

Abbreviations

- BDE: bond dissociation enthalpy
- BSSE: basis set superposition error
- COSMO: conductor-like screening model
- DFT: density functional theory
- DFT-D: Dispersion-corrected DFT
- DMSO: dimethylsulfoxide
- DOPC: 1,2-dioleoyl-sn-glycero-3-phosphocholine
- HAT: hydrogen atom transfer
- HBS: HEPES buffered saline
- HEPES: N-(2-hydroxyethyl)-piperazine-N'-2-ethanesulfonic acid
- LINCS: linear constraint solver
- LPO: lipid peroxidation
- MD: molecular dynamics
- PCM: polarizable continuum model
- PME: particle mesh Ewald
- RESP: restrained fit of electrostatic potential
- ROS: reactive oxygen species
- SPC/E: extended single point charge model
- vitC: vitamin C
- vitE: vitamin E

Methodological comments

When placing several antioxidants in the bilayer (which is modeled in a periodically repeating box of $6\times6\times8\text{ nm}^3$ volume) we definitely model quite high concentrations (one antioxidant molecule in the simulation box corresponds to a concentration of several mM). In our model, the lipid bilayer is too small and the time scale computationally available is limited to several μs . In a real situation, a few μM vitamin and polyphenol concentrations are expected in the organism. Here, we accelerate the diffusion and interacting processes by increasing the initial concentration, corresponding to antioxidant accumulation in the membrane, which has been indeed repeatedly suggested for vitamins and polyphenols.

Our theoretical data provide collective evidence that non-covalent aggregation is likely to occur in a biomembrane. All types of simulations (with DFT-D calculations, and free and constrained MD simulations) clearly show that with regard to the non-covalent association (e.g., quercetin:vitE), the inter-molecular interaction is sufficiently strong to give stable complexes inside lipid bilayers under physiological conditions. This is also supported by the (static) fluorescence quenching.

The occurrence of this association results from a complex phenomenon, in which enthalpy, entropy and solvation effects interplay. QM accurately evaluates the electronic energy of non-covalent association. However, the evaluation of the Gibbs energies of association at the QM level is a more delicate task. In such calculations, the entropy term consists of three major components arising from translational, rotational and vibrational modes. As these contributions are estimated under ideal gas, rigid rotor and harmonic approximations (which are valid only for molecules in gas phase), one might expect that the loss of translational entropy accompanying formation of the non-covalent complexes in the lipid bilayer is dramatically overestimated, as we indeed observed.

In any case, from the different data discussed here, we believe that the difference in Gibbs energy of association is negative but small, as already measured in hetero polyphenol association in water. Therefore the co-existence of non-covalent dimers and free antioxidants is much likely. The association will also be favored in the case of higher concentration, i.e., in the case of antioxidant accumulation in tissues of organs. Such accumulation (local concentration increase) has already been suggested for polyphenols. Here we show again, at a molecular level, that such accumulation may increase the global antioxidant status.

Materials and Methods

Molecular dynamics simulations. The membrane model consisted of a bilayer of 128 DOPC molecules solvated in ca. 5400 water molecules with 20 Na⁺ and 20 Cl⁻ ions (equivalent to 0.9% w/v physiological concentration). Antioxidant molecules and ions were described by the Gromos53a6 force field¹, water by the SPC/E model and DOPC molecules by the Berger force field², which is compatible with Gromos53a6. All MD simulations and analyses were conducted using the GROMACS package version 4.5.5³. The MD calculations were integrated using a 2 fs time step and the leap-frog Verlet scheme. The electrostatic and Van der Waals short-range interaction cutoffs were set to 1.4 nm; PME (particle mesh Ewald) was used for long-range electrostatics. The temperature was kept constant at 310 K with the Nosé-

Hoover thermostat ($\tau_T = 0.5$ ps), and the Parrinello-Rahman barostat was used to maintain the pressure anisotropically at 1 bar ($\tau_p = 5.0$ ps, compressibility = $4.5 \cdot 10^{-5}$ bar $^{-1}$). Periodic boundary conditions were used in every dimension. Bond constraints were handled by LINCS.

Topologies for antioxidant compounds were obtained from the PRODRG webserver. Partial charges were recalculated using RESP and the model of Duan *et al.*⁴. The torsion angle χ between the B and C rings of quercetin was also carefully re-parameterized according to the recent accurate method developed for nucleic acids⁵.

$$E_{\text{dih},\chi}^{\text{solv}} = E^{\text{QM//QM,COSMO}} - E_{-\chi}^{\text{MM//MM,PB}} \quad (1)$$

The following equation was used for describing the dihedral torsion potential V_d :

$$V_d = k_\varphi (1 + \cos(n\varphi - \varphi_s)) \quad (2)$$

The dihedral torsion constant k_φ was determined to be 22.5 kJ.mol $^{-1}$ (Figure S5).

Antioxidant molecules were initially placed in the water phase. The positions of individual compounds (ascorbic acid, ascorbate, quercetin, phenolate form of quercetin, α -tocopherol and α -tocopheroxyl radical) were obtained from simulations of single molecules interacting with the membrane.

The interaction between vitC, vitE and quercetin was assessed by high concentration simulations: 6 molecules of each antioxidant were placed in the water surrounding one bilayer, 3 of each compound close to either one or the other leaflet. The same starting structure was run 6 times for 300 ns to allow better statistical sampling. All molecules converged to their equilibrium positions before 150 ns. Therefore, only data for the last 150 ns were used for analysis. In the high concentration simulations, two molecules were considered to form pairs if the average distance between their centers of mass was less than 10 Å. This cutoff corresponded to the intermolecular distance for which pairs spend more than 90% of the time attached together (Table S2). It is important to note that the difference between this cutoff and distances typical for π - π interactions (3 to 4 Å) is because (i) the intermolecular distances were measured between the centers of mass and not as minimum distances between π -conjugated moieties, and (ii) thermal motion occurs. In order to further assess the relative populations of homo- and hetero-associations (Table S3), one hundred 100 ns long

simulations were conducted. Quercetin and vitE molecules were initially placed in both leaflets of the membrane at their equilibrium depth and at random *x,y*-positions. The concentration was varying from 2 to 4 molecules of each antioxidant per leaflet. The overall simulation time was 13.6 μ s.

The free energy profiles of non-interacting antioxidants and their corresponding radicals were evaluated with COSMOmic⁶ in a DOPC bilayer at 310 K (Figure S1).

Quantum mechanics calculations. The potential energy surface of the various dimers was explored using our previously reported method⁷. Association energies (ΔE) of the complexes were calculated as the difference in energy between the complex and the isolated fragments (Table 1). The association enthalpies (ΔH) were calculated for all conformers of the complexes using a frequency analysis, a temperature of 298 K and a pressure of 1 atm. Negative values indicated that the association was thermodynamically favored compared to the pair of isolated compounds. The calculations were performed with B3P86-D2($s_6=0.78$)/def2-QZVP//B3P86-D2($s_6=0.78$)/def2-SVP. This re-parameterized DFT functional, which includes Grimme's dispersive term with the s_6 parameter adjusted to a value of 0.780, has been validated by high-level SCS-MP2 calculations and experimental values on polyphenol non-covalent complexes^{8,9}. The COSMO implicit solvent was used to model benzene (non-polar) and water (polar) solvation. Bond dissociation enthalpy calculations were performed with B3P86/6-311+G(d,p) as previously reported¹⁰.

Liposome formation and fluorescence. DOPC, vitE and DMSO were purchased from Sigma. Quercetin dihydrate was from Merck Millipore. HBS solution (HEPES 20 mM pH 7.4, NaCl 150 mM) was prepared in Milli-Q water (resistivity higher than 18.2 M Ω .cm) and filtered (0.22 μ M). All chemicals were analytical grade reagents.

VitE and quercetin stock solutions were prepared in ethanol at 10 mM. Further dilutions were carried out directly in the lipid solution or in buffer to the desired concentrations. The samples containing vitE or quercetin were protected from light throughout their preparation.

Liposomes with embedded vitE were obtained by addition of vitE stock solution to a lipid chloroform solution with molar 4:1 lipid:vitE ratio (corresponding to a final vitE concentration of 50 μ M in the liposome suspension). A dried DOPC/vitE-lipid film was formed from a chloroform solution by removing the organic solvent under a nitrogen stream, followed by a minimum of 2 h drying under vacuum. The dried lipid film was then hydrated

in HBS buffer and extruded 19 times through 50 nm size calibrated polycarbonate membranes using a syringe-type extruder (Liposofast, Avestin Inc.)¹¹. The liposomes were separated from free vitE molecules by ultra-centrifugation (200000 g for 2 h at 277 K; Beckman Coulter Optima L-100 XP ultracentrifuge) and re-suspended in buffer prior fluorescence measurement. This procedure was repeated twice in order to remove all non-inserted vitE molecules from the liposome pellet and final suspension. The hydrodynamic mean diameter of the liposomes after centrifugation was determined by quasi-elastic light scattering (Zetasizer, Nano-ZS, Malvern Instruments). Their size found to be homogenous with a diameter of 159 ± 2 nm.

The efficiency of the liposome separation from the non-inserted vitE was checked by adding vitE only after the liposome extrusion step. Pure DOPC liposomes were exposed to 50 μM vitE during 30 min. Again, to discard all non-inserted vitE molecules, the liposomes were submitted to the ultra-centrifugation/re-suspension steps prior to fluorescence measurement. When vitE was incubated in the pre-formed pure DOPC liposomes (latter procedure), the measured vitE fluorescence was very weak (Figure 4A, control), whereas it was much higher when vitE was added prior to liposome formation (former procedure), see Figure 4A, condition: 0 μM quercetin. This shows that under the former procedure, the fluorescence was definitively assigned to vitE molecules embedded in the bilayer and not lying on the liposome surface, supporting the robustness of our cleaning step. Interestingly, this also shows that vitE does not insert easily into liposomes from a buffer solution under our experimental conditions.

To evaluate the effect of quercetin on the fluorescence signal of vitE, different concentrations of quercetin (from 25 μM to 100 μM) were added to the liposome suspension (lipid concentration of 200 μM) and incubated 30 min at 310 K. Emission fluorescence spectra of vitE or quercetin were recorded in buffer (Figures S3A&B and S4) and DOPC liposomes (Figures S3 and 4A) on a Varian Cary Eclipse fluorescence spectrophotometer. Spectra were corrected by subtracting the baseline spectra of the corresponding blank vesicles. The excitation wavelengths of vitE and quercetin were 291 nm and 370 nm, respectively. However, the quercetin emission signal, either in buffer or incubated with liposomes, was too weak for further analysis (Figure S3 B&C). Therefore, only data for vitE emission were employed.

References

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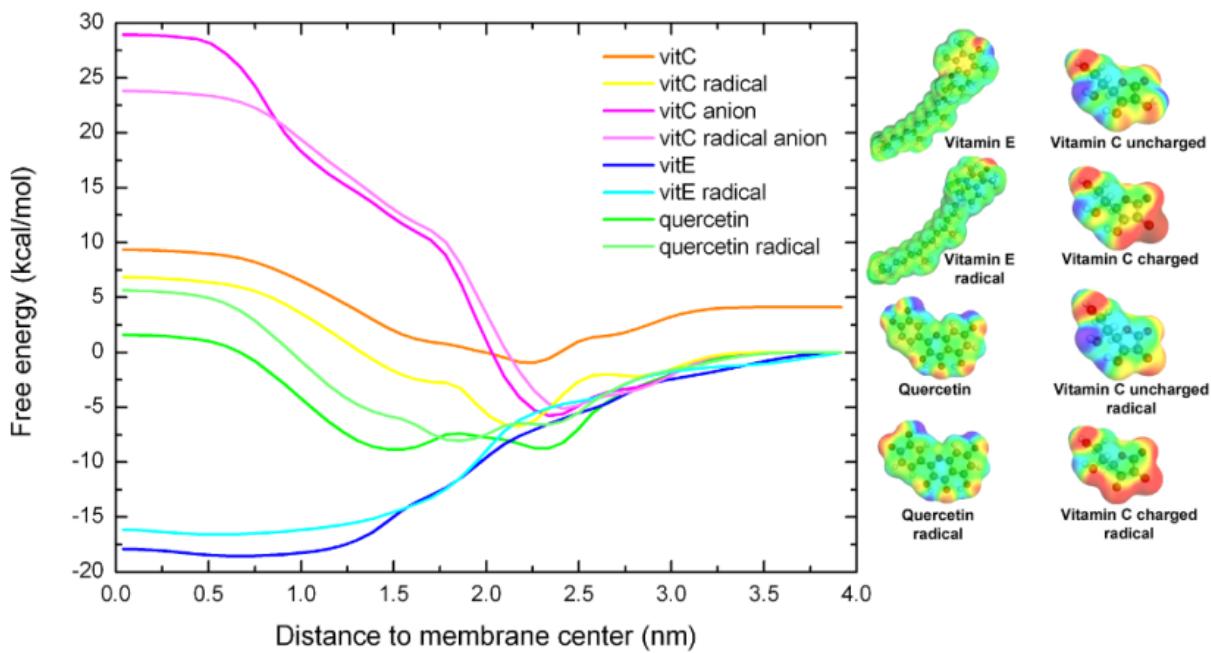


Figure S1: Free energy profiles of antioxidants along bilayer normal calculated with COSMOmic.

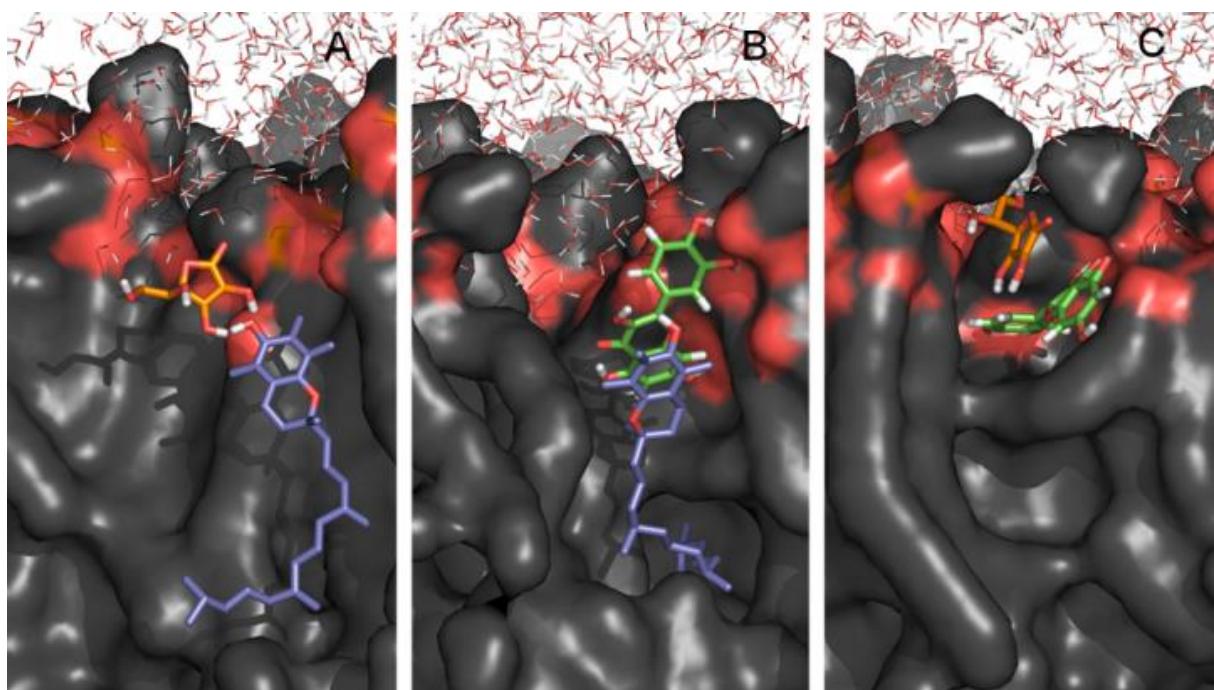


Figure S2. Representative snapshots of the antioxidant complexes.

(A) vitC:vitE, (B) quercetin:vitE, (C) quercetin:vitC.

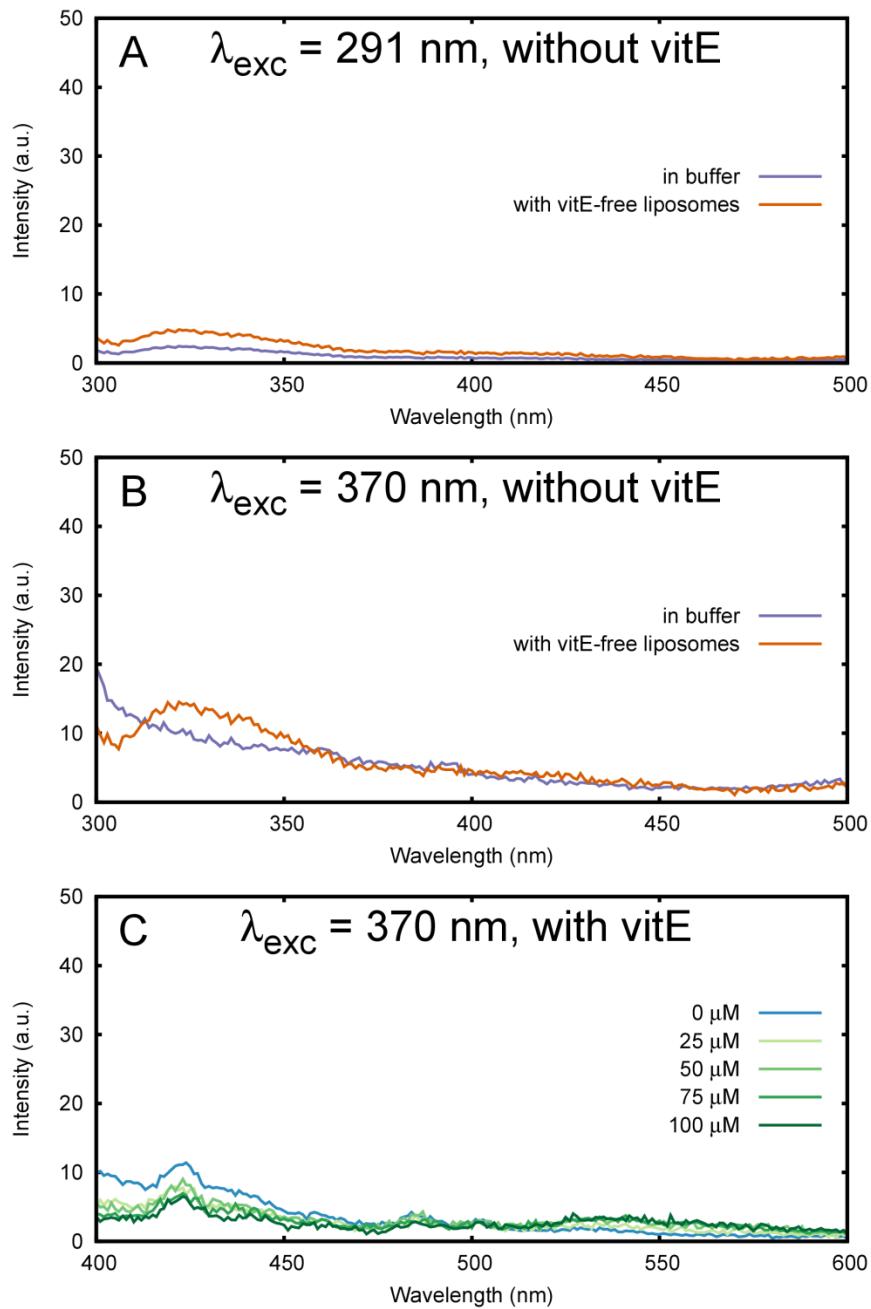


Figure S3: Fluorescence emission spectra of quercetin.

(A) 100 μM , $\lambda_{\text{exc}} = 291 \text{ nm}$, in HBS solution or incubated with vitE-free liposomes, (B) 100 μM , $\lambda_{\text{exc}} = 370 \text{ nm}$, in HBS solution or incubated with vitE-free liposomes, (C) 0 to 100 μM , $\lambda_{\text{exc}} = 370 \text{ nm}$, incubated with liposomes with embedded vitE.

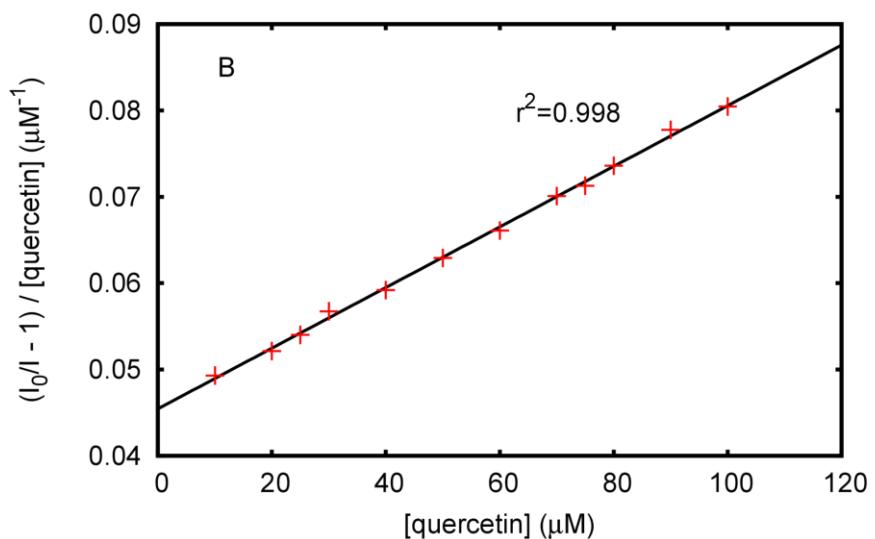


Figure S4: $[I_0/I - 1]/[Q] = f([quercetin])$ plot.

The fluorescence intensity of vitE in liposomes was recorded at $\lambda_{\text{exc}} = 291$ nm in the absence (I_0) and in the presence (I) of increasing concentrations of quercetin.

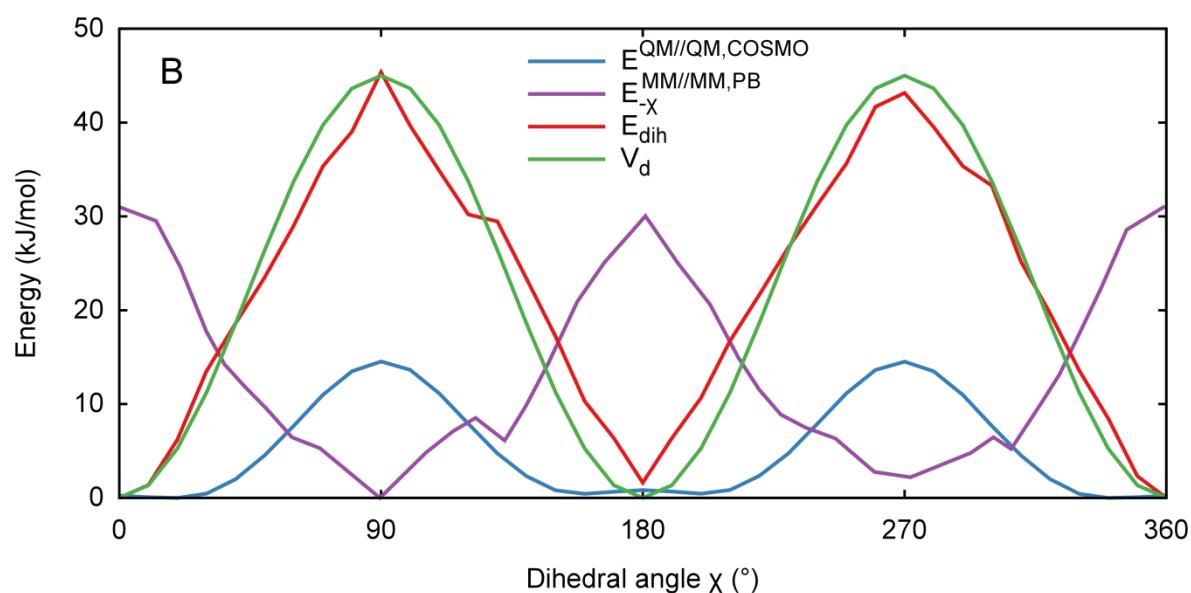
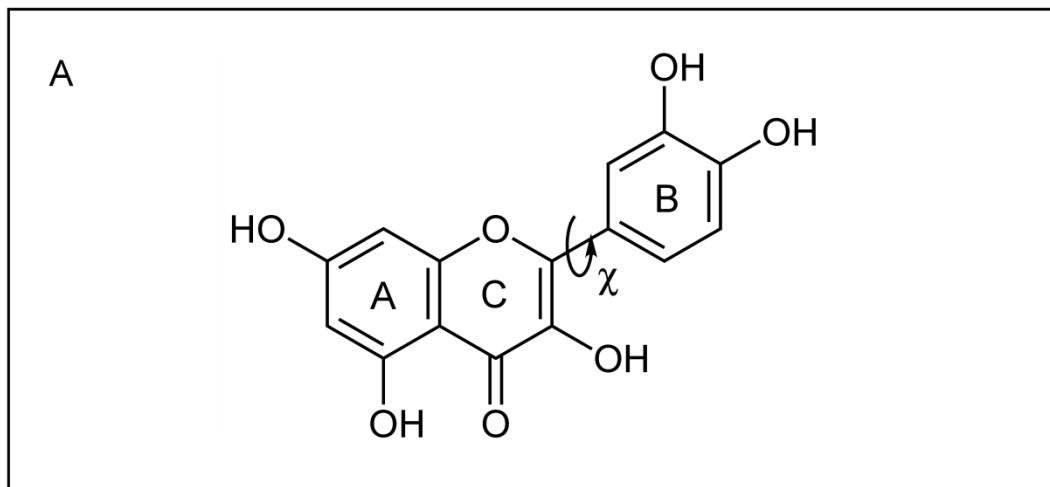


Figure S5: Parameterization of the dihedral angle χ of quercetin.

(A) Dihedral angle χ in the quercetin structure. (B) Determination of dihedral angle potential V_d according to Equation (2).

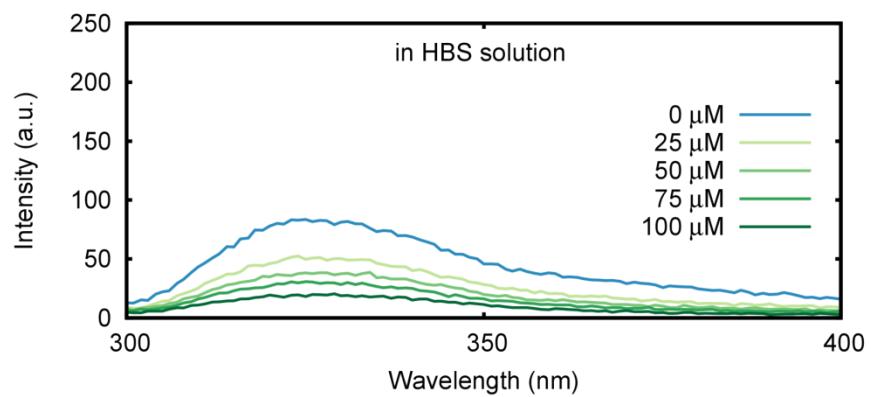


Figure S6: Fluorescence emission spectra of vitE exposed to increasing concentrations of quercetin (0 to 100 μM) in HBS solution.

VitE was excited at $\lambda_{\text{exc}} = 291$ nm.

Table S1: Diffusion coefficients of antioxidants in x,y plane and on z -axis.

	Lateral diffusion coefficient (x,y -plane) in $10^{-8} \text{ cm}^2.\text{s}^{-1}$	Diffusion coefficient on z -axis ($10^{-8} \text{ cm}^2.\text{s}^{-1}$)
vitC	17 ± 2	2 ± 2
quercetin	17 ± 2	1 ± 1
vitE	22 ± 5	3 ± 2

Table S2: Characterization of antioxidant pairs: intermolecular distance, position in the membrane, and ratio of the time spent in contact.

Pairs	Average distance between the centers of mass of each antioxidant (nm)	Average distance between the centers of mass of the pair and bilayer center (nm)	Ratio for the pair of time spent closer than the 10 \AA cutoff
vitC:vitC	0.66 ± 0.12	1.94 ± 0.26	$96 \pm 5 \%$
vitC vitE	0.74 ± 0.16	1.77 ± 0.13	$90 \pm 12 \%$
		1.28 ± 0.12	
vitC quercetin	0.73 ± 0.18	1.88 ± 0.12	$95 \pm 9 \%$
		1.77 ± 0.36	
vitE:vitE	0.77 ± 0.28	1.21 ± 0.06	$87 \pm 14\%$
vitE quercetin	0.72 ± 0.18	1.15 ± 0.07	$93 \pm 13 \%$
		1.49 ± 0.27	
quercetin:quercetin	0.75	2.09 ± 0.14	99%

Table S3: Occurrence of antioxidant pairs involving quercetin and vitE.

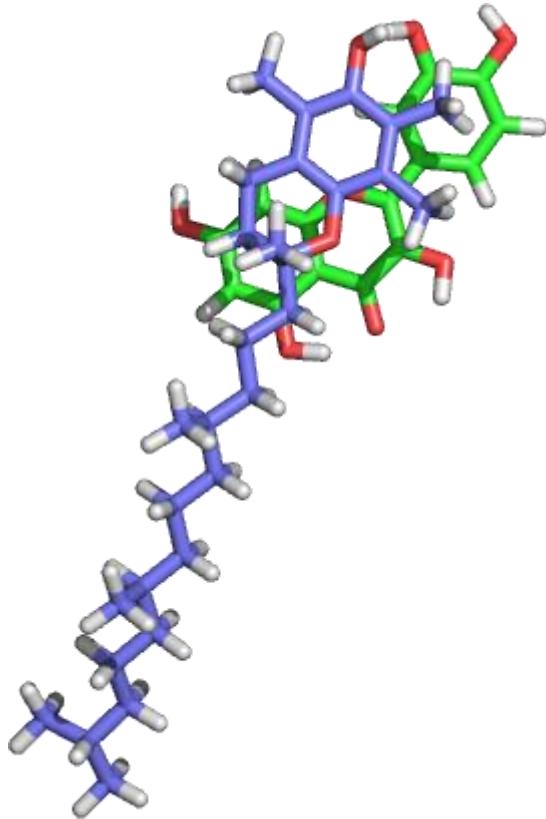
Pairs	Number of complexes observed (ratio)	Number of complexes expected for a random distribution
quercetin:quercetin	51 (27%)	47
quercetin:vitE	87 (45%)	95
vitE:vitE	53 (28%)	49

Dataset S1: Atomic coordinates of stable association-complexes as obtained from quantum DFT-D calculations.

quercetin:vitE 1

$$\Delta E = -13.2 \text{ kcal.mol}^{-1}$$

C	3.175366	5.662592	-1.743688
C	3.201107	4.480652	-2.509445
C	2.366907	4.314760	-3.625569
C	1.490190	5.351767	-3.996910
C	1.482134	6.529372	-3.241825
C	2.311637	6.702537	-2.121130
C	2.371773	3.017619	-4.389567
C	3.521964	2.099472	-3.992542
C	3.814726	2.152590	-2.494574
O	4.084657	3.521048	-2.124556
H	1.400001	2.510338	-4.232253
H	2.426213	3.222732	-5.473032
H	3.299594	1.062443	-4.287883
H	4.438313	2.396958	-4.519381
O	0.677349	7.573440	-3.686927
H	0.216051	7.970635	-2.933621
C	0.589048	5.176744	-5.186982
H	1.176475	5.074704	-6.118131
H	-0.010096	4.253475	-5.094547
H	-0.094258	6.029393	-5.301089
C	2.324737	7.992573	-1.348933
H	3.362481	8.336728	-1.206311
H	1.789076	8.800020	-1.870686
H	1.879944	7.870483	-0.344330
C	4.087869	5.820502	-0.561739
H	4.934074	6.489704	-0.804833
H	3.557724	6.262768	0.298309
H	4.510004	4.850556	-0.264499
C	2.635272	1.648833	-1.667516
H	2.415741	0.597588	-1.915372
H	2.872882	1.720678	-0.593598
H	1.731235	2.247535	-1.866735
C	5.108522	1.420000	-2.144357
H	5.239466	1.464842	-1.047267
H	5.944129	1.991087	-2.578633
C	5.189482	-0.025275	-2.618461
H	5.110498	-0.059626	-3.720636
H	4.330297	-0.597531	-2.224502
C	6.500054	-0.689257	-2.210144
H	7.329980	-0.075651	-2.605144
H	6.595203	-0.678002	-1.105779
C	6.671545	-2.126905	-2.710607
H	6.512235	-2.119421	-3.808437
C	8.104446	-2.605982	-2.457817
H	8.803147	-1.863958	-2.889120
H	8.293308	-2.604721	-1.365455
C	8.432508	-3.983311	-3.025285
H	7.793972	-4.743341	-2.542341
H	8.176104	-4.005621	-4.102830
C	9.899688	-4.363097	-2.854221
H	10.161827	-4.340224	-1.777399
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C	10.282431	-5.731894	-3.427184

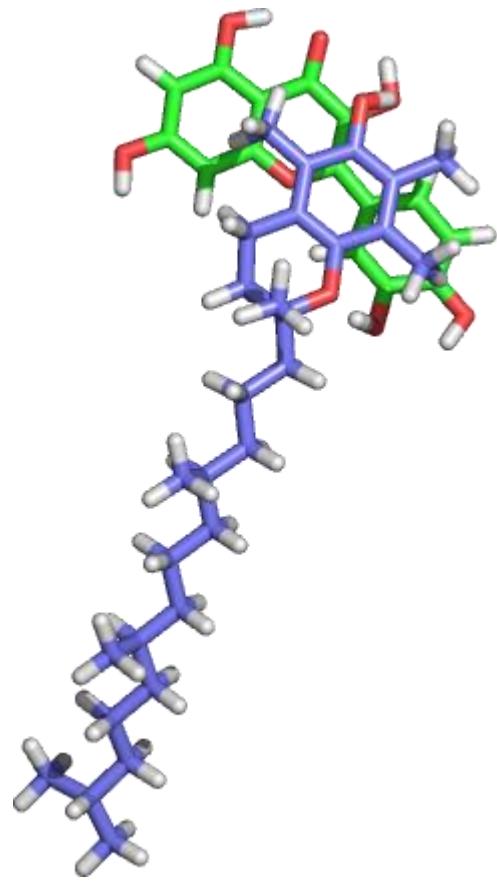


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H	12.166282	-5.866798	-2.379652
H	12.256078	-5.025789	-3.933131
C	12.312865	-7.171868	-4.099245
H	11.953125	-8.061739	-3.550379
H	11.875408	-7.239718	-5.112967
C	13.834029	-7.226664	-4.183934
H	14.252385	-7.074277	-3.170345
H	14.199227	-6.376340	-4.794325
C	14.403803	-8.526742	-4.760188
H	14.031252	-9.360473	-4.131904
C	15.929308	-8.519296	-4.685205
H	16.277775	-8.369360	-3.648437
H	16.355357	-9.466041	-5.060797
H	16.339550	-7.696493	-5.299734
C	5.642547	-3.069757	-2.087555
H	5.796464	-3.130390	-0.993881
H	4.611569	-2.722183	-2.266748
H	5.724662	-4.089918	-2.497105
C	9.591799	-6.869937	-2.676358
H	9.930561	-6.890651	-1.623585
H	8.495652	-6.750982	-2.676822
H	9.820863	-7.850532	-3.124597
C	13.938177	-8.772295	-6.195018
H	12.840348	-8.852986	-6.264078
H	14.258617	-7.939790	-6.849026
H	14.371878	-9.704350	-6.596812
C	6.491444	2.089651	-6.141464
C	7.006743	2.598633	-4.955101
C	6.591789	3.884810	-4.498315
C	5.672981	4.620598	-5.267431
C	5.141252	4.116691	-6.454721
C	5.561348	2.848833	-6.879215
O	5.093966	2.293413	-8.010683
H	6.796787	1.104062	-6.498098
O	7.877201	1.893953	-4.231319
H	8.094701	2.441630	-3.423960
C	7.103134	4.448474	-3.283557
C	6.675518	5.792233	-2.958025
C	5.777526	6.457618	-3.757388
O	5.289781	5.849337	-4.874518
H	4.426190	4.707888	-7.032081
O	7.895654	3.849333	-2.512707
O	7.190266	6.308825	-1.826812
H	7.743010	5.590090	-1.454084
C	5.227390	7.793101	-3.555206
C	4.012992	8.130233	-4.187641
C	3.419200	9.361519	-3.964465
C	4.059917	10.321570	-3.151022
C	5.287232	10.012374	-2.559681
C	5.857615	8.752263	-2.739660
H	6.802091	8.512813	-2.250543
H	3.496125	7.397722	-4.810040
O	2.189909	9.706021	-4.437403
H	1.594204	8.921403	-4.362756
O	3.458099	11.502253	-2.922285
H	2.602383	11.479980	-3.387138

quercetin:vitE 2

$$\Delta E = -12.2 \text{ kcal.mol}^{-1}$$

C	1.994611	8.004963	-0.165542
C	3.366010	8.317610	-0.160145
C	4.321645	7.529949	-0.814997
C	3.897719	6.395046	-1.532622
C	2.521962	6.150639	-1.644758
C	1.566518	6.935922	-0.968122
C	5.779505	7.908267	-0.767529
C	5.977424	9.356894	-0.336430
C	5.088821	9.714286	0.853826
O	3.709576	9.503954	0.459736
H	6.320101	7.227999	-0.081931
H	6.235091	7.750507	-1.760235
H	7.031313	9.545090	-0.079583
H	5.715674	10.039825	-1.165636
O	2.116228	5.092629	-2.411257
H	1.340813	5.362609	-2.930445
C	4.896333	5.457930	-2.153447
H	5.676145	5.995166	-2.717229
H	5.416488	4.876470	-1.369386
H	4.402908	4.749725	-2.833117
C	0.116298	6.591690	-1.168220
H	-0.179131	6.798641	-2.214641
H	-0.066629	5.518160	-0.983279
H	-0.550868	7.179157	-0.523551
C	1.041746	8.831323	0.657835
H	0.574521	9.644118	0.076103
H	0.227447	8.212010	1.064736
H	1.572569	9.299891	1.499599
C	5.372007	8.843420	2.071537
H	6.434400	8.912074	2.354374
H	4.754831	9.172576	2.923734
H	5.137586	7.788582	1.856178
C	5.151517	11.204047	1.180642
H	4.398728	11.408546	1.963901
H	4.834171	11.762482	0.279974
C	6.515010	11.711624	1.636431
H	7.267053	11.535412	0.845133
H	6.848575	11.137248	2.518218
C	6.485856	13.200172	1.967442
H	6.038251	13.744916	1.114632
H	5.809378	13.370541	2.828458
C	7.852606	13.819112	2.277547
H	8.502878	13.652738	1.394245
C	7.709429	15.332085	2.467911
H	7.142202	15.744302	1.611306
H	7.085575	15.519485	3.364970
C	9.022453	16.096174	2.597910
H	9.580005	15.728269	3.476387
H	9.658949	15.882777	1.716341
C	8.815802	17.602388	2.715838
H	8.208578	17.818515	3.617947
H	8.212669	17.946963	1.853797
C	10.100036	18.434803	2.777966
H	10.705121	18.186777	1.881738
C	9.761000	19.926900	2.708927
H	9.150025	20.193851	3.594662
H	9.111934	20.099395	1.828843
C	10.962241	20.862809	2.622577
H	11.581924	20.771263	3.533894
H	11.604919	20.544235	1.780542
C	10.559386	22.323059	2.447265
H	9.857421	22.597513	3.258239
H	9.992394	22.438049	1.501474

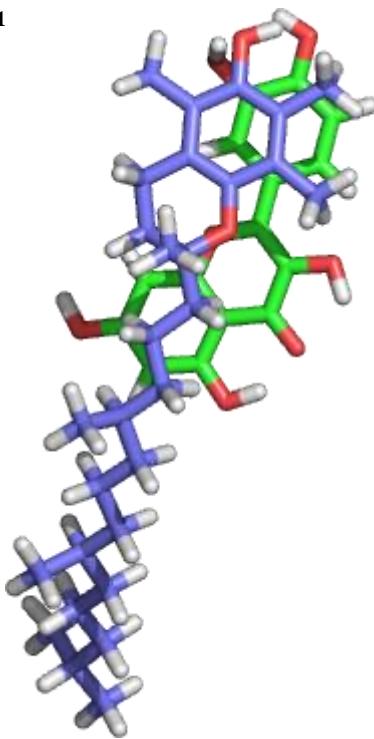


C	11.723007	23.318900	2.446938
H	12.278549	23.181959	3.396463
C	11.198815	24.752931	2.404707
H	10.517959	24.955281	3.249955
H	12.024244	25.484933	2.442860
H	10.635760	24.927972	1.469231
C	8.513841	13.156179	3.485545
H	7.889096	13.297781	4.387097
H	8.647267	12.072496	3.331909
H	9.507882	13.586119	3.690804
C	10.929088	18.102025	4.017753
H	10.358514	18.343888	4.934113
H	11.193071	17.032245	4.055661
H	11.869245	18.677061	4.043821
C	12.691166	23.068370	1.291524
H	13.134808	22.059715	1.337208
H	12.163478	23.163046	0.323948
H	13.515230	23.802668	1.299762
C	6.985741	5.629446	-5.721024
C	5.646934	5.262577	-5.810372
C	4.637095	6.170675	-5.374889
C	5.020923	7.415089	-4.845929
C	6.358415	7.798334	-4.757799
C	7.331695	6.891954	-5.202610
O	8.642159	7.183408	-5.151132
H	7.768177	4.943706	-6.052384
O	5.300135	4.069274	-6.287151
H	4.305250	4.012923	-6.242581
C	3.248936	5.812397	-5.402373
C	2.322236	6.779465	-4.861213
C	2.763204	7.973052	-4.350117
O	4.089598	8.273426	-4.385081
H	6.626947	8.776357	-4.350447
O	2.809908	4.713699	-5.825625
O	1.034771	6.363413	-4.793564
H	1.039422	5.501085	-5.264613
C	1.969849	8.986463	-3.666395
C	2.598697	9.807837	-2.710525
C	1.855766	10.692764	-1.944912
C	0.469321	10.826892	-2.170953
C	-0.150933	10.058585	-3.159757
C	0.587968	9.129649	-3.889132
H	0.089726	8.509814	-4.635613
H	3.665739	9.700645	-2.511826
O	2.368339	11.413575	-0.909257
H	2.929471	10.814000	-0.355451
O	-0.249496	11.654036	-1.388605
H	0.371433	12.049618	-0.749352
H	-1.226796	10.173099	-3.318477
H	8.773599	8.073878	-4.793869

quercetin:vitE 3

$$\Delta E = -10.7 \text{ kcal.mol}^{-1}$$

C	4.191168	5.387801	-1.579930
C	3.926332	4.163841	-2.232653
C	3.129842	4.093468	-3.382344
C	2.584344	5.274400	-3.918185
C	2.896073	6.485633	-3.301869
C	3.664459	6.569112	-2.124511
C	2.906611	2.772248	-4.066638
C	3.907405	1.725780	-3.597355
C	4.083675	1.755450	-2.079671
O	4.522803	3.069221	-1.683877
H	1.872391	2.423557	-3.882737
H	2.987479	2.900352	-5.159771
H	3.587935	0.720463	-3.911480
H	4.891974	1.916721	-4.053233
O	2.496858	7.635489	-3.959821
H	2.809074	8.415297	-3.477046
C	1.754158	5.229018	-5.171973
H	2.390225	5.060789	-6.060836
H	1.021431	4.406147	-5.132301
H	1.207306	6.170809	-5.325470
C	3.876035	7.936394	-1.528576
H	4.424259	8.601798	-2.220713
H	2.908162	8.420205	-1.296461
H	4.457777	7.906012	-0.598953
C	5.067818	5.337743	-0.360594
H	5.078705	6.283517	0.198429
H	4.734472	4.533244	0.315650
H	6.107519	5.094344	-0.645955
C	2.777812	1.442319	-1.355123
H	2.429131	0.430167	-1.618239
H	2.935244	1.492844	-0.265497
H	1.990837	2.164880	-1.627066
C	5.216220	0.834540	-1.623353
H	5.212336	0.798917	-0.518304
H	6.164368	1.312995	-1.919125
C	5.181058	-0.572422	-2.202053
H	5.316905	-0.512335	-3.297570
H	4.189205	-1.031071	-2.033772
C	6.279666	-1.471306	-1.644446
H	7.233781	-0.914829	-1.641569
H	6.069137	-1.720259	-0.585937
C	6.469601	-2.760681	-2.448699
H	6.510243	-2.465996	-3.516324
C	7.809981	-3.422261	-2.122932
H	8.593506	-2.642572	-2.128218
H	7.781190	-3.824934	-1.090558
C	8.211349	-4.526372	-3.095880
H	7.479856	-5.352323	-3.051983
H	8.157354	-4.128753	-4.129640
C	9.617805	-5.059271	-2.844294
H	9.666392	-5.515812	-1.835386
H	10.320304	-4.204331	-2.825597
C	10.115613	-6.077118	-3.874741
H	10.018394	-5.610381	-4.876568
C	11.600511	-6.377606	-3.650155
H	11.721381	-6.870050	-2.664552
H	12.147781	-5.417935	-3.579321
C	12.255046	-7.232365	-4.730288
H	11.777542	-8.229181	-4.769106
H	12.069203	-6.765070	-5.715071
C	13.753772	-7.411653	-4.514103
H	13.921035	-7.822342	-3.499875
H	14.248337	-6.419379	-4.525771

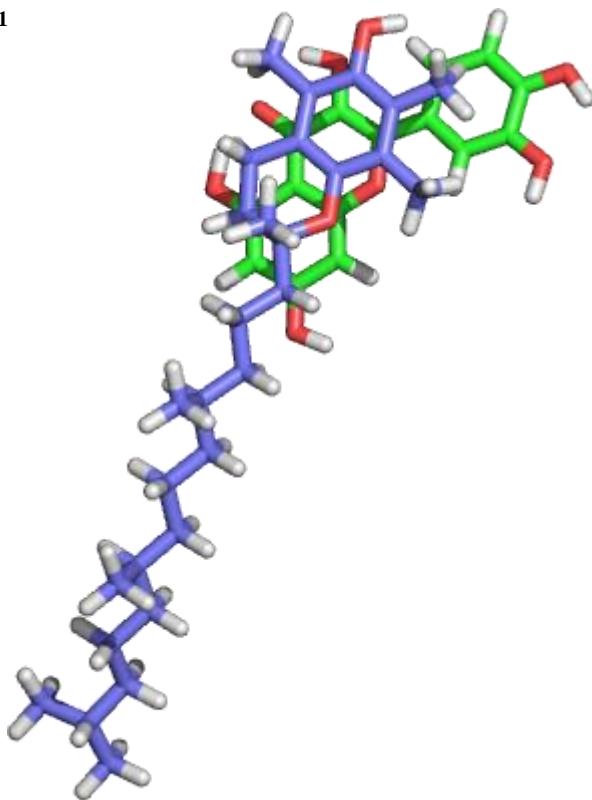


C	14.450593	-8.318457	-5.532939
H	13.939201	-9.301619	-5.508459
C	15.912467	-8.532482	-5.145034
H	16.000190	-8.957023	-4.129661
H	16.420149	-9.214678	-5.849301
H	16.457285	-7.570189	-5.155727
C	5.291972	-3.716858	-2.264685
H	5.227244	-4.042931	-1.209801
H	4.335437	-3.235248	-2.529258
H	5.396975	-4.617124	-2.893040
C	9.273650	-7.352221	-3.861489
H	9.348512	-7.846128	-2.874546
H	8.209384	-7.137969	-4.053912
H	9.612003	-8.070959	-4.626208
C	14.349870	-7.767414	-6.954523
H	13.302552	-7.668542	-7.284919
H	14.817670	-6.766621	-7.011237
H	14.871717	-8.424918	-7.671466
C	8.388024	-0.784640	-4.487236
C	8.780825	0.067817	-3.464762
C	8.309010	1.413229	-3.445855
C	7.469228	1.859663	-4.480973
C	7.062071	1.011972	-5.509874
C	7.524698	-0.311514	-5.493031
O	7.158938	-1.199886	-6.431887
H	8.728792	-1.821388	-4.504784
O	9.571990	-0.365143	-2.483589
H	9.682204	0.392150	-1.841803
C	8.634538	2.302693	-2.371396
C	8.108681	3.648973	-2.455523
C	7.336728	4.041900	-3.523710
O	7.019781	3.131445	-4.489235
H	6.402106	1.377191	-6.300336
O	9.335978	1.980411	-1.379105
O	8.429549	4.449873	-1.422943
H	8.965253	3.881753	-0.828437
C	6.794494	5.371483	-3.788683
C	5.807658	5.546464	-4.780685
C	5.292206	6.806684	-5.048581
C	5.769324	7.930358	-4.344850
C	6.750987	7.769056	-3.366217
C	7.251674	6.502924	-3.082438
H	8.016087	6.391039	-2.314559
H	5.408744	4.693087	-5.330265
O	4.307312	7.004588	-5.979952
H	3.501835	7.286024	-5.490564
O	5.244778	9.153284	-4.584137
H	4.721654	9.097250	-5.402674
H	7.112571	8.649812	-2.828700
H	6.560361	-0.785295	-7.070374

quercetin:vitE 4

$$\Delta E = -10.4 \text{ kcal.mol}^{-1}$$

C	3.879145	5.430056	-0.753585
C	3.863742	4.385348	-1.699222
C	3.113505	4.481075	-2.881017
C	2.362306	5.643723	-3.139449
C	2.384547	6.684650	-2.203521
C	3.114470	6.579719	-1.004185
C	3.085399	3.332500	-3.855895
C	4.110049	2.252499	-3.526747
C	4.269906	2.032285	-2.024609
O	4.620179	3.285464	-1.409699
H	2.064129	2.904944	-3.874635
H	3.265243	3.704692	-4.880235
H	3.836117	1.304807	-4.016567
H	5.099231	2.540517	-3.906880
O	1.660231	7.810677	-2.474754
H	1.946581	8.524142	-1.888889
C	1.568654	5.763361	-4.409876
H	2.222546	5.656754	-5.292918
H	0.809355	4.963658	-4.480390
H	1.059144	6.734834	-4.469959
C	3.023943	7.717358	-0.024064
H	3.447438	8.646602	-0.448630
H	1.969488	7.924997	0.238075
H	3.565533	7.511976	0.908755
C	4.693224	5.290668	0.505446
H	5.264567	6.211146	0.710929
H	4.050607	5.107633	1.386852
H	5.395998	4.450332	0.422089
C	2.991088	1.507750	-1.378941
H	2.696362	0.546742	-1.831327
H	3.147727	1.359523	-0.297645
H	2.165388	2.225087	-1.518084
C	5.475706	1.142485	-1.730593
H	5.612792	1.104496	-0.633674
H	6.361464	1.655768	-2.143948
C	5.413256	-0.272370	-2.290048
H	5.205406	-0.240729	-3.375381
H	4.574779	-0.821141	-1.826288
C	6.725261	-1.017398	-2.068071
H	7.537327	-0.420313	-2.525108
H	6.944719	-1.061877	-0.982198
C	6.779090	-2.436950	-2.638607
H	6.535777	-2.375315	-3.718958
C	8.202371	-2.988524	-2.513843
H	8.900457	-2.263693	-2.975196
H	8.471864	-3.030063	-1.439297
C	8.431929	-4.359993	-3.139393
H	7.792932	-5.107115	-2.637261
H	8.110528	-4.340377	-4.199295
C	9.890496	-4.798333	-3.064065
H	10.211587	-4.812792	-2.003036
H	10.516822	-4.032612	-3.560979
C	10.197995	-6.163441	-3.687494
H	9.828683	-6.147658	-4.733392
C	11.712419	-6.386719	-3.735123
H	12.102900	-6.388364	-2.697630
H	12.180927	-5.517146	-4.234887
C	12.161106	-7.659481	-4.445558
H	11.779547	-8.548344	-3.909955
H	11.704330	-7.688523	-5.452608
C	13.678032	-7.765089	-4.557509
H	14.117128	-7.649482	-3.547740
H	14.063025	-6.914566	-5.155354

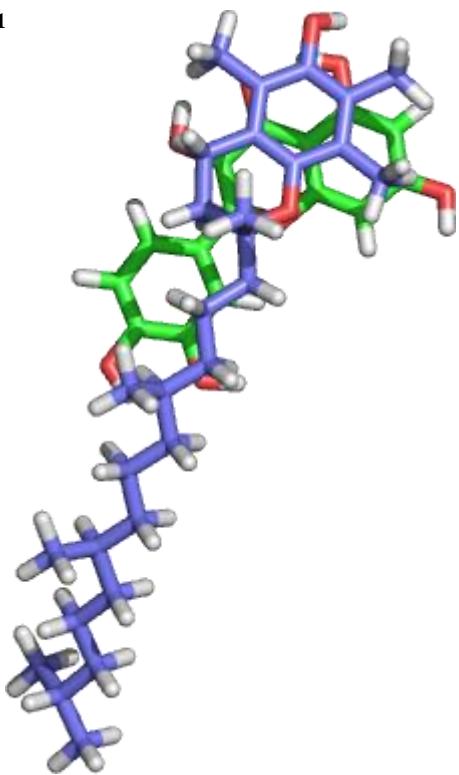


C	14.193668	-9.070633	-5.170377
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C	15.719329	-9.119509	-5.113853
H	16.084105	-9.008029	-4.077880
H	16.107163	-10.071326	-5.516926
H	16.152175	-8.296892	-5.712948
C	5.754297	-3.354205	-1.972168
H	5.979580	-3.457692	-0.894242
H	4.730456	-2.956771	-2.068906
H	5.761609	-4.362481	-2.417634
C	9.485531	-7.295096	-2.947486
H	9.846716	-7.353500	-1.903572
H	8.394530	-7.138855	-2.920244
H	9.670665	-8.271431	-3.424233
C	13.703059	-9.265247	-6.604465
H	12.602177	-9.303719	-6.662146
H	14.046841	-8.430028	-7.242920
H	14.097676	-10.202856	-7.032492
C	7.167546	2.725581	-5.376672
C	6.253879	3.681898	-5.805188
C	5.976746	4.811627	-4.979035
C	6.629961	4.932514	-3.739967
C	7.518911	3.961047	-3.284186
C	7.774358	2.863471	-4.114036
O	8.601532	1.872161	-3.731575
H	7.380257	1.849312	-5.992475
O	5.615173	3.543050	-6.965539
H	5.009122	4.330677	-7.059396
C	5.042178	5.817516	-5.377472
C	4.874448	6.947994	-4.490864
C	5.583517	7.030486	-3.316161
O	6.414605	6.010065	-2.965094
H	7.989697	4.061519	-2.303806
O	4.373364	5.771048	-6.444423
O	4.003887	7.879509	-4.908946
H	3.659860	7.535377	-5.759791
C	5.579681	8.120272	-2.344691
C	6.265783	7.954417	-1.122813
C	6.289467	8.966683	-0.176232
C	5.650217	10.200350	-0.431499
C	4.976897	10.371637	-1.641872
C	4.927832	9.344485	-2.586636
H	4.384033	9.495743	-3.517726
H	6.769097	7.010296	-0.903564
O	6.883048	8.859227	1.041974
H	7.367268	8.024607	1.112305
O	5.678264	11.189611	0.482184
H	6.191522	10.888958	1.250087
H	4.480376	11.327472	-1.830893
H	8.951961	2.052711	-2.847231

quercetin:vitE 5

$$\Delta E = -10.3 \text{ kcal.mol}^{-1}$$

C	6.492903	6.860438	-1.080974
C	5.231754	6.233313	-1.165567
C	4.044727	6.952283	-0.961915
C	4.098759	8.335378	-0.708657
C	5.346258	8.965704	-0.661928
C	6.542893	8.238298	-0.815339
C	2.715471	6.248763	-0.994525
C	2.803721	4.857216	-1.600527
C	4.065926	4.105569	-1.188880
O	5.229235	4.904331	-1.471823
H	2.308795	6.200178	0.034554
H	1.991027	6.847024	-1.572679
H	1.920231	4.261661	-1.321985
H	2.803112	4.925612	-2.696503
O	5.388909	10.315541	-0.427792
H	6.072494	10.701112	-0.997744
C	2.828611	9.113650	-0.519367
H	2.184930	9.017640	-1.410508
H	2.249675	8.731762	0.340696
H	3.039233	10.179622	-0.360511
C	7.841213	8.979795	-0.655989
H	7.903977	9.834804	-1.353225
H	7.931563	9.392228	0.365636
H	8.712885	8.340433	-0.849500
C	7.750206	6.045083	-1.234930
H	8.435385	6.488644	-1.975298
H	8.304045	5.984937	-0.279590
H	7.508318	5.023160	-1.556040
C	4.060860	3.772234	0.298925
H	3.207158	3.118411	0.543195
H	4.996394	3.258635	0.574935
H	3.976567	4.692339	0.901575
C	4.261111	2.868601	-2.067757
H	5.127495	2.297798	-1.685225
H	4.537964	3.239778	-3.070922
C	3.045865	1.961047	-2.205725
H	2.218988	2.529647	-2.668647
H	2.689921	1.640452	-1.209733
C	3.329874	0.748290	-3.086357
H	3.870384	1.089233	-3.988262
H	4.005649	0.044608	-2.561215
C	2.074507	0.006944	-3.548921
H	1.439122	0.748511	-4.070135
C	2.433102	-1.075112	-4.569270
H	3.118136	-0.633157	-5.316381
H	2.997804	-1.883471	-4.063306
C	1.239079	-1.672287	-5.305278
H	0.553980	-2.151301	-4.584297
H	0.652549	-0.856120	-5.773826
C	1.645245	-2.675107	-6.378531
H	2.132716	-3.547934	-5.900096
H	2.416447	-2.211214	-7.023395
C	0.502830	-3.171515	-7.267952
H	0.038031	-2.281301	-7.739006
C	1.055568	-4.054063	-8.391518
H	1.497172	-4.967156	-7.944815
H	1.892520	-3.518890	-8.879877
C	0.042119	-4.449848	-9.458871
H	-0.772492	-5.046506	-9.007828
H	-0.431796	-3.533073	-9.856060
C	0.666864	-5.249628	-10.597825
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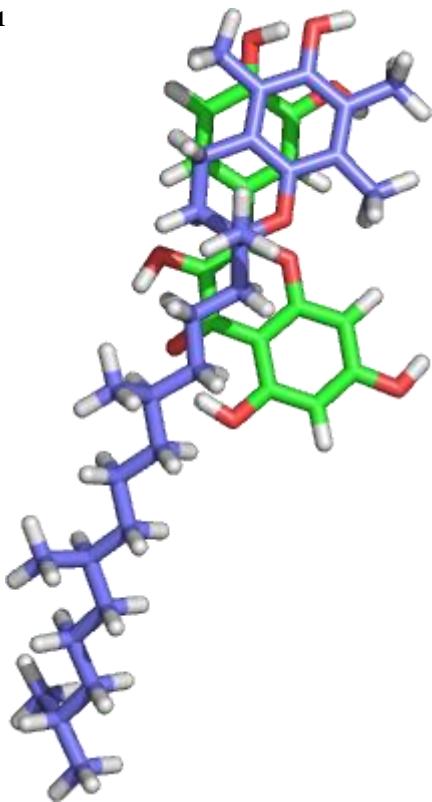


C	-0.317730	-5.719989	-11.671672
H	-1.112077	-6.302323	-11.163529
C	0.381010	-6.639773	-12.671701
H	0.836752	-7.509139	-12.166550
H	-0.323765	-7.014997	-13.434392
H	1.186429	-6.093435	-13.196235
C	1.279869	-0.555258	-2.371537
H	1.892457	-1.285256	-1.810367
H	0.978045	0.242468	-1.672682
H	0.362668	-1.066824	-2.707869
C	-0.572956	-3.893588	-6.457727
H	-0.141895	-4.782643	-5.961217
H	-1.000403	-3.242154	-5.677491
H	-1.403511	-4.232947	-7.098342
C	-0.978665	-4.547262	-12.394634
H	-1.546704	-3.902644	-11.702944
H	-0.211827	-3.922228	-12.889678
H	-1.675364	-4.904157	-13.173017
C	7.769315	8.878430	-3.890256
C	6.441088	9.241521	-3.720679
C	5.409131	8.304945	-4.012159
C	5.759419	7.013897	-4.442489
C	7.089414	6.625657	-4.588081
C	8.081469	7.569060	-4.299700
O	9.389671	7.261900	-4.376867
H	8.572589	9.582842	-3.668059
O	6.1118112	10.458770	-3.268759
H	5.1119151	10.499731	-3.240642
C	4.028308	8.644815	-3.869926
C	3.062067	7.608365	-4.182923
C	3.469767	6.379657	-4.644624
O	4.802727	6.116189	-4.746514
H	7.339073	5.608782	-4.899678
O	3.610196	9.774805	-3.513423
O	1.777214	7.966353	-4.003886
H	1.825442	8.910596	-3.736174
C	2.642520	5.241073	-5.041634
C	3.268856	4.062068	-5.504150
C	2.517137	2.947837	-5.845543
C	1.111684	2.967313	-5.721824
C	0.489007	4.130355	-5.268464
C	1.238460	5.257545	-4.934888
H	0.731041	6.152535	-4.578148
H	4.356260	4.017476	-5.599968
O	3.037609	1.783234	-6.312308
H	4.001117	1.836853	-6.380908
O	0.383394	1.878046	-6.041249
H	0.990700	1.178328	-6.335314
H	-0.600917	4.138330	-5.179910
H	9.499884	6.343019	-4.662464

quercetin:vitE 6

$$\Delta E = -10.0 \text{ kcal.mol}^{-1}$$

C	4.428034	5.609661	-0.999388
C	4.072758	4.446698	-1.717947
C	3.069026	4.454863	-2.691386
C	2.392938	5.657331	-2.972902
C	2.781317	6.819622	-2.301125
C	3.764088	6.811963	-1.288305
C	2.745519	3.196739	-3.450915
C	3.830629	2.138141	-3.287596
C	4.321475	2.045504	-1.842923
O	4.795469	3.336485	-1.414355
H	1.766539	2.801238	-3.117989
H	2.625754	3.438982	-4.520592
H	3.457296	1.153079	-3.607425
H	4.689412	2.381807	-3.929316
O	2.208843	8.001426	-2.710270
H	2.461001	8.714122	-2.107328
C	1.308549	5.687599	-4.011874
H	1.737143	5.616932	-5.028177
H	0.621598	4.833744	-3.887183
H	0.729125	6.620291	-3.959602
C	4.053971	8.119475	-0.596042
H	4.360822	8.896292	-1.322232
H	3.156816	8.502014	-0.072817
H	4.851272	8.041564	0.154804
C	5.529124	5.462431	0.014488
H	5.759842	6.397497	0.542575
H	5.265498	4.693602	0.761405
H	6.448211	5.096123	-0.476827
C	3.202500	1.604385	-0.903609
H	2.860315	0.591272	-1.172882
H	3.570540	1.590786	0.135280
H	2.342732	2.291500	-0.962561
C	5.550739	1.143269	-1.707152
H	5.722832	0.950045	-0.632389
H	6.421593	1.719288	-2.058626
C	5.485528	-0.172423	-2.470282
H	5.531544	0.034206	-3.555301
H	4.515118	-0.668885	-2.286621
C	6.628909	-1.108343	-2.096734
H	7.577636	-0.544361	-2.139438
H	6.509558	-1.430768	-1.043304
C	6.768537	-2.341603	-2.991206
H	6.950665	-1.971588	-4.019055
C	7.992298	-3.159299	-2.569510
H	8.841426	-2.468743	-2.414019
H	7.789494	-3.625861	-1.584202
C	8.416841	-4.234511	-3.563918
H	7.581663	-4.935788	-3.737326
H	8.628573	-3.759421	-4.542209
C	9.648735	-5.006467	-3.105620
H	9.414412	-5.547110	-2.166465
H	10.445470	-4.282158	-2.848600
C	10.207680	-6.004199	-4.124114
H	10.437206	-5.441089	-5.051874
C	11.520835	-6.601821	-3.609865
H	11.311072	-7.189445	-2.693496
H	12.184331	-5.773711	-3.294371
C	12.270857	-7.473612	-4.611603
H	11.654602	-8.348146	-4.892311
H	12.425857	-6.895450	-5.541575
C	13.610396	-7.968216	-4.076081
H	13.436776	-8.494254	-3.117485
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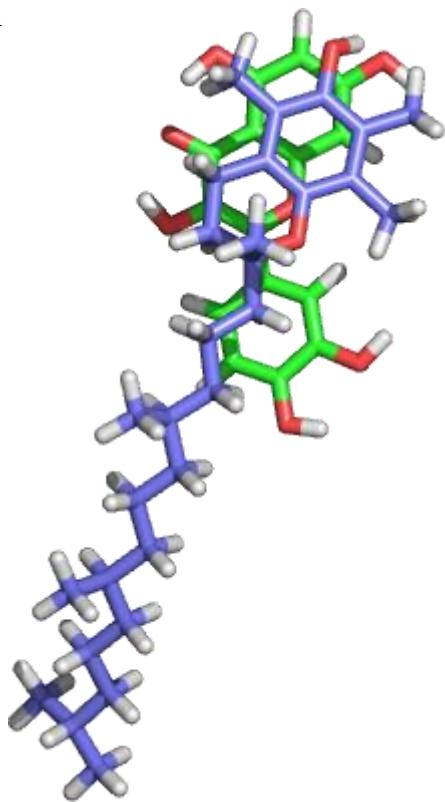


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H	13.711831	-9.753359	-5.259467
C	15.622714	-9.452378	-4.324567
H	15.360061	-9.982667	-3.392458
H	16.171720	-10.152619	-4.978217
H	16.310288	-8.627393	-4.061253
C	5.496520	-3.188974	-2.995189
H	5.264698	-3.534019	-1.970005
H	4.627828	-2.619604	-3.365500
H	5.605700	-4.079724	-3.636191
C	9.190447	-7.091008	-4.469391
H	8.932450	-7.671145	-3.563684
H	8.258682	-6.662484	-4.874077
H	9.587682	-7.793918	-5.220204
C	14.756875	-8.208245	-6.326563
H	13.868544	-7.856838	-6.877407
H	15.398388	-7.330405	-6.122821
H	15.319101	-8.890764	-6.987483
C	10.685476	1.289739	-1.428982
C	9.927915	0.845128	-2.505308
C	8.956262	1.709891	-3.090439
C	8.790330	3.005241	-2.567765
C	9.542798	3.462871	-1.488189
C	10.487329	2.590996	-0.927859
O	11.250847	2.956423	0.115036
H	11.430937	0.637151	-0.969668
O	10.092516	-0.384968	-2.993281
H	9.448538	-0.489493	-3.748489
C	8.147260	1.291523	-4.194479
C	7.186254	2.245921	-4.701168
C	7.075907	3.504343	-4.152078
O	7.884144	3.842290	-3.108305
H	9.392947	4.472454	-1.097785
O	8.214344	0.152725	-4.725654
O	6.413740	1.788687	-5.704100
H	6.738679	0.875672	-5.862941
C	6.166368	4.578058	-4.533620
C	6.197669	5.795748	-3.820226
C	5.323968	6.825950	-4.128956
C	4.342996	6.653358	-5.130000
C	4.343205	5.470967	-5.873103
C	5.239338	4.443750	-5.586341
H	5.202587	3.523348	-6.167159
H	6.916497	5.940412	-3.010523
O	5.331569	8.028648	-3.499362
H	5.866649	7.965614	-2.696169
O	3.419039	7.603360	-5.366182
H	3.265034	8.109515	-4.544917
H	3.601385	5.358075	-6.668661
H	11.035599	3.861157	0.384728

quercetin:vitE 7

$$\Delta E = -9.7 \text{ kcal.mol}^{-1}$$

C	4.649824	5.205622	-1.013924
C	4.348708	4.093311	-1.821669
C	3.490165	4.207753	-2.925085
C	2.882404	5.447478	-3.206244
C	3.140879	6.545571	-2.371380
C	4.021880	6.433109	-1.277755
C	3.205651	3.003511	-3.787757
C	4.091992	1.804315	-3.456700
C	4.357153	1.685297	-1.958074
O	4.945298	2.916490	-1.490815
H	2.137950	2.732651	-3.681020
H	3.331284	3.268902	-4.852077
H	3.626439	0.875128	-3.821235
H	5.064061	1.892783	-3.963398
O	2.502710	7.730561	-2.642792
H	3.127655	8.465220	-2.552532
C	1.979523	5.578981	-4.400220
H	2.485658	5.230458	-5.316438
H	1.072140	4.958087	-4.286153
H	1.675151	6.623322	-4.551903
C	4.317463	7.615260	-0.396183
H	5.350882	7.984675	-0.544175
H	3.620006	8.449407	-0.565664
H	4.247801	7.339518	0.669741
C	5.635643	5.082901	0.115619
H	6.474016	5.792462	-0.014238
H	5.172272	5.327795	1.088883
H	6.042254	4.063384	0.171646
C	3.074375	1.423342	-1.175337
H	2.634487	0.460634	-1.482978
H	3.295399	1.384536	-0.096025
H	2.331532	2.219179	-1.351703
C	5.437536	0.652507	-1.651958
H	5.547007	0.587845	-0.552859
H	6.382804	1.060492	-2.039379
C	5.250615	-0.738872	-2.238647
H	5.258554	-0.671923	-3.342638
H	4.268668	-1.159925	-1.955532
C	6.383674	-1.662659	-1.794025
H	7.328427	-1.089957	-1.810208
H	6.228043	-1.963776	-0.739208
C	6.574564	-2.913648	-2.652226
H	6.705480	-2.572491	-3.700025
C	7.860610	-3.637750	-2.247250
H	8.675246	-2.890692	-2.188773
H	7.740398	-4.039511	-1.220912
C	8.288914	-4.759340	-3.188049
H	7.523569	-5.555318	-3.196753
H	8.334194	-4.365044	-4.222735
C	9.648074	-5.346522	-2.822678
H	9.598230	-5.793489	-1.809407
H	10.380527	-4.519582	-2.755101
C	10.186526	-6.394065	-3.801521
H	10.176030	-5.940184	-4.813850
C	11.641826	-6.732582	-3.465358
H	11.677878	-7.201785	-2.461804
H	12.211760	-5.787381	-3.378939
C	12.346397	-7.633284	-4.474240
H	11.852269	-8.621966	-4.513537
H	12.234533	-7.194360	-5.483019
C	13.824234	-7.829717	-4.153322
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H	14.335577	-6.845935	-4.164021

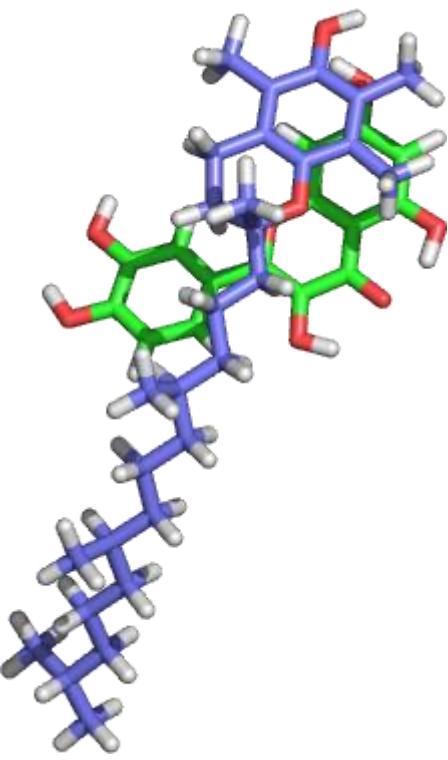


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H	14.048875	-9.756182	-5.067047
C	16.003889	-8.994222	-4.602816
H	16.019782	-9.383101	-3.569649
H	16.548136	-9.706033	-5.247871
H	16.560113	-8.038373	-4.611325
C	5.352681	-3.828841	-2.599187
H	5.192200	-4.188991	-1.565645
H	4.439293	-3.298918	-2.918050
H	5.473301	-4.709794	-3.251794
C	9.307709	-7.643806	-3.831778
H	9.303233	-8.129459	-2.837946
H	8.265031	-7.399947	-4.094787
H	9.674125	-8.379997	-4.566339
C	14.570788	-8.278349	-6.535944
H	13.548083	-8.181871	-6.936655
H	15.052483	-7.284374	-6.596322
H	15.130474	-8.965257	-7.194492
C	4.547166	8.266635	-4.977542
C	4.532590	7.109349	-5.744389
C	5.313417	5.989186	-5.335115
C	6.103064	6.083398	-4.175281
C	6.136063	7.244231	-3.408087
C	5.317195	8.304839	-3.804182
O	5.162518	9.403090	-3.028490
H	3.920766	9.118279	-5.248822
O	3.777453	7.026947	-6.838210
H	3.876955	6.101201	-7.193853
C	5.260167	4.749973	-6.043302
C	6.066827	3.666402	-5.528292
C	6.822709	3.826067	-4.390174
O	6.837831	5.032182	-3.763226
H	6.715553	7.277859	-2.483185
O	4.535581	4.539490	-7.052128
O	5.948340	2.506674	-6.198795
H	5.309200	2.707374	-6.917317
C	7.623228	2.814314	-3.708298
C	8.068915	3.058665	-2.391656
C	8.776548	2.090602	-1.695289
C	9.087663	0.855682	-2.306187
C	8.661589	0.617539	-3.612528
C	7.934941	1.580185	-4.310251
H	7.601659	1.367837	-5.325087
H	7.809217	3.995442	-1.893226
O	9.201553	2.224824	-0.411781
H	8.941638	3.086226	-0.057081
O	9.747862	-0.100254	-1.624521
H	9.934999	0.228752	-0.729587
H	8.901189	-0.345066	-4.072223
H	5.723354	9.337117	-2.241236

quercetin:vitE 8

$$\Delta E = -9.4 \text{ kcal.mol}^{-1}$$

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C	3.920647	4.251921	-2.147510
C	3.435611	4.364010	-3.455587
C	3.103432	5.633910	-3.962516
C	3.267892	6.749581	-3.137700
C	3.699332	6.638106	-1.798896
C	3.266053	3.132464	-4.302124
C	4.028373	1.940477	-3.740385
C	3.904086	1.830081	-2.221101
O	4.323022	3.067079	-1.610351
H	2.187498	2.894374	-4.387700
H	3.605215	3.332622	-5.332780
H	3.670311	1.007734	-4.201845
H	5.094896	2.031178	-3.988798
O	3.037321	7.985613	-3.695822
H	3.033979	8.658532	-3.000473
C	2.608583	5.778820	-5.375179
H	3.402588	5.533459	-6.105986
H	1.774119	5.084034	-5.574839
H	2.266060	6.803156	-5.578121
C	3.788010	7.908374	-0.995917
H	4.504701	8.610466	-1.458936
H	2.805496	8.417192	-0.942707
H	4.113020	7.735818	0.037428
C	4.571977	5.122057	0.085958
H	4.711411	6.043179	0.666723
H	3.892603	4.451696	0.641544
H	5.543805	4.603908	0.041145
C	2.466873	1.547188	-1.796191
H	2.128197	0.583275	-2.210793
H	2.402773	1.504418	-0.696464
H	1.788789	2.339208	-2.155230
C	4.886055	0.804187	-1.652540
H	4.685579	0.693255	-0.571019
H	5.892922	1.243066	-1.738751
C	4.899384	-0.558613	-2.329995
H	5.080706	-0.425949	-3.411500
H	3.916566	-1.055758	-2.231112
C	6.013575	-1.449022	-1.787444
H	6.939740	-0.845467	-1.751972
H	5.798622	-1.744260	-0.741663
C	6.268327	-2.699323	-2.633343
H	6.313638	-2.367293	-3.689895
C	7.627744	-3.316513	-2.299446
H	8.388422	-2.511937	-2.308721
H	7.609321	-3.705487	-1.261737
C	8.075544	-4.418131	-3.254272
H	7.368687	-5.264797	-3.207040
H	8.023756	-4.035927	-4.293602
C	9.493095	-4.906031	-2.974985
H	9.536354	-5.355931	-1.962900
H	10.169701	-4.030568	-2.948129
C	10.041526	-5.913038	-3.990130
H	9.957862	-5.450939	-4.995236
C	11.527165	-6.174682	-3.725994
H	11.634203	-6.665462	-2.737987
H	12.046925	-5.201080	-3.639090
C	12.234074	-7.009307	-4.788667
H	11.782680	-8.017307	-4.844790
H	12.066525	-6.543010	-5.777147
C	13.729404	-7.152098	-4.526948
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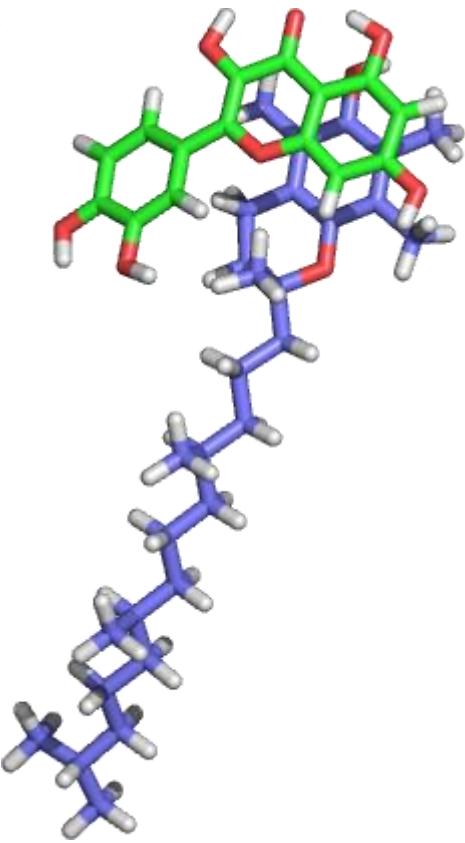


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H	16.000706	-8.642078	-4.080827
H	16.482545	-8.876156	-5.787616
H	16.454921	-7.236494	-5.082072
C	5.127265	-3.706947	-2.501543
H	5.067876	-4.080408	-1.462131
H	4.156457	-3.247505	-2.752251
H	5.268026	-4.574434	-3.167727
C	9.232109	-7.208891	-3.994633
H	9.290181	-7.696649	-3.003519
H	8.168899	-7.022656	-4.219504
H	9.611280	-7.921858	-4.745351
C	14.412550	-7.472106	-6.949121
H	13.374211	-7.396172	-7.312241
H	14.856706	-6.459588	-6.982746
H	14.973155	-8.110272	-7.654231
C	6.985698	7.251429	-1.727023
C	7.470449	6.066531	-1.190736
C	7.454730	4.880141	-1.980885
C	6.954235	4.936927	-3.294999
C	6.429298	6.110130	-3.828145
C	6.435253	7.254633	-3.021468
O	5.907455	8.420260	-3.446287
H	6.971061	8.161341	-1.124297
O	7.930303	6.022446	0.059736
H	8.191209	5.078188	0.241782
C	7.933635	3.635930	-1.465434
C	7.968779	2.515609	-2.384518
C	7.501886	2.642753	-3.669625
O	6.984787	3.837078	-4.078560
H	6.010437	6.126043	-4.835708
O	8.339597	3.465226	-0.287357
O	8.455787	1.373515	-1.866812
H	8.677069	1.600504	-0.937414
C	7.457530	1.616237	-4.708801
C	7.037968	1.968436	-6.012370
C	6.959174	1.013354	-7.015192
C	7.295174	-0.333766	-6.748459
C	7.706547	-0.684595	-5.462667
C	7.789460	0.271944	-4.451616
H	8.109247	-0.028680	-3.455333
H	6.769362	3.002516	-6.242920
O	6.569018	1.267478	-8.290918
H	6.394969	2.211248	-8.413943
O	7.221103	-1.262318	-7.719947
H	6.926880	-0.830608	-8.539233
H	7.959627	-1.730205	-5.266211
H	5.228809	8.258345	-4.123471

quercetin:vitE 9

$$\Delta E = -9.1 \text{ kcal.mol}^{-1}$$

C	6.593495	7.437255	-0.662523
C	5.546100	8.314749	-0.324114
C	4.206208	7.988377	-0.594874
C	3.905611	6.779860	-1.248810
C	4.952123	5.910322	-1.593009
C	6.291910	6.216638	-1.291426
C	3.102864	8.932384	-0.186239
C	3.599046	9.998253	0.782094
C	4.953324	10.555544	0.343450
O	5.899766	9.474839	0.312793
H	2.674331	9.410032	-1.086620
H	2.274862	8.366482	0.272497
H	2.865061	10.815503	0.864967
H	3.733803	9.566362	1.789881
O	4.607125	4.749852	-2.225795
H	5.376168	4.374773	-2.677461
C	2.480197	6.394674	-1.539299
H	2.010477	5.912119	-0.660629
H	1.868875	7.273534	-1.795842
H	2.426394	5.683287	-2.375487
C	7.385128	5.224518	-1.591674
H	7.542897	4.537973	-0.738377
H	7.175464	4.601249	-2.477426
H	8.340723	5.729000	-1.794778
C	8.020273	7.805380	-0.354470
H	8.498058	7.057095	0.302549
H	8.620935	7.844982	-1.280687
H	8.074499	8.784820	0.139391
C	4.890725	11.181437	-1.047286
H	4.094106	11.941437	-1.094325
H	5.856061	11.656164	-1.291907
H	4.675514	10.410136	-1.801717
C	5.519884	11.527458	1.375704
H	6.572318	11.729017	1.104021
H	5.537512	11.011876	2.353735
C	4.765667	12.846319	1.497950
H	3.693788	12.654123	1.691812
H	4.813969	13.386591	0.536369
C	5.316235	13.726521	2.614177
H	5.281224	13.155795	3.562008
H	6.387098	13.938447	2.423662
C	4.575801	15.053176	2.809645
H	3.498037	14.819934	2.930564
C	5.045484	15.732640	4.098962
H	4.971938	15.001315	4.926686
H	6.122427	15.976719	4.002711
C	4.272226	16.990048	4.485610
H	4.409612	17.765913	3.712313
H	3.188498	16.760115	4.501224
C	4.685539	17.538657	5.847086
H	5.757554	17.818823	5.821827
H	4.600528	16.728284	6.596244
C	3.871378	18.741014	6.336263
H	2.801853	18.446705	6.324667
C	4.241508	19.074072	7.784640
H	5.299678	19.402385	7.816951
H	4.193628	18.144605	8.384152
C	3.361104	20.126185	8.451103
H	3.448048	21.090211	7.915893
H	2.303511	19.816947	8.357333
C	3.713035	20.342076	9.919231
H	4.789071	20.590717	9.994597
H	3.580428	19.390587	10.472798

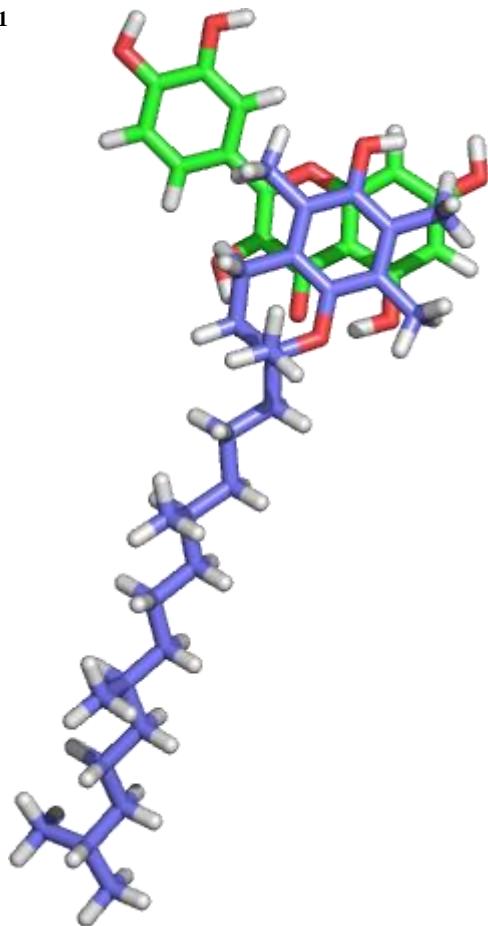


C	2.905939	21.435506	10.625662
H	3.048582	22.375856	10.056337
C	3.430814	21.652928	12.043659
H	4.504386	21.910717	12.038640
H	2.883917	22.464193	12.554975
H	3.307677	20.732511	12.644398
C	4.732498	15.970473	1.596846
H	5.796605	16.238853	1.457697
H	4.381001	15.485706	0.671065
H	4.160576	16.905002	1.718811
C	4.041741	19.950851	5.418058
H	5.100379	20.271016	5.404204
H	3.743821	19.719660	4.382077
H	3.434290	20.806409	5.757188
C	1.411200	21.119051	10.650706
H	0.993795	21.023963	9.634589
H	1.231221	20.165115	11.181112
H	0.847979	21.909683	11.176657
C	7.538560	6.565581	-4.456680
C	6.261811	6.074701	-4.687614
C	5.136055	6.930217	-4.529245
C	5.336714	8.242617	-4.068713
C	6.610019	8.740425	-3.801999
C	7.700283	7.886938	-4.001301
O	8.962830	8.280149	-3.743606
H	8.410611	5.920675	-4.577982
O	6.070828	4.791797	-5.016717
H	5.088667	4.678071	-5.171024
C	3.805384	6.458554	-4.763121
C	2.728430	7.387771	-4.492332
C	2.990976	8.648350	-4.015772
O	4.282383	9.054986	-3.860189
H	6.738699	9.752610	-3.412182
O	3.523516	5.302298	-5.165832
O	1.491309	6.902454	-4.686947
H	1.634753	5.984437	-5.002359
C	2.029409	9.656076	-3.580075
C	2.475333	10.973618	-3.341635
C	1.628919	11.920493	-2.787744
C	0.291340	11.588256	-2.475634
C	-0.162222	10.294075	-2.740655
C	0.690841	9.334534	-3.284379
H	0.323188	8.324748	-3.463333
H	3.506585	11.253023	-3.566511
O	2.001379	13.193078	-2.485034
H	2.893167	13.373912	-2.814027
O	-0.535333	12.503849	-1.937589
H	-0.053291	13.342303	-1.845906
H	-1.200267	10.047163	-2.500952
H	8.971788	9.200166	-3.441565

quercetin:vitE 10

$$\Delta E = -8.9 \text{ kcal.mol}^{-1}$$

C	6.723692	5.783004	-1.072276
C	5.395920	5.382855	-1.316546
C	4.311686	6.210978	-0.983990
C	4.549447	7.468884	-0.400239
C	5.872494	7.880623	-0.188659
C	6.962108	7.053827	-0.523022
C	2.899643	5.736605	-1.215575
C	2.846776	4.495269	-2.099080
C	3.951226	3.504044	-1.737782
O	5.222736	4.158204	-1.888486
H	2.420508	5.535001	-0.237871
H	2.303769	6.540569	-1.679368
H	1.863423	4.004218	-2.020469
H	3.002062	4.781178	-3.151086
O	6.067370	9.114533	0.366301
H	7.015873	9.278642	0.446762
C	3.398494	8.335017	0.027292
H	2.649150	8.436116	-0.773915
H	2.873516	7.888684	0.892400
H	3.736243	9.341081	0.311664
C	8.364633	7.525955	-0.242566
H	8.492795	8.603828	-0.448482
H	8.657037	7.346976	0.809839
H	9.095152	7.017071	-0.886815
C	7.857996	4.854975	-1.408639
H	8.361205	5.171696	-2.340031
H	8.614112	4.836332	-0.606625
H	7.483756	3.834208	-1.569515
C	3.824987	3.009541	-0.298460
H	2.834913	2.556832	-0.126601
H	4.602640	2.256358	-0.089009
H	3.948417	3.845247	0.409547
C	4.023266	2.350911	-2.734580
H	4.914835	1.748838	-2.478903
H	4.213832	2.788941	-3.730875
C	2.800435	1.443133	-2.793326
H	1.913945	2.017851	-3.121043
H	2.570165	1.063534	-1.782598
C	3.024544	0.273020	-3.745717
H	3.343858	0.670019	-4.727936
H	3.874324	-0.333779	-3.374207
C	1.823633	-0.652259	-3.962140
H	0.995156	-0.043148	-4.377928
C	2.189320	-1.718347	-4.999042
H	2.600476	-1.213614	-5.894404
H	3.017863	-2.331596	-4.591182
C	1.057061	-2.640715	-5.435775
H	0.662832	-3.185766	-4.560512
H	0.216162	-2.035855	-5.828383
C	1.509766	-3.633533	-6.500463
H	2.333615	-4.251528	-6.090139
H	1.948346	-3.070290	-7.346786
C	0.426393	-4.567765	-7.046715
H	-0.391175	-3.938003	-7.453465
C	0.998346	-5.392143	-8.203456
H	1.830762	-6.013051	-7.815460
H	1.455206	-4.699187	-8.936076
C	0.000862	-6.287153	-8.932233
H	-0.411095	-7.043035	-8.237880
H	-0.858278	-5.674945	-9.264350
C	0.625516	-7.002855	-10.125101
H	1.530288	-7.539834	-9.781042
H	0.979320	-6.252481	-10.860854

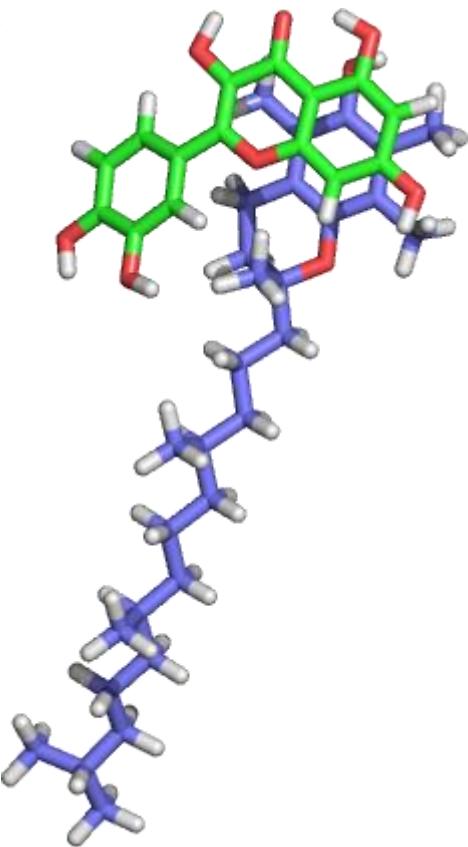


C	-0.294566	-7.997954	-10.839313
H	-0.638818	-8.733839	-10.084812
C	0.473551	-8.752127	-11.923169
H	1.354257	-9.268454	-11.503436
H	-0.164206	-9.503813	-12.420495
H	0.833135	-8.049569	-12.697780
C	1.345244	-1.275955	-2.651844
H	2.150895	-1.887068	-2.203502
H	1.057247	-0.505082	-1.918081
H	0.470661	-1.929147	-2.807705
C	-0.159114	-5.458730	-5.952348
H	0.627144	-6.112388	-5.529849
H	-0.583237	-4.863740	-5.126850
H	-0.962732	-6.104354	-6.343082
C	-1.526461	-7.315642	-11.431658
H	-2.132853	-6.816440	-10.657396
H	-1.221850	-6.549109	-12.168909
H	-2.171881	-8.045020	-11.951661
C	8.287009	7.806483	-3.597309
C	7.119303	7.124935	-3.917959
C	5.856541	7.743270	-3.687118
C	5.814887	9.018274	-3.100395
C	6.978291	9.705773	-2.757192
C	8.204961	9.086306	-3.019978
O	9.373316	9.680846	-2.707090
H	9.262775	7.350307	-3.775499
O	7.167391	5.900313	-4.437069
H	6.225696	5.603974	-4.579233
C	4.634149	7.100705	-4.055746
C	3.408915	7.833421	-3.805639
C	3.435190	9.078770	-3.226163
O	4.633191	9.626077	-2.877387
H	6.920335	10.690494	-2.288379
O	4.562262	5.966316	-4.593543
O	2.284115	7.193676	-4.178083
H	2.606176	6.357640	-4.580339
C	2.302306	9.939309	-2.894339
C	2.528637	11.125297	-2.159254
C	1.474766	11.956863	-1.812213
C	0.151712	11.632397	-2.190854
C	-0.074355	10.464227	-2.919353
C	0.982284	9.623236	-3.268719
H	0.779956	8.717195	-3.837987
H	3.541110	11.393444	-1.847100
O	1.604935	13.108770	-1.104069
H	2.533134	13.270604	-0.883904
O	-0.872284	12.438238	-1.852400
H	-0.518242	13.194236	-1.355321
H	-1.100154	10.222277	-3.211444
H	9.209525	10.565580	-2.349749

quercetin:vitE 11

$$\Delta E = -8.7 \text{ kcal.mol}^{-1}$$

C	4.700850	6.140892	-1.305525
C	5.716370	5.175588	-1.188584
C	6.909977	5.457416	-0.500975
C	7.110128	6.738863	0.042948
C	6.099438	7.707262	-0.086939
C	4.884749	7.412234	-0.732745
C	7.968590	4.390309	-0.360740
C	7.446697	3.013082	-0.752014
C	6.586889	3.088769	-2.014038
O	5.467148	3.949169	-1.744800
H	8.840439	4.654408	-0.988186
H	8.345350	4.369334	0.675866
H	8.283546	2.314024	-0.907534
H	6.813659	2.598689	0.053056
O	6.351198	8.934183	0.461968
H	5.814758	9.613178	0.029445
C	8.372145	7.063711	0.795759
H	8.297147	6.745556	1.853395
H	9.245562	6.554912	0.360718
H	8.569318	8.145289	0.790962
C	3.754938	8.406083	-0.793956
H	2.919847	8.081427	-0.145157
H	4.039324	9.419122	-0.469914
H	3.353321	8.492746	-1.816062
C	3.425502	5.823962	-2.035997
H	2.546995	5.922830	-1.373108
H	3.271341	6.532748	-2.869181
H	3.443160	4.802067	-2.438413
C	7.357847	3.662444	-3.199841
H	8.295508	3.107614	-3.361480
H	6.741976	3.599810	-4.113166
H	7.613300	4.716214	-3.015496
C	5.962385	1.736944	-2.354962
H	5.240508	1.900837	-3.176537
H	5.377972	1.397187	-1.480491
C	6.963846	0.665716	-2.766889
H	7.665305	0.464026	-1.936117
H	7.576491	1.047352	-3.600843
C	6.299098	-0.640601	-3.185923
H	5.674848	-1.012441	-2.351329
H	5.602542	-0.445252	-4.025744
C	7.274475	-1.744911	-3.604074
H	7.980545	-1.904997	-2.763824
C	6.517624	-3.058392	-3.827931
H	5.935658	-3.286172	-2.914221
H	5.772415	-2.909829	-4.634924
C	7.395330	-4.257443	-4.169496
H	7.885716	-4.089720	-5.144323
H	8.211282	-4.337619	-3.424779
C	6.620836	-5.571130	-4.204581
H	5.777226	-5.482922	-4.918213
H	6.163470	-5.739033	-3.210510
C	7.455970	-6.799645	-4.579220
H	8.349116	-6.811048	-3.921571
C	6.665615	-8.081999	-4.303371
H	5.749128	-8.077923	-4.927013
H	6.319202	-8.061357	-3.252059
C	7.433339	-9.377894	-4.541352
H	7.696317	-9.472438	-5.611417
H	8.392902	-9.330301	-3.992806
C	6.650418	-10.615128	-4.115718
H	5.654958	-10.590656	-4.600108
H	6.458844	-10.572480	-3.024559

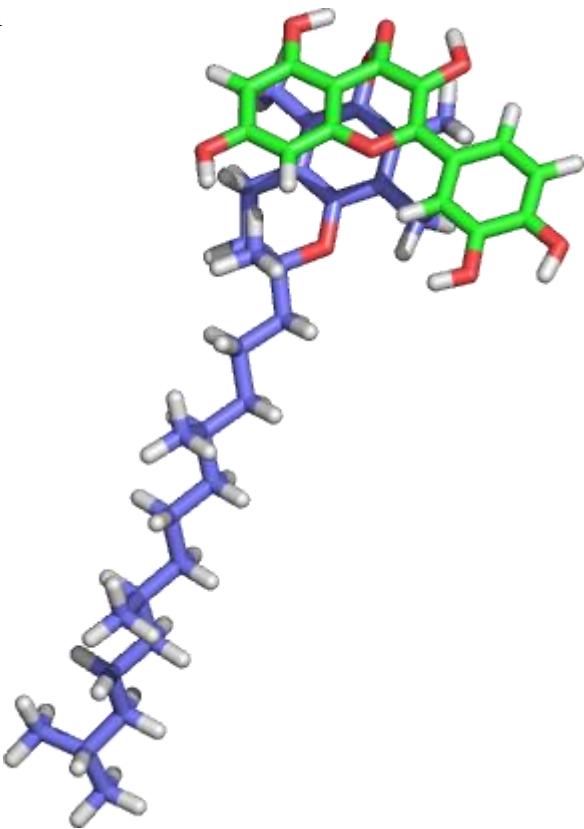


C	7.323691	-11.950216	-4.446022
H	7.496634	-11.973106	-5.540634
C	6.404695	-13.115517	-4.085223
H	5.432482	-13.033828	-4.602004
H	6.858106	-14.085051	-4.355739
H	6.207438	-13.126784	-2.997152
C	8.088082	-1.343341	-4.834081
H	7.416550	-1.171655	-5.696041
H	8.662299	-0.418152	-4.660162
H	8.808258	-2.128090	-5.117659
C	7.933833	-6.733655	-6.029912
H	7.068125	-6.759925	-6.717681
H	8.497594	-5.807876	-6.231284
H	8.590234	-7.583365	-6.279700
C	8.676696	-12.098733	-3.752304
H	9.384037	-11.308260	-4.054836
H	8.553578	-12.040102	-2.654598
H	9.136201	-13.073873	-3.989343
C	5.327959	9.692860	-3.265716
C	6.441823	10.011241	-2.503126
C	7.556453	9.126094	-2.477311
C	7.478466	7.909470	-3.176870
C	6.353510	7.561664	-3.921549
C	5.284965	8.463537	-3.949837
O	4.144844	8.189821	-4.612862
H	4.466785	10.363175	-3.292510
O	6.465794	11.122901	-1.759391
H	7.363268	11.156907	-1.320108
C	8.716694	9.415863	-1.691697
C	9.757806	8.409234	-1.671449
C	9.611482	7.232596	-2.363165
O	8.501642	7.033573	-3.128878
H	6.298837	6.594120	-4.424797
O	8.872246	10.463791	-1.015890
O	10.815335	8.694088	-0.894381
H	10.616623	9.580956	-0.524336
C	10.499697	6.073808	-2.347389
C	10.322053	5.056653	-3.309073
C	11.036461	3.871990	-3.228680
C	11.975907	3.671826	-2.192616
C	12.180643	4.692077	-1.260874
C	11.453566	5.879637	-1.330102
H	11.610771	6.653349	-0.579229
H	9.592008	5.180911	-4.111164
O	10.877727	2.825855	-4.084271
H	10.307180	3.075262	-4.824961
O	12.668123	2.521338	-2.105923
H	12.406781	1.943526	-2.841943
H	12.915161	4.532272	-0.466670
H	4.210740	7.328717	-5.051135

quercetin:vitE 12

$$\Delta E = -8.2 \text{ kcal.mol}^{-1}$$

C	3.994460	5.831388	-1.514683
C	5.164545	5.045696	-1.564660
C	6.290474	5.374298	-0.791450
C	6.259305	6.509807	0.040254
C	5.087950	7.278895	0.111174
C	3.952902	6.941840	-0.653716
C	7.506731	4.488536	-0.844819
C	7.132610	3.086262	-1.309476
C	6.282019	3.128890	-2.578572
O	5.109856	3.931807	-2.351103
H	8.268383	4.932365	-1.516305
H	7.981553	4.436959	0.148527
H	8.033798	2.480644	-1.495617
H	6.547466	2.578629	-0.521595
O	5.054438	8.358091	0.960454
H	4.882680	9.157178	0.422335
C	7.469409	6.877877	0.850304
H	7.686347	6.110283	1.616209
H	8.361080	6.949589	0.204361
H	7.323034	7.843156	1.351656
C	2.678988	7.727883	-0.505798
H	1.982088	7.207996	0.178375
H	2.859957	8.730127	-0.093971
H	2.157037	7.845855	-1.467359
C	2.791082	5.462042	-2.338437
H	1.923707	5.223236	-1.696697
H	2.481684	6.302448	-2.984459
H	2.999802	4.593934	-2.978064
C	7.058061	3.731745	-3.743690
H	7.969339	3.146017	-3.947924
H	6.428311	3.746699	-4.648707
H	7.353775	4.760711	-3.503249
C	5.723077	1.749270	-2.930282
H	5.000898	1.881583	-3.756826
H	5.145634	1.389570	-2.059166
C	6.763921	0.710254	-3.327165
H	7.516019	0.602447	-2.523828
H	7.310910	1.062862	-4.218360
C	6.147824	-0.656166	-3.611750
H	5.616733	-1.001579	-2.704554
H	5.375501	-0.557829	-4.400555
C	7.153224	-1.730346	-4.037508
H	7.967716	-1.743846	-3.285212
C	6.490511	-3.111383	-4.022724
H	6.042025	-3.273898	-3.023660
H	5.646310	-3.109953	-4.740737
C	7.421310	-4.276209	-4.342153
H	7.787966	-4.181411	-5.379065
H	8.316530	-4.216902	-3.692228
C	6.755232	-5.634877	-4.153810
H	5.855133	-5.695471	-4.797914
H	6.389952	-5.709276	-3.111403
C	7.650842	-6.842519	-4.447621
H	8.573129	-6.731403	-3.841057
C	6.956626	-8.133249	-4.001757
H	6.020467	-8.254078	-4.583362
H	6.646204	-8.018551	-2.945452
C	7.797194	-9.399277	-4.131251
H	8.042532	-9.585392	-5.193454
H	8.763454	-9.240857	-3.616333
C	7.099249	-10.631812	-3.565063
H	6.098021	-10.719185	-4.029633
H	6.920366	-10.488315	-2.480364

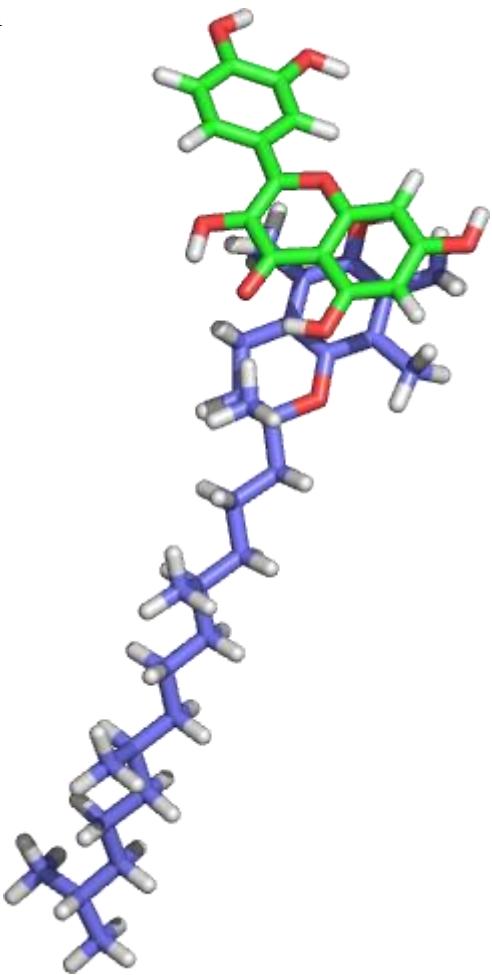


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H	8.016391	-12.070941	-4.860899
C	7.009789	-13.127501	-3.284612
H	6.029855	-13.157833	-3.792497
H	7.520462	-14.089490	-3.465294
H	6.823485	-13.042738	-2.198006
C	7.769523	-1.413599	-5.400295
H	6.988582	-1.426933	-6.183159
H	8.244255	-0.418408	-5.412070
H	8.541094	-2.150427	-5.678388
C	8.054390	-6.899991	-5.920809
H	7.158659	-7.035078	-6.555655
H	8.559254	-5.974108	-6.241576
H	8.740340	-7.739644	-6.119976
C	9.216394	-11.945387	-3.085598
H	9.869675	-11.146036	-3.473659
H	9.098008	-11.787252	-1.997257
H	9.735838	-12.908407	-3.232671
C	8.420743	7.998284	-2.438907
C	7.382414	8.772463	-1.939338
C	6.109455	8.747060	-2.583103
C	5.931514	7.927568	-3.711565
C	6.968145	7.154386	-4.227528
C	8.203870	7.193590	-3.571481
O	9.240494	6.437316	-3.978523
H	9.399223	8.008304	-1.954956
O	7.571021	9.538105	-0.866736
H	6.710693	9.987955	-0.666502
C	5.006488	9.517222	-2.110667
C	3.785938	9.474552	-2.878775
C	3.661683	8.616302	-3.949397
O	4.734872	7.872476	-4.327885
H	6.800888	6.522725	-5.102261
O	5.036301	10.236614	-1.066015
O	2.796360	10.263097	-2.427648
H	3.173719	10.704247	-1.637174
C	2.474893	8.358856	-4.758560
C	2.531657	7.382769	-5.781271
C	1.413994	7.095288	-6.549376
C	0.195026	7.776418	-6.322016
C	0.136137	8.741203	-5.315688
C	1.257365	9.033948	-4.540337
H	1.187048	9.791020	-3.761176
H	3.459935	6.838715	-5.971335
O	1.380156	6.175528	-7.547420
H	2.238165	5.738006	-7.639932
O	-0.890574	7.497308	-7.064539
H	-0.659023	6.805688	-7.706705
H	-0.810349	9.262322	-5.147633
H	8.992269	5.924576	-4.761660

quercetin:vitE 13

$$\Delta E = -7.6 \text{ kcal.mol}^{-1}$$

C	5.748489	7.789483	-1.019604
C	4.787187	8.792603	-0.787348
C	3.418567	8.535406	-0.972960
C	2.993213	7.257631	-1.383128
C	3.952263	6.257059	-1.600732
C	5.326539	6.514076	-1.432624
C	2.422797	9.628929	-0.691883
C	3.004182	10.659720	0.268528
C	4.393063	11.122638	-0.171771
O	5.259876	9.981565	-0.316364
H	2.130279	10.106743	-1.646738
H	1.498736	9.204469	-0.267664
H	2.338684	11.533810	0.350607
H	3.095486	10.214889	1.276105
O	3.497025	5.019106	-1.969586
H	4.246247	4.415922	-2.054498
C	1.524721	6.957006	-1.521164
H	1.031353	6.956392	-0.530686
H	1.011292	7.714655	-2.134960
H	1.357867	5.975418	-1.984389
C	6.343361	5.420928	-1.633968
H	6.595564	4.917287	-0.681634
H	6.002835	4.646738	-2.344470
H	7.279367	5.818774	-2.053550
C	7.209651	8.072555	-0.808947
H	7.652779	7.379112	-0.071845
H	7.768062	7.938152	-1.753127
H	7.365194	9.101222	-0.458615
C	4.343227	11.858404	-1.504615
H	3.719714	12.763427	-1.421840
H	5.361346	12.150531	-1.810034
H	3.910861	11.215128	-2.283193
C	5.072729	11.959142	0.913337
H	6.122816	12.115977	0.605935
H	5.099622	11.350120	1.835953
C	4.422502	13.307847	1.203120
H	3.348551	13.170520	1.429869
H	4.470450	13.941288	0.300462
C	5.081010	14.028703	2.375161
H	5.019719	13.377209	3.267844
H	6.161184	14.164052	2.167792
C	4.465978	15.391578	2.711832
H	3.370722	15.247133	2.814029
C	4.989541	15.892125	4.061709
H	4.849197	15.090690	4.812284
H	6.083944	16.050151	3.985176
C	4.326637	17.166415	4.576261
H	4.522011	17.997008	3.875878
H	3.227698	17.024795	4.586002
C	4.793689	17.551947	5.976365
H	5.881246	17.764585	5.956780
H	4.665744	16.680605	6.647075
C	4.066813	18.750641	6.594466
H	2.982346	18.516839	6.598084
C	4.502851	18.939891	8.050540
H	5.573606	19.225929	8.069110
H	4.439909	17.963763	8.569182
C	3.689233	19.960899	8.839000
H	3.780399	20.960534	8.374750
H	2.619252	19.688685	8.774891
C	4.117282	20.055292	10.299215
H	5.202024	20.272957	10.338910
H	3.986271	19.067469	10.785279

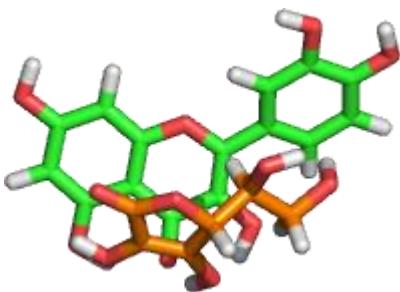


C	3.375010	21.110259	11.125121
H	3.512695	22.087006	10.619373
C	3.976063	21.210518	12.525330
H	5.054060	21.445713	12.483412
H	3.475041	21.991883	13.122797
H	3.860846	20.250319	13.061869
C	4.712407	16.409494	1.597954
H	5.796676	16.601703	1.492283
H	4.336291	16.049079	0.626288
H	4.218003	17.371629	1.810525
C	4.275990	20.023046	5.774600
H	5.351444	20.279005	5.737389
H	3.921589	19.901213	4.737805
H	3.739369	20.881165	6.212154
C	1.875612	20.826120	11.205684
H	1.404625	20.814228	10.208776
H	1.697727	19.840889	11.676063
H	1.360178	21.589473	11.814464
C	7.027450	8.009680	-4.314584
C	5.867581	8.766480	-4.198148
C	4.598380	8.144554	-4.381304
C	4.546696	6.764460	-4.645607
C	5.702569	5.997515	-4.774641
C	6.935376	6.635341	-4.594947
O	8.096209	5.956496	-4.660683
H	8.005770	8.475393	-4.182105
O	5.935478	10.068584	-3.927277
H	5.004064	10.415645	-3.921067
C	3.379948	8.887494	-4.306122
C	2.150179	8.146080	-4.477653
C	2.169968	6.792256	-4.693428
O	3.361414	6.144250	-4.798463
H	5.634009	4.928266	-4.989053
O	3.312788	10.127096	-4.097208
O	1.021438	8.865313	-4.330738
H	1.339168	9.780739	-4.174047
C	1.020712	5.897852	-4.787963
C	1.181762	4.538617	-4.444187
C	0.106819	3.664491	-4.512842
C	-1.161649	4.123821	-4.936228
C	-1.320081	5.468444	-5.274547
C	-0.243798	6.352826	-5.198795
H	-0.385651	7.399845	-5.468220
H	2.150028	4.185803	-4.078541
O	0.161713	2.346957	-4.184671
H	1.055184	2.102069	-3.906942
O	-2.204700	3.274380	-5.006532
H	-1.904562	2.394215	-4.726045
H	-2.306040	5.810351	-5.601833
H	7.926619	5.025842	-4.866199

quercetin:vitC 1

$$\Delta E = -9.2 \text{ kcal.mol}^{-1}$$

C	-0.316430	-0.566167	-1.107130
C	0.871593	-1.089078	-0.613207
C	2.093206	-0.374515	-0.817153
C	2.058611	0.846535	-1.521212
C	0.871472	1.385134	-2.008293
C	-0.312455	0.665025	-1.792560
O	-1.498229	1.111569	-2.228473
H	-1.256546	-1.101308	-0.957760
O	0.875673	-2.248831	0.036960
H	1.784397	-2.376486	0.410700
C	3.338779	-0.842270	-0.300538
C	4.525707	-0.105857	-0.676149
C	4.422933	1.079434	-1.365100
O	3.198789	1.538000	-1.735302
H	0.873621	2.338939	-2.541087
O	3.462273	-1.838317	0.470888
O	5.697771	-0.605221	-0.247432
H	5.470269	-1.414781	0.253727
C	5.506876	1.992921	-1.714081
C	5.214941	3.356345	-1.944244
C	6.227821	4.254236	-2.249489
C	7.569307	3.811293	-2.349698
C	7.857517	2.462458	-2.130592
C	6.842340	1.557818	-1.810481
H	7.091096	0.510519	-1.641078
H	4.186485	3.718446	-1.865881
O	6.047122	5.578293	-2.464160
H	5.115587	5.822619	-2.367846
O	8.550409	4.674941	-2.651091
H	8.167563	5.562908	-2.749904
H	8.896110	2.131267	-2.210537
H	-1.395775	1.968743	-2.668000
C	1.549801	2.044790	2.396272
C	2.092397	0.691119	2.347921
C	3.431446	0.765004	2.504697
C	3.804631	2.207922	2.716298
O	2.561063	2.914851	2.626278
O	0.393698	2.374774	2.265515
C	4.780722	2.785187	1.698982
H	4.340261	2.624418	0.692096
C	6.156526	2.110862	1.769938
H	6.125424	1.091374	1.355661
H	6.468150	2.048197	2.827362
H	4.214292	2.376959	3.729636
O	4.934553	4.154823	1.959430
H	5.817193	4.365413	1.603062
O	7.105060	2.926225	1.107123
H	7.091676	2.694372	0.165616
O	4.357433	-0.193293	2.508337
H	3.995212	-0.997265	2.070097
O	1.321587	-0.393511	2.172362
H	0.409497	-0.092215	2.019731



quercetin:vitC 2

$$\Delta E = -8.4 \text{ kcal.mol}^{-1}$$

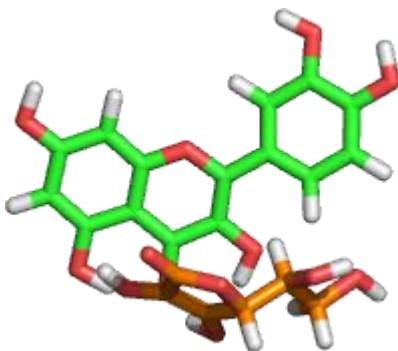
C	-0.268511	-0.178359	0.636874
C	0.025485	0.153649	1.954822
C	1.363977	0.019323	2.433061
C	2.362347	-0.438950	1.551116
C	2.079062	-0.773876	0.229486
C	0.754376	-0.639474	-0.213852
O	0.398691	-0.943547	-1.471728
H	-1.288388	-0.080690	0.259366
O	-0.928065	0.596592	2.771110
H	-0.502651	0.785159	3.650790
C	1.713433	0.365873	3.780342
C	3.103562	0.199542	4.140399
C	4.021300	-0.276664	3.246017
O	3.640068	-0.573426	1.976677
H	2.871579	-1.133104	-0.431617
O	0.908860	0.811817	4.634756
O	3.423803	0.617540	5.394510
H	2.560397	0.880933	5.787533
C	5.453245	-0.437468	3.479137
C	6.356715	-0.147852	2.438375
C	7.723514	-0.166511	2.674300
C	8.218190	-0.582007	3.930776
C	7.325085	-0.907783	4.955585
C	5.951787	-0.813555	4.737465
H	5.257897	-1.033057	5.551362
H	5.994548	0.158932	1.454298
O	8.651125	0.231656	1.758779
H	8.446904	1.164667	1.520043
O	9.542334	-0.588457	4.150143
H	9.966417	-0.245890	3.340792
H	7.725615	-1.188782	5.933595
H	1.168571	-1.247077	-1.975048
C	7.410288	2.886556	3.104573
C	6.091621	2.687573	3.674112
C	6.224311	2.660118	5.021188
C	7.643209	3.031355	5.361240
O	8.294520	3.149223	4.082861
O	7.717633	2.815161	1.923565
C	8.457006	2.068073	6.218089
H	8.757056	1.219362	5.576716
C	7.712128	1.499615	7.416688
H	6.847732	0.900436	7.082576
H	7.336625	2.327566	8.048960
H	7.675144	4.022929	5.849368
O	9.595848	2.775610	6.651353
H	10.019010	2.199018	7.307711
O	8.668774	0.712117	8.099868
H	8.337853	0.527710	8.987740
O	5.338378	2.435892	5.979584
H	4.582143	1.888040	5.647603
O	4.990927	2.507780	2.924278
H	5.267827	2.501068	1.993006



quercetin:vitC 3

$$\Delta E = -6.8 \text{ kcal.mol}^{-1}$$

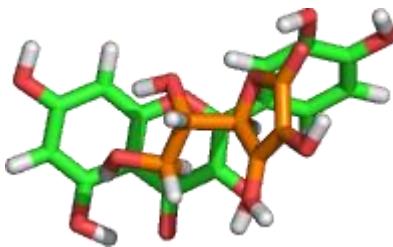
C	0.068404	-0.219466	-0.316342
C	1.352435	-0.700062	-0.090199
C	2.475448	0.015522	-0.613045
C	2.244956	1.19052	-1.342003
C	0.962360	1.690409	-1.571900
C	-0.119908	0.966444	-1.052394
O	-1.387184	1.370694	-1.226219
H	-0.796101	-0.756573	0.079282
O	1.538156	-1.816131	0.605855
H	2.518502	-1.953283	0.685691
C	3.816076	-0.432545	-0.414870
C	4.869192	0.361105	-0.998388
C	4.580604	1.530093	-1.671679
O	3.285594	1.906456	-1.826722
H	0.817340	2.617254	-2.132225
O	4.112828	-1.482578	0.237008
O	6.127004	-0.098493	-0.858341
H	6.055334	-0.953239	-0.393884
C	5.524369	2.467371	-2.270087
C	5.055449	3.426462	-3.197421
C	5.922428	4.353428	-3.754792
C	7.290217	4.363391	-3.390498
C	7.751844	3.423491	-2.468826
C	6.887878	2.479196	-1.918610
H	7.292491	1.770781	-1.198562
H	4.001449	3.443924	-3.487946
O	5.563327	5.298923	-4.659487
H	4.617990	5.243201	-4.857782
O	8.128922	5.268785	-3.922765
H	7.628775	5.831167	-4.537340
H	8.804465	3.443850	-2.174597
H	-1.410579	2.192070	-1.738875
C	4.075754	2.170654	3.112614
C	4.073675	0.795279	2.627630
C	5.356886	0.395781	2.477852
C	6.253873	1.534243	2.889510
O	5.354558	2.579963	3.276085
O	3.111238	2.859887	3.354499
C	7.179727	2.067757	1.802532
H	6.552083	2.319118	0.920111
C	8.229615	1.052103	1.377777
H	7.754194	0.166284	0.930079
H	8.802476	0.739463	2.273874
H	6.860796	1.269751	3.775684
O	7.815838	3.212760	2.311128
H	8.550573	3.389115	1.701505
O	9.059232	1.732958	0.453499
H	9.818486	1.172943	0.248015
O	5.861597	-0.766389	2.073419
H	5.171293	-1.239310	1.534142
O	2.932460	0.114961	2.420110
H	2.193658	0.714070	2.622943



quercetin:vitC 4

$$\Delta E = -6.5 \text{ kcal.mol}^{-1}$$

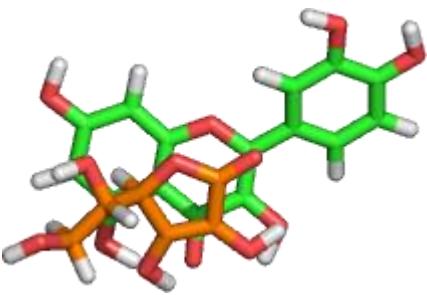
C	0.932167	0.344095	0.914253
C	1.928974	-0.538452	0.509068
C	2.897573	-0.111667	-0.450748
C	2.802485	1.186516	-0.985507
C	1.783385	2.063509	-0.617931
C	0.857835	1.629544	0.340184
O	-0.137814	2.418697	0.767370
H	0.191821	0.035580	1.655252
O	1.997061	-1.765950	1.015182
H	2.782614	-2.213923	0.592642
C	3.951616	-0.985168	-0.884756
C	4.916194	-0.424083	-1.809848
C	4.804731	0.880235	-2.230200
O	3.727482	1.624722	-1.855799
H	1.730415	3.062515	-1.058073
O	4.105610	-2.159811	-0.469330
O	5.941926	-1.221629	-2.150793
H	5.792759	-2.053035	-1.654870
C	5.788119	1.648488	-2.986501
C	5.872008	3.038147	-2.749085
C	6.863518	3.795887	-3.354498
C	7.760307	3.193903	-4.266948
C	7.651064	1.825815	-4.533387
C	6.686540	1.051527	-3.888378
H	6.629628	-0.019671	-4.086691
H	5.194565	3.515796	-2.035812
O	7.056606	5.119251	-3.115446
H	6.792396	5.316250	-2.197520
O	8.719578	3.931685	-4.852052
H	8.658234	4.835346	-4.495680
H	8.353524	1.373071	-5.238591
H	-0.105929	3.275573	0.316661
C	8.069004	5.329395	0.194092
C	8.693205	4.444210	1.168400
C	7.950771	3.318909	1.248684
C	6.765947	3.445509	0.336450
O	6.939387	4.729833	-0.281319
O	8.443563	6.411144	-0.187393
C	5.408835	3.393332	1.032855
H	5.448004	4.067810	1.914002
C	5.077464	1.976297	1.496088
H	5.784725	1.639554	2.274580
H	5.170164	1.300429	0.622062
H	6.797226	2.686842	-0.465923
O	4.425345	3.820753	0.125451
H	3.593187	3.435614	0.456213
O	3.748281	2.021023	1.967581
H	3.323656	1.164556	1.820897
O	9.830848	4.743133	1.817941
H	10.142624	5.606694	1.498873
O	8.120368	2.211404	1.967337
H	8.926937	2.283489	2.503568



quercetin:vitC 5

$$\Delta E = -6.0 \text{ kcal.mol}^{-1}$$

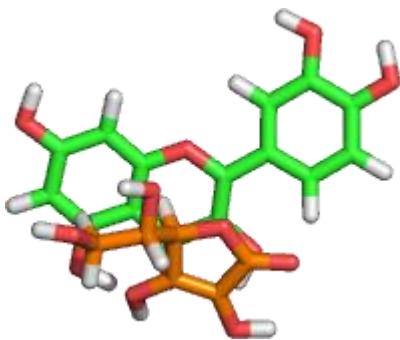
C	-0.166992	-0.213031	-0.968070
C	0.986220	-0.810717	-0.473127
C	2.248176	-0.169005	-0.660826
C	2.292098	1.062329	-1.342380
C	1.141716	1.673027	-1.837075
C	-0.084137	1.020967	-1.643487
O	-1.237943	1.539195	-2.089322
H	-1.137335	-0.695139	-0.833133
O	0.918929	-1.976660	0.165477
H	1.834046	-2.188206	0.486893
C	3.454850	-0.698689	-0.100386
C	4.682738	-0.001772	-0.405147
C	4.658803	1.189329	-1.094545
O	3.468890	1.693503	-1.523140
H	1.205165	2.635163	-2.350462
O	3.490074	-1.706140	0.662156
O	5.806922	-0.531327	0.108763
H	5.501363	-1.277086	0.665420
C	5.793319	2.048015	-1.411952
C	5.569263	3.412757	-1.698202
C	6.629151	4.249383	-2.010073
C	7.949498	3.743559	-2.056637
C	8.171537	2.394032	-1.777747
C	7.109210	1.551073	-1.453994
H	7.304027	0.499269	-1.244800
H	4.559109	3.825249	-1.644683
O	6.513124	5.574441	-2.283212
H	5.595312	5.864003	-2.184968
O	8.977128	4.555325	-2.362682
H	8.630112	5.451867	-2.504854
H	9.196160	2.014876	-1.820981
H	-1.078852	2.389161	-2.525900
C	3.426373	2.755909	1.578851
C	3.502158	1.411277	2.142342
C	2.248791	0.918152	2.218656
C	1.288295	1.971443	1.752563
O	2.124328	3.071501	1.373175
O	4.345875	3.486985	1.292990
C	0.251170	2.441360	2.760520
H	0.790179	2.856924	3.639107
C	-0.639918	1.294587	3.226583
H	-0.062166	0.573348	3.831888
H	-1.033445	0.763975	2.336991
H	0.756150	1.630103	0.846175
O	-0.534470	3.422288	2.136394
H	-1.347709	3.461412	2.668162
O	-1.681469	1.897157	3.969034
H	-2.419476	1.277510	4.023669
O	4.658290	0.789896	2.426153
H	5.385932	1.305876	2.039152
O	1.824091	-0.303429	2.540891
H	2.549521	-0.942376	2.391690



quercetin:vitC 6

$$\Delta E = -4.4 \text{ kcal.mol}^{-1}$$

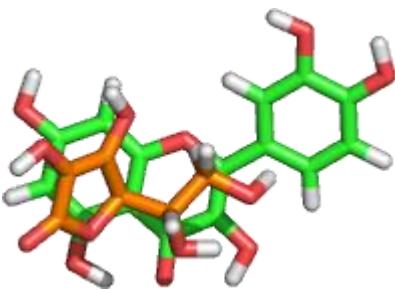
C	0.105248	-0.278689	-0.748566
C	1.335928	-0.855038	-0.459338
C	2.537121	-0.160948	-0.798713
C	2.445175	1.094548	-1.427958
C	1.217207	1.681731	-1.724837
C	0.053126	0.981821	-1.375825
O	-1.168396	1.480621	-1.621037
H	-0.820431	-0.798346	-0.492820
O	1.405298	-2.047423	0.129519
H	2.371229	-2.267866	0.226414
C	3.825024	-0.683537	-0.462483
C	4.971927	0.128243	-0.797096
C	4.818114	1.347629	-1.419646
O	3.564476	1.780825	-1.734055
H	1.174675	2.663278	-2.202943
O	4.002944	-1.778985	0.141469
O	6.163978	-0.373079	-0.431095
H	5.953697	-1.202861	0.048279
C	5.862156	2.280061	-1.828554
C	5.549489	3.307590	-2.748282
C	6.520869	4.206902	-3.159038
C	7.839616	4.113694	-2.655982
C	8.145808	3.107971	-1.738366
C	7.174635	2.197860	-1.326476
H	7.430979	1.438982	-0.589537
H	4.537854	3.399241	-3.152432
O	6.313937	5.215406	-4.044755
H	5.393080	5.227448	-4.341252
O	8.782511	4.985120	-3.054972
H	8.381934	5.605932	-3.685837
H	9.163422	3.054888	-1.341942
H	-1.097518	2.342437	-2.057288
C	5.805209	1.711475	2.039111
C	5.212346	0.400513	2.296404
C	3.871403	0.531039	2.244050
C	3.542551	1.959908	1.919102
O	4.814544	2.609632	1.829611
O	6.982133	1.982694	1.998820
C	2.654943	2.700290	2.907469
H	3.173564	2.712595	3.890352
C	1.298615	2.018595	3.071884
H	1.409605	1.049230	3.588556
H	0.868003	1.827370	2.068322
H	3.061867	2.026758	0.924931
O	2.467183	4.000536	2.414278
H	1.669088	4.323088	2.866919
O	0.502906	2.924914	3.809653
H	-0.425741	2.694930	3.681668
O	5.955242	-0.699734	2.492187
H	6.889026	-0.434018	2.421512
O	2.902579	-0.382243	2.342052
H	3.272196	-1.255949	2.117302



quercetin:vitC 7

$$\Delta E = -4.2 \text{ kcal.mol}^{-1}$$

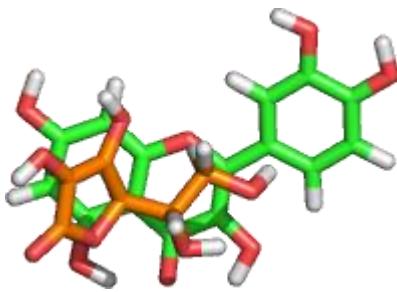
C	0.992652	0.005627	0.100558
C	2.093859	-0.792150	-0.192813
C	3.198400	-0.231598	-0.902965
C	3.156759	1.124282	-1.275243
C	2.053885	1.928378	-0.998853
C	0.977747	1.352265	-0.306188
O	-0.116524	2.063649	0.007559
H	0.143712	-0.407703	0.648937
O	2.128697	-2.063706	0.189265
H	3.008023	-2.434765	-0.093489
C	4.385407	-0.992672	-1.148025
C	5.508987	-0.278352	-1.732360
C	5.401622	1.042592	-2.079450
O	4.214531	1.693947	-1.890957
H	2.047215	2.980166	-1.294185
O	4.528481	-2.200066	-0.852930
O	6.641333	-0.993371	-1.817219
H	6.393172	-1.881828	-1.477868
C	6.461530	1.929569	-2.553402
C	6.249988	3.328916	-2.543376
C	7.250859	4.201707	-2.945992
C	8.504544	3.704128	-3.372272
C	8.715678	2.324586	-3.385458
C	7.712100	1.441910	-2.985583
H	7.901435	0.369341	-3.005526
H	5.290528	3.736649	-2.214960
O	7.133653	5.552240	-2.961324
H	6.251830	5.824653	-2.670784
O	9.477569	4.547330	-3.757006
H	9.149218	5.458523	-3.679715
H	9.686989	1.949854	-3.719893
H	-0.035792	2.968612	-0.327284
C	3.209810	0.968265	4.177631
C	3.256291	2.408881	3.935023
C	3.819740	2.609045	2.726372
C	4.192769	1.277863	2.143663
O	3.755261	0.325501	3.118232
O	2.752499	0.406228	5.145123
C	5.676804	1.063098	1.864983
H	6.208480	1.114359	2.839005
C	6.248179	2.132888	0.924327
H	6.405883	3.077584	1.473290
H	5.528242	2.337801	0.112262
H	3.632382	1.086192	1.211679
O	5.824585	-0.204294	1.283221
H	6.648248	-0.142742	0.763712
O	7.459375	1.618745	0.411072
H	7.540199	1.876223	-0.519484
O	4.041002	3.731012	2.036021
H	3.744716	4.494431	2.556854
O	2.767844	3.311296	4.803155
H	2.400759	2.821154	5.559313



quercetin:vitC 8

$$\Delta E = -4.1 \text{ kcal.mol}^{-1}$$

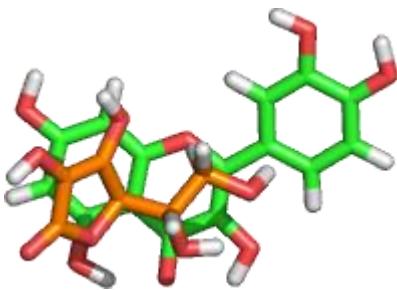
C	0.219760	-0.407433	-0.722718
C	1.416932	-1.111800	-0.644999
C	2.635649	-0.469896	-1.020748
C	2.600917	0.868660	-1.451737
C	1.406994	1.579727	-1.543740
C	0.221871	0.925542	-1.172647
O	-0.967929	1.544851	-1.224188
H	-0.719031	-0.883316	-0.432131
O	1.435392	-2.368797	-0.215772
H	2.385621	-2.666529	-0.210163
C	3.897533	-1.129247	-0.871839
C	5.084282	-0.332901	-1.138694
C	4.982317	0.961261	-1.577543
O	3.745051	1.512205	-1.766788
H	1.406136	2.620549	-1.875818
O	4.038812	-2.312917	-0.491803
O	6.243907	-0.947434	-0.857903
H	5.978659	-1.846150	-0.561429
C	6.065100	1.918940	-1.794161
C	5.756942	3.289862	-1.967501
C	6.764858	4.227982	-2.144704
C	8.121442	3.827261	-2.151921
C	8.428465	2.476638	-1.979449
C	7.420376	1.528914	-1.804420
H	7.686318	0.481281	-1.671558
H	4.716308	3.623476	-1.966289
O	6.558221	5.557244	-2.315406
H	5.613004	5.763654	-2.301508
O	9.099928	4.733077	-2.321292
H	8.697771	5.612266	-2.418446
H	9.479801	2.176736	-1.987038
H	-0.862303	2.446730	-1.560235
C	1.161710	0.766972	3.920300
C	1.062314	2.186973	3.588222
C	1.870259	2.425522	2.535507
C	2.560541	1.147565	2.159549
O	2.028294	0.174702	3.065435
O	0.572133	0.180046	4.797274
C	4.081777	1.151201	2.276981
H	4.329379	1.302172	3.348995
C	4.729419	2.272182	1.454811
H	4.588382	3.244056	1.958438
H	4.242441	2.338850	0.465810
H	2.290385	0.839325	1.133983
O	4.546850	-0.094040	1.827499
H	5.466176	0.072400	1.547494
O	6.098046	1.943019	1.330651
H	6.399521	2.185564	0.442830
O	2.094638	3.541783	1.836912
H	1.571940	4.268358	2.212103
O	0.254023	3.036281	4.246200
H	-0.212980	2.525443	4.929906



quercetin:vitC 9

$$\Delta E = -4.1 \text{ kcal.mol}^{-1}$$

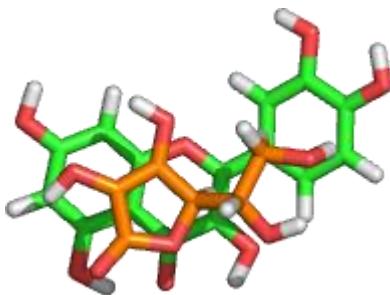
C	0.393895	-0.455924	-0.857444
C	1.613904	-1.089315	-0.642101
C	2.820882	-0.448808	-1.056157
C	2.750725	0.816529	-1.666434
C	1.534333	1.454601	-1.897047
C	0.361716	0.805006	-1.481057
O	-0.847870	1.361151	-1.652574
H	-0.536555	-0.929751	-0.538240
O	1.664460	-2.275853	-0.046741
H	2.624858	-2.523677	0.041049
C	4.101726	-1.014042	-0.754892
C	5.264277	-0.198960	-1.070010
C	5.128631	1.014365	-1.692053
O	3.879927	1.465969	-2.019738
H	1.506911	2.442328	-2.363009
O	4.275799	-2.124090	-0.205350
O	6.432579	-0.703614	-0.643641
H	6.192910	-1.566711	-0.239147
C	6.175375	1.990176	-1.988234
C	5.812155	3.300469	-2.382365
C	6.781887	4.258893	-2.642579
C	8.154219	3.940765	-2.514713
C	8.515488	2.650474	-2.123876
C	7.545991	1.681910	-1.864323
H	7.853528	0.682151	-1.560713
H	4.758720	3.570675	-2.489530
O	6.520307	5.533931	-3.022562
H	5.566926	5.683902	-3.092843
O	9.095917	4.866626	-2.764341
H	8.658758	5.697048	-3.016346
H	9.578559	2.413540	-2.027919
H	-0.764545	2.213443	-2.104409
C	0.960606	1.347006	3.502670
C	0.825799	2.708937	2.989109
C	1.718966	2.868006	1.991502
C	2.489073	1.591558	1.827068
O	1.930532	0.708548	2.805852
O	0.322122	0.835528	4.392502
C	3.996014	1.684184	2.041517
H	4.163553	1.991098	3.095589
C	4.651248	2.714140	1.111627
H	4.446324	3.736455	1.473389
H	4.220834	2.628559	0.098273
H	2.305091	1.152778	0.830692
O	4.541728	0.414551	1.800502
H	5.467171	0.587936	1.545239
O	6.035465	2.431170	1.103365
H	6.377325	2.565688	0.207282
O	1.957640	3.907325	1.186436
H	1.368108	4.641145	1.422930
O	-0.077740	3.584172	3.463255
H	-0.572694	3.138185	4.172019



quercetin:vitC 10

$$\Delta E = -2.2 \text{ kcal.mol}^{-1}$$

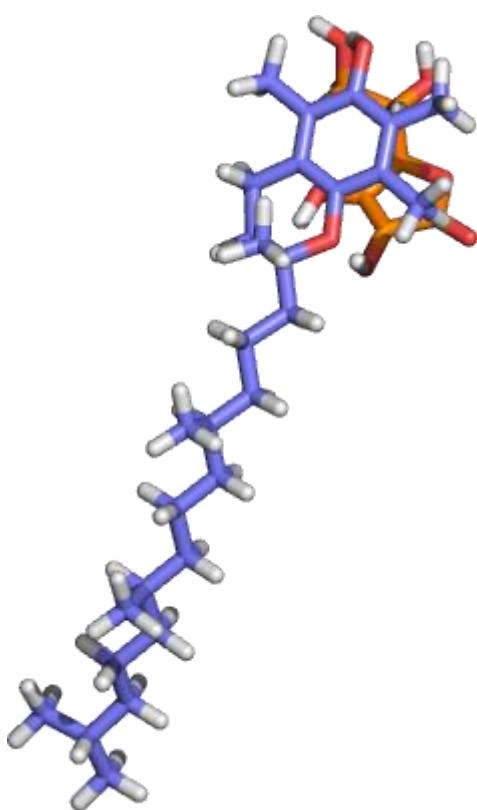
C	0.700175	0.485421	0.642622
C	1.646046	-0.430823	0.196489
C	2.720651	0.015566	-0.631967
C	2.800445	1.379055	-0.970907
C	1.842853	2.299457	-0.552793
C	0.799931	1.836266	0.261780
O	-0.151911	2.660559	0.724834
H	-0.125598	0.157048	1.277192
O	1.554421	-1.712687	0.527728
H	2.325238	-2.185266	0.112015
C	3.717144	-0.893957	-1.113910
C	4.820714	-0.314373	-1.866180
C	4.898100	1.043655	-2.051931
O	3.843091	1.836349	-1.694489
H	1.933918	3.353174	-0.826219
O	3.722826	-2.125644	-0.886511
O	5.781720	-1.174737	-2.228844
H	5.482581	-2.043915	-1.884567
C	6.066500	1.822527	-2.459302
C	5.912915	3.185496	-2.795459
C	7.022603	3.989523	-3.015496
C	8.325956	3.448912	-2.911206
C	8.477513	2.098776	-2.586930
C	7.363554	1.287811	-2.366633
H	7.503834	0.247522	-2.075152
H	4.914909	3.627499	-2.854320
O	6.971920	5.305139	-3.338151
H	6.055717	5.612820	-3.383233
O	9.406461	4.226468	-3.103848
H	9.109921	5.130256	-3.302786
H	9.489880	1.690924	-2.513038
H	0.003384	3.563123	0.411074
C	3.931967	0.378878	2.494837
C	3.519519	1.768222	2.319983
C	4.439253	2.386069	1.552944
C	5.489194	1.391084	1.167062
O	5.106550	0.189028	1.840697
O	3.349126	-0.495613	3.090154
C	6.944176	1.736258	1.441145
H	7.086566	1.861783	2.535326
C	7.337829	3.035506	0.710105
H	7.013614	3.913243	1.293230
H	6.831911	3.078851	-0.270163
H	5.433677	1.182904	0.087904
O	7.715887	0.673343	0.949508
H	8.584968	1.073597	0.766282
O	8.745269	3.050669	0.545801
H	8.933387	3.051323	-0.403042
O	2.389087	2.283416	2.834748
H	1.834347	1.543783	3.136028
O	4.468409	3.631796	1.074018
H	3.675084	4.103147	1.374137



vitC:vitE 1

$$\Delta E = -11.0 \text{ kcal.mol}^{-1}$$

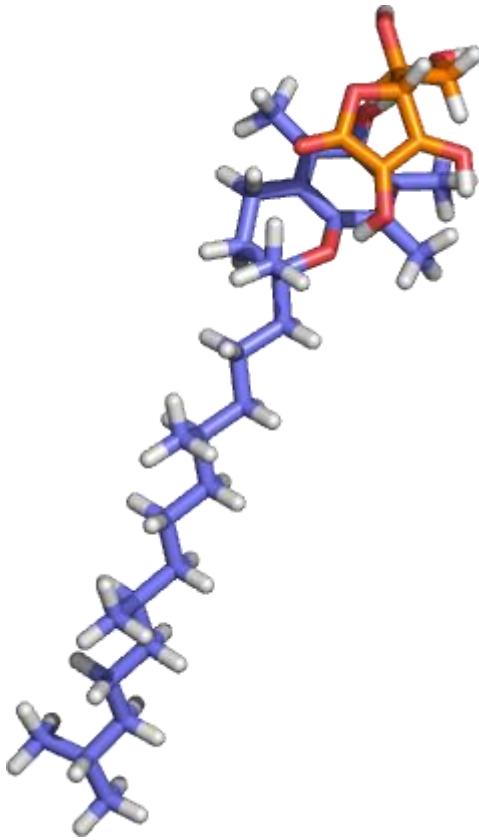
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C	1.430216	-1.000178	-4.735211
C	1.282365	-2.386304	-4.859315
C	-0.002238	-2.947337	-4.739734
C	-1.112540	-2.098068	-4.584622
C	-0.952071	-0.700278	-4.474410
C	2.481992	-3.263212	-5.109226
C	3.704199	-2.453852	-5.525143
C	3.852893	-1.187121	-4.682543
O	2.658937	-0.386589	-4.886866
H	2.708929	-3.848232	-4.197371
H	2.240634	-4.009516	-5.886034
H	4.618758	-3.062904	-5.457606
H	3.609944	-2.118046	-6.573773
O	-2.376997	-2.609313	-4.551530
H	-2.489210	-3.208812	-5.324782
C	-0.173735	-4.441547	-4.765492
H	0.000381	-4.865604	-5.772297
H	0.554200	-4.929812	-4.094838
H	-1.185152	-4.727893	-4.442319
C	-2.155474	0.192701	-4.346552
H	-3.083483	-0.389945	-4.427760
H	-2.161846	0.722298	-3.376201
H	-2.151680	0.968817	-5.131619
C	0.557919	1.336334	-4.391274
H	0.480370	1.835474	-5.375153
H	-0.193203	1.796317	-3.730458
H	1.561599	1.549447	-3.993840
C	3.983426	-1.485145	-3.194784
H	4.837174	-2.157954	-3.016007
H	4.145653	-0.549051	-2.635637
H	3.071602	-1.969123	-2.810190
C	4.984345	-0.300354	-5.195736
H	4.907885	0.674169	-4.680180
H	4.806658	-0.108250	-6.269579
C	6.385893	-0.870546	-5.008751
H	6.445775	-1.883731	-5.448751
H	6.598304	-0.986883	-3.932063
C	7.449471	0.007815	-5.659486
H	7.191813	0.137605	-6.727492
H	7.416523	1.021274	-5.212643
C	8.877517	-0.535788	-5.559976
H	8.865276	-1.578867	-5.937892
C	9.812291	0.268643	-6.468448
H	9.376796	0.291728	-7.485899
H	9.832094	1.321032	-6.121729
C	11.238063	-0.264197	-6.557061
H	11.727658	-0.183738	-5.570876
H	11.208602	-1.345197	-6.798308
C	12.073703	0.456970	-7.609393
H	12.115264	1.538734	-7.371290
H	11.554463	0.379586	-8.584180
C	13.502736	-0.070769	-7.769682
H	13.438561	-1.168402	-7.918032
C	14.150223	0.524508	-9.023561
H	14.220940	1.624068	-8.902340
H	13.471684	0.356113	-9.881930
C	15.525129	-0.039209	-9.368944
H	16.249534	0.207132	-8.570400
H	15.461887	-1.143232	-9.395816
C	16.057921	0.483981	-10.698846
H	16.047204	1.590719	-10.675646
H	15.365538	0.189947	-11.513393



C	17.469908	0.013459	-11.061580
H	18.143782	0.312708	-10.233860
C	17.949170	0.701991	-12.338603
H	17.922573	1.800938	-12.234912
H	18.980852	0.403604	-12.593901
H	17.298278	0.428213	-13.189650
C	9.373387	-0.560185	-4.115089
H	9.424639	0.468856	-3.713563
H	8.703062	-1.145868	-3.463918
H	10.380217	-1.002471	-4.038735
C	14.344022	0.193140	-6.521554
H	14.454923	1.282005	-6.360862
H	13.879152	-0.236242	-5.618594
H	15.354108	-0.238902	-6.613674
C	17.547673	-1.505342	-11.209947
H	17.273205	-2.024938	-10.276586
H	16.857189	-1.846998	-12.003776
H	18.566722	-1.824289	-11.489950
C	0.203932	0.899179	-8.020189
C	1.256009	-0.114637	-7.877378
C	0.745114	-1.297089	-8.278714
C	-0.681751	-1.111297	-8.698837
O	-0.906330	0.290696	-8.531590
C	-1.727067	-1.858140	-7.876333
H	-1.681492	-1.428262	-6.856787
C	-1.462448	-3.350656	-7.773054
H	-0.469112	-3.543723	-7.339137
H	-1.511845	-3.802855	-8.780618
O	0.222580	2.076866	-7.759577
O	2.529130	0.130993	-7.501508
H	2.597514	0.135066	-6.513272
O	1.346092	-2.482317	-8.361473
H	2.277206	-2.375388	-8.101036
O	-2.974726	-1.618637	-8.477455
H	-3.625874	-2.128114	-7.973119
O	-2.493517	-3.878540	-6.943794
H	-2.499315	-4.842235	-7.016286
H	-0.820725	-1.363641	-9.766470

vitC:vitE 2 $\Delta E = -10.0 \text{ kcal.mol}^{-1}$

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C	1.656331	-2.409598	-6.574203
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C	-0.091838	-0.910463	-5.825859
C	-0.421525	-1.842325	-4.821323
C	0.292109	-3.050383	-4.689684
C	1.413778	-0.280362	-7.801861
C	2.936086	-0.352275	-7.898363
C	3.422864	-1.770595	-8.206872
O	2.607426	-2.764729	-7.503419
H	0.957159	-0.585958	-8.761917
H	1.093235	0.753022	-7.601803
H	3.317945	0.319552	-8.683843
H	3.369971	-0.017179	-6.939467
O	-1.460559	-1.550641	-3.983084
H	-2.121436	-2.280989	-4.019152
C	-0.888557	0.354248	-5.987802
H	-0.269398	1.248495	-5.791068
H	-1.270534	0.450024	-7.019135
H	-1.739029	0.365796	-5.292599
C	-0.044355	-4.031351	-3.600570
H	-0.938266	-3.726969	-3.039309
H	-0.216154	-5.042699	-4.010225
H	0.792427	-4.125593	-2.884622
C	2.097119	-4.637318	-5.454135
H	2.501468	-4.766515	-4.434721
H	1.425961	-5.497546	-5.628285
H	2.925709	-4.692159	-6.172800
C	3.271530	-2.106180	-9.683908
H	3.879424	-1.419379	-10.294223
H	3.613835	-3.137425	-9.876462
H	2.217147	-2.026502	-9.990916
C	4.848055	-1.999007	-7.703427
H	5.114937	-3.052395	-7.904419
H	4.838305	-1.873856	-6.604213
C	5.903230	-1.081005	-8.311193
H	5.652941	-0.025673	-8.096611
H	5.893168	-1.187718	-9.410197
C	7.298777	-1.384793	-7.775123
H	7.276361	-1.321910	-6.670084
H	7.561491	-2.433820	-8.016222
C	8.411817	-0.469697	-8.295243
H	8.127666	0.575709	-8.058463
C	9.717955	-0.776254	-7.555573
H	9.522609	-0.733173	-6.466813
H	10.008713	-1.823614	-7.771598
C	10.888884	0.145821	-7.880995
H	11.143227	0.059044	-8.951429
H	10.584322	1.198399	-7.719178
C	12.120382	-0.158772	-7.034038
H	12.431720	-1.208130	-7.207294
H	11.839176	-0.097407	-5.965356
C	13.326220	0.755199	-7.274626
H	12.989977	1.801972	-7.128950
C	14.412683	0.468973	-6.233049
H	14.757291	-0.577008	-6.357427
H	13.956492	0.520808	-5.225762
C	15.615695	1.405448	-6.272273
H	16.142719	1.306220	-7.239501
H	15.258100	2.450732	-6.222489
C	16.603850	1.138188	-5.141645
H	16.886933	0.068246	-5.162792
H	16.100851	1.301241	-4.167073

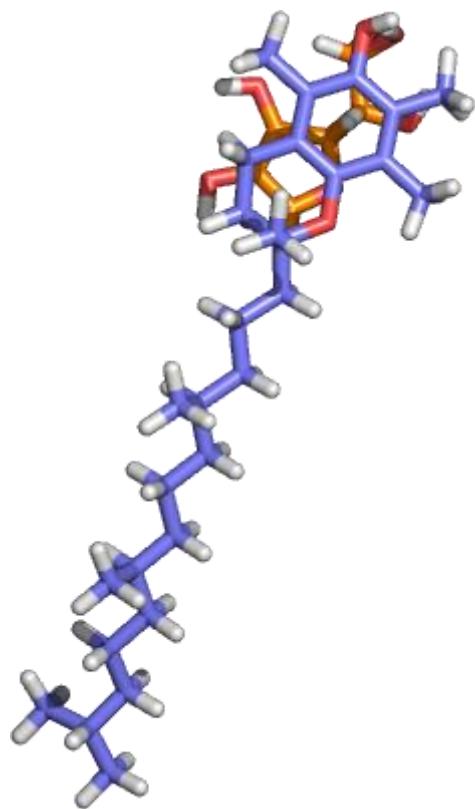


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H	18.366136	1.804169	-6.162240
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H	19.092295	0.470905	-4.172928
H	19.787929	2.118202	-4.123817
H	18.394750	1.705426	-3.087948
C	8.578222	-0.586976	-9.809760
H	8.866238	-1.619371	-10.082920
H	7.644258	-0.342455	-10.342432
H	9.360823	0.092869	-10.184877
C	13.861344	0.621282	-8.699690
H	14.216515	-0.410945	-8.878161
H	13.083957	0.844542	-9.448933
H	14.705661	1.306666	-8.881675
C	17.582846	3.477846	-5.068276
H	16.942728	3.833955	-5.892556
H	17.062198	3.692940	-4.116315
H	18.514728	4.069468	-5.083764
C	-0.601005	-3.128041	-9.260835
C	0.004972	-4.266069	-8.563691
C	-0.957989	-4.851137	-7.822191
C	-2.238777	-4.088534	-7.967742
O	-1.919350	-3.070931	-8.921341
C	-2.730861	-3.394777	-6.701525
H	-1.950923	-2.650410	-6.446771
C	-2.897375	-4.328030	-5.513892
H	-1.955625	-4.850419	-5.285293
H	-3.681017	-5.074863	-5.737777
O	-0.107291	-2.329286	-10.022798
O	1.271155	-4.702617	-8.694676
H	1.889481	-3.992765	-8.378862
O	-0.863740	-5.940103	-7.058796
H	0.047293	-6.276628	-7.128523
O	-3.951128	-2.770790	-7.012238
H	-4.272965	-2.373360	-6.189791
O	-3.298877	-3.500442	-4.425937
H	-3.620869	-4.053820	-3.701785
H	-3.050893	-4.713401	-8.382996

vitC:vitE 3

$$\Delta E = -8.5 \text{ kcal.mol}^{-1}$$

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C	1.726581	-0.947301	-5.167217
C	1.531070	-2.316856	-4.919315
C	0.227816	-2.804007	-4.702133
C	-0.846522	-1.908155	-4.760458
C	-0.665068	-0.549767	-5.072233
C	2.711090	-3.254866	-4.890638
C	3.989656	-2.596452	-5.396810
C	4.115632	-1.151384	-4.921603
O	2.959066	-0.418170	-5.369842
H	2.853505	-3.630153	-3.859026
H	2.494116	-4.145926	-5.506022
H	4.871414	-3.171965	-5.074193
H	3.998210	-2.572755	-6.496172
O	-2.125664	-2.432702	-4.639328
H	-2.676457	-1.833112	-4.115495
C	0.004421	-4.273061	-4.476314
H	0.196769	-4.841264	-5.406433
H	0.695963	-4.671665	-3.714441
H	-1.028084	-4.477131	-4.160421
C	-1.833501	0.371969	-5.287315
H	-2.803240	-0.145851	-5.248613
H	-1.849860	1.190362	-4.545850
H	-1.752861	0.844415	-6.281349
C	0.850564	1.370575	-5.666139
H	0.489221	1.523209	-6.700350
H	0.285975	2.062251	-5.018006
H	1.915918	1.634948	-5.632659
C	4.191853	-1.052969	-3.400592
H	5.045521	-1.635574	-3.017962
H	4.316562	-0.000601	-3.096946
H	3.270724	-1.445045	-2.939141
C	5.277063	-0.439463	-5.610379
H	5.248380	0.621927	-5.301160
H	5.074358	-0.465847	-6.695855
C	6.659461	-1.014722	-5.326718
H	6.719092	-2.057965	-5.690177
H	6.832505	-1.055234	-4.236885
C	7.757611	-0.192631	-5.993195
H	7.520320	-0.090777	-7.068934
H	7.742251	0.836052	-5.580605
C	9.174772	-0.755763	-5.856181
H	9.175268	-1.777710	-6.288043
C	10.148459	0.096614	-6.676007
H	9.747651	0.200823	-7.702484
H	10.164858	1.120628	-6.252016
C	11.575033	-0.434079	-6.758200
H	12.006079	-0.499352	-5.744329
H	11.560869	-1.468633	-7.154059
C	12.467316	0.433091	-7.640063
H	12.504885	1.459338	-7.222886
H	11.996674	0.528812	-8.637533
C	13.901443	-0.072059	-7.822086
H	13.846418	-1.098868	-8.238423
C	14.635884	0.804213	-8.841560
H	14.715175	1.832481	-8.435209
H	14.010418	0.884467	-9.751328
C	16.022495	0.312374	-9.243369
H	16.689487	0.289959	-8.361549
H	15.942753	-0.732967	-9.595808
C	16.663501	1.180244	-10.321456
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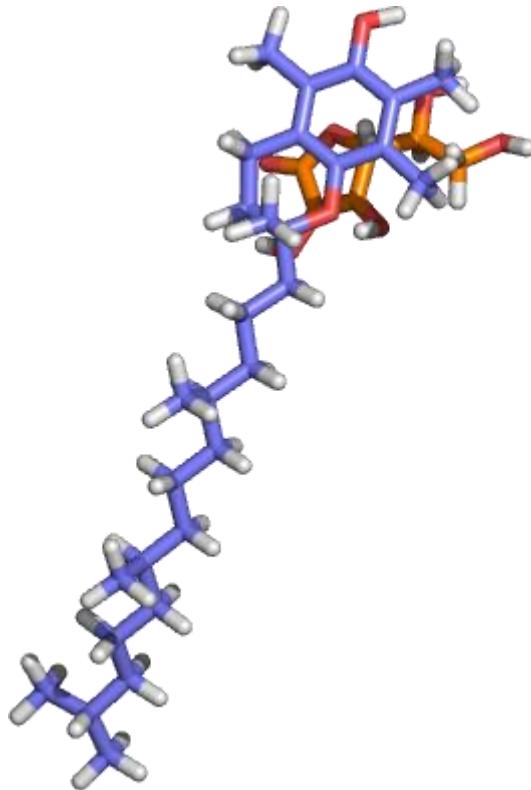


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H	18.702139	0.808636	-9.773094
C	18.684801	1.803786	-11.677125
H	18.662723	2.824522	-11.256604
H	19.730418	1.557496	-11.931524
H	18.101571	1.814520	-12.616495
C	9.604107	-0.857511	-4.393327
H	9.609023	0.145739	-3.927611
H	8.919433	-1.497315	-3.812048
H	10.617291	-1.280515	-4.295258
C	14.650474	-0.137302	-6.491869
H	14.712832	0.870560	-6.040276
H	14.142846	-0.799921	-5.771880
H	15.678553	-0.512695	-6.623630
C	18.167856	-0.621777	-11.283511
H	17.803722	-1.380951	-10.571337
H	17.547484	-0.689938	-12.196682
H	19.204256	-0.884492	-11.558655
C	2.844198	-2.166269	-8.808426
C	2.545974	-3.558678	-8.489666
C	1.223058	-3.752958	-8.657132
C	0.592961	-2.451033	-9.064623
O	1.697666	-1.538262	-9.148936
C	-0.423953	-1.917701	-8.066186
H	0.103859	-1.837178	-7.099887
C	-1.637055	-2.851990	-7.922553
H	-1.365483	-3.756958	-7.353743
H	-1.972201	-3.168265	-8.927380
O	3.930574	-1.631714	-8.785935
O	3.483614	-4.448886	-8.115390
H	4.347547	-4.005230	-8.165296
O	0.482114	-4.852209	-8.503105
H	1.053801	-5.599927	-8.266073
O	-0.871762	-0.657023	-8.495708
H	-1.751489	-0.572371	-8.083412
O	-2.702044	-2.149804	-7.319260
H	-2.625856	-2.269131	-6.350609
H	0.131281	-2.514663	-10.067543

vitC:vitE 4

$\Delta E = -8.2 \text{ kcal.mol}^{-1}$

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C	1.198928	-2.670101	-4.455811
C	-0.051579	-3.292797	-4.292365
C	-1.211374	-2.505129	-4.349112
C	-1.150401	-1.105320	-4.521348
C	2.465299	-3.485686	-4.447200
C	3.663254	-2.720431	-4.999259
C	3.691277	-1.270492	-4.520006
O	2.441356	-0.636051	-4.900739
H	2.666843	-3.817800	-3.410642
H	2.316134	-4.411439	-5.028344
H	4.600526	-3.215360	-4.701767
H	3.640338	-2.710312	-6.100919
O	-2.407100	-3.142193	-4.244501
H	-3.129970	-2.509873	-4.352302
C	-0.138686	-4.782894	-4.117648
H	0.177306	-5.304759	-5.039787
H	0.530653	-5.127484	-3.310308
H	-1.164033	-5.098827	-3.881793
C	-2.455305	-0.371141	-4.675178
H	-2.986496	-0.750488	-5.569387
H	-3.118096	-0.508772	-3.799197
H	-2.318844	0.709518	-4.814074
C	0.256330	1.014274	-4.770602
H	0.272139	1.309489	-5.835057
H	-0.557847	1.562742	-4.273448
H	1.212833	1.342695	-4.337086
C	3.828027	-1.162922	-3.006785
H	4.738947	-1.680480	-2.666697
H	3.887484	-0.104180	-2.706474
H	2.960646	-1.622615	-2.505461
C	4.746381	-0.456079	-5.264178
H	4.631849	0.601695	-4.964057
H	4.514610	-0.515128	-6.343763
C	6.185327	-0.903064	-5.033292
H	6.309182	-1.954913	-5.350747
H	6.411721	-0.874392	-3.953423
C	7.184351	-0.038318	-5.795435
H	6.900166	-0.027173	-6.864442
H	7.105541	1.010653	-5.446830
C	8.641920	-0.494484	-5.679351
H	8.685795	-1.556917	-5.995179
C	9.525879	0.306970	-6.640221
H	9.077499	0.261690	-7.651311
H	9.502017	1.374439	-6.343114
C	10.973340	-0.164989	-6.722149
H	11.458513	-0.044192	-5.738161
H	10.990638	-1.250758	-6.941831
C	11.780896	0.570557	-7.786360
H	11.774078	1.657736	-7.569791
H	11.271923	0.450956	-8.762214
C	13.232768	0.101632	-7.926738
H	13.216579	-0.999875	-8.058257
C	13.868290	0.704268	-9.183265
H	13.895165	1.807420	-9.077157
H	13.205815	0.497421	-10.045733
C	15.267399	0.188811	-9.506234
H	15.971513	0.468922	-8.700778
H	15.244857	-0.916998	-9.522880
C	15.800122	0.718333	-10.833518
H	15.750657	1.824259	-10.821163
H	15.130569	0.392538	-11.654923

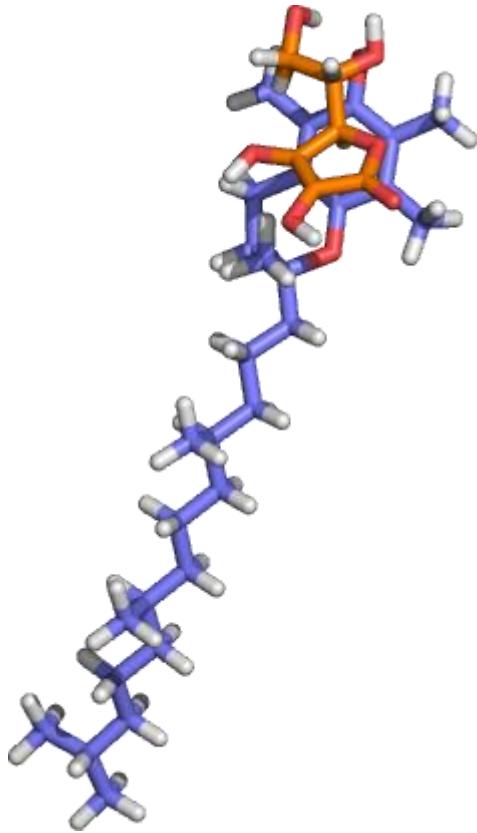


C	17.232940	0.293974	-11.171205
H	17.883785	0.625233	-10.337278
C	17.706712	0.985646	-12.448489
H	17.640696	2.084065	-12.357027
H	18.751645	0.720367	-12.685924
H	17.078300	0.680603	-13.305744
C	9.146839	-0.406550	-4.239868
H	9.127857	0.643752	-3.894401
H	8.523153	-1.001522	-3.552193
H	10.182323	-0.773481	-4.148552
C	14.050631	0.419883	-6.675588
H	14.112006	1.514800	-6.530087
H	13.597510	-0.016356	-5.770097
H	15.079479	0.031405	-6.752806
C	17.366056	-1.222705	-11.302110
H	17.096643	-1.741879	-10.367093
H	16.699825	-1.597024	-12.101917
H	18.399713	-1.508422	-11.563890
C	1.500393	-3.639718	-8.462422
C	2.270431	-2.411402	-8.251166
C	1.434939	-1.461488	-7.784499
C	0.055472	-2.060430	-7.685154
O	0.210029	-3.410153	-8.151045
C	-1.061536	-1.382888	-8.462100
H	-0.854697	-1.512133	-9.545889
C	-1.161104	0.108133	-8.158400
H	-0.283419	0.645657	-8.557586
H	-1.182392	0.248354	-7.061262
O	1.929694	-4.707089	-8.837982
O	3.596116	-2.368571	-8.450685
H	3.873964	-3.251786	-8.751880
O	1.705004	-0.203195	-7.407198
H	2.171181	-0.222976	-6.529174
O	-2.269014	-2.010266	-8.100302
H	-2.963327	-1.393608	-8.387953
O	-2.369747	0.538515	-8.756129
H	-2.616944	1.390721	-8.376792
H	-0.260349	-2.115182	-6.630451

vitC:vitE 5

$$\Delta E = -8.1 \text{ kcal.mol}^{-1}$$

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C	1.762946	-2.995344	-5.354504
C	1.070741	-1.772418	-5.321306
C	-0.315683	-1.762460	-5.076764
C	-0.972904	-2.978956	-4.843895
C	-0.265484	-4.196637	-4.790547
C	1.802229	-0.484347	-5.604416
C	3.314639	-0.674369	-5.616138
C	3.700795	-1.962852	-6.342309
O	3.092302	-3.066150	-5.644752
H	1.460780	-0.084559	-6.578671
H	1.523160	0.278325	-4.856936
H	3.809659	0.188534	-6.089309
H	3.695782	-0.751296	-4.582343
O	-2.345199	-2.990890	-4.738028
H	-2.640359	-3.710223	-5.343724
C	-1.072602	-0.463240	-5.096309
H	-0.897121	0.113875	-4.169177
H	-0.749460	0.174639	-5.935908
H	-2.154879	-0.628879	-5.188151
C	-1.000822	-5.485038	-4.545241
H	-1.943927	-5.307455	-4.005081
H	-1.252238	-5.976794	-5.503154
H	-0.389853	-6.187437	-3.956987
C	1.859830	-5.514020	-5.128642
H	1.862307	-6.016935	-4.144510
H	1.377308	-6.209144	-5.837944
H	2.900834	-5.356991	-5.440514
C	3.218201	-1.972357	-7.791241
H	3.617934	-1.100161	-8.333407
H	3.556219	-2.891360	-8.297532
H	2.118552	-1.931765	-7.841179
C	5.198244	-2.245963	-6.242076
H	5.371135	-3.265803	-6.632070
H	5.464188	-2.268939	-5.169688
C	6.098306	-1.261262	-6.978750
H	5.912113	-0.232753	-6.617511
H	5.843733	-1.263955	-8.052388
C	7.578244	-1.586907	-6.799782
H	7.813094	-1.580401	-5.718622
H	7.774440	-2.620110	-7.148787
C	8.533893	-0.630499	-7.520399
H	8.257158	0.403008	-7.228454
C	9.974096	-0.868115	-7.054608
H	9.998695	-0.818836	-5.948660
H	10.270484	-1.902126	-7.321206
C	10.998435	0.113418	-7.614165
H	11.048440	0.009200	-8.712166
H	10.655749	1.148479	-7.418154
C	12.388976	-0.071992	-7.017283
H	12.748942	-1.097615	-7.233183
H	12.315059	0.000431	-5.914868
C	13.437505	0.933382	-7.504544
H	13.033761	1.950592	-7.323816
C	14.724215	0.797715	-6.685584
H	15.155555	-0.207972	-6.862053
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C	15.780440	1.861694	-6.966635
H	16.117251	1.793890	-8.017545
H	15.318559	2.860496	-6.855644
C	16.995650	1.746533	-6.052761
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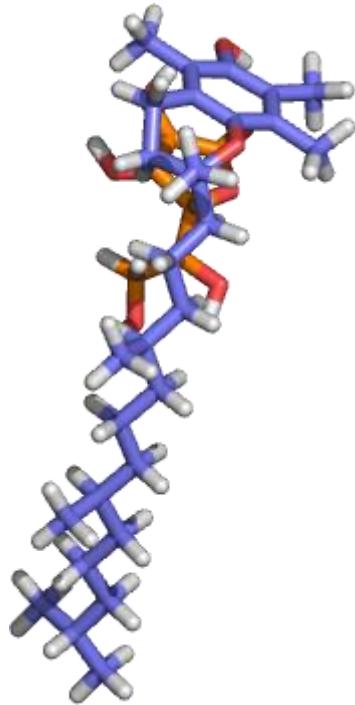


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C	19.338287	2.451305	-5.473142
H	19.693155	1.415260	-5.612498
H	20.173106	3.136365	-5.703711
H	19.081406	2.580411	-4.405613
C	8.404963	-0.748106	-9.039234
H	8.710082	-1.758992	-9.368051
H	7.367760	-0.580246	-9.373151
H	9.042706	-0.015151	-9.560575
C	13.705913	0.788425	-9.002191
H	14.120908	-0.213603	-9.219368
H	12.784328	0.908530	-9.595411
H	14.429927	1.539497	-9.358693
C	17.667398	4.190786	-6.170554
H	16.832169	4.446361	-6.844064
H	17.329330	4.360920	-5.131240
H	18.494462	4.893022	-6.374478
C	0.274168	-5.489006	-9.375485
C	0.639536	-4.165902	-9.875081
C	-0.007400	-3.245323	-9.132554
C	-0.794603	-3.952592	-8.069633
O	-0.575814	-5.343168	-8.329632
C	-2.283691	-3.646502	-8.023787
H	-2.735653	-3.959405	-8.983387
C	-2.524171	-2.134734	-7.775288
H	-2.603992	-1.619184	-8.745090
H	-1.651297	-1.707113	-7.252970
O	0.654428	-6.559657	-9.787774
O	1.493056	-3.973662	-10.895518
H	1.795329	-4.847823	-11.196325
O	0.025458	-1.910582	-9.178095
H	0.613156	-1.624052	-9.895298
O	-2.844743	-4.425046	-6.975578
H	-3.805273	-4.307777	-7.038603
O	-3.706097	-1.910739	-7.048356
H	-3.474447	-2.049069	-6.113232
H	-0.363665	-3.726680	-7.078968

vitC:vitE 6

$$\Delta E = -7.5 \text{ kcal.mol}^{-1}$$

C	1.303596	-0.009265	-5.647315
C	1.863573	-0.914421	-4.736741
C	1.661145	-2.298613	-4.851807
C	0.891063	-2.814308	-5.900087
C	0.360746	-1.906815	-6.836319
C	0.508169	-0.515819	-6.696615
C	2.415922	-3.124698	-3.848727
C	3.835985	-2.556409	-3.782623
C	3.821654	-1.088085	-3.318187
O	2.567750	-0.444104	-3.667382
H	1.941435	-3.055461	-2.850594
H	2.436265	-4.188078	-4.128782
H	4.473891	-3.140666	-3.099049
H	4.280163	-2.639329	-4.790032
O	-0.290501	-2.444398	-7.929565
H	-0.223568	-1.818881	-8.674580
C	0.659913	-4.295815	-6.036358
H	1.533754	-4.804803	-6.480864
H	0.470278	-4.756219	-5.053322
H	-0.203299	-4.507058	-6.684895
C	-0.147408	0.437926	-7.658674
H	0.558211	0.781124	-8.436043
H	-1.007515	-0.022806	-8.171096
H	-0.520961	1.327411	-7.126622
C	1.549102	1.466295	-5.512967
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H	0.615490	2.012155	-5.282576
H	2.270565	1.666104	-4.708055
C	3.896957	-0.998652	-1.802622
H	4.879219	-1.350350	-1.448117
H	3.752321	0.045644	-1.481097
H	3.110874	-1.620552	-1.341817
C	4.917831	-0.262961	-3.995654
H	4.887887	0.760466	-3.580299
H	4.641800	-0.166500	-5.061449
C	6.330681	-0.821958	-3.903445
H	6.351115	-1.850197	-4.313279
H	6.636869	-0.909482	-2.846265
C	7.326486	0.036512	-4.678515
H	6.909289	0.238273	-5.683413
H	7.431426	1.023126	-4.186964
C	8.712176	-0.590025	-4.841434
H	8.565748	-1.582488	-5.320926
C	9.575442	0.263575	-5.774935
H	8.970361	0.541935	-6.657255
H	9.830136	1.211148	-5.262064
C	10.853799	-0.412811	-6.259076
H	11.488889	-0.674332	-5.395054
H	10.602890	-1.378668	-6.745730
C	11.639592	0.447538	-7.242815
H	11.963483	1.378261	-6.736238
H	10.960845	0.763880	-8.057626
C	12.864116	-0.230440	-7.864230
H	12.512815	-1.150737	-8.374118
C	13.485495	0.680445	-8.928333
H	13.884699	1.588255	-8.433787
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C	14.582633	0.035116	-9.767689
H	15.422402	-0.278765	-9.119939
H	14.183678	-0.890153	-10.222988
C	15.118840	0.963595	-10.852671
H	15.462148	1.903450	-10.379216
H	14.292728	1.249662	-11.534620

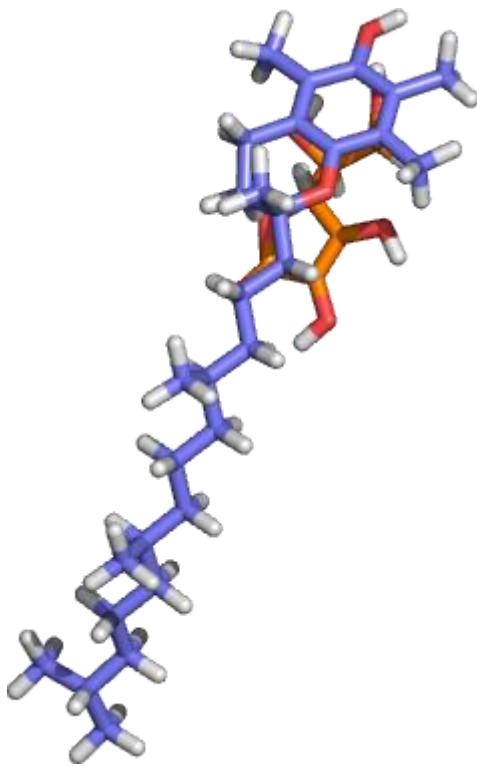


C	16.265865	0.387424	-11.687357
H	17.072389	0.092302	-10.986416
C	16.823484	1.448818	-12.633513
H	17.163197	2.342175	-12.080699
H	17.676397	1.058683	-13.215407
H	16.045644	1.772338	-13.350121
C	9.394936	-0.828613	-3.495737
H	9.527416	0.131976	-2.964762
H	8.797911	-1.494260	-2.850976
H	10.389604	-1.286926	-3.622071
C	13.884813	-0.636210	-6.802285
H	14.238810	0.257105	-6.254819
H	13.450981	-1.334280	-6.067189
H	14.763710	-1.128306	-7.250380
C	15.838631	-0.854657	-12.467874
H	15.497003	-1.663537	-11.800726
H	15.006941	-0.608526	-13.154486
H	16.672720	-1.247516	-13.074770
C	2.345977	-1.449790	-9.129767
C	2.635405	-2.789752	-8.624424
C	3.734138	-2.705127	-7.848106
C	4.216910	-1.289136	-7.830228
O	3.291288	-0.593966	-8.672795
C	5.636626	-1.028123	-8.312054
H	5.665541	-1.252760	-9.399345
C	6.676654	-1.901024	-7.613277
H	6.556494	-2.957603	-7.910753
H	6.540004	-1.832706	-6.516856
O	1.407490	-1.084811	-9.806804
O	1.875189	-3.876721	-8.851867
H	0.944283	-3.615364	-8.661856
O	4.322397	-3.641522	-7.106762
H	3.830181	-4.474727	-7.200695
O	5.913124	0.328962	-8.071018
H	6.877250	0.413553	-8.162383
O	7.931711	-1.381580	-8.006244
H	8.597459	-1.637511	-7.355095
H	4.104136	-0.877719	-6.810378

vitC:vitE 7

$$\Delta E = -5.8 \text{ kcal.mol}^{-1}$$

C	0.327125	-0.435522	-4.854615
C	1.468374	-1.237854	-4.628954
C	1.415760	-2.636561	-4.696855
C	0.207546	-3.268249	-5.055840
C	-0.900204	-2.467413	-5.334241
C	-0.873469	-1.062282	-5.219031
C	2.671264	-3.430916	-4.454013
C	3.911545	-2.593786	-4.736277
C	3.852237	-1.216358	-4.080463
O	2.616122	-0.548309	-4.408702
H	2.689673	-3.799858	-3.410545
H	2.683517	-4.326604	-5.095006
H	4.813492	-3.116565	-4.384853
H	4.028779	-2.456158	-5.823312
O	-2.014318	-3.090670	-5.865906
H	-2.802310	-2.547156	-5.719899
C	0.148346	-4.758141	-5.242170
H	0.656762	-5.033385	-6.185429
H	0.655431	-5.287568	-4.419068
H	-0.891638	-5.109140	-5.301648
C	-2.124069	-0.317304	-5.603133
H	-2.397766	-0.538914	-6.651567
H	-2.985349	-0.610478	-4.971596
H	-2.017503	0.771003	-5.512643
C	0.505773	1.052546	-4.758005
H	1.117484	1.411515	-5.604700
H	-0.445842	1.601261	-4.759104
H	1.059303	1.313578	-3.841331
C	3.936884	-1.315528	-2.562203
H	4.887206	-1.784008	-2.258174
H	3.877248	-0.309431	-2.115912
H	3.106063	-1.922830	-2.165950
C	4.919399	-0.291296	-4.668366
H	4.817915	0.699481	-4.189143
H	4.671214	-0.151011	-5.735544
C	6.355750	-0.784764	-4.550748
H	6.437763	-1.807293	-4.961789
H	6.644712	-0.851994	-3.487057
C	7.330673	0.108444	-5.311597
H	6.991253	0.167726	-6.362755
H	7.281052	1.142585	-4.916582
C	8.783513	-0.373023	-5.282208
H	8.786324	-1.439169	-5.587885
C	9.624854	0.396057	-6.305140
H	9.125499	0.328018	-7.291011
H	9.626093	1.471157	-6.035892
C	11.061193	-0.096529	-6.445127
H	11.602846	0.068440	-5.497512
H	11.054511	-1.192339	-6.608201
C	11.814790	0.570058	-7.590939
H	11.833974	1.667309	-7.433862
H	11.249427	0.405601	-8.528505
C	13.250040	0.069883	-7.786751
H	13.211173	-1.037205	-7.847145
C	13.817741	0.581140	-9.114191
H	13.870860	1.687946	-9.079327
H	13.100459	0.336235	-9.921016
C	15.184984	0.016511	-9.487572
H	15.940941	0.325938	-8.742043
H	15.139732	-1.087606	-9.438195
C	15.648330	0.457198	-10.872067
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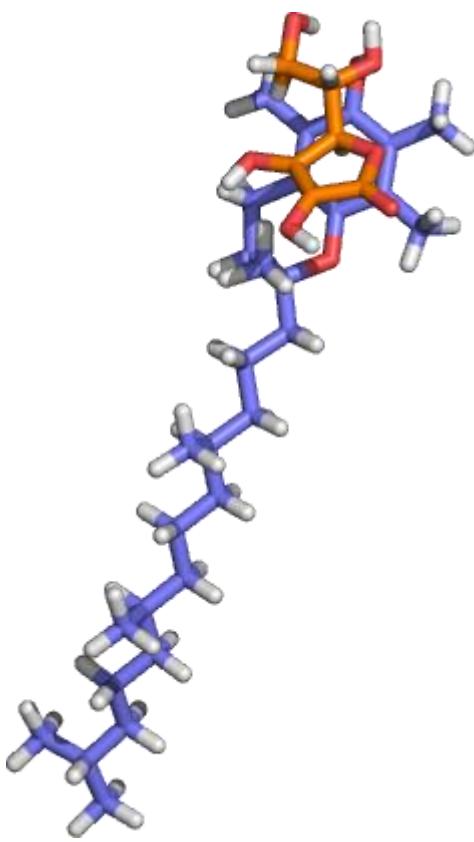


C	17.049345	-0.019858	-11.267706
H	17.755534	0.343220	-10.494280
C	17.459707	0.586358	-12.608728
H	17.421570	1.689525	-12.578147
H	18.483015	0.283505	-12.890875
H	16.775140	0.247830	-13.408465
C	9.375195	-0.280231	-3.876735
H	9.421158	0.775959	-3.552308
H	8.766797	-0.834733	-3.142987
H	10.397755	-0.690183	-3.836962
C	14.145191	0.451509	-6.608303
H	14.234221	1.552059	-6.539498
H	13.738222	0.084569	-5.651636
H	15.160726	0.036953	-6.718713
C	17.143984	-1.544168	-11.317095
H	16.922911	-2.002213	-10.338573
H	16.421779	-1.948538	-12.050977
H	18.153634	-1.868075	-11.624248
C	4.675360	-2.225705	-8.425665
C	4.204150	-0.855629	-8.269094
C	2.882452	-0.890410	-8.001665
C	2.450091	-2.324445	-7.916369
O	3.633595	-3.070591	-8.231483
C	1.284688	-2.774731	-8.786286
H	1.564840	-2.637025	-9.850992
C	0.018274	-1.941324	-8.448594
H	-0.057298	-1.087266	-9.141363
H	0.105252	-1.536280	-7.428743
O	5.802475	-2.586985	-8.675308
O	5.017208	0.214578	-8.360092
H	5.898533	-0.106642	-8.617347
O	2.021035	0.097579	-7.762270
H	2.482596	0.949708	-7.807577
O	1.046237	-4.129248	-8.510246
H	0.075551	-4.214858	-8.593698
O	-1.133020	-2.755556	-8.567298
H	-1.503766	-2.917096	-7.678679
H	2.169734	-2.561995	-6.875032

vitC:vitE 8

$$\Delta E = -5.7 \text{ kcal.mol}^{-1}$$

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C	1.587067	-1.056728	-4.617899
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C	0.170537	-3.026995	-4.669147
C	-0.929664	-2.191748	-4.907184
C	-0.804027	-0.790145	-4.939298
C	2.679607	-3.315967	-4.424108
C	3.916696	-2.568695	-4.899766
C	3.993842	-1.171681	-4.288129
O	2.805920	-0.437937	-4.633397
H	2.812719	-3.649268	-3.377054
H	2.551680	-4.228971	-5.025688
H	4.830391	-3.130177	-4.649268
H	3.876766	-2.463285	-5.998203
O	-2.121273	-2.810423	-5.149210
H	-2.761799	-2.176432	-5.498472
C	-0.040974	-4.516391	-4.646392
H	-0.056889	-4.929576	-5.672579
H	0.746471	-5.035368	-4.079911
H	-1.015685	-4.762728	-4.197485
C	-2.017739	0.032007	-5.276529
H	-2.203768	0.007753	-6.367068
H	-2.923083	-0.345447	-4.767196
H	-1.901651	1.085226	-4.986082
C	0.686085	1.266715	-4.967403
H	0.663814	1.516574	-6.045060
H	-0.097389	1.859577	-4.468622
H	1.664143	1.569058	-4.568799
C	4.101160	-1.218411	-2.767001
H	4.973387	-1.816236	-2.455672
H	4.209617	-0.197312	-2.366106
H	3.195347	-1.670056	-2.330756
C	5.117707	-0.349635	-4.917505
H	5.042173	0.681536	-4.526544
H	4.912318	-0.289995	-6.003008
C	6.529220	-0.881101	-4.701432
H	6.602743	-1.921336	-5.069438
H	6.752261	-0.916678	-3.620821
C	7.569839	-0.031296	-5.423678
H	7.275814	0.054694	-6.487181
H	7.551559	0.999983	-5.018494
C	9.002362	-0.567125	-5.358376
H	8.984649	-1.613429	-5.726711
C	9.903777	0.236295	-6.300382
H	9.430459	0.259496	-7.301025
H	9.936322	1.288801	-5.954934
C	11.326557	-0.292647	-6.445578
H	11.853059	-0.220815	-5.477767
H	11.291167	-1.370836	-6.697848
C	12.115865	0.445905	-7.521432
H	12.164985	1.523989	-7.268484
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H	13.411771	0.412283	-9.851183
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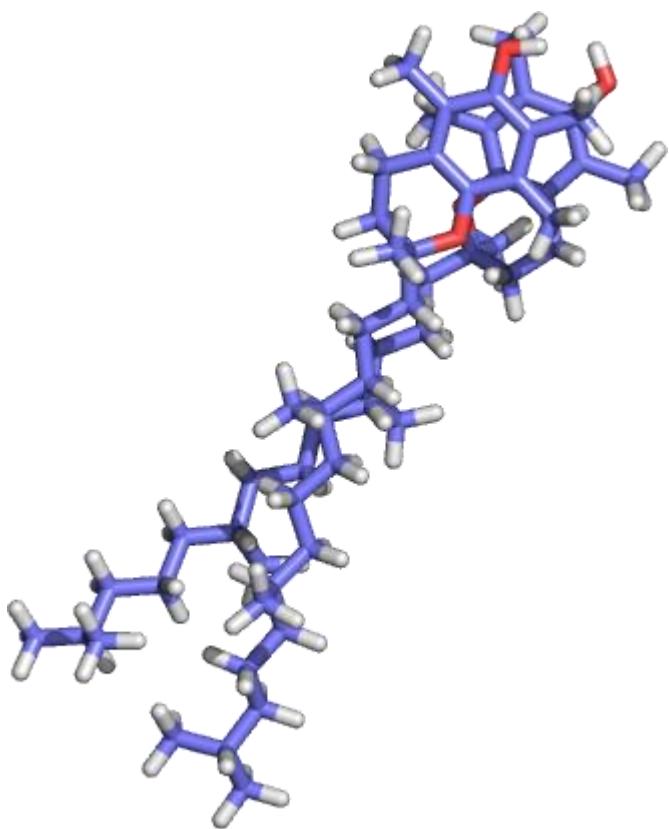


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H	17.705049	1.966308	-12.389965
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H	17.050009	0.603369	-13.337908
C	9.538386	-0.576576	-3.928169
H	9.580962	0.454400	-3.530495
H	8.897116	-1.173111	-3.257929
H	10.555340	-0.999378	-3.879283
C	14.431441	0.162489	-6.537600
H	14.539180	1.246864	-6.346971
H	14.009897	-0.300021	-5.629677
H	15.440299	-0.255724	-6.688592
C	17.436695	-1.365847	-11.416349
H	17.222922	-1.908582	-10.480224
H	16.707650	-1.702345	-12.177189
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C	-0.391113	-3.814999	-8.107103
C	0.754999	-3.153376	-7.850968
C	0.462777	-1.685923	-7.807422
O	-0.928631	-1.593526	-8.137577
C	1.292183	-0.762209	-8.684408
H	1.238985	-1.102326	-9.740545
C	2.746746	-0.761027	-8.211517
H	3.236161	-1.720532	-8.454233
H	2.758792	-0.627003	-7.112556
O	-2.632212	-3.043478	-8.461871
O	-0.594341	-5.146021	-8.154046
H	-1.549752	-5.294855	-8.260302
O	1.978409	-3.617889	-7.586404
H	1.971791	-4.587848	-7.613724
O	0.767323	0.534540	-8.548683
H	1.509033	1.120982	-8.779674
O	3.382842	0.328122	-8.858456
H	4.063298	0.681365	-8.272321
H	0.571730	-1.322216	-6.776230

vitE:vitE 1

$\Delta E = -9.8 \text{ kcal.mol}^{-1}$

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C	-11.214988	1.966530	8.101581
C	-10.322550	1.270253	7.265090
C	-8.849194	3.688832	10.529686
C	-7.362735	3.435690	10.756869
C	-6.610379	3.429667	9.426490
O	-7.124810	2.341573	8.640437
H	-9.037860	4.765180	10.351799
H	-9.415758	3.434589	11.442578
H	-6.931383	4.187145	11.437622
H	-7.234947	2.437577	11.208236
O	-12.569108	1.864342	7.911939
H	-12.741681	1.330000	7.125251
C	-11.725438	3.529871	10.020958
H	-11.708737	3.159106	11.062836
H	-11.458902	4.600306	10.070317
H	-12.755310	3.441208	9.647547
C	-10.892274	0.393255	6.182550
H	-11.455327	-0.454591	6.613213
H	-11.572035	0.957077	5.513491
H	-10.107203	-0.039334	5.547634
C	-7.952939	0.706371	6.568795
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H	-8.127678	0.941225	5.504081
H	-6.923780	0.991814	6.825048
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H	-6.194848	4.716915	7.732033
H	-7.858851	4.868969	8.367728
C	-5.126084	3.101030	9.577474
H	-4.701046	3.051830	8.557986
H	-5.036162	2.085059	9.993786
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H	-4.482288	5.104012	10.060009
C	-2.816990	3.751824	10.335826
H	-2.652436	2.718427	10.696092
H	-2.516599	3.752319	9.269487
C	-1.873184	4.691045	11.096106
H	-2.101215	4.608293	12.178376
C	-0.430499	4.219475	10.878559
H	-0.355168	3.162784	11.199512
H	-0.227000	4.218275	9.789273
C	0.657373	5.028599	11.575797
H	0.636986	6.072305	11.214625
H	0.452012	5.073754	12.663355
C	2.048939	4.445114	11.354265
H	2.197601	4.240899	10.275689
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C	4.446450	4.478075	12.091096
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C	6.797101	4.278796	13.000429
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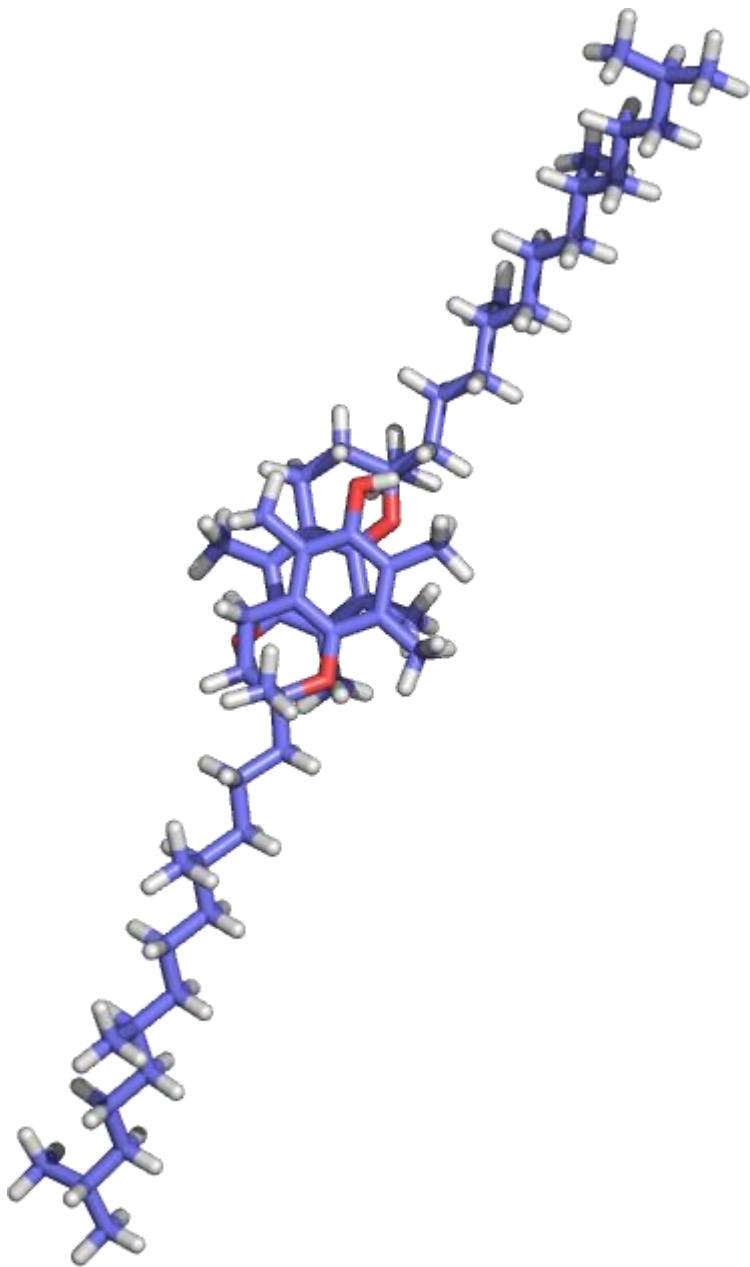
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H	8.892463	3.217113	14.486153
C	-2.059919	6.148896	10.676201
H	-1.851015	6.266494	9.596128
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H	2.536757	7.050186	10.676512
H	4.202098	7.195178	11.291973
C	7.865628	5.786113	14.732531
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C	-9.196724	-2.068063	8.517500
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C	-10.877024	-0.940763	9.899854
C	-6.729920	-1.714172	8.956179
C	-5.816149	-0.777764	9.740931
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H	-6.581980	-1.560326	7.873184
H	-4.766799	-1.105856	9.670161
H	-5.892600	0.243164	9.328357
O	-11.504251	-2.339112	8.036698
H	-12.373362	-2.119079	8.397702
C	-8.845894	-2.979076	7.373813
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H	-9.741147	-3.466671	6.963680
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H	-12.935617	-1.566410	10.229930
H	-12.491728	-0.064610	11.055417
C	-10.188871	0.495852	11.871803
H	-10.610540	1.449835	11.512592
H	-10.931915	0.037151	12.546905
H	-9.283612	0.721218	12.450628
C	-6.257117	-2.089068	11.864782
H	-5.252058	-2.540063	11.817874
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H	-5.804052	0.231871	13.070012
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C	-3.923872	0.085232	12.021335
H	-3.526947	0.251770	11.002143
H	-3.673549	-0.956159	12.289771
C	-3.251394	1.051175	12.990463
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H	-3.616936	0.840957	14.015150
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H	-1.366715	1.347074	12.005441
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H	-1.715703	3.031997	13.813271
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H	0.622844	2.631222	13.072956

C	0.693533	3.300829	15.122438
H	0.483871	2.890431	16.130673
H	0.052804	4.198376	15.021321
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H	2.303814	4.209838	14.059824
C	2.440172	4.818905	16.108317
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H	1.593320	5.530884	16.133748
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H	4.590880	4.927744	15.818464
H	3.655571	6.098019	14.886044
C	3.978602	6.655834	16.954683
H	4.029359	6.147527	17.936976
H	3.111791	7.344714	17.010821
C	5.252192	7.483540	16.760567
H	6.099024	6.776194	16.674424
C	5.500649	8.378733	17.972375
H	5.571110	7.784400	18.900235
H	6.435104	8.956513	17.861379
H	4.671223	9.099567	18.094822
C	-1.171850	-0.362969	13.294718
H	-1.520857	-0.714991	14.283216
H	-1.503683	-1.092667	12.537846
H	-0.069291	-0.371673	13.300948
C	3.123345	2.571932	15.168368
H	2.965806	2.037449	16.123917
H	2.986493	1.849364	14.346803
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vitE:vitE 2

$\Delta E = -8.5 \text{ kcal.mol}^{-1}$

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C	-9.449595	0.250554	3.969099
C	-6.851280	2.375373	6.688325
C	-5.382132	2.230450	6.311360
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H	6.003694	1.993770	5.370336
C	7.472770	3.540794	5.662550
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H	7.294058	3.674893	6.745887
C	8.663570	2.614318	5.438723
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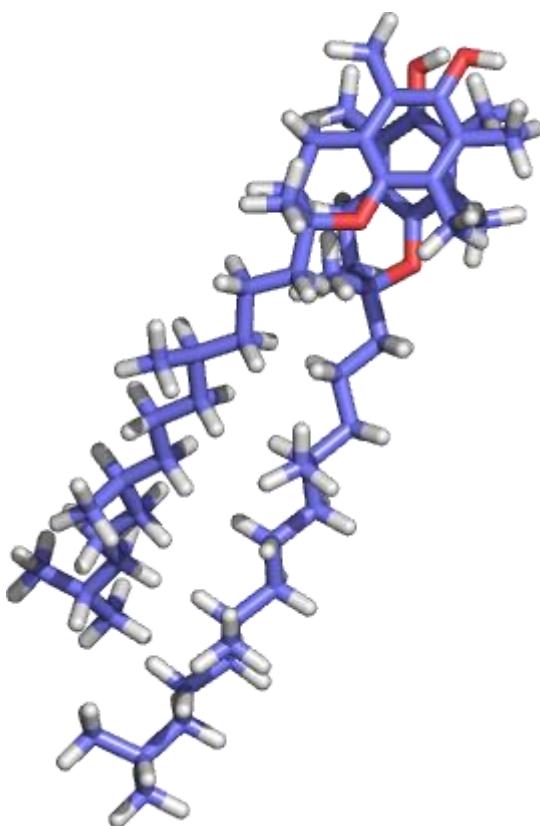
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H	-0.341379	4.939649	3.151199
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C	9.967299	3.335604	7.492155
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C	-6.344677	-1.270779	6.868024
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H	-6.767937	-1.973680	4.276362
H	-7.144586	-3.527179	5.056848
H	-8.465282	-2.472717	4.483426
C	-10.734431	-3.740808	7.970223
H	-11.585932	-3.965006	8.632808
H	-10.574159	-4.596650	7.293489
H	-9.833758	-3.616411	8.593534
C	-12.101858	-2.681195	6.121998
H	-11.757258	-3.461585	5.418561
H	-12.175445	-1.743502	5.543850
C	-13.472961	-3.053161	6.669765
H	-13.828064	-2.269815	7.365125
H	-13.397015	-3.982383	7.260402
C	-14.497076	-3.229086	5.553109
H	-14.486500	-2.324254	4.915849
H	-14.183082	-4.065731	4.897364
C	-15.934499	-3.479390	6.017591
H	-16.235312	-2.622077	6.654187
C	-16.872800	-3.512688	4.807303
H	-16.662599	-2.631458	4.170816
H	-16.623548	-4.399421	4.190264
C	-18.361228	-3.530780	5.136854
H	-18.593131	-4.409631	5.763437
H	-18.610466	-2.641047	5.748345

C	-19.235003	-3.547374	3.887179
H	-19.035078	-4.475897	3.315365
H	-18.929790	-2.712663	3.226796
C	-20.741863	-3.440833	4.138665
H	-20.923197	-2.497090	4.693015
C	-21.487518	-3.346740	2.804229
H	-21.341202	-4.294757	2.248303
H	-21.012359	-2.558076	2.189720
C	-22.979176	-3.048578	2.911720
H	-23.489986	-3.856397	3.467812
H	-23.117996	-2.128249	3.509507
C	-23.645984	-2.892672	1.549371
H	-23.433534	-3.795853	0.944925
H	-23.179914	-2.045771	1.006658
C	-25.161631	-2.676355	1.591535
H	-25.604021	-3.527957	2.146183
C	-25.740438	-2.677444	0.178632
H	-25.498866	-3.614541	-0.352805
H	-26.838562	-2.561619	0.192504
H	-25.320539	-1.839511	-0.407974
C	-16.042777	-4.755171	6.852106
H	-15.726981	-5.629708	6.252954
H	-15.401252	-4.709806	7.747428
H	-17.076559	-4.932674	7.191658
C	-21.257428	-4.598691	4.992037
H	-21.079899	-5.561081	4.476349
H	-20.749943	-4.640879	5.969759
H	-22.339662	-4.510614	5.183222
C	-25.537218	-1.388312	2.322750
H	-25.184574	-1.388731	3.367684
H	-25.088269	-0.514848	1.814032
H	-26.631866	-1.244989	2.335450

vitE:vitE 3

$$\Delta E = -6.4 \text{ kcal.mol}^{-1}$$

C	-8.202765	1.850067	7.629033
C	-6.876089	2.300161	7.499930
C	-6.000263	1.728358	6.560626
C	-6.446837	0.674305	5.744313
C	-7.777677	0.245545	5.853403
C	-8.662359	0.829251	6.780692
C	-4.572659	2.207484	6.460469
C	-4.326461	3.475893	7.272789
C	-5.068993	3.422326	8.606945
O	-6.477401	3.318959	8.321670
H	-3.898741	1.399066	6.804299
H	-4.306580	2.377780	5.402878
H	-3.248309	3.627327	7.446590
H	-4.702366	4.357831	6.725133
O	-8.181615	-0.762487	5.021677
H	-9.108024	-0.971401	5.195751
C	-5.502664	0.033516	4.764221
H	-5.133270	0.770275	4.026988
H	-4.609313	-0.365429	5.276750
H	-5.986488	-0.788522	4.219461
C	-10.098412	0.381245	6.835394
H	-10.728621	0.949516	6.124805
H	-10.227678	-0.693550	6.617312
H	-10.513025	0.525185	7.842662
C	-9.104581	2.434544	8.682371
H	-10.004417	2.898876	8.240372
H	-9.449449	1.639947	9.370338
H	-8.573410	3.195183	9.270040
C	-4.663410	2.210154	9.437841
H	-3.581545	2.193525	9.641436
H	-5.212804	2.221615	10.392322
H	-4.936329	1.287665	8.903667
C	-4.925117	4.720600	9.396564
H	-5.708537	4.723786	10.175677
H	-5.145708	5.566898	8.720416
C	-3.562547	4.910089	10.051350
H	-2.758218	4.767772	9.305192
H	-3.413743	4.119181	10.807233
C	-3.379884	6.275144	10.709200
H	-3.280353	7.046650	9.923116
H	-4.288994	6.538406	11.285721
C	-2.162558	6.318097	11.644485
H	-1.341659	5.763227	11.144709
C	-1.664793	7.746920	11.871548
H	-1.480299	8.216860	10.886173
H	-2.469370	8.338583	12.351652
C	-0.386942	7.827009	12.700742
H	-0.581445	7.452023	13.721011
H	0.364246	7.146624	12.257445
C	0.215784	9.225589	12.764706
H	-0.523585	9.941275	13.176922
H	0.432555	9.564012	11.733417
C	1.504076	9.304769	13.589737
H	2.160287	8.482453	13.246676
C	2.252935	10.611824	13.318567
H	1.635348	11.468775	13.655406
H	2.362324	10.727483	12.222324
C	3.631290	10.697475	13.965269
H	3.538056	10.689814	15.066869
H	4.207695	9.791105	13.698713
C	4.401862	11.946465	13.550589
H	3.743125	12.829016	13.667831
H	4.646179	11.891574	12.470591
C	5.691850	12.196528	14.340003



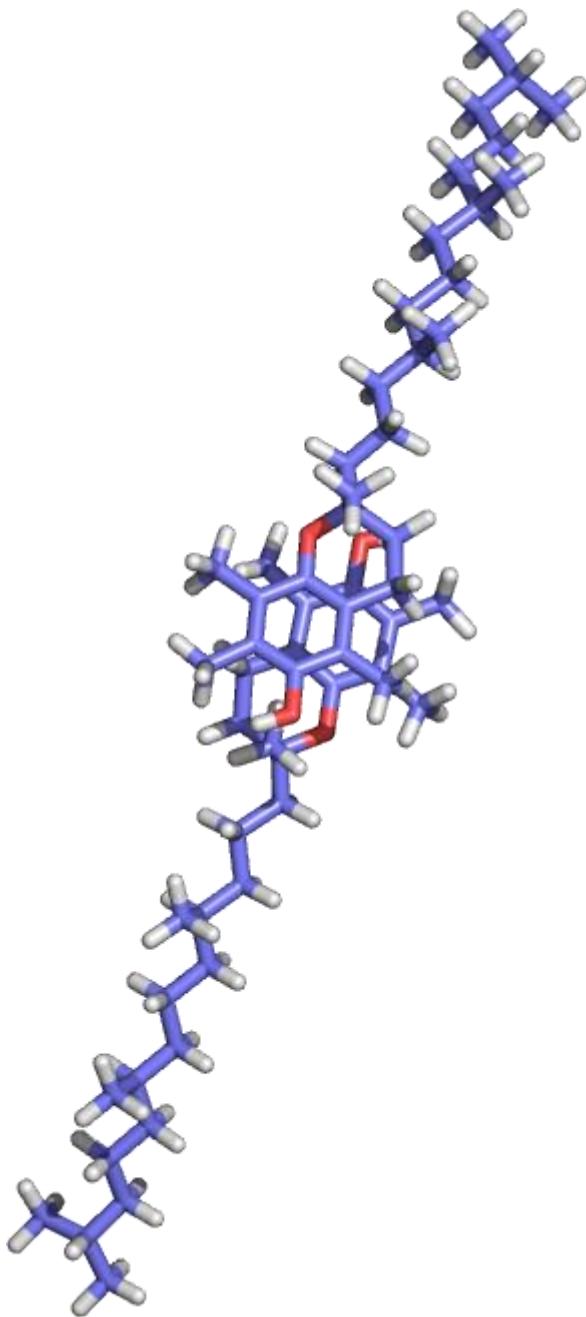
H	5.408378	12.263322	15.409346
C	6.323779	13.524226	13.929711
H	5.620618	14.363594	14.072979
H	7.235105	13.735375	14.516283
H	6.607548	13.501002	12.861429
C	-2.473313	5.611241	12.964203
H	-3.167074	6.223384	13.569620
H	-2.946568	4.631668	12.788504
H	-1.559526	5.429359	13.552476
C	1.232725	9.096832	15.077794
H	0.571732	9.895533	15.463234
H	0.740700	8.128029	15.265007
H	2.163037	9.111576	15.669189
C	6.694754	11.054135	14.185543
H	6.274262	10.087496	14.508828
H	7.000352	10.951214	13.129037
H	7.603091	11.248215	14.782730
C	-9.490143	-0.664799	10.911694
C	-8.149458	-1.063799	10.730116
C	-7.773377	-1.894230	9.662673
C	-8.750856	-2.368416	8.770100
C	-10.084195	-1.990547	8.965031
C	-10.463684	-1.133119	10.013370
C	-6.325038	-2.269296	9.482659
C	-5.387250	-1.399006	10.310089
C	-5.929858	-1.144472	11.715573
O	-7.245838	-0.569337	11.622673
H	-6.184764	-3.335841	9.746820
H	-6.054226	-2.185201	8.416409
H	-4.394596	-1.871075	10.378192
H	-5.243694	-0.419780	9.825766
O	-11.006116	-2.459025	8.069080
H	-11.876918	-2.097376	8.279214
C	-8.382495	-3.230055	7.593067
H	-8.105578	-2.604199	6.722802
H	-7.522106	-3.880119	7.817869
H	-9.229054	-3.862103	7.285705
C	-11.910734	-0.729270	10.114244
H	-12.101166	-0.069977	10.971897
H	-12.239705	-0.185104	9.206816
H	-12.574181	-1.609031	10.222852
C	-9.854820	0.261472	12.041331
H	-10.151625	1.257100	11.662008
H	-10.705621	-0.128537	12.626429
H	-9.000815	0.398966	12.717790
C	-6.012810	-2.431768	12.527959
H	-5.009989	-2.877283	12.638010
H	-6.419198	-2.219559	13.529976
H	-6.667783	-3.166927	12.031831
C	-5.134757	-0.053960	12.435220
H	-5.566043	0.074451	13.445377
H	-5.346092	0.880737	11.889509
C	-3.625474	-0.233599	12.530965
H	-3.215937	-0.524468	11.547241
H	-3.374662	-1.051482	13.229674
C	-2.948486	1.065660	12.960962
H	-3.259371	1.857859	12.253250
H	-3.329333	1.379959	13.952513
C	-1.417910	1.027284	12.999161
H	-1.071191	0.583352	12.044179
C	-0.871162	2.453936	13.066776
H	-1.292301	3.027948	12.219756
H	-1.258896	2.946245	13.980155
C	0.648102	2.590269	13.030311
H	1.087760	2.175058	13.954236
H	1.056017	1.987399	12.194743

C	1.075614	4.044221	12.850881
H	0.636777	4.660025	13.660683
H	0.626885	4.427330	11.914719
C	2.583814	4.300976	12.815887
H	3.031388	3.613532	12.069422
C	2.841222	5.735158	12.348832
H	2.300552	6.417867	13.032366
H	2.369111	5.872237	11.356155
C	4.301457	6.169292	12.259616
H	4.730969	6.261737	13.274959
H	4.887657	5.383311	11.747615
C	4.458623	7.499683	11.526374
H	3.713660	8.217713	11.918430
H	4.204104	7.355729	10.457324
C	5.842101	8.145608	11.624244
H	6.054685	8.317166	12.699031
C	5.839510	9.501460	10.924605
H	5.100769	10.181917	11.381987
H	6.829706	9.986183	10.979373
H	5.581385	9.381942	9.856065
C	-0.902708	0.158252	14.143709
H	-1.191974	0.598097	15.116459
H	-1.320596	-0.861390	14.095088
H	0.196244	0.069885	14.124363
C	3.231681	4.025593	14.172288
H	2.834904	4.724496	14.932447
H	3.028504	2.998401	14.518491
H	4.325216	4.158702	14.130845
C	6.938744	7.242673	11.062584
H	6.981715	6.277375	11.594534
H	6.749687	7.032702	9.993290
H	7.930593	7.721139	11.146183

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$$\Delta E = -5.5 \text{ kcal.mol}^{-1}$$

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C	-8.165967	1.958373	8.896203
C	-8.028960	1.374208	7.626988
C	-9.131739	0.741472	7.025781
C	-10.363416	0.761976	7.688756
C	-10.496748	1.302480	8.981744
C	-6.705732	1.449117	6.912136
C	-5.851704	2.587354	7.459331
C	-5.816365	2.565380	8.987008
O	-7.159311	2.660893	9.494860
H	-6.175173	0.482382	7.019466
H	-6.866901	1.587991	5.830304
H	-4.822811	2.527371	7.069916
H	-6.272295	3.558218	7.140536
O	-11.443874	0.225303	7.037571
H	-12.227025	0.291462	7.599237
C	-8.989541	0.073570	5.687295
H	-8.819757	0.811437	4.880759
H	-8.126388	-0.611166	5.690910
H	-9.885658	-0.510089	5.438376
C	-11.849036	1.249866	9.643252
H	-12.619452	1.751355	9.026003
H	-12.184581	0.207291	9.806293
H	-11.852988	1.748628	10.621667
C	-9.465379	2.455235	10.998418
H	-10.030812	3.405632	11.022672
H	-9.975774	1.758102	11.684374
H	-8.459243	2.656193	11.392046
C	-5.206734	1.272115	9.507656
H	-4.191751	1.126426	9.102333
H	-5.153341	1.281085	10.607422
H	-5.831887	0.419750	9.206661
C	-5.122925	3.799331	9.560399
H	-5.251350	3.767750	10.658257
H	-5.669758	4.691650	9.204231
C	-3.641596	3.935628	9.228405
H	-3.501530	4.015910	8.134003
H	-3.108588	3.022398	9.545042
C	-3.018462	5.153822	9.902688
H	-3.602178	6.051971	9.624356
H	-3.121497	5.052234	11.001547
C	-1.544522	5.404479	9.567980
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H	-1.807677	7.519362	9.906615
H	-1.157490	6.639773	11.295655
C	0.316844	7.178696	9.810722
H	1.049752	6.418031	10.130803
H	0.395972	7.237365	8.707227
C	0.684776	8.529686	10.416200
H	0.642350	8.458422	11.521716
H	-0.086039	9.271098	10.130399
C	2.058747	9.073112	10.011804
H	2.083645	9.130681	8.904162
C	2.240771	10.494609	10.553884
H	2.235340	10.457923	11.662015
H	1.358303	11.097846	10.265725
C	3.499097	11.212897	10.078227
H	4.399283	10.669226	10.420185
H	3.527318	11.189466	8.972570
C	3.578264	12.653155	10.573427
H	3.465598	12.657586	11.675041
H	2.716472	13.226725	10.176575
C	4.869982	13.391685	10.211380



H	5.715420	12.802092	10.619066
C	4.895982	14.772123	10.863378
H	4.788131	14.700486	11.960060
H	5.838642	15.302977	10.643430
H	4.062990	15.391888	10.482851
C	-0.659722	4.238658	10.008309
H	-0.720012	4.108233	11.105152
H	-0.971098	3.291050	9.538840
H	0.396958	4.409080	9.744310
C	3.187690	8.148520	10.465499
H	3.185644	8.057866	11.568063
H	3.078618	7.136064	10.043394
H	4.174861	8.531899	10.159329
C	5.060834	13.508505	8.699761
H	5.115094	12.519687	8.214369
H	4.216061	14.061904	8.248637
H	5.990148	14.053702	8.458925
C	-6.951187	-2.444668	7.839734
C	-8.251525	-2.434669	8.380592
C	-8.479233	-2.087102	9.720680
C	-7.394265	-1.774853	10.557939
C	-6.097821	-1.824204	10.031999
C	-5.866343	-2.136879	8.678572
C	-9.876913	-2.082579	10.281271
C	-10.946004	-2.312153	9.219279
C	-10.483221	-3.285933	8.136439
O	-9.275822	-2.773401	7.545505
H	-9.944641	-2.854455	11.071758
H	-10.062342	-1.119040	10.789524
H	-11.875305	-2.684288	9.679307
H	-11.179638	-1.367950	8.710853
O	-5.058958	-1.532004	10.870511
H	-4.234526	-1.503855	10.368018
C	-7.637912	-1.376249	11.986217
H	-8.230618	-0.443628	12.029468
H	-8.220978	-2.144779	12.524273
H	-6.694539	-1.211463	12.524900
C	-4.445947	-2.123561	8.179641
H	-4.004206	-1.111072	8.259166
H	-3.803387	-2.807667	8.766230
H	-4.370093	-2.428783	7.127117
C	-6.739804	-2.805378	6.392576
H	-6.246534	-1.984220	5.842477
H	-6.092337	-3.694715	6.288818
H	-7.700446	-3.017927	5.904460
C	-10.204393	-4.677259	8.701943
H	-11.104619	-5.083702	9.190233
H	-9.899861	-5.359574	7.890876
H	-9.394065	-4.638369	9.448160
C	-11.469465	-3.325265	6.971140
H	-11.036743	-3.973615	6.186771
H	-11.521898	-2.302699	6.557521
C	-12.870559	-3.811409	7.321229
H	-13.335147	-3.125700	8.054289
H	-12.810644	-4.796708	7.815347
C	-13.770552	-3.905912	6.093393
H	-13.733701	-2.944073	5.547239
H	-13.360957	-4.665604	5.398195
C	-15.234659	-4.243881	6.388844
H	-15.634690	-3.448167	7.050283
C	-16.050309	-4.224203	5.092547
H	-15.812949	-3.297000	4.536110
H	-15.712132	-5.060539	4.448153
C	-17.561051	-4.309901	5.278897
H	-17.815046	-5.229776	5.833526
H	-17.898367	-3.465439	5.911913

C	-18.321361	-4.285465	3.958044
H	-18.032639	-5.169530	3.354667
H	-17.998289	-3.400923	3.375634
C	-19.847394	-4.254342	4.085118
H	-20.115414	-3.357302	4.680332
C	-20.486098	-4.100186	2.701689
H	-20.251828	-5.001124	2.099311
H	-20.000769	-3.251983	2.181944
C	-21.993913	-3.871862	2.706745
H	-22.507433	-4.735466	3.168392
H	-22.220803	-2.999974	3.348660
C	-22.563355	-3.653456	1.309218
H	-22.269327	-4.507654	0.668884
H	-22.095649	-2.756415	0.856098
C	-24.086148	-3.497446	1.251604
H	-24.530439	-4.394982	1.726377
C	-24.563970	-3.441033	-0.197671
H	-24.248811	-4.338273	-0.758436
H	-25.664184	-3.365765	-0.257033
H	-24.137559	-2.557260	-0.706964
C	-15.368810	-5.580402	7.118051
H	-14.947997	-6.395135	6.499527
H	-14.830693	-5.575003	8.080116
H	-16.422698	-5.825143	7.330285
C	-20.380084	-5.485479	4.817341
H	-20.121567	-6.403729	4.257403
H	-19.951861	-5.574872	5.829155
H	-21.476856	-5.450583	4.923689
C	-24.565920	-2.267704	2.021454
H	-24.284324	-2.312320	3.086765
H	-24.122245	-1.350394	1.591438
H	-25.664109	-2.168847	1.965028