Supplementary Information (SI) for New Journal of Chemistry.

Supporting Information

Revolutionizing Fisetin's Anticancer Potential: Nanotechnology and Computational Approaches Unveil Enhanced CT-DNA Interactions and Bioavailability of Nano-Fisetin

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Table S1. Showing the properties of atoms in Fisetin and Nano-Fisetin compounds

Element	Hybridization	Oxidation state	ESP Charges	Mulliken Charges	Hirshfeld_Charges
Fisetin					
O1	Sp2	0	-0.404	-0.491	-0.104
O2	Sp3	0	-0.576	-0.558	-0.192
O3	Sp2	0	-0.589	-0.424	-0.283

O4	Sp3	0	-0.704	-0.56	-0.195
O5	Sp3	0	-0.656	-0.56	-0.195
O6	Sp3	0	-0.64	-0.56	-0.194
C1	Sp2	0	0.227	0.128	0.05
C2	Sp2	0	-0.615	0.053	-0.031
C3	Sp2	0	0.57	0.278	0.076
C4	Sp2	0	-0.015	0	-0.005
C5	Sp2	0	-0.051	0.283	0.043
C6	Sp2	0	0.811	0.244	0.108
C7	Sp2	0	0.204	-0.129	-0.019
C8	Sp2	0	-0.525	-0.179	-0.056
C9	Sp2	0	-0.263	-0.139	-0.044
C10	Sp2	0	-0.163	-0.121	-0.04
C11	Sp2	0	0.649	0.301	0.085
C12	Sp2	0	-0.521	-0.166	-0.065
C13	Sp2	0	0.289	0.249	0.055
C14	Sp2	0	-0.285	-0.126	-0.043
C15	Sp2	0	0.32	0.25	0.059
H1	None	0	0.111	0.149	0.057
H2	None	0	0.234	0.144	0.061
H3	None	0	0.21	0.14	0.059
H4	None	0	0.165	0.124	0.052
H5	None	0	0.188	0.109	0.047
H6	None	0	0.207	0.137	0.06
H7	None	0	0.443	0.356	0.156
H8	None	0	0.48	0.37	0.18
H9	None	0	0.46	0.35	0.164
H10	None	0	0.44	0.35	0.165
Nano-fisetin					
C1	Sp3	0	-0.097	0.104	0.039
C2	Sp3	0	0.307	-0.001	0.049
C3	Sp3	0	-0.034	-0.004	0.07
O1	Sp3	0	-0.473	-0.366	-0.192
C4	Sp3	0	0.288	-0.19	-0.043
O2	Sp3	0	-0.471	-0.377	-0.165
C5	Sp3	0	0.322	-0.047	0.013
O3	Sp3	0	0.156	-0.501	-0.087
C6	Sp3	0	-0.56	0.004	0.072
C7	Sp3	0	-0.107	-0.024	0.031
O4	Sp3	0	-0.197	-0.493	-0.139
O5	Sp3	0	-0.731	-0.585	-0.26
C8	Sp3	0	0.105	-0.05	0.031
C9	Sp3	0	-0.437	-0.186	0.009
O6	Sp3	0	-0.126	-0.243	0.027
C10	Sp3	0	0.063	-0.046	0.03
C11	Sp3	0	-0.567	-0.022	0.004
C12	Sp3	0	0.573	-0.089	0.002
O7	Sp3	0	-0.486	-0.468	-0.158

C13	Sp3	0	-0.136	-0.007	0.02
C14	Sp3	0	-0.082	-0.16	0.027
O8	Sp3	0	-0.641	-0.577	-0.261
O9	Sp3	0	-0.495	-0.437	-0.106
C15	Sp2	0	0.88	0.45	0.194
O10	Sp2	0	-0.585	-0.411	-0.268
C16	Sp3	0	-0.523	-0.286	-0.038
C17	Sp3	0	-0.034	-0.215	-0.042
C18	Sp3	0	0.029	-0.225	-0.042
C19	Sp3	0	-0.26	-0.223	-0.045
C20	Sp3	0	-0.077	-0.223	-0.044
C21	Sp3	0	0.002	-0.2	-0.046
C22	Sp3	0	-0.182	-0.258	-0.045
C23	Sp2	0	-0.204	-0.087	-0.046
C24	Sp2	0	-0.268	-0.096	-0.046
C25	Sp3	0	-0.137	-0.261	-0.047
C26	Sp3	0	-0.102	-0.194	-0.045
C27	Sp3	0	-0.109	-0.225	-0.047
C28	Sp3	0	-0.038	-0.221	-0.046
C29	Sp3	0	-0.126	-0.22	-0.046
C30	Sp3	0	-0.144	-0.217	-0.046
C31	Sp3	0	-0.086	-0.226	-0.042
C32	Sp3	0	-0.518	-0.352	-0.096
C33	Sp3	0	-0.282	0.114	0.042
C34	Sp3	0	0.313	0.005	0.053
C35	Sp3	0	-0.01	-0.007	0.069
O11	Sp3	0	-0.494	-0.369	-0.2
C36	Sp3	0	0.377	-0.186	-0.046
O12	Sp3	0	-0.478	-0.407	-0.183
C37	Sp3	0	0.348	-0.088	-0.01
O13	Sp3	0	0.195	-0.512	-0.083
C38	Sp3	0	-0.532	0.01	0.077
C39	Sp3	0	-0.16	-0.015	0.032
O14	Sp3	0	-0.048	-0.515	-0.107
O15	Sp3	0	-0.734	-0.576	-0.256
C40	Sp3	0	0.152	-0.053	0.031
C41	Sp3	0	-0.473	-0.151	0.015
O16	Sp3	0	-0.172	-0.274	0.031
C42	Sp3	0	0.084	-0.049	0.032
C43	Sp3	0	-0.551	-0.033	0.005
C44	Sp3	0	0.458	-0.047	0.015
O17	Sp3	0	-0.408	-0.461	-0.147
C45	Sp3	0	-0.347	-0.019	0.02
C46	Sp3	0	0.096	-0.145	0.021
O18	Sp3	0	-0.644	-0.575	-0.26
O19	Sp3	0	-0.583	-0.412	-0.144
C47	Sp2	0	0.919	0.438	0.196
O20	Sp2	0	-0.606	-0.415	-0.266

C48	Sp3	0	-0.497	-0.283	-0.037
C49	Sp3	0	0.008	-0.214	-0.041
C50	Sp3	0	0.006	-0.222	-0.041
C51	Sp3	0	-0.226	-0.221	-0.043
C52	Sp3	0	-0.119	-0.221	-0.044
C53	Sp3	0	-0.024	-0.2	-0.045
C54	Sp3	0	-0.168	-0.248	-0.045
C55	Sp2	0	-0.223	-0.09	-0.047
C56	Sp2	0	-0.241	-0.095	-0.045
C57	Sp3	0	-0.203	-0.25	-0.046
C58	Sp3	0	-0.115	-0.195	-0.045
C59	Sp3	0	-0.168	-0.222	-0.046
C60	Sp3	0	0.012	-0.218	-0.045
C61	Sp3	0	-0.152	-0.219	-0.046
C62	Sp3	0	-0.158	-0.213	-0.046
C63	Sp3	0	-0.095	-0.225	-0.042
C64	Sp3	0	-0.525	-0.349	-0.096
H1	None	0	0.024	0.134	0.011
H2	None	0	0.027	0.119	0.017
H3	None	0	0.227	0.185	0.065
H4	None	0	-0.027	0.266	0.007
H5	None	0	0.033	0.124	0.032
H6	None	0	-0.054	0.217	0.025
H7	None	0	0.068	0.121	0.032
H8	None	0	0.235	0.15	0.043
H9	None	0	0.131	0.136	0.034
H10	None	0	0.135	0.162	0.037
H11	None	0	0.506	0.363	0.169
H12	None	0	0.064	0.124	0.03
H13	None	0	0.087	0.14	0.037
H14	None	0	0.214	0.191	0.048
H15	None	0	0.178	0.161	0.039
H16	None	0	0.084	0.122	0.028
H17	None	0	0.179	0.148	0.059
H18	None	0	0.292	0.197	0.018
H19	None	0	0.184	0.118	0.033
H20	None	0	0.024	0.231	0.018
H21	None	0	0.019	0.166	0.027
H22	None	0	0.119	0.131	0.038
H23	None	0	0.196	0.19	0.041
H24	None	0	0.13	0.183	0.051
H25	None	0	0.148	0.151	0.047
H26	None	0	0.38	0.359	0.145
H27	None	0	0.172	0.163	0.051
H28	None	0	0.149	0.156	0.04
H29	None	0	0.05	0.121	0.027
H30	None	0	0.058	0.142	0.03
H31	None	0	0.048	0.122	0.029

H32	None	0	0.042	0.119	0.027
H33	None	0	0.086	0.111	0.025
H34	None	0	0.08	0.113	0.026
H35	None	0	0.038	0.119	0.027
H36	None	0	0.047	0.115	0.026
H37	None	0	0.039	0.115	0.023
H38	None	0	0.038	0.11	0.025
H39	None	0	0.091	0.12	0.031
H40	None	0	0.083	0.12	0.03
H41	None	0	0.161	0.085	0.033
H42	None	0	0.185	0.086	0.034
H43	None	0	0.099	0.114	0.028
H44	None	0	0.076	0.116	0.029
H45	None	0	0.065	0.117	0.023
H46	None	0	0.064	0.109	0.024
H47	None	0	0.049	0.112	0.024
H48	None	0	0.05	0.11	0.024
H49	None	0	0.029	0.114	0.025
H50	None	0	0.034	0.11	0.024
H51	None	0	0.056	0.112	0.024
H52	None	0	0.048	0.11	0.024
H53	None	0	0.074	0.113	0.025
H54	None	0	0.071	0.109	0.024
H55	None	0	0.08	0.115	0.025
H56	None	0	0.074	0.112	0.025
H57	None	0	0.155	0.116	0.029
H58	None	0	0.167	0.112	0.03
H59	None	0	0.149	0.117	0.03
H60	None	0	0.062	0.149	0.017
H61	None	0	0.074	0.145	0.035
H62	None	0	0.174	0.164	0.059
H63	None	0	-0.061	0.268	0.009
H64	None	0	0.017	0.121	0.031
H65	None	0	-0.091	0.238	0.021
H66	None	0	0.034	0.104	0.016
H67	None	0	0.244	0.168	0.052
H68	None	0	0.145	0.141	0.037
H69	None	0	0.142	0.161	0.038
H70	None	0	0.506	0.363	0.17
H71	None	0	0.051	0.128	0.031
H72	None	0	0.073	0.136	0.034
H73	None	0	0.23	0.19	0.054
H74	None	0	0.186	0.163	0.043
H75	None	0	0.073	0.122	0.028
H76	None	0	0.171	0.152	0.061
H77	None	0	0.298	0.214	0.018
H78	None	0	0.171	0.127	0.036
H79	None	0	0.084	0.182	0.03

H80	None	0	0.034	0.161	0.028
H81	None	0	0.166	0.129	0.037
H82	None	0	0.257	0.197	0.043
H83	None	0	0.076	0.166	0.045
H84	None	0	0.117	0.152	0.044
H85	None	0	0.384	0.358	0.144
H86	None	0	0.154	0.162	0.051
H87	None	0	0.136	0.155	0.039
H88	None	0	0.034	0.121	0.027
H89	None	0	0.048	0.142	0.03
H90	None	0	0.041	0.118	0.028
H91	None	0	0.04	0.117	0.026
H92	None	0	0.082	0.11	0.025
H93	None	0	0.079	0.113	0.026
H94	None	0	0.05	0.114	0.026
H95	None	0	0.058	0.114	0.024
H96	None	0	0.044	0.113	0.023
H97	None	0	0.055	0.111	0.025
H98	None	0	0.087	0.116	0.029
H99	None	0	0.082	0.117	0.028
H100	None	0	0.171	0.083	0.033
H101	None	0	0.183	0.084	0.034
H102	None	0	0.12	0.112	0.028
H103	None	0	0.104	0.114	0.028
H104	None	0	0.07	0.115	0.022
H105	None	0	0.079	0.11	0.024
H106	None	0	0.064	0.109	0.024
H107	None	0	0.071	0.111	0.024
H108	None	0	0.02	0.111	0.025
H109	None	0	0.025	0.112	0.024
H110	None	0	0.058	0.109	0.024
H111	None	0	0.057	0.111	0.024
H112	None	0	0.076	0.109	0.025
H113	None	0	0.077	0.11	0.024
H114	None	0	0.087	0.111	0.025
H115	None	0	0.084	0.112	0.025
H116	None	0	0.157	0.115	0.029
H117	None	0	0.168	0.112	0.03
H118	None	0	0.15	0.115	0.03
H119	None	0	0.26	0.279	0.123
H120	None	0	0.379	0.365	0.155
O21	Sp2	0	-0.46	-0.538	-0.137
O22	Sp3	0	-0.603	-0.541	-0.203
O23	Sp2	0	-0.648	-0.528	-0.354
O24	Sp3	0	-0.717	-0.589	-0.233
O25	Sp3	0	-0.684	-0.585	-0.224
O26	Sp3	0	-0.631	-0.586	-0.23
C65	Sp2	0	0.065	0.218	0.025

C66	Sp2	0	-0.582	0.028	-0.034
C67	Sp2	0	0.632	0.276	0.071
C68	Sp2	0	0.123	0.079	-0.009
C69	Sp2	0	0.06	0.166	0.029
C70	Sp2	0	0.611	0.252	0.064
C71	Sp2	0	0.201	-0.162	-0.053
C72	Sp2	0	-0.561	-0.189	-0.064
C73	Sp2	0	-0.296	-0.181	-0.056
C74	Sp2	0	-0.345	-0.189	-0.061
C75	Sp2	0	0.608	0.271	0.068
C76	Sp2	0	-0.547	-0.162	-0.079
C77	Sp2	0	0.302	0.246	0.055
C78	Sp2	0	-0.196	-0.158	-0.048
C79	Sp2	0	0.185	0.219	0.045
H121	None	0	0.064	0.117	0.018
H122	None	0	0.221	0.124	0.051
H123	None	0	0.208	0.14	0.047
H124	None	0	0.205	0.117	0.036
H125	None	0	0.177	0.083	0.033
H126	None	0	0.202	0.122	0.053
H127	None	0	0.422	0.316	0.126
H128	None	0	0.477	0.36	0.169
H129	None	0	0.468	0.349	0.156
H130	None	0	0.438	0.347	0.155

Table S2. Showing the properties of Bonds in Fisetin and Nano-Fisetin compounds

Bond	Order	Type	Length
Fisetin			
O1 - C1	1	Single	1.38593
O1 - C3	1	Single	1.37092
O2 - C5	1	Single	1.37811
O2 - H7	1	Single	0.970644
O3 - C6	2	Double	1.22375
O4 - C11	1	Single	1.36129
O4 - H8	1	Single	0.972779
O5 - C13	1	Single	1.36205
O5 - H9	1	Single	0.970774
O6 - C15	1	Single	1.36228
O6 - H10	1	Single	0.970798
C1 - C4	1	Single	1.4737
C1 - C5	2	Double	1.34557
C2 - C3	2	Double	1.39318
C2 - C6	1	Single	1.47093
C2 - C7	1	Single	1.39712
C3 - C8	1	Single	1.3951
C4 - C9	2	Double	1.3951

C4 - C10	1	Single	1.39509
C5 - C6	1	Single	1.48285
C7 - C12	2	Double	1.39537
C7 - H1	1	Single	1.08631
C8 - C11	2	Double	1.39493
C8 - H2	1	Single	1.08715
C9 - C13	1	Single	1.3949
C9 - H3	1	Single	1.08801
C10 - C14	2	Double	1.3949
C10 - H4	1	Single	1.08731
C11 - C12	1	Single	1.39552
C12 - H5	1	Single	1.08698
C13 - C15	2	Double	1.39487
C14 - C15	1	Single	1.3949
C14 - H6	1	Single	1.08662
Nano-fisetin			
C1 - C2	1	Single	1.52452
C1 - C4	1	Single	1.54903
C1 - O4	1	Single	1.42947
C1 - H1	1	Single	1.07284
C2 - C3	1	Single	1.504
C2 - O2	1	Single	1.42991
C2 - H2	1	Single	1.07071
C3 - O1	1	Single	1.47688
C3 - C6	1	Single	1.53809
C3 - H3	1	Single	1.07146
O1 - C4	1	Single	1.42342
C4 - H4	1	Single	1.07008
C4 - H5	1	Single	1.06994
O2 - C5	1	Single	1.42942
C5 - C9	1	Single	1.5476
C5 - H6	1	Single	1.06926
C5 - H7	1	Single	1.07238
O3 - C6	1	Single	1.42911
O3 - C11	1	Single	1.42456
C6 - C12	1	Single	1.53896
C6 - H8	1	Single	1.07144
C7 - O4	1	Single	1.43775
C7 - C8	1	Single	1.54415
C7 - H9	1	Single	1.07178
C7 - H10	1	Single	1.06848
O5 - C8	1	Single	1.4371
O5 - H11	1	Single	0.963588
C8 - H12	1	Single	1.0683
C8 - H13	1	Single	1.06904
C9 - O6	1	Single	1.43699
C9 - H14	1	Single	1.07407
C9 - H15	1	Single	1.0664

O6 - O16	1	Single	1.32408
O6 - H119	1	Single	0.957361
C10 - C11	1	Single	1.5363
C10 - O8	1	Single	1.43148
C10 - H16	1	Single	1.06977
C10 - H17	1	Single	1.06945
C11 - H18	1	Single	1.07028
C11 - H19	1	Single	1.06942
C12 - O7	1	Single	1.4277
C12 - H20	1	Single	1.06882
C12 - H21	1	Single	1.07024
O7 - C13	1	Single	1.43013
C13 - C14	1	Single	1.53895
C13 - H22	1	Single	1.07024
C13 - H23	1	Single	1.07143
C14 - O9	1	Single	1.42075
C14 - H24	1	Single	1.06941
C14 - H25	1	Single	1.06981
O8 - H26	1	Single	0.959554
O9 - C15	1	Single	1.41917
C15 - O10	2	Double	1.25803
C15 - C16	1	Single	1.5309
C16 - C17	1	Single	1.52991
C16 - H27	1	Single	1.07081
C16 - H28	1	Single	1.06963
C17 - C18	1	Single	1.53414
C17 - H29	1	Single	1.07046
C17 - H30	1	Single	1.06969
C18 - C19	1	Single	1.53101
C18 - H31	1	Single	1.0694
C18 - H32	1	Single	1.06979
C19 - C20	1	Single	1.53641
C19 - H33	1	Single	1.07032
C19 - H34	1	Single	1.06976
C20 - C21	1	Single	1.52977
C20 - H35	1	Single	1.0698
C20 - H36	1	Single	1.07043
C21 - C22	1	Single	1.53751
C21 - H37	1	Single	1.0681
C21 - H38	1	Single	1.07062
C22 - C23	1	Single	1.53072
C22 - H39	1	Single	1.06959
C22 - H40	1	Single	1.0702
C23 - C24	2	Double	1.35086
C23 - H41	1	Single	1.06917
C24 - C25	1	Single	1.53041
C24 - H42	1	Single	1.07013
C25 - C26	1	Single	1.53347

C25 - H43	1	Single	1.06989
C25 - H44	1	Single	1.06997
C26 - C27	1	Single	1.53035
C26 - H45	1	Single	1.06927
C26 - H46	1	Single	1.07
C27 - C28	1	Single	1.53403
C27 - H47	1	Single	1.06901
C27 - H48	1	Single	1.07048
C28 - C29	1	Single	1.53189
C28 - H49	1	Single	1.07054
C28 - H50	1	Single	1.06961
C29 - C30	1	Single	1.53344
C29 - H51	1	Single	1.06885
C29 - H52	1	Single	1.07053
C30 - C31	1	Single	1.53572
C30 - H53	1	Single	1.06982
C30 - H54	1	Single	1.07067
C31 - C32	1	Single	1.53653
C31 - H55	1	Single	1.07037
C31 - H56	1	Single	1.07033
C32 - H57	1	Single	1.07026
C32 - H58	1	Single	1.06957
C32 - H59	1	Single	1.06916
C33 - C34	1	Single	1.51419
C33 - C36	1	Single	1.54733
C33 - O14	1	Single	1.42933
C33 - H60	1	Single	1.069
C34 - C35	1	Single	1.50379
C34 - O12	1	Single	1.43396
C34 - H61	1	Single	1.07329
C35 - O11	1	Single	1.48177
C35 - C38	1	Single	1.54008
C35 - H62	1	Single	1.07013
O11 - C36	1	Single	1.42692
C36 - H63	1	Single	1.06937
C36 - H64	1	Single	1.07077
O12 - C37	1	Single	1.43354
C37 - C41	1	Single	1.54371
C37 - H65	1	Single	1.07445
C37 - H66	1	Single	1.0714
O13 - C38	1	Single	1.43359
O13 - C43	1	Single	1.43257
C38 - C44	1	Single	1.53896
C38 - H67	1	Single	1.07329
C39 - O14	1	Single	1.43044
C39 - C40	1	Single	1.54071
C39 - H68	1	Single	1.06709
C39 - H69	1	Single	1.07145

O15 - C40	1	Single	1.43136
O15 - H70	1	Single	0.958792
C40 - H71	1	Single	1.06764
C40 - H72	1	Single	1.06949
C41 - O16	1	Single	1.43233
C41 - H73	1	Single	1.07094
C41 - H74	1	Single	1.07068
O16 - H120	1	Single	0.957548
C42 - C43	1	Single	1.54374
C42 - O18	1	Single	1.43311
C42 - H75	1	Single	1.06873
C42 - H76	1	Single	1.06993
C43 - H77	1	Single	1.07231
C43 - H78	1	Single	1.07131
C44 - O17	1	Single	1.4268
C44 - H79	1	Single	1.0701
C44 - H80	1	Single	1.06913
O17 - C45	1	Single	1.43549
C45 - C46	1	Single	1.54348
C45 - H81	1	Single	1.07092
C45 - H82	1	Single	1.06989
C46 - O19	1	Single	1.42295
C46 - H83	1	Single	1.07077
C46 - H84	1	Single	1.07089
O18 - H85	1	Single	0.961129
O19 - C47	1	Single	1.42497
C47 - O20	2	Double	1.25796
C47 - C48	1	Single	1.53334
C48 - C49	1	Single	1.53538
C48 - H86	1	Single	1.06912
C48 - H87	1	Single	1.06957
C49 - C50	1	Single	1.53563
C49 - H88	1	Single	1.07013
C49 - H89	1	Single	1.06998
C50 - C51	1	Single	1.53617
C50 - H90	1	Single	1.06944
C50 - H91	1	Single	1.07001
C51 - C52	1	Single	1.5373
C51 - H92	1	Single	1.07056
C51 - H93	1	Single	1.07139
C52 - C53	1	Single	1.53443
C52 - H94	1	Single	1.06873
C52 - H95	1	Single	1.06904
C53 - C54	1	Single	1.54129
C53 - H96	1	Single	1.07034
C53 - H97	1	Single	1.06871
C54 - C55	1	Single	1.53775
C54 - H98	1	Single	1.0693

C54 - H99	1	Single	1.0704
C55 - C56	2	Double	1.35583
C55 - H100	1	Single	1.06875
C56 - C57	1	Single	1.53406
C56 - H101	1	Single	1.06981
C57 - C58	1	Single	1.53845
C57 - H102	1	Single	1.07011
C57 - H103	1	Single	1.069
C58 - C59	1	Single	1.5339
C58 - H104	1	Single	1.06968
C58 - H105	1	Single	1.07041
C59 - C60	1	Single	1.53612
C59 - H106	1	Single	1.07043
C59 - H107	1	Single	1.07048
C60 - C61	1	Single	1.53425
C60 - H108	1	Single	1.0706
C60 - H109	1	Single	1.07074
C61 - C62	1	Single	1.53563
C61 - H110	1	Single	1.06937
C61 - H111	1	Single	1.06995
C62 - C63	1	Single	1.53716
C62 - H112	1	Single	1.07024
C62 - H113	1	Single	1.07005
C63 - C64	1	Single	1.53759
C63 - H114	1	Single	1.0696
C63 - H115	1	Single	1.06996
C64 - H116	1	Single	1.06989
C64 - H117	1	Single	1.07057
C64 - H118	1	Single	1.06941
O21 - C65	1	Single	1.44694
O21 - C67	1	Single	1.44111
O22 - C69	1	Single	1.43153
O22 - H127	1	Single	0.958029
O23 - C70	2	Double	1.25963
O24 - C75	1	Single	1.43023
O24 - H128	1	Single	0.961358
O25 - C77	1	Single	1.43019
O25 - H129	1	Single	0.960291
O26 - C79	1	Single	1.42748
O26 - H130	1	Single	0.958103
C65 - C68	1	Single	1.53556
C65 - C69	2	Double	1.35979
C66 - C67	2	Double	1.39791
C66 - C70	1	Single	1.52121
C66 - C71	1	Single	1.39715
C67 - C72	1	Single	1.40079
C68 - C73	2	Double	1.40104
C68 - C74	1	Single	1.39796

C69 - C70	1	Single	1.52533
C71 - C76	2	Double	1.3987
C71 - H121	1	Single	1.07037
C72 - C75	2	Double	1.40108
C72 - H122	1	Single	1.07013
C73 - C77	1	Single	1.39966
C73 - H123	1	Single	1.07099
C74 - C78	2	Double	1.40121
C74 - H124	1	Single	1.06937
C75 - C76	1	Single	1.40341
C76 - H125	1	Single	1.0692
C77 - C79	2	Double	1.39933
C78 - C79	1	Single	1.40484
C78 - H126	1	Single	1.06935

Table S3. Showing the properties of ADMET in Fisetin and Nano-Fisetin compounds

PARAMETERS	**Fisetin**	**Nano-fisetin**
ADMET Solubility	**-2.594**	**15.537**
ADMET Solubility level	**3**	**5**
ADMET Unknown AlogP98	**0**	**2**
ADMET_BBB	**-1.308**	
ADMET_BBB level	**3**	**4**
ADMET-EXT-CYP2D6	-3.53685	**-0.7648**
ADMET-EXT-CYP2D6#prediction	False	False
ADMET-EXT-CYP2D6-Applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -0.811, 9.062, 3.2351, 1.51. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 114.17, 1297.3, 343.41, 150.3. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 23, 3.7682, 2.694. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 18, 4.8079, 3.38. OPS PC4 out of range. Value: 12.28. Training min, max, SD, explained variance: -5.7693, 6.0734, 2.304, 0.0694. OPS PC8 out of range. Value: -6.3637. Training min, max, SD,

		explained variance: -4.2516, 4.6021, 1.692, 0.0374. OPS PC10 out of range. Value: 7.6899. Training min, max, SD, explained variance: -3.6342, 6.9895, 1.549, 0.0314. OPS PC13 out of range. Value: -5.5322. Training min, max, SD, explained variance: -3.1712, 3.1497, 1.329, 0.0231. OPS PC15 out of range. Value: -3.8657. Training min, max, SD, explained variance: -2.6925, 3.1146, 1.2, 0.0188."
ADMET-EXT-CYP2D6-Applicability#MD	8.44661	49.3605
ADMET-EXT-CYP2D6-Applicability#MDpvalue	0.608177	2.10843e-37
ADMET-EXT- Hepatotoxic	-0.0190081	-27.1524
ADMET-EXT- Hepatotoxic #prediction	True	False
ADMET-EXT- Hepatotoxic Applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -9.291, 11.998, 1.6358, 2.67. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 33, 4.2408, 4.359. OPS PC2 out of range. Value: 10.888. Training min, max, SD, explained variance: -6.6229, 10.715, 2.522, 0.0793. OPS PC9 out of range. Value: -6.6132. Training min, max, SD, explained variance: -5.9126, 6.0586, 1.641, 0.0336. OPS PC11 out of range. Value: 5.36. Training min, max, SD, explained variance: -4.0074, 4.0205, 1.463, 0.0267. OPS PC14 out of range. Value: 6.6022. Training min, max, SD, explained variance: -4.8321, 5.9286, 1.248, 0.0194.
ADMET-EXT- Hepatotoxic Applicability #MD	7.50966	21.673
ADMET-EXT- Hepatotoxic Applicability #MDpvalue	0.970291	4.8014e-32

ADMET_Absorption level	0	3
ADMET-EXT-PPB	-5.40219	-7.733
ADMET-EXT-PPB #Prediction	False	False
ADMET-EXT-PPB- Applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -8.959, 10.25, 1.8512, 2.348. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 32.042, 1463.3, 360.98, 174.2. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 33, 5.1311, 3.823. OPS PC23 out of range. Value: 5.2929. Training min, max, SD, explained variance: -4.2053, 3.3368, 1.203, 0.0120. OPS PC27 out of range. Value: 4.1403. Training min, max, SD, explained variance: -3.2107, 3.3919, 1.129, 0.0105. OPS PC38 out of range. Value: -3.4056. Training min, max, SD, explained variance: -3.1225, 3.1535, 0.9373, 0.0073."
ADMET-EXT-PPB- Applicability #MD	10.5146	31.3855
ADMET-EXT-PPB- Applicability #MDpvalue	0.728974	4.13154e-77
ADMET_AlogP98	1.872	10.207
ADMET PSA 2D	109.492	225.024

Table S4. Toxicity calculations in Fisetin and Nano-Fisetin compounds

PARAMETERS	**Fisetin**	**Nano-fisetin**
TOPKAT Mouse female NTP prediction	Non-Carcinogen	Non-Carcinogen
TOPKAT Mouse female NTP Applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -7.685, 11.179, 1.9974, 2.266. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 0, 959.17, 223.65, 133.5. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.1024, 1.456. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 3.0404, 2.763. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 31, 2.7385, 3.538. OPS PC1 out of range. Value: 7.9532. Training min, max, SD, explained variance: -4.6943, 6.6852, 2.4, 0.0957. OPS PC2 out of range. Value: 13.217. Training min, max, SD,

		explained variance: -6.3771, 8.1586, 2.274, 0.0859. OPS PC8 out of range. Value: -7.0716. Training min, max, SD, explained variance: -4.357, 3.7651, 1.52, 0.0384. OPS PC13 out of range. Value: 8.1429. Training min, max, SD, explained variance: -3.8389, 3.5974, 1.234, 0.0253. OPS PC19 out of range. Value: 3.193. Training min, max, SD, explained variance: -3.4734, 3.1093, 1.012, 0.0170.
TOPKAT mouse female NTP probability	0.151657	0.441527
TOPKAT mouse female NTP enrichment	0.385375	1.12196
TOPKAT mouse female NTP score	-8.04244	-3.31553
TOPKAT mouse male NTP prediction	Carcinogen	Carcinogen
TOPKAT mouse male NTP applicability	All properties and OPS components are within expected ranges.	ALogP out of range. Value: 12.105. Training min, max, mean, SD: -7.685, 11.179, 1.8721, 2.313. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 0, 959.17, 222.11, 135.5. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.1321, 1.491. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 3.03, 2.783. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 31, 2.6997, 3.417. OPS PC1 out of range. Value: 16.731. Training min, max, SD, explained variance: -4.6245, 10.236, 2.634, 0.1116. OPS PC5 out of range. Value: 8.6565. Training min, max, SD, explained variance: -4.0434, 6.9568, 1.871, 0.0563. OPS PC10 out of range. Value: 6.6369. Training min, max, SD, explained variance: -3.7652, 4.2031, 1.428, 0.0328. OPS PC15 out of range. Value: -3.7075. Training min, max, SD, explained variance: -3.6063, 2.7452, 1.167, 0.0219. OPS PC19 out of range. Value: 5.2027. Training min, max, SD, explained variance: -2.8407, 3.4854, 0.9742, 0.0153.
TOPKAT mouse male NTP probability	0.611133	0.716576
TOPKAT mouse male NTP enrichment	0.611133	1.82153
TOPKAT mouse male NTP score	0.471414	3.03147
TOPKAT Rat Female NTP prediction	Non-carcinogen	Non-carcinogen
TOPKAT Rat Female NTP Applicability	All properties and OPS components are within expected ranges.	ALogP out of range. Value: 12.105. Training min, max, mean, SD: -7.685, 11.179, 1.8335, 2.302. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 0, 959.17, 225.46, 143.7. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.1897, 1.516. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 3.1931, 3.123. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 31, 2.9, 3.595. OPS PC1 out of range. Value: 12.052. Training min, max, SD, explained variance: -5.1804, 7.4733, 2.646, 0.1224. OPS PC6 out of range. Value: 4.8698. Training min, max, SD, explained variance: -4.128, 4.0746, 1.639, 0.0470. OPS PC9 out of range. Value: -9.6743. Training min, max, SD, explained variance: -4.6605, 4.2428, 1.417, 0.0351. OPS PC11 out of range. Value: 5.9293. Training min, max, SD, explained variance: -2.3897, 3.1905, 1.314, 0.0302. OPS PC17 out of range. Value: -3.4773. Training min, max, SD, explained variance: -2.3992, 3.4401, 1.019, 0.0182. OPS PC19 out of range. Value: -4.9764. Training min, max, SD, explained variance: -2.8019, 2.8331, 0.9489, 0.0157.
TOPKAT Rat female NTP Probability	0.115579	0.00841509

TOPKAT Rat female NTP enrichment	0.253924	0.0184877
TOPKAT Rat female NTP Score	-12.3774	-21.8014
TOPKAT Rat male NTP prediction	Carcinogen	Non-carcinogen
TOPKAT Rat male NTP Applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -7.685, 11.179, 1.9391, 2.202. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 0, 959.17, 225.88, 137.7. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.1391, 1.472. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 3.1213, 2.995. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 31, 2.7781, 3.523. OPS PC1 out of range. Value: 9.192. Training min, max, SD, explained variance: -4.207, 8.1791, 2.468, 0.1104. OPS PC2 out of range. Value: 13.921. Training min, max, SD, explained variance: -5.1919, 9.0113, 2.183, 0.0864. OPS PC8 out of range. Value: 5.2547. Training min, max, SD, explained variance: -3.1888, 3.6693, 1.511, 0.0414. OPS PC9 out of range. Value: -5.0445. Training min, max, SD, explained variance: -4.6697, 4.43, 1.468, 0.0391. OPS PC11 out of range. Value: -6.0555. Training min, max, SD, explained variance: -4.6713, 4.6443, 1.306, 0.0309. OPS PC12 out of range. Value: -4.025. Training min, max, SD, explained variance: -3.3508, 3.9112, 1.228, 0.0273. OPS PC13 out of range. Value: -7.2105. Training min, max, SD, explained variance: -3.2319, 2.9996, 1.204, 0.0263. OPS PC17 out of range. Value: -3.8511. Training min, max, SD, explained variance: -2.8556, 2.8217, 0.9765, 0.0173.
TOPKAT Rat male NTP Probability	0.719415	0.499233
TOPKAT Rat male NTP enrichment	1.41374	0.981051
TOPKAT Rat male NTP Score	2.65154	-2.7039
TOPKAT mouse female FDA	Non-Carcinogen	Non-Carcinogen
TOPKAT mouse male FDA	Non-Carcinogen	Non-Carcinogen
TOPKAT Rat female FDA	Non-Carcinogen	Non-Carcinogen
TOPKAT Rat male FDA	Non-Carcinogen	Non-Carcinogen
TOPKAT mouse female FDA none vs carcinogen prediction	Non-Carcinogen	Non-Carcinogen
TOPKAT mouse female FDA none vs carcinogen applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -4.311, 10.955, 2.1947, 2.219. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 46.068, 847, 305.71, 119. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.7372, 1.457. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 15, 4.2436, 2.443. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 16, 4.4744, 3.35. OPS PC2 out of range. Value: 8.7727. Training min, max, SD, explained variance: -7.2665, 6.2932, 2.637, 0.0707. OPS PC4 out of range. Value: 6.4173. Training min, max, SD, explained variance: -4.7116, 4.7287, 2.103, 0.0450. OPS PC6 out of range. Value: -6.1738. Training min, max, SD, explained variance: -5.7602, 5.7659, 1.955, 0.0389. OPS PC8 out of range. Value: -5.3599. Training min, max, SD, explained variance: -3.693, 7.8709, 1.782, 0.0323. OPS PC10 out of range. Value: 6.8027. Training min, max, SD, explained variance: -3.226, 5.6767, 1.691, 0.0291.

		OPS PC20 out of range. Value: 4.7199. Training min, max, SD, explained variance: -3.1862, 4.4571, 1.28, 0.0167. OPS PC24 out of range. Value: -5.8769. Training min, max, SD, explained variance: -3.5374, 3.2412, 1.122, 0.0128. OPS PC27 out of range. Value: 3.9393. Training min, max, SD, explained variance: -4.0039, 3.8441, 1.068, 0.0116. OPS PC31 out of range. Value: 5.9073. Training min, max, SD, explained variance: -2.3769, 4.158, 0.968, 0.0095.
TOPKAT mouse female FDA none vs carcinogen probability	0.210921	0.195454
TOPKAT mouse female FDA none vs carcinogen enrichment	0.658072	0.609817
TOPKAT mouse female FDA none vs carcinogen score	-4.17055	-15.5805
TOPKAT mouse male FDA none vs carcinogen prediction	Non-Carcinogen	Non-carcinogen
TOPKAT mouse male FDA none vs carcinogen applicability	"All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -4.311, 10.955, 2.1576, 2.209. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 46.068, 847, 304.63, 118.9. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.7342, 1.449. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 15, 4.2627, 2.435. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 16, 4.443, 3.346. OPS PC2 out of range. Value: 10.887. Training min, max, SD, explained variance: -5.8691, 7.6328, 2.727, 0.0780. OPS PC3 out of range. Value: 6.7919. Training min, max, SD, explained variance: -6.8858, 5.9444, 2.309, 0.0559. OPS PC6 out of range. Value: 6.8629. Training min, max, SD, explained variance: -5.6153, 5.6497, 1.991, 0.0416. OPS PC14 out of range. Value: -5.6926. Training min, max, SD, explained variance: -3.898, 4.688, 1.38, 0.0200. OPS PC18 out of range. Value: -5.3921. Training min, max, SD, explained variance: -3.3103, 3.6362, 1.227, 0.0158.
TOPKAT mouse male FDA none vs carcinogen probability	0.221321	0.16326
TOPKAT mouse male FDA none vs carcinogen enrichment	0.752017	0.554733
TOPKAT mouse male FDA none vs carcinogen score	-3.72908	-7.70369
TOPKAT mouse female FDA single vs multiple prediction	--	--
TOPKAT mouse female FDA single vs multiple applicability	--	--
TOPKAT mouse female FDA single vs multiple probability	--	--
TOPKAT mouse female FDA single vs multiple enrichment	--	--
TOPKAT mouse female FDA single vs multiple score	--	--
TOPKAT mouse male FDA none vs carcinogen prediction	--	--
TOPKAT mouse male FDA none vs carcinogen applicability	--	--
TOPKAT mouse male FDA none vs carcinogen probability	--	--

TOPKAT mouse male FDA none vs carcinogen enrichment	--	--
TOPKAT mouse male FDA none vs carcinogen score	--	--
TOPKAT mouse male FDA single vs multiple prediction	--	--
TOPKAT mouse male FDA single vs multiple applicability	--	--
TOPKAT mouse male FDA single vs multiple probability	--	--
TOPKAT mouse male FDA single vs multiple enrichment	--	--
TOPKAT mouse male FDA single vs multiple score	--	--
TOPKAT rat female FDA none vs carcinogen prediction	Non-carcinogen	Non-carcinogen
TOPKAT rat female FDA none vs carcinogen applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -4.311, 10.955, 2.3055, 2.163. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 46.068, 847, 306.62, 116.4. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 15, 4.2304, 2.314. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 17, 4.4686, 3.355. OPS PC2 out of range. Value: 9.5768. Training min, max, SD, explained variance: -4.3392, 7.7536, 2.634, 0.0729. OPS PC4 out of range. Value: 7.0139. Training min, max, SD, explained variance: -5.3541, 4.9503, 2.055, 0.0443. OPS PC9 out of range. Value: 6.6396. Training min, max, SD, explained variance: -4.3271, 5.5571, 1.739, 0.0317. OPS PC10 out of range. Value: 6.5559. Training min, max, SD, explained variance: -4.8124, 6.2934, 1.592, 0.0266. OPS PC22 out of range. Value: -3.8267. Training min, max, SD, explained variance: -3.7128, 3.0259, 1.157, 0.0141. OPS PC24 out of range. Value: -6.4548. Training min, max, SD, explained variance: -3.884, 4.2254, 1.086, 0.0124. OPS PC26 out of range. Value: 7.1991. Training min, max, SD, explained variance: -3.4786, 3.0719, 1.065, 0.0119.
TOPKAT rat female FDA none vs carcinogen probability	0.24846	0.173722
TOPKAT rat female FDA none vs carcinogen enrichment	0.77164	0.539527
TOPKAT rat female FDA none vs carcinogen score	-2.88336	-11.9705
TOPKAT rat female FDA single vs multiple prediction	--	--
TOPKAT rat female FDA single vs multiple applicability	--	--
TOPKAT rat female FDA single vs multiple probability	--	--
TOPKAT rat female FDA single vs multiple enrichment	--	--
TOPKAT rat female FDA single vs multiple score	--	--
TOPKAT rat male FDA none vs carcinogen prediction	Non-carcinogen	Non-carcinogen
TOPKAT rat male FDA none vs carcinogen applicability	All properties and OPS components are within	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -4.311, 10.955, 2.2335, 2.183.

	expected ranges.	Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 46.068, 847, 305.01, 115.4. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 15, 4.1723, 2.348. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 17, 4.4256, 3.36. OPS PC4 out of range. Value: 7.1377. Training min, max, SD, explained variance: -5.6236, 6.17, 2.327, 0.0505. OPS PC12 out of range. Value: -4.4383. Training min, max, SD, explained variance: -3.9196, 6.4101, 1.581, 0.0233. OPS PC15 out of range. Value: -4.5323. Training min, max, SD, explained variance: -4.0246, 5.5336, 1.388, 0.0180. OPS PC17 out of range. Value: -5.9021. Training min, max, SD, explained variance: -3.8354, 4.9495, 1.344, 0.0168. OPS PC21 out of range. Value: -4.4692. Training min, max, SD, explained variance: -3.3543, 4.5108, 1.198, 0.0134. OPS PC23 out of range. Value: -6.1067. Training min, max, SD, explained variance: -3.6972, 4.7899, 1.135, 0.0120. OPS PC25 out of range. Value: 4.7151. Training min, max, SD, explained variance: -2.9604, 3.8685, 1.096, 0.0112. OPS PC33 out of range. Value: -3.7111. Training min, max, SD, explained variance: -2.8117, 3.0977, 0.9346, 0.0081."
TOPKAT rat male FDA none vs carcinogen probability	0.247513	0.175281
TOPKAT rat male FDA none vs carcinogen enrichment	0.740606	0.524474
TOPKAT rat male FDA none vs carcinogen score	-4.52816	-9.20394
TOPKAT rat male FDA single vs multiple prediction	--	--
TOPKAT rat male FDA single vs multiple applicability	--	--
TOPKAT rat male FDA single vs multiple probability	--	--
TOPKAT rat male FDA single vs multiple enrichment	--	--
TOPKAT rat male FDA single vs multiple score	--	--
TOPKAT WOE Prediction	Non-carcinogen	Non-carcinogen
TOPKAT WOE Applicability	All properties and OPS components are within expected ranges.	ALogP out of range. Value: 12.105. Training min, max, mean, SD: -7.685, 10.955, 2.2018, 2.176. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 46.068, 760.62, 271.86, 116.1. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.3872, 1.332. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 13, 3.6596, 2.328. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 16, 3.8468, 3.473. OPS PC1 out of range. Value: 14.128. Training min, max, SD, explained variance: -4.108, 8.2637, 2.652, 0.1433. OPS PC5 out of range. Value: 10.132. Training min, max, SD, explained variance: -3.6694, 5.9692, 1.498, 0.0457. OPS PC12 out of range. Value: -6.838. Training min, max, SD, explained variance: -3.6396, 3.4437, 1.068, 0.0232. OPS PC14 out of range. Value: -6.5538. Training min, max, SD, explained variance: -3.1618, 3.6024, 1.023, 0.0213. OPS PC16 out of range. Value: -2.9451. Training min, max, SD,

		explained variance: -2.6178, 2.8419, 0.9696, 0.0191. OPS PC18 out of range. Value: -3.8632. Training min, max, SD, explained variance: -3.5049, 2.7579, 0.94, 0.0180. OPS PC19 out of range. Value: -2.8784. Training min, max, SD, explained variance: -2.3106, 4.2584, 0.8979, 0.0164. OPS PC20 out of range. Value: -3.7321. Training min, max, SD, explained variance: -2.4327, 3.0557, 0.8804, 0.0158. OPS PC21 out of range. Value: 4.4104. Training min, max, SD, explained variance: -3.2998, 3.2797, 0.8612, 0.0151.
TOPKAT WOE probability	0.381591	0.18003
TOPKAT WOE enrichment	0.741106	0.349645
TOPKAT WOE score	-4.32541	-12.9636
TOPKAT carcinogenic potency TD50 mouse	76.1931	42.6277
TOPKAT carcinogenic potency TD50 mouse unit	mg/kg_body_weight/day	mg/kg_body_weight/day
TOPKAT carcinogenic potency TD50 mouse applicability	All properties and OPS components are within expected ranges.	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 871.78, 225.83, 133.9. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.1962, 1.306. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 2.8019, 2.374. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 26, 2.6321, 3.34. OPS PC2 out of range. Value: 13.54. Training min, max, SD, explained variance: -5.652, 8.9166, 2.513, 0.0788. OPS PC3 out of range. Value: -8.4269. Training min, max, SD, explained variance: -7.8363, 6.9706, 2.357, 0.0693. OPS PC9 out of range. Value: -4.7785. Training min, max, SD, explained variance: -4.215, 5.5359, 1.562, 0.0304. OPS PC10 out of range. Value: -4.7737. Training min, max, SD, explained variance: -4.4779, 4.3935, 1.47, 0.0270. OPS PC16 out of range. Value: 6.2039. Training min, max, SD, explained variance: -3.1026, 4.016, 1.245, 0.0193. OPS PC19 out of range. Value: -3.5213. Training min, max, SD, explained variance: -3.2253, 3.9514, 1.154, 0.0166. OPS PC21 out of range. Value: 4.5869. Training min, max, SD, explained variance: -3.0727, 3.8003, 1.095, 0.0149. OPS PC22 out of range. Value: 4.0065. Training min, max, SD, explained variance: -3.1587, 3.8589, 1.086, 0.0147.
TOPKAT carcinogenic potency TD50 Rat	54.5438	80.8852
TOPKAT carcinogenic potency TD50 Rat unit	mg/kg_body_weight/day	mg/kg_body_weight/day
TOPKAT carcinogenic potency TD50 Rat applicability	All properties and OPS components are within expected ranges.	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 1255.4, 232.87, 142.7. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 8, 1.0519, 1.223. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 3.4792, 2.825. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 31, 2.9674, 3.409. Num_Atoms out of range. Value: 105. Training min, max, mean, SD: 2, 90, 15.215, 9.324. OPS PC3 out of range. Value: 19.322. Training min, max, SD, explained variance: -4.8735, 15.028, 2.904, 0.0810. OPS PC8 out of range. Value: 7.1724. Training min, max, SD, explained variance: -5.632, 6.1249, 1.814, 0.0316. OPS PC14 out of range. Value: 5.2593. Training min, max, SD, explained variance: -6.3246, 4.7836, 1.48, 0.0210. OPS PC23 out of range. Value: 4.8447. Training min, max, SD,

		explained variance: -2.8727, 4.3064, 1.096, 0.0115. OPS PC24 out of range. Value: -4.0312. Training min, max, SD, explained variance: -3.0088, 7.4204, 1.076, 0.0111. OPS PC26 out of range. Value: 6.4674. Training min, max, SD, explained variance: -2.8903, 4.3012, 1.009, 0.0098."
TOPKAT Ames Prediction	Mutagen	Non-Mutagen
TOPKAT Ames applicability	All properties and OPS components are within expected ranges.	OPS PC4 out of range. Value: -12.092. Training min, max, SD, explained variance: -11.735, 10.368, 1.937, 0.0399.
TOPKAT Ames probability	0.780947	9.94009e-11
TOPKAT Ames enrichment	1.39861	1.78019e-10
TOPKAT Ames score	2.61798	-60.156
TOPKAT DTP prediction	Toxic	Toxic
TOPKAT DTP applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -7.685, 8.435, 2.1067, 2.234. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 32.042, 973.67, 288.22, 157.1. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 9, 1.4481, 1.588. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 16, 3.9037, 3.081. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 19, 3.9704, 3.518. OPS PC1 out of range. Value: 13.47. Training min, max, SD, explained variance: -5.294, 7.595, 2.775, 0.1128. OPS PC5 out of range. Value: -6.2519. Training min, max, SD, explained variance: -5.1315, 4.6227, 1.846, 0.0499. OPS PC10 out of range. Value: 6.4552. Training min, max, SD, explained variance: -4.9641, 4.5475, 1.418, 0.0295. OPS PC12 out of range. Value: 3.5523. Training min, max, SD, explained variance: -3.7514, 3.3159, 1.318, 0.0255. OPS PC17 out of range. Value: 3.4678. Training min, max, SD, explained variance: -2.7025, 2.8536, 1.067, 0.0167. OPS PC19 out of range. Value: -6.8531. Training min, max, SD, explained variance: -2.7817, 3.2747, 1.037, 0.0157."
TOPKAT DTP probability	0.781726	0.582212
TOPKAT DTP enrichment	1.48638	1.10702
TOPKAT DTP score	6.15064	0.904523
TOPKAT rat oral LD50	1.19715	396.484
TOPKAT rat oral LD50 unit	g/kg_body_weight	g/kg_body_weight
TOPKAT rat oral LD50 applicability	All properties and OPS components are within expected ranges.	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 27.025, 835.89, 220.91, 97.79. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 15, 3.0373, 1.958. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 27, 4.0389, 3.433. Molecular_PolarSurfaceArea out of range. Value: 358.64. Training min, max, mean, SD: 0, 331.42, 53.759, 37.5. OPS PC2 out of range. Value: 18.328. Training min, max, SD, explained variance: -7.8566, 12.725, 4.044, 0.0590. OPS PC4 out of range. Value: 13.167. Training min, max, SD, explained variance: -15.374, 12.471, 3.311, 0.0396. OPS PC20 out of range. Value: 6.5584. Training min, max, SD, explained variance: -5.6268, 6.1526, 1.85, 0.0123. OPS PC29 out of range. Value: -9.21. Training min, max, SD, explained variance: -5.8455, 6.6106, 1.515, 0.0083. OPS PC36 out of range. Value: 7.8077. Training min, max, SD, explained variance: -6.2516, 6.4721, 1.37, 0.0068.

		OPS PC43 out of range. Value: -7.0857. Training min, max, SD, explained variance: -5.6417, 5.1926, 1.229, 0.0054.
TOPKAT Rat maximum tolerated dose feed	1.0396	8.9393
TOPKAT Rat maximum tolerated dose feed unit	g/kg_body_weight	g/kg_body_weight
TOPKAT Rat maximum tolerated dose feed applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -4.271, 7.574, 2.3494, 1.981. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 74.122, 731.95, 245.25, 106.4. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 7, 1.2135, 1.216. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 13, 3.2809, 2.199. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 19, 3.0112, 3.203. Molecular_PolarSurfaceArea out of range. Value: 358.64. Training min, max, mean, SD: 0, 201.84, 63.052, 40.7. Molecular_PolarSASA out of range. Value: 459.58. Training min, max, mean, SD: 0, 357.83, 109.38, 65.5. OPS PC1 out of range. Value: 14.343. Training min, max, SD, explained variance: -4.595, 7.2949, 2.487, 0.1398. OPS PC2 out of range. Value: 9.4616. Training min, max, SD, explained variance: -5.6103, 7.6016, 2.34, 0.1237. OPS PC3 out of range. Value: 7.6472. Training min, max, SD, explained variance: -5.5951, 5.5124, 2.075, 0.0973. OPS PC4 out of range. Value: 7.4428. Training min, max, SD, explained variance: -3.4425, 5.5952, 1.755, 0.0696. OPS PC5 out of range. Value: 8.0131. Training min, max, SD, explained variance: -3.3892, 5.0834, 1.644, 0.0611. OPS PC7 out of range. Value: 6.7795. Training min, max, SD, explained variance: -4.36, 3.9384, 1.418, 0.0454. OPS PC8 out of range. Value: 5.7388. Training min, max, SD, explained variance: -3.8548, 3.9137, 1.331, 0.0400. OPS PC9 out of range. Value: 5.1621. Training min, max, SD, explained variance: -2.8548, 3.3954, 1.263, 0.0360. OPS PC11 out of range. Value: 4.5533. Training min, max, SD, explained variance: -3.8346, 3.8752, 1.233, 0.0343. OPS PC13 out of range. Value: 3.4202. Training min, max, SD, explained variance: -2.9619, 2.8704, 1.049, 0.0249.
TOPKAT Rat maximum tolerated dose Gavage	0.000713125	4.59064e-06
TOPKAT Rat maximum tolerated dose Gavage unit	g/kg_body_weight	g/kg_body_weight
TOPKAT Rat maximum tolerated dose Gavage applicability	"Num_H_Donors out of range. Value: 4. Training min, max, mean, SD: 0, 3, 0.4375, 0.8311.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -2.297, 8.698, 1.9556, 1.637. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 68.074, 434.63, 171.13, 85.06. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 3, 0.4375, 0.8311. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 6, 1.6146, 1.644. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 21, 1.8646, 2.793. Molecular_PolarSASA out of range. Value: 459.58. Training min, max, mean, SD: 0, 223.97, 50.816, 55.15. Molecular_PolarSurfaceArea out of range. Value: 358.64. Training min, max, mean, SD: 0, 138.03, 28.978, 32.1. OPS PC1 out of range. Value: 23.397. Training min, max, SD,

		explained variance: -4.0008, 7.9165, 2.861, 0.2531. OPS PC2 out of range. Value: 5.8763. Training min, max, SD, explained variance: -5.7911, 4.8501, 2.284, 0.1613. OPS PC4 out of range. Value: 19.409. Training min, max, SD, explained variance: -2.9402, 6.1938, 1.581, 0.0773. OPS PC5 out of range. Value: -5.109. Training min, max, SD, explained variance: -3.4, 4.1587, 1.489, 0.0686. OPS PC6 out of range. Value: -6.0589. Training min, max, SD, explained variance: -2.4321, 2.9885, 1.256, 0.0488. OPS PC8 out of range. Value: 6.6716. Training min, max, SD, explained variance: -2.2777, 4.3428, 1.076, 0.0358. OPS PC10 out of range. Value: -6.2125. Training min, max, SD, explained variance: -3.9696, 2.3971, 0.982, 0.0298.
TOPKAT Rat inhalational LC50	1348.68	0.0027173
TOPKAT Rat inhalational LC50 unit	mg/m3/h	mg/m3/h
TOPKAT Rat inhalational LC50 applicability	"All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -5.849, 8.536, 2.0945, 1.66. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 27.025, 513.49, 187.96, 100.1. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 16, 2.3423, 1.997. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 20, 2.9474, 2.803. Molecular_PolarSASA out of range. Value: 459.58. Training min, max, mean, SD: 0, 450.97, 66.859, 52.76. Molecular_PolarSurfaceArea out of range. Value: 358.64. Training min, max, mean, SD: 0, 272.06, 40.417, 35.76. OPS PC1 out of range. Value: 20.178. Training min, max, SD, explained variance: -4.4071, 9.1898, 2.877, 0.1148. OPS PC3 out of range. Value: 6.0141. Training min, max, SD, explained variance: -7.0198, 5.7615, 1.996, 0.0553. OPS PC7 out of range. Value: 11.757. Training min, max, SD, explained variance: -3.6077, 7.268, 1.655, 0.0380. OPS PC12 out of range. Value: -5.22. Training min, max, SD, explained variance: -4.808, 4.6082, 1.396, 0.0270. OPS PC15 out of range. Value: -3.4165. Training min, max, SD, explained variance: -3.2797, 5.4, 1.258, 0.0220. OPS PC17 out of range. Value: 5.6635. Training min, max, SD, explained variance: -3.9061, 5.5073, 1.195, 0.0198. OPS PC19 out of range. Value: 4.1704. Training min, max, SD, explained variance: -3.716, 3.6677, 1.125, 0.0176. OPS PC20 out of range. Value: 4.8593. Training min, max, SD, explained variance: -3.5716, 3.7345, 1.071, 0.0159.
TOPKAT chronic LOAEL	0.186139	0.218457
TOPKAT chronic LOAEL Unit	g/kg_body_weight	g/kg_body_weight
TOPKAT chronic LOAEL Applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -4.271, 10.946, 2.3349, 2.023. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 60.098, 959.17, 240.83, 125.5. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 9, 1.0902, 1.316. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 22, 3.1211, 2.47. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 21, 3.1289, 3.293. Num_Atoms out of range. Value: 105. Training min, max, mean, SD: 3, 60, 15.593, 8.2. OPS PC2 out of range. Value: -12.618. Training min, max, SD,

		explained variance: -11.826, 8.5031, 4.271, 0.0798. OPS PC13 out of range. Value: -6.0131. Training min, max, SD, explained variance: -5.6594, 6.6668, 2.119, 0.0196. OPS PC16 out of range. Value: 7.6914. Training min, max, SD, explained variance: -5.2665, 7.0934, 1.905, 0.0159. OPS PC28 out of range. Value: -5.4077. Training min, max, SD, explained variance: -3.911, 3.7469, 1.37, 0.0082."
TOPKAT Skin irritancy	None	Mild
TOPKAT Skin irritancy none vs irritant prediction	Non-irritant	Irritant
TOPKAT Skin irritancy none vs irritant applicability	All properties and OPS components are within expected ranges.	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 984.97, 196.73, 90.86. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 32, 4.3015, 4.265. OPS PC2 out of range. Value: -9.4602. Training min, max, SD, explained variance: -8.4513, 10.425, 2.399, 0.0728. OPS PC3 out of range. Value: 10.146. Training min, max, SD, explained variance: -8.0457, 9.6394, 2.076, 0.0545. OPS PC4 out of range. Value: 14.248. Training min, max, SD, explained variance: -4.3157, 9.5869, 1.948, 0.0480. OPS PC10 out of range. Value: 9.1434. Training min, max, SD, explained variance: -5.7292, 8.2109, 1.529, 0.0296. OPS PC12 out of range. Value: 6.8637. Training min, max, SD, explained variance: -3.0857, 5.2897, 1.358, 0.0233. OPS PC15 out of range. Value: 5.8057. Training min, max, SD, explained variance: -5.1621, 5.0139, 1.212, 0.0186. OPS PC16 out of range. Value: 9.6652. Training min, max, SD, explained variance: -4.158, 4.7984, 1.178, 0.0175."
TOPKAT Skin irritancy none vs irritant Probability	0.945231	0.999452
TOPKAT Skin irritancy none vs irritant enrichment	1.02641	1.08529
TOPKAT Skin irritancy none vs irritant score	-2.00969	1.59821
TOPKAT Skin irritancy mild vs moderate severe prediction	--	Mild
TOPKAT Skin irritancy mild vs moderate severe applicability	--	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 45.084, 984.97, 199.3, 94.47. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 32, 4.5791, 4.371. OPS PC2 out of range. Value: -10.346. Training min, max, SD, explained variance: -9.5281, 9.4053, 2.411, 0.0785. OPS PC4 out of range. Value: 17.107. Training min, max, SD, explained variance: -4.2367, 10.085, 1.947, 0.0512. OPS PC7 out of range. Value: 5.4218. Training min, max, SD, explained variance: -4.7717, 5.3182, 1.704, 0.0392. OPS PC8 out of range. Value: -7.6577. Training min, max, SD, explained variance: -7.3411, 6.8287, 1.559, 0.0328. OPS PC12 out of range. Value: 8.4333. Training min, max, SD, explained variance: -2.9627, 5.5422, 1.315, 0.0234. OPS PC18 out of range. Value: -9.1512. Training min, max, SD, explained variance: -3.918, 4.482, 1.084, 0.0159."
TOPKAT Skin irritancy mild vs moderate severe probability	--	0.0397363
TOPKAT Skin irritancy mild vs moderate severe enrichment	--	0.10794
TOPKAT Skin irritancy mild vs moderate severe score	---	-11.7196
TOPKAT Skin Sensitization	Strong	None

TOPKAT Skin Sensitization none vs sensitizer prediction	Irritant	Non-Irritant
TOPKAT Skin Sensitization none vs sensitizer applicability	"All properties and OPS components are within expected ranges.	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 959.12, 217.67, 105.5. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 19, 3.2194, 2.113. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 36, 4.574, 5.139. OPS PC1 out of range. Value: 12.1. Training min, max, SD, explained variance: -3.2732, 11.551, 2.954, 0.1979. OPS PC3 out of range. Value: 11.219. Training min, max, SD, explained variance: -4.6819, 6.3422, 1.904, 0.0822. OPS PC6 out of range. Value: -6.2726. Training min, max, SD, explained variance: -4.4824, 3.7178, 1.466, 0.0487. OPS PC7 out of range. Value: 6.5199. Training min, max, SD, explained variance: -3.3757, 5.1803, 1.33, 0.0401. OPS PC8 out of range. Value: -5.3868. Training min, max, SD, explained variance: -3.5152, 4.75, 1.283, 0.0373. OPS PC11 out of range. Value: -5.1029. Training min, max, SD, explained variance: -2.5901, 5.0746, 1.087, 0.0268. OPS PC15 out of range. Value: -4.6668. Training min, max, SD, explained variance: -3.7293, 3.5535, 0.908, 0.0187.
TOPKAT Skin Sensitization none vs sensitizer probability	0.832846	0.000376443
TOPKAT Skin Sensitization none vs sensitizer enrichment	1.21366	0.000548571
TOPKAT Skin Sensitization none vs sensitizer score	0.967505	-22.1948
TOPKAT Skin Sensitization weak vs strong prediction	Strong	--
TOPKAT Skin Sensitization weak vs strong applicability	All properties and OPS components are within expected ranges.	--
TOPKAT Skin Sensitization weak vs strong probability	0.992668	--
TOPKAT Skin Sensitization weak vs strong enrichment	1.28054	--
TOPKAT Skin Sensitization weak vs strong score	4.30492	--
TOPKAT ocular irritancy	Moderate	None
TOPKAT ocular irritancy none vs irritant prediction	Irritant	Non-Irritant
TOPKAT ocular irritancy none vs irritant applicability	"All properties and OPS components are within expected ranges.	Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 1199.5, 199.38, 124.7. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 6, 0.68472, 0.8931. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 24, 2.7745, 2.283. OPS PC12 out of range. Value: -5.4887. Training min, max, SD, explained variance: -5.4138, 5.3465, 1.17, 0.0167.
TOPKAT ocular irritancy none vs irritant probability	0.999883	0
TOPKAT ocular irritancy none vs irritant enrichment	1.17553	0
TOPKAT ocular irritancy none vs irritant score	1.43623	-60.3116
TOPKAT ocular irritancy mild vs moderate severe prediction	Moderate-Severe	--

TOPKAT ocular irritancy mild vs moderate severe applicability	"All properties and OPS components are within expected ranges.	--
TOPKAT ocular irritancy mild vs moderate severe probability	0.835183	--
TOPKAT ocular irritancy mild vs moderate severe enrichment	1.21224	--
TOPKAT ocular irritancy mild vs moderate severe score	0.923834	--
TOPKAT ocular irritancy moderate vs severe prediction	Single	--
TOPKAT ocular irritancy moderate vs severe applicability	All properties and OPS components are within expected ranges.	--
TOPKAT ocular irritancy moderate vs severe probability	0.655911	--
TOPKAT ocular irritancy moderate vs severe enrichment	1.05812	--
TOPKAT ocular irritancy moderate vs severe score	-0.975184	--
TOPKAT Aerobic Biodegradability prediction	Non-Degradable	Degradable
TOPKAT Aerobic Biodegradability applicability	All properties and OPS components are within expected ranges.	"Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 959.17, 193.39, 118.3. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 6, 0.69786, 0.8466. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 12, 1.9188, 1.701. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 54, 3.9515, 6.48. OPS PC3 out of range. Value: 12.292. Training min, max, SD, explained variance: -4.8703, 8.6267, 2.463, 0.0697. OPS PC7 out of range. Value: 8.6251. Training min, max, SD, explained variance: -5.3302, 7.0026, 1.868, 0.0401. OPS PC16 out of range. Value: 4.9189. Training min, max, SD, explained variance: -3.0094, 4.2513, 1.289, 0.0191. OPS PC17 out of range. Value: -5.0741. Training min, max, SD, explained variance: -3.6883, 4.4684, 1.261, 0.0182. OPS PC19 out of range. Value: 3.3213. Training min, max, SD, explained variance: -3.6376, 3.3142, 1.187, 0.0162. OPS PC20 out of range. Value: 6.61. Training min, max, SD, explained variance: -3.5628, 4.5498, 1.102, 0.0139. OPS PC21 out of range. Value: -4.1002. Training min, max, SD, explained variance: -3.7241, 4.0586, 1.073, 0.0132. OPS PC23 out of range. Value: 6.5382. Training min, max, SD, explained variance: -3.0961, 3.4354, 1.042, 0.0125."
TOPKAT Aerobic Biodegradability probability	0.414286	0.999312
TOPKAT Aerobic Biodegradability enrichment	0.94954	2.29041
TOPKAT Aerobic Biodegradability score	-1.60653	35.0114
TOPKAT Fathead Minnow LC50	0.0406162	1.96818e-13
TOPKAT Fathead Minnow LC50 unit	g/l	g/l
TOPKAT Fathead Minnow LC50 applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -3.709, 7.307, 2.0523, 1.462. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 766.9, 168.84, 77.75. Num_H_Donors out of range. Value: 10. Training min, max, mean, SD: 0, 4, 0.5729, 0.6807. Num_H_Acceptors out of range. Value: 26. Training min, max, mean,

		SD: 0, 10, 1.8601, 1.463. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 21, 2.4256, 2.639. Molecular_PolarSurfaceArea out of range. Value: 358.64. Training min, max, mean, SD: 0, 242.45, 35.359, 30. Molecular_PolarSASA out of range. Value: 459.58. Training min, max, mean, SD: 0, 259.02, 65.335, 44.32. OPS PC2 out of range. Value: 17.626. Training min, max, SD, explained variance: -5.6178, 6.9053, 2.377, 0.0973. OPS PC3 out of range. Value: -11.455. Training min, max, SD, explained variance: -5.951, 6.9816, 2.181, 0.0819. OPS PC4 out of range. Value: 11.099. Training min, max, SD, explained variance: -4.3057, 6.1463, 1.927, 0.0639. OPS PC5 out of range. Value: -6.042. Training min, max, SD, explained variance: -4.3062, 6.9049, 1.75, 0.0527. OPS PC7 out of range. Value: 10.318. Training min, max, SD, explained variance: -4.0218, 6.8974, 1.591, 0.0436. OPS PC8 out of range. Value: 5.3485. Training min, max, SD, explained variance: -4.2029, 4.1447, 1.474, 0.0374. OPS PC9 out of range. Value: -15.987. Training min, max, SD, explained variance: -4.4045, 4.4278, 1.418, 0.0346. OPS PC11 out of range. Value: -8.2947. Training min, max, SD, explained variance: -3.2871, 6.0547, 1.313, 0.0297. OPS PC12 out of range. Value: 7.1291. Training min, max, SD, explained variance: -3.3233, 3.4374, 1.268, 0.0277. OPS PC15 out of range. Value: -3.7764. Training min, max, SD, explained variance: -2.9985, 5.0192, 1.089, 0.0204. OPS PC16 out of range. Value: -8.7504. Training min, max, SD, explained variance: -3.5859, 4.6043, 1.06, 0.0194. OPS PC17 out of range. Value: -3.4224. Training min, max, SD, explained variance: -3.2639, 3.1779, 1.02, 0.0179.
TOPKAT Daphnia EC50	6.20004	3.46187e-10
TOPKAT Daphnia EC50 unit	mg/l	mg/l
TOPKAT Daphnia EC50 applicability	All properties and OPS components are within expected ranges.	"ALogP out of range. Value: 12.105. Training min, max, mean, SD: -6.264, 10.795, 2.4862, 2.177. Molecular_Weight out of range. Value: 1495.9. Training min, max, mean, SD: 30.026, 777.96, 236.08, 114.5. Num_H_Acceptors out of range. Value: 26. Training min, max, mean, SD: 0, 17, 2.9862, 2.091. Num_RotatableBonds out of range. Value: 66. Training min, max, mean, SD: 0, 24, 3.5275, 3.621. Molecular_PolarSurfaceArea out of range. Value: 358.64. Training min, max, mean, SD: 0, 299.12, 58.748, 42.2. Num_Atoms out of range. Value: 105. Training min, max, mean, SD: 1, 39, 14.852, 7.318. NPlusO_Count out of range. Value: 26. Training min, max, mean, SD: 0, 17, 3.3456, 2.375. OPS PC2 out of range. Value: 19.367. Training min, max, SD, explained variance: -7.9801, 12.527, 4.84, 0.0787. OPS PC34 out of range. Value: -5.6772. Training min, max, SD, explained variance: -4.9766, 4.3675, 1.405, 0.0066. OPS PC42 out of range. Value: -7.1717. Training min, max, SD, explained variance: -4.0993, 5.5834, 1.254, 0.0053."

Figure S1: Fluorescence displacement assay results showing the competition between Fisetin/Nano- Fisetin and EtBr for binding to CT-DNA. The reduction in fluorescence intensity upon addition of Fisetin/Nano-Fisetin (80µM) suggests their ability to displace EtBr, indicating the interaction with CT-DNA.