Supplementary Materials

Antioxidant properties of ethenyl indole: A DPPH assay and TDDFT studies

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List of supporting Table

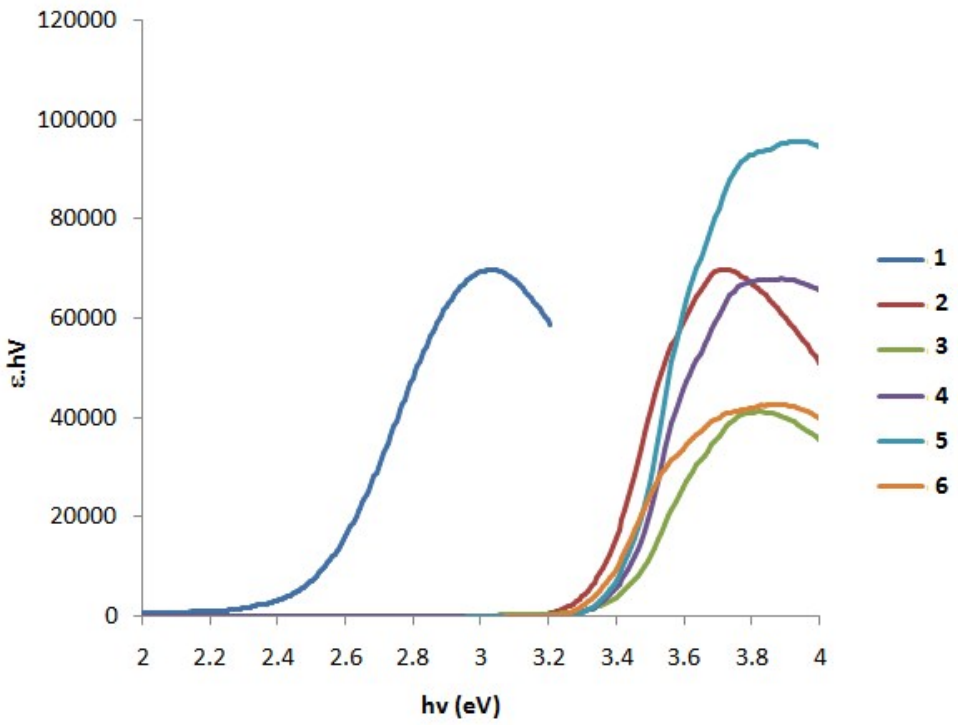


Figure S7. Experimentally determined optical band gap of ethenyls **1**-**6** in methanol using Tauc plot, εhv *vs*. hv**.**

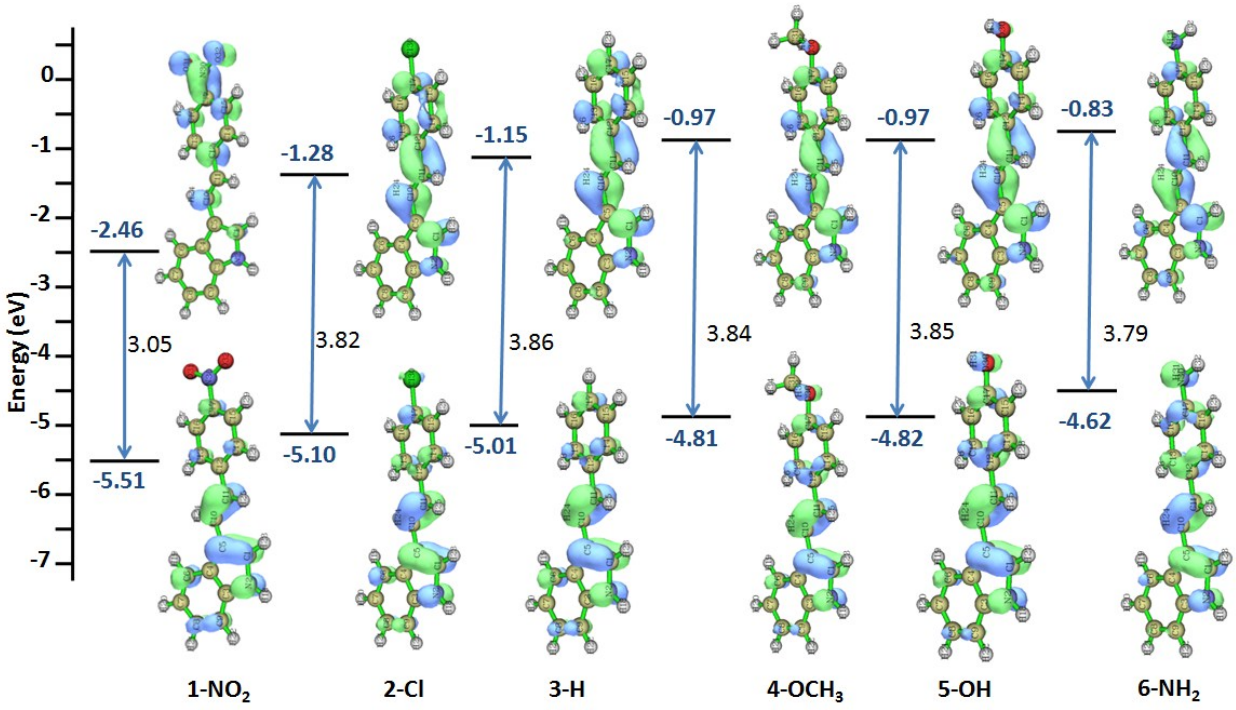


Figure S8. TDDFT computed HOMO-LUMO energy of ethenyls **1-6.**

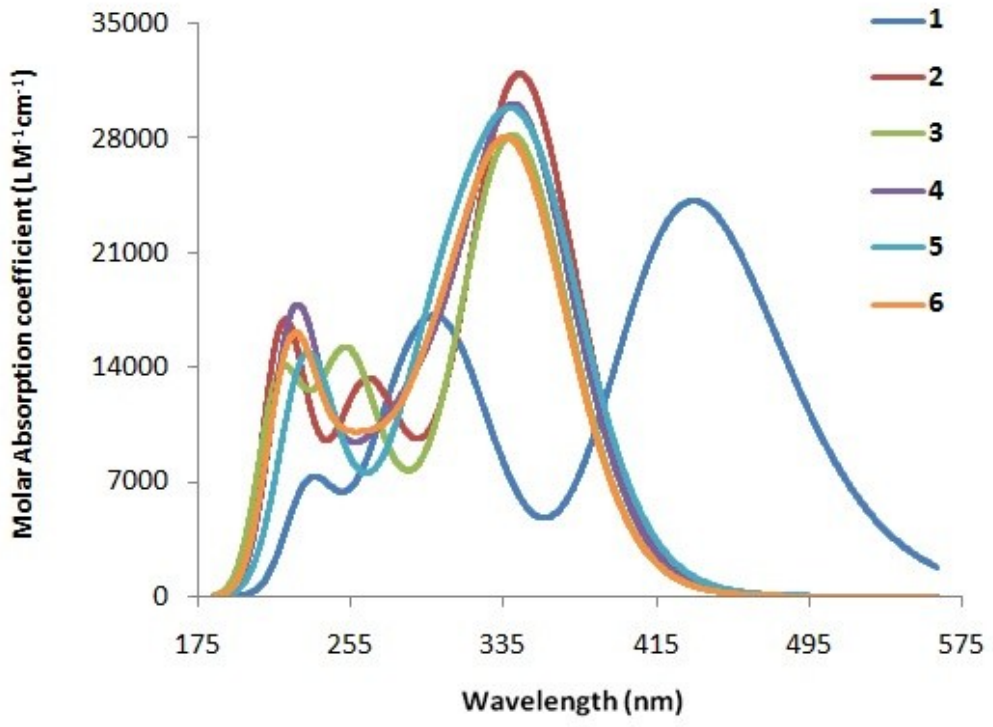


Figure S9. TDDFT computed UV-Vis absorption spectra of ethenyls **1-6.**

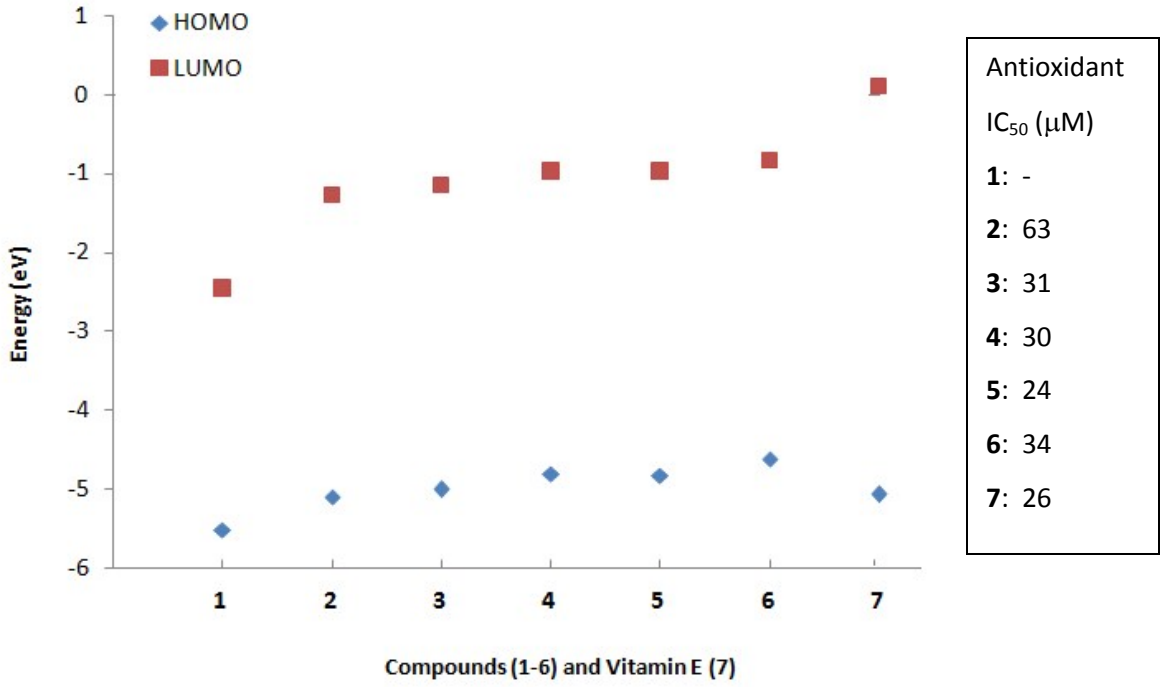


Figure S10. HOMO and LUMO energy of **1-6** and vitamin E (**7**).

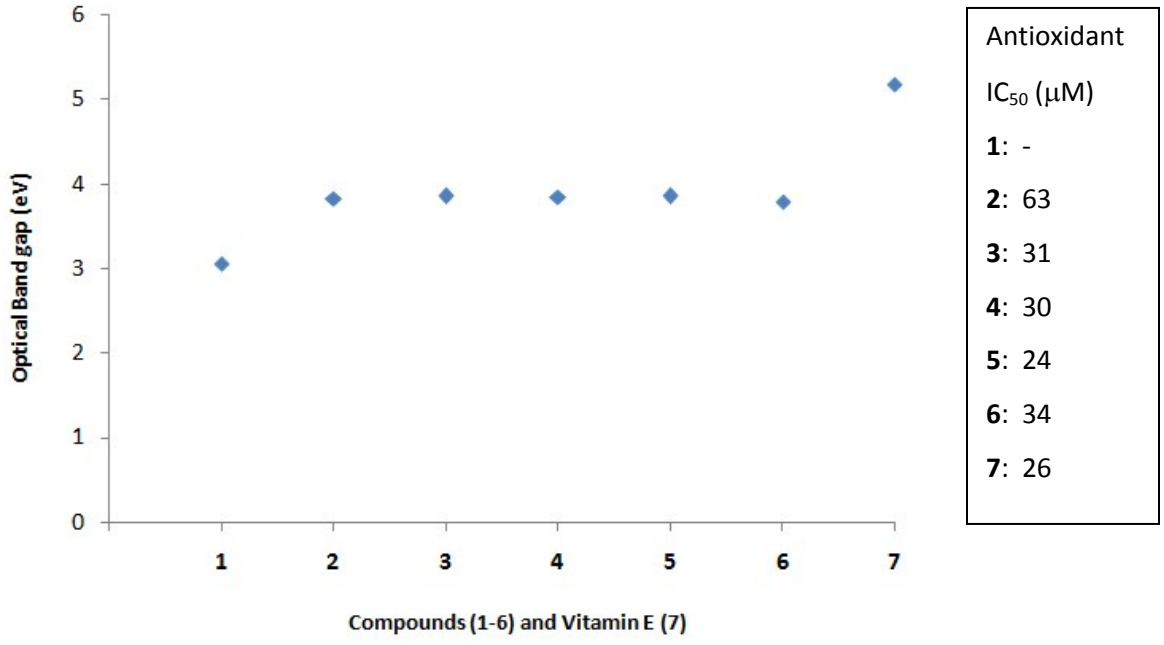


Figure S11. Optical band gap of **1-6** and vitamin E (**7**).

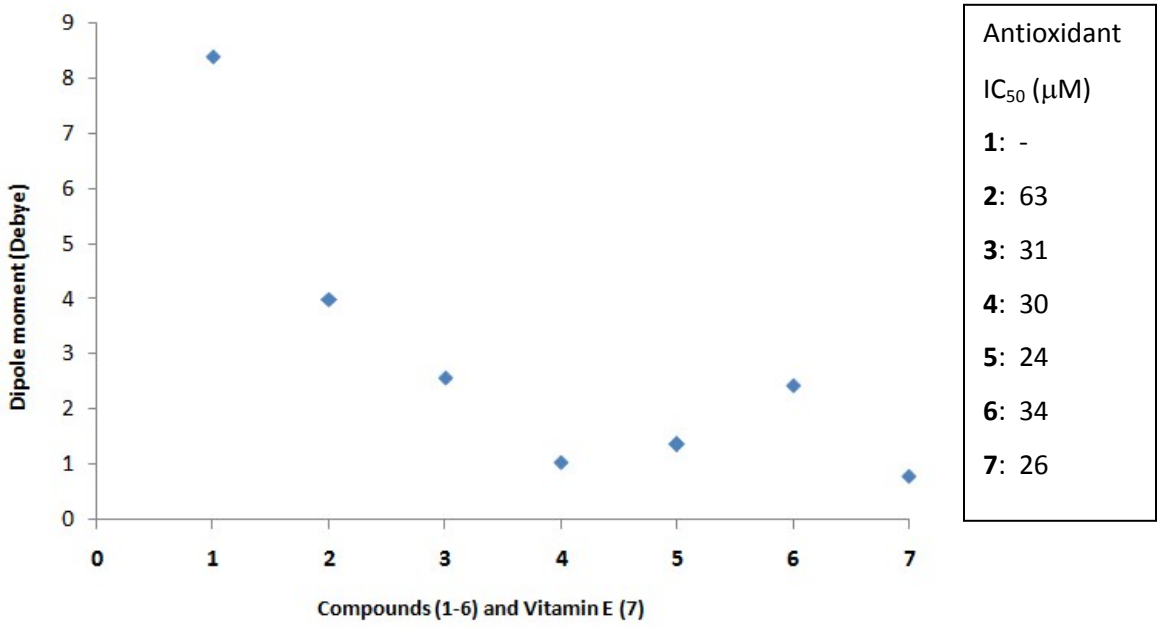
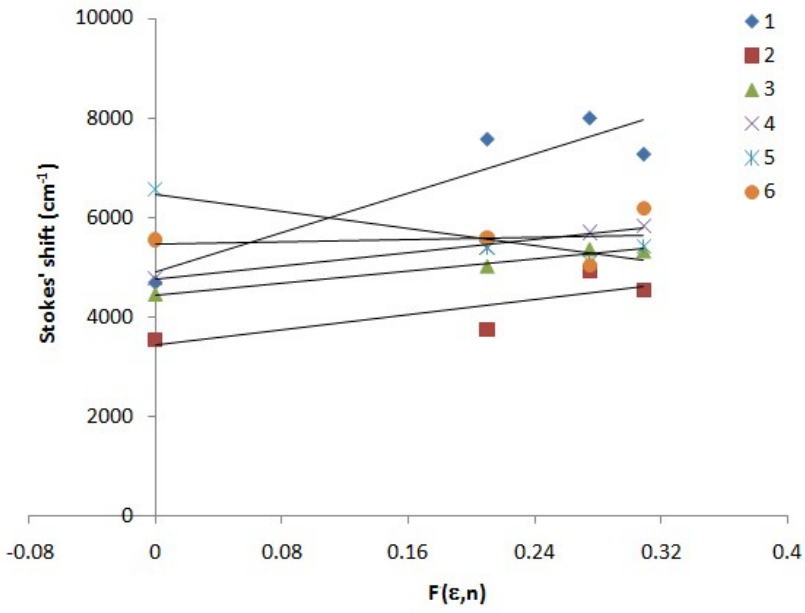


Figure S12. Ground state dipole moment of **1-6** and vitamin E (**7**).



Comp	Slope	R^2	Δμ (Debye)
1	10170	0.92	15.25
2	3743	0.86	9.07
3	3087	0.98	7.99
4	3352	0.99	8.81
5	-4362	0.99	9.66
6	1772	0.85	6.20

Figure S13. Lippert-Mataga plot, Stokes' shift vs. solvent polarity parameter

Change of excited state dipole moment is calculated from the absorption and fluorescence spectral data of the compound using Lippert-Mataga equation [Ref N Mataga, Y Kaifu, M Koizumi Solvent effects upon fluorescence spectra and the dipole moments of excited molecules, Bull Chem Soc Jpn 1956, 29, 465–470, E Lippert Spectroscopic determination of dipole moment of aromatic compounds in the first excited singlet state. Z Elektrochem 1957, 61, 962–975]

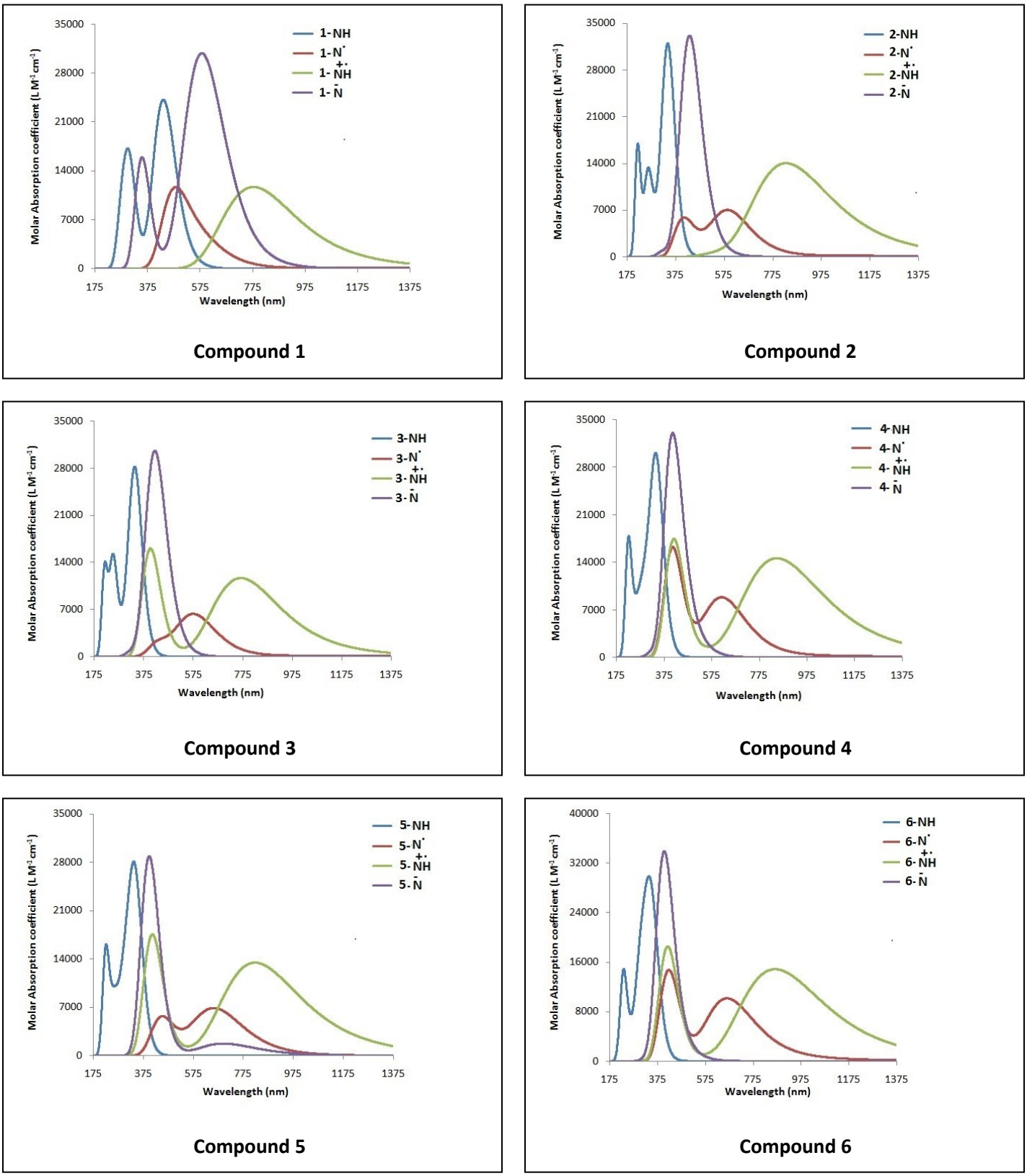
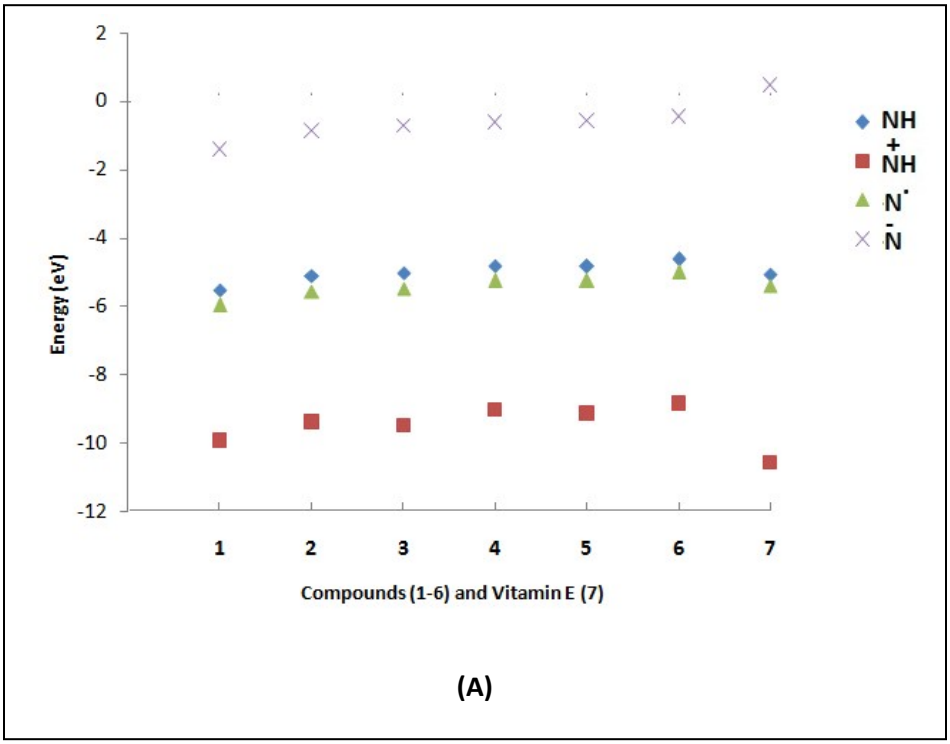


Figure S14. TDDFT computed UV-Visible absorption spectra of neutral (NH), cationic radical ($NH^{+\cdot}$), radical ((NH·) and anion (N-) of compound **1-6.**



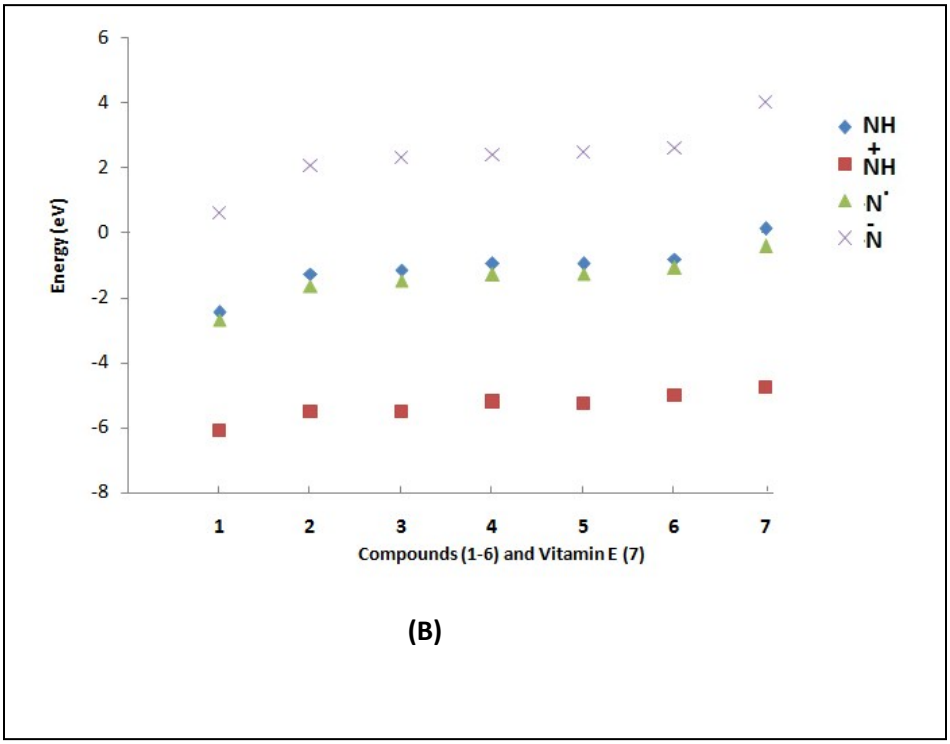
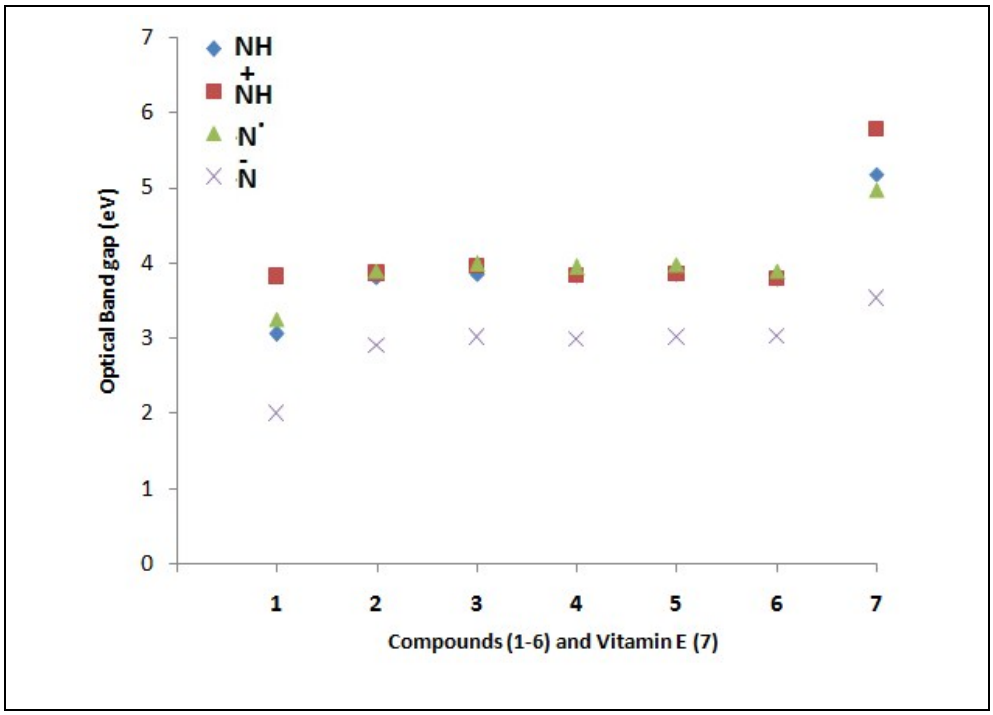


Figure S15. A correlation plot of (A) HOMO energy and (B) LUMO energy of neutral (NH), cationic radical ($NH^{+\cdot}$), radical ($NH^{\cdot}$) and anion (N-) of compound **1-6** and vitamin E (**7**).



Antioxidant IC_{50} (μM)
1: -
2: 63
3: 31
4: 30
5: 24
6: 34
7: 26

Figure S16. A correlation plot of optical band gap of neutral (NH), cationic radical ($NH^{+\cdot}$), radical ($NH^{\cdot}$) and anion (N-) of compound **1-6** and vitamin E (**7**).

Table S1. TDDFT computed absorption wavelength, energy of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), ground state dipole moment and optical band gap of indolic ethenyls (**1-6**).

Compound	λ_{abs} (nm) S_o-S_1	μ_g (Debye)	HOMO (eV)	LUMO (eV)	Band Gap (eV)
Vitamin E	274.0	0.80	-5.06	0.10	5.17
1	434.3	8.39	-5.51	-2.46	3.05
2	343.4	3.99	-5.10	-1.28	3.82
3	339.4	2.57	-5.01	-1.15	3.86
4	339.8	1.05	-4.81	-0.97	3.84
5	336.2	1.37	-4.82	-0.97	3.85
6	338.6	2.44	-4.62	-0.83	3.79

Table S2. Absorption and fluorescence wavelength and optical band gap in methanol of compound **1-6**.

Compounds	λ_{abs} (nm)	λ_{em} (nm)	λ_{ex} (nm)	Band Gap[a] (nm)(eV)	Band Gap[b] (eV)	IC_{50} (μM)
1	413	590	423	518 (2.39)	2.37	-
2	335	395	346	370 (3.35)	3.24	63
3	327	396	349	367 (3.37)	3.31	31
4	327	404	344	369 (3.36)	3.30	30
5	322	390	328	363 (3.41)	3.30	24
6	324	405	339	370 (3.35)	3.24	34

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a: using intersection of absorption and fluorescence spectra

b**:** using Tauc plot