Supporting Information

Tautomerism of Warfarin: Combined Chemoinformatics, Quantum Chemical, and NMR Investigation

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CONTENT

Tautomer	Type	SMILES	InChIKey	FICuS	FICuu
T0R	open form	C3=C([C@H](C1=C(OC2=C(C1=O)C=CC=C2)O)CC(=O)C)C=CC=C3	InChIKey=QTXVAVXCBMYBJW-OAHLLOKOSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T0S	open form	C3=C([C@@H](C1=C(OC2=C(C1=O)C=CC=C2)O)CC(=O)C)C=CC=C3	InChIKey=QTXVAVXCBMYBJW-HNNXBMFYSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T1R_R	open form	C3=C([C@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(=O)C)C=CC=C3	InChIKey=FQEPJUOLUDFINX-NVXWUHKLSA-N	380FDC3B980D4B88-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T1R_S	open form	C3=C([C@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(=O)C)C=CC=C3	InChIKey=FQEPJUOLUDFINX-WBVHZDCISA-N	8CBCEB9521DB22A3-FICuS-01-7D	D76B88C0354759F1-FICuu-01-77
T1S_R	open form	C3=C([C@@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(=O)C)C=CC=C3	InChIKey=FQEPJUOLUDFINX-DOTOQJQBSA-N	D0B10E66C94D0FC3-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T1S_S	open form	C3=C([C@@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(=O)C)C=CC=C3	InChIKey=FQEPJUOLUDFINX-RDJZCZTQSA-N	2092FDA4C9743762-FICuS-01-4C	D76B88C0354759F1-FICuu-01-77
T2R_E	open form	C3=C([C@H](C1=C(OC2=C(C1=O)C=CC=C2)O)\C=C(\O)C)C=CC=C3	InChIKey=VWSXIGYSLWNCBN-AYJWMTRPSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T2R_Z	open form	C3=C([C@H](C1=C(OC2=C(C1=O)C=CC=C2)O)\C=C(/O)C)C=CC=C3	InChIKey=VWSXIGYSLWNCBN-QYMJWVLRSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T2S_E	open form	C3=C([C@@H](C1=C(OC2=C(C1=O)C=CC=C2)O)\C=C(\O)C)C=CC=C3	InChIKey=VWSXIGYSLWNCBN-RUMSDORHSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T2S_Z	open form	C3=C([C@@H](C1=C(OC2=C(C1=O)C=CC=C2)O)\C=C(/O)C)C=CC=C3	InChIKey=VWSXIGYSLWNCBN-SSCKCOOKSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T3R	open form	C3=C([C@H](C1=C(OC2=C(C1=O)C=CC=C2)O)CC(O)=C)C=CC=C3	InChIKey=GRAAPKVUSREWIL-OAHLLOKOSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T3S	open form	C3=C([C@@H](C1=C(OC2=C(C1=O)C=CC=C2)O)CC(O)=C)C=CC=C3	InChIKey=GRAAPKVUSREWIL-HNNXBMFYSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T4R	open form	C3=C([C@H](C1=C(C2=C(OC1=O)C=CC=C2)O)CC(=O)C)C=CC=C3	InChIKey=PJVWKTKQMONHTI-OAHLLOKOSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T4S	open form	C3=C([C@@H](C1=C(C2=C(OC1=O)C=CC=C2)O)CC(=O)C)C=CC=C3	InChIKey=PJVWKTKQMONHTI-HNNXBMFYSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T5R_RE	open form	C3=C([C@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(\O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-DEOOBNHLSA-N	380FDC3B980D4B88-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T5R_RZ	open form	C3=C([C@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(/O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-MUEZYAOPSA-N	380FDC3B980D4B88-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T5R_SE	open form	C3=C([C@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(\O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-GMZAYQHBSA-N	8CBCEB9521DB22A3-FICuS-01-7D	D76B88C0354759F1-FICuu-01-77
T5R_SZ	open form	C3=C([C@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(/O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-IHCBKXQLSA-N	8CBCEB9521DB22A3-FICuS-01-7D	D76B88C0354759F1-FICuu-01-77
T5S_RE	open form	C3=C([C@@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(\O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-ZEERGYAVSA-N	D0B10E66C94D0FC3-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T5S_RZ	open form	C3=C([C@@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(/O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-VTCQZUJXSA-N	D0B10E66C94D0FC3-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T5S_SE	open form	C3=C([C@@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(\O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-ATOWBYMVSA-N	2092FDA4C9743762-FICuS-01-4C	D76B88C0354759F1-FICuu-01-77
T5S_SZ	open form	C3=C([C@@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)\C=C(/O)C)C=CC=C3	InChIKey=UCKRWKACBKRIKB-PDOXMOPTSA-N	2092FDA4C9743762-FICuS-01-4C	D76B88C0354759F1-FICuu-01-77
T6R_R	open form	C3=C([C@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(O)=C)C=CC=C3	InChIKey=NNLYDNMZCAHUOV-NVXWUHKLSA-N	380FDC3B980D4B88-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77
T6R_S	open form	C3=C([C@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(O)=C)C=CC=C3	InChIKey=NNLYDNMZCAHUOV-WBVHZDCISA-N	8CBCEB9521DB22A3-FICuS-01-7D	D76B88C0354759F1-FICuu-01-77
T6S_R	open form	C3=C([C@@H]([C@@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(O)=C)C=CC=C3	InChIKey=NNLYDNMZCAHUOV-DOTOQJQBSA-N	D0B10E66C94D0FC3-FICuS-01-6F	D76B88C0354759F1-FICuu-01-77

T6S_S	open form	C3=C([C@@H]([C@H]1C(C2=C(OC1=O)C=CC=C2)=O)CC(O)=C)C=CC=C3	InChIKey=NNLYDNMZCAHUOV-RDJZCZTQSA-N	2092FDA4C9743762-FICuS-01-4C	D76B88C0354759F1-FICuu-01-77
T7R_E	open form	C3=C([C@H](C1=C(C2=C(OC1=O)C=CC=C2)O)\C=C(\O)C)C=CC=C3	InChIKey=FVSFCRPKSVCTBA-AYJWMTRPSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T7R_Z	open form	C3=C([C@H](C1=C(C2=C(OC1=O)C=CC=C2)O)\C=C(/O)C)C=CC=C3	InChIKey=FVSFCRPKSVCTBA-QYMJWVLRSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T7S_E	open form	C3=C([C@@H](C1=C(C2=C(OC1=O)C=CC=C2)O)\C=C(\O)C)C=CC=C3	InChIKey=FVSFCRPKSVCTBA-RUMSDORHSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T7S_Z	open form	C3=C([C@@H](C1=C(C2=C(OC1=O)C=CC=C2)O)\C=C(/O)C)C=CC=C3	InChIKey=FVSFCRPKSVCTBA-SSCKCOOKSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T8R	open form	C3=C([C@H](C1=C(C2=C(OC1=O)C=CC=C2)O)CC(O)=C)C=CC=C3	InChIKey=BBOSKMPTDUUMKL-OAHLLOKOSA-N	F827AE327B01E945-FICuS-01-5A	D76B88C0354759F1-FICuu-01-77
T8S	open form	C3=C([C@@H](C1=C(C2=C(OC1=O)C=CC=C2)O)CC(O)=C)C=CC=C3	InChIKey=BBOSKMPTDUUMKL-HNNXBMFYSA-N	E1587768B6305F57-FICuS-01-48	D76B88C0354759F1-FICuu-01-77
T9R_R	close form	C4=C([C@H]1C[C@@](OC2=C1C(C3=C(O2)C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=PIBBOXWKSPNJFI-AUUYWEPGSA-N	B2E54FE6EA5F22C5-FICuS-01-87	8F5519DD1E62B6B2-FICuu-01-8D
T9R_S	close form	C4=C([C@H]1C[C@](OC2=C1C(C3=C(O2)C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=PIBBOXWKSPNJFI-KUHUBIRLSA-N	868767C8AAA56BF2-FICuS-01-74	8F5519DD1E62B6B2-FICuu-01-8D
T9S_R	close form	C4=C([C@@H]1C[C@@](OC2=C1C(C3=C(O2)C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=PIBBOXWKSPNJFI-IFXJQAMLSA-N	3425AD28840DCB8E-FICuS-01-66	8F5519DD1E62B6B2-FICuu-01-8D
T9S_S	close form	C4=C([C@@H]1C[C@](OC2=C1C(C3=C(O2)C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=PIBBOXWKSPNJFI-LIRRHRJNSA-N	FB6B6F37AB71AFD4-FICuS-01-97	8F5519DD1E62B6B2-FICuu-01-8D
T10R_R	close form	C4=C([C@H]1C[C@@](OC2=C1C(OC3=C2C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=LSCYDZJASSKSMJ-AUUYWEPGSA-N	AEEF4BBFC9F12FC8-FICuS-01-BC	09BB2FAADA1508A7-FICuu-01-9B
T10R_S	close form	C4=C([C@H]1C[C@](OC2=C1C(OC3=C2C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=LSCYDZJASSKSMJ-KUHUBIRLSA-N	54A13A91AF246CC8-FICuS-01-61	09BB2FAADA1508A7-FICuu-01-9B
T10S_R	close form	C4=C([C@@H]1C[C@@](OC2=C1C(OC3=C2C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=LSCYDZJASSKSMJ-IFXJQAMLSA-N	42F64A70CED6F76E-FICuS-01-7F	09BB2FAADA1508A7-FICuu-01-9B
T10S_S	close form	C4=C([C@@H]1C[C@](OC2=C1C(OC3=C2C=CC=C3)=O)(O)C)C=CC=C4	InChIKey=LSCYDZJASSKSMJ-LIRRHRJNSA-N	86BE245036F78F2B-FICuS-01-5F	09BB2FAADA1508A7-FICuu-01-9B

Table SI2: Cartesian coordinates and absolute energies of the optimized geometry (B3LYP/6-311**G(d,p) of the twenty (S)-Warfarin tautomers at aqueous phase.

Tautomer **T0S**
Energy (B3LYP/6-311++G(d,p) = -1034.8618245 hartrees

C	-1.86345174	-1.72523652	1.38922039
C	-2.08276736	-0.90258533	0.27608597
C	-1.45321928	0.49602673	0.27873832
C	0.07248427	0.41932332	0.24552661
C	0.82353505	1.08323432	1.17874712
O	2.15495214	0.95256827	1.32081170
C	2.85076263	0.12315206	0.47492869
C	2.21293700	-0.51505508	-0.58952281
C	0.75518843	-0.34643854	-0.78248964
O	0.17087957	-0.84034307	-1.75513862
C	2.98851004	-1.32165893	-1.43839197
C	4.34663789	-1.47770068	-1.21486778
C	4.95958383	-0.82472729	-0.13426819
C	4.21664863	-0.01982729	0.71681747
O	0.36936436	1.94840654	2.07605344
C	-2.02555030	1.45094586	-0.78026262
C	-1.79997472	2.91805977	-0.48822593
O	-1.34263877	3.31509938	0.57936730
C	-2.17738461	3.89236728	-1.56837532
C	-2.88647526	-1.39113798	-0.75733988
C	-3.45414481	-2.66478546	-0.68158986
C	-3.22538604	-3.47440123	0.42917296
C	-2.42449640	-2.99789876	1.46807370
H	-1.24633668	-1.36399601	2.20588417
H	-1.72836902	0.91628420	1.24969806
H	2.49437145	-1.81816000	-2.26439907
H	4.93780352	-2.10385687	-1.87223122
H	6.02222162	-0.94590798	0.03962737
H	4.66961313	0.49754659	1.55333400
H	-0.40355136	2.43145732	1.68245619
H	-1.64457493	1.22781239	-1.78101079
H	-3.11536026	1.33893433	-0.84881996
H	-1.39451775	3.87163036	-2.33495879
H	-3.11035666	3.60247683	-2.05606881
H	-2.25170907	4.90148082	-1.16556681
H	-3.06983716	-0.79146696	-1.63985188
H	-4.07279167	-3.02306440	-1.49715369
H	-3.66618451	-4.46328185	0.48661609
H	-2.24150244	-3.61367520	2.34183130

Tautomer **T1S_R**
Energy (B3LYP/6-311++G(d,p) = -1034.85901688 hartrees

C	0.02916314	1.76573314	-1.34827179
C	0.59832965	1.54514853	-0.08692968
C	1.54691648	0.38337614	0.18579347
C	0.78731860	-0.97527563	0.49694970
C	0.11942896	-0.84951845	1.85489004
O	-1.23895799	-0.75705871	1.92441073
C	-2.05981729	-0.94252720	0.82445520
C	-1.56564500	-1.29452606	-0.43508350
C	-0.11736617	-1.43338421	-0.64231397
O	0.36859813	-1.88044822	-1.66868108
C	-2.47938868	-1.51181588	-1.47936454
C	-3.84031995	-1.36384935	-1.26766797
C	-4.30846568	-1.00293879	0.00205554
C	-3.42335527	-0.79578926	1.05414190
O	0.73858730	-0.79184763	2.88489142
C	2.60584402	0.20785531	-0.92478115
C	3.78877561	-0.68617790	-0.57205311
O	4.13252567	-1.58187174	-1.32326383
C	4.54418000	-0.40033277	0.70517471
C	0.28386385	2.43260276	0.95001241
C	-0.58196597	3.50534006	0.73865014
C	-1.14534980	3.71093309	-0.51941988
C	-0.83463963	2.83869305	-1.56244464
H	0.26085701	1.10704294	-2.17709243
H	2.07038379	0.61541309	1.11514375
H	1.55423157	-1.74451153	0.62116591
H	-2.09073388	-1.78892877	-2.45149122
H	-4.53953900	-1.52546415	-2.07856755
H	-5.37198311	-0.88673580	0.17386236
H	-3.77144210	-0.52875812	2.04380589
H	2.16709004	-0.17077713	-1.84658524
H	3.02215062	1.20068789	-1.13345630
H	3.96741981	-0.75555772	1.56563899
H	4.69795041	0.67299288	0.84235048
H	5.50166578	-0.91953748	0.69278497
H	0.72610198	2.29012386	1.93062175
H	-0.80844726	4.18195771	1.55492468
H	-1.81514766	4.54648437	-0.68793082
H	-1.26162397	2.99409891	-2.54679039

Tautomer **T1S_S**
Energy (B3LYP/6-311++G(d,p) = -1034.85956927 hartrees

C	0.00210025	2.01526152	-1.41583205
C	-0.62999899	1.49931443	-0.27758491
C	-1.48283308	0.24174777	-0.39804446
C	-0.72483615	-1.06914949	0.07108334
C	-0.27786454	-0.98788840	1.51647559
O	1.04931695	-0.81626625	1.78952606
C	2.03604166	-0.93062044	0.82620425
C	1.75774428	-1.24681545	-0.50730668
C	0.36632802	-1.40895768	-0.94361561
O	0.05106859	-1.76679960	-2.06648449
C	2.82946676	-1.38708201	-1.40480204
C	4.13432920	-1.20524212	-0.97773057
C	4.38557616	-0.88292377	0.36212724
C	3.34139651	-0.74805993	1.27008123
O	-1.03496504	-1.04282086	2.45011973
C	-2.86075322	0.39872855	0.28441582
C	-3.88665691	-0.67241690	-0.06530088
O	-4.45826211	-1.29420579	0.81309034
C	-4.19680887	-0.90984073	-1.52533074
C	-0.46103130	2.17103558	0.94072403
C	0.32582417	3.31934835	1.01799686
C	0.95342468	3.82024561	-0.12224087
C	0.78768124	3.16496340	-1.34130092
H	-0.12698835	1.51830790	-2.37155585
H	-1.65130100	0.07156237	-1.46304629
H	-1.44960085	-1.88678186	0.03208231
H	2.60600496	-1.63287844	-2.43556815
H	4.95649204	-1.30957357	-1.67467607
H	5.40445814	-0.73925700	0.70180636
H	3.52206037	-0.50987915	2.31050491
H	-2.77218676	0.43482383	1.36947165
H	-3.27958690	1.35471835	-0.05082750
H	-5.12195519	-1.47699679	-1.62020621
H	-4.27288485	0.03336050	-2.07189556
H	-3.38780576	-1.48550484	-1.98748636
H	-0.94767356	1.80933392	1.83908151
H	0.44282320	3.82518442	1.96976524
H	1.56180053	4.71541932	-0.06142273
H	1.26429769	3.54901132	-2.23615205

Tautomer **T2S_E**
Energy (B3LYP/6-311++G(d,p) = -1034.83868495 hartrees

C	2.91951413	-1.60768818	-0.87141924
C	1.95019202	-1.05458377	-0.02714767

C	1.31210864	0.29004348	-0.39488160
C	-0.17761245	0.33806331	-0.05482449
C	-0.71638479	1.07045689	0.96762301
O	-2.02121044	1.09869172	1.28635502
C	-2.91900511	0.35332823	0.56130362
C	-2.50203125	-0.40566745	-0.53196708
C	-1.07212010	-0.42888415	-0.90579326
O	-0.67239384	-1.07114864	-1.88668925
C	-3.47140915	-1.13655201	-1.23849775
C	-4.80108624	-1.09898978	-0.85259779
C	-5.18975288	-0.32606839	0.25252446
C	-4.25198317	0.40525136	0.96676290
O	-0.06456004	1.86850707	1.80640493
C	2.18253673	1.41476251	0.16500302
C	2.37082279	2.61932878	-0.40934062
O	3.25014085	3.53874303	0.09037688
C	1.68184238	3.15302611	-1.62348898
C	1.63591202	-1.72487543	1.15851387
C	2.27583737	-2.91925169	1.49405639
C	3.23922466	-3.46253725	0.64499547
C	3.55891033	-2.80169069	-0.54186786
H	3.17286637	-1.10105727	-1.79734900
H	1.34752229	0.34526172	-1.48572962
H	-3.14901749	-1.72744547	-2.08677930
H	-5.54307120	-1.66590862	-1.40186243
H	-6.23011848	-0.29670062	0.55395103
H	-4.52925821	1.00953602	1.82146009
H	0.84703280	1.98995759	1.45557237
H	2.79735961	1.16387608	1.02790456
H	3.72068441	3.17420943	0.85190074
H	0.98363628	2.43501378	-2.04809816
H	1.13278961	4.06413958	-1.36834849
H	2.42348477	3.42042637	-2.38170611
H	0.88287101	-1.31952029	1.82555499
H	2.01798507	-3.42532713	2.41793867
H	3.73369291	-4.39224062	0.90312445
H	4.30263224	-3.21739748	-1.21285286

Tautomer **T2S_Z**
Energy (B3LYP/6-311++G(d,p) = -1034.84056762 hartrees

C	2.97996681	-1.57195241	-0.89382615
C	2.00527051	-1.03131673	-0.04782495
C	1.32602134	0.28695029	-0.43339028
C	-0.15994937	0.31090289	-0.07541186
C	-0.67971720	0.98038163	0.99979555

O	-1.97702983	0.98288511	1.34389751
C	-2.88547856	0.27193111	0.59633081
C	-2.48574495	-0.43257773	-0.53930769
C	-1.06292539	-0.43325308	-0.93826589
O	-0.67341625	-1.03840248	-1.94608715
C	-3.46511059	-1.13258382	-1.26298246
C	-4.78810444	-1.11706986	-0.85337105
C	-5.15937015	-0.39868616	0.29363277
C	-4.21118791	0.30035306	1.02632440
O	-0.01207654	1.72638258	1.87221378
C	2.15899167	1.46024256	0.07806998
C	2.16440177	2.69647467	-0.45943912
O	1.34794502	3.08575616	-1.47910188
C	3.05599998	3.81377571	-0.02047848
C	1.71874062	-1.69091982	1.15056582
C	2.39314007	-2.86256436	1.49785930
C	3.36217872	-3.39373154	0.64760846
C	3.65334617	-2.74376052	-0.55227633
H	3.21069908	-1.07375942	-1.83016655
H	1.34379253	0.30828147	-1.52984321
H	-3.15573109	-1.68182186	-2.14347495
H	-5.53819303	-1.65913659	-1.41647159
H	-6.19449580	-0.38659253	0.61365695
H	-4.47512665	0.86176081	1.91380804
H	0.89131396	1.88247896	1.51206401
H	2.89295103	1.25547638	0.84909119
H	0.77444665	2.36185739	-1.76274061
H	3.68480315	4.13771899	-0.85523009
H	2.46008972	4.67518059	0.29457334
H	3.69637297	3.50348381	0.80407399
H	0.96191694	-1.29576177	1.81919587
H	2.15734347	-3.36073606	2.43179443
H	3.88282405	-4.30632482	0.91503041
H	4.40079917	-3.15065173	-1.22441619

Tautomer **T3S**
Energy (B3LYP/6-311++G(d,p) = -1034.83438085 hartrees

C	2.41676682	-1.25870104	-1.33560894
C	2.43567509	-0.26658912	-0.34079103
C	1.28865754	0.74922498	-0.29980694
C	-0.05649901	0.08488752	-0.02435531
C	-0.25716654	-0.73371048	1.05095942
O	-1.42744369	-1.29630726	1.38568480
C	-2.53916869	-1.06112250	0.61219018
C	-2.45712525	-0.28523888	-0.54420453

C	-1.16622265	0.32247487	-0.93465382
O	-1.05662776	0.98667569	-1.97314379
C	-3.62674011	-0.09927231	-1.29953132
C	-4.82233635	-0.67246970	-0.89902661
C	-4.87281698	-1.44650200	0.27050907
C	-3.73199978	-1.64654731	1.03377801
O	0.65391370	-1.11255541	1.94809892
C	1.55609588	1.95043935	0.64993716
C	0.60556077	3.09829092	0.46057776
O	0.84550757	3.74722224	-0.72558619
C	-0.33946094	3.46567873	1.33105528
C	3.49861497	-0.26862571	0.57158664
C	4.50791546	-1.23637175	0.49650606
C	4.47416885	-2.20980541	-0.49509132
C	3.42231707	-2.21481012	-1.41616372
H	1.60385334	-1.27485800	-2.05388449
H	1.19451908	1.15739000	-1.30876022
H	-3.56546761	0.50369502	-2.19688451
H	-5.72030525	-0.52404388	-1.48655847
H	-5.80832786	-1.89485802	0.58330466
H	-3.74658454	-2.24237792	1.93777203
H	1.55240850	-0.94746797	1.61179675
H	2.56704790	2.32299077	0.45642924
H	1.51715461	1.63761194	1.69488556
H	0.20168141	4.45637053	-0.84846064
H	-0.47522648	2.91485604	2.25151363
H	-0.99077493	4.31304639	1.14619325
H	3.56457822	0.48883986	1.34348179
H	5.31919795	-1.21656863	1.21530367
H	5.25704274	-2.95697137	-0.55575756
H	3.38898759	-2.96531725	-2.19800089

Tautomer **T4S**
Energy (B3LYP/6-311++G(d,p) = -1034.86734476 hartrees

C	-3.16565740	-0.88939427	-0.82558246
C	-2.31144175	-0.52875965	0.22339262
C	-1.39829590	0.70302755	0.18692983
C	0.08176098	0.34345922	0.28027539
C	0.69278791	-0.64004390	-0.45530876
C	2.11709841	-0.87903301	-0.35341103
C	2.84679254	-0.08206132	0.53565743
O	2.23264136	0.88127354	1.28423629
C	0.87756247	1.14154507	1.19184854
O	0.45501318	2.03877973	1.89894932
C	4.22199107	-0.24121467	0.69629463

C	4.87604086	-1.21419487	-0.04723058
C	4.16578273	-2.02483487	-0.94400515
C	2.79847777	-1.86046192	-1.09567434
O	0.05594916	-1.44574956	-1.32104296
C	-1.68767374	1.65168723	-1.01355952
C	-0.96534176	2.98572460	-0.89351090
O	0.10031384	3.17316801	-1.45461569
C	-1.64403434	4.06694824	-0.08934535
C	-2.29916891	-1.33145339	1.37625906
C	-3.11120821	-2.45534934	1.47540988
C	-3.95573455	-2.80826626	0.41924935
C	-3.97931331	-2.02385093	-0.72842246
H	-3.21579023	-0.29159135	-1.72763889
H	-1.61805711	1.26431234	1.09779981
H	4.75214251	0.39402964	1.39469085
H	5.94520267	-1.34513649	0.07016582
H	4.68620665	-2.78123951	-1.51854109
H	2.23998222	-2.48097215	-1.78380075
H	-0.90866645	-1.36755289	-1.23117722
H	-1.37965249	1.19100226	-1.95461423
H	-2.76391466	1.84015843	-1.05100831
H	-2.48030591	4.46009646	-0.67855746
H	-2.06497101	3.67100822	0.83744001
H	-0.94907512	4.87716199	0.12735386
H	-1.64772624	-1.06730380	2.20259667
H	-3.08896727	-3.05619606	2.37756410
H	-4.58815173	-3.68514060	0.49585794
H	-4.63214533	-2.28325143	-1.55394379

Tautomer **T5S_RE**
Energy (B3LYP/6-311++G(d,p) = -1034.84263653 hartrees

C	-2.99375353	-0.02454982	-1.12591229
C	-2.45604030	0.05965620	0.16151965
C	-1.00303254	0.45310782	0.42653325
C	-0.13960861	-0.81574947	0.87070559
C	0.03297514	-1.79736181	-0.26420676
O	1.20969270	-1.78052729	-0.96910790
C	2.34435478	-1.13878768	-0.50510754
C	2.37693096	-0.44415669	0.70877930
C	1.15232533	-0.32019196	1.50969012
O	1.12299592	0.18698788	2.61931683
C	3.58882854	0.13176783	1.12383189
C	4.72550608	0.02507336	0.33929050
C	4.66456934	-0.66836672	-0.87621701
C	3.47855490	-1.25599130	-1.30203406

O	-0.81473030	-2.57226127	-0.61994890
C	-0.34376109	1.22125264	-0.68800612
C	0.03015745	2.50851605	-0.64780355
O	0.62480774	3.12352754	-1.72399911
C	-0.11283610	3.48327235	0.47846032
C	-3.29275396	-0.21162422	1.25259853
C	-4.62696529	-0.56383845	1.06413039
C	-5.15094365	-0.65174790	-0.22670067
C	-4.32996422	-0.37949725	-1.31911890
H	-2.37603829	0.19346039	-1.98839186
H	-1.00512349	1.06328917	1.33056015
H	-0.71461400	-1.32913421	1.64246921
H	3.60619673	0.66602430	2.06577409
H	5.65580162	0.47621250	0.66128080
H	5.55021398	-0.75498191	-1.49454195
H	3.42102004	-1.80583389	-2.23283529
H	-0.16296799	0.68286138	-1.61638628
H	0.71783986	2.49800766	-2.45426954
H	-0.70772333	4.34035405	0.14934554
H	0.87116041	3.86214307	0.76999755
H	-0.59095772	3.04718621	1.35256397
H	-2.89909875	-0.13972019	2.26203372
H	-5.25788490	-0.76320969	1.92318162
H	-6.18949010	-0.92393922	-0.37730520
H	-4.72772177	-0.43923233	-2.32615964

Tautomer **T5S_RZ**
Energy (B3LYP/6-311++G(d,p) = -1034.84513288 hartrees

C	2.92155793	-0.83959348	0.82961473
C	1.90730940	-0.65336910	-0.11851560
C	0.87328705	0.45842666	0.02511726
C	-0.05648751	0.20332380	1.30201704
C	-1.01174551	1.36097285	1.46435828
O	-2.14477252	1.35056050	0.68887095
C	-2.60852705	0.18679626	0.09661882
C	-2.00631480	-1.05648654	0.32079175
C	-0.78435050	-1.12440545	1.14303202
O	-0.35027866	-2.15568525	1.62447978
C	-2.58347567	-2.19986799	-0.25172735
C	-3.71894507	-2.09491412	-1.04042786
C	-4.29958156	-0.83915925	-1.25464945
C	-3.75390987	0.30564323	-0.68271293
O	-0.82954546	2.30762272	2.18113509
C	1.52529427	1.81529870	0.07946619
C	1.31989697	2.79169460	-0.81397090

O	0.43766595	2.59048558	-1.85026376
C	1.99519844	4.12879096	-0.78043198
C	1.87307952	-1.49499419	-1.23470118
C	2.82802360	-2.49890130	-1.40424534
C	3.83165419	-2.67615818	-0.45407515
C	3.87441774	-1.84209279	0.66472576
H	2.97521270	-0.20202040	1.70561872
H	0.22611459	0.42495506	-0.85247703
H	0.57217590	0.16862279	2.19076617
H	-2.11275484	-3.15889540	-0.07248575
H	-4.15434744	-2.97856892	-1.49018691
H	-5.18836833	-0.75210626	-1.86837835
H	-4.20424447	1.27985365	-0.82496880
H	2.22520271	2.01038634	0.88253515
H	0.39100127	3.37890077	-2.40272893
H	2.67269049	4.20199271	0.06969241
H	2.57127598	4.29423117	-1.69747682
H	1.25603460	4.93363202	-0.70431313
H	1.09573732	-1.36414240	-1.98028886
H	2.78515380	-3.13957254	-2.27801209
H	4.57460820	-3.45518170	-0.58235636
H	4.65166364	-1.97198329	1.40957947

Tautomer **T5S_SE**
Energy (B3LYP/6-311++G(d,p) = -1034.8423851 hartrees

C	-3.33855279	-0.14121400	0.96843164
C	-2.31184923	-0.09766964	0.01577014
C	-1.04488045	0.69410247	0.33596955
C	-0.09905450	-0.13333103	1.33142571
C	0.94212479	0.82395562	1.87060298
O	2.20440646	0.78772397	1.34971560
C	2.62244470	-0.20704101	0.48182838
C	1.82047641	-1.30437075	0.15199436
C	0.45787363	-1.39855646	0.70080566
O	-0.21387866	-2.41567911	0.64818075
C	2.34805887	-2.29539739	-0.69083880
C	3.63213327	-2.17798303	-1.19885809
C	4.41341751	-1.06747480	-0.85645373
C	3.91665803	-0.08116030	-0.01118239
O	0.70673503	1.65409187	2.70967610
C	-0.30076983	1.20602971	-0.86786758
C	-0.13782340	2.49390160	-1.20665256
O	0.55274541	2.86096704	-2.33712476
C	-0.63717725	3.71493493	-0.50014926
C	-2.50118659	-0.76748300	-1.19697588

C	-3.68113196	-1.46959092	-1.44726182
C	-4.69307420	-1.51005944	-0.48995030
C	-4.51839330	-0.83947769	0.72153698
H	-3.21764521	0.38274273	1.91180391
H	-1.35763001	1.54086040	0.94765688
H	-0.72348038	-0.42541381	2.17655908
H	1.72314508	-3.14462324	-0.93889058
H	4.03053418	-2.94036410	-1.85671077
H	5.41924917	-0.97212948	-1.24807704
H	4.51460660	0.77548185	0.27287542
H	0.13857318	0.46268585	-1.52860109
H	0.86806104	2.07558744	-2.80300019
H	-1.29222220	4.28311737	-1.16720019
H	-1.18884564	3.48047782	0.40736775
H	0.20429695	4.36341023	-0.23941278
H	-1.73333644	-0.74246630	-1.96031495
H	-3.80818011	-1.98198930	-2.39447262
H	-5.61080700	-2.05257763	-0.68690826
H	-5.30214712	-0.85431918	1.47069411

Tautomer **T5S_SZ**
Energy (B3LYP/6-311++G(d,p) = -1034.84504702 hartrees

C	3.17996922	-0.05827489	0.80401033
C	2.17435161	-0.12228906	-0.16906897
C	0.78665806	0.46395172	0.07310474
C	0.02323145	-0.31491616	1.24162187
C	-0.01953442	-1.79032693	0.92120891
O	-0.99525477	-2.21041088	0.05058107
C	-2.12570218	-1.44781360	-0.19621033
C	-2.37943716	-0.24841714	0.47885807
C	-1.36887873	0.27606516	1.41471516
O	-1.59454579	1.14544454	2.23720888
C	-3.58734528	0.42174760	0.23407526
C	-4.50106977	-0.08515695	-0.67716100
C	-4.21977644	-1.28166562	-1.34751872
C	-3.03690204	-1.97282606	-1.10600476
O	0.76222833	-2.60809465	1.32552374
C	0.85631532	1.93961120	0.36631266
C	0.33951916	2.89257960	-0.41981023
O	-0.33433565	2.53643918	-1.56535426
C	0.44255802	4.36330547	-0.15240178
C	2.47156747	-0.71537573	-1.40022959
C	3.74265450	-1.23160361	-1.65783459
C	4.73495451	-1.16424374	-0.68204396
C	4.44814766	-0.57571038	0.55126245

H	2.97857736	0.39748214	1.76743315
H	0.20470347	0.32241596	-0.83867616
H	0.58191117	-0.19036178	2.16846020
H	-3.77909542	1.34736776	0.76322420
H	-5.42687356	0.44183266	-0.87179146
H	-4.93114405	-1.68258831	-2.05985337
H	-2.81656218	-2.90946744	-1.60227628
H	1.38562259	2.25596030	1.25670440
H	-0.66296060	3.32344721	-2.01405104
H	0.95972046	4.87091745	-0.97409822
H	-0.55330210	4.81087171	-0.06162729
H	0.99084773	4.55402719	0.76961187
H	1.70531052	-0.77206058	-2.16647496
H	3.95388037	-1.68499443	-2.61992558
H	5.72293622	-1.56504426	-0.87842699
H	5.21400533	-0.51867622	1.31677907

Tautomer **T6S_R**
Energy (B3LYP/6-311++G(d,p) = -1034.84076089 hartrees

C	-2.58009409	0.88672558	1.07953210
C	-1.65875405	0.61858124	0.05935369
C	-0.73829703	-0.59162490	0.11651405
C	0.28567013	-0.46840312	1.32215813
C	1.19756707	-1.67532759	1.35823105
O	2.26775475	-1.67655861	0.50223700
C	2.73949739	-0.50635567	-0.07456412
C	2.22428660	0.75004649	0.26261610
C	1.07881761	0.82936850	1.18693482
O	0.74999039	1.84389115	1.77281970
C	2.81146036	1.89367830	-0.29857211
C	3.86905562	1.77598401	-1.18776779
C	4.36090162	0.50711732	-1.51552233
C	3.80590882	-0.63951828	-0.95578851
O	1.02284105	-2.64657088	2.04460500
C	-1.52883541	-1.92440688	0.19350320
C	-2.40917523	-2.15499238	-1.00312336
O	-1.67014986	-2.18193533	-2.16036613
C	-3.73138574	-2.33786537	-0.96023224
C	-1.60712025	1.48320751	-1.03822154
C	-2.45406774	2.58967262	-1.11890923
C	-3.36570620	2.84729648	-0.09728973
C	-3.42578800	1.99080829	1.00339351
H	-2.64401557	0.23549487	1.94460159
H	-0.15458699	-0.60844589	-0.80641247
H	-0.26805476	-0.45089678	2.26038840

H	2.40937454	2.86350541	-0.03189005
H	4.31155265	2.66047012	-1.62879548
H	5.18815811	0.41039685	-2.20863610
H	4.19074218	-1.62522624	-1.18454113
H	-0.82524574	-2.75988458	0.25333829
H	-2.13939189	-1.95329244	1.09696147
H	-2.25125597	-2.32364085	-2.91854894
H	-4.25721308	-2.29966085	-0.01635331
H	-4.31062108	-2.53019683	-1.85682804
H	-0.90127402	1.29017679	-1.83914649
H	-2.39953992	3.24701866	-1.97947995
H	-4.02418876	3.70652250	-0.15622694
H	-4.13157906	2.18309561	1.80373033

Tautomer **T6S_S**
Energy (B3LYP/6-311++G(d,p) = -1034.83845687 hartrees

C	-2.21182471	-1.13488240	-0.84409066
C	-2.11234973	-0.27250513	0.25347080
C	-0.91561463	0.63825198	0.48265406
C	0.20032152	-0.08206868	1.36110448
C	1.15854118	0.97206258	1.88142444
O	2.38546694	1.09888632	1.29082159
C	2.86059514	0.19181578	0.35639013
C	2.16824574	-0.97692841	0.02506918
C	0.86750075	-1.25404363	0.65619695
O	0.32859537	-2.34710713	0.62001766
C	2.74842850	-1.86642871	-0.89292228
C	3.97476906	-1.58060523	-1.47162123
C	4.64626216	-0.40168518	-1.12523051
C	4.09733435	0.48673053	-0.20648407
O	0.88195610	1.73865899	2.76607326
C	-0.34286598	1.28449273	-0.80090166
C	-1.32313146	2.18504479	-1.50360052
O	-1.79645716	3.15623908	-0.65684067
C	-1.66877648	2.08471688	-2.78955250
C	-3.16262230	-0.25196459	1.18027280
C	-4.27876938	-1.07138386	1.02118165
C	-4.36464831	-1.92742168	-0.07671762
C	-3.32799673	-1.95433762	-1.00878514
H	-1.42032507	-1.17680385	-1.58201198
H	-1.25686285	1.45077746	1.12636771
H	-0.32038572	-0.47491997	2.23546394
H	2.20931598	-2.77244002	-1.14116586
H	4.41284333	-2.26490524	-2.18749025
H	5.60681420	-0.17485838	-1.57238407

H	4.61135168	1.39520800	0.08061457
H	0.52323938	1.89921078	-0.53037087
H	0.01278785	0.53506462	-1.50811253
H	-2.42825998	3.71916199	-1.12202128
H	-1.26337520	1.29271694	-3.40370582
H	-2.35624392	2.78393496	-3.25304213
H	-3.10796024	0.41603088	2.03433638
H	-5.08111430	-1.03637585	1.74965698
H	-5.23246845	-2.56417479	-0.20661922
H	-3.38623877	-2.61420642	-1.86724017

Tautomer **T7S_E**
Energy (B3LYP/6-311++G(d,p) = -1034.85084167 hartrees

C	-1.84147930	-1.54408196	-1.14549431
C	-2.19831570	-0.74776937	-0.05293433
C	-1.32520773	0.42126772	0.41748186
C	0.16394272	0.07184139	0.40314433
C	1.08882505	0.50236267	-0.51481359
C	2.47112878	0.07133151	-0.44831233
C	2.83759591	-0.78456413	0.59558978
O	1.92485591	-1.18604521	1.52795140
C	0.59641677	-0.79208299	1.48512279
O	-0.11172180	-1.21140257	2.38212667
C	4.14338634	-1.25393990	0.72882947
C	5.09705457	-0.85748846	-0.19892931
C	4.75362501	0.00159124	-1.25241696
C	3.45287751	0.46321772	-1.37603397
O	0.81109358	1.32800042	-1.53551762
C	-1.73157872	1.68359736	-0.34251684
C	-1.67068082	2.93873291	0.14186312
O	-2.14690847	4.01597220	-0.55290338
C	-1.09265696	3.36928859	1.45117750
C	-3.41505300	-0.99999691	0.59016185
C	-4.25625859	-2.02281525	0.15406626
C	-3.89222318	-2.81050207	-0.93851936
C	-2.68194245	-2.56694873	-1.58688994
H	-0.89961300	-1.37425666	-1.65575576
H	-1.57258613	0.57120257	1.47087873
H	4.38886408	-1.91484849	1.55068222
H	6.11482684	-1.21696771	-0.10355587
H	5.50577219	0.30523984	-1.97023271
H	3.17573748	1.12678367	-2.18442480
H	-0.08644210	1.70014710	-1.40561103
H	-2.22479913	1.53207038	-1.30112109
H	-2.54786261	3.72906125	-1.38419489

H	-0.26403644	4.06321612	1.28177359
H	-1.85072114	3.90184369	2.03267456
H	-0.72526478	2.52793960	2.03481949
H	-3.70541636	-0.39299228	1.44178657
H	-5.19241692	-2.20636571	0.66977217
H	-4.54345088	-3.60774007	-1.27870953
H	-2.38788204	-3.17478020	-2.43549427

Tautomer **T7S_Z**
Energy (B3LYP/6-311++G(d,p) = -1034.85257261 hartrees

C	-3.45041989	-0.97963089	0.58116238
C	-2.22517671	-0.73009544	-0.04653132
C	-1.34799706	0.42386776	0.45076595
C	0.14154305	0.07355529	0.43505890
C	1.04975339	0.46809299	-0.51689943
C	2.43004267	0.02991685	-0.46247774
C	2.80940271	-0.79943203	0.59836825
O	1.91111967	-1.17120167	1.55720875
C	0.58470415	-0.77312255	1.52637876
O	-0.11444023	-1.17331308	2.43887826
C	4.11450032	-1.27309157	0.72168347
C	5.05353838	-0.90903325	-0.23376445
C	4.69678660	-0.07757764	-1.30489470
C	3.39705606	0.38895106	-1.41848659
O	0.75448614	1.25813419	-1.55882702
C	-1.73389524	1.71224981	-0.27347241
C	-1.52555492	2.95683758	0.19846037
O	-0.85270919	3.23165974	1.35226986
C	-1.99545736	4.21076948	-0.46711352
C	-1.86190448	-1.51631061	-1.14389144
C	-2.70644423	-2.52636191	-1.60651926
C	-3.92571364	-2.76726923	-0.97432795
C	-4.29532166	-1.98987072	0.12356341
H	-3.74476661	-0.38092305	1.43724765
H	-1.60272594	0.54326631	1.51027024
H	4.37062557	-1.91274834	1.55695002
H	6.07061546	-1.27245179	-0.14642287
H	5.43791278	0.20077206	-2.04404871
H	3.10936893	1.03163461	-2.23995791
H	-0.13928150	1.64161063	-1.42796498
H	-2.32591145	1.62059049	-1.17682540
H	-0.54280098	2.42169623	1.77748822
H	-2.67342614	4.75426172	0.19786070
H	-1.14817679	4.86886482	-0.68033346
H	-2.51615600	3.98890247	-1.39759147

H	-0.91333851	-1.34930783	-1.64207625
H	-2.40813735	-3.12645938	-2.45905741
H	-4.57975363	-3.55480853	-1.33121176
H	-5.23835150	-2.17180390	0.62705834

Tautomer **T8S**
Energy (B3LYP/6-311++G(d,p) = -1034.8466979 hartrees

C	-2.33578511	-1.30347341	1.34811915
C	-2.32648414	-0.48199644	0.20824875
C	-1.39333997	0.73584871	0.19266296
C	0.07510614	0.33843485	0.31775877
C	0.68644875	-0.58665413	-0.48884640
C	2.10317678	-0.86382434	-0.38428892
C	2.82798470	-0.16408075	0.58681412
O	2.21141540	0.72515491	1.41919927
C	0.85518577	1.00353141	1.34398409
O	0.42980878	1.79190736	2.16742815
C	4.19897866	-0.35516806	0.75007631
C	4.85242647	-1.26391509	-0.07137816
C	4.14580429	-1.97982949	-1.04812639
C	2.78300121	-1.78304470	-1.20339484
O	0.04946644	-1.29621053	-1.43776534
C	-1.62720502	1.68742897	-1.01609028
C	-0.96619947	3.02831122	-0.86571277
O	-1.59306029	3.78018221	0.09681659
C	0.07919681	3.45639918	-1.57949299
C	-3.17652056	-0.81775121	-0.85288237
C	-4.00551211	-1.94322400	-0.78043406
C	-4.00278442	-2.74496524	0.35515019
C	-3.16326616	-2.41786867	1.42380025
H	-1.68814171	-1.06143043	2.18416811
H	-1.62170352	1.30983123	1.09259948
H	4.72607775	0.20422596	1.51276381
H	5.91800974	-1.41972017	0.04847614
H	4.66539612	-2.68811739	-1.68175541
H	2.22707762	-2.32950486	-1.95364812
H	-0.91449925	-1.22539124	-1.34040661
H	-1.28134709	1.23054916	-1.94504139
H	-2.70346271	1.86024615	-1.11339616
H	-1.13136845	4.62068745	0.20960876
H	0.52563326	2.81827271	-2.32945844
H	0.50660559	4.44257469	-1.43276343
H	-3.21351031	-0.20639871	-1.74644757
H	-4.65364613	-2.18181150	-1.61601106
H	-4.64668997	-3.61495901	0.41294440

H	-3.15674923	-3.03227835	2.31713333

Tautomer **T9S_R**
Energy (B3LYP/6-311++G(d,p) = -1034.85863101 hartrees

C	3.33685297	-1.23991493	-0.85163189
C	2.10147629	-0.86697770	-0.30086617
C	1.17624139	0.05110511	-1.11174011
C	-0.24393147	0.11403986	-0.60429827
C	-0.67572927	1.22860475	0.05511494
O	-1.92476376	1.40403299	0.51809565
C	-2.85878718	0.40979208	0.33405358
C	-2.53808573	-0.77058900	-0.34010610
C	-1.16972419	-0.96752860	-0.86543380
O	-0.84751127	-1.98826604	-1.48850741
C	-3.54350642	-1.73900471	-0.49367680
C	-4.81445845	-1.52241679	0.01276758
C	-5.10646102	-0.32652276	0.68598914
C	-4.13187689	0.64719227	0.85002308
O	0.03298740	2.31272213	0.33643053
C	1.48298150	2.35538985	-0.01346758
C	1.71703016	1.49263141	-1.25371920
O	2.20497905	1.94147665	1.10806252
C	1.76925254	3.82815533	-0.22947473
C	1.76963103	-1.35058587	0.96943553
C	2.65322919	-2.16961730	1.67864382
C	3.87873715	-2.52515472	1.12313520
C	4.21640437	-2.05878701	-0.14979412
H	3.60885443	-0.89043968	-1.84252698
H	1.13680761	-0.37196852	-2.11965585
H	-3.29572400	-2.65464534	-1.01631859
H	-5.58430892	-2.27481264	-0.10893771
H	-6.10047550	-0.15671354	1.08246577
H	-4.33581391	1.57740163	1.36546455
H	2.78694617	1.49189433	-1.46763071
H	1.21465026	1.97369727	-2.09613991
H	2.28052841	0.97621417	1.13003482
H	1.15047728	4.22559070	-1.03409908
H	2.82105865	3.95688122	-0.48906220
H	1.56253714	4.37983127	0.68916820
H	0.81113461	-1.09941150	1.40941840
H	2.37426836	-2.53211943	2.66165561
H	4.56343717	-3.16299260	1.67028384
H	5.16443495	-2.33700083	-0.59649509

Tautomer **T9S_S**

Energy (B3LYP/6-311++G(d,p) = -1034.85713997 hartrees

C	3.26548185	-1.28492885	-0.90128352
C	2.23306493	-0.78535346	-0.10248017
C	1.39708261	0.39627683	-0.58970187
C	-0.09045365	0.25460995	-0.32088169
C	-0.78491408	1.28609464	0.24370227
O	-2.08842393	1.25000511	0.56552987
C	-2.81362579	0.10791975	0.31522596
C	-2.23869835	-0.97926279	-0.34511242
C	-0.81736757	-0.92523652	-0.75328838
O	-0.29626367	-1.83104688	-1.41464063
C	-3.04334898	-2.10315373	-0.59367322
C	-4.36698585	-2.12597887	-0.18597306
C	-4.91605550	-1.01816959	0.47750565
C	-4.14391833	0.10611372	0.73172504
O	-0.30605792	2.48675527	0.55135003
C	0.98337045	2.87393893	-0.07631097
C	1.93634112	1.69204665	0.06096086
O	0.73463679	3.24672722	-1.40201539
C	1.41800343	4.11177970	0.67958247
C	2.03864190	-1.34116530	1.16659914
C	2.85057559	-2.37926808	1.62114991
C	3.87702566	-2.87353905	0.81503187
C	4.08297003	-2.32097563	-0.44852919
H	3.42839497	-0.86547665	-1.88910283
H	1.54457088	0.45019801	-1.67527574
H	-2.59887114	-2.94719284	-1.10643375
H	-4.98017232	-2.99827092	-0.37756484
H	-5.95185882	-1.03559987	0.79512010
H	-4.54798043	0.97352019	1.23855869
H	2.09727615	1.52237920	1.12788449
H	2.89917644	1.95965440	-0.37783433
H	0.67178849	2.47070761	-1.97294788
H	2.37270748	4.46112169	0.28434892
H	0.67302011	4.89922202	0.55387787
H	1.52986807	3.88969965	1.74086210
H	1.24278309	-0.96813099	1.80290950
H	2.68105703	-2.80253622	2.60516934
H	4.50774238	-3.68164350	1.16800356
H	4.87623057	-2.69766721	-1.08485841

Tautomer **T10S_R**
Energy (B3LYP/6-311++G(d,p) = -1034.87149432 hartrees

C	2.08731961	-0.99246098	1.06323563

C	2.34854705	-0.48219640	-0.21301086
C	1.24742097	0.03349406	-1.14945722
C	-0.15259206	-0.36189416	-0.75024293
C	-1.01831862	0.54188993	-0.19506526
C	-2.37509417	0.15908611	0.14552619
C	-2.75747164	-1.16192334	-0.11953154
O	-1.88834734	-2.05417316	-0.68385775
C	-0.58914061	-1.71060308	-1.02330616
O	0.08537498	-2.58479591	-1.53542922
C	-4.03996647	-1.61986141	0.17816502
C	-4.95195873	-0.74238904	0.74897470
C	-4.59068130	0.58410458	1.02303563
C	-3.31330866	1.03102669	0.72477331
O	-0.71440160	1.81890743	0.06787213
C	0.64862491	2.33867766	-0.18387686
C	1.27608676	1.56734778	-1.34415798
O	1.37550877	2.24623709	1.01097740
C	0.44435471	3.81301197	-0.47706569
C	3.68047720	-0.43709524	-0.65120603
C	4.71849155	-0.87603712	0.16504025
C	4.44639349	-1.37218595	1.44226092
C	3.12894322	-1.42982084	1.88704691
H	1.06606307	-1.06151341	1.42137704
H	1.44805461	-0.41218525	-2.12771083
H	-4.30019232	-2.64788710	-0.04086106
H	-5.95093456	-1.09081451	0.98320081
H	-5.30987564	1.26001357	1.46917123
H	-3.02060210	2.05164072	0.93264598
H	2.29766028	1.92546553	-1.48017903
H	0.71841957	1.81327798	-2.25100900
H	1.76006890	1.36333216	1.10947221
H	-0.01293112	4.29742718	0.38747648
H	1.40980252	4.28131526	-0.67431568
H	-0.20185847	3.94556198	-1.34506177
H	3.90508784	-0.05955917	-1.64376902
H	5.74020396	-0.83457534	-0.19556290
H	5.25442999	-1.71390661	2.07883593
H	2.90276177	-1.82002394	2.87296097

Tautomer **T10S_S**
Energy (B3LYP/6-311++G(d,p) = -1034.86995111 hartrees

C	3.72670105	-0.22336280	-0.72422400
C	2.51389110	-0.19384821	-0.03037317
C	1.33605716	0.60210749	-0.58755168
C	-0.00328611	-0.10465901	-0.48276400

C	-1.12018788	0.53194003	-0.00831586
C	-2.37186989	-0.17730435	0.16546273
C	-2.40955340	-1.52145151	-0.22345576
O	-1.32049476	-2.12325148	-0.78831269
C	-0.11849744	-1.45765062	-0.98441311
O	0.74566587	-2.07513587	-1.57509566
C	-3.56196625	-2.29048275	-0.07044844
C	-4.69362183	-1.70247383	0.47865036
C	-4.68058507	-0.35609604	0.86904844
C	-3.53106865	0.40157401	0.71125229
O	-1.15955170	1.82952730	0.33217410
C	-0.05193425	2.69817025	-0.10275557
C	1.25811476	1.96121046	0.14574012
O	-0.25462739	3.03718850	-1.45058592
C	-0.20730371	3.96498090	0.71410715
C	2.43123550	-0.84516132	1.20519077
C	3.53291170	-1.51976043	1.72892681
C	4.73924445	-1.54589000	1.02763811
C	4.83306086	-0.89328565	-0.20095760
H	3.80618200	0.27572020	-1.68474957
H	1.55479601	0.77636527	-1.64849462
H	-3.55452719	-3.32667899	-0.38460317
H	-5.59400678	-2.29269332	0.60157027
H	-5.57023942	0.09302724	1.29332063
H	-3.50795155	1.44167382	1.00820763
H	1.34543757	1.79775183	1.22221597
H	2.09032721	2.59847878	-0.15824292
H	0.04178883	2.32605110	-2.03197650
H	-0.14498282	3.74075819	1.77922830
H	-1.17475125	4.42283526	0.50084385
H	0.58340746	4.66822534	0.44950827
H	1.49875595	-0.83448883	1.76004023
H	3.44904178	-2.02552360	2.68454839
H	5.59598099	-2.07128982	1.43428502
H	5.76475265	-0.90817980	-0.75568583

SI3: Determination of activation energies. We calculated the transition states (TS) at the B3LYP/6-311++ G(d,p) level of theory using the self-consistent reaction field theory (SCRF) polarizable continuum model (PCM). We verified the TSs by examining the vibrational frequencies and calculating the intrinsic reaction coordinate (IRC). A TS is characterized by only one imaginary frequency. Table 1 shows the one imaginary frequency for each calculated TS. The movement of the hydrogen in each of the prototropic reactions had a similar frequency of around -2100 cm^{-1}, which was visualized in GaussView and corresponds to O-H bond stretching. The vibration mode for ring-chain equilibrium is a combination of several vibrational modes: O-H stretching, H-O-C bending and C=O stretching.

Table 1. Tautomeric equilibrium reactions of warfarin, the corresponding tautomerization equilibrium constants and energy barriers in solution.

Reaction	Equilibrium	Rule	pK_T	Transition State Energy (au)	Energy Barrier (kcal/mol)	Frequency
A	T0 ↔ T1	prototropic (Rule 6)	1.04		-	-
B	**T0 ↔ T2**	prototropic (Rule 6)	9.78	-1034.744266	60.43	-2147.12
C	**T0 ↔ T3**	prototropic (Rule 6)	12.62	-1034.748671	53.78	-2181.05
D	**T1 ↔ T4**	prototropic (Rule 6)	-3.58	-1034.759637	62.71	-2155.26
E	**T1 ↔ T5**	prototropic (Rule 6)	6.64	-1034.747541	61.24	-2196.1
F	**T1 ↔ T6**	prototropic (Rule 6)	8.65	-1034.750981	56.34	-2187.97
G	**T4 ↔ T7**	prototropic (Rule 6)	6.80	-1034.754283	61.68	-2066.03
H	**T4 ↔ T8**	prototropic (Rule 6)	9.50	-1034.756171	56.81	-2197
I	T5 ↔ T2	prototropic (Rule 6)	2.10		-	-
J	T5 ↔ T7	prototropic (Rule 6)	-3.42		-	-
K	T6 ↔ T3	prototropic (Rule 6)	2.93		-	-
L	T6 ↔ T8	prototropic (Rule 6)	-2.73		-	-
M	**T0 ↔ T4**	prototropic (Rule 7)	-2.54	-1034.754900 // -1034.759637	65.68 // 62.71	-2135.84 // -2155.26
N	T2 ↔ T7	prototropic (Rule 7)	-5.52		-	-
O	T3 ↔ T8	prototropic (Rule 7)	-5.67		-	-
P	**T0 ↔ T9**	ring chain	1.47	-1034.827955	30.23	-159.4
Q	**T4 ↔ T10**	ring chain	-1.91	-1034.829285	23.88	-186.32

Figure 1 shows the reaction **D** from T1 to T4 as a prototropic example and the reaction **Q** from T4 to T10 as a ring-chain example. The other reactions had similar profiles. Reaction **D**, through 161 points on the reaction path, shows the movement of the hydrogen from the hydroxy group (D1) to the keto group (D3) with an energy barrier of 62.71 kcal/mol. Reaction **Q,** starting with the open-chain form

(Q1), shows the movement of the proton from the hydroxyl group of the coumarin moiety to the side-chain keto group (Q2), and at the same time the approach of the side-chain moiety to close the ring and form a new six-membered ring (Q4).

Figure 1. Intrinsic reaction coordinates (IRC) for the prototropic tautomerism reaction **D** equivalent to T1↔T4 (panel **a**) and the ring-chain tautomerism reaction **Q** equivalent to T4↔T10 (panel **b**). The structures corresponding to the labels D*x* and Q*x* along the IRC are shown in the panels **c** and **d**, respectively. The orange circles in the structures D1 and Q1 indicate where the reactions are taking place.

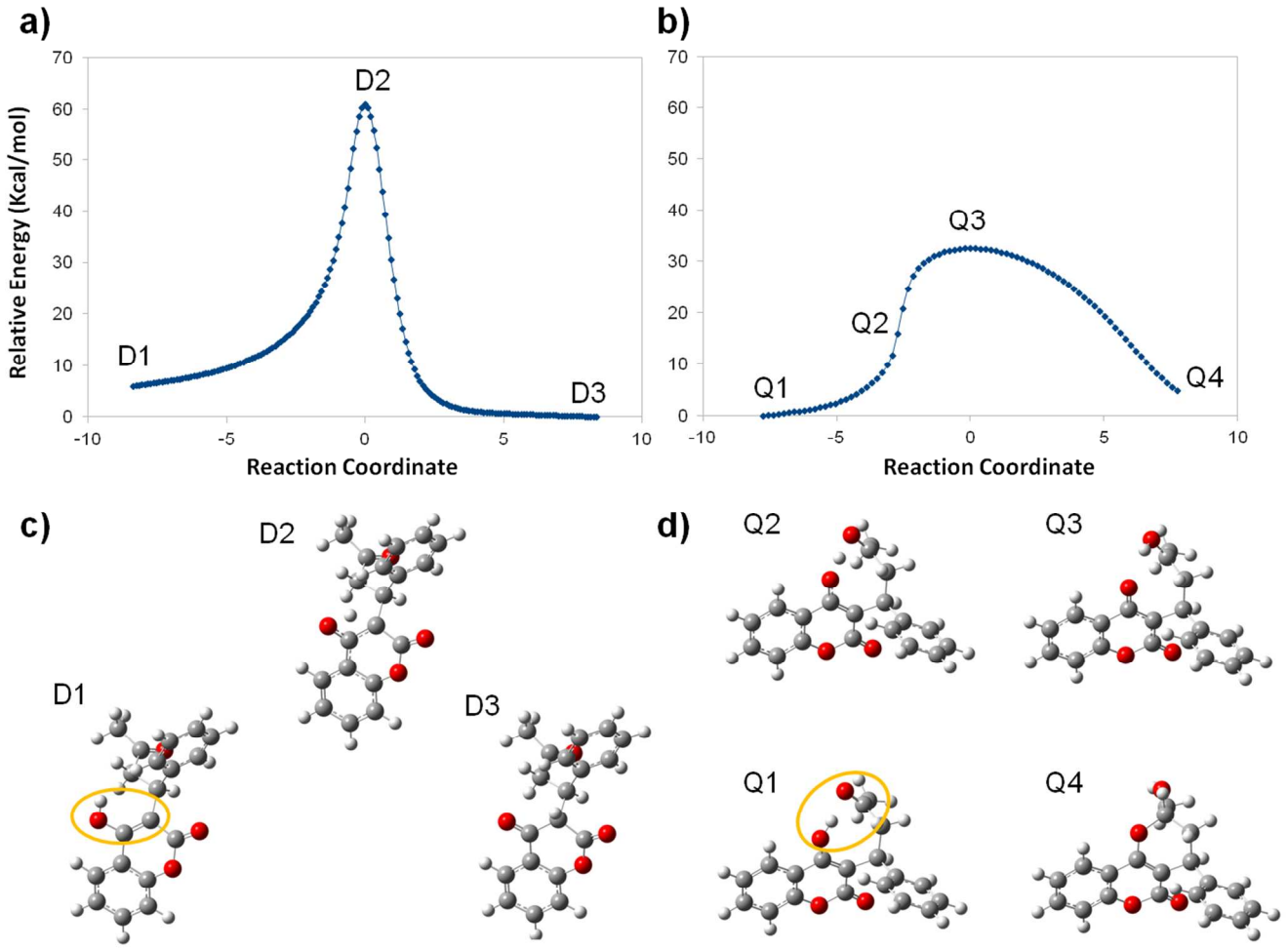

Table 1 shows the transition states and energy barriers for the most favorable equilibria. The order of the TS energies indicates that T4↔T10 TS is the most energetically favorable transition (-1034.829285 au), whereas T0↔T2 TS is the least favorable one (-1034.744266 au). The TS involved in ring-chain tautomerism are much lower in energy than the ones involved in prototropic reactions. One TS was obtained for each of the reactions except for the reaction **M**, which corresponds to the equilibrium of T0↔T4. Two TS were calculated for T0↔T4 due to the existence of an intermediate (T1) along the reaction path. This reaction corresponds to the prototropic transformation Rule 7 (1.5 shift) where the hydrogen first moves by one position (1.3 shift), which is the first equilibrium (T0↔T1), and after that does the second movement (1.3 shift), which is the equilibrium (T1↔T4).

At the B3LYP level of theory in solution, the energy barriers for prototropic tautomerization are predicted to be between 53.78-65.68 kcal/mol for the reactions **B**, **C**, **D**, **E**, **F**, **G**, **H** and **M**. In contrast, the barriers for ring-chain tautomerization are predicted to be between 23.88 and 30.23 kcal/mol corresponding to the equilibria **P** and **Q,** respectively. Thus our results suggest that the barrier height for prototropic reactions is much higher than for ring-chain reactions. One would think that the process of opening or closing a ring would be much more energetically expensive than the movement of a proton, however our results show that proton transfer reactions from carbon atoms are intrinsically slow with high energy barriers. It would be interesting to analyze other molecules that have both types of tautomerism, and see if the energy barriers follow the same tendency. The results also suggest that tautomeric energy barriers may be somewhat independent of the overall structure of the tautomers themselves, because the energy barriers for each type of tautomeric reaction were of the same order of magnitude. This opens up the interesting possibility that types of tautomerism could be categorized by the value of their energy barriers.