Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical Design and Investigation of 1,8-Naphthalimide-Based Two-photon Fluorescent Probes for Detecting Cytochrome P450 1A with Separated Fluorescence Signal

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Supporting Information

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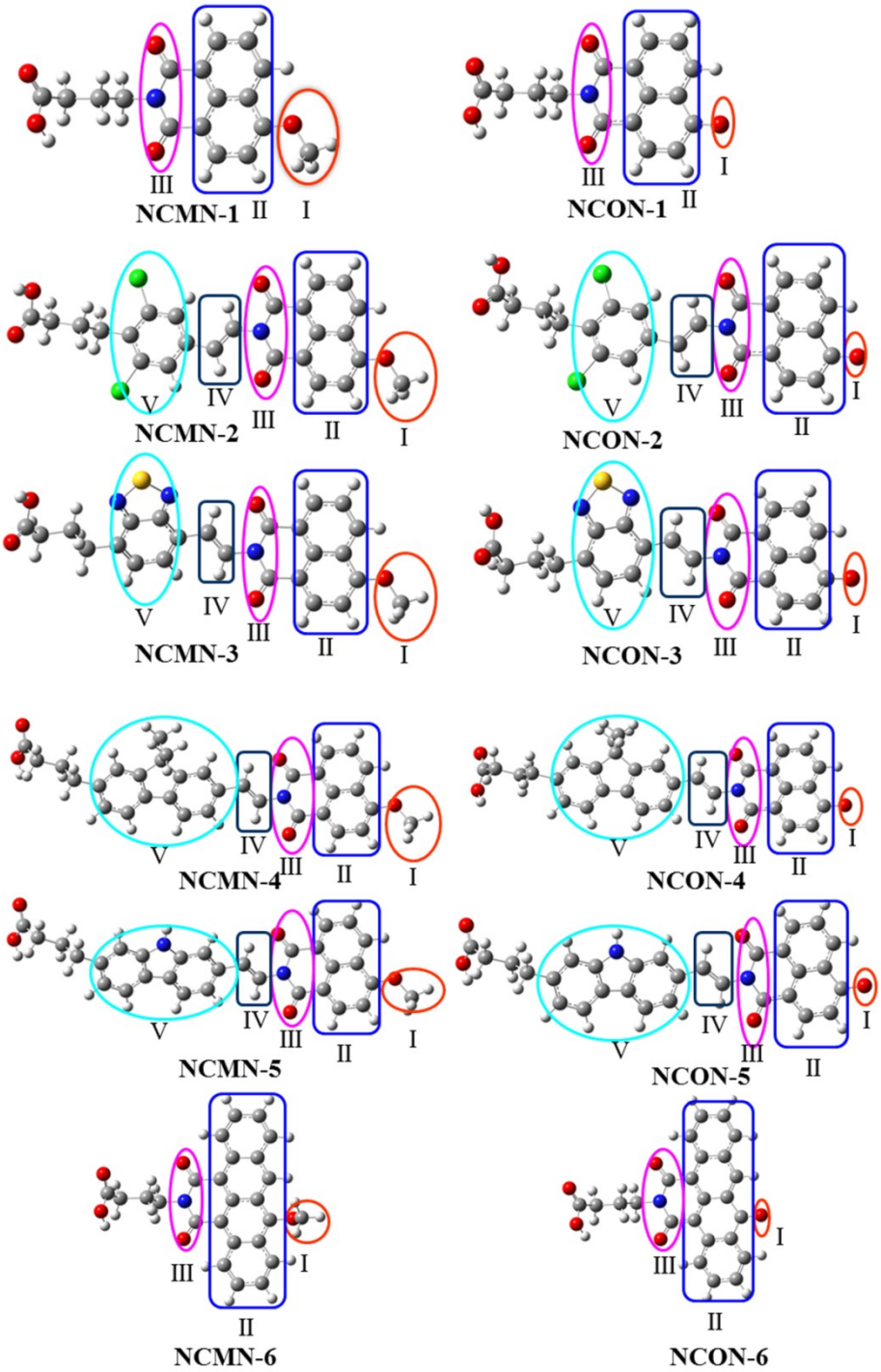
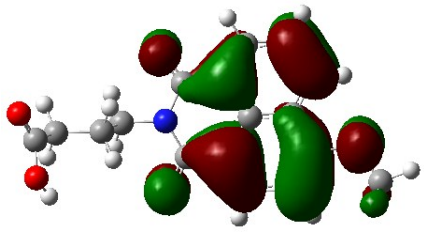


Figure S1. The partition diagrams of all investigated chromophores.

Table S1. The calculated frontier molecular orbital energy of all investigated molecules at the DFT//B3LYP/6-31+G(d) level.

Mol.	H-3	H-2	H-1	H	L	L+1	L+2	L+3	ΔE_{L-H}
NCMN-1	-7.69	-7.65	-7.42	-6.37	-2.67	-1.06	-0.98	-0.46	3.70
NCON-1	-7.09	-6.94	-6.48	-5.21	-2.01	-0.60	-0.47	-0.31	3.20
NCMN-2	-7.48	-7.08	-6.44	-6.26	-2.75	-1.94	-1.06	-0.99	3.51
NCON-2	-7.01	-6.52	-6.14	-5.26	-2.13	-1.63	-0.92	-0.57	3.13
NCMN-3	-7.46	-7.41	-6.42	-6.03	-2.74	-2.72	-1.58	-1.05	3.29
NCON-3	-7.01	-6.54	-5.87	-5.28	-2.66	-2.07	-1.26	-0.51	2.62
NCMN-4	-6.94	-6.90	-6.38	-5.72	-2.69	-1.82	-1.05	-0.99	3.03
NCON-4	-6.73	-6.52	-5.57	-4.75	-2.07	-1.61	-0.81	-0.62	2.68
NCMN-5	-6.96	-6.38	-5.87	-5.52	-2.69	-1.74	-1.05	-0.98	2.83
NCON-5	-6.52	-5.81	-5.57	-4.95	-2.37	-1.54	-0.79	-0.48	2.58
NCMN-6	-7.28	-7.18	-6.87	-5.76	-3.34	-1.52	-1.15	-0.92	2.42
NCON-6	-6.81	-6.66	-6.28	-5.00	-2.68	-0.96	-0.63	-0.52	2.32

Table S2. The mainly involved molecular orbital plots of the studied products.



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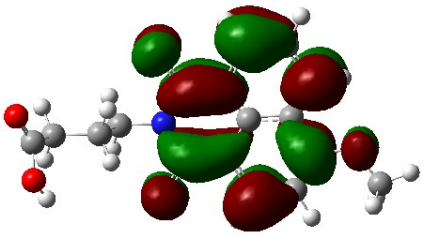

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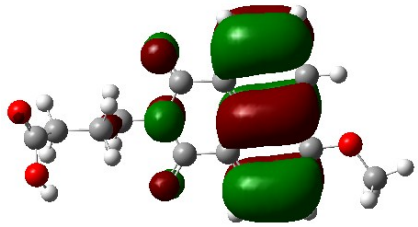

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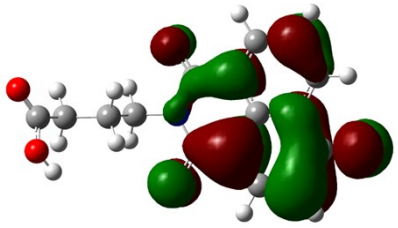

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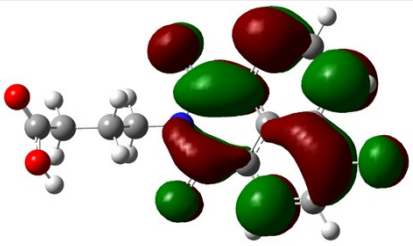

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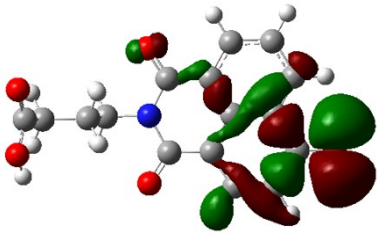

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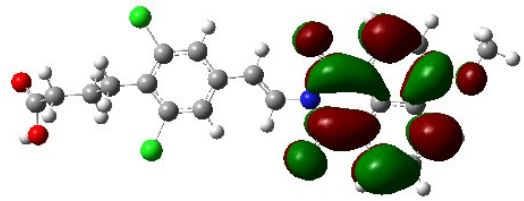
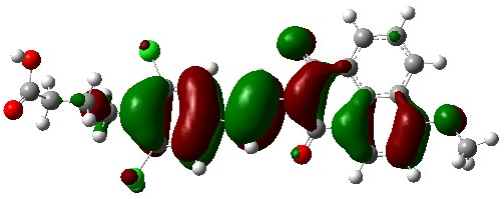
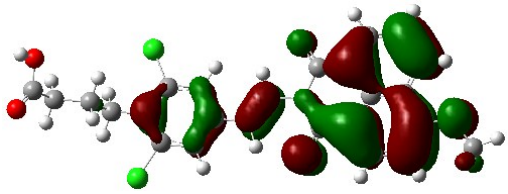
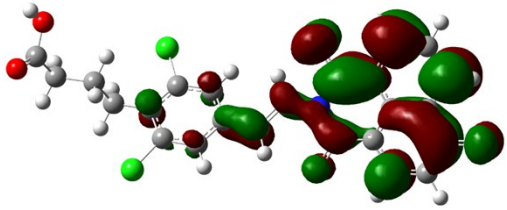
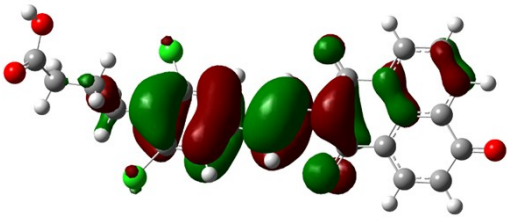
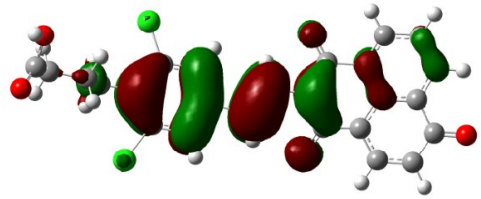
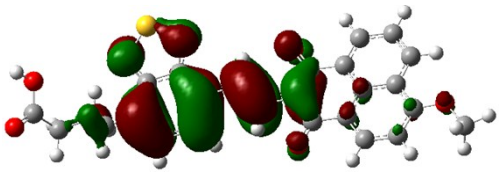
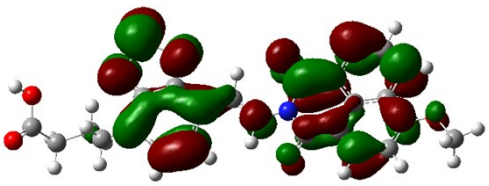
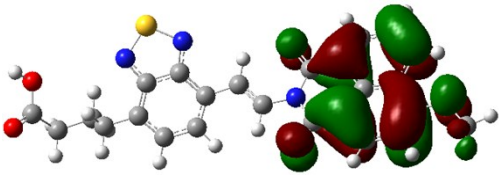
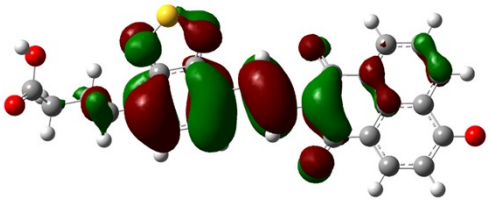
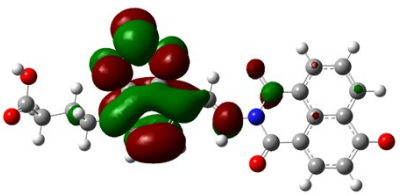
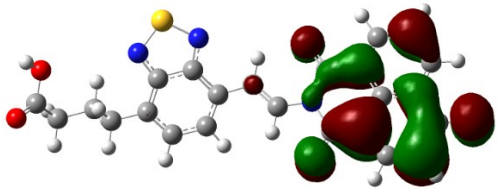
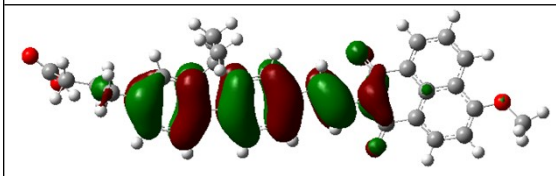
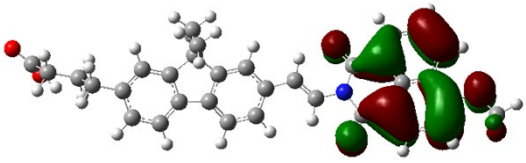
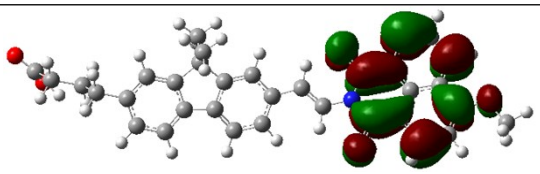
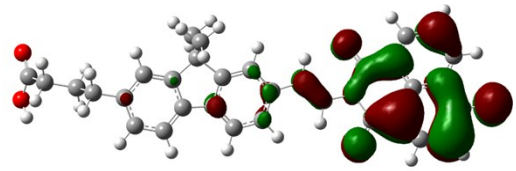
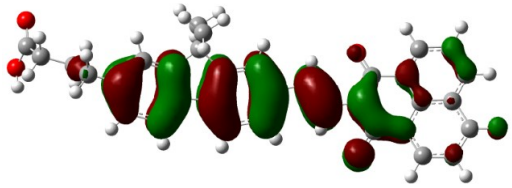
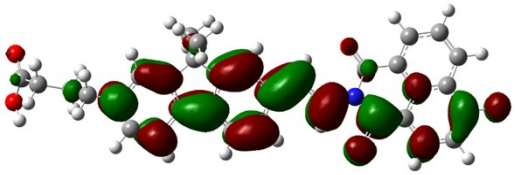
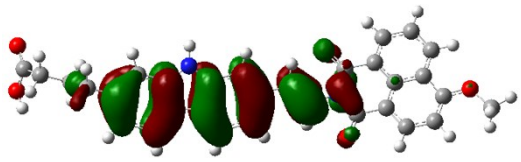
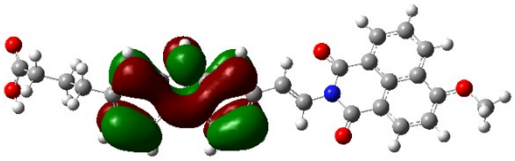
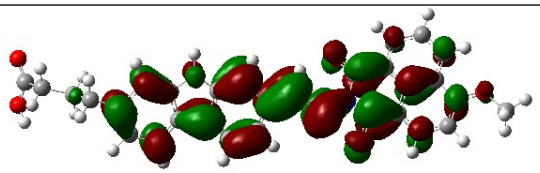
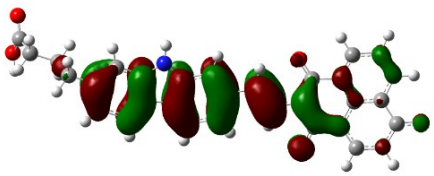
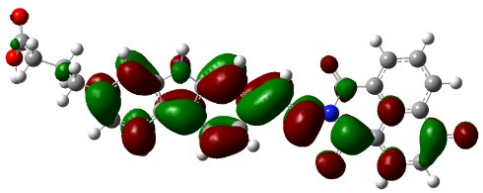
 NCMN-2-HOMO	 NCMN-2-LUMO
 NCMN-2-HOMO-1	
 NCON-2-HOMO	 NCON-2-LUMO
 NCON-2-HOMO-1	
 NCMN-3-HOMO	 NCMN-3-LUMO
 NCMN-3-HOMO-1	
 NCON-3-HOMO	 NCON-3-LUMO

 NCON-3-HOMO-1	
 NCMN-4-HOMO  NCMN-4-HOMO-1	 NCMN-4-LUMO
 NCON-4-HOMO  NCON-4-HOMO-1	 NCON-4-LUMO
 NCMN-5-HOMO  NCMN-5-HOMO-1	 NCMN-5-LUMO
 NCON-5-HOMO	 NCON-5-LUMO

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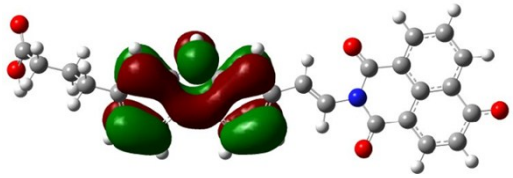
<tr><td> 
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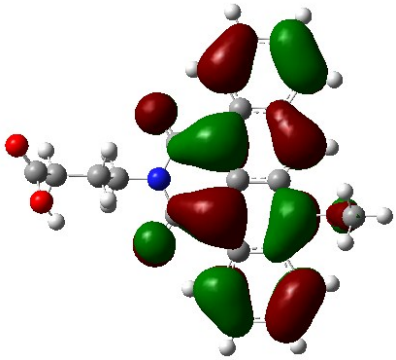
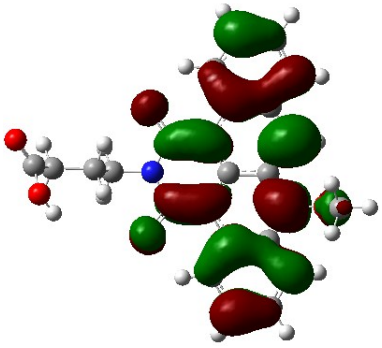
<tr><td> 
NCMN-6-HOMO</td><td> 
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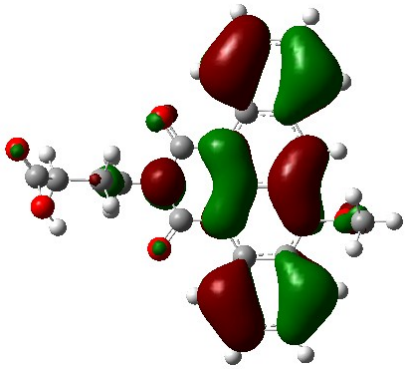
<tr><td> 
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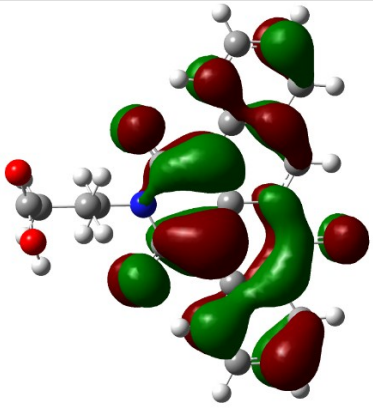
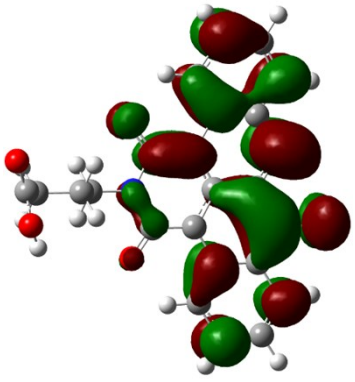
<tr><td> 
NCON6-HOMO</td><td> 
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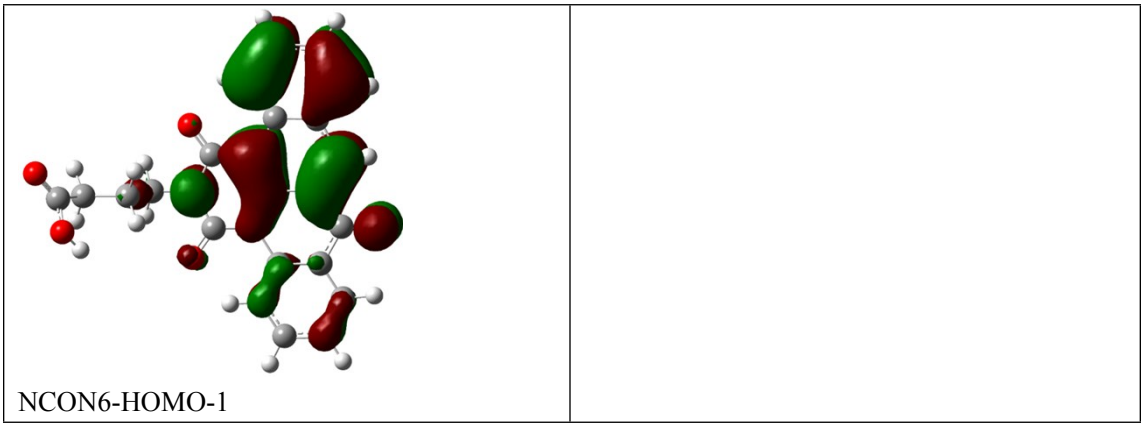

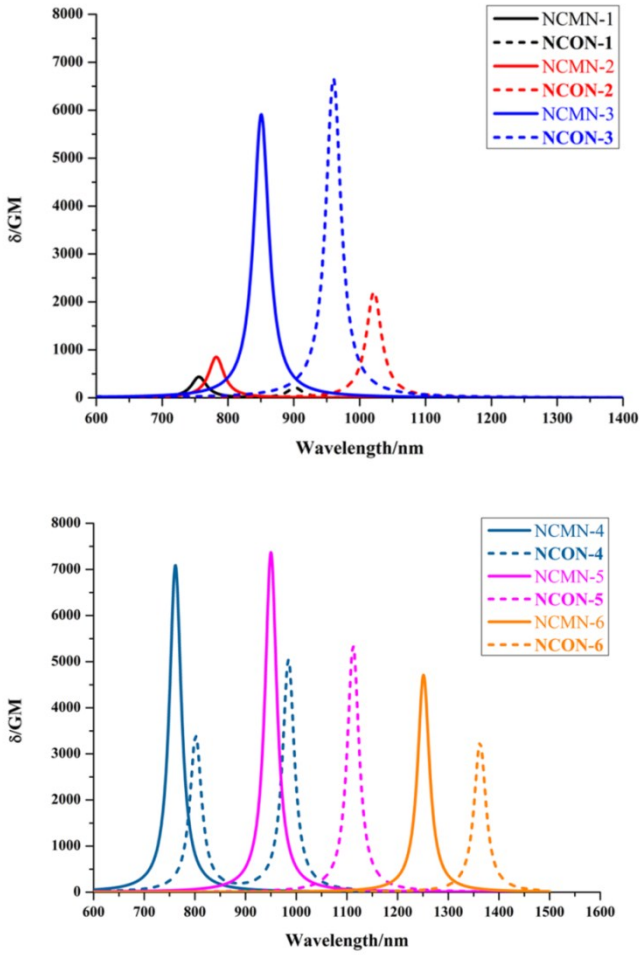

Figure S2. Simulated two-photon absorption spectra of the studied molecules by TDDFT//B3LYP/6-31+G(d).

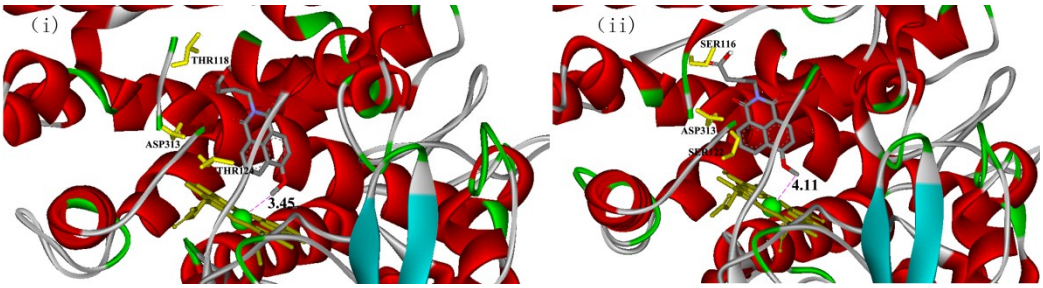

Figure S3. Docking simulation of synthesized NCMN-1 into reported CYP1A2 (i) andCYP1A1 (ii).

Table S3. All the energy parameters (Kcal/mol) during the docking simulations of NCMN-3 and NCMN-5 with CYP1A1.

	Binding Affinity Energy	Intermolecular Energy	Internal Energy	Torsional Energy	Unbound Extended Energy
NCMN-3	-12.42	-14.81	-1.50	2.39	-1.50
NCMN-5	-6.77	-9.16	-0.62	2.39	-0.62