Supporting Information

In Silico Studies with Substituted Adenines to Achieve Remarkable Stability of Mispairs with Thymine Nucleobase

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The M06-2X/6-31+G(d,p) level of theory optimized Cartesian coordinates and zero-point corrected electronic energies free energies and zero-point corrections of studied mispairs. All the energy values are given in Hatree.

A-T

E=-920.939329
G=-920.985368
ZPE= 0.230922

N	4.94651600	0.55970800	0.00027500
C	5.20824100	-0.79128700	0.00034900
H	6.22048500	-1.17117500	0.00050200
N	4.12870300	-1.52642500	0.00019700
C	3.09975200	-0.60724000	0.00000900
C	1.69548900	-0.75632100	-0.00018700
N	1.09167900	-1.95116200	-0.00019000
H	0.07386800	-2.01695600	-0.00038800
H	1.65969500	-2.78336000	-0.00023600
N	0.95539100	0.36774800	-0.00031800
C	1.56012000	1.57118700	-0.00021000
H	0.88185200	2.42175300	-0.00028500
N	2.86021300	1.82847900	0.00000600
C	3.58165400	0.69811200	0.00010000
H	5.61574500	1.31472700	0.00035300
N	-3.81150500	1.60210800	0.00031000
C	-4.54470400	0.43724000	0.00044700
H	-5.62221800	0.56647700	0.00081100
C	-3.96648500	-0.78128700	0.00017000
C	-4.71827600	-2.07639500	0.00029700
H	-4.45699400	-2.67230900	-0.87871800
H	-4.45568000	-2.67283000	0.87856000
H	-5.79667400	-1.90147000	0.00113900
C	-2.50162500	-0.83452200	-0.00020200
O	-1.86480200	-1.88617000	-0.00034300
N	-1.84770700	0.38259200	-0.00060200
H	-0.79524400	0.36712200	-0.00051300
C	-2.42601100	1.62966800	-0.00009300
O	-1.79215300	2.66936300	-0.00012000
H	-4.26116100	2.50621600	0.00065000

ANH_2-T

E= -976.283210
G= -976.328225
ZPE= 0.247751

N	-4.99138400	0.20361500	0.00024900
C	-5.14536400	-1.17069300	0.00093900
H	-6.12429500	-1.62939300	0.00137700
N	-4.01024100	-1.81129300	0.00098200
C	-3.05915500	-0.80794400	0.00036100
C	-1.64732500	-0.83889600	-0.00004500
N	-0.98462900	-2.00424500	0.00005500
H	0.03182800	-2.04209300	-0.00021600
H	-1.52414800	-2.85544300	0.00077600
N	-0.97616100	0.32429800	-0.00065100
C	-1.68559500	1.48982700	-0.00084900
N	-3.01742900	1.63091800	-0.00070100
C	-3.64271500	0.45191400	-0.00009000
H	-5.71883300	0.90193300	0.00008300
N	3.95787100	1.44650000	0.00094300
C	4.66314700	0.26386700	0.00070500
H	5.74329300	0.36573800	0.00111200
C	4.04943600	-0.93520600	0.00000600
C	2.58315900	-0.94975000	-0.00056000
O	1.92768100	-1.98506900	-0.00140200
N	1.95407800	0.28818400	-0.00000900
H	0.90612500	0.30276900	-0.00025300
C	2.57976000	1.51005100	0.00067000
O	1.98780300	2.57947400	0.00103100
H	4.42832900	2.34019100	0.00150200
N	-0.95961100	2.63098900	-0.00120700
H	0.05369100	2.62663400	-0.00115500
H	-1.46445200	3.50065900	-0.00181300
C	4.76040200	-2.25279000	-0.00029500
H	4.47941900	-2.84045500	0.87796800
H	4.47981000	-2.83983300	-0.87909500
H	5.84338400	-2.11098800	0.00000900

AOH-T

E= -996.157780
G= -996.204027
ZPE= 0.235945

N	4.95346000	0.21447900	0.00065000
C	5.11538400	-1.15688300	0.00016700
H	6.09711600	-1.60972300	0.00027700
N	3.98475200	-1.80686300	-0.00032400
C	3.02791400	-0.80999600	-0.00026100
C	1.61854200	-0.84711500	-0.00076700
N	0.95153700	-2.00994200	-0.00174600
H	-0.06520500	-2.05559500	-0.00076000
H	1.48989200	-2.86228600	-0.00110800
N	0.95146100	0.32238000	-0.00036100
C	1.65734700	1.48351700	0.00044900
N	2.97399600	1.63153900	0.00076400
C	3.60416900	0.45365500	0.00042700
H	5.67547900	0.91906700	0.00101800
N	-3.83341700	1.50824100	-0.00047200
C	-4.60381500	0.36473200	0.00000400
H	-5.67628600	0.52792600	-0.00006800
C	-4.06046100	-0.86879100	0.00044400
C	-2.59788600	-0.96843200	0.00041000
O	-1.99306700	-2.03436500	0.00060200
N	-1.90614800	0.23382900	0.00004800
H	-0.85567500	0.21603600	-0.00001700
C	-2.45780400	1.48541800	-0.00045600
O	-1.79131300	2.51425100	-0.00087100
H	-4.25298200	2.42724700	-0.00070900
C	-4.84808200	-2.14231200	0.00084500

$^{Br}ANH_2$-T

E= -3547.494917
G= -3547.543179
ZPE= 0.237558

N	3.55823300	1.11836400	0.00020500
C	3.89690300	-0.21753900	-0.00024600
N	2.88742300	-1.02504300	-0.00039900
C	1.79538100	-0.17072000	-0.00005900
C	0.40509600	-0.41529400	0.00000700
N	-0.07709100	-1.66524400	-0.00029500
H	-1.07736300	-1.85265100	0.00000500
H	0.58058800	-2.42881100	-0.00059100
N	-0.43037400	0.63646000	0.00042000
C	0.09506200	1.89453700	0.00076500
N	1.39328500	2.23344000	0.00077000
C	2.18321000	1.16221500	0.00036200
H	4.19199000	1.90326500	0.00035700
N	-5.47622800	1.01253900	-0.00035500
C	-5.99754400	-0.26226500	-0.00014800
H	-7.08078900	-0.32223900	-0.00031300
C	-5.21280500	-1.35691000	0.00024300
C	-3.76114700	-1.15368100	0.00043800
O	-2.95812400	-2.07947300	0.00086200
N	-3.32408100	0.16404700	0.00014400
H	-2.29131800	0.33408400	0.00026200
C	-4.12342400	1.27991200	-0.00023200
O	-3.69523000	2.42494900	-0.00045700
H	-6.07461300	1.82620500	-0.00067200
N	-0.79077700	2.91402400	0.00117900
H	-1.79263000	2.75896600	0.00083700

H	-4.60137300	-2.74482600	-0.87769000
H	-4.60146000	-2.74422100	0.87981900
H	-5.92089800	-1.93756900	0.00071700
O	0.96604700	2.61690500	0.00040100
H	-0.00328200	2.47122000	-0.00001800

H	-0.42107400	3.84928800	0.00130800
C	-5.72096100	-2.76529800	0.00050300
H	-5.35590000	-3.30448000	-0.87806400
H	-5.35613900	-3.30406700	0.87942100
H	-6.81304500	-2.78544900	0.00035600
Br	5.69073700	-0.71793600	-0.00079000

^{Br}AOH-T

E= -3567.368880
G= -3567.418175
ZPE= 0.225748

N	3.52502700	1.11631000	0.00050900
C	3.87183700	-0.21606600	0.00014200
N	2.86735600	-1.03159700	-0.00041400
C	1.77087300	-0.18445600	-0.00032900
C	0.38406300	-0.43429800	-0.00068500
N	-0.10412100	-1.68192500	-0.00129800
H	-1.10374300	-1.87583300	-0.00093600
H	0.55165600	-2.44757800	-0.00107200
N	-0.44794200	0.62491400	-0.00048900
C	0.07460300	1.87752900	0.00004400
N	1.35676800	2.22084200	0.00042600
C	2.15121500	1.15124300	0.00021800
H	4.15205700	1.90727300	0.00094400
N	-5.35444300	1.09507300	-0.00033400
C	-5.94803200	-0.14944700	0.00003800
H	-7.03280100	-0.14570300	0.00013600
C	-5.23016600	-1.29005500	0.00025800
C	-3.76906400	-1.17453300	0.00008300
O	-3.01311500	-2.13926500	0.00021000
N	-3.26226000	0.11668300	-0.00024900
H	-2.22198200	0.25236600	-0.00041100
C	-3.99107200	1.27409400	-0.00050200
O	-3.48135500	2.38931300	-0.00084700
H	-5.90485300	1.94225700	-0.00051500
C	-5.82455800	-2.66428700	0.00063800
H	-5.49434500	-3.22496100	-0.87822100
H	-5.49406400	-3.22459300	0.87962500
H	-6.91571100	-2.61649700	0.00079900
O	-0.77574400	2.89472400	0.00014900
H	-1.71415800	2.60874700	-0.00033800
Br	5.66682200	-0.70554600	0.00049800

^{COOH}ANH$_2$-T

E= -1164.789386
G= -1164.839222
ZPE= 0.262760

N	3.97822400	0.99533800	0.00012000
C	4.29969300	-0.34826700	-0.00039600
N	3.24910500	-1.13033600	-0.00060200
C	2.19326400	-0.25948500	-0.00018400
C	0.79090800	-0.47201100	-0.00010600
N	0.28596800	-1.71043200	-0.00048800
H	-0.71836600	-1.87863700	-0.00013300
H	0.92975400	-2.48628900	-0.00073100
N	-0.01733900	0.59630000	0.00034000
C	0.53999800	1.84493900	0.00074300
N	1.84331100	2.15749700	0.00073600
C	2.61668800	1.07220900	0.00027000
H	4.64454100	1.75544400	0.00034700
N	-5.05303700	1.08062000	-0.00034800
C	-5.60194100	-0.18265300	-0.00012400
H	-6.68621700	-0.21887500	-0.00024900
C	-4.84160300	-1.29458600	0.00022700
C	-3.38611700	-1.12344500	0.00034800
O	-2.60241000	-2.06589100	0.00062700
N	-2.92082300	0.18447800	0.00012200
H	-1.88546900	0.33269900	0.00022200
C	-3.69499000	1.31795200	-0.00023000
O	-3.24024300	2.45273900	-0.00043100
H	-5.63374600	1.90706500	-0.00062400
N	-0.32543300	2.87910600	0.00128300
H	-1.33044500	2.74323000	0.00070700
H	0.06227500	3.80737100	0.00122800
C	-5.38099900	-2.69137600	0.00047700
H	-5.02833300	-3.23860600	-0.87817100
H	-5.02848800	-3.23823000	0.87942000
H	-6.47323500	-2.68703800	0.00037800
O	6.61498100	0.08037900	-0.00042800
O	5.91234500	-2.05769100	-0.00119300
C	5.71843800	-0.73627400	-0.00065700
H	6.87047100	-2.20443000	-0.00133800

^{COOH}AOH-T

E= -1184.662519
G= -1184.713294
ZPE= 0.250938

N	3.94281000	0.99555700	0.00073100
C	4.27153800	-0.34375100	0.00028800
N	3.22845100	-1.13520200	-0.00040000
C	2.16580500	-0.27053200	-0.00042900
C	0.76736400	-0.48847200	-0.00091000
N	0.25649100	-1.72443300	-0.00164400
H	-0.74733000	-1.89908800	-0.00114000
H	0.89825300	-2.50238400	-0.00127100
N	-0.03771200	0.58717500	-0.00070400
C	0.51625900	1.83069000	-0.00004100
N	1.80327500	2.14762900	0.00049000
C	2.58106000	1.06296000	0.00028100
H	4.60262200	1.76203900	0.00126300
N	-4.93356400	1.15779000	-0.00028600
C	-5.55195100	-0.07458900	0.00017900
H	-6.63642900	-0.04889700	0.00032400
C	-4.85760000	-1.22984500	0.00041900
C	-3.39458900	-1.14386400	0.00016700
O	-2.65730200	-2.12322700	0.00029600
N	-2.86221300	0.13676200	-0.00023100
H	-1.82009200	0.25178100	-0.00043700
C	-3.56691600	1.30912400	-0.00051200
O	-3.03300100	2.41292700	-0.00093400

^{NO2}ANH$_2$-T

E= -1180.708242
G= -1180.759850
ZPE= 0.250454

N	4.00772700	0.94481100	0.00011900
C	4.29167800	-0.39829600	-0.00037900
N	3.25557700	-1.17969000	-0.00056500
C	2.20771600	-0.29850100	-0.00018000
C	0.80213100	-0.50093600	-0.00010700
N	0.28424400	-1.73164600	-0.00045100
H	-0.72342000	-1.88630800	-0.00012700
H	0.91534800	-2.51819900	-0.00071500
N	0.00752800	0.57683400	0.00031400
C	0.57390500	1.82034300	0.00069300
N	1.88297500	2.12206300	0.00070500
C	2.64212800	1.03170700	0.00026500
H	4.68873700	1.69202100	0.00033800
N	-5.02562400	1.11433100	-0.00039600
C	-5.58647300	-0.14410600	-0.00016400
H	-6.67100300	-0.16950200	-0.00029300
C	-4.83774400	-1.26424400	0.00019800
C	-3.38126200	-1.10768300	0.00033100
O	-2.60393900	-2.05568600	0.00064300
N	-2.90457900	0.19605700	0.00007700
H	-1.87015000	0.33344500	0.00017800
C	-3.66619600	1.33788800	-0.00029100
O	-3.19648600	2.46694300	-0.00051800

H	-5.46705100	2.01576700	-0.00045600
C	-5.47975400	-2.59170400	0.00088900
H	-5.16115800	-3.15902700	-0.87796900
H	-5.16084800	-3.15856400	0.87993400
H	-6.56969200	-2.52168400	0.00106200
O	-0.31466400	2.86185200	0.00010200
H	-1.25865400	2.59417400	-0.00043100
O	6.58431000	0.10060900	0.00132200
O	5.89550100	-2.04250700	0.00010800
C	5.69626200	-0.72338700	0.00065300
H	6.85399500	-2.18807200	0.00037400

H	-5.59903500	1.94599300	-0.00068900
N	-0.27984400	2.86047300	0.00115200
H	-1.28703000	2.73386000	0.00067700
H	0.11564000	3.78580300	0.00119500
C	-5.39201600	-2.65524400	0.00045700
H	-5.04554400	-3.20617000	-0.87830500
H	-5.04565400	-3.20579400	0.87949600
H	-6.48406500	-2.63905800	0.00038200
N	5.66822200	-0.82991400	-0.00064200
O	6.50252300	0.06996700	-0.00031600
O	5.89907700	-2.01933600	-0.00096400

^{NO2}AOH-T

E= -1200.580482
G= -1200.630589
ZPE= 0.238519

N	3.97157100	0.94642900	0.00052600
C	4.26286200	-0.39267300	0.00012900
N	3.23511700	-1.18362100	-0.00042200
C	2.17983300	-0.30862500	-0.00036700
C	0.77814900	-0.51695800	-0.00071400
N	0.25493700	-1.74539000	-0.00134700
H	-0.75221800	-1.90716700	-0.00082900
H	0.88446600	-2.53363600	-0.00102100
N	-0.01334500	0.56794000	-0.00051500
C	0.54918800	1.80666500	0.00000500
N	1.84141200	2.11298300	0.00040300
C	2.60563300	1.02310400	0.00019300
H	4.64570800	1.70065500	0.00092400
N	-4.90412900	1.19058500	-0.00033100
C	-5.53471600	-0.03607700	0.00004600
H	-6.61882400	0.00096800	0.00007100
C	-4.85301600	-1.19920500	0.00034900
C	-3.38974300	-1.12826300	0.00025100
O	-2.65901800	-2.11276300	0.00044900
N	-2.84586500	0.14740900	-0.00006300
H	-1.80517400	0.25023300	-0.00020600
C	-3.53688800	1.32763800	-0.00041100
O	-2.98798200	2.42455600	-0.00076400
H	-5.42978800	2.05352400	-0.00055000
C	-5.48994100	-2.55422700	0.00072600
H	-5.17760500	-3.12485900	-0.87819200
H	-5.17751000	-3.12442400	0.87989200
H	-6.57896900	-2.47232600	0.00076300
O	-0.27023100	2.84300000	0.00023600
H	-1.21881100	2.58677000	-0.00012000
N	5.64655800	-0.81683600	0.00037500
O	6.47332900	0.08779100	0.00094100
O	5.88099700	-2.00439800	0.00009300

^{OH}ANH$_2$-T

E= -1051.487729
G= -1051.536213
ZPE= 0.252526

N	4.61727000	0.57604700	0.05583100
C	4.84016900	-0.76896400	-0.10415800
N	3.76803600	-1.49320900	-0.17614200
C	2.74352100	-0.55394800	-0.05654900
C	1.34403800	-0.67207900	-0.04785400
N	0.73752500	-1.86514800	-0.19190100
H	-0.25942900	-1.96505400	-0.01490900
H	1.32058800	-2.68701800	-0.20495000
N	0.60303100	0.44313800	0.09144300
C	1.23144200	1.63913700	0.22367900
N	2.55363900	1.85921000	0.22933000
C	3.24526500	0.73170800	0.08922400
H	5.31751500	1.29813800	0.13088900
N	-4.34273900	1.27692900	-0.28818200
C	-4.98697600	0.06816000	-0.14710600
H	-6.06918100	0.10674700	-0.21483700
C	-4.31599100	-1.08143600	0.05949100
C	-2.85295900	-1.01316100	0.12574000
O	-2.14570400	-2.00045700	0.29255200
N	-2.28861600	0.24702600	-0.01457400
H	-1.24254500	0.32098400	0.03437900
C	-2.97156100	1.41870600	-0.22487800
O	-2.43271400	2.50904400	-0.34880900
H	-4.85626300	2.13320100	-0.43955500
N	0.43416400	2.72768000	0.40261000
H	-0.54222700	2.68300400	0.12921000
H	0.89918600	3.61872100	0.33296000
C	-4.96147900	-2.42315700	0.21746000
H	-4.59325700	-3.11702100	-0.54324700
H	-4.71352800	-2.85651100	1.19051400
H	-6.04770100	-2.34513400	0.13116300
O	6.10797600	-1.19679000	-0.17012500
H	6.08139200	-2.15594600	-0.28976900

^{OH}AOH-T

E= -1071.410693
G= -1071.362864
ZPE= 0.240335

N	-4.59885900	0.58407300	-0.00362800
C	-4.82734800	-0.76839300	-0.00102400
N	-3.75738300	-1.50170700	0.00205100
C	-2.73038100	-0.55946000	0.00165000
C	-1.33249000	-0.67982100	0.00382200
N	-0.72758600	-1.87967400	0.00793400
H	0.28484700	-1.97848900	0.00432500
H	-1.30753600	-2.70350500	0.00533900
N	-0.59349700	0.45027400	0.00245100
C	-1.22388400	1.64804200	-0.00082400
N	-2.53301000	1.87188500	-0.00309900
C	-3.22718500	0.73650000	-0.00176100
H	-5.29479500	1.31467300	-0.00542500
N	4.25595500	1.35509700	0.00084900
C	4.95921000	0.16939600	-0.00123300
H	6.03929400	0.27067500	-0.00197800
C	4.34607200	-1.03081300	-0.00225300
C	2.87971400	-1.04652000	-0.00107000

^{OMe}ANH$_2$-T

E= -1090.741214
G= -1090.791602
ZPE= 0.280962

N	4.23098700	1.04336800	-0.11061000
C	4.56141300	-0.28519400	0.03633400
N	3.54497600	-1.08795300	0.12564100
C	2.45254900	-0.22561900	0.03243000
C	1.06666700	-0.45021400	0.04553000
N	0.55551600	-1.68757600	0.19511400
H	-0.43015100	-1.86484500	0.01644900
H	1.20257200	-2.46016000	0.18518300
N	0.23950300	0.60507500	-0.07716300
C	0.77325400	1.84578500	-0.21481500
N	2.07436800	2.16644300	-0.24113700
C	2.85309500	1.09480900	-0.11726800
H	4.87373900	1.81512600	-0.20147100
N	-4.74923600	1.05126200	0.30475400
C	-5.30204300	-0.19922000	0.13991900
H	-6.38471500	-0.24124800	0.19708700
C	-4.54630000	-1.29348400	-0.07527200
C	-3.09161200	-1.11677400	-0.12681300

O	2.21482800	-2.07588900	-0.00182800
N	2.25821600	0.19377800	0.00107700
H	1.20874600	0.23614500	0.00172500
C	2.88119000	1.41160000	0.00210200
O	2.27553200	2.47725200	0.00400800
H	4.72765500	2.24845800	0.00157200
C	5.05969400	-2.34700900	-0.00440900
H	4.78041100	-2.93558600	0.87383400
H	4.77925900	-2.93340400	-0.88374600
H	6.14241500	-2.20329500	-0.00494200
O	-0.47093800	2.74270800	-0.00204400
H	0.48818800	2.54198000	0.00071500
O	-6.09540900	-1.19562400	-0.00199200
H	-6.07498400	-2.16244100	-0.00001200

O	-2.31221900	-2.04668400	-0.30133800
N	-2.62251100	0.17911500	0.03671100
H	-1.58414200	0.33271500	-0.00857500
C	-3.39164600	1.29413800	0.25619600
O	-2.93594900	2.41956200	0.39912400
H	-5.32547000	1.86567600	0.46170800
N	-0.10828000	2.87031800	-0.37768000
H	-1.07370300	2.74769800	-0.08976100
H	0.28724600	3.79431800	-0.30881800
C	-5.08837500	-2.67720500	-0.25808900
H	-4.78318900	-3.08275500	-1.22675800
H	-4.69017900	-3.34902100	0.50743800
H	-6.17917500	-2.67987100	-0.19985600
O	5.85710300	-0.59956300	0.06913500
C	6.12344500	-1.99444800	0.21427500
H	5.68682900	-2.54992900	-0.61941900
H	7.20803300	-2.08665500	0.21537900
H	5.70086400	-2.36338500	1.15207500

^{OMe}AOH-T

E= -1110.616520
G= -1110.666867
ZPE= 0.268761

N	-4.21387000	1.05157800	-0.00003800
C	-4.54835900	-0.28304200	-0.00014900
N	-3.53341200	-1.09493700	-0.00021300
C	-2.44018000	-0.23126800	-0.00006600
C	-1.05587900	-0.45865300	0.00000100
N	-0.54602600	-1.70243700	-0.00032900
H	0.45541700	-1.88033300	0.00065900
H	-1.18982100	-2.47744400	0.00034600
N	-0.23129500	0.61085300	0.00020800
C	-0.76843500	1.85336500	0.00023900
N	-2.05625600	2.17763600	0.00017200
C	-2.83667700	1.09892900	0.00004400
H	-4.85290300	1.83236900	-0.00008800
N	4.67276600	1.13488500	-0.00102000
C	5.28135700	-0.10199000	-0.00109500
H	6.36597600	-0.08560300	-0.00192100
C	4.57626200	-1.25024000	-0.00022600
C	3.11338900	-1.15152800	0.00076600
O	2.37137200	-2.12681900	0.00144700
N	2.59003700	0.13311000	0.00092800
H	1.54647800	0.25728200	0.00099000
C	3.30646400	1.29856500	-0.00001500
O	2.78683300	2.40862700	0.00007200
H	5.21259100	1.98883100	-0.00161400
C	5.18460600	-2.61834500	-0.00027900
H	4.86017100	-3.18160600	0.87897900
H	4.85846500	-3.18228700	-0.87846500
H	6.27523500	-2.56018200	-0.00135100
O	-5.84297500	-0.59676300	-0.00022300
C	-6.11306800	-1.99906200	-0.00047600
H	-5.68491900	-2.46466900	0.89033800
H	-7.19775500	-2.08725900	-0.00075600
H	-5.68446300	-2.46444100	-0.89118800
O	0.06697900	2.88714100	0.00037300
H	1.00737400	2.61265400	0.00031800

ANHLi-T

E= -983.267754
G= -983.315038
ZPE= 0.237068

N	-4.82284200	-0.03175200	0.52785600
C	-4.96355400	-1.28176800	-0.05111800
H	-5.91117000	-1.80236700	-0.04678100
N	-3.85970300	-1.72918000	-0.57667700
C	-2.94279600	-0.71702600	-0.34431500
C	-1.55848900	-0.62904400	-0.56472000
N	-0.88652000	-1.65429900	-1.16760700
H	0.05305900	-1.82180400	-0.82135100
H	-1.44332100	-2.49407500	-1.26168500
N	-0.90588600	0.47545500	-0.18768400
C	-1.60434500	1.52225900	0.41861400
N	-2.91950600	1.46083500	0.75538400
C	-3.51351700	0.34814800	0.35006700
H	-5.53172600	0.50905000	0.99807300
N	3.96496200	1.16113700	-0.35665100
C	4.54059500	-0.02689600	0.04704000
H	5.62459100	-0.03332800	0.07996300
C	3.79089300	-1.09605400	0.36782500
C	2.33146200	-0.96647600	0.25913700
O	1.56863500	-1.89916200	0.46104900
N	1.83500000	0.28681400	-0.10468100
H	0.73728900	0.40343200	-0.14282800
C	2.61125100	1.34639600	-0.43149300
O	2.16629300	2.45097200	-0.79106000
H	4.52736600	1.96445800	-0.59880800
N	-0.90847700	2.63384100	0.65137700
H	-1.52019400	3.27690300	1.14546700
C	4.34071400	-2.41989500	0.79774000
H	3.95501000	-2.69107400	1.78429100
H	4.02397800	-3.20550900	0.10619700
H	5.43200800	-2.39633400	0.83575800
Li	0.50040200	3.05945100	-0.44002800

AOLi-T

E= -1003.168181
G= -1003.215434
ZPE= 0.224575

N	4.90016300	0.20218300	-0.14041600
C	5.08206100	-1.11393400	0.24089600
H	6.06948500	-1.54386100	0.33642500
N	3.96203500	-1.74278600	0.46140800
C	2.98983600	-0.78810600	0.21666500
C	1.58473600	-0.83952900	0.23832500
N	0.93376200	-1.97486300	0.59218200

NLiANH2-T

E= -983.274565
G= -983.321542
ZPE= 0.237569

N	4.89932600	0.40794700	0.07809500
C	5.17213000	-0.83776100	-0.45224800
H	6.18477600	-1.15873900	-0.65258000
N	4.09528800	-1.54164300	-0.66997700
C	3.06112600	-0.71532900	-0.27521000
C	1.65252700	-0.94487300	-0.21059000
N	1.07165700	-2.09357800	-0.50927500

H	-0.01060000	-2.09992900	0.24014000
H	1.51347100	-2.79873900	0.66353700
N	0.89772800	0.26788000	-0.07213600
C	1.56866300	1.43642600	-0.41924000
N	2.90850000	1.55056300	-0.48808200
C	3.54492600	0.42903800	-0.16449600
H	5.61086600	0.87882400	-0.37210700
N	-3.89629300	1.25372300	0.48330300
C	-4.55180100	0.07147100	0.21116500
H	-5.63030200	0.09657300	0.32312700
C	-3.87644700	-1.02776200	-0.16609600
C	-2.41385700	-0.93265800	-0.26165700
O	-1.72151100	-1.89381000	-0.56614800
N	-1.83155100	0.30607600	0.01437100
H	-0.71555900	0.34534300	-0.03771700
C	-2.53866100	1.40347700	0.37451000
O	-2.04442400	2.52197600	0.60688100
H	-4.40113100	2.08670900	0.75044400
C	-4.50843200	-2.34818800	-0.47642000
H	-4.25984200	-2.65871200	-1.49490600
H	-4.12335100	-3.12125600	0.19421000
H	-5.59459800	-2.29507900	-0.37408000
O	0.84062300	2.45248000	-0.67566400
Li	-0.48749900	3.22804100	0.04468400

H	1.77833700	-2.73136600	-0.86794400
N	0.89836900	0.11265800	0.24157000
C	1.50874300	1.25858600	0.63953800
N	2.81309800	1.52317100	0.67054900
C	3.53588500	0.49472700	0.19821300
H	5.56004100	1.12643500	0.33047900
N	-3.65019300	1.49895400	-0.75583000
C	-4.50803000	0.49133000	-0.40443600
H	-5.56194700	0.68908700	-0.57039600
C	-4.06002700	-0.67174400	0.11303400
C	-2.61786900	-0.81964800	0.26257700
O	-2.12816600	-1.87968200	0.69700000
N	-1.81392200	0.22854600	-0.09208700
H	-0.71164800	0.14580100	0.04433300
C	-2.27707500	1.42673600	-0.58984300
O	-1.55764800	2.37173900	-0.86610100
H	-3.98884300	2.37764800	-1.12269300
N	0.67569300	2.25910200	1.10593100
H	-0.16616400	2.38937800	0.55409700
H	1.18638900	3.12234300	1.23420600
C	-4.94110000	-1.81472600	0.51454300
H	-4.69294400	-2.71308500	-0.05746000
H	-4.80057800	-2.05723100	1.57146400
H	-5.99229600	-1.57034000	0.34621600
Li	-0.46389200	-2.50875600	0.42893000

NLiAOH-T

E= -1003.149767
G= -1003.196877
ZPE= 0.224217

N	4.90542200	0.37716400	0.13084500
C	5.16959400	-0.90365500	-0.30906600
H	6.18127300	-1.26082600	-0.44105800
N	4.08604300	-1.59625700	-0.53373200
C	3.05728400	-0.72342000	-0.23764100
C	1.64343600	-0.91836300	-0.22160900
N	1.05926700	-2.07343400	-0.48924300
H	1.78184300	-2.72828100	-0.78283400
N	0.89993400	0.18298700	0.13802500
C	1.52938400	1.33917200	0.47782700
N	2.82601500	1.57604200	0.55264700
C	3.54108500	0.50158700	0.18192800
H	5.57077900	1.09701400	0.36783400
N	-3.64165200	1.54519100	-0.59556200
C	-4.50749100	0.51955000	-0.32247100
H	-5.55994600	0.73741100	-0.47062100
C	-4.06528400	-0.68260500	0.10188600
C	-2.62377200	-0.85143000	0.24016800
O	-2.14606600	-1.94522500	0.59588100
N	-1.81114900	0.21415600	-0.03551200
H	-0.68783900	0.13764500	0.05265500
C	-2.27406200	1.44239800	-0.44039700
O	-1.54533600	2.40236500	-0.65333800
H	-3.97245400	2.45474400	-0.88746000
C	-4.95322400	-1.84752300	0.41515900
H	-4.70782300	-2.70210700	-0.22143900
H	-4.81674100	-2.16868500	1.45142800
H	-6.00268900	-1.58611400	0.26296900
O	0.75138100	2.37900600	0.80666800
H	-0.08968700	2.35733600	0.30898200
Li	-0.51514100	-2.62083500	0.29295200

ANHLi-T-2W

E= -1136.062689
G= -1136.115877
ZPE= 0.288820

N	4.60587500	-0.59167000	-1.19175600
C	4.87443600	-1.75758600	-0.49355500
H	5.77253100	-2.33073800	-0.67805300
N	3.95072800	-2.06050600	0.37160400
C	3.02492800	-1.03710100	0.24723500
C	1.77476900	-0.81156400	0.84168200
N	1.25896500	-1.65910200	1.77881700
H	0.24952000	-1.76016300	1.73759100
H	1.75725500	-2.53667900	1.85175300
N	1.07723600	0.27351100	0.48957200
C	1.57098000	1.15460600	-0.47389400
N	2.74789700	0.96745300	-1.12965900
C	3.40422300	-0.11156700	-0.72825400
H	5.16390200	-0.16857400	-1.91696900
N	-4.01596100	0.52359500	-0.78342300
C	-4.42910900	-0.78903400	-0.69365400
H	-5.46812700	-0.96761700	-0.94944400
C	-3.59857500	-1.77491100	-0.30532600
C	-2.21794900	-1.41019500	0.03025000
O	-1.39585100	-2.19942600	0.46830000
N	-1.87184500	-0.07654300	-0.18567200
H	-0.88725100	0.16292700	0.01376500
C	-2.73698300	0.93653400	-0.49234300
O	-2.43798100	2.12745900	-0.52029300
H	-4.66308000	1.26364500	-1.01489400
N	0.79997100	2.20882500	-0.73055800
H	1.20765800	2.68696400	-1.53208700
C	-3.99222300	-3.21252900	-0.16694100
H	-3.36757100	-3.84339100	-0.80530300
H	-3.84101500	-3.55196000	0.86151300
H	-5.03989000	-3.35860600	-0.43916100
Li	-0.81717600	2.80757800	0.24528400
O	-0.67027200	1.74242600	1.88172200
H	-0.48762200	1.97748400	2.79484600
O	0.11302700	4.54437500	0.56651000
H	0.35248600	4.96634800	1.39608800
H	0.05802800	1.13028800	1.55800300
H	0.85629700	3.96981000	0.29291400

AOLi-T-2W

E= -1155.965923
G= -1156.019548

NLiANH2-T-2W

E= -1136.070900
G= -1136.123687

ZPE= 0.276502			
N	4.82128200	0.33025300	0.84961400
C	5.06675000	1.60932900	0.38350500
H	6.02970800	2.08296700	0.51465300
N	4.03712200	2.14587900	-0.20630400
C	3.05953700	1.16782600	-0.12909600
C	1.71859600	1.13071300	-0.54535500
N	1.13937800	2.16713400	-1.20289800
H	0.13378300	2.26024100	-1.08899400
H	1.67134600	3.02625300	-1.20360500
N	1.00613900	0.01996900	-0.30922900
C	1.57521000	-1.05886800	0.36950800
N	2.85218600	-1.08848900	0.80615300
C	3.51963700	0.02774800	0.53032800
H	5.45503000	-0.27282900	1.35111400
N	-4.02571800	-0.82117400	0.51642800
C	-4.57977500	0.44019800	0.53579000
H	-5.64698200	0.47676500	0.72629800
C	-3.84187200	1.54600900	0.32394600
C	-2.40883200	1.36956000	0.06889000
O	-1.65478700	2.29747100	-0.18695300
N	-1.92754500	0.06373800	0.13654700
C	-2.69059200	-1.06078800	0.28763800
O	-2.26383400	-2.21083400	0.23446400
H	-4.59410100	-1.64777900	0.63471500
C	-4.38497000	2.94096000	0.31422000
H	-3.87811700	3.55416300	1.06430300
H	-4.20744300	3.41310500	-0.65596200
H	-5.45773300	2.94330100	0.51937700
O	0.81021000	-2.05681200	0.55244700
Li	-0.57757600	-2.74941600	-0.46725200
H	-0.89996100	-0.04350900	0.00191400
O	0.30446400	-4.49006000	-0.12885000
H	0.78777400	-5.14381300	-0.63960100
O	-0.45707300	-1.57486200	-2.03851900
H	-0.16982400	-1.71734700	-2.94427600
H	0.95226700	-3.92198700	0.33574300
H	0.12311500	-0.87781200	-1.64305000

ZPE= 0.290053			
N	4.73598500	-0.75760100	-0.84728800
C	4.77598500	0.34347300	-1.67834600
H	5.64873400	0.57557600	-2.27222700
N	3.66929400	1.03595200	-1.65103800
C	2.86047700	0.35497100	-0.76320700
C	1.54152100	0.64144500	-0.28111300
N	0.80450000	1.67648700	-0.60744900
H	1.30243700	2.21668400	-1.31284800
N	1.04692600	-0.26778000	0.63621600
C	1.78888800	-1.33925500	1.01589700
N	3.02098200	-1.65375500	0.63567200
C	3.50252000	-0.75753900	-0.24928400
H	5.46207400	-1.44083900	-0.69693000
N	-3.36379200	-2.18465100	-0.51062500
C	-4.26699300	-1.21817500	-0.88499600
H	-5.21792400	-1.58578900	-1.25586400
C	-3.98911300	0.09720600	-0.78810600
C	-2.67278800	0.47748200	-0.27543200
O	-2.35260300	1.65489000	-0.11300000
N	-1.80524800	-0.55475300	0.02917600
H	-0.81472200	-0.34968700	0.29481000
C	-2.10574800	-1.89998600	-0.01713700
O	-1.34171400	-2.77425700	0.35212100
H	-3.59495800	-3.16707400	-0.55479600
N	1.18418100	-2.17032400	1.94356000
H	0.20898400	-2.35369600	1.72847600
H	1.71344400	-3.02327300	2.06891000
C	-4.93691900	1.19327900	-1.16665100
H	-5.15491900	1.82848300	-0.30357600
H	-4.49454500	1.83585000	-1.93282700
H	-5.87399700	0.78167200	-1.54806100
Li	-0.69134100	2.35377900	0.44961500
O	-0.24900600	1.45473500	2.21222100
H	-0.77163300	1.07726700	2.92574600
O	-0.02153200	4.02197300	1.29637200
H	0.27872200	3.45996800	2.02832200
H	0.28775200	0.70788700	1.80339700
H	0.77664600	4.29446300	0.82959300

NLiAOH-T-2W E= -1155.944665 G= -1155.998045 ZPE= 0.276987			
N	-4.84473200	-0.70267700	-0.70558200
C	-4.93923300	0.46993900	-1.42520700
H	-5.85667600	0.76244500	-1.91631600
N	-3.82315200	1.14871900	-1.43385500
C	-2.95110600	0.38103700	-0.68855300
C	-1.59277900	0.61259900	-0.29684300
N	-0.87604500	1.67344800	-0.58148700
H	-1.43025100	2.27985700	-1.18387100
N	-1.03679200	-0.38578100	0.48725400
C	-1.76379700	-1.48610400	0.81029100
N	-3.02098300	-1.75171700	0.52289200
C	-3.56347400	-0.76867400	-0.22422700
H	-5.56339500	-1.39455900	-0.55729500
N	3.46250800	-2.11826200	-0.39634400
C	4.35597300	-1.14255800	-0.77396500
H	5.33490100	-1.49817200	-1.07732100
C	4.03594000	0.16678000	-0.75773800
C	2.68624500	0.53057300	-0.32660200
O	2.32486700	1.70185100	-0.21941300
N	1.82980800	-0.51503800	-0.03416100
H	0.81759600	-0.33703300	0.16787000
C	2.17479400	-1.84541400	0.00953500
O	1.41517100	-2.72517200	0.38593300
H	3.72431800	-3.09410300	-0.37462300
C	4.97070800	1.27209000	-1.14206600
H	4.55768500	1.85256600	-1.97169500
H	5.11199300	1.96361400	-0.30696600
H	5.94263000	0.87274600	-1.43994300

AOLi-T-2W-COOH E= -1344.470035 G= -1344.527785 ZPE= 0.291733			
N	3.98782900	0.66709700	-0.60756700
C	4.43572800	-0.54726600	-0.11153200
N	3.48360800	-1.25867600	0.43547300
C	2.36710000	-0.47885500	0.29870000
C	1.01749300	-0.68844300	0.65895200
N	0.61775100	-1.81371600	1.29055600
H	-0.35511400	-2.08341300	1.17076100
H	1.29978000	-2.55743000	1.34034800
N	0.13271800	0.27483000	0.38538900
C	0.52763700	1.43744100	-0.28825000
N	1.79604300	1.69989800	-0.67227200
C	2.64553100	0.72942000	-0.35562500
H	4.54839300	1.36204400	-1.07917500
N	-4.92821300	0.20957500	-0.63397800
C	-5.24260100	-1.13154800	-0.67510500
H	-6.27239100	-1.36049400	-0.92796300
C	-4.33099000	-2.08628000	-0.40997300
C	-2.97166600	-1.65351400	-0.07206400
O	-2.07801900	-2.42847100	0.23829400
N	-2.73137100	-0.28212900	-0.12497700
C	-3.67321300	0.68582700	-0.33654000
O	-3.46158900	1.89415100	-0.27740900
H	-5.62753900	0.91935600	-0.79998400
C	-4.61255100	-3.55658300	-0.42300800
H	-3.95584700	-4.06544000	-1.13404200
H	-4.41649600	-3.99253400	0.56050900
H	-5.65166700	-3.75203700	-0.69686600
O	-0.39640100	2.27316400	-0.51641200

O	-1.12739600	-2.41692800	1.54051900
H	-0.18373700	-2.42497700	1.29667100
Li	0.65750900	2.32810600	0.42207100
O	0.28397900	1.30106900	2.14596000
H	0.83290500	0.90274800	2.82806200
O	0.06165200	3.92732600	1.42887500
H	-0.26506500	3.32649800	2.11673200
H	-0.25954400	0.57073200	1.73488200
H	-0.71598400	4.34570400	1.04384000

Li	-1.92241600	2.75148700	0.43109700
H	-1.74687900	0.00864400	0.05243900
O	-1.35317800	4.60085100	0.05654200
H	-1.04416700	5.37872100	0.52664500
O	-1.62553100	1.66492700	2.05776900
H	-1.41714600	1.86958600	2.97321900
H	-0.58578700	4.17001900	-0.36823200
H	-0.92382700	1.06468600	1.71454000
C	5.84648700	-0.95811800	-0.21250200
O	6.31739600	-1.99002300	0.18867100
O	6.57996400	-0.00012000	-0.83434900
H	7.49251600	-0.32265400	-0.87701800

AOLi-T-2W-NO2

E= -1360.392652
G= -1360.450273
ZPE= 0.279283

N	4.02981400	0.69073200	-0.60226000
C	4.44679300	-0.53144400	-0.13401000
N	3.51439300	-1.26813900	0.38775100
C	2.39898400	-0.48272100	0.26535100
C	1.04588000	-0.70170700	0.61615100
N	0.64414200	-1.84158600	1.21282000
H	-0.33467000	-2.09833600	1.10995300
H	1.32112000	-2.58971900	1.25783100
N	0.16591100	0.27073600	0.36485900
C	0.56410800	1.44973800	-0.27820300
N	1.83820400	1.72155300	-0.65005700
C	2.68178000	0.74530200	-0.35569700
H	4.61436600	1.38400900	-1.04818200
N	-4.91563000	0.21944300	-0.63629300
C	-5.24006000	-1.12001100	-0.65349100
H	-6.27343300	-1.34510800	-0.89468600
C	-4.33359200	-2.07774400	-0.38063800
C	-2.96859000	-1.65044000	-0.06179000
O	-2.07680500	-2.42672400	0.25165900
N	-2.71923800	-0.28192400	-0.13800500
C	-3.65582800	0.69054300	-0.35476900
O	-3.43195000	1.89736000	-0.31323100
H	-5.61183500	0.93142500	-0.80661700
C	-4.62680200	-3.54578900	-0.36744800
H	-3.97825200	-4.07173400	-1.07346200
H	-4.42886300	-3.96670200	0.62222300
H	-5.66886700	-3.73750600	-0.63222700
O	-0.35251000	2.29162700	-0.49196800
Li	-1.90250900	2.75054800	0.42572800
H	-1.73476600	0.00668900	0.03084500
O	-1.35490300	4.60115500	0.08513700
H	-1.12164100	5.43225500	0.50455100
O	-1.62702800	1.64756300	2.04460000
H	-1.43646000	1.86162800	2.96195800
H	-0.55895500	4.22306800	-0.33296900
H	-0.91541500	1.05305800	1.71860400
O	6.18218600	-1.98612100	0.15932500
O	6.56293600	-0.05854700	-0.77073100
N	5.83437100	-0.89931800	-0.25110900

AOLi-T-2W-OH

E= -1231.171134
G= -1231.226491
ZPE= 0.280788

N	4.52090500	0.19170200	-0.79427000
C	4.87646900	-1.02758700	-0.27193800
N	3.92754800	-1.65574500	0.34404500
C	2.84217000	-0.78150700	0.22734300
C	1.51004800	-0.86251900	0.63732200
N	1.02379300	-1.92244300	1.34293700
H	0.03974100	-2.12643300	1.19003300
H	1.63304900	-2.72842900	1.36572600
N	0.68701800	0.16330900	0.35571700
C	1.14085800	1.26006900	-0.36570400
N	2.41369000	1.39595500	-0.80744600
C	3.18451400	0.36987500	-0.48238900
H	5.10943900	0.81615900	-1.32414900
N	-4.37632500	0.47937900	-0.51832300
C	-4.78765700	-0.83423300	-0.57805500
H	-5.83900600	-0.98340000	-0.80017400
C	-3.93820200	-1.85696400	-0.36631600
C	-2.54020000	-1.53021200	-0.06691000
O	-1.69494100	-2.37560100	0.19015100
N	-2.20414600	-0.17825200	-0.09223100
C	-3.08031900	0.85826700	-0.25501100
O	-2.78272200	2.04752400	-0.18249900
H	-5.02623400	1.24154100	-0.64780400
C	-4.32348100	-3.30291100	-0.40292100
H	-3.72886400	-3.83826400	-1.14832900
H	-4.12499500	-3.77616500	0.56274300
H	-5.38265800	-3.41842600	-0.64382700
O	0.28522900	2.17297700	-0.59066900
Li	-1.14262400	2.77550400	0.43198200
H	-1.19391500	0.03505100	0.06181700
O	-0.45309400	4.57338400	-0.01328500
H	-0.04366000	5.30948800	0.44753000
O	-0.86108700	1.69930500	2.06585400
H	-0.55209800	1.91066300	2.95062700
H	0.24845700	4.05695800	-0.45897900
H	-0.24115200	1.03139300	1.68287600
O	6.13976200	-1.44468900	-0.44216600
H	6.21199500	-2.31084600	-0.01864300

AOLi-T-2W-OMe

E= -1270.423866
G= -1270.480434
ZPE= 0.309837

N	4.16801700	0.74467000	-0.82648100
C	4.64990600	-0.43812700	-0.31114400
N	3.77029600	-1.15535000	0.31576600
C	2.60599000	-0.38807300	0.21270400
C	1.29417400	-0.59715300	0.64067600
N	0.92497300	-1.69799400	1.35582500
H	-0.03411400	-2.00304300	1.21226900
H	1.61402300	-2.43721500	1.37078800
N	0.36972400	0.34178300	0.36820800
C	0.70585100	1.47514700	-0.36054300

N	1.95426500	1.73643900	-0.81455900
C	2.82657000	0.79114800	-0.49958500
H	4.68706600	1.42235600	-1.36325500
N	-4.68731900	0.11910600	-0.54410400
C	-4.95967300	-1.23020400	-0.59991900
H	-5.98678600	-1.48811700	-0.83532700
C	-4.01242400	-2.15827900	-0.36904300
C	-2.66011300	-1.68673500	-0.05238500
O	-1.73633100	-2.43812900	0.22486600
N	-2.46498900	-0.30726200	-0.08501900
C	-3.44105100	0.63184500	-0.26735100
O	-3.26999400	1.84601100	-0.19982800
H	-5.41121700	0.80882500	-0.68674600
C	-4.24691900	-3.63656200	-0.39982300
H	-3.58793800	-4.11303000	-1.13091300
H	-4.01779900	-4.08075500	0.57290200
H	-5.28445000	-3.86140400	-0.65698400
O	-0.23903500	2.29721400	-0.58121700
Li	-1.72803100	2.75026800	0.43151600
H	-1.48368200	0.01112500	0.07747700
O	-1.19613500	4.61277300	0.02201200
H	-0.84428300	5.36442500	0.50467300
O	-1.34349500	1.69919100	2.06667900
H	-1.07070800	1.93465800	2.95726400
H	-0.45319100	4.15970000	-0.42645600
H	-0.64668500	1.11049900	1.68422200
O	5.94179300	-0.71536200	-0.50469100
C	6.36572900	-1.95901400	0.05076300
H	7.42742500	-2.03541400	-0.17788300
H	6.19843000	-1.96697600	1.13069200
H	5.81054600	-2.78371600	-0.40338600

Table S1: The M06-2X-D3 level of theory calculated energies and free energies for representative system

Name	ΔE_{M062X}	$\Delta E_{M062X-D3}$	ΔG_{M062X}	$\Delta G_{M062X-D3}$
A-T	-16.4	-16.9	-3.3	-3.9
ANH_2-T	-19.3	-19.9	-5.3	-5.9
AOH-T	-20.3	-20.8	-7.0	-7.6
ANHLi-T	-25.1	-25.7	-13.0	-13.7
AoLi-T	-28.6	-29.2	-16.4	-17.0
ANHLi-T-2W	-60.7	-61.9	-24.9	-26.1
AoLi-T-2W	-66.0	-67.2	-30.3	-31.1
AoLi-T-2W-COOH	-64.9	-66.1	-29.0	-30.1
AoLi-T-2W-NO_2	-67.0	-68.1	-30.0	-31.2

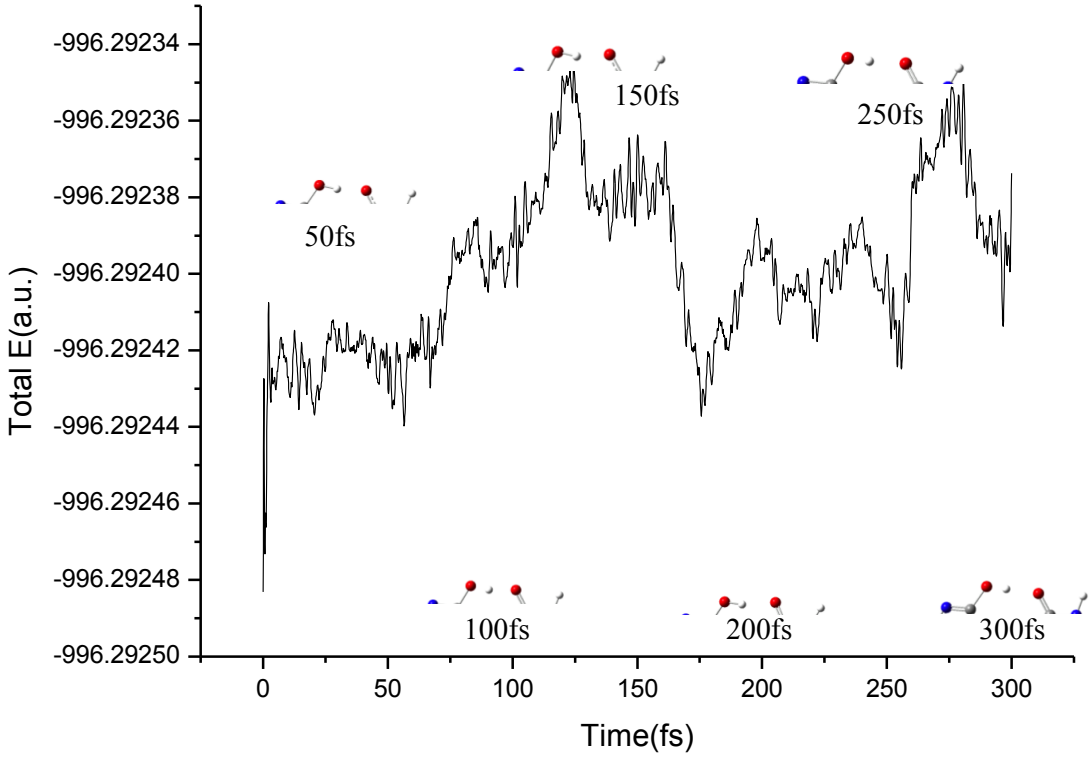

Figure S1: Trajectory analysis of AOH-T mispair with time.

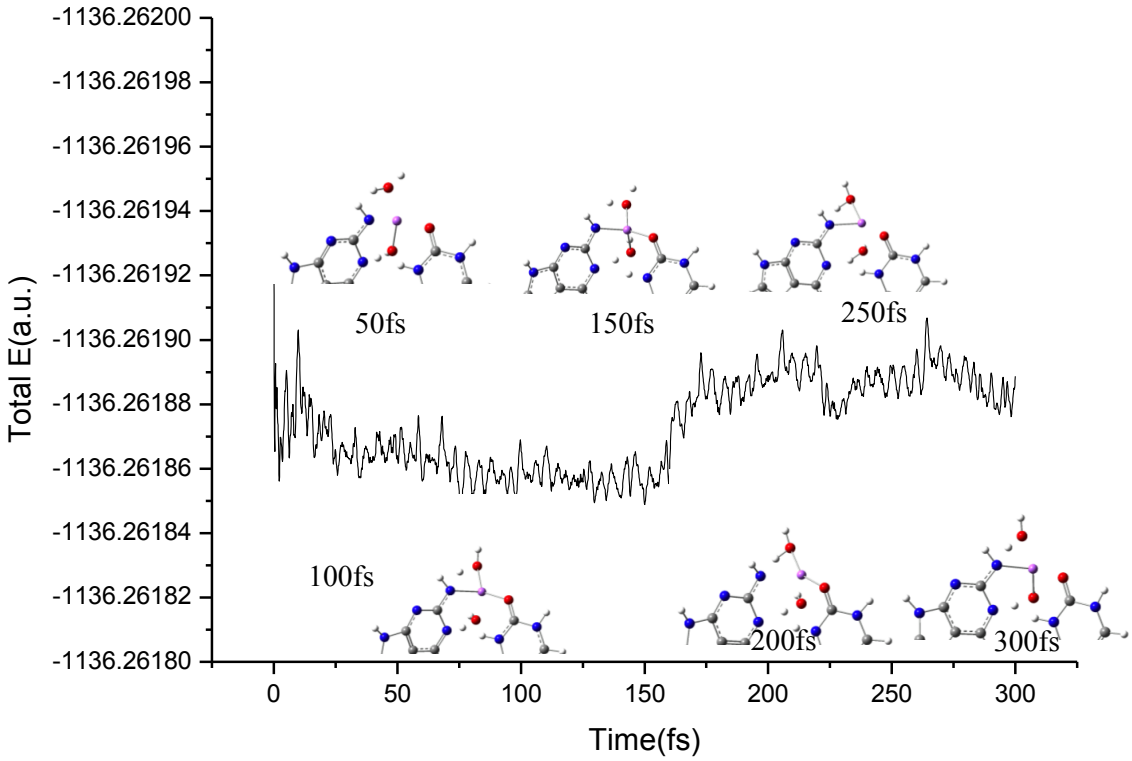

Figure S2: Trajectory analysis of ANHLi-T mispair with time.

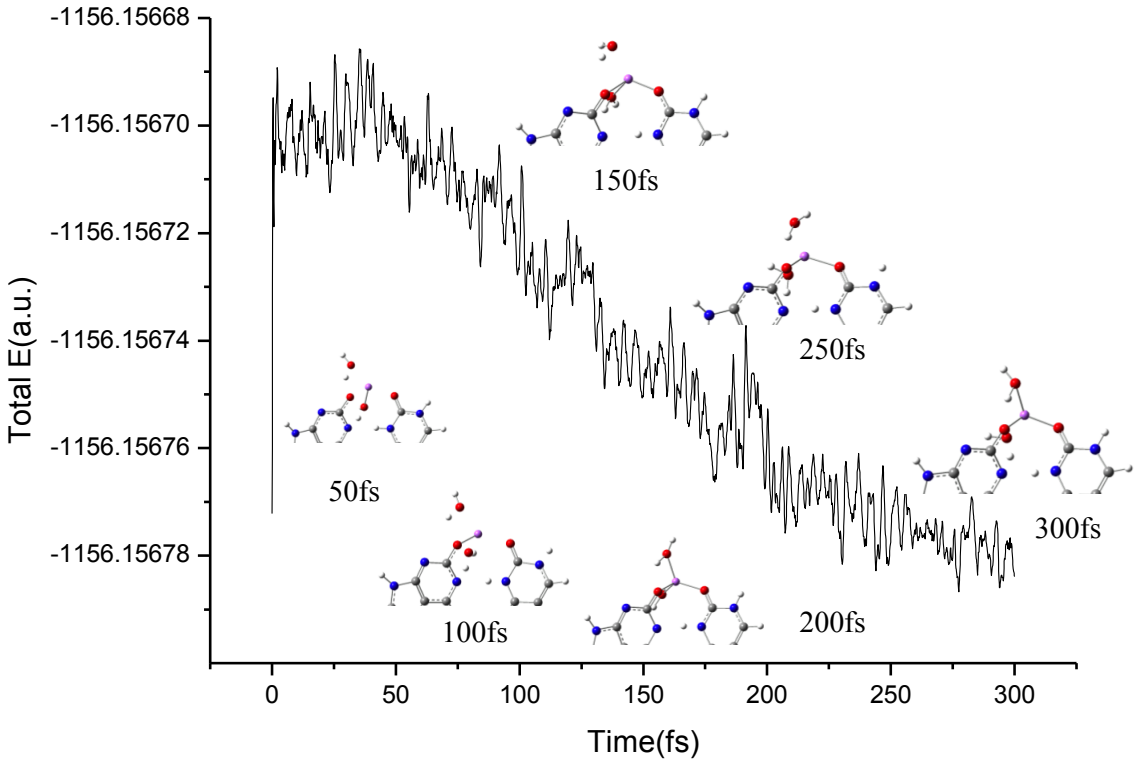

Figure S3: Trajectory analysis of AOLi-T mispair with time.

Table S2: Solvation free energies of representative system. Energy values are given in kcal/mol.

Name	$\Delta G_{Solvation}$
A-T	2.82
ANH_2-T	2.22
AOH-T	-0.25
$^{Br}ANH_2$-T	2.07
^{Br}AOH-T	-0.89
$^{NO2}ANH_2$-T	0.12
^{NO2}AOH-T	-0.99

Table S3:H-Bond Energy Calculations using three different methods*.

		$E_{HB}=0.33*\sqrt{(\Delta\nu-40)}$	$E_{HB}=-2.03+225*\rho$	$E_{HB}=1/2(V(r))$
A-T	N---H-N	8.6	8.6	10.68
	N-H---O	4.0	3.5	6.10
	C-H---O	-	-	1.23
ANH2-T	N---H-N	8.0	5.9	7.23
	N-H---O(CH3)	3.7	4.1	6.79
	N-H---O	3.0	3.6	6.28
AOH-T	N---H-N	8.4	7.3	8.89
	N-H---O(CH3)	3.7	3.8	6.40
	O-H---O	5.6	5.5	8.01

*Hydrogen bonding strengths are in good agreement the literature. H. Szatyłowicz, and N. Sadlej-Sosnowska, *J. Chem. Inf. Model.*, **2010**, *50*, 2151–2161

Table S4: The deprotonation energies of the ANH2 and AOH nucleobases before and after lithiation.

Base	Deprotonation Energy	
ANH2	612.779	
ANHLi	590.34	
AOH	620.599	
AOLi	597.632	

Table S5: Topological analysis of noncovalent hydrogen bonding interactions calculated using the M06-2X/6-31+G** level of theory obtained wave function.[a]

$^{Br}ANH_2$-T	N---H-N	0.0349	0.0816	1.058	7.19
	N-H---O(CH3)	0.0274	0.0885	0.990	6.81
	N-H---O	0.0251	0.0810	0.996	6.31
^{Br}AOH-T	N---H-N	0.0413	0.0937	1.092	8.84
	N-H---O(CH3)	0.0259	0.0804	1.007	6.39
	O-H---O	0.0340	0.1137	0.955	8.15
$^{COOH}ANH_2$-T	N---H-N	0.0348	0.0817	1.057	7.18
	N-H---O(CH3)	0.0275	0.0886	0.990	6.81
	N-H---O	0.0251	0.0808	0.997	6.30
^{COOH}AOHT	N---H-N	0.0348	0.0814	1.058	7.17
	N-H---O(CH3)	0.0273	0.0882	0.991	6.79
	O-H---O	0.0251	0.0810	0.996	6.31
$^{OH}ANH_2$-T	N---H-N	0.0378	0.0865	1.074	7.87
	N-H---O(CH3)	0.0265	0.0847	0.997	6.60
	N-H---O	0.0240	0.0759	1.008	6.05
^{OH}AOH-T	N---H-N	0.0411	0.0926	1.093	8.76
	N-H---O(CH3)	0.0256	0.0797	1.007	6.35
	O-H---O	0.0333	0.1119	0.954	8.01
$^{OMe}ANH_2$-T	N---H-N	0.0383	0.0871	1.078	7.98
	N-H---O(CH3)	0.0262	0.0834	0.999	6.54
	N-H---O	0.0242	0.0769	1.007	6.11
^{OMe}AOH-T	N---H-N	0.0414	0.0927	1.096	8.82
	N-H---O(CH3)	0.0256	0.0800	1.007	6.36
	O-H---O	0.0331	0.1112	0.955	7.97
AOLi-T-2W	N---H-N	0.0313	0.0764	1.051	6.64
	O-Li-O	0.0303	0.2219	0.757	10.61
	N-H---O	0.0218	0.0694	1.012	5.57
	(A)N---OH(W)	0.0371	0.0968	1.058	8.52
AOLi-T	N---H-N	0.0667	0.0929	1.394	16.75
	O-Li-O	0.0407	0.3215	0.781	16.15
	N-H---O	0.0272	0.0883	0.999	6.91
ANHLi-T-2W	N---H-N	0.0253	0.0642	1.046	5.52
	N-Li-O	0.0296	0.2130	0.760	10.24
	N-H---O	0.0176	0.0570	1.002	4.49
	(A)N---OH(W)	0.0517	0.1119	1.179	12.61
ANHLi-T	N---H-N	0.0623	0.0964	1.333	15.11
	N-Li-O	0.0405	0.3129	0.785	15.88
	N-H---O	0.0235	0.0725	1.028	6.02
AOLi-T-2W-COOH	N---H-N	0.0315	0.0775	1.048	6.70
	O-Li-O	0.0307	0.2257	0.758	10.80
	N-H---O	0.0224	0.0716	1.008	5.71
	(A)N---OH(W)	0.0336	0.0914	1.038	7.74
AOLi-T-2W-NO_2	N---H-N	0.0301	0.0747	1.043	6.38
	O-Li-O	0.0305	0.2241	0.757	10.71
	N-H---O	0.0232	0.0748	1.003	5.90
	(A)N---OH(W)	0.0314	0.0870	1.029	7.23
AOLi-T-2W-OH	N---H-N	0.0330	0.0799	1.056	7.01
	O-Li-O	0.0310	0.2277	0.758	10.91
	N-H---O	0.0213	0.0673	1.015	5.45
	(A)N---OH(W)	0.0368	0.0965	1.056	8.47
AOLi-T-2W-OMe	N---H-N	0.0332	0.0803	1.057	7.06
	O-Li-O	0.0310	0.2283	0.758	10.94
	N-H---O	0.0215	0.0678	1.015	5.48
	(A)N---OH(W)	0.0373	0.0973	1.059	8.59

a: W in parenthesis indicates that the corresponding group/atom participates from the water molecule and A indicates adenine unit.