**LETTER TO THE EDITOR**

**Exploration of binding studies of β-ODAP (β-Oxalyldiamino propionic acid) a non-protein amino acid with human serum albumin-biophysical and computational approach**

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**Supplementary data**

**S Figure 1.**

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**S Figure 1.** β-ODAP appears to be stabilized by hydrogen bonding between the residues Lys195 and Lys199 of HSA, as the hydrogen bonds are intact throughout the 50 ns simulations, compared to the other residues in the binding pocket.

**S Table1. Percentage change of CD**

Table 1. Secondary structural analysis of HSA and HSA with different concentrations of ODAP (0.001mM, 0.005mM and 0.009mM). Data was analyzed by web based software CDNN 2.2, on the basis of Fig. 4.

HSA HSA+0.001mM ODAP HSA+0.005mM ODAP HSA+0.007mM ODAP HSA+0.009mM ODAP

α-Helix% 58.80 58.20 56.80 55.20 52.70

β-Sheet% 13.40 13.00 13.20 13.30 13.70

Random coils% 16.60 17.50 18.30 19.80 20.40

**S Table 2. Docking conformers and their binding energy in 50 Runs**

| | | | | |

Rank | Sub- | Run | Binding | Cluster | Reference |

| Rank | | Energy | RMSD | RMSD |

1 1 25 -5.74 0.00 52.15

1 2 43 -4.98 1.16 52.05

1 3 31 -4.58 1.28 52.22

1 4 19 -3.97 1.35 52.86

1 5 32 -3.77 1.34 51.85

2 1 36 -5.41 0.00 38.81

2 2 8 -5.31 1.23 38.18

2 3 29 -5.30 0.65 38.73

2 4 30 -5.12 1.35 38.48

2 5 35 -4.94 0.89 39.07

2 6 17 -4.83 1.09 38.30

2 7 40 -4.69 1.79 38.89

3 1 23 -4.58 0.00 38.31

4 1 5 -4.53 0.00 37.29

4 2 46 -4.29 1.10 36.90

5 1 18 -4.06 0.00 37.36

5 2 49 -4.01 1.14 37.32

5 3 50 -3.80 1.36 37.04

5 4 48 -3.69 1.53 36.81

6 1 45 -3.98 0.00 37.66

7 1 33 -3.87 0.00 64.98

8 1 21 -3.73 0.00 40.75

9 1 15 -3.32 0.00 43.30

10 1 24 -3.18 0.00 16.17

10 2 22 -2.73 1.89 15.96

11 1 16 -3.07 0.00 19.13

12 1 34 -2.99 0.00 32.55

13 1 47 -2.92 0.00 46.62

14 1 9 -2.89 0.00 34.89

15 1 37 -2.88 0.00 25.86

16 1 42 -2.81 0.00 48.73

17 1 10 -2.61 1.45 21.20

17 3 41 -2.17 1.78 21.79

18 1 39 -2.66 0.00 35.13

19 1 13 -2.65 0.00 21.02

19 2 7 1.98 1.96 22.38

20 1 4 -2.59 0.00 30.54

21 1 44 -2.46 0.00 25.63

22 1 3 -2.40 0.00 18.00

23 1 38 -2.34 0.00 22.72

24 1 6 -2.31 0.00 18.80

25 1 28 -2.29 0.00 49.63

26 1 2 -2.27 0.00 56.77

27 1 20 -2.25 0.00 14.59

28 1 11 -2.10 0.00 31.00

29 1 26 -2.01 0.00 64.48

30 1 1 -1.70 0.00 53.32

31 1 14 -1.34 0.00 65.26

32 1 12 -1.33 0.00 68.48