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Supplementary material

SUPPLEMENTARY MATERIAL TO

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

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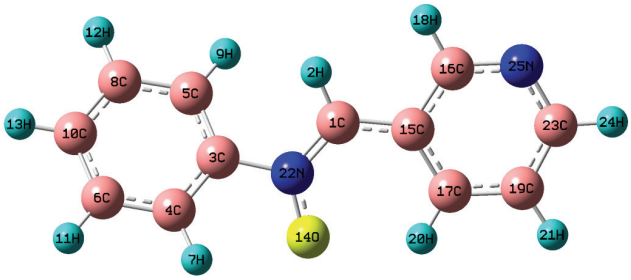

Fig. S-1. B3LYP/6-311G(d,p) calculated Optimized geometry of **1** (gas phase).

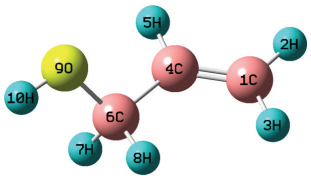

Fig. S-2. B3LYP/6-311G(d,p) calculated Optimized geometry of **2** (gas phase).

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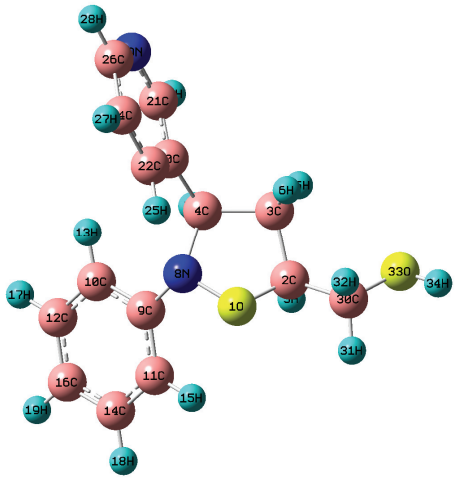

Fig. S-3. B3LYP/6-311G(d,p) calculated Optimized geometry of **CAox** (gas phase).

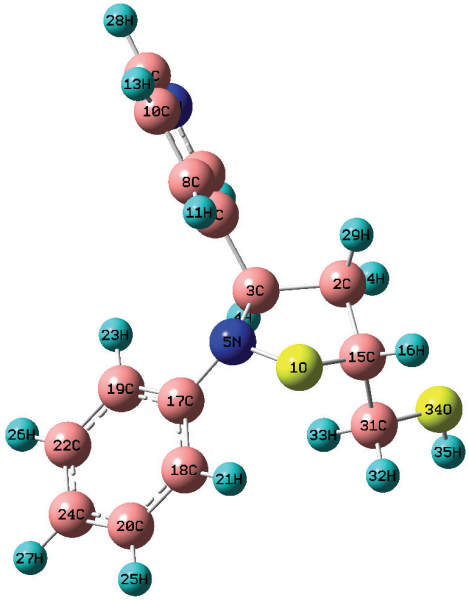

Fig. S-4. B3LYP/6-311G(d,p) calculated Optimized geometry of **CAon** (gas phase).

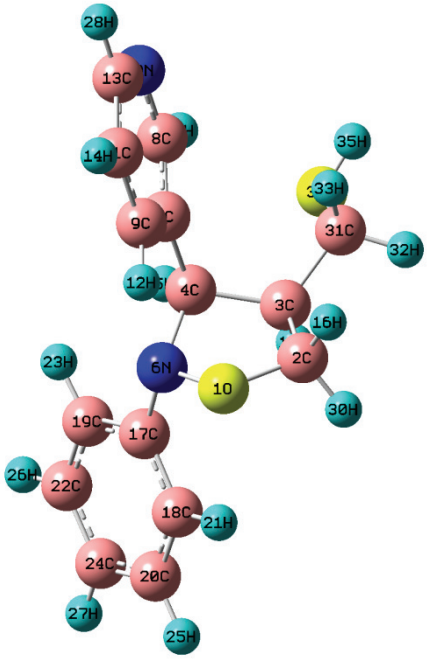

Fig. S-5. B3LYP/6-311G(d,p) calculated Optimized geometry of **CAmx** (gas phase) .

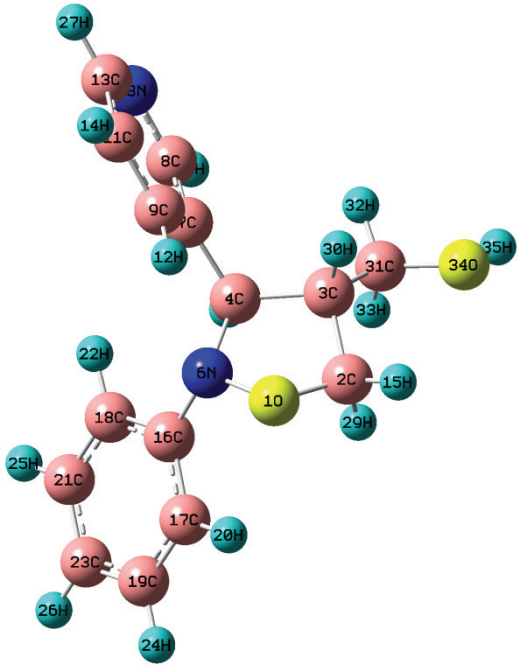

Fig. S-6. B3LYP/6-311G(d,p) calculated Optimized geometry of **CAmn** (gas phase).

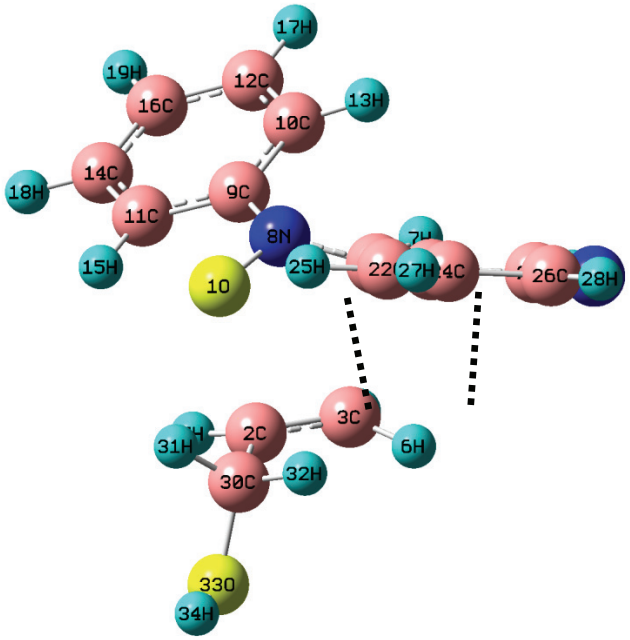

Fig. S-7. B3LYP/6-311G(d,p) calculated Optimized geometry of **TSox** (gas phase).

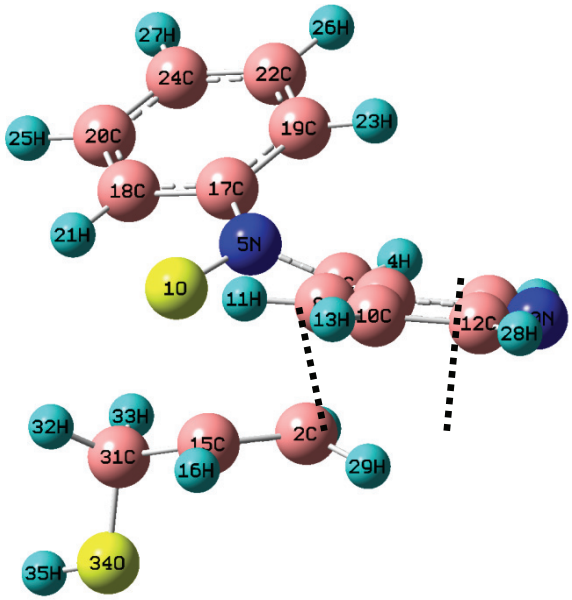

Fig. S-8. B3LYP/6-311G(d,p) calculated Optimized geometry of **TSon** (gas phase).

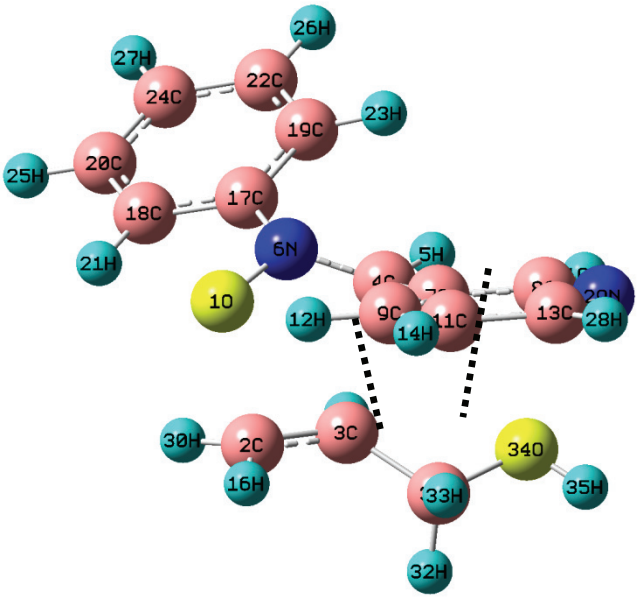

Fig. S-9. B3LYP/6-311G(d,p) calculated Optimized geometry of **TSmx** (gas phase).

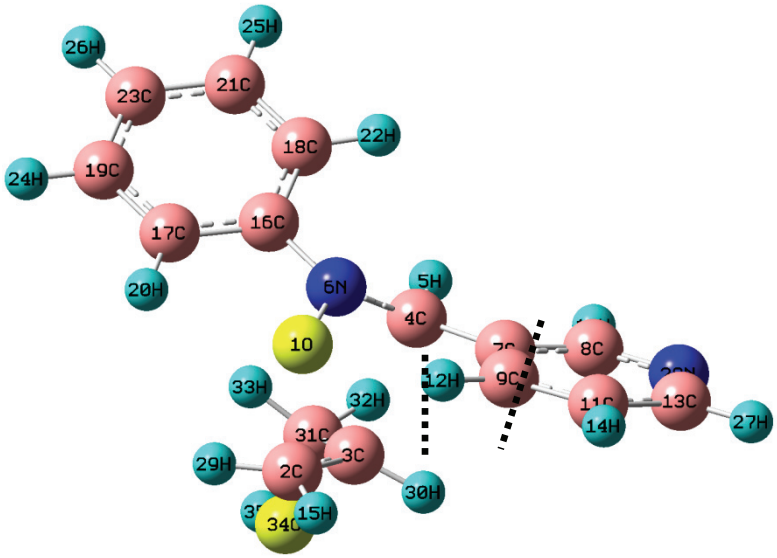

Fig. S-10. B3LYP/6-311G(d,p) calculated Optimized geometry of **TSmn** (gas phase).

TABLE S-I. B3LYP/6-311G(d,p) calculated total energies of **1** (gas phase)

E(RB+HF-LYP) / a. u.	–648.112015191
Zero-point correction, hartree particle^{-1}	0.195476
Thermal correction to energy, a. u.	0.207040
Thermal correction to enthalpy, a. u.	0.207984
Thermal correction to Gibbs free energy, a. u.	0.156565
Sum of electronic and zero-point energies, a. u.	–647.916539
Sum of electronic and thermal energies, a. u.	–647.904975
Sum of electronic and thermal enthalpies, a. u.	–647.904031
Sum of electronic and thermal free energies, a. u.	–647.955450

TABLE S-II. B3LYP/6-311G(d,p) calculated total energies of **2** (gas phase)

E(RB+HF-LYP) / a. u.	–193.172620669
Zero-point correction, hartree particle^{-1}	0.084534
Thermal correction to energy, a. u.	0.089613
Thermal correction to enthalpy, a. u.	0.090557
Thermal correction to Gibbs free energy, a. u.	0.057258
Sum of electronic and zero-point energies, a. u.	–193.088087
Sum of electronic and thermal energies, a. u.	–193.083008
Sum of electronic and thermal enthalpies, a. u.	–193.082064
Sum of electronic and thermal free energies, a. u.	–193.115363

TABLE S-III. B3LYP/6-311G(d,p) calculated total energies of **CAox**(gas phase)

E(RB+HF-LYP) / a. u.	–841.315703960
Zero-point correction, hartree particle^{-1}	0.286112
Thermal correction to energy, a. u.	0.302332
Thermal correction to enthalpy, a. u.	0.303277
Thermal correction to Gibbs free energy, a. u.	0.240118
Sum of electronic and zero-point energies, a. u.	–841.029592
Sum of electronic and thermal energies, a. u.	–841.013372
Sum of electronic and thermal enthalpies, a. u.	–841.012427
Sum of electronic and thermal free energies, a. u.	–841.075586

TABLE S-IV. B3LYP/6-311G(d,p) calculated total energies of **CAon** (gas phase)

E(RB+HF-LYP) / a. u.	–841.315289247
Zero-point correction, hartree particle-1	0.286270
Thermal correction to energy, a. u.	0.302420
Thermal correction to enthalpy, a. u.	0.303364
Thermal correction to Gibbs free energy, a. u.	0.240719
Sum of electronic and zero-point energies, a. u.	–841.029019
Sum of electronic and thermal energies, a. u.	–841.012869
Sum of electronic and thermal enthalpies, a. u.	–841.011925
Sum of electronic and thermal free energies, a. u.	–841.074570

TABLE S-V. B3LYP/6-311G(d,p) calculated total energies of **CAmx** (gas phase)

E(RB+HF-LYP) / a. u.	–841.311621374
Zero-point correction, hartree particle-1	0.286658
Thermal correction to energy, a. u.	0.302687
Thermal correction to enthalpy, a. u.	0.303631
Thermal correction to Gibbs free energy, a. u.	0.241688
Sum of electronic and zero-point energies, a. u.	–841.024963
Sum of electronic and thermal energies, a. u.	–841.008935
Sum of electronic and thermal enthalpies, a. u.	–841.007990
Sum of electronic and thermal free energies, a. u.	–841.069934

TABLE S-VI. B3LYP/6-311G(d,p) calculated total energies of **CAmx** (gas phase)

E(RB+HF-LYP) / a. u.	–841.313379546
Zero-point correction, hartree particle-1	0.286499
Thermal correction to energy, a. u.	0.302575
Thermal correction to enthalpy, a. u.	0.303519
Thermal correction to Gibbs free energy, a. u.	0.241023
Sum of electronic and zero-point energies, a. u.	–841.026881
Sum of electronic and thermal energies, a. u.	–841.010805
Sum of electronic and thermal enthalpies, a. u.	–841.009860
Sum of electronic and thermal free energies, a. u.	–841.072357

TABLE S-VII. B3LYP/6-311G(d,p) calculated total energies of **TSox** (gas phase)

E(RB+HF-LYP) / a. u.	–841.256198482
Zero-point correction, hartree particle-1	0.282033
Thermal correction to energy, a. u.	0.298772
Thermal correction to enthalpy, a. u.	0.299716
Thermal correction to Gibbs free energy, a. u.	0.236319
Sum of electronic and zero-point energies, a. u.	–840.974166
Sum of electronic and thermal energies, a. u.	–840.957426
Sum of electronic and thermal enthalpies, a. u.	–840.956482
Sum of electronic and thermal free energies, a. u.	–841.019880

TABLE S-VIII. B3LYP/6-311G(d,p) calculated total energies of **TSon** (gas phase)

E(RB+HF-LYP) / a. u.	–841.253804119
Zero-point correction, hartree particle-1	0.281991
Thermal correction to energy, a. u.	0.298725
Thermal correction to enthalpy, a. u.	0.299669
Thermal correction to Gibbs free energy, a. u.	0.236427
Sum of electronic and zero-point energies, a. u.	–840.971813
Sum of electronic and thermal energies, a. u.	–840.955079
Sum of electronic and thermal enthalpies, a. u.	–840.954135
Sum of electronic and thermal free energies, a. u.	–841.017377

TABLE S-IX. B3LYP/6-311G(d,p) calculated total energies of **TSmx**(gas phase)

E(RB+HF-LYP) / a. u.	–841.255014509
Zero-point correction, hartree particle^{-1}	0.282365
Thermal correction to energy, a. u.	0.298776
Thermal correction to enthalpy, a. u.	0.299720
Thermal correction to Gibbs free energy, a. u.	0.237783
Sum of electronic and zero-point energies, a. u.	–840.972650
Sum of electronic and thermal energies, a. u.	–840.956238
Sum of electronic and thermal enthalpies, a. u.	–840.955294
Sum of electronic and thermal free energies, a. u.	–841.017232

TABLE S-X. B3LYP/6-311G(d,p) calculated total energies of **TSmn**(gas phase)

E(RB+HF-LYP) / a. u.	–841.252610554
Zero-point correction, hartree particle^{-1}	0.282064
Thermal correction to energy, a. u.	0.298738
Thermal correction to enthalpy, a. u.	0.299682
Thermal correction to Gibbs free energy, a. u.	0.23658
Sum of electronic and zero-point energies, a. u.	–840.970547
Sum of electronic and thermal energies, a. u.	–840.953872
Sum of electronic and thermal enthalpies, a. u.	–840.952928
Sum of electronic and thermal free energies, a. u.	–841.016024

TABLE S-XI. B3LYP/6-311G(d,p) calculated total and relative energies in toluene at 383 K

Cmpd.	*E* a.u.	*H* a.u.	*G* a.u.	*S* cal mol^{-1} K^{-1}	Δ*E* kcal mol^{-1}	Δ*H* kcal mol^{-1}	Δ*G* kcal mol^{-1}	Δ*S* cal mol^{-1} K^{-1}
1	–648.12	–647.905123	–647.979715	122.211				
2	–193.177	–193.084501	–193.130422	75.238				
CAox	–841.326	–841.013701	–841.106485	152.017	–18.0668	–15.1086	2.291667	–45.432
TSox	–841.267	–840.957725	–841.050907	152.671	19.14445	20.01694	37.16742	–44.778
CAon	–841.326	–841.013168	–841.105378	151.078	–17.7746	–14.7741	2.98632	–46.371
TSon	–841.264	–840.955335	–841.048375	152.437	20.65847	21.51669	38.75627	–45.012
CAmx	–841.322	–841.00928	–841.100612	149.639	–15.5143	–12.3343	5.977033	–47.81
TSmx	–841.265	–840.95558	–841.046863	149.559	20.50558	21.36295	39.70507	–47.89
CAmn	–841.324	–841.011122	–841.103101	150.699	–16.6151	–13.4902	4.41516	–46.75
TSmn	–841.263	–840.95406	–841.046937	152.17	21.45408	22.31677	39.65863	–45.279