"Supporting Information"

Decoding the [3+2] Cycloaddition of a Furan-Imine Oxide with Styrene: Mechanism, Selectivity and Bioactivity

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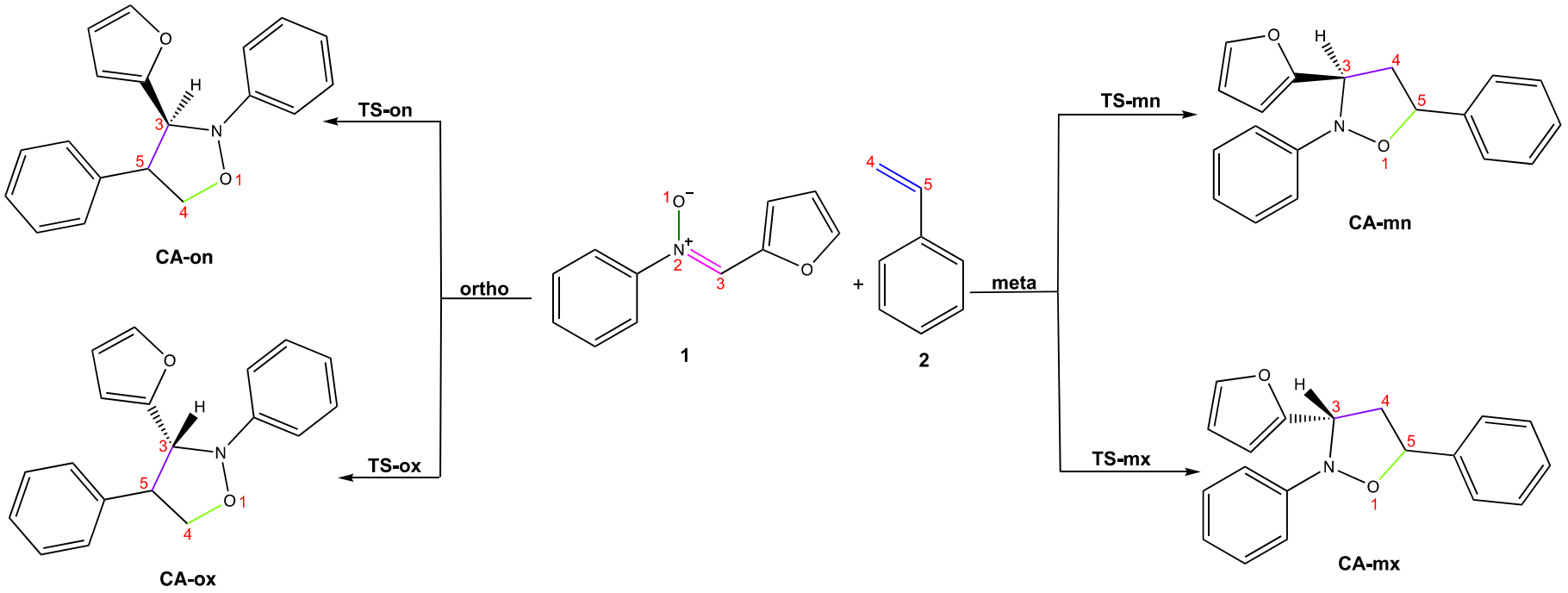
S1 General Aspects of Thermodynamics and Kinetics

In this work, DFT at the M06-2X-D3/6–311G(d,p) level of approximation, in benzene at ambient temperature, is employed to describe the 32CA reaction between 1-(furan-2-yl)-N-phenylmethanimine oxide **1** and styrene **2** (**Scheme S1**).



Scheme S1. 32CA reaction of 1-(furan-2-yl)-N-phenylmethanimine oxide **1** with styrene **2** for synthesis 3-(furan-2-yl)-2,5-diphenylisoxazolidine **3**.

S2 Local reactivity indices

Table S1 IEFPCM(benzene)/M06-2X-D3/6–311G(d,p) local reactivity descriptors namely the nucleophilic and electrophilic indices (N_k, ω_k), and Local reactivity difference index (R_k), in eV. k corresponds to each of the two reactive centers of **1** and **2**.

Reactants	k	P_k^-	N_k	P_k^+	ω_k	R_k
1	O1	0.48	1.77	0.13	0.17	-1.60
	N2	0.05	0.18	0.19	0.25	0.07
	C3	0.02	0.07	0.23	0.31	0.24
2	C4	0.47	1.38	0.41	0.43	-0.95
	C5	-0.04	-0.18	0.05	0.05	0.23

S3 Thermodynamic data

Table S2 Energies, enthalpies, entropies, and Gibbs enthalpies of reactants, transition states, and products were calculated at the DFT level using different exchange-correlation functionals (M06-2X-D3, B3LYP, and ωB97X-D) with the 6-311G(d,p) basis set, considering benzene as the solvent at ambient temperature.

Systems	**E (a.u.)**	**H^0 (a.u.)**	**S^0 (cal mol^{-1} K^{-1})**	**G^0 (a.u.)**
M06-2X-D3/6-311G(d,p)				
nitrone 1	-629.598186	-629.407142	103.760	-629.456442
styrene 2	-309.580983	-309.440067	77.307	-309.476798
CA-on	-939.229126	-938.891192	137.078	-938.956322
CA-ox	-939.228721	-938.890880	137.580	-938.956249
CA-mn	-939.232591	-938.894865	136.754	-938.959841
CA-mx	-939.229607	-938.891816	135.857	-938.956367
TS-on	-939.163319	-938.829332	136.157	-938.894024
TS-ox	-939.163496	-938.829596	136.050	-938.894238
TS-mn	-939.164953	-938.831105	138.590	-938.896954
TS-mx	-939.162166	-938.828325	138.091	-938.893936
B3LYP/6-311G(d,p)				

nitrone 1	-629.858747	-629.670102	104.504	-629.719755
styrene 2	-309.728734	-309.588211	82.737	-309.627522
CA-on	-939.602064	-939.268046	140.700	-939.334897
CA-ox	-939.600122	-939.266241	138.803	-939.332191
CA-mn	-939.606651	-939.272923	141.687	-939.340244
CA-mx	-939.601050	-939.267310	140.650	-939.334138
TS-on	-939.550271	-939.220191	140.923	-939.287148
TS-ox	-939.549632	-939.219578	139.101	-939.285669
TS-mn	-939.555590	-939.225420	141.579	-939.292689
TS-mx	-939.552869	-939.222806	142.249	-939.290393
	ωB97X-D/6-311G(d,p)			
nitrone 1	-629.632716	-629.441862	104.197	-629.491369
styrene 2	-309.610501	-309.469638	77.241	-309.506337
CA-on	-939.288705	-938.950832	138.156	-939.016474
CA-ox	-939.288777	-938.950988	138.606	-939.016845
CA-mn	-939.292399	-938.954648	136.927	-939.019706
CA-mx	-939.290135	-938.952400	137.264	-939.017618
TS-on	-939.224221	-938.890269	137.766	-938.955726
TS-ox	-939.223351	-938.889544	136.350	-938.954328
TS-mn	-939.226817	-938.893005	138.941	-938.959020
TS-mx	-939.224084	-938.890135	139.007	-938.956181

Table S3 Maxwell−Boltzmann weight (P in %) for the all the studied TSs and cycloadducts involved in the 32CA reaction between nitrone **1** and styrene **2**.

Structures	**CA-on**	**TS-on**	**CA-ox**	**TS-ox**	**CA-mn**	**TS-mn**	**CA-mx**	**TS-mx**
P	1.50	6.15	3.04	5.00	93.08	85.42	2.37	3.43

Table S4 Calculated relative energies (ΔE), enthalpies (ΔH) and Gibbs free energies (ΔG), in kcal mol^{-1}, and relative entropies (ΔS), in cal mol^{-1} K^{-1}, for the stationary points involved in the 32CA between nitrone **1** and styrene **2** using different exchange-correlation functionals (B3LYP, and ωB97X-D) with the 6-311G(d,p) basis set, considering benzene as the solvent at ambient temperature.

Species	ΔE	ΔH	ΔS	ΔG
B3LYP/6-311G(d,p)				
CA-on	-9.2	-6.1	-46.5	7.8
CA-ox	-7.9	-5.0	-48.4	9.5
CA-mn	-12.0	-9.2	-45.6	4.4
CA-mx	-8.5	-5.7	-46.6	8.3
TS-on	23.4	23.9	-46.3	37.8
TS-ox	23.8	24.4	-48.1	38.7
TS-mn	20.0	20.7	-45.7	34.3
TS-mx	21.7	22.3	-45.0	35.7
ωB97X-D/6-311G(d,p)				
CA-on	-28.6	-24.7	-43.3	-11.8
CA-ox	-28.6	-24.8	-42.8	-12.0
CA-mn	-30.9	-27.1	-44.5	-13.8
CA-mx	-29.5	-25.7	-44.2	-12.5
TS-on	11.9	13.4	-43.7	26.4
TS-ox	12.5	13.8	-45.1	27.2
TS-mn	10.3	11.6	-42.5	24.3
TS-mx	12.0	13.4	-42.4	26.1

S4 DIAS Analysis

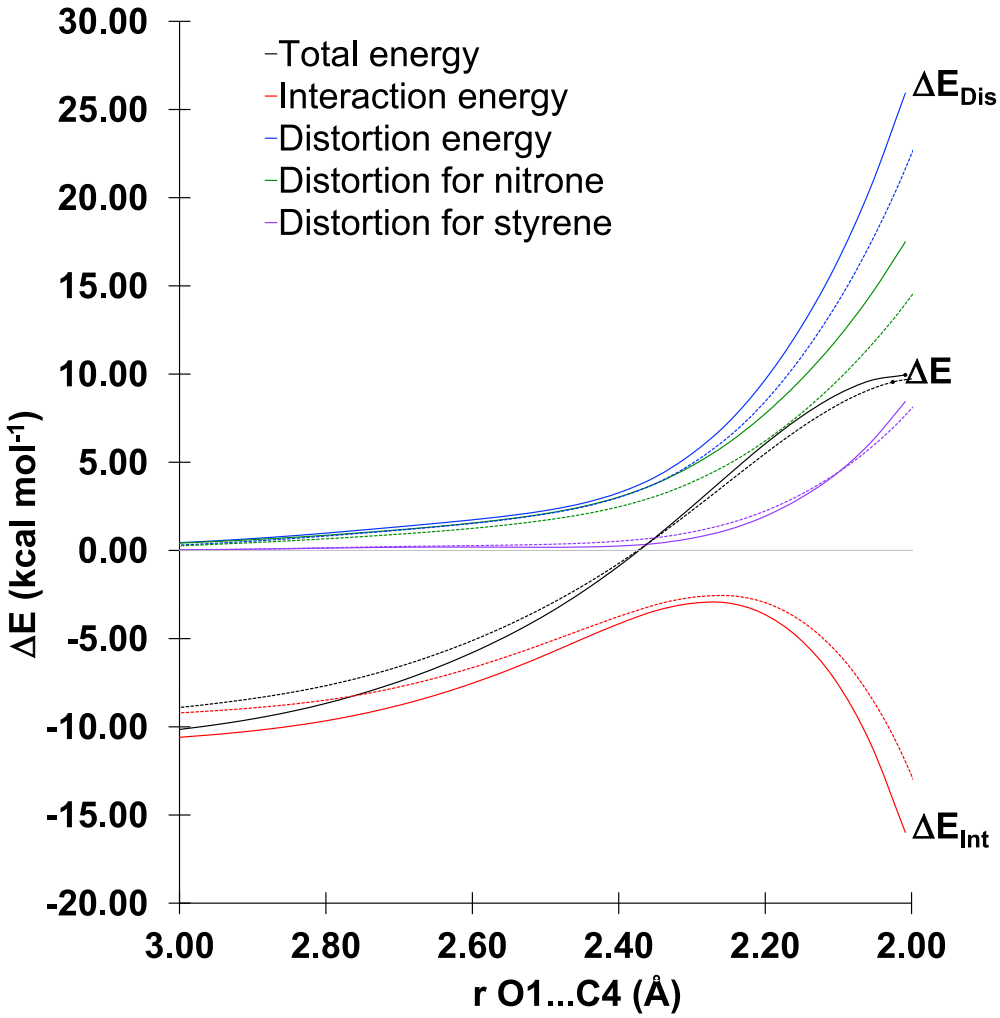


Fig. S1 Comparative DIAS diagrams for the **TS-on** (solid lines) and **TS-ox** (dashed lines) approaches of the 32CA reaction between **1** and **2** along the reaction coordinate projected onto the forming O1···C4 bond distances. The transition states are indicated by a dot.

S5 BET Analysis

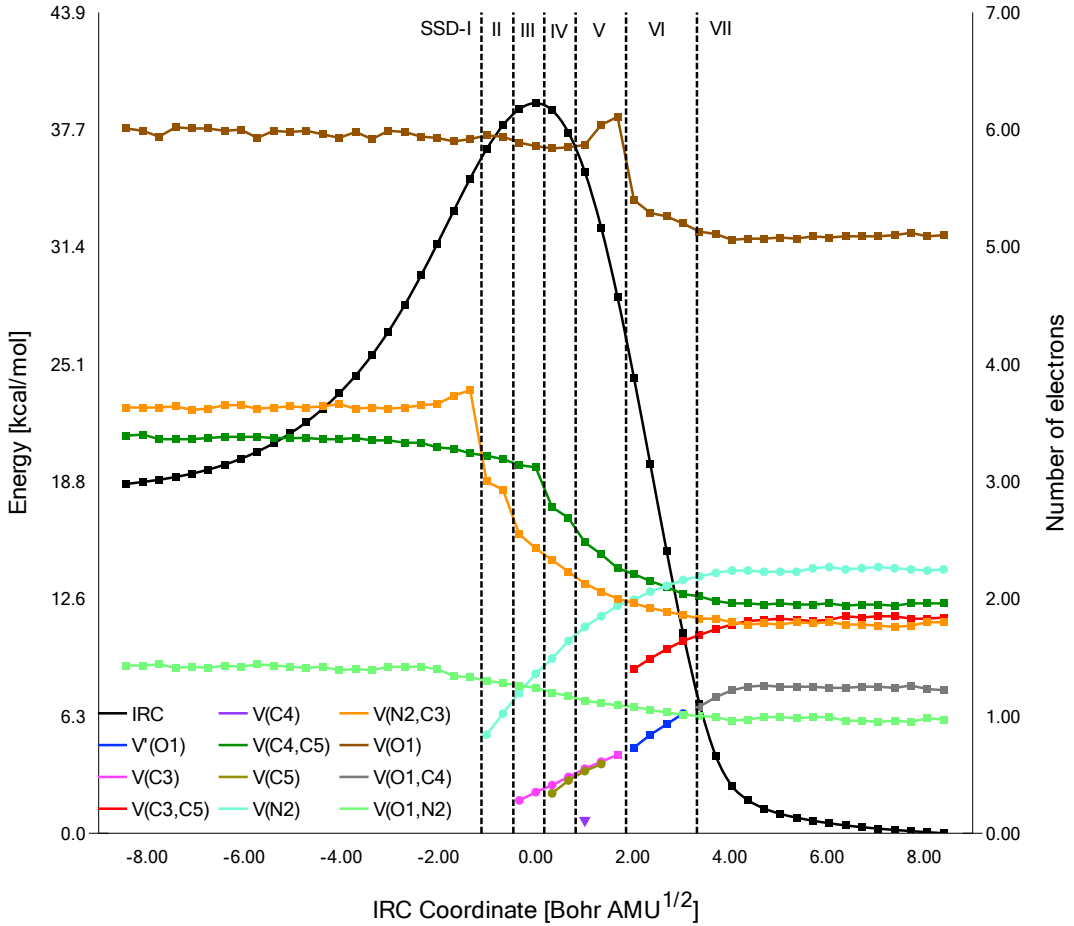


Fig. S2 Electron populations (e) evolution for selected basins along the IRC associated to the **TS-on** pathway of the 32CA reaction between **1** and **2** as calculated at the IEFPCM(benzene)/M06-2X-D3/6–311G(d,p) level of approximation. These evolutions are depicted on top of the potential energy surface.

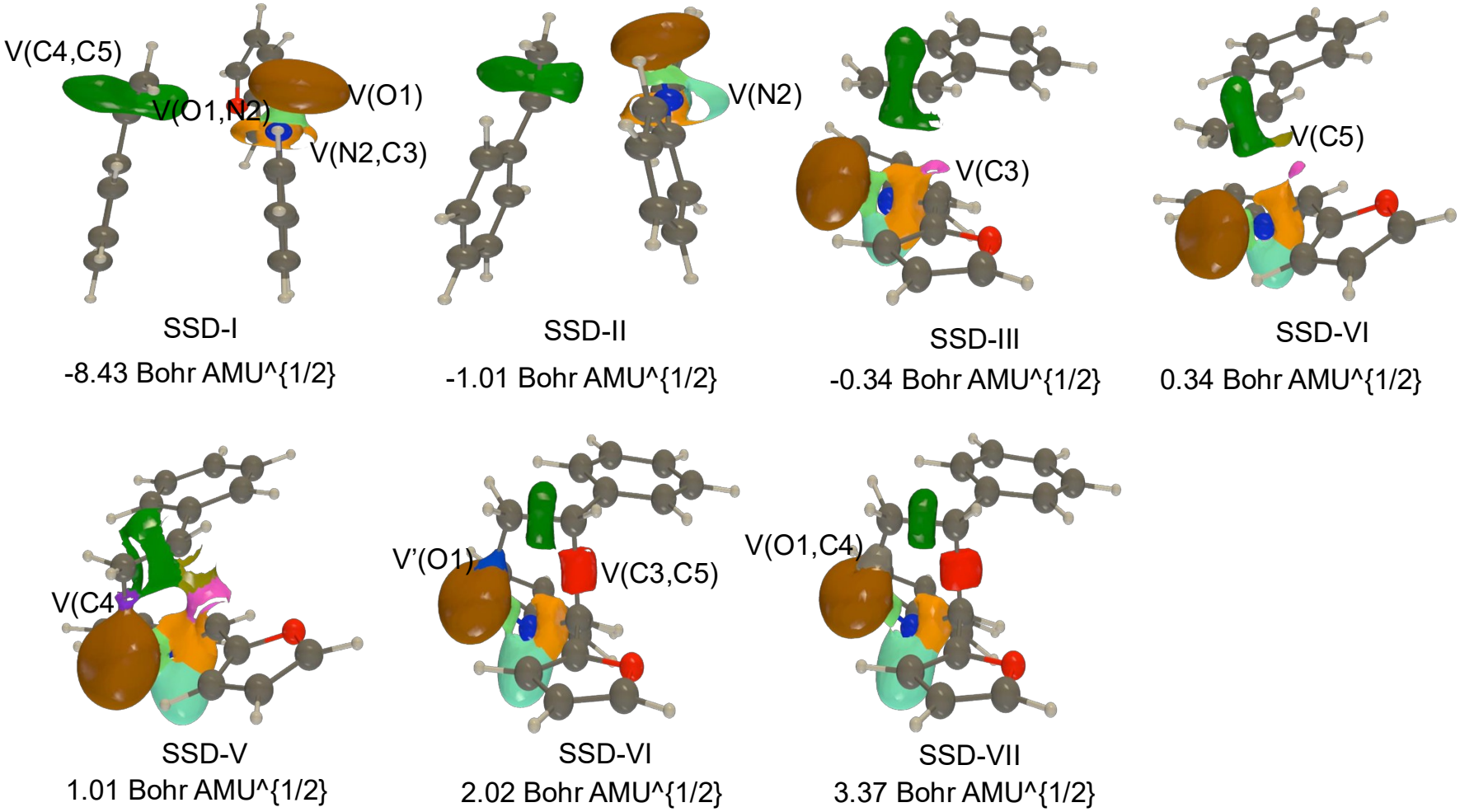


Fig. S3 ELF basin isosurfaces (η = 0.75) for specific points of the successive SSDs and Lewis structures along the IRC for the **TS-on** of the 32CA reaction between **1** and **2**. The color labeling of the basins was performed according to Fig. S2, and, for each point, the corresponding intrinsic reaction coordinate is provided.

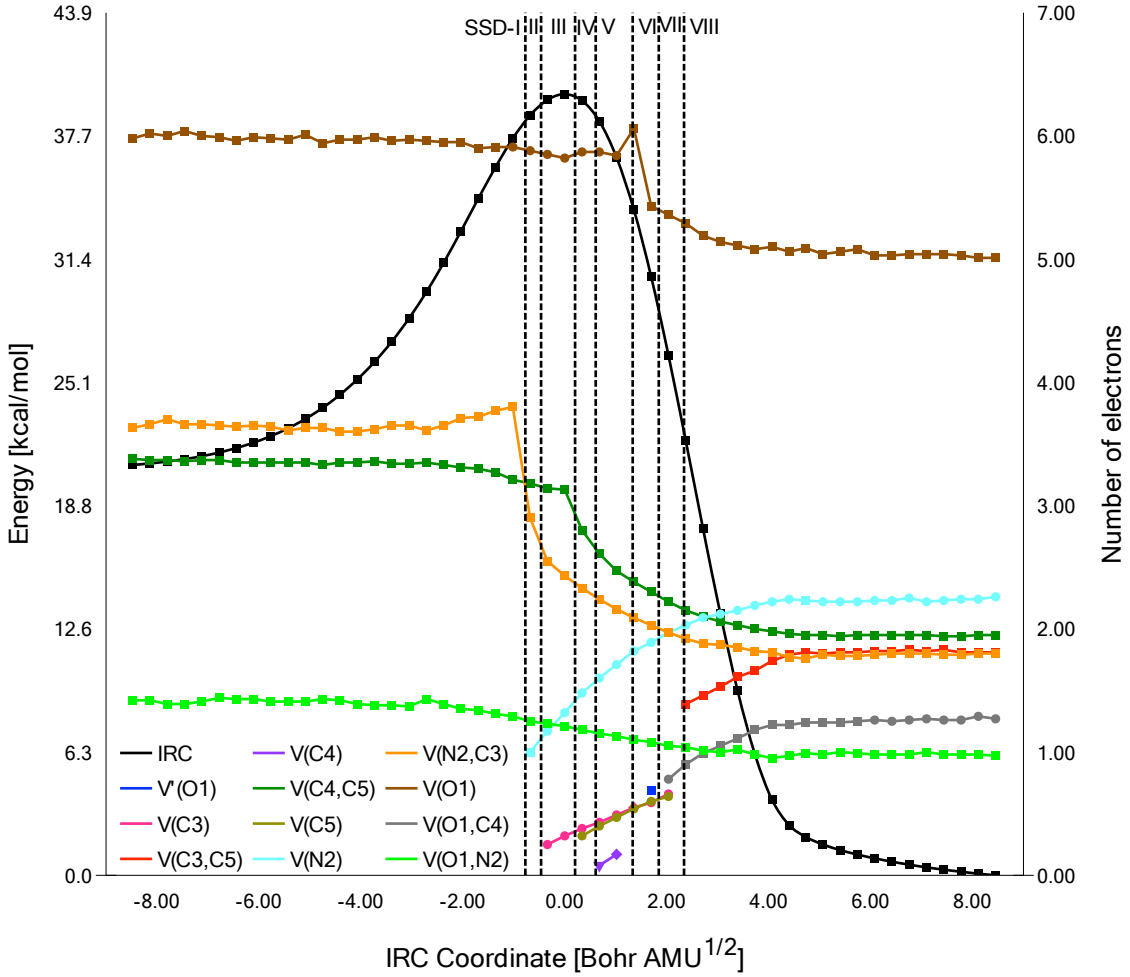


Fig. S4 Electron populations (e) evolution for selected basins along the IRC associated to the **TS-ox** pathway of the 32CA reaction between **1** and **2** as calculated at the IEFPCM(benzene)/M06-2X-D3/6–311G(d,p) level of approximation. These evolutions are depicted on top of the potential energy surface.

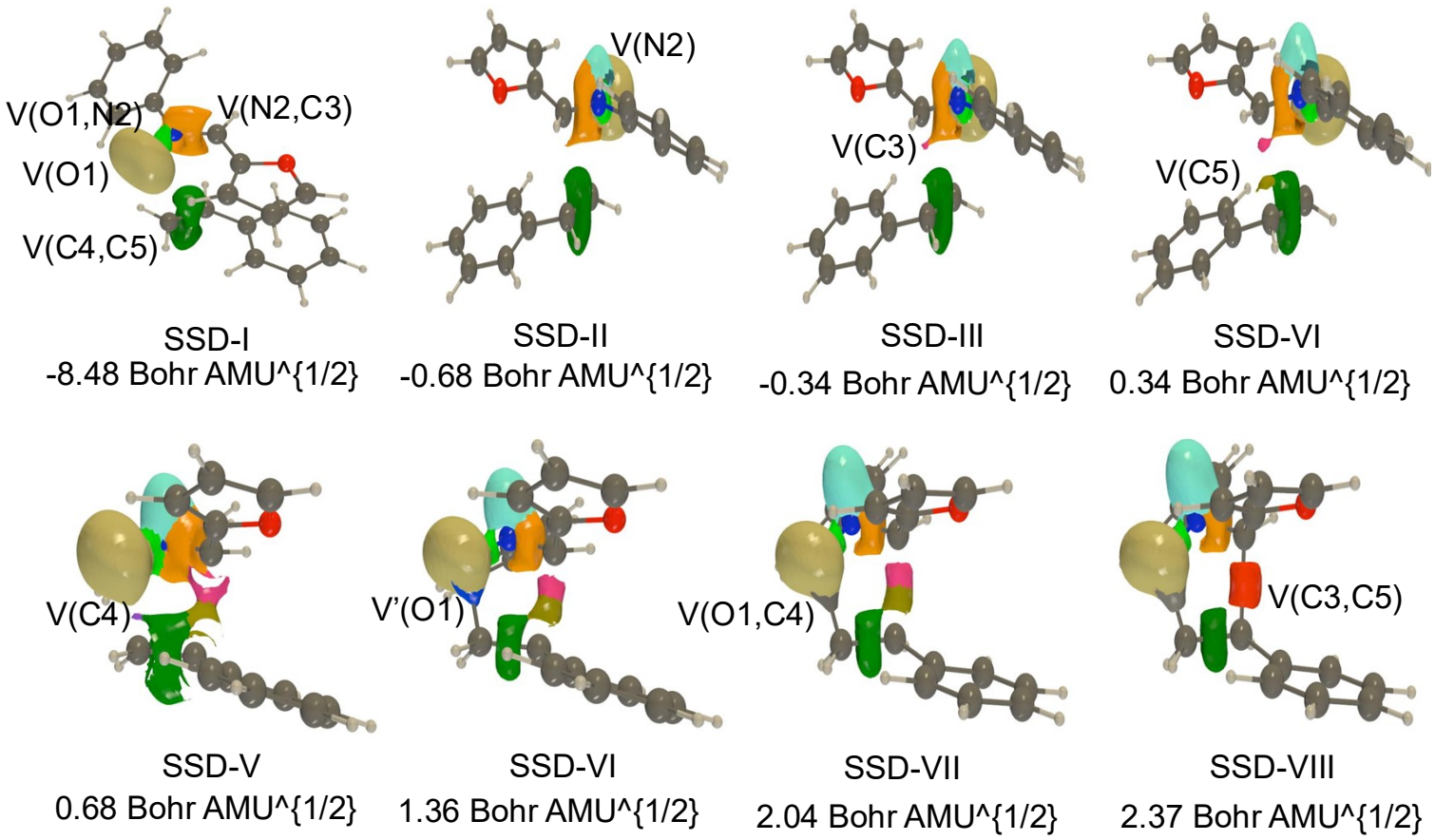


Fig. S5 ELF basin isosurfaces (η = 0.75) for specific points of the successive SSDs and Lewis structures along the IRC for the **TS-ox** of the 32CA reaction between **1** and **2**. The color labeling of the basins was performed according to Fig. S4, and, for each point, the corresponding intrinsic reaction coordinate is provided.

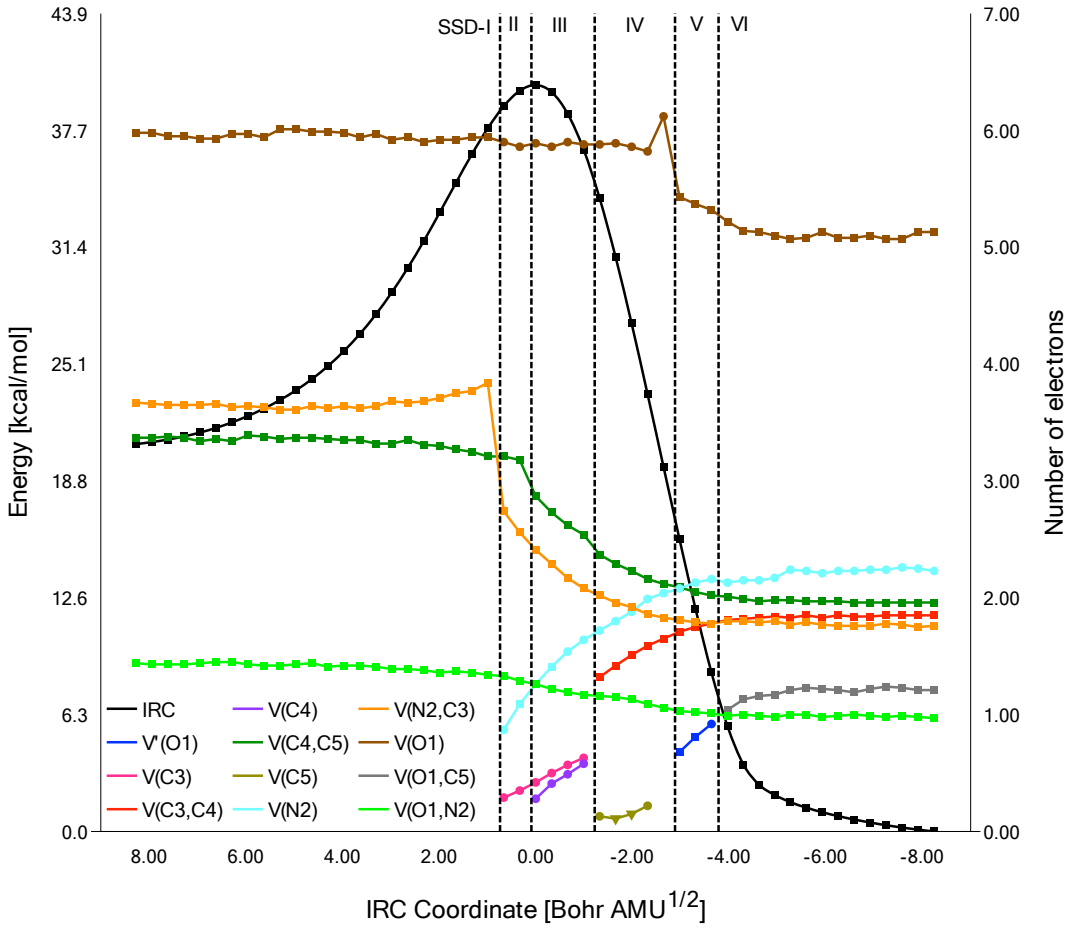


Fig. S6 Electron populations (e) evolution for selected basins along the IRC associated to the **TS-mx** pathway of the 32CA reaction between **1** and **2** as calculated at the IEFPCM(benzene)/M06-2X-D3/6–311G(d,p) level of approximation. These evolutions are depicted on top of the potential energy surface.

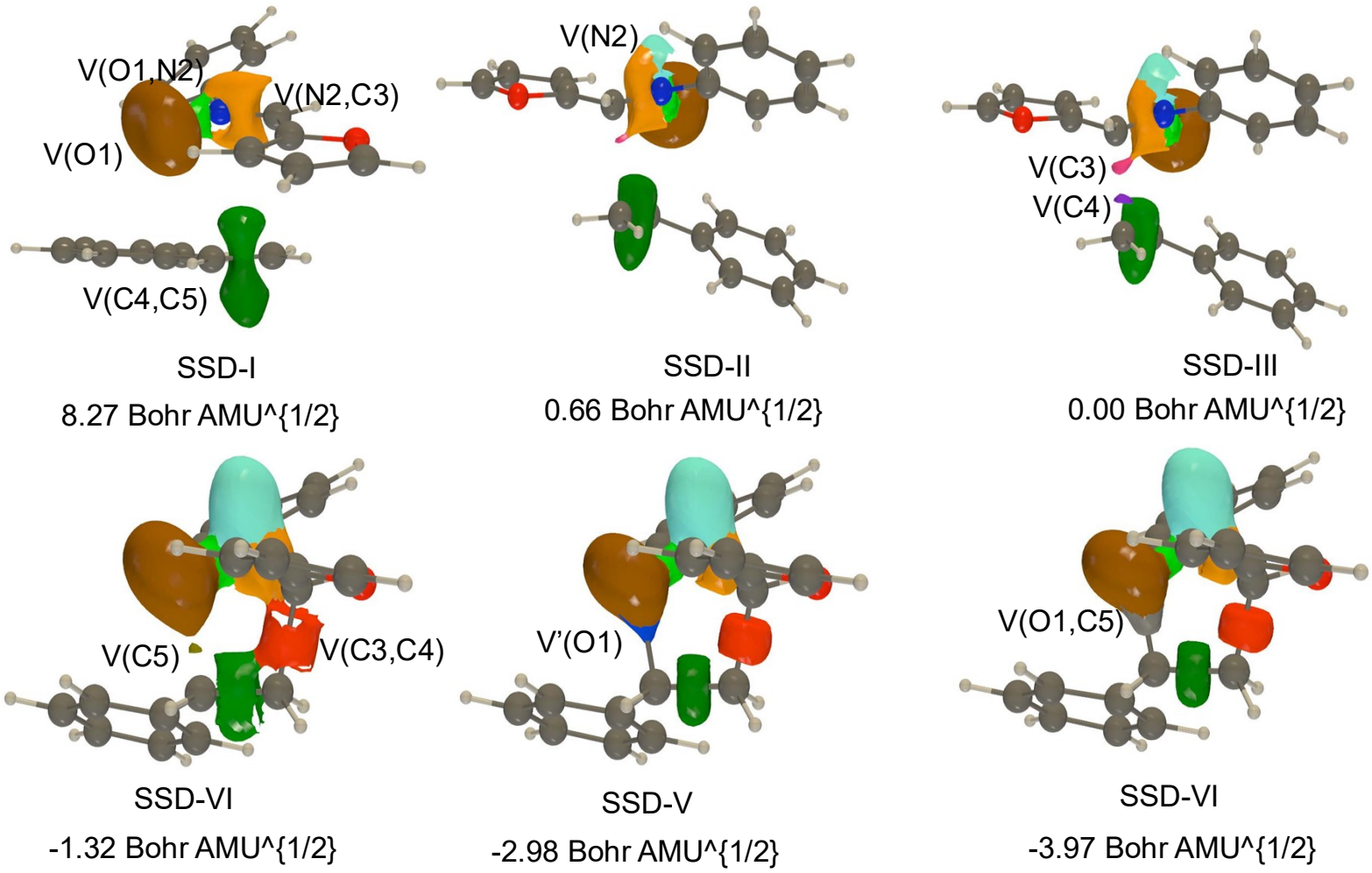


Fig. S7 ELF basin isosurfaces (η = 0.75) for specific points of the successive SSDs and Lewis structures along the IRC for the **TS-mx** of the 32CA reaction between **1** and **2**. The color labeling of the basins was performed according to Fig. S6, and, for each point, the corresponding intrinsic reaction coordinate is provided.

Table S5 Table Basin Populations (in e), IRC coordinates (RX, Bohr $AMU^{1/2}$), relative electronic energies (ΔE in kcal/mol) and C3-C5/O1-C4 bond lengths (in Å) along the **TS-on** regio-isomeric channel of 32CA reaction.

	SSD-I		**SSD-II**		**SSD-III**		**SSD-IV**		**SSD-V**		**SSD-VI**		**SSD-VII**	
Basins	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last
V(N2,C3)	3.63	3.78	3.00	2.93	2.55	2.43	2.33	2.23	2.13	2.00	1.96	1.86	1.83	1.80
V(O1,N2)	1.43	1.33	1.30	1.28	1.26	1.24	1.20	1.17	1.13	1.09	1.08	1.01	1.00	0.97
V(C4,C5)	3.39	3.24	3.22	3.19	3.14	3.12	2.78	2.69	2.48	2.26	2.21	2.04	2.02	1.96
V(O1)	6.01	5.92	5.95	5.94	5.89	5.86	5.84	5.85	5.87	6.11	5.40	5.20	5.13	5.10
V(N2)	---	---	0.84	1.02	1.20	1.36	1.49	1.64	1.76	1.94	1.99	2.16	2.19	2.25
V(C3)	---	---	---	---	0.28	0.35	0.41	0.48	0.55	0.67	---	---	---	---
V(C4)	---	---	---	---	---	---	0.34	0.45	0.53	0.59	---	---	---	---
V(C3,C5)	---	---	---	---	---	---	---	---	---	---	1.40	1.64	1.69	1.84
V(C5)	---	---	---	---	---	---	---	---	0.11	0.11	---	---	---	---
V'(O1)	---	---	---	---	---	---	---	---	---	---	0.73	1.02	---	---
V(O1,C4)	---	---	---	---	---	---	---	---	---	---	---	---	1.08	1.22
d(C3,C5)	3.057	2.381	2.333	2.285	2.237	2.187	2.138	2.087	2.036	1.955	1.865	1.736	1.667	1.561
d(O1,C4)	3.056	2.204	2.154	2.105	2.056	2.009	1.961	1.914	1.868	1.775	1.728	1.586	1.540	1.448
RX	-8.43	-1.35	-1.01	-0.67	-0.34	0.00	0.34	0.67	1.01	1.69	2.02	3.03	3.37	8.40
E	18.69	35.04	36.59	37.88	38.75	39.01	38.69	37.49	35.39	28.68	24.37	10.69	6.93	0.00

Table S6 Table Basin Populations (in e), IRC coordinates (RX, Bohr $AMU^{1/2}$), relative electronic energies (ΔE in kcal/mol) and C3-C5/O1-C4 bond lengths (in Å) along the **TS-ox** regio-isomeric channel of 32CA reaction.

	SSD-I		**SSD-II**		**SSD-III**		**SSD-IV**		**SSD-V**		**SSD-VI**		**SSD-VII**		**SSD-VIII**	
Basins	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last
V(N2,C3)	3. 63	3.80	2.90	2.90	2.55	2.43	2.33	2.33	2.24	2.16	2.09	2.03	1.97	1.97	1.92	1.80
V(O1,N2)	1.42	1.29	1.25	1.25	1.23	1.21	1.18	1.18	1.15	1.13	1.10	1.08	1.05	1.05	1.04	0.97
V(C4,C5)	3.38	3.21	3.18	3.18	3.14	3.13	2.80	2.80	2.61	2.47	2.38	2.30	2.22	2.22	2.15	1.95
V(O1)	5.98	5.91	5.88	5.88	5.85	5.82	5.87	5.87	5.87	6.06	5.43	5.43	5.36	5.36	5.29	5.01
V(N2)	---	---	1.00	1.00	1.17	1.32	1.48	1.48	1.60	1.71	1.82	1.89	1.97	1.97	2.03	2.26
V(C3)	---	---	---	---	0.25	0.32	0.38	0.38	0.43	0.49	0.55	0.59	0.66	0.66	---	---
V(C4)	---	---	---	---	---	---	---	---	0.08	0.17	---	---	---	---	---	---
V(C3,C5)	---	---	---	---	---	---	---	---	---	---	---	---	---	---	1.39	1.81
V(C5)	---	---	---	---	---	---	0.32	0.32	0.40	0.47	0.54	0.60	0.64	0.64	---	---
V'(O1)	---	---	---	---	---	---	---	---	---	---	0.69	0.69	---	---	---	---
V(O1,C4)	---	---	---	---	---	---	---	---	---	---	---	---	0.78	0.78	0.90	1.27
d(C3,C5)	3.146	2.420	2.347	2.347	2.328	2.281	2.235	2.235	2.187	2.138	2.089	2.039	1.987	1.987	1.935	1.576
d(O1,C4)	3.037	2.128	2.077	2.077	2.026	1.975	1.924	1.924	1.847	1.825	1.777	1.723	1.682	1.682	1.637	1.448
RX	-8.48	-1.02	-0.68	-0.68	-0.34	0.00	0.34	0.34	0.68	1.02	1.36	1.69	2.04	2.04	2.37	8.45
E	20.89	37.52	38.70	38.70	39.48	39.77	39.45	39.45	38.40	36.55	33.88	30.48	26.49	26.49	22.13	0.00

Table S7 Table Basin Populations (in e), IRC coordinates (RX, Bohr $AMU^{1/2}$), relative electronic energies (ΔE in kcal/mol) and C3-C4/O1-C5 bond lengths (in Å) along the **TS-mn** regio-isomeric channel of 32CA reaction.

	SSD-I		**SSD-II**		**SSD-III**		**SSD-IV**		**SSD-V**		**SSD-VI**		**SSD-VII**		**SSD-VIII**	
Basins	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last
V(N2,C3)	3.65	3.87	2.96	2.96	2.56	2.56	2.40	2.20	2.10	2.02	1.97	1.84	1.83	1.82	1.80	1.80
V(O1,N2)	1.42	1.31	1.29	1.29	1.27	1.27	1.25	1.19	1.17	1.16	1.13	1.08	1.09	1.06	1.02	0.98
V(C4,C5)	3.36	3.22	3.17	3.17	3.16	3.16	2.88	2.64	2.57	2.48	2.32	2.13	2.08	2.06	2.02	1.95
V(O1)	5.97	5.94	5.92	5.92	5.92	5.92	5.93	5.96	5.91	5.91	5.86	5.93	6.13	5.42	5.33	5.13
V(N2)	---	---	0.98	0.98	1.14	1.14	1.31	1.58	1.70	1.78	1.87	2.05	2.08	2.13	2.17	2.22
V(C3)	---	---	---	---	0.32	0.32	0.41	0.56	---	---	---	---	---	---	---	---
V(C4)	---	---	---	---	---	---	0.25	0.47	---	---	0.13	0.12	---	---	---	---
V(C3,C4)	---	---	---	---	---	---	---	---	1.17	1.33	1.41	1.66	1.71	1.75	1.77	1.83
V(C5)	---	---	---	---	---	---	---	---	---	---	0.13	0.12	---	---	---	---
V'(O1)	---	---	---	---	---	---	---	---	---	---	---	---	0.74	0.74	---	---
V(O1,C5)	---	---	---	---	---	---	---	---	---	---	---	---	---	---	0.86	1.18
d(C3,C4)	3.091	2.256	2.199	2.199	2.141	2.141	2.083	1.965	1.906	1.850	1.795	1.658	1.627	1.602	1.583	1.542
d(O1,C5)	3.095	2.316	2.276	2.276	2.236	2.236	2.197	2.121	2.082	2.042	1.999	1.847	1.789	1.728	1.666	1.465
RX	8.47	1.02	0.68	0.68	0.34	0.34	0.34	0.00	-0.68	-1.02	-1.36	-1.69	-3.05	-3.39	-3.73	-8.45
E	23.44	37.69	38.78	38.78	39.55	39.55	39.45	39.84	38.38	36.50	33.94	30.87	16.54	12.99	9.65	0.00

Table S8 Table Basin Populations (in e), IRC coordinates (RX, Bohr $AMU^{1/2}$), relative electronic energies (ΔE in kcal/mol) and C3-C4/O1-C5 bond lengths (in Å) along the **TS-mx** regio-isomeric channel of 32CA reaction.

	SSD-I		**SSD-II**		**SSD-III**		**SSD-IV**		**SSD-V**		**SSD-VI**	
Basins	First	Last	First	Last	First	Last	First	Last	First	Last	First	Last
V(N2,C3)	3. 67	3.84	2.74	2.56	2.41	2.08	2.02	1.83	1.81	1.78	1.80	1.76
V(O1,N2)	1.44	1.34	1.33	1.29	1.26	1.17	1.16	1.06	1.03	1.01	0.99	0.97
V(C4,C5)	3.37	3.21	3.21	3.18	2.87	2.54	2.37	2.12	2.09	2.02	2.01	1.96
V(O1)	5.98	5.94	5.90	5.86	5.89	5.88	5.88	6.12	5.43	5.32	5.22	5.13
V(N2)	---	---	0.97	1.09	1.26	1.64	1.72	2.04	2.08	2.16	2.13	2.23
V(C3)	---	---	0.29	0.35	0.42	0.63	---	---	---	---	0.21	0.34
V(C4)	---	---	---	---	0.28	0.58	---	---	---	---	---	---
V(C3,C4)	---	---	---	---	---	---	1.32	1.65	1.71	1.78	1.81	1.85
V(C5)	---	---	---	---	---	---	0.13	0.22	---	---	---	---
V'(O1)	---	---	---	---	---	---	---	---	0.68	0.92	---	---
V(O1,C5)	---	---	---	---	---	---	---	---	---	---	1.04	1.21
d(C3,C4)	3.119	2.250	2.195	2.139	2.083	1.916	1.852	1.677	1.646	1.534	1.577	1.548
d(O1,C5)	3.025	2.285	2.244	2.205	1.166	2.048	2.006	1.814	1.733	1.640	1.580	1.466
RX	8.27	0.99	0.66	0.33	0.00	-0.99	-1.32	-2.65	-2.98	-3.64	-3.97	-8.24
E	20.81	37.77	38.95	39.78	40.09	36.62	34.01	19.58	15.70	8.54	5.66	0.00

S6 ADMET and Docking Analysis

Table S9 ADMET/pharmacokinetic features of the best-hit compounds.

Property	CA-on	CA-ox	CA-mn	CA-mx
Caco-2 Permeability	-4.681	-4.768	-4.772	-4.739
MDCK Permeability	-4.427	-4.384	-4.683	-4.652
Pgp-inhibitor	0.985	0.992	0.991	0.979
Pgp-substrate	0.174	0.104	0.027	0.118
HIA	0.000	0.000	0.000	0.000
$F_{20\%}$	0.004	0.005	0.00	0.000
$F_{30\%}$	0.045	0.05	0.014	0.024

Table S10 Compounds **3**, **4**, **5** and **6** Metabolism SwissADME-Computed Drug-Likeness Predictions.

Property	CA-on	CA-ox	CA-mn	CA-mx
CYP1A2 inhibitor	0.894	0.894	0.856	0.765
CYP1A2 substrate	0.005	0.158	0.006	0.001
CYP2C19 inhibitor	1.000	1.000	1.000	1.000
CYP2C19 substrate	0.315	0.872	0.899	0.366
CYP2C9 inhibitor	0.997	1.000	1.000	1.000
CYP2C9 substrate	0.275	0.579	0.000	0.000
CYP2D6 inhibitor	0.188	0.130	0.009	0.011
CYP2D6 substrate	0.566	0.620	0.000	0.000
CYP3A4 inhibitor	0.624	0.863	0.936	0.964
CYP3A4 substrate	0.992	0.944	0.982	0.939
CYP2B6 inhibitor	1.000	1.000	1.000	0.994
CYP2B6 substrate	0.003	0.026	0.003	0.002
CYP2C8 inhibitor	0.818	0.702	0.996	0.995
HLM Stability	0.567	0.758	0.942	0.849

Table S11 Compounds **CA-on**, **CA-ox**, **CA-mn** and **CA-mx** predicted toxicity was calculated using OSIRIS Property Explorer and PreADMET.

Property	CA-on	CA-ox	CA-mn	CA-mx
AMES Mutagenicity	0.802	0.685	0.655	0.655
Rat Oral Acute Toxicity	0.357	0.482	0.680	0.569
Skin Sensitization	0.920	0.576	0.272	0.201
Carcinogenicity	0.704	0.503	0.656	0.647
Respiratory	0.199	0.153	0.148	0.337
Human Hepatotoxicity	0.700	0.724	0.695	0.828
Hematotoxicity	0.241	0.205	0.270	0.229

Table S12 Main features of the five drug-likeness rules evaluated throughout this work.

Lipinski	Ghose	Veber	Egan	Muegge
MW ≤ 500 Da MLOGP ≤ 4.15 #H-bond donors ≤ 5 #H-bond acceptors ≤ 10	160 Da ≤ MW ≤ 480 Da -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ #atoms ≤ 70	#Rotatable bonds ≤ 10 TPSA ≤ 140 $Å^2$	WLOGP ≤ 5.88 TPSA ≤ 131.6 $Å^2$	200 Da ≤ MW ≤ 600 Da -2 ≤ XLOGP3 ≤ 5 TPSA ≤ 150 Å2 #Rings ≤ 7 #Carbons > 4 #Heteroatoms > 1 #Rotatable bonds ≤ 15 #H-bond donors ≤ 5 #H-bond acceptors ≤ 10

Table S13 PASS prediction of the main potential activities of **CA-on** and **CA-ox** compounds. The results are expressed for a molecule's probability of being active Pa > 0.59.

Biological Activity	Pa	Pi
Antiallergic	0.737	0.007
Phobic disorders treatment	0.699	0.077
Vasoprotector	0.594	0.021

S7 Cartesian Coordinates of all the Stationary Points as Computed at the M06-2X-D3/6–311G(d,p) level of approximation, in benzene at ambient temperature.

1 (Electronic Energy = -629.598186 Hartree; Vibrational frequency = 53.28 cm^{-1}**)**

C	-0.74181100	-0.46774900	-0.13771100
N	0.15941400	0.44534700	0.11859000
C	1.57116200	0.11164400	0.05421800
C	2.03544000	-1.15146000	0.40160500
C	3.39783300	-1.41331600	0.31513500
C	4.27857500	-0.42140600	-0.10318500
C	3.79739800	0.84433800	-0.42583600
C	2.43956000	1.12017400	-0.34186800
O	-2.96067600	-1.23112000	-0.34713400
C	-2.13856800	-0.17914200	-0.06197000
C	-2.88519400	0.93047400	0.23314600
C	-4.24905000	0.52443400	0.12355200
C	-4.22925200	-0.78626300	-0.22885500
O	-0.13023400	1.65212300	0.39691400
H	-0.41328200	-1.45225000	-0.43090500
H	1.35613200	-1.91113400	0.76673900
H	3.77043600	-2.39171200	0.59176100
H	5.33933900	-0.63074300	-0.16497600
H	4.48166500	1.62193500	-0.74188000
H	2.03233400	2.09608800	-0.56702100
H	-2.48343800	1.89357600	0.48931400
H	-5.12646900	1.12881800	0.28432500
H	-5.00189400	-1.51039400	-0.42511800

2 (Electronic Energy = -309.580983 Hartree; Vibrational frequency = 37.90 cm^{-1}**)**

C	-0.51033400	-0.22299700	-0.00000100
C	-0.01349400	1.08643100	-0.00000100

C	1.35242300	1.32611800	0.00000000
C	2.25438100	0.26380500	0.00000100
C	1.77603100	-1.04067800	0.00000100
C	0.40624000	-1.27853200	0.00000000
H	-0.69864700	1.92575100	-0.00000200
H	1.71807700	2.34615100	-0.00000100
H	3.32069500	0.45475500	0.00000100
H	2.46795300	-1.87445500	0.00000100
H	0.03595900	-2.29835000	0.00000000
C	-1.95184200	-0.53330200	-0.00000100
H	-2.18815300	-1.59461700	-0.00000300
C	-2.95801800	0.33823300	0.00000100
H	-3.98491200	-0.00479500	0.00000100
H	-2.80329600	1.41109800	0.00000400

CA-mn (Electronic Energy = -939.232591 Hartree; Vibrational frequency = 14.13 cm^{-1}**)**

C	-0.60774100	1.01382000	0.70800700
N	-1.25895200	0.47158500	-0.49351400
C	-2.58457700	-0.01725700	-0.29735400
C	-3.55891900	0.86416700	0.18259800
C	-4.86611300	0.43116900	0.35059500
C	-5.22708800	-0.87460900	0.02822100
C	-4.26312900	-1.73773300	-0.47651300
C	-2.94634800	-1.31896400	-0.64282300
O	1.56868500	2.03576100	1.09626900
C	0.49992800	1.92234100	0.27070600
C	0.68487800	2.67142300	-0.84430600
C	1.97117600	3.28915500	-0.69744800
C	2.45716700	2.86485800	0.49354000
O	-0.37977600	-0.54738300	-0.91032500
H	-1.34118500	1.55449900	1.30604800
H	-3.29739200	1.89360900	0.39730300

H	-5.60995400	1.12444800	0.72485900
H	-6.24935300	-1.20756700	0.15630200
H	-4.53153400	-2.75184500	-0.74822600
H	-2.20375400	-1.98546600	-1.05861800
H	0.00114300	2.73890400	-1.67413600
H	2.46419900	3.95241800	-1.38917700
H	3.36970100	3.04947400	1.03394500
C	1.66901800	-1.41908100	0.01157800
C	2.29831200	-2.49420100	0.63766900
C	3.66799800	-2.68955600	0.49970300
C	4.42034300	-1.81286000	-0.27533600
C	3.79418000	-0.74563100	-0.91143600
C	2.42472800	-0.54688800	-0.77075100
H	1.71149800	-3.18365000	1.23660700
H	4.14537400	-3.52937700	0.99053100
H	5.48724300	-1.96459800	-0.38768300
H	4.37247300	-0.06246300	-1.52252400
H	1.93517200	0.27791200	-1.27379500
C	0.19504800	-1.19302800	0.24960400
H	-0.30213100	-2.15637000	0.39806600
C	-0.11136400	-0.24817600	1.43046100
H	-0.91730800	-0.64914000	2.04586800
H	0.76221000	-0.06259400	2.05140000

TS-mn (Electronic Energy = -939.164953 Hartree; Imaginary vibrational frequency = -486.28 cm^{-1}**)**

C	-0.70416800	1.26322500	0.21890900
N	-1.28150900	0.30912500	-0.53931900
C	-2.65276400	-0.03252900	-0.33168600
C	-3.61018400	0.95874000	-0.11464100
C	-4.93196300	0.59363300	0.10140500
C	-5.30534400	-0.74745900	0.08578000
C	-4.34704500	-1.72503100	-0.15885100

C	-3.01918100	-1.37535100	-0.37251000
O	1.00183900	2.88283400	0.52971700
C	0.57365900	1.81879900	-0.20438300
C	1.48461900	1.51273100	-1.16763100
C	2.54048800	2.46884500	-1.02640800
C	2.19816000	3.26262900	0.01704200
O	-0.48410500	-0.62354700	-0.94066000
H	-1.36732200	1.94910700	0.73150300
H	-3.33479200	2.00548900	-0.14692900
H	-5.67566000	1.36349600	0.26688700
H	-6.33916300	-1.02559700	0.24844800
H	-4.63215300	-2.76976700	-0.18608600
H	-2.26016000	-2.11506000	-0.58371900
H	1.41107100	0.68673700	-1.85377800
H	3.43915600	2.54025400	-1.61677400
H	2.66766200	4.10546900	0.49506600
C	1.72661300	-1.36058700	0.60490900
C	2.77968500	-0.49922500	0.93214500
C	4.06950800	-0.75073400	0.48303700
C	4.33548300	-1.86928000	-0.30127100
C	3.29809000	-2.73641500	-0.63297800
C	2.00976200	-2.48260100	-0.18336200
H	2.59631700	0.38248900	1.53572100
H	4.86958800	-0.06823400	0.74511800
H	5.34240800	-2.06376400	-0.65077600
H	3.49341900	-3.60826000	-1.24616200
H	1.19776600	-3.14809100	-0.45649200
C	0.34046400	-1.12722600	1.03297500
H	-0.31012900	-1.99230300	0.98415100
C	-0.09399000	-0.01767000	1.74346300
H	-1.03895500	-0.08612000	2.27175300
H	0.61828900	0.67901600	2.16917700

CA-mx (Electronic Energy = -939.229607 Hartree; Vibrational frequency = 32.80 cm^{-1}**)**

C	-1.39009700	-0.44965800	0.28151700
N	-0.66551000	0.22477000	-0.80849500
C	0.21916100	1.27448300	-0.47118600
C	-0.19764700	2.22804400	0.46421000
C	0.63969600	3.28528200	0.79854600
C	1.88678800	3.42007300	0.19900400
C	2.27966100	2.48848400	-0.75760800
C	1.45525500	1.42687200	-1.10417300
O	-3.65049600	-0.86758500	1.03299600
C	-2.85900200	-0.22904600	0.13479700
C	-3.60881700	0.50144100	-0.72488500
C	-4.97462500	0.29623900	-0.32723600
C	-4.93603500	-0.53770000	0.73690400
O	-0.08741400	-0.77434700	-1.61518100
H	-1.06259100	-0.03739200	1.24112600
H	-1.18191500	2.15328600	0.91261500
H	0.30566500	4.01188800	1.52995300
H	2.53757500	4.24372200	0.46425900
H	3.24438000	2.58335500	-1.24246200
H	1.76614800	0.70169600	-1.84214400
H	-3.22784300	1.09980100	-1.53559300
H	-5.85881300	0.71548700	-0.77869300
H	-5.69091200	-0.97361900	1.36870600
C	1.58552700	-1.64763400	-0.08019700
C	1.72063600	-1.13448800	1.20784100
C	2.97767000	-0.82526800	1.71802300
C	4.11462000	-1.03488900	0.94709400
C	3.99219200	-1.56752700	-0.33359900
C	2.73553500	-1.87179400	-0.83929400
H	0.84695700	-0.95521400	1.82392100

H	3.06562000	-0.41390600	2.71628700
H	5.09278600	-0.79006700	1.34322400
H	4.87523000	-1.74352200	-0.93627100
H	2.63813400	-2.27270600	-1.84333400
C	0.24323700	-1.87473600	-0.74347400
H	0.30202800	-2.73835600	-1.40674300
C	-0.97573600	-1.93724000	0.17232900
H	-1.76804900	-2.50540500	-0.31386200
H	-0.77067600	-2.38262200	1.14426400

TS-mx (Electronic Energy = -939.162166 Hartree; Imaginary vibrational frequency = -510.64 cm^{-1}**)**

C	-1.67030300	0.66854400	0.37295700
N	-0.67873200	0.72727500	-0.53812900
C	0.41876000	1.63239300	-0.37983700
C	0.21033900	2.91522900	0.12663400
C	1.29094100	3.77567000	0.27414900
C	2.56824800	3.37282000	-0.10127700
C	2.75733200	2.10332700	-0.63976500
C	1.68881100	1.22971500	-0.78747200
O	-3.97070500	0.32826500	0.83054400
C	-2.93750200	0.05660500	-0.01117600
C	-3.35236300	-0.76038800	-1.01765100
C	-4.74666000	-0.99155200	-0.78500400
C	-5.06076300	-0.31538200	0.34606500
O	-0.47295700	-0.37276600	-1.17660600
H	-1.75084400	1.49864900	1.06329100
H	-0.78690100	3.25574400	0.37491200
H	1.12710700	4.77055000	0.66981400
H	3.40709100	4.04824200	0.01248600
H	3.74629500	1.78237400	-0.94421500
H	1.82110500	0.23928700	-1.20088100
H	-2.72803400	-1.14019900	-1.80730600

H	-5.41873300	-1.58728200	-1.38055900
H	-5.96935300	-0.19156000	0.91012900
C	1.21874500	-1.82261200	0.40398900
C	2.12828800	-1.34739900	1.35344700
C	3.49798900	-1.45981000	1.14460100
C	3.98631700	-2.06707200	-0.00737100
C	3.08984100	-2.57875700	-0.94422700
C	1.72367400	-2.46125600	-0.73642700
H	1.76955600	-0.88046500	2.26260100
H	4.18610400	-1.07470200	1.88802700
H	5.05407300	-2.15354000	-0.16916600
H	3.45889000	-3.06349600	-1.84050800
H	1.02592800	-2.83001700	-1.48052500
C	-0.24137000	-1.66235700	0.54812700
H	-0.84111500	-2.41277400	0.04566300
C	-0.85819800	-0.87434200	1.51239300
H	-1.82201300	-1.18150700	1.89870800
H	-0.25149700	-0.29447100	2.19999500

CA-on (Electronic Energy = -939.229126 Hartree; Vibrational frequency = 29.23 cm^{-1}**)**

C	-0.24239000	0.78767900	0.02296900
N	-0.91698000	-0.17774400	-0.87478900
C	-1.49892600	-1.32337300	-0.30226900
C	-2.23122100	-1.18908300	0.88414400
C	-2.85230800	-2.29721200	1.44224500
C	-2.76147000	-3.54577900	0.83360700
C	-2.04111300	-3.67074200	-0.34840500
C	-1.41104300	-2.57235700	-0.92323700
O	-0.65484700	2.95705600	1.00880300
C	-1.09556100	2.00661800	0.14703400
C	-2.25561300	2.39712800	-0.43626700
C	-2.55434800	3.69236600	0.10925200

C	-1.55293000	3.97616100	0.97331200
O	-0.00002200	-0.53586600	-1.90556300
H	-0.07443100	0.35156800	1.01396500
H	-2.32939400	-0.21679500	1.35287500
H	-3.41497600	-2.17958700	2.36078200
H	-3.24849900	-4.40676400	1.27375600
H	-1.96230800	-4.63559500	-0.83563700
H	-0.85127100	-2.67169600	-1.84184900
H	-2.81934800	1.82590300	-1.15491400
H	-3.40159300	4.31913300	-0.11565400
H	-1.33761300	4.81489000	1.61306400
C	2.26453400	0.28954300	-0.09182300
C	2.13028400	-1.06101100	0.24308800
C	3.21535000	-1.77400400	0.74021400
C	4.44805000	-1.15138600	0.90927300
C	4.58965000	0.19220400	0.58068800
C	3.50361300	0.90549800	0.08451500
H	1.17641300	-1.56212500	0.11596600
H	3.09533500	-2.81975100	0.99727900
H	5.29110000	-1.70901500	1.29914300
H	5.54379000	0.68798000	0.71475800
H	3.61680200	1.95544300	-0.16502600
C	1.11285600	1.07592900	-0.66998900
H	1.33634300	2.14237800	-0.62818100
C	0.76975000	0.63334400	-2.09820600
H	0.17700300	1.39797200	-2.61246000
H	1.63746300	0.35161900	-2.69114700

TS-on (Electronic Energy = -939.163319 Hartree; Imaginary vibrational frequency = -507.19 cm^{-1}**)**

C	1.21856700	-0.23234700	-0.51426000
N	0.55980300	-1.32688400	-0.09952000
C	-0.82825100	-1.51147600	-0.40271700

C	-1.38671300	-1.01318500	-1.57957600
C	-2.74962200	-1.15205600	-1.79665500
C	-3.55218100	-1.80898800	-0.86765600
C	-2.97471300	-2.34789300	0.27596800
C	-1.61283500	-2.20684400	0.51302200
O	3.23377900	0.84541900	-1.11107300
C	2.66513600	-0.18428300	-0.42552800
C	3.62646500	-0.91230400	0.20951500
C	4.87241200	-0.29397700	-0.12506000
C	4.57129300	0.76368500	-0.91783400
O	0.98052800	-1.79235600	1.03849200
H	0.77341400	0.35248100	-1.30802000
H	-0.77557900	-0.52215400	-2.32531900
H	-3.18489300	-0.74722100	-2.70203200
H	-4.61544400	-1.91329600	-1.04467300
H	-3.58603300	-2.88006300	0.99492600
H	-1.14567100	-2.61152500	1.39948100
H	3.44543300	-1.76849900	0.83564100
H	5.85777700	-0.59621500	0.18939800
H	5.16431900	1.51806400	-1.40608200
C	-0.58174700	1.51104000	0.84350100
C	-1.83255600	1.05493400	1.27426300
C	-3.00548500	1.60245800	0.77021500
C	-2.95985000	2.63039100	-0.16682900
C	-1.72362700	3.11360500	-0.58537200
C	-0.55233900	2.56029000	-0.08444100
H	-1.89898000	0.25129100	1.99708800
H	-3.96091400	1.22051700	1.11121000
H	-3.87575200	3.05383800	-0.56086900
H	-1.67111000	3.92149700	-1.30608000
H	0.40970900	2.93168600	-0.42622000
C	0.69950200	0.90549000	1.28008200

H	1.56687100	1.54647300	1.16005700
C	0.80421400	-0.15041400	2.18185600
H	1.74627800	-0.32072400	2.68433500
H	-0.06852200	-0.54122600	2.68947500

CA-ox (Electronic Energy = -939.228721 Hartree; Vibrational frequency = 21.26 cm^{-1}**)**

C	-0.27939800	0.18043300	-0.63292300
N	-1.14895900	-0.37069800	0.43077200
C	-2.54515000	-0.26534400	0.21782400
C	-3.06616900	0.96464100	-0.20117600
C	-4.43505300	1.11449500	-0.37437200
C	-5.30235200	0.05412500	-0.12791300
C	-4.78036800	-1.15978100	0.30337900
C	-3.41153700	-1.32761500	0.48256800
O	1.28372000	1.97496900	-1.02245800
C	0.42275100	1.40127700	-0.14790200
C	0.40839800	2.08125600	1.02368300
C	1.34625100	3.15778200	0.86288000
C	1.84388400	3.03886900	-0.38950300
O	-0.74226700	-1.70245000	0.66915900
H	-0.89513700	0.43962000	-1.50176600
H	-2.40037600	1.80444600	-0.36595100
H	-4.82485700	2.07216800	-0.69866500
H	-6.36970100	0.17628300	-0.26253100
H	-5.44317100	-1.99288100	0.50640700
H	-3.00835300	-2.26841500	0.82921700
H	-0.18523300	1.83105500	1.88736400
H	1.61122500	3.91052900	1.58697000
H	2.56456400	3.59935200	-0.95986600
C	2.03382700	-0.97187000	-0.42618600
C	2.21453100	-0.92197700	0.95965400
C	3.49448800	-0.90836000	1.50065300

C	4.61103000	-0.94171100	0.67005300
C	4.44029400	-0.98744000	-0.70830900
C	3.15848200	-0.99951900	-1.24930900
H	1.34930500	-0.89093300	1.61130300
H	3.62018300	-0.86686500	2.57612000
H	5.60722400	-0.92819400	1.09588000
H	5.30255400	-1.00960800	-1.36418100
H	3.02921400	-1.02537800	-2.32629200
C	0.65523100	-0.99886400	-1.04492500
H	0.75287700	-1.01131200	-2.13085500
C	-0.20190700	-2.17117200	-0.56173900
H	-1.01132100	-2.38889700	-1.26880600
H	0.36868700	-3.07159100	-0.34198300

TS-ox (Electronic Energy = -939.163496 Hartree; Imaginary vibrational frequency = 474.54 cm^{-1}**)**

C	0.37967100	0.56554800	0.51387100
N	1.44194500	0.82527900	-0.26314500
C	2.72909700	0.29768600	0.05807900
C	3.15232800	0.21932700	1.38534600
C	4.40216200	-0.31197000	1.67218600
C	5.23745100	-0.74601400	0.64678300
C	4.81886900	-0.63178800	-0.67405200
C	3.56844000	-0.10637100	-0.97709600
O	-1.74339300	1.16144200	1.36471700
C	-0.82707400	1.34687900	0.37714700
C	-1.29044800	2.25992800	-0.52594700
C	-2.56981900	2.67366200	-0.04423200
C	-2.79292700	1.96626400	1.09247500
O	1.16724700	1.00573100	-1.52159900
H	0.56536100	0.13070900	1.48722700
H	2.52916800	0.59745400	2.18569900
H	4.72944900	-0.37174300	2.70290300

H	6.21365300	-1.15439600	0.87643500
H	5.46933600	-0.95043300	-1.47944800
H	3.23657800	0.01318700	-1.99831400
H	-0.77078700	2.57364100	-1.41490900
H	-3.23892900	3.38918900	-0.49308700
H	-3.61307400	1.92085800	1.78862900
C	-1.60532800	-1.35497200	-0.42522900
C	-2.61420500	-0.68166900	-1.12479700
C	-3.93953400	-0.76386600	-0.71764300
C	-4.29394800	-1.52753000	0.39066200
C	-3.30403100	-2.21692800	1.08495300
C	-1.97883600	-2.12841600	0.68119500
H	-2.36430000	-0.07053300	-1.98347200
H	-4.70074600	-0.22382900	-1.26918000
H	-5.32887600	-1.58985600	0.70495600
H	-3.56423300	-2.82082600	1.94661700
H	-1.20988200	-2.65668400	1.23618500
C	-0.17693300	-1.23826000	-0.76719800
H	0.47470400	-1.92012300	-0.22708700
C	0.30850000	-0.71686200	-1.96376600
H	1.23617300	-1.10585400	-2.36254800
H	-0.36863700	-0.30299000	-2.69994500