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Antioxidant Activity in Curcuminoids				
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Optimized geometries for TSS at the B3LYP/6-31G* level of theory				
Antioxidants: Curcuminoids in the diketo form Model substrate: NO. radical				

2ts				
C	2.320985	-1.742574	0.275563	
H	2.367492	-2.092671	1.306431	
C	1.240439	-2.145053	-0.436646	
O	0.242607	-3.338443	1.364757	
C	0.210129	-3.001606	0.188390	
C	-0.934189	-3.455937	-0.729588	
H	-1.550964	-4.159837	-0.165537	
H	-0.513208	-3.949770	-1.612045	
C	-1.748150	-2.254351	-1.224770	
C	-2.847009	-1.802586	-0.353304	
H	-3.002443	-2.344067	0.575945	
C	-3.617553	-0.750830	-0.713101	
H	-3.365307	-0.291694	-1.669077	
H	1.082264	-1.859841	-1.472463	
O	-1.447985	-1.698761	-2.277301	
C	3.416566	-0.907647	-0.168686	
C	4.462331	-0.632294	0.743966	
C	3.481305	-0.345834	-1.473101	
C	5.544950	0.148987	0.374707	
H	4.400594	-1.054507	1.741279	
C	4.536381	0.452571	-1.845872	
H	2.681514	-0.541804	-2.179930	
C	5.628460	0.710596	-0.959933	
H	4.596520	0.889762	-2.837595	
C	-4.734180	-0.156850	0.004543	
C	-5.403771	0.937578	-0.590603	
C	-5.179878	-0.612045	1.258564	
C	-6.473954	1.544352	0.048158	
H	-5.065915	1.294781	-1.557621	
C	-6.252863	-0.005196	1.901899	
H	-4.682064	-1.447694	1.739618	
C	-6.907018	1.072758	1.306488	
H	-6.600561	-0.351246	2.869943	
O	-7.953407	1.665937	1.932163	
H	-8.260581	2.387648	1.354358	
O	-7.206052	2.607774	-0.418733	
O	6.650735	1.396948	-1.322317	
O	6.578992	0.494206	1.176444	
C	-6.858102	3.161087	-1.680955	
H	-7.557543	3.980284	-1.854567	
H	-5.832442	3.550667	-1.673402	
H	-6.959763	2.416797	-2.480653	
C	6.565143	0.055402	2.531016	
H	7.468131	0.465417	2.984789	
H	5.681443	0.432222	3.060428	

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H	6.588932	-1.039505	2.590882	
N	7.231090	3.320543	0.300042	
O	8.414685	3.415602	0.405515	
H	6.969554	2.501994	-0.445705	

4ts				
C	-1.963024	-1.157597	0.008647	
C	-0.800784	-0.412083	-0.113744	
C	0.487293	-1.048763	-0.099691	
H	-0.872677	0.664059	-0.220596	
C	4.191187	-0.026331	-0.346466	
C	4.287988	1.385520	-0.491861	
C	5.380957	-0.788592	-0.314534	
C	5.511225	2.001258	-0.596446	
H	3.383290	1.984546	-0.515899	
C	6.624889	-0.185254	-0.432678	
H	5.298773	-1.863772	-0.197771	
C	6.731124	1.253250	-0.597785	
H	5.598179	3.077342	-0.711830	
H	2.979015	-1.805598	-0.115748	
C	2.926993	-0.723466	-0.226160	
C	1.680912	-0.193021	-0.234110	
H	1.512282	0.875581	-0.339151	
O	7.812784	-0.826306	-0.403739	
O	7.877266	1.814714	-0.757134	
H	8.544841	1.853067	0.471174	
C	7.818805	-2.235560	-0.204409	
H	7.296812	-2.753435	-1.018436	
H	8.869226	-2.529355	-0.200256	
H	7.357495	-2.503010	0.754325	
O	7.695148	1.291101	2.067389	
N	8.736153	1.614985	1.582215	
O	0.609886	-2.299888	0.023157	
O	-1.920374	-2.481207	0.141830	
H	-0.936311	-2.723280	0.127416	
C	-3.276605	-0.545040	-0.001282	
H	-3.286709	0.535945	-0.110592	
C	-4.421302	-1.258242	0.116718	
H	-4.317071	-2.336134	0.221810	
C	-5.788296	-0.760568	0.120906	
C	-6.842048	-1.679974	0.255871	
C	-6.108264	0.612843	-0.005015	
C	-8.172623	-1.266321	0.267249	
H	-6.611782	-2.737235	0.353486	
C	-7.428779	1.026725	0.006017	
H	-5.314092	1.342437	-0.110422	
C	-8.476874	0.084825	0.143000	
H	-8.986228	-1.976736	0.371515	
O	-9.767075	0.503327	0.152321	
H	-9.754218	1.472342	0.053987	
O	-7.876533	2.319940	-0.106618	
C	-6.915190	3.356211	-0.248859	
H	-6.318811	3.220604	-1.159886	
H	-6.247885	3.399226	0.621127	
H	-7.481513	4.286157	-0.319593	

5ts				
C	7.914631	1.632787	0.008715	
C	7.884429	0.226091	0.118937	
C	6.671597	-0.446032	0.122224	
C	5.452523	0.262784	0.016543	
C	5.503520	1.664067	-0.091742	
C	6.718477	2.341073	-0.095609	
H	6.642374	-1.527272	0.205804	
H	4.584135	2.234532	-0.174960	

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H	6.762843	3.422262	-0.179371	
C	9.218985	-1.755227	0.332113	
H	10.283279	-1.987615	0.394140	
H	8.785910	-2.253370	-0.544315	
H	8.713395	-2.109122	1.239267	
O	9.131315	-0.341620	0.214274	
O	9.101330	2.290791	0.004463	
H	9.800777	1.617641	0.085691	
C	4.211256	-0.498149	0.023326	
H	4.313135	-1.579643	0.106884	
C	2.944209	-0.036297	-0.061835	
H	2.724210	1.024844	-0.147461	
C	1.797453	-0.956294	-0.043109	
C	0.472472	-0.388128	-0.133589	
H	0.349214	0.686078	-0.209800	
C	-0.649994	-1.195665	-0.125097	
C	-1.987119	-0.644828	-0.215869	
H	-2.042695	0.437582	-0.288072	
C	-3.106658	-1.415165	-0.211776	
H	-2.960540	-2.490159	-0.134768	
O	1.966429	-2.203321	0.048548	
O	-0.555129	-2.521828	-0.033460	
H	0.436880	-2.715773	0.019999	
C	-4.479700	-0.971294	-0.297742	
C	-4.846541	0.393925	-0.405730	
C	-5.506499	-1.952322	-0.267654	
C	-6.175528	0.767273	-0.487245	
H	-4.070853	1.149860	-0.423365	
C	-6.834036	-1.598200	-0.338493	
H	-5.225318	-2.998604	-0.182584	
C	-7.232432	-0.233696	-0.476037	
H	-7.625014	-2.341402	-0.321015	
O	-6.626944	2.037383	-0.580722	
C	-5.677720	3.095899	-0.583705	
H	-5.001458	3.020244	-1.444494	
H	-6.259033	4.015953	-0.658087	
H	-5.090044	3.106071	0.342920	
O	-8.465306	0.102825	-0.611981	
N	-8.991269	1.035066	1.644774	
O	-7.931963	0.820771	2.153340	
H	-8.900119	0.806842	0.524727	

6ts				
C	-2.918393	-1.912200	-0.527823	
H	-2.909770	-2.426427	-1.488308	
C	-1.859721	-2.152205	0.286270	
O	-0.746080	-3.588045	-1.248548	
C	-0.776545	-3.065122	-0.143051	
C	0.329357	-3.334065	0.887411	
H	0.998435	-4.087702	0.466086	
H	-0.129862	-3.715986	1.806284	
C	1.072566	-2.043099	1.255315	
C	2.288851	-1.738967	0.484010	
H	2.580404	-2.443774	-0.289679	
C	3.001750	-0.618182	0.742214	
H	2.612205	0.010761	1.542778	
H	-1.756371	-1.693283	1.264764	
O	0.625377	-1.307525	2.131154	
C	-4.053007	-1.057331	-0.267232	
C	-5.072745	-0.956986	-1.252350	
C	-4.202008	-0.303537	0.931958	
C	-6.179513	-0.161935	-1.064153	
H	-4.965031	-1.529654	-2.170371	
C	-5.296140	0.501137	1.132503	
H	-3.433773	-0.362312	1.696906	
C	-6.339550	0.597792	0.145096	
H	-5.415966	1.079707	2.043414	

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C	4.215087	-0.147489	0.094702	
C	4.790792	1.061202	0.551683	
C	4.843770	-0.830421	-0.962348	
C	5.947158	1.557580	-0.029343	
H	4.311941	1.594486	1.366087	
C	6.003592	-0.334850	-1.547190	
H	4.422396	-1.758506	-1.334493	
C	6.563872	0.857137	-1.089024	
H	6.492638	-0.856661	-2.363423	
O	7.694560	1.342003	-1.657688	
H	7.913426	2.172416	-1.197572	
O	-7.378538	1.322893	0.352074	
N	-7.433528	3.660337	-0.807603	
O	-8.380537	4.293739	-0.444956	
H	-7.471587	2.628623	-0.394593	
H	-6.961981	-0.092570	-1.813974	
O	6.604238	2.711649	0.317810	
C	6.067693	3.500549	1.371649	
H	6.735346	4.356946	1.477444	
H	5.057245	3.851752	1.128052	
H	6.041639	2.938058	2.313277	

7ts				
C	-4.151952	-0.641967	-0.820149	
H	-3.849513	-0.590833	-1.866079	
C	-3.390138	-1.429959	-0.028692	
O	-1.873224	-2.056878	-1.754137	
C	-2.229749	-2.150214	-0.584169	
C	-1.428254	-3.010817	0.400408	
H	-0.923543	-3.788731	-0.182083	
H	-2.072156	-3.466273	1.156803	
C	-0.379971	-2.160588	1.132204	
C	0.692688	-1.590433	0.288989	
H	0.627087	-1.770074	-0.780065	
C	1.695878	-0.871554	0.848518	
H	1.648833	-0.752248	1.930566	
H	-3.594821	-1.557728	1.030928	
O	-0.454256	-1.973227	2.339521	
C	-5.320967	0.143714	-0.456498	
C	-5.973417	0.893567	-1.452624	
C	-5.845271	0.201120	0.853588	
C	-7.094213	1.665236	-1.167126	
H	-5.590802	0.867978	-2.469790	
C	-6.960568	0.965517	1.152072	
H	-5.368354	-0.362117	1.649932	
C	-7.593107	1.704117	0.139699	
H	-7.361829	1.009387	2.159435	
C	2.817967	-0.245454	0.181354	
C	3.752888	0.465113	0.968843	
C	3.018040	-0.316714	-1.225221	
C	4.845656	1.095205	0.392481	
H	3.594698	0.507008	2.041044	
C	4.099493	0.293329	-1.811752	
H	2.309108	-0.861289	-1.840285	
C	5.047429	1.044694	-1.045466	
H	4.263155	0.252558	-2.884174	
O	6.022023	1.668948	-1.601771	
H	7.252875	1.058169	-1.246311	
O	5.793107	1.785551	1.060789	
O	-8.684778	2.436837	0.493008	
H	-9.027043	2.899356	-0.288292	
C	5.694462	1.878648	2.477617	
H	6.555659	2.467336	2.796189	
H	4.770917	2.388631	2.778069	
H	5.733388	0.886745	2.944539	
H	-7.581563	2.236468	-1.954952	
N	7.957794	0.187589	-1.025201	

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O	7.338125	-0.652834	-0.445349	

8ts				
C	8.270908	1.305276	-0.130325	
C	8.150677	-0.044868	-0.476610	
C	6.891302	-0.632400	-0.529325	
C	5.723008	0.097163	-0.241265	
C	5.873877	1.457902	0.104545	
C	7.121712	2.056362	0.160563	
H	6.805533	-1.681925	-0.798943	
H	4.996864	2.056172	0.332740	
H	7.234726	3.102491	0.426559	
O	9.470498	1.947348	-0.058176	
H	10.180425	1.323613	-0.278047	
C	4.435644	-0.579321	-0.312538	
H	4.462982	-1.629591	-0.601885	
C	3.207669	-0.075277	-0.063779	
H	3.063390	0.960905	0.232879	
C	2.001873	-0.925418	-0.191991	
C	0.729038	-0.262727	0.083626	
H	0.771331	0.737954	0.506221	
C	-0.582256	-0.809415	-0.191345	
C	-1.731315	0.088605	0.041958	
H	-1.516449	1.090091	0.406662	
C	-2.995381	-0.323639	-0.198555	
H	-3.094646	-1.343448	-0.569322	
O	2.079194	-2.123266	-0.511281	
O	-0.747875	-1.985235	-0.593606	
H	0.349308	-3.041669	0.430786	
C	-4.236671	0.417522	-0.027456	
C	-5.448873	-0.219974	-0.379627	
C	-4.295391	1.731204	0.471465	
C	-6.661931	0.436525	-0.238495	
H	-5.414001	-1.233994	-0.763610	
C	-5.510698	2.392095	0.615155	
H	-3.382126	2.244476	0.754701	
C	-6.699800	1.755085	0.263468	
H	-5.560701	3.405357	1.000820	
H	9.038869	-0.631586	-0.703638	
O	-7.902111	-0.068137	-0.543865	
C	-7.981203	-1.388610	-1.063758	
H	-7.587558	-2.120770	-0.347683	
H	-9.041076	-1.582003	-1.236539	
H	-7.433982	-1.474620	-2.010793	
O	-7.886850	2.397359	0.403383	
H	-8.580764	1.781494	0.106499	
N	0.366513	-3.332162	1.464571	
O	0.558288	-2.354864	2.139337	

9ts				
C	7.588815	0.152972	-0.542029	
C	7.240453	-1.220693	-0.314659	
C	5.923227	-1.603306	-0.204352	
C	4.863772	-0.659962	-0.291177	
C	5.203598	0.705867	-0.505017	
C	6.512550	1.103800	-0.626319	
H	5.673353	-2.649076	-0.042410	
H	4.412981	1.446788	-0.576769	
H	6.771925	2.144451	-0.798229	
O	8.815662	0.512236	-0.684229	
H	9.434547	1.247951	0.443889	
C	3.503947	-1.128921	-0.158023	
H	3.372562	-2.197789	0.003414	
C	2.363954	-0.395379	-0.209607	
H	2.380412	0.679859	-0.367651	

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C	1.040760	-1.028323	-0.053387	
C	-0.118171	-0.183877	-0.128210	
H	-0.004647	0.880993	-0.294331	
C	-1.392693	-0.714225	0.008135	
C	-2.581491	0.110311	-0.065503	
H	-2.408495	1.169316	-0.234144	
C	-3.831799	-0.392931	0.064451	
H	-3.909621	-1.465487	0.231714	
O	0.949192	-2.273256	0.138546	
O	-1.575843	-2.016207	0.213529	
H	-0.647001	-2.421718	0.233944	
C	-5.094115	0.328777	0.006685	
C	-6.291237	-0.406714	0.170778	
C	-5.188540	1.716381	-0.204633	
C	-7.523998	0.225839	0.123379	
H	-6.229647	-1.477392	0.334499	
C	-6.423723	2.353568	-0.252573	
H	-4.288574	2.308754	-0.333977	
C	-7.597614	1.619221	-0.090377	
H	-6.501145	3.423728	-0.415744	
H	8.050373	-1.940531	-0.247014	
O	-8.752132	-0.370902	0.266314	
C	-8.796652	-1.774453	0.485784	
H	-8.279429	-2.046381	1.414407	
H	-9.853277	-2.033741	0.568082	
H	-8.349826	-2.320830	-0.354229	
O	-8.803172	2.238980	-0.137885	
H	-9.482528	1.553513	-0.005146	
N	9.940845	1.632250	1.364354	
O	11.099527	1.837165	1.154868	

10ts				
C	-9.058893	0.880742	0.041538	
C	-8.840539	-0.487422	0.235517	
C	-7.540375	-0.980764	0.259098	
C	-6.427140	-0.136719	0.091702	
C	-6.676699	1.239433	-0.102122	
C	-7.966119	1.744731	-0.127785	
H	-7.378499	-2.045053	0.410070	
H	-5.844580	1.924239	-0.235308	
H	-8.154848	2.803029	-0.277047	
O	-10.303329	1.434526	0.007080	
H	-10.966546	0.738002	0.135078	
C	-5.091863	-0.717064	0.124917	
H	-5.043323	-1.794031	0.281699	
C	-3.903632	-0.090140	-0.014907	
H	-3.835290	0.982907	-0.175780	
C	-2.637526	-0.837043	0.044061	
C	-1.407151	-0.097335	-0.113543	
H	-1.436663	0.974954	-0.268924	
C	-0.182545	-0.737593	-0.070022	
C	1.063608	-0.014209	-0.227085	
H	0.968334	1.057077	-0.377373	
C	2.277823	-0.622331	-0.193230	
H	2.280068	-1.699466	-0.041278	
O	-2.628906	-2.085198	0.226346	
O	-0.089143	-2.053806	0.118368	
H	-1.043564	-2.379758	0.205452	
C	3.575037	0.000403	-0.338867	
C	4.723216	-0.825214	-0.285927	
C	3.749760	1.399121	-0.529152	
C	5.997323	-0.297331	-0.425157	
H	4.582354	-1.889811	-0.133490	
C	5.005553	1.940057	-0.659876	
H	2.881863	2.049661	-0.566735	
C	6.182244	1.126242	-0.640325	
H	5.152966	3.005223	-0.809486	

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H	-9.684656	-1.161796	0.367291	
O	7.146651	-1.004682	-0.377277	
C	7.071758	-2.406478	-0.145632	
H	6.517752	-2.912231	-0.946162	
H	8.103335	-2.760892	-0.137163	
H	6.599522	-2.624849	0.820216	
O	7.351878	1.626054	-0.828650	
N	8.303828	1.591919	1.479157	
O	7.345668	1.153955	2.042401	
H	8.109383	1.536046	0.349476	

12ts				
C	-2.167866	-1.742685	-0.742710	
H	-2.082070	-2.106008	-1.766266	
C	-1.116255	-2.006559	0.073310	
O	0.173887	-3.093395	-1.603774	
C	0.060147	-2.745866	-0.436359	
C	1.154889	-3.065257	0.591863	
H	1.902496	-3.689122	0.096756	
H	0.706287	-3.613591	1.427856	
C	1.765436	-1.780972	1.167500	
C	2.959635	-1.254198	0.484428	
H	3.327284	-1.806517	-0.376047	
C	3.559084	-0.124313	0.924010	
H	3.103005	0.342639	1.796927	
H	-1.086409	-1.690986	1.111744	
O	1.237203	-1.227522	2.127306	
C	-3.384918	-1.039574	-0.410892	
C	-4.379878	-0.886296	-1.414478	
C	-3.639527	-0.486467	0.876720	
C	-5.561461	-0.228843	-1.161893	
H	-4.191562	-1.305997	-2.399721	
C	-4.809761	0.179884	1.143500	
H	-2.892141	-0.588584	1.657596	
C	-5.827999	0.327985	0.136057	
H	-5.010265	0.605568	2.121982	
C	4.731861	0.544995	0.384441	
C	5.196894	1.714928	1.013500	
C	5.439479	0.086204	-0.748581	
C	6.312088	2.400072	0.544834	
H	4.670544	2.090826	1.887174	
C	6.551375	0.758701	-1.226264	
H	5.109845	-0.811398	-1.262827	
C	6.995229	1.923126	-0.579638	
H	7.093779	0.405735	-2.097395	
O	8.093271	2.540498	-1.094678	
H	8.297436	3.327607	-0.565213	
O	-6.935610	0.920209	0.399678	
N	-7.175710	3.391604	-0.415170	
O	-8.187277	3.879430	-0.004628	
H	-7.129089	2.312486	-0.155313	
H	6.652711	3.302634	1.048541	
H	-6.324390	-0.119477	-1.926917	

14ts				
C	-6.910161	-0.482839	-0.710900	
C	-6.647216	0.895287	-0.396351	
C	-5.357688	1.347966	-0.242701	
C	-4.241314	0.477322	-0.373776	
C	-4.493712	-0.891028	-0.674412	
C	-5.774379	-1.360799	-0.831490	
H	-5.173108	2.394849	-0.014095	
H	-3.658327	-1.576865	-0.779279	
H	-5.970944	-2.402704	-1.066337	
O	-8.106318	-0.914387	-0.896968	

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C	-2.914338	1.019701	-0.194517	
H	-2.851077	2.081819	0.037005	
C	-1.730876	0.361998	-0.277737	
H	-1.679759	-0.699848	-0.504053	
C	-0.451034	1.062470	-0.060397	
C	0.759081	0.294513	-0.159534	
H	0.713876	-0.763359	-0.390521	
C	1.995051	0.889437	0.041806	
C	3.233527	0.140804	-0.045038	
H	3.127384	-0.914102	-0.282089	
C	4.447278	0.704874	0.155254	
H	4.460481	1.767763	0.388059	
O	-0.437934	2.296581	0.205681	
O	2.096885	2.184688	0.327932	
H	1.146279	2.534919	0.348164	
C	5.750738	0.058505	0.098035	
C	6.906462	0.831507	0.335174	
C	5.931998	-1.310398	-0.182742	
C	8.178799	0.279249	0.296167	
H	6.794584	1.890437	0.554300	
C	7.198762	-1.876090	-0.224798	
H	5.071518	-1.945305	-0.371189	
C	8.330987	-1.083359	0.014752	
H	7.315519	-2.936122	-0.443256	
O	9.597851	-1.583260	-0.013042	
H	9.563985	-2.531256	-0.216541	
H	-7.498233	1.563311	-0.302745	
H	9.062918	0.881030	0.479759	
N	-8.703457	-1.641818	1.460717	
O	-7.658780	-1.322166	1.944669	
H	-8.706315	-1.298218	0.390845	

15ts				
C	6.896160	-0.483323	-0.713162	
C	6.636491	0.894806	-0.399872	
C	5.348620	1.349434	-0.241764	
C	4.229305	0.480352	-0.365676	
C	4.479967	-0.889217	-0.663910	
C	5.759622	-1.359893	-0.826115	
H	5.167456	2.397416	-0.015106	
H	3.644944	-1.576188	-0.764384	
H	5.953669	-2.402454	-1.060066	
O	8.092192	-0.916808	-0.906597	
C	2.907098	1.026546	-0.184010	
H	2.855960	2.090335	0.037340	
C	1.722997	0.359832	-0.257634	
H	1.683034	-0.703796	-0.473092	
C	0.442627	1.006317	-0.056390	
C	-0.746024	0.303981	-0.134676	
H	-0.718122	-0.757473	-0.352351	
C	-2.014987	0.965338	0.070107	
C	-3.238191	0.154906	-0.027023	
H	-3.112233	-0.901863	-0.249466	
C	-4.458061	0.706750	0.153948	
H	-4.466939	1.773988	0.372247	
O	0.467550	2.312074	0.208390	
O	-2.071034	2.198937	0.324470	
C	-5.760338	0.058038	0.094878	
C	-6.918786	0.830346	0.319261	
C	-5.936107	-1.313329	-0.176323	
C	-8.189536	0.274324	0.277889	
H	-6.810099	1.891148	0.530553	
C	-7.201004	-1.882949	-0.220860	
H	-5.071567	-1.945429	-0.355403	
C	-8.336363	-1.090887	0.006456	
H	-7.314112	-2.944822	-0.432181	
O	-9.601848	-1.594183	-0.024355	

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H	-9.564591	-2.543526	-0.220847
H	7.488429	1.562380	-0.311686
H	-9.076465	0.874884	0.451682
N	8.708186	-1.660006	1.426686
O	7.669482	-1.353188	1.929773
H	8.693053	-1.299612	0.355046
H	-0.501391	2.582173	0.316728