Supplementary File

Interaction studies unveil potential binding sites on bovine serum albumin for gut metabolite trimethylamine n-oxide (TMAO)

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The detail information for bond length, bond angle and dihedral angle for each atom of TMAO molecule has been mentioned below.

Table S1: Detail of Bond length (Å) for each atom of TMAO molecule

		C-H (CH3 Group)	C-H (CH3 Group)	C-H (CH3 Group)	N-O	N-C
		1.07	1.07	1.07		1.47
	Unoptimized	1.07	1.07	1.07	1.36	1.47
		1.07	1.07	1.07		1.47
Bond length (Å)						
		1.08717	1.08716	1.08717	1.35851	1.50291
	Optimized	1.09395	1.09397	1.094		1.50291
		1.08715	1.08717	1.08716		1.50288

Table S2: Detail of Bond angle (°) for each atom of TMAO molecule

		H-C-H (CH3)	H-C-H (CH3)	H-C-H (CH3)	C-N-C	O-N-C
	Unoptimized	**109.47122**	**109.47122**	**109.47122**	**109.47122**	**109.47122**
		109.47122	**109.47122**	**109.47122**	**109.47122**	**109.47122**
		109.47122	**109.47122**	**109.47122**	**109.47122**	**109.47122**
Bond Angle (°)						
		111.25714	**111.26552**	**111.25639**	**109.44178**	**109.50281**
	Optimized	**111.25799**	**111.26319**	**111.26253**	**109.44996**	**109.49708**
		109.09407	**109.10266**	**109.11291**	**109.44996**	**109.4932**

Table S3: Rank wise confirmation of TMAO-BSA complex with corresponding energy

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-3.6	0.000	0.000
2	-3.5	18.072	18.499
3	-3.3	16.954	17.320
4	-3.2	60.654	60.995
5	-3.2	13.014	13.176
6	-3.2	67.847	67.998
7	-3.1	56.876	57.191
8	-3.1	61.565	61.896
9	-3.0	62.772	63.108

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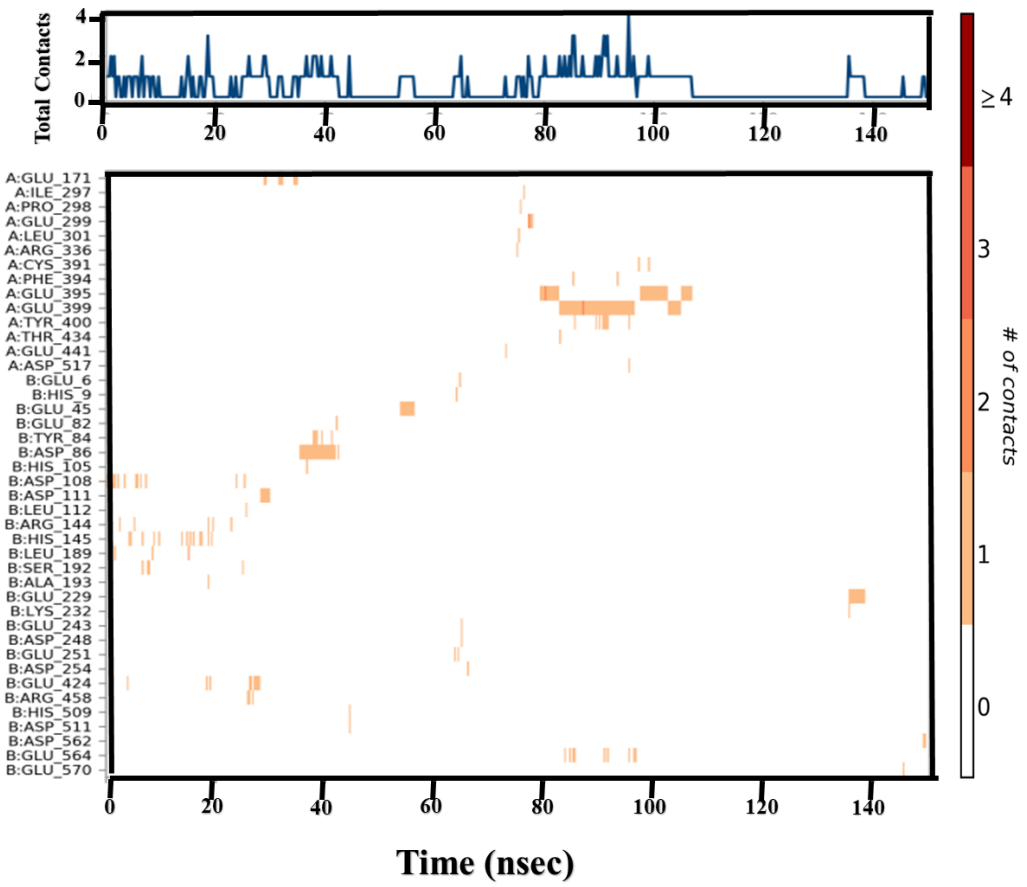
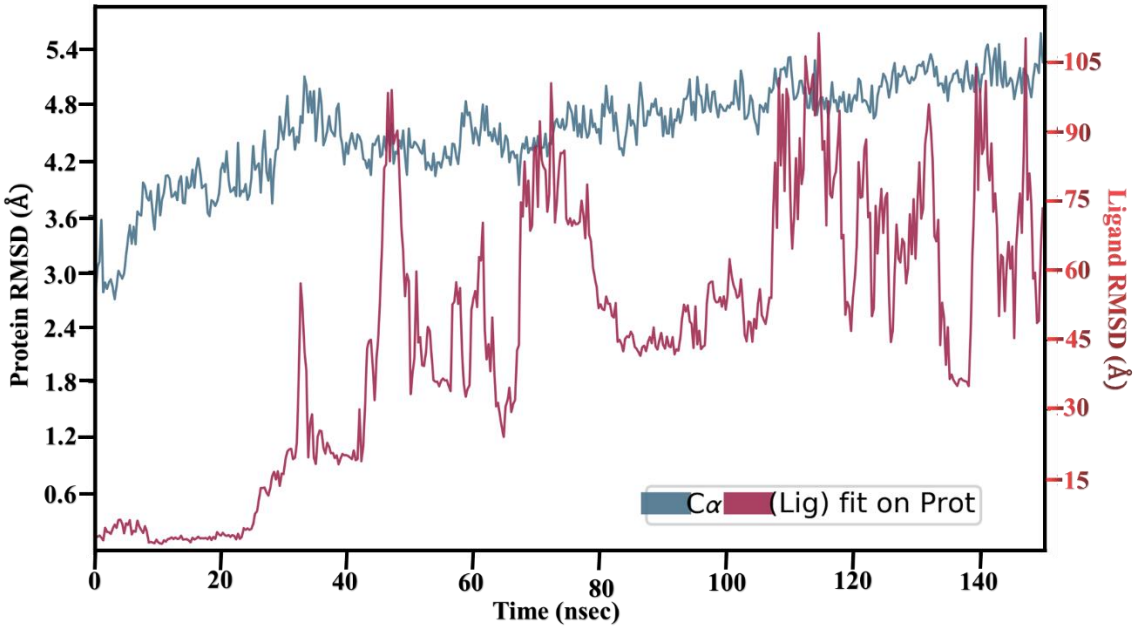


Figure_S1: showing a timeline representation of the interactions and contacts between TMAO and BSA.



Figure_S2: RMSD value for TMAO as ligand and BSA protein for TMAO-BSA complex for 150ns of simulation.