Understanding the regio- and diastereoselective synthesis of a potent antinociceptive isoxazolidine from *C*-(pyridin-3-yl)-*N*-phenyl nitrone in the light of molecular electron density theory

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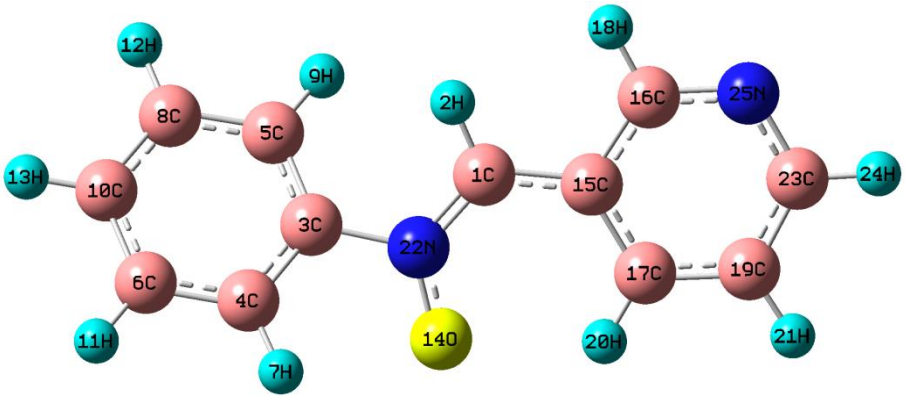

Fig. S1- B3LYP/6-311G(d,p) calculated Optimized geometry of **1**

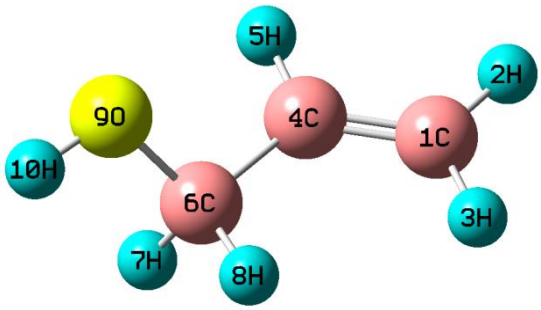

Fig. S2 - B3LYP/6-311G(d,p) calculated Optimized geometry of **2**

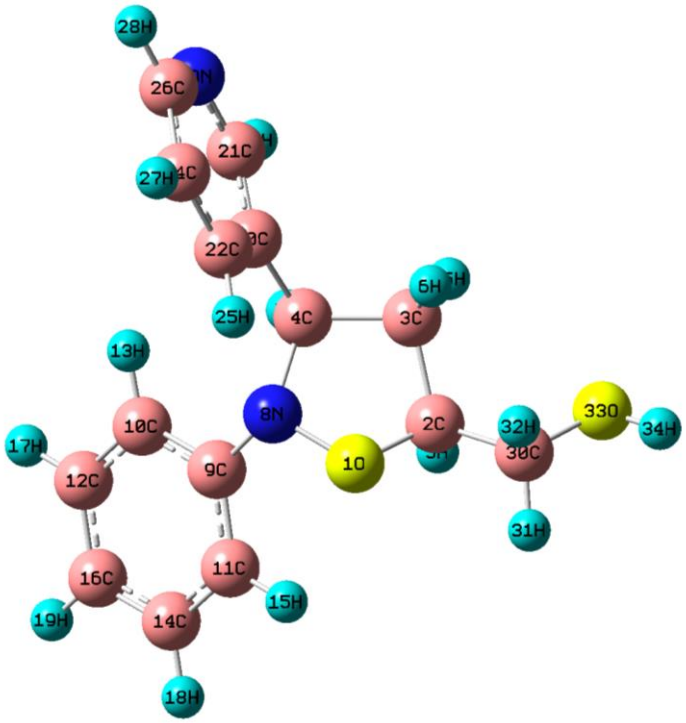

Fig. S3 - B3LYP/6-311G(d,p) calculated Optimized geometry of **CAox**

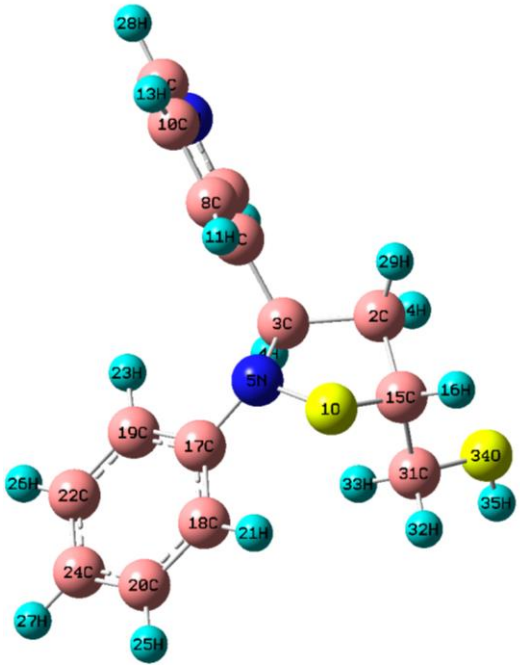

Fig. S4 - B3LYP/6-311G(d,p) calculated Optimized geometry of CAon

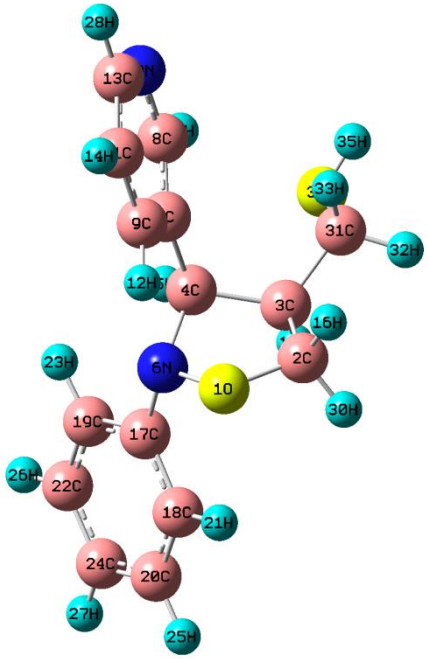

Fig. S5 - B3LYP/6-311G(d,p) calculated Optimized geometry of CAmx

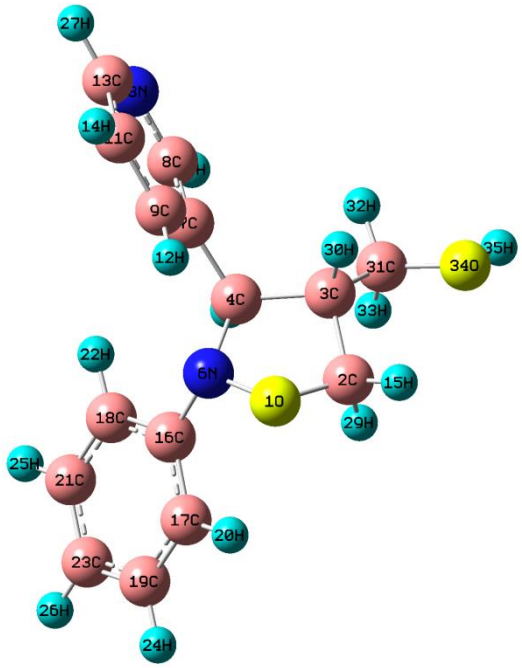

Fig. S6 - B3LYP/6-311G(d,p) calculated Optimized geometry of CAmn

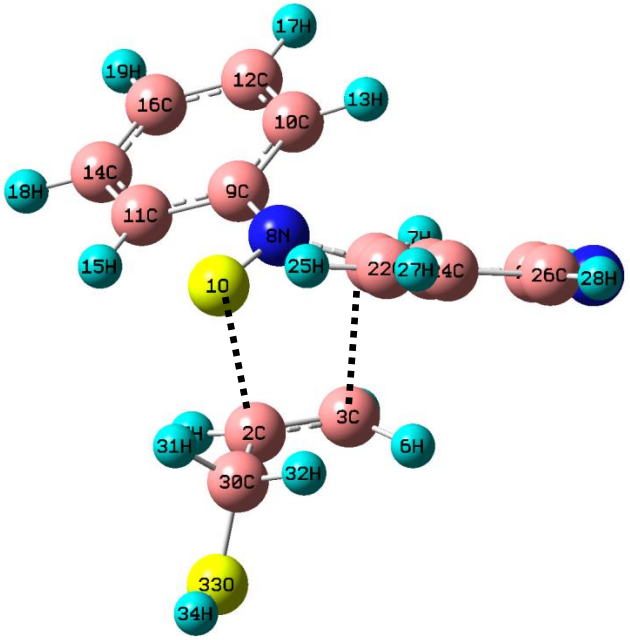

Fig. S7 - B3LYP/6-311G(d,p) calculated Optimized geometry of TSox

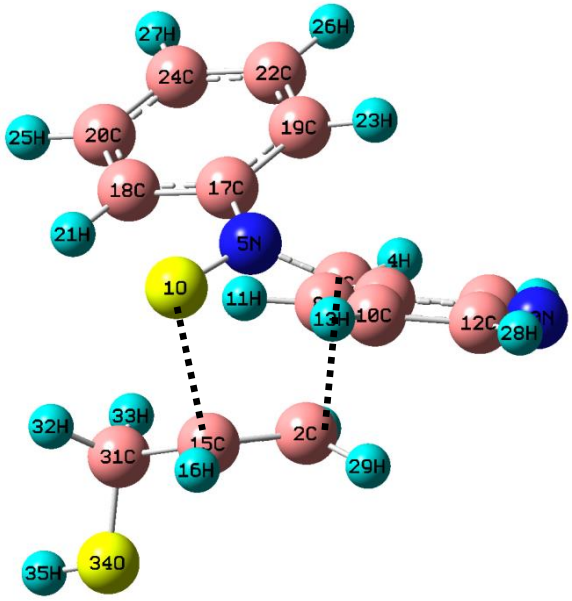

Fig. S8 - B3LYP/6-311G(d,p) calculated Optimized geometry of TSon

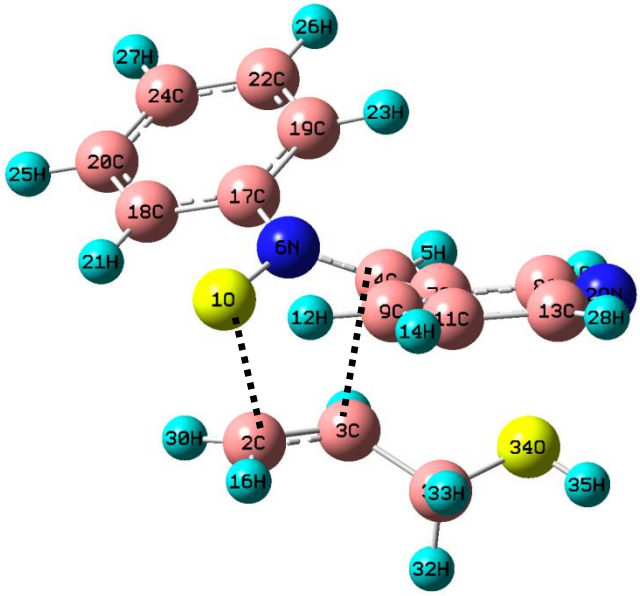

Fig. S9 - B3LYP/6-311G(d,p) calculated Optimized geometry of **TSmx**

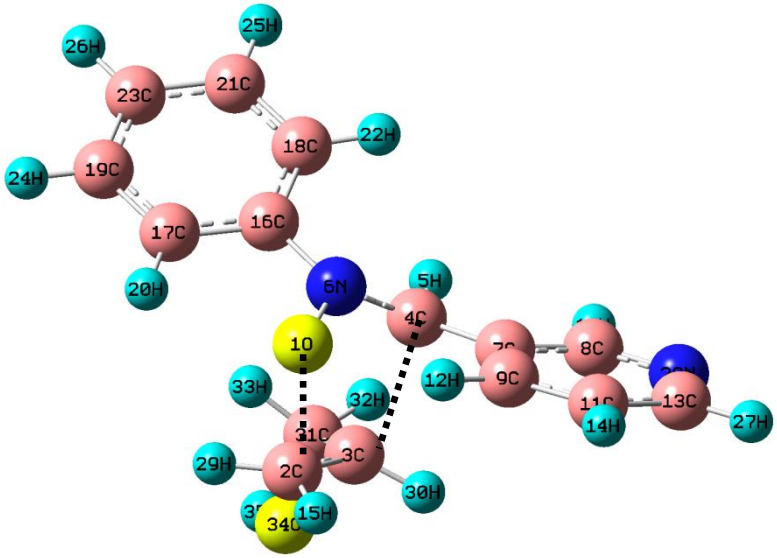

Fig. S10 - B3LYP/6-311G(d,p) calculated Optimized geometry of **TSmn**

Table S1 : B3LYP/6-311G(d,p) calculated total energies of **1**

E(RB+HF-LYP)	-648.112015191 A.U.
Zero-point correction=	0.195476 Hartree/Particle)
Thermal correction to Energy=	0.207040
Thermal correction to Enthalpy=	0.207984
Thermal correction to Gibbs Free Energy=	0.156565
Sum of electronic and zero-point Energies=	-647.916539
Sum of electronic and thermal Energies=	-647.904975
Sum of electronic and thermal Enthalpies=	-647.904031
Sum of electronic and thermal Free Energies=	-647.955450

Table S2 : B3LYP/6-311G(d,p) calculated total energies of **2**

E(RB+HF-LYP)	-193.172620669 A.U.
Zero-point correction=	0.084534 (Hartree/Particle)
Thermal correction to Energy=	0.089613
Thermal correction to Enthalpy=	0.090557
Thermal correction to Gibbs Free Energy=	0.057258
Sum of electronic and zero-point Energies=	-193.088087
Sum of electronic and thermal Energies=	-193.083008
Sum of electronic and thermal Enthalpies=	-193.082064
Sum of electronic and thermal Free Energies=	-193.115363

Table S3 : B3LYP/6-311G(d,p) calculated total energies of **CAox**

E(RB+HF-LYP)	-841.315703960 A.U
Zero-point correction=	0.286112 (Hartree/Particle)
Thermal correction to Energy=	0.302332
Thermal correction to Enthalpy=	0.303277
Thermal correction to Gibbs Free Energy=	0.240118
Sum of electronic and zero-point Energies=	-841.029592
Sum of electronic and thermal Energies=	-841.013372
Sum of electronic and thermal Enthalpies=	-841.012427
Sum of electronic and thermal Free Energies=	-841.075586

Table S4 : B3LYP/6-311G(d,p) calculated total energies of **CAon**

E(RB+HF-LYP)	-841.315289247 A.U.
Zero-point correction=	0.286270 (Hartree/Particle)
Thermal correction to Energy=	0.302420
Thermal correction to Enthalpy=	0.303364
Thermal correction to Gibbs Free Energy=	0.240719
Sum of electronic and zero-point Energies=	-841.029019
Sum of electronic and thermal Energies=	-841.012869
Sum of electronic and thermal Enthalpies=	-841.011925
Sum of electronic and thermal Free Energies=	-841.074570

Table S5 : B3LYP/6-311G(d,p) calculated total energies of **CAmx**

E(RB+HF-LYP)	-841.311621374 A.U.
Zero-point correction=	0.286658 (Hartree/Particle)
Thermal correction to Energy=	0.302687
Thermal correction to Enthalpy=	0.303631
Thermal correction to Gibbs Free Energy=	0.241688
Sum of electronic and zero-point Energies=	-841.024963
Sum of electronic and thermal Energies=	-841.008935
Sum of electronic and thermal Enthalpies=	-841.007990
Sum of electronic and thermal Free Energies=	-841.069934

Table S6 : B3LYP/6-311G(d,p) calculated total energies of **CAmx**

E(RB+HF-LYP)	-841.313379546 A.U.
Zero-point correction=	0.286499 (Hartree/Particle)
Thermal correction to Energy=	0.302575
Thermal correction to Enthalpy=	0.303519
Thermal correction to Gibbs Free Energy=	0.241023
Sum of electronic and zero-point Energies=	-841.026881
Sum of electronic and thermal Energies=	-841.010805
Sum of electronic and thermal Enthalpies=	-841.009860
Sum of electronic and thermal Free Energies=	-841.072357

Table S7 : B3LYP/6-311G(d,p) calculated total energies of **TSox**

E(RB+HF-LYP)	-841.256198482 A.U.
Zero-point correction=	0.282033 (Hartree/Particle)
Thermal correction to Energy=	0.298772
Thermal correction to Enthalpy=	0.299716
Thermal correction to Gibbs Free Energy=	0.236319
Sum of electronic and zero-point Energies=	-840.974166
Sum of electronic and thermal Energies=	-840.957426
Sum of electronic and thermal Enthalpies=	-840.956482
Sum of electronic and thermal Free Energies=	-841.019880

Table S8 : B3LYP/6-311G(d,p) calculated total energies of **TSon**

E(RB+HF-LYP)	-841.253804119 A.U.
Zero-point correction=	0.281991 (Hartree/Particle)
Thermal correction to Energy=	0.298725
Thermal correction to Enthalpy=	0.299669
Thermal correction to Gibbs Free Energy=	0.236427
Sum of electronic and zero-point Energies=	-840.971813
Sum of electronic and thermal Energies=	-840.955079
Sum of electronic and thermal Enthalpies=	-840.954135
Sum of electronic and thermal Free Energies=	-841.017377

Table S10 : B3LYP/6-311G(d,p) calculated total energies of **TSmx**

E(RB+HF-LYP)	-841.255014509 A.U.
Zero-point correction=	0.282365 (Hartree/Particle)
Thermal correction to Energy=	0.298776
Thermal correction to Enthalpy=	0.299720
Thermal correction to Gibbs Free Energy=	0.237783
Sum of electronic and zero-point Energies=	-840.972650
Sum of electronic and thermal Energies=	-840.956238
Sum of electronic and thermal Enthalpies=	-840.955294
Sum of electronic and thermal Free Energies=	-841.017232

Table S10 : B3LYP/6-311G(d,p) calculated total energies of **TSmn**

E(RB+HF-LYP)	-841.252610554 A.U.
Zero-point correction=	0.282064 (Hartree/Particle)
Thermal correction to Energy=	0.298738
Thermal correction to Enthalpy=	0.299682
Thermal correction to Gibbs Free Energy=	0.236587
Sum of electronic and zero-point Energies=	-840.970547
Sum of electronic and thermal Energies=	-840.953872
Sum of electronic and thermal Enthalpies=	-840.952928
Sum of electronic and thermal Free Energies=	-841.016024