Supporting Information

for

Interaction of Nucleobases and Aromatic Amino Acids with Graphene oxide and Graphene Flakes

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Table S1: Calculated binding energy (in kJ/mol) of G and GO with nucleobases and amino acids using M052X and M062X level of theory (BE is corrected with basis set super position error (BSSE)).

Complex	M052X		M062X		M062X	
	6-311++G(d,p)		6-31+G(d,p)		6-311++G(d,p)	
	G	GO	G	GO	G	GO
A	16.70	30.88	52.19	46.92	44.23	43.53
G	27.23	46.70	65.08	62.09	57.46	58.60
T	19.64	28.27	52.93	42.96	46.23	39.06
C	20.50	54.57	51.02	69.41	45.10	66.09
U	13.93	33.06	46.36	48.66	35.00	45.47
TYR	11.48	36.55	33.14	49.25	28.75	48.14
TRP	16.34	40.69	45.11	48.61	38.62	46.70
PHE	9.60	17.18	28.15	28.82	23.80	26.33
HIS	10.35	85.73	25.23	93.52	21.81	92.81

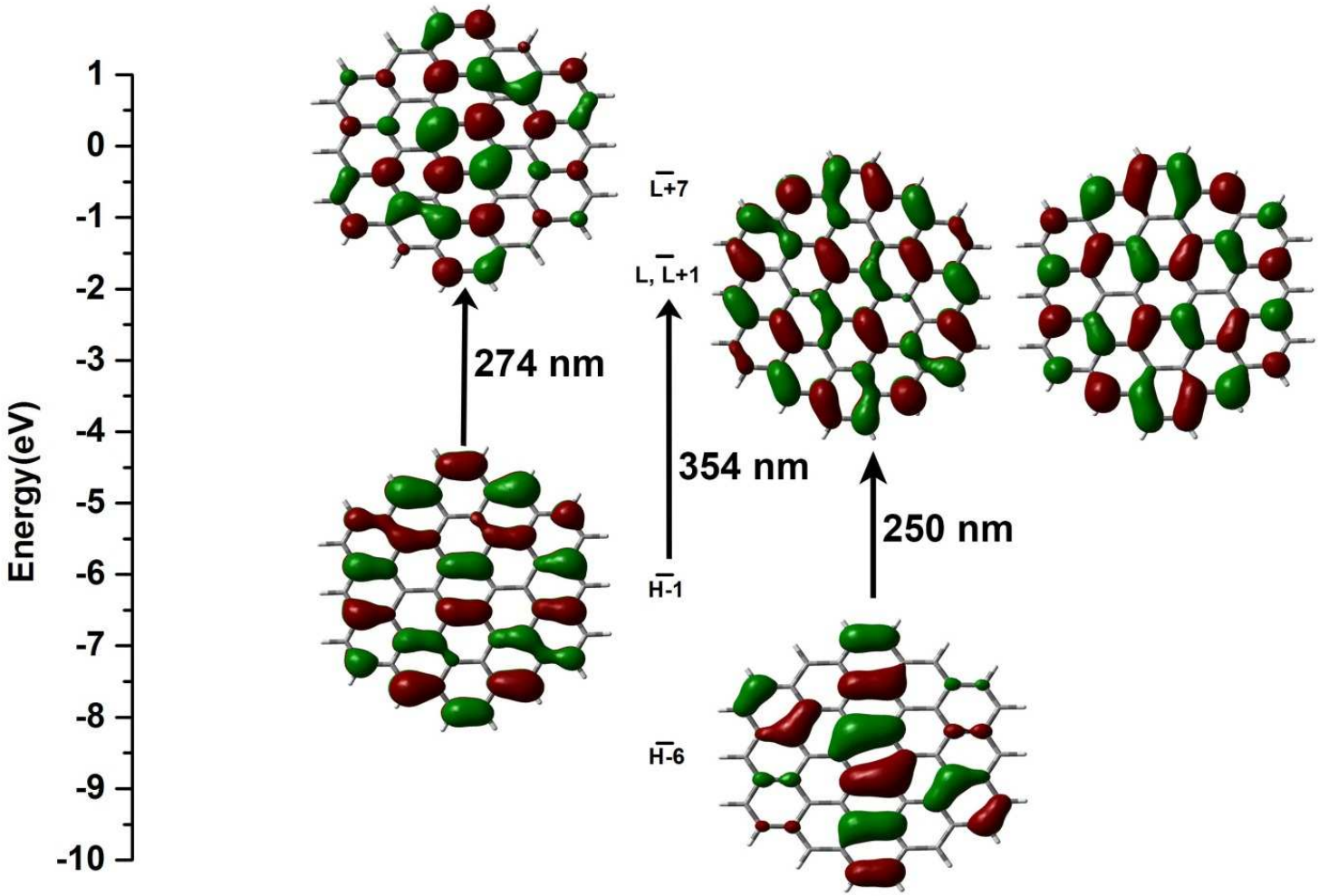


Figure S1. Frontier molecular orbitals involved in the vertical excitation of G flake.

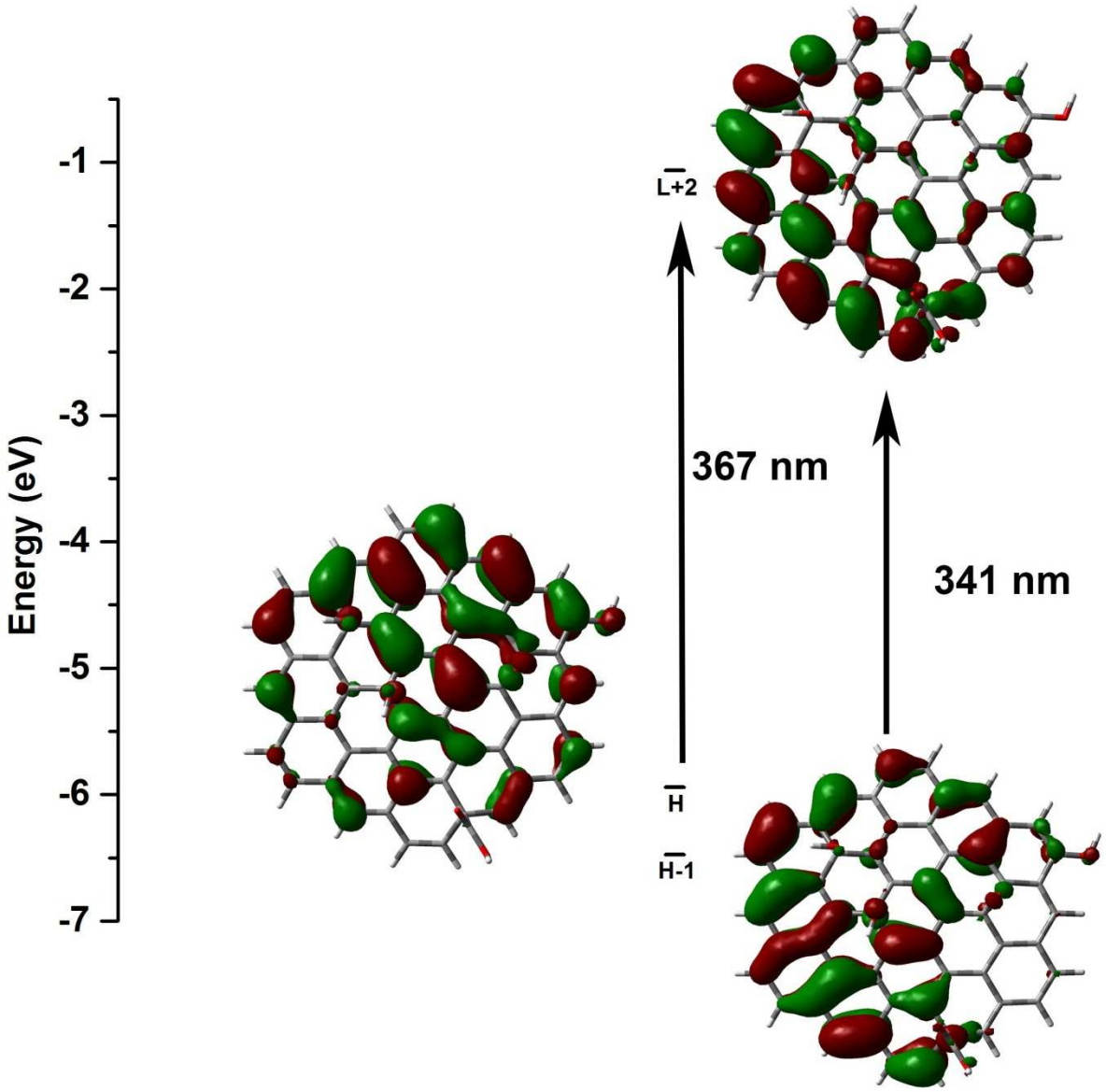


Figure S2. Frontier molecular orbitals involved in the vertical excitation of GO flake.

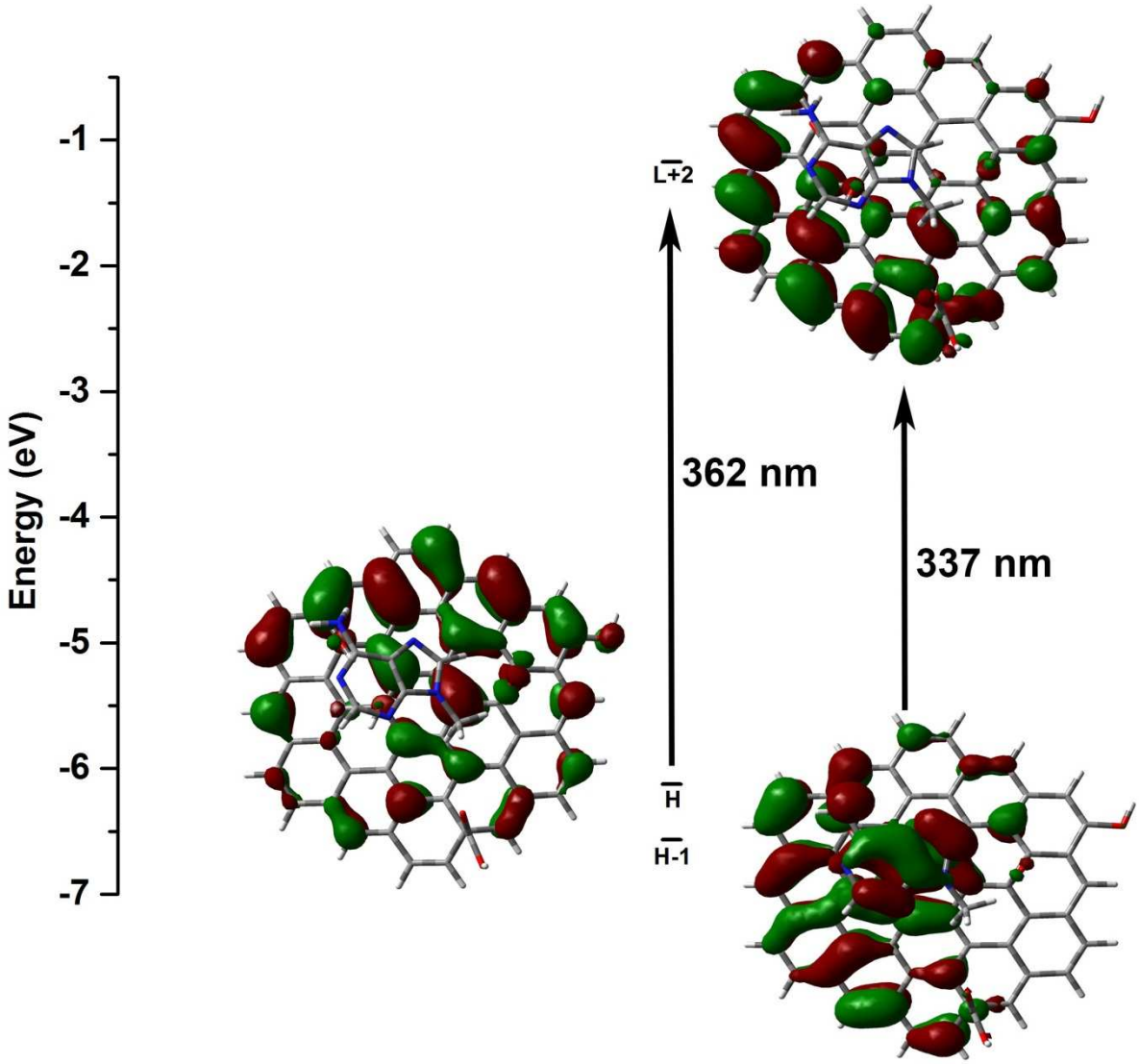
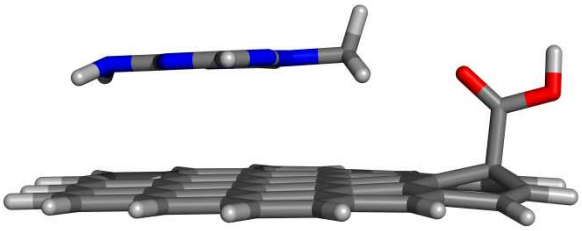
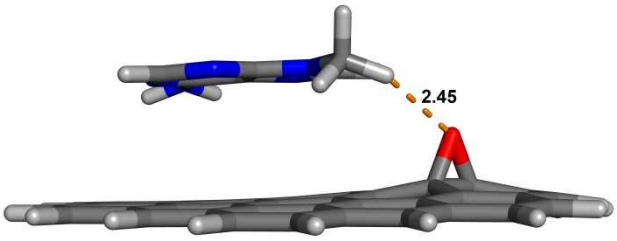


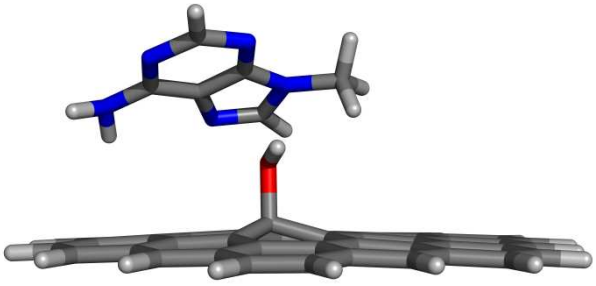
Figure S3. Frontier molecular orbitals involved in the vertical excitation of GO-A.



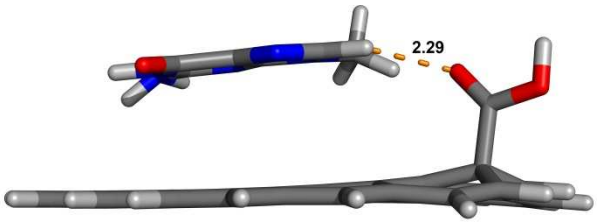
GO-A-CAR



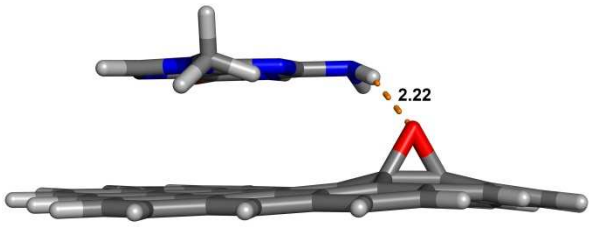
GO-A-EPO



GO-A-OH



GO-G-CAR



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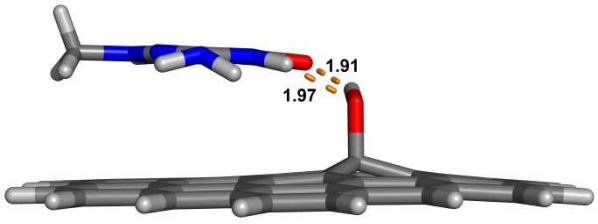
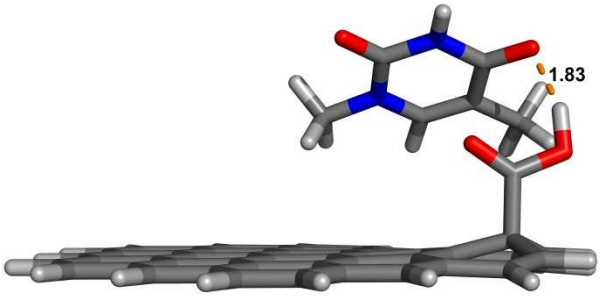
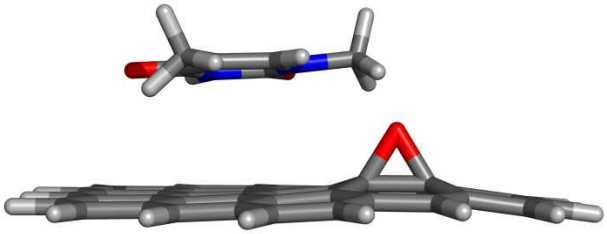


GO-G-OH



GO-T-CAR



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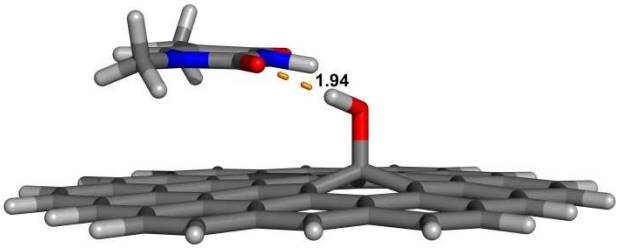

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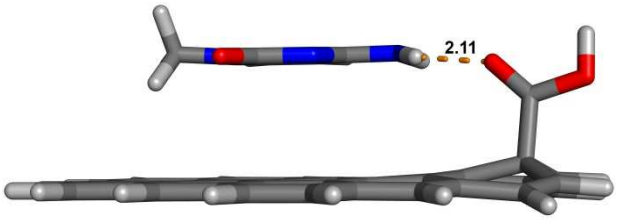
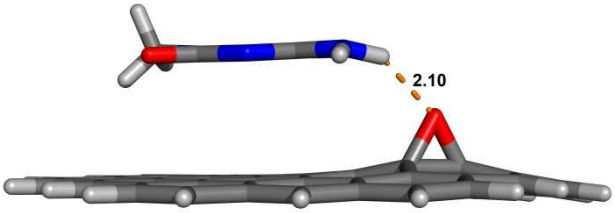


GO-C-CAR



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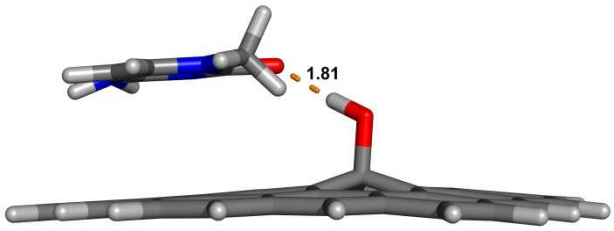

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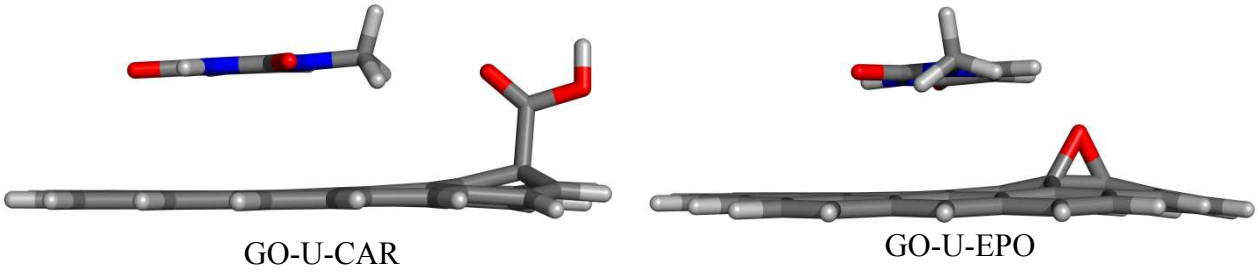
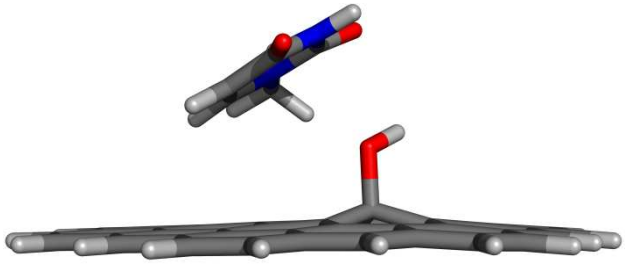
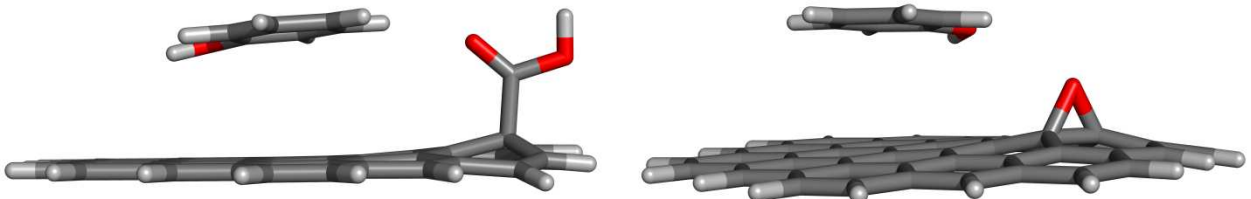


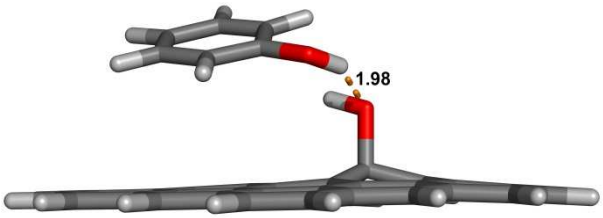
GO-U-CAR GO-U-EPO



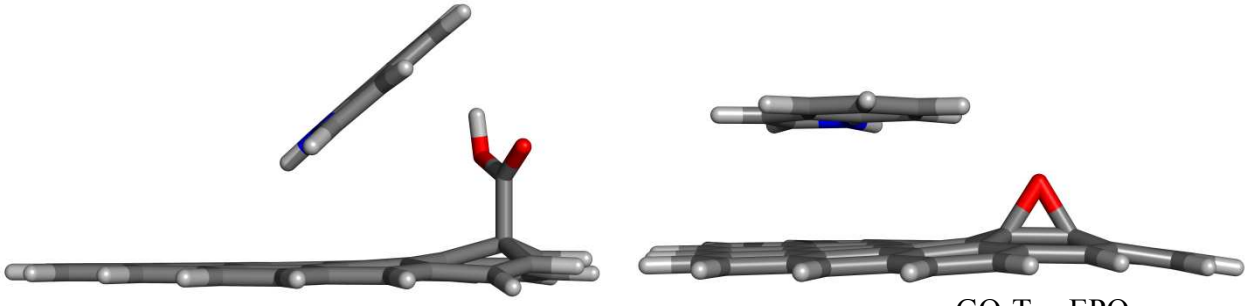
GO-U-OH



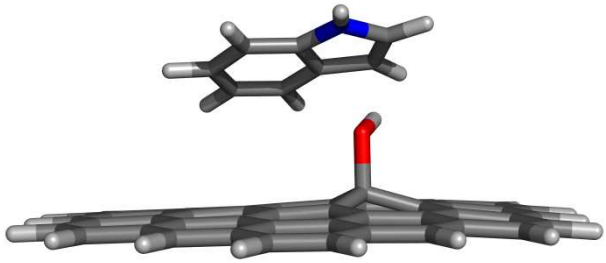
GO-Tyr-CAR GO-Tyr-EPO



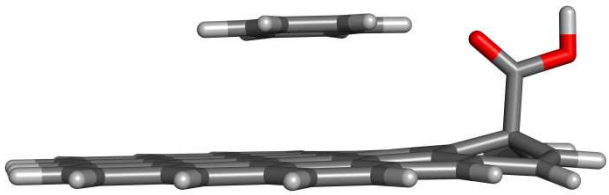
GO-Tyr-OH



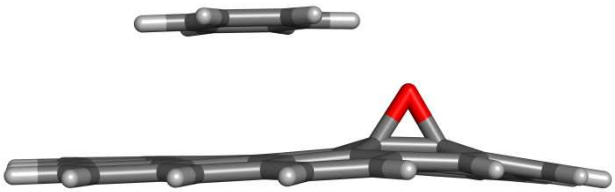
GO-Trp-CAR GO-Trp-EPO



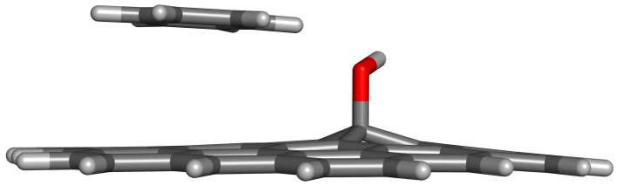
GO-Trp-OH



GO-Phe-CAR



GO-Phe-EPO



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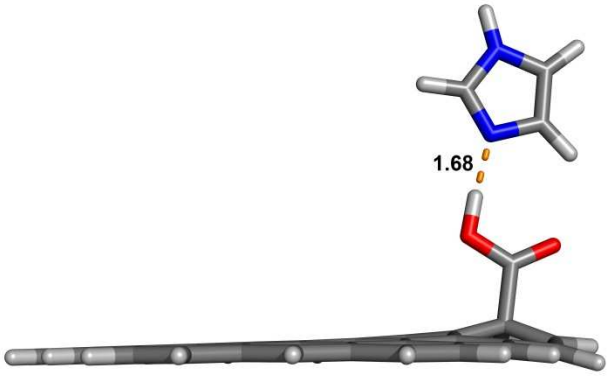
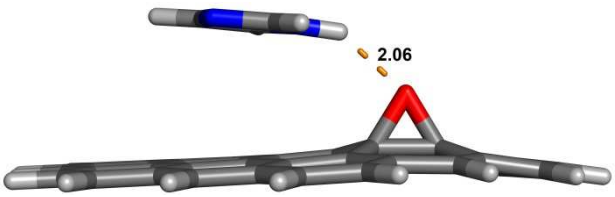
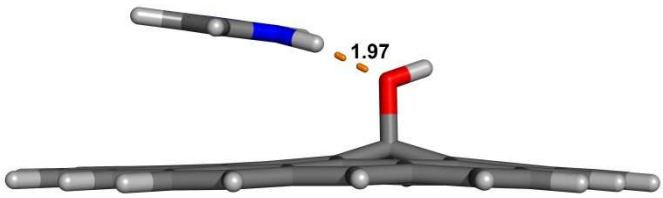


GO-His-CAR



GO-His-EPO



GO-His-OH

Figure S4. Optimized geometries (bond lengths in Å) of mono carboxyl or epoxy or hydroxy GO with DNA bases and aromatic amino acids using M05-2X/6-31G (d) level of theory.