 105.5/109.4 |
| C8-C9-H11 | 110.2/109.4 | C8-C9-C12 | 113.3/111.3 |
| H10-C9-H11 | 107.9/ 108.0 | H10-C9-C12 | 109.2/109.4 |
| H11-C9-C12 | 110.5/109.4 | C9-C12-C13 | 120.4/116.8 |
| C9-C12-C14 | 122.6 /123.9 | C13-C12-C14 | 117.1/119.2 |
| O2-C13-O3 | 121.1/123.3 | O2-C13-C12 | 126.5/120.9 |
| O3-C13-C12 | 112.3/115.7 | C12-C14-H15 | 121.3/118.9 |
| C12-C14-H16 | 120.8/122.5 | H15-C14-H16 | 117.9 /118.5 |
| N6-C17-C18 | 117.1/117.6 | N6-C17-C25 | 123.7/122.6 |
| C18-C17-C25 | 119.2 /119.6 | C17-C18-H19 | 119.6/ 120.0 |
| C17-C18-C20 | 120.7/120.0 | H19-C18-C20 | 119.7 /120.0 |
| C18-C20-H21 | 120.6 /119.4 | C18-C20-C22 | 120.8 /121.1 |
| H21-C20-C22 | 118.6/119.4 | C20-C22-C23 | 118.1/118.1 |
| C20-C22-C27 | 118.7 /118.7 | C23-C22-C27 | 123.2 /123.1 |
| C22-C23-H24 | 120.3 /119.3 | C22-C23-C25 | 121.8/121.3 |
| H24-C23-C25 | 117.9 /119.3 | C17-C25-C23 | 119.4/119.6 |
| C17-C25-H26 | 119.9/120.2 | C23-C25-H26 | 120.7/120.2 |
| O5-C27-C22 | 120.8/120.3 | O5-C27-C28 | 120.4/121.3 |
| C22-C27-C28 | 118.8 /118.3 | C27-C28-H29 | 111.2/109.5 |
| C27-C28-H30 | 111.3/109.5 | C27-C28-H31 | 108.9/109.5 |

| | | | | |
|---|---|---|---|---|
| H29-C28-H30 | 107.3/109.5 | H29-C28-H31 | 109.1/109.5 |
| H30-C28-H31 | 109.1/109.5 | | |

Dihedral angles (°) DFT/XRD

| | | | |
|---|---|---|---|
| C17-N6-C8-O1 | 1.0/-5.0 | C17-N6-C8-C9 | -178.8/-174.0 |
| C8-N6-C17-C18 | 178.5/148.4 | C8-N6-C17-C25 | -1.7/-34.2 |
| O1-C8-C9-C12 | -101.7/-35.3 | N6-C8-C9-C12 | 78.1/145.7 |
| C8-C9-C12-C13 | -88.6/-68.8 | C8-C9-C12-C14 | 91.6/ 111.3 |
| C9-C12-C13-O2 | -176.0/-177.0 | C9-C12-C13-O3 | 3.6/-3.0 |
| C14-C12-C13-O2 | 3.8/-3.1 | C14-C12-C13-O3 | -176.6/-176.9 |
| N6-C17-C18-C20 | 179.9/177.5 | C25-C17-C18-C20 | 0.1/0.0 |
| N6-C17-C25-C23 | -179.9/-177.5 | C18-C17-C25-C23 | -0.1/-0.1 |
| C17-C18-C20-C22 | -0.0/0.0 | C18-C20-C22-C23 | -0.0/0.1 |
| C18-C20-C22-C27 | 179.9/179.3 | C20-C22-C23-C25 | 0.0/-0.2 |
| C27-C22-C23-C25 | -179.9/-179.2 | C20-C22-C27-O5 | 0.2/0.6 |
| C20-C22-C27-C28 | -179.8/-179.8 | C23-C22-C27-O5 | -179.9/-178.8 |
| C23-C22-C27-C28 | 0.2/0.4 | C22-C23-C25-C17 | 0.0/ 0.2 |

**Table 2**

**Calculated (scaled) wavenumbers, observed IR, Raman bands and vibrational assignments of 4-((4-acetylphenyl)amino)-2-methylene-4-oxobutanoic acid**

| B3LYP/6-311++G(d) (5D, 7F) | | | IR | Raman | Assignments[a] |
|---|---|---|---|---|---|
| $\upsilon(cm^{-1})$ | $IR_I$ | $R_A$ | $\upsilon(cm^{-1})$ | $\upsilon(cm^{-1})$ | - |
| 3587 | 64.56 | 89.25 | 3564 | - | υOH(100) |
| 3434 | 109.55 | 206.49 | 3297 | - | υNH(98) |
| 3122 | 2.49 | 46.33 | - | - | υCH(98) |
| 3121 | 0.41 | 60.90 | - | - | $\upsilon CH_2$(100) |
| 3078 | 3.18 | 79.24 | 3075 | 3079 | υCH(97) |
| 3066 | 8.29 | 67.42 | 3064 | 3062 | υCH(98) |
| 3033 | 3.02 | 93.81 | - | - | $\upsilon CH_2$(98) |
| 3031 | 18.36 | 76.99 | - | 303 | υCH(97) |
| 3024 | 17.50 | 114.53 | 3025 | - | $\upsilon CH_3$(99) |
| 3012 | 4.01 | 51.44 | 3008 | 3009 | $\upsilon CH_2$(99) |
| 2974 | 10.44 | 42.85 | 2972 | 2970 | $\upsilon CH_3$(100) |
| 2956 | 7.94 | 99.41 | 2954 | 2950 | $\upsilon CH_2$(99) |
| 2920 | 3.68 | 161.22 | 2928 | 2930 | $\upsilon CH_3$(100) |
| 1737 | 298.26 | 16.87 | 1744 | - | υC=O(75) |
| 1694 | 228.66 | 72.25 | 1695 | - | υC=O(72) |
| 1672 | 248.51 | 123.30 | 1665 | 1661 | υC=O(78) |
| 1617 | 39.39 | 93.90 | 1610 | 1600 | υC=C(65), δOH(15) |
| 1586 | 56.67 | 471.00 | 1590 | - | υPh(60), δNH(10) |
| 1574 | 283.25 | 191.24 | 1580 | - | υPh(47), δNH(22) |
| 1508 | 532.16 | 199.86 | 1505 | 1506 | υPh(41), δNH(24) |
| 1483 | 2.23 | 3.21 | - | - | υPh(30), δNH(48) |
| 1440 | 35.98 | 11.78 | - | 1438 | $\delta CH_2$(91) |
| 1440 | 12.31 | 10.45 | - | 1438 | $\delta CH_3$(94) |
| 1431 | 19.60 | 5.29 | 1433 | - | $\delta CH_3$(90) |
| 1389 | 47.41 | 3.94 | - | - | υPh(57), $\delta CH_2$(14) |
| 1386 | 10.63 | 32.59 | 1383 | 1381 | $\delta CH_2$(58), υPh(10) |
| 1346 | 52.41 | 1.75 | 1345 | 1355 | $\delta CH_3$(94) |
| 1308 | 132.82 | 26.16 | - | 1308 | δOH(41), υCC(24) |
| 1300 | 71.32 | 94.23 | 1302 | - | υPh(56), δCH(22) |
| 1288 | 23.56 | 7.36 | 1285 | - | υPh(17), δCH(68) |
| 1277 | 3.01 | 5.69 | 1273 | 1274 | $\delta CH_2$(85) |
| 1238 | 6.43 | 12.83 | 1240 | - | $\delta CH_2$(35), δNH(45) |
| 1234 | 241.44 | 42.46 | - | - | υCO(46), υCN(40) |
| 1231 | 159.86 | 153.86 | 1225 | - | υCN(47), υPh(22) |
| 1205 | 5.92 | 21.57 | 1198 | 1198 | υCC(42), $\delta CH_2$(15) |
| 1159 | 121.53 | 128.73 | 1157 | 1162 | δCH(68) |
| 1110 | 246.32 | 12.17 | 1112 | 1115 | υCN(11), $\delta CH_2$(47) |
| 1105 | 101.86 | 0.97 | - | - | $\delta CH_2$(41), δCH(40) |
| 1082 | 116.72 | 4.15 | 1090 | 1084 | υCC(48), $\delta CH_2$(10) |
| 1052 | 2.09 | 69.75 | 1050 | - | $\delta CH_3$(55), υPhI(25) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 139 | 1011 | 0.89 | 0.29 | 1013 | 1008 | δ$CH_3$(70), δCH(19) |
| 140 | 990 | 0.80 | 12.19 | 988 | - | δCH(53), υPhI(34) |
| 141 | 965 | 34.88 | 4.10 | 964 | - | γOH(95) |
| 142 | 943 | 1.34 | 0.20 | 945 | 946 | γCHI(53), τPhI(29) |
| 143 | 941 | 0.23 | 0.17 | - | - | γCHI(73), τPhI(14) |
| 144 | 940 | 11.51 | 4.15 | - | - | υCC(43), δ$CH_2$(23) |
| 145 | 932 | 18.42 | 4.66 | - | - | δ$CH_2$(44), υCC(10) |
| 146 | 924 | 34.87 | 19.37 | 927 | 921 | υCC(35), δ$CH_3$(22), |
| 147 | | | | | | δ$CH_2$(21) |
| 148 | 911 | 6.59 | 2.12 | - | - | δ$CH_2$(39), υCC(19) |
| 149 | 835 | 4.98 | 8.70 | 836 | - | υPh(43), δC=O(14) |
| 150 | 826 | 48.32 | 0.29 | - | 824 | γCHI(71), γCN(10), τPhI(10) |
| 151 | 807 | 34.36 | 0.50 | 810 | - | γCHI(66) |
| 152 | 801 | 21.74 | 2.30 | 798 | 798 | γC=O(40), τ$CH_2$(18), |
| 153 | | | | | | γCHI(15) |
| 154 | 775 | 2.47 | 14.08 | 774 | - | γC=O(17), δ$CH_2$(26), |
| 155 | | | | | | υCC(10) |
| 156 | 739 | 8.24 | 4.58 | 739 | 739 | υCC(48), δCO(10), δPhI(10) |
| 157 | 719 | 0.18 | 1.22 | 721 | - | τPhI(66), γCN(14), γCC(11) |
| 158 | 685 | 19.02 | 28.63 | - | - | δCC(24), γC=O(40) |
| 159 | 661 | 81.02 | 1.00 | 670 | 664 | γNH(49), τC=O(29) |
| 160 | 659 | 80.06 | 2.12 | - | - | τ$CH_2$(25), τOH(24), |
| 161 | | | | | | γC=O(13), γNH(13) |
| 162 | 624 | 0.08 | 8.62 | 625 | - | δPhI(75) |
| 163 | 613 | 5.21 | 2.71 | 613 | 615 | τOH(34), δC=O(37) |
| 164 | 591 | 60.07 | 3.71 | 589 | 593 | τOH(22), δC=O(20), |
| 165 | | | | | | τ$CH_2$(10), δCC(12) |
| 166 | 579 | 12.59 | 0.46 | - | 572 | γC=O(37), δ$CH_3$(13), |
| 167 | | | | | | γCC(10), γCN(10), τPhI(13) |
| 168 | 558 | 7.08 | 1.86 | 552 | - | γNH(30), τPhI(13) |
| 169 | 519 | 7.37 | 5.96 | 517 | - | δC=O(35), δCC(17) |
| 170 | 501 | 7.96 | 2.37 | 501 | - | δCO(31), γCN(10), δCC(10) |
| 171 | 484 | 20.07 | 0.38 | - | 480 | τPhI(34), δCC(13), |
| 172 | | | | | | δC=O(10) |
| 173 | 458 | 7.05 | 0.55 | 464 | 458 | δCC(40), δC=O(10) |
| 174 | 411 | 1.24 | 1.09 | - | - | δCC(36), τCC(11), δC=O(19) |
| 175 | 404 | 0.05 | 0.08 | - | - | τPhI(91) |
| 176 | 386 | 19.05 | 2.33 | - | - | γCC(22), δCN(11), |
| 177 | | | | | | γC=O(11) |
| 178 | 361 | 4.53 | 1.89 | - | 367 | δCC(44), δC=O(13) |
| 179 | 331 | 0.48 | 1.60 | - | 331 | δCN(28), δC=O(18), |
| 180 | | | | | | δCC(20) |
| 181 | 294 | 0.59 | 1.32 | - | - | τPhI(29), γCC(27) |
| 182 | 284 | 0.21 | 0.59 | - | 282 | δCC(16), γCC(11), δCO(10), |
| 183 | | | | | | τPhI(10) |
| 184 | 226 | 0.96 | 3.57 | - | 230 | δNH(26), δCC(28), δPhI(19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 185 | 204 | 1.26 | 0.84 | - | 202 | δCC(53), δC=O(17) |
| 186 | 163 | 0.07 | 0.18 | - | 168 | $\tau CH_3$(90) |
| 187 | 154 | 0.40 | 0.61 | - | - | $\delta CH_2$(18), γNH(13), |
| 188 | | | | | | γCC(21), τC=O(11) |
| 189 | 120 | 9.26 | 0.28 | - | - | τCC(31), δCC(18), δCN(17), |
| 190 | | | | | | δNH(10) |
| 191 | 103 | 2.78 | 0.77 | - | - | $\delta CH_2$(30), τCC(16), |
| 192 | | | | | | τC=O(10) |
| 193 | 72 | 2.19 | 1.28 | - | 75 | τC=O(49), $\tau CH_2$(11) |
| 194 | 64 | 1.84 | 1.19 | - | - | τC=O(59), τNH(10) |
| 195 | 54 | 6.72 | 0.47 | - | - | $\tau CH_2$(37), τNH((21), |
| 196 | | | | | | τC=O(14) |
| 197 | 46 | 4.16 | 3.23 | - | - | τCC(54), τC=O(33) |
| 198 | 28 | 0.17 | 3.34 | - | - | τC=O(40), τNH(22) |
| 199 | 23 | 0.32 | 3.84 | - | - | $\tau CH_2$(38), τPh(31) |

200 [a]υ-stretching; δ-in-plane deformation; γ-out-of-plane deformation; τ-torsion; Ph-phenyl ring;
201 potential energy distribution (%) is given in brackets in the assignment column; $IR_I$-IR intensity;
202 $R_A$-Raman activity
203

204 **Table 3**
205 **Second order perturbation theory analysis of Fock matrix in NBO basis corresponding to the**
206 **intramolecular bonds of the title compound**
207

| Donor(i) | Type | ED/e | Acceptor(j) | Type | ED/e | E(2)[a] | E(i)-E(j)[b] | F(i,j)[c] |
|---|---|---|---|---|---|---|---|---|
| 208 O2-C8 | π | 1.98727 | C9-C12 | σ* | 0.02577 | 1.62 | 0.76 | 0.031 |
| 209 O2-C13 | σ | 1.99679 | C9-C12 | σ* | 0.02577 | 1.02 | 1.50 | 0.035 |
| 210 - | - | - | C12-C13 | σ* | 0.07375 | 1.70 | 1.52 | 0.046 |
| 211 - | π | 1.98705 | C12-C14 | π* | 0.04522 | 3.72 | 0.43 | 0.036 |
| 212 O2-C13 | σ | 1.99593 | C12-C14 | σ* | 0.01274 | 1.42 | 1.57 | 0.042 |
| 213 N6-C8 | σ | 1.98983 | N6-C17 | σ* | 0.02954 | 1.96 | 1.26 | 0.045 |
| 214 - | - | - | C17-C18 | σ* | 0.02094 | 1.53 | 1.38 | 0.041 |
| 215 C9-C9 | σ | 1.97042 | N6-C17 | σ* | 0.02954 | 4.49 | 1.06 | 0.062 |
| 216 - | - | - | C12-C14 | π* | 0.04522 | 2.69 | 0.66 | 0.038 |
| 217 C12-C13 | σ | 1.97498 | O2-C13 | σ* | 0.01831 | 1.02 | 1.29 | 0.032 |
| 218 - | - | - | C12-C14 | σ* | 0.01274 | 1.85 | 1.33 | 0.044 |
| 219 C17-C25 | σ | 1.97418 | N6-C17 | σ* | 0.02954 | 1.31 | 1.13 | 0.034 |
| 220 - | - | - | C17-C18 | σ* | 0.02094 | 3.72 | 1.25 | 0.061 |
| 221 - | - | - | C23-C25 | σ* | 0.01459 | 2.40 | 1.29 | 0.050 |
| 222 C23-C27 | σ | 1.98068 | C18-C20 | σ* | 0.01261 | 2.25 | 1.25 | 0.047 |
| 223 - | - | - | C20-C22 | σ* | 0.02187 | 1.96 | 1.22 | 0.044 |
| 224 - | - | - | C22-C23 | σ* | 0.02298 | 2.29 | 1.23 | 0.047 |
| 225 - | - | - | C23-C25 | σ* | 0.01459 | 2.07 | 1.24 | 0.045 |
| 226 C27-C28 | σ | 1.99071 | C20-C22 | σ* | 0.02187 | 2.35 | 1.20 | 0.048 |
| 227 LP1 N6 | σ | 1.97381 | N6-C8 | σ* | 0.07744 | 2.30 | 1.13 | 0.046 |
| 228 - | - | - | C8-C9 | σ* | 0.06928 | 1.91 | 1.03 | 0.040 |
| 229 LP1 N6 | π | 1.85987 | N6-C8 | σ* | 0.07744 | 26.63 | 0.71 | 0.124 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| - | 231 | - | - | C8-C9 | σ* | 0.06928 | 21.51 | 0.61 | 0.104 |
| LP | 232 | σ | 1.97599 | O3-C13 | σ* | 0.11051 | 1.20 | 1.01 | 0.032 |
| - | 233 | - | - | C12-C13 | σ* | 0.07375 | 2.88 | 1.10 | 0.051 |
| LP | 234 | π | 1.83353 | O3-C13 | σ* | 0.11051 | 36.97 | 0.59 | 0.133 |
| - | 235 | - | - | C12-C13 | σ* | 0.07375 | 19.40 | 0.68 | 0.105 |
| LP | 236 | σ | 1.96940 | O2-C13 | σ* | 0.01831 | 6.36 | 1.24 | 0.079 |
| LP | 237 | π | 1.83540 | O2-C13 | π* | 0.23906 | 40.87 | 0.35 | 0.109 |
| LP | 238 | σ | 1.97772 | C22-C27 | σ* | 0.06682 | 2.05 | 1.12 | 0.043 |
| - | 239 | - | - | C27-C28 | σ* | 0.05316 | 1.49 | 1.07 | 0.036 |
| LP | 240 | π | 1.89069 | C22-C27 | σ* | 0.06682 | 19.90 | 0.70 | 0.106 |
| - | 241 | - | - | C27-C28 | σ* | 0.05316 | 20.48 | 0.64 | 0.104 |
| LP | 242 | σ | 1.65329 | O1-C8 | π* | 0.26733 | 60.78 | 0.28 | 0.118 |
| - | 243 | - | - | C17-C25 | π* | 0.37737 | 36.48 | 0.30 | 0.094 |

[a] E(2) means energy of hyper-conjugative interactions (stabilization energy in kJ/mol).
[b] Energy difference (a.u.) between donor and acceptor i and j NBO orbitals.
[c] F(i,j) is the Fock matrix elements (a.u.) between i and j NBO orbitals.

**Table 4**

**NBO results showing the formation of Lewis and non-Lewis orbitals.**

| Bond (A–B) | ED/e[a] | EDA% | EDB % | NBO | s% | p% |
|---|---|---|---|---|---|---|
| σ O1-C8 | 1.98727 | 69.04 | 30.96 | $0.8309(sp^{1.00})O$ | 0.01 | 99.99 |
| | -0.37501 | - | - | $+0.5564(sp^{1.00})C$ | 0.01 | 99.99 |
| σ O2-C13 | 1.99679 | 65.83 | 34.17 | $0.8114(sp^{1.35})O$ | 42.30 | 57.70 |
| | -1.11704 | - | - | $+0.5845(sp^{1.95})C$ | 33.90 | 66.10 |
| σ O2-C13 | 1.98705 | 69.09 | 30.91 | $0.8312(sp^{99.99})O$ | 0.06 | 99.94 |
| | -0.40395 | - | - | $+0.5560(sp^{99.99})C$ | 0.05 | 99.95 |
| σ O3-C13 | 1.99593 | 69.34 | 30.66 | $0.8327(sp^{1.95})O$ | 33.83 | 66.17 |
| | -0.93837 | - | - | $+0.5537(sp^{2.82})C$ | 26.14 | 73.86 |
| σ N6-C8 | 1.98983 | 63.40 | 36.60 | $0.7962(sp^{1.77})N$ | 36.08 | 63.92 |
| | -0.83404 | - | - | $+0.6050(sp^{2.14})C$ | 31.81 | 68.19 |
| σ C8-C9 | 1.97042 | 48.03 | 51.97 | $0.6930(sp^{1.83})C$ | 35.36 | 64.66 |
| | -0.63420 | - | - | $+0.7209(sp^{2.98})C$ | 25.10 | 75.90 |
| σ C12-C13 | 1.97498 | 51.68 | 48.32 | $0.7189(sp^{2.42})C$ | 29.21 | 70.89 |
| | -0.69404 | - | - | $+0.6951(sp^{1.50})C$ | 39.90 | 60.10 |
| σ C17-C25 | 1.97418 | 51.50 | 48.50 | $0.7176(sp^{1.70})C$ | 37.04 | 62.96 |
| | -0.70144 | - | - | $+0.6964(sp^{2.00})C$ | 33.33 | 66.67 |
| σ C22-C27 | 1.98068 | 52.58 | 47.42 | $0.7251(sp^{2.18})C$ | 31.42 | 68.58 |
| | -0.64905 | - | - | $+0.6886(sp^{1.84})C$ | 35.15 | 64.85 |
| σ C27-C28 | 1.99071 | 48.58 | 51.42 | $0.6970(sp^{1.90})C$ | 34.51 | 65.49 |
| | -0.62679 | - | - | $+0.7171(sp^{2.70})C$ | 27.04 | 72.96 |
| LP O1 | 1.97381 | - | - | $sp^{0.73}$ | 57.74 | 42.26 |
| | -0.68016 | - | - | - | - | - |
| LP O1 | 1.85987 | - | - | $sp^{99.99}$ | 0.02 | 99.98 |
| | -0.25478 | - | - | - | - | - |
| LP O2 | 1.97599 | - | - | $sp^{0.74}$ | 57.60 | 42.40 |
| | -0.70320 | - | - | - | - | - |
| LP O2 | 1.83353 | - | - | $sp^{1.00}$ | 0.00 | 100.00 |
| | -0.27969 | - | - | - | - | - |
| LP O3 | 1.96940 | - | - | $sp^{1.27}$ | 44.08 | 55.92 |
| | -0.64024 | - | - | - | - | - |
| LP O3 | 1.83540 | - | - | $sp^{99.99}$ | 0.06 | 99.94 |
| | -0.36214 | - | - | - | - | - |
| LP O5 | 1.97772 | - | - | $sp^{0.76}$ | 56.80 | 43.20 |
| | -0.66999 | - | - | - | - | - |
| LP O5 | 1.89069 | - | - | $sp^{99.99}$ | 0.02 | 99.98 |
| | -0.24789 | - | - | - | - | - |
| LP N6 | 1.65329 | - | - | $sp^{99.99}$ | 0.06 | 99.94 |
| | -0.26843 | - | - | - | - | - |

[a] ED/e is expressed in a.u.

**Table 5**

**Binding affinity of different poses of the title compound as predicted by Autodock Vina.**

| Mode | Affinity | Distance from best mode | |
|---|---|---|---|
| | (kcal/mol) | RMSD 1.b. | RMSD u.b. |
| 1 | -10.2 | 0.000 | 0.000 |
| 2 | -10.0 | 2.008 | 8.346 |
| 3 | -9.9 | 2.373 | 4.794 |
| 4 | -9.5 | 2.236 | 5.186 |
| 5 | -9.0 | 2.376 | 3.548 |
| 6 | -8.4 | 12.047 | 14.496 |
| 7 | -8.1 | 4.790 | 8.273 |
| 8 | -7.6 | 2.719 | 9.762 |
| 9 | -7.5 | 3.384 | 8.217 |