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Supplementary Information

For the Manuscript Entitled

Ex-vivo binding studies of anti-cancer drug Noscapine with Human Hemoglobin:

Spectroscopic and molecular docking study

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Table S1: Varied emission ranges inflicted by microenvironment of Trp in a protein

S.No.	Trp microenvironment in the protein	Emission Range
1	Trp in hydrophilic environment	350-353 nm
2	Trp in a hydrophobic environment	330–332 nm
3	Trp in a limited water accessibility	340–342 nm

Table S2: Change in % α-helicity in Hb structure upon increasing concentration of Nos

S.No.	Samples	% α- helicity
1	Hb (2.2 μM)	19.3
2	Hb + Nos 0.5 μM	18.9
3	Hb +Nos 1.5 μM	18.9
4	Hb + Nos 2.5 μM	18.8
5	Hb + Nos 4.5 μM	18.3
6	Hb + Nos 5.5 μM	17.9

Table S3. Fluorescence lifetime parameters for Hb and HB + Nos in aqueous medium (λ_{ex} = 280 nm)

	T1 (ns)	T2 (ns)	T3 (ns)	B1	B2	B3	Average Lifetime τ_{av} (ns)
Hb	1.2831	0.1948	4.1782	0.0849	0.5299	0.0158	1.56
Hb + Nos	0.1934	1.1742	4.1427	0.5798	0.0825	0.01178	1.18

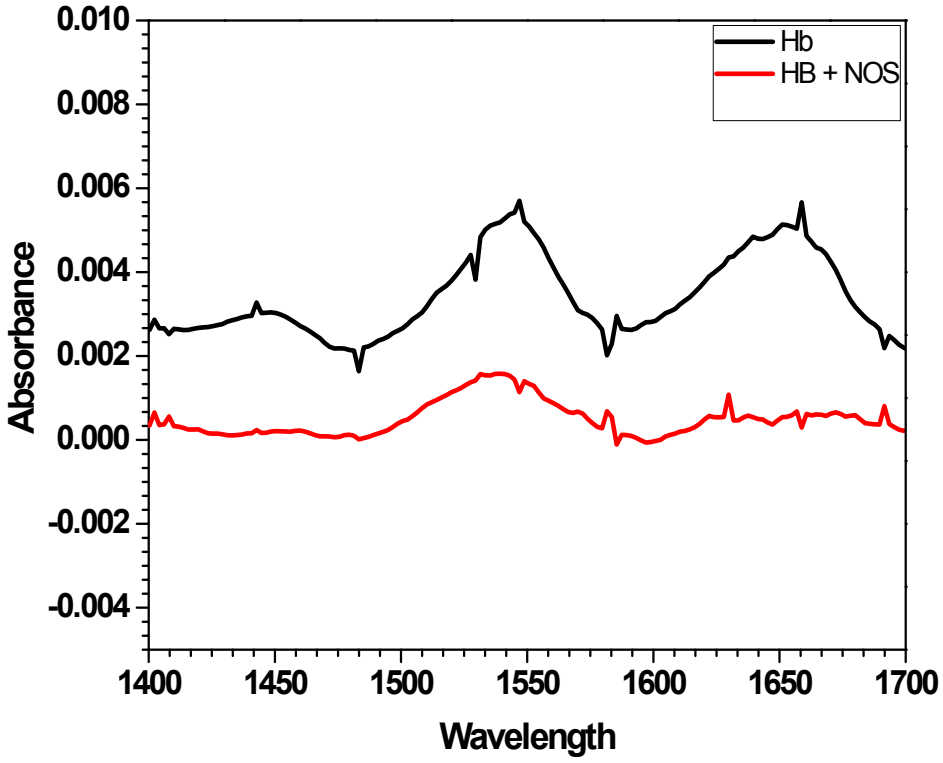

Figure S1: FTIR Spectroscopy: FTIR Spectra of Hb and Hb-Nos Complex (1:1) molar ratio.

Structural quality assessment of Hb structure

The structural quality assessment of Hb structure depicted the stable composition of 3D structure with minimal variations of residues, in comparison with the native structures (0.5-0.9 Å deviations). The differently colored lines are depicting the four chains of Hb structure. Also, verify 3D server showed the high quality of Hb structure, which indicated more than 80% residues with good 3D/1D profile.

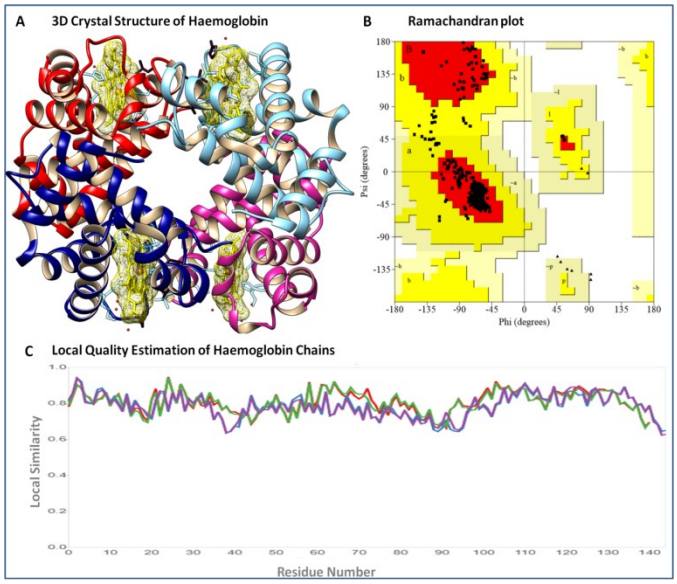

Figure S2: Ramachandran Plot: (A) 3D crystal structure of Hb retrieved from the protein data bank. (B) Stereochemical parameter analysis of Hb structure by Ramachandran plot. (C) Local quality estimation of Hb protein for all chains (the different colored lines), minima fluctuations of residues (<1 Å).

Protein-ligand docked file through molecular docking

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NOscapine.pdb
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REMARK    Solution 1, from model "FromOB NOscapine", ID:
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REMARK    Energy -2.218015e+002, RMS  -1.00
REMARK    Overlap Volume 0.0, Clash Volume 0.0
REMARK    Box_min: -19.361 -26.843 -16.721
REMARK    Box_max: 49.523 30.722 43.319
REMARK    Cube_min: -19.361 -32.503 -21.143
REMARK    Cube_max: 49.523 36.382 47.741
REMARK    Symmetry Type: Default
REMARK    Symmetry Matrix: 0
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HETATM 5923  C   UNL     1      23.719  14.628  15.854  1.00 99.99
HETATM 5924  C   UNL     1      23.199  13.991  15.802  1.00 99.99
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HETATM 5928  C   UNL     1      22.492  13.031  15.013  1.00 99.99
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HETATM 5943  C   UNL     1      21.871  12.639  17.792  1.00 99.99
HETATM 5944  O   UNL     1      22.364  13.382  18.909  1.00 99.99
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HETATM 5948  C   UNL     1      23.050  13.995  17.223  1.00 99.99
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