Supplementary Information

for

Multiple Reactivities of Flavonoids towards Pathological Elements in Alzheimer's Disease: Structure-Activity Relationship

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Materials and Methods. All reagents were purchased from commercial suppliers and used as received unless noted otherwise. NMR and high-resolution mass spectrometric analyses of small molecules were conducted on an Agilent 400-MR DD2 NMR spectrometer (UNIST Central Research Facilities, Ulsan, Republic of Korea) and Q exactive plus orbitrap mass spectrometer (HRMS; Thermo Fisher Scientific, Waltham, MA, USA), respectively. Absorbance and fluorescence values for biological assays were measured on a Molecular Devices SpectraMax M5e microplate reader (Sunnyvale, CA, USA). Trace metal contamination was removed from buffers and solutions used in metal binding and Aβ aggregation experiments by treating with Chelex overnight (Sigma-Aldrich, St. Louis, MO, USA). Optical spectra were recorded on an Agilent 8453 UV−Vis spectrophotometer (Santa Clara, CA, USA). $A\beta_{42}$ (DAEFRHDSGYEVHH-QKLVFFAEDVGSNKGAIIGLMVGGVVIA) was purchased from AnaSpec (Fremont, CA, USA) and Peptide Institute (Osaka, Japan). Double-distilled H_2O (ddH_2O) was obtained from a Milli-Q Direct 16 system (18.2 MΩ·cm; Merck KGaA, Darmstadt, Germany). Morphologies of peptide aggregates were taken by a JEOL JEM-2100 transmission electron microscope (200 kV; 25,000x magnification; UNIST Central Research Facility, Ulsan, Republic of Korea) and a Tecnai F30 (FEI) transmission electron microscope (KAIST Analysis Center for Research Advancement, Daejeon, Republic of Korea).

Synthesis of 5-Hydroxyisoflavone (HIF)

1-[2-Hydroxy-6-(methoxymethoxy)phenyl]ethanone (2). 2,6-Dihydroxyaceto-phenone (303 mg, 2.0 mmol) was dissolved with CH_2Cl_2 (10 mL) in a flame-dried flask. The resultant mixture was cooled to 0 °C, and *N*,*N*-diisopropylethylamine (450 μL, 3 mmol) was slowly introduced. After 20 min, methyl chloromethyl ether (MOMCl; 159 μL, 2 mmol) was added dropwise. The reaction mixture was maintained at 0 °C for 20 min and then brought to room temperature followed by being quenched with H_2O (40 mL). The aqueous collection was extracted with $CHCl_3$ (3 × 40 mL). The combined organic layers were dried using magnesium sulfate ($MgSO_4$) and concentrated to obtain the product [yield: 316 mg (82%)].^{1}H NMR [400 MHz; $CDCl_3$, δ (ppm)]: 13.12 (s, 1H), 8.36 (t, J = 8.4 Hz, 1H), 6.62 (m, 2H), 5.30 (s, 2H), 3.54 (s, 3H), 2.74 (s, 3H). ^{13}C NMR [100 MHz; $CDCl_3$, δ (ppm)]: 205.0, 164.4, 158.9, 136.1, 111.7, 111.6, 104.0, 94.5, 56.7, 33.7.

3-(Dimethylamino)-1-[2-hydroxy-6-(methoxymethoxy)phenyl]prop-2-en-1-one (3). 2 (316 mg, 1.6 mmol) was dissolved in *N*,*N*-dimethylformamide (DMF) (10 mL), and the solution

was heated to 74 °C in an oil bath. *N*,*N*-dimethylformamide dimethyl acetal (DMF-DMA; 700 μL, 8.0 mmol) was then added dropwise to the flask. After the mixture was stirred for 4.5 h, it was cooled to room temperature. The reaction was quenched with H_2O (100 mL) and the mixture was extracted with ethyl acetate (EtOAc; 100 mL). The extracts were washed with H_2O (50 mL), dried with $MgSO_4$, and concentrated under reduced pressure. The resultant residues were purified by column chromatography (SiO_2; EtOAc) to give a yellow solid [yield: 337 mg (83%)]. [400 MHz; $CDCl_3$, δ (ppm)]: 14.24 (s, 1H), 7.98 (d, *J* = 12.3 Hz, 1H), 7.21 (t, *J* = 8.3 Hz, 1H), 6.62 (d, *J* = 8.3 Hz, 1H), 6.53 (d, *J* = 8.3 Hz, 1H), 6.31 (d, *J* = 12.3 Hz, 1H), 5.25 (s, 2H), 3.54 (s, 3H), 3.20 (s, 3H), 2.96 (s, 3H). ^{13}C NMR [100 MHz; $CDCl_3$, δ (ppm)]: 190.6, 164.3, 157.4, 154.8, 133.1, 112.7, 111.9, 104.8, 97.6, 95.2, 56.6, 45.3, 37.3.

3-Iodo-5-(methoxymethoxy)-4*H*-chromen-4-one (4). A solution of **3** (337 mg, 1.3 mmol) and I_2 (399 mg, 1.9 mmol) in CH_3OH (30 mL) was stirred at room temperature for 6 h followed by being concentrated under reduced pressure to give a red-black residue. To remove the remaining I_2, the residue was treated with saturated aqueous sodium sulfite (Na_2SO_3) until the mixture became clear. The mixture was then extracted with $CHCl_3$ (3 × 40 mL), and the extracts were dried with $MgSO_4$ and concentrated under reduced pressure. The resulting off-white solid was purified by chromatography [SiO_2; EtOAc/hexanes (1:1)] to give a white solid [yield: 271 mg (61%)]. [400 MHz; $CDCl_3$, δ (ppm)]: 8.19 (s, 1H), 7.58 (t, *J* = 8.4 Hz, 1H), 7.12 (m, 2H), 5.35 (s, 2H), 3.57 (s, 3H). ^{13}C NMR [100 MHz; $CDCl_3$, δ (ppm)]: 172.0, 158.0, 157.0, 156.1, 134.0, 113.6, 111.9, 111.2, 95.5, 89.2, 56.7.

5-(Methoxymethoxy)-3-phenyl-4*H*-chromen-4-one (5). PEG 10000 (6.7 g), ground to a fine consistency in a mortar, and palladium acetate [$Pd(OAc)_2$; 7.9 mg, 0.04 mmol] were added to a solution of sodium carbonate (Na_2CO_3; 174 mg, 2.0 mmol) in CH_3OH (10 mL). The reaction mixture was heated to 50 °C in a water bath. When the mixture turned black, **4** (271 mg, 0.82 mmol) and phenylboronic acid (209 mg, 2.1 mmol) were added. After being stirred for 3 h, the resulting mixture was filtered, washed with CH_3OH (40 mL), and concentrated under reduced pressure. The mixture was extracted with H_2O and EtOAc (3 × 40 mL), and the extracts were dried with $MgSO_4$ and concentrated under reduced pressure. The white solid was used in the next reaction without further purification [yield: 181 mg (80%)]. [400 MHz; $CDCl_3$, δ (ppm)]: 7.80 (s, 1H), 7.46 (m, 3H), 7.32(m, 3H), 7.02 (m, 2H), 5.26 (s, 2H), 3.47 (s, 3H). ^{13}C NMR [100 MHz; $CDCl_3$, δ (ppm)]: 175.9, 158.2, 157.6, 151.3, 133.6, 131.8, 192.2, 128.4, 128.1, 126.5, 111.7, 111.6, 95.5, 56.6.

5-Hydroxy-3-phenyl-4*H*-chromen-4-one (HIF). A solution of **5** (181 mg, 0.99 mmol) in $CHCl_3$ (2 mL) / CH_3OH (2 mL) with concentrated HCl (36%, 0.5 mL) was refluxed for 1 h. The reaction was quenched with H_2O, and the mixture was extracted with $CHCl_3$ (2 × 10 mL). The extracts were washed with H_2O (10 mL) and purified by column chromatography to give the final product [SiO_2; EtOAc/hexanes (1:4); yield: 84 mg (35%)]. [400 MHz; $CDCl_3$, δ (ppm)]: 12.68 (s, 1H), 8.02 (s, 1H), 7.57 (m, 3H), 7.48 (m, 3H), 6.96 (d, J = 8.4 Hz, 1H), 6.86 (d, J = 8.3 Hz, 1H). ^{13}C NMR [100 MHz; $CDCl_3$, δ (ppm)]: 181.8, 161.4, 156.6, 153.9, 135.6, 130.6, 124.4, 111.5, 107.1. HRMS: Calcd for $[M+Na]^+$, 261.0522; found, 261.0529.

UV–Vis Measurements. The interaction of compounds with Cu(II) was detected by UV–Vis spectroscopy. The experiments were carried out in 20 mM HEPES, pH 7.4, 150 mM NaCl for most of compounds. In the case of chrysin (**Chr**) and 5-hydroxyflavone (**HF**), their Cu(II) interaction was monitored in ethanol (EtOH). The solutions of compounds were titrated up to 5 equiv of $CuCl_2$ at room temperature. The mixture solution was allowed to equilibrate for 5 min after the addition of $CuCl_2$ at room temperature before the spectra were recorded.

Aβ Aggregation Experiments. $A\beta_{42}$ was dissolved in ammonium hydroxide [1% v/v NH_4OH (aq)]. The resulting solution was aliquoted, lyophilized overnight, and stored at −80 °C. A stock solution of $A\beta_{42}$ was then prepared by dissolving the lyophilized peptide using 1% v/v NH_4OH (aq) (10 μL) and diluting with ddH_2O. All $A\beta_{42}$ samples were prepared following previously reported procedures.[1] The concentration of the peptide solution was determined by measuring the absorbance of the solution at 280 nm (ε = 1,490 $M^{-1}cm^{-1}$). The buffered solution [20 mM 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES), pH 7.4, 150 mM NaCl] was used for the preparation of $A\beta_{42}$ samples. For the inhibition studies, compounds (final concentration, 50 μM; 1% v/v DMSO) were added to the samples of $A\beta_{42}$ (25 μM) in the absence and presence of Cu(II) or Zn(II) (25 μM) followed by incubation for 24 h at 37 °C with constant agitation. For the disaggregation studies, $A\beta_{42}$ (25 μM) was incubated with and without Cu(II) or Zn(II) (25 μM) for 24 h at 37 °C with constant agitation to generate preformed $A\beta_{42}$ aggregates. The resulting $A\beta_{42}$ aggregates were then treated with compounds (50 μM) and incubated for an additional 24 h with constant agitation.

Gel/Western Blot. The resultant $A\beta_{42}$ species from the inhibition and disaggregation experiments

were analyzed through gel/Western blot using an anti-Aβ antibody (6E10).[1] The samples (10 μL) were separated on a 10-20% Tris-tricine gel (Invitrogen, Carlsbad, CA, USA). Following separation, the proteins were transferred onto nitrocellulose membranes and blocked with bovine serum albumin (BSA; 3% w/v; Sigma-Aldrich) in Tris-buffered saline (TBS) containing 0.1% v/v Tween-20 (Sigma-Aldrich) (TBS-T) for 4 h at room temperature or overnight at 4 °C. The membranes were incubated with 6E10 (1:2,000, Covance, Princeton, NJ, USA) in a solution of BSA (2% w/v in TBS-T) for 2 h at room temperature or overnight at 4 °C. After washing with TBS-T (3x, 10 min each), a horseradish peroxidase-conjugated goat anti-mouse secondary antibody (1:5,000 in 2% w/v BSA in TBS-T; Cayman Chemical Company, Ann Arbor, MI, USA) was added for 2 h at room temperature. Lastly, a homemade ECL kit[2] was used to visualize gel/Western blots on a ChemiDoc MP Imaging System (Bio-Rad, Hercules, USA). The amounts of Aβ species observed in the gel/Western blots were quantified by the ImageJ software (National Institutes of Health, Bethesda, MD, USA).

TEM. Samples for TEM were prepared following previously reported methods.[1] Glow-discharged grids (Formvar/Carbon 300-mesh, Electron Microscopy Sciences, Hatfield, PA, USA) were treated with Aβ samples (5 μL, 25 μM) for 2 min at room temperature. Excess sample was removed using filter paper followed by washing twice with ddH_2O. Each grid, incubated with uranyl acetate (5 μL, 1% w/v in ddH_2O) for 1 min, was blotted off and dried for 15 min at room temperature. Images for each sample were taken on a transmission electron microscope. For the TEM studies, we randomly selected the locations of samples on the grids for imaging and collected more than 25 images from each grid (sample).

TEAC Assay. The free radical scavenging capacities of compounds were determined by the TEAC assay based on the decolorization of ABTS [2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)diammonium salt] cation radical in comparison to that of the vitamin E analog, Trolox, known for its antioxidant properties.[3] The TEAC assay was conducted in EtOH following previously reported methods.[4] Blue $ABTS^{\bullet+}$ cation radicals were generated by dissolving ABTS (7.0 mM) with potassium persulfate (2.5 mM) in H_2O (5 mL) and incubating the solution for 16 h at room temperature in the dark. Then the solution was diluted with EtOH to an absorbance of *ca*. 0.7 at 734 nm. The $ABTS^{\bullet+}$ solution (200 μL) was then added to a clear 96 well plate. Various concentrations of compounds or Trolox were added to the 96 well plate and incubated at 25 ºC for various time periods (1, 3, 6, and 10 min). Percent inhibition was calculated based on the measured absorbance at 734 nm [% inhibition = 100 x $(A_0 - A)/A_0$; A_0 = absorbance of control

well without compounds; A = absorbance of wells treated with compounds] and plotted as a function of compounds' concentration. The TEAC values of each time point were calculated as the ratio between the slope of compounds and the slope of Trolox. All measurements were carried out in triplicate.

Calculation of Redox Potentials. All calculations were performed based on the density functional theory (DFT)[5] with the Jaguar 9.1 suite[6] at the B3LYP-D3[7-9] level of theory. The optimization of compounds' structures were carried out with the 6-31G** basis set.[10-12] Following geometry optimization, the electronic energies of the optimized flavonoid structures were recalculated with a high quality triple-ζ basis set cc-pVTZ(-f).[13] Vibrational frequencies for the optimized structures were calculated at the same level of theory as the geometry optimization procedure. Vibrational entropy correction along with the zero point vibrational energies were considered for proper thermodynamic approximations. Based on the optimized gas phase geometries, solvation correction energies were deduced. Self-consistent reaction field (SCRF)[14-16] approximations were considered to calculate the linearized Poisson-Boltzmann equations with the dielectric constant ε. The solvation energy used in the system was treated with ethanol (ε = 24.5). The Gibbs free energies in solution phase were computed as the following equations:

$$G(sol) = G(gas) + G(solv) \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

G(sol) represents the Gibbs free energy with solvation correction G(solv) from the gas phase free energy G(gas); H(gas) is the enthalpy of the molecule in gas phase; T is the temperature (298.15 K); S(gas) is the entropy of the molecule in the gas phase; E(SCF) is the self-consistent field converged electronic energy; ZPE represents the vibrational zero-point energy. To calculate the redox potential, the free energy of the one-electron oxidized form of the flavonoid was deduced by the free energy of its neutral form. Note that the dihedral angle was defined as the angle between two planes: A mean plane calculated from ten carbon coordinates of the A/C rings using the least-squares method and another mean plane consisted of six carbon coordinates of the B ring.

AChE Activity Assay. The activity of AChE was determined by a change in fluorescence of Amplex Red under optimized conditions. *Electrophorus electricus* acetylcholinesterase (*ee*AChE)

was dissolved and diluted to 400 mU/mL in 50 mM Tris-HCl, pH 7.4. The *ee*AChE solution (50 μL) was first added to a 96 well plate. Varying concentrations of compounds (1 μL) in dimethyl sulfoxide (DMSO) were then introduced to the 96 well plate. After shaking, the mixtures of *ee*AChE and compounds were pre-incubated for 15 min. A reaction mixture solution (50 μL) containing 500 μM acetylcholine, 50 μM Amplex Red, 1 U/mL horseradish peroxidase, and 250 mU/mL choline oxidase in 50 mM Tris-HCl, pH 7.4 was added to each well to initiate the catalytic reaction yielding a fluorescence readout ($\lambda_{ex}/\lambda_{em}$ = 540/590 nm). The inhibitory activities of compounds against *ee*AChE was calculated by measuring fluorescence intensities from each well following a 10 min incubation period. The measured values were normalized to that of the compound-untreated control containing 1% v/v DMSO. All experiments were performed in triplicate.

Docking Studies. Ligand docking studies were carried out to obtain plausible ligand bound conformations. With Autodock Vina,[17] the aforementioned DFT optimized structures of quercetin (**Que**), luteolin (**Lut**), orobol (**Oro**), 3,5-dihydroxylflavone (**DHF**), and **HF** were docked to the catalytic active site (CAS) near the S203 of *ee*AChE (PDB 1C2O[18]). The tetrameric structure was simplified to the dimeric form using PyMOL[19] to reduce the computational cost that resulted in a model with 1078 residues in total (Fig. 6b). The docking grid for the ligand binding region was set as 20 x 30 x 20 $Å^3$ in dimension with a 0.375 Å grid spacing. Four ligand-bound structures with the highest binding affinity were chosen for each compound for further MD simulations.

MD Simulation. Both *apo* and ligand-bound dimer models were simulated with the Amber16[20] software package. We considered the docked structures selected from the initial docking studies as the structural models of *holo* state. The Amber FF99SB force field[21] was used for the *ee*AChE dimer and the Generalized Amber Force Field (GAFF)[22] was used to parameterize the covalent bonding parameters of the ligands. Atomic partial charges of the ligands were computed as follows. First, we used the Gaussian09 software[23] to achieve ESP potentials around each molecule at HF/6-31G(d) level of theory. Then atomic partial charges were retrieved based on the Merz-Singh-Kollman algorithm. All simulation systems were immersed in octahedral solvation boxes filled with TIP3P[24] water molecules with a margin of 12 Å from the solvation boundary. Sodium ions (Na^+) were added to achieve electrostatic neutrality of the solvated simulation system which consists of approximately 285,000 atoms in total. The integration time step was 2 fs for all MD simulations. The preliminary procedure was initiated by the energy minimization for 4,000 cycles. Next, the solvated system was equilibrated with the Berendsen thermostat at 300 K using

the NVT ensemble for 5 ns. During these two steps, all carbons in the ligand as well as the C_α of the hydrophobic pocket residues present within 5.0 Å from the docked ligand were restrained with a restraint force constant of 5.0 kcal/mol/Å^2. As the third step, an isobaric ensemble (NPT) was used for 10 ns where the pressure was controlled to maintain 1 atm with a relatively weaker restraint force constant (0.1 kcal/mol/Å^2). At last, a 100 ns equilibrium step was performed without any restraints with the Langevin thermostat and the Monte Carlo barostat to keep the temperature at 300 K and the pressure at 1 atm. In addition, the particle mesh Ewald method[25] was used to treat the long-range electrostatic interactions and the SHAKE algorithm was employed to constrain the hydrogens.

aMD Simulation. aMD simulation is a promising method to add a non-negative boost potential to the system and therefore accelerates the conformational sampling of the protein–ligand complex.[26] From the initial unbiased MD simulations (100 ns) mentioned above, the parameter sets were obtained for the aMD calculations. The detailed parameters used for the simulations are listed: α_D = 0.2, α_P = 0.2, and $E_{PerResidue}$ = 3.5. aMD simulations were then performed for *ca*. 150 ns for each ligand-bound case by boosting both the torsional and non-bonded degrees of freedom of the model systems.

Analysis of the Conformations Sampled from the aMD Simulations. The trajectories were merged with the VMD software[27] and the backbone coordinates of the seven residues in the hydrophobic pocket (*i.e.*, W86, G121, G122, S203, F297, F338, and H447) were aligned. For each aligned trajectory, the coordinates were clustered based on the RMSD metric of the ligand with a cutoff of 1.5 Å. In-house scripts for VMD and CPPTRAJ[28] were used to conduct clustering analysis. For each ligand-bound aMD simulation, the most populated major clusters were presented in the manuscript (Fig. 6c). Detailed analyses of each cluster were conducted as explained in the following sections.

Hydrogen Bond Analysis. To assess the interactions between the ligand and the enzyme, the number of intermolecular hydrogen bonding was determined. Hydrogen bonds that fell within the criteria (D–A lower than the cutoff distance 3.0 Å and A–D–H lower than the cutoff angle 30 ^{o} (D: H-bond donor; A: H-bond acceptor; H: Hydrogen) were counted using the VMD hbonds function.

Solvent Accessible Surface Area (SASA). The SASA values of the chosen hydrophobic residues (Ala, Ile, Leu, Phe, Val, Pro, Gly, Met, and Trp) residing within 6.0 Å from S203 in the AChE dimer

model were calculated. The selected hydrophobic residues are W117, G120, G121, G122, F123, G201, S203, A204, G205, A206, A207, V209, G230, W236, F295, F297, F338, V407, G448, and I451.

Water Molecules in the Binding Pocket. To determine the presence of water molecules within the binding site, we counted the number of water molecules within 8.0 Å from the C_α atom of S203 in both *apo* and *holo* cases for each frame.

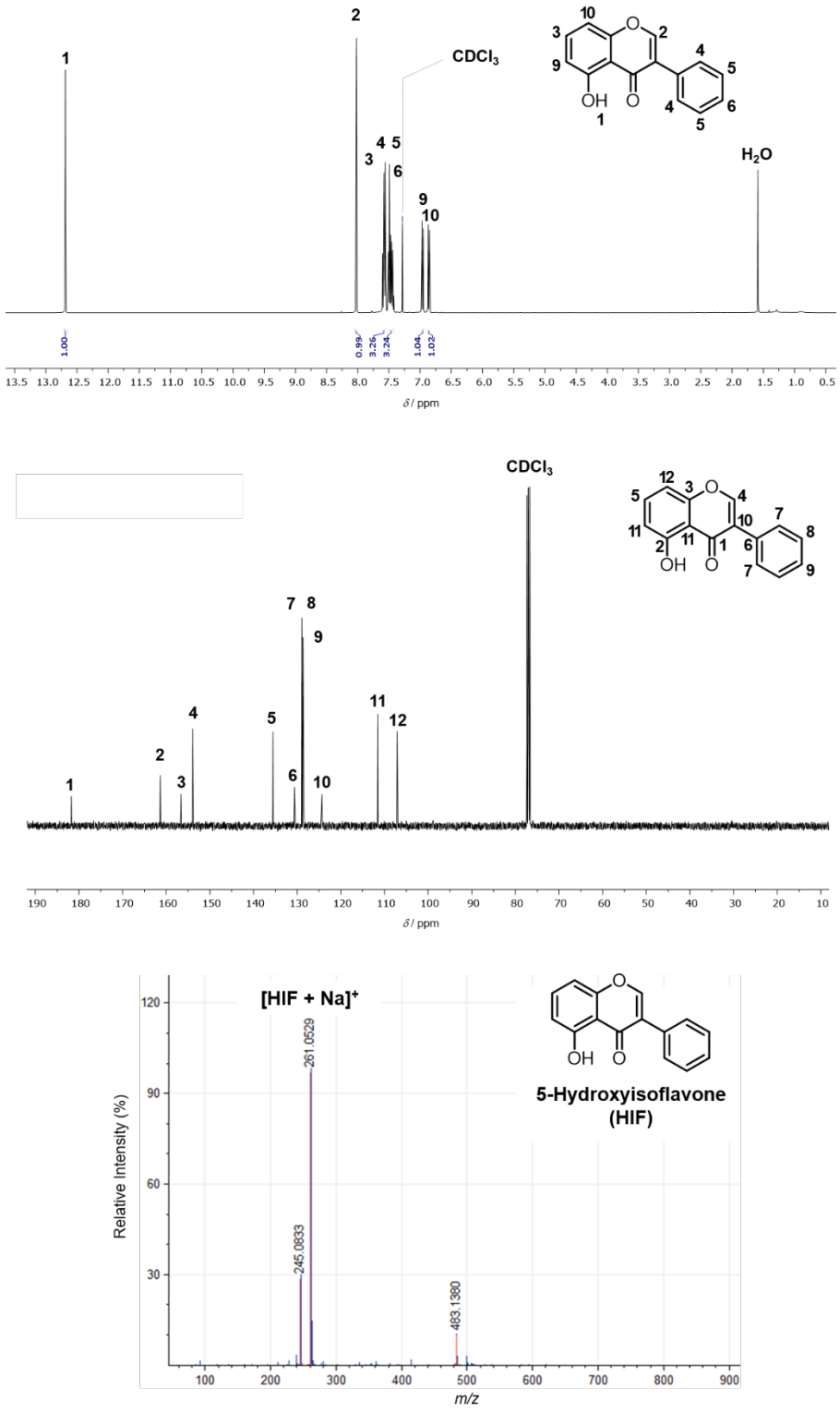


Fig. S1 NMR [^{1}H (400 MHz) and ^{13}C (100 MHz)] spectra and high resolution-mass spectrometric spectrum of **HIF**.

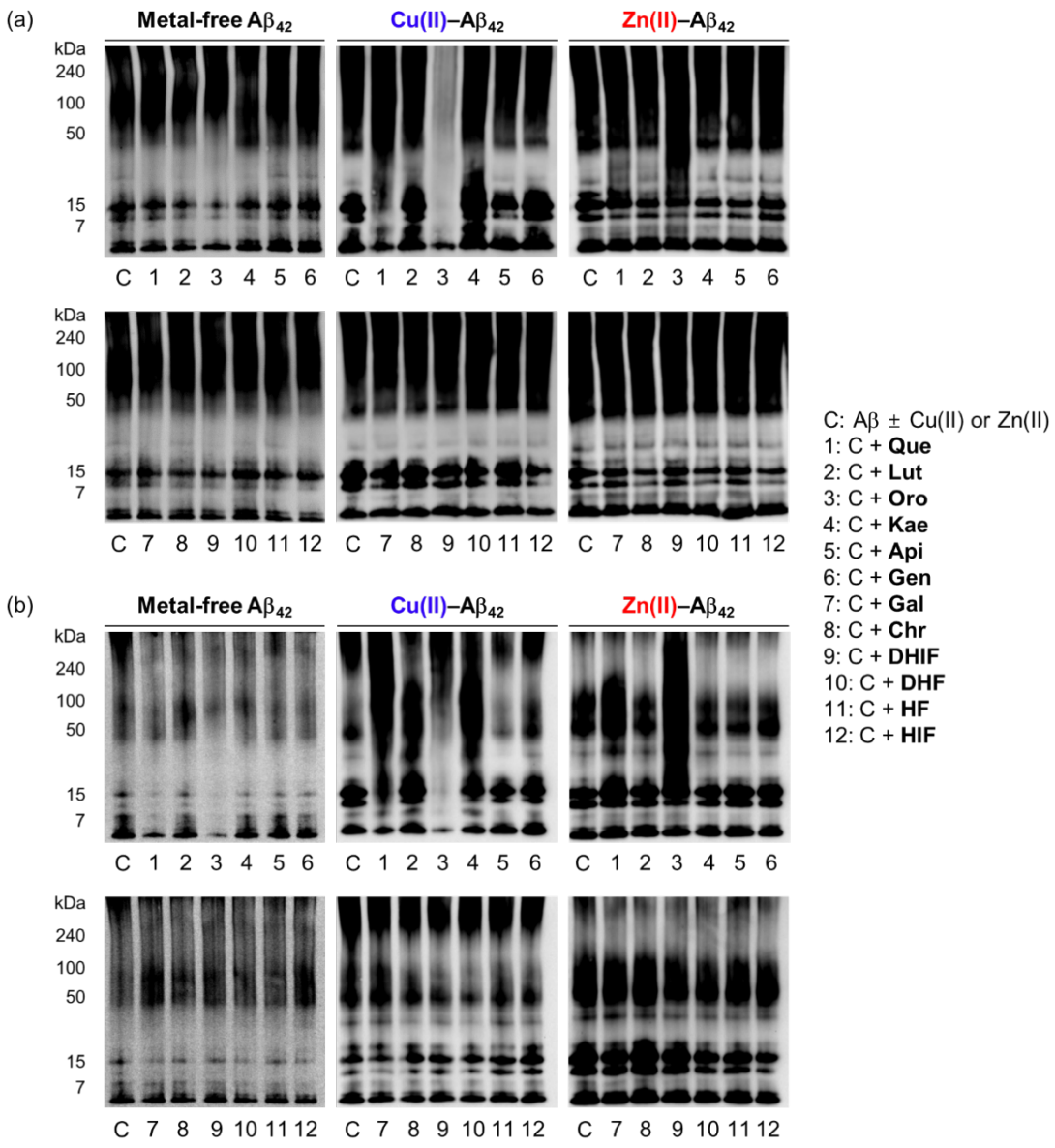


Fig. S2 Original gel/Western blot images of Fig. 3 and 4. Detailed conditions are described in Fig. 3 and 4 and experimental section in Supporting Information.

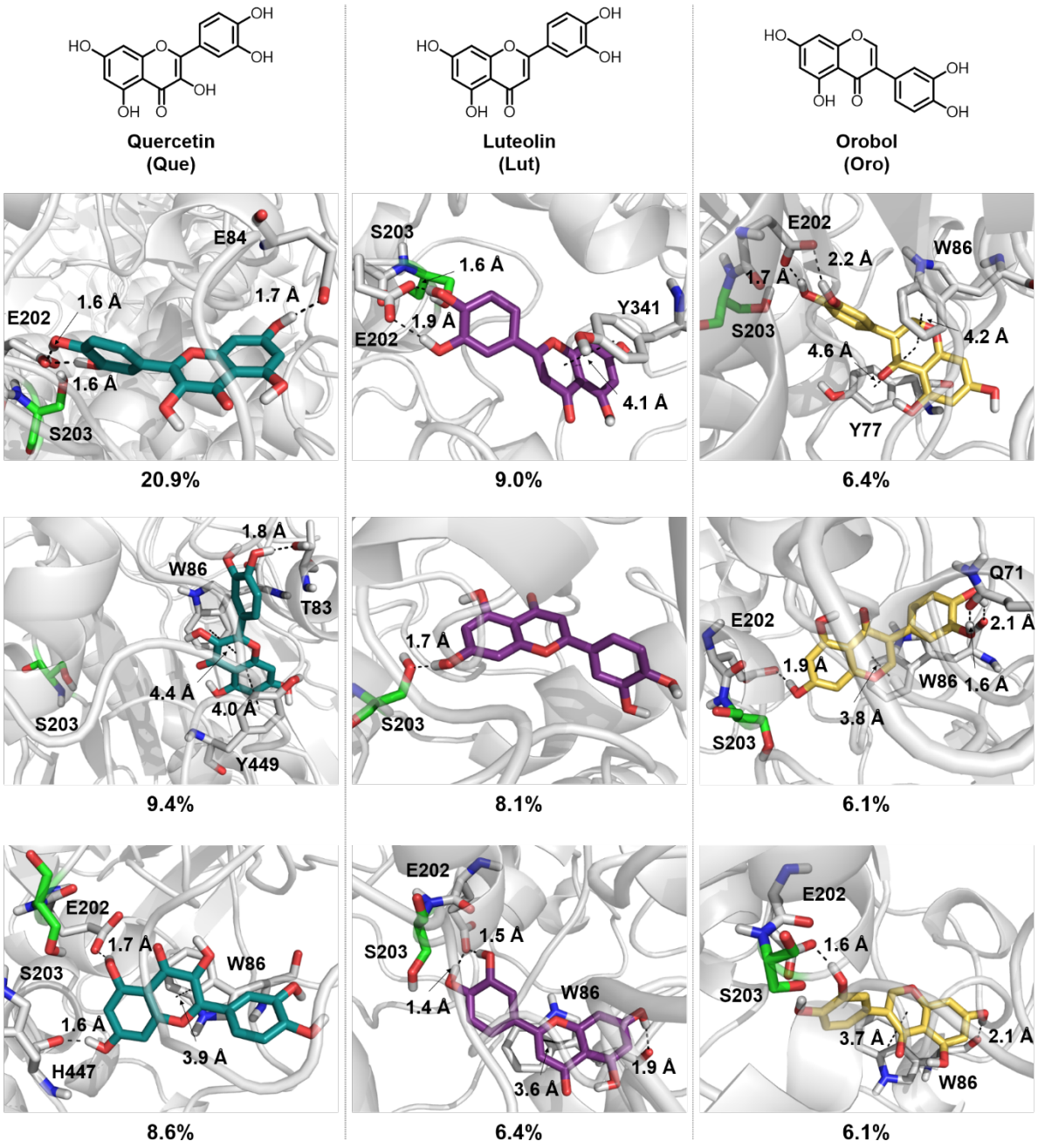
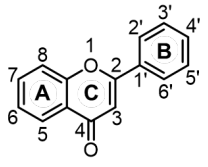
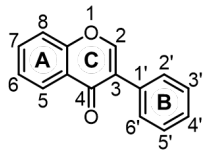
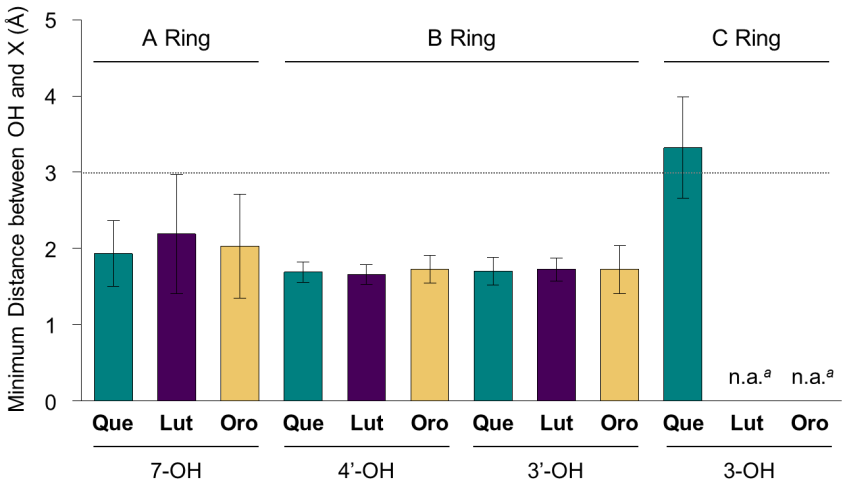


Fig. S3 Alternative binding modes of **Que**, **Lut**, and **Oro** against AChE (PDB 1C2O[18]) modeled through aMD simulations and their % populations (# of snapshots for each cluster / # of snapshots in the total simulation × 100).

(a)







(b)

	Minimum Distance from S203 (Å)	Number of Hydrogen Bonds	Hydrophobic Residue SASA in the Pocket (nm^2)	Number of Water Molecules in the Pocket
Apo	n.a.[a]	n.a.[a]	1.44	22
Que	2.38	2.7	0.88	14
Lut	2.44	2.4	0.54	12
Oro	2.37	2.5	0.49	7
DHF	2.49	0.4	0.97	14
HF	5.11	0.1	1.23	16

Fig. S4 Computational parameters of the interactions between the selected flavonoids and AChE (PDB 1C2O[18]). (a) Closest distance between hydroxyl groups in the flavonoids and the heteroatom (X = O or N) in the binding pocket. [a]n.a., not available. Error bars represent the standard deviation. (b) Calculated mean values for the selected binding determinants: the minimum distance from S203, the number of hydrogen bonds, the SASA of the hydrophobic residues in the binding pocket, and the number of water molecules in the binding pocket.

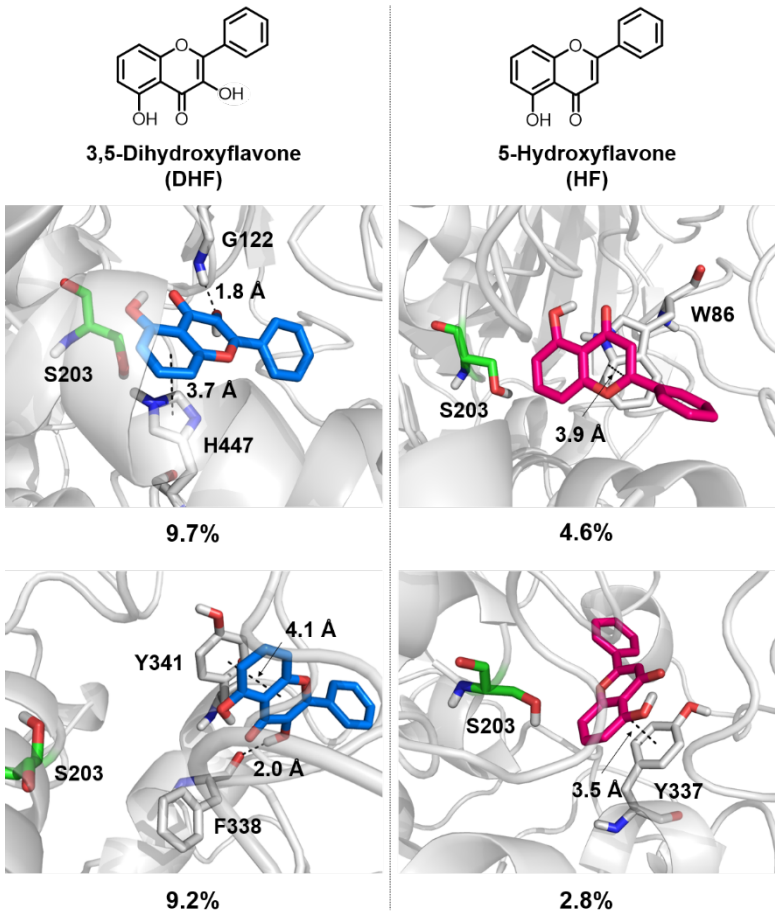


Fig. S5 Possible binding modes of **DHF** and **HF** against AChE (PDB 1C2O[18]) generated by aMD simulations and their % populations (# of snapshots for each cluster / # of snapshots in the total simulation × 100).

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Appendix A. Cartesian coordinates of the optimized flavonoid geometries.

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Que

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C	-2.254538774	0.530205131	-4.686897755
C	-1.680854917	1.790954828	-4.563512325
C	-1.166833043	2.203252077	-3.322434425
C	-1.211934686	1.381177902	-2.193386555
C	-1.788600683	0.123882644	-2.331024408
C	-2.315962791	-0.330022931	-3.554015875
C	-2.896259308	-1.638349891	-3.627007246
C	-2.905093193	-2.420321465	-2.402049541
C	-2.370751619	-1.932146907	-1.237801909
O	-1.827459574	-0.667715430	-1.227896929
H	-1.641524911	2.438399315	-5.434006691
H	-0.809387922	1.715211630	-1.246214390
O	-3.398049831	-2.137880802	-4.671174526
O	-2.745833158	0.134363994	-5.869112015
H	-3.104770422	-0.780116618	-5.741874695
O	-3.461077213	-3.650934458	-2.518159151
H	-3.729363680	-3.699607611	-3.458718777
C	-2.295143366	-2.575842381	0.077635914
C	-2.807268620	-3.871570110	0.298277438
C	-1.689077973	-1.895434976	1.151122212
H	-3.277335405	-4.430938244	-0.496954501
H	-1.287410617	-0.901529312	1.004959226
C	-2.720443010	-4.461398602	1.551814437
C	-1.602302909	-2.490711212	2.406697512
H	-1.135056376	-1.957462192	3.231571198
C	-2.113440514	-3.767950296	2.614451647
O	-0.598420084	3.426749229	-3.159929514
H	-0.618488908	3.905812263	-3.998827934
O	-2.078705311	-4.439184666	3.811397314
H	-1.625390768	-3.906883478	4.476523876
O	-3.223604441	-5.713421345	1.738722324
H	-3.069397688	-5.961608410	2.661855698

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C	-2.248536348	0.521037936	-4.702561855
C	-1.757437825	1.818530917	-4.567617893
C	-1.298017025	2.255563498	-3.320788145
C	-1.316451192	1.415251493	-2.178640366
C	-1.806529045	0.137523994	-2.328052282
C	-2.280069113	-0.350000173	-3.565356016
C	-2.773794413	-1.677236557	-3.660551071
C	-2.753890276	-2.470928907	-2.418100357
C	-2.277145863	-1.938604474	-1.209403396
O	-1.816350341	-0.664057255	-1.213556528
H	-1.741315365	2.465628624	-5.438143730
H	-0.952682495	1.784045219	-1.228584409
O	-3.227887154	-2.235842228	-4.685363770
O	-2.681374311	0.106366538	-5.886576176
H	-2.990471125	-0.827183962	-5.812139034
O	-3.229511976	-3.695516825	-2.541396618
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C	-2.234988928	-2.587186337	0.073199593
C	-2.592519045	-3.945280313	0.247814149
C	-1.815533280	-1.829573512	1.211205602
H	-2.906915426	-4.563943863	-0.578874588
H	-1.545448542	-0.788996458	1.090439916
C	-2.540441036	-4.528657436	1.498651385
C	-1.765381575	-2.406279325	2.461831093
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O	-2.111780643	-4.415874004	3.788815022
H	-1.821280479	-3.861405849	4.527729988
O	-2.879078150	-5.819937706	1.641179204
H	-2.791494608	-6.090469837	2.568110466

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C	-1.727045178	0.122767121	-2.353719711
C	-2.233041048	-0.355279028	-3.573410988
C	-2.805537701	-1.687267303	-3.658487082
C	-2.809497595	-2.435235977	-2.418638945
C	-2.292843342	-1.917642951	-1.270926476
O	-1.762761593	-0.661354899	-1.229923129
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H	-0.788253188	1.734598160	-1.264919996
O	-3.265986919	-2.146670103	-4.729888916
O	-2.631582260	0.079848871	-5.894365311
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C	-2.231517792	-2.582810163	0.040916078
C	-2.617842913	-3.929488420	0.183532134
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H	-1.474726200	-0.846384466	1.076301336
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H	-0.592113674	3.907764196	-4.031761169
O	-2.121711493	-4.537321568	3.724178791
H	-1.817169189	-3.976076841	4.448543549
O	-2.958538055	-5.852990150	1.534941792
H	-2.862853050	-6.114507675	2.462552071

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C	-2.173606157	0.495660186	-4.712446690
C	-1.635497093	1.785458803	-4.613668442
C	-1.145521402	2.222072124	-3.385684490
C	-1.179900646	1.389833450	-2.229984522
C	-1.716895103	0.116549246	-2.348516464
C	-2.220925331	-0.366691291	-3.559222937
C	-2.778295279	-1.701642990	-3.657920122
C	-2.766620874	-2.446491003	-2.412968874
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H	-0.791827679	1.757593274	-1.288468599
O	-3.233738899	-2.162169218	-4.723316669
O	-2.639624357	0.062104944	-5.863293171
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C	-2.544234037	-3.954154730	0.159102738
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H	-3.192911625	-3.440354109	-2.429856300
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O	-2.141917229	-4.529544830	3.697252274
H	-1.883135200	-3.993376493	4.461324692
O	-2.829727173	-5.877182007	1.489089608
H	-2.758247137	-6.176699162	2.409265041

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C	-2.113533735	0.650545776	-4.704410076
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C	-2.141041756	2.534752846	-3.184942722
C	-2.117318630	1.690562725	-2.070248365
C	-2.092568398	0.323105067	-2.300749302
C	-2.089085817	-0.241311342	-3.590424299
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C	-2.033926487	-1.829487443	-1.366049647
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H	-2.115496397	2.091547966	-1.065341830
O	-2.035174847	-2.184372663	-4.930384636
O	-2.113126755	0.180698574	-5.956140518
H	-2.094114304	-0.813664258	-5.875932217
H	-1.978026509	-2.333059311	-0.408379525
C	-2.085086823	-3.967017412	-2.581295729
C	-2.795894146	-4.692503452	-1.612733960
C	-1.369071007	-4.682569981	-3.559296608
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C	-1.356133580	-6.068859577	-3.545658588
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H	-2.177257299	4.353773117	-3.771611452
O	-2.039415121	-8.148983002	-2.544884205
H	-1.504188538	-8.444587708	-3.296477318
O	-0.683234334	-6.845131874	-4.461959362
H	-0.268938690	-6.280433655	-5.125813484

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C	-2.076664925	0.654263616	-4.711667061
C	-2.123145342	2.036349773	-4.489610195
C	-2.163484097	2.535672426	-3.186672688
C	-2.158430576	1.667281985	-2.070067883
C	-2.116092205	0.309783101	-2.316280603
C	-2.072979212	-0.252713352	-3.603834152
C	-2.022682190	-1.680625796	-3.806216002
C	-2.062198162	-2.505548716	-2.569088697
C	-2.086073160	-1.832566738	-1.363405466
O	-2.108989239	-0.516523957	-1.215318561
H	-2.127167940	2.696413517	-5.350573540
H	-2.184921265	2.062273264	-1.062598467
O	-1.965163469	-2.183416128	-4.947607994
O	-2.037546158	0.208958507	-5.959193230
H	-2.005393982	-0.783188105	-5.922692299
H	-2.055795908	-2.323326349	-0.398051113
C	-2.059397697	-3.957376480	-2.588859558
C	-2.554410934	-4.700630665	-1.464107871
C	-1.572226167	-4.675630093	-3.706758738
H	-2.988183022	-4.180664063	-0.618371248
H	-1.218672633	-4.137598991	-4.576375961
C	-2.545902252	-6.074498653	-1.445531130
C	-1.556647778	-6.054417610	-3.693153143
H	-2.931726456	-6.640433311	-0.605328321
C	-2.041441679	-6.779765606	-2.554855824
O	-2.206974745	3.845691442	-2.899838448
H	-2.206128597	4.382161140	-3.705623150
O	-2.030385971	-8.103758812	-2.536482096
H	-1.661880851	-8.449163437	-3.369341135
O	-1.101683021	-6.848774433	-4.684631824
H	-0.807703614	-6.340618610	-5.454487801

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C	-1.791880131	1.844137430	-4.492059708
C	-1.382821679	2.275115967	-3.218768597
C	-1.385849953	1.421025515	-2.112774372
C	-1.810771823	0.112094127	-2.307443857
C	-2.227983475	-0.362670720	-3.564960480
C	-2.657496452	-1.723981619	-3.695867300
C	-2.630665779	-2.536330700	-2.493129015
C	-2.209344149	-2.025753498	-1.293318033
O	-1.808454275	-0.710862875	-1.226142883
H	-1.787174821	2.516438007	-5.344220638
H	-1.065674186	1.770335197	-1.139995813
O	-3.055807352	-2.246507645	-4.773089886
O	-2.607658625	0.119401395	-5.885789871
H	-2.869432926	-0.831562221	-5.799049377
O	-3.052520990	-3.814469814	-2.660783291
H	-3.283223867	-3.859911203	-3.611471891
C	-2.124291897	-2.697547197	0.004103499
C	-2.495037556	-4.048755169	0.176563919
C	-1.649090290	-1.995608807	1.129281402
H	-2.859185219	-4.616897106	-0.667607188
H	-1.353388906	-0.958562315	1.027975440
C	-2.400639534	-4.663357735	1.416711569
C	-1.554150462	-2.608891726	2.371844053
H	-2.683794022	-5.702101707	1.547727823
H	-1.188299894	-2.045908689	3.227792263
C	-1.930217266	-3.948809624	2.524020195
O	-0.962489128	3.548654795	-3.000591040
H	-0.998472154	4.046484947	-3.827932835
O	-1.861429453	-4.606631279	3.714887619
H	-1.523861051	-4.008065701	4.394071102

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C	-2.220370054	0.529465973	-4.687655926
C	-1.793876886	1.845930338	-4.514511585
C	-1.384051800	2.274654150	-3.248142958
C	-1.387941599	1.407445669	-2.124110222
C	-1.812198520	0.111582428	-2.311929226
C	-2.234291792	-0.366962343	-3.569388390
C	-2.663705111	-1.712126017	-3.706193924
C	-2.633278847	-2.532238960	-2.482912064
C	-2.201271534	-2.010907650	-1.245513558
O	-1.810340166	-0.713983655	-1.214131951
H	-1.789866447	2.512567282	-5.370083809
H	-1.064116001	1.769588709	-1.157065511
O	-3.063255787	-2.265670300	-4.756605148
O	-2.609459162	0.117047183	-5.885986805
H	-2.877400160	-0.833167970	-5.836480618
O	-3.038125515	-3.776034594	-2.646491289
H	-3.273502111	-3.848293543	-3.605015993
C	-2.119766235	-2.689038515	0.014053444
C	-2.491853237	-4.057620525	0.176315323
C	-1.647625446	-1.980599046	1.158097625
H	-2.853717804	-4.626427650	-0.667341650
H	-1.359001517	-0.941741109	1.060296297
C	-2.398434639	-4.672821045	1.402034163
C	-1.552729845	-2.594815731	2.384691954
H	-2.678337336	-5.711358547	1.536190748
H	-1.191166162	-2.043002844	3.247740984
C	-1.928096056	-3.951996565	2.521941423
O	-0.961702108	3.520831108	-3.001157999
H	-0.979713500	4.065914154	-3.801637650
O	-1.863273740	-4.612112045	3.676936626
H	-1.532037735	-4.053859234	4.396970272

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C	-2.178973675	0.539583087	-4.680978298
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C	-1.626458526	2.355904341	-3.182835817
C	-1.642724872	1.502848625	-2.073266506
C	-1.930271029	0.163969472	-2.296314240
C	-2.202543974	-0.352447361	-3.573137760
C	-2.489082098	-1.765818119	-3.746860981
C	-2.472337246	-2.550888300	-2.531199694
C	-2.203866482	-1.989088893	-1.319936514
O	-1.941098571	-0.656021476	-1.197488546
H	-1.875411749	2.557004213	-5.333231926
H	-1.437818289	1.879440546	-1.079760313
O	-2.730308533	-2.263032436	-4.872342587
O	-2.431811333	0.090720661	-5.914205551
H	-2.610418320	-0.889326632	-5.817926884
C	-2.153409004	-2.679453850	-0.022192536
C	-2.357465267	-4.070526600	0.080025241
C	-1.896268010	-1.961369514	1.159426093
H	-2.568716526	-4.660063267	-0.806195915
H	-1.731409788	-0.891393065	1.109896541
C	-2.310417175	-4.716741085	1.304836035
C	-1.846781492	-2.601868629	2.392308712
H	-1.646783113	-2.027421236	3.294715881
C	-2.052491903	-3.984405518	2.472529888
H	-2.475186825	-5.786330223	1.383481026
H	-2.671240330	-3.609734535	-2.623152494
O	-1.340649247	3.662601948	-2.937178850
H	-1.356387377	4.155813694	-3.767927408
O	-2.019203901	-4.672585011	3.645231724
H	-1.832448840	-4.064100266	4.373293877

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C	-2.069326878	0.524863601	-4.690642357
C	-1.984106064	1.913244963	-4.504138470
C	-1.912922502	2.414943933	-3.208760262
C	-1.925883889	1.553397417	-2.069774866
C	-2.010997057	0.183966309	-2.275815964
C	-2.082839251	-0.365957648	-3.556493044
C	-2.172375441	-1.798496246	-3.752216578
C	-2.182056427	-2.568202496	-2.527035475
C	-2.108198166	-1.968029380	-1.281285524
O	-2.020055294	-0.617348969	-1.167097926
H	-1.974599600	2.560176373	-5.374414921
H	-1.870387793	1.977168083	-1.074702144
O	-2.239512205	-2.313083649	-4.888516903
O	-2.137416124	0.018655971	-5.898661137
H	-2.193039656	-0.992787063	-5.803551674
C	-2.122553110	-2.662465334	-0.011867839
C	-2.135558605	-4.083017826	0.051229928
C	-2.128849745	-1.934583306	1.205764532
H	-2.114880562	-4.676550388	-0.854812324
H	-2.122767448	-0.851854801	1.182656407
C	-2.155912399	-4.740114689	1.259352803
C	-2.152585983	-2.585292816	2.421236753
H	-2.162797689	-2.016761303	3.346861839
C	-2.167141438	-3.997852325	2.461158752
H	-2.159860373	-5.822464466	1.317649961
H	-2.264265299	-3.642273664	-2.622040749
O	-1.828717828	3.717462063	-2.916636944
H	-1.823214650	4.263409138	-3.717276573
O	-2.190103769	-4.696021080	3.597696066
H	-2.193843842	-4.119057655	4.376607418

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Gen

C	-2.464015484	0.664266050	-4.646642685
C	-2.386328936	2.037229776	-4.418819427
C	-2.012308121	2.518249989	-3.156564713
C	-1.708401442	1.651507854	-2.102060318
C	-1.792889953	0.288807362	-2.346134424
C	-2.164829969	-0.249600664	-3.592695951
C	-2.245043039	-1.684322596	-3.800976515
C	-1.942420006	-2.514262199	-2.625228882
C	-1.563557029	-1.881792903	-1.483686805
O	-1.486653566	-0.545066595	-1.304000616
H	-2.619714022	2.714169264	-5.234763622
H	-1.417505264	2.031914711	-1.131838918
O	-2.554361105	-2.170361757	-4.912897110
O	-2.821333408	0.219237402	-5.856127262
H	-2.809702158	-0.776808321	-5.801014900
H	-1.275108695	-2.406437874	-0.580487847
C	-2.046400309	-3.989614248	-2.656578779
C	-2.557269573	-4.693635464	-1.550791502
C	-1.626384854	-4.732182026	-3.771627903
H	-2.930516005	-4.143607140	-0.691459417
H	-1.252571702	-4.214486599	-4.645941257
C	-2.617583990	-6.082046509	-1.536030769
C	-1.688202500	-6.122537613	-3.768436193
H	-3.013069630	-6.621607780	-0.682172239
H	-1.354124784	-6.680902958	-4.640445232
C	-2.177930593	-6.805129051	-2.649125099
O	-1.924369454	3.848178148	-2.893934250
H	-2.154014111	4.349326611	-3.687534094
O	-2.260658741	-8.166343689	-2.587416887
H	-1.941115260	-8.543133736	-3.417487383

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C	-2.164937973	0.644992411	-4.715845585
C	-2.155559063	2.029656410	-4.488639832
C	-2.088009596	2.523149490	-3.186451197
C	-2.028185368	1.646687746	-2.073835135
C	-2.039764643	0.288148284	-2.325278044
C	-2.103785515	-0.267357111	-3.612596273
C	-2.108364820	-1.693900585	-3.827836275
C	-2.079425573	-2.527012110	-2.595720768
C	-2.006584406	-1.857507229	-1.385805607
O	-1.981783867	-0.542354047	-1.231696367
H	-2.203968763	2.691960096	-5.346572876
H	-1.975962162	2.038963795	-1.066085339
O	-2.156161308	-2.184007645	-4.973871708
O	-2.231401205	0.201522782	-5.959677219
H	-2.235594034	-0.795714855	-5.926424980
H	-1.923262358	-2.356091022	-0.427537173
C	-2.122004509	-3.973477840	-2.618920088
C	-2.586605549	-4.711902618	-1.486667633
C	-1.694774508	-4.714899540	-3.761761665
H	-2.973945856	-4.192683697	-0.617350221
H	-1.346347809	-4.183732033	-4.635876656
C	-2.613284826	-6.083463669	-1.482946992
C	-1.706979513	-6.091579437	-3.761823177
H	-2.985076904	-6.646782875	-0.634545684
H	-1.360827923	-6.640181541	-4.633482456
C	-2.166981697	-6.794835091	-2.625185728
O	-2.074557066	3.829848051	-2.888106585
H	-2.116793394	4.375060081	-3.687162876
O	-2.215458870	-8.123079300	-2.555503845
H	-1.900882363	-8.540473938	-3.372688770

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C	-2.208289146	0.542062581	-4.677214146
C	-1.822389483	1.865434170	-4.495783806
C	-1.435138583	2.309725285	-3.219908476
C	-1.423577547	1.458087921	-2.111921787
C	-1.812095284	0.138523042	-2.307392597
C	-2.206234694	-0.350074321	-3.567047834
C	-2.595561504	-1.721636534	-3.698497057
C	-2.555853605	-2.532784700	-2.491460562
C	-2.163871765	-2.005612850	-1.289336801
O	-1.796853662	-0.681810915	-1.225136995
H	-1.827944636	2.536198616	-5.349183559
H	-1.121354103	1.817466259	-1.137045145
O	-2.970888615	-2.257170439	-4.776712418
O	-2.579017878	0.115678377	-5.892504215
H	-2.814752102	-0.842367589	-5.804675102
O	-2.943198681	-3.819484711	-2.661896467
H	-3.162929296	-3.874472618	-3.614833355
C	-2.082921505	-2.666490316	0.019146552
C	-2.313004971	-4.048236370	0.173172027
C	-1.759016752	-1.907067657	1.162536144
H	-2.556606770	-4.652994156	-0.688148081
H	-1.576394796	-0.844363928	1.064549685
C	-2.223892212	-4.639296055	1.430759311
C	-1.674080253	-2.508351088	2.413742065
H	-2.402781487	-5.705987930	1.529472113
H	-1.425777912	-1.904161215	3.281561136
C	-1.906190872	-3.877643347	2.555903673
H	-1.839397430	-4.345659733	3.533803701
O	-1.052075744	3.594153881	-3.001060009
H	-1.097648025	4.090680599	-3.828819513

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C	-2.102857351	0.528221846	-4.704397678
C	-2.042141676	1.906785965	-4.486433506
C	-1.984917879	2.393679380	-3.178666592
C	-1.986783862	1.522066712	-2.054176807
C	-2.047423124	0.166012838	-2.289487600
C	-2.105680704	-0.372433424	-3.589254379
C	-2.168783188	-1.779350638	-3.767227173
C	-2.167015553	-2.590857983	-2.536186457
C	-2.106170893	-2.002235889	-1.253241658
O	-2.047460318	-0.656013548	-1.191673398
H	-2.041133881	2.572357655	-5.342839718
H	-1.942057371	1.928392172	-1.051801085
O	-2.228119612	-2.393445253	-4.855978489
O	-2.157102585	0.067157596	-5.943816185
H	-2.196364641	-0.919308722	-5.929669380
O	-2.233545065	-3.888912201	-2.738744736
H	-2.265540361	-3.996951818	-3.723703146
C	-2.103232622	-2.660439014	0.028830191
C	-2.103533983	-4.076313496	0.149374053
C	-2.097249031	-1.869365931	1.210369706
H	-2.102403641	-4.702836990	-0.730061650
H	-2.100087643	-0.789388478	1.134617448
C	-2.098866701	-4.664904594	1.404165030
C	-2.095105648	-2.472960234	2.454584360
H	-2.096747160	-5.746410370	1.487828255
H	-2.093898773	-1.861797690	3.350815058
C	-2.095641375	-3.872324467	2.558073759
H	-2.093455315	-4.341806412	3.536917210
O	-1.925203800	3.695486307	-2.880828619
H	-1.926478744	4.245547771	-3.678446293

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C	-2.194408178	0.546688974	-4.679461479
C	-1.945961356	1.904474854	-4.479604244
C	-1.696944952	2.383572340	-3.186267614
C	-1.687655687	1.533860326	-2.074254751
C	-1.937089324	0.187038690	-2.293017864
C	-2.194650173	-0.342389196	-3.568506718
C	-2.452256203	-1.761249781	-3.736833572
C	-2.433574438	-2.538251877	-2.513228893
C	-2.160616636	-1.965214968	-1.310842872
O	-1.918085217	-0.629416108	-1.191791058
H	-1.950077653	2.569665670	-5.337544918
H	-1.490753531	1.917777419	-1.081992984
O	-2.683577776	-2.269854069	-4.858004093
O	-2.432190657	0.088395081	-5.912855625
H	-2.581060886	-0.895654500	-5.821920872
C	-2.106857061	-2.653558016	-0.008182595
C	-2.015303135	-4.053947926	0.066138729
C	-2.146379709	-1.912776589	1.185835123
H	-1.954815984	-4.644946575	-0.840839326
H	-2.208757639	-0.832184970	1.141033530
C	-1.984700084	-4.695330143	1.300496936
C	-2.112638950	-2.559415102	2.418828487
H	-2.149223566	-1.973334551	3.332227468
C	-2.034858227	-3.951478958	2.482017994
H	-1.913995981	-5.778027058	1.340375543
H	-2.010072231	-4.454262733	3.444291115
H	-2.654368162	-3.594352961	-2.587765455
O	-1.450718284	3.698320866	-2.944753647
H	-1.480291009	4.188900948	-3.776667356

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C	-2.088867903	0.537009895	-4.688344002
C	-2.059590578	1.936011553	-4.506514549
C	-2.029988050	2.440476894	-3.214294195
C	-2.029489517	1.572589517	-2.072799206
C	-2.058186769	0.189122260	-2.275722980
C	-2.086154938	-0.354452670	-3.550178289
C	-2.120449781	-1.790661097	-3.751064062
C	-2.120751381	-2.562110662	-2.535015583
C	-2.089860201	-1.963194966	-1.288719773
O	-2.055066586	-0.605011225	-1.175049067
H	-2.061082840	2.579167366	-5.379514217
H	-2.007418394	1.997543693	-1.076066256
O	-2.150436401	-2.281162977	-4.903470993
O	-2.118607044	0.014660744	-5.879664898
H	-2.137730837	-1.019381762	-5.755851746
C	-2.093415260	-2.648307323	-0.004822709
C	-2.011418343	-4.059198856	0.061115388
C	-2.185765982	-1.909674525	1.196259141
H	-1.921608567	-4.654372215	-0.839826584
H	-2.253813982	-0.829253078	1.163496971
C	-2.022579193	-4.704178810	1.289167643
C	-2.199643373	-2.564331532	2.419569016
H	-2.274940252	-1.989901423	3.336898565
C	-2.118554354	-3.961450815	2.471279383
H	-1.954430223	-5.786128044	1.328998923
H	-2.128445387	-4.469493389	3.430545330
H	-2.163991213	-3.638566256	-2.628045321
O	-2.000975609	3.739420414	-2.908965826
H	-2.002430916	4.299263000	-3.700512171

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C	-2.486022472	0.611625493	-4.647647858
C	-2.383364677	1.990508795	-4.470166683
C	-1.964023590	2.508266211	-3.237417459
C	-1.639446616	1.674207568	-2.162143946
C	-1.749708533	0.305928171	-2.355366230
C	-2.166316748	-0.268664598	-3.571350098
C	-2.271311045	-1.707879901	-3.728175879
C	-1.938181281	-2.499244690	-2.533716679
C	-1.524027586	-1.836164355	-1.423707366
O	-1.422537088	-0.496301562	-1.293223381
H	-2.632731915	2.642676592	-5.301420212
H	-1.313219190	2.084618330	-1.215694666
O	-2.625165224	-2.226883173	-4.811190605
O	-2.885038376	0.128739759	-5.828553677
H	-2.880504131	-0.866125345	-5.739427090
H	-1.219290972	-2.336608887	-0.511886299
C	-2.043555021	-3.977632284	-2.515727520
C	-2.538547277	-4.636358738	-1.378083348
C	-1.630861998	-4.748613834	-3.615508556
H	-2.900209904	-4.051540375	-0.536673903
H	-1.269322157	-4.251971722	-4.507284164
C	-2.596880674	-6.028336525	-1.328164697
C	-1.695531011	-6.139389992	-3.563910723
H	-2.984720707	-6.520000935	-0.440487444
H	-1.370331645	-6.722422123	-4.420761108
C	-2.173613071	-6.784597874	-2.421359539
H	-2.224273205	-7.869095802	-2.387086630
O	-1.849442482	3.844579458	-3.023293972
H	-2.095303297	4.322217941	-3.826502562

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C	-2.547933102	0.620444715	-4.629520416
C	-2.425575495	2.012323856	-4.458026886
C	-1.946996570	2.523186445	-3.255294323
C	-1.578453422	1.656851292	-2.188656092
C	-1.712332129	0.288369834	-2.382693291
C	-2.183336258	-0.278650820	-3.570380688
C	-2.306765795	-1.709497690	-3.739288807
C	-1.931265950	-2.520687819	-2.553470850
C	-1.467128754	-1.838229179	-1.442837358
O	-1.353358507	-0.517723858	-1.338844419
H	-2.712756157	2.658198833	-5.280877590
H	-1.206034660	2.061760187	-1.255697370
O	-2.720930576	-2.203532696	-4.805657864
O	-3.000237226	0.155608714	-5.773635387
H	-3.021226883	-0.846358955	-5.711759567
H	-1.116065264	-2.328309298	-0.542935014
C	-2.024926662	-3.972378016	-2.523811340
C	-2.210775137	-4.655641079	-1.288693786
C	-1.914998531	-4.743776321	-3.714498758
H	-2.354625940	-4.094806671	-0.371109992
H	-1.780131817	-4.244450092	-4.662849426
C	-2.273952961	-6.035430431	-1.246582389
C	-1.965356827	-6.127193451	-3.658207417
H	-2.436116695	-6.543001175	-0.301566213
H	-1.863153815	-6.705936909	-4.570187092
C	-2.144846678	-6.780579090	-2.431452274
H	-2.190736532	-7.864656448	-2.395435095
O	-1.794941306	3.827535629	-3.001793623
H	-2.057535887	4.373744488	-3.757513523

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C	-2.089842319	0.535476446	-4.658763885
C	-1.753421545	1.872745037	-4.451969147
C	-1.439732075	2.317890406	-3.163414717
C	-1.449795961	1.468241572	-2.059029579
C	-1.787064195	0.132030845	-2.269243956
C	-2.107360125	-0.355948716	-3.548877478
C	-2.449024200	-1.744371176	-3.698913574
C	-2.435396671	-2.558575392	-2.495672941
C	-2.113778830	-2.025088072	-1.273858666
O	-1.795248747	-0.692753375	-1.188792467
H	-1.742163062	2.545604706	-5.301691532
H	-1.179581046	3.362461329	-3.018802643
H	-1.206758261	1.812093973	-1.060756087
O	-2.758341074	-2.288270712	-4.792481899
O	-2.391255379	0.101281047	-5.891316891
H	-2.598694086	-0.862654030	-5.820753098
O	-2.770364761	-3.856586933	-2.687541962
H	-2.945119858	-3.913016319	-3.650173664
C	-2.064939976	-2.694529772	0.030665994
C	-2.272249460	-4.081780434	0.164271370
C	-1.797104239	-1.939532161	1.190858364
H	-2.474303246	-4.683166981	-0.710355818
H	-1.634311318	-0.871953428	1.109157801
C	-2.215641499	-4.683099747	1.418986201
C	-1.743743777	-2.550670624	2.438934088
H	-2.376615047	-5.754098415	1.501139760
H	-1.538206458	-1.949253798	3.319803953
C	-1.952784300	-3.925920725	2.561251163
H	-1.910411239	-4.401716709	3.536602497

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$DHF^{\bullet+}$

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C	-2.089985132	0.532412946	-4.667171955
C	-1.616960526	1.848641872	-4.478180885
C	-1.190263987	2.248507500	-3.220812559
C	-1.211071491	1.381008267	-2.110363483
C	-1.677726150	0.089953899	-2.302313328
C	-2.121450424	-0.362287402	-3.555562019
C	-2.594146013	-1.701848865	-3.693494081
C	-2.577159166	-2.528277874	-2.473966360
C	-2.115730524	-2.020912886	-1.237241268
O	-1.690680861	-0.742692590	-1.216057181
H	-1.598860383	2.519824266	-5.328899384
H	-0.827377200	3.261578560	-3.081835032
H	-0.875344515	1.698906422	-1.130357981
O	-3.019559145	-2.225445747	-4.745000839
O	-2.494231462	0.148924068	-5.864523411
H	-2.789862156	-0.794958651	-5.829111099
O	-3.025892496	-3.755995512	-2.626137733
H	-3.278873682	-3.837656260	-3.577663422
C	-2.044735193	-2.696234941	0.035139609
C	-2.377513885	-4.069317341	0.181801870
C	-1.622918725	-1.965301275	1.179037690
H	-2.696153164	-4.651957989	-0.669672072
H	-1.367468238	-0.917473674	1.084161162
C	-2.288745403	-4.674777508	1.426084638
C	-1.542111278	-2.584208250	2.413419247
H	-2.541973829	-5.724351883	1.529870033
H	-1.222654700	-2.017656326	3.281673908
C	-1.874078870	-3.940814734	2.543185711
H	-1.808790565	-4.422393799	3.513952732

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HF

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C	-2.123996735	0.540588796	-4.655328274
C	-1.846872211	1.895860076	-4.448645592
C	-1.591368318	2.363613129	-3.159204721
C	-1.601010561	1.517621517	-2.049190521
C	-1.876073837	0.170910820	-2.263974190
C	-2.138841629	-0.345817327	-3.543253183
C	-2.422288179	-1.766927958	-3.712751865
C	-2.423585176	-2.543323040	-2.490363121
C	-2.142847538	-1.975513697	-1.287431479
O	-1.874799609	-0.647884190	-1.162606120
H	-1.837121725	2.560291290	-5.305180550
H	-1.402125120	1.874827743	-1.045763373
O	-2.656192780	-2.270438194	-4.833591461
O	-2.373551130	0.091069624	-5.891016483
H	-2.550851822	-0.885518909	-5.804675579
C	-2.107292891	-2.670835733	0.008680208
C	-1.978640676	-4.066954136	0.070733570
C	-2.201604366	-1.941047668	1.204479694
H	-1.875118017	-4.643164158	-0.842569351
H	-2.291635275	-0.861682475	1.164163709
C	-1.965411305	-4.718697071	1.300670862
C	-2.186687469	-2.597572565	2.432447195
H	-2.267638445	-2.021583319	3.349218845
C	-2.070986032	-3.987414598	2.485696316
H	-1.377691388	3.418635130	-3.014068842
H	-1.864629030	-5.798970699	1.334204316
H	-2.059558630	-4.498008251	3.444068193
H	-2.664232969	-3.595799208	-2.562616825

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$HF^{\bullet+}$

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C	-2.055895329	0.528817892	-4.645491600
C	-2.199377060	1.939850807	-4.442294598
C	-2.331151009	2.424005985	-3.151779652
C	-2.327734709	1.560856700	-2.039396524
C	-2.185368538	0.169579849	-2.250655413
C	-2.049608231	-0.357720852	-3.521039248
C	-1.908793926	-1.790251493	-3.728336811
C	-1.925935626	-2.574218273	-2.522466421
C	-2.060160637	-1.988237739	-1.278914332
O	-2.182534933	-0.631406665	-1.163616300
H	-2.200835943	2.590837240	-5.309284687
H	-2.431197166	1.937821150	-1.027811646
O	-1.791247845	-2.257349968	-4.885368824
O	-1.930535316	0.038205002	-5.840235233
H	-1.843429446	-0.999530137	-5.723605633
C	-2.100303888	-2.678094387	0.002847633
C	-1.813916326	-4.059020519	0.085647643
C	-2.435367823	-1.972308278	1.178835273
H	-1.531570911	-4.622243881	-0.796329975
H	-2.662250042	-0.914384723	1.130852938
C	-1.864639401	-4.709699631	1.310668468
C	-2.487406015	-2.633469582	2.398440838
H	-2.751586437	-2.085783005	3.297001362
C	-2.203066111	-4.001952171	2.468499660
H	-2.440347433	3.490403414	-2.986746788
H	-1.637298822	-5.768913269	1.366425037
H	-2.243959427	-4.515269756	3.424079657
H	-1.849370241	-3.648555279	-2.618787527

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HIF

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C	-1.755083799	0.617453456	-4.632616043
C	-1.866749763	1.997639298	-4.439548492
C	-2.214849234	2.502075195	-3.186106682
C	-2.460138321	1.664592385	-2.098105669
C	-2.348593712	0.292796016	-2.298779964
C	-2.000809431	-0.266006708	-3.541439533
C	-1.895693660	-1.711190224	-3.708957195
C	-2.202653408	-2.511113644	-2.516777039
C	-2.507617712	-1.854102373	-1.366773725
O	-2.589198828	-0.517435074	-1.218075037
H	-1.676036239	2.653066158	-5.281636715
H	-2.729339600	2.044377565	-1.119785070
O	-1.568310976	-2.222078085	-4.800990105
O	-1.420470476	0.147185206	-5.840506554
H	-1.395033717	-0.843081355	-5.761187077
H	-2.296410084	3.576917648	-3.053275108
H	-2.709797382	-2.359841824	-0.429779500
C	-2.200939655	-3.990321875	-2.546877384
C	-3.192830563	-4.714031219	-1.863728404
C	-1.204968691	-4.699604511	-3.237258911
H	-3.996043205	-4.181461334	-1.362008810
H	-0.447801143	-4.153450966	-3.785898447
C	-3.176436186	-6.107345104	-1.847375512
C	-1.195237994	-6.092600822	-3.224064589
H	-3.954516888	-6.648889542	-1.317038894
H	-0.417003393	-6.626651287	-3.761730671
C	-2.175164700	-6.802294254	-2.527194977
H	-2.163996220	-7.888398170	-2.522332907

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$HIF^{\bullet+}$

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C	-1.659466386	0.616252303	-4.600123882
C	-1.787657738	2.019221067	-4.407521248
C	-2.223035574	2.515063047	-3.188259602
C	-2.546252489	1.655354738	-2.125263691
C	-2.419316053	0.277285308	-2.329852819
C	-1.983898044	-0.277406633	-3.535586596
C	-1.857624412	-1.713962436	-3.712685823
C	-2.250722170	-2.534347534	-2.542591333
C	-2.656180382	-1.859492421	-1.406419516
O	-2.740225077	-0.536317587	-1.285352349
H	-1.538524508	2.671830654	-5.236709595
H	-2.887398005	2.026147842	-1.165529728
O	-1.462888598	-2.194575071	-4.790326118
O	-1.241957784	0.168984741	-5.762925148
H	-1.214450836	-0.833936155	-5.715831757
H	-2.317682266	3.586453676	-3.048689842
H	-2.918368578	-2.350678444	-0.477326661
C	-2.228171587	-3.988714933	-2.555309534
C	-3.110036850	-4.725584030	-1.717113018
C	-1.320766807	-4.703794003	-3.384234190
H	-3.852074623	-4.209153652	-1.116776943
H	-0.643124163	-4.161971092	-4.028954983
C	-3.077550173	-6.107345581	-1.700921416
C	-1.287405014	-6.088671684	-3.349573612
H	-3.769086838	-6.658440113	-1.072476029
H	-0.579440713	-6.624325275	-3.973075390
C	-2.161054134	-6.797670364	-2.513398647
H	-2.134701014	-7.882728577	-2.496158600

Appendix B. Vibrational frequencies of the optimized flavonoid structures.

Que

11.98 38.60 80.65 89.22 112.19 145.02
200.70 213.10 220.54 230.17 247.06 255.78
284.24 297.93 310.35 340.82 346.69 370.26
371.08 403.38 403.53 407.07 453.65 461.11
490.31 525.46 545.44 571.72 596.04 597.83
603.30 619.34 644.17 645.41 664.81 685.29
695.24 707.50 722.48 733.83 804.53 806.79
809.38 818.13 824.16 854.52 900.32 927.90
949.13 1019.89 1034.31 1115.54 1133.77 1159.05
1184.26 1187.15 1207.40 1227.91 1237.10 1275.62
1285.77 1302.46 1330.03 1359.45 1364.36 1377.66
1387.99 1426.84 1447.26 1479.40 1511.69 1529.70
1552.02 1561.39 1621.81 1646.35 1656.28 1670.38
1679.32 1708.21 3171.29 3199.76 3242.70 3245.65
3273.17 3341.13 3600.77 3793.22 3822.03 3842.30

Lut

7.40 42.26 84.60 103.34 114.34 173.52
208.69 215.71 231.56 247.45 253.81 261.28
288.84 311.00 342.64 352.54 360.25 372.98
407.31 417.13 451.25 489.00 495.17 517.11
566.28 572.65 595.86 603.08 623.27 641.34
643.03 667.75 690.40 696.24 711.87 747.19
752.99 805.22 811.72 813.60 820.14 851.98
870.77 884.93 901.43 935.10 960.23 1019.17
1054.16 1125.38 1133.84 1143.57 1180.44 1186.64
1212.29 1230.96 1240.55 1270.18 1298.23 1310.99
1338.33 1348.37 1361.08 1387.63 1411.62 1435.55
1474.59 1508.68 1516.48 1553.91 1562.24 1629.23
1642.71 1656.96 1672.02 1679.26 1718.59 3158.07
3171.38 3198.28 3221.19 3236.81 3244.39 3253.50
3791.16 3821.95 3834.96

$Que^{\bullet+}$

21.58 38.58 79.50 88.92 107.19 137.08
194.44 215.79 220.05 236.96 252.05 278.26
300.10 319.03 330.26 342.59 355.38 397.53
398.91 401.11 432.92 457.86 459.08 463.63
483.91 517.56 542.19 565.41 592.82 594.77
606.40 638.19 643.83 655.64 690.52 694.53
711.59 719.85 736.16 756.40 777.53 806.07
817.39 831.11 846.36 851.55 900.46 947.26
959.69 1003.16 1028.03 1103.39 1134.64 1154.93
1184.52 1191.81 1218.75 1231.30 1256.14 1265.71
1301.53 1302.57 1350.14 1365.60 1385.82 1402.75
1410.00 1427.29 1456.02 1476.79 1519.76 1530.67
1540.59 1548.86 1566.12 1601.50 1608.94 1661.59
1667.30 1699.27 3198.25 3216.41 3251.86 3252.48
3283.49 3428.82 3458.12 3782.34 3801.52 3803.92

$Lut^{\bullet+}$

13.96 43.30 82.34 105.22 110.91 163.72
199.77 215.85 226.51 243.99 257.43 281.08
318.64 325.08 341.10 355.31 399.79 402.34
450.78 465.25 468.81 476.63 487.38 509.44
553.80 564.95 591.96 594.47 597.56 629.94
635.07 638.38 683.14 688.98 712.43 731.27
736.63 805.51 819.14 826.78 843.49 864.38
867.15 884.88 947.99 954.08 958.66 1009.44
1049.04 1114.98 1131.03 1146.12 1183.28 1187.40
1219.75 1227.90 1254.19 1256.65 1297.70 1314.55
1329.63 1359.11 1372.85 1400.53 1418.28 1434.26
1467.66 1509.88 1513.76 1527.01 1543.66 1557.87
1596.89 1610.11 1620.10 1658.18 1709.62 2998.33
3199.42 3220.65 3237.26 3248.17 3248.73 3260.30
3772.05 3796.18 3801.37

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Oro

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32.41 45.80 65.86 110.29 130.84 181.11
206.84 210.59 221.91 236.03 243.54 283.03
308.24 311.43 349.63 375.03 377.21 409.90
417.68 427.61 448.84 462.79 484.26 503.22
522.41 580.96 593.24 601.05 621.46 629.43
638.89 649.86 669.67 695.32 709.61 785.59
797.66 804.04 815.52 824.19 832.23 857.00
860.93 884.59 919.98 941.57 958.55 1014.19
1077.29 1086.13 1140.49 1174.40 1186.52 1201.83
1210.86 1232.46 1251.31 1271.82 1308.53 1329.03
1350.05 1360.32 1367.29 1401.21 1419.86 1441.89
1469.56 1483.42 1507.84 1554.62 1578.02 1626.56
1645.46 1653.82 1673.11 1674.87 1711.39 3190.58
3198.64 3200.19 3214.86 3217.70 3235.78 3247.02
3783.89 3821.41 3843.00

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$Oro^{\bullet+}$

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31.76 38.84 74.76 109.38 122.70 176.97
202.67 223.85 229.08 242.55 273.07 298.75
317.27 349.16 360.86 366.08 396.67 417.93
442.21 451.52 455.41 466.83 499.94 516.41
570.50 582.15 588.30 601.36 621.34 625.58
633.44 641.54 664.14 685.89 713.88 776.75
789.44 804.45 829.05 832.60 847.62 851.23
858.04 887.17 929.16 949.46 972.62 1010.40
1060.07 1074.99 1151.51 1176.08 1182.55 1205.59
1212.02 1247.74 1269.41 1289.67 1310.80 1349.55
1370.29 1375.63 1396.19 1409.90 1423.22 1438.44
1460.63 1504.64 1516.77 1546.04 1556.41 1566.85
1583.65 1606.70 1650.97 1668.60 1693.19 3215.59
3220.88 3235.67 3243.21 3244.35 3250.57 3284.13
3720.63 3805.82 3809.06

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Kae

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12.48 38.96 79.51 94.87 110.89 145.07
222.41 237.60 239.98 247.56 282.61 304.31
322.67 343.51 359.13 371.16 371.92 404.10
405.27 419.00 440.46 463.86 507.40 526.39
572.68 585.04 591.18 611.44 631.87 645.48
647.87 653.18 684.07 693.04 723.72 730.69
733.19 808.16 816.80 817.42 822.69 838.26
853.10 897.64 955.10 979.95 998.81 1029.80
1035.96 1114.96 1147.68 1162.40 1186.02 1200.76
1213.06 1221.21 1244.41 1277.07 1300.16 1323.29
1346.72 1359.87 1377.87 1388.42 1424.18 1445.91
1473.59 1490.34 1529.74 1551.82 1560.84 1620.86
1632.61 1656.56 1671.99 1680.93 1708.03 3168.87
3201.11 3214.04 3231.17 3245.24 3263.75 3349.26
3598.93 3820.20 3822.30

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$Kae^{\bullet+}$

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28.82 39.48 75.89 96.54 104.39 136.00
216.79 237.15 237.82 240.80 274.04 298.79
306.42 345.61 356.30 391.66 400.32 404.91
443.30 463.92 465.66 500.41 504.36 519.45
568.44 587.30 598.09 615.26 636.95 641.33
649.95 683.88 697.09 719.39 726.46 739.95
755.86 791.23 814.80 832.17 841.50 847.73
861.52 886.79 982.44 983.33 995.60 1014.84
1027.97 1102.00 1153.66 1161.71 1185.64 1195.81
1219.57 1232.13 1258.72 1273.46 1303.25 1352.83
1366.25 1383.66 1403.20 1409.46 1427.31 1459.14
1479.95 1508.57 1528.45 1540.39 1551.36 1577.31
1581.83 1606.68 1663.52 1666.85 1699.53 3196.34
3218.61 3231.60 3243.85 3251.39 3277.65 3393.94
3454.34 3786.14 3798.71

Api	Gen
13.79 42.99 90.08 102.10 112.93 174.78	33.11 57.69 67.82 112.29 136.29 190.43
224.71 237.29 248.51 256.52 284.19 336.00	216.05 228.99 240.50 279.63 290.94 341.41
348.41 354.89 373.40 382.06 416.24 416.75	352.34 373.50 375.92 404.71 415.77 426.27
445.91 500.34 515.71 517.56 570.75 583.47	436.24 471.36 497.00 520.85 542.20 574.87
617.85 639.97 641.66 653.87 662.20 670.95	600.71 624.09 629.68 648.45 650.91 660.25
695.13 733.72 750.65 751.93 811.35 818.65	694.45 730.04 788.79 798.25 815.31 819.40
820.44 842.12 848.41 851.94 903.91 919.54	824.20 840.57 848.13 884.17 896.80 918.33
962.29 966.34 999.03 1029.38 1052.95 1128.24	951.56 964.71 1010.04 1031.06 1071.96 1085.20
1138.80 1153.69 1180.71 1201.06 1212.56 1218.15	1145.54 1175.00 1197.78 1203.50 1216.88 1232.38
1267.42 1281.17 1303.97 1328.60 1338.46 1358.28	1266.19 1294.88 1315.33 1334.89 1349.46 1364.94
1385.88 1406.35 1435.37 1474.41 1487.38 1510.41	1381.40 1405.75 1437.75 1465.66 1482.17 1507.70
1554.74 1561.33 1624.07 1637.72 1651.63 1667.65	1551.92 1564.48 1625.94 1638.35 1649.11 1673.55
1679.38 1719.07 3149.52 3166.79 3198.47 3199.52	1675.33 1710.85 3167.17 3184.34 3199.51 3204.03
3216.65 3227.56 3244.28 3251.21 3809.65 3821.80	3215.09 3233.36 3238.35 3246.75 3821.97 3822.93

$Api^{\bullet+}$	$Gen^{\bullet+}$
17.27 43.63 90.38 104.52 108.81 168.91	32.47 51.65 73.41 110.26 131.11 186.86
217.51 237.73 246.35 249.36 273.09 317.38	216.75 232.59 245.06 264.77 279.77 351.68
328.24 360.92 396.84 403.50 444.32 474.50	365.56 381.56 395.31 417.24 441.01 448.34
492.55 494.76 506.79 508.31 568.24 580.61	457.46 494.53 514.03 516.67 540.41 567.05
588.37 619.83 632.11 633.13 641.11 656.63	599.98 615.45 625.11 635.62 637.41 652.65
691.09 724.84 736.44 739.87 812.29 827.01	681.49 731.40 778.21 796.13 809.81 833.03
844.04 845.67 857.04 859.73 904.31 978.32	839.22 854.00 858.76 872.15 885.43 925.91
981.23 989.91 994.70 1015.33 1046.93 1115.27	984.07 987.53 1004.93 1011.46 1060.19 1077.17
1136.66 1158.69 1184.03 1196.06 1220.07 1227.43	1155.47 1182.63 1193.52 1206.49 1228.38 1247.73
1256.59 1283.85 1299.45 1325.34 1354.43 1374.04	1273.58 1309.06 1341.51 1351.29 1373.30 1386.34
1400.42 1417.77 1435.94 1473.46 1500.64 1514.62	1397.37 1403.02 1437.02 1462.89 1504.59 1513.19
1518.81 1545.82 1562.66 1585.10 1600.23 1617.52	1539.31 1548.94 1560.43 1569.07 1599.50 1650.98
1664.46 1707.82 2838.83 3196.10 3222.68 3222.85	1672.57 1694.39 3195.38 3205.36 3213.70 3216.38
3236.82 3239.81 3247.03 3261.88 3787.17 3793.44	3233.53 3243.51 3249.64 3269.21 3778.93 3803.56

Gal

19.65 46.71 79.93 108.62 127.08 172.81
227.19 252.95 257.86 260.93 285.02 314.75
352.80 374.85 380.52 398.02 408.87 411.95
460.15 470.51 527.06 585.73 589.64 612.73
621.81 632.95 634.60 646.35 649.15 685.83
703.01 716.87 723.80 735.66 786.01 809.68
818.50 824.03 859.39 892.54 939.67 984.66
999.16 1007.37 1014.39 1031.81 1065.53 1109.10
1132.92 1155.43 1186.18 1200.91 1213.54 1229.48
1246.00 1278.00 1300.62 1344.88 1355.45 1375.70
1379.16 1425.37 1447.68 1477.33 1494.91 1530.94
1540.04 1553.01 1622.66 1629.90 1656.77 1660.96
1679.47 1709.02 3180.52 3191.99 3201.04 3205.26
3234.83 3245.53 3266.96 3344.67 3597.06 3821.26

Chr

26.61 51.53 97.13 105.81 139.43 201.37
232.81 256.61 258.29 271.50 294.77 352.15
369.45 376.45 410.59 427.77 469.65 506.30
518.52 569.87 618.89 622.31 632.50 641.14
642.44 664.37 675.15 702.20 720.55 748.74
755.65 788.49 813.20 821.71 851.21 864.13
894.49 919.68 940.90 981.17 1000.60 1007.51
1015.50 1050.28 1064.50 1120.30 1128.19 1139.90
1180.85 1200.61 1212.93 1226.78 1265.34 1278.15
1304.61 1339.71 1358.75 1371.77 1405.17 1435.13
1472.53 1492.43 1510.84 1539.20 1556.95 1624.93
1637.17 1654.08 1661.72 1677.35 1719.15 3176.98
3184.47 3195.29 3199.26 3206.27 3216.98 3231.08
3245.43 3250.18 3822.21

$Gal^{\bullet+}$

21.32 46.47 77.39 110.11 123.95 158.39
218.37 243.00 254.63 262.26 277.15 314.52
347.79 366.45 384.41 396.05 400.23 449.28
469.51 472.44 519.87 582.97 596.73 613.64
617.57 620.14 639.87 644.26 671.74 686.26
716.99 719.76 729.25 771.79 785.65 794.69
834.65 844.13 852.70 887.98 968.02 980.50
1001.36 1008.31 1026.43 1029.33 1052.76 1103.01
1137.64 1154.34 1185.74 1208.89 1219.97 1241.23
1254.79 1279.72 1302.92 1358.71 1364.56 1390.53
1406.98 1424.03 1456.66 1475.11 1491.81 1523.07
1528.01 1539.47 1581.18 1594.68 1603.29 1643.72
1658.43 1698.31 3205.85 3217.35 3219.88 3224.77
3242.93 3250.36 3278.01 3407.18 3437.94 3795.81

$Chr^{\bullet+}$

13.45 53.08 103.04 105.96 137.94 189.05
227.73 249.34 258.89 259.25 276.55 332.64
379.59 396.34 405.99 451.98 479.35 501.97
508.56 565.84 578.33 611.12 618.81 625.62
630.15 636.53 668.21 683.61 712.77 724.60
740.52 792.89 823.30 839.72 850.28 867.27
904.96 955.58 988.23 993.70 1010.82 1026.64
1041.41 1058.34 1091.36 1114.97 1130.04 1146.38
1181.61 1208.46 1222.36 1233.92 1261.09 1275.25
1295.58 1308.35 1356.93 1384.74 1410.46 1436.50
1464.02 1490.13 1512.27 1523.35 1540.68 1557.42
1582.75 1608.45 1625.08 1649.19 1711.60 2458.64
3203.70 3213.02 3220.12 3225.97 3228.96 3237.09
3242.59 3262.71 3789.21

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DHIF

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37.85 60.69 85.91 114.36 154.87 212.04
232.60 244.09 253.57 285.11 337.48 363.78
378.84 399.33 420.81 421.69 451.91 504.67
520.73 539.32 584.33 600.84 629.67 631.00
639.05 649.51 687.65 695.11 713.51 766.43
797.88 806.44 815.81 824.70 859.93 890.41
893.96 919.45 938.15 977.53 1000.88 1010.10
1016.39 1052.51 1078.21 1085.48 1119.27 1175.05
1198.08 1203.37 1225.55 1233.42 1266.21 1293.84
1334.86 1346.90 1365.54 1370.27 1406.62 1437.84
1468.80 1489.90 1507.84 1540.63 1555.53 1625.50
1635.84 1649.27 1661.69 1676.06 1712.25 3174.80
3183.44 3185.26 3193.70 3199.80 3205.26 3231.91
3235.96 3247.02 3821.82

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$DHIF^{\bullet+}$

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38.15 56.61 93.58 114.09 152.76 201.59
224.58 247.10 257.68 272.18 336.83 353.08
380.89 397.60 419.08 443.43 457.25 498.76
507.50 525.22 572.20 602.83 607.36 621.18
625.93 630.91 669.91 683.81 684.21 766.19
796.98 803.21 832.15 837.57 857.16 862.81
924.87 929.35 960.33 997.66 1002.21 1006.38
1022.50 1041.44 1065.11 1086.83 1130.94 1182.25
1202.63 1204.67 1235.48 1239.98 1268.29 1306.01
1330.64 1340.40 1371.82 1387.70 1402.25 1431.60
1463.30 1480.87 1503.27 1519.06 1542.47 1563.74
1568.62 1586.50 1632.77 1657.99 1694.04 3089.23
3200.58 3207.68 3218.47 3219.92 3225.76 3247.75
3248.53 3271.76 3798.81

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DHF

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16.69 47.30 97.76 118.67 131.59 187.25
242.76 261.07 276.63 281.32 327.54 381.90
386.34 411.52 433.78 457.79 460.95 502.83
514.68 565.63 594.99 619.19 631.82 640.98
641.53 673.62 697.79 700.47 703.21 744.95
785.93 789.71 805.92 806.68 860.17 879.40
896.14 940.89 983.23 985.57 996.17 1008.03
1014.62 1065.01 1087.68 1099.57 1124.16 1161.54
1196.54 1200.73 1228.67 1246.27 1277.23 1285.65
1342.86 1355.94 1362.86 1377.03 1388.11 1436.94
1473.61 1495.14 1522.98 1529.99 1540.90 1619.77
1629.55 1649.53 1660.96 1677.19 1698.74 3181.26
3191.83 3193.34 3205.99 3223.96 3229.45 3232.19
3265.18 3381.19 3589.59

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$DHF^{\bullet+}$

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14.87 47.45 92.69 119.08 132.43 176.26
233.62 247.72 274.49 279.20 323.81 361.73
372.94 394.37 425.50 447.89 458.58 488.54
507.08 554.10 606.28 617.48 625.72 626.34
669.55 673.77 690.55 695.73 733.87 746.12
794.55 803.59 804.85 815.94 844.38 889.63
910.03 967.80 979.00 1001.18 1008.72 1009.37
1029.69 1053.30 1079.97 1098.47 1136.51 1146.43
1201.30 1209.85 1238.05 1247.39 1272.71 1274.17
1357.47 1360.20 1381.56 1391.57 1403.24 1434.08
1470.91 1489.37 1512.92 1520.35 1526.78 1563.49
1595.84 1602.21 1634.91 1649.39 1694.89 3205.75
3217.29 3217.35 3224.87 3236.38 3239.95 3242.18
3277.63 3375.91 3484.96

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HF

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25.06 51.33 102.41 133.08 142.66 210.09

247.65 260.18 279.23 302.27 370.17 411.21

458.80 468.93 486.23 491.03 509.35 569.08

623.59 626.26 633.06 660.61 666.76 684.62

703.79 722.51 760.30 787.12 795.16 822.19

854.51 864.33 876.65 881.47 917.98 942.80

982.22 982.35 1007.63 1016.00 1023.45 1062.99

1084.30 1108.84 1122.69 1139.70 1195.68 1200.25

1226.40 1262.54 1283.88 1290.50 1336.38 1359.34

1367.33 1373.79 1425.94 1449.66 1492.58 1510.75

1529.69 1542.27 1628.47 1635.62 1656.26 1662.67

1669.50 1716.35 3185.59 3192.11 3196.21 3205.23

3214.85 3222.23 3226.16 3227.78 3231.84 3245.30

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$HF^{\bullet+}$

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17.62 53.50 108.61 140.68 145.85 201.24

217.63 237.45 271.13 273.62 354.69 398.24

450.63 458.09 461.44 481.98 507.55 549.96

597.00 607.10 624.36 637.76 659.38 669.70

686.98 710.09 715.73 791.88 801.98 819.56

842.17 870.01 900.88 909.18 954.39 992.60

1003.66 1011.49 1017.53 1026.64 1058.02 1078.58

1095.26 1111.76 1117.78 1130.20 1195.67 1208.38

1232.00 1232.89 1262.56 1282.65 1308.70 1357.99

1383.23 1394.90 1419.94 1431.61 1487.46 1491.13

1521.11 1538.97 1556.76 1584.66 1613.29 1619.30

1647.76 1707.43 2368.48 3203.31 3211.90 3218.81

3222.48 3227.42 3233.85 3236.28 3240.39 3262.32

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HIF

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44.99 60.92 88.90 131.82 161.34 233.40

246.14 252.02 277.39 345.55 398.34 419.90

438.38 453.31 489.28 501.29 520.64 541.63

563.58 604.40 633.40 637.61 672.75 706.85

713.47 738.07 768.40 788.39 809.56 825.96

857.85 859.53 882.51 889.66 922.16 939.23

977.42 984.72 1001.31 1016.48 1037.36 1062.43

1075.08 1099.97 1119.61 1193.52 1198.29 1216.69

1226.85 1254.24 1284.57 1329.27 1338.13 1360.04

1370.13 1389.97 1427.07 1442.15 1490.66 1508.37

1525.53 1543.82 1624.80 1634.43 1650.83 1661.28

1669.15 1707.81 3175.65 3183.92 3193.84 3194.17

3205.86 3223.29 3229.77 3232.26 3235.97 3272.37

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$HIF^{\bullet+}$

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45.04 59.08 96.93 140.70 159.10 222.04

232.36 255.48 276.79 332.40 380.36 397.57

440.05 446.54 479.10 493.81 514.69 521.44

555.21 591.71 609.14 631.34 663.35 676.40

682.35 730.46 766.56 795.30 816.03 817.63

839.33 869.24 912.33 925.83 934.06 960.66

997.78 1005.83 1006.90 1022.06 1031.56 1053.31

1073.74 1096.99 1131.09 1194.90 1202.22 1218.58

1224.13 1246.01 1288.30 1327.50 1343.38 1370.46

1382.74 1388.30 1425.43 1435.38 1480.80 1501.53

1508.66 1523.19 1560.67 1567.89 1594.62 1620.71

1655.39 1695.41 3089.04 3199.56 3208.17 3218.97

3221.67 3226.46 3234.84 3239.65 3248.86 3264.65