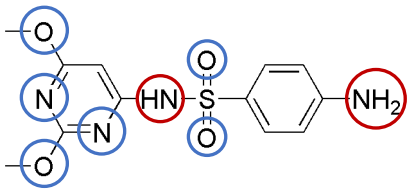
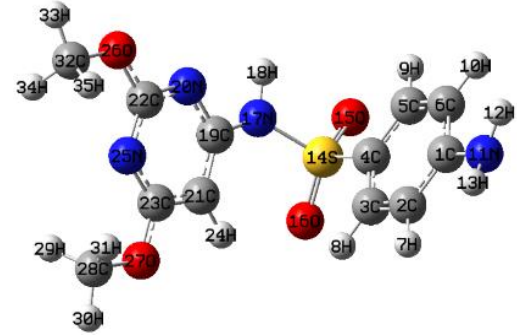
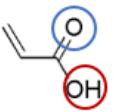
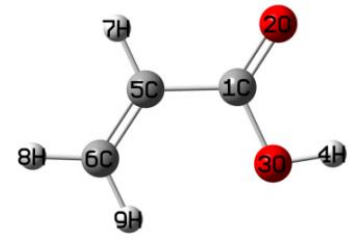

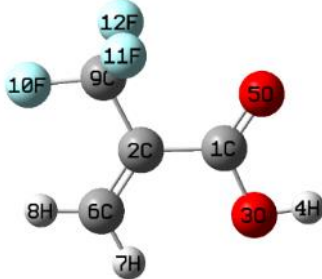
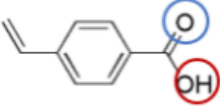
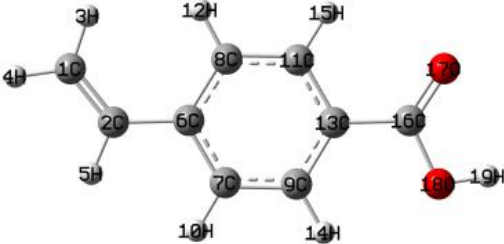
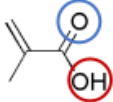
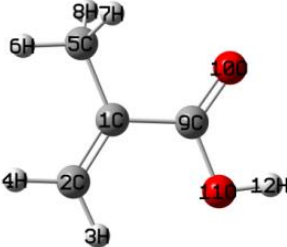
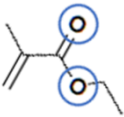
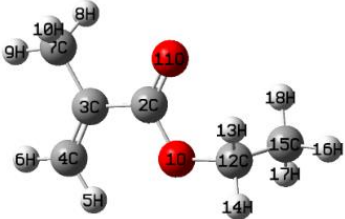
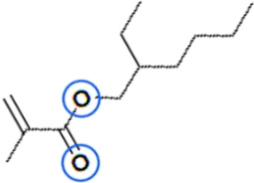
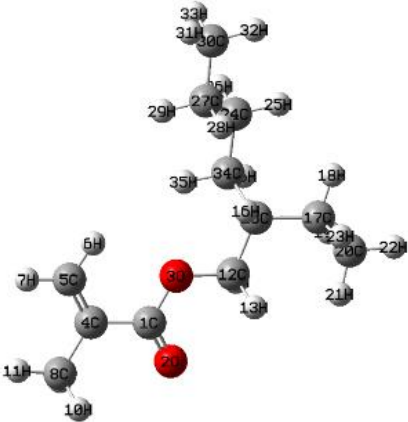
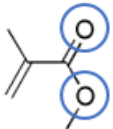
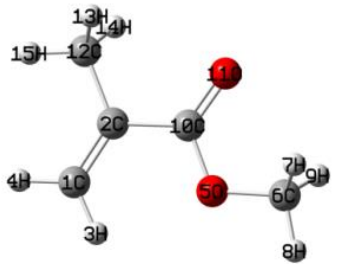


Table S1 Electron donor/acceptor atoms and optimized conformations of the template and functional monomers

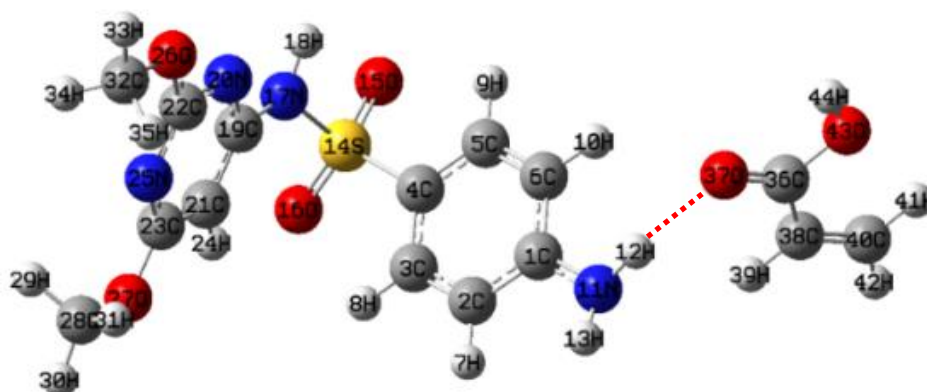
Abbreviation of chemical name	Chemical structure and hydrogen bond donor (○) or acceptor(○)	The NBO charge of hydrogen bond donor	The NBO charge of hydrogen bond acceptor		Optimized conformation	
SDM		17N-18H	-0.864	15O	-0.918	
			+0.432	16O	-0.931	
		11N-12H	-0.798	27O	-0.534	
			+0.387	25N	-0.588	
		11N-13H	-0.798	26O	-0.536	
			+0.386	20N	-0.564	
AA		3O-4H	-0.714	2O	-0.598	
		+0.495				

Abbreviation of chemical name	Chemical structure and hydrogen bond donor (○) or acceptor(○)	The NBO charge of hydrogen bond donor	The NBO charge of hydrogen bond acceptor		Optimized conformation
TFMAA		3O-4H -0.708 +0.501	5O	-0.572	
4-VBA		18O-19H -0.710 +0.495	17O	-0.611	
MAA		11O-12H -0.710 +0.493	10O	-0.607	

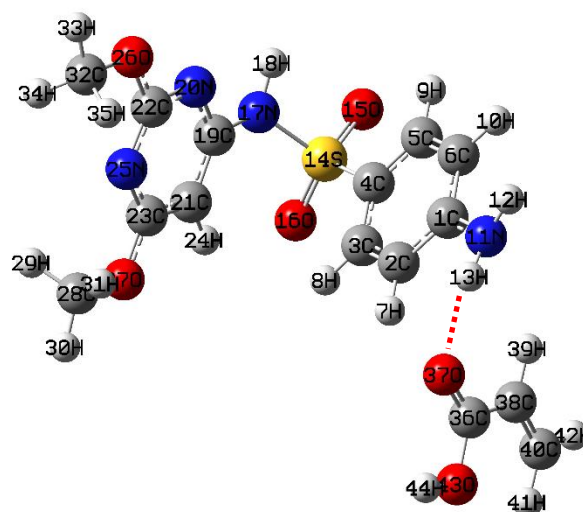
Abbreviation of chemical name	Chemical structure and hydrogen bond donor (○) or acceptor(○)	The NBO charge of hydrogen bond donor	The NBO charge of hydrogen bond acceptor		Optimized conformation
EMA		/	11O	-0.570	
			1O	-0.587	
EHMA		/	3O	-0.590	
			2O	-0.572	

Abbreviation of chemical name	Chemical structure and hydrogen bond donor (○) or acceptor(○)	The NBO charge of hydrogen bond donor	The NBO charge of hydrogen bond acceptor		Optimized conformation
MMA		/	11O	-0.606	
			5O	-0.575	

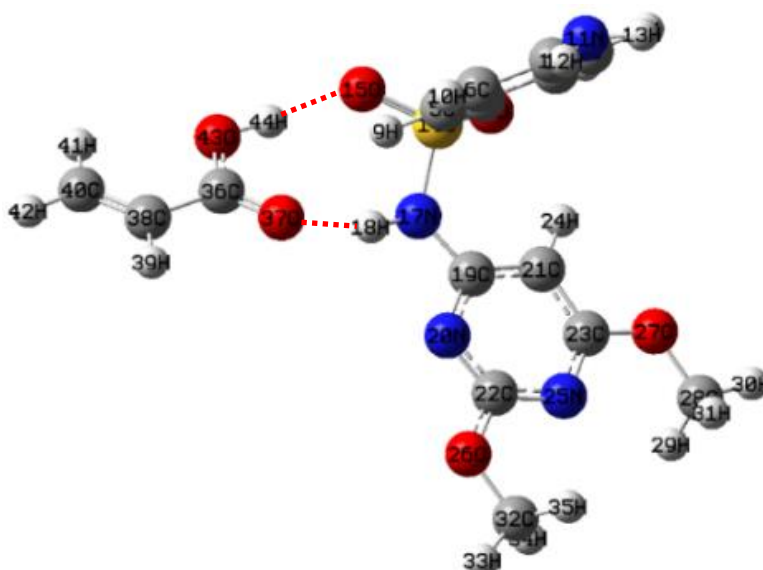
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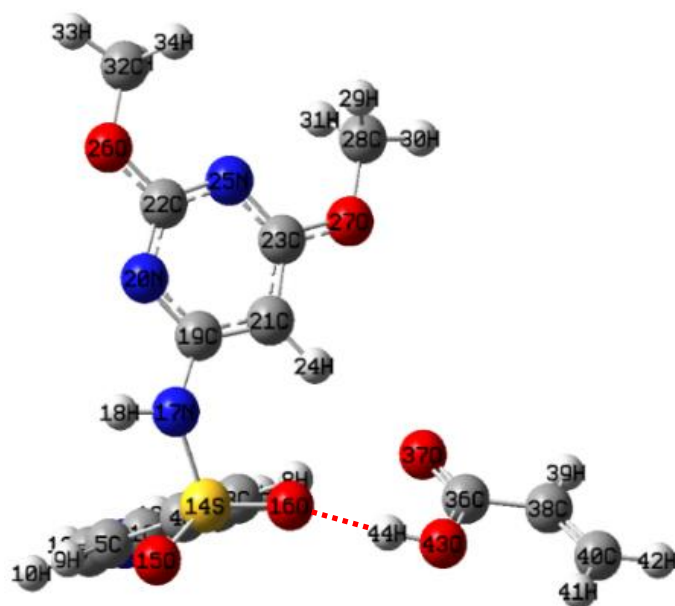
2) SDM-AA②



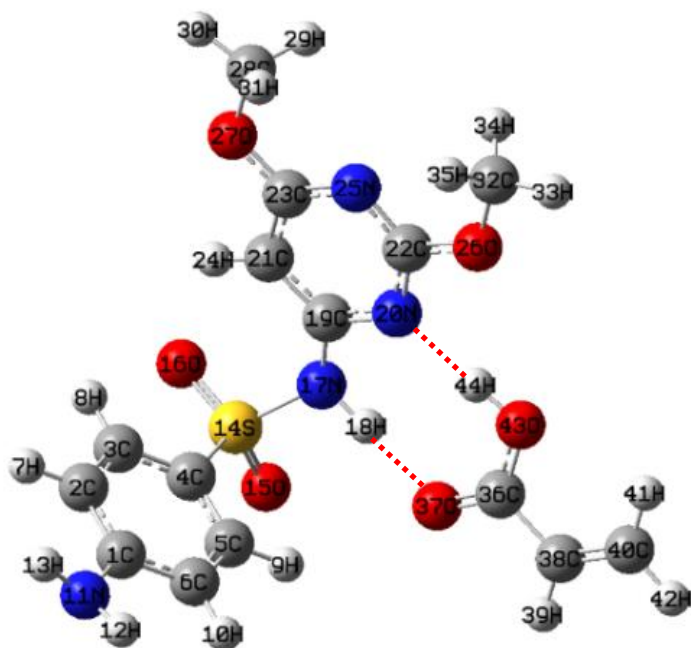
3) SDM-AA③



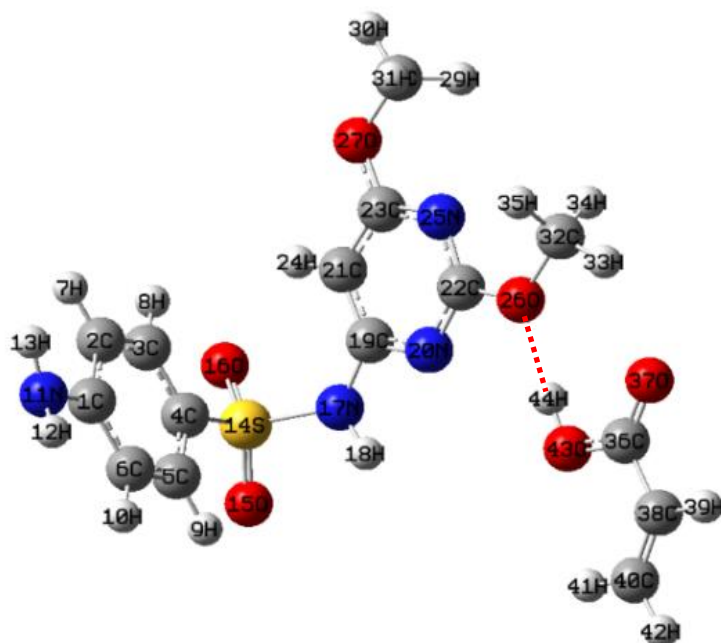
4) SDM-AA④



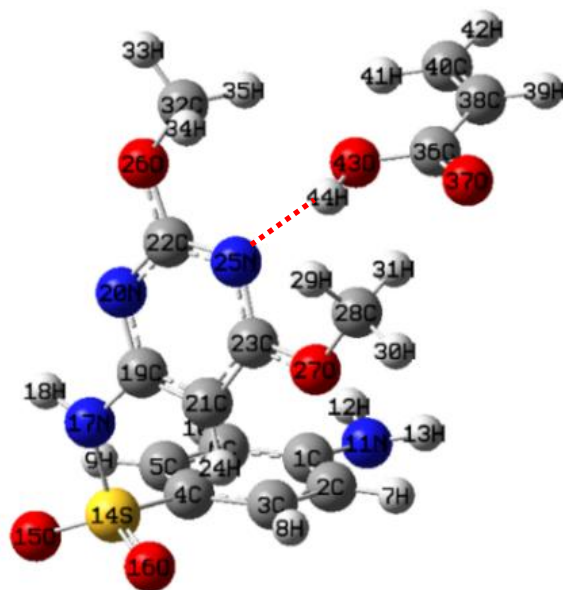
5) SDM-AA⑤



6) SDM-AA⑥



7) SDM-AA⑦



8) SDM-AA⑧

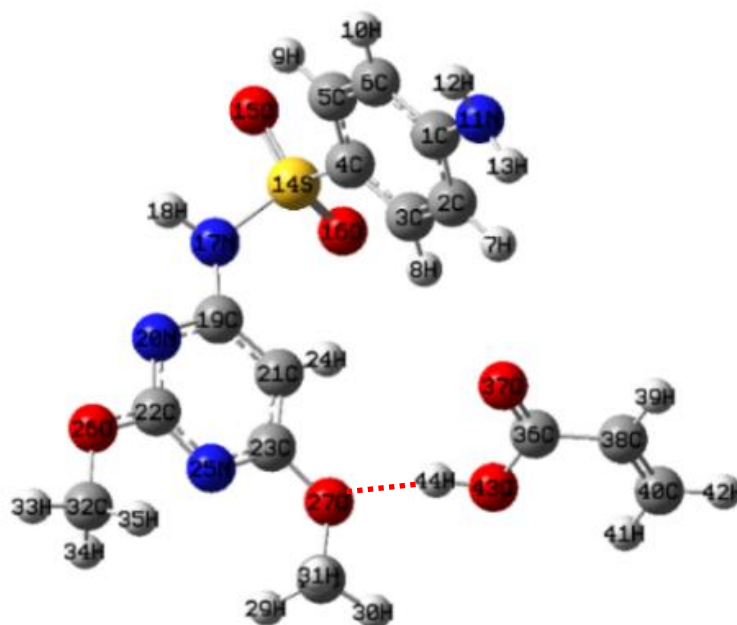
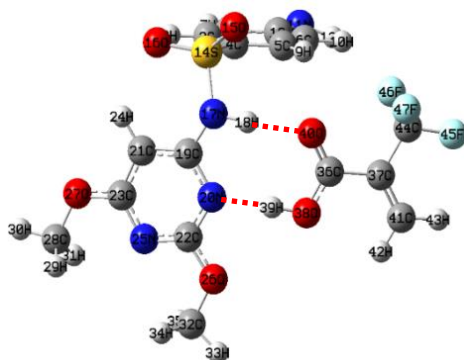
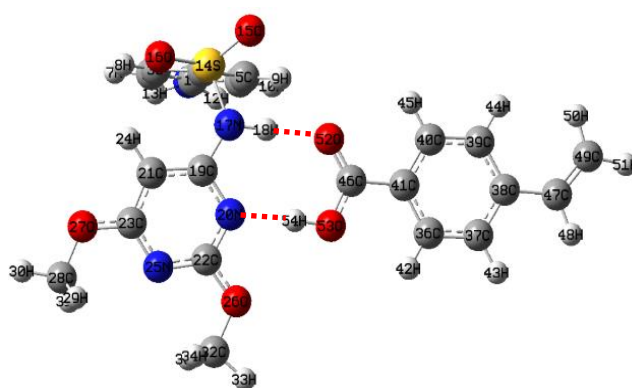


Figure S1. Possible complex formed between SDM and AA at the mole ratio of 1:1.
(The dotted red lines are hydrogen bonds)

1) SDM-TFMAA⑤



2) SDM-4-VBA⑤



3) SDM-MAA⑤

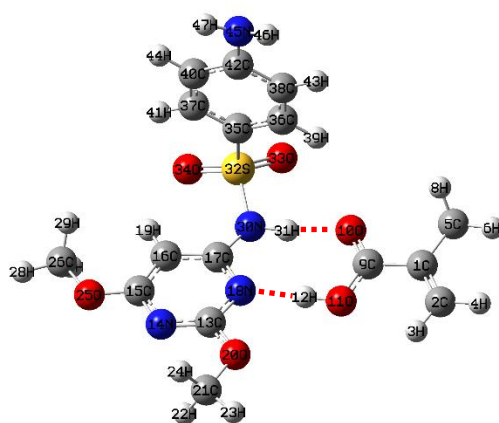
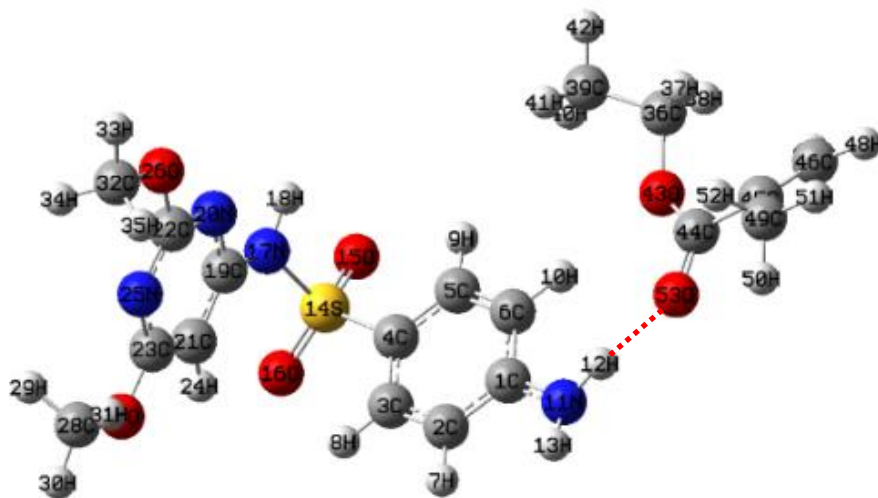
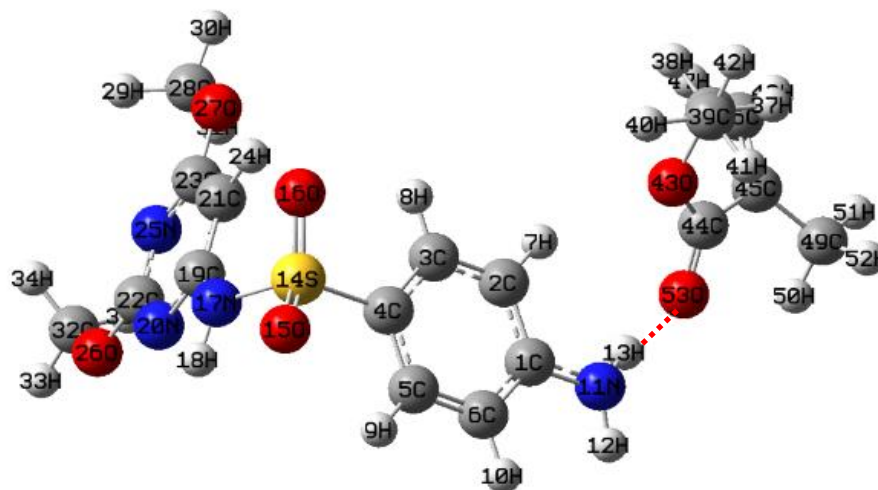


Figure S2. Structures of SDM-TFMAA⑤, SDM-4-VBA⑤ and SDM-MAA⑤.
(The dotted red lines are hydrogen bonds)

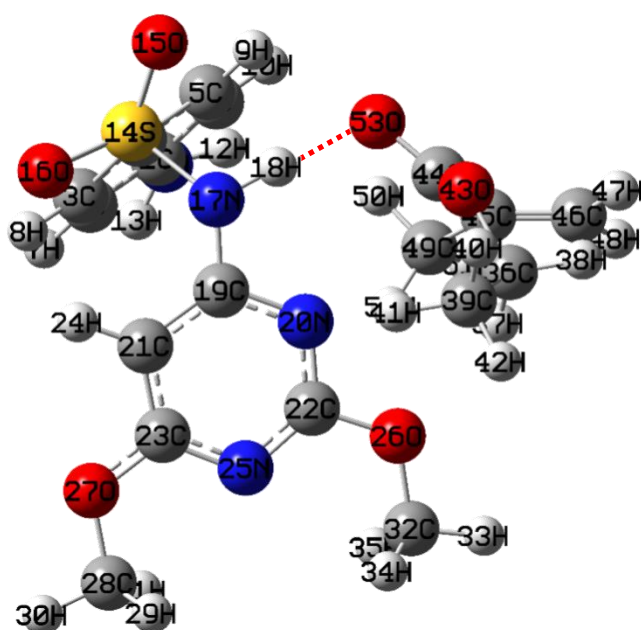
1)SDM-EMA①



2)SDM-EMA②



3)SDM-EMA③



4)SDM-EMA④

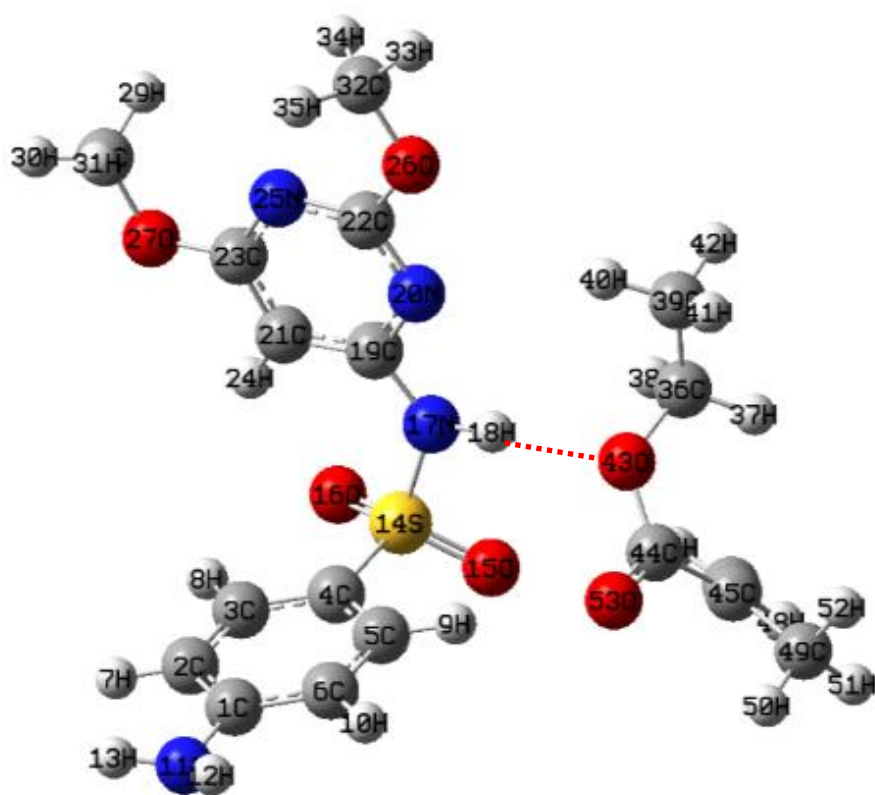


Figure S3. Possible complex formed between SDM and EMA at the mole ratio of 1:1.
(The dotted red lines are hydrogen bonds)

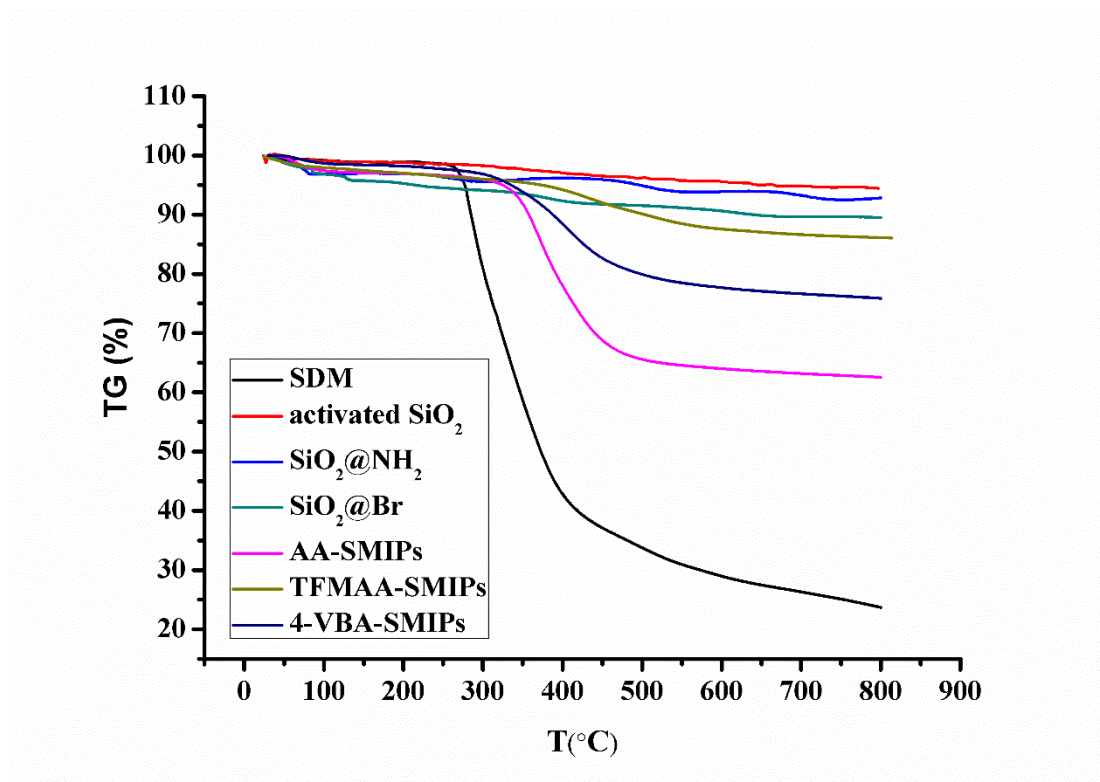


Figure S4 Thermogravimetric curves of SDM and products of each stage.

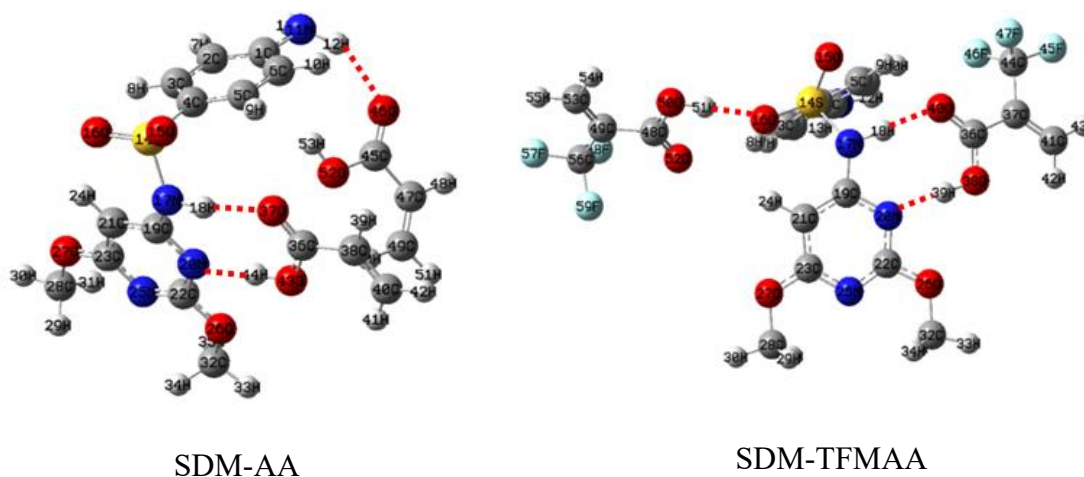
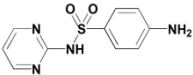
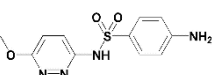
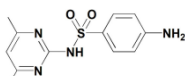
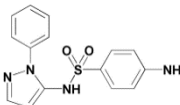
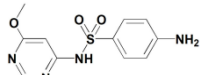
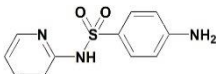


Figure S5 The complexes formed between SDM and AA and TFMAA at the mole ratio of 1:2.

Table S2 The chemical structure of sulfonamides.

Drug	Chemical structure	Drug	Chemical structure
SD		SMP	
SM2		SPA	
SMM		SPD	

AA

TFMAA

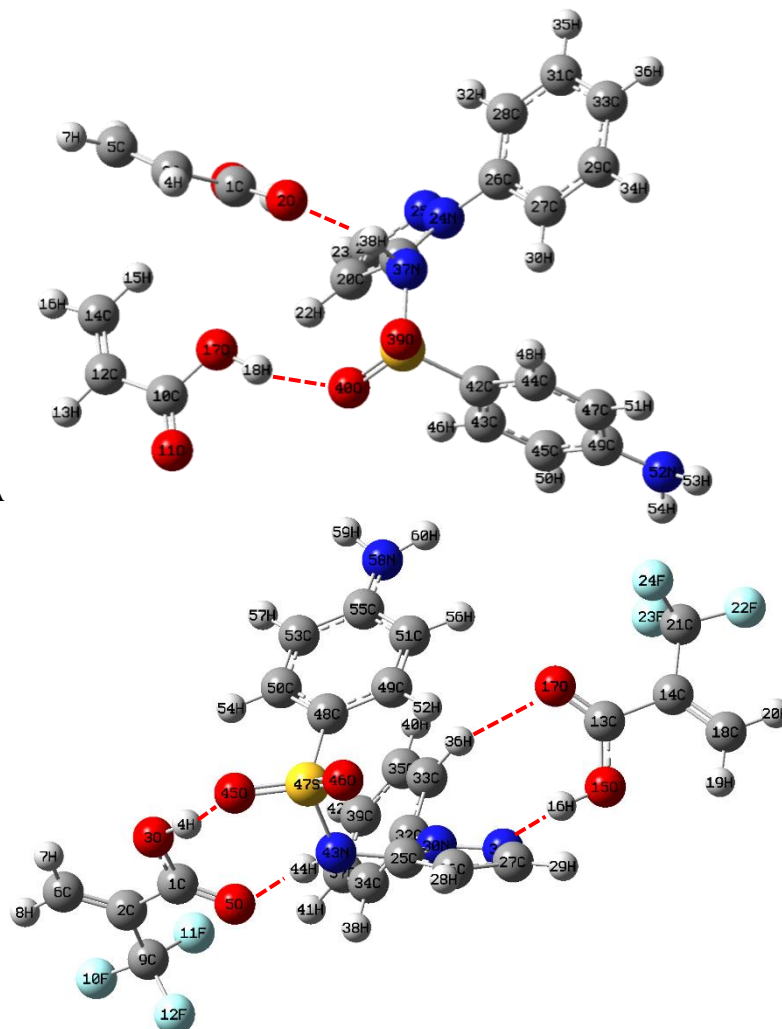


Figure S6 The complexes formed between SPA and “holes” of SDM-AA and SDM-TFMAA SMIPs.