Supporting Information

S1. AM1 optimized structure of the neutral, base pairing form of 1,3-diaza-2-oxopheno-thiazine, tC. (Numbering is not according to IUPAC)

			Coordinates (Å)		
Number	Atom	Charge	x	y	z
1	C	0.499102	-7.35718	-1.06502	-0.51018
2	N	-0.18225	-7.40107	0.32093	-0.13673
3	C	0.13146	-6.25547	0.97022	0.21671
4	C	-0.01853	-5.03785	0.32331	0.24756
5	C	0.348815	-5.01823	-1.08123	-0.17038
6	N	-0.44267	-6.12495	-1.73993	-0.53985
7	N	-0.22226	-3.81382	-1.78105	-0.16075
8	C	0.098008	-2.55616	-1.15767	-0.12781
9	C	0.026654	-2.40115	0.18161	0.29397
10	S	-0.05055	-3.68336	1.15665	0.80515
11	C	-0.03648	-1.40995	-1.90246	-0.49129
12	C	-0.01689	-0.14947	-1.32342	-0.41834
13	C	-0.02769	0	0	0
14	C	-0.02179	-1.12108	0.74489	0.34494
15	O	-0.58669	-8.4433	-1.59791	-0.80528
16	H	0.048503	-6.34392	2.03953	0.49222
17	H	0.172669	-3.82813	-2.7292	-0.48015
18	H	0.026305	-1.50897	-2.94633	-0.82722
19	H	0.024681	0.73586	-1.91531	-0.69659
20	H	0.023969	1.00058	0.45317	0.053
21	H	0.023786	-1.01036	1.79318	0.66661
22	H	0.181847	-8.27957	0.78773	-0.13912