Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry


# Absolute Stereochemistry and Preferred Conformations of Urate Degradation Intermediates from Computed and Experimental Circular Dichroism Spectra

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April 18, 2011

SUPPORTING INFORMATION

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# 1 Coordinates

## 1.1 Coordinates of optimized HIU tautomers - B3LYP/6-31G**

Data in Å

| HIU-21 | | | |
|---|---|---|---|
| $E_{el}$= -712.2835439170 Hartree | | | |
| $\Delta E_{el}$= 40.49 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.035491 | -0.007622 | 0.055157 |
| C | 0.055023 | -0.003794 | 1.431681 |
| N | 1.111281 | -0.126336 | 2.148384 |
| C | 2.280602 | -0.300665 | 1.396843 |
| C | 2.229683 | -0.902643 | -0.014738 |
| C | 1.043100 | -0.326917 | -0.804361 |
| N | 3.521859 | -0.742415 | -0.527217 |
| C | 4.280179 | -0.264562 | 0.490223 |
| N | 3.458998 | 0.033653 | 1.743034 |
| O | -1.153872 | 0.201279 | 2.014692 |
| O | 0.904942 | -0.198346 | -2.002927 |
| O | 1.835586 | -2.321493 | 0.086812 |
| H | 2.598039 | -2.717302 | -0.366181 |
| H | -0.910934 | 0.253539 | -0.379263 |
| O | 5.485482 | -0.037042 | 0.514919 |
| H | -0.950314 | 0.225622 | 2.963632 |

HIU-31

$E_{el}$= -712.3193828740 Hartree

$\Delta E_{el}$= 18.00 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | -1.386319 | -1.519842 | -0.191709 |
| C | -0.298300 | -0.929239 | 0.081189 |
| C | -0.447764 | 0.566045 | 0.339449 |
| N | -1.770365 | 0.849248 | -0.025131 |
| C | -2.377095 | -0.340112 | -0.252851 |
| C | 0.700081 | 1.352775 | -0.304349 |
| N | 1.895983 | 0.603493 | -0.345950 |
| C | 2.108775 | -0.755406 | -0.107156 |
| N | 0.972496 | -1.488731 | 0.167855 |
| O | 3.225842 | -1.252561 | -0.177862 |
| O | -0.196515 | 0.800378 | 1.772822 |
| O | 0.703125 | 2.506805 | -0.680535 |
| O | -3.547624 | -0.582210 | -0.515566 |
| H | -1.046838 | 1.205477 | 2.009447 |
| H | 1.082670 | -2.492228 | 0.115668 |
| H | 2.727518 | 1.107342 | -0.626275 |

HIU-32

| $E_{el}$= -712.2798303520 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 42.82 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -1.375248 | -1.530952 | -0.235825 |
| C | -0.300213 | -0.928348 | 0.049606 |
| C | -0.446843 | 0.557027 | 0.350129 |
| N | -1.789132 | 0.830354 | 0.033116 |
| C | -2.388259 | -0.348930 | -0.231410 |
| C | 0.697208 | 1.354122 | -0.316995 |
| N | 1.962721 | 0.703329 | -0.291655 |
| C | 2.019754 | -0.570580 | -0.098163 |
| N | 0.992311 | -1.451739 | 0.094564 |
| O | 3.227640 | -1.188594 | -0.101204 |
| O | -0.168833 | 0.753487 | 1.785126 |
| O | 0.598499 | 2.473021 | -0.775365 |
| O | -3.559552 | -0.604292 | -0.481692 |
| H | -1.036275 | 1.093374 | 2.057894 |
| H | 3.850484 | -0.463271 | -0.271978 |
| H | 1.150473 | -2.438732 | -0.058571 |

HIU-61

$E_{el}$= -712.2769521260 Hartree

$\Delta E_{el}$= 44.63 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | -1.269845 | -1.588396 | -0.249698 |
| C | -0.179225 | -1.028640 | 0.124138 |
| C | -0.382098 | 0.422941 | 0.504361 |
| N | -1.714814 | 0.733002 | 0.169328 |
| C | -2.269856 | -0.454445 | -0.240306 |
| C | 0.626538 | 1.199202 | -0.310550 |
| N | 1.808882 | 0.735364 | -0.564841 |
| C | 1.990466 | -0.599648 | -0.148832 |
| N | 1.119719 | -1.524527 | 0.099318 |
| O | 3.301013 | -0.935286 | -0.130453 |
| O | -0.062085 | 0.697133 | 1.896168 |
| O | 0.179285 | 2.352274 | -0.778740 |
| O | -3.418819 | -0.659816 | -0.606739 |
| H | -0.951679 | 0.872213 | 2.241526 |
| H | -0.803817 | 2.254503 | -0.593288 |
| H | 3.756331 | -0.127622 | -0.414845 |

HIU-62

| $E_{el}$= -712.3047274980 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 27.20 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -1.284710 | -1.580409 | -0.265328 |
| C | -0.193538 | -1.003824 | 0.061594 |
| C | -0.366924 | 0.433694 | 0.478887 |
| N | -1.699556 | 0.750910 | 0.152067 |
| C | -2.282400 | -0.430463 | -0.227161 |
| C | 0.670404 | 1.231464 | -0.275653 |
| N | 1.870700 | 0.815890 | -0.499529 |
| C | 2.180144 | -0.516342 | -0.176304 |
| N | 1.113700 | -1.431714 | 0.035728 |
| O | 3.324534 | -0.940746 | -0.171805 |
| O | -0.066099 | 0.607691 | 1.891343 |
| O | 0.226424 | 2.398773 | -0.728711 |
| O | -3.441757 | -0.634649 | -0.553205 |
| H | -0.956870 | 0.779803 | 2.235405 |
| H | -0.754612 | 2.314651 | -0.567515 |
| H | 1.345508 | -2.404447 | -0.114066 |

HIU-71

$E_{el}$= -712.3480708920 Hartree

$\Delta E_{el}$= 0.00 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | -0.024478 | 0.007433 | -0.003642 |
| C | 0.002952 | -0.049807 | 1.447111 |
| N | 1.207662 | -0.113199 | 2.076984 |
| C | 2.282806 | -0.312938 | 1.329684 |
| C | 2.190844 | -0.852240 | -0.117061 |
| C | 0.997142 | -0.270595 | -0.867360 |
| N | 3.490592 | -0.510980 | -0.584616 |
| C | 4.329055 | -0.337710 | 0.555465 |
| N | 3.547604 | -0.163962 | 1.698947 |
| O | -1.088931 | 0.045687 | 1.998800 |
| O | 0.934939 | -0.130398 | -2.081100 |
| O | 1.923728 | -2.269646 | -0.107764 |
| H | 2.458912 | -2.636031 | 0.611806 |
| H | -0.921671 | 0.257897 | -0.398350 |
| O | 5.548613 | -0.317447 | 0.479675 |
| H | 3.873690 | -0.989773 | -1.387385 |

HIU-72

| $E_{el}$= -712.3253224350 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 14.27 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.029508 | 0.062422 | -0.049714 |
| C | 0.107671 | -0.025789 | 1.282082 |
| N | 1.186689 | -0.122472 | 2.068196 |
| C | 2.300490 | -0.369713 | 1.362100 |
| C | 2.171067 | -0.985390 | -0.035276 |
| C | 1.064420 | -0.240301 | -0.809077 |
| N | 3.518351 | -0.889574 | -0.488353 |
| C | 4.313741 | -0.319441 | 0.533879 |
| N | 3.544756 | -0.120759 | 1.702092 |
| O | -1.058552 | 0.114093 | 1.958891 |
| O | 1.185654 | -0.014756 | -2.011286 |
| O | 1.703966 | -2.343497 | 0.038351 |
| H | 2.401216 | -2.822111 | 0.510187 |
| H | -1.710780 | 0.222860 | 1.247402 |
| O | 5.492143 | -0.037337 | 0.391376 |
| H | 3.711176 | -0.676215 | -1.457162 |

HIU-73

| $E_{el}$= -712.3388736520 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 5.77 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.045790 | 0.067128 | -0.071863 |
| C | -0.085272 | 0.014041 | 1.272975 |
| N | 1.180208 | -0.207782 | 2.027441 |
| C | 2.330194 | -0.402460 | 1.374570 |
| C | 2.168197 | -1.007147 | -0.001982 |
| C | 1.067822 | -0.232607 | -0.773223 |
| N | 3.518811 | -0.908266 | -0.465377 |
| C | 4.322693 | -0.325158 | 0.538961 |
| N | 3.556414 | -0.120913 | 1.720913 |
| O | -1.057661 | 0.214332 | 1.993754 |
| O | 1.265181 | 0.004618 | -1.968893 |
| O | 1.711535 | -2.361982 | 0.069234 |
| H | 2.473098 | -2.866790 | 0.390852 |
| H | 1.182314 | 0.187618 | 2.958971 |
| O | 5.494383 | -0.028925 | 0.394919 |
| H | 3.669993 | -0.659193 | -1.434552 |

HIU-76

| $E_{el}$= -712.3117885840 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 22.77 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.036436 | 0.113843 | -0.119423 |
| C | -0.000416 | -0.036345 | 1.335016 |
| N | 1.206319 | -0.010536 | 2.006850 |
| C | 2.287499 | -0.270687 | 1.307750 |
| C | 2.195771 | -0.871493 | -0.119645 |
| C | 0.983478 | -0.268697 | -0.775815 |
| N | 3.492837 | -0.532419 | -0.607913 |
| C | 4.334607 | -0.343425 | 0.544356 |
| N | 3.561554 | -0.129829 | 1.674608 |
| O | -1.081718 | -0.094820 | 1.903815 |
| O | 1.020688 | -0.166087 | -2.125901 |
| O | 1.942745 | -2.289229 | -0.077769 |
| H | 2.449806 | -2.624848 | 0.676455 |
| H | 0.162246 | 0.229117 | -2.358324 |
| O | 5.554829 | -0.349859 | 0.456199 |
| H | 3.884377 | -1.097040 | -1.350603 |

HIU-79

$E_{el}$= -712.3276375120 Hartree

$\Delta E_{el}$= 12.82 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | 0.023534 | 0.015517 | -0.084721 |
| C | -0.000744 | 0.036100 | 1.292015 |
| N | 1.256483 | 0.138572 | 2.058948 |
| C | 2.264287 | -0.349969 | 1.465029 |
| C | 2.233884 | -1.033100 | 0.120569 |
| C | 1.111054 | -0.397670 | -0.736247 |
| N | 3.586526 | -0.808955 | -0.345147 |
| C | 4.397042 | -0.277236 | 0.625866 |
| N | 3.609546 | -0.203736 | 1.800695 |
| O | -1.034841 | 0.081070 | 1.946061 |
| O | 1.286287 | -0.461122 | -1.970728 |
| O | 1.947288 | -2.423122 | 0.268151 |
| H | 1.565644 | -2.689786 | -0.581839 |
| H | 3.902767 | 0.422541 | 2.537060 |
| O | 5.559705 | 0.082230 | 0.535403 |
| H | 3.780749 | -0.705010 | -1.329993 |

HIU-81

$E_{el}$= -712.3177930690 Hartree

$\Delta E_{el}$= 19.00 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | -0.119121 | -0.138058 | 0.043659 |
| C | -0.066814 | -0.008138 | 1.372771 |
| C | 1.413218 | 0.103547 | 1.808365 |
| N | 2.158936 | -0.215173 | 0.620523 |
| C | 1.209157 | -0.260846 | -0.281811 |
| C | 1.666754 | -0.719398 | 3.073203 |
| N | 0.531409 | -0.776031 | 3.843509 |
| C | -0.788522 | -0.271746 | 3.521021 |
| N | -1.081961 | -0.011113 | 2.214460 |
| O | -1.579723 | -0.211483 | 4.457286 |
| O | 1.659303 | 1.471139 | 2.217896 |
| O | 2.747463 | -1.167900 | 3.433313 |
| O | 1.513338 | -0.464157 | -1.583269 |
| H | 2.606419 | 1.575620 | 2.043684 |
| H | 2.480363 | -0.539383 | -1.587495 |
| H | 0.628763 | -1.113782 | 4.792168 |

HIU-82

$E_{el}$= -712.2923326630 Hartree

$\Delta E_{el}$= 34.98 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | -0.056729 | -0.029644 | 0.008054 |
| C | 0.098882 | 0.005572 | 1.336099 |
| N | 1.184119 | -0.006719 | 2.120176 |
| C | 2.299664 | -0.244222 | 1.423659 |
| C | 2.258823 | -0.879280 | 0.028813 |
| C | 1.033068 | -0.352442 | -0.760815 |
| N | 3.595043 | -0.658664 | -0.487964 |
| C | 4.206370 | -0.170244 | 0.549482 |
| N | 3.534156 | 0.110567 | 1.735076 |
| O | -1.065507 | 0.178059 | 2.013819 |
| O | 1.015007 | -0.397731 | -1.988955 |
| O | 1.992885 | -2.290568 | 0.175536 |
| H | 2.014191 | -2.616434 | -0.737088 |
| H | -1.723341 | 0.207803 | 1.299616 |
| O | 5.525851 | 0.126489 | 0.516288 |
| H | 5.796070 | -0.120698 | -0.381943 |

HIU-83

| $E_{el}$= -712.3047320340 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 27.20 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.052098 | -0.001177 | -0.003438 |
| C | -0.063934 | 0.065555 | 1.337331 |
| N | 1.180706 | -0.230490 | 2.100621 |
| C | 2.337434 | -0.360954 | 1.440376 |
| C | 2.276542 | -0.928866 | 0.040983 |
| C | 1.024393 | -0.390427 | -0.725314 |
| N | 3.607677 | -0.631935 | -0.475509 |
| C | 4.217107 | -0.160410 | 0.562166 |
| N | 3.535983 | 0.048998 | 1.773280 |
| O | -1.004304 | 0.398884 | 2.054089 |
| O | 1.039235 | -0.512008 | -1.954247 |
| O | 2.061840 | -2.344328 | 0.110585 |
| H | 1.886353 | -2.583352 | -0.813425 |
| H | 1.189323 | 0.219418 | 3.008601 |
| O | 5.518598 | 0.200524 | 0.541749 |
| H | 5.803319 | 0.006905 | -0.364986 |

HIU-86

$E_{el}$= -712.2831354400 Hartree

$\Delta E_{el}$= 40.75 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | 2.029284 | 0.608287 | -0.404916 |
| C | 2.141037 | -0.712261 | -0.173893 |
| C | 0.749227 | -1.359761 | -0.379512 |
| N | -0.164843 | -0.245051 | -0.469919 |
| C | 0.670707 | 0.761839 | -0.542094 |
| C | 0.608939 | -2.381780 | 0.724468 |
| N | 1.611154 | -3.003358 | 1.212650 |
| C | 2.941769 | -2.654539 | 0.720830 |
| N | 3.190057 | -1.382562 | 0.226261 |
| O | 3.818724 | -3.494255 | 0.865757 |
| O | 0.711919 | -2.115267 | -1.614808 |
| O | -0.643124 | -2.689750 | 1.129216 |
| O | 0.219311 | 2.022496 | -0.737039 |
| H | -0.043911 | -1.705111 | -2.062036 |
| H | -0.508135 | -3.403392 | 1.778021 |
| H | 1.030650 | 2.553774 | -0.729116 |

HIU-87

$E_{el}$= -712.2832201340 Hartree

$\Delta E_{el}$= 40.69 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | 0.010599 | -0.034748 | -0.093766 |
| C | 0.023673 | -0.098925 | 1.290066 |
| N | 1.271849 | 0.189579 | 2.010779 |
| C | 2.315890 | -0.204336 | 1.401629 |
| C | 2.243294 | -0.975836 | 0.093388 |
| C | 1.128849 | -0.313686 | -0.756864 |
| N | 3.589312 | -0.782770 | -0.447319 |
| C | 4.263167 | -0.098728 | 0.562111 |
| N | 3.652430 | 0.163376 | 1.671173 |
| O | -0.986201 | -0.258506 | 1.963533 |
| O | 1.363971 | -0.189775 | -1.980084 |
| O | 1.952113 | -2.346292 | 0.320747 |
| H | 1.469827 | -2.655186 | -0.458820 |
| H | 3.535012 | -0.358584 | -1.376789 |
| O | 5.552981 | 0.237767 | 0.355163 |
| H | 5.843963 | -0.242769 | -0.433253 |

HIU-89

| $E_{el}$= -712.2830435530 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 40.81 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -1.440351 | -1.442432 | 0.196263 |
| C | -0.123049 | -0.937204 | 0.245652 |
| C | -0.271953 | 0.564967 | 0.379581 |
| N | -1.649212 | 0.827960 | -0.094774 |
| C | -2.200357 | -0.322811 | -0.143955 |
| C | 0.901229 | 1.260322 | -0.375702 |
| N | 2.028848 | 0.558936 | -0.564551 |
| C | 2.134864 | -0.754841 | -0.200849 |
| N | 0.927738 | -1.588888 | -0.020053 |
| O | 3.203967 | -1.347407 | -0.094370 |
| O | -0.154999 | 0.978335 | 1.739381 |
| O | 0.752487 | 2.476473 | -0.584662 |
| O | -3.485467 | -0.556842 | -0.493022 |
| H | 0.033002 | 1.928454 | 1.657731 |
| H | -3.843409 | 0.323822 | -0.688039 |
| H | -1.608649 | -2.333829 | -0.252124 |

HIU-91

| $E_{el}$= -712.3349901260 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 8.21 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.029810 | 0.009262 | 0.041224 |
| C | -0.047476 | 0.063784 | 1.466236 |
| N | 1.162112 | 0.029334 | 2.136418 |
| C | 2.198989 | -0.287919 | 1.411157 |
| C | 2.217309 | -0.867689 | -0.011918 |
| C | 1.024015 | -0.316832 | -0.801595 |
| N | 3.521221 | -0.675431 | -0.529457 |
| C | 4.319827 | -0.330886 | 0.482447 |
| N | 3.484258 | -0.160845 | 1.725303 |
| O | -1.128654 | 0.229224 | 2.014403 |
| O | 0.920313 | -0.254442 | -2.013830 |
| O | 1.899801 | -2.292383 | 0.108447 |
| H | 2.623192 | -2.668013 | -0.418615 |
| H | 3.829913 | 0.269409 | 2.570777 |
| O | 5.525849 | -0.123359 | 0.564743 |
| H | -0.920740 | 0.201966 | -0.398652 |

HIU-92

$E_{el}$= -712.3013817820 Hartree

$\Delta E_{el}$= 29.30 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| N | -0.158555 | -0.059208 | 0.011326 |
| C | -0.010489 | 0.002672 | 1.301022 |
| N | 1.123758 | 0.033250 | 2.096507 |
| C | 2.200363 | -0.284311 | 1.417667 |
| C | 2.197555 | -0.855761 | -0.000730 |
| C | 0.987425 | -0.269982 | -0.766682 |
| N | 3.512523 | -0.688337 | -0.514830 |
| C | 4.319060 | -0.349013 | 0.482624 |
| N | 3.472112 | -0.150693 | 1.744568 |
| O | -1.139821 | 0.150809 | 2.036332 |
| O | 0.986996 | -0.092495 | -1.971497 |
| O | 1.871339 | -2.279458 | 0.129693 |
| H | 2.599299 | -2.661711 | -0.385087 |
| H | 3.819651 | 0.278950 | 2.590140 |
| O | 5.525506 | -0.153983 | 0.580522 |
| H | -0.816808 | 0.214260 | 2.949044 |

HIU-96

| $E_{el}$= -712.3105595830 Hartree | | | |
|---|---|---|---|
| $\Delta E_{el}$= 23.54 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.101064 | 0.168757 | -0.048085 |
| C | -0.081010 | 0.028422 | 1.383322 |
| N | 1.160843 | 0.115325 | 2.075345 |
| C | 2.170257 | -0.298016 | 1.387019 |
| C | 2.076518 | -0.964142 | 0.023077 |
| C | 0.930121 | -0.258049 | -0.672636 |
| N | 3.336780 | -0.811402 | -0.617659 |
| C | 4.208956 | -0.366647 | 0.308876 |
| N | 3.495922 | -0.178003 | 1.601947 |
| O | -1.131429 | -0.032704 | 1.993540 |
| O | 1.094561 | -0.101172 | -1.992082 |
| O | 1.700996 | -2.356622 | 0.152582 |
| H | 2.506643 | -2.794288 | -0.161768 |
| H | 3.902497 | 0.375321 | 2.342488 |
| O | 5.404550 | -0.111187 | 0.243913 |
| H | 2.043525 | -0.331774 | -2.121274 |

## 1.2 Coordinates of optimized HIU tautomers in solution - PCM/B3LYP/6-31+G**

Data in Å

HIU-71

| $G_{PCM}$= -712.4207880000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 0.00 kcal/mol | | | |
| Atom | X | Y | Z |
| N | 1.951622 | 0.557829 | -0.347803 |
| C | 2.061635 | -0.855386 | -0.098599 |
| N | 0.927058 | -1.610471 | -0.047364 |
| C | -0.232392 | -0.969562 | -0.024870 |
| C | -0.333636 | 0.524571 | 0.342394 |
| C | 0.813630 | 1.312944 | -0.289336 |
| N | -1.652927 | 0.798837 | -0.124811 |
| C | -2.332721 | -0.427908 | -0.282911 |
| N | -1.425689 | -1.491941 | -0.263322 |
| O | 3.201896 | -1.310506 | -0.031296 |
| O | 0.742658 | 2.485226 | -0.628622 |
| O | -0.139221 | 0.741041 | 1.742560 |
| H | -0.748253 | 0.154977 | 2.218180 |
| H | 2.814221 | 1.018860 | -0.613251 |
| O | -3.542084 | -0.511807 | -0.459414 |
| H | -2.161596 | 1.605502 | 0.211254 |

HIU-72

| $G_{PCM}$= -712.3994600000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 13.38 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.099109 | 0.029929 | -0.042610 |
| C | 0.067402 | -0.019190 | 1.282757 |
| N | 1.178634 | -0.076115 | 2.039620 |
| C | 2.284389 | -0.313146 | 1.326755 |
| C | 2.178786 | -0.874915 | -0.096366 |
| C | 0.989377 | -0.224050 | -0.828795 |
| N | 3.505323 | -0.593836 | -0.552263 |
| C | 4.322100 | -0.332937 | 0.556562 |
| N | 3.528826 | -0.114585 | 1.702953 |
| O | -1.059109 | 0.098842 | 2.008353 |
| O | 1.022945 | -0.035936 | -2.043450 |
| O | 1.845399 | -2.266762 | -0.090837 |
| H | 2.489806 | -2.721002 | 0.474191 |
| H | -1.785412 | 0.173794 | 1.367032 |
| O | 5.542972 | -0.256834 | 0.512129 |
| H | 3.890170 | -1.041236 | -1.372342 |

HIU-73

| $G_{PCM}$= -712.4126080000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 5.13 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.061212 | 0.063262 | -0.056022 |
| C | -0.072387 | -0.000024 | 1.295927 |
| N | 1.179199 | -0.183983 | 2.022386 |
| C | 2.328814 | -0.373406 | 1.360295 |
| C | 2.173334 | -0.965690 | -0.027451 |
| C | 1.045198 | -0.218506 | -0.777451 |
| N | 3.520491 | -0.820869 | -0.476538 |
| C | 4.329106 | -0.319793 | 0.537305 |
| N | 3.550908 | -0.104412 | 1.714535 |
| O | -1.066688 | 0.161595 | 2.003886 |
| O | 1.181881 | 0.003769 | -1.986058 |
| O | 1.727462 | -2.319996 | 0.017584 |
| H | 2.431569 | -2.839181 | 0.436614 |
| H | 1.183428 | 0.154906 | 2.977215 |
| O | 5.519345 | -0.070153 | 0.435256 |
| H | 3.781669 | -0.801004 | -1.450784 |

HIU-76

| $G_{PCM}$= -712.4055030000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 9.59 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.053550 | -0.031774 | -0.049026 |
| C | -0.023299 | 0.012927 | 1.322822 |
| N | 1.225397 | 0.142101 | 2.057779 |
| C | 2.253517 | -0.264291 | 1.423842 |
| C | 2.226792 | -0.931070 | 0.063365 |
| C | 1.038992 | -0.376255 | -0.747647 |
| N | 3.557479 | -0.619399 | -0.410275 |
| C | 4.399130 | -0.287573 | 0.624801 |
| N | 3.577363 | -0.120887 | 1.761639 |
| O | -1.055184 | 0.048413 | 1.998125 |
| O | 1.129647 | -0.405857 | -1.988343 |
| O | 2.027392 | -2.331152 | 0.255642 |
| H | 1.752308 | -2.694075 | -0.600865 |
| H | 3.903198 | 0.390554 | 2.570826 |
| O | 5.606047 | -0.122841 | 0.596538 |
| H | 3.923982 | -0.982500 | -1.278102 |

HIU-91

| $G_{PCM}$= -712.4074560000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 8.37 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.035275 | 0.000065 | 0.031319 |
| C | -0.045281 | 0.037807 | 1.453033 |
| N | 1.162686 | 0.015028 | 2.129186 |
| C | 2.206434 | -0.280276 | 1.406393 |
| C | 2.212231 | -0.866873 | -0.008925 |
| C | 1.030255 | -0.295331 | -0.797145 |
| N | 3.519082 | -0.684949 | -0.529426 |
| C | 4.308922 | -0.325441 | 0.485725 |
| N | 3.492080 | -0.135600 | 1.712504 |
| O | -1.123687 | 0.176918 | 2.016076 |
| O | 0.964288 | -0.199968 | -2.012230 |
| O | 1.868226 | -2.278611 | 0.124907 |
| H | 2.590420 | -2.711138 | -0.358279 |
| H | 3.848988 | 0.279003 | 2.563216 |
| O | 5.522686 | -0.122442 | 0.540732 |
| H | -0.921935 | 0.216987 | -0.409996 |

## 1.3 Coordinates of Optimized OHCU tautomers in solution - PCM/B3LYP/6-31G**

| OHCU-182 | | | |
|---|---|---|---|
| $G_{PCM}$= -788.8197040000 Hartree | | | |
| $\Delta G_{PCM}$= 40.67 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.099338 | 0.110979 | 0.035230 |
| N | -0.019086 | 0.259090 | 1.297832 |
| C | 1.334813 | 0.053747 | 1.847249 |
| C | 2.185990 | -0.390532 | 0.646537 |
| N | 1.358475 | -0.261965 | -0.434569 |
| O | 1.370469 | -0.856085 | 2.900297 |
| C | 1.882594 | 1.458164 | 2.385982 |
| O | 2.135418 | 1.426511 | 3.622521 |
| N | 3.417457 | -0.769942 | 0.750289 |
| C | 4.189797 | -1.145064 | -0.336010 |
| O | 3.597863 | -1.063355 | -1.568201 |
| O | -0.842926 | 0.258831 | -0.901290 |
| N | 5.400946 | -1.555432 | -0.267395 |
| O | 1.990935 | 2.387040 | 1.567315 |
| H | 1.610328 | -0.479941 | -1.388650 |
| H | 4.258781 | -1.359111 | -2.214509 |
| H | 5.685468 | -1.555525 | 0.712251 |
| H | -1.663838 | 0.519032 | -0.452945 |
| H | 1.680587 | -0.260047 | 3.630706 |

OHCU-183

| $G_{PCM}$= -788.8525770000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 20.05 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.035013 | 0.058532 | -0.055361 |
| N | 0.021066 | 0.102557 | 1.308884 |
| C | 1.364534 | 0.011750 | 1.884211 |
| C | 2.175841 | -0.411766 | 0.654614 |
| N | 1.341014 | -0.322715 | -0.420008 |
| O | 1.454209 | -0.891827 | 2.935129 |
| C | 1.860973 | 1.439425 | 2.402844 |
| O | 2.211472 | 1.411956 | 3.613955 |
| N | 3.415402 | -0.759066 | 0.760288 |
| C | 4.193805 | -1.142027 | -0.320819 |
| O | 3.582035 | -1.153654 | -1.544652 |
| O | -0.874448 | 0.276417 | -0.839838 |
| N | 5.425982 | -1.480019 | -0.248489 |
| O | 1.835426 | 2.375383 | 1.585678 |
| H | 1.616384 | -0.530803 | -1.369925 |
| H | 4.249682 | -1.439738 | -2.188542 |
| H | 5.721325 | -1.417702 | 0.725887 |
| H | -0.708477 | 0.630942 | 1.766493 |
| H | 1.801274 | -0.293660 | 3.647005 |

OHCU-21

| $G_{PCM}$= -788.8516550000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 20.62 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.122991 | 0.067383 | 0.033682 |
| N | -0.009390 | 0.257633 | 1.290398 |
| C | 1.335843 | 0.054652 | 1.865642 |
| C | 2.191129 | -0.432956 | 0.688784 |
| N | 1.383431 | -0.333179 | -0.405104 |
| O | 1.347951 | -0.824596 | 2.945739 |
| C | 1.889477 | 1.468918 | 2.370779 |
| O | 2.119995 | 1.472680 | 3.612149 |
| N | 3.421731 | -0.826109 | 0.778385 |
| C | 4.069028 | -1.224845 | -0.401490 |
| O | 3.581879 | -1.238184 | -1.546096 |
| O | -0.808754 | 0.195507 | -0.916492 |
| N | 5.349610 | -1.609322 | -0.167874 |
| O | 2.022080 | 2.371523 | 1.526665 |
| H | 1.696654 | -0.600625 | -1.332342 |
| H | 5.904161 | -1.971576 | -0.926670 |
| H | 5.705230 | -1.646282 | 0.773535 |
| H | -1.630683 | 0.477954 | -0.483738 |
| H | 1.648187 | -0.208852 | 3.663739 |

OHCU-26

| $G_{PCM}$= -788.8469880000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 23.55 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.068839 | 0.067387 | 0.068803 |
| N | -0.039501 | 0.195060 | 1.347744 |
| C | 1.336032 | 0.034992 | 1.815511 |
| C | 2.059979 | -0.393242 | 0.546079 |
| N | 1.301889 | -0.306195 | -0.507043 |
| O | 1.530569 | -0.850411 | 2.878408 |
| C | 1.885758 | 1.477353 | 2.287403 |
| O | 2.232435 | 1.464392 | 3.501910 |
| N | 3.357786 | -0.793634 | 0.638234 |
| C | 4.236994 | -1.126544 | -0.408269 |
| O | 3.971526 | -0.949943 | -1.588339 |
| O | -0.934010 | 0.240576 | -0.806373 |
| N | 5.434120 | -1.611206 | 0.037909 |
| O | 1.905122 | 2.396793 | 1.455376 |
| H | 3.668326 | -0.920793 | 1.595381 |
| H | 6.041198 | -1.992369 | -0.672180 |
| H | 5.537780 | -1.993693 | 0.966246 |
| H | -1.720198 | 0.490971 | -0.295626 |
| H | 1.837405 | -0.213096 | 3.577987 |

OHCU-283

$G_{PCM}$= -788.8168120000 Hartree

$\Delta G_{PCM}$= 42.49 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.229471 | -0.263786 | 0.105348 |
| N | 0.117031 | 0.000668 | 1.430477 |
| C | 1.489091 | 0.129332 | 1.960187 |
| C | 2.267495 | -0.375071 | 0.731712 |
| N | 1.426990 | -0.558792 | -0.351043 |
| O | 1.709798 | -0.612846 | 3.111631 |
| C | 1.816983 | 1.656486 | 2.270086 |
| O | 2.248534 | 1.823733 | 3.444020 |
| N | 3.533526 | -0.590213 | 0.791025 |
| C | 4.213160 | -1.067041 | -0.326299 |
| O | 4.580352 | -0.068399 | -1.172042 |
| O | -0.816975 | -0.270710 | -0.712661 |
| N | 4.596114 | -2.266092 | -0.557357 |
| O | 1.611394 | 2.477485 | 1.359155 |
| H | -1.643201 | -0.120129 | -0.227872 |
| H | 5.109861 | -0.487844 | -1.870199 |
| H | 4.247454 | -2.877146 | 0.181396 |
| H | -0.618515 | 0.603917 | 1.777387 |
| H | 2.008957 | 0.106809 | 3.726106 |

OHCU-28

| $G_{PCM}$= -788.8154970000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 43.31 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.188604 | 0.216844 | -0.022790 |
| N | -0.005418 | 0.243829 | 1.251400 |
| C | 1.332915 | -0.002038 | 1.797287 |
| C | 2.160242 | -0.300162 | 0.543745 |
| N | 1.448703 | -0.113591 | -0.543211 |
| O | 1.381204 | -1.014682 | 2.762456 |
| C | 1.864619 | 1.346714 | 2.481602 |
| O | 2.117575 | 1.189754 | 3.710737 |
| N | 3.479491 | -0.594395 | 0.660702 |
| C | 4.170842 | -1.226892 | -0.241107 |
| O | 3.604738 | -1.894653 | -1.259155 |
| O | -0.762727 | 0.475435 | -0.941097 |
| N | 5.522461 | -1.243515 | -0.162741 |
| O | 1.964247 | 2.365164 | 1.775428 |
| H | 4.269324 | -2.303835 | -1.833966 |
| H | 6.062238 | -1.961248 | -0.624448 |
| H | 5.926802 | -0.845518 | 0.671981 |
| H | -1.573214 | 0.689349 | -0.452210 |
| H | 1.679459 | -0.486810 | 3.547114 |

OHCU-31

| $G_{PCM}$= -788.8845220000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 0.00 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.056029 | -0.004077 | -0.054739 |
| N | 0.028310 | 0.096827 | 1.308829 |
| C | 1.364893 | 0.009933 | 1.903542 |
| C | 2.176206 | -0.471493 | 0.699072 |
| N | 1.358958 | -0.417375 | -0.386646 |
| O | 1.431834 | -0.855281 | 2.988972 |
| C | 1.875148 | 1.449164 | 2.373671 |
| O | 2.209279 | 1.463764 | 3.589705 |
| N | 3.412682 | -0.839762 | 0.792525 |
| C | 4.066114 | -1.255445 | -0.380514 |
| O | 3.575400 | -1.310426 | -1.521290 |
| O | -0.845117 | 0.195441 | -0.853832 |
| N | 5.349354 | -1.619716 | -0.135823 |
| O | 1.873918 | 2.353612 | 1.521266 |
| H | 1.691262 | -0.685565 | -1.307094 |
| H | 5.943221 | -1.886152 | -0.904629 |
| H | 5.741295 | -1.513715 | 0.785766 |
| H | -0.694077 | 0.661853 | 1.732797 |
| H | 1.774944 | -0.234274 | 3.682828 |

OHCU-32

| $G_{PCM}$= -788.8470840000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 23.49 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.287604 | -0.282070 | 0.058939 |
| N | 0.119741 | -0.092530 | 1.383696 |
| C | 1.461547 | 0.103457 | 1.961874 |
| C | 2.312851 | -0.301436 | 0.739553 |
| N | 1.513010 | -0.481773 | -0.378376 |
| O | 1.694336 | -0.666451 | 3.093306 |
| C | 1.682083 | 1.634829 | 2.337143 |
| O | 2.060349 | 1.786364 | 3.531812 |
| N | 3.584325 | -0.447572 | 0.833621 |
| C | 4.345557 | -0.740619 | -0.312227 |
| O | 4.602315 | 0.076843 | -1.197197 |
| O | -0.787193 | -0.288871 | -0.718154 |
| N | 4.898972 | -1.988060 | -0.282800 |
| O | 1.458336 | 2.475347 | 1.448280 |
| H | -0.491350 | -0.434710 | -1.632231 |
| H | 5.401216 | -2.304784 | -1.097926 |
| H | 4.565966 | -2.677093 | 0.373233 |
| H | -0.687075 | 0.410474 | 1.729154 |
| H | 1.928203 | 0.046858 | 3.742082 |

OHCU-38

| $G_{PCM}$= -788.8447770000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 24.94 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.144799 | 0.209087 | -0.125336 |
| N | 0.038343 | 0.103374 | 1.250998 |
| C | 1.363324 | -0.028313 | 1.833159 |
| C | 2.151678 | -0.306221 | 0.550623 |
| N | 1.446771 | -0.155888 | -0.541165 |
| O | 1.473550 | -1.057083 | 2.775433 |
| C | 1.843144 | 1.326413 | 2.520049 |
| O | 2.226022 | 1.159359 | 3.712514 |
| N | 3.469292 | -0.588961 | 0.677000 |
| C | 4.165640 | -1.242438 | -0.209813 |
| O | 3.597468 | -1.982649 | -1.171958 |
| O | -0.760808 | 0.550842 | -0.879694 |
| N | 5.513056 | -1.210985 | -0.152971 |
| O | 1.782745 | 2.365532 | 1.837577 |
| H | 4.256044 | -2.418908 | -1.733682 |
| H | 6.088728 | -1.879730 | -0.642389 |
| H | 5.928770 | -0.729602 | 0.630150 |
| H | -0.672326 | 0.658071 | 1.709057 |
| H | 1.824967 | -0.544564 | 3.546886 |

OHCU-63

| $G_{PCM}$= -788.8756320000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 5.58 kcal/mol | | | |
| Atom | X | Y | Z |
| N | 0.220218 | -0.158888 | -0.328995 |
| C | -0.011864 | -0.284305 | 1.098577 |
| C | 1.442490 | -0.379743 | 1.543364 |
| N | 2.313786 | -0.084225 | 0.631057 |
| C | 1.551957 | 0.175404 | -0.542129 |
| O | -0.761536 | -1.390544 | 1.505554 |
| N | 1.654901 | -0.780436 | 2.825943 |
| C | 2.884981 | -0.891671 | 3.504806 |
| N | 2.752246 | -1.430573 | 4.751345 |
| O | 2.016790 | 0.599842 | -1.590109 |
| O | 3.944592 | -0.498490 | 3.040935 |
| H | 0.810587 | -1.099196 | 3.288891 |
| H | 3.612673 | -1.649191 | 5.230480 |
| H | 1.936325 | -1.958090 | 5.024327 |
| C | -0.715999 | 1.027669 | 1.694771 |
| O | -0.192116 | 2.121270 | 1.430180 |
| O | -1.748729 | 0.747012 | 2.363754 |
| H | -0.463499 | 0.311989 | -0.907448 |
| H | -1.506264 | -0.929145 | 1.976527 |

OHCU-682

| $G_{PCM}$= -788.8179430000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 41.78 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.077627 | 0.069620 | 0.057204 |
| N | -0.038100 | 0.199041 | 1.335428 |
| C | 1.334508 | 0.041874 | 1.811269 |
| C | 2.064735 | -0.391593 | 0.547704 |
| N | 1.313536 | -0.307209 | -0.510259 |
| O | 1.527002 | -0.837898 | 2.878798 |
| C | 1.880650 | 1.488243 | 2.279242 |
| O | 2.219084 | 1.481217 | 3.495860 |
| N | 3.362551 | -0.791884 | 0.659830 |
| C | 4.298977 | -1.160266 | -0.306016 |
| O | 3.875720 | -0.911619 | -1.556706 |
| O | -0.919065 | 0.243166 | -0.824142 |
| N | 5.451091 | -1.661740 | -0.082795 |
| O | 1.904869 | 2.402724 | 1.442148 |
| H | 3.647916 | -0.937964 | 1.621602 |
| H | 4.595715 | -1.198334 | -2.142131 |
| H | 5.623667 | -1.795469 | 0.912424 |
| H | -1.707853 | 0.496176 | -0.318681 |
| H | 1.828186 | -0.196709 | 3.577523 |

OHCU-863

$G_{PCM}$= -788.8466250000 Hartree

$\Delta G_{PCM}$= 23.78 kcal/mol

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.018424 | 0.008093 | -0.017499 |
| N | 0.006122 | -0.001910 | 1.372022 |
| C | 1.375230 | -0.001906 | 1.855437 |
| C | 2.057974 | -0.413150 | 0.557215 |
| N | 1.304842 | -0.367495 | -0.495607 |
| O | 1.660822 | -0.881251 | 2.902152 |
| C | 1.832132 | 1.466030 | 2.313296 |
| O | 2.307147 | 1.469680 | 3.482370 |
| N | 3.360344 | -0.796671 | 0.667410 |
| C | 4.288581 | -1.190101 | -0.298923 |
| O | 3.852614 | -0.981345 | -1.551823 |
| O | -0.938462 | 0.265746 | -0.732796 |
| N | 5.444994 | -1.676450 | -0.069060 |
| O | 1.659868 | 2.390068 | 1.502969 |
| H | 3.655711 | -0.917016 | 1.629876 |
| H | 4.569696 | -1.279265 | -2.135402 |
| H | 5.627518 | -1.778362 | 0.928171 |
| H | -0.683384 | 0.585335 | 1.823255 |
| H | 1.989137 | -0.235561 | 3.584123 |

OHCU-86

| $G_{PCM}$= -788.7918780000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 58.13 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -0.031089 | 1.625272 | 0.022598 |
| C | -1.541702 | 1.741552 | -0.153914 |
| N | -2.110961 | 0.590396 | -0.505240 |
| C | -1.090118 | -0.418561 | -0.466549 |
| C | 0.162836 | 0.393051 | -0.210302 |
| O | -2.053273 | 2.861620 | 0.023811 |
| O | -0.911047 | -1.203410 | -1.643344 |
| C | -1.346957 | -1.455588 | 0.719469 |
| O | -1.331148 | -1.032238 | 1.890592 |
| N | 1.381728 | -0.304386 | -0.330610 |
| C | 2.612507 | 0.061503 | 0.024257 |
| N | 3.661840 | -0.694485 | -0.269629 |
| O | -1.556847 | -2.636089 | 0.303456 |
| O | 2.732629 | 1.188767 | 0.683833 |
| H | 3.652694 | 1.392084 | 0.917629 |
| H | 4.594492 | -0.444461 | 0.027462 |
| H | 3.558362 | -1.560172 | -0.781091 |
| H | -1.198304 | -2.087038 | -1.290856 |
| H | 1.260222 | -1.178930 | -0.837518 |

## 1.4 Coordinates of Optimized Allantoin conformers in solution - PCM/B3LYP/6-31G**

Data in Å

ALL-C1

| $G_{PCM}$= -600.7925850000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 3.28 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.906275 | 1.196246 | 0.230207 |
| C | 0.016100 | -0.074276 | 0.305238 |
| C | 2.259978 | -0.656979 | -0.121657 |
| N | 0.972784 | -1.115016 | -0.056242 |
| N | 2.184562 | 0.743515 | 0.036717 |
| H | 2.991824 | 1.342586 | -0.074160 |
| H | 0.793466 | -2.099904 | 0.078134 |
| O | 3.284111 | -1.292047 | -0.290322 |
| O | 0.523047 | 2.344184 | 0.319777 |
| H | -0.316612 | -0.180403 | 1.343294 |
| N | -1.139205 | 0.021368 | -0.538061 |
| H | -1.043502 | 0.497242 | -1.424943 |
| C | -2.457479 | -0.206364 | -0.185171 |
| O | -3.374782 | 0.172653 | -0.911516 |
| N | -2.673484 | -0.833715 | 1.022074 |
| H | -3.637650 | -1.105414 | 1.155189 |
| H | -2.008381 | -1.517268 | 1.355850 |

ALL-C2

| $G_{PCM}$= -600.7942050000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 2.26 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.527605 | 1.263366 | -0.032535 |
| C | 0.055602 | 0.225615 | 1.023682 |
| C | 2.028312 | -0.504815 | -0.031778 |
| N | 0.959879 | -0.891139 | 0.753561 |
| N | 1.714080 | 0.773379 | -0.523583 |
| H | 2.275312 | 1.232116 | -1.229563 |
| H | 1.118902 | -1.608194 | 1.449967 |
| O | 3.036912 | -1.134794 | -0.281407 |
| O | -0.031532 | 2.297421 | -0.329089 |
| H | 0.251525 | 0.658774 | 2.011215 |
| N | -1.346215 | -0.096816 | 0.991132 |
| H | -1.913709 | 0.325384 | 1.711817 |
| C | -2.082021 | -0.442180 | -0.135769 |
| O | -3.302726 | -0.301965 | -0.163965 |
| N | -1.346124 | -0.927149 | -1.189750 |
| H | -1.907410 | -1.322003 | -1.931463 |
| H | -0.494179 | -1.431221 | -0.977411 |

ALL-C3

| $G_{PCM}$= -600.7960360000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 1.11 kcal/mol | | | |
| Atom | X | Y | Z |
| N | 1.959026 | 0.873210 | -0.316209 |
| C | 0.636263 | 1.101245 | -0.062527 |
| C | 0.066718 | -0.229600 | 0.483284 |
| N | 1.216225 | -1.098873 | 0.400945 |
| C | 2.356086 | -0.443091 | 0.003187 |
| O | 0.003377 | 2.129387 | -0.230423 |
| N | -1.039844 | -0.721069 | -0.324076 |
| C | -2.370723 | -0.413015 | -0.106861 |
| N | -2.582223 | 0.739813 | 0.615078 |
| O | 3.486825 | -0.879245 | -0.070804 |
| O | -3.275199 | -1.138245 | -0.521731 |
| H | 2.602081 | 1.555151 | -0.697063 |
| H | 1.289521 | -1.961411 | 0.921846 |
| H | -0.267366 | -0.067763 | 1.516802 |
| H | -0.878887 | -1.586165 | -0.820991 |
| H | -3.551647 | 1.023635 | 0.643220 |
| H | -1.916080 | 1.496577 | 0.487188 |

ALL-C4

| $G_{PCM}$= -600.7916320000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 3.88 kcal/mol | | | |
| Atom | X | Y | Z |
| N | -1.804966 | 0.714947 | 0.338176 |
| C | -0.680491 | 1.201419 | -0.269590 |
| C | -0.077221 | 0.009294 | -1.050303 |
| N | -0.867175 | -1.105046 | -0.524980 |
| C | -1.955652 | -0.681376 | 0.190711 |
| O | -0.234131 | 2.332463 | -0.214942 |
| N | 1.355476 | -0.122294 | -0.965403 |
| C | 2.095096 | -0.319391 | 0.203787 |
| N | 1.633611 | 0.335335 | 1.320535 |
| O | -2.876303 | -1.339909 | 0.635199 |
| O | 3.093018 | -1.034979 | 0.201521 |
| H | -2.407797 | 1.262463 | 0.938478 |
| H | -0.906273 | -1.999419 | -0.994549 |
| H | -0.304664 | 0.176982 | -2.110034 |
| H | 1.762221 | -0.644474 | -1.731117 |
| H | 2.267537 | 0.273508 | 2.105677 |
| H | 1.219286 | 1.250067 | 1.191393 |

ALL-T1

| $G_{PCM}$= -600.7978080000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 0.00 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.965327 | 1.220978 | 0.099389 |
| C | 0.022184 | 0.016010 | 0.333631 |
| C | 2.220312 | -0.725054 | -0.080250 |
| N | 0.914843 | -1.108567 | 0.069963 |
| N | 2.214284 | 0.684755 | -0.091439 |
| H | 3.047064 | 1.226782 | -0.279290 |
| H | 0.700583 | -2.051803 | 0.361419 |
| O | 3.208435 | -1.427231 | -0.193691 |
| O | 0.651241 | 2.393830 | 0.088997 |
| H | -0.323457 | 0.024678 | 1.372853 |
| N | -1.154374 | 0.064166 | -0.479165 |
| H | -1.032591 | 0.059919 | -1.482877 |
| C | -2.393402 | -0.243470 | 0.059559 |
| O | -2.557230 | -0.446351 | 1.263420 |
| N | -3.408731 | -0.329799 | -0.856750 |
| H | -4.337080 | -0.332952 | -0.460316 |
| H | -3.322768 | 0.126737 | -1.753836 |

ALL-T2

| $G_{PCM}$= -600.7973760000 Hartree | | | |
|---|---|---|---|
| $\Delta G_{PCM}$= 0.27 kcal/mol | | | |
| Atom | X | Y | Z |
| C | 0.630648 | 1.247626 | 0.093767 |
| C | 0.070916 | 0.180559 | 1.071553 |
| C | 1.942503 | -0.659390 | -0.087438 |
| N | 0.919831 | -0.965209 | 0.766387 |
| N | 1.744160 | 0.679200 | -0.473490 |
| H | 2.313529 | 1.126227 | -1.178929 |
| H | 0.976075 | -1.783438 | 1.355093 |
| O | 2.858456 | -1.373269 | -0.457734 |
| O | 0.202004 | 2.369930 | -0.076893 |
| H | 0.244910 | 0.537995 | 2.092249 |
| N | -1.343672 | -0.023943 | 0.939222 |
| H | -1.848132 | -0.266537 | 1.779733 |
| C | -1.899075 | -0.316467 | -0.293200 |
| O | -1.245492 | -0.232313 | -1.334151 |
| N | -3.207579 | -0.722700 | -0.259454 |
| H | -3.678035 | -0.712623 | -1.152641 |
| H | -3.787217 | -0.501810 | 0.537973 |

# 2 Rotatory Strenghts

HIU[7,1] B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 300.51000 | -84.21630 |
| 285.11000 | 92.10690 |
| 268.19000 | -14.80810 |
| 258.03000 | 43.13640 |
| 243.04000 | -69.64620 |
| 235.62000 | -23.03660 |
| 224.03000 | 21.86800 |
| 216.72000 | 4.84290 |
| 211.27000 | -27.42100 |
| 207.54000 | -0.90470 |
| 202.00000 | 0.91480 |
| 192.52000 | 4.85090 |
| 191.65000 | -8.28980 |
| 190.98000 | 4.64160 |
| 190.69000 | 9.40590 |
| 187.16000 | 59.82430 |
| 184.30000 | 5.40680 |
| 182.37000 | -12.93080 |
| 181.22000 | -28.72870 |
| 180.28000 | -3.83190 |

HIU[7,1] CAM-B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 276.81000 | -98.75560 |
| 260.98000 | 104.25590 |
| 243.46000 | -17.40050 |
| 229.45000 | 30.45770 |
| 216.11000 | 12.12740 |
| 213.88000 | -133.79960 |
| 204.35000 | 132.04770 |
| 199.77000 | -50.31200 |
| 191.91000 | -18.78150 |
| 187.34000 | 8.84830 |
| 179.93000 | 13.28490 |
| 174.62000 | -20.78030 |
| 173.64000 | 7.40820 |
| 171.25000 | 5.76650 |
| 169.98000 | 10.96710 |
| 168.20000 | 1.57980 |
| 166.51000 | -45.41790 |
| 166.09000 | -6.18710 |
| 165.29000 | 19.99080 |
| 164.38000 | 25.56130 |

OHCU$^{1,3}$ B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 265.124 | -58.86740 |
| 256.03 | 20.10610 |
| 239.63 | 4.79500 |
| 223.251 | -48.24290 |
| 222.661 | 158.22100 |
| 218.563 | -30.84610 |
| 211.12 | -23.91560 |
| 209.908 | 8.36090 |
| 201.613 | 17.85560 |
| 199.726 | -3.73920 |
| 198.584 | -81.58710 |
| 193.254 | -21.98870 |
| 190.571 | 6.26030 |
| 189.337 | 8.12120 |
| 187.485 | -10.09190 |

OHCU$^{1,3}$ CAM-B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 245.398 | -27.52440 |
| 229.857 | -36.95570 |
| 208.419 | 93.80950 |
| 201.048 | -67.42260 |
| 199.981 | 86.09680 |
| 195.703 | -8.89980 |
| 189.415 | -11.39490 |
| 188.813 | -11.91580 |
| 185.933 | -11.44580 |
| 181.302 | -25.06620 |
| 180.842 | 2.21220 |
| 177.064 | 13.41930 |
| 174.127 | 0.64110 |
| 172.691 | -6.59440 |
| 171.679 | -1.46440 |

OHCU[3,6] B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 260.189 | -20.99930 |
| 244.57 | 6.73810 |
| 233.7 | -10.43620 |
| 225.197 | 130.50230 |
| 216.245 | -12.40120 |
| 213.77 | 34.96760 |
| 211.037 | -5.15050 |
| 209.097 | 13.10540 |
| 206.661 | -89.48660 |
| 199.504 | -18.29070 |
| 197.988 | -65.28870 |
| 195.92 | -31.02550 |
| 187.434 | -5.39340 |
| 185.23 | 0.23270 |
| 182.764 | -13.05980 |

OHCU[3,6] CAM-B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 234.331 | -43.42230 |
| 217.474 | -32.72080 |
| 212.786 | 178.38010 |
| 202.817 | 42.74550 |
| 196.959 | 8.39390 |
| 193.934 | -114.91920 |
| 191.301 | -46.07830 |
| 189.303 | 2.97370 |
| 183.832 | 10.52760 |
| 181.608 | -1.43700 |
| 179.937 | -23.44510 |
| 172.602 | -90.69750 |
| 171.38 | 38.28610 |
| 169.187 | 0.59650 |
| 168.163 | -16.59410 |

ALL-T1 B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 233.726 | 6.63300 |
| 220.801 | -3.13310 |
| 205.974 | 17.41610 |
| 198.305 | -7.87300 |
| 192.548 | -4.46500 |
| 190.574 | -24.12930 |
| 188.836 | -28.09260 |
| 184.549 | -17.27400 |
| 182.407 | -22.46510 |
| 181.645 | -7.69460 |
| 181.016 | 22.43760 |
| 178.158 | 37.54770 |
| 176.549 | -24.78250 |
| 174.829 | -4.28160 |
| 173.98 | -14.37120 |
| 171.817 | -1.91630 |
| 169.731 | 25.16570 |
| 168.637 | -29.15040 |
| 167.792 | 22.57010 |
| 167.082 | -19.74920 |

ALL-T1 CAM-B3LYP

| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 224.106 | 3.56570 |
| 198.374 | 12.08860 |
| 188.723 | -2.24280 |
| 179.848 | -4.52270 |
| 178.834 | -39.38100 |
| 175.559 | 39.26310 |
| 172.427 | -3.64820 |
| 171.713 | -94.09190 |
| 168.104 | -60.59340 |
| 166.606 | 66.45650 |
| 163.443 | -21.73280 |
| 162.197 | 16.71530 |
| 160.835 | -5.18210 |
| 159.402 | 71.51960 |
| 158.916 | 16.67160 |
| 157.948 | -79.52770 |
| 155.455 | 64.01050 |
| 154.563 | -1.69960 |
| 153.205 | 7.10690 |
| 152.564 | -0.95810 |

ALL-T2 B3LYP

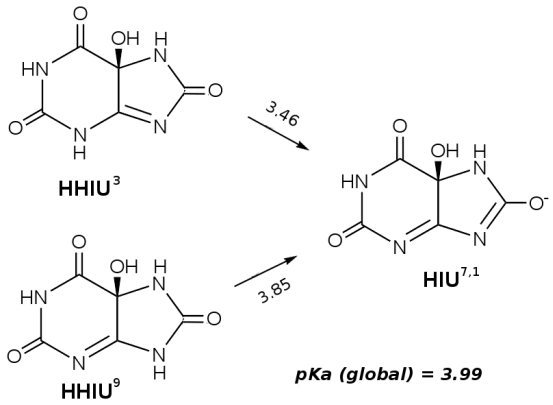
| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 230.433 | 5.91820 |
| 217.574 | 3.86380 |
| 209.429 | 14.52940 |
| 200.068 | -6.27430 |
| 194.906 | -5.99720 |
| 190.829 | 8.74110 |
| 188.62 | 4.16680 |
| 187.055 | 17.03080 |
| 182.791 | -15.83810 |
| 181.821 | -138.19160 |
| 181.053 | 78.41030 |
| 177.645 | 50.69460 |
| 177.327 | -67.60240 |
| 173.433 | 64.48740 |
| 172.283 | -15.71770 |
| 172.085 | 46.28370 |
| 170.534 | -6.40030 |
| 170.076 | 7.33950 |
| 168.91 | 37.61680 |
| 167.999 | -4.15410 |

ALL-T2 CAM-B3LYP

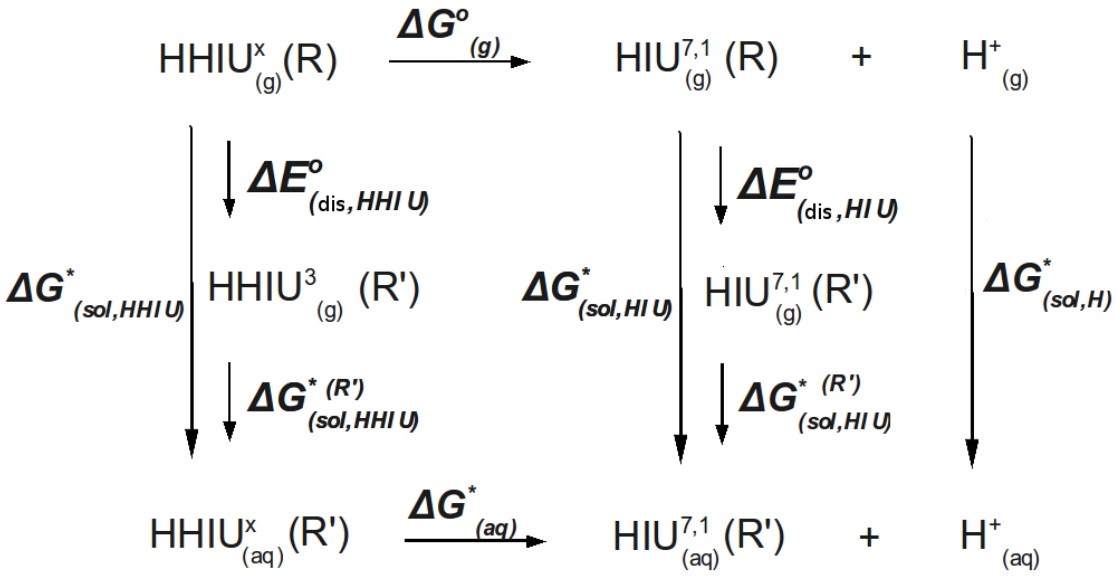
| $\lambda_{0i}(nm)$ | $R_{0i}$ $(10^{-40}esu^2cm^2)$ |
|---|---|
| 221.607 | 3.49600 |
| 195.963 | 25.38270 |
| 189.819 | 0.64050 |
| 181.493 | 23.66830 |
| 179.952 | 13.94390 |
| 177.413 | -31.68460 |
| 173.634 | 15.93840 |
| 171.53 | -3.12700 |
| 167.615 | -26.69250 |
| 167.405 | -47.22110 |
| 164.486 | 4.31180 |
| 162.686 | -83.37610 |
| 161.658 | 44.32490 |
| 160.055 | 19.37930 |
| 158.981 | -10.48410 |
| 157.962 | 34.09320 |
| 156.98 | 44.41360 |
| 155.905 | -12.75620 |
| 154.217 | -12.30290 |
| 152.752 | -25.10990 |

# 3 pKa Calculations for the protonated species of HIU

Global pKa value have been computed for the neutral HIU species (HHIU) taking into account two protonation sites: N3 and N9. The used protocol is described in the work of Verdolino et. al (manuscript ref. 33, in particular equations (1) and (15)). Calculated quantities are shown in Table S1. The global pKa value obtained for HHIU is 0.95.




Scheme S1: Protonation of HIU, local and global values of pKa




Scheme S2: Thermodynamic cycle for the protonation of HIU. The upscript 'x' refers to the N3 and N9 sites of protonation

Table S1: Energetic data for the protonation of HIU

| Isomer | $E^\circ(R)$[a] Hartree | ZPE(R) + $G^\circ_{th}(R)$ Hartree | $G^\circ_{(g)}(R)$[b] kcal/mol | $E^\circ(R')$[a] Hartree | $\Delta E^\circ_{dis}$[a] kcal/mol | $\Delta G^{R'}_{sol}$[c] kcal/mol | $G^*_{(aq)}$[c] kcal/mol | $\Delta G^\circ_{(g,taut)}$[d] kcal/mol | $pop_{(g)}$ kcal/mol | $\Delta G^*_{(aq,taut)}$[d] | $pop_{(aq)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $HHIU^3$ | -712.9909 | 0.0757 | -447360.69 | -712.9901 | 0.49 | -15.12 | 447373.43 | 0.43 | 0.33 | 0.52[e] | 0.30 |
| $HHIU^9$ | -712.9920 | 0.0761 | -447361.12 | -712.9912 | 0.52 | -15.24 | 447373.96 | 0.00 | 0.67 | 0.00 | 0.70 |
| $HIU^{71}$ | -712.4767 | 0.0636 | -447045.66 | -712.4756 | 0.74 | 55.36 | 447098.39 | 0.00 | 1.00 | 0.00 | 1.00 |

| Reaction | $\Delta_{reax}G^*$ kcal/mol | $pKa$ local | $pKa$ global | Gas Phase Basicity (GB) [e] kcal/mol |
|---|---|---|---|---|
| $HHIU^3 \rightarrow HIU^{7,1}$ | 4.75 | 3.46 | 3.99 | 308.75 |
| $HHIU^9 \rightarrow HIU^{7,1}$ | 5.28 | 3.85 | 3.99 | 309.18 |

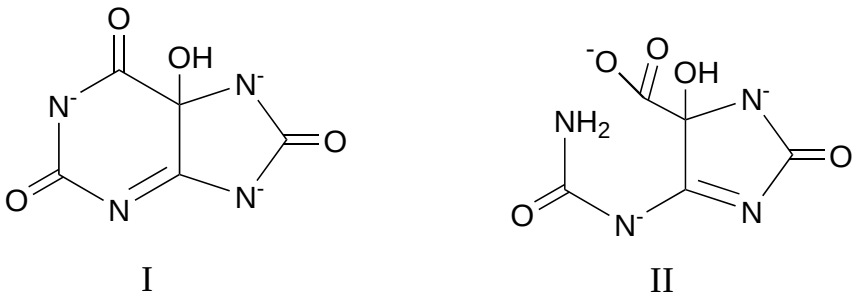
[a] Calculations at B3LYP/aug-cc-pVDZ//B3LYP/6-31+G(d,p) and IEFPCM/B3LYP/aug-cc-pVDZ//B3LYP/6-31+G(d,p) levels of theory respectively in gas phase and solution.

[b] Zero Point Energy and thermal contributions calculated at the B3LYP/6-31+G(d,p) level of theory

[c] Free energies of solvation calculated at the IEFPCM-B3LYP/aug-cc-pVDZ level of theory with UFF radii and scaling factors $\alpha = 0.90$ for anions and $\alpha = 0.91$ for neutral species. The scaling factor for the anions has been specifically reoptimized on the basis of the agreement between computed and excperimental pKa value of uric acid [36].

[d] Gibbs energy difference between the most stable tautomer and the one to which is referred.

[e] See manuscript ref. 36 for a comparison of the calculated Gibbs free energy difference between the two isomers, and the definitions of GB and PA.




I II

Scheme S3: HIU (I) and OHCU (II) deprotonated tri-anionc species used as a starting point for the selection of the tautomeric structures in gas phases.

# 4 Additional Computed ECD and ORD Spectra

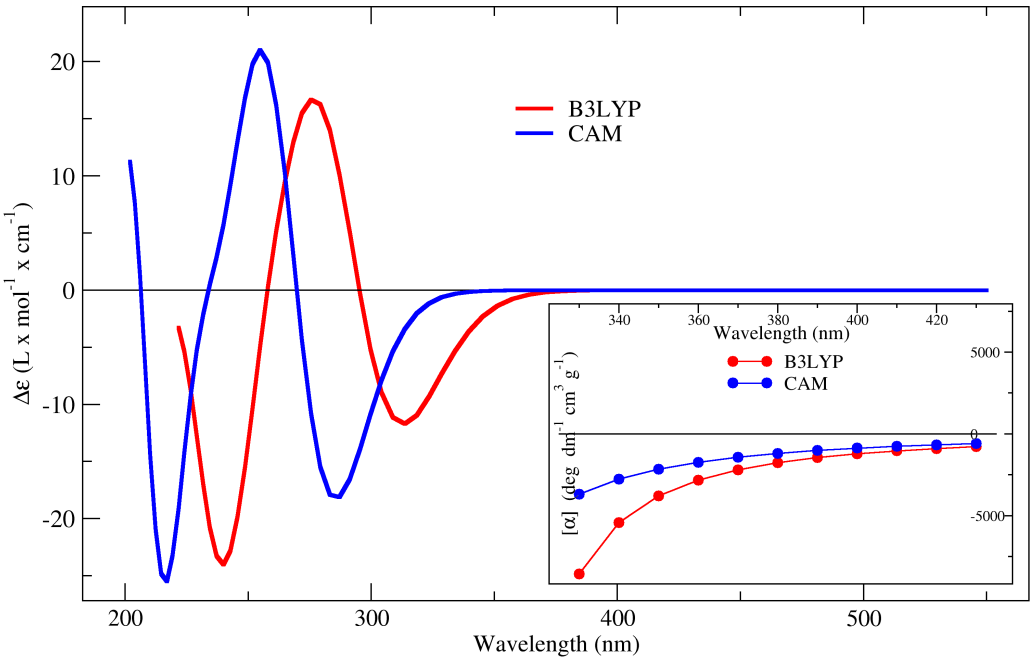



Figure S1: Computed spectra of (*S*)-HIU. Main figure: ECD spectra calculated using PCM/TDDFT/B3LYP (red) and PCM/TDDFT/CAM-B3LYP (blue). Inset: ORD spectra calculated using PCM/TDDFT/B3LYP (red) and PCM/TDDFT/CAM-B3LYP (blue)

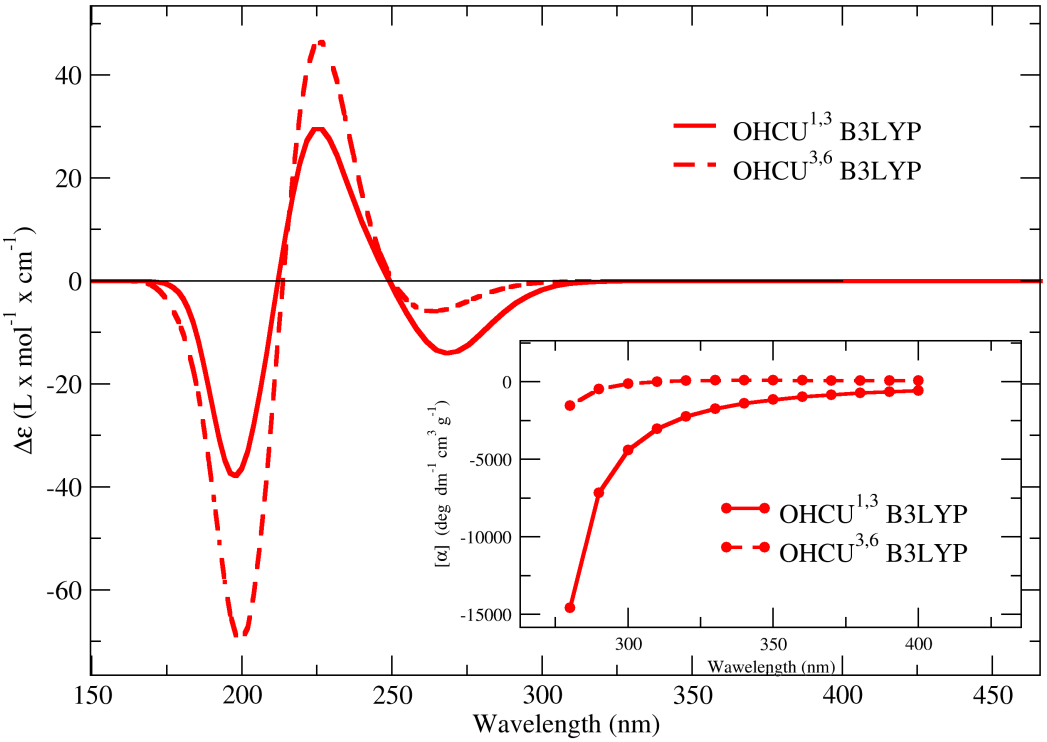



Figure S2: Computed spectra of (*S*)-*OHCU*$^{1,3}$ (solid line) and (*S*)-*OHCU*$^{3,6}$ (dashed line). Main figure: ECD spectra calculated using PCM/TDDFT/B3LYP. Inset: ORD spectra calculated using PCM/TDDFT/B3LYP.

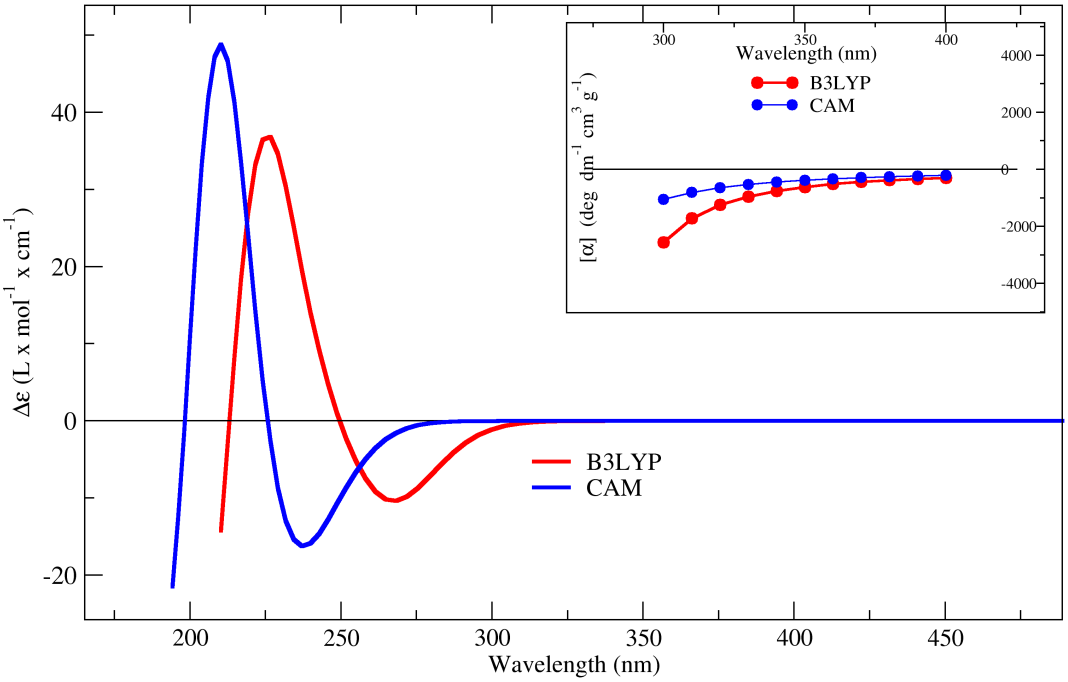



Figure S3: Computed spectra of (*S*)-OHCU. Main figure: ECD spectra calculated using PCM/TDDFT/B3LYP (solid red) and PCM/TDDFT/CAM-B3LYP (solid blue). Inset: ORD spectra calcutated using PCM/TDDFT/B3LYP (solid red) and PCM/TDDFT/CAM-B3LYP (solid blue).

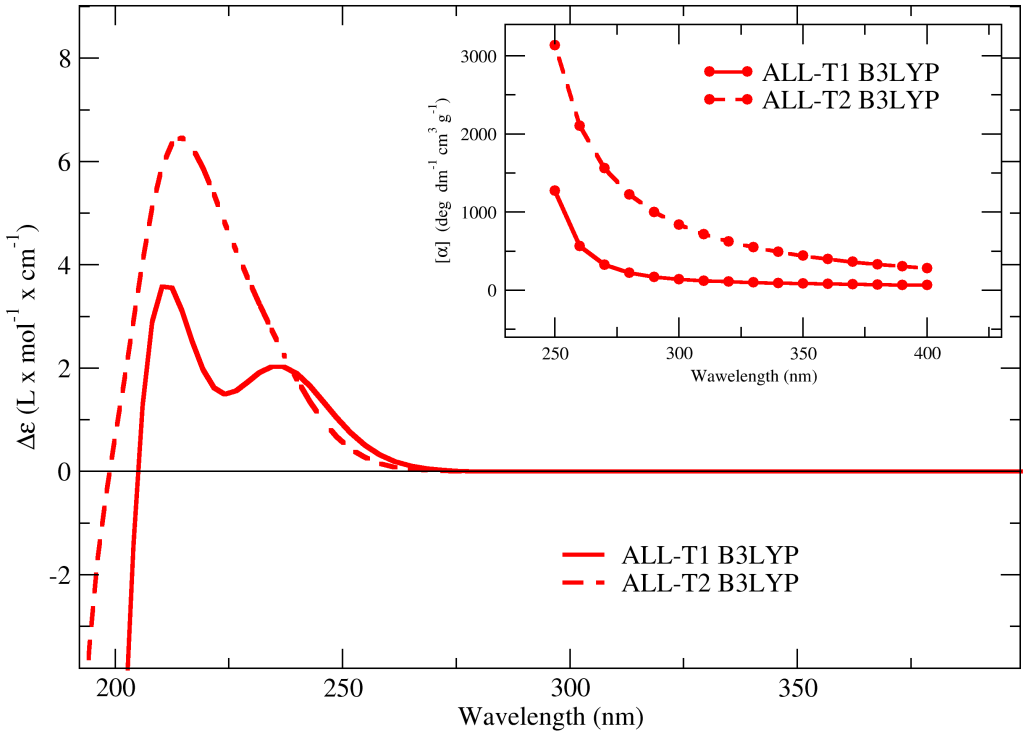



Figure S5: Computed Spectra of (*S*)-ALL-T1 (solid line) and (*S*)-ALL-T2 (dashed line). Main figure: ECD spectra calculated using PCM/TDDFT/B3LYP. Inset: ORD spectra calculated using PCM/TDDFT/B3LYP.

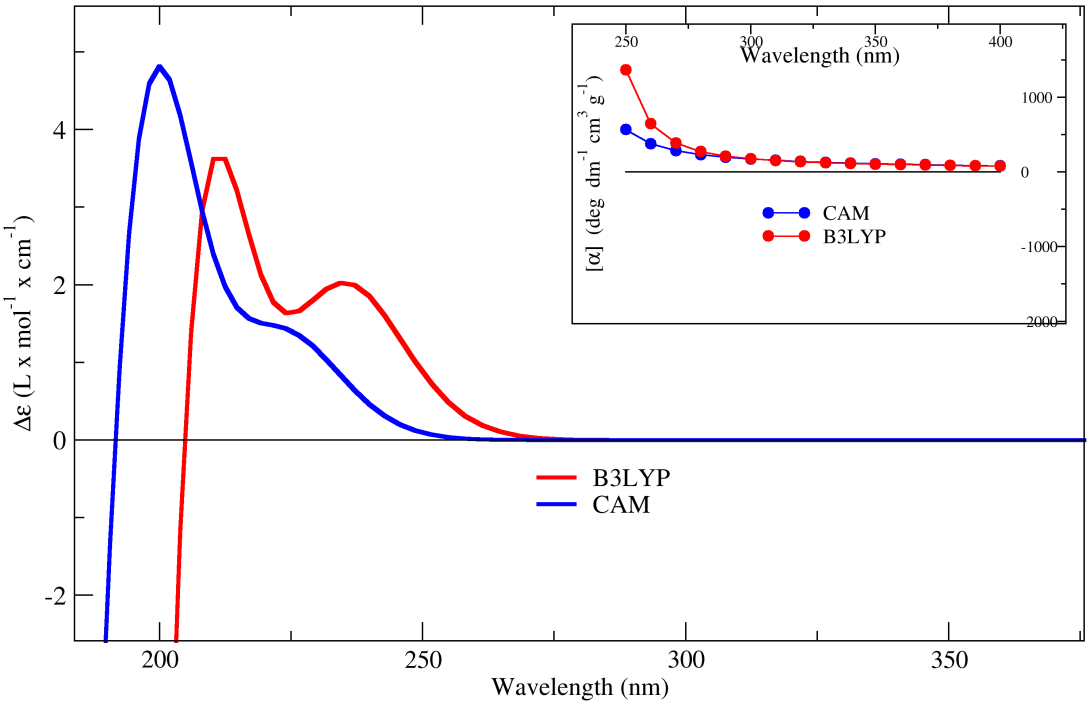



Figure S4: Computed Spectra of (*S*)-Allantoin. Main figure: ECD spectra calculated using PCM/TDDFT/B3LYP (solid red) and PCM/TDDFT/CAM-B3LYP (solid blue). Inset: ORD spectra calculated using PCM/TDDFT/B3LYP (solid red/blue) and PCM/TDDFT/CAM-B3LYP (solid blue).