SUPPORTING INFORMATION

Evaluation of (Z)-5-(Azulen-1-Ylmethylene)-2-Thioxothiazolidin-4-Ones Properties Using Quantum Mechanical Calculations

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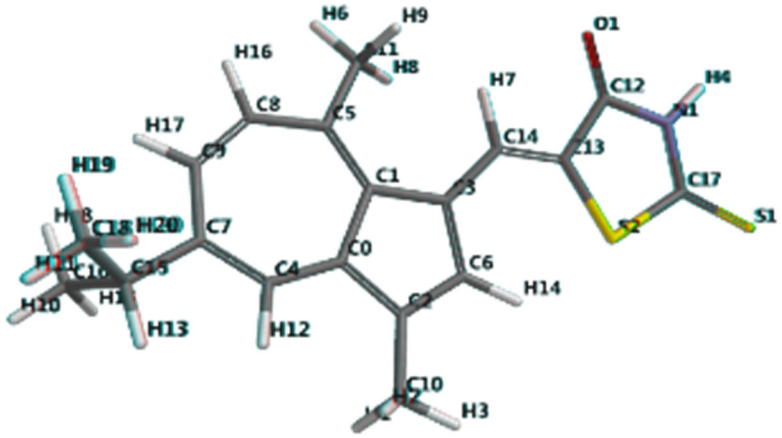
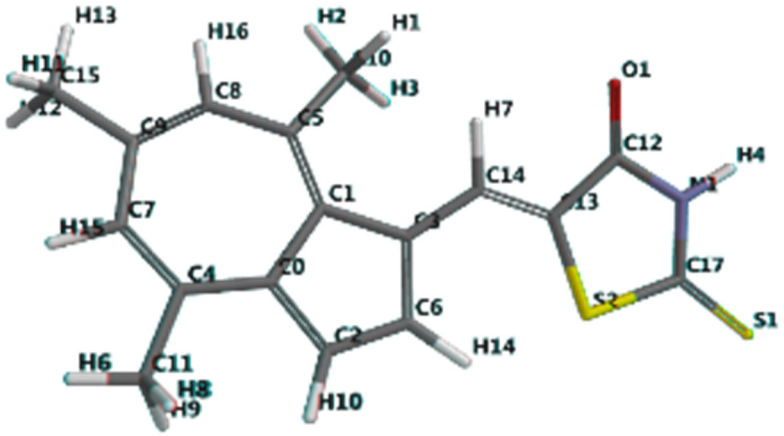
T1



T2



T3

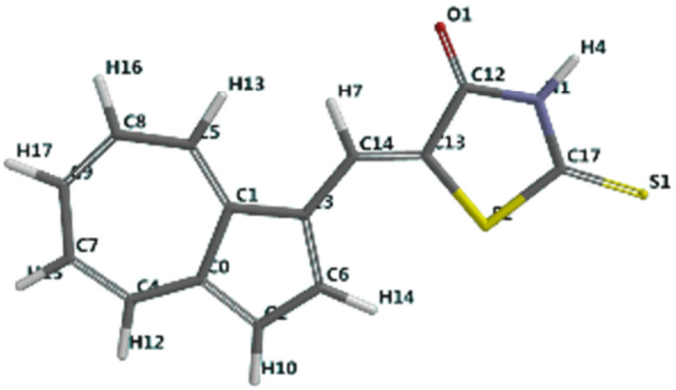


Figure S1. Atomic numbering scheme for the optimized geometries of **T1**-**T3**.

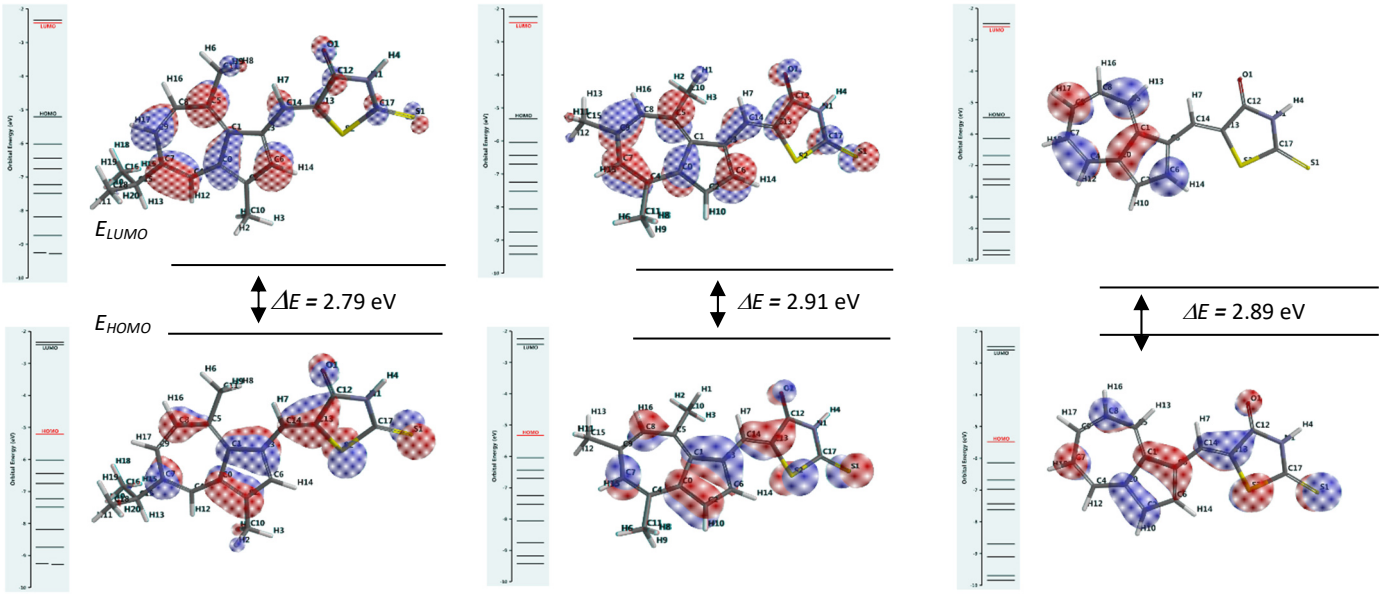


Figure S2. HOMO (down) and LUMO (up) frontier molecular orbitals and their energy gaps for **T1** - **T3** calculated using B3LYP/6-31+G (d,p).

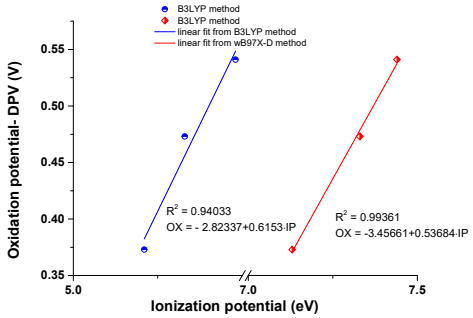


Figure S3. Correlation between ionization potentials calculated using B3LYP/6-31G (d,p) (blue line) or wB97X-D/6-311++G (d,p) (red line) density functional models and experimental oxidation potentials.

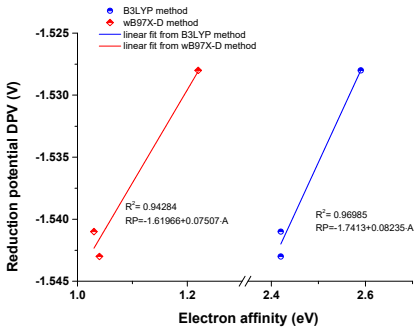


Figure S4. Correlation between electron affinity calculated using B3LYP/6-31G (d,p) (blue line) or wB97X-D/6-311++G (d,p) (red line) density functional models and experimental reduction potentials.

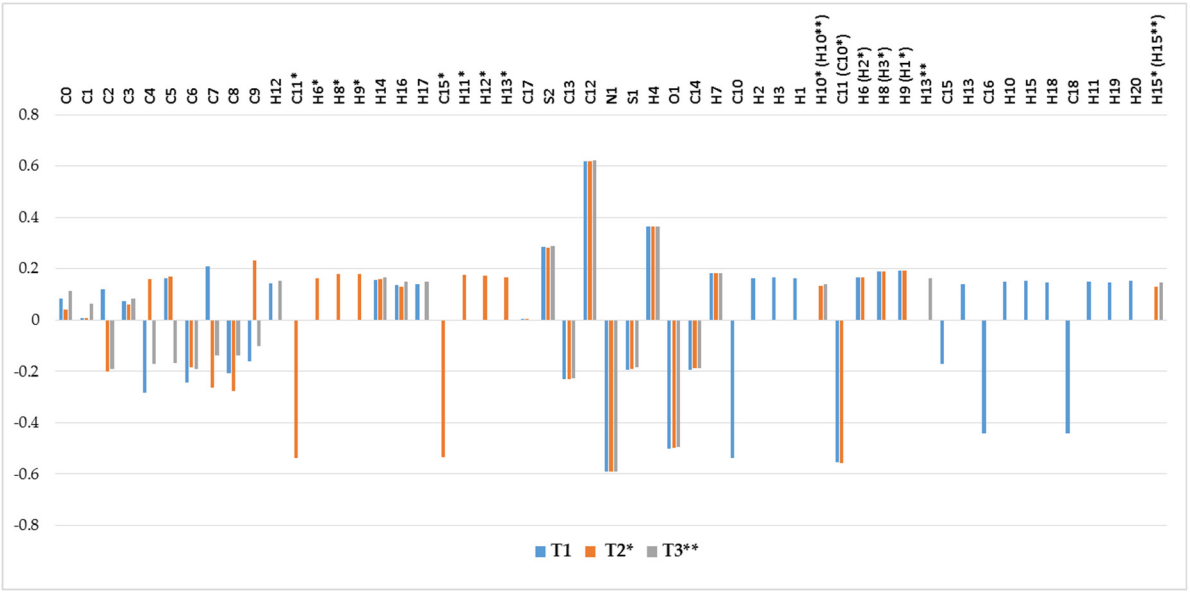


Figure S5. Mulliken population diagram for **T1**-**T3** (using B3LYP/6-31G(d) functional)**.**

Table S1. Atom labelling and predicted bond lengths (*Å*) for **T1** - **T3** compounds (using B3LYP/6-31G(d) functional).

T1		**T2**	**T3**
Cycle of 7 atoms (I)			
C5-C1	1.409	1.407	1.390
C5-C8	1.411	1.411	1.400
C8-C9	1.393	1.394	1.396
C9-C7	1.398	1.403	1.398
C7-C4	1.399	1.393	1.396
C4-C0	1.392	1.412	1.393
C0-C1	1.493	1.492	1.484
Substituents (methyl and isopropyl) of cycle I			
C5-C11: 1.519		C5-C10: 1.520	-
C7-C15: 1.530		C9-C15: 1.518	-
C15-C18: 1.541		C4-C11: 1.518	-
C15-C16: 1.541		-	-
Cycle of 5 atoms (II)			
C1-C3	1.438	1.446	1.433
C3-C6	1.428	1.419	1.425
C6-C2	1.381	1.385	1.388
C2-C0	1.426	1.411	1.413
Substituents of cycle II			
C2-C10: 1.502		-	**-**
Chain between cycle II and cycle III			
C3-C14	1.431	1.435	1.428
C14-C13	1.364	1.362	1.361
Cycle III			
C13-S2	1.777	1.777	1.775
S2-C17	1.777	1.777	1.778
C17-N1	1.366	1.366	1.366
N1-C12	1.406	1.405	1.405
C12-C13	1.475	1.476	1.476
Functional groups (C=O and C=S) of cycle III			
C12-O1	1.220	1.220	1.219
C17-S1	1.648	1.647	1.646

Table S2. Angles and dihedral angles (°) prediction for **T1** - **T3** optimized conformers (using B3LYP/6-31G(d) functional).

T1	**T2**	**T3**
Dihedral (C11, C5, C1, C3): 1.95	Dihedral (C10, C5, C1, C3): 2.81	Dihedral (H13, C5, C1, C3): -0.06
Dihedral (H7, C14, C3, C1): 10.08	Dihedral (H7, C14, C3, C1): 16.73	Dihedral (H7, C14, C3, C1): 0.11
Dihedral (H7, C14, C13, C12): -0.10	Dihedral (H7, C14, C13, C12): 0.10	Dihedral (H7, C14, C13, C12): -0.11
Dihedral (O1, C12, C13, C14): 1.33	Dihedral (O1, C12, C13, C14): 2.11	Dihedral (O1, C12, C13, C14): 0.20
Dihedral (O1, C12, N1, H4): 0.21	Dihedral (O1, C12, N1, H4): 0.05	Dihedral (O1, C12, N1, H4): 0.01
Dihedral (H4, N1, C17, S1): 0.06	Dihedral (C6, C3, C14, C13): 19.84	Dihedral (H4, N1, C17, S1): -0.01
Dihedral (C6, C3, C14, C13): 12.27	Dihedral (H14, C6, C3, C14): -1.71	Dihedral (C6, C3, C14, C13): 0.09
Dihedral (H14, C6, C3, C14): -1.67	Dihedral (S1, C17, N1, H4): 0.22	Dihedral (H14, C6, C3, C14): 0.09
Dihedral (C3, C14, C13, S2): 3.56	Dihedral (C11, C4, C0, C2): -0.37	Dihedral (C3, C14, C13, S2): -0.04
Dihedral (C10, C2, C6, H14): -1.37	Dihedral (C11, C4, C7, H15): 0.92	Dihedral (S1, C17, N1, H4): -0.01
Dihedral (C10, C2, C0, C4): 0.88	Dihedral (C15, C9, C8, H16): -1.99	Angle (S2, C17, S1): 124.84
Dihedral (C11, C5, C1, C3): 1.95	Dihedral (C15, C9, C7, H15): 0.73	Angle (C14, C13, S2):129.50
Dihedral (C11, C5, C8, H16): -1.11	Dihedral (C10, C5, C8, H16): -1.97	Angle (H4, N1, C17): 120.09
Dihedral (C15, C7, C9, H17): -0.48	Dihedral (C10, C5, C1, C3): 2.81	Angle (H4, N1, C12): 120.13
Dihedral (C15, C7, C4, H12): 1.21	Angle (O1, C12, N1): 123.16	Angle (O1, C12, N1): 123.26
Angle (O1, C12, N1): 123.06	Angle (O1, C12, C13): 127.92	Angle (O1, C12, C13): 127.88
Angle (O1, C12, C13): 127.97	Angle (C10, C5, C1): 120.68	Angle (H13, C5, C1): 116.10
Angle (C11, C5, C1): 120.65	Angle (C10, C5, C8): 113.08	Angle (H13, C5, C8):114.65
Angle (C11, C5, C8): 113.55	Angle (H7, C14, C3): 118.79	Angle (H7, C14, C3): 117.25
Angle (H7, C14, C3): 118.46	Angle (H7, C14, C13):111.30	Angle (H7, C14, C13): 119.97
Angle (H7, C14, C13): 110.83	Angle (C12, C13, C14): 119.95	Angle (C12, C13, C14): 120.33
Angle (C12, C13, C14): 119.49	Angle (C11, C4, C0): 117.20	Angle (H12, C4, C0): 115.10
Angle (H12, C4, C0): 113.97	Angle (C11, C4, C7): 116.07	Angle (H12, C4, C7): 115.75
Angle (H12, C4, C7):114.75	Angle (C0, C2, H10): 125.70	Angle (C0, C2, H10): 124.94
Angle (C0, C2, C10): 126.60	Angle (H15, C7, C9): 114.58	Angle (H15, C7, C9): 115.85
Angle (C15, C7, C9): 118.48	Angle (H15, C7, C4): 115.15	Angle (H15, C7, C4): 115.77
Angle (C15, C7, C4): 118.00	Angle (C15, C9, C8): 117.27	Angle (H17, C9, C8): 115.28
Angle (H17, C9, C8): 113.69	Angle (C15, C9, C7): 115.59	Angle (H17, C9, C7):115.33
Angle (C7, C9, H17):115.41	Angle (C9, C8, H16): 113.64	Angle (C9, C8, H16): 115.64
Angle (C9, C8, H16): 113.19	Angle (H16, C8, C5): 113.55	Angle (H16, C8, C5): 115.32
Angle (H16, C8, C5): 113.71	Angle (C8, C5, C10): 113.07	Angle (H10, C2, C6): 126.13
Angle (C8, C5, C11): 113.55	Angle (H10, C2, C6): 125.10	Angle (H10, C2, C0):124.94
Angle (C11, C5, C1): 120.95	Angle (H10, C2, C0): 125.70	Angle (C2, C6, H14): 124.37
Angle (C10, C2, C6): 125.84	Angle (C2, C6, H14): 124.47	Angle (H14, C6, C3): 125.23
Angle (C2, C6, H14): 123.61	Angle (H14, C6, C3): 124.90	Angle (C3, C14, C13): 130.77
Angle (H14, C6, C3): 124.70	Angle (C3, C14, C13): 129.88	
Angle (C3, C14, C13): 130.68		

Table S3. Mulliken charges for **T1**-**T3** (using B3LYP/6-31G(d) functional).

Atom labelling	**T1**	**T2***	**T3****
C0	+0.083	+0.041	+0.113
C1	+0.006	+0.009	+0.063
C2	**+0.119**	**-0.201**	**-0.190**
C3	+0.072	+0.060	+0.083
C4	-0.282	**+0.158**	**-0.171**
C5	**+0.161**	**+0.168**	**-0.169**
C6	-0.242	-0.183	-0.192
C7	**+0.208**	**-0.264**	**-0.137**
C8	-0.207	-0.277	-0.138
C9	-0.161	**+0.233**	-0.102
H12	+0.142	-	+0.152
C11*	-	-0.538	-
H6*	-	+0.163	-
H8*	-	+0.178	-
H9*	-	+0.178	-
H14	+0.157	+0.160	+0.166
H16	+0.135	+0.129	+0.149
H17	+0.141	-	+0.151
C15*	-	-0.535	-
H11*	-	+0.175	-
H12*	-	+0.174	-
H13*	-	+0.166	-
C17	+0.001	+0.004	-0.000
S2	**+0.284**	**+0.283**	**+0.289**
C13	-0.231	-0.230	-0.227
C12	+0.619	+0.619	+0.621
N1	-0.591	-0.591	-0.591
S1	**-0.193**	**-0.190**	**-0.183**
H4	+0.363	+0.363	+0.364
O1	-0.501	-0.498	-0.494
C14	-0.195	-0.188	-0.187
H7	+0.181	+0.183	+0.181
C10	-0.539	-	-
H2	+0.162	-	-
H3	+0.167	-	-
H1	+0.162	-	-
H10* (H10**)	-	+0.133	+0.140
C11 (C10*)	-0.554	-0.556	0
H6 (H2*)	+0.165	+0.166	0
H8 (H3*)	+0.189	+0.190	0
H9 (H1*)	+0.193	+0.191	0
H13**	-	-	+0.163
C15	-0.170	-	-
H13	+0.139	-	-
C16	-0.441	-	-
H10	+0.150	-	-
H15	+0.154	-	-
H18	+0.146	-	-
C18	-0.442	-	-
H11	+0.150	-	-
H19	+0.146	-	-
H20	+0.154	-	-
H15* (H15**)	-	+0.129	+0.147