# The Ability of Chlorophyll to Trap Carcinogen Aflatoxin $B_1$, a Theoretical Approach.

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**Table S1.** Natural atomic charges ($e^-$) for **chl a 1**, **chl a 2**, $AFB_1$ and their complexes.
**Table S2.** Interaction energy, in kcal/mol, of complexes **chl a 1**-$AFB_1$, and **chl a 2**-$AFB_1$ in the gas phase.
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**Table S4.** Cartesian coordinates for the more stable optimized geometries.

**$AFB_1$** = aflatoxin $B_1$
**chl a 2 =** folded chlorophyll a.
**chl a 1**-α-E-$AFB_1$ = **$AFB_1$** coordinated to unfolded chlorophyll a.
**chl a 2**-β-E-$AFB_1$ = **$AFB_1$** coordinated to folded chlorophyll a.
**chl a 1**-D-$2AFB_1$ = **$2AFB_1$** coordinate to unfolded chlorophyll a.
**chl a 2**-E-$2AFB_1$ = **$2AFB_1$** coordinate to folded chlorophyll a.
**chl a 2**-$AFB_1$c = an intermolecular hydrogen bond between **$AFB_1$** and chlorophyll a.

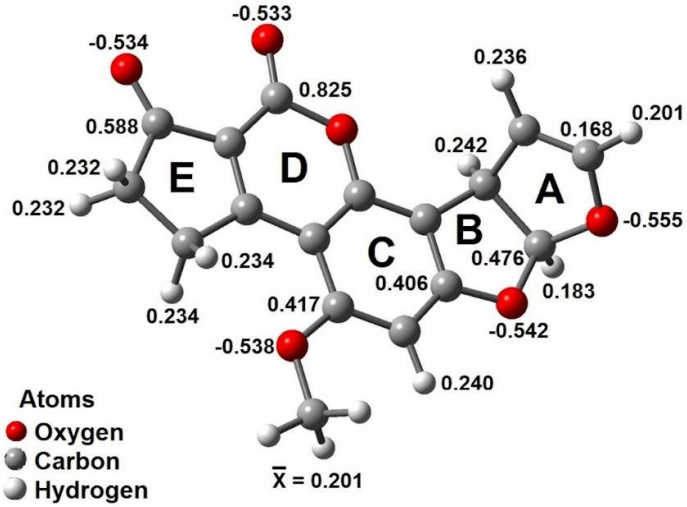


**Figure S1.** M06-2X/6-311G(d,p) optimized geometries of $AFB_1$. Atomic charges of selected atoms are in electron units.

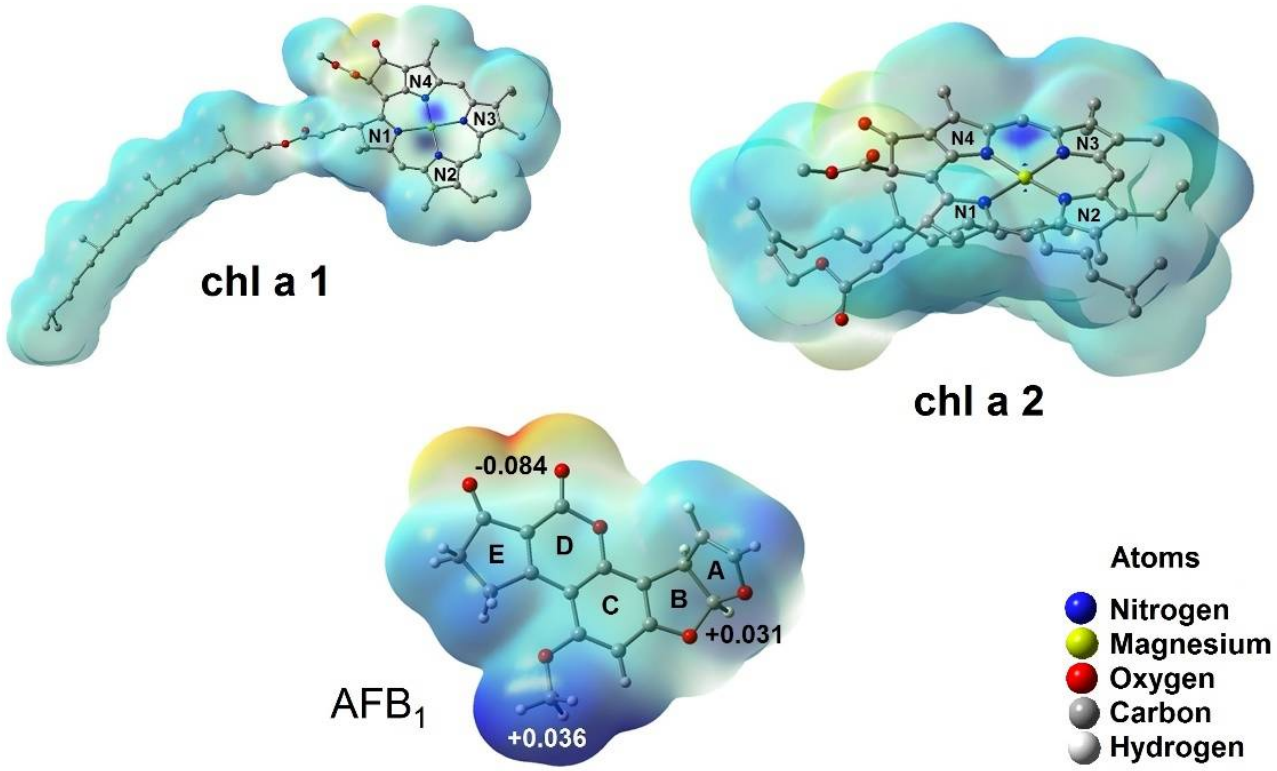


**Figure S2.** Reactive sites attained in the electrostatic potential map. The total electron density isosurface mapped with the molecular electrostatic potential of $AFB_1$, **chl a 1**, and **chl a 2**. The density = 0.0004 and isovalue = 0.02, at a level of calculation M06-2X/6-311G(d,p). The color scheme for the MEP is as follows: blue for electron-deficient, partially positive charge; light blue for the slightly electron-deficient region; yellow for a slightly electron-rich region and red for electron-rich, partial negative charge [1].

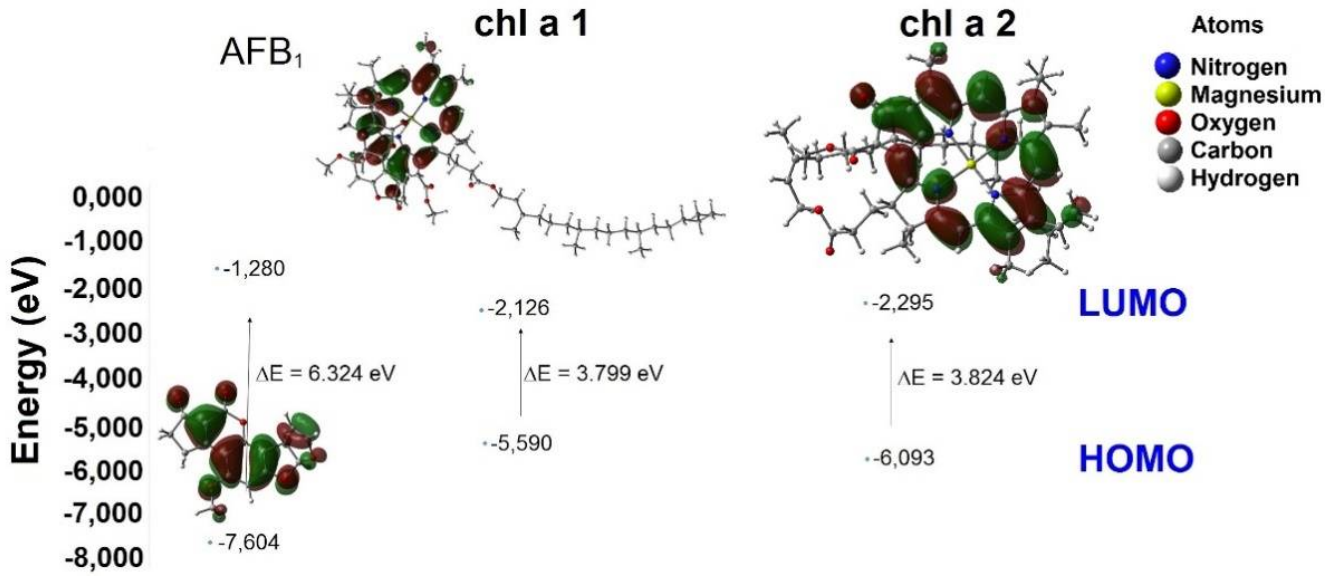


**Figure S3.** HOMO (eV), LUMO (eV) and the inter-frontier molecular orbital energy gaps of the target molecules.

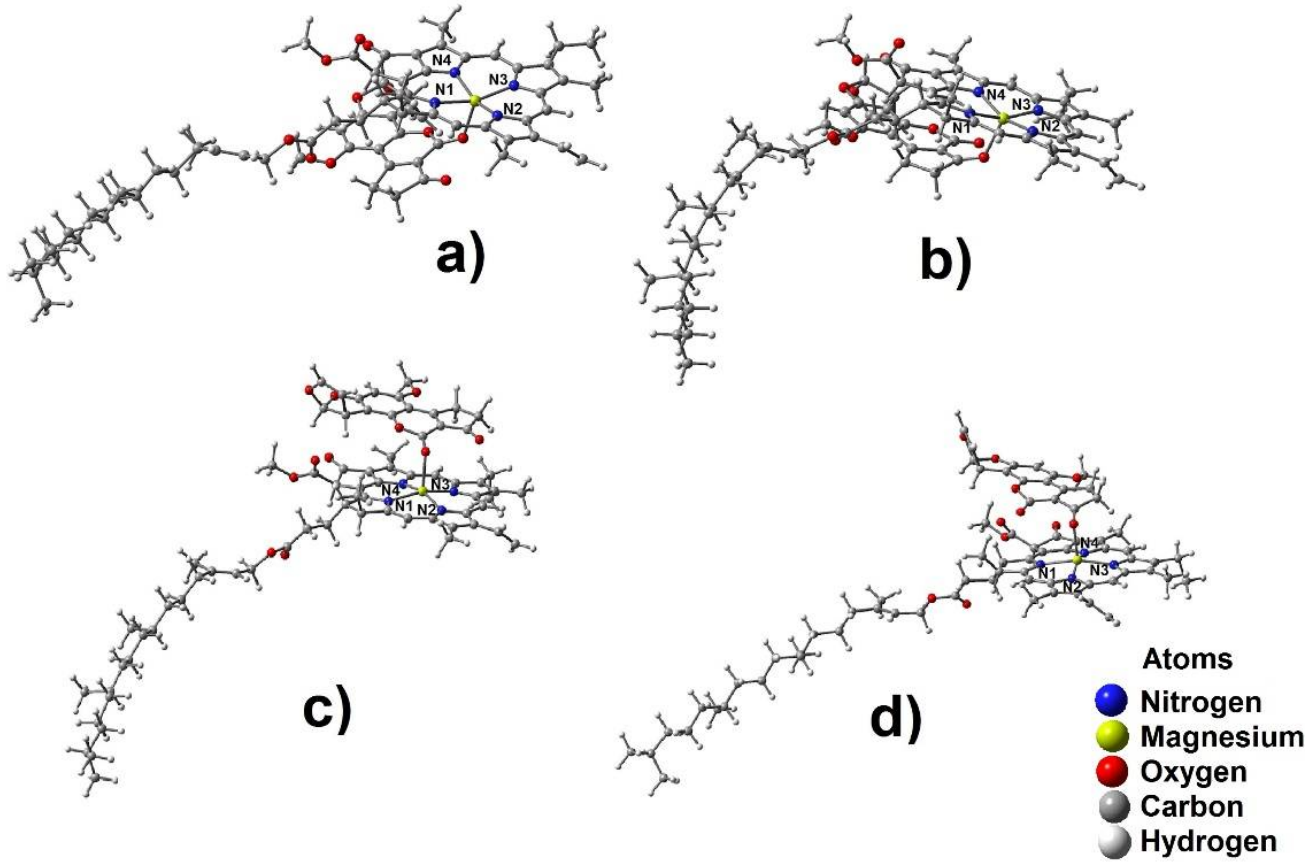


**Figure S4.** Optimized geometry: a) **chl a 1**-α-D-AFB$_1$, b) **chl a 1**-α-E-AFB$_1$, c) **chl a 1**-β-D-AFB$_1$, and d) **chl a 1**-β-E-AFB$_1$.

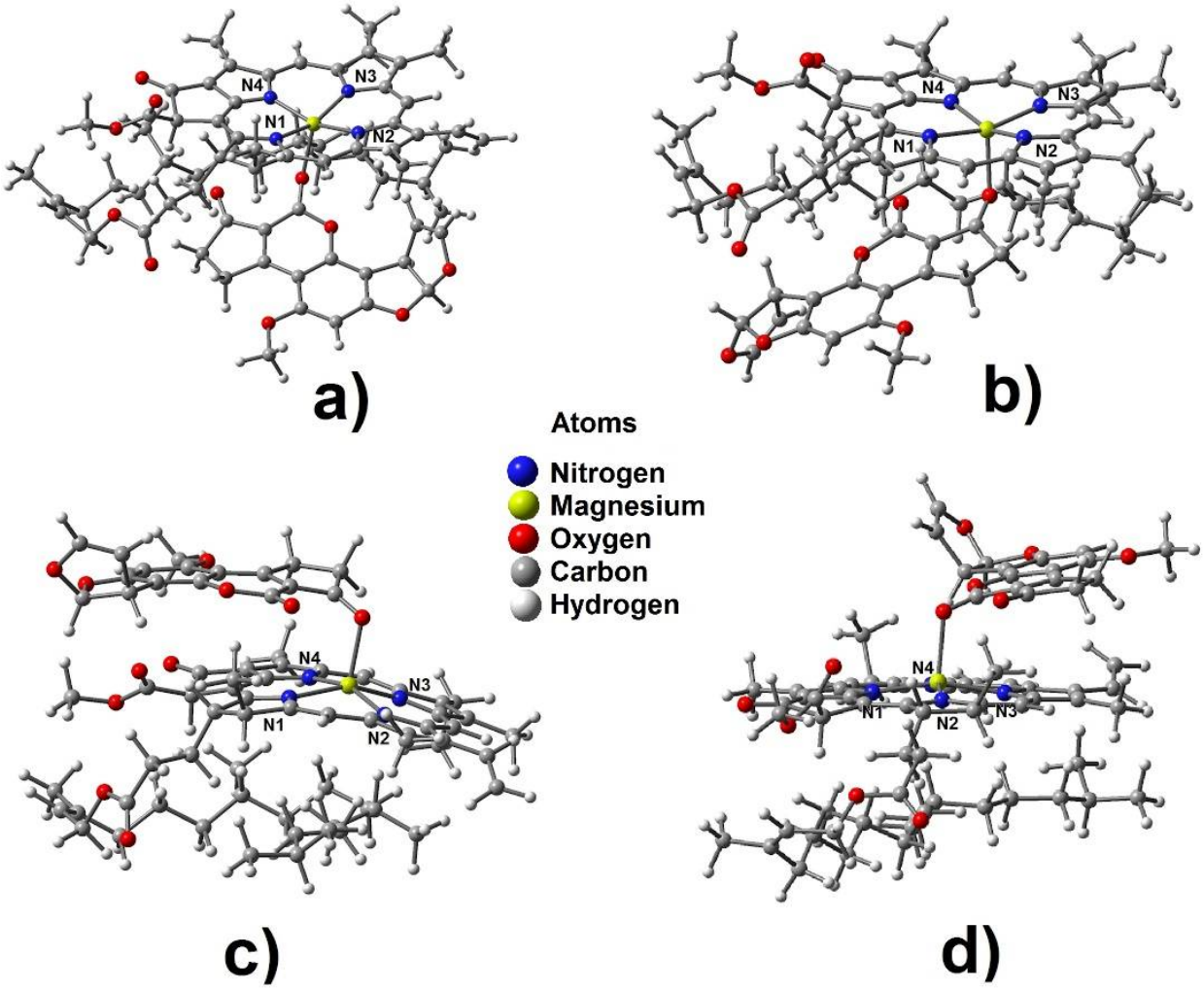


**Figure S5.** Optimized geometry: a) **chl a 2**-α-D-AFB$_1$, b) **chl a 2**-α-E-AFB$_1$, c) **chl a 2**-β-E-AFB$_1$, and d) **chl a 2**-β-D-AFB$_1$.

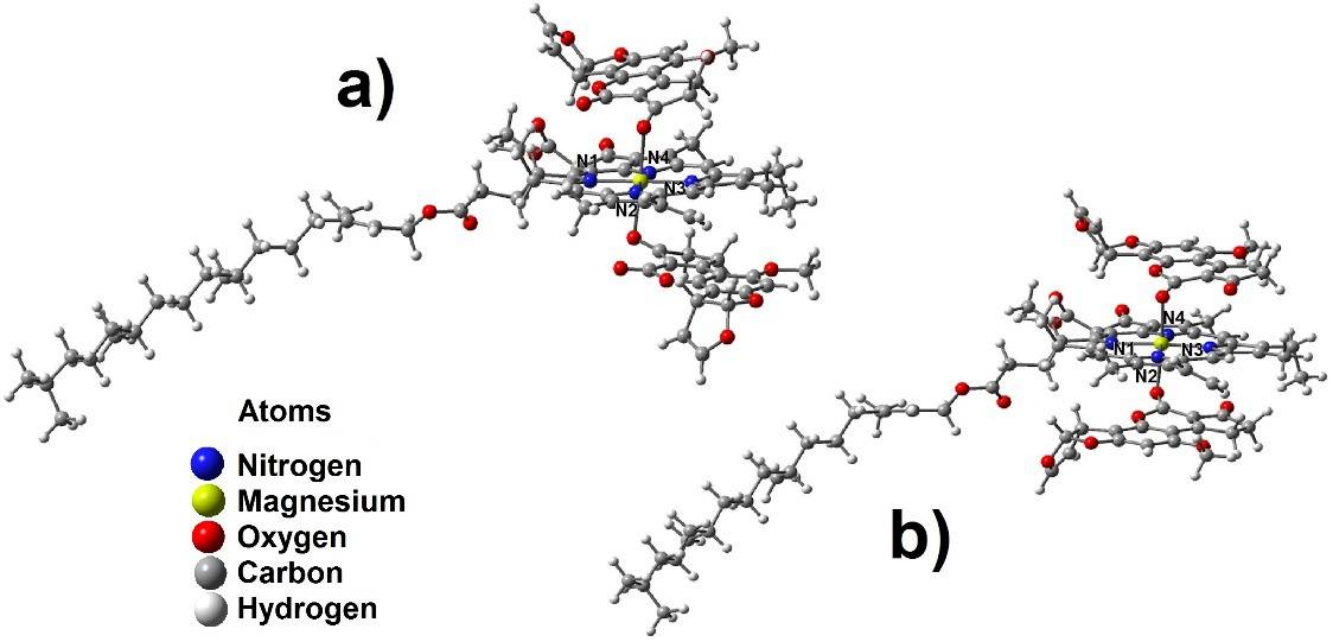


**Figure S6.** Optimized geometry of a) **chl a 1**-E-2AFB$_1$, and b) **chl a 1**-D-2AFB$_1$.

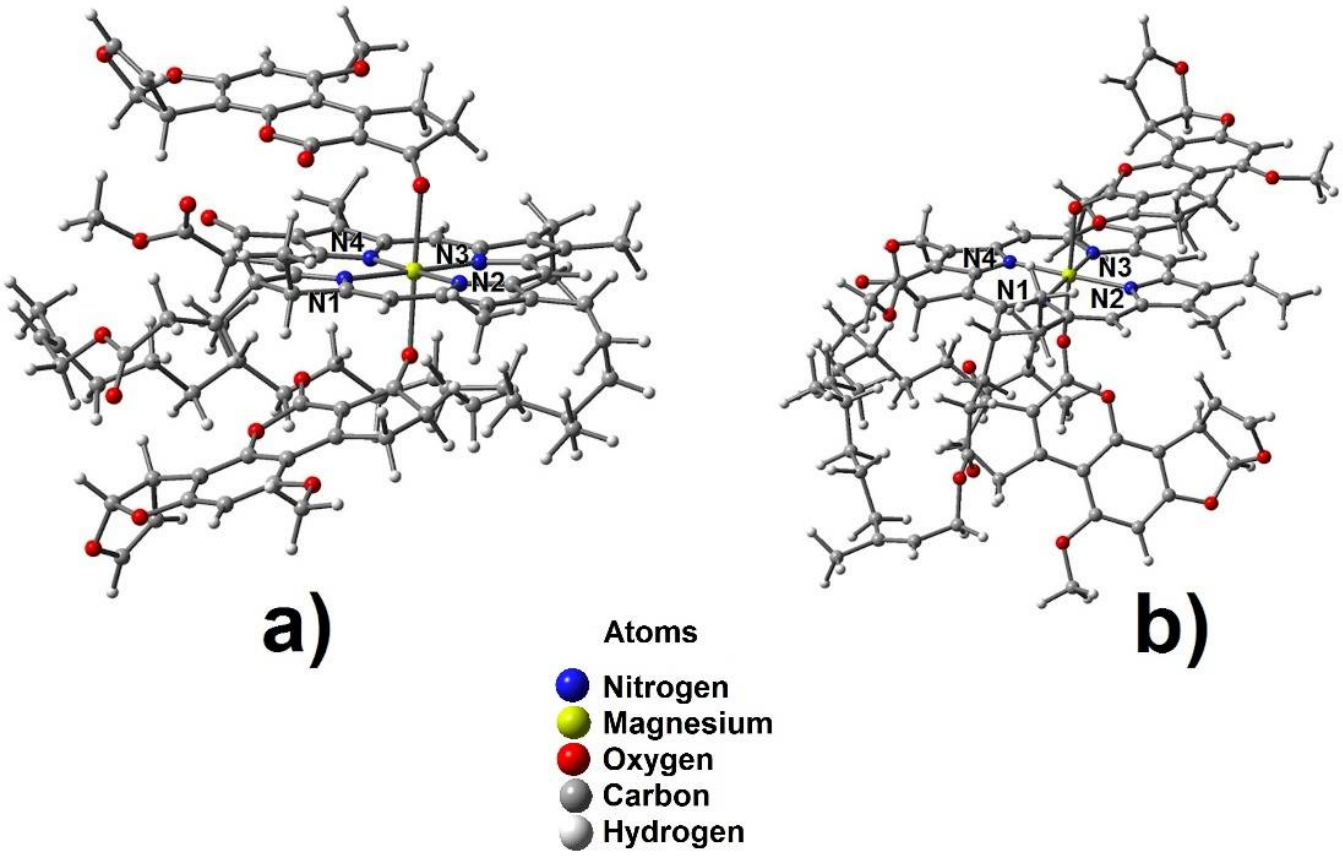


**Figure S7.** Optimized geometry of a) **chl a 2**-E-2AFB$_1$, and b) **chl a 2**-D-2AFB$_1$.

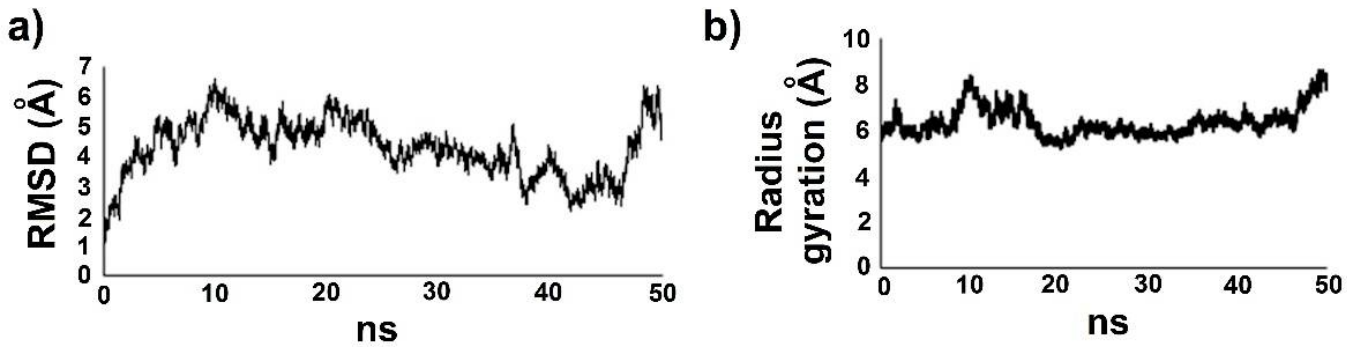


**Figure S8.** a) RMSD, and b) radius of gyration of **chl a 2**, obtained by MD simulation.

**Table S1.** Natural atomic charges ($e^-$) for **chl a 1**, **chl a 2**, $AFB_1$ and their complexes.

| | $Mg^{2+}$ | N1 | N2 | N3 | N4 | O* | C* |
|---|---|---|---|---|---|---|---|
| **chl a 2** | 1.762 | -0.796 | -0.745 | -0.770 | -0.726 | | |
| **chl a 1** | 1.758 | -0.792 | -0.744 | -0.769 | -0.725 | | |
| **chl a 1**-α-D-$AFB_1$ | 1.759 | -0.763 | -0.708 | -0.730 | -0.693 | -0.697 | 0.873 |
| **chl a 1**-α-E-$AFB_1$ | 1.760 | -0.698 | -0.760 | -0.706 | -0.734 | -0.695 | 0.646 |
| **chl a 1**-β-E-$AFB_1$ | 1.758 | -0.767 | -0.716 | -0.744 | -0.691 | -0.695 | 0.641 |
| **chl a 1**-β-D-$AFB_1$ | 1.757 | -0.763 | -0.712 | -0.745 | -0.694 | -0.699 | 0.868 |
| **chl a 2**-α-D-$AFB_1$ | 1.760 | -0.763 | -0.723 | -0.737 | -0.690 | -0.686 | 0.877 |
| **chl a 2**-α-E-$AFB_1$ | 1.765 | -0.746 | -0.721 | -0.742 | -0.695 | -0.687 | 0.648 |
| **chl a 2**-β-E-$AFB_1$ | 1.766 | -0.779 | -0.718 | -0.755 | -0.704 | -0.697 | 0.643 |
| **chl a 2**-β-D-$AFB_1$ | 1.762 | -0.768 | -0.715 | -0.747 | -0.691 | -0.691 | 0.870 |
| **chl a 1**-D-2$AFB_1$ | 1.753 | -0.763 | -0.713 | -0.727 | -0.672 | -0.664 | 0.869 |
| | | | | | | -0.612 | 0.853 |
| **chl a 1**-E-2$AFB_1$ | 1.753 | -0.751 | -0.723 | -0.737 | -0.662 | -0.650 | 0.638 |
| | | | | | | -0.622 | 0.624 |
| **chl a 2**-D-2$AFB_1$ | 1.749 | -0.737 | -0.693 | -0.711 | -0.669 | -0.631 | 0.866 |
| | | | | | | -0.640 | 0.865 |
| **chl a 2**-E-2$AFB_1$ | 1.756 | -0.737 | -0.703 | -0.726 | -0.673 | -0.643 | 0.638 |
| | | | | | | -0.644 | 0.642 |
| | | | | E | | D | |
| | | | | O | C | O | C |
| $AFB_1$ | | | | -0.534 | 0.588 | -0.533 | 0.825 |

E= specific oxygen atom of carbonyl group on ring E, D = specific oxygen atom of lactone group on ring D, O* and C*= atoms of $AFB_1$ when have coordinated to the $Mg^{2+}$ ion.

**Table S2.** Interaction energy, in kcal/mol, of complexes **chl a 1**-$AFB_1$, and **chl a 2**-$AFB_1$ in the gas phase.

| Molecule | Interaction energy | Energy differences between chlorophylls | Energy difference considering carbonylic interaction |
|---|---|---|---|
| | kcal/mol | | |
| **chl a 1**-α-D-$AFB_1$ | -32.1 | 4.3 | 3.6 |
| **chl a 1**-α-E-$AFB_1$ | -36.4 | 0.0 | 0.0 |
| **chl a 1**-β-E-$AFB_1$ | -35.5 | 0.9 | 0.9 |
| **chl a 1**-β-D-$AFB_1$ | -35.7 | 0.7 | 0.0 |
| **chl a 2**-α-D-$AFB_1$ | -33.3 | 5.9 | 0.0 |
| **chl a 2**-α-E-$AFB_1$ | -36.5 | 2.7 | 2.7 |
| **chl a 2**-β-E-$AFB_1$ | -39.2 | 0.0 | 0.0 |
| **chl a 2**-β-D-$AFB_1$ | -32.8 | 6.4 | 0.4 |
| **chl a 1**-$AFB_1$a | -17.0 | | |
| **chl a 1**-$AFB_1$b | -15.6 | | |
| **chl a 2**-$AFB_1$c | -29.6 | | |
| **chl a 2**-$AFB_1$d | -20.4 | | |
| **chl a 1**-E-2$AFB_1$ | -60.0 | 2.2 | 20.1 |
| **chl a 1**-D-2$AFB_1$ | -62.3 | 0.0 | 11.2 |
| **chl a 2**-E-2$AFB_1$ | -64.8 | 0.0 | 0.0 |
| **chl a 2**-D-2$AFB_1$ | -58.0 | 6.7 | 0.0 |

a and b = three hydrogen bond interactions, c = one hydrogen bond interaction, d = two hydrogen bond interactions.

**Table S3.** Interaction energy, in kcal/mol, of complexes **chl a 1**-2$AFB_1$, and **chl a 2**-2$AFB_1$ in water as solvent.

| Chemical system | Interaction energy | Energy differences between chlorophylls | Energy difference considering carbonylic interaction |
|---|---|---|---|
| | | kcal/mol | kcal/mol |
| **chl a 1**-α-D-$AFB_1$ | -22.6 | 3.9 | 3.8 |
| **chl a 1**-α-E-$AFB_1$ | -26.5 | 0.0 | 0.0 |
| **chl a 1**-β-E-$AFB_1$ | -23.6 | 2.9 | 2.9 |
| **chl a 1**-β-D-$AFB_1$ | -26.4 | 0.1 | 0.0 |
| **chl a 2**-α-D-$AFB_1$ | -23.4 | 4.5 | 3.3 |
| **chl a 2**-α-E-$AFB_1$ | -27.6 | 0.3 | 0.3 |
| **chl a 2**-β-E-$AFB_1$ | -27.9 | 0.0 | 0.0 |
| **chl a 2**-β-D-$AFB_1$ | -26.6 | 1.3 | 0.0 |
| **chl a 1**-$AFB_1$a | -10.3 | | |
| **chl a 1**-$AFB_1$b | -11.2 | | |
| **chl a 2**-$AFB_1$c | -23.0 | | |
| **chl a 2**-$AFB_1$d | -14.4 | | |
| **chl a 1**-E-2$AFB_1$ | -45.9 | 3.1 | 13.1 |
| **chl a 1**-D-2$AFB_1$ | -49.0 | 0.0 | 8.7 |
| **chl a 2**-E-2$AFB_1$ | -47.6 | 0.0 | 0.0 |
| **chl a 2**-D-2$AFB_1$ | -46.3 | 1.3 | 0.0 |

a and b = three hydrogen bond interactions, c = one hydrogen bond interaction, d = two hydrogen bond interactions.

**Table S4.** Cartesian coordinate

| $AFB_1$ | | | | chl a 2 | | | | chl a 1-α-E-$AFB_1$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 1 | | | | 0 1 | | | | 0 1 | | | |
| C | 3.97611200 | -1.04111100 | 0.09524100 | Mg | -1.74528200 | -0.15458700 | -1.10972300 | Mg | -5.04151200 | 2.62023600 | 0.24818000 |
| O | 4.66777900 | -2.02098700 | 0.08248700 | N | -3.08417400 | -1.65161200 | -0.97566800 | N | -4.55355000 | 4.59721000 | 0.30025000 |
| C | 4.47256400 | 0.39949900 | 0.25212600 | C | -4.45654900 | -1.52295200 | -1.02086700 | C | -5.38757900 | 5.62853700 | -0.06678300 |
| H | 5.17443000 | 0.61354400 | -0.55520400 | C | -5.05786300 | -2.85027100 | -0.88980800 | C | -4.61690200 | 6.87719900 | -0.08268400 |
| H | 5.02225400 | 0.47604600 | 1.19130600 | C | -4.03165600 | -3.72964200 | -0.69769600 | C | -3.35579000 | 6.56230200 | 0.32406000 |
| C | 3.22487300 | 1.29017000 | 0.21338200 | C | -2.80105500 | -2.95694400 | -0.77370300 | C | -3.33745700 | 5.11927200 | 0.54529200 |
| H | 3.23447600 | 2.01391400 | -0.60315100 | C | -6.48461100 | -3.17542400 | -0.95313400 | C | -5.10438100 | 8.20610900 | -0.46202000 |
| H | 3.07767600 | 1.86641100 | 1.12835500 | H | -6.83396100 | -3.94041600 | -0.26300600 | H | -4.75319100 | 9.03663200 | 0.14574500 |
| C | 2.07363000 | 0.32835700 | 0.02858700 | C | -7.35461500 | -2.62735000 | -1.80074200 | C | -5.90202200 | 8.46382900 | -1.49768800 |
| C | 2.50221600 | -0.96072200 | -0.03402800 | H | -8.39701900 | -2.92165600 | -1.79818600 | O | -6.21359700 | 9.47648700 | -1.72307600 |
| C | 1.60577700 | -2.09327600 | -0.22051100 | H | -7.04371800 | -1.89267700 | -2.53511700 | H | -6.24334900 | 7.67694900 | -2.16088100 |
| O | 1.86985100 | -3.24957000 | -0.25583500 | C | -4.09854200 | -5.20664400 | -0.48434900 | C | -2.17689000 | 7.46533400 | 0.49010400 |
| O | 0.25228000 | -1.73577100 | -0.30526000 | H | -3.62961900 | -5.48519300 | 0.46385600 | H | -1.35837600 | 7.16499900 | -0.17009100 |
| C | 0.67733000 | 0.63841400 | -0.07842100 | H | -3.57636900 | -5.74148900 | -1.28252400 | H | -1.79966900 | 7.43468800 | 1.51615800 |
| C | -0.18872800 | -0.46145400 | -0.25480300 | H | -5.13086800 | -5.55612500 | -0.46985300 | H | -2.43436200 | 8.49724600 | 0.25088300 |
| C | -1.25721300 | 2.14418100 | -0.13468800 | C | -5.13612200 | -0.32542000 | -1.04273700 | C | -6.73985700 | 5.51419100 | -0.29551000 |
| C | -1.54953100 | -0.27026500 | -0.38316400 | H | -6.21658400 | -0.38066700 | -0.97696400 | H | -7.27187800 | 6.43012800 | -0.52177400 |
| H | -1.71504200 | 3.12013600 | -0.09099000 | N | -3.25886600 | 1.23974400 | -1.22711000 | C | -7.05078500 | 3.11842900 | 0.09254400 |
| C | -2.05129200 | 1.01495000 | -0.31129700 | C | -4.57763000 | 0.97493800 | -1.10088000 | H | -7.52610700 | 4.33463400 | -0.21926200 |
| C | 0.11250400 | 1.94021400 | -0.01976300 | C | -3.13268500 | 2.60776700 | -1.29470300 | C | -8.12147000 | 2.25635000 | 0.08753500 |
| O | 0.99362100 | 2.94701000 | 0.15263600 | C | -4.43573800 | 3.22236200 | -1.17464600 | H | -9.32719000 | 2.98062300 | -0.26769400 |
| C | 0.49297100 | 4.27122500 | 0.21944200 | C | -5.34005900 | 2.11946700 | -1.04577700 | C | -8.95616700 | 4.28272300 | -0.45665600 |
| H | -0.01818500 | 4.54745300 | -0.70826600 | C | -6.82388200 | 2.27612400 | -0.86439900 | H | -9.80315400 | 5.45194600 | -0.85120400 |
| H | 1.36150800 | 4.91008700 | 0.35814700 | H | -7.13381000 | 1.77141600 | 0.05502200 | H | -9.46211900 | 5.88447400 | -1.79619700 |
| H | -0.18832300 | 4.38899400 | 1.06649900 | H | -7.35240400 | 1.79906900 | -1.69477600 | C | -9.78760100 | 6.24239500 | -0.09627400 |
| O | -3.39296700 | 1.07027500 | -0.44604000 | H | -7.16066600 | 3.31142400 | -0.80498200 | H | -10.84510600 | 5.15716000 | -0.97882900 |
| O | -4.80161600 | -0.57873700 | 0.38475400 | C | -4.68631900 | 4.69785000 | -1.11731800 | H | -10.67380700 | 2.35621400 | -0.46629700 |
| C | -3.03731200 | -1.97129500 | 0.75221800 | H | -5.72142100 | 4.90625600 | -1.39810300 | C | -11.45287300 | 3.11305700 | -0.34665600 |
| H | -2.40863500 | -2.71018300 | 1.22159900 | H | -4.06282000 | 5.20952300 | -1.85628300 | H | -10.85474900 | 1.60838500 | 0.31133500 |
| C | -4.20450000 | -1.52249000 | 1.18749400 | C | -4.40502100 | 5.26504400 | 0.28065700 | C | -10.78951700 | 1.70391900 | -1.85129700 |
| H | -4.77845600 | -1.78905500 | 2.06201400 | H | -4.56874600 | 6.34414200 | 0.31160600 | C | -11.76190400 | 1.22389300 | -1.98238000 |
| C | -2.69127000 | -1.23606600 | -0.52301500 | H | -3.37276400 | 5.06102900 | 0.57702700 | H | -10.00545200 | 0.95632300 | -1.99255900 |
| H | -2.58178100 | -1.90080300 | -1.38165300 | H | -5.05683900 | 4.79397100 | 1.01970700 | H | -10.66705500 | 2.45662300 | -2.63331100 |
| C | -3.89967800 | -0.25926300 | -0.64292000 | C | -1.92818800 | 3.29299400 | -1.47065500 | C | -8.08147600 | 0.90346700 | 0.39707900 |
| H | -4.44188700 | -0.25572600 | -1.58587500 | H | -1.98606200 | 4.37288900 | -1.56932600 | H | -8.98969800 | 0.34383700 | 0.33498000 |
| | | | | C | -0.65904600 | 2.72024800 | -1.53535300 | C | -6.91759700 | 0.18398500 | 0.76427900 |
| | | | | N | -0.45931500 | 1.35904700 | -1.34977800 | N | -5.67273200 | 0.78492200 | 0.86350500 |
| | | | | C | -1.51552100 | -3.50395900 | -0.65682600 | C | -2.20408000 | 4.40350700 | 0.96211900 |
| | | | | C | -1.46629700 | -4.56980500 | -0.46862100 | C | -1.30279400 | 4.98459800 | 1.12042200 |
| | | | | C | -0.29809200 | -2.84551200 | -0.77250800 | C | -2.10649700 | 3.04045500 | 1.21759600 |
| | | | | N | -0.12118200 | -1.52865300 | -0.98851500 | N | -3.07939900 | 2.12895600 | 1.06892000 |
| | | | | C | 1.22357200 | -1.23803800 | -1.07905500 | C | -2.61299500 | 0.87492500 | 1.39400300 |
| | | | | C | 0.84848200 | 1.16621200 | -1.45065200 | C | -4.82453900 | -0.18631200 | 1.15706200 |
| | | | | C | 1.68421600 | 0.02973700 | -1.31192100 | C | -3.42010800 | -0.22924600 | 1.37263100 |
| | | | | C | 0.60002000 | 3.38035500 | -1.77633700 | H | -6.81668000 | -1.22331500 | 1.01438200 |
| | | | | C | 1.54421000 | 2.36830000 | -1.72630300 | C | -5.48456700 | -1.44447200 | 1.26163100 |
| | | | | C | 0.82060300 | 4.83874900 | -2.01229200 | C | -7.92176400 | -2.22652300 | 0.96862600 |
| | | | | H | 0.25679000 | 5.18665000 | -2.88149400 | H | -8.69766700 | -2.00329800 | 1.70543700 |
| | | | | H | 1.87878600 | 5.03111000 | -2.18712100 | H | -7.52390600 | -3.22050600 | 1.17958300 |
| | | | | H | 0.49932300 | 5.42890100 | -1.14904400 | H | -8.38891000 | -2.23272700 | -0.02134800 |
| | | | | C | 2.97261000 | 2.06607200 | -1.83412900 | C | -4.46840200 | -2.45813100 | 1.57123000 |
| | | | | O | 3.90143000 | 2.76643700 | -2.13928700 | O | -4.57059300 | -3.64678700 | 1.74838100 |
| | | | | C | 3.10640100 | 0.56038400 | -1.38711400 | C | -3.07759400 | -1.69164300 | 1.60297800 |
| | | | | H | 3.53555600 | 0.64680800 | -0.38694400 | H | -2.49516600 | -2.12864400 | 0.78620500 |
| | | | | C | 4.12158000 | -0.21789200 | -2.18328700 | C | -2.34770400 | -2.00434800 | 2.88432900 |
| | | | | O | 5.35114500 | 0.09034700 | -1.75840500 | H | -1.66853300 | -3.15893300 | 2.77203600 |
| | | | | C | 6.42484500 | -0.61887300 | -2.37709900 | C | -1.02774800 | -3.60236900 | 3.96820500 |
| | | | | H | 6.45642100 | -1.63728300 | -1.98571700 | H | -0.52882300 | -4.53295000 | 3.71114900 |
| | | | | H | 7.32930800 | -0.08425500 | -2.09826900 | C | -1.76787400 | -3.76727100 | 4.75136200 |
| | | | | H | 6.29774600 | -0.63529900 | -3.45882000 | H | -0.30672100 | -2.85968400 | 4.31183800 |
| | | | | O | 3.88604800 | -1.02546500 | -3.04160300 | O | -2.35288500 | -1.34040400 | 3.88432000 |
| | | | | C | 1.02523700 | -3.58727500 | -0.65911800 | C | -0.80797800 | 2.41590500 | 1.71439300 |
| | | | | H | 1.12300900 | -3.94385300 | 0.37410700 | C | -0.04082300 | 2.55638300 | 0.94199900 |
| | | | | C | 2.06736400 | -2.48702600 | -0.93738900 | H | -1.16543600 | 0.92103000 | 1.84976200 |
| | | | | H | 2.55636500 | -2.66706500 | -1.90162700 | H | -1.51412400 | 0.62994400 | 2.90721400 |
| | | | | C | 1.13643200 | -4.77971100 | -1.60949800 | C | -0.31643700 | 3.03799300 | 3.02259200 |
| | | | | H | 0.39109600 | -5.54638200 | -1.39079600 | H | -0.08731400 | 4.09827000 | 2.90326000 |
| | | | | | | | | H | 0.58648900 | 2.53098400 | 3.37276800 |
| | | | | | | | | H | -1.08381700 | 2.94036500 | 3.79407200 |
| | | | | | | | | C | -0.22896800 | -0.01327800 | 1.08303300 |
| | | | | | | | | H | -0.17461100 | 0.29856500 | 0.03424700 |
| | | | | | | | | H | -0.61007100 | -1.03747800 | 1.08407000 |
| | | | | | | | | C | 1.17521200 | -0.03952700 | 1.67038800 |
| | | | | | | | | H | 1.67412700 | 0.93127200 | 1.60771900 |
| | | | | | | | | H | 1.14359100 | -0.29971400 | 2.73504800 |
| | | | | | | | | C | 2.04843400 | -1.06280800 | 0.98422400 |
| | | | | | | | | O | 1.65254400 | -1.93016800 | 0.24824700 |
| | | | | | | | | O | 3.33534000 | -0.89961200 | 1.30176900 |
| | | | | | | | | C | 4.25819500 | -1.82377300 | 0.68963600 |
| | | | | | | | | H | 4.13357300 | -1.75293000 | -0.39531200 |
| | | | | | | | | H | 3.99177400 | -2.83902600 | 0.98466100 |
| | | | | | | | | C | 5.62970600 | -1.41755600 | 1.11507100 |
| | | | | | | | | C | 6.61030900 | -2.21622300 | 1.53886200 |
| | | | | | | | | H | 5.82159300 | -0.35032000 | 1.03686400 |
| | | | | | | | | C | 6.49358500 | -3.71184600 | 1.67969400 |
| | | | | | | | | H | 6.96154800 | -4.21739300 | 0.82976700 |
| | | | | | | | | H | 5.46154600 | -4.05418300 | 1.74152200 |
| | | | | | | | | H | 7.01901200 | -4.04542500 | 2.57864900 |
| | | | | | | | | C | 7.96261100 | -1.64028700 | 1.87880100 |
| | | | | | | | | H | 7.91615500 | -0.54855300 | 1.83306700 |
| | | | | | | | | H | 8.21533100 | -1.90779500 | 2.91304700 |
| | | | | | | | | C | 9.08215800 | -2.13734200 | 0.95534600 |
| | | | | | | | | H | 8.81804300 | -1.90032700 | -0.08263800 |
| | | | | | | | | H | 9.15319700 | -3.22682700 | 1.02286500 |
| | | | | | | | | C | 10.42934800 | -1.50455200 | 1.30075100 |
| | | | | | | | | H | 10.29413700 | -0.42028400 | 1.39277400 |
| | | | | | | | | H | 10.75472300 | -1.85868500 | 2.28812200 |
| | | | | | | | | C | 11.54747100 | -1.76853300 | 0.28476900 |
| | | | | | | | | H | 11.21615600 | -1.37289600 | -0.68554100 |
| | | | | | | | | C | 12.80947400 | -1.00226500 | 0.69890200 |
| | | | | | | | | H | 12.53565900 | 0.04204300 | 0.89177100 |
| | | | | | | | | H | 13.17134300 | -1.40533800 | 1.65454000 |
| | | | | | | | | C | 13.94821400 | -1.02513300 | -0.32045000 |
| | | | | | | | | H | 13.57169700 | -0.68048300 | -1.29240000 |
| | | | | | | | | H | 14.29573200 | -2.05161900 | -0.46355900 |
| | | | | | | | | C | 15.11913400 | -0.14235700 | 0.11183600 |
| | | | | | | | | H | 14.73214800 | 0.85004500 | 0.37260000 |
| | | | | | | | | H | 15.55808300 | -0.55140100 | 1.03182900 |
| | | | | | | | | C | 16.23007700 | 0.03019400 | -0.93077500 |
| | | | | | | | | H | 15.77811900 | 0.45756200 | -1.83668400 |
| | | | | | | | | C | 17.26860000 | 1.03043100 | -0.40855500 |
| | | | | | | | | H | 16.74977900 | 1.95493000 | -0.12663800 |
| | | | | | | | | H | 17.70910800 | 0.63301300 | 0.51562200 |
| | | | | | | | | C | 18.38787100 | 1.38126800 | -1.38894800 |
| | | | | | | | | H | 17.94534700 | 1.64186500 | -2.35721800 |
| | | | | | | | | H | 19.02823500 | 0.50902200 | -1.56177800 |
| | | | | | | | | C | 19.25233600 | 2.53482700 | -0.88091400 |
| | | | | | | | | H | 18.64908500 | 3.45197500 | -0.84536800 |
| | | | | | | | | H | 19.55007500 | 2.32331100 | 0.15347500 |
| | | | | | | | | C | 20.51317600 | 2.80502800 | -1.70791900 |
| | | | | | | | | H | 21.12154200 | 1.89149300 | -1.69903600 |
| | | | | | | | | C | 21.82057500 | -3.26489900 | 0.12352400 |
| | | | | | | | | H | 10.93114900 | -3.80343100 | -0.20892800 |
| | | | | | | | | C | 12.14064200 | -3.69624900 | 1.07838700 |
| | | | | | | | | H | 12.60535300 | -3.45322600 | -0.61085100 |
| | | | | | | | | C | 16.87370700 | -1.30649100 | -1.30218200 |
| | | | | | | | | H | 16.14231900 | -2.00801400 | -1.70724700 |
| | | | | | | | | C | 17.33029200 | -1.76567700 | -0.41848100 |
| | | | | | | | | H | 17.65278500 | -1.17912500 | -2.05583100 |
| | | | | | | | | C | 21.33049000 | 3.93046500 | -1.07373300 |
| | | | | | | | | H | 20.75808100 | 4.86380700 | -1.07712100 |
| | | | | | | | | H | 22.25886100 | 4.10596100 | -1.62247500 |
| | | | | | | | | H | 21.58729600 | 3.69883800 | -0.03695800 |
| | | | | | | | | C | 20.18106200 | 3.14352700 | -3.16189500 |
| | | | | | | | | H | 19.51309400 | 4.01046300 | -3.20617000 |
| | | | | | | | | H | 19.69078000 | 2.31346600 | -3.67400800 |
| | | | | | | | | C | 21.08686000 | 3.39134000 | -3.72042900 |
| | | | | | | | | C | -3.94776700 | 0.91150300 | -1.92018900 |
| | | | | | | | | O | -4.49740700 | 1.97605600 | -1.68154000 |
| | | | | | | | | C | -2.45018800 | 0.73739100 | -2.07751400 |
| | | | | | | | | H | -1.93653700 | 1.37447600 | -1.35551500 |
| | | | | | | | | O | -2.17632300 | 1.07868300 | -3.07976900 |
| | | | | | | | | C | -2.20501000 | -0.76206900 | -1.88157100 |
| | | | | | | | | H | -1.67968800 | -0.97315200 | -0.95173200 |
| | | | | | | | | H | -1.61803900 | -1.23069400 | -2.67375300 |
| | | | | | | | | C | -3.58635900 | -1.36549600 | -1.84311100 |
| | | | | | | | | C | -4.55499900 | -0.40919400 | -1.99364300 |
| | | | | | | | | C | -5.97250800 | -0.71988800 | -2.09754400 |
| | | | | | | | | H | -6.87498600 | 0.02276100 | -2.32181900 |
| | | | | | | | | O | -6.26488300 | -2.08283000 | -1.97696000 |
| | | | | | | | | C | -3.95045800 | -2.72211400 | -1.62192500 |
| | | | | | | | | C | -5.33533000 | -3.01695300 | -1.66813600 |
| | | | | | | | | C | -3.48297300 | -5.03512300 | -0.96395300 |
| | | | | | | | | C | -5.78177300 | -4.28893800 | -1.39158700 |
| | | | | | | | | H | -2.82269200 | -5.82691600 | -0.84675500 |
| | | | | | | | | C | -4.85198100 | -5.26138300 | -1.05231500 |
| | | | | | | | | C | -3.04184300 | -3.75430500 | -1.25269300 |
| | | | | | | | | O | -1.75456600 | -3.37759800 | -1.16027600 |
| | | | | | | | | C | -0.84521500 | -4.23271700 | -0.46996200 |
| | | | | | | | | H | -1.23805300 | -4.46326500 | 0.52447400 |
| | | | | | | | | H | 0.07830200 | -3.66416700 | -0.38302000 |
| | | | | | | | | C | -0.67334500 | -5.15066400 | -1.03823500 |
| | | | | | | | | O | -5.40917200 | -6.45756700 | -0.79507100 |
| | | | | | | | | O | -7.30299800 | -7.26614400 | -1.86175300 |
| | | | | | | | | C | -7.63021500 | -5.23601100 | -2.83795300 |
| | | | | | | | | H | -7.87965900 | -4.49738900 | -3.58219600 |
| | | | | | | | | C | -7.66533200 | -6.55240600 | -2.97939000 |
| | | | | | | | | C | -7.94978600 | -7.16140000 | -3.82404700 |
| | | | | | | | | C | -7.14385600 | -4.92046000 | -1.44090000 |
| | | | | | | | | H | -7.88459300 | -4.38645800 | -0.84571400 |
| | | | | | | | | C | -6.83734500 | -6.34937200 | -0.90605900 |
| | | | | | | | | H | -7.25362900 | -6.61667100 | 0.06254200 |

**chl a 2-β-E-AFB$_1$**

| O 1 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Mg | 2.35799400 | -0.91822900 | -0.94294600 | H | -6.50999900 | 1.47613200 | 4.57445000 | H | 15.97800000 | -0.61800000 | 0.32700000 |
| N | 3.69081000 | 0.40553000 | -1.70689000 | H | -5.55632900 | 1.55005100 | 6.06630900 | C | 16.48800000 | 1.07700000 | 1.56200000 |
| C | 5.05630800 | 0.33218000 | -1.61401900 | C | -3.18853700 | 2.49872600 | 4.88717900 | H | 15.99000000 | 1.98800000 | 1.91600000 |
| C | 5.65223600 | 1.35760700 | -2.48003600 | H | -2.77241300 | 3.50933200 | 4.89376900 | H | 16.68600000 | 0.46900000 | 2.45500000 |
| C | 4.62172300 | 1.99807400 | -3.09885900 | H | -3.17936700 | 2.15249700 | 5.92599900 | C | -3.05500000 | 5.87300000 | 0.72500000 | C | 17.82600000 | 1.47000000 | 0.92300000 |
| C | 3.39165000 | 1.40167300 | -2.56600700 | C | -2.28208700 | 1.58467300 | 4.05138100 | C | -2.81700000 | 4.45400000 | 0.46600000 | H | 17.60600000 | 2.03200000 | 0.00500000 |
| C | 7.08951100 | 1.57966000 | -2.63145600 | H | -2.30576900 | 1.94599000 | 3.01615900 | C | -4.92800000 | 7.47600000 | 0.17700000 | C | 18.59800000 | 2.40100000 | 1.86600000 |
| H | 7.72363600 | 0.69720800 | -2.59923100 | H | -2.71047100 | 0.57585400 | 4.03573600 | H | -4.83200000 | 8.07200000 | 1.08100000 | H | 17.95700000 | 3.25700000 | 2.11200000 |
| C | 7.65304400 | 2.77585400 | -2.79589300 | C | -0.83712100 | 1.55755800 | 4.55518300 | C | -5.58600000 | 7.98800000 | -0.86200000 | H | 18.78400000 | 1.87500000 | 2.81200000 |
| H | 8.72443100 | 2.88075100 | -2.91562400 | H | -0.38046100 | 2.53378500 | 4.35474000 | H | -6.03700000 | 8.97100000 | -0.80800000 | C | 19.92200000 | 2.92600000 | 1.31300000 |
| H | 7.06020300 | 3.88398000 | -2.79238300 | H | -0.83088300 | 1.43189700 | 5.64596900 | H | -5.67100000 | 7.45000000 | -1.79900000 | H | 19.75500000 | 3.31500000 | 0.30200000 |
| C | 4.66913200 | 3.04898900 | -4.15994100 | C | 0.02350900 | 0.44901900 | 3.93092200 | C | -2.08800000 | 6.78900000 | 1.40000000 | H | 20.64400000 | 2.10700000 | 1.21700000 |
| H | 4.52075000 | 4.05223100 | -3.74985300 | H | -0.15158000 | 0.44674800 | 2.84366600 | H | -1.14600000 | 6.84000000 | 0.84500000 | C | 20.52800000 | 4.01400000 | 2.19900000 |
| H | 3.88829100 | 2.87688100 | -4.90385800 | C | 1.52173500 | 0.71609000 | 4.12197200 | H | -1.85600000 | 6.44000000 | 2.41000000 | H | 19.87400000 | 4.89700000 | 2.18800000 |
| H | 5.63606000 | 3.03220900 | -4.66541500 | H | 1.72157500 | 1.76073100 | 3.87503400 | H | -2.48700000 | 7.80100000 | 1.47100000 | H | 20.54400000 | 3.65700000 | 3.23600000 |
| C | 5.75675900 | -0.54380600 | -0.81755900 | H | 1.78085400 | 0.59867200 | 5.18288100 | C | -6.04900000 | 4.73800000 | -0.91600000 | C | 21.94500000 | 4.44500000 | 1.80800000 |
| H | 6.83650500 | -0.44733500 | -0.81227000 | C | 2.41748000 | -0.19745400 | 3.27077900 | H | -6.70500000 | 5.60000000 | -0.91400000 | H | 22.59100000 | 3.56000000 | 1.86300000 |
| N | 3.90435200 | -1.82239500 | 0.15070100 | H | 1.96302500 | -0.33428400 | 2.28078600 | N | -5.92500000 | 2.37900000 | -1.56700000 | C | 13.52200000 | -1.85500000 | -0.22400000 |
| C | 5.21200100 | -1.54602800 | 0.02767900 | H | 2.44270000 | -1.19586300 | 3.71829500 | C | -6.56800000 | 3.55400000 | -1.50300000 | H | 12.78600000 | -2.24500000 | -0.90800000 |
| C | 3.79537000 | -2.82755700 | 1.08868900 | C | 3.85764300 | 0.30746800 | 3.09138500 | C | -6.75000000 | 1.50700000 | -2.24400000 | H | 13.67400000 | -2.59400000 | 0.57000000 |
| C | 5.11986300 | -3.21013500 | 1.55780900 | H | 4.17625300 | 0.83624000 | 4.00096700 | C | -7.97500000 | 2.19000000 | -2.62000000 | H | 14.45200000 | -1.76800000 | -0.78700000 |
| C | 6.00394400 | -2.39096400 | 0.90541900 | H | 4.52951100 | -0.55308400 | 2.98178600 | C | -7.86500000 | 3.46800000 | -2.15000000 | C | 18.65600000 | 0.24200000 | 0.54700000 |
| C | 7.49155600 | -2.32186800 | 1.04879300 | C | 4.08942200 | 1.21727100 | 1.87291000 | C | -8.85800000 | 4.58300000 | -2.21900000 | H | 18.10900000 | -0.42900000 | -0.11800000 |
| H | 7.80948000 | -1.33623400 | 1.40101400 | H | 3.93056700 | 0.60678100 | 0.97743200 | H | -8.42900000 | 5.47300000 | -2.68800000 | H | 18.92600000 | -0.32100000 | 1.44700000 |
| H | 7.99176400 | -2.50663400 | 0.09406100 | C | 3.09823900 | 2.37975000 | 1.78535500 | H | -9.18800000 | 4.86200000 | -1.21400000 | H | 19.57900000 | 0.52300000 | 0.03600000 |
| H | 7.85254100 | -3.09137100 | 1.76456600 | H | 2.08492900 | 1.96960400 | 1.67549000 | H | -9.73700000 | 4.29600000 | -2.79800000 | C | 22.47300000 | 5.48500000 | 2.79600000 |
| C | 5.40201800 | -4.19723300 | 2.63982200 | H | 3.11054400 | 2.95087700 | 2.72349400 | C | -9.09000000 | 1.59000000 | -3.42200000 | H | 21.85700000 | 6.38900000 | 2.76200000 |
| H | 6.40419200 | -4.61164600 | 2.50512900 | C | 3.35171600 | 3.34654800 | 0.62707600 | H | -10.02600000 | 2.10900000 | -3.19400000 | H | 23.50000000 | 5.77300000 | 2.55800000 |
| H | 4.71103400 | -5.04116100 | 2.55866300 | H | 3.64518700 | 2.78155500 | -0.26567200 | H | -9.24200000 | 0.54500000 | -3.12900000 | H | 22.45600000 | 5.10600000 | 3.82000000 |
| C | 5.28753600 | -3.56376600 | 4.03322000 | H | 4.19371500 | 4.00483000 | 0.87212900 | C | -8.81700000 | 1.66300000 | -4.93000000 | C | 22.00200000 | 4.99100000 | 0.38100000 |
| H | 5.46665300 | -4.29928300 | 4.82028600 | C | 2.11076600 | 4.18494400 | 0.32600600 | H | -9.63400000 | 1.21900000 | -5.50300000 | H | 21.31100000 | 5.83400000 | 0.26900000 |
| H | 4.29314800 | -3.13394800 | 4.17833800 | H | 1.41559300 | 3.56969500 | -0.26584800 | H | -7.89200000 | 1.13700000 | -5.17700000 | H | 21.73200000 | 4.23400000 | -0.35800000 |
| H | 6.01357500 | -2.75506200 | 4.14318500 | H | 1.58947200 | 4.41452000 | 1.26648600 | H | -8.69900000 | 2.70200000 | -5.24100000 | H | 23.00600000 | 5.34800000 | 0.14000000 |
| C | 2.60561000 | -3.34755900 | 1.57179300 | C | 2.35911300 | 5.49933500 | -0.41585400 | C | -6.46000000 | 0.17200000 | -2.49500000 | C | -8.10700000 | 1.27400000 | 0.63200000 |
| H | 2.68288400 | -4.13636500 | 2.31449200 | H | 2.97258500 | 6.13521900 | 0.23551800 | H | -7.20500000 | -0.40300000 | -3.03800000 | O | -7.96100000 | 2.43900000 | 0.88300000 |
| C | 1.31008100 | -2.88409400 | 1.27819100 | C | -0.36120400 | -0.91960200 | 4.49985800 | C | -5.29500000 | -0.50700000 | -2.11100000 | C | -9.39300000 | 0.62300000 | 0.11800000 |
| N | 1.08962400 | -1.84249400 | 0.38536100 | H | -1.39791100 | -1.19138200 | 4.28258200 | N | -4.25400000 | 0.13200000 | -1.44900000 | H | -9.74200000 | 1.17100000 | -0.75800000 |
| C | 2.10887500 | 1.88055200 | -2.82962400 | H | -0.23588500 | -0.90970700 | 5.58797100 | C | -1.65200000 | 3.77000000 | 0.83400000 | H | -10.15300000 | 0.72200000 | 0.89700000 |
| H | 2.03427200 | 2.71007800 | -3.52253600 | H | 0.27403200 | -1.70664300 | 4.09269400 | H | -0.89200000 | 4.35400000 | 1.34200000 | C | -9.04600000 | -0.84400000 | -0.16300000 |
| C | 0.92146700 | 1.51036800 | -2.19449500 | C | 5.54181600 | 1.69449400 | 1.85157100 | C | -1.33600000 | 2.43400000 | 0.59600000 | H | -9.02600000 | -1.07400000 | -1.23300000 |
| N | 0.75229300 | 0.48721500 | -1.34874900 | H | 6.22205000 | 0.84352200 | 1.95627800 | N | -2.11100000 | 1.52400000 | -0.00900000 | H | -9.73400000 | -1.55900000 | 0.29100000 |
| C | -0.52120700 | 0.53208400 | -0.80998800 | H | 5.73510000 | 2.38767900 | 2.67817000 | C | -1.43300000 | 0.32900000 | -0.13600000 | C | -7.65000000 | -1.02200000 | 0.38200000 |
| C | -0.18369700 | -1.49718400 | 0.54652600 | H | 5.78920800 | 2.19963700 | 0.91455400 | C | -3.30600000 | -0.78100000 | -1.30000000 | C | -7.12800000 | 0.17200000 | 0.79500000 |
| C | -0.97578500 | -0.40723100 | 0.07519700 | C | 1.03601700 | 6.21634200 | -0.68494900 | C | -1.99500000 | -0.76200000 | -0.74100000 | C | -5.75200000 | 0.29200000 | 1.18300000 |
| C | 0.10015700 | -3.23759000 | 1.95197400 | H | 0.41752300 | 5.62350500 | -1.36835100 | C | -4.97700000 | -1.88600000 | -2.33900000 | O | -5.10000000 | 1.31300000 | 1.29000000 |
| C | -0.84574600 | -2.33268000 | 1.47254900 | H | 1.19575500 | 7.19328100 | -1.14786700 | C | -3.69700000 | -2.04100000 | -1.81600000 | O | -5.09600000 | -0.88000000 | 1.41500000 |
| C | -0.09083700 | -4.29937800 | 2.98714000 | H | 0.46083200 | 6.36279000 | 0.23270500 | C | -5.83700000 | -2.90400000 | -3.01800000 | C | -6.87300000 | -2.21400000 | 0.45200000 |
| H | -0.05493100 | -5.29937800 | 2.54352200 | C | 3.12438300 | 5.27511100 | -1.71783800 | H | -6.87200000 | -2.84000000 | -2.67000000 | C | -5.59400000 | -2.08500000 | 1.03400000 |
| H | -1.06094600 | -4.17600700 | 3.46986100 | H | 2.53930100 | 4.63006400 | -2.38480800 | H | -5.45900000 | -3.90600000 | -2.81400000 | C | -6.43700000 | -4.60400000 | 0.12700000 |
| H | 0.68606800 | -4.25176800 | 3.75505800 | H | 4.08232500 | 4.77566200 | -1.53794900 | H | -5.84000000 | -2.75300000 | -4.10100000 | C | -4.77400000 | -3.17300000 | 1.20400000 |
| C | -2.20468600 | -1.85139900 | 1.66009400 | H | 3.31599200 | 6.21596700 | -2.23438600 | C | -2.64100000 | -3.00000000 | -1.54200000 | H | -6.69800000 | -5.58600000 | -0.23700000 |
| O | -3.14078100 | -2.34786700 | 2.23970200 | C | 1.81868100 | -3.05783900 | -2.36538600 | O | -2.64100000 | -4.20600000 | -1.59900000 | C | -5.20200000 | -4.40600000 | 0.74500000 |
| C | -2.20692700 | -0.42618600 | 0.98567900 | O | 2.19538800 | -2.37920500 | -2.47073000 | C | -1.39900000 | -2.12300000 | -1.08600000 | C | -7.26500000 | -3.50000000 | -0.01100000 |
| H | -1.97383200 | 0.20084200 | 1.85716300 | C | 1.11124300 | -4.43644700 | -1.74553500 | H | -0.78700000 | -2.05800000 | -1.99500000 | O | -8.47100000 | -3.55000000 | -0.62000000 |
| C | -3.55502000 | 0.08240600 | 0.55340500 | H | 1.84742700 | -4.52250600 | -0.94583300 | C | -0.55300000 | -2.83100000 | -0.06000000 | C | -8.89200000 | -4.79200000 | -1.15900000 |
| O | -4.36904800 | 0.16061400 | 1.60279600 | H | 1.35764400 | -5.16673300 | -2.52234300 | O | 0.15900000 | -3.80500000 | -0.62900000 | H | -8.19300000 | -5.13700000 | -1.92600000 |
| C | -5.68331800 | 0.64871700 | 1.32286100 | C | -0.34630500 | -4.56440400 | -1.27778900 | C | 0.93200000 | -4.60400000 | 0.27000000 | H | -9.98500000 | -4.60600000 | -1.60800000 |
| H | -5.62273100 | 1.66660600 | 0.93433700 | H | -0.42940900 | -4.46798300 | -0.19402800 | H | 1.40900000 | -5.35900000 | -0.34800000 | H | -8.98500000 | -5.54700000 | -0.37400000 |
| H | -6.20498900 | 0.63745600 | 2.27590500 | H | -0.82801900 | -5.50501500 | -1.54890600 | H | 0.28300000 | -5.06600000 | 1.01600000 | O | -4.29400000 | -5.37700000 | 0.91900000 |
| H | -6.17701800 | -0.00713200 | 0.60326000 | C | -1.05452600 | -3.40787200 | -1.93646500 | H | 1.67700000 | -3.99000000 | 0.77600000 | O | -7.66300000 | -5.44900000 | 2.57300000 |
| O | -3.87606600 | 0.44048800 | -0.55420600 | C | -0.17713700 | -2.63714200 | -2.65352100 | O | -0.50600000 | -2.58900000 | 1.12000000 | C | -3.37500000 | -3.41500000 | 3.30300000 |
| C | -0.33966400 | 2.34327400 | -2.36313000 | C | -0.57207900 | -1.48674600 | -3.44095300 | C | 0.00500000 | 1.85500000 | 1.02000000 | H | -3.63700000 | -2.61600000 | 3.97700000 |
| H | -0.09700500 | 3.38362600 | -2.11419600 | O | 0.11594300 | -0.78492800 | -4.11723700 | H | 0.80100000 | 2.41900000 | 0.52000000 | C | -2.96200000 | -4.62900000 | 3.63600000 |
| C | -1.28458200 | 1.74052200 | -1.30841200 | O | -1.94089500 | -1.23302500 | -3.42411500 | C | -0.05300000 | 0.40900000 | 0.48600000 | H | -2.79700000 | -5.07500000 | 4.60500000 |
| H | -2.21624100 | 1.40223300 | -1.76786800 | C | -2.42000400 | -3.02296800 | -1.84592600 | H | -0.02000000 | -0.29900000 | 1.32100000 | C | -3.40800000 | -3.31900000 | 1.79400000 |
| C | -0.90788200 | 2.29871700 | -3.78366900 | C | -2.80921300 | -1.90899100 | -2.63059200 | C | 0.21400000 | 1.92600000 | 2.53400000 | H | -2.70300000 | -2.57700000 | 1.41900000 |
| H | -0.18734500 | 2.67667600 | -4.51201900 | C | -4.66422700 | -3.08991800 | -0.86385900 | H | 0.23300000 | 2.95700000 | 2.89200000 | C | -3.08400000 | -4.78700000 | 1.40600000 |
| H | -1.80742500 | 2.91850900 | -3.83809500 | C | -4.09887900 | -1.44487600 | -2.59067200 | H | 1.15900000 | 1.45100000 | 2.80900000 | H | -2.31900000 | -4.94400000 | 0.63000000 |
| H | -1.16104000 | 1.27516300 | -4.06235200 | H | -5.38914800 | -3.45975400 | -0.15420800 | H | -0.59500000 | 1.40200000 | 3.04700000 | C | -5.82400000 | 2.85500000 | -3.63000000 |
| C | -1.63232000 | 2.89292900 | -0.16191200 | C | -4.98471400 | -2.02208700 | -1.69530200 | C | 1.08500000 | 0.06300000 | -0.47600000 | O | -5.94000000 | 1.66100000 | -3.63900000 |
| H | -0.72193200 | 3.17351000 | 0.21289000 | C | -3.37332300 | -3.59749100 | -0.95595500 | H | 1.11600000 | 0.79200000 | -1.29300000 | C | -6.86800000 | 3.85700000 | -4.13300000 |
| H | -2.05649900 | 2.13114800 | 0.67180500 | O | -2.92203400 | -4.61701100 | -0.21193900 | H | 0.92400000 | -0.91000000 | -0.94600000 | H | -7.79200000 | 3.70300000 | -3.57500000 |
| C | -2.65585700 | 3.75576700 | -0.57687500 | C | -3.78383200 | -5.15282800 | 0.78594700 | C | 2.42700000 | 0.02300000 | 0.24400000 | H | -7.07900000 | 3.64000000 | -5.18100000 |
| H | -2.23758700 | 4.46360300 | -1.29401600 | H | -4.05487500 | -4.37761600 | 1.50490500 | H | 2.71100000 | 0.99700000 | 0.65200000 | C | -6.26400000 | 5.25000000 | -3.91900000 |
| H | -3.52402000 | 3.25359200 | -1.01345700 | H | -3.20658400 | -5.92957400 | 1.28152000 | H | 2.38100000 | -0.66200000 | 1.09800000 | H | -6.85700000 | 5.88200000 | -3.25700000 |
| C | -3.09207100 | 4.51871500 | 0.64646700 | H | -4.67389900 | -5.59311400 | 0.32784900 | C | 3.54400000 | -0.45500000 | -0.65200000 | H | -6.13900000 | 5.81300000 | -4.84600000 |
| O | -2.75325400 | 5.63000200 | 0.94731200 | O | -6.16590800 | -1.37713500 | -1.63714300 | O | 3.40200000 | -0.92200000 | -1.74900000 | C | -4.91000000 | 4.98900000 | -3.29900000 |
| O | -3.88284000 | 3.75160800 | 1.42244900 | O | -7.13762200 | -0.21752900 | -3.39762200 | O | 4.73700000 | -0.31500000 | -0.05700000 | C | -4.67700000 | 3.65800000 | -3.14500000 |
| C | -4.25239800 | 4.32729800 | 2.69690500 | C | -5.25788200 | -0.52035000 | -4.64562200 | C | 5.86800000 | -0.77200000 | -0.82300000 | O | -3.45000000 | 3.12200000 | -2.57900000 |
| H | -4.81587000 | 5.24288100 | 2.50504200 | H | -4.62922200 | -0.71086900 | -5.50015700 | H | 5.90100000 | -0.19700000 | -1.75400000 | O | -3.14000000 | 1.98800000 | -2.41100000 |
| H | -3.33902400 | 4.60267500 | 3.22520900 | C | -6.58233100 | -0.49380700 | -4.62526700 | H | 5.71500000 | -1.81700000 | -1.09300000 | O | -2.52600000 | 4.10600000 | -2.19200000 |
| C | -5.06605000 | 3.30888700 | 3.42554200 | H | -7.30218300 | -0.63386400 | -5.41738400 | C | 7.08800000 | -0.54000000 | 0.00500000 | C | -3.93000000 | 5.95300000 | -2.89100000 |
| C | -4.61242100 | 2.49327800 | 4.38045200 | C | -4.75602300 | -0.26667600 | -3.24247600 | C | 8.06400000 | -1.41400000 | 0.25600000 | C | -2.74500000 | 5.43100000 | -2.32900000 |
| H | -6.09884400 | 3.21047800 | 3.10054100 | H | -4.15397300 | 0.63881100 | -3.14663600 | H | 7.16500000 | 0.46300000 | 0.41800000 | C | -3.05100000 | 8.22100000 | -2.58300000 |
| C | -5.49804200 | 1.43593100 | 4.98000500 | C | -6.09552100 | -0.19396300 | -2.45891200 | C | 8.09300000 | -2.83200000 | -0.25400000 | C | -1.74500000 | 6.27400000 | -1.89100000 |
| H | -5.08129300 | 0.44230200 | 4.78099100 | H | -6.22705800 | 0.65926700 | -1.79834300 | H | 8.73900000 | -2.91400000 | -1.13400000 | H | -3.11700000 | 9.29500000 | -2.66200000 |
| | | | | | | | | H | 7.10800000 | -3.20300000 | -0.53000000 | H | -1.91200000 | 7.63800000 | -2.03400000 |
| | | | | | | | | H | 8.50600000 | -3.49600000 | 0.50900000 | C | -4.05700000 | 7.36300000 | -3.00800000 |
| | | | | | | | | C | 9.26300000 | -1.00200000 | 1.07500000 | O | -5.21100000 | 7.79700000 | -3.55600000 |
| | | | | | | | | H | 9.11600000 | 0.01300000 | 1.45500000 | C | -5.39900000 | 9.19400000 | -3.70100000 |
| | | | | | | | | H | 9.34300000 | -1.66400000 | 1.94700000 | H | -5.38000000 | 9.69300000 | -2.72900000 |
| | | | | | | | | C | 10.58000000 | -1.06700000 | 0.29100000 | H | -6.38000000 | 9.31500000 | -4.15500000 |
| | | | | | | | | H | 10.49900000 | -0.42800000 | -0.59600000 | H | -4.63600000 | 9.62500000 | -4.35500000 |
| | | | | | | | | H | 10.73500000 | -2.08900000 | -0.06700000 | O | -0.86500000 | 8.35400000 | -1.57400000 |
| | | | | | | | | C | 11.77300000 | -0.62600000 | 1.13800000 | O | 1.32900000 | 7.61300000 | -1.74800000 |
| | | | | | | | | H | 11.54400000 | 0.34800000 | 1.58600000 | C | 0.63100000 | 5.52400000 | -2.32800000 |
| | | | | | | | | H | 11.90200000 | -1.32700000 | 1.97400000 | H | 0.59800000 | 4.56500000 | -2.81900000 |
| | | | | | | | | C | 13.10000000 | -0.51300000 | 0.37700000 | C | 1.51800000 | 6.48800000 | -2.51700000 |
| | | | | | | | | H | 12.95500000 | 0.20200000 | -0.44500000 | H | 2.38100000 | 6.53200000 | -3.16400000 |
| | | | | | | | | C | 14.17900000 | 0.05600000 | 1.30700000 | C | -0.38400000 | 6.00400000 | -1.31500000 |
| | | | | | | | | H | 13.80600000 | 0.99100000 | 1.74100000 | H | -0.41800000 | 5.38300000 | -0.41800000 |
| | | | | | | | | H | 14.32300000 | -0.63700000 | 2.14700000 | C | 0.12300000 | 7.45400000 | -1.04700000 |
| | | | | | | | | C | 15.52700000 | 0.32700000 | 0.64000000 | H | 0.28900000 | 7.73700000 | -0.01000000 |
| | | | | | | | | H | 15.36800000 | 0.91700000 | -0.27300000 | | | | |

**chl a 1-D-2AFB$_1$**

| O 1 | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Mg | -4.16600000 | 1.94300000 | -0.51100000 | H | 15.97800000 | -0.61800000 | 0.32700000 |
| N | -3.87000000 | 3.91900000 | -0.17900000 | C | 16.48800000 | 1.07700000 | 1.56200000 |
| C | -4.80500000 | 4.90900000 | -0.35500000 | H | 15.99000000 | 1.98800000 | 1.91600000 |
| C | -4.27700000 | 6.16300000 | 0.20000000 | H | 16.68600000 | 0.46900000 | 2.45500000 |
| C | -3.05500000 | 5.87300000 | 0.72500000 | C | 17.82600000 | 1.47000000 | 0.92300000 |
| C | -2.81700000 | 4.45400000 | 0.46600000 | H | 17.60600000 | 2.03200000 | 0.00500000 |
| C | -4.92800000 | 7.47600000 | 0.17700000 | C | 18.59800000 | 2.40100000 | 1.86600000 |
| H | -4.83200000 | 8.07200000 | 1.08100000 | H | 17.95700000 | 3.25700000 | 2.11200000 |
| C | -5.58600000 | 7.98800000 | -0.86200000 | H | 18.78400000 | 1.87500000 | 2.81200000 |
| H | -6.03700000 | 8.97100000 | -0.80800000 | C | 19.92200000 | 2.92600000 | 1.31300000 |
| H | -5.67100000 | 7.45000000 | -1.79900000 | H | 19.75500000 | 3.31500000 | 0.30200000 |
| C | -2.08800000 | 6.78900000 | 1.40000000 | H | 20.64400000 | 2.10700000 | 1.21700000 |
| H | -1.14600000 | 6.84000000 | 0.84500000 | C | 20.52800000 | 4.01400000 | 2.19900000 |
| H | -1.85600000 | 6.44000000 | 2.41000000 | H | 19.87400000 | 4.89700000 | 2.18800000 |
| H | -2.48700000 | 7.80100000 | 1.47100000 | H | 20.54400000 | 3.65700000 | 3.23600000 |
| C | -6.04900000 | 4.73800000 | -0.91600000 | C | 21.94500000 | 4.44500000 | 1.80800000 |
| H | -6.70500000 | 5.60000000 | -0.91400000 | H | 22.59100000 | 3.56000000 | 1.86300000 |
| N | -5.92500000 | 2.37900000 | -1.56700000 | C | 13.52200000 | -1.85500000 | -0.22400000 |
| C | -6.56800000 | 3.55400000 | -1.50300000 | H | 12.78600000 | -2.24500000 | -0.90800000 |
| C | -6.75000000 | 1.50700000 | -2.24400000 | H | 13.67400000 | -2.59400000 | 0.57000000 |
| C | -7.97500000 | 2.19000000 | -2.62000000 | H | 14.45200000 | -1.76800000 | -0.78700000 |
| C | -7.86500000 | 3.46800000 | -2.15000000 | C | 18.65600000 | 0.24200000 | 0.54700000 |
| C | -8.85800000 | 4.58300000 | -2.21900000 | H | 18.10900000 | -0.42900000 | -0.11800000 |
| H | -8.42900000 | 5.47300000 | -2.68800000 | H | 18.92600000 | -0.32100000 | 1.44700000 |
| H | -9.18800000 | 4.86200000 | -1.21400000 | H | 19.57900000 | 0.52300000 | 0.03600000 |
| H | -9.73700000 | 4.29600000 | -2.79800000 | C | 22.47300000 | 5.48500000 | 2.79600000 |
| C | -9.09000000 | 1.59000000 | -3.42200000 | H | 21.85700000 | 6.38900000 | 2.76200000 |
| H | -10.02600000 | 2.10900000 | -3.19400000 | H | 23.50000000 | 5.77300000 | 2.55800000 |
| H | -9.24200000 | 0.54500000 | -3.12900000 | H | 22.45600000 | 5.10600000 | 3.82000000 |
| C | -8.81700000 | 1.66300000 | -4.93000000 | C | 22.00200000 | 4.99100000 | 0.38100000 |
| H | -9.63400000 | 1.21900000 | -5.50300000 | H | 21.31100000 | 5.83400000 | 0.26900000 |
| H | -7.89200000 | 1.13700000 | -5.17700000 | H | 21.73200000 | 4.23400000 | -0.35800000 |
| H | -8.69900000 | 2.70200000 | -5.24100000 | H | 23.00600000 | 5.34800000 | 0.14000000 |
| C | -6.46000000 | 0.17200000 | -2.49500000 | C | -8.10700000 | 1.27400000 | 0.63200000 |
| H | -7.20500000 | -0.40300000 | -3.03800000 | O | -7.96100000 | 2.43900000 | 0.88300000 |
| C | -5.29500000 | -0.50700000 | -2.11100000 | C | -9.39300000 | 0.62300000 | 0.11800000 |
| N | -4.25400000 | 0.13200000 | -1.44900000 | H | -9.74200000 | 1.17100000 | -0.75800000 |
| C | -1.65200000 | 3.77000000 | 0.83400000 | H | -10.15300000 | 0.72200000 | 0.89700000 |
| H | -0.89200000 | 4.35400000 | 1.34200000 | C | -9.04600000 | -0.84400000 | -0.16300000 |
| C | -1.33600000 | 2.43400000 | 0.59600000 | H | -9.02600000 | -1.07400000 | -1.23300000 |
| N | -2.11100000 | 1.52400000 | -0.00900000 | H | -9.73400000 | -1.55900000 | 0.29100000 |
| C | -1.43300000 | 0.32900000 | -0.13600000 | C | -7.65000000 | -1.02200000 | 0.38200000 |
| C | -3.30600000 | -0.78100000 | -1.30000000 | C | -7.12800000 | 0.17200000 | 0.79500000 |
| C | -1.99500000 | -0.76200000 | -0.74100000 | C | -5.75200000 | 0.29200000 | 1.18300000 |
| C | -4.97700000 | -1.88600000 | -2.33900000 | O | -5.10000000 | 1.31300000 | 1.29000000 |
| C | -3.69700000 | -2.04100000 | -1.81600000 | O | -5.09600000 | -0.88000000 | 1.41500000 |
| C | -5.83700000 | -2.90400000 | -3.01800000 | C | -6.87300000 | -2.21400000 | 0.45200000 |
| H | -6.87200000 | -2.84000000 | -2.67000000 | C | -5.59400000 | -2.08500000 | 1.03400000 |
| H | -5.45900000 | -3.90600000 | -2.81400000 | C | -6.43700000 | -4.60400000 | 0.12700000 |
| H | -5.84000000 | -2.75300000 | -4.10100000 | C | -4.77400000 | -3.17300000 | 1.20400000 |
| C | -2.64100000 | -3.00000000 | -1.54200000 | H | -6.69800000 | -5.58600000 | -0.23700000 |
| O | -2.64100000 | -4.20600000 | -1.59900000 | C | -5.20200000 | -4.40600000 | 0.74500000 |
| C | -1.39900000 | -2.12300000 | -1.08600000 | C | -7.26500000 | -3.50000000 | -0.01100000 |
| H | -0.78700000 | -2.05800000 | -1.99500000 | O | -8.47100000 | -3.55000000 | -0.62000000 |
| C | -0.55300000 | -2.83100000 | -0.06000000 | C | -8.89200000 | -4.79200000 | -1.15900000 |
| O | 0.15900000 | -3.80500000 | -0.62900000 | H | -8.19300000 | -5.13700000 | -1.92600000 |
| C | 0.93200000 | -4.60400000 | 0.27000000 | H | -9.98500000 | -4.60600000 | -1.60800000 |
| H | 1.40900000 | -5.35900000 | -0.34800000 | H | -8.98500000 | -5.54700000 | -0.37400000 |
| H | 0.28300000 | -5.06600000 | 1.01600000 | O | -4.29400000 | -5.37700000 | 0.91900000 |
| H | 1.67700000 | -3.99000000 | 0.77600000 | O | -7.66300000 | -5.44900000 | 2.57300000 |
| O | -0.50600000 | -2.58900000 | 1.12000000 | C | -3.37500000 | -3.41500000 | 3.30300000 |
| C | 0.00500000 | 1.85500000 | 1.02000000 | H | -3.63700000 | -2.61600000 | 3.97700000 |
| H | 0.80100000 | 2.41900000 | 0.52000000 | C | -2.96200000 | -4.62900000 | 3.63600000 |
| C | -0.05300000 | 0.40900000 | 0.48600000 | H | -2.79700000 | -5.07500000 | 4.60500000 |
| H | -0.02000000 | -0.29900000 | 1.32100000 | C | -3.40800000 | -3.31900000 | 1.79400000 |
| C | 0.21400000 | 1.92600000 | 2.53400000 | H | -2.70300000 | -2.57700000 | 1.41900000 |
| H | 0.23300000 | 2.95700000 | 2.89200000 | C | -3.08400000 | -4.78700000 | 1.40600000 |
| H | 1.15900000 | 1.45100000 | 2.80900000 | H | -2.31900000 | -4.94400000 | 0.63000000 |
| H | -0.59500000 | 1.40200000 | 3.04700000 | C | -5.82400000 | 2.85500000 | -3.63000000 |
| C | 1.08500000 | 0.06300000 | -0.47600000 | O | -5.94000000 | 1.66100000 | -3.63900000 |
| H | 1.11600000 | 0.79200000 | -1.29300000 | C | -6.86800000 | 3.85700000 | -4.13300000 |
| H | 0.92400000 | -0.91000000 | -0.94600000 | H | -7.79200000 | 3.70300000 | -3.57500000 |
| C | 2.42700000 | 0.02300000 | 0.24400000 | H | -7.07900000 | 3.64000000 | -5.18100000 |
| H | 2.71100000 | 0.99700000 | 0.65200000 | C | -6.26400000 | 5.25000000 | -3.91900000 |
| H | 2.38100000 | -0.66200000 | 1.09800000 | H | -6.85700000 | 5.88200000 | -3.25700000 |
| C | 3.54400000 | -0.45500000 | -0.65200000 | H | -6.13900000 | 5.81300000 | -4.84600000 |
| O | 3.40200000 | -0.92200000 | -1.74900000 | C | -4.91000000 | 4.98900000 | -3.29900000 |
| O | 4.73700000 | -0.31500000 | -0.05700000 | C | -4.67700000 | 3.65800000 | -3.14500000 |
| C | 5.86800000 | -0.77200000 | -0.82300000 | O | -3.45000000 | 3.12200000 | -2.57900000 |
| H | 5.90100000 | -0.19700000 | -1.75400000 | O | -3.14000000 | 1.98800000 | -2.41100000 |
| H | 5.71500000 | -1.81700000 | -1.09300000 | O | -2.52600000 | 4.10600000 | -2.19200000 |
| C | 7.08800000 | -0.54000000 | 0.00500000 | C | -3.93000000 | 5.95300000 | -2.89100000 |
| C | 8.06400000 | -1.41400000 | 0.25600000 | C | -2.74500000 | 5.43100000 | -2.32900000 |
| H | 7.16500000 | 0.46300000 | 0.41800000 | C | -3.05100000 | 8.22100000 | -2.58300000 |
| C | 8.09300000 | -2.83200000 | -0.25400000 | C | -1.74500000 | 6.27400000 | -1.89100000 |
| H | 8.73900000 | -2.91400000 | -1.13400000 | H | -3.11700000 | 9.29500000 | -2.66200000 |
| H | 7.10800000 | -3.20300000 | -0.53000000 | H | -1.91200000 | 7.63800000 | -2.03400000 |
| H | 8.50600000 | -3.49600000 | 0.50900000 | C | -4.05700000 | 7.36300000 | -3.00800000 |
| C | 9.26300000 | -1.00200000 | 1.07500000 | O | -5.21100000 | 7.79700000 | -3.55600000 |
| H | 9.11600000 | 0.01300000 | 1.45500000 | C | -5.39900000 | 9.19400000 | -3.70100000 |
| H | 9.34300000 | -1.66400000 | 1.94700000 | H | -5.38000000 | 9.69300000 | -2.72900000 |
| C | 10.58000000 | -1.06700000 | 0.29100000 | H | -6.38000000 | 9.31500000 | -4.15500000 |
| H | 10.49900000 | -0.42800000 | -0.59600000 | H | -4.63600000 | 9.62500000 | -4.35500000 |
| H | 10.73500000 | -2.08900000 | -0.06700000 | O | -0.86500000 | 8.35400000 | -1.57400000 |
| C | 11.77300000 | -0.62600000 | 1.13800000 | O | 1.32900000 | 7.61300000 | -1.74800000 |
| H | 11.54400000 | 0.34800000 | 1.58600000 | C | 0.63100000 | 5.52400000 | -2.32800000 |
| H | 11.90200000 | -1.32700000 | 1.97400000 | H | 0.59800000 | 4.56500000 | -2.81900000 |
| C | 13.10000000 | -0.51300000 | 0.37700000 | C | 1.51800000 | 6.48800000 | -2.51700000 |
| H | 12.95500000 | 0.20200000 | -0.44500000 | H | 2.38100000 | 6.53200000 | -3.16400000 |
| C | 14.17900000 | 0.05600000 | 1.30700000 | C | -0.38400000 | 6.00400000 | -1.31500000 |
| H | 13.80600000 | 0.99100000 | 1.74100000 | H | -0.41800000 | 5.38300000 | -0.41800000 |
| H | 14.32300000 | -0.63700000 | 2.14700000 | C | 0.12300000 | 7.45400000 | -1.04700000 |
| C | 15.52700000 | 0.32700000 | 0.64000000 | H | 0.28900000 | 7.73700000 | -0.01000000 |
| H | 15.36800000 | 0.91700000 | -0.27300000 | | | | |

| chl a 2-E-2AFB$_1$ | | chl a 2-AFB$_1$c | |
|---|---|---|---|
| 0 1 | | 0 1 | |
| Mg -2.50645900 -0.47135500 -0.88531700 | H -0.64367300 1.62994100 3.89463700 | Mg -4.27683300 0.06861500 -1.14368300 | H 6.03349300 3.25088200 -2.64852600 |
| N -3.40087500 -1.91114200 -1.99757600 | C -1.47517200 -0.01772200 4.99614000 | N -5.32605000 -1.64703700 -1.05747600 | H 6.30728900 3.84132100 -1.00768900 |
| C -4.72343600 -2.24999900 -1.93675700 | H -1.13066500 -1.00887800 5.32192700 | C -6.64745500 -1.77465200 -0.68413400 | C 4.33159700 2.12150200 0.20909900 |
| C -4.95352800 -3.40813600 -2.80987500 | H -1.44820200 0.61767100 5.88977600 | C -7.02686900 -3.18491800 -0.77329300 | H 4.60590900 1.26396400 0.84992200 |
| C -3.75269500 -3.70992600 -3.38565100 | C -2.92732400 -0.16331500 4.51619900 | C -5.90359600 -3.87263300 -1.13188000 | H 4.70840000 3.01569900 0.75430000 |
| C -2.78793800 -2.74276500 -2.85264600 | H -3.22836400 0.78178600 4.04070600 | C -4.85235200 -2.88469400 -1.31966000 | C 2.86547700 2.18468700 -0.00906600 |
| C -6.24847400 -4.06131000 -2.99602000 | C -3.02786600 -1.28232200 3.46156700 | C -8.35500500 -3.75116200 -0.52669800 | H 2.57865100 1.27765800 -0.55476500 |
| H -7.12019600 -3.41152100 -3.01266000 | H -2.59024900 -0.93721700 2.51891800 | H -8.38046900 -4.70687400 -0.00769800 | H 2.62588100 3.02626400 -0.66892300 |
| C -6.42454500 -5.37571600 -3.13000400 | H -2.40163200 -2.12163700 3.79875500 | C -9.50403900 -3.19658700 -0.91149500 | C 2.07566800 2.26749600 1.30068400 |
| H -7.41128700 -5.79870600 -3.27405600 | C -4.43267500 -1.82502800 3.18963200 | H -10.45235200 -3.67606900 -0.70223200 | H 2.17716300 1.31022200 1.82664800 |
| H -5.59026700 -6.06608300 -3.07365300 | H -5.08020700 -1.01418000 2.83357800 | H -9.52602400 -2.26675900 -1.46873700 | H 2.52058300 3.02951900 1.95496200 |
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| C -2.22925300 1.95008500 1.05736600 | C -1.85387600 -4.42499900 -0.15437000 | C -3.70864800 3.11612600 -1.04071500 | C 0.40845800 4.07615000 0.73214400 |
| N -1.66207600 0.98897700 0.24075900 | H -2.84939400 -4.29429900 -0.88702300 | N -3.30578000 1.81136400 -1.29593300 | H 0.92066800 4.34692900 -0.18994700 |
| C -1.41734800 -2.72038400 -3.16515300 | H -2.28886600 -4.91276100 0.72459600 | C -3.54184300 -3.19016100 -1.71473400 | H 0.80440600 4.69387200 1.54028700 |
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| C -1.46644600 4.17163700 2.24204800 | C 1.93343600 -4.77452500 -0.04969100 | C -2.68869000 5.52724900 -1.27685100 | H -4.96583900 -5.14207100 2.75734400 |
| H -2.29031900 4.77232100 1.84009800 | C 2.77773500 -3.90887900 0.88310400 | H -3.49416800 5.95821300 -1.87691400 | C -7.56750400 -2.85012500 2.94409700 |
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| H -1.71296600 3.91658500 3.27782400 | C 4.12519100 -4.15284600 0.77409800 | H -2.85045500 5.83010400 -0.23820800 | H -7.72579900 -1.86755100 3.39485000 |
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| C 7.08418000 0.91895500 0.43277700 | C -1.30491800 5.20458800 -1.16661200 | C 5.35571700 0.90854500 -1.76474000 | H 8.78070600 -6.14656000 0.76754000 |
| C 6.59249000 1.36771900 1.59048600 | C 0.01343300 4.87220100 -1.55570600 | C 5.13202700 2.04655300 -1.10151400 | C 6.91136300 -3.48663900 -0.10934000 |
| H 7.62780100 1.61061700 -0.20495000 | C -0.45609700 7.23554600 -0.09159800 | H 5.88151900 0.95301300 -2.71446800 | H 6.70831900 -3.19648500 -1.14137400 |
| C 8.76697800 2.81070600 1.98066100 | C 1.07003900 5.68599500 -1.21237800 | C 5.57368700 3.36688200 -1.66673300 | C 5.96287000 -4.61531600 0.38831300 |
| H 5.78747500 3.29251600 2.07471600 | H -0.57984600 8.14740300 0.47186600 | H 4.71819500 4.04490000 -1.75367400 | H 5.14324500 -4.88813900 -0.26847900 |
| H 7.35530900 3.36251800 1.24631000 | C 0.81530600 8.84554400 -0.50586900 | | |
| H 7.26095100 2.89173200 2.95313300 | C -1.51039300 6.39534500 -0.42341700 | | |
| C 5.77315300 0.55367200 2.56638800 | O -2.78842800 6.63263900 -0.05133100 | | |
| H 6.05524000 -0.50371400 2.55889900 | C -3.04309200 7.76736500 0.75753100 | | |
| H 5.98439200 0.92138000 3.57619300 | H -2.48785200 7.70563200 1.69815200 | | |
| C 4.26615700 0.70203600 2.29170800 | H -4.11117200 7.75502900 0.95998900 | | |
| H 4.03052500 0.11080100 1.39802900 | H -2.78042800 8.68956400 0.23218500 | | |
| H 4.06276300 1.74329500 2.02093300 | O 1.92846000 7.55340700 -0.22723700 | | |
| C 3.35766500 0.26942000 3.45262600 | O 3.70832200 7.63812600 -1.72527900 | | |
| H 3.22176300 -0.81685000 3.44469100 | C 2.97271100 5.81630300 -2.88181300 | | |
| H 3.84672700 0.49590700 4.40992100 | H 2.76862900 5.14674200 -3.70216500 | | |
| C 1.97862400 0.95191200 3.43366700 | C 3.58154600 8.99236900 -2.93239000 | | |
| H 1.58497900 0.88465800 2.41471300 | H 4.01185700 7.52620200 -3.76638200 | | |
| C 0.96034600 0.22943200 4.32405900 | C 2.54677600 5.56971900 -1.45508600 | | |
| H 1.09786100 -0.85280000 4.22738800 | H 2.95681500 4.66135500 -1.01338400 | | |
| H 1.15310800 0.48150800 5.37667600 | C 3.06742400 6.85223200 -0.74605000 | | |
| C -0.49502700 0.54631700 3.96583200 | H 3.75298900 6.70643400 0.08572300 | | |

**Reference**

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