Supporting information

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Transient species of esculetin produced in pulse radiolysis: experimental and quantum chemical investigations

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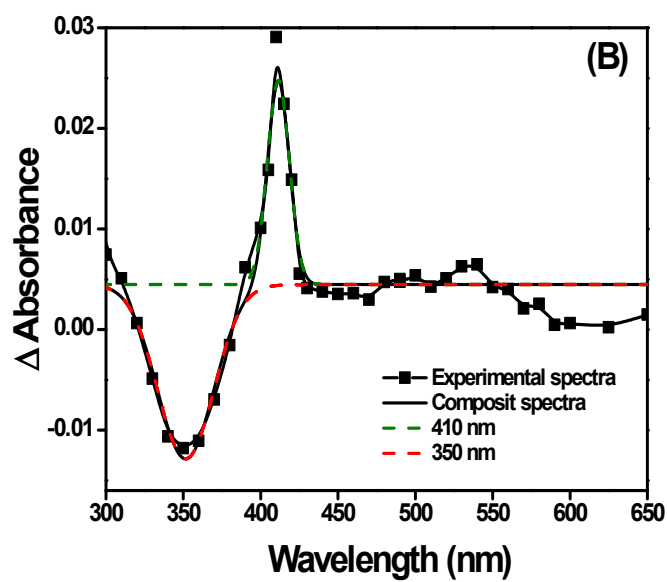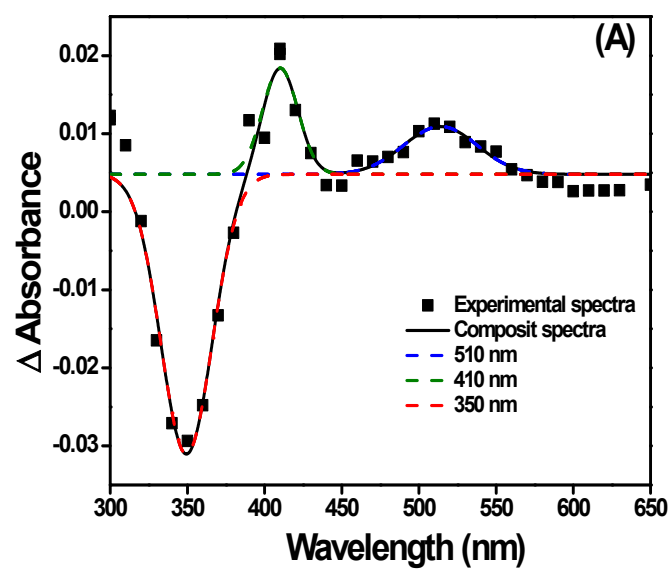Corresponding author's email: atanu@barc.gov.in

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Figure S1 *Deconvolution of the transient spectra obtained during the reaction of **E** with •OH radical (**A**) and with N₃• radical (**B**) after 20 μs of pulse.*
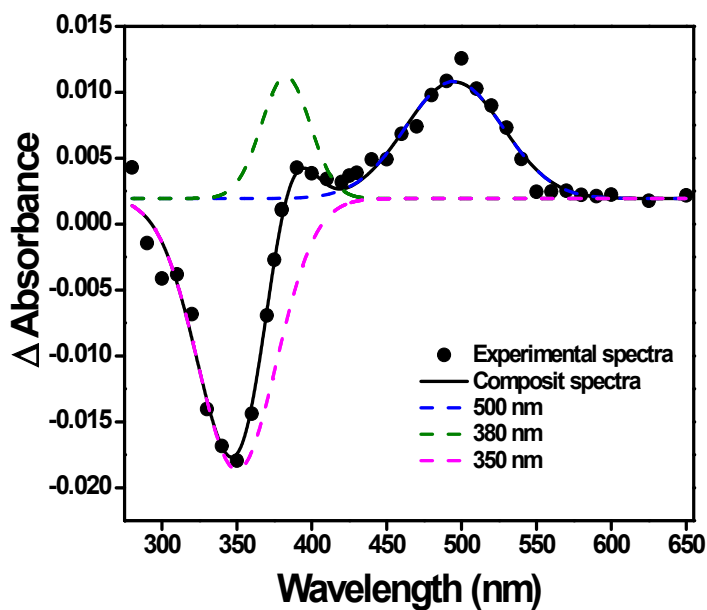
Figure S2. *Deconvolution of the transient spectra obtained during the reaction of **E** with H• atom after 20 μs of pulse.*
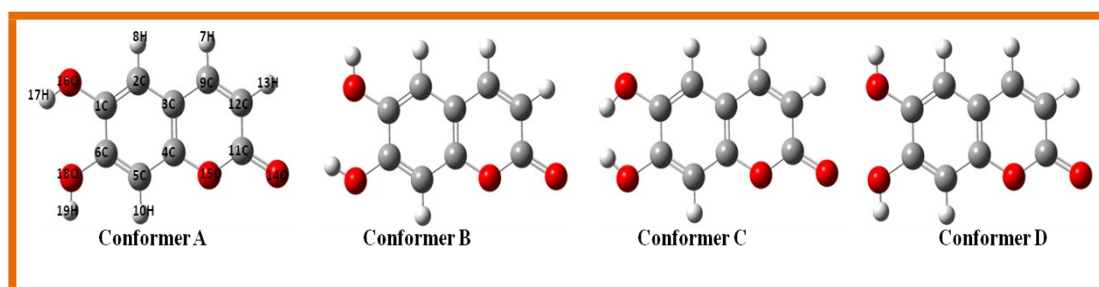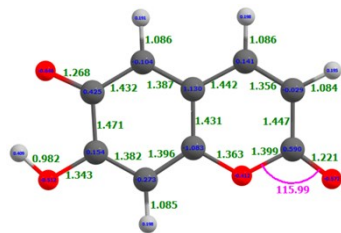

Figure S3 *Possible ground state conformers of **E** used for energy optimization.*
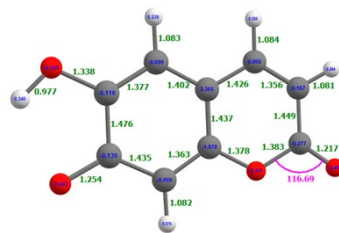
Table ST1. *Energy calculation of the conformers of **E** using B3LYP/6-311++G(d,p) basis set in water phase.*

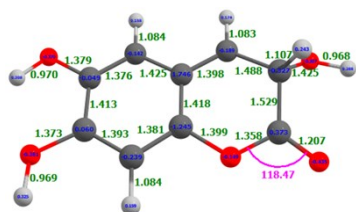| Conformer	E_0 (Hartree)	ΔE_0 (kcal/mol)
A	-647.2222	0.00
B	-647.2219	[#]0.21
C	-647.2211	[#]0.67
D	-647.2195	[#]1.68

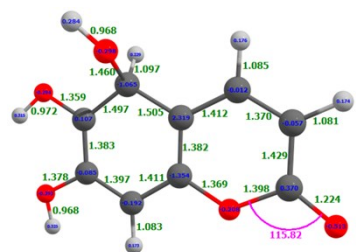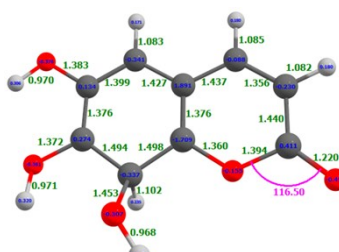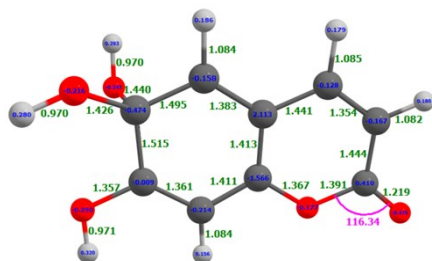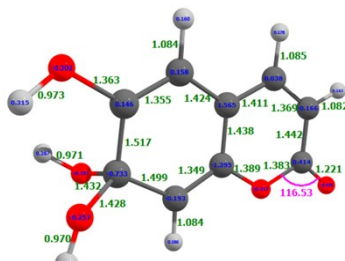# ΔE_0 was calculated with respect to the conformer A
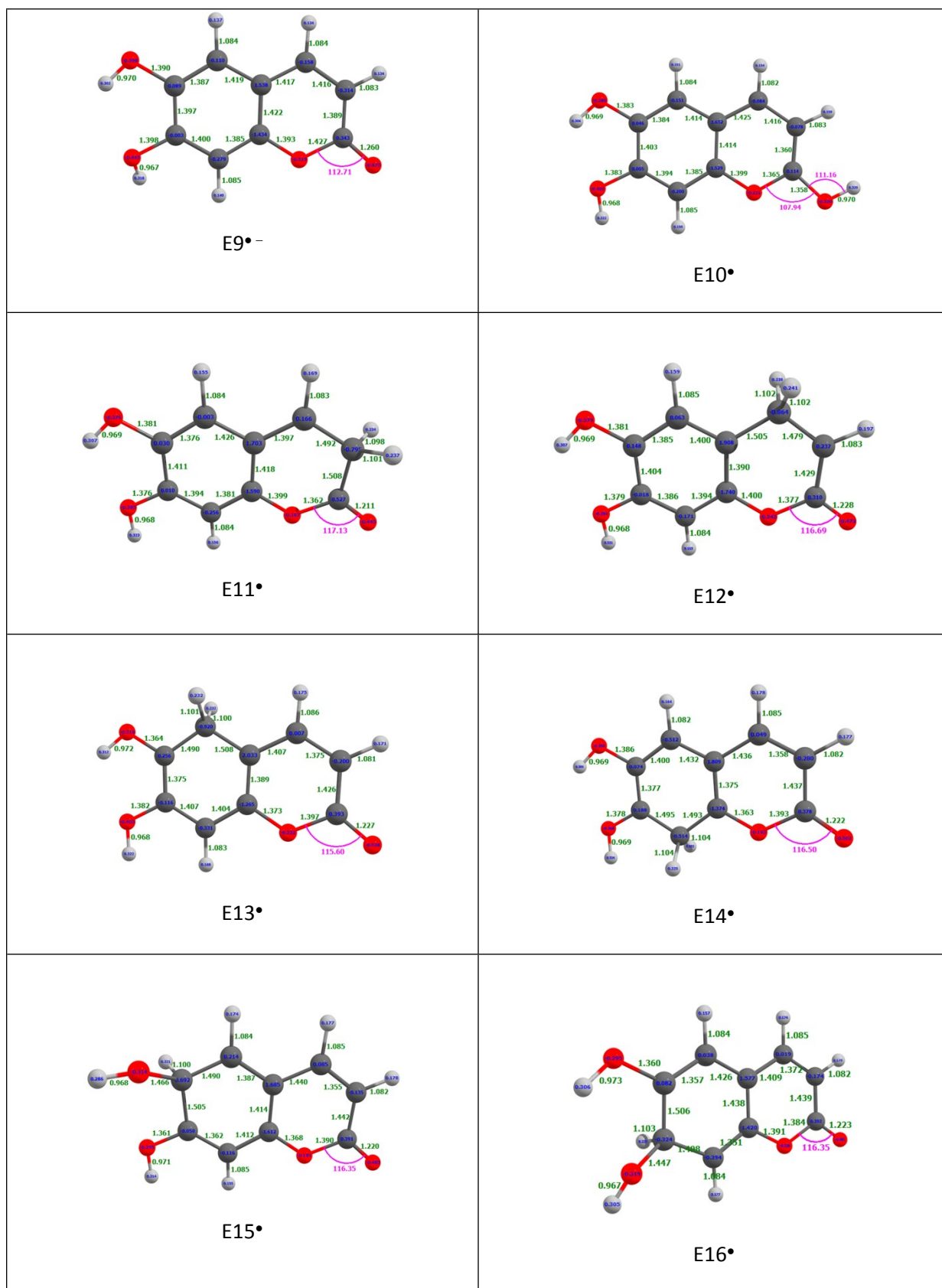
E1•

E2•

E3•
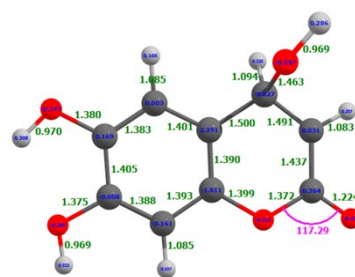
E4•

E5•

E6•

E7•

E8•

Figure S4. *Optimized structures of different transients of* **E** *with atomic charges, bond length and bond angles.*