Supporting Information for:

,5-Didehydro-3-picoline Diradicals from Skipped Aza-Enediynes: Computational and Trapping Studies of an Aza-Myers-Saito Cyclization.

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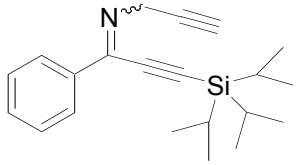
A. Experimental Section

1. General methods

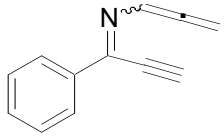
All commercial chemicals were used without further purification unless otherwise noted. Tetrahydrofuran (THF) was re-distilled from Na/benzophenone prior to use. All reactions were performed under argon. Unless otherwise noted, organic extracts were dried with Na_2SO_4, filtered through a fritted glass funnel, and concentrated with a rotary evaporator (20-30 mmHg). Thin-layer chromatography (TLC) was performed on silica gel TLC plates using the indicated mobile phase. Flash chromatography was performed with EM silica gel. ^{1}H NMR spectra were recorded at 500 and 300 MHz and ^{13}C NMR spectra were recorded at 100 and 75 MHz. All mass spectra were obtained by chemical ionization with methane as the ionizing gas. Melting points are uncorrected.

2. Preparation of 1-triisopropylsilyl-3-phenyl-3-ene-4-aza-1,6-diyne (**7**)



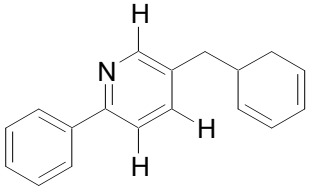
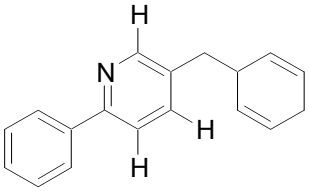
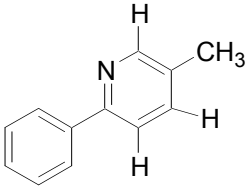
Propargylamine (200.0 mg, 3.49 mmol) was added dropwise to a mixture of 1-phenyl-3-(triisopropylsilyl)-propynone[1] (500.0 mg, 1.75 mmol) and titanium(IV) ethoxide (600.0 mg, 2.62 mmol) in 10 mL dry THF. The resulting yellow mixture was heated to reflux under argon for 1.5 h and then cooled to room temperature. The mixture was poured into water (30 mL), and the water layer was extracted by CH_2Cl_2 (2 x 20 mL). The residue upon drying and concentration of the organic layer was purified by flash chromatography (0-2% ethyl acetate in hexanes) to afford 290.0 mg (52%) of compound **7** as a yellow oil: R_f 0.50 (ethyl acetate : hexanes 1:9); ^{1}H NMR ($CDCl_3$) □ 1.12-1.21 (m, 21H), 2.28 (t, 1H, J = 2.8 Hz), 4.58 (d, 2H, J = 2.8 Hz), 7.36-7.44 (m, 3H), 8.07 (dd, 2H, J = 8.0, 1.6 Hz); ^{13}C NMR ($CDCl_3$) _ 11.09, 18.61, 45.07, 70.87, 81.26, 97.15, 105.18, 127.69, 128.24, 130.92, 136.59, 153.72; HRMS *m/z* 324.2153 (calc'd 324.2147, $C_{21}H_{29}NSi$).

3. Preparation of (1-phenyl-prop-2-ynylidene)-propa-1,2-dienyl-amine (aza-enyne allene **3d**)



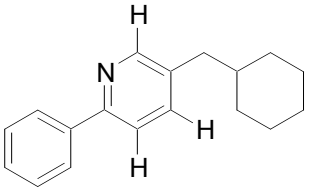
A 1 M solution of TBAF (1.46 mmol) was slowly added to a solution of the compound **7** (130.0 mg, 0.40 mmol) in dry THF (3 mL) cooled to -78 °C. After being stirred at -78 °C for 5 min, the mixture was poured into ice-water (10 mL) and extracted by CH_2Cl_2 (2 x 15 mL). The organic layer upon drying, concentration, and removal of trace of solvent under vacuum (0.05-0.1 mmHg/5min) afforded aza-enyne allene **3d** as a yellow oil. R_f 0.45 (ethyl acetate : hexanes 1:9); ^{1}H NMR ($CDCl_3$) □ 3.82 (s, 1H), 5.36 (d, 2H, J = 6.0 Hz), 7.38-7.41 (m, 3H), 7.60 (t, 1H, J = 6.0 Hz), 8.07 (dd, 2H, J = 7.6, 2.0 Hz); ^{13}C NMR ($CDCl_3$) □ 75.35, 81.06, 89.72, 110.11, 127.99, 128.54, 131.12, 136.72, 147.10, 213.72; CI-MS *m/z* 168(MH^+).

4. Preparation of 5-cyclohexa-2,4-dienylmethyl-2-phenylpyridine (**10a**), 5-cyclohexa-2,5-dienylmythyl-2-phenylpyridine (**10b**) and 6-phenyl-3-picoline (**9**)

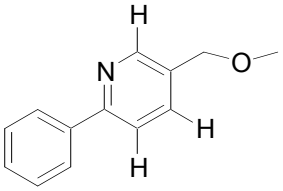
Compound **3d** (0.40 mmol) prepared as above was placed in a round bottle flask that was then cooled to 0 °C. To this was added freshly distilled 1,4-chd (2 mL). The reaction mixture was then kept at 4 °C for 8 h. The residue upon concentration was purified by flash chromatography (0-2% ethyl acetate in hexanes) to afford 16.5 mg (17%) of 1:1 ratio mixture of **10a** and **10b** as a yellow oil and 13.0 mg (20%) of compound **9** as a light yellow solid: R_f (**10a/10b**) 0.40 (ethyl acetate : hexanes 1:9); ^{1}H NMR ($CDCl_3$) (**10a/10b**) □ 1.98-2.08 (m, 0.5H), 2.20-2.31 (m, 0.5H), 2.50-2.70 (m, 1.5H), 2.72 (d, 2H, J = 6.9 Hz), 2.97-3.10 (m, 0.5H), 5.58-5.78 (m, 3H), 5.88-5.94 (m, 1H), 7.37-7.48 (m, 3H), 7.52-7.58 (m, 1H), 7.63 (dd, 1H, J = 8.4, 1.8 Hz), 7.96 (d, 2H, J = 7.2 Hz), 8.49 (brs, 1H); CI-MS *m/z* (**10a/10b**) 248; R_f (**9**) 0.36 (ethyl acetate : hexanes, 1:9); mp (**9**) 52-54 °C, Lit:[2] mp 56 °C; ^{1}H NMR ($CDCl_3$) (**9**) □ 2.35 (s, 3H), 7.35-7.40 (m, 1H), 7.41-7.47 (m, 2H), 7.54 (dd, 1H, J = 7.6, 2.0 Hz), 7.60 (d, 1H, J = 7.6 Hz), 7.93 (dd, 2H, J = 8.4, 1.6 Hz), 8.50 (brs, 1H); ^{13}C NMR ($CDCl_3$) (6b) □ 17.67, 120.09, 126.68, 128.58, 128.68, 131.61, 137.34, 139.36, 150.02, 154.80; CI-MS *m/z* (**9**) 170.

5. Preparation of 5-cyclohexylmethyl-2-phenylpyridine (**11**)



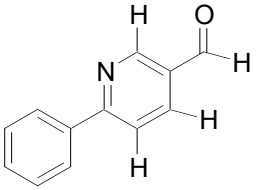
A 5 mL empty round bottle flask was charged with 10% palladium on activated carbon (10.0 mg, 0.0063 mmol); the flask was purged and then filled with hydrogen gas (this process was repeated three times). To this flask was added **10a/10b** (15.0 mg, 0.063 mmol) in degassed ethyl acetate (1 mL). The reaction mixture was stirred under an atmosphere of H_2 at room temperature for 2 h. The reaction mixture was filtered, concentrated, and purified by flash chromatography (0.5% ethyl acetate in hexanes) to afford 13.0 mg (87%) of compound 11 as a white solid: mp 60-62 °C; R_f 0.47 (ethyl acetate : hexanes, 1:9); ^{1}H NMR ($CDCl_3$) □ 0.90-1.02 (m, 2H), 1.14-1.1.24 (m, 4H), 1.48-1.58 (m, 1H), 1.60-1.74 (m, 4H), 2.50 (d, 2H, J = 7.2 Hz), 7.37 (t, 1H, J = 7.2 Hz), 7.40-7.48 (m, 2H), 7.51 (dd, 1H, J = 8.0, 2.0 Hz), 7.63 (d, 1H, J = 8.0 Hz), 7.96 (dd, 2H, J = 8.8, 1.6 Hz), 8.46 (d, 1H, J = 2.0 Hz); ^{13}C NMR ($CDCl_3$) □ 26.19, 26.42, 32.96, 39.53, 40.69, 119.98, 126.68, 128.62, 128.69, 134.99, 137.42, 139.29, 150.23, 154.89; HRMS *m/z* 252.1747 (calc'd 252.1752, $C_{18}H_{21}N$).

6. Preparation of 5-methoxymethyl-2-phenylpyridine (**12**)



Compound **3d** (0.17 mmol) prepared as above was placed in a round bottle flask that was then cooled to 0 °C. To this was added freshly distilled methanol (2 mL). The reaction mixture was then kept at 0 °C for 14 h. The residue upon concentration was purified by flash chromatography (0-10% ethyl acetate in hexanes) to afford 6.7 mg (20%) of compound **12** as a yellow oil: R_f 0.20 (ethyl acetate : hexanes, 1:9); ^{1}H NMR ($CDCl_3$) □ 3.41 (s, 3H), 4.50 (s, 2H), 7.38-7.49 (m, 3H), 7.71-7.74 (m, 2H), 7.94-7.99 (m, 2H), 8.62 (brs, 1H); ^{13}C NMR ($CDCl_3$) □ 58.32, 71.97, 120.32, 126.91, 128.75, 128.98, 131.94, 136.41, 139.09, 149.05, 156.97; HRMS *m/z* 200.1074 (calc'd 200.1075, $C_{13}H_{13}NO$).

7. Isolation of 6-phenylpyridine-3-carbaldehyde (**8**)



Compound **3d** (0.31 mmol) prepared above was dissolved in 1 mL of $CDCl_3$. The solution was stored at 10 °C in a fridge for 12 h. The residue upon concentration was purified by flash chromatography (10% ethyl acetate in hexanes) to afford 1.0 mg (1.8%) of compound **8** as a yellow wax product:[3] R_f 0.12 (ethyl acetate : hexanes, 1:9); ^{1}H NMR ($CDCl_3$) □ 7.45-7.52 (m, 3H), 7.90 (d, 1H, J = 8.4 Hz), 8.03-8,08 (m, 2H), 8.22 (dd, 1H, J = 8.4, 2.0 Hz), 9.11 (dd, 1H, J = 2.0, 0.4 Hz), 10.13 (s, 1H); HRMS *m/z* 184.0765 (calc'd 184.0762, $C_{12}H_9NO$).

References

1. 1-Phenyl-3-(triisopropylsilyl)-propynone was prepared according to the procedure published previously: Feng, L.; Kumar, D.; Kerwin, S.M.; *J. O. Chem.* **2003**, 68, 2234.
2. The melting point and NMR data reported here are in agreement with the data published previously: Kagabu, S.; Ando, C.; Ando, J.; *J. Chem. Soc. Perkin Trans 1*, **1994**, 6, 739.
3. ^{1}H NMR data reported here is in agreement with the data published previously: Tanaka, A.; Terasawa, T.; Hagihara, H.; Sakuma, Y.; Ishibe, N.; Sawada, M.; Takasugi, H.; Tanaka, H. *J. Med. Chem.* **1998**, 41, 2390.

B. Energies calculated at the (U)B3LYP/6-31G* level of theory

1. Table 1. (U)B3LYP/6-31G* Energies for Myers-Saito and Schmittel cyclizations.

	Electronic energy[a]	ZPE[b]	Relative energy[c]	Enthalpy[f]
(*Z*)-Enyne allene (s-cis) **3a**	-270.20169	62.2	4.0	-270.09411
(*Z*)-Enyne allene (s-trans) **3a**	-270.20832	62.3	0	-270.10066
(*E*)-Enyne allene (s-cis) **3a**	-270.20436	62.1	-2.2	-270.09685
(*E*)-Enyne allene (s-*trans*) **3a**	-270.20816	62.1	-0.1	-270.10063
□,3-Didehydrotoluene triplet diradical **4a••**	-270.22722	64.0	-10.2	-270.11871
□,3-Didehydrotoluene singlet diradical **4a••**	-270.22906	63.7	-11.6	-270.12080
Zwitterion[d] **4a±**	-270.17919	65.0	20.9	-270.06906
Cyclic allene **5a**	-270.21139	64.4	0.1	-270.10217
Myers-Saito transition state[e] **TS1a**	-270.16603	62.1	26.3	-270.05996
Schmittel triplet diradical **6a**, anti-addition	-270.19203	62.6	10.5	-270.08531
Schmittel singlet diradical **6a**, anti-addition	-270.18754	62.4	13.1	-270.08105
Schmittel transition state[e] **TS2a**, anti-addition	-270.1521095	61.5	34.5	-270.04694

[a]Absolute energies in Hartrees; [b]ZPE in kcal/mol; [c]ZPE-corrected energies relative to (*Z*)-enyne allene (s-tran*s*) **3a** in kcal/mol; [d]1 imaginary frequency at the HF/6-31G* level; [e]1 imaginary frequency at the B3LYP/6-31G* level; [f]Enthalpy in Hartrees.

2. Table 2. (U)B3LYP/6-31G* Energies for aza-Myers-Saito and aza-Schmittel cyclizations.

	Electronic energy[a]	ZPE[b]	Relative energy[c]	Enthalpy[f]
(*Z*)-Aza-enyne allene (s-cis) **3b**	-286.23233	54.7	3.5	-286.13682
(*Z*)-Aza-enyne allene (s-trans) **3b**	-286.23795	54.8	0	-286.14245
(*E*)-Aza-enyne allene (s-cis) **3b**	-286.23454	54.7	-2.0	-286.13911
(*E*)-Aza-enyne allene (s-trans) **3b**	-286.23766	54.5	-0.1	-286.14245
□,5-Didehydro-3-picoline triplet diradical **4b••**	-286.26314	56.6	-14.0	-286.16652
□,5-Didehydro-3-picoline singlet diradical **4b••**	-286.26503	56.4	-15.4	-286.16863
Aza-zwitterion[d] **4b±**	-286.21523	57.0	16.5	-286.11834
Aza-cyclic allene **5b**	-286.24552	56.9	-2.6	-286.14828
(*Z*)-Aza-skipped enediyne **2b**	-286.21899	54.9	12.0	-286.12314
(*E*)-Aza-skipped enediyne **2b**	-286.22186	54.7	10.1	-286.12616
Aza-Myers transition state[d] **TS1b**	-286.20081	54.6	23.2	-286.10671
Aza-Schmittel singlet diradical **6b**, syn-addition	-286.22656	54.8	7.2	-286.13216
Aza-Schmittel triplet diradical **6b**, syn-addition	-286.23075	55.0	4.8	-286.13612
Aza-Schmittel transition state[d] **TS2b**, syn-addition,	-286.18804	53.8	30.4	-286.09493
Aza-Schmittel singlet diradical **6b**, anti-addition	-286.22630	54.8	7.3	-286.13194
Aza-Schmittel triplet diradical **6b**, anti-addition	-286.23001	54.9	5.2	-286.13546
Aza-Schmittel transition state[d] **TS2b**, anti-addition	-286.19269	54.1	27.7	-286.09936

[a]Absolute energies in Hartrees; [b]ZPE in kcal/mol; [c]ZPE-corrected energies relative to (*Z*)-aza-enyne allene (s-trans) **3b** in kcal/mol; [d]1 imaginary frequency at the B3LYP/6-31G* level; [f]Enthalpy in Hartrees.

3. Table 3. B3LYP/6-31G* Energies for 7-methyl-4-aza-3-ene-1,6-diyne and corresponding aza-enyne allene.

	Electronic energy[a]	ZPE[b]	Relative energy[c]	Enthalpy[d]
(*Z*)-7-Methyl-4-aza-3-ene-1,6-diyne (Skipped aza-enediyne) **2c**	-325.54547	73.0	7.3	-325.41895
(*Z*)-7-Methyl-aza-enyne allene (S-*cis*) **3c**	-325.55124	72.7	3.5	-325.42551
(*Z*)-7-Methyl-aza-enyne allene (S-*trans*) **3c**	-325.55682	72.8	0	-325.43107
(*E*)-7-Methyl-4-aza-3-ene-1,6-diyne (Skipped aza-enediyne) **2c**	-325.54553	72.8	7.1	-325.41923
(*E*)-7-Methyl-aza-enyne allene (S-*cis*) **3c**	-325.55353	72.6	2.0	-325.42790
(*E*)-7-Methyl-aza-enyne allene (S-*trans*) **3c**	-325.55668	72.5	-0.1	-325.43125

[a]Absolute energies in Hartrees; [b]ZPE in kcal/mol; [c]ZPE-corrected energies relative to (*Z*)-7-methyl-aza-enyne allene (S-*trans*) in kcal/mol; [d]Enthalpy in Hartrees.

4. Table 4. B3LYP/6-31G* Energies for **3d.**

	Electronic energy[a]	Relative energy[b]
(*Z*)-Aza-enyne allene (s-cis) **3d**	-517.28537	10.2
(*Z*)-Aza-enyne allene (s-trans) **3d**	-517.29068	6.9
(*E*)-Aza-enyne allene (s-cis) **3d**	-517.29516	4.1
(*E*)-Aza-enyne allene (s-trans) **3d**	-517.30170	0

[a]Absolute energies in Hartrees; [b]Energies relative to (*E*)-Aza-enyne allene (s-trans) **3d** in kcal/mol.

C. Geometries of optimized structures

1. (*Z*)-Enyne allene (s-cis) **3a** (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
C,2,R6,1,A6,3,D6,0
H,2,R7,1,A7,6,D7,0
H,3,R8,1,A8,5,D8,0
C,5,R9,3,A9,1,D9,0
C,6,R10,2,A10,1,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
H,10,R13,6,A13,2,D13,0
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R2=1.35435293
R3=1.4606302
R4=1.08764492
R5=1.32004743
R6=1.41703157
R7=1.08908998
R8=1.09126467
R9=1.30379976
R10=1.21211324
R11=1.0892296
R12=1.08922695
R13=1.06599533
A3=129.90582854
A4=116.10696354
A5=128.85935362
A6=127.17683104
A7=117.35814566
A8=114.85119979
A9=176.32487253
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A11=121.66788997
A12=121.67288725
A13=177.78144733

D4=-179.99962644
D5=0.01078714
D6=-0.00146632
D7=179.99843995
D8=179.99087542
D9=-179.63755671
D10=-179.71713604
D11=90.41938093
D12=178.42699276
D13=-179.59336829

2. (*Z*)-Enyne allene (s-trans) **3a** (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,5,R9,2,A9,1,D9,0
C,6,R10,3,A10,1,D10,0
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H,10,R12,6,A12,3,D12,0
H,10,R13,6,A13,12,D13,0
Variables:
R2=1.35464299
R3=1.4539973
R4=1.08703751
R5=1.41974808
R6=1.3190197
R7=1.08830654
R8=1.09015262
R9=1.21217104
R10=1.30447578
R11=1.06612227
R12=1.08938959
R13=1.08938995
A3=124.7983083
A4=118.29629726
A5=124.94399323
A6=123.68015552
A7=118.6478819
A8=117.14671634
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A10=179.98458325
A11=179.70783901
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D4=-179.99955689
D5=-0.000088
D6=179.99084197
D7=179.9990002
D8=-179.98330137
D9=179.99896024
D10=2.67350912

D11=-179.99431806
D12=87.37871767
D13=179.90262026

3. (*E*)-Enyne allene (s-cis) **3a** (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,5,R9,2,A9,1,D9,0
C,6,R10,3,A10,1,D10,0
H,9,R11,5,A11,2,D11,0
H,10,R12,6,A12,3,D12,0
H,10,R13,6,A13,12,D13,0
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R2=1.35195854
R3=1.46436942
R4=1.08727074
R5=1.41743547
R6=1.31863436
R7=1.08999235
R8=1.09020939
R9=1.21217663
R10=1.30463842
R11=1.06601555
R12=1.08966478
R13=1.08966386
A3=125.72734893
A4=118.66470139
A5=123.82993498
A6=126.14349357
A7=119.27815684
A8=116.16349668
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D11=179.96654786
D12=88.71446297
D13=179.84383076

4. (*E*)-Enyne allene (s-trans) **3a** (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,5,R9,2,A9,1,D9,0
C,6,R10,3,A10,1,D10,0
H,9,R11,5,A11,2,D11,0
H,10,R12,6,A12,3,D12,0
H,10,R13,6,A13,12,D13,0
Variables:
R2=1.35296656
R3=1.45389435
R4=1.0872234
R5=1.41788842
R6=1.31935145
R7=1.09032713
R8=1.09139623
R9=1.21193295
R10=1.30431446
R11=1.06605234
R12=1.08945389
R13=1.08945519
A3=123.2195093
A4=119.53948928
A5=124.13649114
A6=124.14396675
A7=119.18500344
A8=117.2241877
A9=178.43204818
A10=179.94116709
A11=179.2237779
A12=121.69482917
A13=121.69496562
D4=179.99782009
D5=-179.99632648
D6=179.98987947
D7=-179.99775496
D8=-179.98774586
D9=177.65645804
D10=4.87250218

D11=178.02806761
D12=85.18332759
D13=179.96336135

5. ,3-Didehydrotoluene singlet diradical **4a** (UB3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,5,R9,2,A9,1,D9,0
C,6,R10,3,A10,1,D10,0
H,9,R11,5,A11,2,D11,0
H,10,R12,6,A12,3,D12,0
H,10,R13,6,A13,12,D13,0
Variables:
R2=1.41179989
R3=1.3861233
R4=1.08766692
R5=1.38410465
R6=1.43048007
R7=1.08608682
R8=1.08700414
R9=1.36644477
R10=1.4031425
R11=1.0874807
R12=1.08527944
R13=1.08502071
A3=120.71579118
A4=119.46908567
A5=116.12798742
A6=121.86266422
A7=121.1808466
A8=119.79230796
A9=126.29836707
A10=121.60227699
A11=122.56417418
A12=121.15906477
A13=121.26236447
D4=180.
D5=0.00027383
D6=-0.00005858
D7=-179.99970672
D8=180.
D9=-0.00031875
D10=-179.9998868

D11=179.99923512
D12=0.00103497
D13=179.99986118

6. ,3-Didehydrotoluene triplet diradical **4a** (UB3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,180.,0
C,2,R5,1,A5,3,0.,0
C,3,R6,1,A6,2,0.,0
H,2,R7,1,A7,3,180.,0
H,3,R8,1,A8,2,180.,0
C,5,R9,2,A9,1,0.,0
C,6,R10,3,A10,1,180.,0
H,9,R11,5,A11,2,180.,0
H,10,R12,6,A12,3,0.,0
H,10,R13,6,A13,3,180.,0
Variables:
R2=1.41008462
R3=1.38692278
R4=1.08782306
R5=1.3834044
R6=1.42741908
R7=1.08615738
R8=1.08698539
R9=1.36609832
R10=1.40728249
R11=1.08743091
R12=1.08521497
R13=1.08499176
A3=120.68863933
A4=119.49375088
A5=116.13943302
A6=121.81553083
A7=121.27358414
A8=119.7576058
A9=126.2833208
A10=121.53543297
A11=122.45861333
A12=121.11395479
A13=121.21669778

7. Myers-Saito cyclization transition state **TS1a** (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
C,2,R6,1,A6,3,D6,0
H,2,R7,1,A7,6,D7,0
H,3,R8,1,A8,5,D8,0
C,5,R9,3,A9,1,D9,0
C,6,R10,2,A10,1,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
H,10,R13,6,A13,2,D13,0
Variables:
R2=1.37893284
R3=1.42386909
R4=1.0877046
R5=1.36470871
R6=1.39451169
R7=1.08599197
R8=1.08974723
R9=1.33296087
R10=1.25473952
R11=1.08955136
R12=1.08705034
R13=1.07065311
A3=123.19861446
A4=118.83188488
A5=128.46381404
A6=115.63397585
A7=121.11167331
A8=115.74596183
A9=144.32760353
A10=141.36172849
A11=120.91214259
A12=122.34488859
A13=147.2992386
D4=168.00730212
D5=-10.94531231
D6=9.93058943
D7=-172.05241849
D8=169.5314398
D9=-157.69364639
D10=-6.66337974

D11=42.17189702
D12=173.03156209
D13=153.78772215

8. Zwitterion **4a**$^{\pm}$ (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,180.,0
C,2,R5,1,A5,3,0.,0
C,3,R6,1,A6,2,0.,0
H,2,R7,1,A7,3,180.,0
H,3,R8,1,A8,2,180.,0
C,5,R9,2,A9,1,0.,0
C,6,R10,3,A10,1,180.,0
H,9,R11,5,A11,2,180.,0
H,10,R12,6,A12,3,0.,0
H,10,R13,6,A13,3,180.,0
Variables:
R2=1.44047943
R3=1.36180028
R4=1.08776836
R5=1.42510105
R6=1.45157087
R7=1.09605155
R8=1.087909
R9=1.39693271
R10=1.35701805
R11=1.09716453
R12=1.08798208
R13=1.08869463
A3=119.36919328
A4=119.97483941
A5=128.14502268
A6=117.8413066
A7=113.91275696
A8=122.64560181
A9=109.72163828
A10=120.49219989
A11=120.16704291
A12=122.26186185
A13=121.02922967

9. Cyclic allene **5a** (B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,5,R9,2,A9,1,D9,0
C,6,R10,3,A10,1,D10,0
H,9,R11,5,A11,2,D11,0
H,10,R12,6,A12,3,D12,0
H,10,R13,6,A13,12,D13,0

Variables:
R2=1.45963558
R3=1.36205113
R4=1.08777047
R5=1.34332238
R6=1.47084705
R7=1.08936975
R8=1.08756447
R9=1.33885197
R10=1.35567393
R11=1.08750297
R12=1.08683277
R13=1.08616841
A3=116.70120185
A4=121.23685425
A5=114.92021611
A6=122.92247397
A7=119.30823379
A8=119.9619726
A9=129.2861384
A10=121.28854375
A11=124.58398437
A12=121.7453485
A13=121.38364897
D4=-166.97793163
D5=-25.95117323
D6=12.14888867
D7=165.39522956
D8=-178.36024495
D9=16.8524053
D10=178.09107528

D11=-156.60797534
D12=-3.4108762
D13=-177.1502566

10. Schmittel singlet diradical **6a**, anti-addition (UB3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,6,R9,3,A9,1,D9,0
C,5,R10,2,A10,1,D10,0
H,9,R11,6,A11,3,D11,0
H,9,R12,6,A12,11,D12,0
H,10,R13,5,A13,2,D13,0
Variables:
R2=1.38388933
R3=1.41154062
R4=1.0847301
R5=1.46551115
R6=1.43500838
R7=1.08208264
R8=1.0838981
R9=1.35824699
R10=1.32322244
R11=1.08579954
R12=1.0853888
R13=1.08204034
A3=110.37731788
A4=124.95990296
A5=108.79519203
A6=109.72842095
A7=127.2356703
A8=126.00667825
A9=127.89327352
A10=127.10834976
A11=121.00552453
A12=121.97422283
A13=137.98406559
D4=179.999475
D5=-0.00104315
D6=-0.00340131
D7=-179.99762508
D8=-179.99488571
D9=-179.9946227
D10=-179.99411979

D11=0.00034469
D12=179.99979192
D13=179.99225993

11. Schmittel triplet diradical **6a**, anti-addition (UB3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,5,D7,0
H,3,R8,1,A8,6,D8,0
C,5,R9,2,A9,1,D9,0
C,6,R10,3,A10,1,D10,0
H,9,R11,5,A11,2,D11,0
H,10,R12,6,A12,3,D12,0
H,10,R13,6,A13,12,D13,0
Variables:
R2=1.40403281
R3=1.39339885
R4=1.08482765
R5=1.443223
R6=1.44644563
R7=1.08239978
R8=1.08356813
R9=1.33591259
R10=1.34954212
R11=1.08177853
R12=1.08619612
R13=1.08578344
A3=110.45094544
A4=124.58511224
A5=109.05026452
A6=109.24370625
A7=126.61124572
A8=126.52172545
A9=127.50271948
A10=127.77120251
A11=137.46001613
A12=121.13259696
A13=121.97238736
D4=179.99080004
D5=0.00970542
D6=-0.01643357
D7=179.99704533
D8=-179.98899865
D9=179.99700032
D10=-179.99087791

D11=-179.99915901
D12=0.00394572
D13=-179.99704284

12. Schmittel transition state **TS2a**, anti-addition (UB3LYP/6-31G* or B3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
C,2,R6,1,A6,3,D6,0
H,2,R7,1,A7,6,D7,0
H,3,R8,1,A8,5,D8,0
C,5,R9,3,A9,1,D9,0
C,6,R10,2,A10,1,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
H,10,R13,6,A13,2,D13,0
Variables:
R2=1.37407346
R3=1.42231214
R4=1.08492866
R5=1.37654462
R6=1.4314474
R7=1.08483904
R8=1.08718082
R9=1.32938322
R10=1.27640036
R11=1.08771129
R12=1.08721258
R13=1.07926069
A3=112.87374917
A4=123.30243171
A5=112.24499006
A6=114.90914413
A7=124.52189167
A8=123.19542084
A9=143.37020474
A10=142.96187825
A11=121.47269745
A12=121.13684811
A13=137.25714292
D4=175.9181467
D5=-14.69804802
D6=-1.30557285
D7=177.87864768
D8=167.08956863
D9=-143.93048208

D10=-165.64338644
D11=12.56129317
D12=175.51481282
D13=-159.97500344

13. (*Z*)-Aza-enyne allene (s-cis) **3b** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
Variables:
R2=1.28476995
R3=1.40622899
R4=1.43228117
R5=1.3184056
R6=1.09243585
R7=1.08964298
R8=1.21108996
R9=1.30503751
R10=1.06683246
R11=1.08961369
R12=1.08938791
A3=122.48726921
A4=128.75646962
A5=126.93648631
A6=116.09702405
A7=113.29400917
A8=174.70359674
A9=176.15005057
A10=178.10749202
A11=121.90440161
A12=121.48192595
D4=-4.4010003
D5=-41.78801498
D6=-178.33974458
D7=-172.92659791
D8=-159.05950885
D9=-97.42271726
D10=168.74258496
D11=12.32635156
D12=179.21976296

14. (*Z*)-Aza-enyne allene (s-trans) **3b** (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
Variables:
R2=1.29017902
R3=1.3980595
R4=1.43220943
R5=1.32077131
R6=1.09129672
R7=1.09372504
R8=1.21151882
R9=1.3025963
R10=1.06691835
R11=1.08925244
R12=1.08925131
A3=119.22092221
A4=127.58596822
A5=120.83485171
A6=116.54385886
A7=119.78604622
A8=177.96605898
A9=178.54553036
A10=179.78318554
A11=121.64312827
A12=121.64270874
D4=-0.00392729
D5=179.99762932
D6=-179.99064184
D7=-179.9945638
D8=-179.99553024
D9=179.90380198
D10=179.97578068
D11=-90.2384614
D12=-179.32725266

15. (*E*)-Aza-enyne allene (s-cis) **3b** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,3,R4,1,A4,2,D4,0
C,2,R5,1,A5,3,D5,0
H,2,R6,1,A6,5,D6,0
H,3,R7,1,A7,4,D7,0
C,4,R8,3,A8,1,D8,0
C,5,R9,2,A9,1,D9,0
H,8,R10,4,A10,3,D10,0
H,8,R11,4,A11,10,D11,0
H,9,R12,5,A12,2,D12,0
Variables:
R2=1.28494486
R3=1.40859294
R4=1.31938881
R5=1.42559306
R6=1.09877275
R7=1.08890615
R8=1.30589568
R9=1.21033597
R10=1.08988907
R11=1.0895419
R12=1.06667349
A3=118.91895827
A4=126.17834717
A5=121.62632264
A6=122.13324893
A7=113.83922077
A8=176.57091074
A9=176.62529259
A10=121.83106114
A11=121.71735637
A12=178.33365323
D4=33.32720992
D5=-176.6446117
D6=-179.98528345
D7=175.31903608
D8=85.13284921
D9=-179.03343808
D10=2.30377025
D11=179.68834672
D12=-179.31722621

16. (*E*)-Aza-enyne allene (s-trans) **3b** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,3,R4,1,A4,2,D4,0
C,2,R5,1,A5,3,D5,0
H,2,R6,1,A6,5,D6,0
H,3,R7,1,A7,4,D7,0
C,4,R8,3,A8,1,D8,0
C,5,R9,2,A9,1,D9,0
H,8,R10,4,A10,3,D10,0
H,8,R11,4,A11,10,D11,0
H,9,R12,5,A12,2,D12,0
Variables:
R2=1.2880837
R3=1.39692642
R4=1.32051889
R5=1.42407762
R6=1.10062029
R7=1.09695505
R8=1.30255443
R9=1.21050997
R10=1.08936981
R11=1.08931638
R12=1.06662571
A3=116.62748175
A4=121.70179904
A5=121.97869127
A6=122.06894842
A7=119.04225961
A8=179.89990061
A9=176.79850531
A10=121.64045728
A11=121.69990118
A12=178.37824016
D4=179.54280352
D5=-179.97564768
D6=-179.87389947
D7=-179.6927511
D8=88.05263305
D9=-178.7865389
D10=1.83546381
D11=-179.79743543
D12=-175.60486661

17. □,5-Didehydro-3-picoline singlet diradical **4b** (UB3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
Variables:
R2=1.35604129
R3=1.32385811
R4=1.38638582
R5=1.43337228
R6=1.08584452
R7=1.08982153
R8=1.3659569
R9=1.40112926
R10=1.08787056
R11=1.08514743
R12=1.08489046
A3=118.75502045
A4=119.242019
A5=125.30629935
A6=117.05160575
A7=116.05768578
A8=124.29835213
A9=121.68012343
A10=122.83787498
A11=120.98197886
A12=121.31336396
D4=0.01125829
D5=0.00014723
D6=179.9620728
D7=179.98634036
D8=-0.01659363
D9=-179.99863098
D10=-179.9951681
D11=0.00055537
D12=-179.99846988

18. ,5-Didehydro-3-picoline triplet diradical **4b** (UB3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
C,1,R4,2,A4,3,180.,0
N,2,R5,1,A5,3,0.,0
C,3,R6,1,A6,2,0.,0
H,2,R7,1,A7,3,180.,0
H,3,R8,1,A8,2,180.,0
H,4,R9,1,A9,2,180.,0
H,4,R10,1,A10,2,0.,0
C,5,R11,2,A11,1,0.,0
H,11,R12,5,A12,2,180.,0
Variables:
R2=1.43040274
R3=1.43371197
R4=1.4044846
R5=1.32441119
R6=1.36614641
R7=1.09004449
R8=1.08713385
R9=1.08424075
R10=1.08457595
R11=1.3556054
R12=1.08500737
A3=115.33667699
A4=121.69258164
A5=125.32997022
A6=117.06675729
A7=118.62864838
A8=120.10020852
A9=121.30799644
A10=120.92143355
A11=118.69220844
A12=117.05320932

19. Aza-zwitterion **4b**$^{\pm}$ (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,0.,0
C,3,R5,1,A5,2,0.,0
H,2,R6,1,A6,3,180.,0
H,3,R7,1,A7,2,180.,0
C,4,R8,2,A8,1,0.,0
C,5,R9,3,A9,1,180.,0
H,8,R10,4,A10,2,180.,0
H,9,R11,5,A11,3,0.,0
H,9,R12,5,A12,3,180.,0
Variables:
R2=1.39898535
R3=1.29832392
R4=1.42323751
R5=1.45941632
R6=1.0933092
R7=1.09171516
R8=1.39391894
R9=1.35561978
R10=1.09635441
R11=1.08919466
R12=1.08749667
A3=115.6831741
A4=131.28270149
A5=122.43195163
A6=109.9442855
A7=118.47866936
A8=109.49917315
A9=119.52384424
A10=121.09341916
A11=121.92939105
A12=121.34355271

20. Aza-cyclic allene **5b** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,4,R9,2,A9,8,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,4,A11,2,D11,0
H,9,R12,4,A12,11,D12,0

Variables:

R2=1.29417374
R3=1.42533087
R4=1.4878505
R5=1.33914917
R6=1.09161371
R7=1.08574953
R8=1.47180662
R9=1.35281314
R10=1.08796767
R11=1.08606553
R12=1.08739217
A3=113.49132815
A4=126.7072403
A5=118.30018294
A6=116.706455
A7=114.78355405
A8=112.3967447
A9=120.16246712
A10=119.47956683
A11=121.68710378
A12=121.44051947
D4=-10.12271075
D5=26.40599928
D6=177.97757293
D7=-173.62744659
D8=-15.16477689
D9=-168.07513548
D10=-138.75790482
D11=-177.40666947
D12=-178.04402584

21. (*Z*)-Aza-skipped enediyne **2b** (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,3,R4,1,A4,2,D4,0
C,2,R5,1,A5,3,D5,0
H,2,R6,1,A6,5,D6,0
H,3,R7,1,A7,4,D7,0
H,3,R8,1,A8,4,D8,0
C,4,R9,3,A9,1,D9,0
C,5,R10,2,A10,1,D10,0
H,9,R11,4,A11,3,D11,0
H,10,R12,5,A12,2,D12,0
Variables:
R2=1.27862971
R3=1.46660881
R4=1.46535335
R5=1.43844397
R6=1.09305539
R7=1.10059544
R8=1.09946244
R9=1.20655858
R10=1.21047305
R11=1.0662979
R12=1.06715399
A3=118.72571677
A4=110.89229037
A5=128.21228815
A6=116.56709603
A7=113.20071556
A8=106.61903525
A9=178.95283246
A10=177.13799576
A11=179.46444114
A12=179.3792483
D4=126.22999992
D5=-0.42304612
D6=179.85440163
D7=-123.88713078
D8=118.54820828
D9=-160.64512671
D10=-179.47024795
D11=153.41901575
D12=175.22680349

22. (*E*)-Aza-skipped enediyne **2b** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
H,3,R8,1,A8,5,D8,0
C,4,R9,2,A9,1,D9,0
C,5,R10,3,A10,1,D10,0
H,9,R11,4,A11,2,D11,0
H,10,R12,5,A12,3,D12,0

Variables:

R2=1.27767274
R3=1.46356425
R4=1.43112873
R5=1.46919623
R6=1.09765884
R7=1.09890207
R8=1.09890195
R9=1.20940006
R10=1.20808755
R11=1.06664605
R12=1.06673242
A3=119.07573933
A4=121.13597259
A5=118.57616075
A6=122.83990623
A7=106.55408455
A8=106.55460644
A9=176.59988773
A10=179.05307316
A11=178.44784333
A12=178.83149888
D4=179.99706351
D5=0.02756129
D6=-179.9992193
D7=-124.01050329
D8=124.00408318
D9=179.98319715
D10=-4.26310889
D11=179.91352068
D12=173.6592272

23. Aza-Myers transition state **TS1b** (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
Variables:
R2=1.30889318
R3=1.36237976
R4=1.4148098
R5=1.36542039
R6=1.08710195
R7=1.08975013
R8=1.25527859
R9=1.33140704
R10=1.07098832
R11=1.08912934
R12=1.08772109
A3=122.08352238
A4=119.55163963
A5=130.78400676
A6=117.8652432
A7=113.20023633
A8=136.41242464
A9=145.22187689
A10=148.23619991
A11=121.07806402
A12=122.22056765
D4=5.69743127
D5=-16.44564464
D6=-178.29751109
D7=172.769366
D8=0.8214244
D9=-152.49896757
D10=160.3210533
D11=46.23086162
D12=173.54549976

24. Aza-Schmittel singlet diradical **6b**, syn-addition (UB3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
Variables:
R2=1.32055453
R3=1.36203344
R4=1.4816384
R5=1.43483205
R6=1.0841264
R7=1.08411572
R8=1.3207959
R9=1.35990626
R10=1.08241816
R11=1.08577038
R12=1.08482638
A3=107.96659394
A4=112.20663617
A5=113.19381572
A6=122.38343484
A7=120.64290565
A8=127.57077775
A9=128.53988339
A10=137.27527353
A11=120.94728957
A12=121.62972876
D4=-0.007071
D5=0.00182166
D6=-179.99139115
D7=-179.99935822
D8=-179.99136304
D9=-179.99725131
D10=0.0012988
D11=0.00047901
D12=179.99985387

25. Aza-Schmittel triplet diradical **6b**, syn-addition (UB3LYP/6-31G*)

C
C,1,R2
C,1,R3,2,A3
C,1,R4,2,A4,3,180.,0
N,2,R5,1,A5,3,0.,0
C,3,R6,1,A6,2,0.,0
C,3,R7,1,A7,6,180.,0
H,2,R8,1,A8,5,180.,0
H,4,R9,1,A9,2,0.,0
H,4,R10,1,A10,9,180.,0
H,6,R11,3,A11,1,180.,0
H,7,R12,3,A12,1,180.,0
Variables:
R2=1.45211889
R3=1.50158026
R4=1.34779011
R5=1.33485674
R6=1.45353193
R7=1.33388382
R8=1.08488174
R9=1.0863196
R10=1.08553556
R11=1.08336456
R12=1.08211823
A3=103.39742579
A4=128.17969661
A5=112.87058361
A6=103.26329094
A7=128.19058081
A8=125.71536253
A9=121.06521822
A10=121.70048275
A11=126.07995833
A12=136.86506867

26. Aza-Schmittel cyclization transition state **TS2b**, syn-addition (B3LYP/6-31G*)

```
N
 C,1,R2
 C,1,R3,2,A3
 C,2,R4,1,A4,3,D4,0
 C,3,R5,1,A5,2,D5,0
 H,2,R6,1,A6,4,D6,0
 H,3,R7,1,A7,5,D7,0
 C,4,R8,2,A8,1,D8,0
 C,5,R9,3,A9,1,D9,0
 H,8,R10,4,A10,2,D10,0
 H,9,R11,5,A11,3,D11,0
 H,9,R12,5,A12,11,D12,0
     Variables:
 R2=1.30546656
 R3=1.36293407
 R4=1.46032731
 R5=1.38361367
 R6=1.08659073
 R7=1.08629641
 R8=1.25798151
 R9=1.32792599
 R10=1.07121429
 R11=1.08698813
 R12=1.08737959
 A3=110.48390769
 A4=118.0458579
 A5=114.71914562
 A6=120.89286528
 A7=118.98141986
 A8=145.82830199
 A9=143.31710331
 A10=155.34715473
 A11=121.67424727
 A12=120.03078809
 D4=-2.72261391
 D5=-16.925332
 D6=174.60797084
 D7=166.73942114
 D8=-177.12795281
 D9=-141.56854923
 D10=42.74921397
 D11=10.37308439
 D12=175.72257079
```

27. Aza-Schmittel singlet diradical **6b**, anti-addition (UB3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,5,R8,3,A8,1,D8,0
C,4,R9,2,A9,1,D9,0
H,8,R10,5,A10,3,D10,0
H,8,R11,5,A11,10,D11,0
H,9,R12,4,A12,2,D12,0
Variables:
R2=1.32158351
R3=1.36149401
R4=1.47551483
R5=1.43553092
R6=1.08389799
R7=1.08447298
R8=1.35923872
R9=1.3199704
R10=1.08571812
R11=1.08529244
R12=1.08215111
A3=107.74060436
A4=112.57193921
A5=113.4521757
A6=122.30897666
A7=120.70852415
A8=128.46230206
A9=127.07205945
A10=120.89708414
A11=122.02847005
A12=138.60501194
D4=0.01245682
D5=-0.00696582
D6=179.98765209
D7=-179.99765545
D8=-179.99852366
D9=179.99266132
D10=-0.0011495
D11=179.99990119
D12=179.99692378

28. Aza-Schmittel triplet diradica **6b**, anti-addition (UB3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,0.,0
C,3,R5,1,A5,2,0.,0
H,2,R6,1,A6,3,180.,0
H,3,R7,1,A7,2,180.,0
C,5,R8,3,A8,1,180.,0
C,4,R9,2,A9,1,180.,0
H,8,R10,5,A10,3,0.,0
H,8,R11,5,A11,3,180.,0
H,9,R12,4,A12,2,180.,0
Variables:
R2=1.34861596
R3=1.33551526
R4=1.44898447
R5=1.45277115
R6=1.08291182
R7=1.08573708
R8=1.34715441
R9=1.33242823
R10=1.08682657
R11=1.0852009
R12=1.08344128
A3=107.89554924
A4=112.76414877
A5=113.019771
A6=121.41460742
A7=121.45179036
A8=128.05785223
A9=127.89967396
A10=120.96324647
A11=122.16871889
A12=138.03028149

29. Aza-Schmittel cyclization transition state **TS2b**, anti-addition (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
H,8,R10,4,A10,2,D10,0
H,9,R11,5,A11,3,D11,0
H,9,R12,5,A12,11,D12,0
Variables:
R2=1.30551349
R3=1.36779373
R4=1.45202167
R5=1.37771052
R6=1.08635512
R7=1.08686694
R8=1.26947278
R9=1.32896011
R10=1.07698742
R11=1.08744553
R12=1.08772106
A3=110.02462607
A4=118.39920384
A5=116.18146647
A6=120.73480058
A7=118.52608266
A8=140.27296353
A9=143.89690255
A10=141.39897389
A11=121.75410437
A12=120.87743866
D4=-2.07834764
D5=-16.12116311
D6=175.69089151
D7=167.06125247
D8=-170.32121858
D9=-142.81993065
D10=-161.28459702
D11=15.80349329
D12=175.45920522

30. (*Z*)-7-methyl-4-aza-3-ene-1,6-diyne **2c** (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
H,3,R8,1,A8,5,D8,0
C,4,R9,2,A9,1,D9,0
C,5,R10,3,A10,1,D10,0
C,10,R11,5,A11,3,D11,0
H,9,R12,4,A12,2,D12,0
H,11,R13,10,A13,5,D13,0
H,11,R14,10,A14,13,D14,0
H,11,R15,10,A15,13,D15,0
Variables:
R2=1.27843143
R3=1.46793141
R4=1.43900017
R5=1.46534818
R6=1.0932846
R7=1.10086713
R8=1.09973387
R9=1.2105557
R10=1.20879502
R11=1.46057906
R12=1.06705318
R13=1.09683949
R14=1.09681275
R15=1.09688317
A3=118.81258344
A4=128.26474183
A5=110.9200742
A6=116.6377717
A7=112.94382072
A8=106.37925469
A9=176.9016751
A10=179.36789903
A11=179.67551232
A12=179.19260376
A13=111.41324923
A14=110.98950821
A15=111.42142769
D4=-0.27570254
D5=124.72406704

D6=179.86774279
D7=-124.03849666
D8=118.79014107
D9=-179.54329857
D10=-145.00159597
D11=131.90806048
D12=179.8782276
D13=131.62616383
D14=-119.84041393
D15=120.28850041

31. (*Z*)-7-methyl-aza-enyne allene (s-cis) **3c** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,3,R4,1,A4,2,D4,0
C,2,R5,1,A5,3,D5,0
H,2,R6,1,A6,5,D6,0
H,3,R7,1,A7,4,D7,0
C,4,R8,3,A8,1,D8,0
C,5,R9,2,A9,1,D9,0
C,8,R10,4,A10,3,D10,0
H,8,R11,4,A11,10,D11,0
H,9,R12,5,A12,2,D12,0
H,10,R13,8,A13,4,D13,0
H,10,R14,8,A14,13,D14,0
H,10,R15,8,A15,13,D15,0
Variables:
R2=1.28465883
R3=1.40724832
R4=1.31898445
R5=1.43273357
R6=1.09258165
R7=1.08997016
R8=1.30733752
R9=1.21123864
R10=1.5106164
R11=1.09277897
R12=1.06676246
R13=1.09760579
R14=1.09308157
R15=1.09763585
A3=122.45593674
A4=126.89180843
A5=128.8209564
A6=116.14384908
A7=112.99405658
A8=175.98426733
A9=174.47279585
A10=125.37873839
A11=118.24667093
A12=178.14192432
A13=110.65982473
A14=111.37385742
A15=110.61845287
D4=41.27668886

D5=4.43148371
D6=178.32498121
D7=173.19236516
D8=93.22270087
D9=160.74061719
D10=-7.74181867
D11=-179.45865709
D12=-168.00282324
D13=121.07757465
D14=-120.79235492
D15=118.48357445

32. (*Z*)-7-methyl-aza-enyne allene (s-trans) **3c** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
C,9,R10,5,A10,3,D10,0
H,8,R11,4,A11,2,D11,0
H,9,R12,5,A12,10,D12,0
H,10,R13,9,A13,5,D13,0
H,10,R14,9,A14,13,D14,0
H,10,R15,9,A15,13,D15,0
Variables:
R2=1.29018608
R3=1.39902204
R4=1.43255906
R5=1.32129294
R6=1.09139264
R7=1.09397717
R8=1.2116155
R9=1.30494988
R10=1.51094205
R11=1.06685379
R12=1.09261198
R13=1.0971994
R14=1.09295479
R15=1.09736536
A3=119.27823852
A4=127.62399372
A5=120.89599112
A6=116.58476603
A7=119.42712678
A8=177.80562564
A9=178.82349093
A10=125.23333514
A11=179.60140766
A12=118.30531515
A13=110.47697759
A14=111.39499689
A15=110.60201991
D4=0.0203996

D5=-179.90352634
D6=179.97138841
D7=179.91345499
D8=179.72417438
D9=-174.36354854
D10=84.57559954
D11=-177.19925987
D12=179.56637636
D13=120.26355099
D14=-120.62656653
D15=118.51717726

33. (*E*)-7-methyl-4-aza-3-ene-1,6-diyne **2c** (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
H,3,R8,1,A8,5,D8,0
C,4,R9,2,A9,1,D9,0
C,5,R10,3,A10,1,D10,0
C,10,R11,5,A11,3,D11,0
H,9,R12,4,A12,2,D12,0
H,11,R13,10,A13,5,D13,0
H,11,R14,10,A14,13,D14,0
H,11,R15,10,A15,13,D15,0
Variables:
R2=1.27683959
R3=1.46585713
R4=1.43117713
R5=1.46554379
R6=1.10171609
R7=1.10508329
R8=1.09947434
R9=1.20927893
R10=1.20876047
R11=1.46046181
R12=1.06670739
R13=1.0967487
R14=1.09671986
R15=1.09681189
A3=116.13759445
A4=121.9872683
A5=111.41092224
A6=122.49091291
A7=112.1919278
A8=106.93724413
A9=176.80968407
A10=179.52665553
A11=179.65162464
A12=178.39328333
A13=111.39586436
A14=110.95233112
A15=111.40141399
D4=179.50186862

D5=120.21398237
D6=-179.9348679
D7=-123.65399715
D8=119.42886446
D9=-177.78384965
D10=-127.99342606
D11=130.70536545
D12=-179.20296625
D13=116.3778018
D14=-119.84724299
D15=120.29188282

34. (*E*)-7-methyl-aza-enyne allene (s-trans) **3c** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,3,R5,1,A5,2,D5,0
H,2,R6,1,A6,4,D6,0
H,3,R7,1,A7,5,D7,0
C,4,R8,2,A8,1,D8,0
C,5,R9,3,A9,1,D9,0
C,9,R10,5,A10,3,D10,0
H,8,R11,4,A11,2,D11,0
H,9,R12,5,A12,10,D12,0
H,10,R13,9,A13,5,D13,0
H,10,R14,9,A14,13,D14,0
H,10,R15,9,A15,13,D15,0
Variables:
R2=1.28785722
R3=1.39803422
R4=1.42445189
R5=1.32084948
R6=1.10080179
R7=1.09750938
R8=1.2106261
R9=1.30504964
R10=1.51079572
R11=1.06657067
R12=1.09268198
R13=1.09716458
R14=1.09288895
R15=1.09735732
A3=116.64379464
A4=122.02041872
A5=121.90449792
A6=122.0561959
A7=118.63931793
A8=176.76821375
A9=178.80750065
A10=125.24892866
A11=178.30512461
A12=118.35465003
A13=110.45573585
A14=111.42400313
A15=110.60071958
D4=-179.97492485

D5=-179.92090574
D6=179.98912091
D7=179.93309467
D8=-179.68221482
D9=-173.45035498
D10=83.78413864
D11=-179.62539091
D12=179.37695509
D13=120.07369879
D14=-120.62680895
D15=118.47384765

35. (*E*)-7-methyl-aza-enyne allene (s-cis) **3c** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,3,R4,1,A4,2,D4,0
C,2,R5,1,A5,3,D5,0
H,2,R6,1,A6,5,D6,0
H,3,R7,1,A7,4,D7,0
C,4,R8,3,A8,1,D8,0
C,5,R9,2,A9,1,D9,0
C,8,R10,4,A10,3,D10,0
H,8,R11,4,A11,10,D11,0
H,9,R12,5,A12,2,D12,0
H,10,R13,8,A13,4,D13,0
H,10,R14,8,A14,13,D14,0
H,10,R15,8,A15,13,D15,0
Variables:
R2=1.28470679
R3=1.40978284
R4=1.32000048
R5=1.42608504
R6=1.09883111
R7=1.08925592
R8=1.30838631
R9=1.2103972
R10=1.5110524
R11=1.09291633
R12=1.0666115
R13=1.09749101
R14=1.09295976
R15=1.09744319
A3=118.81612805
A4=126.27076372
A5=121.68837883
A6=122.04875443
A7=113.51224986
A8=176.26016717
A9=176.66501773
A10=125.32412125
A11=118.47507109
A12=178.50649862
A13=110.53668984
A14=111.3835453
A15=110.625166
D4=33.2340497

D5=-176.64577724
D6=179.95156822
D7=175.52108033
D8=94.20634205
D9=-179.69825844
D10=-6.49884198
D11=179.76722259
D12=179.38627095
D13=120.67166871
D14=-120.78564046
D15=118.41336954

36. (*Z*)-Aza-enyne allene (s-cis) **3d** (B3LYP/6-31G*)
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,4,D5,0
C,3,R6,1,A6,2,D6,0
H,3,R7,1,A7,6,D7,0
C,5,R8,2,A8,1,D8,0
C,4,R9,2,A9,1,D9,0
C,4,R10,2,A10,9,D10,0
C,6,R11,3,A11,1,D11,0
C,9,R12,4,A12,2,D12,0
C,10,R13,4,A13,2,D13,0
H,8,R14,5,A14,2,D14,0
H,9,R15,4,A15,12,D15,0
H,10,R16,4,A16,13,D16,0
H,11,R17,6,A17,3,D17,0
H,11,R18,6,A18,17,D18,0
C,12,R19,9,A19,4,D19,0
H,12,R20,9,A20,19,D20,0
H,13,R21,10,A21,4,D21,0
H,19,R22,12,A22,9,D22,0
Variables:
R2=1.28978309
R3=1.40484842
R4=1.50068184
R5=1.44092086
R6=1.31813848
R7=1.09039113
R8=1.20981216
R9=1.40330006
R10=1.40183613
R11=1.30529423
R12=1.3929088
R13=1.39472366
R14=1.06663494
R15=1.08509569
R16=1.0860498
R17=1.08988216
R18=1.08995369
R19=1.39751609
R20=1.08669827
R21=1.08664025
R22=1.08669366
A3=124.29005748

A4=128.3931599
A5=116.32171594
A6=126.89807596
A7=113.22331631
A8=177.85633765
A9=120.92871197
A10=119.96224668
A11=177.5769618
A12=120.36513546
A13=120.51187055
A14=178.50911936
A15=119.66030474
A16=119.39036129
A17=122.06401721
A18=121.41647177
A19=120.25055244
A20=119.64881229
A21=119.71014753
A22=120.10304048
D4=8.96136801
D5=178.12581078
D6=46.6262053
D7=170.32820681
D8=167.57923929
D9=44.93721158
D10=176.65256599
D11=94.0859331
D12=177.51254277
D13=-178.3929201
D14=179.0915658
D15=-179.48638705
D16=-179.94517941
D17=-11.95366321
D18=-179.36381888
D19=0.38129062
D20=-179.69110226
D21=-179.25241157
D22=179.77180577

37. (*Z*)-Aza-enyne allene (s-trans) **3d** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,4,D5,0
C,3,R6,1,A6,2,D6,0
H,3,R7,1,A7,6,D7,0
C,5,R8,2,A8,1,D8,0
C,4,R9,2,A9,1,D9,0
C,4,R10,2,A10,9,D10,0
C,6,R11,3,A11,1,D11,0
C,9,R12,4,A12,2,D12,0
C,10,R13,4,A13,2,D13,0
H,8,R14,5,A14,2,D14,0
H,9,R15,4,A15,12,D15,0
H,10,R16,4,A16,13,D16,0
H,11,R17,6,A17,3,D17,0
H,11,R18,6,A18,17,D18,0
C,12,R19,9,A19,4,D19,0
H,12,R20,9,A20,19,D20,0
H,13,R21,10,A21,4,D21,0
H,19,R22,12,A22,9,D22,0
Variables:
R2=1.29617872
R3=1.3946655
R4=1.49847398
R5=1.43814963
R6=1.32247916
R7=1.09274032
R8=1.21030754
R9=1.40439515
R10=1.40403652
R11=1.30285849
R12=1.39459997
R13=1.39330033
R14=1.06654
R15=1.0857841
R16=1.08606032
R17=1.08964315
R18=1.0895576
R19=1.39592645
R20=1.08663081
R21=1.08664042
R22=1.08663741

A3=121.33331601
A4=127.82771074
A5=116.62891186
A6=120.90172297
A7=120.47683517
A8=177.65569781
A9=121.16143583
A10=119.96609351
A11=178.27400719
A12=120.4809619
A13=120.57064804
A14=178.29496803
A15=119.62421998
A16=119.26236207
A17=121.82628212
A18=121.63185182
A19=120.19200432
A20=119.66119795
A21=119.73375327
A22=120.11031644
D4=6.46447476
D5=179.67725259
D6=-171.26212416
D7=-177.83964158
D8=172.83602514
D9=46.53842623
D10=177.87024999
D11=154.91392084
D12=178.84047954
D13=-179.57066829
D14=-175.50205478
D15=-178.60478473
D16=-179.91545955
D17=-63.32031184
D18=-179.25355707
D19=0.23395526
D20=-179.63278161
D21=-179.24347073
D22=179.80434998

38. (*E*)-Aza-enyne allene (s-cis) **3d** (B3LYP/6-31G*)

N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,4,D5,0
C,3,R6,1,A6,2,D6,0
H,3,R7,1,A7,6,D7,0
C,5,R8,2,A8,1,D8,0
C,6,R9,3,A9,1,D9,0
C,4,R10,2,A10,1,D10,0
C,4,R11,2,A11,10,D11,0
C,10,R12,4,A12,2,D12,0
C,11,R13,4,A13,2,D13,0
H,8,R14,5,A14,2,D14,0
H,9,R15,6,A15,3,D15,0
H,9,R16,6,A16,15,D16,0
H,10,R17,4,A17,12,D17,0
H,11,R18,4,A18,13,D18,0
C,12,R19,10,A19,4,D19,0
H,12,R20,10,A20,19,D20,0
H,13,R21,11,A21,4,D21,0
H,19,R22,12,A22,10,D22,0
Variables:
R2=1.29337023
R3=1.39790761
R4=1.48925989
R5=1.44224903
R6=1.32017458
R7=1.09045294
R8=1.21006733
R9=1.30492827
R10=1.40588284
R11=1.40294864
R12=1.39046444
R13=1.39469368
R14=1.06688997
R15=1.08972105
R16=1.08985265
R17=1.08432856
R18=1.08510545
R19=1.3989648
R20=1.08680133
R21=1.08668177
R22=1.08678407

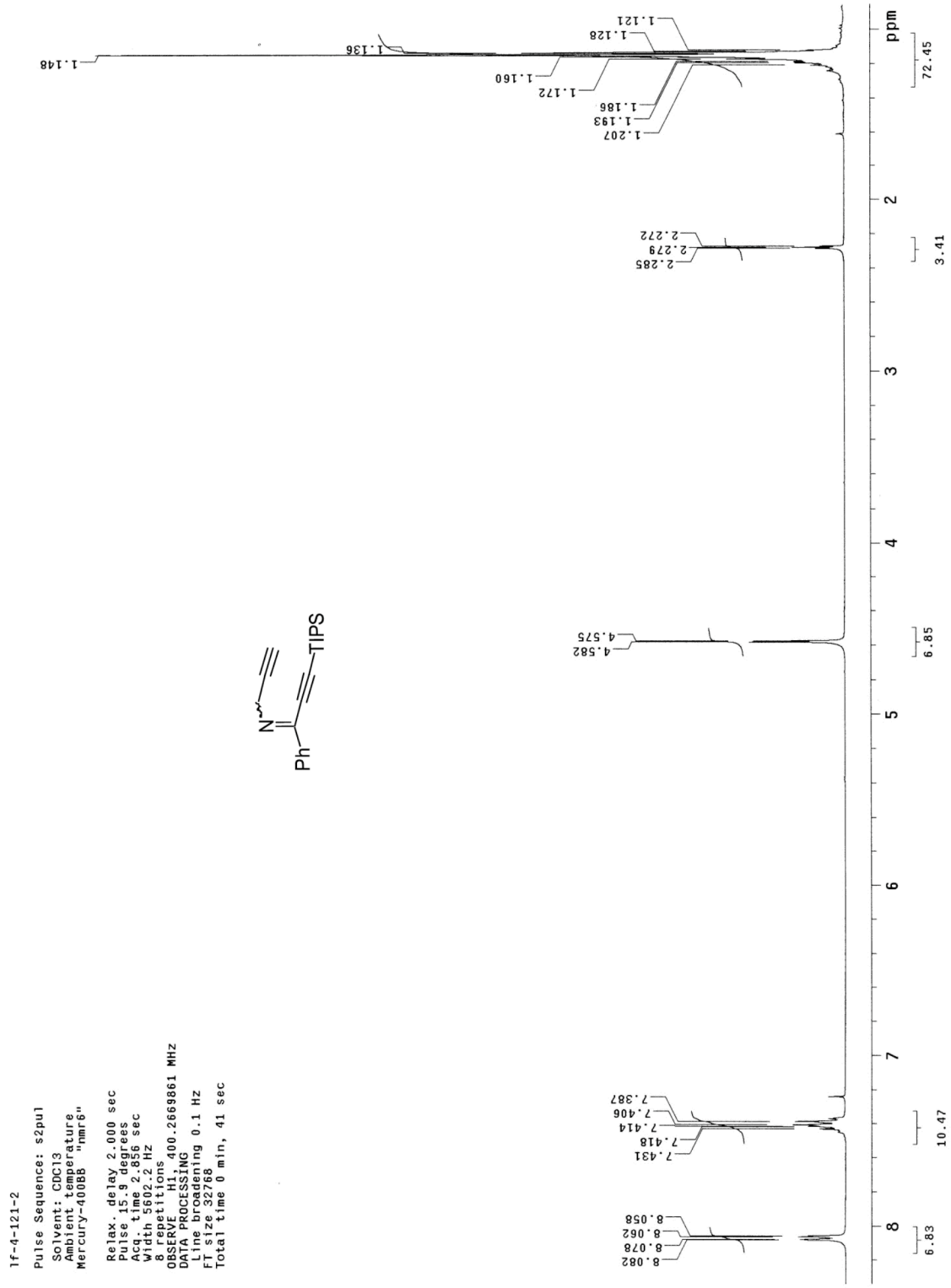
A3=124.17172109
A4=118.53714541
A5=123.99808097
A6=127.69709319
A7=113.22527357
A8=177.44270823
A9=175.88553853
A10=119.73035688
A11=121.34081776
A12=120.40053238
A13=120.51186951
A14=178.49941362
A15=121.56327591
A16=121.94628785
A17=118.56694983
A18=119.54848375
A19=120.32053372
A20=119.66579584
A21=119.64043678
A22=120.14951225
D4=-176.62591721
D5=-178.16937886
D6=41.0805814
D7=172.8115088
D8=124.91552061
D9=105.90115728
D10=0.86903653
D11=179.98452355
D12=-179.88085308
D13=179.92492178
D14=-147.60008084
D15=159.98922185
D16=179.08951489
D17=179.91305189
D18=179.98145325
D19=-0.10398817
D20=-179.94878822
D21=179.99000519
D22=-179.91324673

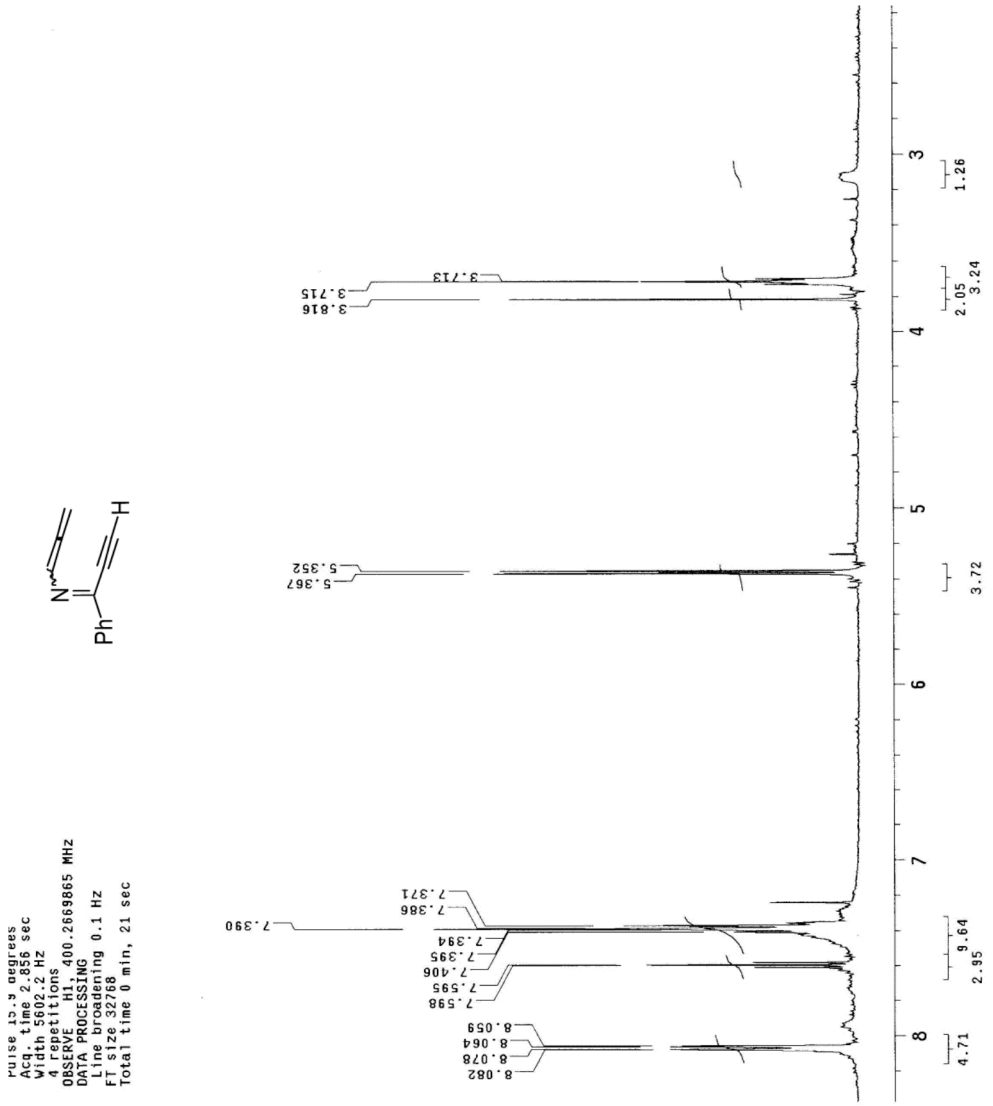
39. (*E*)-Aza-enyne allene (s-trans) **3d** (B3LYP/6-31G*)

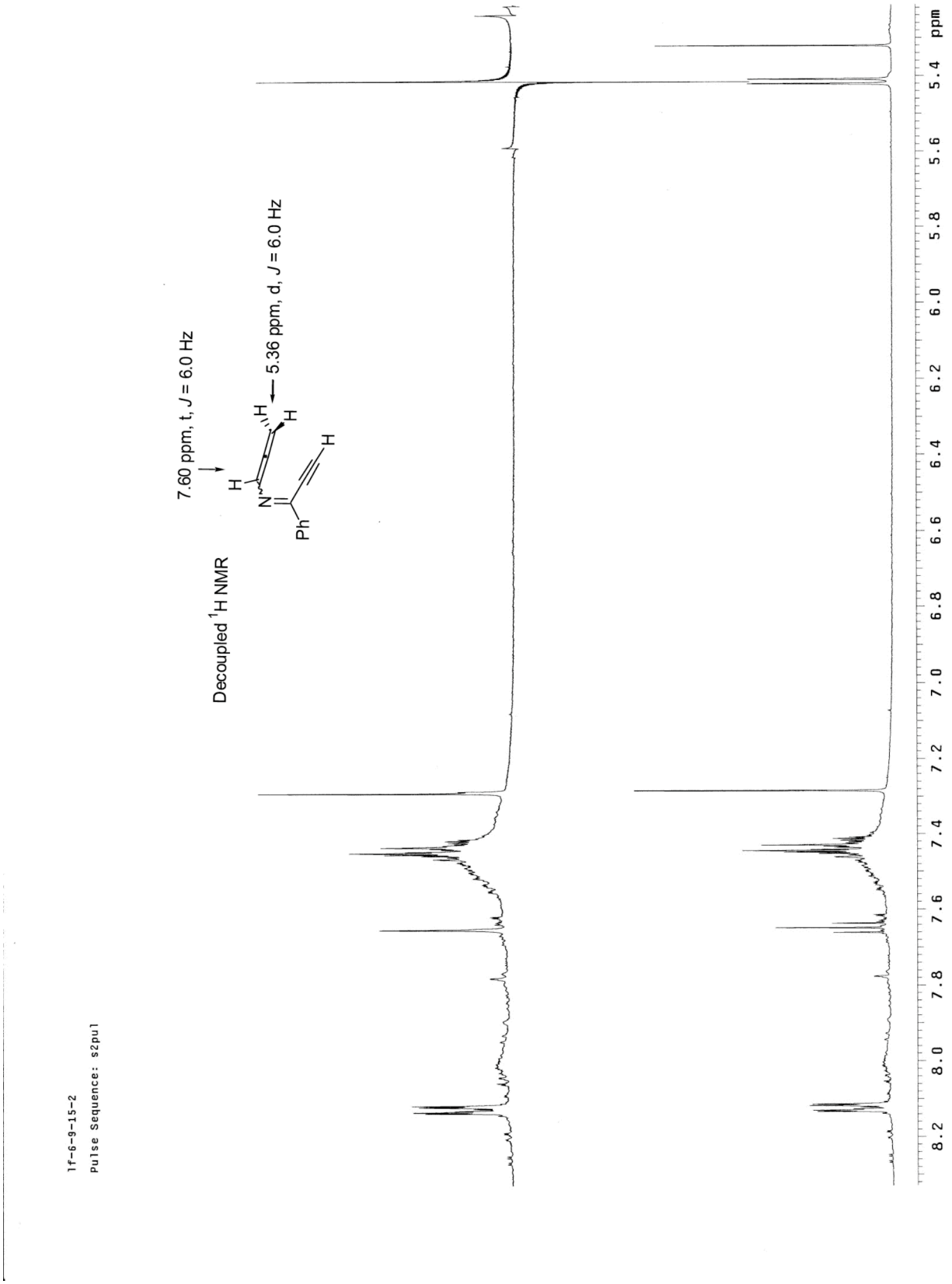
N
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,4,D5,0
C,3,R6,1,A6,2,D6,0
H,3,R7,1,A7,6,D7,0
C,5,R8,2,A8,1,D8,0
C,6,R9,3,A9,1,D9,0
C,4,R10,2,A10,1,D10,0
C,4,R11,2,A11,10,D11,0
C,10,R12,4,A12,2,D12,0
C,11,R13,4,A13,2,D13,0
H,8,R14,5,A14,2,D14,0
H,9,R15,6,A15,3,D15,0
H,9,R16,6,A16,15,D16,0
H,10,R17,4,A17,12,D17,0
H,11,R18,4,A18,13,D18,0
C,12,R19,10,A19,4,D19,0
H,12,R20,10,A20,19,D20,0
H,13,R21,11,A21,4,D21,0
H,19,R22,12,A22,10,D22,0
Variables:
R2=1.29876794
R3=1.38957279
R4=1.48456048
R5=1.44262179
R6=1.32294319
R7=1.09347187
R8=1.21070155
R9=1.30265371
R10=1.40619532
R11=1.40344613
R12=1.39043639
R13=1.39440569
R14=1.06704055
R15=1.08965293
R16=1.08965315
R17=1.08433801
R18=1.08545594
R19=1.39904461
R20=1.08681986
R21=1.08670734
R22=1.08678864

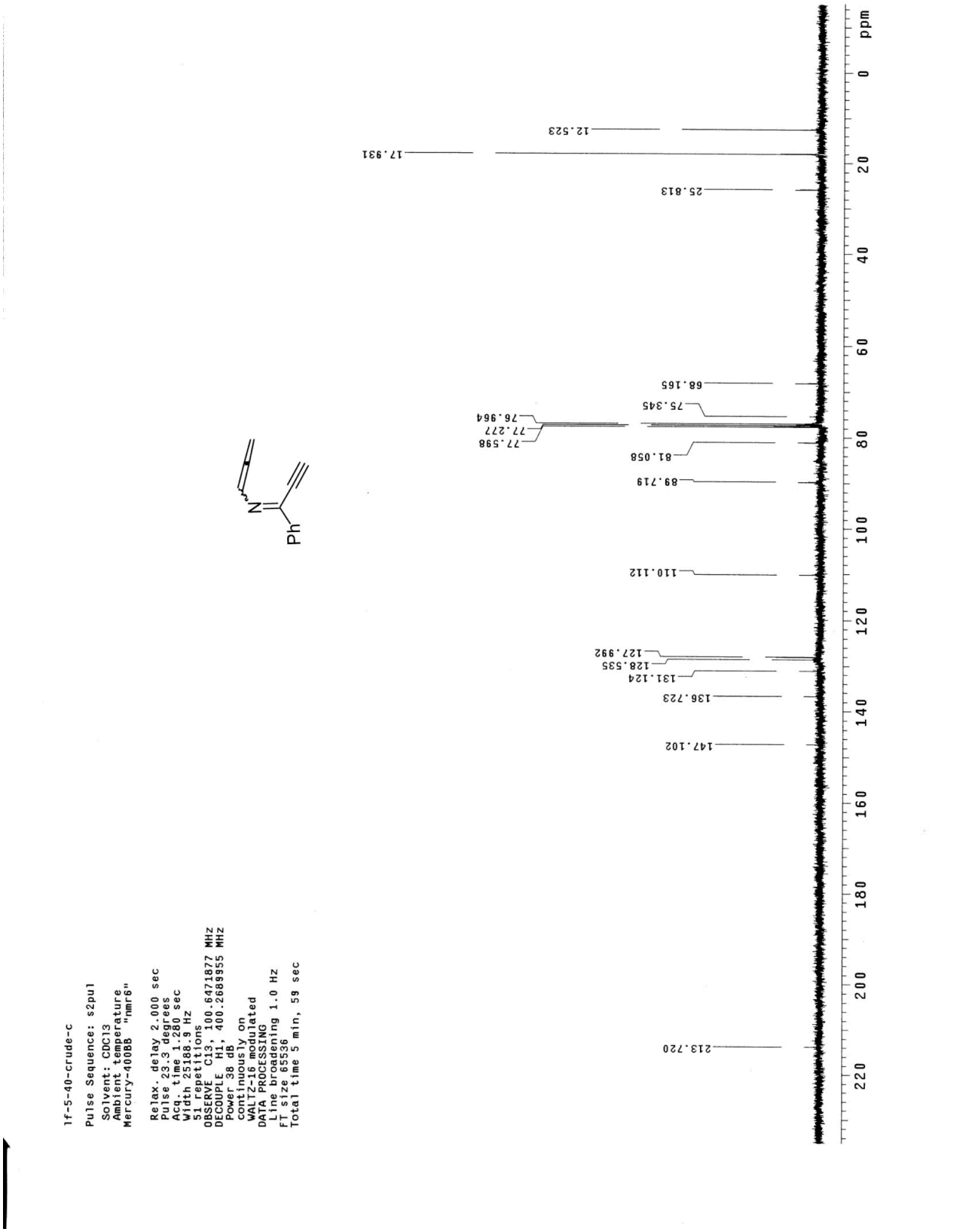
A3=120.72979337
A4=118.95632876
A5=123.09054417
A6=121.04472341
A7=119.91998607
A8=178.63044296
A9=178.48884371
A10=119.83248526
A11=121.22665207
A12=120.36730789
A13=120.5094836
A14=179.7459828
A15=121.72502318
A16=121.72506863
A17=118.54001404
A18=119.5452563
A19=120.34297787
A20=119.64504574
A21=119.65176927
A22=120.15550071
D4=179.99546523
D5=-179.99503863
D6=-179.99416833
D7=179.98759851
D8=-0.54097139
D9=179.98108396
D10=0.00297418
D11=-179.99989872
D12=179.99983122
D13=-179.99985489
D14=178.83666448
D15=90.31250121
D16=179.40527417
D17=-179.99980464
D18=179.9997657
D19=0.00014808
D20=180.
D21=179.99988857
D22=180.

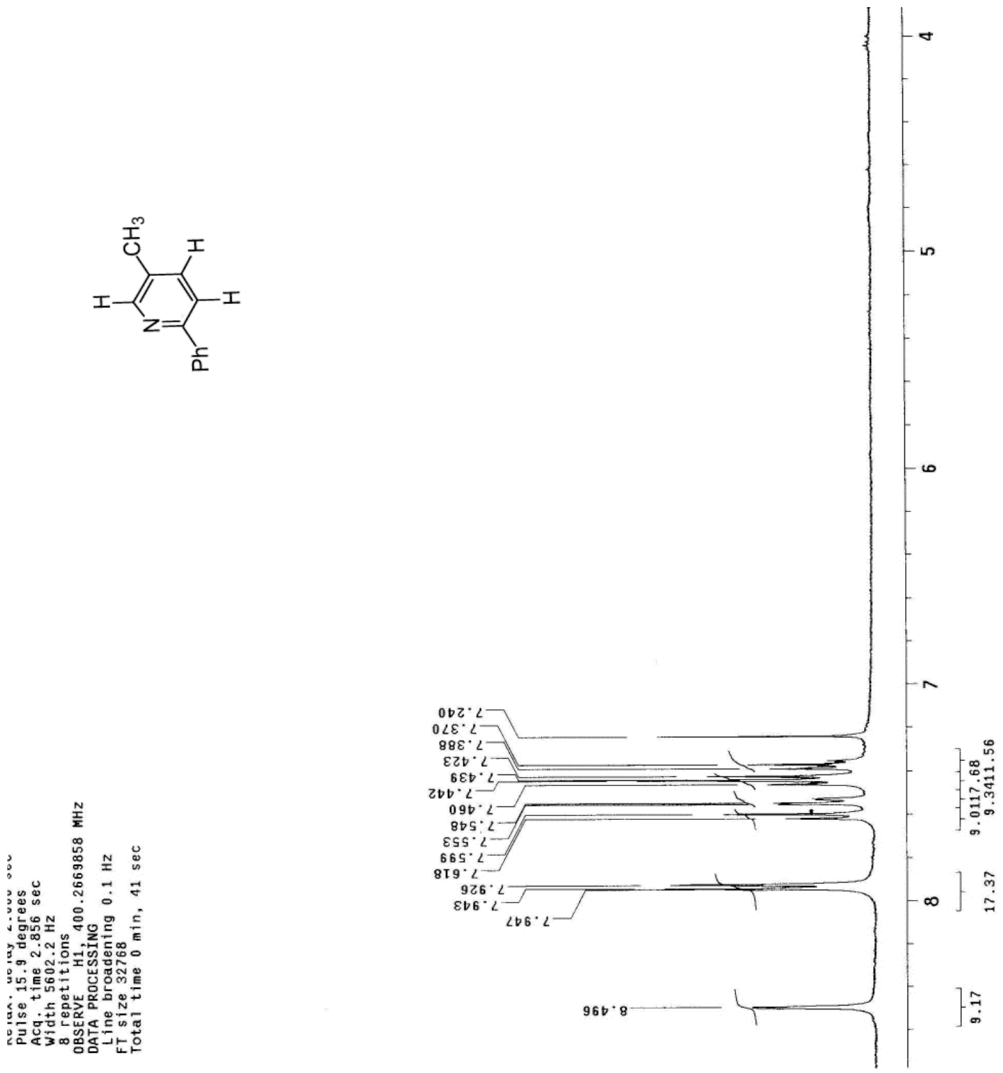
D. NMRs for all compounds.

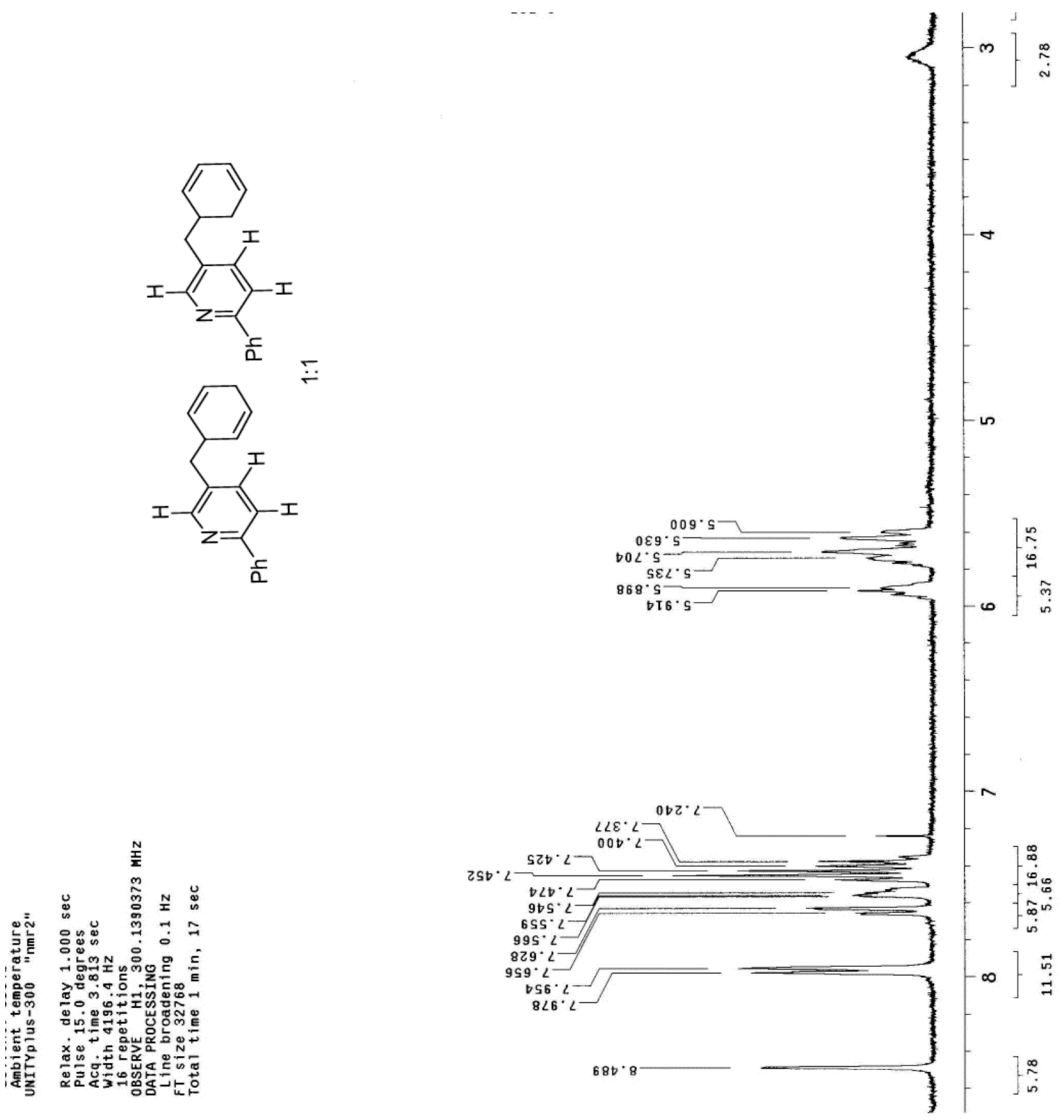


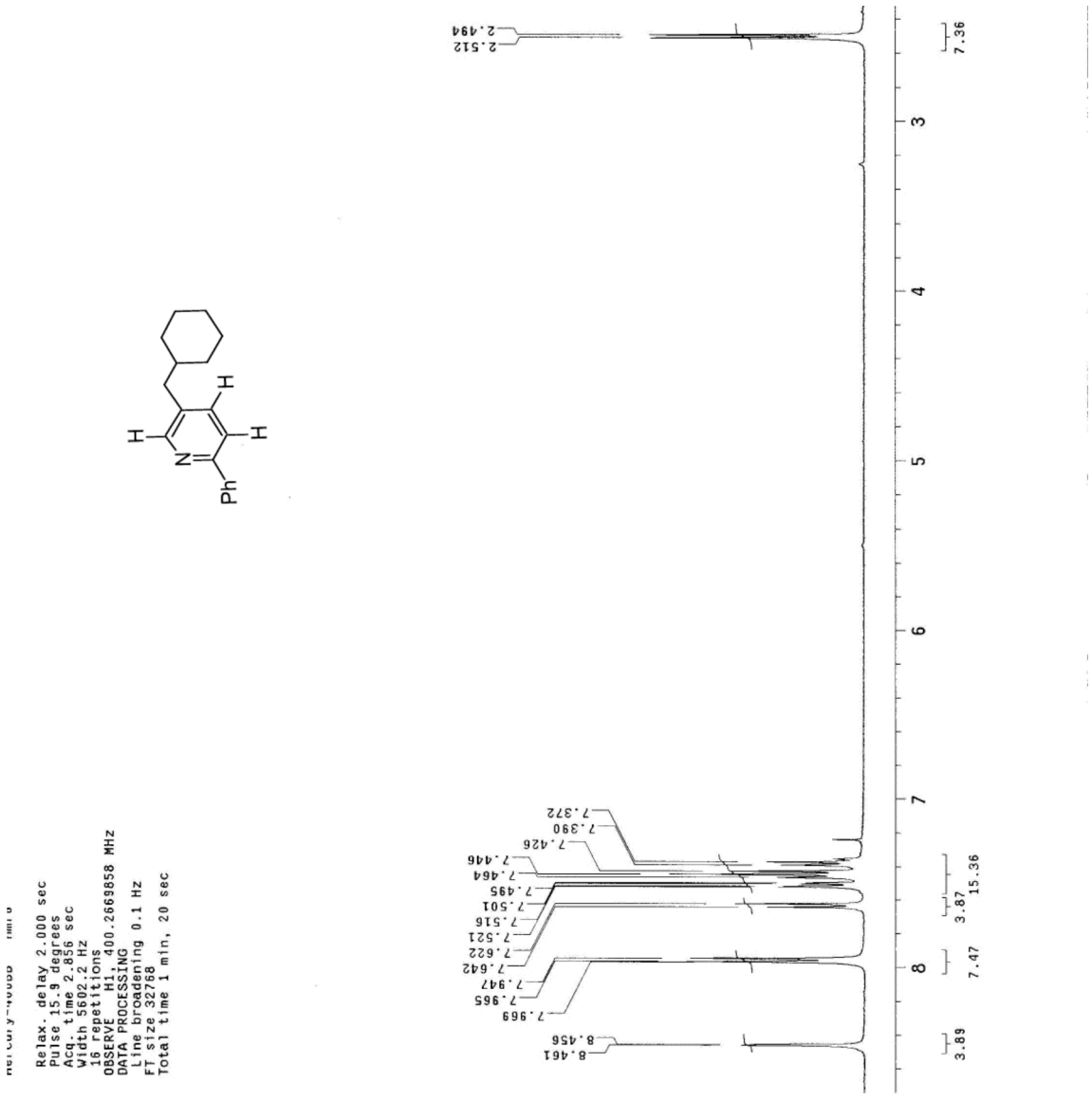

Pulse 45.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
4 repetitions
OBSERVE H1, 400.2669865 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 21 sec
Ph
N
H
8.082
8.078
8.064
8.059
7.598
7.595
7.406
7.395
7.394
7.390
7.386
7.371
5.367
5.352
3.816
3.715
3.713
4.71
2.95
9.64
3.72
2.05
3.24
1.26

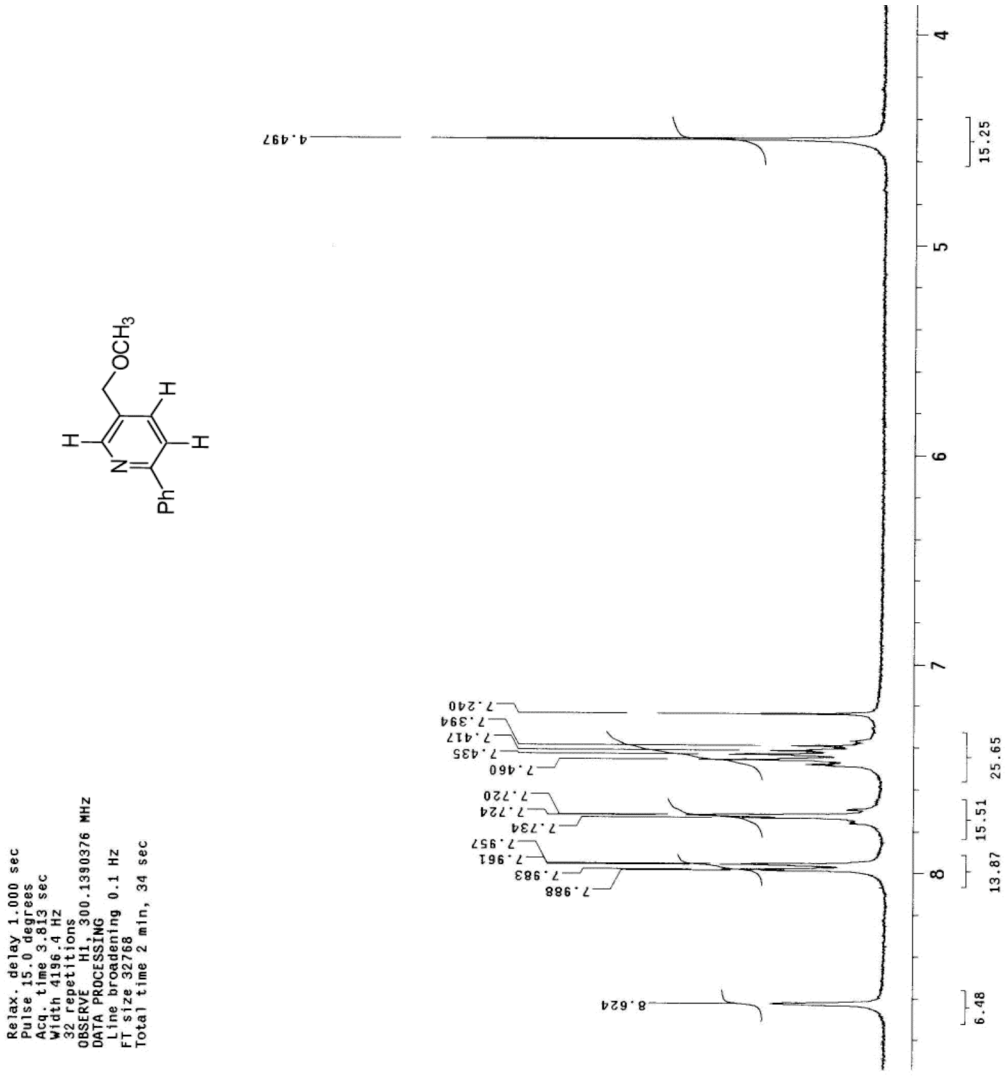

1f-6-9-15-2
Pulse Sequence: s2pul
Decoupled ^{1}H NMR
7.60 ppm, t, J = 6.0 Hz
5.36 ppm, d, J = 6.0 Hz
H
H
H
H
N
Ph
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
ppm

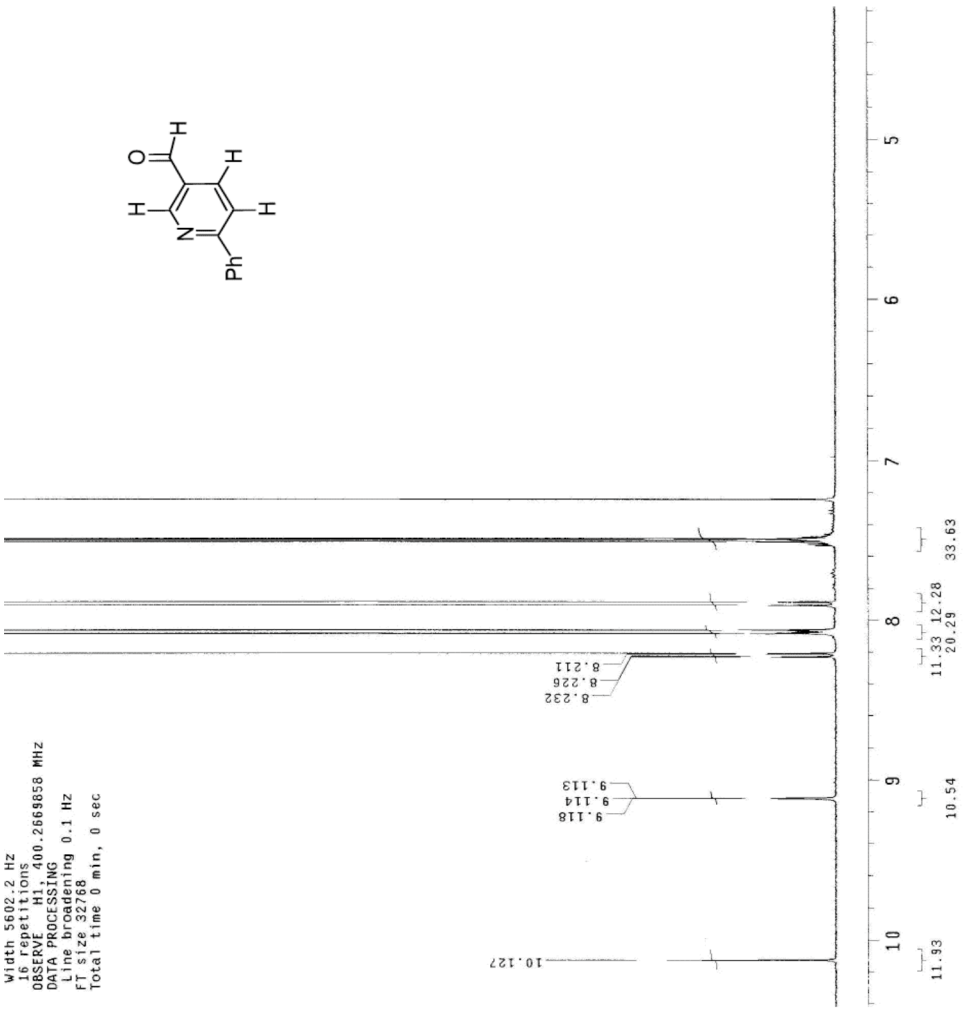

1f-5-40-crude-c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"
Relax. delay 2.000 sec
Pulse 23.3 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
51 repetitions
OBSERVE C13, 100.6471877 MHz
DECOUPLE H1, 400.2689955 MHz
Power 38 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 5 min, 59 sec
N
Ph
12.523
17.931
25.813
68.165
75.345
76.964
77.277
77.598
81.058
89.719
110.112
127.992
128.535
131.124
136.723
147.102
213.720
ppm
0
20
40
60
80
100
120
140
160
180
200
220


Pulse 15.9 degrees
Acq time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1 400.2669858 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 41 sec
CH3
H
H
H
N
Ph
8.496
7.947
7.943
7.926
7.618
7.599
7.553
7.548
7.460
7.442
7.439
7.423
7.388
7.370
7.240
8
7
6
5
4
9.17
17.37
9.0117.68
9.3411.56


Ambient temperature
UNITYplus-300 "nmr2"
Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4186.4 Hz
16 repetitions
OBSERVE H1, 300.1380373 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 17 sec
1:1
Ph
8.489
7.978
7.954
7.656
7.628
7.566
7.559
7.546
7.474
7.452
7.425
7.400
7.377
7.240
5.914
5.898
5.735
5.704
5.630
5.600
5.78
11.51
5.87
5.66
16.88
5.37
16.75
2.78


Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
16 repetitions
OBSERVE H1, 400.2669858 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 20 sec
H
H
H
N
Ph
2.512
2.494
7.372
7.390
7.426
7.446
7.464
7.495
7.501
7.516
7.521
7.622
7.642
7.947
7.965
7.969
8.456
8.461
7.36
3.87
15.36
7.47
3.89
1
2
3
4
5
6
7
8


Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
32 repetitions
OBSERVE H1, 300.1390376 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 2 min, 34 sec
OCH3
H
H
H
N
Ph
8.624
7.988
7.983
7.961
7.957
7.734
7.724
7.720
7.460
7.435
7.417
7.394
7.240
4.497
6.48
13.87
15.51
25.65
15.25
8
7
6
5
4


Width 5602.2 Hz
16 repetitions
OBSERVE H1, 400.2669658 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec
10.127
9.118
9.114
9.113
8.232
8.226
8.211
11.93
10.54
11.33
12.28
20.29
33.63
10
9
8
7
6
5
O
H
H
H
N
Ph