SUPPLEMENTARY INFORMATION

The amidine formed by tacrine and saccharin revisited: An ab initio Investigation of Structural, Electronic and Spectroscopic Properties

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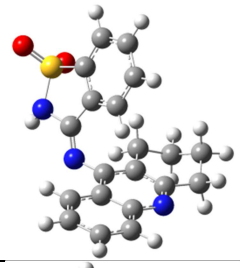
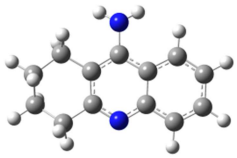
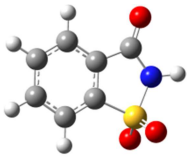
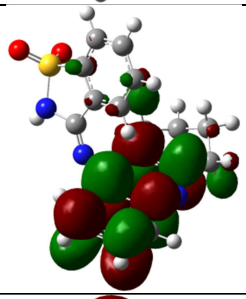
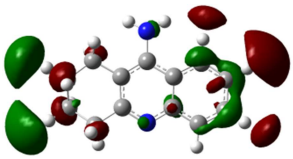
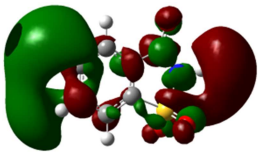
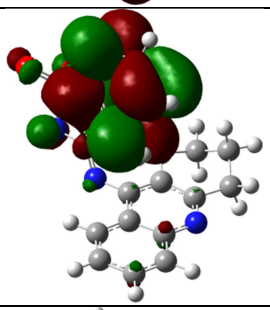
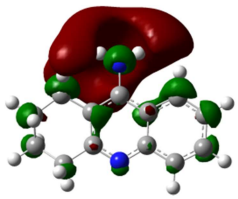
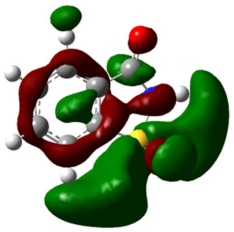
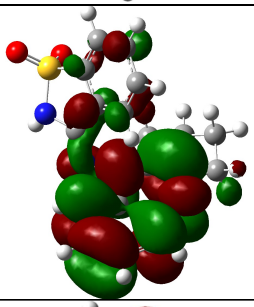
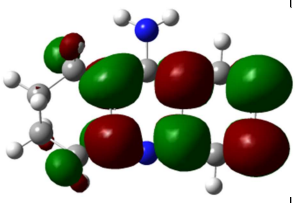
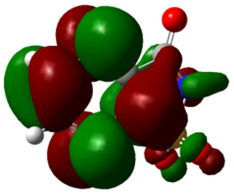
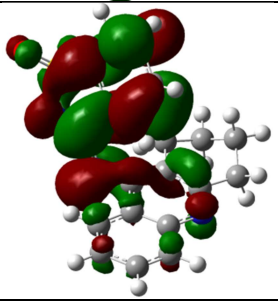
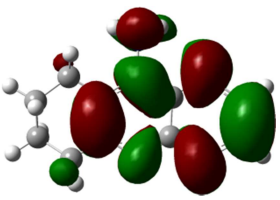
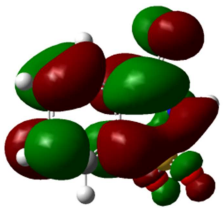
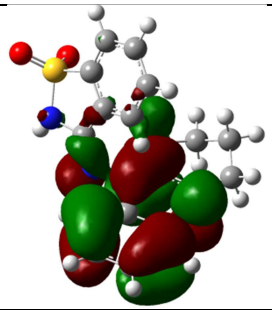
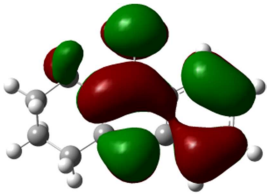
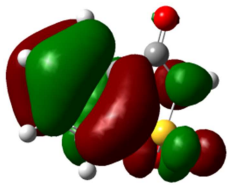
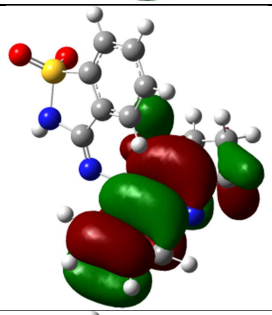
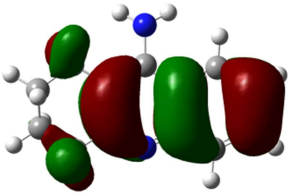
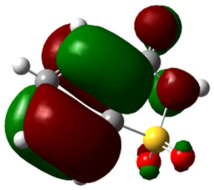
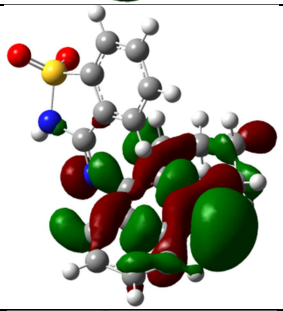
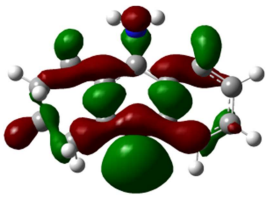
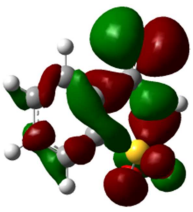
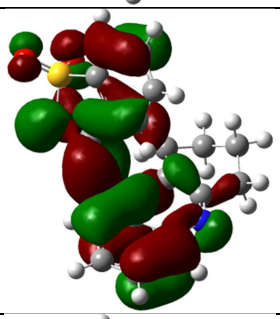
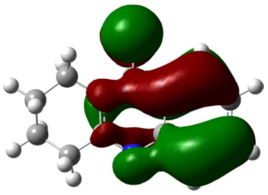
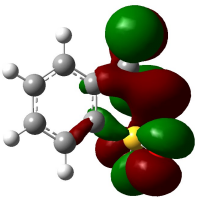
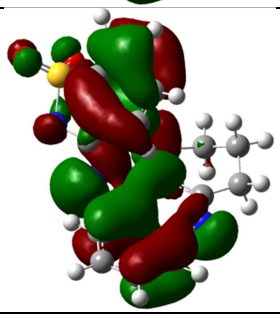
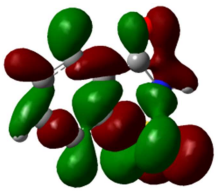
	TacSac	Tac	Sac
			
LUMO+3			
LUMO+2			
LUMO+1			
LUMO			

HOMO			
HOMO-1			
HOMO-2			
HOMO-3			
HOMO-4			

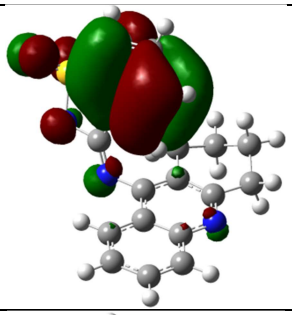
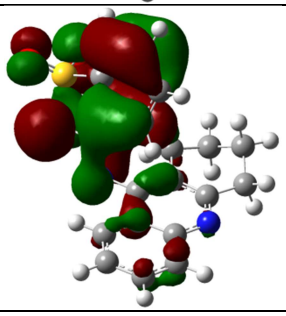
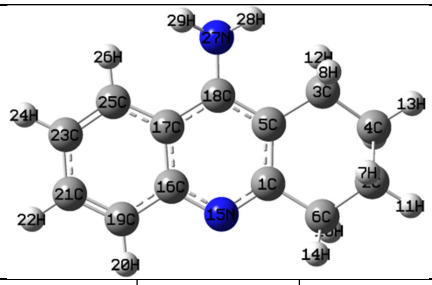
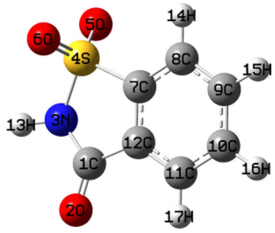
HOMO-5			
HOMO-6			

Fig. S1. Molecular orbitals contributing to the listed electronic transitions for Tac, Sac and TacSac.

Table S1. APT charges for atoms of Tac and Sac calculated in gas phase and in H2O at MP2/6-311++G(d,p)

Tac				**Sac**			
	GAS (ATP)	H2O	H2O (SMD)		GAS (ATP)	H2O	H2O (SMD)
C(1)	0.304	0.470	0.526	C(1)	1.145	1.682	1.885
C(2)	0.090	0.018	0.121	O(2)	-0.705	-1.021	-1.154
C(3)	0.127	0.152	0.138	N(3)	-0.992	-1.397	-1.507
C(4)	0.112	0.144	0.143	S(4)	2.185	3.101	3.298
C(5)	-0.180	-0.262	-0.278	O(5)	-0.808	-1.153	-1.245
C(6)	0.071	0.100	0.084	O(6)	-0.825	-1.166	-1.255
H(7)	-0.029	-0.043	-0.047	C(7)	-0.219	-0.299	-0.319
H(8)	-0.064	-0.074	-0.069	C(8)	-0.035	-0.056	-0.076
H(9)	-0.026	-0.043	-0.046	C(9)	-0.009	-0.009	-0.020
H(10)	-0.048	-0.068	-0.065	C(10)	-0.026	-0.033	-0.045
H(11)	-0.045	-0.057	-0.054	C(11)	0.001	0.003	0.005
H(12)	-0.040	-0.055	-0.052	C(12)	-0.207	-0.302	-0.340
H(13)	-0.046	-0.056	-0.054	H(13)	0.232	0.313	0.367

H(14)	-0.046	-0.039	-0.041	H(14)	0.077	0.099	0.120
N(15)	-0.460	-0.683	-0.747	H(15)	0.054	0.072	0.092
C(16)	0.134	0.205	0.221	H(16)	0.054	0.073	0.091
C(17)	-0.080	-0.101	-0.106	H(17)	0.079	0.093	0.111
C(18)	0.470	0.753	0.825				
C(19)	0.036	0.061	0.058				
H(20)	0.055	0.060	0.072				
C(21)	-0.104	-0.157	-0.184				
H(22)	0.034	0.047	0.063				
C(23)	0.004	0.006	0.000				
H(24)	0.030	0.045	0.059				
C(25)	-0.085	-0.125	-0.150				
H(26)	0.031	0.049	0.067				
N(27)	-0.654	-0.984	-1.093				
H(28)	0.189	0.268	0.305				
H(29)	0.190	0.268	0.305				

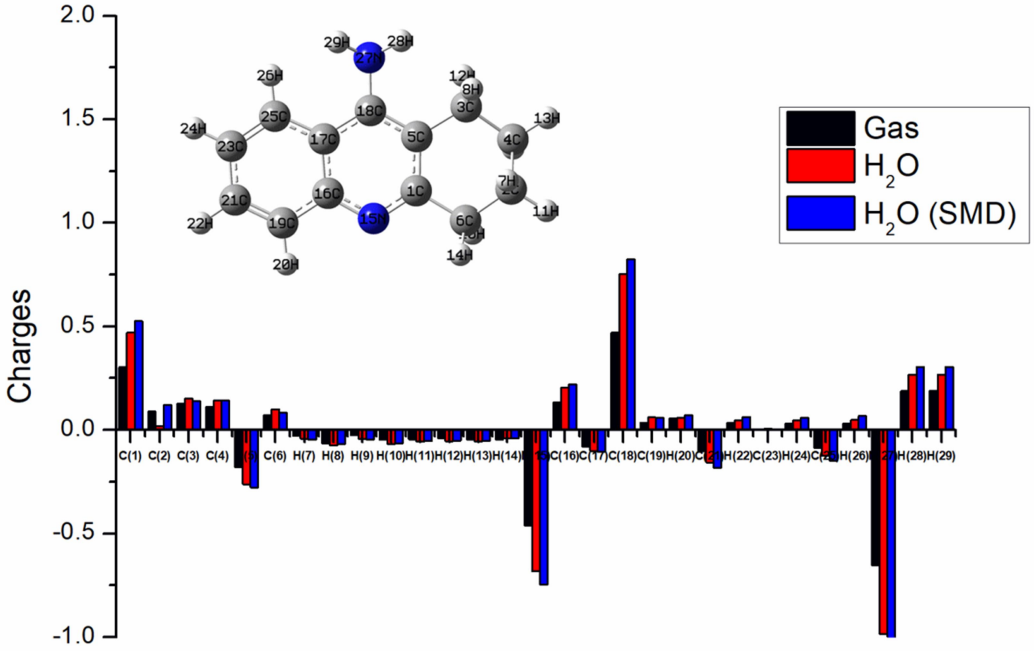


Fig. S2. APT charges for atoms of Tac calculated in gas phase and in H_2O at MP2/6-311++G(d,p)

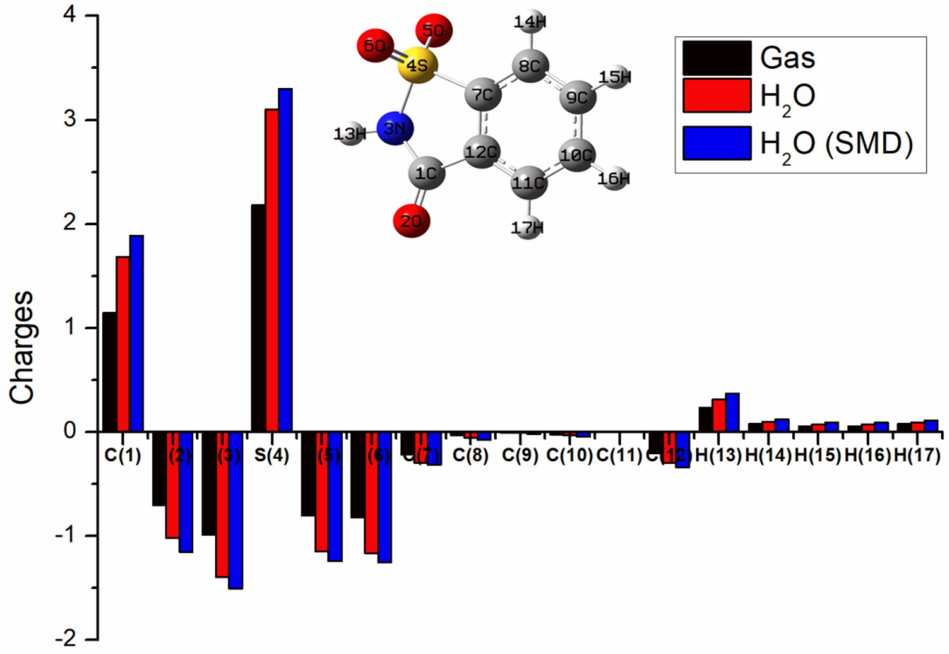
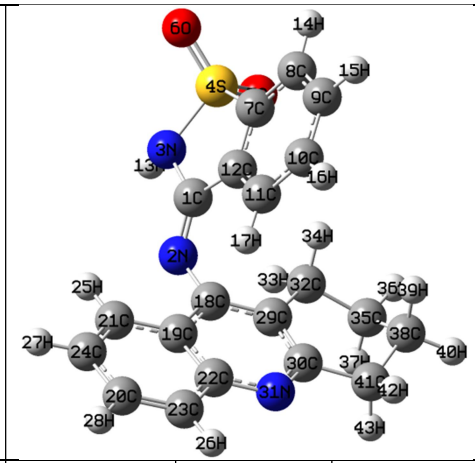


Fig. S3. APT charges for atoms of Sac calculated in gas phase and in H_2O at MP2/6-311++G(d,p)

Table S2. APT charges for atoms of TacSac calculated in gas phase and in H2O at MP2/6-311++G(d,p)

TacSac			
	GAS (ATP)	H2O	H2O (SMD)
C(1)	0.898	1.307	1.349
N(2)	-0.726	-1.058	-1.088
N(3)	-0.996	-1.403	-1.115
S(4)	2.177	3.168	3.330
O(5)	-0.820	-1.199	-1.288
O(6)	-0.819	-1.182	-1.265

C(7)	-0.201	-0.293	-0.319
C(8)	-0.034	-0.063	0.038
C(9)	-0.013	-0.024	0.059
C(10)	-0.030	-0.037	0.039
C(11)	-0.007	-0.013	0.096
C(12)	-0.141	-0.213	-0.229
H(13)	0.212	0.297	0.000
H(14)	0.075	0.096	0.000
H(15)	0.049	0.071	0.000
H(16)	0.054	0.073	0.000
H(17)	0.065	0.096	0.000
C(18)	0.408	0.598	0.611
C(19)	-0.086	-0.104	-0.098
C(20)	-0.090	-0.149	-0.117
C(21)	-0.092	-0.121	-0.051
C(22)	0.106	0.161	0.169
C(23)	0.022	0.045	0.117
C(24)	0.014	0.013	0.066
H(25)	0.058	0.075	0.000
H(26)	0.052	0.059	0.000
H(27)	0.033	0.045	0.000
H(28)	0.032	0.046	0.000
C(29)	-0.158	-0.192	-0.178
C(30)	0.249	0.360	0.385
N(31)	-0.375	-0.538	-0.572
C(32)	0.095	0.125	0.025
H(33)	-0.020	-0.036	0.000
H(34)	-0.053	-0.058	0.000
C(35)	0.105	0.140	0.041
H(36)	-0.034	-0.054	0.000
H(37)	-0.029	-0.045	0.000
C(38)	0.083	0.114	0.023
H(39)	-0.029	-0.040	0.000
H(40)	-0.042	-0.053	0.000
C(41)	0.061	0.087	-0.028
H(42)	-0.015	-0.038	0.000
H(43)	-0.041	-0.063	0.000

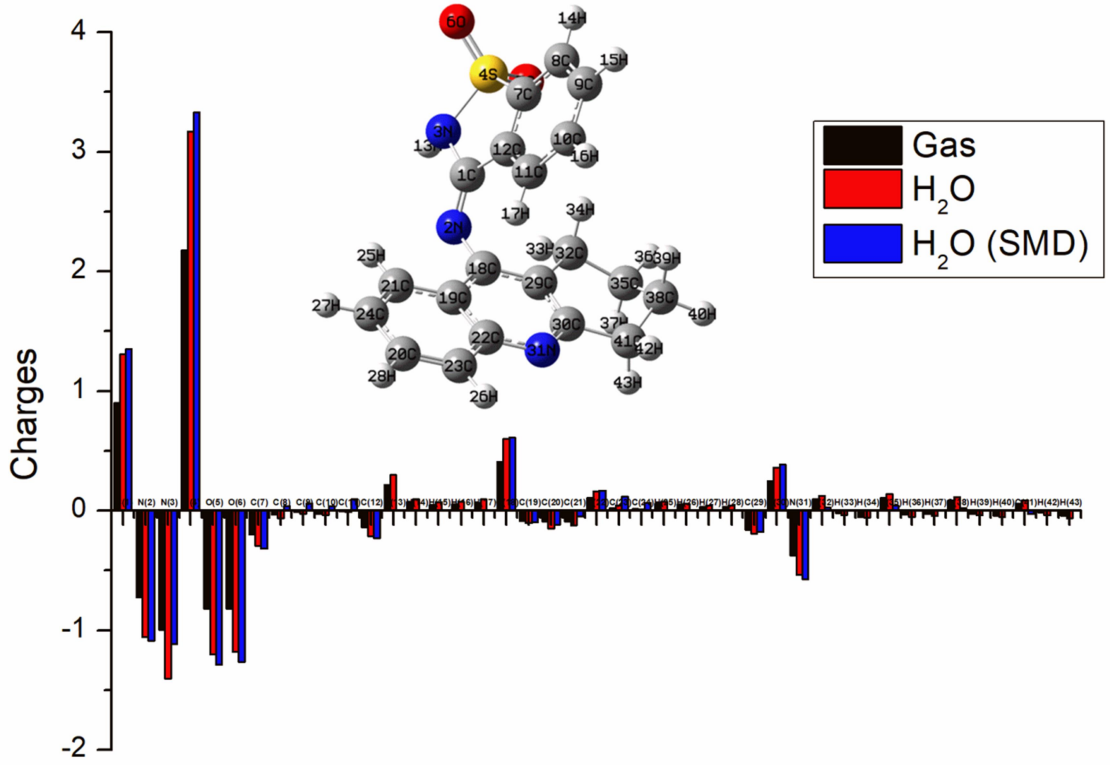


Fig S4. Presentation of APT charges for atoms of TacSac calculated in gas phase and in H_2O at MP2/6-311++G(d,p)