

Supporting Information For:

**Mechanism of Epoxide Hydrolysis in Microsolvated Nucleotide
Bases Adenine, Guanine and Cytosine: A DFT Study**

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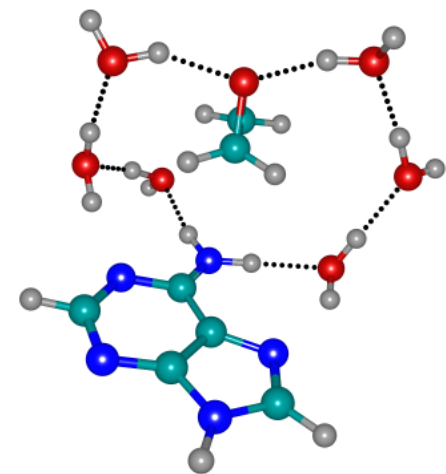
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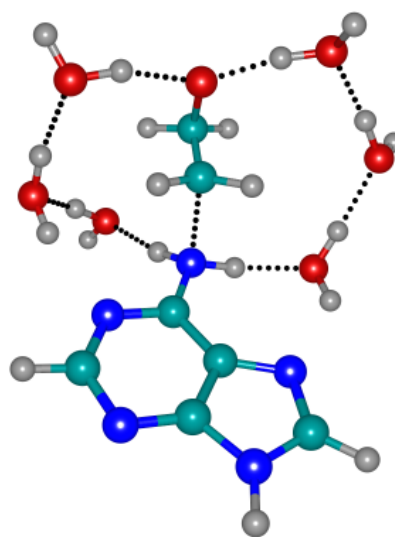
Table S1. Cartesian coordinates of all the optimized geometries (in Å), SCF energy (in a.u) and number of imaginary frequencies (N_{img}) computed at MPWB1K /6-31++G(d,p) level of theory.

EAw			
At. No	X	Y	Z
6	1.588937000	0.006011000	-0.670396000
6	2.644278000	-0.188926000	0.300003000
8	2.946009000	-0.127297000	-1.100522000
1	1.167957000	0.991772000	-0.805557000
1	0.959084000	-0.829612000	-0.939854000
1	2.997562000	0.658933000	0.867915000
1	2.781580000	-1.161566000	0.746615000
8	3.831005000	2.460863000	-1.498581000
1	3.642581000	1.511644000	-1.500882000
1	3.935044000	2.732002000	-2.406220000
8	2.486904000	-2.800454000	-1.735890000
1	3.137795000	-3.425394000	-2.042174000
1	2.910181000	-1.935166000	-1.694642000
8	2.190360000	3.776446000	0.312093000
1	2.776889000	3.374577000	-0.344853000
1	2.723273000	4.380163000	0.821775000
8	0.796928000	-3.439215000	0.475266000
1	1.317284000	-3.293885000	-0.322121000
1	-0.051841000	-2.980192000	0.368688000
7	-3.847884000	1.102587000	-1.129702000
6	-3.293940000	2.155430000	-0.470588000
7	-2.319381000	1.808631000	0.311020000
6	-2.223290000	0.447814000	0.157628000
6	-1.386773000	-0.526303000	0.742661000
7	-0.468033000	-0.243528000	1.651692000
7	-1.552988000	-1.792832000	0.325595000
6	-2.509673000	-2.079825000	-0.554738000
7	-3.366930000	-1.265390000	-1.132657000
6	-3.168251000	-0.010809000	-0.739896000
8	1.521762000	-2.177167000	2.712004000
8	0.069022000	2.587186000	1.778773000
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1	-3.649192000	3.160748000	-0.606082000
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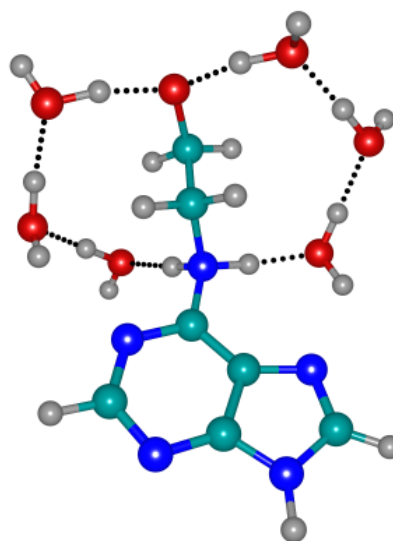


The image shows a 3D ball-and-stick model of a complex organic molecule. The structure features a central ring system with various substituents. Dotted lines indicate hydrogen bonding interactions between several atoms, forming a network of interactions. The atoms are color-coded: carbon (grey), oxygen (red), nitrogen (blue), and hydrogen (white).

1	1.364780000	-2.799309000	1.977425000	
1	-0.745804000	2.713417000	1.283048000	
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8	3.747817000	2.320444000	-1.407539000	
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1	2.972811000	-1.745822000	-1.549984000	
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8	0.979472000	-3.471447000	0.386424000	
1	1.594170000	-3.297733000	-0.344289000	
1	0.139840000	-3.060197000	0.156883000	
7	-4.107221000	1.051163000	-0.874262000	
6	-3.454590000	2.137390000	-0.378857000	
7	-2.320043000	1.849094000	0.176537000	
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7	-1.453185000	-1.724644000	0.123610000	
6	-2.569713000	-2.077534000	-0.512689000	
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6	-3.322402000	-0.028919000	-0.617346000	
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1	-4.993590000	1.035584000	-1.340824000	
1	-3.867175000	3.127150000	-0.456026000	
1	-0.028043000	0.848375000	1.417323000	
1	0.284631000	-0.819585000	1.690426000	
1	-2.674025000	-3.131097000	-0.723999000	
1	0.942177000	-2.531065000	3.444996000	
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1	-0.676915000	2.854557000	1.163782000	

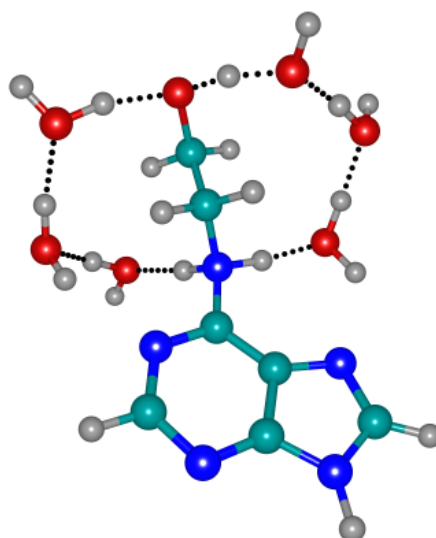


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1	1.001201000	0.756892000	-0.965112000	
1	0.986424000	-1.016409000	-0.927448000	
1	2.676022000	0.784488000	0.858344000	
1	2.609707000	-0.971807000	0.960834000	
8	3.591182000	2.148564000	-1.480905000	
1	3.606203000	1.141696000	-1.253553000	
1	3.634179000	2.238960000	-2.427153000	
8	3.186749000	-2.670207000	-1.268853000	
1	4.023225000	-3.124563000	-1.294865000	
1	3.381528000	-1.673652000	-1.139339000	
8	2.220966000	3.658557000	0.157857000	
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1	2.875689000	4.153753000	0.641991000	
8	1.210178000	-3.500422000	0.294133000	
1	1.987695000	-3.267312000	-0.266421000	
1	0.431519000	-3.269554000	-0.210682000	
7	-4.248453000	1.133047000	-0.492304000	
6	-3.551937000	2.184057000	0.019208000	
7	-2.343831000	1.885528000	0.379068000	
6	-2.225859000	0.551453000	0.087543000	
6	-1.218057000	-0.389332000	0.211071000	
7	0.078438000	-0.083834000	0.726441000	
7	-1.419999000	-1.630984000	-0.172691000	
6	-2.607296000	-1.964440000	-0.675275000	
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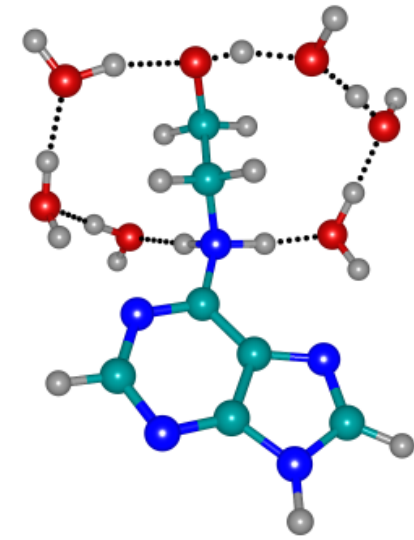


EAW-TS2

At. No	X	Y	Z
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1	2.548252000	1.117873000	1.035726000
1	2.734291000	-0.635154000	1.077061000
8	2.828012000	2.311932000	-1.578252000
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1	3.318085000	2.693422000	-2.299384000
8	3.406654000	-2.222613000	-1.266819000
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1	2.421701000	4.238384000	0.606494000
8	1.540120000	-3.283498000	0.394736000
1	2.274956000	-2.988189000	-0.177279000
1	0.730768000	-3.051298000	-0.063227000
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6	-3.780239000	1.700972000	-0.067077000
7	-2.556867000	1.569451000	0.336699000
6	-2.239294000	0.272679000	0.027972000
6	-1.112754000	-0.516661000	0.174331000
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7	-1.123832000	-1.768149000	-0.231964000
6	-2.232542000	-2.257610000	-0.784637000
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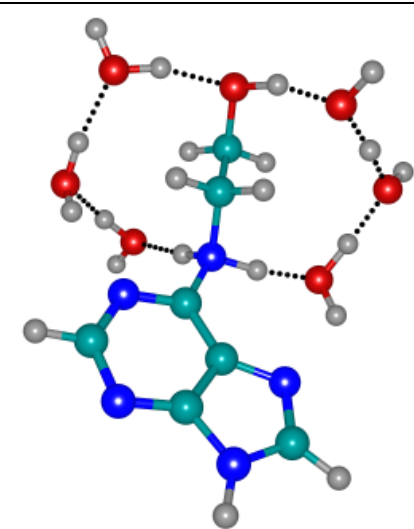


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1	-4.356979000	2.604828000	0.015001000	
1	-0.001482000	0.948586000	1.145559000	
1	0.394516000	-0.688084000	1.505161000	
1	-2.191848000	-3.289041000	-1.097975000	
1	0.629689000	-2.354763000	3.301493000	
1	1.311672000	-2.538817000	1.899115000	
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8	2.766614000	2.341208000	-1.552434000	
1	3.368149000	1.150822000	-1.087785000	
1	3.147592000	2.772161000	-2.310713000	
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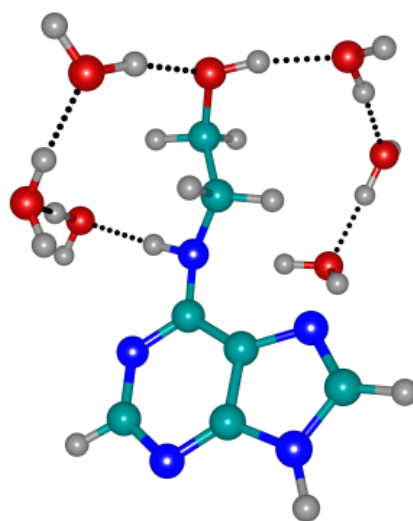


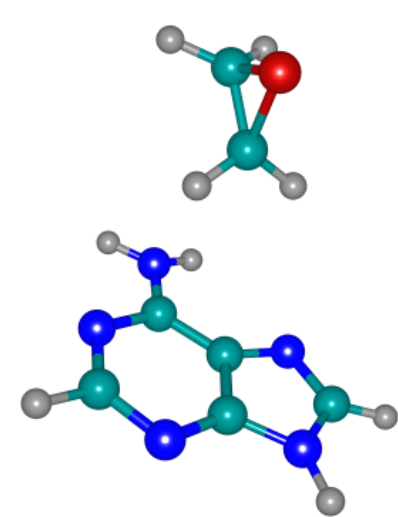
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6	-3.316581000	-0.369748000	-0.581521000
8	1.008288000	-1.855439000	2.574379000
8	0.007267000	2.446605000	1.512146000
1	-5.217763000	0.443464000	-0.998859000
1	-4.359219000	2.599540000	0.018043000
1	0.014398000	0.982164000	1.116468000
1	0.402203000	-0.659249000	1.491270000
1	-2.172032000	-3.282525000	-1.112968000
1	0.660310000	-2.296340000	3.343526000
1	1.296252000	-2.531264000	1.926374000
1	-0.855439000	2.773018000	1.256539000
1	0.696058000	2.994082000	1.016607000
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1	1.035205000	0.924659000	-0.950175000
1	1.201897000	-0.842016000	-0.897516000

1	2.564757000	1.133674000	0.982396000
1	2.750782000	-0.623063000	1.035737000
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1	3.380678000	1.144894000	-1.108722000
1	3.091344000	2.866762000	-2.300045000
8	3.390011000	-2.284317000	-1.292358000
1	4.206468000	-2.713763000	-1.529270000
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1	0.698854000	-3.017540000	-0.002252000
7	-4.307007000	0.544128000	-0.605727000
6	-3.789163000	1.684938000	-0.071944000
7	-2.559376000	1.570946000	0.316059000
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6	-1.095801000	-0.501643000	0.161771000
7	0.124673000	-0.000317000	0.708483000
7	-1.102663000	-1.759940000	-0.226586000
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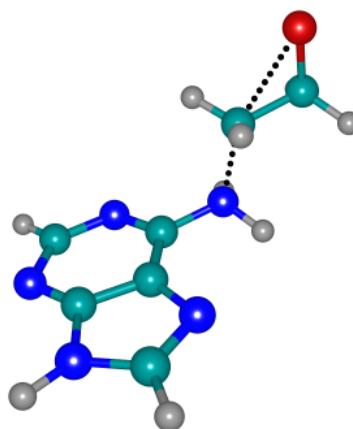


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E(RmPW+HF-B95) = -1079.30824051				N _{img} = 1
EAW-3				
At. No	X	Y	Z	
6	1.041666000	0.146180000	-0.141165000	
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6	-3.032643000	1.443889000	-1.331616000	
7	-1.874979000	1.261405000	-0.775721000	
6	-1.969367000	0.022205000	-0.186817000	
6	-1.096866000	-0.737608000	0.604920000	

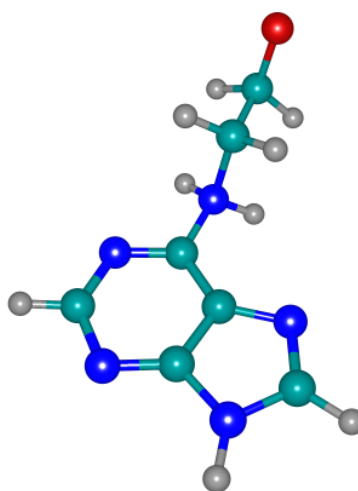


7	0.172231000	-0.365613000	0.910292000	
7	-1.553514000	-1.885220000	1.106374000	
6	-2.796250000	-2.270856000	0.834562000	
7	-3.696104000	-1.661648000	0.084961000	
6	-3.230107000	-0.518885000	-0.391262000	
8	1.610945000	-2.456609000	2.414702000	
8	-0.441476000	2.581159000	1.423308000	
1	-4.833208000	0.332256000	-1.468756000	
1	-3.317812000	2.320736000	-1.884379000	
1	-0.192029000	1.701089000	1.718652000	
1	0.623462000	-1.063256000	1.500706000	
1	-3.100139000	-3.208472000	1.276499000	
1	1.020070000	-2.917440000	3.004292000	
1	1.631195000	-2.971489000	1.592786000	
1	-0.960046000	2.420372000	0.625970000	
1	0.913058000	3.617978000	1.037116000	
E(RmPW+HF-B95) = -1079.35776085 N _{img} = 0				
EA				
At. No	X	Y	Z	
6	1.381117000	0.108762000	-0.677563000	
6	2.723791000	-0.008517000	-0.132211000	
8	2.513698000	0.159772000	-1.513393000	
1	0.844316000	1.042222000	-0.573110000	
1	0.769726000	-0.777534000	-0.779069000	
1	3.171094000	0.837448000	0.371841000	
1	3.095738000	-0.980388000	0.162039000	
7	-3.453122000	1.124509000	-1.318124000	
6	-2.980787000	2.136913000	-0.535959000	
7	-2.225075000	1.729519000	0.435017000	
6	-2.199081000	0.368597000	0.281914000	
6	-1.565230000	-0.652648000	0.996553000	

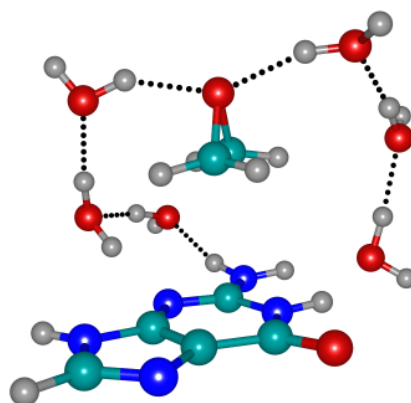
7	-0.782133000	-0.402256000	2.056137000	
7	-1.723293000	-1.907326000	0.590040000	
6	-2.482789000	-2.142692000	-0.477804000	
7	-3.133714000	-1.276833000	-1.231611000	
6	-2.954546000	-0.033753000	-0.804563000	
1	-4.045097000	1.204411000	-2.121792000	
1	-3.230899000	3.163524000	-0.734150000	
1	-0.741547000	0.521394000	2.436273000	
1	-0.432198000	-1.175270000	2.584820000	
1	-2.574337000	-3.181465000	-0.759325000	
E(RmPW+HF-B95) =			-620.860928142	N _{img} = 0
EA-TS1				
At. No	X	Y	Z	
6	-2.376109000	-0.037771000	-0.299451000	
6	-3.779062000	-0.287020000	0.161649000	
8	-4.281779000	-0.490036000	-1.049380000	
1	-1.929274000	-0.908734000	-0.758788000	
1	-2.285522000	0.857768000	-0.898069000	
1	-3.810393000	-1.144895000	0.869116000	
1	-4.163753000	0.592187000	0.724674000	
7	2.911443000	-1.050387000	-0.408186000	
6	2.145026000	-2.094540000	0.018469000	
7	0.969882000	-1.743401000	0.439815000	
6	0.960452000	-0.387333000	0.277859000	
6	0.024464000	0.599846000	0.525105000	
7	-1.274857000	0.288523000	0.968876000	
7	0.292676000	1.862257000	0.278818000	
6	1.491091000	2.163121000	-0.222750000	
7	2.472450000	1.328975000	-0.513923000	
6	2.164458000	0.073744000	-0.247962000	
1	3.842377000	-1.093949000	-0.776836000	



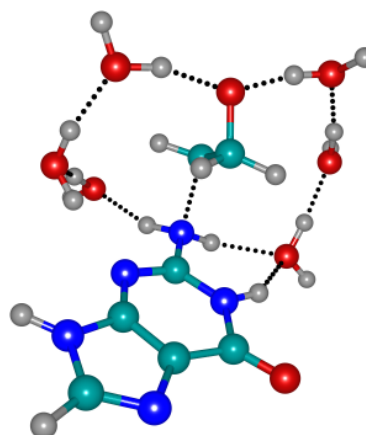
1	2.510971000	-3.105238000	-0.005033000	
1	-1.290735000	-0.542545000	1.547152000	
1	-1.675952000	1.073928000	1.466741000	
1	1.673425000	3.209708000	-0.409239000	
E(RmPW+HF-B95) = -620.778088454				N _{img} = 1
EA-1				
At. No	X	Y	Z	
6	-2.296539000	-0.057244000	-0.378461000	
6	-3.711011000	-0.243150000	0.207853000	
8	-4.557812000	-0.522551000	-0.729717000	
1	-1.934807000	-0.961950000	-0.853884000	
1	-2.248405000	0.790222000	-1.052492000	
1	-3.572150000	-1.022828000	1.020470000	
1	-3.888174000	0.714504000	0.791334000	
7	2.941017000	-1.030857000	-0.334094000	
6	2.150791000	-2.091753000	-0.002869000	
7	0.943504000	-1.761540000	0.337296000	
6	0.936841000	-0.402122000	0.220977000	
6	-0.014630000	0.575903000	0.421566000	
7	-1.355792000	0.246659000	0.784767000	
7	0.257557000	1.844954000	0.247526000	
6	1.488652000	2.170610000	-0.150140000	
7	2.492539000	1.347725000	-0.393458000	
6	2.176556000	0.083590000	-0.195086000	
1	3.898846000	-1.058575000	-0.628562000	
1	2.524543000	-3.099551000	-0.030849000	
1	-1.389133000	-0.568518000	1.394827000	
1	-1.779945000	1.030155000	1.282972000	
1	1.678416000	3.223530000	-0.284408000	
E(RmPW+HF-B95) = -620.780945488				N _{img} = 0
EGw				



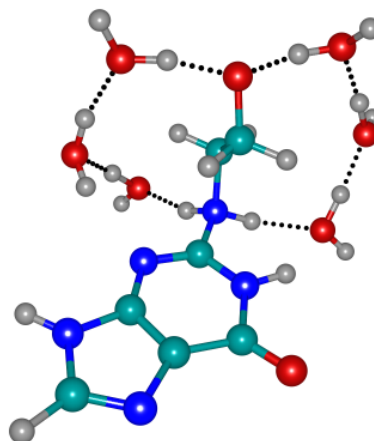
At. No	X	Y	Z
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6	1.099406000	-0.063900000	-0.187952000
8	1.840919000	-0.133032000	-1.408320000
1	0.081666000	0.969373000	-1.837782000
1	-0.096132000	-0.857478000	-1.848876000
1	1.260622000	0.841280000	0.379801000
1	1.081036000	-0.983762000	0.379288000
8	2.926154000	2.431424000	-1.334611000
1	2.683331000	1.516236000	-1.529440000
1	2.874410000	2.923603000	-2.149322000
8	1.500989000	-2.895772000	-1.645047000
1	2.135788000	-3.567524000	-1.877698000
1	1.948652000	-2.044118000	-1.694799000
8	2.147292000	3.302505000	1.151791000
1	2.415385000	3.087529000	0.244687000
1	2.938962000	3.290429000	1.682209000
8	-0.337294000	-3.372786000	0.515931000
1	0.246379000	-3.257516000	-0.241745000
1	-0.992801000	-2.656857000	0.494029000
8	0.501522000	-2.378214000	2.883785000
8	-0.326714000	2.858254000	2.241894000
1	0.478052000	-2.967113000	3.632265000
1	0.311314000	-2.912934000	2.092696000
1	-0.636047000	3.659323000	2.656789000
1	0.539752000	3.063233000	1.852124000
7	-3.286795000	-1.952143000	-1.393566000
6	-3.883690000	-1.339322000	-2.464051000
7	-3.808865000	-0.051083000	-2.409360000
6	-3.136070000	0.206025000	-1.245783000
6	-2.725442000	1.441701000	-0.654428000
8	-2.852974000	2.577341000	-1.051612000
7	-2.063162000	1.201427000	0.561856000
6	-1.763715000	-0.007757000	1.104367000
7	-1.068220000	0.000752000	2.243841000
7	-2.119892000	-1.143096000	0.545895000
6	-2.802897000	-0.965772000	-0.600147000
1	-4.354847000	-1.905966000	-3.246193000
1	-1.674575000	2.021660000	1.012132000
1	-0.705723000	0.875258000	2.583163000
1	-0.670773000	-0.864264000	2.586711000
1	-3.223882000	-2.935288000	-1.210961000
E(RmPW+HF-B95) = -1154.54237064			N _{img} = 0
EGw-TS1			



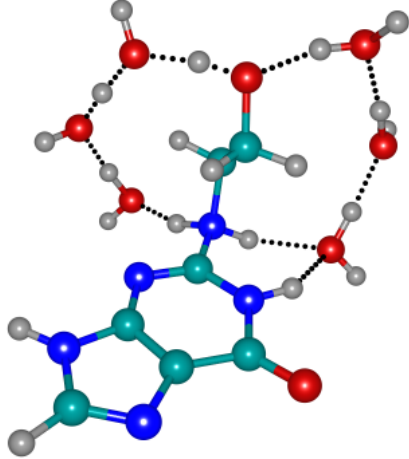
At. No	X	Y	Z
6	-1.442432000	0.230710000	-1.169340000
6	-1.816860000	0.646197000	0.178594000
8	-2.546942000	0.969681000	-1.558018000
1	-1.516958000	-0.840471000	-1.366512000
1	-0.487761000	0.616086000	-1.532481000
1	-2.668194000	0.154134000	0.619005000
1	-1.653359000	1.678658000	0.435651000
8	-4.465237000	-0.754820000	-1.769708000
1	-3.791898000	-0.023571000	-1.770245000
1	-4.552153000	-1.071450000	-2.663768000
8	-1.310162000	3.289491000	-1.658716000
1	-1.727690000	4.018935000	-2.105899000
1	-1.903341000	2.506610000	-1.737170000
8	-4.032867000	-2.217639000	0.390604000
1	-4.213571000	-1.754786000	-0.456945000
1	-4.841647000	-2.195015000	0.893782000
8	0.335100000	3.359544000	0.560330000
1	-0.205913000	3.445705000	-0.241272000
1	0.835763000	2.540808000	0.474770000
8	-0.813854000	2.477245000	2.802907000
8	-1.644559000	-2.630738000	1.526913000
1	-0.598778000	2.917929000	3.619515000
1	-0.442104000	3.007380000	2.070886000
1	-1.637435000	-3.495880000	1.928999000
1	-2.513637000	-2.532015000	1.086600000
7	3.677990000	0.998533000	-0.332293000
6	4.544657000	0.169303000	-0.986514000
7	4.114103000	-1.048379000	-1.064133000
6	2.904749000	-1.025494000	-0.433606000
6	1.953149000	-2.073026000	-0.205980000
8	1.981390000	-3.237885000	-0.512940000
7	0.839568000	-1.561005000	0.496460000
6	0.675624000	-0.290106000	0.910614000
7	-0.531139000	-0.004855000	1.530218000
7	1.524476000	0.666108000	0.699630000
6	2.617380000	0.239722000	0.028423000
1	5.477365000	0.527508000	-1.381976000
1	0.089980000	-2.220305000	0.683908000
1	-0.970919000	-0.826683000	1.932199000
1	-0.484180000	0.792822000	2.171004000
1	3.790879000	1.977907000	-0.153341000
E(RmPW+HF-B95) = -1154.49858336			N _{img} = 1
EGw-1			
At. No	X	Y	Z



6	-1.543301000	0.156193000	-1.048318000
6	-1.669870000	0.627301000	0.391912000
8	-2.470225000	0.836314000	-1.772812000
1	-1.681316000	-0.937409000	-1.089885000
1	-0.515433000	0.348308000	-1.396170000
1	-2.638931000	0.354905000	0.796284000
1	-1.558949000	1.702589000	0.434541000
8	-4.412481000	-0.701982000	-1.748517000
1	-3.659091000	0.002368000	-1.820795000
1	-4.539777000	-1.078359000	-2.614138000
8	-1.587718000	3.208262000	-1.475079000
1	-1.762657000	3.791286000	-2.206752000
1	-2.015863000	2.313597000	-1.679185000
8	-4.007194000	-2.180065000	0.315951000
1	-4.161814000	-1.656840000	-0.522401000
1	-4.813820000	-2.127101000	0.820271000
8	0.184929000	3.454576000	0.550197000
1	-0.453135000	3.515873000	-0.189097000
1	0.757433000	2.717463000	0.329802000
8	-0.574265000	2.290083000	2.813011000
8	-1.699918000	-2.467689000	1.475276000
1	-0.172734000	2.622060000	3.610664000
1	-0.343197000	2.899098000	2.077178000
1	-1.715894000	-3.265800000	1.997809000
1	-2.581035000	-2.398597000	1.020377000
7	3.694778000	1.024588000	-0.292620000
6	4.600397000	0.182907000	-0.868795000
7	4.174979000	-1.037973000	-0.949022000
6	2.928275000	-1.002598000	-0.404149000
6	1.969103000	-2.054829000	-0.217550000
8	2.026963000	-3.224707000	-0.485621000

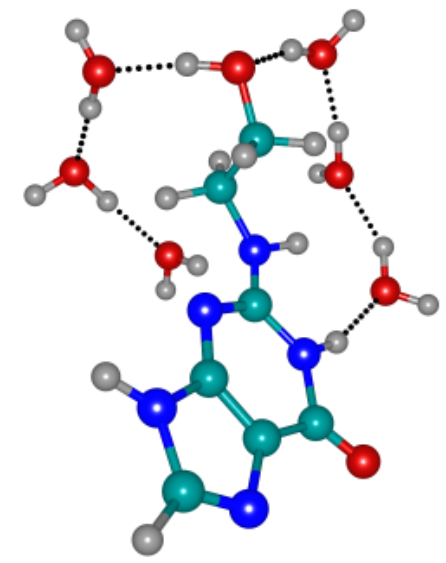


7	0.803766000	-1.528226000	0.394391000	
6	0.627205000	-0.249236000	0.749801000	
7	-0.643238000	0.047311000	1.349181000	
7	1.473087000	0.704540000	0.601188000	
6	2.612302000	0.272107000	0.009983000	
1	5.557817000	0.532274000	-1.209273000	
1	0.038802000	-2.181936000	0.542945000	
1	-1.036912000	-0.822228000	1.735599000	
1	-0.507441000	0.765457000	2.097173000	
1	3.797265000	2.008464000	-0.131628000	
E(RmPW+HF-B95) = -1154.52174655 N _{img} = 0				
EGw-TS2				
At. No	X	Y	Z	
6	-1.442587000	-0.048474000	-1.020557000	
6	-1.606654000	0.506902000	0.380309000	
8	-2.462018000	0.469431000	-1.801383000	
1	-1.507444000	-1.138766000	-1.026385000	
1	-0.462601000	0.228731000	-1.419268000	
1	-2.528741000	0.151508000	0.827889000	
1	-1.636255000	1.586289000	0.323217000	
8	-4.385437000	-1.302508000	-1.658123000	
1	-3.761958000	-0.553335000	-1.797232000	
1	-4.497758000	-1.737688000	-2.498228000	
8	-2.151304000	2.894845000	-1.462961000	
1	-2.764612000	3.508327000	-1.855935000	
1	-2.402109000	1.511002000	-1.747634000	
8	-3.782533000	-2.518243000	0.615141000	
1	-4.000658000	-2.134074000	-0.262518000	
1	-4.569097000	-2.438646000	1.147539000	
8	-0.912577000	3.789735000	0.391470000	
1	-1.516385000	3.419836000	-0.489098000	



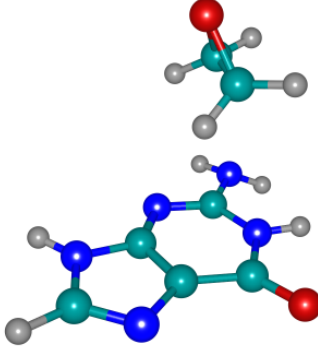
1	-0.099042000	4.139438000	0.039715000
8	-0.664951000	2.438004000	2.492139000
8	-1.374008000	-2.462774000	1.704993000
1	-0.122789000	2.872751000	3.143339000
1	-0.751063000	3.052483000	1.673815000
1	-1.269750000	-3.241694000	2.246470000
1	-2.266613000	-2.519810000	1.293962000
7	3.761786000	1.221952000	-0.404931000
6	4.692059000	0.393121000	-0.958403000
7	4.318482000	-0.847702000	-0.972318000
6	3.081006000	-0.838065000	-0.405480000
6	2.171102000	-1.918311000	-0.146613000
8	2.276548000	-3.098965000	-0.353834000
7	0.994387000	-1.409367000	0.450524000
6	0.771568000	-0.117932000	0.750891000
7	-0.504020000	0.155740000	1.346888000
7	1.574392000	0.857567000	0.546296000
6	2.717134000	0.441265000	-0.045395000
1	5.627383000	0.765081000	-1.334641000
1	0.271296000	-2.089150000	0.668291000
1	-0.802074000	-0.667399000	1.877274000
1	-0.424057000	1.034157000	1.973295000
1	3.817595000	2.216390000	-0.297121000
E(RmPW+HF-B95) = -1154.51529192 N _{img} =1			
EGw-2			
At. No	X	Y	Z
6	-1.470900000	0.147263000	-1.714498000
6	-1.244088000	0.694294000	-0.315635000
8	-2.582986000	0.756933000	-2.324305000
1	-1.694795000	-0.917011000	-1.650553000
1	-0.576496000	0.267786000	-2.323999000

1	-2.213058000	0.869814000	0.147850000
1	-0.712740000	1.640246000	-0.355284000
8	-4.485898000	-0.753320000	-1.169474000
1	-3.933209000	-0.132535000	-1.680785000
1	-5.006102000	-1.254017000	-1.791158000
8	-2.477734000	3.402664000	-1.559985000
1	-3.156600000	4.016366000	-1.826099000
1	-2.552508000	1.715701000	-2.171799000
8	-3.160027000	-1.657759000	1.010671000
1	-3.661620000	-1.436841000	0.204070000
1	-3.626220000	-1.239901000	1.730952000
8	-1.907221000	3.874672000	1.095490000
1	-2.304213000	3.569412000	-0.618401000
1	-1.226575000	4.522353000	1.256802000
8	-1.265193000	1.651103000	2.643507000
8	-0.976658000	-3.083123000	1.837893000
1	-0.884837000	1.619818000	3.517208000
1	-1.720869000	3.130863000	1.687987000
1	-0.879356000	-4.030204000	1.888385000
1	-1.875467000	-2.887363000	1.545658000
7	3.786640000	0.768194000	-1.070184000
6	4.950318000	0.073704000	-0.882190000
7	4.788734000	-0.990880000	-0.166567000
6	3.456052000	-1.003007000	0.135454000
6	2.675844000	-1.945415000	0.880350000
8	3.003246000	-2.971695000	1.428450000
7	1.332844000	-1.530232000	0.920773000
6	0.817448000	-0.425188000	0.332430000
7	-0.516032000	-0.206397000	0.551556000
7	1.513076000	0.425283000	-0.360815000
6	2.815172000	0.083977000	-0.419482000

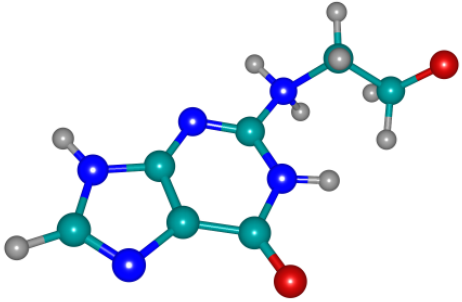


The image shows a 3D ball-and-stick model of a complex organic molecule. The structure features a central core with several nitrogen (blue) and oxygen (red) atoms. The molecule is surrounded by several water molecules (grey and red spheres) which are connected to the main structure via hydrogen bonds, represented by dashed lines. The overall structure is highly branched and appears to be a part of a larger assembly or a specific conformation of a molecule.

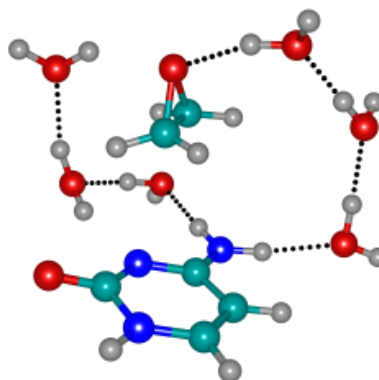
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1	0.692669000	-2.162038000	1.390064000	
1	-1.049135000	-1.021603000	0.817071000	
1	-0.850944000	0.947953000	2.124186000	
1	3.657766000	1.614438000	-1.589115000	
E(RmPW+HF-B95) = -1154.57702323 N _{img} = 0				
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At. No	X	Y	Z	
6	-2.149279000	-1.047496000	1.099677000	
6	-3.008456000	-0.850981000	-0.058401000	
8	-3.076959000	-2.030495000	0.705423000	
1	-2.378490000	-0.545673000	2.029833000	
1	-1.109764000	-1.310073000	0.954562000	
1	-3.869234000	-0.201003000	0.020026000	
1	-2.592787000	-0.966298000	-1.050194000	
7	1.805373000	-1.322341000	-1.308613000	
6	2.695778000	-1.614828000	-0.311589000	
7	2.576447000	-0.834053000	0.711993000	
6	1.560347000	0.015819000	0.377908000	
6	0.956477000	1.080829000	1.115213000	
8	1.182256000	1.510717000	2.219800000	
7	-0.078091000	1.664692000	0.348198000	
6	-0.468261000	1.298876000	-0.898101000	
7	-1.522369000	1.970932000	-1.433844000	
7	0.074694000	0.326659000	-1.562865000	
6	1.066584000	-0.274598000	-0.877094000	
1	3.404763000	-2.416804000	-0.405531000	
1	-0.575490000	2.388681000	0.836849000	
1	-1.671934000	2.921997000	-1.158349000	
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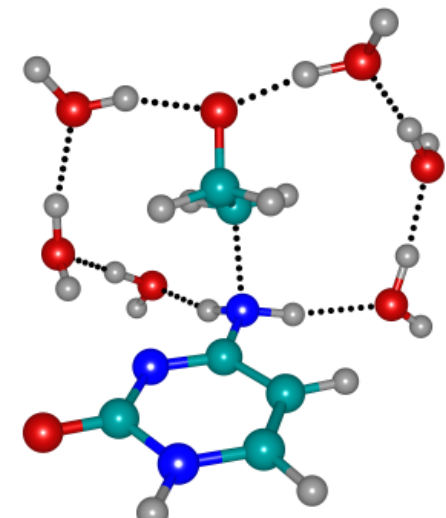
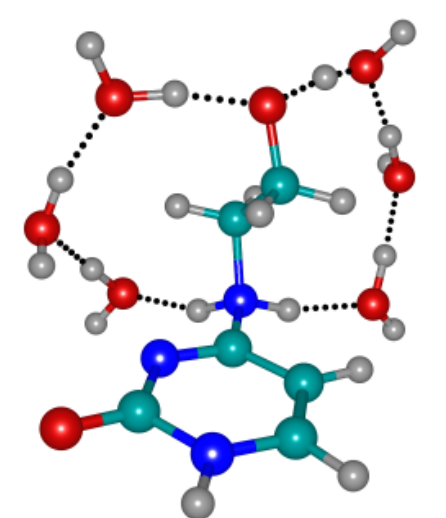
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6	-2.911165000	-0.737051000	0.428473000				
8	-4.568334000	0.436394000	0.938030000				
1	-4.216258000	0.063548000	-1.082060000				
1	-3.161172000	1.279972000	-0.337612000				
1	-3.475598000	-1.648941000	0.561099000				
1	-2.343400000	-0.456524000	1.305241000				
7	2.941980000	-1.348920000	0.277855000				
6	3.806950000	-0.306525000	0.440388000				
7	3.237084000	0.848246000	0.297335000				
6	1.935721000	0.556993000	0.029329000				
6	0.824074000	1.435468000	-0.208246000				
8	0.762418000	2.632789000	-0.237128000				
7	-0.349674000	0.662682000	-0.429067000				
6	-0.398846000	-0.679050000	-0.438835000				
7	-1.678095000	-1.248760000	-0.669214000				
7	0.582608000	-1.477815000	-0.228654000				
6	1.732539000	-0.804852000	0.013586000				
1	4.846111000	-0.464544000	0.663454000				
1	-1.204426000	1.197514000	-0.519393000				
1	-2.060673000	-0.975250000	-1.569320000				
1	-1.562361000	-2.255253000	-0.658576000				
1	3.148773000	-2.327094000	0.343228000				
E(RmPW+HF-B95) = -695.984090531				N _{img} = 1			
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6	-2.790647000	-0.769341000	0.574131000				

8	-4.752488000	0.551967000	0.486189000	
1	-3.911731000	-0.385422000	-1.165144000	
1	-3.039650000	1.036673000	-0.558495000	
1	-3.336302000	-1.650639000	0.890538000	
1	-2.290409000	-0.309168000	1.419061000	
7	2.950010000	-1.369404000	0.130432000	
6	3.838304000	-0.341334000	0.246515000	
7	3.272559000	0.823365000	0.186742000	
6	1.950190000	0.554164000	0.024943000	
6	0.836273000	1.455367000	-0.102612000	
8	0.794749000	2.652394000	-0.101988000	
7	-0.363896000	0.703211000	-0.251208000	
6	-0.424208000	-0.632127000	-0.271332000	
7	-1.734893000	-1.204928000	-0.429741000	
7	0.550274000	-1.454330000	-0.164408000	
6	1.730190000	-0.804294000	-0.012876000	
1	4.890899000	-0.516076000	0.373379000	
1	-1.221891000	1.241944000	-0.335863000	
1	-2.164947000	-0.944194000	-1.334994000	
1	-1.589983000	-2.209630000	-0.439217000	
1	3.150095000	-2.351117000	0.149723000	
E(RmPW+HF-B95) = -695.989319193 N _{img} = 0				
ECw				
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6	2.409733000	-0.387897000	-0.082027000	
8	3.075433000	-0.302367000	-1.349368000	
1	1.144683000	0.527860000	-1.613458000	
1	1.241120000	-1.305175000	-1.695138000	
1	2.460986000	0.515586000	0.508684000	
1	2.567269000	-1.315938000	0.444905000	
8	3.531520000	2.405210000	-1.311229000	
1	3.526164000	1.448340000	-1.465595000	
1	3.744575000	2.832642000	-2.135324000	

8	3.106546000	-3.143004000	-1.404384000
1	3.337667000	-3.705100000	-2.138325000
1	3.422190000	-2.257801000	-1.608387000
8	2.340978000	3.500401000	0.934528000
1	2.704241000	3.163438000	0.102493000
1	3.079150000	3.579634000	1.531997000
8	0.777378000	-3.364765000	0.328190000
1	1.467383000	-3.425296000	-0.337889000
1	0.072105000	-2.804317000	-0.027764000
8	1.210937000	-1.978128000	2.555538000
8	-0.210818000	3.006806000	1.931729000
1	1.031194000	-2.468715000	3.352012000
1	1.116179000	-2.604698000	1.809333000
1	-0.427067000	3.713707000	2.532513000
1	0.667032000	3.205343000	1.571785000
7	-1.105369000	-1.180443000	-0.277535000
6	-1.727981000	-1.352909000	-1.465795000
7	-2.532775000	-0.308879000	-1.921766000
6	-2.609927000	0.881199000	-1.290093000
6	-1.939541000	1.083988000	-0.144655000
6	-1.181474000	-0.025869000	0.361968000
7	-0.530569000	0.129286000	1.506491000
8	-1.613492000	-2.347014000	-2.158018000
1	-3.224665000	1.635490000	-1.754140000
1	-1.953775000	2.023477000	0.378616000
1	0.031701000	-0.618475000	1.897254000
1	-0.489710000	1.047598000	1.918704000
1	-2.994717000	-0.473710000	-2.795776000
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ECw-TS1			
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6	-1.153618000	0.620975000	0.210798000
8	-1.886343000	1.563812000	-1.287254000
1	-0.981330000	-0.263368000	-1.756575000
1	0.140299000	1.101910000	-1.453149000
1	-2.042026000	0.078111000	0.487751000
1	-0.893914000	1.483575000	0.800403000
8	-4.049962000	0.178043000	-1.554768000
1	-3.264520000	0.788530000	-1.511640000
1	-4.323367000	0.110401000	-2.463985000
8	-0.474316000	3.742372000	-0.783909000
1	-0.438281000	4.400953000	-1.470179000
1	-1.127554000	3.058855000	-1.051273000
8	-4.167359000	-1.632568000	0.390778000

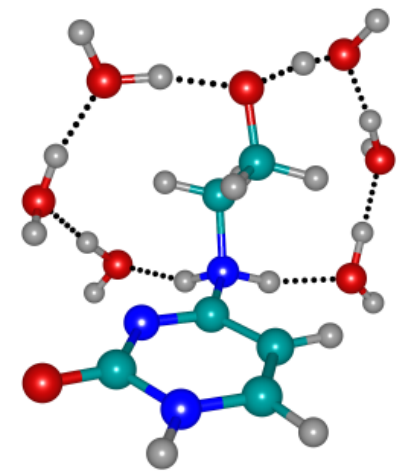


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1	-4.851166000	-1.304833000	0.968158000
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1	0.895939000	3.179040000	0.261657000
1	1.910627000	2.008384000	0.493657000
8	0.471400000	1.519646000	3.017208000
8	-1.875406000	-2.694829000	1.368243000
1	0.947425000	1.655420000	3.830925000
1	0.857487000	2.123489000	2.347485000
1	-2.087272000	-3.396035000	1.977947000
1	-2.724294000	-2.364307000	1.017061000
7	2.068367000	-0.147781000	0.237157000
6	3.107948000	-0.468271000	-0.586620000
7	3.059551000	-1.733971000	-1.175761000
6	2.047636000	-2.598864000	-0.998048000
6	1.013965000	-2.272216000	-0.194406000
6	1.096566000	-0.993786000	0.422390000
7	0.053173000	-0.584135000	1.228142000
8	4.038433000	0.262020000	-0.832419000
1	2.115435000	-3.539386000	-1.520357000
1	0.175663000	-2.923502000	-0.020153000
1	0.327360000	0.053863000	1.984414000
1	-0.560951000	-1.341516000	1.518741000
1	3.834276000	-1.952090000	-1.775548000
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ECw-1			
At. No	X	Y	Z
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6	-0.927028000	0.497910000	0.373111000
8	-1.873299000	1.274879000	-1.599865000
1	-1.596452000	-0.736794000	-1.256137000
1	-0.136525000	0.189658000	-1.597560000
1	-1.883634000	0.501738000	0.884726000
1	-0.436646000	1.449739000	0.525874000
8	-4.192574000	0.468827000	-1.334521000
1	-3.249934000	0.883744000	-1.483151000
1	-4.590612000	0.341640000	-2.190156000
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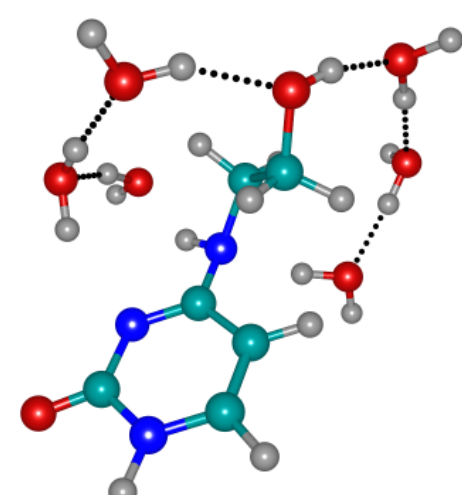
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1	-4.174745000	-0.727121000	-0.300423000
1	-4.754135000	-1.127849000	1.090142000
8	1.369490000	2.979849000	1.050668000
1	0.754504000	3.222370000	0.332949000
1	2.052234000	2.450262000	0.638977000
8	0.531684000	1.304393000	2.976446000
8	-1.886123000	-2.575517000	1.117232000
1	1.098340000	1.361294000	3.740324000
1	0.816542000	2.009506000	2.354230000
1	-2.099778000	-3.303125000	1.694638000
1	-2.744171000	-2.166666000	0.841939000
7	2.057730000	-0.081450000	0.367029000
6	3.197316000	-0.353563000	-0.346121000
7	3.194104000	-1.559204000	-1.051643000
6	2.168207000	-2.421476000	-1.064048000
6	1.048309000	-2.146749000	-0.354314000
6	1.083598000	-0.920031000	0.338693000
7	-0.081706000	-0.531896000	1.086769000
8	4.160658000	0.367771000	-0.392629000
1	2.288230000	-3.311907000	-1.659167000
1	0.182164000	-2.784724000	-0.338258000
1	0.225663000	-0.058268000	1.961794000
1	-0.678629000	-1.354859000	1.281774000
1	4.029913000	-1.741521000	-1.578872000
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At. No	X	Y	Z
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6	-0.936703000	0.499124000	0.376122000

8	-1.882236000	1.284468000	-1.592264000
1	-1.599627000	-0.728652000	-1.262644000
1	-0.141973000	0.204779000	-1.594797000
1	-1.894767000	0.501757000	0.884763000
1	-0.447086000	1.450502000	0.533722000
8	-4.198284000	0.470976000	-1.346883000
1	-3.254635000	0.888671000	-1.487690000
1	-4.600818000	0.371034000	-2.204052000
8	-0.375465000	3.282932000	-1.021311000
1	-0.462329000	4.021718000	-1.615005000
1	-1.032526000	2.575194000	-1.310136000
8	-4.158084000	-1.439079000	0.384388000
1	-4.189973000	-0.751443000	-0.339122000
1	-4.771125000	-1.142204000	1.051012000
8	1.376959000	2.980411000	1.055678000
1	0.746946000	3.221981000	0.351176000
1	2.062718000	2.471663000	0.623553000
8	0.526004000	1.305642000	2.976571000
8	-1.899616000	-2.577920000	1.085218000
1	1.079123000	1.342366000	3.751556000
1	0.849250000	1.997217000	2.357638000
1	-2.134437000	-3.314739000	1.642317000
1	-2.747905000	-2.148223000	0.810322000
7	2.052012000	-0.091689000	0.386908000
6	3.191371000	-0.359610000	-0.328041000
7	3.182208000	-1.554210000	-1.051739000
6	2.149496000	-2.408194000	-1.082543000
6	1.028325000	-2.136167000	-0.373780000
6	1.071246000	-0.921625000	0.339605000
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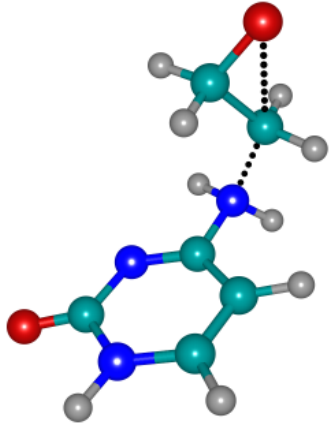
The image shows a 3D ball-and-stick model of a complex organic molecule. The structure features a central core with several nitrogen (blue) and oxygen (red) atoms. The molecule is surrounded by a network of hydrogen bonds, represented by dashed lines connecting hydrogen atoms (grey) to oxygen atoms (red) of neighboring molecules. The overall structure is highly symmetrical and appears to be a dimer or a small cluster of molecules.

1	2.265476000	-3.289901000	-1.691308000	
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1	0.218994000	-0.058556000	1.962440000	
1	-0.691301000	-1.353240000	1.286337000	
1	4.018474000	-1.734407000	-1.578978000	
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ECw-2				
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6	-1.057437000	0.408506000	0.264877000	
8	-2.143228000	1.157694000	-1.711765000	
1	-1.658042000	-0.821359000	-1.419272000	
1	-0.336620000	0.298187000	-1.761237000	
1	-1.967318000	0.161074000	0.807605000	
1	-0.887761000	1.474030000	0.401959000	
8	-4.542968000	0.171686000	-0.831747000	
1	-3.047712000	0.938869000	-1.436703000	
1	-5.218928000	-0.121839000	-1.435608000	
8	-0.143064000	3.069208000	-1.484974000	
1	-0.143353000	3.874728000	-1.993637000	
1	-0.994854000	2.634809000	-1.631266000	
8	-4.198534000	-1.738997000	1.097191000	
1	-4.463960000	-0.509180000	-0.142707000	
1	-4.456022000	-1.520704000	1.988754000	
8	1.440912000	2.716920000	0.881882000	
1	0.977896000	2.880479000	0.051935000	
1	1.996981000	1.941763000	0.756490000	
8	0.034278000	1.722995000	2.979937000	
8	-1.579684000	-2.598513000	1.163938000	
1	0.463103000	1.853847000	3.820520000	
1	0.508807000	2.276867000	2.336614000	



The image shows a 3D ball-and-stick model of a complex organic molecule. The structure features a central ring system with several nitrogen atoms (blue) and oxygen atoms (red). The molecule is surrounded by several water molecules (red and white spheres) which are connected to the main structure via hydrogen bonds, indicated by dashed lines. The overall structure is highly branched and complex.

1	-1.257189000	-3.357111000	1.642668000
1	-3.301264000	-2.104078000	1.146074000
7	2.324144000	-0.169154000	0.626379000
6	3.512399000	-0.565452000	0.082891000
7	3.435603000	-1.507473000	-0.945642000
6	2.278765000	-2.030159000	-1.384538000
6	1.110533000	-1.645380000	-0.833545000
6	1.193583000	-0.675969000	0.210719000
7	0.057634000	-0.311872000	0.898329000
8	4.596016000	-0.147672000	0.416479000
1	2.345195000	-2.765884000	-2.169584000
1	0.175148000	-2.087494000	-1.122761000
1	0.313340000	0.200844000	1.738820000
1	-0.915330000	-1.892977000	1.252124000
1	4.316751000	-1.776599000	-1.343163000
E(RmPW+HF-B95) = -1006.98458497 N _{img} = 0			
EC			
At. No	X	Y	Z
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6	-1.259117000	0.676312000	-0.443183000
8	-1.718860000	1.138524000	-1.691022000
1	-0.060561000	-0.098994000	-2.110339000
1	0.340518000	1.618708000	-1.617298000
1	-1.621931000	-0.300632000	-0.151957000
1	-1.221539000	1.415601000	0.344886000
7	2.052998000	-0.246019000	0.600963000
6	2.713301000	-0.291371000	-0.583188000
7	2.486305000	-1.423001000	-1.383237000
6	1.631371000	-2.403046000	-1.050387000
6	0.946655000	-2.336561000	0.107595000
6	1.211315000	-1.190564000	0.921618000

7	0.539734000	-1.044549000	2.079602000	
8	3.472795000	0.556194000	-0.994205000	
1	1.527194000	-3.218178000	-1.748378000	
1	0.247120000	-3.101011000	0.395055000	
1	0.822373000	-0.293171000	2.678467000	
1	0.019418000	-1.800703000	2.472907000	
1	3.001415000	-1.445308000	-2.243740000	
E(RmPW+HF-B95) = -548.498718124			N _{img} = 0	
EC-TS1				
At. No	X	Y	Z	
6	2.424864000	-0.501289000	-0.895565000	
6	2.420695000	-0.000412000	0.513318000	
8	3.624208000	-0.011683000	-1.199507000	
1	1.556144000	-0.088990000	-1.454702000	
1	2.309521000	-1.603632000	-0.924515000	
1	2.473265000	1.079372000	0.546302000	
1	3.183868000	-0.468036000	1.121347000	
7	-0.985690000	-0.903224000	0.494378000	
6	-2.145197000	-0.650867000	-0.197154000	
7	-2.338478000	0.683794000	-0.576397000	
6	-1.496012000	1.681059000	-0.282051000	
6	-0.365606000	1.425720000	0.418090000	
6	-0.184745000	0.068173000	0.756678000	
7	1.017042000	-0.312590000	1.428807000	
8	-2.972589000	-1.475856000	-0.477612000	
1	-1.760499000	2.664052000	-0.635681000	
1	0.353177000	2.191692000	0.643726000	
1	0.958995000	-1.310806000	1.600631000	
1	1.117885000	0.172687000	2.312069000	
1	-3.179408000	0.853806000	-1.099632000	
E(RmPW+HF-B95) = -548.408576524			N _{img} = 1	

EC-1

At. No	X	Y	Z
6	3.218236000	0.063425000	0.288972000
6	2.110508000	-0.600204000	-0.566058000
8	4.231191000	0.448961000	-0.392963000
1	3.395312000	-0.727735000	1.095937000
1	2.645648000	0.863811000	0.872871000
1	2.461081000	-1.507693000	-1.043545000
1	1.701140000	0.078654000	-1.305906000
7	-1.267813000	-1.010172000	0.099633000
6	-2.504884000	-0.434527000	-0.085286000
7	-2.510429000	0.964815000	-0.107393000
6	-1.420808000	1.730108000	0.035035000
6	-0.206778000	1.154846000	0.215116000
6	-0.241960000	-0.250754000	0.229846000
7	1.002148000	-0.968389000	0.405104000
8	-3.530965000	-1.043281000	-0.218849000
1	-1.565942000	2.797358000	-0.003330000
1	0.705190000	1.715200000	0.327714000
1	0.761761000	-1.954984000	0.378971000
1	1.417462000	-0.769343000	1.328183000
1	-3.416689000	1.378140000	-0.243554000
E(RmPW+HF-B95) = -548.417156543			N _{img} = 0

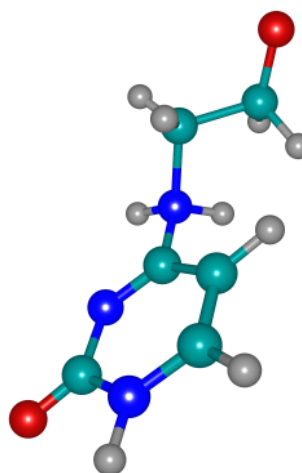


Table S2. Zero-point energy (ZPE) corrected SCF energies (E+ZPE), enthalpies (H), free energies (G), ZPE and thermal correction to Gibb's free energy (G_{corr}) computed at MPWB1K/6-31++G(d,p) level of theory. All the energies are given in atomic units (a.u).

System	E+ZPE	H	G	ZPE	G_{corr}
EAw	-1078.9889	-1078.9602	-1079.0500	0.34	0.27
EAw-TS1	-1078.9461	-1078.9198	-1079.0014	0.34	0.28
EAw-1	-1078.9742	-1078.9484	-1079.0297	0.34	0.28
EAw-TS2	-1078.9754	-1078.9504	-1079.0292	0.33	0.28
EAw-2	-1078.9742	-1078.9487	-1079.0285	0.33	0.28
EAw-TS3	-1078.9756	-1078.9507	-1079.0293	0.33	0.28
EAw-3	-1079.0187	-1078.9913	-1079.0757	0.34	0.28
EA	-620.6843	-620.6719	-620.7259	0.18	0.14
EA-TS1	-620.6012	-620.5897	-620.6390	0.18	0.14
EA-1	-620.6033	-620.5917	-620.6417	0.18	0.14
EGw	-1154.2019	-1154.1721	-1154.2621	0.34	0.28
EGw-TS1	-1154.1584	-1154.1306	-1154.2157	0.34	0.28
EGw-1	-1154.1804	-1154.1534	-1154.2370	0.34	0.28
EGw-TS2	-1154.1782	-1154.1520	-1154.2338	0.34	0.28
EGw-2	-1154.2352	-1154.2057	-1154.2967	0.34	0.28
EG	-695.8906	-695.8770	-695.9309	0.18	0.14
EG-TS1	-695.8028	-695.7904	-695.8415	0.18	0.14
EG-1	-695.8075	-695.7951	-695.8458	0.18	0.14
ECw	-1006.6421	-1006.6135	-1006.7019	0.32	0.26
ECw-TS1	-1006.5975	-1006.5711	-1006.6531	0.32	0.27
ECw-1	-1006.6232	-1006.5972	-1006.6788	0.32	0.27
ECw-TS2	-1006.6232	-1006.5970	-1006.6784	0.32	0.27
ECw-2	-1006.6610	-1006.6336	-1006.7182	0.32	0.27
EC	-548.3349	-548.3239	-548.3711	0.16	0.13
EC-TS1	-548.2458	-548.2351	-548.2824	0.16	0.13
EC-1	-548.2509	-548.2429	-548.2903	0.16	0.13

Table S3. Single point SCF energies (in a.u.) of MPWB1K/6-31+G(d,p) optimized geometries at seven different DFT functionals using 6-311++G(3df,2p) basis set.

System	MPWB1K	M05	B3LYP	PBE0	TPSS	BP86	PBE
EAw	-1079.6474	-1079.5498	-1080.1939	-1078.9819	-1080.2949	-1080.1993	-1078.9632
EAw-TS1	-1079.6025	-1079.4992	-1080.1603	-1078.9471	-1080.2677	-1080.1751	-1078.9372
EAw-1	-1079.6291	-1079.5175	-1080.1802	-1078.9729	-1080.2818	-1080.1939	-1078.9565
EAw-TS2	-1079.6262	-1079.5133	-1080.1768	-1078.9702	-1080.2782	-1080.1912	-1078.9540
EAw-2	-1079.6260	-1079.5114	-1080.1759	-1078.9697	-1080.2777	-1080.1907	-1078.9533
EAw-TS3	-1079.6257	-1079.5113	-1080.1757	-1078.9699	-1080.2768	-1080.1907	-1078.9534
EAw-3	-1079.6796	-1079.5706	-1080.2233	-1079.0146	-1080.3162	-1080.2273	-1078.9909
EA	-621.0334	-620.9208	-621.3325	-620.6290	-621.4315	-621.3407	-620.6079
EA-TS1	-620.9485	-620.8366	-621.2602	-620.5547	-621.3650	-621.2777	-620.5442
EA-1	-620.9528	-620.8381	-621.2598	-620.5571	-621.3624	-621.2787	-620.5461
EGw	-1154.8924	-1154.7954	-1155.4636	-1154.1791	-1155.5697	-1155.4715	-1154.1622
EGw-TS1	-1154.8457	-1154.7451	-1155.4295	-1154.1432	-1155.5430	-1155.4487	-1154.1371
EGw-1	-1154.8685	-1154.7588	-1155.4454	-1154.1649	-1155.5539	-1155.4638	-1154.1527
EGw-TS2	-1154.8604	-1154.7498	-1155.4400	-1154.1599	-1155.5488	-1155.4602	-1154.1486
EGw-2	-1154.9252	-1154.8186	-1155.4970	-1154.2138	-1155.5966	-1155.5044	-1154.1938
EG	-696.2735	-696.1628	-696.5985	-695.8222	-696.7044	-696.6114	-695.8054
EG-TS1	-696.1832	-696.0734	-696.5208	-695.7429	-696.6328	-696.5452	-695.7381
EG-1	-696.1903	-696.0764	-696.5238	-695.7480	-696.6323	-696.5470	-695.7407
ECw	-1007.2725	-1007.2030	-1007.7904	-1006.6576	-1007.8691	-1007.7880	-1006.6404
ECw-TS1	-1007.2241	-1007.1511	-1007.7548	-1006.6202	-1007.8408	-1007.7633	-1006.6132
ECw-1	-1007.2491	-1007.1681	-1007.7723	-1006.6438	-1007.8531	-1007.7797	-1006.6307
ECw-TS2	-1007.2490	-1007.1679	-1007.7721	-1006.6436	-1007.8529	-1007.7795	-1006.6305
ECw-2	-1007.2923	-1007.2139	-1007.8102	-1006.6800	-1007.8841	-1007.8087	-1006.6602
EC	-548.6573	-548.5746	-548.9283	-548.3043	-549.0069	-548.9307	-548.2870
EC-TS1	-548.5655	-548.4826	-548.8490	-548.2233	-548.9305	-548.8631	-548.2181
EC-1	-548.5757	-548.4888	-548.8549	-548.2317	-548.9367	-548.8681	-548.2238

Table S4. Zero-point-energy (ZPE) corrected activation energies (E_{act}) are given with respect to the pre-reactant complex at seven different DFT functionals using 6-311++G(3df,2p) basis set (kcal/mol).

System	MPWB1K	M05	B3LYP	PBE0	TPSS	BP86	PBE
EAw	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EAw-TS1	28.94	32.56	21.88	22.70	17.90	16.01	17.13
EAw-1	11.75	20.58	8.80	5.95	8.50	3.70	4.47
EAw-TS2	11.54	21.17	8.96	5.64	8.77	3.40	4.06
EAw-2	12.59	23.26	10.43	6.86	10.02	4.62	5.42
EAw-TS3	11.88	22.44	9.67	5.86	9.68	3.69	4.45
EAw-3	-17.92	-10.74	-16.20	-18.21	-11.04	-15.28	-15.06
EA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EA-TS1	53.51	53.06	45.59	46.78	41.92	39.75	40.18
EA-1	51.24	52.54	46.30	45.77	44.00	39.54	39.41
EGw	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EGw-TS1	29.12	31.40	21.19	22.37	16.59	14.16	15.54
EGw-1	15.52	23.53	11.98	9.47	10.47	5.38	6.46
EGw-TS2	17.98	26.49	12.69	9.95	11.02	5.02	6.40
EGw-2	-19.75	-13.72	-20.09	-20.91	-16.03	-19.78	-19.03
EG	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EG-TS1	55.76	55.21	47.86	48.88	44.00	40.63	41.29
EG-1	51.68	53.70	46.39	46.02	44.67	39.86	40.05
ECw	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ECw-TS1	30.28	32.46	22.27	23.37	17.64	15.40	16.97
ECw-1	14.73	21.95	11.42	8.71	10.06	5.23	6.13
ECw-TS2	14.68	21.93	11.43	8.71	10.06	5.25	6.13
ECw-2	-10.68	-5.09	-10.66	-12.33	-7.67	-11.23	-10.70
EC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EC-TS1	56.93	57.03	49.04	50.17	47.26	41.74	42.56
EC-1	50.98	53.59	45.84	45.35	43.81	39.06	39.45

Table S5. Single point MPWB1K-PCM/6-311++G(3df,2p) ZPE corrected SCF energies (in a.u) of MPWB1K/6-31+G(d,p) optimized geometries of reactants, intermediates and transition states of **EAw**, **EGw** and **ECw** systems.

System	MPWB1K-PCM
EAw	-1079.3512
EAw-TS1	-1079.3064
EAw-1	-1079.3429
EAw-TS2	-1079.3395
EAw-2	-1079.3370
EAw-TS3	-1079.3357
EAw-3	-1079.3798
EGw	-1154.6007
EGw-TS1	-1154.5551
EGw-1	-1154.5829
EGw-TS2	-1154.5782
EGw-2	-1154.6366
ECw	-1006.9938
ECw-TS1	-1006.9486
ECw-1	-1006.9800
ECw-TS2	-1006.9800
ECw-2	-1007.0148

Figure S1. Relative energy (E_{act}) profiles at seven different DFT functionals using 6-311++G(3df,2p) basis set (kcal/mol). The corresponding numerical values are given in Table S4.

