Supporting Information for the Manuscript: Challenging 50 years of established views on Ugi reaction: a theoretical approach.

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1. Computational details.

Quantum mechanics calculations were performed with the Gaussian09 software package.[23] Energy and forces were computed by density functional theory with the M06-2X[24] exchange-correlation functional including ZPE corrections. A polarizable continuum model[25] (PCM) of solvent was used as implemented in Gaussian09 to describe the medium (methanol or toluene). Transition states were localized using the string theory[15] as implemented in Opt'n Path.[16] All structures were optimized and frequency calculations were performed to ensure the absence of any imaginary frequencies on local minima, and the presence of only one imaginary frequency on transition states. Reactants and products were re-localized starting from the transition states (IRC calculations followed by optimizations) to ensure that no TS were forgotten.

(23) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision A.02*, Gaussian, Inc., Wallingford CT, **2009**.

(24) (a) Zhao, Y.; Truhlar, D. G. *Theor Chem Account* **2008**, *120*, 215–241. (b) Zhao, Y.; Truhlar, D. G. *Theor Chem Account* **2008**, *119*, 525–525. (c) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.***2008**, *41*, 157–167.

(25) (a) Mierts, S.; Scrocco, E.; Tomasi, J. *Chem. Phys.* **1981**, *55*, 117–129. (b) Cossi, M.; Mennucci, B.; Tomasi, J. *Chem. Phys. Lett.* **1994**, *228*, 165–170. (c) Mennucci, B.; Cancès, E.; Tomasi, J. *J. Phys. Chem. B* **1997**, *101*, 10506–10517.

2. Systematic analysis of the possible reaction paths for the Ugi reaction.

The unbiased study of the mechanism of a system as complex as a multicomponent reaction requires a systematic procedure without any assumption. The only certitude used here was the fact that the imidate can be isolated with some examples for both Ugi and Ugi-Smiles couplings.[8] Moreover, in some cases the isolated imidate can lead to the corresponding Ugi product under extreme microwave heating. This confirms that the mechanism involves the formation of this structure.

Naming (A) the amine, (B) the aldehyde, (C) the isocyanide and (D) the acid, the imidate can be written as (A-B-C-D). Thus, we investigated all the possibilities to construct the structure (A-B-C-D) from the four isolated bricks (A), (B), (C) and (D). 12 possible pathways can lead to (A-B-C-D); the first six are the linear formation of the structure:

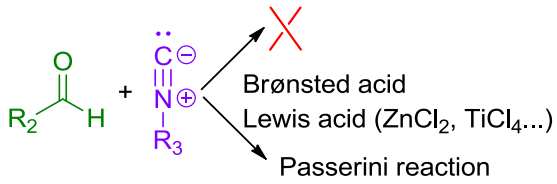
1. A + B + C + D → A-B + C + D → A-B-C + D → A-B-C-D
2. A + B + C + D → A-B + C + D → A-B + C-D → A-B-C-D
3. A + B + C + D → A + B-C + D → A-B-C + D → A-B-C-D
4. A + B + C + D → A + B-C + D → A + B-C-D → A-B-C-D
5. A + B + C + D → A + B + C-D → A-B + C-D → A-B-C-D
6. A + B + C + D → A + B + C-D → A + B-C-D → A-B-C-D

The next six are due to the possible insertion of one of the brick in a pre-formed structure. Even if it can sound like odd possibilities, they have to be considered to be exhaustive, and some of them are chemically possible since isocyanides are known to insert into some structures (such as in acyl chlorides in the Nef-Isocyanide reaction[10]):

7. A + B + C + D → A-B + D + C → A-B-D + C → A-B-C-D
8. A + B + C + D → A + B-D + C → A-B-D + C → A-B-C-D
9. A + B + C + D → A + C-D + B → A-C-D + B → A-B-C-D
10. A + B + C + D → A-C + D + B → A-C-D + B → A-B-C-D
11. A + B + C + D → A-D + B + C → A-B-D + C → A-B-C-D
12. A + B + C + D → A-D + C + B → A-C-D + B → A-B-C-D

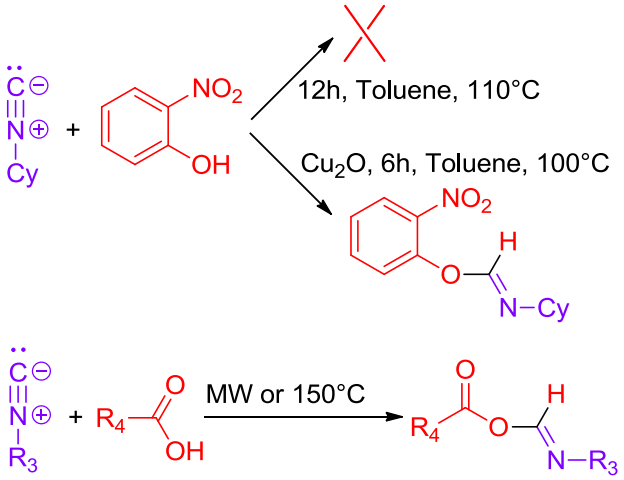
We then considered the possible formation of some intermediates.

- No reaction occurs between an aldehyde (B) and an isocyanide (C) unless an acid is added (a Lewis or a Brønsted one), leading to a Passerini reaction (see Scheme SI-1). When performing a Ugi reaction, a Passerini reaction could occur. However this has never been observed as the imine formation is faster than the addition of the isocyanide onto the aldehyde and the iminium is more electrophilic than the aldehyde. Thus, the two possible pathways involving the (B-C) structure (3 and 4) do not need to be computationally considered.



Scheme SI-1. Possible reaction between an aldehyde and an isocyanide.

- When an isocyanide (C) and a nitrophenol (D) are put together in toluene, no reaction occurs after 12 hours at reflux (see Scheme SI-2). If copper oxide is added, an insertion of the isocyanide is observed. A similar reaction can occur between an isocyanide (C) and a carboxylic acid (D) without metals but with strong conditions (microwave irradiation or heating at 150°C for example). As the Ugi reaction is done between room temperature and 60°C without cupper, the four possible pathways involving the (C-D) structure (2, 5, 6 and 9) do not need to be computationally considered.



Scheme SI-2. Possible reaction between an isocyanide and an acid.

- An aldehyde (B) and an acid (D) (such as a carboxylic acid or a phenol) don't react together, so no (B-D) structure can be observed (as in the pathway 8).
- And finally, the insertion of an aldehyde (B) into an (A-D) or an (A-C-D) structure (as in pathways 10, 11 and 12) is not realistic.

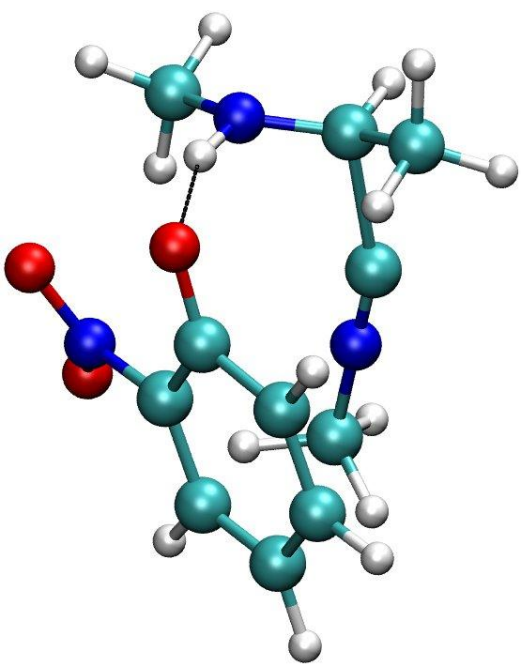
Therefore, only two of the pathways (1 and 7) are possible:

1. A-B + C + D → A-B-C + D → A-B-C-D

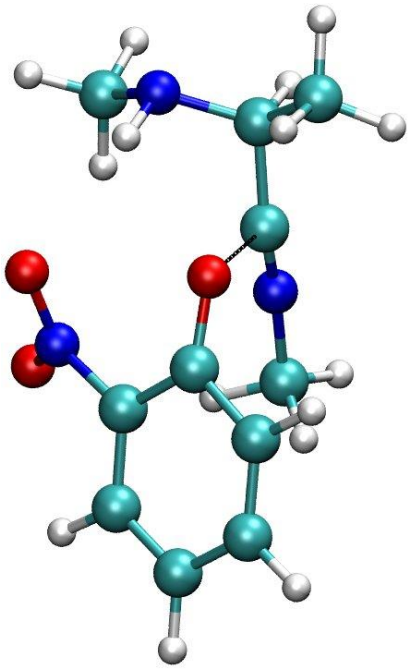
7. A-B + D + C → A-B-D + C → A-B-C-D

The first one is the mechanism proposed by Ugi: (A) and (B) react to form the imine (A- B); the imine then reacts with (C) to form the nitrilium (A-B-C) which finally reacts with (D) to form the imidate. The second one is the formation of a hemiaminal (A-B-D) in which the isocyanide (C) inserts. In both cases, an imine is first formed and can then be used as a starting point for a computational study.

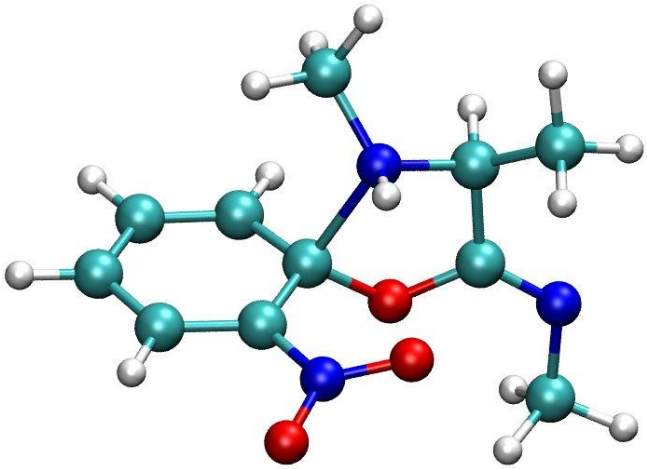
3. Cartoons of the optimized transition states structures in methanol.



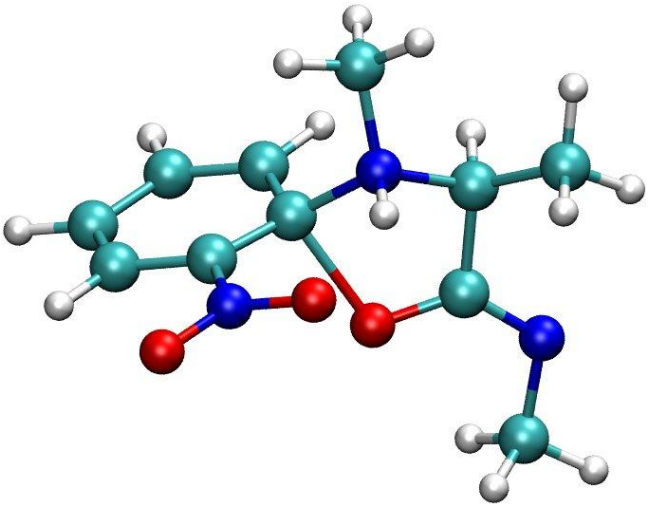
(**TS-1**)



(**TS-2**)

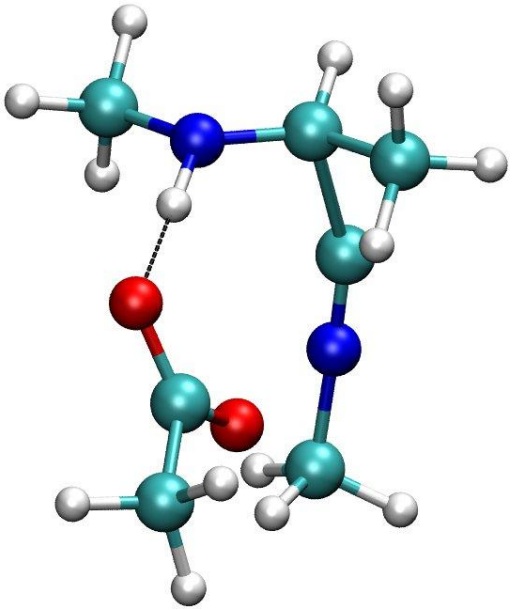


(**TS-3**)

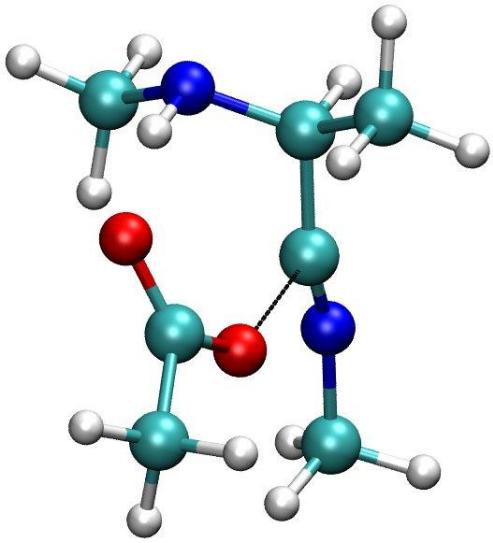


(**TS-4**)

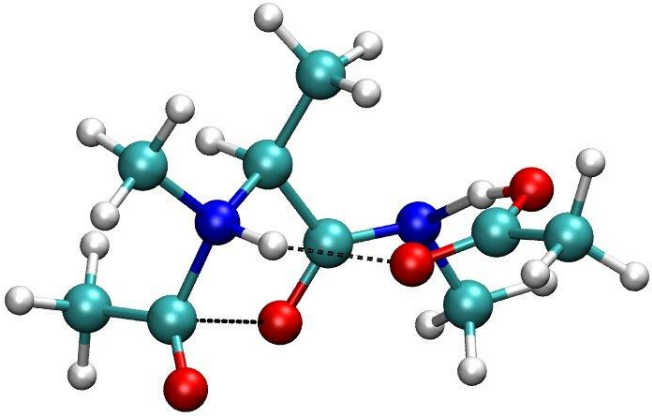
Scheme SI-3. Optimized structures of the transition states for the Ugi-Smiles reaction in methanol. When they exist, structures in toluene are very close. Interactive 3D structures are given below.



(**TS-1'**)



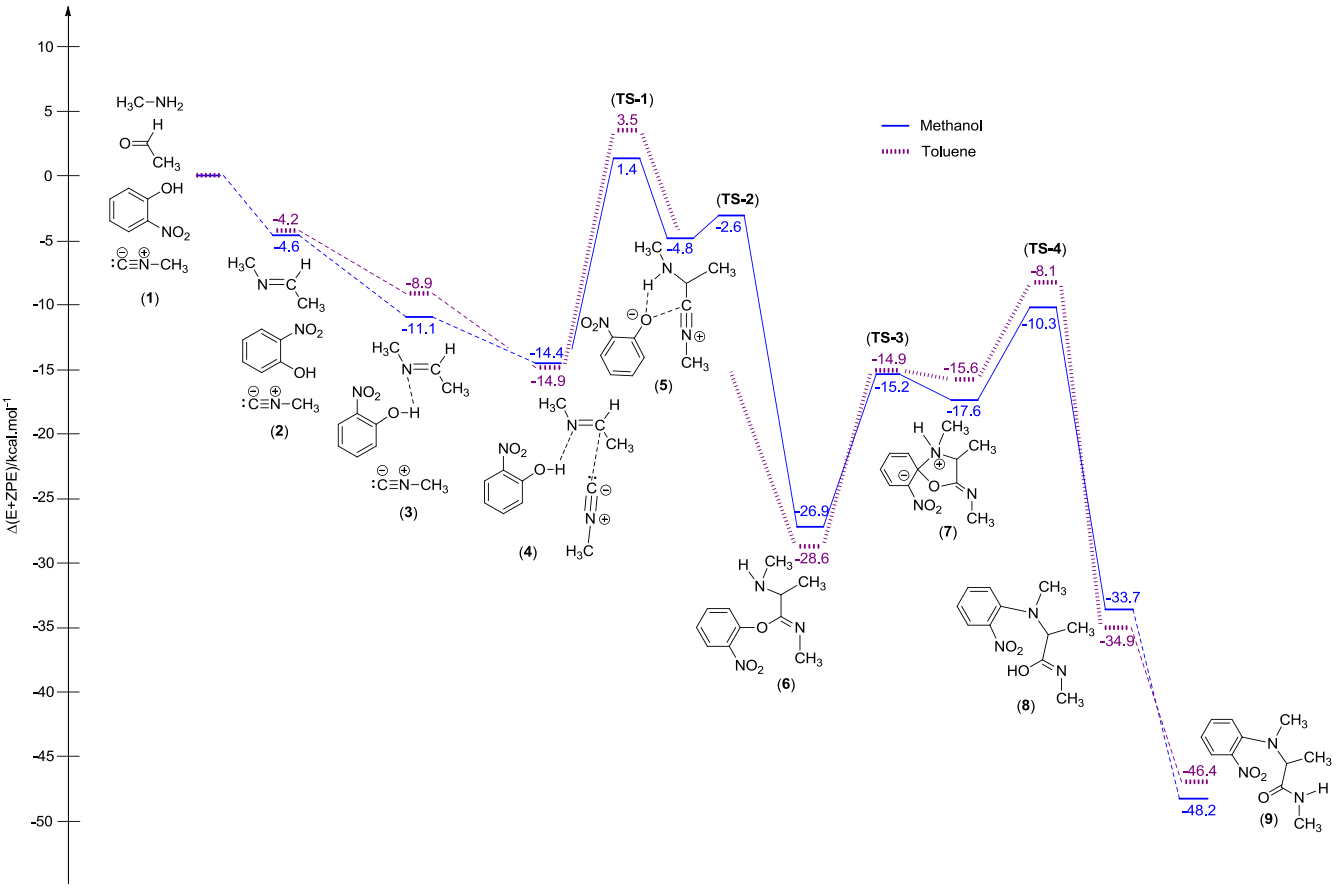
(**TS-2'**)



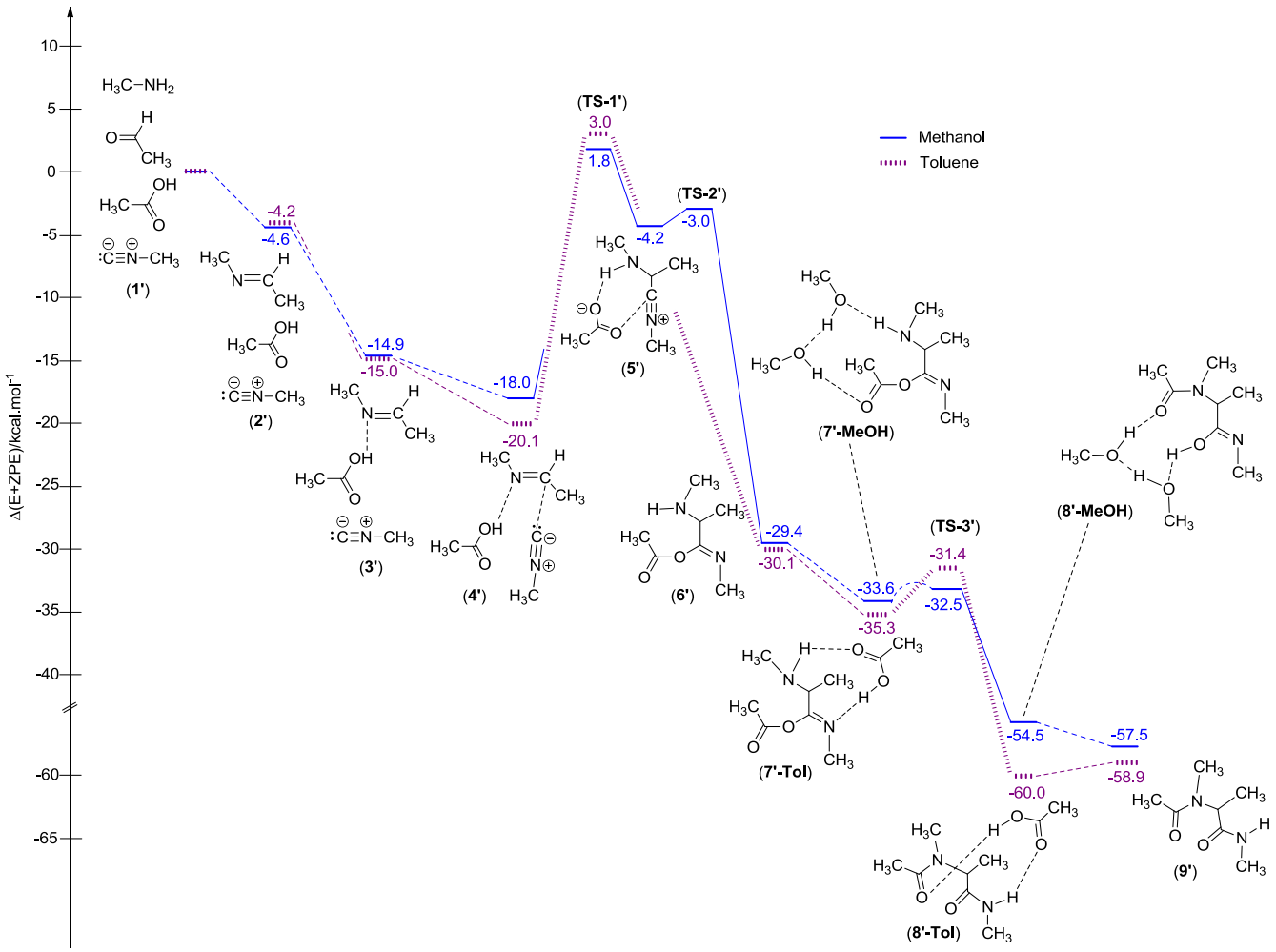
(**TS-3'-AcOH**)

Scheme SI-4. Optimized structures of some transition states for the Ugi-Mumm reaction in methanol. When they exist, structures in toluene are very close. Interactive 3D structures are given below.

4. Full energy profiles.

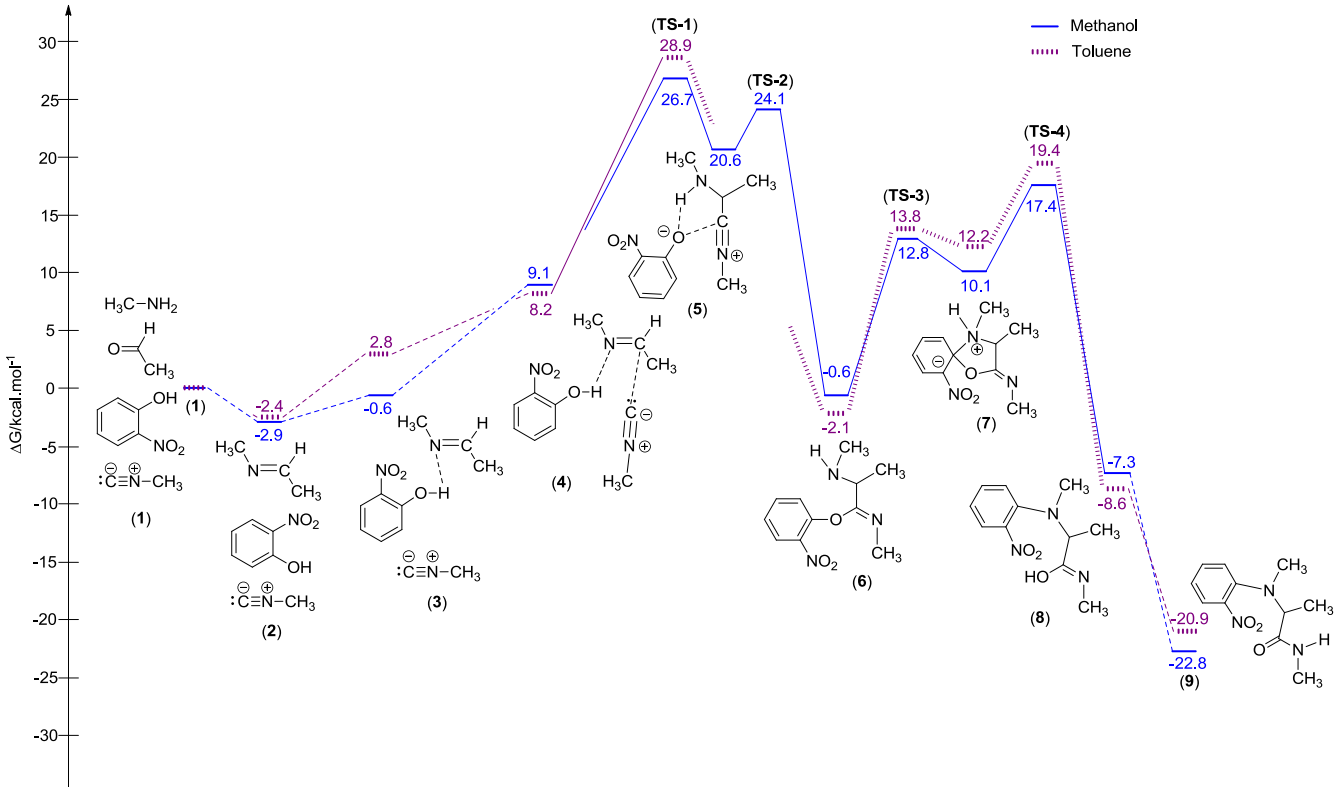


Scheme SI-5. Full energy profile of the Ugi-Smiles reaction in methanol and in toluene (at the M06-2X/6-31+G(d,p) level of theory, including ZPE corrections). The energy reference is the sum of the four reactants energies computed separately. For the sake of clarity, the water molecule released in the imine formation is not displayed in the scheme.

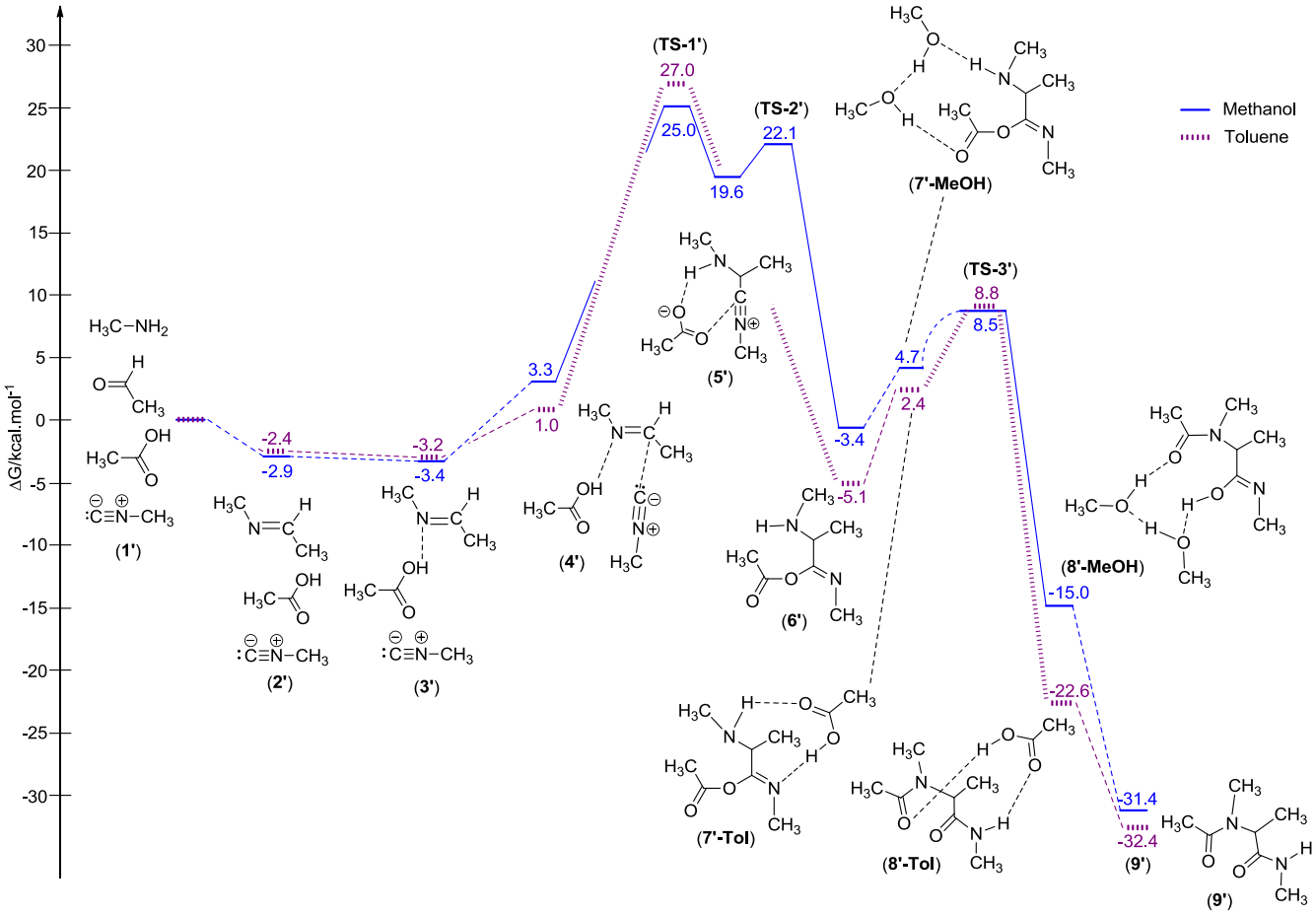


Scheme SI-6. Full energy profile of the Ugi reaction in methanol and in toluene (at the M06-2X/6-31+G(d,p) level of theory, including ZPE corrections). The energy reference is the sum of the four reactants energies computed separately. For the sake of clarity, the water molecule released in the imine formation is not displayed in the scheme. When an extra carboxylic acid is involved, its energy reference is the one computed separately. When two methanol molecules are involved, their energy reference is a hydrogen bonded methanol dimer computed separately.

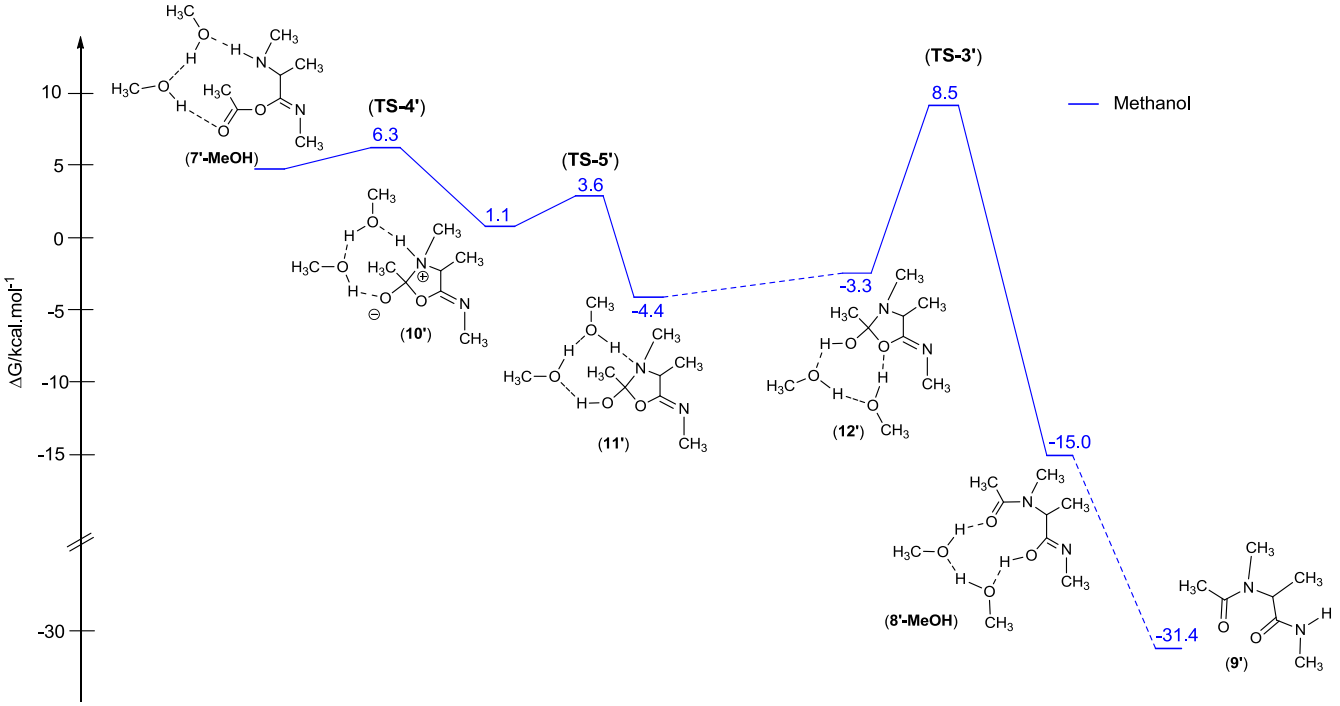
5. Gibbs free energy profiles.



Scheme SI-7. Gibbs free energy profile (at 298 K and 1 atm) of the Ugi-Smiles reaction in methanol and in toluene (at the M06-2X/6-31+G(d,p) level of theory). The energy reference is the sum of the four reactants energy computed separately.



Scheme SI-8. Gibbs free energy profile (at 298 K and 1 atm) of the Ugi reaction in methanol and in toluene (at the M06-2X/6-31+G(d,p) level of theory). The energy reference is the sum of the four reactants energy computed separately.



Scheme SI-9. Gibbs free energy profile (at 298 K and 1 atm) of the Mumm rearrangement in methanol with explicit solvation by two molecules (at the M06-2X/6-31+G(d,p) level of theory). The energy reference is the sum of the four reactants and two hydrogen bonded methanol molecules energies computed separately.

6. Comparison of energy profiles between E+ZPE and G energies by considering (4) as the reference.

In the Ugi-Smiles reaction, after the formation of (**4**), only intramolecular reactions occur. Thus, the energy profiles in electronic plus ZPE corrections and in Gibbs free energies are very similar and are just shifted. We present in Table SI-1 and Table SI-2 the respective energies in methanol and toluene by taking (**4**) as the reference. Slight variations are observed, but no significant differences appear.

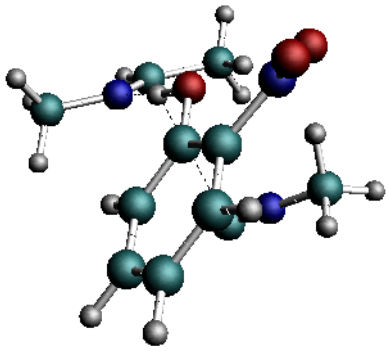
	(**4**)	(**TS-1**)	(**5**)	(**TS-2**)	(**6**)	(**TS-3**)	(**7**)	(**TS-4**)	(**8**)	(**9**)
E+ZPE	0.0	15.7	9.6	11.8	-12.5	-0.9	-3.2	4.1	-19.3	-33.8
G	0.0	17.6	11.5	15.0	-9.7	3.7	1.0	8.3	-16.4	-31.9

Table SI-1. Comparison of electronic energies plus ZPE corrections and Gibbs free energies in methanol for the Ugi-Smiles reactions by considering (**4**) as the reference.

	(**4**)	(**TS-1**)	(**6**)	(**TS-3**)	(**7**)	(**TS-4**)	(**8**)	(**9**)
E+ZPE	0.0	18.4	-13.7	0.0	-0.7	6.8	-20.0	-31.5
G	0.0	20.7	-10.3	5.6	4.0	11.1	-16.8	-29.1

Table SI-2. Comparison of electronic energies plus ZPE corrections and Gibbs free energies in toluene for the Ugi-Smiles reactions by considering (**4**) as the reference.

7. Interactive 3D structures of the reaction intermediates. These structures can only be manipulated with Adobe Reader.



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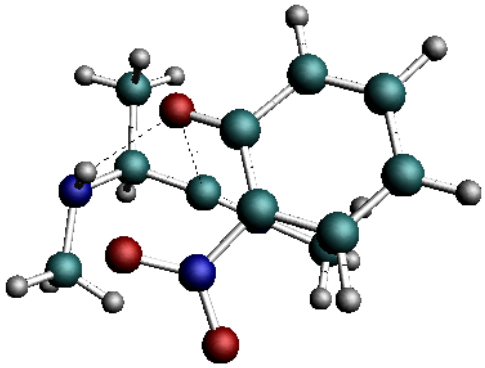

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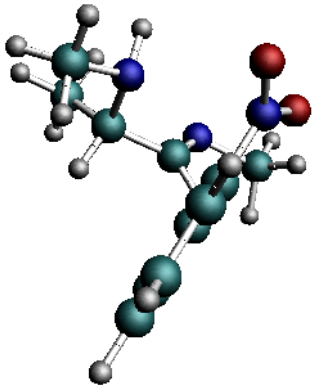

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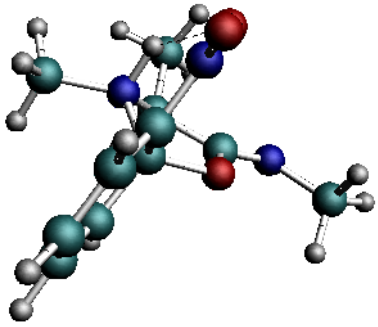

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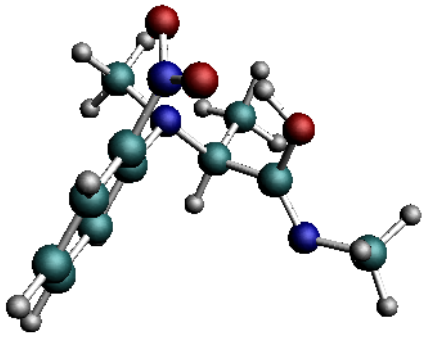

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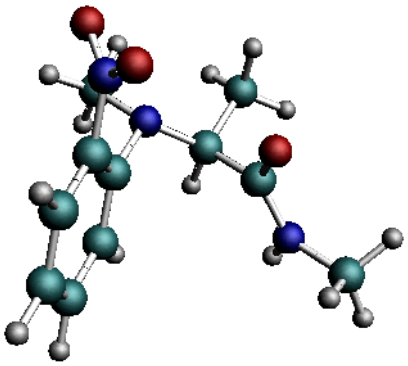

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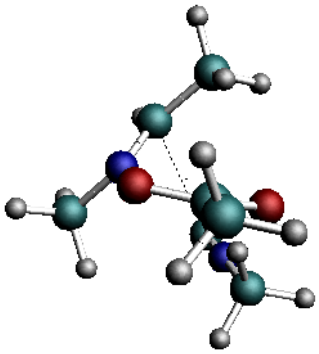

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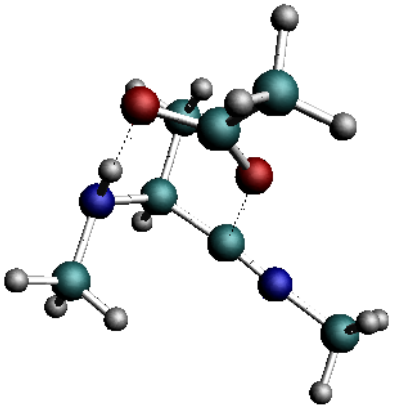

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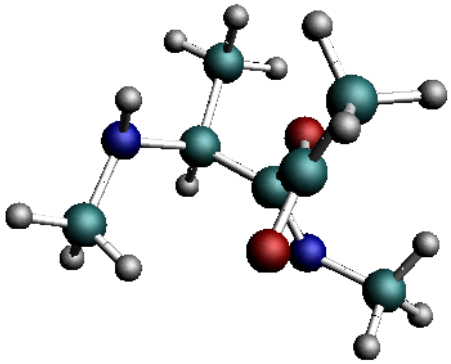

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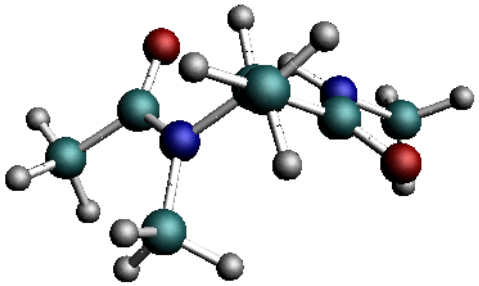

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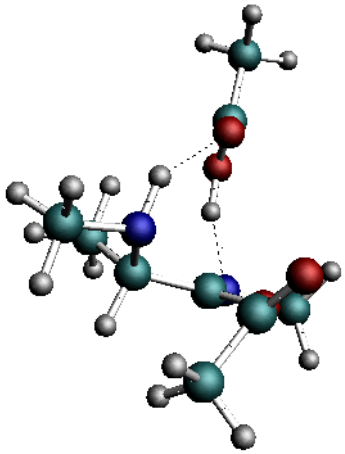
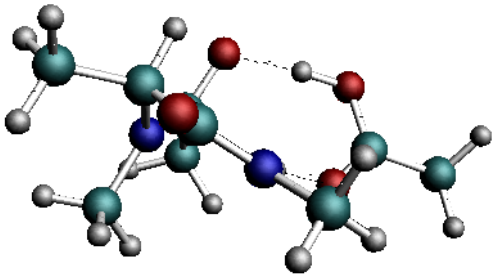


(7’-Tol)



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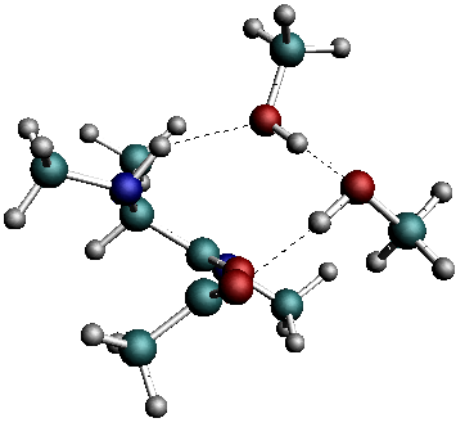

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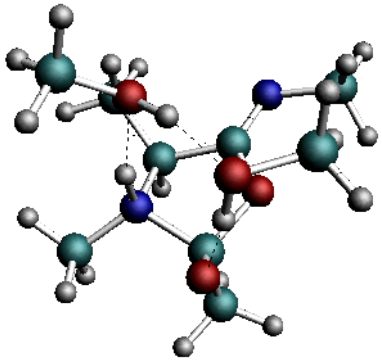

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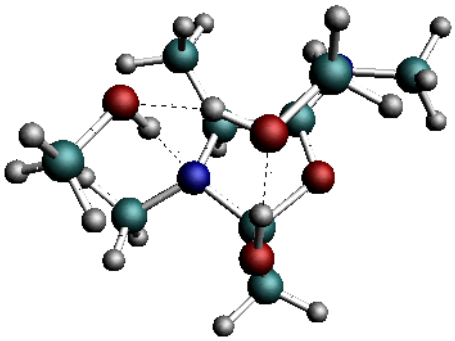

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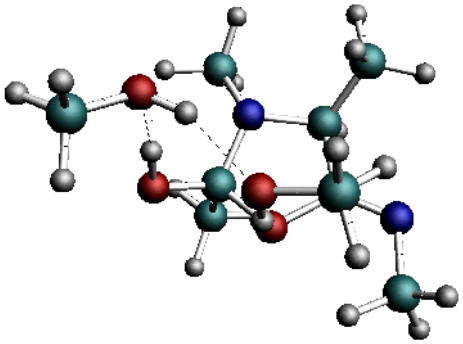

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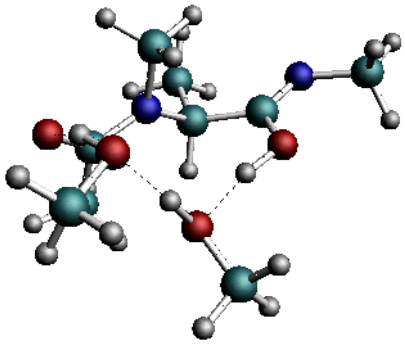
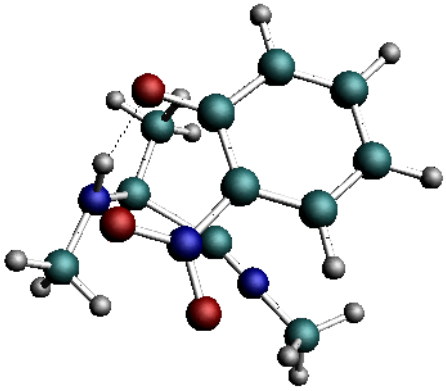
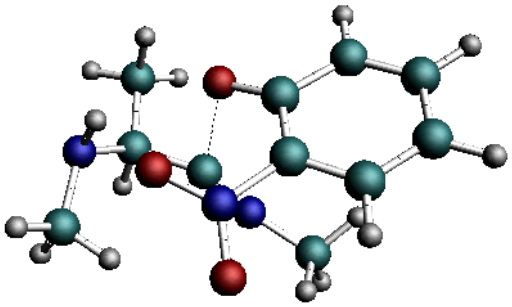


(8'-MeOH)

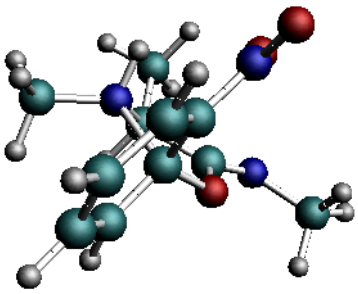
8. Interactive 3D structures of the transition states in methanol. These structures can only be manipulated with Adobe Reader.



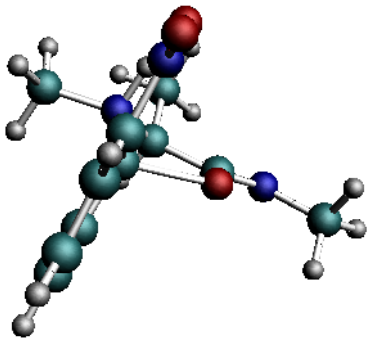
(TS-1)



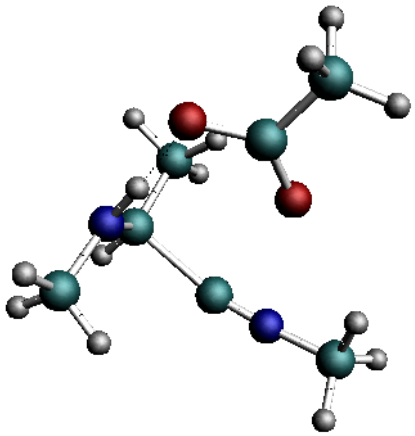
(TS-2)



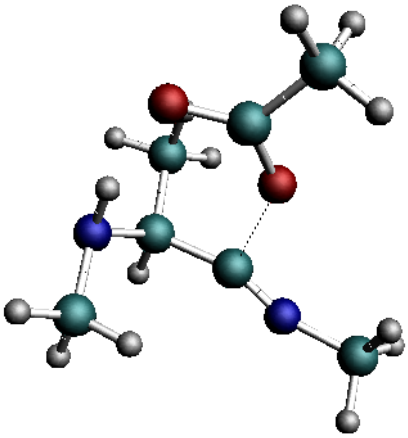
(TS-3)



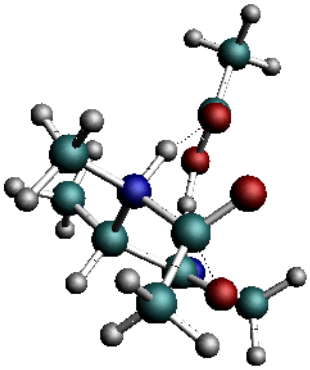
(TS-4)



(TS-1')



(TS-2')



(TS-3'-AcOH)

9. Cartesian coordinates for the structures discussed in the text.

Below are given the optimized geometries of the structures discussed in the text at the M06-2X/6-31+G(d,p) level of theory in methanol and in toluene.

Ugi-Smiles reaction in methanol

(**2**)-MeOH. Energy: -173.18876426 a.u.

C	-3.073396	0.230410	-1.419313
N	-2.132223	1.315645	-1.193074
C	-1.010965	1.021772	-0.677392
C	0.041198	2.047634	-0.395294
H	-3.999159	0.439714	-0.875581
H	-0.300180	3.040558	-0.692759
H	-3.324884	0.190069	-2.483084
H	0.287003	2.051449	0.671563
H	-2.687624	-0.749584	-1.105299
H	0.961363	1.801843	-0.935148
H	-0.767129	-0.019549	-0.413595

(**3**)-MeOH. Energy: -685.00105641 a.u.

C	1.642999	-1.439083	0.546384
C	0.678007	-0.420188	0.687116
C	0.787340	0.675428	-0.194044
C	1.797710	0.739947	-1.140053
C	2.740353	-0.288438	-1.263248
C	2.649250	-1.383487	-0.422253
O	-0.303730	-0.511779	1.576778
N	1.624905	-2.613034	1.406661
O	2.081670	-3.657368	0.953922
O	1.182388	-2.511440	2.539483
N	-1.968744	1.515931	1.518005
C	-1.674634	2.616938	2.080976
C	-0.368104	2.840696	2.768622
C	-3.254381	1.371697	0.851277
H	-3.081286	1.130548	-0.201158
H	-3.862726	2.280136	0.920389
H	1.850011	1.602906	-1.796611
H	-3.796458	0.535602	1.299749
H	0.051905	1.470181	-0.121004
H	-2.388951	3.450009	2.067834
H	3.529045	-0.232374	-2.004095
H	-0.950393	0.286784	1.519286
H	0.165653	3.665921	2.286616
H	-0.541620	3.133990	3.808318
H	0.252468	1.942602	2.744452
H	3.354174	-2.204367	-0.484648

(**4**)-MeOH. Energy: -817.68244167 a.u.

C	1.805137	-3.013731	0.964975
C	2.439265	-2.160641	0.079188
C	1.896007	-0.899875	-0.183451
C	0.727243	-0.436275	0.454978
C	0.108469	-1.324274	1.356491
C	0.633052	-2.582931	1.600766
N	2.590305	-0.075038	-1.160556
O	1.942977	0.711412	-1.835045
O	0.253368	0.782584	0.228869
C	-2.907339	-0.996605	-0.384883
C	-2.708296	2.196886	0.973708
C	-2.650545	2.398283	-0.504063
O	3.800020	-0.228952	-1.281406
N	-2.060484	-0.981436	-1.188656
C	-1.025994	-0.973266	-2.171747
N	-1.816870	1.558141	1.616998
C	-1.950681	1.409747	3.058912
H	-0.409067	-1.865287	-2.043937
H	-0.409014	-0.081565	-2.037871
H	-3.542520	1.965172	-0.967899
H	-1.040601	1.774613	3.541367
H	0.121625	-3.240678	2.296646
H	-1.475829	-0.977217	-3.165062
H	-0.802073	-1.000192	1.849653
H	2.209495	-4.000310	1.158096
H	-2.057468	0.349293	3.305232
H	-2.815786	1.954157	3.452937
H	-3.565138	2.628570	1.506811
H	3.346223	-2.452661	-0.437494
H	-0.560557	1.012311	0.823333
H	-2.655173	3.469262	-0.729682
H	-1.759434	1.936114	-0.933235

(**TS-1**)-MeOH. Energy: -817.65933018 a.u.

C	6.170877	4.183375	-1.810115
C	5.549447	4.106503	-0.586686
C	5.320136	5.266158	0.182912
C	5.711358	6.584909	-0.257351
C	6.343547	6.594193	-1.556778
C	6.562148	5.456311	-2.292291
N	4.629666	5.082685	1.420716
O	4.714978	5.931561	2.305664
O	5.487615	7.668937	0.363047
C	2.301070	5.768014	-1.226501
C	2.201131	7.566217	-0.592559
C	2.937779	8.345865	-1.647738
O	3.947066	4.057780	1.571217
N	2.344020	4.613536	-1.195195
C	2.390849	3.186071	-1.159742
N	2.680403	7.571035	0.654340
C	1.931296	6.950641	1.734316
H	2.797519	2.892473	-0.191179
H	3.035940	2.840512	-1.967406
H	2.545882	8.110164	-2.637270
H	2.329569	7.292130	2.688777
H	7.048621	5.534093	-3.261200
H	1.378587	2.804042	-1.289745
H	6.644327	7.568499	-1.931976
H	6.366355	3.286971	-2.387423
H	2.012233	5.855158	1.695334
H	0.879017	7.234176	1.659066
H	1.113359	7.590286	-0.656248
H	5.246102	3.149955	-0.175157
H	3.704187	7.654744	0.760827

H	2.776411	9.408078	-1.444404
H	4.008551	8.139083	-1.610240

(**5**)-MeOH. Energy: -817.67134820 a.u.

C	2.541805	-2.200358	-1.239354
C	1.875982	-2.082744	-0.041281
C	1.301565	-0.854351	0.341527
C	1.338118	0.326308	-0.487725
C	2.042035	0.129014	-1.733693
C	2.615856	-1.067689	-2.087262
N	0.582684	-0.839713	1.578248
O	0.439205	0.217121	2.188708
O	0.752113	1.419167	-0.231477
C	-1.806599	0.525788	-0.658741
C	-2.214367	1.895373	-0.190453
C	-1.745007	2.950370	-1.190111
O	0.114380	-1.904788	2.002095
N	-1.559477	-0.558560	-0.939482
C	-1.237220	-1.901448	-1.314283
N	-1.741056	2.132066	1.148070
C	-2.376325	1.290005	2.159276
H	-1.070851	-2.471592	-0.398696
H	-0.325155	-1.876953	-1.913862
H	-2.102747	2.723409	-2.196891
H	-1.940671	1.521366	3.131874
H	3.133047	-1.147664	-3.039920
H	-2.074266	-2.306141	-1.882186
H	2.090100	0.988797	-2.395763
H	3.003409	-3.138469	-1.524585
H	-2.244026	0.210616	1.983346
H	-3.447090	1.510652	2.194053
H	-3.310923	1.848772	-0.182017
H	1.786984	-2.925435	0.635966
H	-0.726771	2.005330	1.153756
H	-2.161942	3.907216	-0.871686
H	-0.655739	2.997155	-1.187844

(**TS-2**)-MeOH. Energy: -817.66764514 a.u.

C	2.636546	-2.245586	-1.259579
C	1.925382	-2.111971	-0.083039
C	1.257125	-0.911641	0.191684
C	1.209591	0.188420	-0.715892
C	1.963953	-0.002667	-1.912892
C	2.655487	-1.169375	-2.169059
N	0.522008	-0.840855	1.433418
O	0.447726	0.229626	2.023526
O	0.461203	1.223791	-0.547036
C	-1.519007	0.539745	-0.734206
C	-2.126547	1.843781	-0.274976
C	-1.718550	3.007451	-1.168416
O	-0.000969	-1.871812	1.858805
N	-1.560058	-0.589425	-1.005495
C	-1.334031	-1.954758	-1.366534
N	-1.817262	2.082300	1.114029
C	-2.439929	1.130120	2.032470
H	-1.187713	-2.522600	-0.445136
H	-0.435032	-2.018352	-1.983581
H	-1.873457	2.768766	-2.223487
H	-2.117016	1.359353	3.049034
H	3.211400	-1.264974	-3.097596
H	-2.204239	-2.327020	-1.906478
H	1.951637	0.809838	-2.633256
H	3.176143	-3.161033	-1.473183
H	-2.182661	0.079005	1.828442
H	-3.527004	1.239857	1.980592
H	-3.205463	1.663168	-0.367805
H	1.881103	-2.913925	0.646347
H	-0.802548	2.059569	1.217070
H	-2.338074	3.866246	-0.903402
H	-0.667513	3.245572	-1.008245

(**6**)-MeOH. Energy: -817.70882721 a.u.

H	3.755361	2.446531	1.125775
H	1.976827	2.498642	1.261603
C	2.862647	1.859879	1.344898
H	2.925465	1.506081	2.380348
N	2.795079	0.735034	0.419397
C	1.742488	0.042662	0.406071
O	0.733752	0.321628	1.314978
H	3.415261	-2.106283	-0.254402
C	-0.537783	-0.164520	1.164907
C	1.505704	-1.109207	-0.550413
H	-0.232167	-1.568495	2.735121
C	-0.953194	-1.176436	2.025506
H	3.395413	-0.935949	-1.584181
O	-0.185693	2.168262	-0.393356
H	0.953877	-1.882270	0.000742
C	-1.457884	0.346097	0.238622
C	-2.254567	-1.669378	1.964943
C	-2.753117	-0.155296	0.160778
H	-2.558704	-2.456036	2.647240
N	-1.093853	1.413157	-0.694633
C	-3.157152	-1.160676	1.032536
C	2.810728	-1.703397	-1.070984
O	-1.744153	1.507003	-1.722991
H	-3.429992	0.256028	-0.578607
H	-4.170287	-1.542494	0.980460
N	0.607470	-0.617239	-1.598787
H	1.151911	-0.117477	-2.298223
H	-0.914477	-2.040594	-1.474931
H	2.589667	-2.512865	-1.771877
C	-0.208432	-1.653882	-2.219769
H	-0.788148	-1.210482	-3.032535
H	0.366601	-2.500585	-2.622534

(**TS-3**)-MeOH. Energy: -817.69046568 a.u.

H	3.762051	2.234734	1.906644
H	2.022054	2.415486	1.574881
C	2.815167	1.700975	1.823524
H	2.574786	1.260891	2.797729
N	2.936046	0.670429	0.796912
C	1.896405	0.024947	0.503552
O	0.701461	0.220175	1.126170
H	3.802394	-0.808108	-1.342163
C	-0.473583	-0.324891	0.567828
C	1.841789	-1.097707	-0.510961
H	-0.396758	-1.979768	1.958833
C	-1.072739	-1.346917	1.392017
H	2.514253	0.048084	-2.207930
O	0.278816	1.661750	-1.112478
H	2.091613	-2.028409	0.013881
C	-1.414359	0.598311	-0.015003
C	-2.429226	-1.507819	1.466987
C	-2.809312	0.410162	0.076124
H	-2.824914	-2.304573	2.090568
N	-0.921094	1.672335	-0.784476
C	-3.327956	-0.641386	0.788258
C	2.772550	-0.882675	-1.694091
O	-1.681733	2.577908	-1.134424
H	-3.448778	1.120823	-0.435045
H	-4.398168	-0.792285	0.856773
N	0.428180	-1.173231	-0.879277
H	0.249888	-0.533760	-1.654912
H	0.006611	-3.139179	-0.295225
H	2.696882	-1.717156	-2.395170
C	-0.114385	-2.500683	-1.171832
H	-1.178429	-2.400148	-1.395184
H	0.398496	-2.949579	-2.026236

(**7**)-MeOH. Energy: -817.69556783 a.u.

N	0.968549	0.900637	-0.303232
C	-0.312514	0.017016	-0.502647
O	0.214895	-1.267107	-0.060285
C	1.570056	-1.324345	-0.106455
C	2.129936	0.004657	-0.568752
C	-1.433303	0.476402	0.348169
C	-2.731236	0.738488	-0.177433
C	-2.993539	0.623341	-1.506414
C	-1.931991	0.205390	-2.385210
C	-0.684471	-0.062623	-1.939881
N	2.262170	-2.331175	0.193857
C	1.538025	-3.535137	0.593951
C	3.395111	0.434567	0.147341
N	-1.212222	0.622102	1.698368
O	-2.145312	0.889234	2.474200
C	0.942426	2.181611	-1.043882
O	-0.032864	0.499571	2.146952
H	2.256011	-4.319880	0.831240
H	0.915744	-3.345073	1.475343
H	0.881494	-3.886713	-0.209455
H	4.156619	-0.329975	-0.013472
H	0.086667	-0.413256	-2.620624
H	3.218816	0.524388	1.222953
H	2.281160	-0.019862	-1.653781
H	-2.140154	0.088721	-3.445077
H	-3.496594	1.041905	0.527463
H	-3.978868	0.833692	-1.903278
H	0.948705	1.078703	0.718745
H	1.006790	1.979152	-2.112514
H	3.764898	1.384093	-0.244089
H	0.004817	2.688911	-0.813027
H	1.785117	2.789540	-0.716815

(**8**)-MeOH. Energy: -817.72048647 a.u.

N	0.963413	1.003307	-0.257325
C	-0.354541	0.709096	-0.735148
O	1.226717	-1.051016	1.441382
C	1.581602	-1.278077	0.152777
C	1.945707	-0.028233	-0.631031
C	-1.455805	0.634990	0.130740
C	-2.736219	0.303413	-0.304125
C	-2.951103	0.065725	-1.655023
C	-1.880150	0.140748	-2.545619
C	-0.602863	0.449356	-2.087115
N	1.651244	-2.437319	-0.350428
C	1.336336	-3.554867	0.534650
C	3.372763	0.392187	-0.272313
N	-1.303684	0.889606	1.565760
O	-1.975720	0.215275	2.331462
C	1.333373	2.395968	-0.532976
O	-0.528531	1.761228	1.924689
H	1.390733	-4.485553	-0.031111
H	2.043662	-3.612062	1.370201
H	0.330338	-3.458168	0.959087
H	4.040829	-0.454997	-0.441582
H	0.222755	0.497511	-2.790322
H	3.447022	0.692922	0.777548
H	1.914758	-0.289817	-1.696517
H	-2.039104	-0.041915	-3.603172
H	-3.543625	0.247749	0.416912
H	-3.947056	-0.175688	-2.009010
H	1.159166	-0.083879	1.557236
H	1.539330	2.572069	-1.599228
H	3.707758	1.219778	-0.900368
H	0.505062	3.033954	-0.221171
H	2.210407	2.670457	0.054253

(**TS-4**)-MeOH. Energy: -817.68281124 a.u.

N	0.631575	0.832621	0.089265
C	-0.723507	0.260620	-0.207821
O	-0.130022	-1.417534	0.445674
C	1.155816	-1.477254	0.244970
C	1.717891	-0.147405	-0.259211
C	-1.830897	0.605735	0.621698
C	-3.154300	0.533262	0.142154
C	-3.406521	0.240805	-1.175504
C	-2.312451	0.025992	-2.043609
C	-1.017496	0.073991	-1.591575
N	1.945303	-2.473621	0.401166
C	1.297748	-3.703739	0.842027
C	3.047592	0.247088	0.353713
N	-1.650956	0.879273	2.010310
O	-2.630469	1.029452	2.727016
C	0.805469	2.185265	-0.514479
O	-0.497210	0.963532	2.470046
H	2.045743	-4.494538	0.926356
H	0.813766	-3.579428	1.819376
H	0.522364	-4.031561	0.137440
H	3.740813	-0.578345	0.188165
H	-0.197424	-0.084521	-2.283410
H	2.952230	0.397408	1.433481
H	1.791213	-0.164965	-1.351465
H	-2.490819	-0.163730	-3.097463
H	-3.959557	0.726901	0.840028
H	-4.423322	0.200197	-1.546057
H	0.625022	0.936769	1.120514
H	0.860266	2.084350	-1.598017
H	3.461053	1.146995	-0.105432
H	-0.050772	2.798567	-0.234935
H	1.722707	2.621115	-0.122339

(**9**)-MeOH. Energy: -817.74350052 a.u.

N	0.584946	1.104179	0.067687
C	-0.730260	0.741803	-0.343240
O	0.519913	-1.297731	1.523735
C	1.070453	-1.253480	0.423925
C	1.581722	0.061436	-0.172576
C	-1.819754	0.902481	0.523198
C	-3.111027	0.500602	0.202549
C	-3.350746	-0.059997	-1.046987
C	-2.291734	-0.232305	-1.937384
C	-1.000713	0.156573	-1.584738
N	1.307286	-2.356324	-0.309511
C	0.945642	-3.675813	0.179094
C	2.909747	0.403148	0.509766
N	-1.620974	1.483132	1.851594
O	-2.180426	0.938096	2.792342
C	0.975562	2.424671	-0.433482
O	-0.935016	2.484417	1.949952
H	1.268192	-4.418377	-0.548952
H	1.431914	-3.872584	1.137906
H	-0.136457	-3.750535	0.316969
H	3.588563	-0.451353	0.445060
H	-0.185421	0.006547	-2.286048
H	2.732741	0.638439	1.562716
H	1.775282	-0.081113	-1.250301
H	-2.469694	-0.672701	-2.913033
H	-3.906944	0.633330	0.926859
H	-4.355353	-0.363126	-1.319317
H	1.735485	-2.266243	-1.219310
H	1.238370	2.399091	-1.503566
H	3.397577	1.252256	0.027791
H	0.143641	3.114282	-0.288078
H	1.827904	2.802023	0.134517

(2)-Tol. Energy: -173.18626947 a.u.

C	-3.071865	0.231856	-1.419101
N	-2.129210	1.312362	-1.191207
C	-1.009650	1.017712	-0.676184
C	0.040723	2.046701	-0.395070
H	-3.997174	0.444903	-0.876035
H	-0.309093	3.035583	-0.694994
H	-3.322982	0.195692	-2.483121
H	0.287036	2.055341	0.671817
H	-2.691156	-0.751805	-1.106854
H	0.961672	1.806170	-0.936315
H	-0.764298	-0.024556	-0.411911

(3)-Tol. Energy: -684.99246692 a.u.

H	-0.917773	1.400656	3.572736
H	-2.242848	2.550486	3.234049
C	-1.232123	2.238747	2.944743
H	-0.238200	-3.120424	0.935781
H	-0.534472	3.061655	3.118581
H	-0.540244	-0.688225	1.211259
H	-3.145567	2.235723	1.248095
C	0.523506	-2.442842	0.562034
N	-1.151504	1.839881	1.548866
C	0.342840	-1.076291	0.713225
C	-2.192148	1.892570	0.822521
H	1.810312	-4.023519	-0.165331
C	1.670602	-2.954795	-0.052500
H	0.299602	1.384202	0.881779
H	-2.883394	0.669323	-0.780757
C	1.299347	-0.156787	0.240110
C	-2.184716	1.496370	-0.618181
O	1.163981	1.155423	0.406532
C	2.633749	-2.072167	-0.514478
H	-2.526219	2.332511	-1.236016
H	-1.185187	1.197960	-0.940208
C	2.439430	-0.697362	-0.384692
H	3.543513	-2.421538	-0.989177
N	3.480988	0.172124	-0.926376
O	3.159903	1.257532	-1.375025
O	4.628262	-0.256501	-0.923765

(4)-Tol. Energy: -817.67445156 a.u.

C	1.820129	-3.050877	0.898822
C	2.455575	-2.193107	0.015983
C	1.915708	-0.931598	-0.235923
C	0.756420	-0.465994	0.413945
C	0.132690	-1.357107	1.307040
C	0.651693	-2.621442	1.538872
N	2.600644	-0.103410	-1.223286
O	1.931065	0.637394	-1.924758
O	0.296232	0.761144	0.197190
C	-2.933190	-0.873558	-0.346245
C	-2.620925	2.244241	1.009160
C	-2.534230	2.497641	-0.459614
O	3.813917	-0.223053	-1.318980
N	-2.096289	-0.894715	-1.161518
C	-1.073381	-0.930690	-2.155039
N	-1.751032	1.570901	1.644339
C	-1.918452	1.365074	3.073894
H	-0.489133	-1.845040	-2.028822
H	-0.418582	-0.064269	-2.033818
H	-3.419586	2.084501	-0.953707
H	-1.011140	1.688110	3.590461
H	0.137200	-3.283796	2.228203
H	-1.533070	-0.923520	-3.144214
H	-0.778194	-1.033062	1.800099
H	2.222828	-4.039571	1.085196
H	-2.054411	0.297339	3.270267
H	-2.780568	1.910045	3.475758
H	-3.484235	2.666108	1.541863
H	3.363468	-2.479726	-0.502687
H	-0.488262	0.999658	0.809422
H	-2.526574	3.575629	-0.649488
H	-1.637084	2.045624	-0.886908

(TS-1)-Tol. Energy: -817.64737285 a.u.

C	6.807273	3.694753	-1.534983
C	5.995793	3.676357	-0.427303
C	5.346479	4.849099	0.016064
C	5.484904	6.121298	-0.657999
C	6.341174	6.062884	-1.825049
C	6.968094	4.916580	-2.237647
N	4.468988	4.708919	1.131035
O	4.102082	5.703947	1.752873
O	4.902224	7.196799	-0.347402
C	1.956393	6.030336	-0.869296
C	1.842632	7.845161	-0.286492
C	2.409839	8.543176	-1.495946
O	4.072841	3.573276	1.436250
N	2.338435	4.979626	-1.164408
C	2.793284	3.682615	-1.562482
N	2.497802	7.929527	0.875543
C	1.852234	7.425822	2.077671
H	3.075440	3.128887	-0.664636
H	3.663356	3.808393	-2.209272
H	1.865587	8.254602	-2.396870
H	2.488051	7.632795	2.937333
H	7.604868	4.944728	-3.118424
H	1.983567	3.181179	-2.092967
H	6.467820	6.997853	-2.362942
H	7.323170	2.797302	-1.856671
H	1.704823	6.339574	2.019267
H	0.889873	7.925596	2.212742
H	0.757670	7.879803	-0.189012
H	5.841168	2.764789	0.139544
H	3.510853	7.763997	0.793909
H	2.280867	9.617644	-1.335965
H	3.472462	8.316838	-1.597453

(6)-Tol. Energy: -817.70246921 a.u.

C	-2.712727	-0.071174	0.140159
C	-3.181424	-0.999613	1.063289
C	-2.321549	-1.490183	2.044058
C	-0.999407	-1.057559	2.097892
C	-0.517251	-0.124221	1.183269
C	-1.396641	0.372451	0.211199
O	0.774418	0.297813	1.331484
C	1.772458	-0.041243	0.425552
N	2.837897	0.625735	0.394332
C	2.935400	1.804535	1.245064
N	-0.970523	1.368601	-0.777324
O	-0.024097	2.084737	-0.506684
C	1.506952	-1.233112	-0.472207
C	2.800883	-1.889554	-0.945297
N	0.634297	-0.763976	-1.549281
C	-0.163546	-1.803813	-2.182284
O	-1.612774	1.439275	-1.811514
H	3.842114	2.352258	0.986832

H	2.064058	2.455602	1.117912
H	2.990727	1.517274	2.301366
H	3.383741	-2.269090	-0.102018
H	-0.310149	-1.432516	2.847403
H	3.415489	-1.160261	-1.478528
H	0.922000	-1.959774	0.108826
H	-2.675800	-2.215586	2.769017
H	-3.351573	0.324392	-0.640569
H	-4.211087	-1.335313	1.013940
H	1.184344	-0.247877	-2.232062
H	-0.872723	-2.200378	-1.445404
H	2.569008	-2.723989	-1.612927
H	-0.742441	-1.360129	-2.995634
H	0.419959	-2.644857	-2.586196

(TS-3)-Tol. Energy: -817.68035599 a.u.

C	-2.871202	0.428314	0.108196
C	-3.340610	-0.592834	0.896330
C	-2.393860	-1.423084	1.552859
C	-1.046334	-1.260115	1.387752
C	-0.498200	-0.262971	0.489672
C	-1.489041	0.616067	-0.085035
O	0.670269	0.363265	0.997874
C	1.875083	-0.024347	0.502108
N	2.964960	0.528895	0.796469
C	2.908172	1.662388	1.713471
N	-1.054780	1.662140	-0.935615
O	0.120546	1.635748	-1.345379
C	1.747077	-1.220680	-0.417967
C	2.782538	-1.238353	-1.529144
N	0.361911	-1.117294	-0.884191
C	-0.317794	-2.351337	-1.274445
O	-1.842614	2.541767	-1.271550
H	3.902470	2.100602	1.798693
H	2.207000	2.424286	1.355551
H	2.576325	1.344718	2.708328
H	3.781349	-1.249732	-1.090189
H	-0.334848	-1.857294	1.951572
H	2.692935	-0.335440	-2.140224
H	1.812706	-2.132525	0.190239
H	-2.743242	-2.190202	2.238724
H	-3.542489	1.120416	-0.387933
H	-4.403134	-0.740064	1.043902
H	0.314378	-0.411474	-1.624303
H	-0.282376	-3.054573	-0.440465
H	2.659904	-2.121854	-2.160654
H	-1.361519	-2.115847	-1.495458
H	0.154786	-2.794632	-2.154312

(7)-Tol. Energy: -817.68302511 a.u.

C	-2.838395	0.429471	0.252567
C	-3.191428	-0.480942	1.203241
C	-2.180067	-1.363138	1.710135
C	-0.896216	-1.324540	1.279303
C	-0.419975	-0.335980	0.282399
C	-1.512739	0.501302	-0.247896
O	0.666834	0.463868	0.842426
C	1.892105	-0.044996	0.563823
N	2.985705	0.397745	0.998674
C	2.921878	1.543764	1.900919
N	-1.220392	1.419723	-1.246603
O	-0.079576	1.379229	-1.798534
C	1.762154	-1.232173	-0.369564
C	2.809359	-1.269253	-1.466213
N	0.381071	-1.033520	-0.879914
C	-0.290185	-2.215894	-1.450450
O	-2.060011	2.242382	-1.614215
H	3.926299	1.771674	2.257200
H	2.522550	2.421482	1.380925
H	2.272566	1.342541	2.760048
H	3.794859	-1.292005	-0.998182
H	-0.142901	-1.974699	1.717124
H	2.748345	-0.368371	-2.083495
H	1.767135	-2.161055	0.212912
H	-2.444370	-2.084496	2.478941
H	-3.558427	1.122352	-0.167773
H	-4.207000	-0.540325	1.573271
H	0.405682	-0.249184	-1.573992
H	-0.306319	-3.013783	-0.707172
H	2.695764	-2.154587	-2.095879
H	-1.311816	-1.935680	-1.712164
H	0.251321	-2.532544	-2.341906

(TS-4)-Tol. Energy: -817.67014966 a.u.

N	0.624611	0.827567	0.094384
C	-0.735374	0.288679	-0.220994
O	-0.130458	-1.423439	0.483607
C	1.143681	-1.489177	0.244858
C	1.704442	-0.155674	-0.263477
C	-1.839174	0.636840	0.603951
C	-3.158856	0.535815	0.134136
C	-3.410733	0.217018	-1.180632
C	-2.320565	0.000057	-2.045455
C	-1.022626	0.073373	-1.595285
N	1.948757	-2.477835	0.362811
C	1.326537	-3.715221	0.815650
C	3.037894	0.228069	0.349011
N	-1.659640	0.954118	1.993505
O	-2.637256	1.068825	2.709702
C	0.819404	2.192441	-0.465417
O	-0.507329	1.122319	2.430275
H	2.084299	-4.499412	0.870458
H	0.871319	-3.598628	1.807601
H	0.529839	-4.042452	0.134895
H	3.707286	-0.622193	0.212053
H	-0.202047	-0.103443	-2.282176
H	2.937705	0.400903	1.425538
H	1.774696	-0.168624	-1.356335
H	-2.499137	-0.218482	-3.093816
H	-3.963509	0.728486	0.833137
H	-4.428627	0.154091	-1.545175
H	0.598756	0.909870	1.130324
H	0.865202	2.127626	-1.552805
H	3.479752	1.108464	-0.123551
H	-0.024620	2.812797	-0.163203
H	1.746619	2.600519	-0.065494

(8)-Tol. Energy: -817.71360404 a.u.

N	0.970388	0.958574	-0.216976
C	-0.342101	0.611632	-0.647912
O	1.161581	-1.337118	1.250186
C	1.636220	-1.358840	-0.020427
C	2.017108	-0.005531	-0.587727
C	-1.481849	0.893314	0.133634
C	-2.769199	0.550446	-0.272825
C	-2.960395	-0.089892	-1.488616
C	-1.851557	-0.412262	-2.268527
C	-0.569563	-0.072749	-1.849627
N	1.801186	-2.425428	-0.677835
C	1.457170	-3.670778	-0.000870
C	3.374172	0.415369	-0.013825
N	-1.377333	1.502109	1.465362
O	-2.237504	1.206590	2.281705
C	1.316856	2.350518	-0.540672
O	-0.451394	2.260812	1.697494
H	1.629126	-4.505367	-0.681330
H	2.065204	-3.817650	0.899304
H	0.405564	-3.676520	0.309025

H	4.088484	-0.395290	-0.173001
H	0.276183	-0.346007	-2.469465
H	3.301910	0.618087	1.059423
H	2.129299	-0.123879	-1.674214
H	-1.980928	-0.930289	-3.213215
H	-3.601793	0.784199	0.379790
H	-3.961646	-0.348103	-1.814133
H	1.048741	-0.409484	1.519751
H	1.669236	2.434850	-1.580166
H	3.757484	1.307170	-0.513303
H	0.438369	2.979256	-0.412343
H	2.090100	2.711956	0.138598

(9)-Tol. Energy: -817.73116870 a.u.

O	2.309917	-0.140795	-2.912318
O	1.239717	1.684306	-2.486779
N	1.774316	0.644345	-2.146560
H	-2.619247	-3.636834	-0.151352
H	-2.680584	0.649738	-1.885340
H	3.805390	-0.430095	-0.946668
C	1.816178	0.317049	-0.718059
C	-2.170327	-3.301091	0.786938
H	-2.749569	-3.688248	1.624700
C	2.991034	-0.260128	-0.251413
O	-0.950843	-1.633533	-1.040311
H	-2.637936	-1.382139	1.610233
C	-2.919786	0.809589	-0.830743
N	-2.161972	-1.850087	0.854123
C	-1.549542	-1.118815	-0.106468
H	-1.150667	-3.691982	0.838398
H	-3.790325	0.202893	-0.566720
N	-0.506423	1.067525	-0.427622
H	-3.183660	1.857418	-0.675373
C	0.700444	0.539038	0.102728
C	-1.718226	0.398886	0.027987
H	0.401262	2.945613	-0.571845
H	-1.284405	2.912783	-1.079494
C	-0.577717	2.527568	-0.342109
C	3.091197	-0.614118	1.088736
H	4.007950	-1.053636	1.465494
H	-1.947603	0.642779	1.083331
C	0.825839	0.152791	1.442657
H	-0.884448	2.860761	0.664229
C	2.001608	-0.409781	1.932764
H	-0.017917	0.296218	2.110905
H	2.065657	-0.688940	2.97974

Ugi reaction in methanol

(3′)-MeOH. Energy: -402.21573515 a.u.

C	-0.538017	2.785174	4.734330
C	-0.714081	2.712841	3.240163
O	0.012942	1.763775	2.675875
O	-1.453207	3.453074	2.608178
N	-0.364896	1.682380	0.082761
C	-0.593306	2.950998	-0.592033
C	-0.404730	0.601328	-0.583151
C	-0.183130	-0.737025	0.041169
H	-1.421753	3.463238	-0.097836
H	-0.812888	2.821319	-1.657663
H	0.296258	3.576808	-0.478518
H	-0.608728	0.626364	-1.661578
H	-0.145412	1.744815	1.650520
H	-1.058653	-1.372364	-0.123989
H	0.667388	-1.232318	-0.437114
H	0.003976	-0.646995	1.112517
H	-1.135113	3.598676	5.142706
H	-0.843987	1.836468	5.182419
H	0.517321	2.937856	4.972331

(4′)-MeOH. Energy: -534.89591773 a.u.

O	0.954860	-1.089443	1.458567
C	0.252716	-0.517078	2.280162
H	0.915188	-1.687107	3.944705
O	-0.565997	0.471104	1.966452
H	1.788087	1.177790	0.362308
C	0.234077	-0.861614	3.745606
H	-0.781383	-1.133280	4.043889
H	0.145693	-1.387597	-0.691071
H	2.423618	0.887408	-1.275927
C	1.781497	1.534798	-0.668581
H	-0.532862	0.683921	0.951893
H	0.526928	0.014388	4.329569
C	-0.098508	-0.684835	-3.734313
H	2.201213	2.543933	-0.720515
H	0.638281	-2.845343	-1.595520
C	-0.103023	-2.048261	-1.526429
C	0.400813	1.526856	-1.233920
N	-0.607764	1.124932	-0.572778
N	-0.099683	-1.300998	-2.742568
H	-1.092944	-2.482192	-1.377982
H	0.276791	1.869844	-2.268901
H	-2.288448	0.083462	-1.232286
C	-1.915681	1.112542	-1.210320
H	-2.612019	1.705779	-0.612034
H	-1.884664	1.505052	-2.233045

(TS-1′)-MeOH. Energy: -534.86654214 a.u.

O	0.461336	-0.316875	1.201998
C	0.207388	0.477276	2.139247
H	0.757201	-1.008935	3.630876
O	-0.288578	1.637734	1.991405
H	1.919950	1.637207	0.151812
C	0.531978	0.056533	3.571046
H	-0.301557	0.300864	4.233925
H	0.215375	-2.260621	-0.094743
H	2.695882	1.874877	-1.440615
C	1.887894	2.199492	-0.784300
H	-0.447876	1.940880	0.326467
H	1.402473	0.622786	3.917582
C	0.632339	0.165600	-1.861255
H	2.009642	3.264859	-0.570800
H	1.181004	-2.883982	-1.476957
C	0.310081	-2.299733	-1.181428
C	0.547636	2.011835	-1.449353
N	-0.535509	2.185295	-0.689372
N	0.486449	-0.954307	-1.619935
H	-0.589684	-2.706659	-1.641831
H	0.458795	2.364959	-2.474965
H	-2.110142	1.044564	-1.506716
C	-1.857317	2.089704	-1.277370
H	-2.593269	2.480514	-0.574435
H	-1.903066	2.672445	-2.200731

(5′)-MeOH. Energy: -534.87856971 a.u.

O	0.298301	-0.588174	1.108285
C	0.041050	0.097573	2.135922

H	0.412130	-1.630349	3.412128
O	-0.345304	1.299381	2.125174
H	1.786326	1.288629	0.171470
C	0.223275	-0.560052	3.503766
H	-0.663354	-0.389727	4.119758
H	0.052924	-3.332233	-0.524826
H	2.567556	1.040059	-1.414354
C	1.737424	1.521800	-0.893760
H	-0.589836	1.556825	0.251765
H	1.070151	-0.090049	4.013383
C	0.326761	-0.441096	-1.411996
H	1.803551	2.601557	-1.037599
H	1.020303	-3.407695	-2.033120
C	0.129127	-2.998077	-1.559361
C	0.389217	1.064118	-1.447010
N	-0.705112	1.686601	-0.762759
N	0.237654	-1.575436	-1.551933
H	-0.761091	-3.272698	-2.123310
H	0.325634	1.279847	-2.522945
H	-2.219271	0.182591	-1.020057
C	-2.026136	1.252725	-1.198995
H	-2.781926	1.826153	-0.659333
H	-2.148520	1.449570	-2.268904

(TS-2')-MeOH. Energy: -534.87612424 u.a

C	-0.007707	-0.578668	3.362516
C	0.118116	-0.025774	1.947774
O	-0.075788	1.193381	1.753608
O	0.445235	-0.878978	1.055527
C	0.880858	-0.960462	-0.994853
N	0.659406	-2.064640	-1.286359
C	0.251648	-3.420081	-1.081220
C	1.288307	0.458915	-1.303400
N	0.221160	1.403530	-1.123453
C	-0.996088	1.085092	-1.861344
C	2.524086	0.841651	-0.496822
H	-0.523896	0.128138	4.012810
H	2.262115	0.924182	0.559572
H	0.997238	-0.756079	3.758102
H	-0.196595	-3.504291	-0.090577
H	3.320833	0.104283	-0.617156
H	0.029065	1.479698	-0.117821
H	-0.532441	-1.536062	3.352075
H	2.876318	1.809307	-0.858864
H	1.131903	-4.057850	-1.159307
H	-0.463304	-3.691484	-1.856843
H	1.539987	0.396303	-2.371462
H	-1.459127	0.131997	-1.559279
H	-1.725996	1.880947	-1.702396
H	-0.776369	1.033107	-2.932572

(6')-MeOH. Energy: -534.92142778 a.u.

C	-0.023891	-0.685403	3.251238
C	-0.383939	-0.933569	1.817966
O	-1.448973	-1.318769	1.402190
O	0.669678	-0.664016	0.999325
C	0.547656	-0.897118	-0.382501
N	0.431588	-2.038037	-0.897017
C	0.375596	-3.231626	-0.068834
C	0.661546	0.389968	-1.175833
N	-0.424780	1.323925	-0.911400
C	-1.750127	0.816460	-1.263600
C	2.005065	1.064039	-0.902846
H	-0.908771	-0.800219	3.873827
H	2.066879	1.388381	0.140390
H	0.393696	0.317459	3.360014
H	0.850108	-3.108257	0.911413
H	2.833747	0.379030	-1.101134
H	-0.399076	1.618879	0.062504
H	0.742407	-1.403297	3.555462
H	2.107071	1.940009	-1.547029
H	0.867340	-4.046818	-0.601950
H	-0.672031	-3.508013	0.084088
H	0.601496	0.095538	-2.229224
H	-2.026020	-0.111229	-0.743675
H	-2.496029	1.580104	-1.032367
H	-1.780240	0.629168	-2.341541

(7'-MeOH). Energy: -766.29447580 a.u.

C	-0.018757	-0.123472	-0.032553
C	-0.147309	-0.070410	1.460233
N	2.405253	0.064909	1.651659
C	2.502109	-1.369035	1.425138
C	3.706661	-2.049189	2.082250
O	-0.699053	0.840012	2.045029
C	1.201951	-2.035825	1.869039
O	0.146492	-1.186727	2.184988
N	1.086965	-3.279380	2.018756
C	-0.190692	-3.837286	2.438959
C	3.336405	0.861136	0.864779
O	-0.613860	0.260542	4.779132
C	-1.501146	-0.829484	5.002754
O	1.932596	-0.755577	4.478912
C	2.641614	-0.554639	5.688916
H	-2.545185	-0.500664	4.974442
H	-1.284453	-1.230007	5.994831
H	-1.349485	-1.618388	4.257435
H	-0.729192	0.563825	3.857684
H	-1.027199	-0.245190	-0.439586
H	0.599946	-0.947700	-0.382508
H	0.384705	0.826430	-0.383609
H	-0.259506	-4.866046	2.082223
H	-0.233054	-3.860013	3.533672
H	-1.050659	-3.266675	2.074131
H	2.578744	-1.517259	0.338449
H	3.634383	-1.944704	3.168238
H	4.629852	-1.579224	1.732606
H	3.737578	-3.109898	1.827725
H	3.195729	1.916910	1.106560
H	4.394506	0.609322	1.027734
H	3.116104	0.725119	-0.199818
H	2.507236	0.238596	2.651666
H	1.022159	-0.411917	4.591140
H	2.710806	0.508867	5.947604
H	2.175602	-1.090787	6.524403
H	3.653308	-0.943857	5.550586

(TS-3')-MeOH. Energy: -766.29290256 a.u.

H	-0.817302	2.323911	3.856173
H	0.149605	3.621204	3.115147
H	0.935665	2.100217	3.626850
C	0.027719	2.538788	3.201141
O	-0.264260	1.972430	1.922077
H	-0.369469	0.493807	1.989437
O	-0.277227	-0.518641	2.182039
C	-0.199489	-1.335964	1.168745
C	0.252870	-2.708583	1.578184
H	1.128235	-2.605756	2.218009
H	0.494201	-3.354169	0.738047
H	-0.560211	-3.161088	2.154454
O	1.454589	-0.835834	0.173140
C	1.129941	-1.202823	-1.038548
N	1.874257	-1.216871	-2.085242
C	3.253082	-0.797454	-1.863604
H	3.820572	-0.910123	-2.789916
H	3.321414	0.254836	-1.553829
H	3.740296	-1.392860	-1.080044
C	-0.330157	-1.707454	-1.132706

H	-0.307174	-2.797417	-1.044729
C	-1.022246	-1.368144	-2.441581
H	-0.988480	-0.297911	-2.659380
H	-2.061987	-1.705561	-2.432585
H	-0.494257	-1.886606	-3.242645
N	-0.992723	-1.170987	0.069674
C	-1.659031	0.121832	-0.084097
H	-2.150060	0.390056	0.850867
H	-0.958648	0.921644	-0.362557
H	-2.421556	0.032135	-0.855601
H	1.836851	0.856352	0.278319
O	1.780101	1.840735	0.305284
H	0.519022	2.086725	1.315997
C	1.603400	2.334817	-1.021190
H	1.098700	1.594716	-1.653286
H	0.990937	3.237790	-0.971768
H	2.569474	2.585588	-1.469705

(8′)-MeOH. Energy: -766.32835871 a.u.

H	-1.976327	3.478640	3.156574
H	-0.292435	3.906712	2.776151
H	-0.653421	2.350785	3.563936
C	-1.008448	3.085447	2.832560
O	-1.101591	2.510976	1.530844
H	-1.683156	1.724626	1.573413
O	-2.030364	-0.039130	1.655781
C	-1.225070	-0.779726	1.063170
C	-0.462362	-1.837951	1.822664
H	0.591184	-1.551213	1.892206
H	-0.526912	-2.819944	1.348972
H	-0.880780	-1.891517	2.826340
O	1.313767	0.449628	-1.468729
C	0.706608	-0.624644	-1.994045
N	0.798863	-0.928715	-3.223759
C	1.622493	-0.048464	-4.044159
H	1.634298	-0.421379	-5.069306
H	1.231778	0.976307	-4.047651
H	2.653846	-0.001673	-3.674433
C	-0.092176	-1.491639	-1.028328
H	0.638101	-1.898128	-0.321892
C	-0.828227	-2.635055	-1.715323
H	-1.559126	-2.249078	-2.430440
H	-1.349660	-3.234401	-0.964573
H	-0.125295	-3.268919	-2.257422
N	-1.012343	-0.640237	-0.262583
C	-1.822639	0.333026	-0.994103
H	-2.868789	0.245318	-0.696501
H	-1.482685	1.355067	-0.795761
H	-1.731437	0.133835	-2.062735
H	1.155718	0.583639	-0.487474
O	1.122514	1.055754	1.052743
H	0.335522	1.632543	1.205320
C	2.300048	1.788730	1.385572
H	2.375604	2.705691	0.792106
H	2.307901	2.042215	2.449839
H	3.158108	1.151373	1.166613

(9′)-MeOH. Energy: -534.96789924 a.u.

C	0.027465	-2.354078	2.276456
N	-0.072561	-1.492380	1.112566
C	-0.569633	-1.943624	-0.052993
C	-0.519043	-0.923145	-1.202524
N	0.875787	-0.767058	-1.640445
C	1.629039	0.210046	-1.075661
O	1.191507	0.907214	-0.148830
O	-1.008415	-3.085721	-0.199294
C	-1.444037	-1.309835	-2.345552
C	3.026795	0.430381	-1.607718
H	0.452514	-1.781015	3.099253
H	0.667500	-3.216692	2.069366
H	-0.960837	-2.719627	2.566925
H	-2.476113	-1.302411	-1.988340
H	-1.230317	-2.311304	-2.722913
H	-0.818493	0.048537	-0.803482
H	-1.351901	-0.587462	-3.160457
H	0.314512	-0.554461	1.130911
H	3.695648	-0.364178	-1.263336
H	3.384655	1.379783	-1.212567
H	3.052928	0.451929	-2.699112
C	1.401000	-1.759073	-2.573952
H	2.488174	-1.758393	-2.556156
H	1.061598	-2.752940	-2.268663
H	1.059378	-1.566137	-3.595072

Ugi reaction in toluene

(3′)-Tol. Energy: -402.21070376 a.u.

C	-0.554769	2.814264	4.736656
C	-0.689747	2.730567	3.238197
O	-0.003926	1.723620	2.714565
O	-1.356130	3.503238	2.572352
N	-0.356927	1.663298	0.081363
C	-0.611066	2.940795	-0.564058
C	-0.405735	0.594139	-0.599824
C	-0.165060	-0.752901	0.001529
H	-1.433005	3.434501	-0.041098
H	-0.847031	2.830251	-1.629460
H	0.273002	3.574267	-0.450449
H	-0.634149	0.633420	-1.674412
H	-0.134109	1.709378	1.699526
H	-1.040692	-1.391559	-0.151143
H	0.679602	-1.239566	-0.496109
H	0.041701	-0.671648	1.069974
H	-1.129212	3.658796	5.113039
H	-0.911841	1.885127	5.187542
H	0.499077	2.926425	5.002896

(4′)-Tol. Energy: -534.89039709 a.u.

O	0.693592	-1.043332	1.633845
C	0.057774	-0.317493	2.382043
H	0.582280	-1.375715	4.164213
O	-0.646130	0.719652	1.961683
H	1.766679	0.591598	0.106069
C	-0.003710	-0.505191	3.875014
H	-1.044109	-0.629869	4.184834
H	0.201626	-1.460920	-0.552701
H	2.242296	0.267921	-1.581342
C	1.781978	0.999031	-0.906677
H	-0.584386	0.820322	0.941716
H	0.381944	0.389694	4.369760
C	-0.462472	-0.956341	-3.572813
H	2.401975	1.900433	-0.942141
H	1.158521	-2.641577	-1.487828
C	0.175724	-2.181106	-1.375353
C	0.401099	1.305193	-1.383620
N	-0.625401	1.155647	-0.650053
N	-0.173294	-1.516895	-2.588992

H	-0.565567	-2.952748	-1.163070
H	0.289590	1.649562	-2.420405
H	-2.521000	0.496807	-1.201620
C	-1.938297	1.422771	-1.216877
H	-2.457699	2.155500	-0.593831
H	-1.881505	1.789939	-2.248285

(TS-1′)-Tol. Energy: -534.85560318 a.u.

O	0.763777	-0.256548	1.150898
C	0.306711	0.463555	2.071175
H	0.926130	-0.985315	3.568674
O	-0.269149	1.581623	1.901475
H	1.979498	1.605392	0.064383
C	0.444464	-0.008300	3.516135
H	-0.544466	-0.054104	3.980677
H	0.410882	-2.137819	0.019205
H	2.704759	1.877898	-1.547878
C	1.913629	2.183081	-0.860884
H	-0.391834	1.931510	0.346393
H	1.032071	0.722385	4.078959
C	0.596067	0.197949	-1.855549
H	2.023890	3.246627	-0.634758
H	1.067049	-2.875793	-1.491831
C	0.297836	-2.233215	-1.063814
C	0.550362	1.983186	-1.484098
N	-0.505031	2.190486	-0.681547
N	0.451708	-0.915136	-1.586168
H	-0.692581	-2.603240	-1.328530
H	0.434178	2.356086	-2.502454
H	-2.091865	1.061087	-1.499896
C	-1.840066	2.099168	-1.230528
H	-2.557414	2.443139	-0.484991
H	-1.932180	2.722609	-2.125497

(6′)-Tol. Energy: -534.91625572 a.u.

O	1.694999	-1.182108	1.025704
C	1.264109	-1.238858	-0.097227
H	2.440477	-2.878641	-0.767650
O	0.283730	-0.410063	-0.552414
H	-1.379273	-1.785549	1.117059
C	1.701037	-2.190412	-1.172107
H	2.129576	-1.623870	-2.003066
H	2.512930	1.387720	1.003666
H	-1.033146	-0.758442	2.518868
C	-1.689662	-0.882094	1.654414
H	-2.306691	-0.710435	-0.862595
H	0.837665	-2.740032	-1.553430
C	-0.190461	0.593806	0.319204
H	-2.717310	-1.022915	1.996260
H	2.054010	2.828877	0.082112
C	1.852680	1.765030	0.216716
C	-1.623207	0.338595	0.739806
N	-2.527766	0.161639	-0.387877
N	0.476263	1.603929	0.650115
H	2.084003	1.235190	-0.715437
H	-1.933081	1.233875	1.289637
H	-1.527551	1.440859	-1.806908
C	-2.509465	1.267455	-1.338844
H	-3.240180	1.076372	-2.127728
H	-2.801120	2.186462	-0.821289

(7′)-Tol. Energy: -763.92912583 a.u.

N	-0.077252	-1.468506	-0.148647
C	0.960627	-0.641009	-2.325427
C	-0.379592	-0.668860	-3.000846
O	1.878495	-1.357476	-2.599401
C	-0.440163	-0.097997	0.173600
C	0.673205	0.797296	-0.341114
O	1.232257	0.492010	-1.541611
N	1.098632	1.807164	0.298855
C	2.158036	2.605069	-0.312587
C	-1.166231	-2.429013	-0.052421
C	-0.809610	0.177488	1.630286
O	2.256210	1.207646	2.681105
C	2.688370	-0.045497	2.564006
C	3.678612	-0.418914	3.632015
O	2.307546	-0.801852	1.688040
H	3.055350	1.998431	-0.480000
H	1.843176	3.008455	-1.280034
H	2.403265	3.431450	0.355341
H	-0.269353	-0.164486	-3.966186
H	1.658407	1.433507	1.909676
H	-0.658507	-1.707395	-3.178612
H	0.721382	-1.745277	0.421580
H	3.991328	-1.452779	3.498686
H	4.542753	0.247315	3.576247
H	-1.155144	-0.158027	-2.433601
H	-0.004901	-0.139008	2.297299
H	3.221179	-0.285388	4.615359
H	-1.323777	0.145550	-0.436271
H	-0.810187	-3.406014	-0.386448
H	-1.007246	1.239555	1.789000
H	-1.976952	-2.117707	-0.721459
H	-1.712004	-0.383426	1.886426
H	-1.582288	-2.539641	0.958947

(TS-3′)-Tol. Energy: -763.92236158 a.u.

C	-2.205375	-0.215355	-0.853111
N	-1.276626	-0.873043	0.203807
C	-1.929516	-2.085473	0.759852
O	-2.006817	-0.574116	-1.981513
C	-0.773071	0.095264	1.234425
C	-0.298110	1.260869	0.362838
O	-1.145012	1.560981	-0.535042
C	-3.508673	0.311130	-0.323130
N	0.868224	1.791115	0.590775
C	1.210921	2.901640	-0.293528
C	0.209080	-0.532932	2.205751
O	2.843004	0.208296	0.371567
C	2.552896	-0.800054	-0.408655
C	3.762360	-1.526626	-0.936871
O	1.405042	-1.146772	-0.691514
H	1.218414	2.589475	-1.345630
H	0.487912	3.719082	-0.200884
H	2.201845	3.273560	-0.025206
H	-3.825464	1.109517	-0.993603
H	1.986990	0.821203	0.591918
H	-4.248995	-0.494627	-0.358988
H	-0.437380	-1.150081	-0.341323
H	3.457362	-2.404645	-1.503495
H	4.332360	-0.849186	-1.577911
H	-3.435743	0.706088	0.688737
H	0.983221	-1.101244	1.688175
H	4.409581	-1.813270	-0.104776
H	-1.654129	0.446162	1.783846
H	-2.328563	-2.673614	-0.067194
H	0.692595	0.271823	2.762838
H	-2.731742	-1.779123	1.433578
H	-0.302476	-1.185624	2.917437
H	-1.189285	-2.671241	1.303139

(8′)-Tol. Energy: -763.97036590 a.u.

C	-1.779697	0.080606	-0.514461
N	-1.179331	-0.398751	0.663608
C	-1.582133	-1.746017	1.105846
O	-2.009883	1.267424	-0.650111
C	-1.072522	0.616672	1.734936
C	-0.200407	1.827509	1.374051
O	-0.294012	2.832903	2.070904
C	-2.075709	-0.915412	-1.610872

N	0.723971	1.699864	0.398193
C	1.527210	2.854824	0.031827
C	-0.497064	0.033260	3.027470
O	1.198490	-0.278686	-1.795200
C	1.733320	-1.227893	-1.253226
C	2.890211	-2.002145	-1.809845
O	1.321873	-1.686674	-0.066821
H	0.900906	3.671311	-0.342069
H	2.077185	3.215061	0.903172
H	2.231263	2.551440	-0.743459
H	-2.229251	-0.350594	-2.528985
H	0.600766	0.995946	-0.320026
H	-1.255260	-1.623083	-1.751466
H	0.560266	-1.131843	0.223262
H	3.731295	-1.943669	-1.114748
H	2.613040	-3.054487	-1.906226
H	-2.987434	-1.475827	-1.382358
H	0.476224	-0.437150	2.848800
H	3.172430	-1.594634	-2.778280
H	-2.067888	1.033873	1.932561
H	-1.628700	-2.416473	0.249934
H	-0.359122	0.853770	3.733063
H	-2.561329	-1.726133	1.599599
H	-1.168282	-0.697101	3.483067
H	-0.843657	-2.148634	1.798886

(9′)-Tol. Energy: -534.96110188 a.u.

C	0.022391	-2.342269	2.274898
N	-0.112628	-1.466630	1.125943
C	-0.544862	-1.940384	-0.060795
C	-0.517460	-0.910404	-1.201810
N	0.872463	-0.758613	-1.658565
C	1.642562	0.198108	-1.073449
O	1.219122	0.884145	-0.137606
O	-0.901398	-3.103142	-0.233028
C	-1.457350	-1.301230	-2.331074
C	3.043865	0.407976	-1.605281
H	0.285374	-1.741034	3.144776
H	0.796439	-3.098419	2.109276
H	-0.921872	-2.857608	2.464442
H	-2.485265	-1.286327	-1.961957
H	-1.254812	-2.310608	-2.693280
H	-0.807146	0.062272	-0.798286
H	-1.371661	-0.588851	-3.155830
H	0.255917	-0.521517	1.150481
H	3.704919	-0.396954	-1.269583
H	3.409341	1.348744	-1.196966
H	3.071146	0.443168	-2.696509
C	1.383039	-1.758952	-2.589247
H	2.470811	-1.755775	-2.590869
H	1.049079	-2.750804	-2.269962
H	1.025133	-1.576538	-3.607309

Mumm rearrangement with explicit solvation of methanol

(7′-MeOH). Energy: -766.29447580 a.u.

C	-0.018757	-0.123472	-0.032553
C	-0.147309	-0.070410	1.460233
N	2.405253	0.064909	1.651659
C	2.502109	-1.369035	1.425138
C	3.706661	-2.049189	2.082250
O	-0.699053	0.840012	2.045029
C	1.201951	-2.035825	1.869039
O	0.146492	-1.186727	2.184988
N	1.086965	-3.279380	2.018756
C	-0.190692	-3.837286	2.438959
C	3.336405	0.861136	0.864779
O	-0.613860	0.260542	4.779132
C	-1.501146	-0.829484	5.002754
O	1.932596	-0.755577	4.478912
C	2.641614	-0.554639	5.688916
H	-2.545185	-0.500664	4.974442
H	-1.284453	-1.230007	5.994831
H	-1.349485	-1.618388	4.257435
H	-0.729192	0.563825	3.857684
H	-1.027199	-0.245190	-0.439586
H	0.599946	-0.947700	-0.382508
H	0.384705	0.826430	-0.383609
H	-0.259506	-4.866046	2.082223
H	-0.233054	-3.860013	3.533672
H	-1.050659	-3.266675	2.074131
H	2.578744	-1.517259	0.338449
H	3.634383	-1.944704	3.168238
H	4.629852	-1.579224	1.732606
H	3.737578	-3.109898	1.827725
H	3.195729	1.916910	1.106560
H	4.394506	0.609322	1.027734
H	3.116104	0.725119	-0.199818
H	2.507236	0.238596	2.651666
H	1.022159	-0.411917	4.591140
H	2.710806	0.508867	5.947604
H	2.175602	-1.090787	6.524403
H	3.653308	-0.943857	5.550586

(TS-4′)-MeOH. Energy: -766.29411914 a.u.

H	2.634519	-3.118157	1.840365
H	1.933124	-2.114423	3.129418
H	2.384352	-1.368992	1.575996
C	1.975747	-2.268479	2.049733
O	0.651643	-2.525721	1.598172
H	0.660045	-2.530776	0.619045
O	0.660854	-2.170899	-1.138698
C	0.806578	-0.989414	-1.401200
C	1.095067	-0.494811	-2.788878
H	2.122597	-0.787000	-3.028695
H	1.014165	0.587409	-2.882229
H	0.419984	-0.986344	-3.489699
O	1.153527	-0.154331	-0.353169
C	0.683597	1.141684	-0.282742
N	1.309472	2.027125	0.357527
C	2.583316	1.674086	0.970738
H	3.141330	2.587208	1.181984
H	2.404559	1.158301	1.921397
H	3.189327	1.016551	0.338484
C	-0.657719	1.389427	-0.964284
H	-0.450524	1.892937	-1.918760
C	-1.552861	2.300734	-0.124829
H	-1.739437	1.834273	0.845478
H	-2.503319	2.460768	-0.641375
H	-1.075286	3.269416	0.031702
N	-1.224423	0.088139	-1.281699
C	-2.197249	0.078834	-2.364685
H	-2.526008	-0.948023	-2.540160
H	-3.081856	0.698294	-2.164254
H	-1.720351	0.447912	-3.278649
H	-1.591301	-0.329439	-0.424112
O	-1.057435	-0.376745	1.633963

H	-0.409532	-1.109994	1.692875
C	-2.052294	-0.567649	2.624994
H	-2.565511	-1.529170	2.504613
H	-1.630571	-0.515791	3.635595
H	-2.788114	0.233048	2.516044

(10′)-MeOH. Energy: -766.30420241 a.u.

H	-3.723101	-1.859814	0.120897
H	-3.044073	-2.441263	-1.414405
H	-2.696912	-0.783322	-0.862481
C	-2.847840	-1.819497	-0.537855
O	-1.695193	-2.323015	0.117748
H	-1.408154	-1.665881	0.829977
O	-0.811125	-0.653925	1.858622
C	-0.296299	0.430743	1.410188
C	-0.294779	1.621186	2.359469
H	-1.340205	1.869592	2.552209
H	0.202431	2.505453	1.952437
H	0.173509	1.338297	3.304232
O	-0.899368	0.865867	0.122991
C	0.006635	1.391106	-0.730451
N	-0.260937	1.934320	-1.838357
C	-1.671831	2.026120	-2.200844
H	-1.777250	2.689920	-3.059709
H	-2.060514	1.039743	-2.479500
H	-2.285947	2.406174	-1.376657
C	1.412445	1.223834	-0.182212
H	1.711430	2.141950	0.336034
C	2.453234	0.838572	-1.217339
H	2.171044	-0.094516	-1.710152
H	3.437391	0.731209	-0.754953
H	2.508329	1.630504	-1.966073
N	1.177799	0.184247	0.850896
C	2.209097	0.047875	1.895559
H	1.830738	-0.641140	2.651945
H	3.121615	-0.353792	1.454233
H	2.411990	1.023735	2.338167
H	1.070308	-0.721823	0.337625
O	0.677507	-1.887059	-0.936043
H	-0.240639	-2.164113	-0.679278
C	1.525226	-3.024613	-1.015873
H	1.510157	-3.601194	-0.084278
H	1.233897	-3.676323	-1.845993
H	2.543525	-2.669372	-1.191415

(TS-5′)-MeOH. Energy: -766.29511082 a.u.

H	-3.613392	-1.742607	-0.276584
H	-2.606406	-2.146035	-1.682147
H	-2.610164	-0.485838	-1.039428
C	-2.652288	-1.548801	-0.764829
O	-1.587633	-1.898178	0.099925
H	-1.335708	-0.999717	0.944894
O	-1.016151	-0.215742	1.722385
C	-0.379595	0.850058	1.255229
C	-0.281055	1.947582	2.300811
H	-1.299630	2.262714	2.532902
H	0.283045	2.814532	1.948875
H	0.178238	1.556344	3.210129
O	-1.031118	1.384036	0.064624
C	-0.120681	1.872430	-0.819100
N	-0.404033	2.470263	-1.891442
C	-1.821754	2.680402	-2.172930
H	-1.922589	3.232439	-3.107593
H	-2.350438	1.725456	-2.271379
H	-2.308366	3.248600	-1.372171
C	1.279931	1.576513	-0.322121
H	1.659643	2.450305	0.223596
C	2.262140	1.175547	-1.408379
H	1.907050	0.289071	-1.938863
H	3.248812	0.977681	-0.982624
H	2.352154	2.000105	-2.117635
N	0.986699	0.498190	0.653511
C	2.039282	0.232032	1.648729
H	1.644567	-0.473288	2.382054
H	2.897591	-0.215566	1.145576
H	2.347146	1.157451	2.141073
H	0.823357	-0.477223	0.006084
O	0.579783	-1.508754	-0.809804
H	-0.479713	-1.805326	-0.451989
C	1.525086	-2.562643	-0.724502
H	1.566383	-2.985097	0.287414
H	1.266236	-3.360931	-1.427053
H	2.518503	-2.182553	-0.986377

(11′)-MeOH. Energy: -766.31699195 a.u.

H	-3.029768	-1.018272	-1.009639
H	-2.428184	-2.128339	-2.265334
H	-1.482874	-0.679602	-1.820868
C	-2.135678	-1.474085	-1.438418
O	-1.495798	-2.216737	-0.405930
H	-1.054987	-1.288709	0.970928
O	-0.790482	-0.747368	1.757932
C	-0.193775	0.408378	1.330320
C	-0.041455	1.347254	2.514100
H	-1.036483	1.596720	2.885938
H	0.467467	2.267109	2.213998
H	0.525226	0.864823	3.312663
O	-1.038824	1.044479	0.344828
C	-0.291318	1.540618	-0.676018
N	-0.758161	2.163652	-1.668756
C	-2.200069	2.392503	-1.686700
H	-2.476701	2.852067	-2.636020
H	-2.761768	1.458801	-1.569084
H	-2.500339	3.063329	-0.873520
C	1.162921	1.222699	-0.421979
H	1.637465	2.110747	0.032655
C	1.923919	0.822893	-1.674707
H	1.438968	-0.030321	-2.157599
H	2.956141	0.557110	-1.432681
H	1.937308	1.660102	-2.375462
N	1.042941	0.144235	0.566443
C	2.234280	-0.047008	1.394100
H	2.024652	-0.800655	2.157218
H	3.050554	-0.413547	0.766365
H	2.559280	0.882613	1.880342
H	1.131971	-1.468460	-0.295188
O	1.179824	-2.378949	-0.679730
H	-0.599836	-2.475508	-0.708785
C	1.615908	-3.274035	0.338653
H	0.984830	-3.198503	1.233219
H	1.543754	-4.288181	-0.057580
H	2.656430	-3.077807	0.618673

(12′)-MeOH. Energy: -766.31004365 a.u.

H	-0.795236	2.765015	3.533681
H	-0.065309	4.005300	2.489433
H	0.926669	2.651583	3.096350
C	-0.068457	2.939665	2.738960
O	-0.462736	2.153040	1.619331
H	-0.139611	0.465800	1.907337
O	0.149702	-0.445587	2.161098
C	0.134197	-1.254446	1.057128
C	0.128252	-2.705174	1.509679
H	1.018630	-2.892370	2.112963
H	0.135399	-3.377862	0.647807
H	-0.758167	-2.904835	2.114841
O	1.353083	-1.045522	0.275305
C	1.054350	-1.105573	-1.055950

N	1.895134	-1.041623	-1.993525
C	3.313069	-0.946482	-1.669899
H	3.790682	-0.263776	-2.376483
H	3.517257	-0.604958	-0.648557
H	3.776732	-1.930014	-1.797153
C	-0.443368	-1.236723	-1.216531
H	-0.678606	-2.296548	-1.430994
C	-1.002941	-0.361102	-2.325811
H	-0.771522	0.688497	-2.122794
H	-2.086548	-0.479262	-2.402943
H	-0.555283	-0.645933	-3.280442
N	-0.898860	-0.853353	0.114280
C	-2.247769	-1.278713	0.455749
H	-2.455893	-1.019221	1.496463
H	-2.962709	-0.745209	-0.173928
H	-2.397901	-2.361168	0.317418
H	1.927642	0.919166	0.263731
O	1.780541	1.865887	0.114702
H	0.213789	2.252860	0.921031
C	2.340699	2.265016	-1.133140
H	1.932518	1.672801	-1.958987
H	2.077967	3.313398	-1.278552
H	3.431255	2.170761	-1.121027

(TS-3′)-MeOH. Energy: -766.29290256 a.u.

H	-0.817302	2.323911	3.856173
H	0.149605	3.621204	3.115147
H	0.935665	2.100217	3.626850
C	0.027719	2.538788	3.201141
O	-0.264260	1.972430	1.922077
H	-0.369469	0.493807	1.989437
O	-0.277227	-0.518641	2.182039
C	-0.199489	-1.335964	1.168745
C	0.252870	-2.708583	1.578184
H	1.128235	-2.605756	2.218009
H	0.494201	-3.354169	0.738047
H	-0.560211	-3.161088	2.154454
O	1.454589	-0.835834	0.173140
C	1.129941	-1.202823	-1.038548
N	1.874257	-1.216871	-2.085242
C	3.253082	-0.797454	-1.863604
H	3.820572	-0.910123	-2.789916
H	3.321414	0.254836	-1.553829
H	3.740296	-1.392860	-1.080044
C	-0.330157	-1.707454	-1.132706
H	-0.307174	-2.797417	-1.044729
C	-1.022246	-1.368144	-2.441581
H	-0.988480	-0.297911	-2.659380
H	-2.061987	-1.705561	-2.432585
H	-0.494257	-1.886606	-3.242645
N	-0.992723	-1.170987	0.069674
C	-1.659031	0.121832	-0.084097
H	-2.150060	0.390056	0.850867
H	-0.958648	0.921644	-0.362557
H	-2.421556	0.032135	-0.855601
H	1.836851	0.856352	0.278319
O	1.780101	1.840735	0.305284
H	0.519022	2.086725	1.315997
C	1.603400	2.334817	-1.021190
H	1.098700	1.594716	-1.653286
H	0.990937	3.237790	-0.971768
H	2.569474	2.585588	-1.469705

(8′)-MeOH. Energy: -766.32835871 a.u.

H	-1.976327	3.478640	3.156574
H	-0.292435	3.906712	2.776151
H	-0.653421	2.350785	3.563936
C	-1.008448	3.085447	2.832560
O	-1.101591	2.510976	1.530844
H	-1.683156	1.724626	1.573413
O	-2.030364	-0.039130	1.655781
C	-1.225070	-0.779726	1.063170
C	-0.462362	-1.837951	1.822664
H	0.591184	-1.551213	1.892206
H	-0.526912	-2.819944	1.348972
H	-0.880780	-1.891517	2.826340
O	1.313767	0.449628	-1.468729
C	0.706608	-0.624644	-1.994045
N	0.798863	-0.928715	-3.223759
C	1.622493	-0.048464	-4.044159
H	1.634298	-0.421379	-5.069306
H	1.231778	0.976307	-4.047651
H	2.653846	-0.001673	-3.674433
C	-0.092176	-1.491639	-1.028328
H	0.638101	-1.898128	-0.321892
C	-0.828227	-2.635055	-1.715323
H	-1.559126	-2.249078	-2.430440
H	-1.349660	-3.234401	-0.964573
H	-0.125295	-3.268919	-2.257422
N	-1.012343	-0.640237	-0.262583
C	-1.822639	0.333026	-0.994103
H	-2.868789	0.245318	-0.696501
H	-1.482685	1.355067	-0.795761
H	-1.731437	0.133835	-2.062735
H	1.155718	0.583639	-0.487474
O	1.122514	1.055754	1.052743
H	0.335522	1.632543	1.205320
C	2.300048	1.788730	1.385572
H	2.375604	2.705691	0.792106
H	2.307901	2.042215	2.449839
H	3.158108	1.151373	1.166613