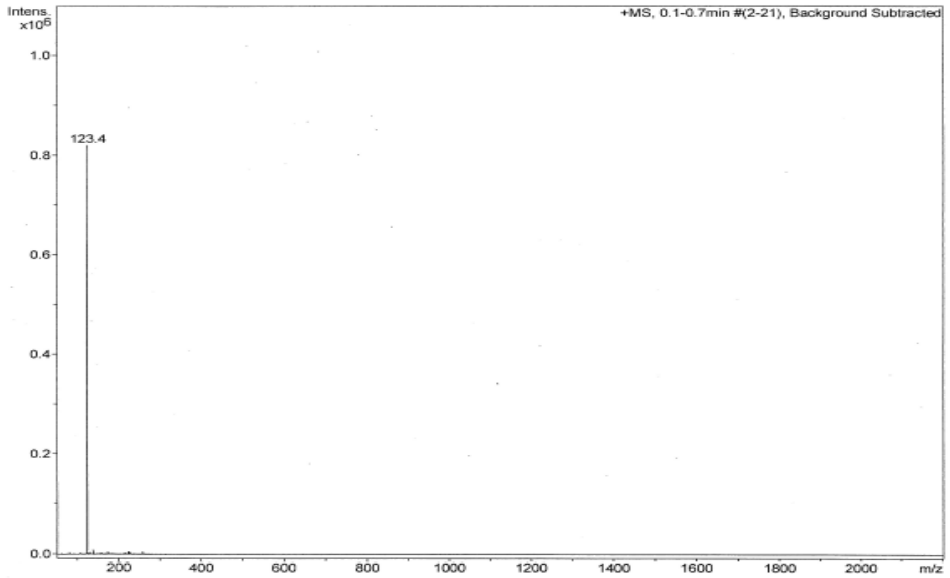
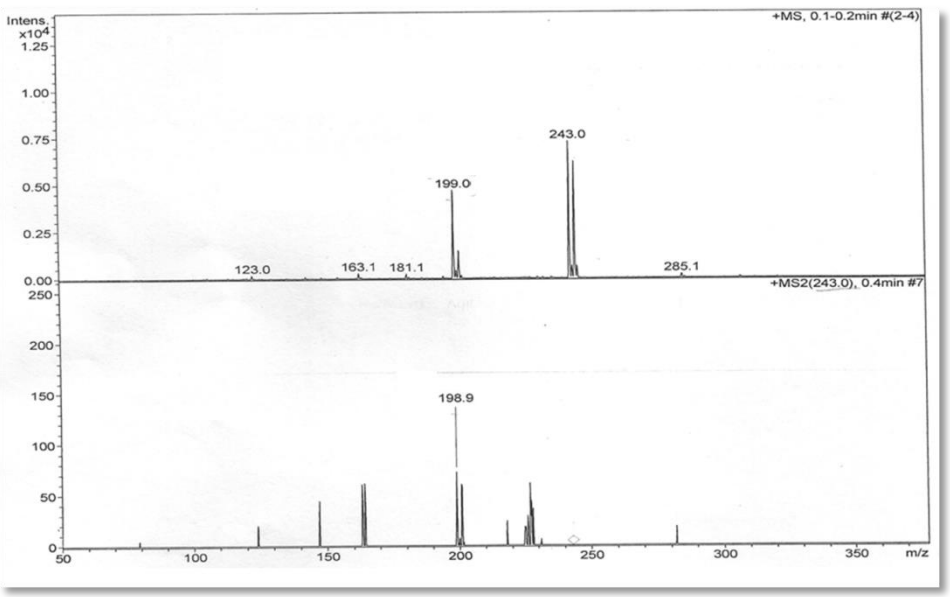
Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION:

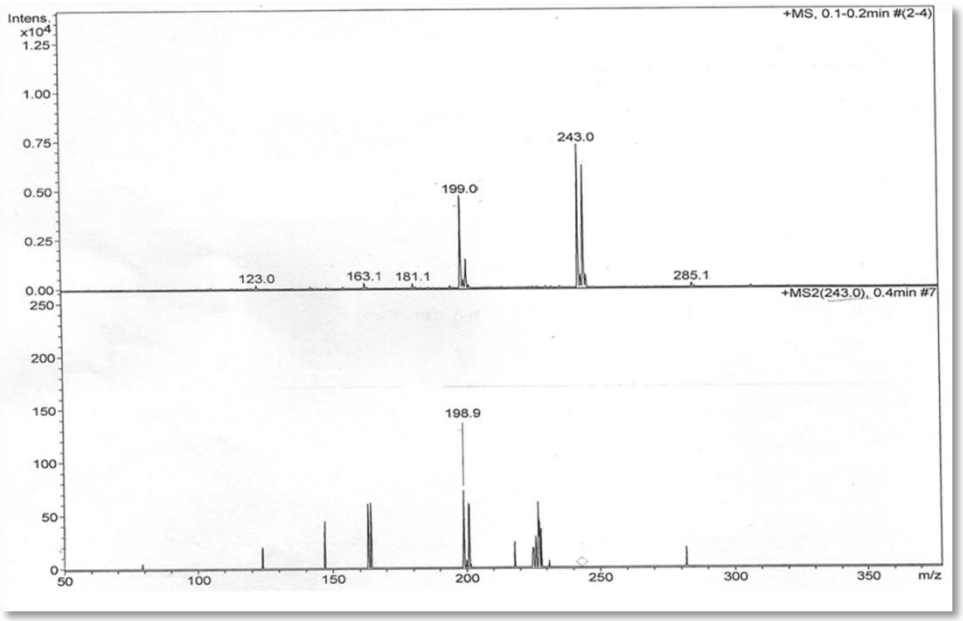
S1: Mass spectra of 4P



S2: Mass spectra of 4PBP



S3: Mass spectra of 4PBB



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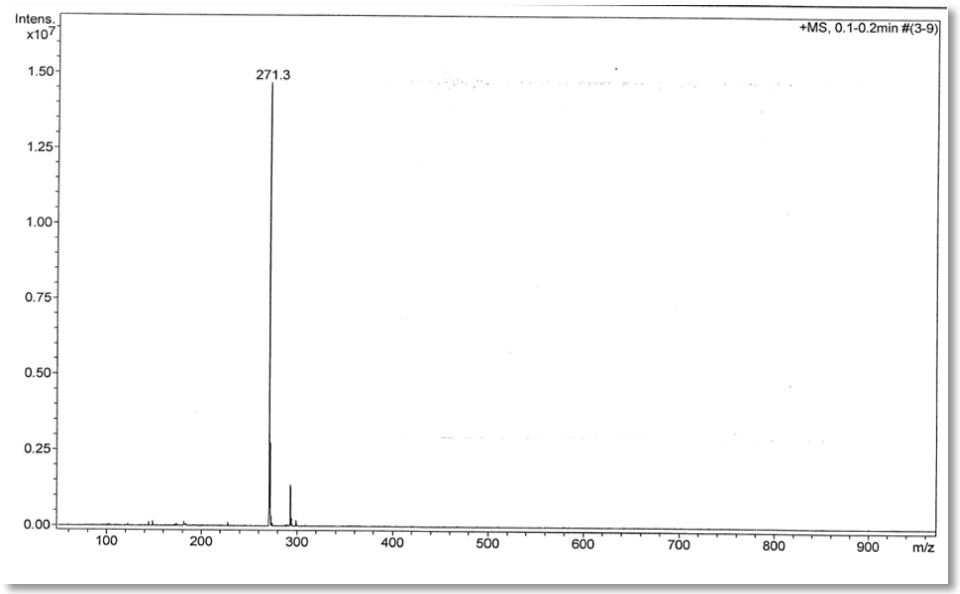
S4: Mass spectra of 4PCB



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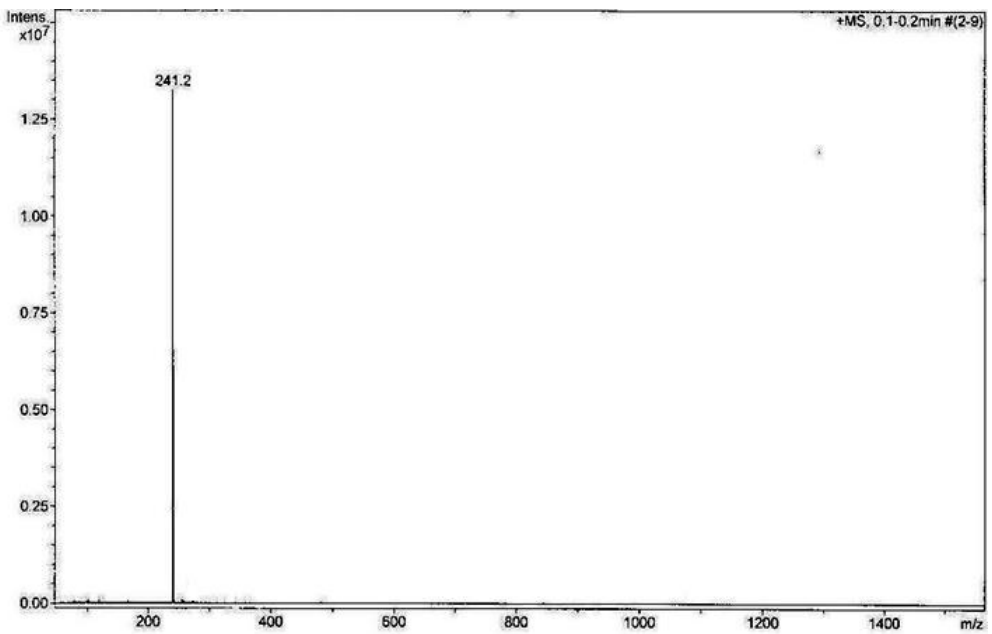
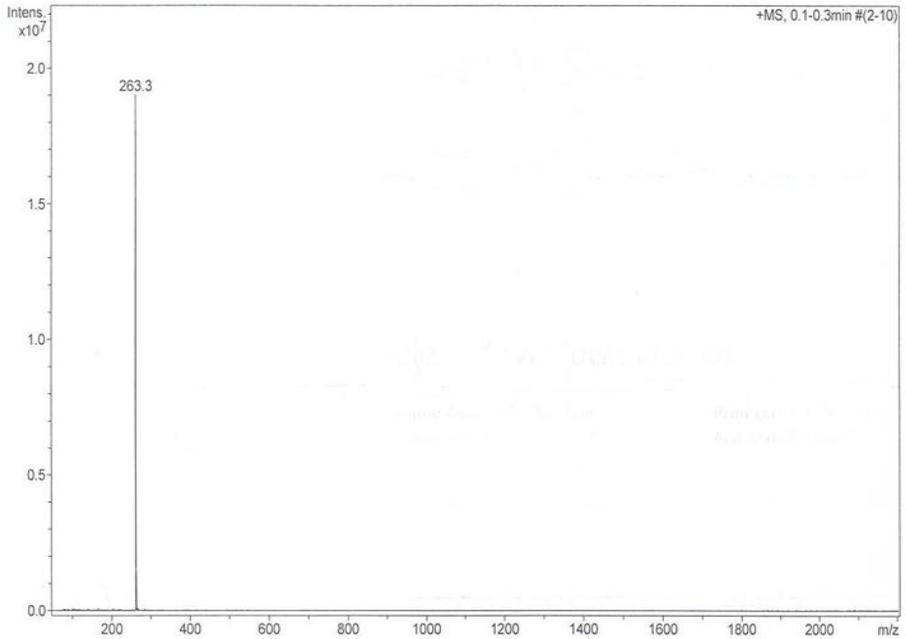
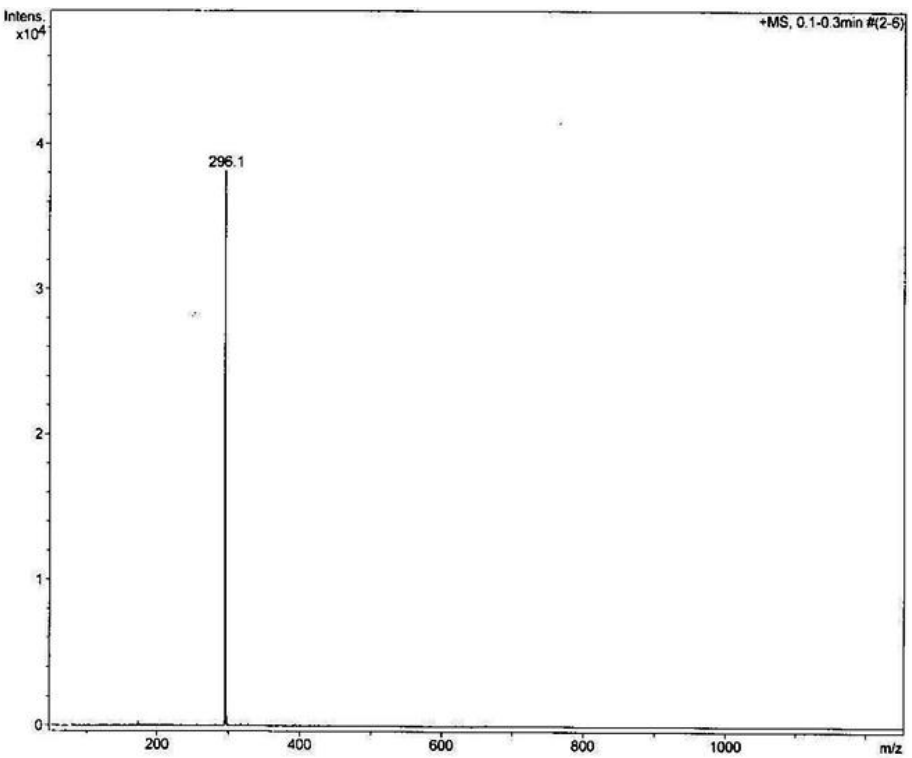
S5: Mass spectra of 4OA



S6: Mass spectra of 4ON



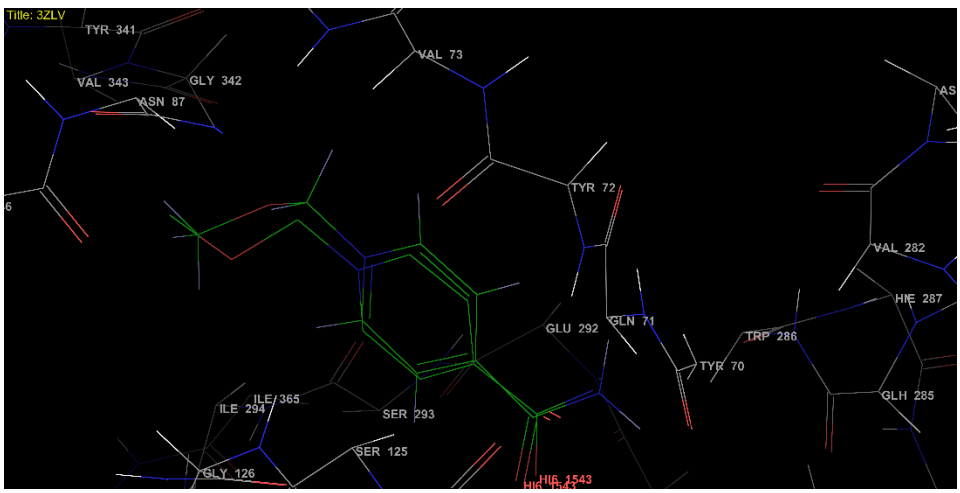
S7: Mass spectra of 4OPh



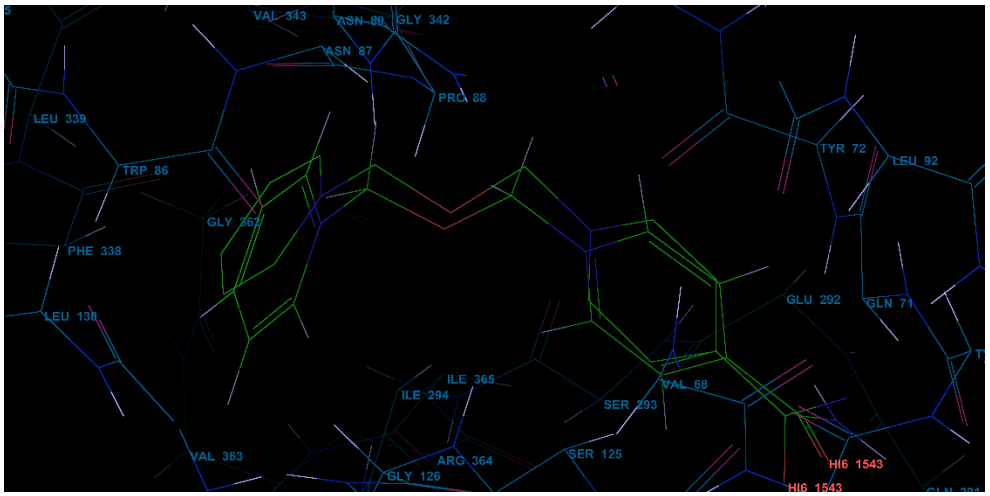
S8: Glide Gscore for synthesized oxime and reference molecule

s.no.	Oxime	Glide Gscore 2WHP (XP mode)	Glide Gscore 3ZLV(XP mode)
1	4PBP	-9.920	-11.021
2	4PBB	-10.793	-10.902
3	4PCB	-9.951	-9.760
4	4OA	-10.250	-8.927
5	4ON	-8.639	-8.261
6	4OPh	-9.202	-8.244
Reference Oxime	2-PAM	-9.455	-9.517

S9- Validation of docking accuracy (Docked HI-6 ligand superimposed on co-crystallized HI-6 ligand with PDB 3ZLV and 2WHP).



[A]



[B]

S10: MMGBSA energy profile of Ligand-protein docking complex (pdb: 3ZLV) done in XP mode:

Ligand-Protein complex	MMGBSA_ Binding	MMGBSA_ Hbond	MMGBSA_ Coulomb
4PBB	-73.0957508	-0.257383263	-1.667295743
4PCB	-23.86986501	-0.827651401	30.969615
4PBP	-64.44832657	-0.304917754	-12.30799023
4OA	-67.19469439	-1.025290219	-48.59183187

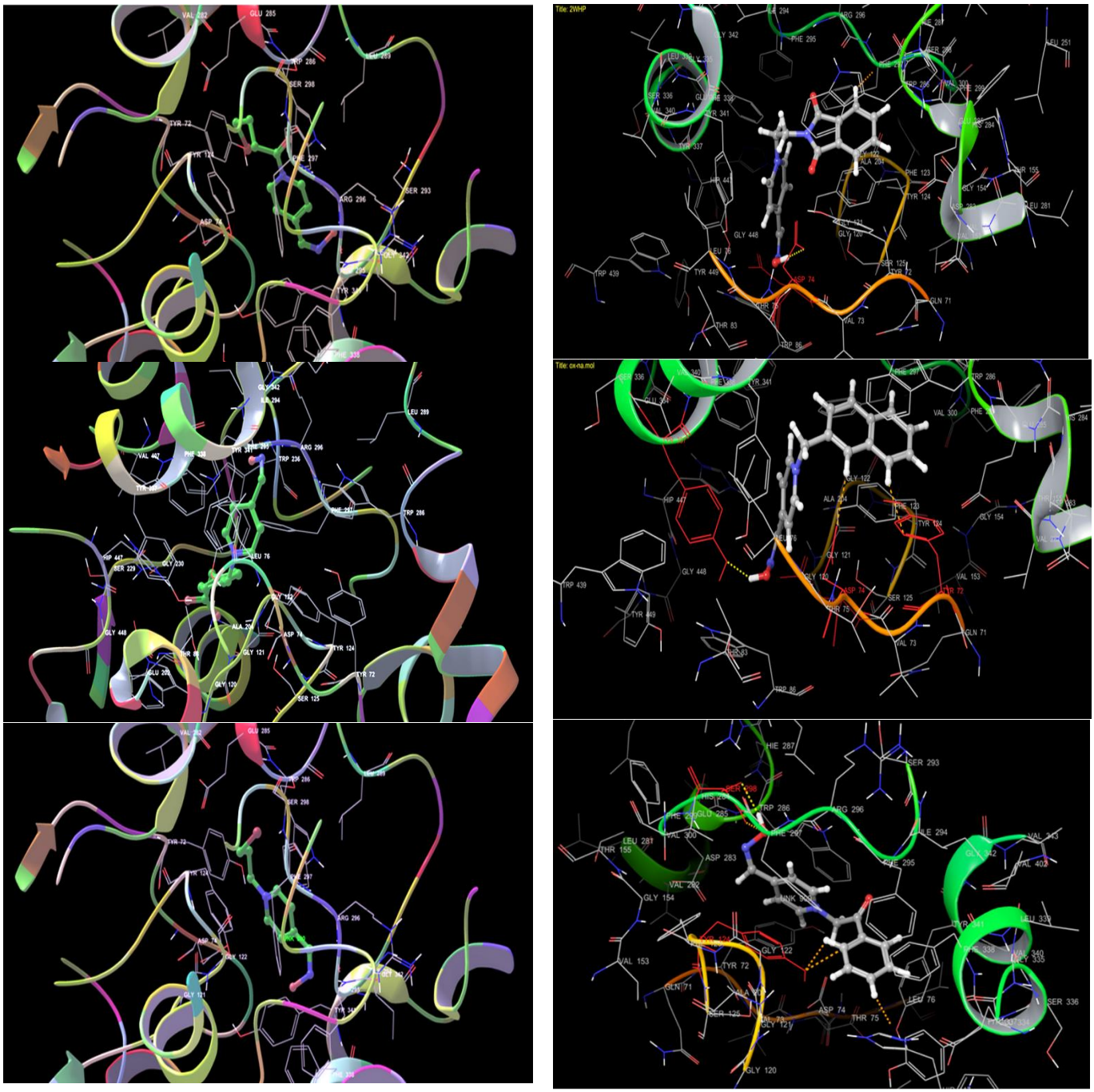
4OPh	-47.45964083	-0.00686598	16.35570336
4ON	-51.84705515	-0.022923585	-10.28341714

S11: MMGBSA energy profile of Ligand-protein docking complex (pdb: 2WHP) done in XP mode:

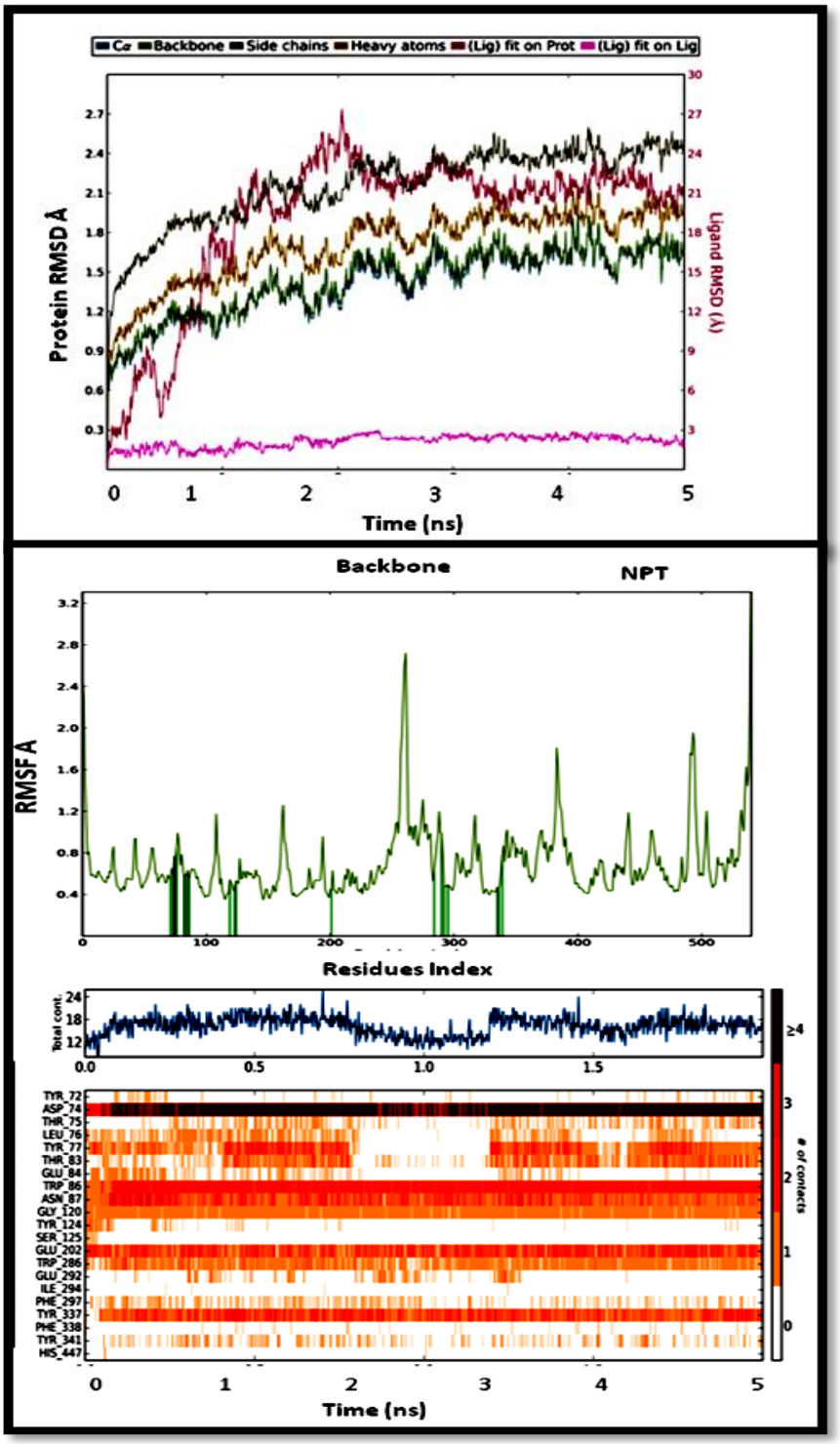
Ligand-Protein complex	MMGBSA_ Binding	MMGBSA_ Hbond	MMGBSA_ Coulomb
4PBB	-52.14055814	-0.101971335	4.889751361
4PAC	-46.03521123	-4.693521679	17.63214105
4PBP	-65.17012026	-0.206345754	-13.55154512
4OA	-70.55233863	-0.695850438	-53.50737842

4OPh	-64.74743373	-0.591874874	-39.79861635
4ON	-63.77068228	-0.23301724	-32.1453338
2-PAM	-44.87880233	-0.468150942	-6.851267661

S12- 3D interactive diagram of Oxime derivatives



S13- Timeline representation of Simulation Interactions for the NPT ensemble of 4PBB-2WHP system.


Cα
Backbone
Side chains
Heavy atoms
(Lig) fit on Prot
(Lig) fit on Lig
Protein RMSD Å
Ligand RMSD (Å)
Time (ns)
Backbone
NPT
RMSF Å
Residues Index
Total cont.
TYR_72
ASP_74
THR_75
LEU_76
TYR_77
THR_83
GLU_84
TRP_86
ASN_87
GLY_120
TYR_124
SER_125
GLU_202
TRP_286
GLU_292
ILE_294
PHE_297
TYR_337
PHE_338
TYR_341
HIS_447
# of contacts
Time (ns)