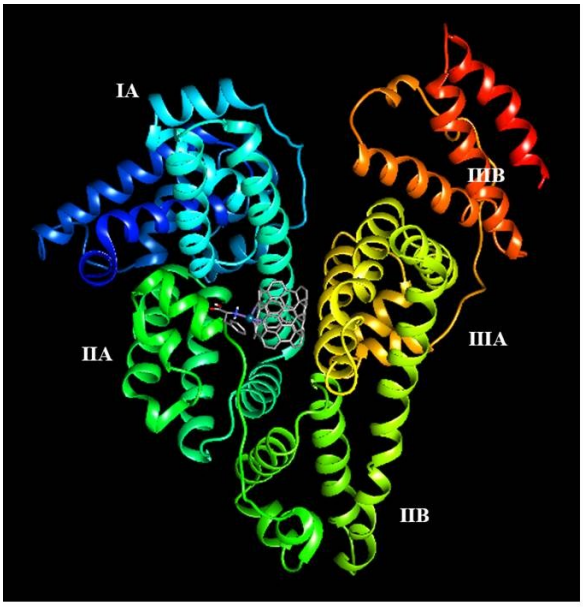
Electronic Supplementary Material (ESI) for RSC Advances.

Table 1. The binding free energies of the purposed binding to HAS. The binding free energies (kcal.mol^{-1}) and Inhibition Constant of the biosensor-HAS complex were estimated by the scoring function of AUTODOCK.

Number	Binding site	$\Delta G_{binding}$	ΔG_{nes}	ΔG_{es}	ΔG_{tor}	K_i
1	IIA	-10.05	-11.70	-0.27	1.92	42.68
2	IB	-10.05	-11.71	-0.27	1.92	42.81



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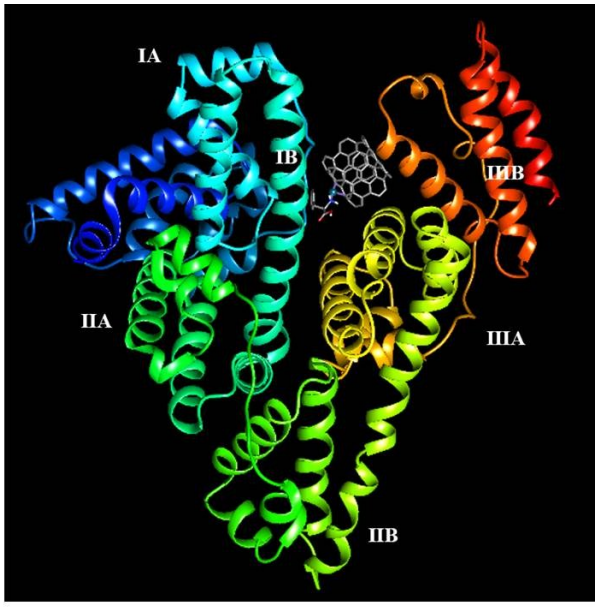

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Table 2. Hydrogen bonding parameters

Hydrogen bonding interaction	**Bond length (Å)**	**Bond angles (°)**
Phe-Pd/SWCNT … Glu292	2.76	127
Phe-Pd/SWCNT … Lys190	2.45	145
Phe-Pd/SWCNT … Glu425	2.47	136