Supporting Information for

Quantum Chemical Characterization of the Cyclization of the Neocarzinostatin Chromophore to the 1,5-Didehydroindene Biradical

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All geometries optimized at the BPW91/cc-pVDZ level of theory

Cartesian coordinates (ang) for Cyclonona-1,2,3,7-tetraen-5-yne:

C	2.272604	0.539208	0.000000
C	1.396199	1.609380	0.000000
C	1.911299	-0.864606	0.000000
C	0.000000	1.422583	0.000000
C	0.626975	-1.283533	0.000000
C	-0.616246	-1.577496	0.000000
C	-1.920821	-1.273374	0.000000
C	-2.332217	0.210614	0.000000
C	-1.200528	1.122627	0.000000
H	3.349147	0.765116	0.000000
H	1.804488	2.630985	0.000000
H	2.731351	-1.600059	0.000000
H	-2.733921	-2.012482	0.000000
H	-2.987329	0.392010	0.881867
H	-2.987329	0.392010	-0.881867

Cartesian coordinates (ang) for reaction **b** cyclization transition state structure:

C	1.356506	1.199507	0.000000
C	2.325214	0.148886	0.000000
C	1.972205	-1.195835	0.000000
C	0.594176	-1.466761	0.000000
C	-0.542609	-0.900519	0.000000
C	0.000000	1.002880	0.000000
C	-2.015316	-0.794152	0.000000
C	-2.357889	0.688859	0.000000
C	-1.256326	1.472772	0.000000
H	1.708814	2.241142	0.000000
H	-2.440305	-1.316754	0.886567
H	-2.440305	-1.316754	-0.886567
H	3.389218	0.424212	0.000000
H	-3.402285	1.024844	0.000000
H	2.729091	-1.990513	0.000000

Cartesian coordinates (ang) for 1,5-Didehydroindene singlet (unrestricted DFT):

C	0.424289	-1.691142	0.000000
C	1.807448	-1.438836	0.000000
C	2.300821	-0.113820	0.000000
C	1.358485	0.907589	0.000000
C	0.000000	0.762193	0.000000
C	-0.475268	-0.614220	0.000000
C	-1.167832	1.723374	0.000000
C	-2.370914	0.783135	0.000000
C	-1.913753	-0.484221	0.000000
H	0.044953	-2.720490	0.000000
H	-1.156243	2.390440	0.889381
H	-1.156243	2.390440	-0.889381
H	2.517551	-2.278182	0.000000
H	-3.410850	1.127905	0.000000
H	3.381171	0.085580	0.000000

Cartesian coordinates (ang) for 1,5-Didehydroindene triplet (unrestricted DFT):

C	-1.120003	1.327479	0.000000
C	-2.250219	0.492420	0.000000
C	-2.116537	-0.917688	0.000000
C	-0.829252	-1.441065	0.000000
C	0.321611	-0.680049	0.000000
C	0.158085	0.744479	0.000000
C	1.802731	-1.013570	0.000000
C	2.480153	0.353703	0.000000
C	1.511807	1.290089	0.000000
H	-1.232018	2.419717	0.000000
H	2.090190	-1.611570	0.891148
H	2.090190	-1.611570	-0.891148
H	-3.257229	0.934196	0.000000
H	3.566427	0.495187	0.000000
H	-3.007818	-1.560746	0.000000

Cartesian coordinates (ang) for hepta-1,2,4-trien-6-yne :

C	1.826437	-1.696282	0.000000
C	0.606610	-1.551317	0.000000
C	-0.808983	-1.494629	0.000000
C	-1.596328	-0.375465	0.000000
C	-1.216339	1.034121	0.000000
C	0.000000	1.577775	0.000000
C	1.158495	2.197310	0.000000
H	-1.320931	-2.470476	0.000000
H	-2.682325	-0.549995	0.000000
H	-2.060564	1.745883	0.000000
H	2.900293	-1.785106	0.000000
H	1.672086	2.455310	0.939991
H	1.672086	2.455310	-0.939991

Cartesian coordinates (ang) for reaction **c** cyclization transition state structure:

H	0.985412	2.293439	0.125558
C	0.190063	1.578008	-0.037868
C	-1.038273	1.278130	0.013441
C	-1.911197	0.177988	0.031980
C	-1.304769	-1.065481	0.073576
C	1.115240	-0.335664	-0.085211
C	0.109421	-1.260743	-0.062820
C	2.432479	-0.108069	0.048718
H	-2.998400	0.283402	-0.078924
H	-1.935916	-1.965810	0.064150
H	0.432387	-2.287942	-0.299085
H	2.965281	-0.422058	0.961720
H	2.993450	0.513959	-0.664317