Supporting Information
For

Experimental and computational studies of the recognition of amino acids by galactosyl-imine & -amine derivatives: An attempt to understand the lectin – carbohydrate interactions

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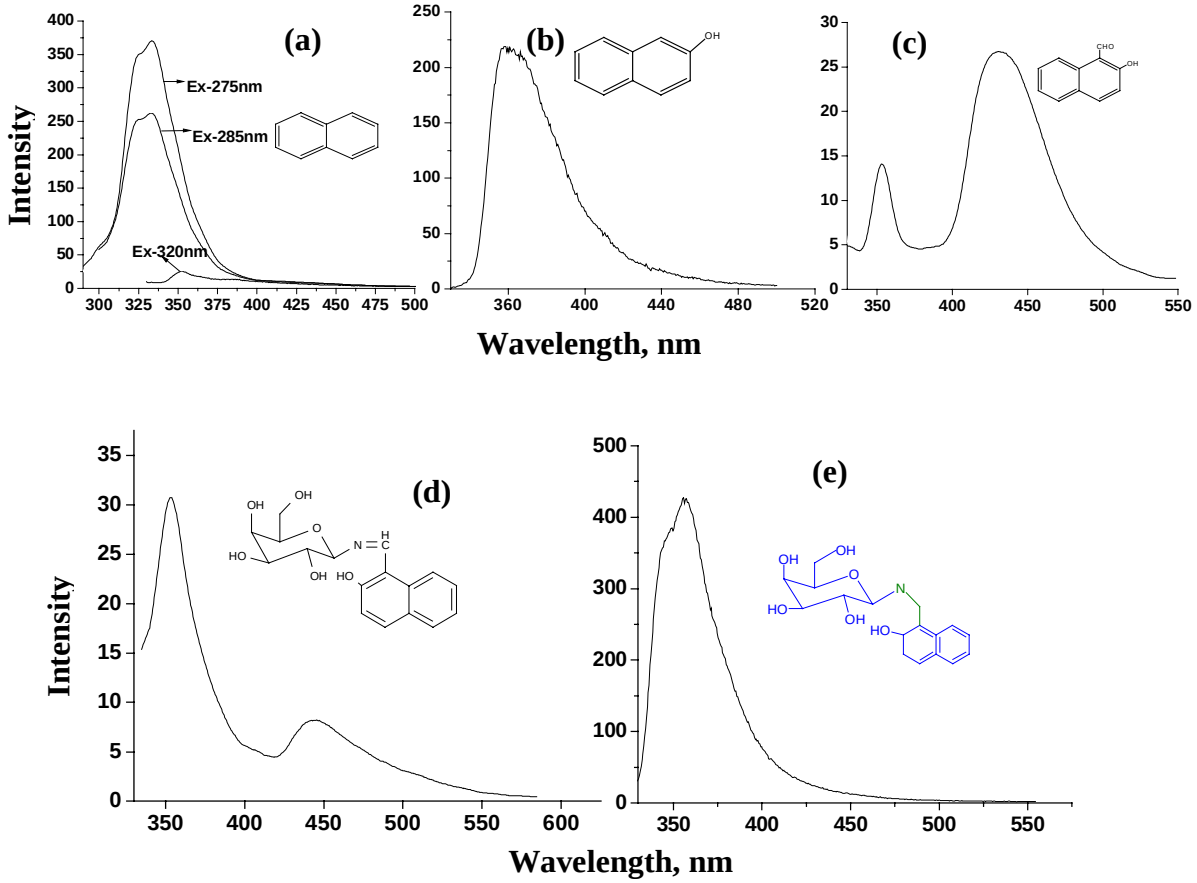
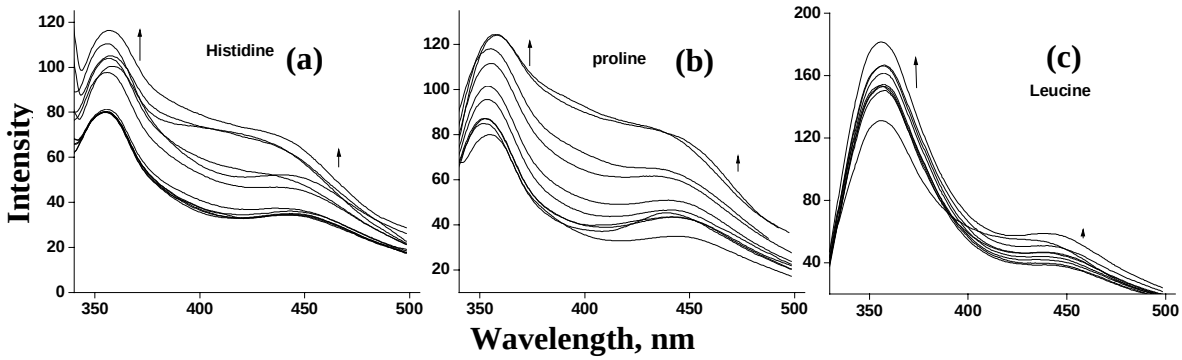


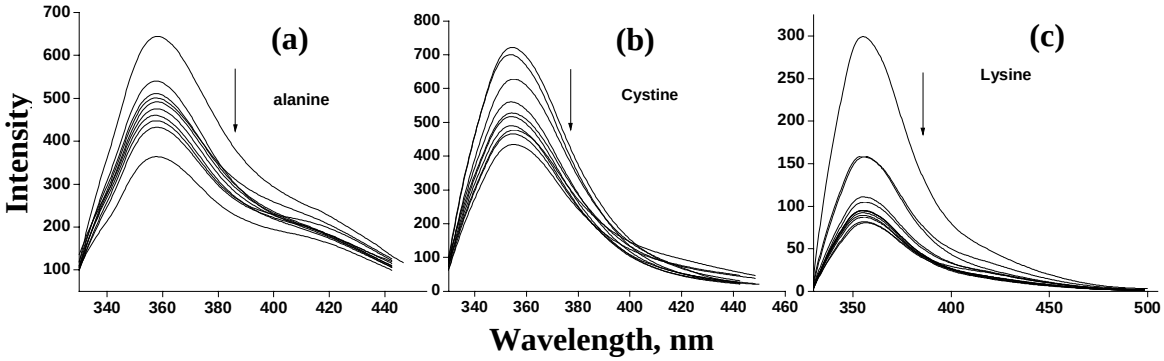
S1. Fluorescence spectral traces of (a) naphthalene; (b) β-Napthol; (c) 2-Hydroxy Naphthaldehyde; (d) **GNI**; and (e)**GNA** in MeOH. The λ_{exc} at 320 nm is common in all the cases.

S2

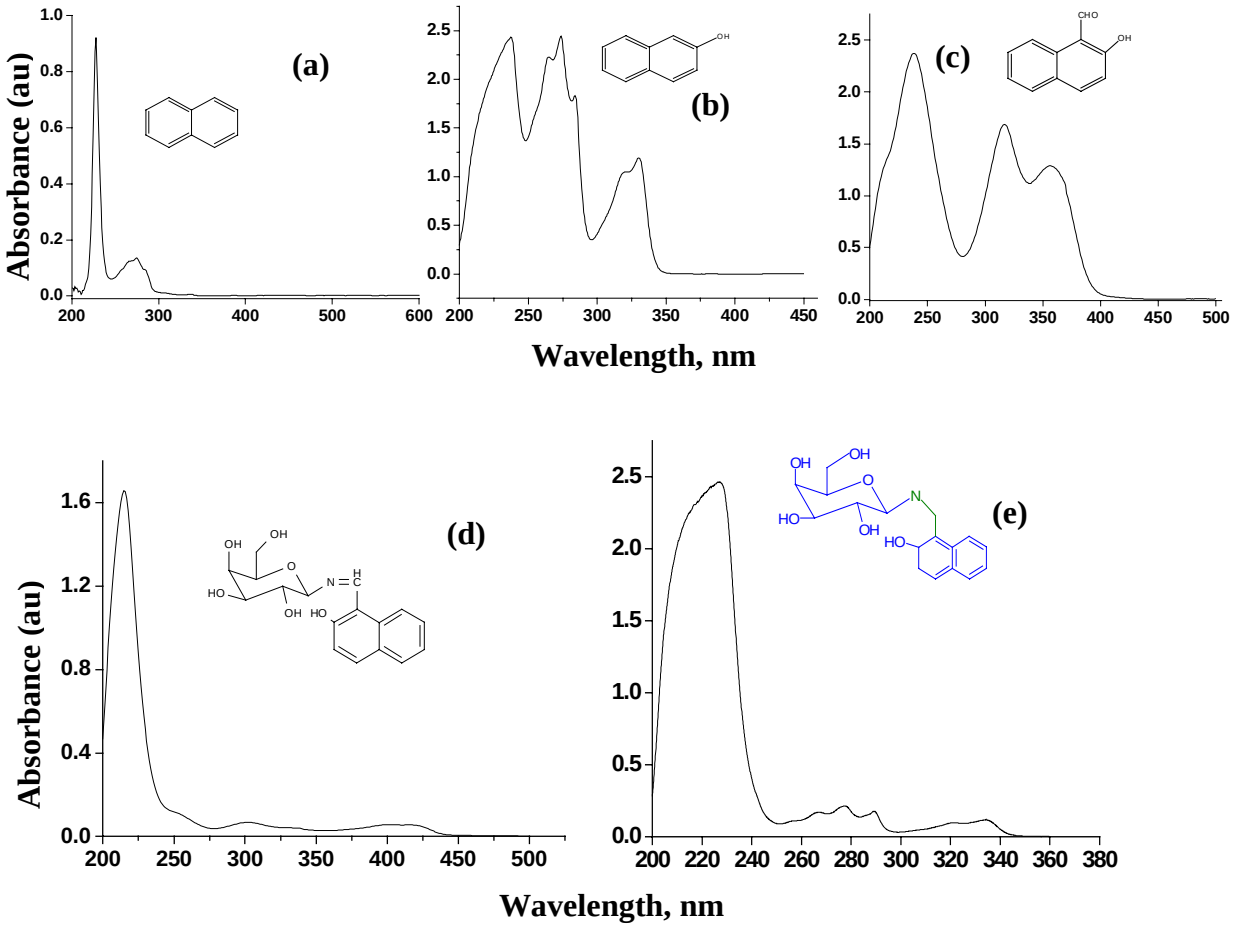


S2. Fluorescence spectral traces of **GNI** titration with (a)His; (b)Pro; and (c)Leu in MeOH while exciting at 320 nm.

S3

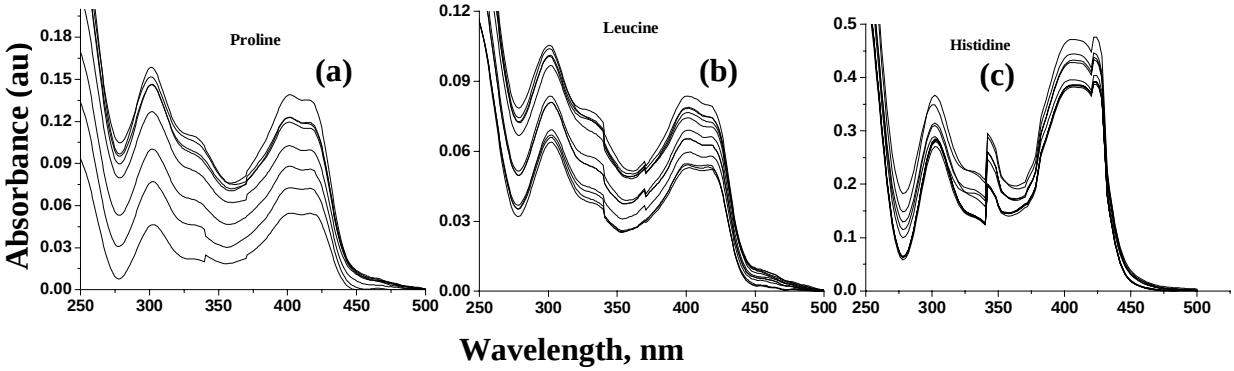


S3. Fluorescence spectral traces of **GNA** titration with (a)Ala; (b)Cys; and (c)Lys in MeOH

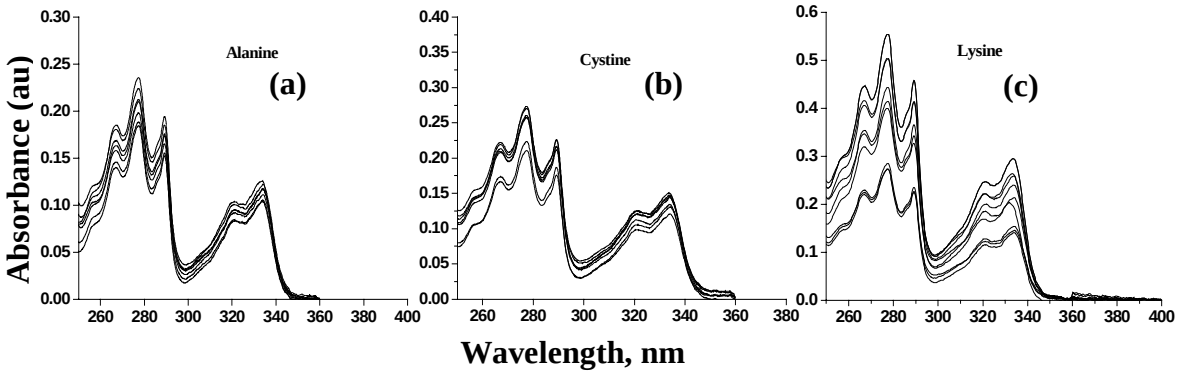


S4. Absorption spectra of (a) naphthalene; (b) β-Napthol; (c) 2-Hydroxy Naphthaldehyde; (d) **GNI**; and (e)**GNA** in MeOH

S5

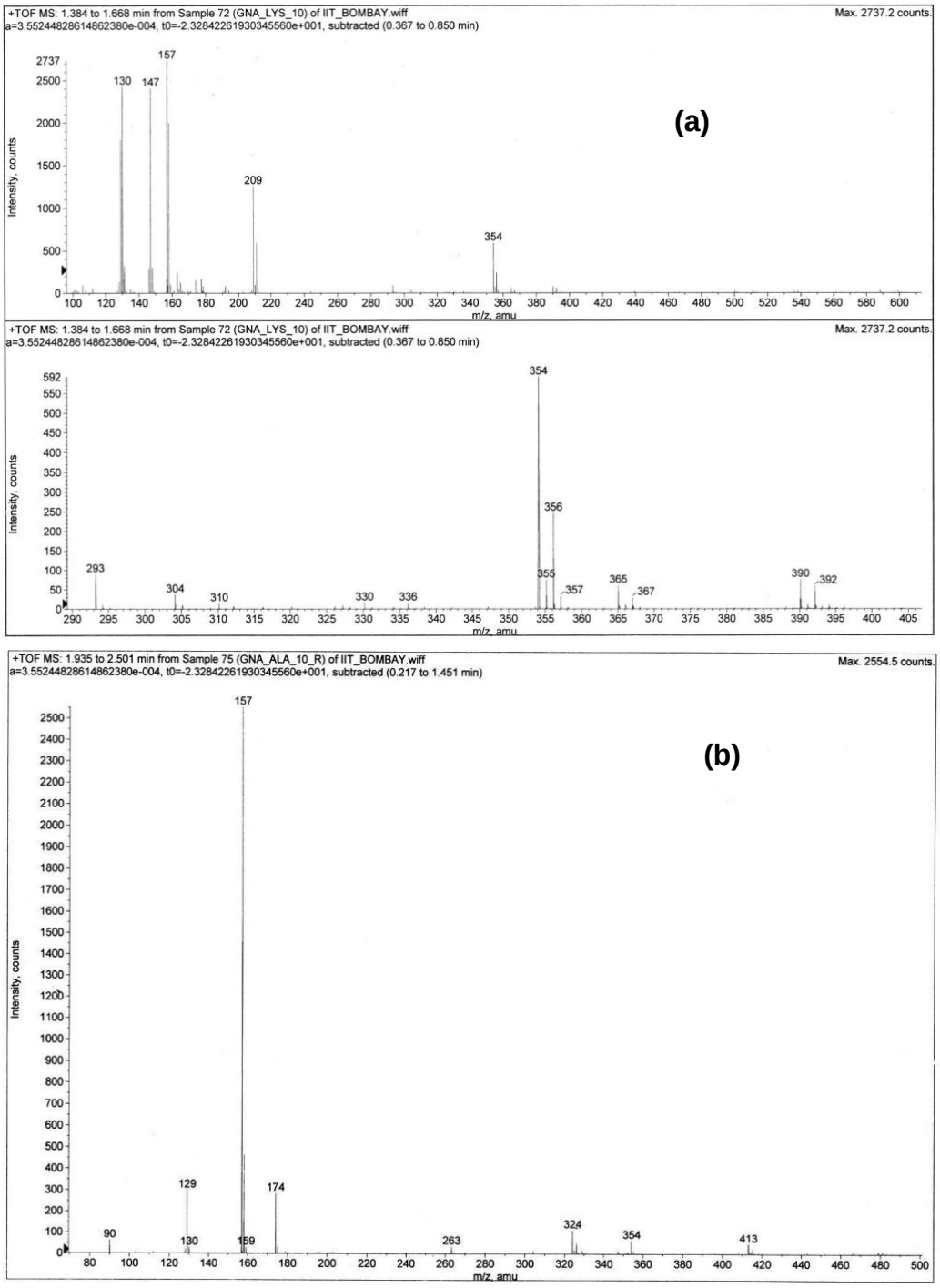


S5. Absorption spectra obtained in the titration of **GNI** with (a) Pro; (b) Leu; and (c) His in MeOH.

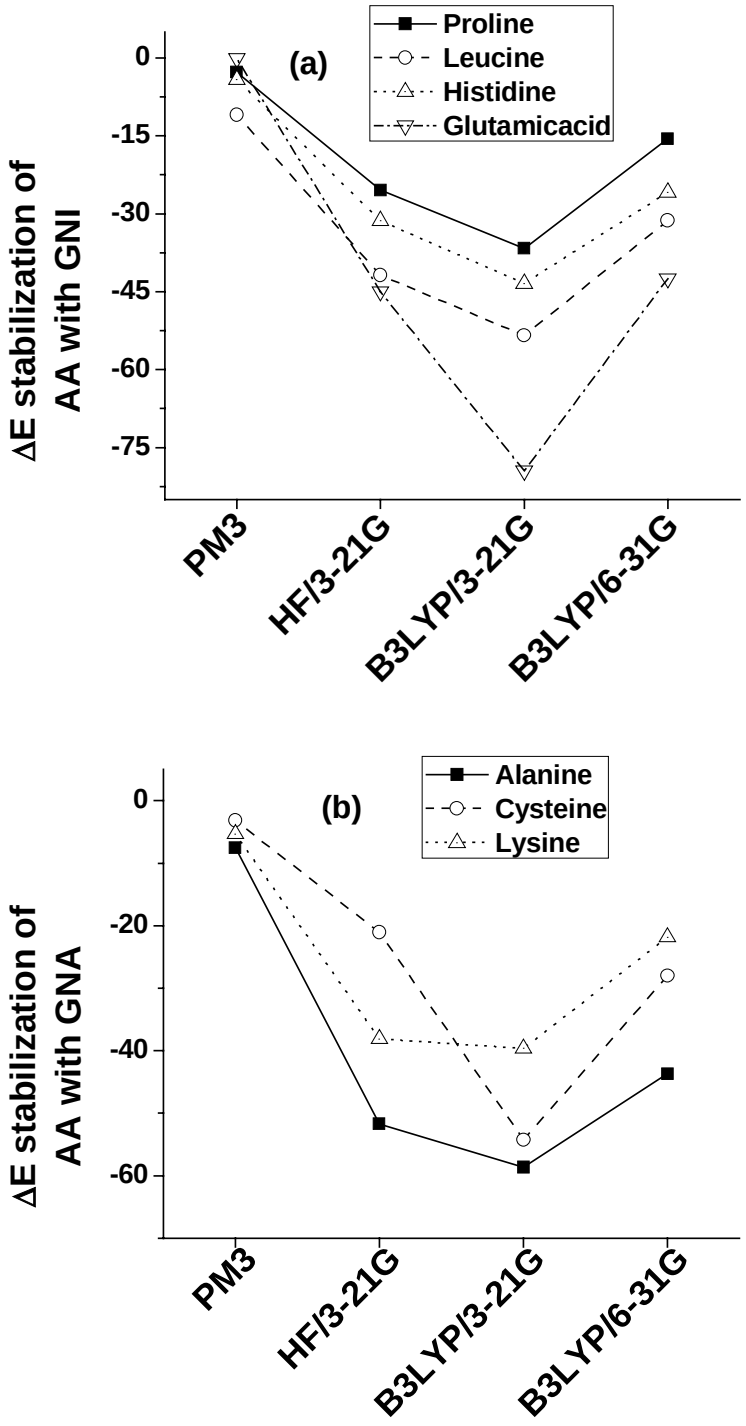


S6. Absorption spectra obtained in the titration of **GNA** with (a) Ala; (b) Cys; and (c) Lys in MeOH.

S7



S7. ESI/MS spectra for the titration mixtures of (a) **GNA +** Lys and (b) **GNA +** Ala.



S8. Plot of theories/basis set Vs. stabilization energies in case of the amino acid complexes of (a) **GNI** and (b) **GNA**

S9

(a) Cremer-Pople ring puckering parameters for **GNI** and its Amino Acid complexes obtained from B3LYP/6-311G calculations

Parameters	**GNI-Free**	**GNI-GLU**		**GNI-HIS**	**GNI-LEU**	**GNI-PRO**
		GNI(a)	**GNI(b)**			
Q2(Å)	0.0628	0.0388	0.0360	0.6724	0.0655	0.0575
Q3(Å)	0.5612	0.5745	0.5548	0.1174	0.5295	0.5732
Q(Å) Total puckering amplitude	0.5647	0.5758	0.5560	0.6826	0.5330	0.5761
θ (˚) theta	6.39	3.87	3.71	80.09	7.06	5.73
ϕ (˚) phi	76.3515	162.4654	352.6975	279.6152	159.5974	30.6901
ΔCs(C-1, C-4) (˚)	0	0	0	0	0	0
ΔCs(C-2, C-5) (˚)	0	0	0	0	0	0
ΔCs(O, C-3) (˚)	0	0	0	0	0	0
ΔCs(C-3, C-5) (˚)	0.96	-0.92	8.16	-0.34	-3.66	6.61

(b) Cremer-Pople ring puckering parameters for **GNA** and its Amino Acid complexes obtained from B3LYP/6-311G calculations

Parameters	**GNA-Free**	**GNA-ALA**	**GNA-LYS**	**GNA-CYS**
Q2(Å)	0.1583	0.0590	0.5560	0.0206
Q3(Å)	0.4789	0.5636	0.2642	0.5570
Q(Å) puckering amplitude	0.5044	0.5667	0.6156	0.5574
θ (˚) theta	18.29	5.98	64.58	2.12
ϕ (˚) phi	160.0197	351.7573	318.3207	357.0444
ΔCs(C-1, C-4) (˚)	0	0	0	0
ΔCs(C-2, C-5) (˚)	0	0	0	0
ΔCs(O, C-3) (˚)	0	0	0	0
ΔCs(C-3, C-5) (˚)	2.35	10.03	-7.61	6.8

S9. (a) & (b) are the Cremer-Pople parameters for the **GNI** and **GNA**…aa complexes.

(c) Dihedral angles present in the optimized structure of **GNI** and its Amino acid complexes obtained from B3LYP/6-311G calculations

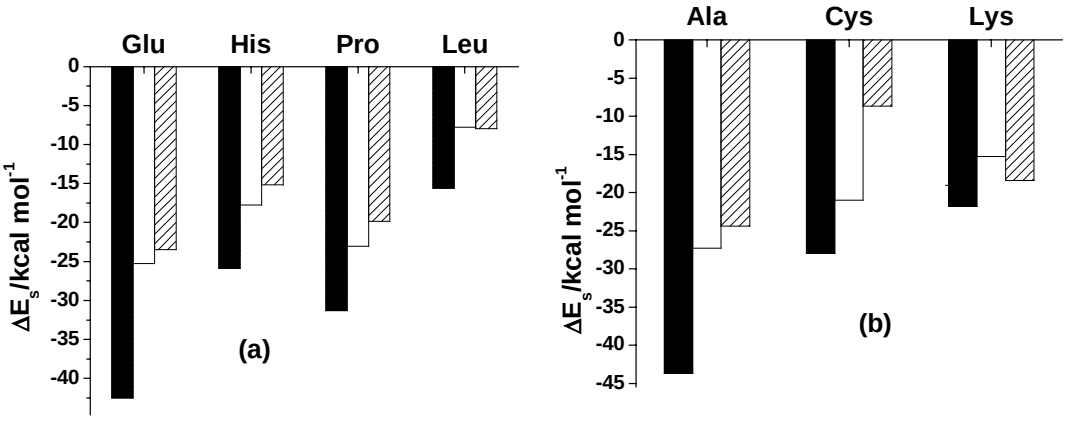
Dihedral angle	**GNI**	**GNI** (a) -Glu	**GNI** (b) – Glu	**GNI** -His	**GNI** -Leu	**GNI** -Pro
$C2_{nap}$-$C1_{nap}$-C_{im}-N	0.824	0.70	4.83	2.74	1.37	0.56
$C1_{nap}$-C_{im}-N-$C1_{gal}$	-178.53	176.50	179.80	179.81	179.29	178.92
C_{im}-N-$C1_{gal}$- $C2_{gal}$	17.890	-99.96	-86.80	-66.50	-90.87	15.2
C_{im}-N-$C1_{gal}$- O_{gal}	135.860	139.96	153.56	172.87	148.54	-106.88

(d) Dihedral angles present in the optimized structure of **GNA** and its Amino acid complexes obtained from B3LYP/6-311G calculations

Dihedral angle	**GNA**	**GNA** -Ala	**GNA** -Lys	**GNA** -Cys
$C2_{nap}$-$C1_{nap}$-C_{im}-N	7.895	98.22	34.08	45.15
$C1_{nap}$-C_{im}-N-$C1_{gal}$	96.950	152.25	-165.37	-165.35
C_{im}-N-$C1_{gal}$- $C2_{gal}$	168.660	-171.17	-74.83	-107.68
C_{im}-N-$C1_{gal}$- O_{gal}	-72.300	68.33	165.15	131.93

S9. (c) & (d) list of certain relevant dihedral angles obtained in the optimized structures of the amino acid complexes of **GNI** and **GNA**.

S10.



S10. Computed stabilization energies, viz., ΔE_s^p (completely filled), ΔE_s^q (unfilled) and ΔE_s^r (partially filled): (a) in case of **GNI**…aa complexes; (b) **GNA**…aa complexes.