**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**

**VeerababuNagati1, Monika Kallubai1 Dinesh Chinthapalli and Rajagopal Subramanyam \***

Department of Plant Sciences, School of Life Sciences, University of Hyderabad, Hyderabad 500046, India

\*Corresponding author

Rajagopal Subramanyam

Department of Plant Sciences

School of Life Sciences

University of Hyderabad 500 046 India

Tel: +91-40-23134572

Fax: +91-40-23010120

Email: srgsl@uohyd.ernet.in

**Supplementary data**

**S Figure 1.**

******

**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