Supporting Information (SI)

Substitution effects on the antiradical activity of hydralazine: a DFT analysis

Houssem Boulebd[1,*], Nguyen Minh Tam[2,3] Adam Mechler[4] and Quan V. Vo[5,6*]

[1]Laboratory of Synthesis of Molecules with Biological Interest, University of Frères Mentouri Constantine 1, Constantine, Algeria.
[2]Computational Chemistry Research Group, Ton Duc Thang University, Ho Chi Minh City, Vietnam.
[3]Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam
[4]Department of Chemistry and Physics, La Trobe University, Victoria 3086, Australia
[5]Institute of Research and Development, Duy Tan University, Danang 550000, Vietnam
[6]The University of Danang - University of Technology and Education, 48 Cao Thang, Danang 550000, Vietnam.
*Corresponding authors: boulebd.houssem@umc.edu.dz; vovanquan2@duytan.edu.vn; vvquan@ute.udn.vn

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Table S1. The method to calculate rate constant following the conventional transition state theory

The rate constant (k) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):[1-5]

$$k = \sigma\kappa \frac{k_B T}{h} e^{-(\Delta G^{\neq})/RT} \quad (1)$$

Where: σ is the reaction symmetry number ,[6, 7]

κ contains the tunneling corrections calculated using the Eckart barrier,[8]

k_B is the Boltzmann constant,

h is the Planck constant,

$\Delta G^{\neq}$ is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.[9-12] The free energy of reaction $\Delta G^{\neq}$ for the SET pathway was computed following the equations (2,3).

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{SET}^{0}}{\lambda}\right)^2 \quad (2)$$

$$\lambda \approx \Delta E_{SET} - \Delta G_{SET}^{0} \quad (3)$$

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{SET} is the non-adiabatic energy difference between reactants and vertical products for SET.[13, 14]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[15]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[16] the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).[15, 17]

$$k_{app} = \frac{k_{TST} k_D}{k_{TST} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

where R_{AB} is the reaction distance, N_A is the Avogadro constant, and $D_{AB} = D_A + D_B$ (D_{AB} is the mutual diffusion coefficient of the reactants A and B),[16, 18] where D_A or D_B is estimated using the Stokes–Einstein formulation (6).[19, 20]

$$D_{A\ or\ B} = \frac{k_B T}{6\pi\eta a_{A\ or\ B}} \quad (6)$$

η is the viscosity of the solvents (i.e. $\eta(H_2O) = 8.91\times10^{-4}$ Pa s, η(pentyl ethanoate) = 8.62×10^{-4} Pa s) and a is the radius of the solute.

The kinetic study requires different considerations. Water (dielectric constants, $\varepsilon = 78.35$) and pentyl ethanoate ($\varepsilon = 4.73$) are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body.[15, 21-23] Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno,[24] adjusted with the free volume theory according to the Benson correction[15, 25-27] to reduce over-penalizing entropy losses in solution. For the species that have multiple conformers, all of these were investigated and the conformer with the lowest electronic energy was included in the analysis.[22, 23] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy.[23, 28] All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex.

Table S2: Relative bond dissociation enthalpies (ΔBDEs) of monosubstituted hydralazine (compared with HZ, BDE(N9–H)= 69.9 kcal/mol and BDE(N10–H)= 79.7 kcal/mol)[29] calculated in the gas-phase.

R	Substitution position						
	4	**5**	**6**	**7**	**8**	**10**	
	N9–H	N9–H	N9–H	N9–H	N9–H	N9–H	N10–H
NO_2	0.3	-1.0	-0.9	-0.5	0.7	19.1	10.4
CN	0.1	-0.8	-0.5	-0.4	1.2	2.4	0.4
CF_3	0.3	-0.5	-0.6	-0.4	0.0	5.1	11.2
COOH	0.4	-0.4	-0.8	-1.2	-5.0	-0.3	14.4
COOMe	0.4	-0.4	-0.1	0.0	-1.9	1.7	8.6
F	-0.4	-0.1	-0.3	-0.3	3.9	9.8	3.8
Cl	-0.2	-0.3	-0.2	-0.4	2.2	7.3	5.1
Br	-0.1	-0.3	-0.3	-0.4	1.8	6.4	6.3
Ethinyl	-0.2	-0.3	-0.2	-0.1	4.0	-1.2	-2.9
Ethenyl	-0.1	0.0	0.0	-0.1	1.3	-5.5	-3.0
Ethanyl	-0.2	0.2	0.1	0.0	-1.0	-1.9	4.1
Ph	-0.3	-0.1	0.0	0.0	3.1	-5.8	-1.8
OMe	-0.7	0.2	0.1	0.2	7.0	3.5	-2.9

Table S3: Relative ionization potentials (IPs) of monosubstituted hydralazine (compared with HZ, IP= 176.9 kcal/mol)[29] calculated in the gas-phase.

R	Substitution position					
	4	**5**	**6**	**7**	**8**	**10**
NO_2	11.5	8.4	8.9	8.5	-1.6	22.2
CN	9.6	7.3	7.9	7.8	-0.3	17.2
CF_3	7.7	5.5	5.9	5.7	-1.7	15.7
COOH	4.4	7.2	6.5	7.6	0.1	21.8
COOMe	2.5	1.1	1.7	1.9	-2.2	1.9
F	3.0	3.0	3.2	2.6	-0.9	21.4
Cl	3.0	2.8	13.3	2.5	-2.8	12.4
Br	2.9	2.7	2.9	2.4	-3.7	10.2
Ethinyl	0.1	0.5	0.8	0.6	-4.8	-1.2
Ethenyl	-4.1	-1.4	-1.4	7.5	-4.3	-10.1
Ethanyl	-3.5	-2.0	-2.3	-2.8	-4.5	-9.2
Ph	-4.6	-2.7	7.4	-2.5	-9.2	-12.9
OMe	-6.3	-3.5	-2.3	-4.2	-8.2	0.8

Table S4: Relative ionization potentials (IPs) of monosubstituted hydralazine (compared with phenol, IP= 196.9 kcal/mol) calculated in the gas-phase.

R	Substitution position					
	4	**5**	**6**	**7**	**8**	**10**
NO_2	-8.5	-11.6	-11.1	-11.5	-21.6	2.1
CN	-10.5	-12.7	-12.1	-12.2	-20.3	-2.8
CF_3	-12.3	-14.5	-14.1	-14.3	-21.7	-4.3
COOH	-15.6	-12.8	-13.5	-12.4	-19.9	1.8
COOMe	-17.5	-18.9	-18.3	-18.2	-22.2	-18.1
F	-17.0	-17.0	-16.8	-17.4	-20.9	1.4
Cl	-17.0	-17.2	-6.7	-17.5	-22.8	-7.6
Br	-17.1	-17.3	-17.1	-17.6	-23.7	-9.2
Ethinyl	-19.9	-19.5	-19.2	-19.4	-24.8	-21.3
Ethenyl	-24.1	-21.4	-21.4	-12.5	-24.3	-30.1
Ethanyl	-23.5	-22.1	-22.3	-22.9	-24.5	-29.2
Ph	-24.6	-22.7	-12.6	-22.5	-29.2	-32.9
OMe	-26.3	-23.6	-22.3	-24.2	-28.2	-19.3

Table S5: The Cartesian coordinates and energies of TS of the reaction between selected compounds with HOO• at the M06-2X/6-311++G(d,p) calculating method following the FHT mechanism

Name				**TS-10-Ete-HZ-N9-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	2.69927200	1.91812500	-0.65886300	Zero-point correction= 0.204072 (Hartree/Particle)
C	3.82069700	1.11728500	-0.35990100	Thermal correction to Energy= 0.218748
C	3.65940500	-0.19460800	0.01531500	Thermal correction to Enthalpy= 0.219692
C	2.36211000	-0.73926700	0.10275100	Thermal correction to Gibbs Free Energy= 0.160363
C	1.24833700	0.06115800	-0.19468400	Sum of electronic and zero-point Energies= -756.602135
C	1.42555400	1.40475800	-0.58165200	Sum of electronic and thermal Energies= -756.587459
C	2.10485300	-2.09165900	0.48817400	Sum of electronic and thermal Enthalpies= -756.586515
N	0.91746600	-2.61002700	0.58131900	Sum of electronic and thermal Free Energies= -756.645844
N	-0.16434600	-1.84590300	0.29872900	
C	-0.02295200	-0.60024300	-0.07391000	
N	-1.17169000	0.11568500	-0.39280200	
N	-2.34491000	-0.48894900	-0.03623400	
C	-3.46433200	-0.29217200	-0.83605000	
C	-4.56752900	-1.03651800	-0.76751100	
H	2.84478500	2.95028500	-0.95337100	
H	4.81404600	1.54413500	-0.42832400	
H	4.51490900	-0.81905400	0.24688800	
H	0.57141100	2.02935500	-0.81371000	
H	2.93139100	-2.75332100	0.72972400	
H	-1.13332800	1.13250100	0.00166900	
H	-2.20665400	-1.39392000	0.40942200	
H	-3.37419200	0.55979800	-1.49923700	
H	-5.41429500	-0.80329700	-1.39553900	
H	-4.64703500	-1.88127000	-0.09351800	
O	-2.68961400	2.07297600	1.07180300	
H	-2.79887500	1.63188400	1.92789300	
O	-1.35417200	2.21778500	0.91682300	

Name				**TS-10-Ete-HZ-N10-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	-3.15039400	-1.51995800	-0.84573500	Zero-point correction= 0.202986 (Hartree/Particle)
C	-4.02341700	-0.62115100	-0.19886400	Thermal correction to Energy= 0.217564
C	-3.53577000	0.52850100	0.37241500	Thermal correction to Enthalpy= 0.218508
C	-2.15348700	0.80381500	0.32089500	Thermal correction to Gibbs Free Energy= 0.158950
C	-1.28209200	-0.10076900	-0.30591900	Sum of electronic and zero-point Energies= -756.590551
C	-1.79986900	-1.26844400	-0.90457700	Sum of electronic and thermal Energies= -756.575973
C	-1.57296400	1.99115400	0.86112000	Sum of electronic and thermal Enthalpies= -756.575029
N	-0.30594400	2.27043800	0.80418600	Sum of electronic and thermal Free Energies= -756.634588
N	0.55082600	1.38568400	0.23924000	
C	0.10690700	0.27342800	-0.27190200	
N	1.03735500	-0.59665500	-0.85662700	
N	2.38942200	-0.42088300	-0.65915200	
C	2.93137200	0.75875500	-1.15100900	
C	4.16596800	1.16354700	-0.83446100	
H	-3.55155900	-2.41462800	-1.30623700	
H	-5.08371900	-0.83996400	-0.16253600	
H	-4.19848900	1.23321600	0.86203900	
H	-1.15012100	-1.95859200	-1.42846600	
H	-2.20291100	2.73238200	1.34404600	
H	0.80365300	-1.57436100	-0.74819800	
H	2.64928200	-0.65357500	0.39387100	
H	2.30002400	1.31218900	-1.83565000	

H	4.56757600	2.06825400	-1.26643600
H	4.77391200	0.61729200	-0.12316100
O	1.87719100	-2.34968300	1.33251300
H	2.61939000	-2.96306700	1.23214000
O	2.45453800	-1.16063000	1.67914600

Name	**TS-10-Ph-HZ-N9-H-OOH** (gas)
Cartesian Coordinates	Frequency and Energy

C	-3.48918400	-2.01732300	-0.70529700	Zero-point correction= 0.252485 (Hartree/Particle)
C	-4.65939600	-1.23096400	-0.67833300	Thermal correction to Energy= 0.269376
C	-4.58650300	0.11779000	-0.42653000	Thermal correction to Enthalpy= 0.270320
C	-3.33143500	0.71547400	-0.19185100	Thermal correction to Gibbs Free Energy= 0.205191
C	-2.16927300	-0.07058200	-0.21813600	Sum of electronic and zero-point Energies= -910.187466
C	-2.25548300	-1.45245500	-0.48041900	Sum of electronic and thermal Energies= -910.170575
C	-3.16593900	2.10956900	0.07891600	Sum of electronic and thermal Enthalpies= -910.169630
N	-2.01960400	2.67771300	0.30257800	Sum of electronic and thermal Free Energies= -910.234760
N	-0.89199600	1.92755900	0.28266000	
C	-0.94723100	0.64524800	0.03134600	
N	0.25088400	-0.05781500	-0.01905000	
N	1.33372300	0.62404000	0.45257500	
H	-3.56506900	-3.07896200	-0.90632500	
H	-5.61986700	-1.69838000	-0.85902100	
H	-5.48003300	0.73144100	-0.40458100	
H	-1.36297400	-2.06595100	-0.50468300	
H	-4.03311500	2.76249700	0.11068200	
H	0.17620900	-1.02570200	0.47546400	
H	1.11092500	1.57726500	0.72993300	
O	1.38481300	-1.61915200	2.13943200	
H	1.11862200	-1.14991400	2.94435900	
O	0.22633900	-1.98917700	1.55043200	
C	2.59949200	0.35512200	-0.06887900	
C	3.64240300	1.23586300	0.23628100	
C	2.84926000	-0.78335200	-0.83695400	
C	4.92131500	0.97997700	-0.23276600	
H	3.44163300	2.11618800	0.83743000	
C	4.13726000	-1.02606700	-1.29712600	
H	2.04178800	-1.46516300	-1.06852300	
C	5.17877200	-0.15273600	-1.00171600	
H	5.72202200	1.67085400	0.00293000	
H	4.32607700	-1.91060500	-1.89387300	
H	6.17916900	-0.35079200	-1.36526900	

Name	**TS-10-Ph-HZ-N9-H-OOH** (water)
Cartesian Coordinates	Frequency and Energy

C	-3.29573700	-2.30759800	-0.19626800	Zero-point correction= 0.252186 (Hartree/Particle)
C	-4.52830100	-1.62868700	-0.09718300	Thermal correction to Energy= 0.269146
C	-4.56830500	-0.25446400	-0.08881700	Thermal correction to Enthalpy= 0.270090
C	-3.36355100	0.47219100	-0.17441200	Thermal correction to Gibbs Free Energy= 0.204872
C	-2.13725200	-0.20487800	-0.26360100	Sum of electronic and zero-point Energies= -910.217157
C	-2.10983500	-1.61351700	-0.27979300	Sum of electronic and thermal Energies= -910.200196
C	-3.32131600	1.89817800	-0.18970000	Sum of electronic and thermal Enthalpies= -910.199252
N	-2.22428900	2.59100000	-0.27536700	Sum of electronic and thermal Free Energies= -910.264471
N	-1.02486200	1.94763200	-0.34014700	
C	-0.97780200	0.64177700	-0.33847900	
N	0.26910100	0.02439000	-0.43131500	
N	1.33694100	0.86585800	-0.33663000	
H	-3.28508100	-3.39085100	-0.20991800	
H	-5.44660900	-2.19969900	-0.03231600	

H	-5.50752900	0.28239000	-0.01972000
H	-1.17142900	-2.14810500	-0.36435600
H	-4.24515700	2.46438500	-0.13145500
H	0.35169700	-0.74718800	0.31467500
H	1.19497800	1.70459800	0.22455200
O	1.03325500	0.08791900	2.31310500
H	0.26181700	0.60395400	2.60531200
O	0.53398800	-1.07050400	1.82107300
C	2.61167300	0.31539800	-0.36499500
C	3.68733900	1.11682400	0.04462800
C	2.83871000	-0.99553600	-0.79635100
C	4.97479600	0.60783200	0.01409800
H	3.49671400	2.12884000	0.38581800
C	4.13991300	-1.49035700	-0.81726300
H	2.01312600	-1.61706800	-1.11862600
C	5.21128000	-0.69965600	-0.41651200
H	5.80070600	1.23280400	0.33309800
H	4.31103200	-2.50669600	-1.15253600
H	6.21988800	-1.09388100	-0.43584300

Name	**TS-10-Ph-HZ-N9-H-OOH** (pentyl ethanoate)
Cartesian Coordinates	Frequency and Energy

C	-3.47534400	-2.02686100	-0.71767500
C	-4.64760000	-1.24391200	-0.68950300
C	-4.57806600	0.10694800	-0.44322500
C	-3.32342800	0.70548000	-0.21073400
C	-2.15902700	-0.07829600	-0.22820200
C	-2.24164100	-1.45943600	-0.49287000
C	-3.16283300	2.10402500	0.03844800
N	-2.01507800	2.67523000	0.24735600
N	-0.88184100	1.92603400	0.24802300
C	-0.93701200	0.63931900	0.02467500
N	0.25587500	-0.07472500	0.01051700
N	1.34863100	0.60423600	0.44988300
H	-3.54831700	-3.08821600	-0.92323600
H	-5.60693600	-1.71471600	-0.86913900
H	-5.47156900	0.72112300	-0.42662700
H	-1.34844700	-2.07154100	-0.53119900
H	-4.03306200	2.75341000	0.05780700
H	0.17018200	-1.02191200	0.54227800
H	1.15950100	1.53502300	0.81270000
O	1.32258400	-1.46531800	2.32178100
H	0.98658200	-0.91785000	3.05104500
O	0.22128600	-1.92756900	1.68816700
C	2.60321800	0.33085200	-0.08517400
C	3.66949600	1.16687700	0.26988000
C	2.82243600	-0.76560600	-0.92355800
C	4.94050600	0.90647700	-0.21784900
H	3.48871000	2.01304900	0.92441700
C	4.10499900	-1.01334800	-1.40020300
H	1.99747700	-1.40934800	-1.20088300
C	5.16894100	-0.18600800	-1.05435200
H	5.75950000	1.56112700	0.05730900
H	4.27008200	-1.86425800	-2.05130100
H	6.16436600	-0.38729000	-1.43116100

Zero-point correction= 0.251847 (Hartree/Particle)
Thermal correction to Energy= 0.268839
Thermal correction to Enthalpy= 0.269784
Thermal correction to Gibbs Free Energy= 0.204473
Sum of electronic and zero-point Energies= -910.216653
Sum of electronic and thermal Energies= -910.199661
Sum of electronic and thermal Enthalpies= -910.198717
Sum of electronic and thermal Free Energies= -910.264027

Name	**TS-10-Ph-HZ-N10-H-OOH**
Cartesian Coordinates	Frequency and Energy

C	3.99532200	0.01791000	-1.61058200
C	4.73200500	-0.63473300	-0.59989700
C	4.11359500	-1.04206100	0.55655300
C	2.73699500	-0.79337800	0.73844200
C	2.00977000	-0.12346100	-0.25811200
C	2.65328100	0.26990100	-1.45062500
C	2.00912000	-1.21559100	1.89121500
N	0.73632800	-1.01680600	2.06085700
N	0.03371900	-0.33389100	1.12485500
C	0.62314500	0.09486000	0.04746500
N	-0.15132600	0.79826000	-0.89496200
N	-1.45318800	1.13099200	-0.61050900
C	-2.35715500	0.07600000	-0.46960700
C	-3.55856500	0.33922200	0.19962600
C	-4.52509600	-0.64800100	0.29858700
C	-4.31418000	-1.90141900	-0.27211700
C	-3.12021400	-2.15790100	-0.94130500
C	-2.13915800	-1.18288800	-1.03988200
H	4.49371600	0.31547300	-2.52523400
H	5.78888000	-0.82159300	-0.74676300
H	4.66659700	-1.55723000	1.33394900
H	2.09443600	0.74643700	-2.24669400
H	2.51728500	-1.75002000	2.68859400
H	0.32643700	1.60135700	-1.28431000
H	-1.47884000	1.88218700	0.23078600
H	-3.70954800	1.31313900	0.65191700
H	-5.44743900	-0.44030200	0.82762900
H	-5.07150500	-2.67140000	-0.19311700
H	-2.94962100	-3.12956300	-1.38958000
H	-1.21228200	-1.37974200	-1.56332200
O	-0.26238300	3.53733400	0.18966800
H	-0.85875800	4.18850400	-0.20641800
O	-1.04652700	2.84543000	1.07562200

Zero-point correction=	0.250996 (Hartree/Particle)
Thermal correction to Energy=	0.267809
Thermal correction to Enthalpy=	0.268754
Thermal correction to Gibbs Free Energy=	0.203727
Sum of electronic and zero-point Energies=	-910.175527
Sum of electronic and thermal Energies=	-910.158714
Sum of electronic and thermal Enthalpies=	-910.157769
Sum of electronic and thermal Free Energies=	-910.222796

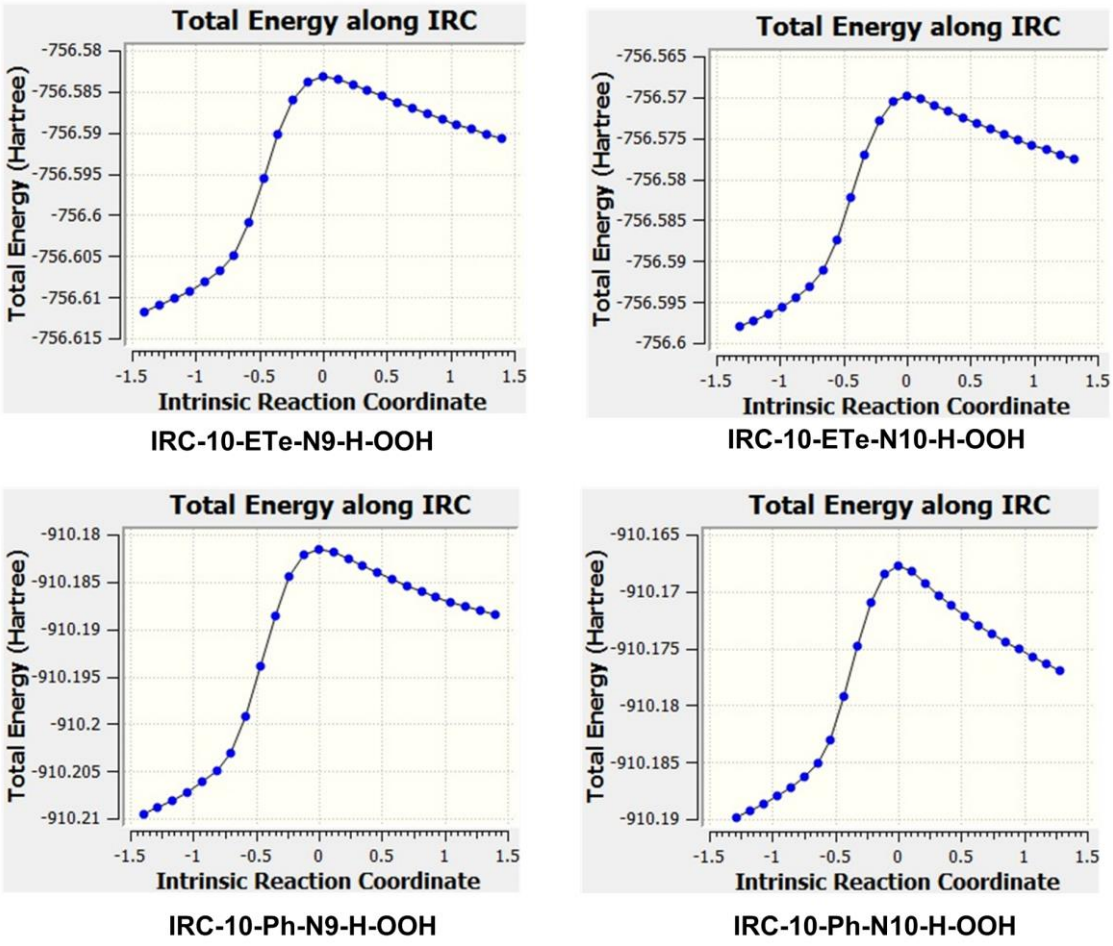

Figure S1. IRC plots for the transition states related to the reaction of HOO• radical with the selected HZs .

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