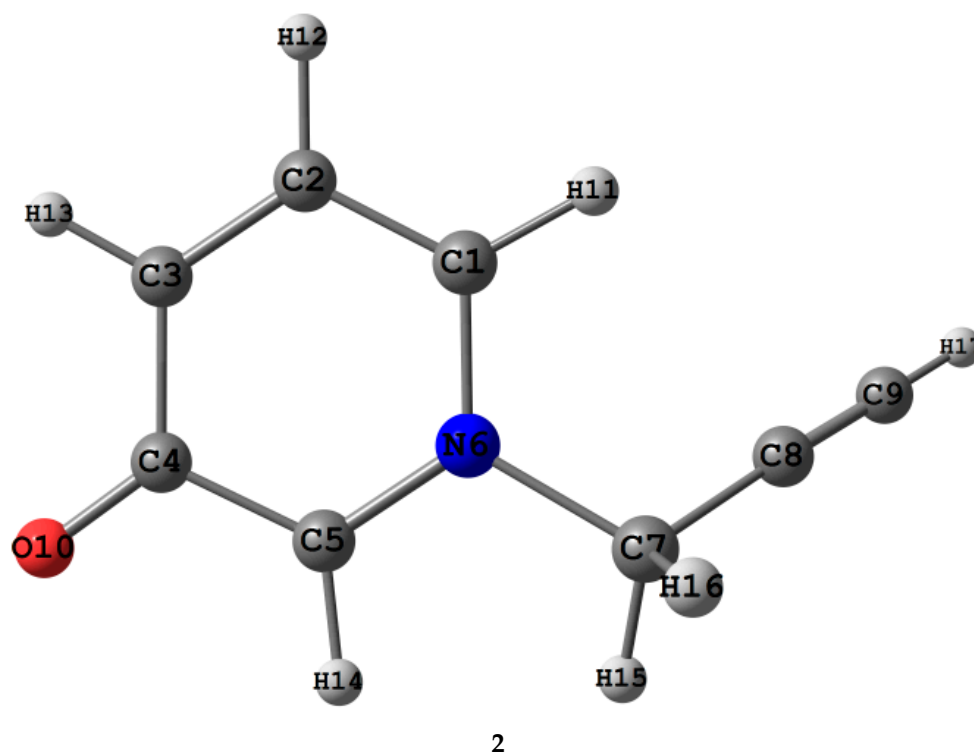
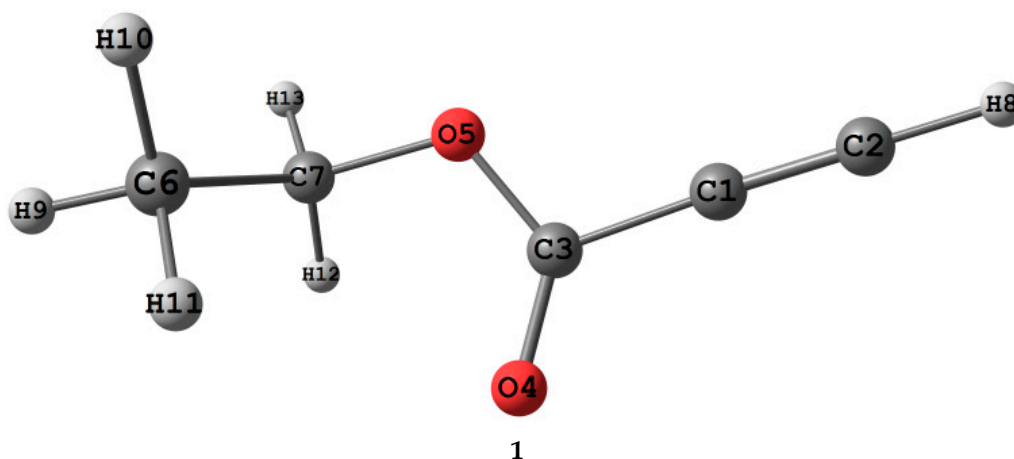
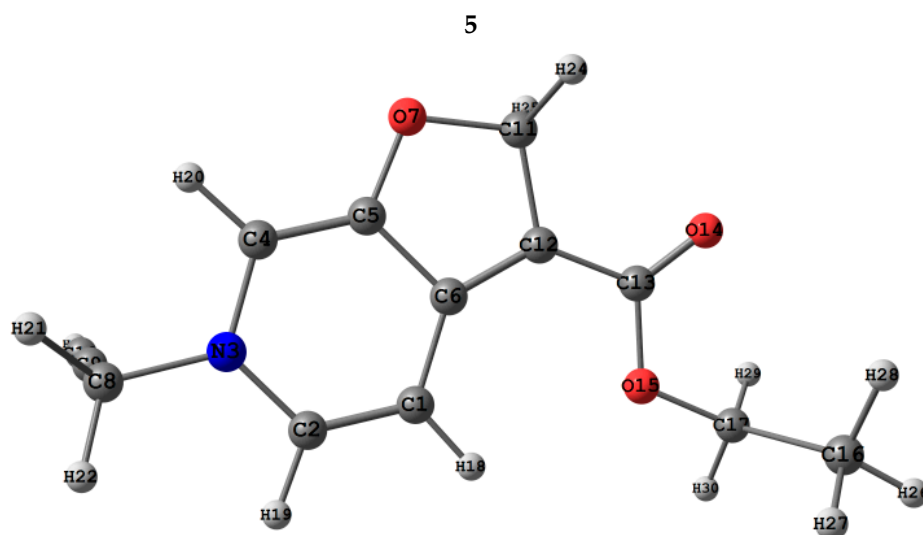
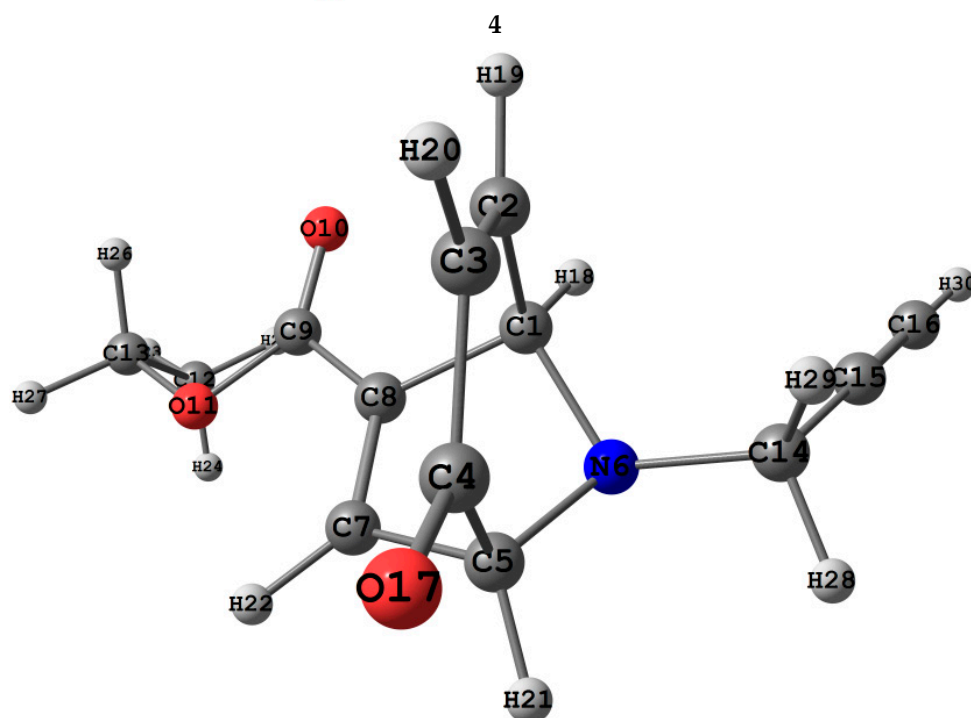
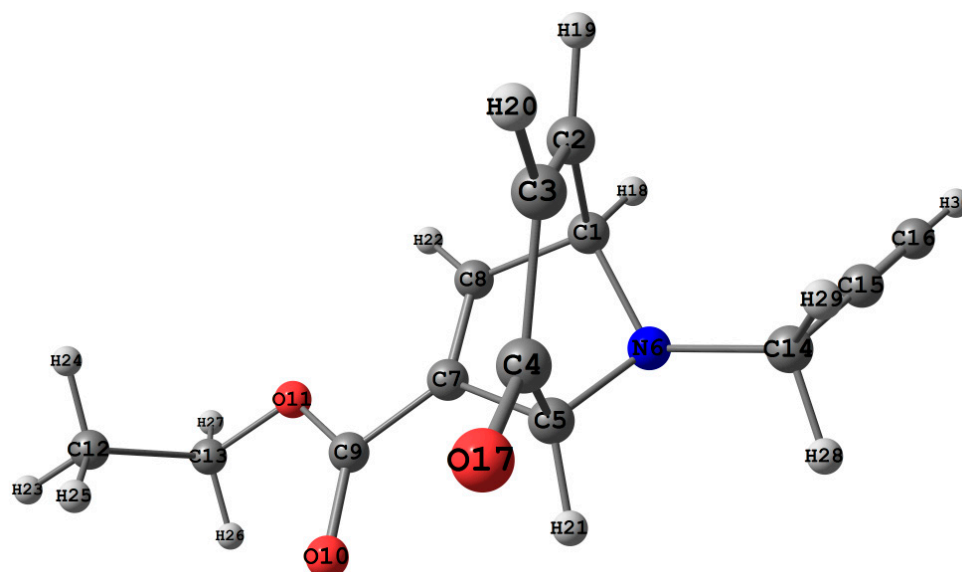
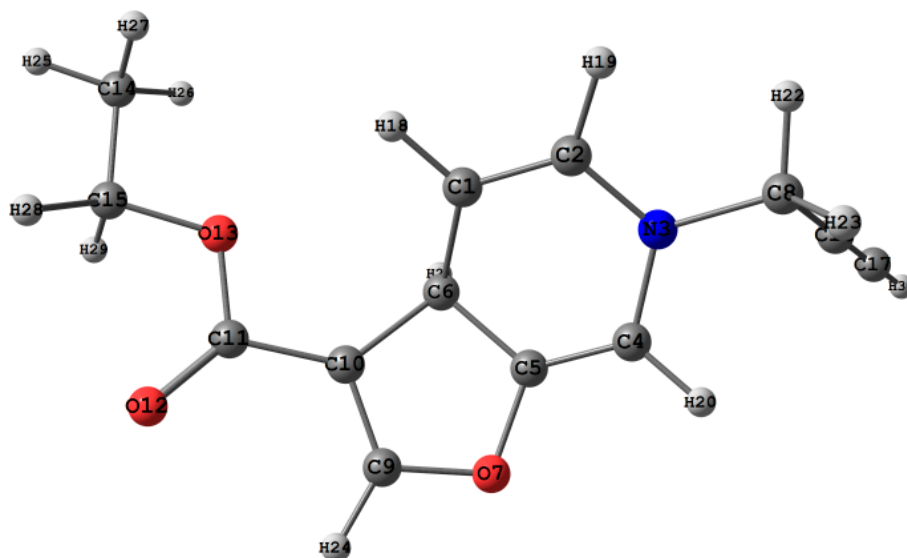


Supplementary Materials: Ultrasonic Synthesis, Molecular Structure and Mechanistic Study of 1,3-Dipolar Cycloaddition Reaction of 1-Alkynylpyridinium-3-olate and Acetylene Derivatives

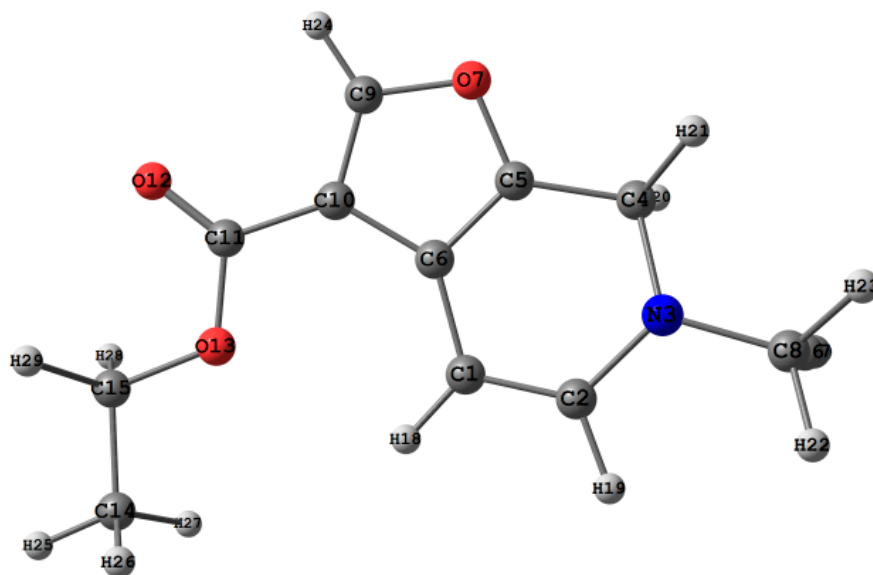
AsmaaAbolnaga, Mohamed Hagar and Saied M. Soliman







8



9

Figure S1. The optimized structure of the reactants.

Reactant # 1

C	-1.89700000	-0.14859000	0.08683200
C	-3.03751500	-0.50152500	0.26666500
C	-0.54673700	0.34024000	-0.11832600
O	-0.23852600	1.51291000	-0.07314000
O	0.29810000	-0.67943100	-0.36577200
C	2.43791800	-0.18463100	0.72962600
C	1.68773300	-0.31875600	-0.58598100
H	-4.04483100	-0.81296200	0.42587400
H	3.49729800	0.00860700	0.53164700
H	2.35986400	-1.10353700	1.31744600
H	2.04194800	0.64762600	1.31618100
H	1.72261000	0.60971400	-1.16032300
H	2.08012300	-1.13770800	-1.19241900

Reactant # 2

C	0.331636000	1.131793000	0.288948000
C	-0.902033000	1.762697000	0.108643000
C	-2.056684000	1.040155000	-0.102323000
C	-2.053251000	-0.413583000	-0.149350000
C	-0.729572000	-0.977774000	0.046332000
N	0.368429000	-0.222946000	0.247123000
C	1.655590000	-0.921754000	0.527091000
C	2.809968000	-0.306756000	-0.117636000
C	3.793986000	0.173064000	-0.624165000
O	-3.050215000	-1.130587000	-0.334578000
H	1.269346000	1.644405000	0.441680000
H	-0.925802000	2.847797000	0.137268000
H	-3.010020000	1.539687000	-0.243503000
H	-0.599435000	-2.052781000	0.033637000
H	1.540272000	-1.953287000	0.185996000
H	1.795136000	-0.945127000	1.613877000
H	4.655390000	0.597579000	-1.087434000

Product # 4

C	-1.448143000	-0.774501000	0.949078000
C	-1.631456000	0.460599000	1.828593000
C	-1.266778000	1.662622000	1.348240000
C	-0.665288000	1.778915000	-0.012035000
C	-0.517982000	0.430806000	-0.767190000
N	-1.672719000	-0.444224000	-0.477145000
C	0.588334000	-0.386951000	-0.101562000
C	0.046975000	-1.096372000	0.895810000
C	1.995388000	-0.316635000	-0.537941000
O	2.375189000	0.345045000	-1.484702000
O	2.800866000	-1.085721000	0.230544000
C	4.945253000	0.075357000	0.501517000
C	4.205748000	-1.096661000	-0.124593000
C	-2.988995000	0.072620000	-0.858158000
C	-4.044642000	-0.910032000	-0.601027000
C	-4.927407000	-1.699848000	-0.368057000
O	-0.314702000	2.846462000	-0.481498000
H	-2.082871000	-1.604158000	1.269895000
H	-2.040233000	0.350139000	2.831049000
H	-1.366612000	2.582741000	1.917196000
H	-0.364941000	0.613505000	-1.832994000
H	0.562484000	-1.748786000	1.588396000
H	6.014963000	-0.001181000	0.280329000
H	4.818917000	0.080802000	1.588084000
H	4.578617000	1.021342000	0.096428000
H	4.292963000	-1.081772000	-1.213426000
H	4.571969000	-2.052847000	0.256315000
H	-2.946985000	0.288860000	-1.933161000
H	-3.261104000	1.019003000	-0.358268000
H	-5.705000000	-2.403871000	-0.180630000

Product # 5

C	0.608749000	0.582260000	0.419466000
C	1.102176000	-0.211794000	1.624367000
C	1.708434000	-1.397391000	1.426360000
C	1.854039000	-1.940938000	0.049438000
C	1.304561000	-1.011181000	-1.071148000
N	1.524272000	0.407238000	-0.731242000
C	-0.215987000	-1.060301000	-1.013244000
C	-0.629599000	-0.124924000	-0.150097000
C	-1.987185000	0.180643000	0.330326000
O	-2.211996000	0.961166000	1.238183000
O	-2.935608000	-0.506709000	-0.341737000
C	-4.892028000	0.942532000	-0.637057000
C	-4.308305000	-0.275154000	0.061990000
C	2.918560000	0.823440000	-0.567125000
C	3.022731000	2.265221000	-0.331088000
C	3.121273000	3.447662000	-0.109457000
O	2.336812000	-3.034353000	-0.188771000
H	0.448621000	1.634797000	0.656981000
H	0.939368000	0.182535000	2.624671000
H	2.075247000	-2.018588000	2.238612000
H	1.744172000	-1.296535000	-2.031278000
H	-0.825294000	-1.781203000	-1.542288000
H	-5.949633000	1.048639000	-0.374011000
H	-4.816509000	0.841676000	-1.723539000
H	-4.369462000	1.850764000	-0.327752000
H	-4.340858000	-0.161472000	1.147978000
H	-4.830427000	-1.191120000	-0.223642000
H	3.439213000	0.569401000	-1.499437000
H	3.451209000	0.294852000	0.243206000
H	3.206284000	4.494317000	0.071406000

Product # 8

C	1.219083000	-2.842613000	-0.777985000
C	-1.057957000	-2.635522000	-0.094333000
N	0.119174000	-3.396575000	-0.101460000
C	-1.076557000	-1.309201000	-0.308841000
C	1.260115000	-1.517776000	-0.946340000
C	0.229011000	-0.548782000	-0.415329000
O	2.127133000	-0.874723000	-1.835898000
C	0.029280000	-4.852797000	-0.011722000
C	1.528524000	0.313279000	-2.134198000
C	0.404792000	0.570626000	-1.436750000
C	-0.355146000	1.810718000	-1.582430000
O	-0.118289000	2.693641000	-2.388580000
O	-1.381738000	1.870095000	-0.692290000
C	-3.265931000	2.944744000	0.308999000
C	-2.187542000	3.067100000	-0.750381000
C	1.148840000	-5.451688000	0.720059000
C	2.076575000	-5.964868000	1.296444000
H	-2.014033000	-0.768094000	-0.323989000
H	0.086716000	-1.966437000	-3.200653000
H	1.949901000	-3.525716000	-1.192291000
H	0.509041000	-0.156667000	0.581371000
H	-0.907706000	-5.095359000	0.499817000
H	-0.029968000	-5.311961000	-1.013068000
H	2.025413000	0.909895000	-2.886403000
H	-3.896160000	3.839451000	0.302920000
H	-2.825768000	2.840597000	1.304820000
H	-3.902868000	2.075296000	0.121848000
H	-2.607735000	3.163855000	-1.756508000
H	-1.543643000	3.936119000	-0.581745000
H	2.892600000	-6.407070000	1.820182000

Product # 9

C	-0.259705000	-1.046552000	-0.224994000
C	-1.553582000	-1.325787000	-0.498612000
N	-2.536300000	-0.357759000	-0.697055000
C	-2.366050000	1.01919	-0.200306000
C	-0.902265000	1.28977	-0.138958000
C	0.09004	0.35625	-0.101748000
O	-0.405919000	2.55795	-0.014678000
C	-3.922294000	-0.787122000	-0.823933000
C	0.94081	2.43141	0.09408
C	1.31377	1.11357	0.04849
C	2.71559	0.68083	0.13945
O	3.6641	1.43391	0.26029
O	2.83737	-0.667191000	0.07417
C	4.11389	-2.686924000	0.05685
C	4.18795	-1.175434000	0.15438
C	-4.641215000	-0.920970000	0.45584
C	-5.214596000	-1.016073000	1.51462
H	0.48153	-1.827171000	-0.141279000
H	-1.895966000	-2.344717000	-0.646437000
H	-2.848804000	1.14972	0.78861
H	-2.876538000	1.70867	-0.889003000
H	-3.941159000	-1.742695000	-1.359436000
H	-4.452548000	-0.064955000	-1.459499000
H	1.51158	3.34077	0.19019
H	5.1206	-3.112604000	0.11241
H	3.6622	-2.996117000	-0.890128000
H	3.51964	-3.103440000	0.87528
H	4.63468	-0.845325000	1.09747
H	4.77865	-0.739264000	-0.657225000
H	-5.718248000	-1.108764000	2.44929

Product # 6

C	0.33516	-1.137479000	-0.169259000
C	1.64893	-1.429496000	-0.410245000
N	2.59966	-0.467889000	-0.614485000
C	2.25685	0.88635	-0.546867000
C	0.96338	1.21655	-0.306868000
C	-0.071972000	0.23223	-0.105042000
O	0.47574	2.47677	-0.233058000
C	4.01263	-0.831552000	-0.753393000
C	4.77358	-0.736878000	0.49676
C	5.40177	-0.656076000	1.52391
C	-0.959060000	2.39535	0.03329
C	-1.249301000	0.91374	0.102
C	-2.586844000	0.43888	0.34544
O	-3.556716000	1.16995	0.50885
O	-2.670695000	-0.930036000	0.38127
C	-4.776768000	-1.601857000	-0.679382000
C	-3.984937000	-1.475427000	0.61439
H	-0.384277000	-1.932928000	-0.033994000
H	2.00641	-2.451798000	-0.458003000
H	3.04981	1.60616	-0.693327000
H	4.46077	-0.181146000	-1.514133000
H	4.05996	-1.851933000	-1.147149000
H	5.9473	-0.583359000	2.43683
H	-1.487520000	2.91597	-0.775521000
H	-1.163240000	2.93357	0.96766
H	-5.738023000	-2.090047000	-0.485226000
H	-4.229781000	-2.199928000	-1.414631000
H	-4.972341000	-0.613732000	-1.102293000
H	-4.511668000	-0.840451000	1.33078
H	-3.802119000	-2.454722000	1.06546

Product # 7

C	-1.822425000	-0.462961000	-0.630678000
C	-1.947799000	-1.779417000	-0.384559000
N	-0.880902000	-2.593888000	-0.010409000
C	0.42018	-2.089871000	-0.153952000
C	0.58544	-0.774784000	-0.337760000
C	-0.531860000	0.2464	-0.277009000
O	1.74615	-0.201434000	-0.841104000
C	-1.112568000	-3.843105000	0.70166
C	-1.208806000	-3.706490000	2.16297
C	-1.287325000	-3.585943000	3.36178
C	1.34113	0.99176	-1.413916000
C	0.05199	1.2971	-1.202400000
C	2.39673	1.72267	-2.150602000
O	3.54958	1.35908	-2.239296000
O	1.89517	2.85221	-2.701738000
C	2.93755	3.17653	-4.897413000
C	2.82748	3.6605	-3.459919000
H	-2.662777000	0.09488	-1.029267000
H	-2.890189000	-2.303175000	-0.517952000
H	1.2248	-2.811939000	-0.236990000
H	-0.621262000	0.69778	0.7323
H	-0.299779000	-4.537113000	0.45243
H	-2.035451000	-4.291956000	0.31399
H	-1.353267000	-3.469404000	4.41896
H	-0.441363000	2.19331	-1.548885000
H	3.58847	3.84894	-5.465990000
H	1.95571	3.15949	-5.379227000
H	3.36747	2.17278	-4.932604000
H	3.79882	3.63866	-2.960460000
H	2.41403	4.67028	-3.406700000

TS #4

C	-2.024449000	0.67658	0.75245
C	-1.556519000	2.0214	1.00447
C	-0.504093000	2.53572	0.32266
C	0.20423	1.7113	-0.656746000
C	-0.444104000	0.42	-0.928341000
N	-1.681706000	0.13727	-0.470396000
C	0.35648	-0.617064000	1.20388
C	-0.669721000	-0.399894000	1.88074
C	1.59453	-1.129311000	0.67288
O	1.70043	-2.208363000	0.11246
O	2.6005	-0.250452000	0.85843
C	3.88159	-0.295808000	-1.237569000
C	3.87509	-0.589452000	0.25541
C	-2.252151000	-1.177879000	-0.843122000
C	-3.701509000	-1.239883000	-0.688787000
C	-4.898072000	-1.327423000	-0.561073000
O	1.24342	2.04389	-1.234581000
H	-3.003940000	0.38589	1.11518
H	-2.047363000	2.58257	1.79407
H	-0.130441000	3.53834	0.50114
H	-0.070778000	-0.166746000	-1.760280000
H	-1.144002000	-0.524571000	2.83734
H	4.90169	-0.382897000	-1.627046000
H	3.50622	0.71251	-1.428393000
H	3.24921	-1.009570000	-1.770663000
H	4.09616	-1.640249000	0.46057
H	4.58887	0.04071	0.79045
H	-1.761791000	-1.943362000	-0.226398000
H	-1.977719000	-1.364281000	-1.885338000
H	-5.956862000	-1.399539000	-0.459464000

TS #5

C	0.75873	0.14962	1.4051
C	1.28174	-1.160670000	1.55156
C	2.39446	-1.566881000	0.86725
C	2.97092	-0.714028000	-0.159618000
C	2.21783	0.55567	-0.365974000
N	1.43816	1.04469	0.65814
C	0.87304	-0.220459000	-1.603504000
C	-0.207006000	-0.561662000	-1.083170000
C	-1.465613000	-1.068497000	-0.633297000
O	-1.644484000	-2.190795000	-0.186794000
O	-2.459359000	-0.146420000	-0.784389000
C	-3.981674000	-0.377277000	1.12747
C	-3.776602000	-0.570932000	-0.367953000
C	1.02406	2.46443	0.65502
C	-0.235021000	2.72883	-0.038296000
C	-1.282126000	2.96937	-0.585827000
O	3.92913	-1.000224000	-0.880685000
H	-0.020051000	0.53418	2.0512
H	0.78214	-1.823670000	2.24973
H	2.8468	-2.538101000	1.03499
H	2.73177	1.30938	-0.954895000
H	1.45907	-0.266801000	-2.507668000
H	-5.013881000	-0.622862000	1.39895
H	-3.788442000	0.66058	1.41556
H	-3.314737000	-1.033947000	1.6912
H	-3.920874000	-1.616374000	-0.650190000
H	-4.458641000	0.05642	-0.947620000
H	1.84167	3.03461	0.20462
H	0.95314	2.78301	1.70076
H	-2.203701000	3.14511	-1.091107000

TS #6

C	-0.683193000	-1.396893000	-0.410911000
C	-1.903594000	-1.486157000	0.22524
N	-2.623337000	-0.356063000	0.46834
C	-2.139856000	0.87161	0.13498
C	-0.929322000	1.02137	-0.539196000
C	-0.171419000	-0.158121000	-0.818086000
O	-0.494054000	2.21977	-0.823635000
C	-3.977666000	-0.465032000	1.05952
C	1.1102	2.3984	-0.327741000
C	1.7392	1.41175	0.14217
C	2.68737	0.54163	0.71416
O	2.8776	0.33565	1.90699
O	3.39039	-0.133835000	-0.266864000
C	5.06694	-1.664694000	-0.985930000
C	4.38642	-1.045059000	0.22199
C	-5.026830000	-0.601753000	0.05215
C	-5.899294000	-0.714822000	-0.773048000
H	-0.139811000	-2.311884000	-0.618204000
H	-2.360046000	-2.422089000	0.51901
H	-2.741176000	1.73203	0.39816
H	0.69038	-0.108731000	-1.465525000
H	-3.974204000	-1.324465000	1.73676
H	-4.142682000	0.4256	1.6735
H	1.21297	3.44857	-0.550189000
H	5.83846	-2.371645000	-0.663692000
H	5.53996	-0.895361000	-1.603197000
H	4.34541	-2.203148000	-1.608227000
H	3.91364	-1.805480000	0.85441
H	5.10015	-0.505485000	0.85416
H	-6.664970000	-0.811468000	-1.508920000

TS #7

C	-1.939153000	2.12427	-0.007136000
C	-2.816499000	1.23253	-0.550298000
N	-2.560028000	-0.116338000	-0.514743000
C	-1.412280000	-0.597902000	0.03711
C	-0.465282000	0.23985	0.6576
C	-0.675926000	1.70418	0.55665
O	0.61195	-0.187271000	1.14976
C	-3.591787000	-1.059594000	-0.987097000
C	-4.569766000	-1.408841000	0.04371
C	-5.382874000	-1.698807000	0.88652
C	1.79475	1.36416	-0.219226000
C	0.81449	2.12696	-0.419345000
C	2.97818	0.58745	0.00103
O	3.79908	0.81831	0.87157
O	3.08163	-0.414112000	-0.910859000
C	3.92077	-2.375073000	0.29352
C	4.21237	-1.297839000	-0.740878000
H	-2.211747000	3.17505	-0.009803000
H	-3.770205000	1.52058	-0.973995000
H	-1.277851000	-1.672170000	0.04559
H	-0.350178000	2.26847	1.43101
H	-3.081163000	-1.956396000	-1.351578000
H	-4.091099000	-0.605921000	-1.849401000
H	-6.092812000	-1.952445000	1.64032
H	0.63719	3.02463	-0.990403000
H	4.76495	-3.070490000	0.3554
H	3.02396	-2.939590000	0.02313
H	3.76666	-1.926548000	1.27725
H	5.08744	-0.707468000	-0.457528000
H	4.37181	-1.726772000	-1.733523000
