Electronic Supplementary Material (ESI) for Chemical Science.

On the Factors That Control the Reactivity of *meta*–Benzynes

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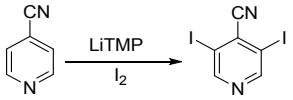
I. Synthesis of precursors

Methods and materials. All reagents were used as received. Commercially available chemicals were purchased from Sigma-Aldrich Chemical Company (Milwaukee, WI), Alfa Aesar (Ward Hill, MA), or Acros Organics (Pittsburgh, PA). ^{1}H and ^{13}C NMR spectra were acquired on either a Varian Inova (300 MHz; 75 MHz) or a Bruker ARX (400 MHz; 100 MHz) and chemical shifts are reported relative to the residual solvent peak. In reporting spectral data the format (δ) chemical shift (multiplicity, J values in Hz, integration) was used with the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Infrared spectra were recorded on a Thermo Nicolet FT-IR spectrophotometer with Thermo Scientific Smart iTR sampling accessory. Peaks are reported in wavenumbers (cm^{-1}). High resolution mass spectra are reported in units of m/z, and were acquired on a Thermo-Fisher Scientific 7 Tesla LQIT/FT-ICR Mass Spectrometer.

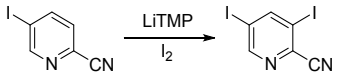
Representative procedure for synthesis of cyano-subsitituted diiodopyridines: 4-cyano-3,5-diiodopyridine



To a stirred solution of 2,2,6,6-tetramethylpiperidine (22.2 mmol, 3.74 mL) in THF (50 mL) under Ar at -30 ºC was added 2.5 M *n*-butyllithium (22.0 mmol, 8.80 mL).[1] The solution was allowed to reach 0 ºC, stirred for 15 min and then cooled to -78 ºC. 4-Cyanopyridine (10.0 mmol, 1.04 g) in THF (20 mL) was slowly added to the mixture over 15 min. After 30 min of stirring at -78 ºC, a solution of I_2 (22.2 mmol, 5.63 g) in THF (10 mL) was slowly added over 15 min and the resulting mixture was stirred for 30 min. The solution was then allowed to warm slowly to room temperature. The mixture was quenched with 20 mL of a saturated $Na_2S_2O_3$ solution. The solution was extracted with EtOAc (3 × 100 mL), the combined organic layers were washed with brine (2 × 100 mL), dried with $MgSO_4$, filtered and evaporated under reduced pressure. The product was purified by silica gel chromatography using EtOAc/hexanes (1:3) as the eluent to afford 4-cyano-3,5-diiodopyridine (2.49 g, Yield: 70%) as pale orange powder.

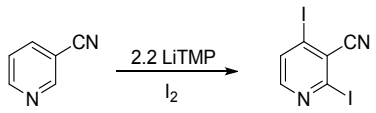
4-Cyano-3,5-diiodopyridine: ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.98 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 156.3, 156.2, 134.3, 118.3, 97.2; IR : 2926, 2232, 1892, 1835, 1783, 1540, 1495, 1423, 1390, 1400, 1361, 1338, 1223, 1245, 1182, 1050, 1033, 1006, 891 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_6H_2I_2N_2$, 356.8386; found 356.8356; Melting Point: 156.0-157.0 ºC.

2-Cyano-3,5-diiodopyridine



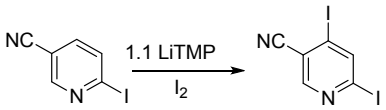
2-Cyano-3,5-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86 (d, J = 1.6 Hz, 1H), 8.61 (d, J = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 156.2, 134.3, 118.3, 97.2; IR: 3079, 3031, 2925, 2853, 2479, 2234, 2050, 1823, 1793, 1723, 1528, 1489, 1479, 1407, 1360, 1342, 1288, 1273, 1232, 1178, 1120, 1083, 898, 890, 876, 843, 807 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_6H_2I_2N_2$, 356.8386; found 356.8299. Melting Point: 131.0-132.0 ºC.

3-Cyano-2,4-diiodopyridine



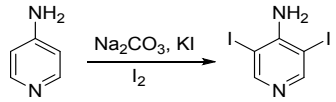
3-Cyano-2,4-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, J = 5.0, 1H), 7.85 (d, J = 5.3, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.6, 133.1, 127.1, 120.9, 119.0, 110.5; IR: 3099, 3051, 2939, 2739, 2605, 2273, 2225, 2051, 1946, 1809, 1673, 1531, 1517, 1483, 1072, 1415, 1343, 1213, 1191, 1180, 1077, 1062, 958, 836 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_6H_2I_2N_2$, 356.8386; found 356.8392. Melting Point: 200.0-201.0 ºC.

5-Cyano-2,4-diiodopyridine



5-Cyano-2,4-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86 (d, J = 1.6 Hz, 1H), 8.61 (d, J = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 156.2, 134.3, 118.3, 97.2; IR: 3082, 2967, 2576, 2230, 2082, 1866, 1721, 1540, 1507, 1479, 1433, 1379, 1290, 1277, 1232, 1199, 1122, 1083, 1063, 1041, 935, 928, 891, 861, 801 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_6H_2I_2N_2$, 356.8386; found 356.8396. Melting Point: 159.0-160.0 ºC.

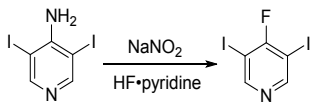
Synthesis of 4-amino-3,5-diiodopyridine



To a stirred solution of 4-aminopyridine (10.0 mmol, 0.941 g) in H_2O (50 mL) was added at room temperature Na_2CO_3 (20.0 mmol, 2.12 g), KI (20.0 mmol, 3.32 g) and I_2 (22.0 mmol, 5.58 g).[2] The solution was allowed to reflux for 5 h. The solution was extracted with EtOAc (3 × 50 mL), the combined organic layers were washed with brine (2 × 100 mL), dried with $MgSO_4$, filtered and evaporated under reduced pressure. The product was purified by silica gel chromatography using EtOAc/hexanes (1:3) as the eluent to afford 4-amino-3,5-diiodopyridine (2.42 g, Yield: 70%) as white powder.

4-Amino-3,5-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.6, 155.2, 79.4; IR: 3454, 3347, 2713, 2531, 2284, 2063, 1831, 1601, 1545, 1456, 1404, 1317, 1253, 1153, 1029, 1007, 940, 896, 852 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_5H_5I_2N_2$, 346.8542; found 346.8553. Melting Point: 134.0-135.0 ºC.

Synthesis of 4-fluoro-3,5-diiodopyridine

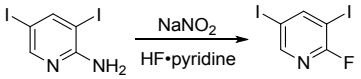


Sodium nitrite (6.00 mmol, 0.414 g) was added in small portions to a solution of 4-amino-3,5-diiodopyridine (5.00 mmol, 1.73 g) in an HF/pyridine mixture (25 mL) in a polyethylene reaction vessel cooled with an ice/salt bath.[3] The resulting

solution was stirred at 0 °C for 30 min, then heated to 50-60 °C and stirred at this temperature for 2 h. The reaction mixture was poured onto crushed ice (100 g), partially neutralized with sodium bicarbonate (pH 5), and extracted with ether (3 × 100 mL). The combined organic layers were washed with brine (2 × 100 mL), dried with $MgSO_4$, filtered and evaporated under reduced pressure. The product was purified by silica gel chromatography using EtOAc/hexanes (1:3) as the eluent to afford 4-fluoro-3,5-diiodopyridine (1.57 g, Yield: 90%) as white needles.

4-Fluoro-3,5-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73 (d, J = 7.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 164.9, 158.2, 80.7, 80.5; IR: 3084, 3045, 2925, 2454, 2271, 2096, 1875, 1827, 1786, 1541, 1465, 1438, 1394, 1235, 1149, 1134, 1053, 928, 893, 829 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_5H_3FI_2N$, 349.8339; found 349.8269. Melting Point: 143.0-144.0 ºC.

Synthesis of 2-fluoro-3,5-diiodopyridine



The procedure used to synthesize 4-fluoro-3,5-diiodopyridine was used.

2-Fluoro-3,5-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (dd, J = 7.5, 2.2 Hz, 1H), 8.33 (d, J = 1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2, 160.9, 156.79, 156.77, 153.2, 153.0, 87.61, 87.65; IR: 3079, 3046, 3024, 2952, 2779, 2499, 2461, 2269, 2090, 1880, 1843, 1802, 1723, 1555, 1537, 1467, 1421, 1362, 1276, 1267, 1249, 1221, 1166, 1102, 1078, 1032, 943, 900, 847 cm^{-1}; HRMS (m/z): $[M+D]^+$ calculated for $C_5H_2DFI_2N$, 350.8402; found 350.8420. Melting Point: 100.5-101.0 ºC.

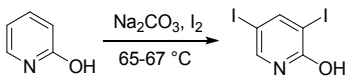
Synthesis of 4-hydroxy-3,5-diiodopyridine and 4-chloro-3,5-diiodopyridine

4-Hydroxy-3,5-diiodopyridine and 4-chloro-3,5-diiodopyridine were synthesized according to a procedure reported by Kay.[4]

4-Hydroxy-3,5-diiodopyridine: ^{1}H NMR (400 MHz, DMSO): δ 8.22 (s, 1H); IR: 3272, 2954, 2161, 2035, 1642, 1047, 1088, 1015 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_5H_4I_2NO$, 347.8382; found 347.8541.

4-Chloro-3,5-diiodopyridine: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 150.9, 97.1; IR: 3073, 3030, 2734, 2411, 2232, 2119, 1984, 1867, 1816, 1770, 1531, 1502, 1420, 1391, 1242, 1212, 1168, 1101, 1096, 1062, 1028, 1008, 956, 934 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_5H_3ClI_2N$, 365.8043; found 365.8190. Melting Point: 177.5-178.0 ºC.

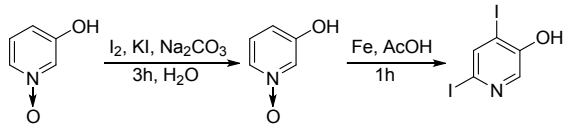
Synthesis of 2-hydroxy-3,5-diiodopyridine



2-Hydroxy-3,5-diiodopyridine was synthesized according to a procedure reported by Koch.[5]

2-Hydroxy-3,5-diiodopyridine: ^{1}H NMR (400 MHz, DMSO): δ 8.21 (d, *J* = 1.4, 1H), 7.69 (d, *J* = 1.4 Hz, 1H); IR: 3262, 3161, 3084, 3029, 2963, 2905, 2835, 2659, 1889, 1804, 1623, 1594, 1523, 1499, 1457, 1409, 1365, 1307, 1247, 1183, 1148, 1091, 1025, 959, 862, 824 cm^{-1}; HRMS (m/z): $[M+H]^+$ calculated for $C_5H_4I_2NO$, 347.8382; found 347.8281.

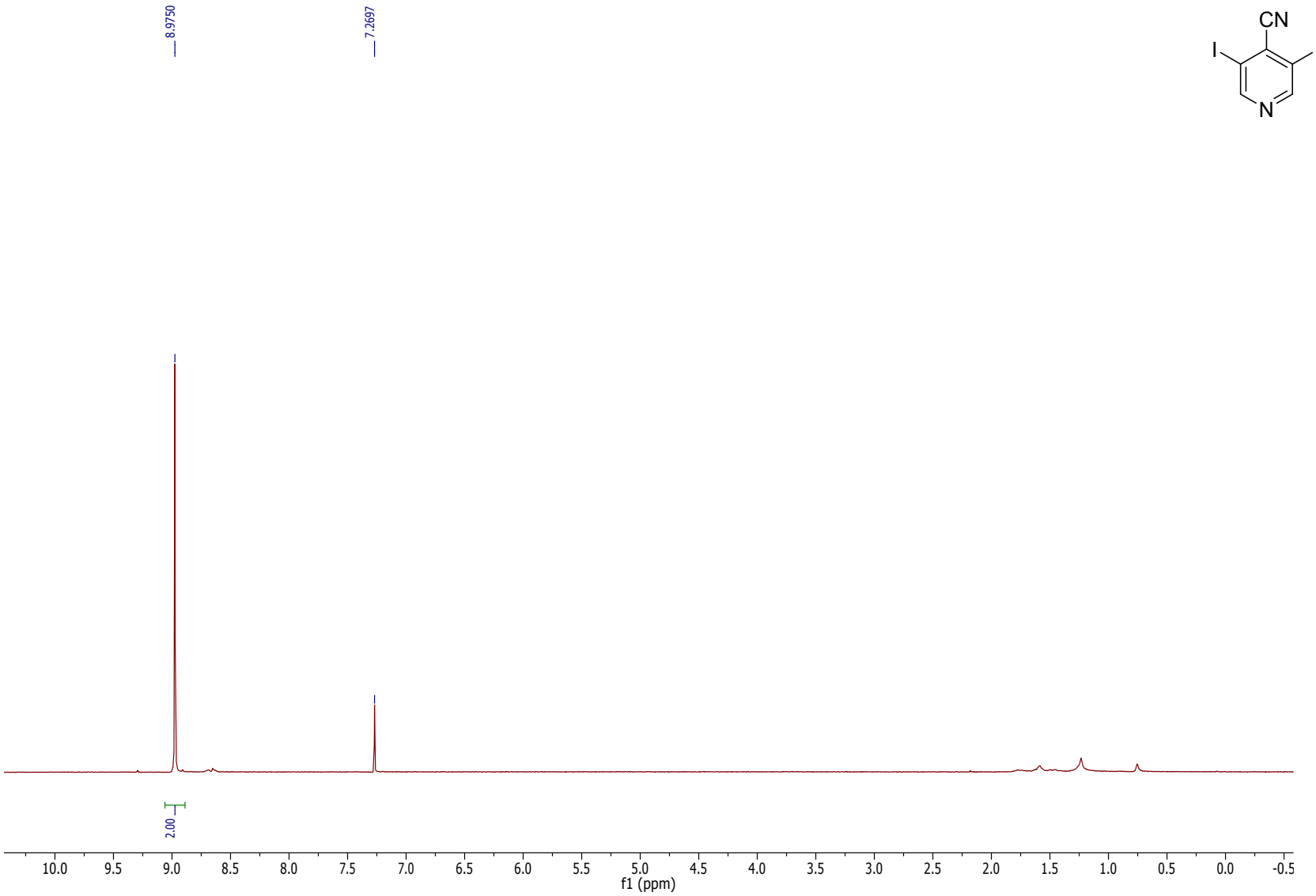
Synthesis of 5-hydroxy-2,4-diiodopyridine



5-Hydroxy-2,4-diiodopyridine was synthesized according to a procedure reported by Lewicka. [6]

5-Hydroxy-2,4-diiodopyridine: ^{1}H NMR (400 MHz, Acetone): δ 8.12 (s, 1H), 7.95 (s, 1H); HRMS (m/z): $[M+H]^+$ calculated for $C_5H_4I_2NO$, 347.8382; found 347.8361.

II. ^{1}H and ^{13}C NMR spectra of synthesized precursors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7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
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0.5
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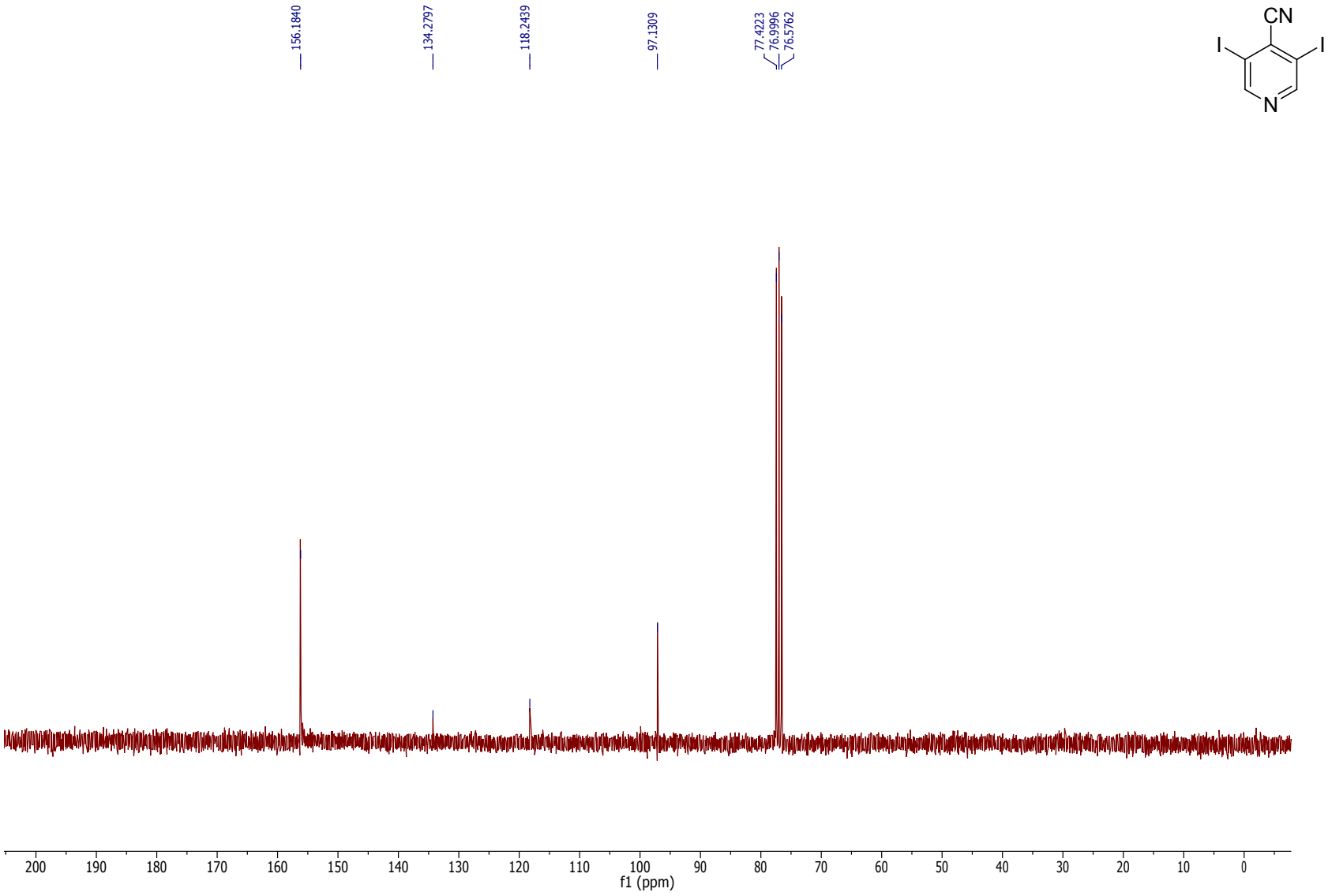
-0.5
f1 (ppm)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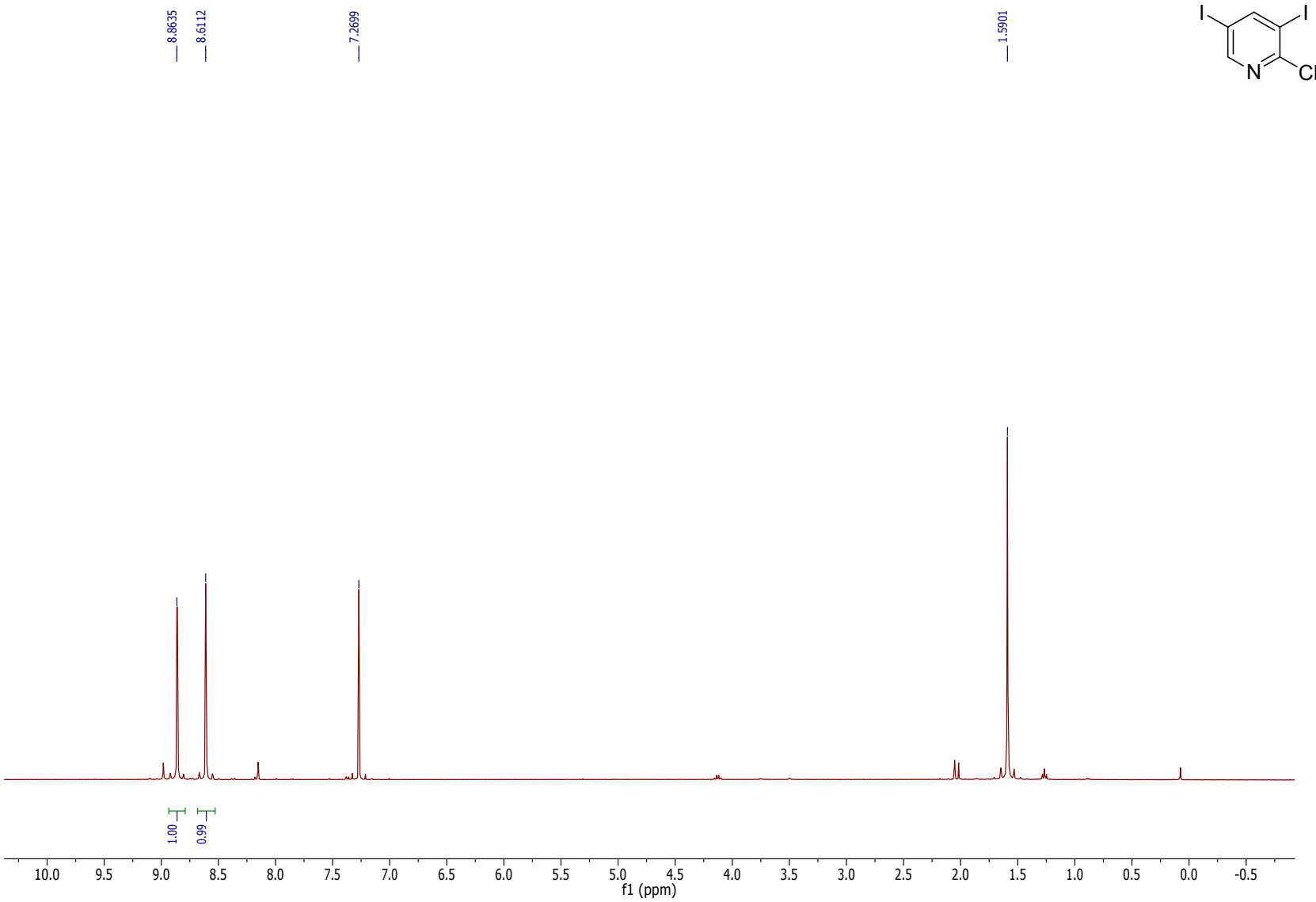
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7.0
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5.5
5.0
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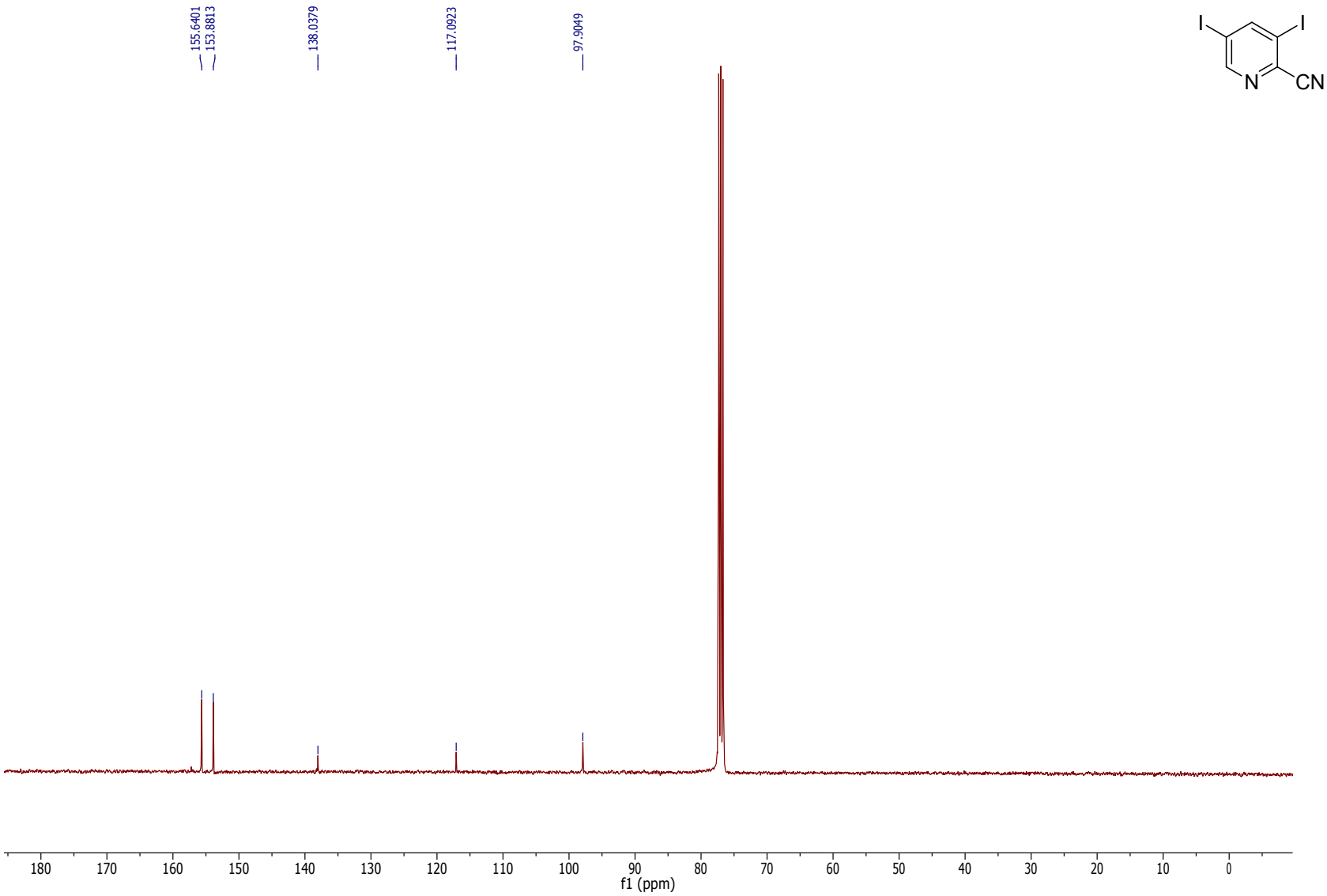
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10
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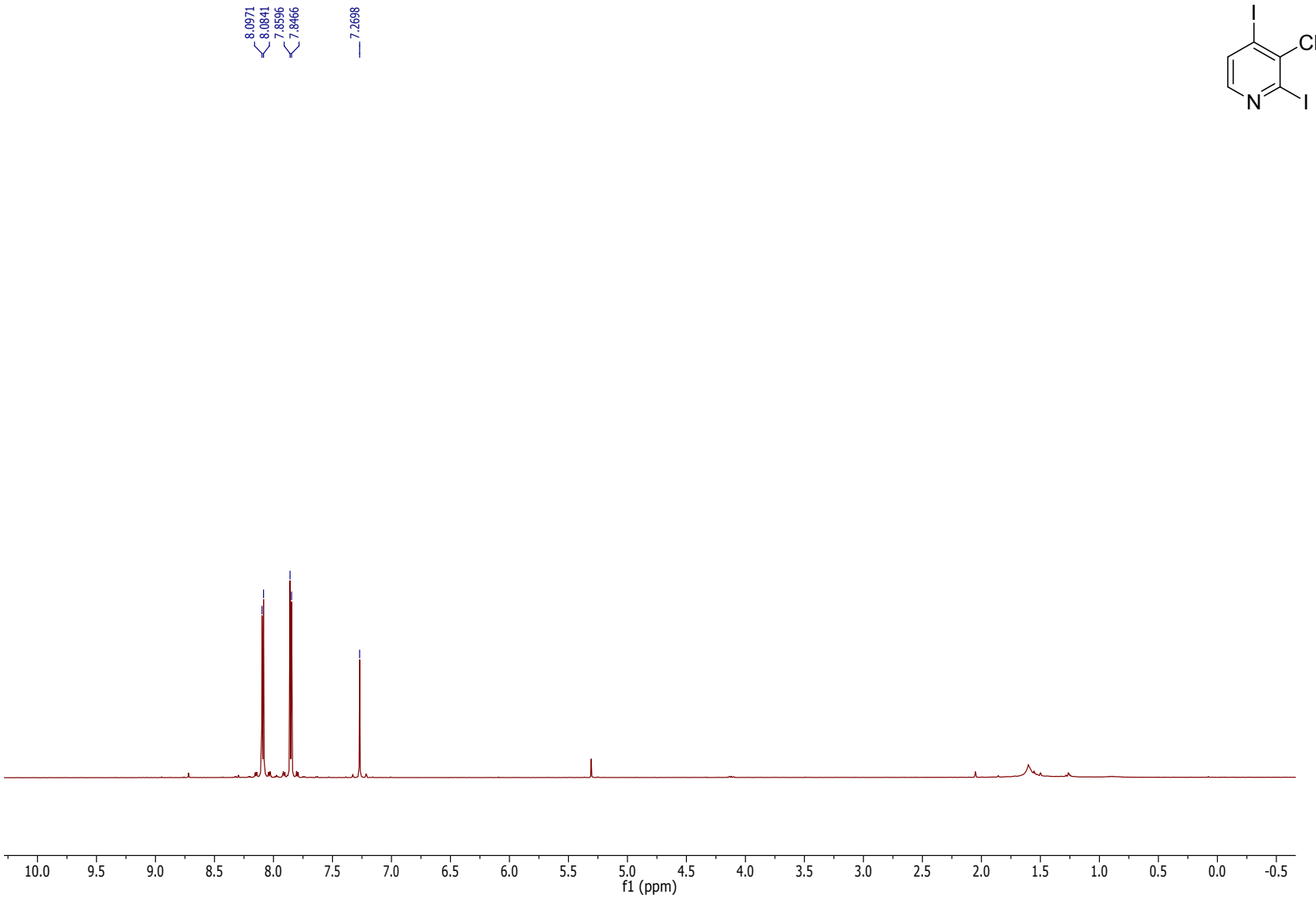
f1 (ppm)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6.0
5.5
5.0
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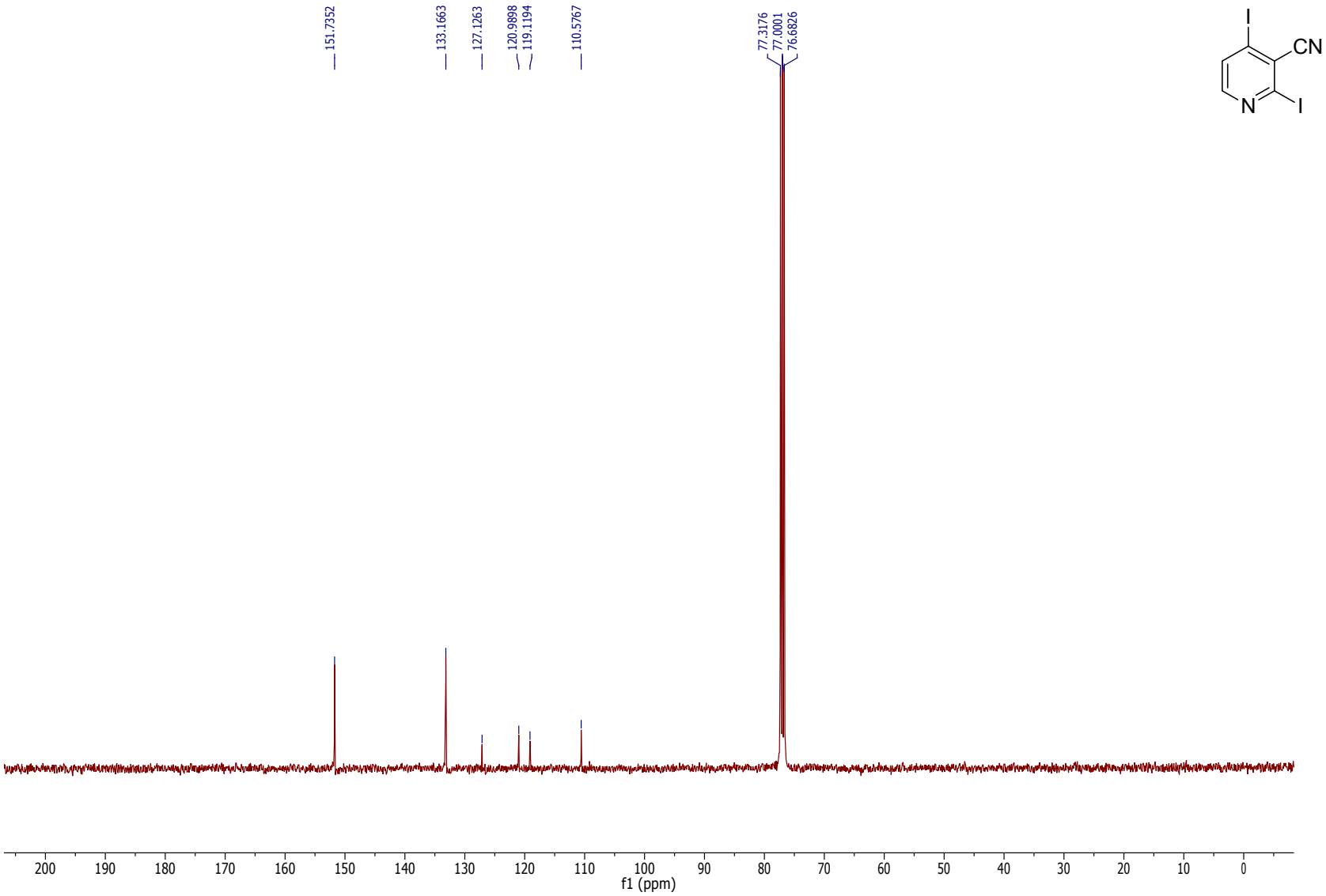
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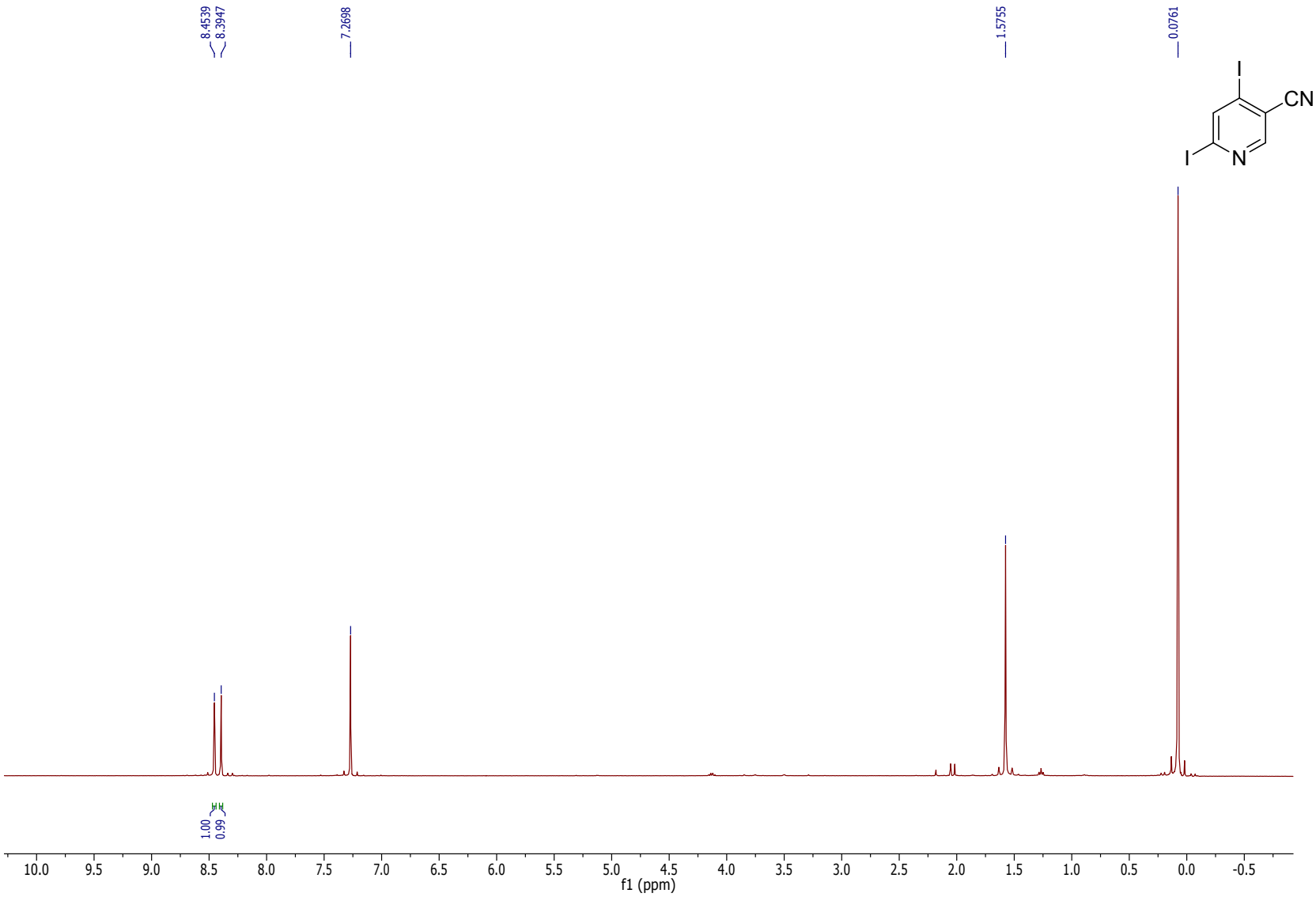
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
1.5
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0.5
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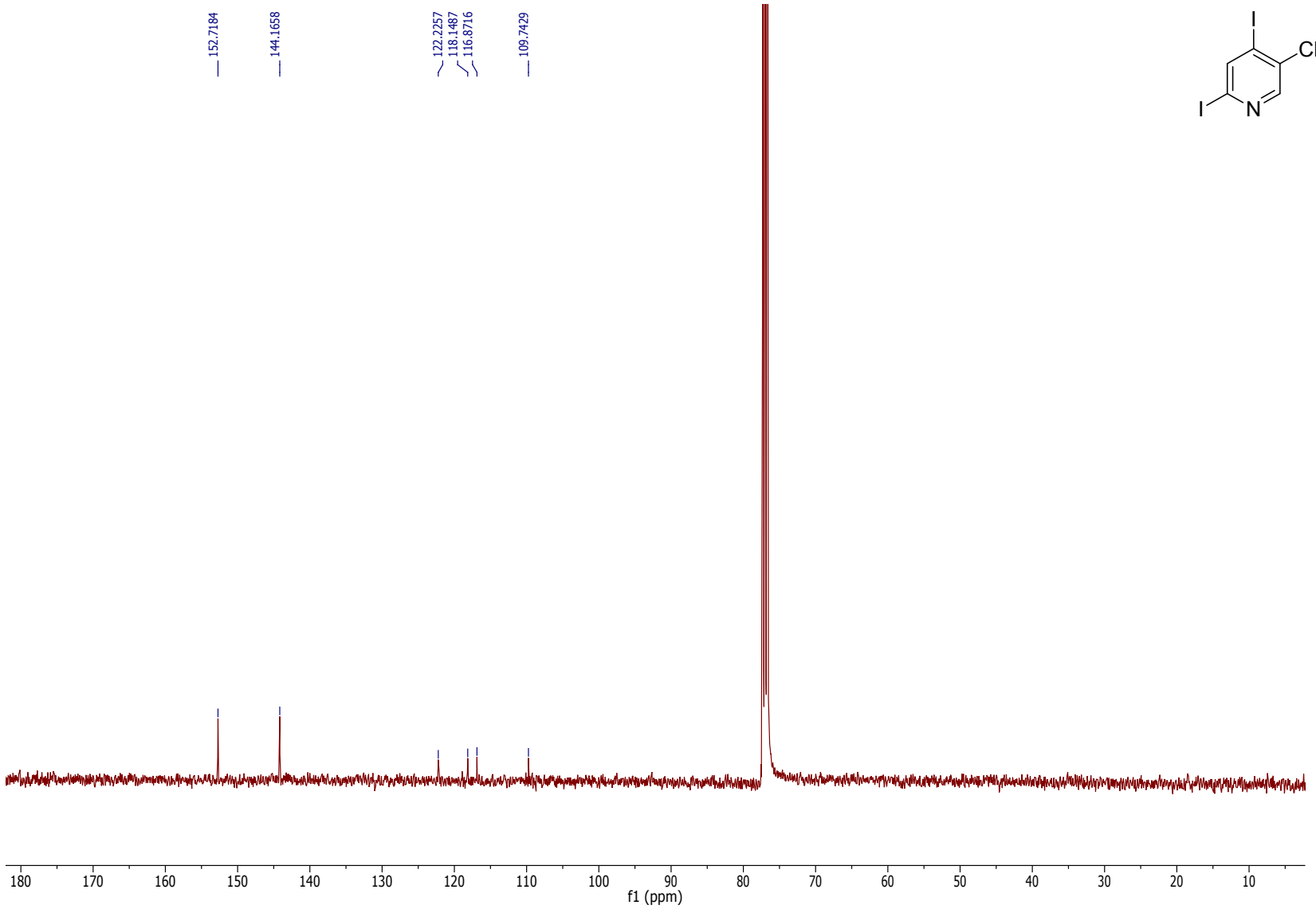
-0.5
f1 (ppm)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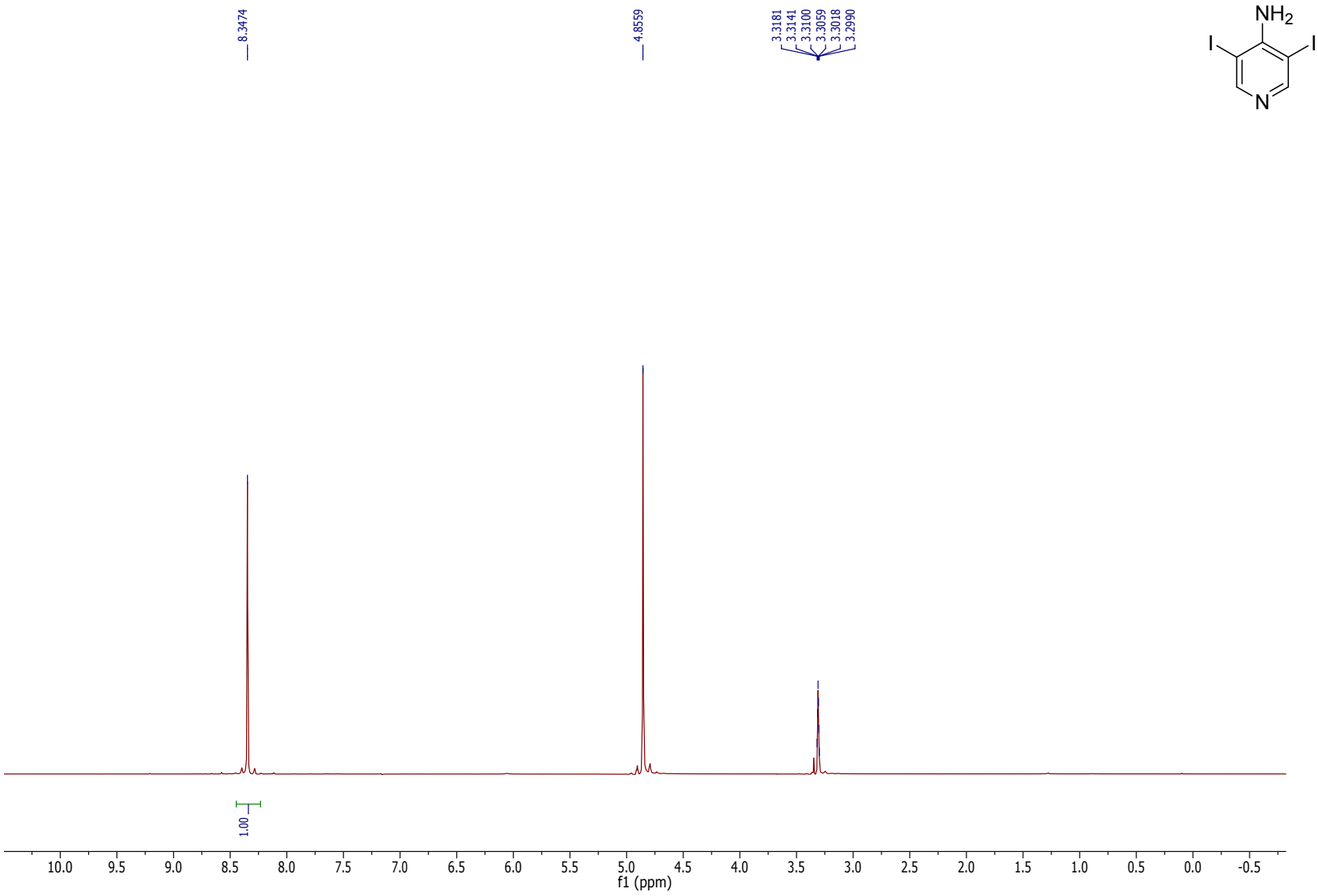
f1 (ppm)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10.0
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8.0
7.5
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5.5
5.0
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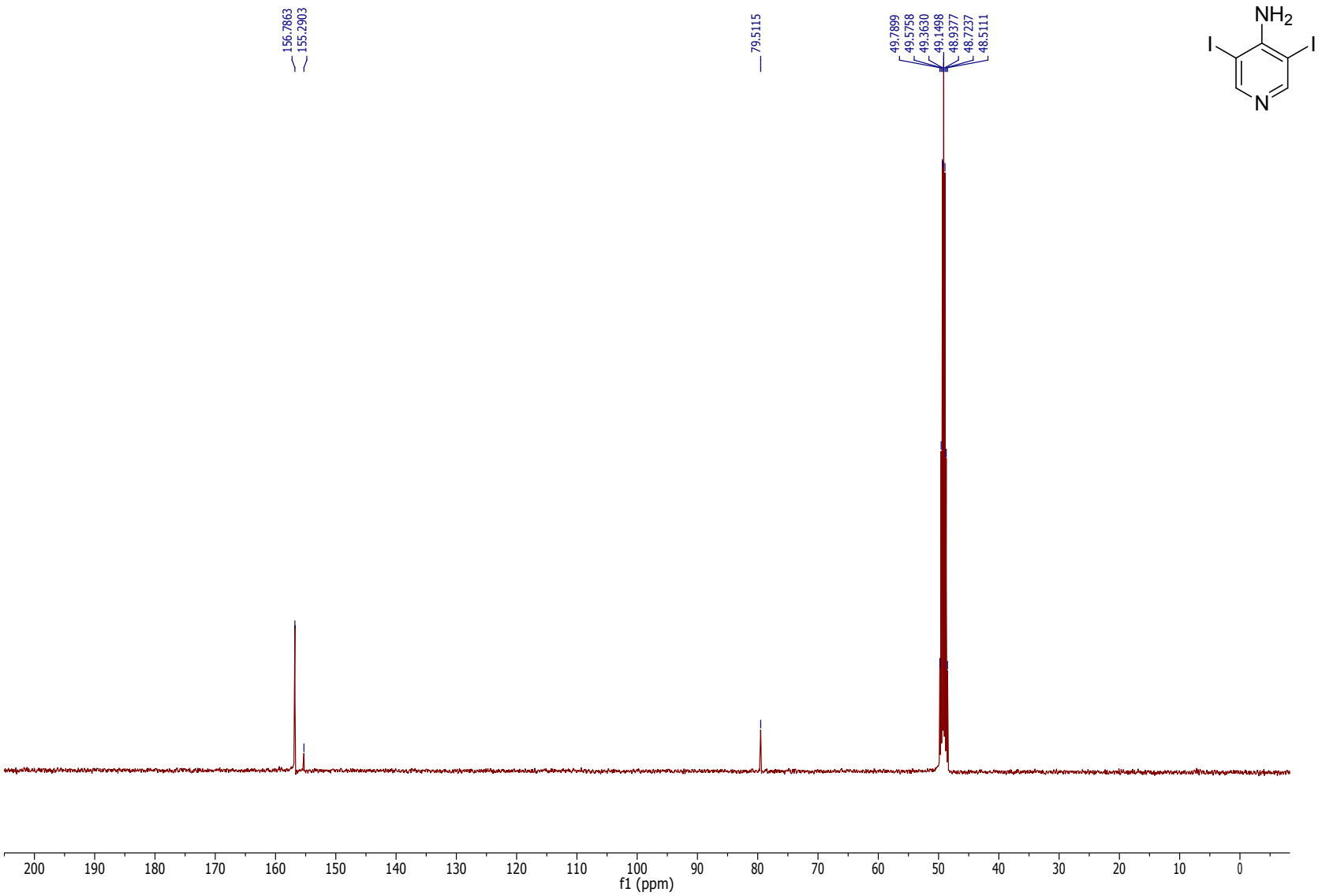
-0.5
f1 (ppm)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N
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180
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50
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10
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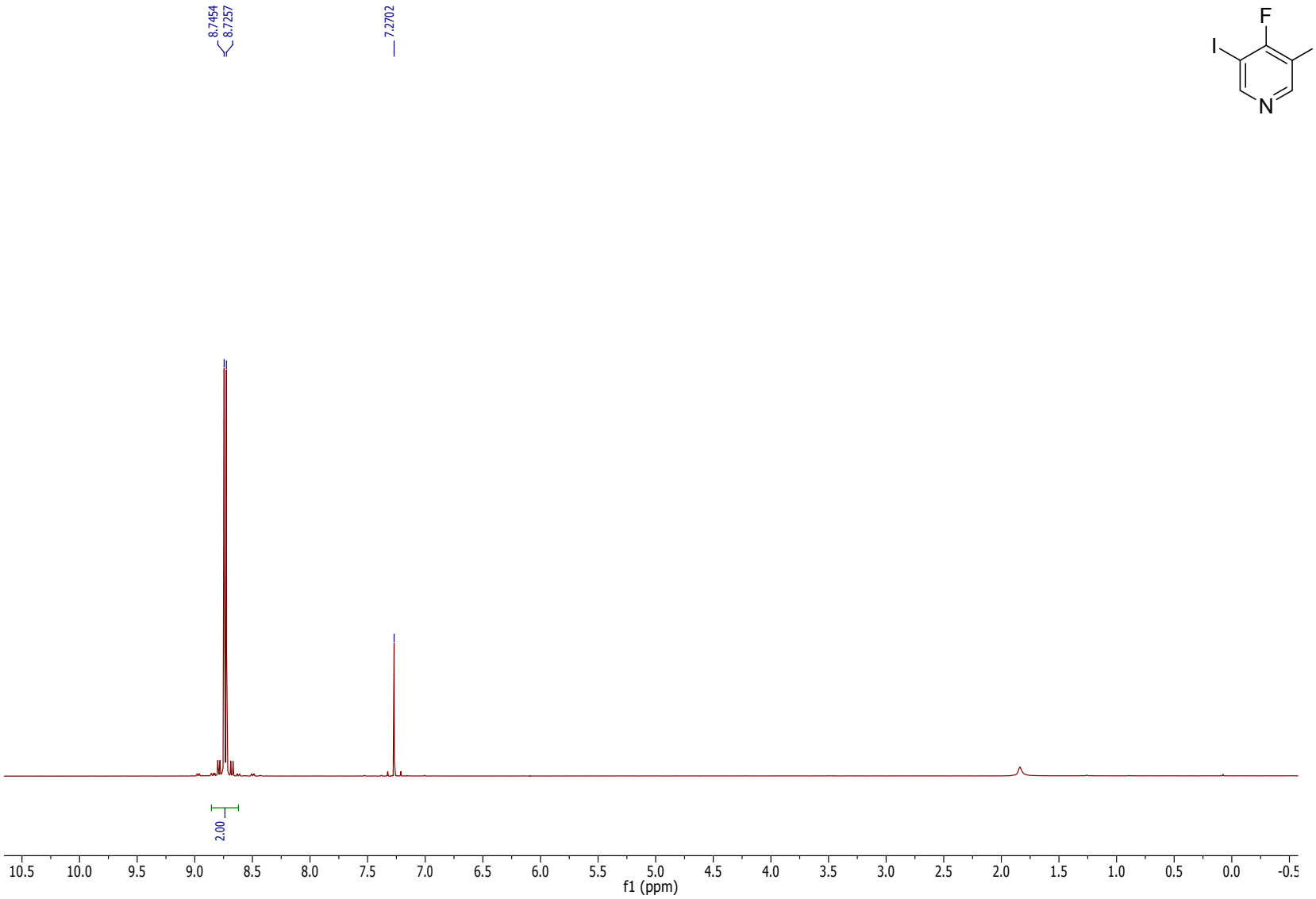
f1 (ppm)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7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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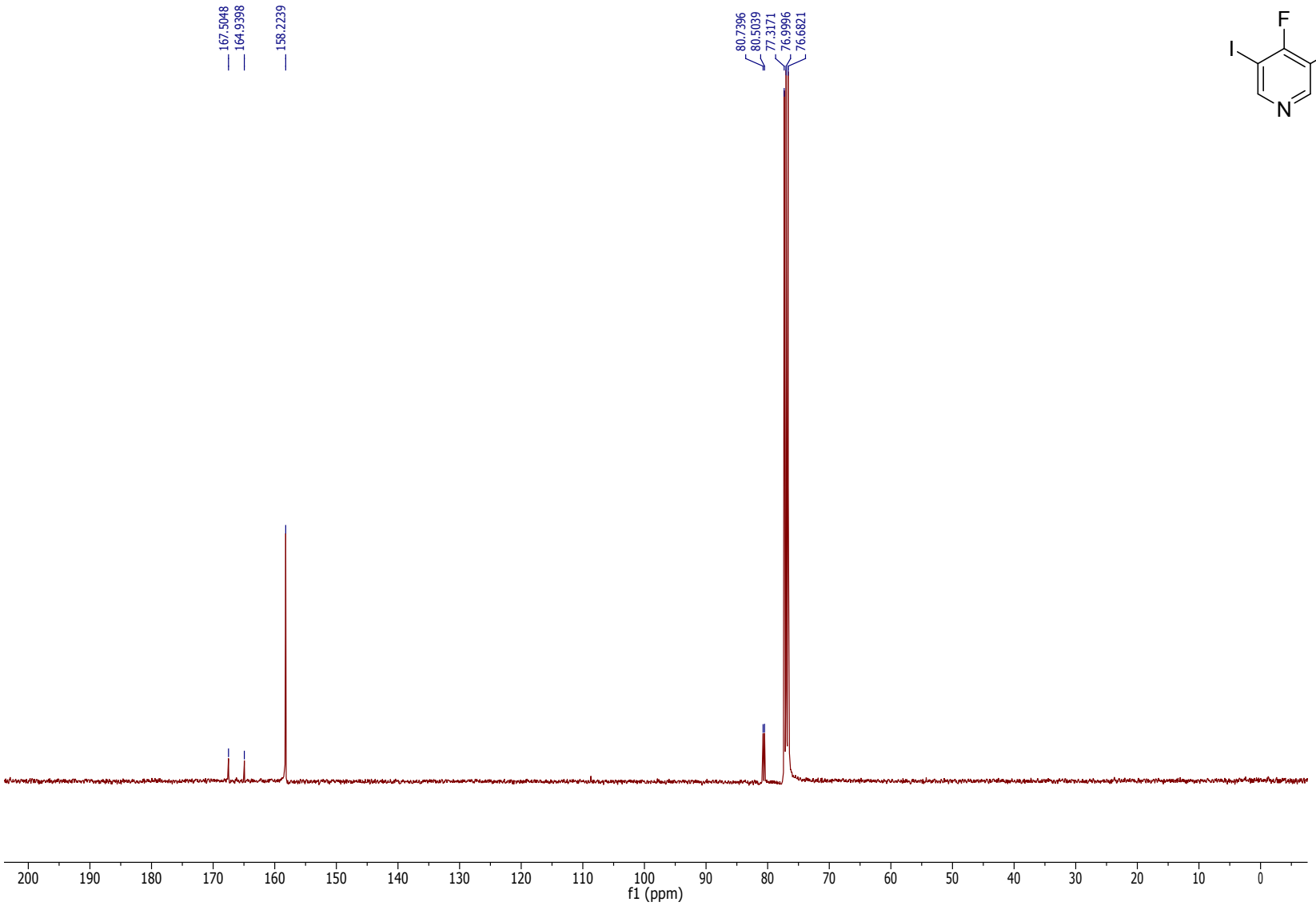
0.0
f1 (ppm)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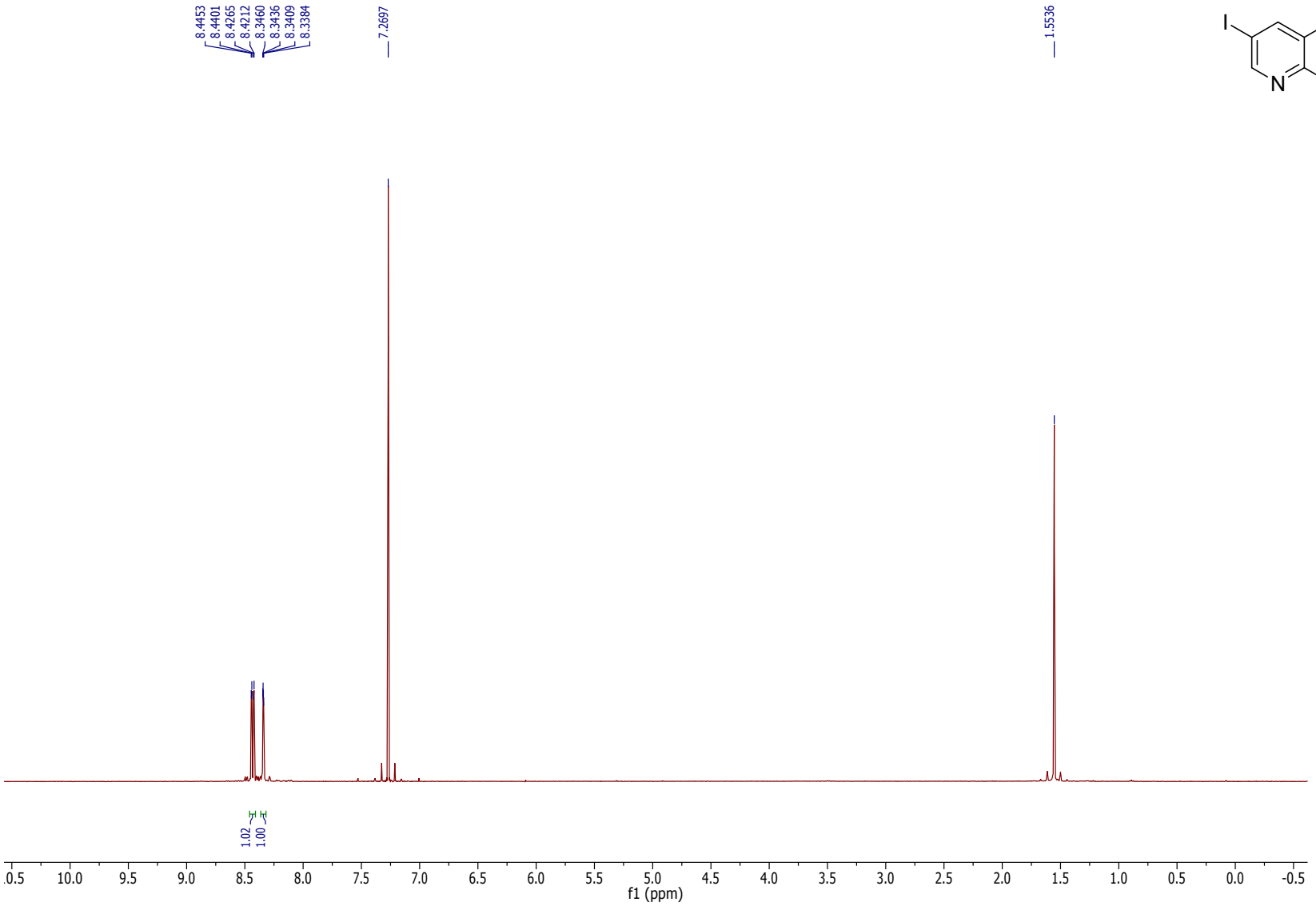
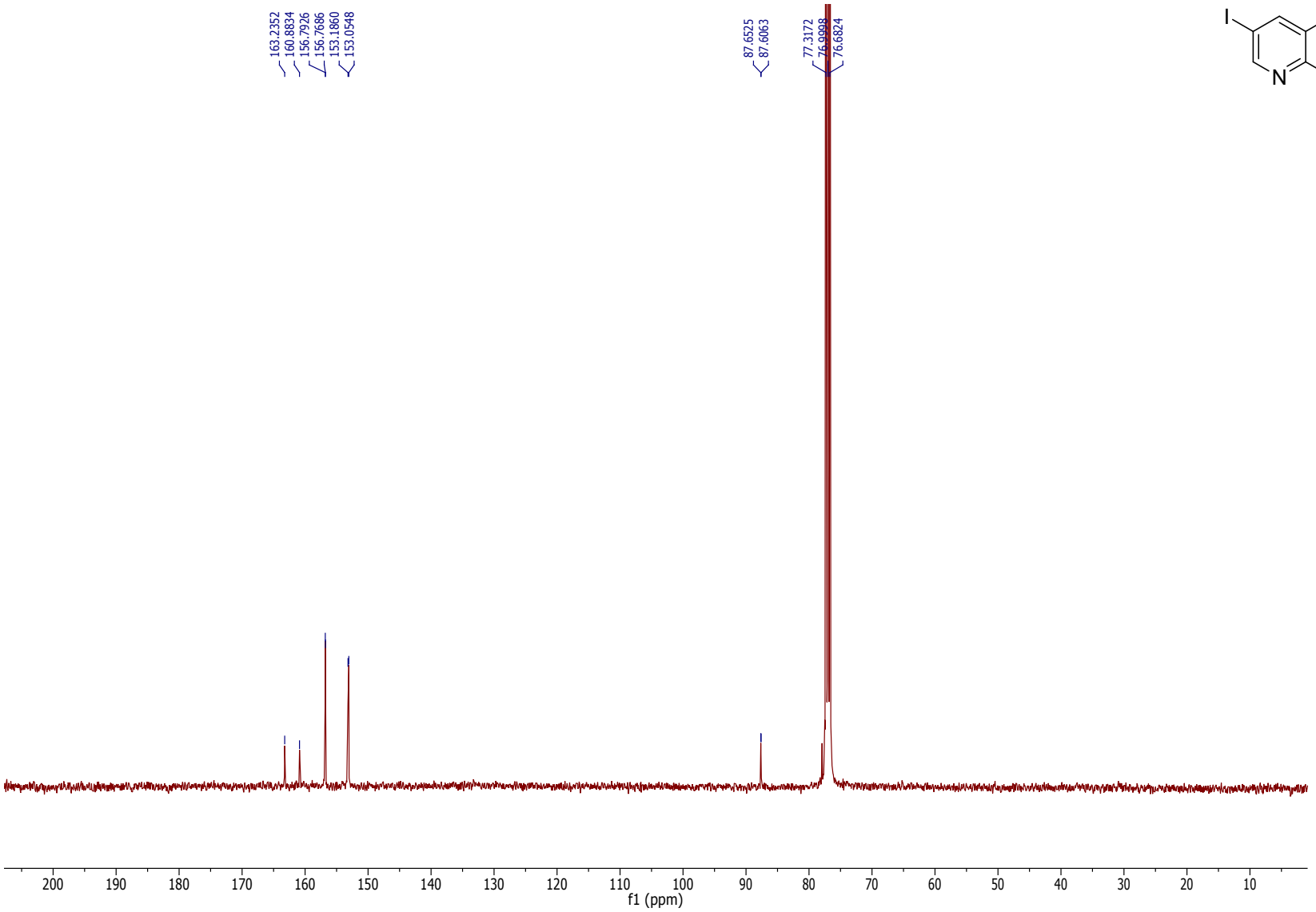
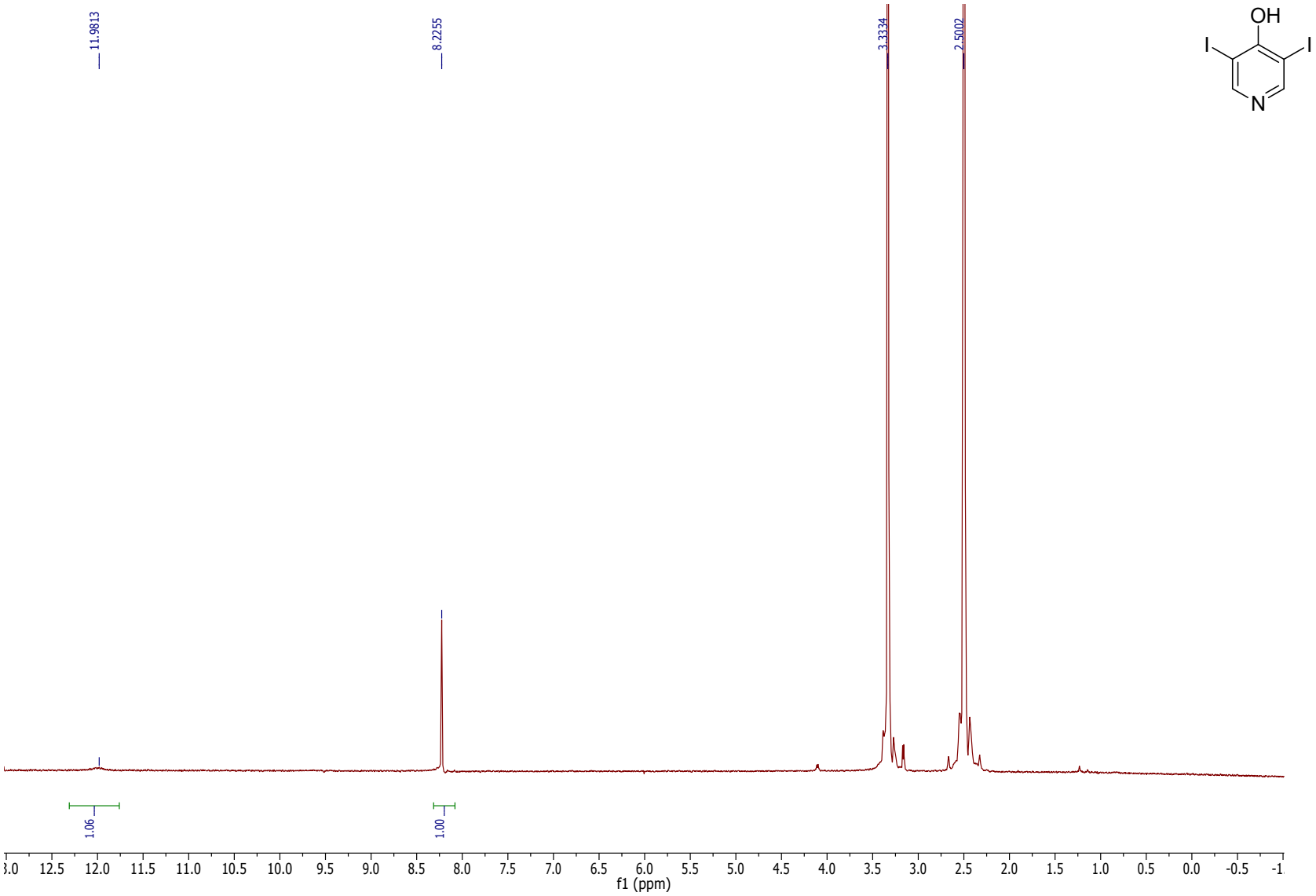
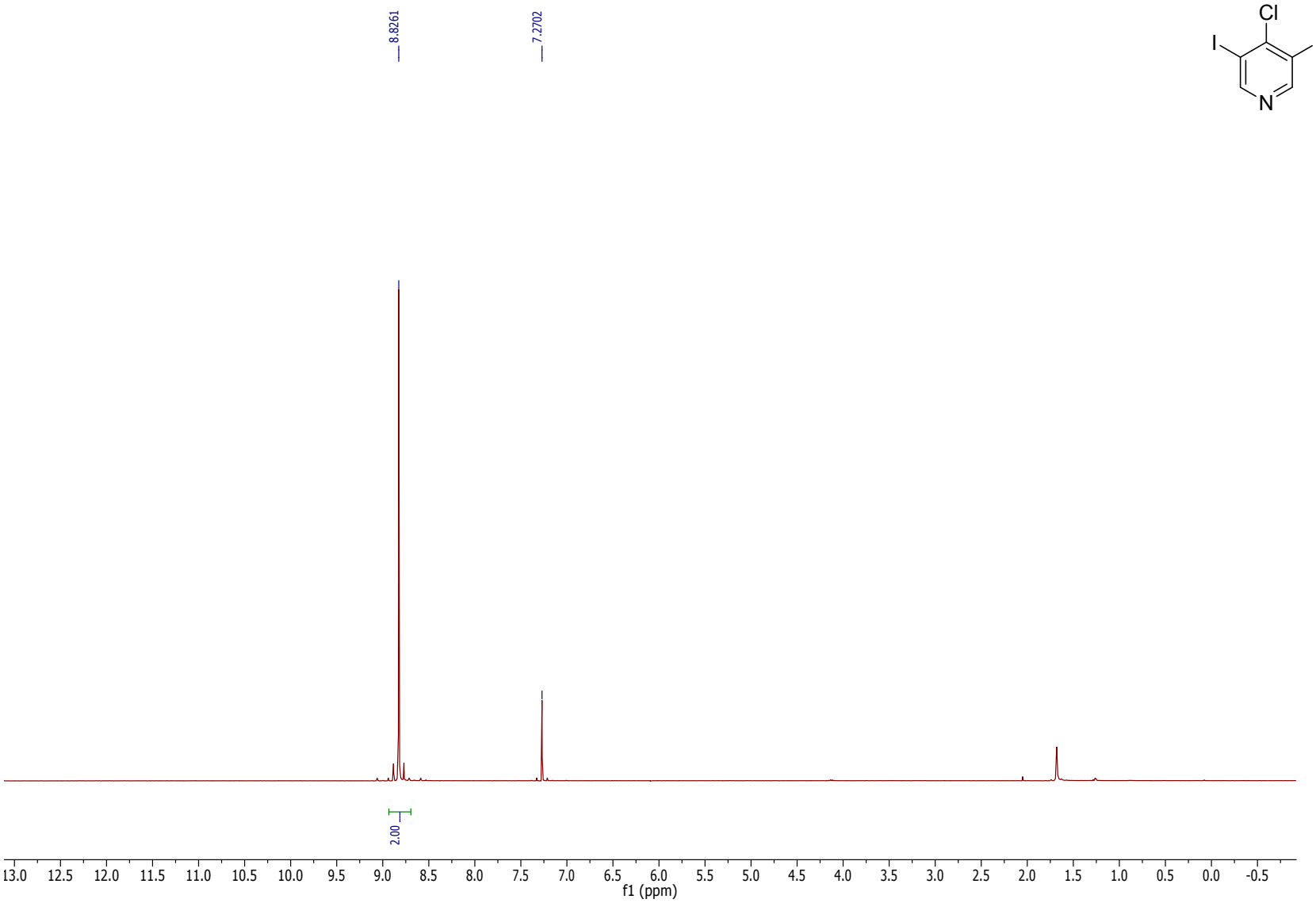
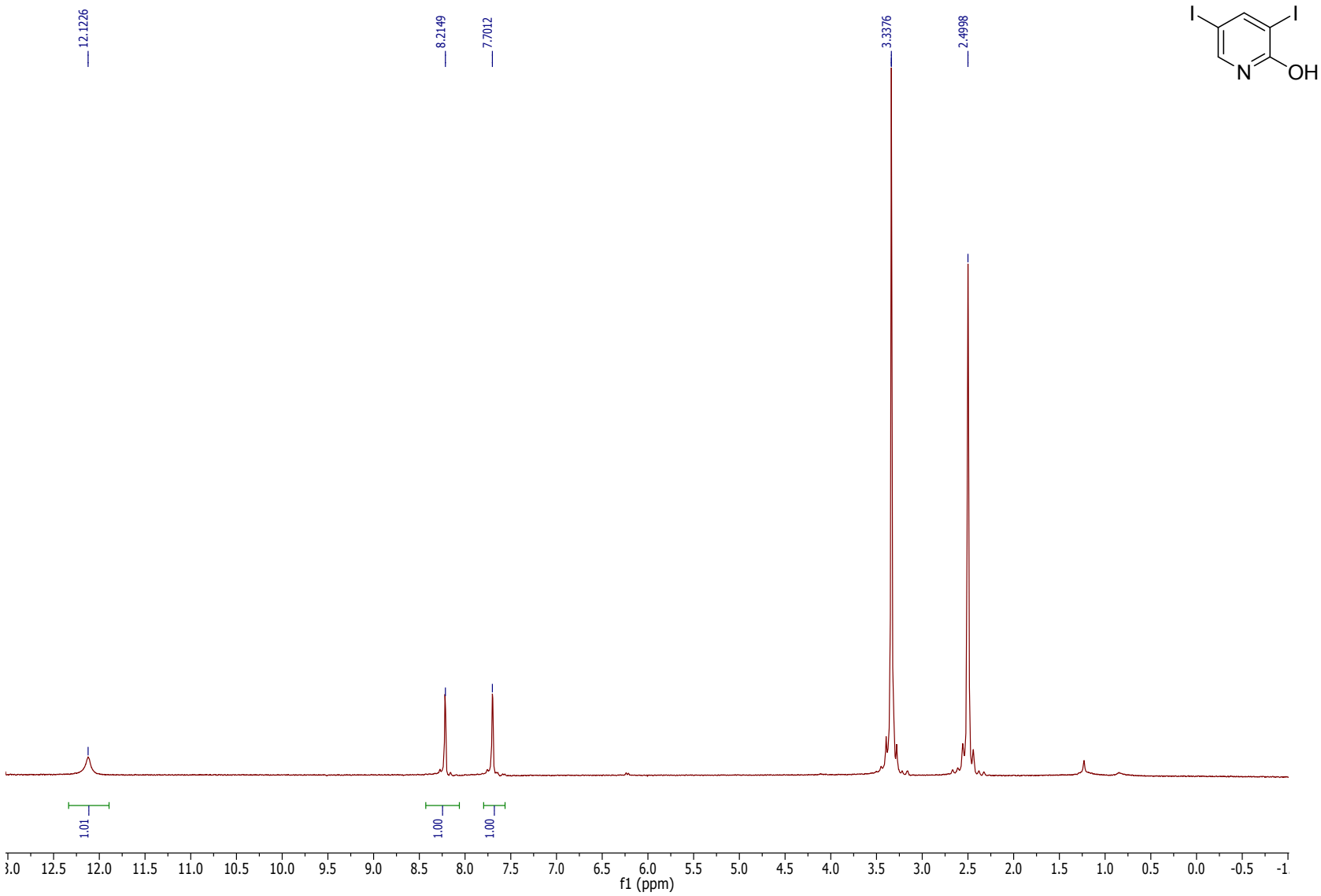
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

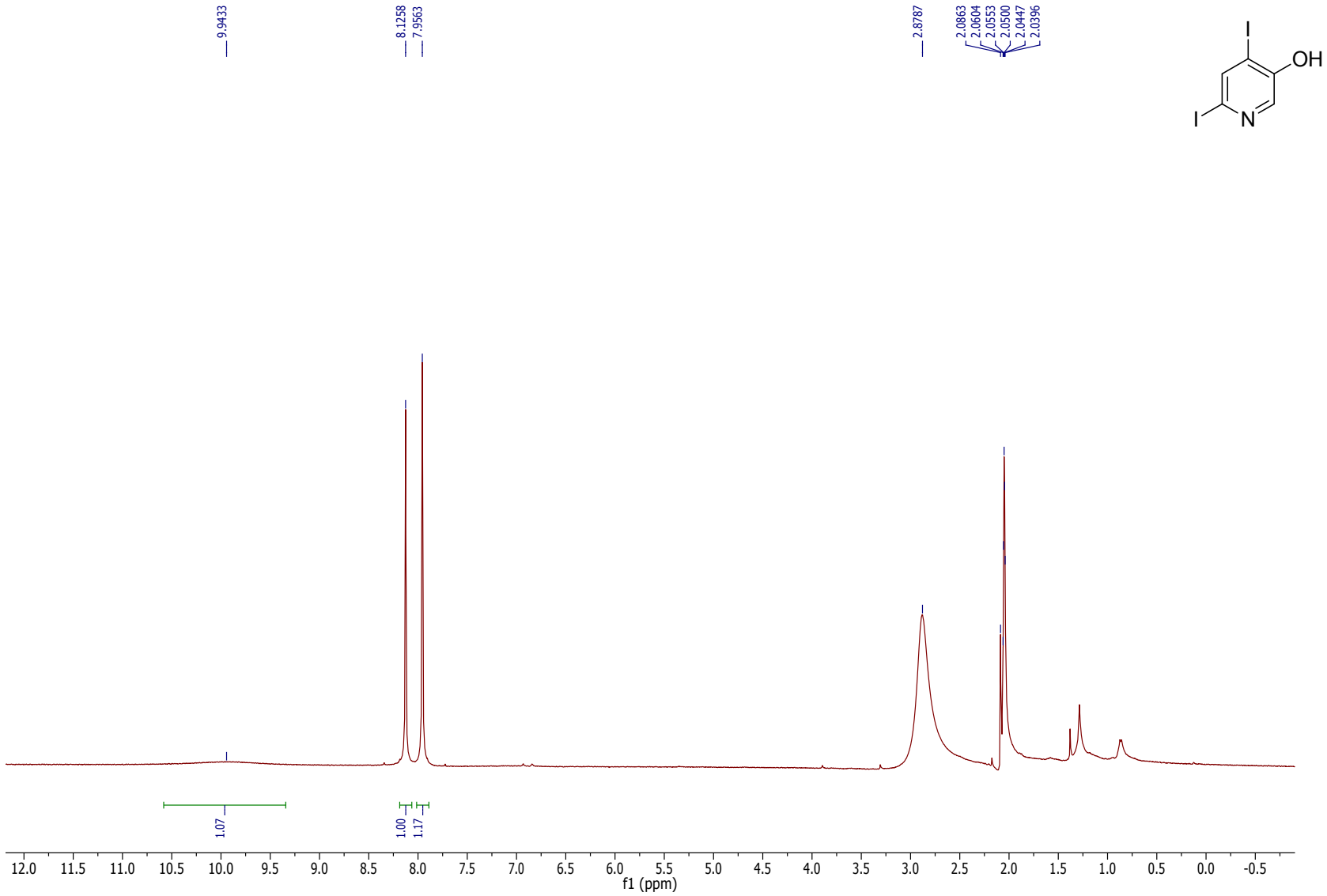

8.4453
8.4401
8.4265
8.4212
8.3460
8.3436
8.3409
8.3384
7.2697
1.5536
I
I
N
F
1.02
1.00
f1 (ppm)

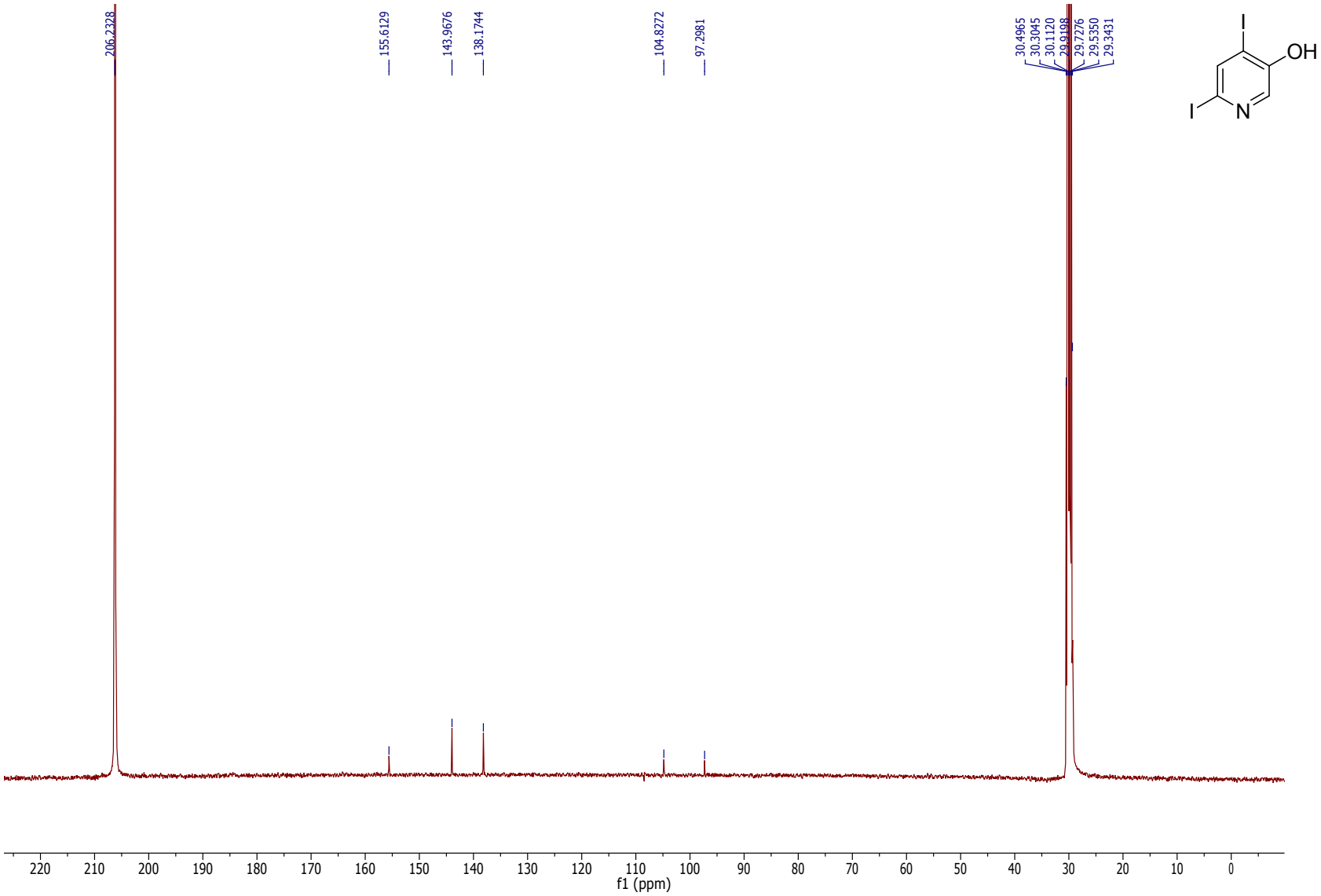

163.2352
160.8834
156.7926
156.7686
153.1860
153.0548
87.6525
87.6063
77.3172
76.9998
76.6824
I
I
N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


11.9813
8.2255
3.3334
2.5002
OH
I
I
N
1.06
1.00
f1 (ppm)


8.8261
7.2702
Cl
I
I
N
2.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


12.1226
8.2149
7.7012
3.3376
2.4998
I
I
N
OH
1.01
1.00
1.00
f1 (ppm)


9.9433
8.1258
7.9563
2.8787
2.0863
2.0604
2.0553
2.0500
2.0447
2.0396
I
OH
I
N
1.07
1.00
1.17
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


206.2328
155.6129
143.9676
138.1744
104.8272
97.2981
30.4965
30.3045
30.1120
29.9198
29.7276
29.5350
29.3431
I
OH
I
N
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

III. Experimental methods

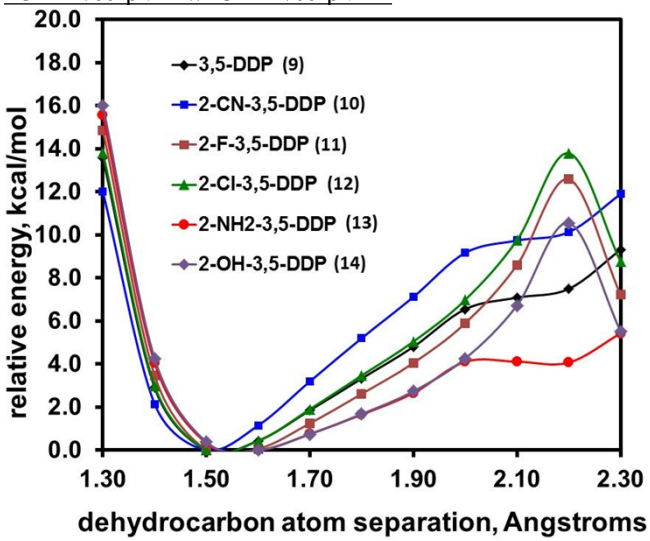
All experiments were carried out in a Finnigan FTMS 2001 dual–cell FT–ICR mass spectrometer equipped with an Odyssey data station and a SWIFT (Stored Waveform Inverse Fourier Transform) cell controller, as described previously.[7-11] Briefly, the biradical precursors and other reagents were introduced into the dual cell through two variable leak valves. An electron beam of 20–30 eV kinetic energy was used to ionize all reagents (the filament current was 7 uA and ionization time 0.02–1 s). The biradical precursors were allowed to react with ions formed upon electron ionization or their reaction products (reaction times: 5–20 s) to yield protonated biradical precursors. These ions were transferred into the analyzer cell by slightly increasing the voltage of the source cell trapping plate (2.1 V) and slightly decreasing the voltage of the analyzer trapping plate (1.9 V) while grounding the conductance limit plate for 183–189 μs. The technique of sustained off–resonance irradiated collision–activated dissociation [12] (SORI–CAD) with argon target gas was used to homolytically cleave either C–I or C–NO_2 bonds in the protonated precursors. During SORI–CAD, the nominal pressure of argon in the cell was increased to 1×10^{-5} Torr. The biradical precursor ions were kinetically excited by using an RF pulse with a frequency 1000 Hz above the cyclotron frequency of the ions and collisionally activated with argon for 0.3 s.

The charged biradicals of interest were isolated by ejecting all the other ions via the application of a series of SWIFT excitation pulses[13] to the excitation plates of the analyzer cell. The isolated charged biradicals were allowed to react with cyclohexane for a variable period of time (typically 0.05–1000 s). Detection was performed by using "chirp" excitation of 124 V amplitude, 2.7 MHz bandwidth, and 3.2 kHz/μs sweep rate. All of the spectra are the average of five transients, which were recorded as 128 k data points and subjected to one zero fill prior to Fourier transformation. Each reaction spectrum was background corrected by using a procedure described previously.[14]

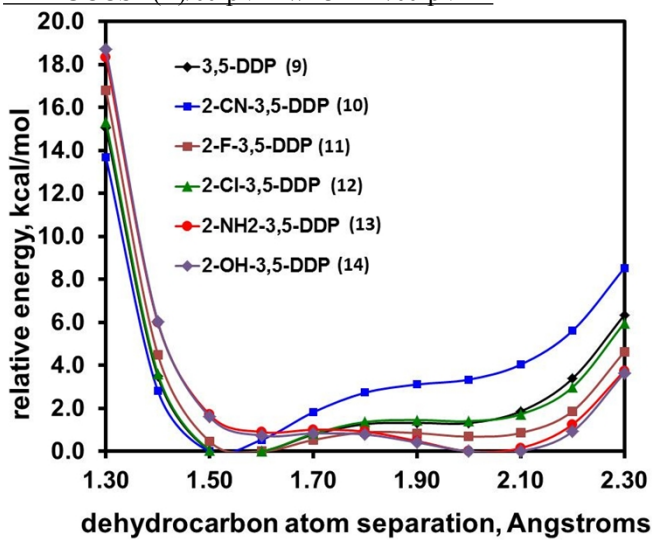
In the FT–ICR mass spectrometer, the concentration of ions (in this case, charged biradicals) inside the cell is much smaller than that of the neutral reagent. Hence, the concentration of the neutral reagent can be assumed to be constant. Indeed, all the reactions studied followed pseudo–first–order kinetics, which allowed for the derivation of the second–order reaction rate constant (k_{exp}) from a semilogarithmic plot of the relative abundance of the reactant ion versus reaction time and the concentration of the neutral reagent. The pressure inside each side of the dual cell was measured by an ionization gauge located about one meter above each cell. The ion gauge pressure readings were corrected for the sensitivity of the ion gauges toward each neutral reagent and for the pressure gradient between the ion gauge and the cell. The correction factors were obtained by measuring the rate of an exothermic electron transfer from the reagent to the radical cation of CS_2. Such reactions are highly exothermic and have low barriers and hence can be expected to occur at the collision rate.[15] The accuracy of the measured rate constants is estimated to be about 50%, with the precision estimated to be better than 10%. The theoretical collision rate constants (k_{coll}) were calculated using a parameterized trajectory theory.[16] The efficiency of each reaction (i.e., the fraction of collisions that leads to reaction) is given by k_{exp}/k_{coll}. The relative abundances of the primary products are reported as branching ratios, which are given as the ratio of the abundance of a primary product ion to the sum of the abundance of all primary products.

IV. Calculated potential energy surfaces for biradicals 4–20

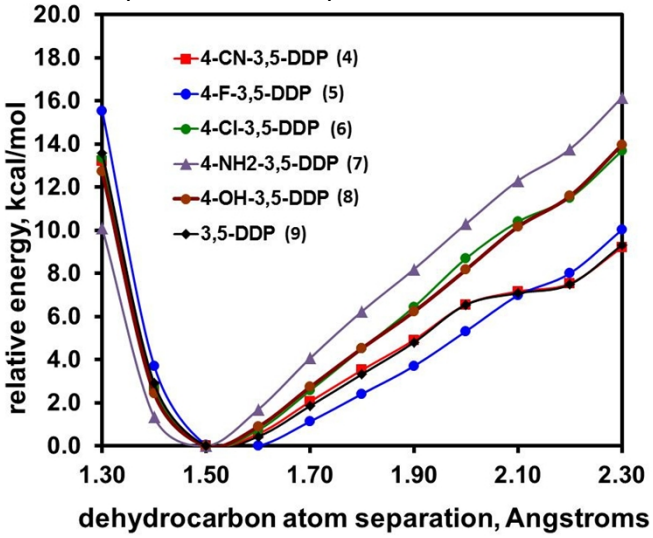
B3LYP/cc-pVTZ//B3LYP/cc-pVTZ



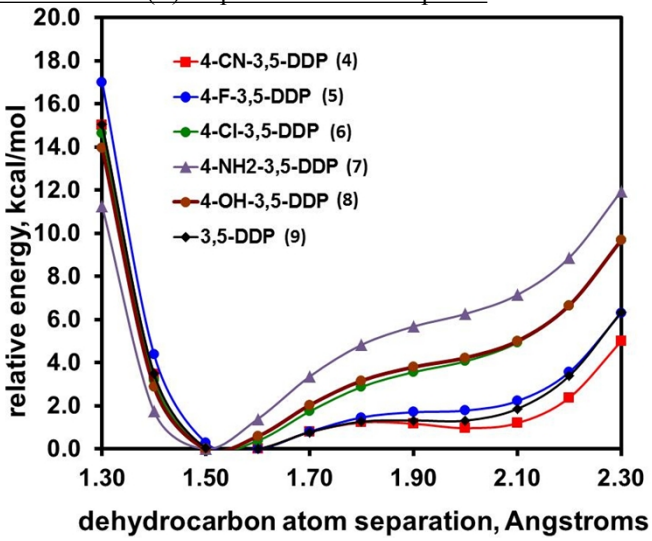
RHF-UCCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ



B3LYP/cc-pVTZ//B3LYP/cc-pVTZ

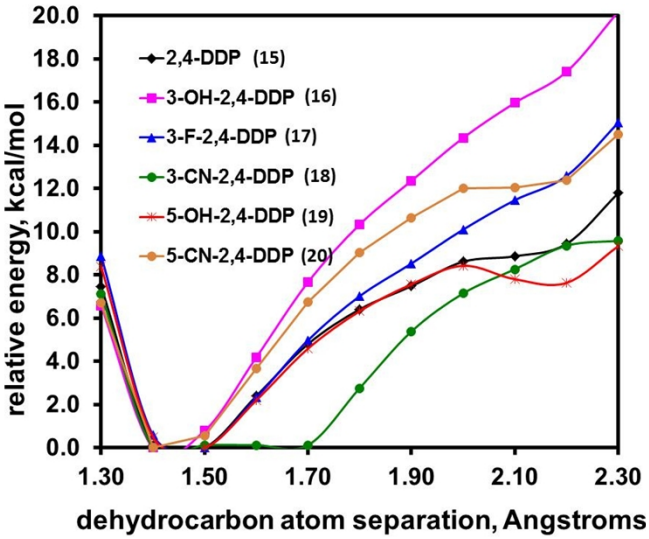


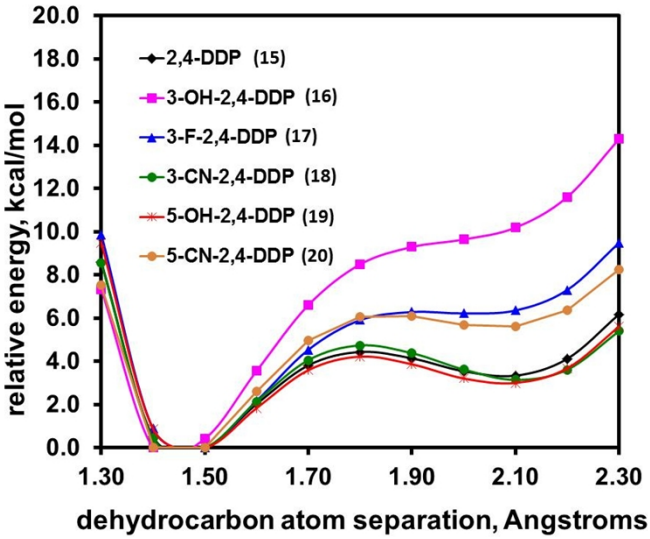
RHF-UCCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ



B3LYP/cc-pVTZ//B3LYP/cc-pVTZ

RHF-UCCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ





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Minimum Energy Geometries

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
3B2 triplet state (C2v)

6	-1.177395	-1.089323	0.000000
6	-1.159082	0.264485	0.000000
6	0.000000	1.045448	0.000000
6	1.173527	0.282998	0.000000
6	1.204271	-1.069429	0.000000
1	0.025408	-2.747936	0.000000
1	-2.073545	-1.693097	0.000000
1	2.108108	-1.661732	0.000000
7	0.017515	-1.735002	0.000000
8	0.049987	2.359806	0.000000
1	-0.830400	2.764267	0.000000

E = -339.5851957 au
ZPVE = 0.074763 au
(H298 - E0) = 4.4 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -338.8659662 au

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

6	0.000000	0.000000	0.915832
6	0.000000	0.000000	2.320019
6	0.000000	0.759513	-0.203846
6	0.000000	-0.759513	-0.203846
6	0.000000	1.146774	-1.520024
6	0.000000	-1.146774	-1.520024
7	0.000000	0.000000	-2.257446
1	0.000000	2.120760	-1.979002
1	0.000000	-2.120760	-1.979002
1	0.000000	0.000000	-3.275559
7	0.000000	0.000000	3.472431

E = -339.6173916 au
ZPVE = 0.074541 au
(H298 - E0) = 4.5 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -338.9009579 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
3B2 triplet state (C2v)

6	0.000000	1.193125	-1.063939
6	0.000000	1.171956	0.294592
6	0.000000	0.000000	1.037039
6	0.000000	-1.171956	0.294592
6	0.000000	-1.193125	-1.063939
1	0.000000	2.090674	-1.666128
1	0.000000	-2.090674	-1.666128
1	0.000000	0.000000	-2.724834
9	0.000000	0.000000	2.337506
7	0.000000	0.000000	-1.710077

E = -346.6005879 au
ZPVE = 0.068847 au
(H298 - E0) = 3.8 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -345.9175865 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

6	0.000000	0.000000	1.276225
9	0.000000	0.000000	2.549722

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
3B2 triplet state (C2v)

6	0.000000	1.192709	-1.515726
6	0.000000	1.163202	-0.156722

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

6	0.000000	0.000000	0.818364
17	0.000000	0.000000	2.478477

6	0.000000	0.773558	0.182956	6	0.000000	0.000000	0.595626	6	0.000000	0.757265	-0.302049
6	0.000000	-0.773558	0.182956	6	0.000000	-1.163202	-0.156722	6	0.000000	-0.757265	-0.302049
6	0.000000	1.147007	-1.135858	6	0.000000	-1.192709	-1.515726	6	0.000000	1.146186	-1.617080
6	0.000000	-1.147007	-1.135858	1	0.000000	2.090672	-2.116600	6	0.000000	-1.146186	-1.617080
7	0.000000	0.000000	-1.869772	1	0.000000	-2.090672	-2.116600	7	0.000000	0.000000	-2.355878
1	0.000000	2.119728	-1.597370	1	0.000000	0.000000	-3.178252	1	0.000000	2.120032	-2.075510
1	0.000000	-2.119728	-1.597370	17	0.000000	0.000000	2.297229	1	0.000000	-2.120032	-2.075510
1	0.000000	0.000000	-2.886878	7	0.000000	0.000000	-2.163686	1	0.000000	0.000000	-3.372572

E = -346.6391302 au
ZPVE = 0.069009 au
(H298 - E0) = 3.8 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -345.9605143 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
3B2 triplet state (C2v)

6	0.000000	1.190089	-1.096951
6	0.000000	1.165355	0.250425
6	0.000000	0.000000	1.042692
6	0.000000	-1.165355	0.250425
6	0.000000	-1.190089	-1.096951
1	0.000000	2.091479	-1.692419
1	0.000000	-2.091479	-1.692419
1	0.000000	0.000000	-2.773340
7	0.000000	0.000000	-1.762086
7	0.000000	0.000000	2.373235
1	0.000000	-0.862919	2.891145

E = -706.9625547 au
ZPVE = 0.067022 au
(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -705.9242048 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

6	0.000000	0.000000	1.286369
7	0.000000	0.000000	2.592551
6	0.000000	0.738878	0.135984
6	0.000000	-0.738878	0.135984
6	0.000000	1.142961	-1.172471
6	0.000000	-1.142961	-1.172471
7	0.000000	0.000000	-1.922084
1	0.000000	2.118799	-1.625389
1	0.000000	-2.118799	-1.625389
1	0.000000	0.868254	3.106576
1	0.000000	-0.868254	3.106576

E = -707.0034839 au
ZPVE = 0.067301 au
(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -705.9688342 au

4-hydroxy-3,5-didehydropyridinium cation (8)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	-1.177395	-1.089323	0.000000
6	-1.159082	0.264485	0.000000
6	0.000000	1.045448	0.000000
6	1.173527	0.282998	0.000000
6	1.204271	-1.069429	0.000000
1	0.025408	-2.747936	0.000000
1	-2.073545	-1.693097	0.000000
1	2.108108	-1.661732	0.000000
7	0.017515	-1.735002	0.000000
8	0.049987	2.359806	0.000000
1	-0.830400	2.764267	0.000000

1	0.000000	0.862919	2.891145	1	0.000000	0.000000	-2.936010				

E = -302.7466751 au
ZPVE = 0.093759 au
(H298 - E0) = 4.2 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -302.0990459 au

E = -302.7955456 au
ZPVE = 0.094200 au
(H298 - E0) = 4.1 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -302.1516436 au

E = -322.5989712 au
ZPVE = 0.081394 au
(H298 - E0) = 3.9 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9351730 au

4-hydroxy-3,5-didehydropyridinium cation (8)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

1	-2.842883	-0.617226	0.000000	1	0.000000	0.000000	2.262334	6	0.000000	0.000000	-1.794778
7	-1.850350	-0.402816	0.000000	7	0.000000	0.000000	1.246634	6	0.000000	0.762159	-0.682891
6	-1.367089	0.873268	0.000000	6	0.000000	1.194437	0.606286	6	0.000000	-0.762159	-0.682891
6	0.000000	0.770006	0.000000	6	0.000000	-1.194437	0.606286	6	0.000000	1.144286	0.636395
6	1.260131	0.260614	0.000000	6	0.000000	1.158763	-0.757990	6	0.000000	-1.144286	0.636395
6	0.315627	-0.704005	0.000000	6	0.000000	-1.158763	-0.757990	7	0.000000	0.000000	1.374139
6	-0.884623	-1.365233	0.000000	6	0.000000	0.000000	-1.500908	1	0.000000	2.117872	1.096364
1	-1.123912	-2.414463	0.000000	1	0.000000	2.088641	1.212167	1	0.000000	-2.117872	1.096364
8	2.529655	0.463373	0.000000	1	0.000000	-2.088641	1.212167	1	0.000000	0.000000	-2.877408
1	-2.020888	1.728019	0.000000	1	0.000000	0.000000	-2.587218	1	0.000000	0.000000	2.392321
1	2.758617	1.408502	0.000000								

E = -322.6441216 au
ZPVE = 0.081579 au
(H298 - E0) = 3.9 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9843142 au

E = -247.3405281 au
ZPVE = 0.076317 au
(H298 - E0) = 3.3 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -246.7998388 au

E = -247.3701202 au
ZPVE = 0.075776 au
(H298 - E0) = 3.4 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -246.8339053 au

2-cyano-3,5-didehydropyridinium cation (10)

2-cyano-3,5-didehydropyridinium cation (10)

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

3A' triplet state (Cs)

1	-1.982130	0.041307	0.000000
7	-1.033973	-0.328044	0.000000
6	0.000000	0.566762	0.000000
6	1.265314	0.036489	0.000000
6	1.540069	-1.310977	0.000000
6	0.430905	-2.125054	0.000000
6	-0.857621	-1.667605	0.000000
1	2.555212	-1.698911	0.000000
1	-1.743163	-2.287139	0.000000
6	-0.306851	1.954231	0.000000
7	-0.574716	3.073996	0.000000

E = -339.58517 au

ZPVE = 0.074347 au

(H298 - E0) = 4.4 kcal/mol

RHF-UCCSD(T)/cc-pVTZ E = -338.8656114 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

1	-2.092302	0.783361	0.000000
7	-1.218045	0.259587	0.000000
6	0.000000	0.861212	0.000000
6	0.979890	-0.090893	0.000000
6	1.535824	-1.321440	0.000000
6	0.193125	-1.418099	0.000000

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

1	-2.161616	0.221627	0.000000
7	-1.236794	-0.206967	0.000000
6	-0.076025	0.535899	0.000000
6	-0.076025	1.947474	0.000000
6	0.958762	-0.376046	0.000000
6	1.661960	-1.529845	0.000000
6	0.329182	-1.737527	0.000000
6	-1.037500	-1.546833	0.000000
1	2.646127	-1.981597	0.000000
1	-1.856907	-2.246110	0.000000
7	-0.076025	3.099444	0.000000

E = -339.6178472 au

ZPVE = 0.074145 au

(H298 - E0) = 4.4 kcal/mol

RHF-UCCSD(T)/cc-pVTZ E = -338.9020869 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

3A' triplet state (Cs)

7	-1.021815	-0.410047	0.000000
6	0.000000	0.483476	0.000000
6	1.268185	-0.033891	0.000000
6	1.552271	-1.374756	0.000000
6	0.448493	-2.204942	0.000000
6	-0.835938	-1.758797	0.000000

UB3LYP/cc-pVTZ

3A' triplet state (Cs)

7	-1.090980	0.101712	0.000000
6	0.000000	0.894156	0.000000
6	1.233742	0.302601	0.000000
6	1.402474	-1.056415	0.000000
6	0.235709	-1.799113	0.000000
6	-1.010916	-1.261338	0.000000
9	-0.219094	2.175800	0.000000
1	2.386867	-1.517221	0.000000
1	-1.940985	-1.810326	0.000000
1	-2.003235	0.554020	0.000000

E = -346.6029122 au

ZPVE = 0.068211 au

(H298 - E0) = 3.8 kcal/mol

RHF-UCCSD(T)/cc-pVTZ E = -345.9199162 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

1	2.097587	0.469202	0.000000
7	1.250547	-0.095647	0.000000
6	0.000000	0.456973	0.000000
6	-0.898973	-0.583022	0.000000
6	-1.407734	-1.829430	0.000000
6	-0.057469	-1.856154	0.000000

6	-1.137553	-1.105918	0.000000	1	2.570461	-1.753684	0.000000	6	1.253305	-1.461499	0.000000
1	-2.016720	-1.727618	0.000000	1	-1.721116	-2.377842	0.000000	1	2.169924	-2.026587	0.000000
1	2.475051	-1.859539	0.000000	1	-1.970506	-0.044072	0.000000	1	-2.315089	-2.419745	0.000000
9	0.081397	2.159723	0.000000	17	-0.372012	2.139964	0.000000	17	-0.237707	2.134438	0.000000

E = -346.6271945 au
ZPVE = 0.067690 au
(H298 - E0) = 3.8 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -345.9484353 au

E = -706.9626072 au
ZPVE = 0.066568 au
(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -705.9245953 au

E = -706.989824 au
ZPVE = 0.066215 au
(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -705.9562055 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

1	-2.015055	0.509476	0.000000
7	-1.094638	0.086470	0.000000
6	0.000000	0.898243	0.000000
6	1.227552	0.229499	0.000000
6	1.375753	-1.115485	0.000000
6	0.191733	-1.853572	0.000000
6	-1.029768	-1.290561	0.000000
1	2.352905	-1.589515	0.000000
1	-1.972750	-1.815696	0.000000
7	-0.135663	2.226797	0.000000
1	-1.030651	2.686271	0.000000
1	0.686041	2.807855	0.000000

E = -302.740769 au
ZPVE = 0.092604 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

1	2.100161	0.784947	0.000000
7	1.225487	0.270234	0.000000
6	0.000000	0.862505	0.000000
7	-0.203955	2.187252	0.000000
1	-1.142942	2.545715	0.000000
6	-0.950982	-0.161274	0.000000
6	-1.483626	-1.379269	0.000000
6	-0.123614	-1.488189	0.000000
6	1.171137	-1.124500	0.000000
1	-2.411552	-1.935261	0.000000
1	2.076179	-1.706357	0.000000
1	0.549946	2.852913	0.000000

E = -302.7625241 au
ZPVE = 0.091567 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

7	-1.091785	0.097295	0.000000
6	0.000000	0.898441	0.000000
6	1.227493	0.264893	0.000000
6	1.384239	-1.088882	0.000000
6	0.208012	-1.824921	0.000000
6	-1.025824	-1.268863	0.000000
8	-0.258631	2.189694	0.000000
1	2.363537	-1.559500	0.000000
1	-1.963629	-1.804007	0.000000
1	0.547906	2.725823	0.000000
1	-1.999788	0.555064	0.000000

E = -322.6023095 au
ZPVE = 0.080624 au

(H298 - E0) = 4.3 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -302.0937347 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

1	-2.086543	0.795375	0.000000
7	-1.218548	0.263932	0.000000
6	0.000000	0.863974	0.000000
8	0.047912	2.184039	0.000000
1	0.955429	2.517038	0.000000
6	0.972591	-0.117384	0.000000
6	1.504320	-1.350445	0.000000
6	0.158056	-1.455423	0.000000
6	-1.154019	-1.110730	0.000000
1	2.437527	-1.898272	0.000000
1	-2.045560	-1.713928	0.000000

(H298 - E0) = 4.5 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -302.1195786 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

1	0.031680	2.294703	0.000000
7	0.000000	1.279176	0.000000
6	-1.173263	0.659988	0.000000
6	-1.318510	-0.697779	0.000000
6	-0.120099	-1.376833	0.000000
6	1.133264	-0.803661	0.000000
6	1.166824	0.576536	0.000000
1	-2.288364	-1.181016	0.000000
1	2.050109	-1.375909	0.000000
1	2.077276	1.158482	0.000000

(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9388794 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

1	2.090111	0.873648	0.000000
7	1.199431	0.392399	0.000000
6	0.000000	0.950642	0.000000
6	-1.330230	1.205621	0.000000
6	-0.995136	-0.101506	0.000000
6	-0.301533	-1.328525	0.000000
6	1.031861	-0.996574	0.000000
1	-2.097363	1.968129	0.000000
1	-0.715096	-2.322279	0.000000
1	1.896557	-1.644231	0.000000

E = -322.6237464 au
ZPVE = 0.079756 au
(H298 - E0) = 4.1 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9467011 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	0.033111	-1.787262	0.000000
6	1.234833	-1.100094	0.000000

E = -247.3425822 au
ZPVE = 0.076031 au
(H298 - E0) = 3.3 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -246.8019729 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

6	-1.915478	-0.382242	0.000000
6	-0.968381	-1.379475	0.000000

E = -247.3772836 au
ZPVE = 0.076087 au
(H298 - E0) = 3.3 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -246.8409199 au

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	-1.143282	0.258162	0.000000
6	0.000000	1.027220	0.000000

6	1.160062	0.267615	0.000000
6	0.000000	1.033533	0.000000
6	-1.143148	0.246908	0.000000
7	-1.123900	-1.076040	0.000000
1	-0.055130	-2.862871	0.000000
1	2.173259	-1.637135	0.000000
8	-0.091266	2.357995	0.000000
1	0.779671	2.779312	0.000000
1	-2.009521	-1.575180	0.000000

E = -322.5910116 au
ZPVE = 0.080614 au
(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9276163 au

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

6	0.000000	0.713215	0.000000
6	1.258743	0.239546	0.000000
6	0.312161	-0.712010	0.000000
6	-0.916329	-1.401994	0.000000
6	-1.884298	-0.425384	0.000000
1	-1.833774	1.721010	0.000000
1	-1.075320	-2.466349	0.000000
1	-2.958392	-0.534920	0.000000
9	2.497096	0.539146	0.000000
7	-1.318292	0.849674	0.000000

6	0.276053	-0.709182	0.000000
6	1.269108	0.221554	0.000000
6	0.000000	0.694222	0.000000
7	-1.317278	0.876530	0.000000
1	-2.991272	-0.466478	0.000000
1	-1.151785	-2.439506	0.000000
8	2.511272	0.566979	0.000000
1	3.113081	-0.195964	0.000000
1	-1.807069	1.761143	0.000000

E = -322.6451904 au
ZPVE = 0.081501 au
(H298 - E0) = 3.9 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9857547 au

3-cyano-2,4-didehydropyridinium cation (18)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	-1.126632	-0.114719	0.000000
6	0.000000	0.680299	0.000000
6	1.179258	-0.056011	0.000000
6	1.274679	-1.426713	0.000000
6	0.080628	-2.122663	0.000000
1	-1.972986	-1.953620	0.000000
1	2.218966	-1.953411	0.000000
1	0.009648	-3.201057	0.000000
7	-1.096563	-1.436841	0.000000
6	-0.056060	2.104487	0.000000

6	1.174647	0.297179	0.000000
6	1.250984	-1.072904	0.000000
6	0.050928	-1.762273	0.000000
1	-1.996772	-1.576067	0.000000
1	2.190645	-1.608287	0.000000
1	-0.028461	-2.839240	0.000000
9	-0.039166	2.334252	0.000000
7	-1.116082	-1.066997	0.000000

E = -346.5957396 au
ZPVE = 0.068334 au
(H298 - E0) = 3.8 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -345.9128424 au

3-cyano-2,4-didehydropyridinium cation (18)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

6	0.000000	0.722498	0.000000
6	0.854722	-0.333705	0.000000
6	-0.466494	-0.643763	0.000000
6	-1.873599	-0.605177	0.000000
6	-2.199234	0.732183	0.000000
1	-1.033959	2.542352	0.000000
1	-2.560940	-1.433572	0.000000
1	-3.174363	1.196830	0.000000
7	-1.046744	1.529524	0.000000
6	2.193208	-0.755878	0.000000

7	-0.098704	3.253985	0.000000

E = -346.6419252 au
ZPVE = 0.069193 au
(H298 - E0) = 3.7 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -345.9635040 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	-1.143095	0.144039	0.000000
6	0.000000	0.941914	0.000000
6	1.200646	0.245301	0.000000
6	1.345501	-1.116800	0.000000
6	0.161895	-1.806155	0.000000
8	-0.155856	2.263461	0.000000
7	-1.019488	-1.208027	0.000000
1	-1.864748	-1.771731	0.000000
1	2.307952	-1.615207	0.000000
1	0.691965	2.728783	0.000000
1	-2.141590	0.556866	0.000000

E = -322.5949484 au
ZPVE = 0.080401 au
(H298 - E0) = 4.0 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9314187 au

5-cyano-2,4-didehydropyridinium cation (20)

7	3.292122	-1.101318	0.000000

E = -339.5858617 au
ZPVE = 0.074456 au
(H298 - E0) = 4.5 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -338.8671485 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

6	-1.189293	0.206094	0.000000
6	0.000000	0.928074	0.000000
6	1.147904	0.150072	0.000000
6	1.375791	-1.185588	0.000000
6	0.116303	-1.752982	0.000000
8	-0.050190	2.259516	0.000000
7	-1.053594	-1.144398	0.000000
1	-1.890598	-1.722444	0.000000
1	2.311388	-1.721240	0.000000
1	0.829343	2.660670	0.000000
1	-2.177686	0.643644	0.000000

E = -322.6098036 au
ZPVE = 0.079909 au
(H298 - E0) = 4.1 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -321.9631662 au

E = -339.6236332 au
ZPVE = 0.074815 au
(H298 - E0) = 4.4 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -338.9071107 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	0.273339	-2.124762	0.000000
6	1.432241	-1.399790	0.000000
6	1.232466	-0.041261	0.000000
6	0.000000	0.599404	0.000000
6	-1.111828	-0.236527	0.000000
1	2.412245	-1.863653	0.000000
1	-2.129508	0.127967	0.000000
1	-1.757563	-2.184989	0.000000
7	-0.937972	-1.582524	0.000000
6	-0.151109	2.016939	0.000000
7	-0.287146	3.159190	0.000000

E = -339.5882342 au
ZPVE = 0.074290 au
(H298 - E0) = 4.4 kcal/mol
RHF-UCCSD(T)/cc-pVTZ E = -338.8695142 au

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

6	-0.095347	-2.071087	0.000000
6	-1.372383	-1.546093	0.000000
6	-1.127110	-0.217448	0.000000
6	0.000000	0.584778	0.000000
6	1.201894	-0.108208	0.000000
1	-2.301018	-2.094309	0.000000
1	2.188933	0.334979	0.000000
1	1.915164	-2.038401	0.000000
7	1.076928	-1.459925	0.000000
6	-0.057804	2.008989	0.000000
7	-0.091010	3.158802	0.000000

E = -339.6058811 au

ZPVE = 0.073473 au

(H298 - E0) = 4.4 kcal/mol

RHF-UCCSD(T)/cc-pVTZ E = -338.9104748 au

Transition States and Auxillary Geometries

methane

MPW1K/6-31+G(d,p)

1A' singlet state (Cs)

6	0.000000	0.000000	0.000000
1	0.626865	0.626865	0.626865
1	-0.626865	-0.626865	0.626865

4-cyano-3,5-didehydropyridinium cation (4)

MPW1K/6-31+G(d,p)

1A1 singlet state (C2v)

6	0.000000	1.167440	-1.444469
6	0.000000	1.115965	-0.085098
6	0.000000	0.000000	0.724353

4-cyano-3,5-didehydropyridinium cation (4) + methane TS

MPW1K/6-31+G(d,p)

1A singlet state (C1)

1	-3.132446	1.125620	0.000000
7	-2.253773	0.623304	0.000000

1	-0.626865	0.626865	-0.626865
1	0.626865	-0.626865	-0.626865

E = -40.5126335 au
ZPVE = 0.045985 au
(H298 - E0) = 2.4 kcal/mol

6	0.000000	-1.115965	-0.085098
6	0.000000	-1.167440	-1.444469
1	0.000000	0.000000	-3.121294
1	0.000000	2.084486	-2.012935
1	0.000000	-2.084486	-2.012935
7	0.000000	0.000000	-2.108196
6	0.000000	0.000000	2.143322
7	0.000000	0.000000	3.293326

E = -339.3780338 au
ZPVE = 0.077481 au
(H298 - E0) = 4.4 kcal/mol

6	-1.102601	1.313859	0.000000
6	0.084994	0.635968	0.000000
6	0.172048	-0.750275	0.000000
6	-1.065183	-1.357188	0.000000
6	-2.266619	-0.719425	0.000000
1	-1.172282	2.390316	0.000000
6	1.410313	-1.453653	0.000000
1	-3.221515	-1.221142	0.000000
1	1.336093	1.479048	0.000000
6	2.324498	2.159116	0.000000
1	2.277745	2.753051	-0.905279
1	3.148920	1.455584	-0.000002
1	2.277747	2.753048	0.905282
7	2.416779	-2.009866	0.000000

E = -379.8876126 au
ZPVE = 0.120610 au
(H298 - E0) = 6.3 kcal/mol

4-fluoro-3,5-didehydropyridinium cation (5)
MPW1K/6-31+G(d,p)
1A1 singlet state (C2v)

6	0.000000	1.142382	-1.137602
6	0.000000	0.749279	0.175863
6	0.000000	0.000000	1.283729
6	0.000000	-0.749279	0.175863
6	0.000000	-1.142382	-1.137602
1	0.000000	0.000000	-2.872952

4-fluoro-3,5-didehydropyridinium cation (5)
+ methane TS
MPW1K/6-31+G(d,p)
1A singlet state (C1)

6	-1.372680	1.080321	-0.000122
6	-2.212215	0.015235	-0.000184
6	-0.004489	1.005589	0.000088
6	0.477581	-0.283808	0.000270
6	-0.332387	-1.380232	0.000216

4-chloro-3,5-didehydropyridinium cation (6)
MPW1K/6-31+G(d,p)
1A1 singlet state (C2v)

6	0.000000	1.141088	-1.614341
6	0.000000	0.739308	-0.303503
6	0.000000	0.000000	0.825853
6	0.000000	-0.739308	-0.303503
6	0.000000	-1.141088	-1.614341
1	0.000000	0.000000	-3.354171

1	0.000000	2.114246	-1.596321
1	0.000000	-2.114246	-1.596321
7	0.000000	0.000000	-1.860381
9	0.000000	0.000000	2.547418

E = -346.41265 au
ZPVE = 0.072103 au
(H298 - E0) = 3.6 kcal/mol

7	-1.666281	-1.214419	-0.000026
1	-2.269114	-2.025841	-0.000096
1	-3.288247	0.092921	-0.000362
1	0.038806	-2.393116	0.000401
6	3.123145	-0.826877	-0.000128
1	3.624711	0.131944	-0.058683
1	3.312330	-1.345044	0.932590
1	3.290457	-1.443436	-0.875439
1	1.957568	-0.559797	0.000362
9	0.769301	2.042437	0.000063

E = -386.9074483 au
ZPVE = 0.114567 au
(H298 - E0) = 5.7 kcal/mol

1	0.000000	2.113874	-2.070799
1	0.000000	-2.113874	-2.070799
7	0.000000	0.000000	-2.341961
17	0.000000	0.000000	2.467559

E = -706.8162283 au
ZPVE = 0.070298 au
(H298 - E0) = 3.8 kcal/mol

4-chloro-3,5-didehydropyridinium cation (6) + methane TS
MPW1K/6-31+G(d,p)
1A singlet state (C1)

6	-1.117092	-1.269227	0.000009
6	-2.301129	-0.606805	0.000012
6	0.133246	-0.698241	-0.000005
6	0.079324	0.685809	-0.000020
6	-1.088245	1.393019	-0.000014
7	-2.261003	0.737446	0.000001
1	-3.125407	1.261304	0.000004
1	-3.266561	-1.087696	0.000026
1	-1.126935	2.470987	-0.000019

4-amino-3,5-didehydropyridinium cation (7)
MPW1K/6-31+G(d,p)
1A1 singlet state (C2v)

6	0.000000	1.138161	-1.172816
6	0.000000	0.724806	0.131505
6	0.000000	0.000000	1.288430
6	0.000000	-0.724806	0.131505
6	0.000000	-1.138161	-1.172816
1	0.000000	0.000000	-2.920291
1	0.000000	2.112071	-1.625759
1	0.000000	-2.112071	-1.625759
7	0.000000	0.000000	-1.910712
1	0.000000	-0.865261	3.098577

4-amino-3,5-didehydropyridinium cation (7) + methane TS
MPW1K/6-31+G(d,p)
1A singlet state (C1)

6	-1.385258	1.059182	0.000029
6	-2.211736	-0.002063	0.000029
6	0.009635	1.036268	-0.000008
6	0.481495	-0.289531	-0.000036
6	-0.326771	-1.377758	-0.000033
7	-1.668058	-1.239762	-0.000004
1	-2.261772	-2.053768	-0.000007
1	-3.287495	0.075458	0.000054
1	0.057090	-2.385626	-0.000055

6	2.271316	2.223306	0.000016
1	3.113649	1.542200	-0.001297
1	2.198472	2.812749	-0.906173
1	2.199768	2.810877	0.907523
1	1.291609	1.494079	-0.000014
17	1.569289	-1.578458	-0.000003

E = -747.3037935 au
ZPVE = 0.112168 au
(H298 - E0) = 5.9 kcal/mol

1	0.000000	0.865261	3.098577
7	0.000000	0.000000	2.587827

E = -302.6073387 au
ZPVE = 0.098115 au
(H298 - E0) = 3.9 kcal/mol

6	3.054301	-0.945725	0.000036
1	3.469420	-0.528764	-0.909685
1	3.469129	-0.529458	0.910207
1	3.025948	-2.028539	-0.000394
1	1.836502	-0.581053	-0.000019
1	0.381151	3.028471	0.000001
1	1.780588	2.029843	-0.000054
7	0.782264	2.109932	-0.000017

E = -343.0830973 au
ZPVE = 0.139683 au
(H298 - E0) = 6.0 kcal/mol

4-hydroxy-3,5-didehydropyridinium cation (8)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

6	1.264770	0.259628	0.000000
6	0.000000	0.751581	0.000000
6	0.306836	-0.688301	0.000000
6	-1.365686	0.868796	0.000000
6	-0.886961	-1.360078	0.000000
7	-1.840109	-0.399581	0.000000
1	-2.017186	1.723040	0.000000
1	-1.125664	-2.407563	0.000000
1	-2.828608	-0.611956	0.000000
8	2.522981	0.463130	0.000000
1	2.754617	1.398754	0.000000

4-hydroxy-3,5-didehydropyridinium cation (8)
+ methane TS
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-2.287557	-2.021800	0.000000
7	-1.678627	-1.216813	0.000000
6	-0.342119	-1.384561	0.000000
6	0.475581	-0.300207	0.000000
6	0.025216	1.015229	0.000000
6	-1.356106	1.075878	0.000000
6	-2.204509	0.023104	0.000000
1	0.024839	-2.398849	0.000000
8	0.861275	2.015770	0.000000
1	-3.279259	0.116041	0.000000
1	1.888912	-0.586626	0.000000

3,5-didehydropyridinium cation (9)
MPW1K/6-31+G(d,p)
1A1 singlet state (C2v)

6	0.000000	0.000000	-1.557346
6	0.000000	1.109904	-0.747966
6	0.000000	-1.109904	-0.747966
6	0.000000	1.166551	0.613136
6	0.000000	-1.166551	0.613136
7	0.000000	0.000000	1.277485
1	0.000000	2.082205	1.182839
1	0.000000	-2.082205	1.182839
1	0.000000	0.000000	-2.636078
1	0.000000	0.000000	2.290038

E = -247.2033553 au

E = -322.4345464 au
ZPVE = 0.085114 au
(H298 - E0) = 3.8 kcal/mol

6	3.076286	-0.886044	0.000000
1	3.234859	-1.456337	0.907281
1	3.585055	0.070234	-0.000017
1	3.234852	-1.456365	-0.907265
1	0.412389	2.864840	0.000000

ZPVE = 0.078908 au
(H298 - E0) = 3.2 kcal/mol

E = -362.9198007 au
ZPVE = 0.127065 au
(H298 - E0) = 5.8 kcal/mol

3,5-didehydropyridinium cation (9) + methane TS
MPW1K/6-31+G(d,p)
1A singlet state (C1)

6	-1.384381	1.250189	0.000100
6	-2.114917	0.101205	0.000227
6	-0.014525	1.338462	-0.000186
6	0.601227	0.097056	-0.000420
6	-0.093403	-1.083968	-0.000243
7	-1.435102	-1.056854	0.000066
1	-1.947077	-1.929155	0.000184
1	-3.192363	0.057881	0.000474
1	0.530172	2.271196	-0.000179
1	0.377073	-2.054352	-0.000273
6	3.268323	-0.120189	0.000379
1	3.601645	0.424893	-0.874603
1	3.592507	0.322359	0.934622
1	3.469173	-1.183297	-0.059608

2-cyano-3,5-didehydropyridinium cation (10)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

1	2.092721	0.518884	0.000000
7	1.241879	-0.034303	0.000000
6	0.000000	0.535697	0.000000
6	-0.886583	-0.516202	0.000000
6	-1.434958	-1.751251	0.000000
6	-0.089626	-1.745195	0.000000
6	1.241952	-1.377163	0.000000
1	-2.343520	-2.336447	0.000000
1	2.149564	-1.954113	0.000000
6	-0.193719	1.934800	0.000000
7	-0.344902	3.075382	0.000000

E = -339.3921433 au
ZPVE = 0.077420 au
(H298 - E0) = 4.3 kcal/mol

2-cyano-3,5-didehydropyridinium cation (10) + methane TS (3-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.347884	-2.124162	-0.000001
7	-1.257137	-1.114705	0.000000
6	-0.021219	-0.565527	0.000000
6	0.107972	0.802535	0.000000
6	-0.974404	1.667766	0.000000
6	-2.173988	1.004848	0.000000
6	-2.353224	-0.348846	0.000000
1	-0.874516	2.743308	0.000001
1	1.527817	1.316554	0.000000
6	2.673066	1.677854	0.000000
1	3.112257	1.272571	0.903914
1	2.629252	2.760843	-0.000009
1	3.112262	1.272557	-0.903906
6	1.091228	-1.455574	0.000000

1	2.040642	-0.008080	-0.000228

E = -287.7091092 au
ZPVE = 0.121583 au
(H298 - E0) = 5.2 kcal/mol

2-cyano-3,5-didehydropyridinium cation (10)
+ methane TS (5-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.134709	-1.941217	-0.000307
7	-0.621748	-1.067117	-0.000435
6	0.714793	-1.078920	-0.000880
6	1.402317	0.110435	-0.001096
6	0.786720	1.348573	-0.000725
6	-0.583761	1.254303	-0.000212
6	-1.310556	0.097166	-0.000066
1	1.195046	-2.045115	-0.000948
1	1.324832	2.285210	-0.000767
6	-2.732034	0.040411	0.000526
1	2.870267	-0.001875	-0.000337
6	4.080293	-0.130395	0.001471
1	4.325107	-0.601433	0.946089
1	4.469016	0.877761	-0.081614
1	4.314003	-0.744410	-0.860249
7	-3.879710	-0.029793	0.001010

2-fluoro-3,5-didehydropyridinium cation (11)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

7	-1.207670	0.264446	0.000000
6	0.000000	0.859283	0.000000
6	0.960458	-0.110599	0.000000
6	1.535845	-1.330239	0.000000
6	0.191889	-1.391118	0.000000
6	-1.142020	-1.092691	0.000000
9	0.089105	2.147886	0.000000
1	2.470989	-1.871202	0.000000
1	-2.021785	-1.709927	0.000000
1	-2.074484	0.791221	0.000000

E = -346.4011276 au
ZPVE = 0.070768 au
(H298 - E0) = 3.7 kcal/mol

7	1.979767	-2.185400	0.000000
1	-3.314185	-0.839267	0.000000

E = -379.884641 au
ZPVE = 0.120262 au
(H298 - E0) = 6.3 kcal/mol

2-fluoro-3,5-didehydropyridinium cation (11)
+ methane TS (3-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	1.826955	1.820883	0.000494
7	1.429321	0.888486	0.000233
6	0.100125	0.758223	-0.000236
6	-0.491835	-0.477206	-0.000624
6	0.247631	-1.638274	-0.000416
6	1.609983	-1.413247	0.000094
6	2.223372	-0.204556	0.000437
9	-0.566456	1.871315	-0.000322
1	-0.196813	-2.622832	-0.000600
1	3.290396	-0.050344	0.000873
1	-2.043117	-0.471887	-0.000210
6	-3.224480	-0.434251	0.000584
1	-3.511629	0.028851	0.937349
1	-3.552245	-1.464949	-0.072475
1	-3.509463	0.154907	-0.863200

E = -386.9024395 au

E = -379.8831909 au
ZPVE = 0.119937 au
(H298 - E0) = 6.4 kcal/mol

2-fluoro-3,5-didehydropyridinium cation (11)
+ methane TS (5-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.496790	-1.935083	0.000043
7	-0.968004	-1.070145	-0.000155
6	0.382161	-1.080881	-0.000647
6	1.054734	0.104457	-0.000896
6	0.426287	1.346982	-0.000518
6	-0.936732	1.259842	-0.000014
6	-1.634660	0.087076	0.000163
1	0.860074	-2.047500	-0.000689
1	0.966080	2.282806	-0.000542
9	-2.925409	0.002368	0.000677
1	2.530430	0.003608	-0.000383
6	3.735338	-0.118374	0.000965
1	3.985943	-0.583763	0.946853
1	4.122222	0.890114	-0.087157
1	3.973995	-0.735098	-0.857454

E = -386.9001327 au
ZPVE = 0.113558 au
(H298 - E0) = 5.7 kcal/mol

2-chloro-3,5-didehydropyridinium cation (12)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

7	1.242899	-0.082180	0.000000
6	0.000000	0.460059	0.000000
6	-0.875270	-0.599455	0.000000
6	-1.394793	-1.840298	0.000000
6	-0.046163	-1.827892	0.000000
6	1.266422	-1.437321	0.000000
1	-2.295876	-2.436285	0.000000
1	2.186369	-1.993166	0.000000
1	2.080595	0.488561	0.000000
17	-0.257209	2.116799	0.000000

E = -706.8033185 au
ZPVE = 0.069242 au
(H298 - E0) = 3.9 kcal/mol

ZPVE = 0.114253 au
(H298 - E0) = 5.7 kcal/mol

2-chloro-3,5-didehydropyridinium cation (12)
+ methane TS (3-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.539190	-1.945362	-0.000032
7	-1.358914	-0.948786	-0.000017
6	-0.083707	-0.521675	0.000003
6	0.171216	0.828960	0.000027
6	-0.826032	1.782366	0.000025
6	-2.092284	1.242120	0.000001
6	-2.389748	-0.082525	-0.000020
1	-0.625155	2.843776	0.000044
1	-3.387358	-0.491958	-0.000038
1	1.595955	1.241985	0.000020
6	2.759295	1.576583	-0.000025
1	3.185014	1.160271	0.905135
1	2.744932	2.660277	-0.000739
1	3.185284	1.159099	-0.904518
17	1.124734	-1.702445	0.000011

E = -747.2987095 au
ZPVE = 0.111849 au
(H298 - E0) = 5.9 kcal/mol

2-chloro-3,5-didehydropyridinium cation (12) + methane TS (5-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.018193	-1.948625	-0.000168
7	-0.508591	-1.073400	-0.000315
6	0.837321	-1.079873	-0.000730
6	1.516335	0.105311	-0.000956
6	0.882356	1.341550	-0.000605
6	-0.481475	1.240691	-0.000181
6	-1.201727	0.079409	-0.000037
1	1.315964	-2.046425	-0.000747
1	1.413428	2.282178	-0.000587
1	2.975272	0.007952	-0.000283
6	4.190549	-0.109680	0.001200
1	4.440932	-0.570275	0.949418
1	4.570260	0.901071	-0.091122
1	4.429205	-0.728944	-0.855308
17	-2.883934	0.008966	0.000521

E = -747.2981136 au
ZPVE = 0.111732 au
(H298 - E0) = 5.9 kcal/mol

2-amino-3,5-didehydropyridinium cation (13)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.150801	1.909298	0.002899
7	-0.487493	1.147853	0.000767
6	-0.848514	-0.149424	-0.000222
6	0.346472	-0.877154	-0.001696
6	1.629070	-1.217419	0.001216
6	1.456322	0.137360	-0.001780
6	0.887726	1.354975	0.000025
1	2.340935	-2.028996	0.005052
1	1.295843	2.348012	0.000714
7	-2.103806	-0.597633	0.000097
1	-2.896881	0.013887	-0.001026
1	-2.276462	-1.583768	0.001059

E = -302.5722304 au
ZPVE = 0.095579 au
(H298 - E0) = 4.3 kcal/mol

2-amino-3,5-didehydropyridinium cation (13) + methane TS (3-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	1.875001	1.753821	0.012381
7	1.446914	0.836503	0.007438
6	0.107909	0.772304	0.007093
6	-0.511408	-0.467842	0.000411
6	0.199281	-1.641365	-0.005915
6	1.573255	-1.469938	-0.004993
6	2.212207	-0.280476	0.001417
1	-0.275507	-2.611739	-0.011144
1	3.282202	-0.150083	0.002118
1	-1.954651	-0.478204	0.000361
6	-3.193926	-0.483774	0.000338
1	-3.501046	0.015740	0.912270
1	-3.452686	-1.536140	-0.005316
1	-3.501056	0.025513	-0.906170
1	-1.491039	2.006841	0.013745
7	-0.490067	1.960816	0.013498
1	-0.003060	2.819563	-0.154908

E = -343.0323524 au
ZPVE = 0.141717 au
(H298 - E0) = 5.8 kcal/mol

2-amino-3,5-didehydropyridinium cation (13) + methane TS (5-position)

2-hydroxy-3,5-didehydropyridinium cation (14) MPW1K/6-31+G(d,p)

2-hydroxy-3,5-didehydropyridinium cation (14) + methane TS (3-position)

MPW1K/6-31+G(d,p)

1A singlet state (C1)

1	-1.409359	-1.972308	0.000139
7	-0.931504	-1.083432	-0.000138
6	0.432141	-1.077161	-0.000749
6	1.101214	0.094927	-0.001145
6	0.445065	1.340128	-0.000598
6	-0.899712	1.237306	-0.000032
6	-1.646275	0.059825	0.000166
1	0.908380	-2.044140	-0.000522
1	0.974992	2.281188	-0.000422
7	-2.976468	0.032188	0.000703
1	2.538274	0.013442	0.000131
6	3.763751	-0.094939	0.001418
1	4.074426	0.158572	1.007795
1	4.111306	0.608850	-0.745393
1	3.972541	-1.125075	-0.261856
1	-3.485504	0.895293	0.000859
1	-3.506353	-0.817641	0.000959

E = -343.0717459 au

ZPVE = 0.138664 au

(H298 - E0) = 6.2 kcal/mol

2-hydroxy-3,5-didehydropyridinium cation (14)

+ methane TS (5-position)

MPW1K/6-31+G(d,p)

1A singlet state (C1)

1A' singlet state (Cs)

1	-2.066602	0.807929	0.000000
7	-1.207963	0.270514	0.000000
6	0.000000	0.863354	0.000000
6	0.947556	-0.141930	0.000000
6	1.505533	-1.361631	0.000000
6	0.156638	-1.423622	0.000000
6	-1.160198	-1.097394	0.000000
1	2.434601	-1.912407	0.000000
1	-2.052141	-1.696027	0.000000
8	0.060326	2.171497	0.000000
1	0.960102	2.502271	0.000000

E = -322.4132739 au

ZPVE = 0.083276 au

(H298 - E0) = 4.0 kcal/mol

2,4-didehydropyridinium cation (15)

MPW1K/6-31+G(d,p)

1A' singlet state (Cs)

1	2.085658	0.861139	0.000000

MPW1K/6-31+G(d,p)

1A singlet state (C1)

1	-1.872463	1.782187	-0.000003
7	-1.448866	0.862774	-0.000002
6	-0.110191	0.792028	0.000001
6	0.503056	-0.451149	0.000002
6	-0.213362	-1.621200	0.000002
6	-1.586482	-1.443055	0.000000
6	-2.219611	-0.250466	-0.000002
8	0.484666	1.960098	0.000002
1	0.256676	-2.593898	0.000004
1	-3.288955	-0.114842	-0.000004
1	1.946231	-0.468567	0.000001
6	3.185464	-0.480196	-0.000003
1	3.495049	0.022717	-0.909229
1	3.439075	-1.533830	-0.000019
1	3.495054	0.022691	0.909237
1	1.440812	1.887576	0.000006

E = -362.9136106 au

ZPVE = 0.126239 au

(H298 - E0) = 5.8 kcal/mol

2,4-didehydropyridinium cation (15)

+ methane TS (2-position)

MPW1K/6-31+G(d,p)

1A singlet state (C1)

1	-1.458851	-1.950189	0.000035
7	-0.943045	-1.078860	-0.000142
6	0.409965	-1.075471	-0.000538
6	1.074889	0.108489	-0.000747
6	0.427636	1.347353	-0.000439
6	-0.927162	1.242172	-0.000023
6	-1.643088	0.064469	0.000131
1	0.893778	-2.038977	-0.000530
1	0.957181	2.288787	-0.000460
8	-2.942627	-0.081547	0.000553
1	2.531252	0.019856	-0.000243
6	3.744784	-0.102440	0.000840
1	3.993805	-0.572974	0.944470
1	4.129481	0.907264	-0.081596
1	3.982373	-0.714376	-0.861153
1	-3.408830	0.757574	0.000710

E = -362.9144223 au
ZPVE = 0.126403 au
(H298 - E0) = 5.9 kcal/mol

2,4-didehydropyridinium cation (15)
+ methane TS (4-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	2.056556	-2.006014	0.000328
6	0.060521	-1.132197	-0.000493
6	-0.601307	0.086311	-0.000780
7	1.197713	0.384511	0.000000
6	0.000000	0.937533	0.000000
6	-1.322461	1.212039	0.000000
6	-0.984756	-0.093024	0.000000
6	-0.306510	-1.326141	0.000000
6	1.022597	-0.992131	0.000000
1	-2.083388	1.977602	0.000000
1	-0.722289	-2.317048	0.000000
1	1.882804	-1.642919	0.000000

E = -247.2272093 au
ZPVE = 0.079097 au
(H298 - E0) = 3.2 kcal/mol

3-hydroxy-2,4-didehydropyridinium cation (16)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

6	-1.904145	-0.372741	0.000000
6	-0.968121	-1.375069	0.000000
6	0.271368	-0.701610	0.000000
6	1.266893	0.220676	0.000000
1	-1.802605	-2.137832	0.000215
6	0.565441	0.171070	-0.000650
6	-0.110517	1.371339	-0.000304
6	-1.467103	1.191437	0.000204
6	-2.166513	0.007649	0.000412
1	0.502104	-1.839148	-0.000488
1	0.392443	2.324571	-0.000393
1	-3.244252	-0.037795	0.000843
1	2.027931	0.052889	-0.000358
6	3.244464	-0.101153	0.000565
1	3.481134	-0.601549	0.932344
1	3.640428	0.906298	-0.050775
1	3.473256	-0.689628	-0.880392
7	-0.062605	-1.001449	-0.000411
6	-1.404472	-1.134954	0.000087

E = -287.7141742 au
ZPVE = 0.121446 au
(H298 - E0) = 5.2 kcal/mol

3-hydroxy-2,4-didehydropyridinium cation (16)
+ methane TS (2-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-2.162698	-2.259381	0.000009
6	0.462507	-0.247390	0.000041
6	-0.051460	1.035980	0.000008

6	0.008589	1.323652	-0.000409
6	1.371983	1.208400	0.000220
1	-0.476826	-2.067492	-0.000600
1	-0.507976	2.269186	-0.000490
1	3.057639	0.117273	0.000946
1	-2.001543	0.019874	-0.000551
6	-3.251175	-0.105481	0.000668
1	-3.472245	-0.726567	-0.858699
1	-3.620534	0.908628	-0.091247
1	-3.485048	-0.568625	0.951409
7	2.047120	0.075693	0.000438
6	1.431412	-1.126704	0.000099

E = -287.7116794 au
ZPVE = 0.121254 au
(H298 - E0) = 5.2 kcal/mol

6	0.000000	0.684460	0.000000
7	-1.310435	0.875836	0.000000
1	-2.978558	-0.455163	0.000000
1	-1.155557	-2.432764	0.000000
8	2.500999	0.557764	0.000000
1	3.099000	-0.197313	0.000000
1	-1.795807	1.757976	0.000000

E = -322.4390801 au
ZPVE = 0.084905 au
(H298 - E0) = 3.8 kcal/mol

6	-1.423098	1.010489	-0.000040
6	-2.254398	-0.077244	-0.000040
1	0.165864	-2.226892	0.000127
1	-3.329407	0.016754	-0.000076
1	1.911026	-0.536438	0.000108
6	3.090657	-0.829948	-0.000018
1	3.264602	-1.384291	0.914870
1	3.589908	0.131551	-0.015344
1	3.258787	-1.410013	-0.899944
7	-0.301159	-1.330572	0.000044
6	-1.647254	-1.312796	0.000004
8	0.758787	2.075408	0.000017
1	0.278008	2.904906	0.000069

E = -362.9125543 au
ZPVE = 0.126527 au
(H298 - E0) = 5.9 kcal/mol

3-hydroxy-2,4-didehydropyridinium cation (16)
+ methane TS (4-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-2.461834	-2.026393	0.000000
6	-0.354865	-1.441725	0.000006
6	0.461104	-0.331909	0.000006
6	0.060657	0.983550	0.000002
6	-1.313910	1.063206	-0.000004
1	0.053486	-2.440048	0.000010

3-fluoro-2,4-didehydropyridinium cation (17)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

6	0.000000	0.699168	0.000000
6	1.258238	0.238531	0.000000
6	0.305673	-0.703401	0.000000
6	-0.916907	-1.398850	0.000000
6	-1.874100	-0.417072	0.000000
1	-1.822463	1.717319	0.000000
1	-1.079234	-2.460975	0.000000

3-fluoro-2,4-didehydropyridinium cation (17)
+ methane TS (2-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-2.140028	-2.264101	-0.000023
6	0.464492	-0.230266	-0.000083
6	-0.079204	1.028083	-0.000014
6	-1.442441	1.013559	0.000059
6	-2.259647	-0.086751	0.000067
1	0.187881	-2.217446	-0.000025

1	-3.127867	0.223888	-0.000009
1	1.818312	-0.587428	0.000008
6	3.031443	-0.900032	-0.000006
1	3.169276	-1.469231	0.910676
1	3.525417	0.063316	-0.000175
1	3.169191	-1.469507	-0.910528
7	-2.134576	0.032066	-0.000005
6	-1.716057	-1.248244	0.000000
8	0.914271	1.986810	0.000003
1	0.471656	2.837386	0.000001

E = -362.9104617 au
ZPVE = 0.126216 au
(H298 - E0) = 5.9 kcal/mol

3-fluoro-2,4-didehydropyridinium cation (17)
+ methane TS (4-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-2.420084	-2.055328	-0.000002
6	-0.327119	-1.436399	0.000006
6	0.472236	-0.310601	0.000007
6	0.023217	0.978717	0.000002
6	-1.340994	1.053514	-0.000004
1	0.094552	-2.429418	0.000010
1	-3.141236	0.178392	-0.000009
1	1.901860	-0.551743	0.000005
6	3.087619	-0.825805	-0.000005
1	-2.946846	-0.524710	0.000000
9	2.488524	0.535785	0.000000
7	-1.312229	0.848008	0.000000

E = -346.4191795 au
ZPVE = 0.072078 au
(H298 - E0) = 3.7 kcal/mol

3-cyano-2,4-didehydropyridinium cation (18)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

6	0.000000	0.714096	0.000000
6	0.847586	-0.339036	0.000000
6	-0.473552	-0.629680	0.000000
6	-1.877536	-0.584522	0.000000
6	-2.179036	0.754557	0.000000
1	-1.004635	2.543868	0.000000
1	-2.573956	-1.403075	0.000000
1	-3.148205	1.228197	0.000000
7	-1.029799	1.535721	0.000000
6	2.183026	-0.777251	0.000000
1	-3.336124	-0.009318	0.000128
1	1.974283	-0.504472	0.000086
6	3.135128	-0.771566	0.000126
1	3.326131	-1.310874	0.920834
1	3.630284	0.192145	-0.030633
1	3.315577	-1.362819	-0.890357
7	-0.285739	-1.323949	-0.000066
6	-1.632859	-1.312353	-0.000008
9	0.658817	2.100033	-0.000049

E = -386.903917 au
ZPVE = 0.114247 au
(H298 - E0) = 5.7 kcal/mol

3-cyano-2,4-didehydropyridinium cation (18)
+ methane TS (2-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-3.130124	1.339658	-0.000003
6	0.088528	0.593427	-0.000008
6	0.136671	-0.788502	0.000000
6	-1.122636	-1.339305	0.000007
6	-2.328895	-0.685482	0.000007
1	-0.998364	2.278291	-0.000014
1	-3.273761	-1.206780	0.000014
1	1.363945	1.482218	-0.000003
6	2.327275	2.176529	0.000008

1	3.251123	-1.393271	0.908154
1	3.578882	0.139662	-0.000590
1	3.250895	-1.394251	-0.907592
7	-2.143026	0.009246	-0.000005
6	-1.689838	-1.261885	0.000000
9	0.792718	2.028443	0.000003

E = -386.9026283 au
ZPVE = 0.113714 au
(H298 - E0) = 5.7 kcal/mol

7	3.276066	-1.135432	0.000000

E = -339.3999505 au
ZPVE = 0.078005 au
(H298 - E0) = 4.3 kcal/mol

1	2.277065	2.770671	-0.905419
1	3.162614	1.485594	-0.000044
1	2.277105	2.770584	0.905495
7	-1.050824	1.268057	-0.000009
6	-2.270211	0.687635	-0.000002
6	1.362628	-1.512289	-0.000002
7	2.359589	-2.084102	-0.000004

E = -379.8917588 au
ZPVE = 0.120725 au
(H298 - E0) = 6.3 kcal/mol

3-cyano-2,4-didehydropyridinium cation (18)
+ methane TS (4-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	3.278042	1.097820	0.000136
6	1.113730	1.366022	0.000090
6	-0.071229	0.655726	0.000026
6	-0.183656	-0.722548	-0.000039
6	1.053044	-1.323060	-0.000032
1	1.125546	2.444877	0.000139
1	3.053746	-1.240519	0.000025
1	-1.299896	1.455574	0.000032
6	-2.297991	2.150193	0.000042
1	-2.238393	2.739600	0.907225
1	-3.119063	1.443181	-0.000089
1	-2.238275	2.739803	-0.907001

5-hydroxy-2,4-didehydropyridinium cation (19)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

6	1.255301	0.344582	0.000000
6	0.000000	0.914492	0.000000
6	-0.900713	-0.170191	0.000000
6	-1.447951	-1.407581	0.000000
6	-0.103752	-1.359764	0.000000
8	-0.211904	2.220531	0.000000
7	1.169867	-1.041252	0.000000
1	1.953753	-1.674328	0.000000
1	-2.335687	-2.021097	0.000000
1	-1.140346	2.449126	0.000000
1	2.211133	0.841594	0.000000

E = -322.4151467 au

5-hydroxy-2,4-didehydropyridinium cation (19)
+ methane TS (2-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.324347	-2.132759	-0.000044
6	1.051709	0.179670	-0.000768
6	0.363906	1.377697	-0.000445
6	-0.986140	1.198760	-0.000019
6	-1.692265	0.008717	0.000143
1	0.987794	-1.825902	-0.000616
1	0.861061	2.334209	-0.000496
1	2.544204	0.057022	-0.000240
6	3.740872	-0.106085	0.000857
1	3.978952	-0.608972	0.931051
1	4.153286	0.894912	-0.050114
1	3.970514	-0.696411	-0.878768

7	2.204945	-0.688140	0.000027
6	2.291328	0.660932	0.000090
6	-1.415153	-1.436602	-0.000104
7	-2.419538	-1.995333	-0.000156

E = -379.8895476 au
ZPVE = 0.120017 au
(H298 - E0) = 6.3 kcal/mol

5-hydroxy-2,4-didehydropyridinium cation (19)
+ methane TS (4-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.926640	1.937258	0.000340
6	-0.042832	0.826095	-0.000136
6	0.449686	-0.482869	-0.000363
6	-0.308409	-1.620855	-0.000287
6	-1.655481	-1.339728	0.000042
1	0.085573	-2.623838	-0.000457
1	-3.176323	-0.039416	0.000521
1	1.906832	-0.565557	-0.000166
6	3.125283	-0.581527	0.000339
1	3.417061	-0.049718	-0.896808
1	3.393417	-1.631330	-0.014239
1	3.415958	-0.075093	0.912424
7	-2.169338	-0.132561	0.000259
6	-1.412152	0.988789	0.000159
8	0.837161	1.818594	-0.000241

ZPVE = 0.083107 au
(H298 - E0) = 4.1 kcal/mol

5-cyano-2,4-didehydropyridinium cation (20)
MPW1K/6-31+G(d,p)
1A' singlet state (Cs)

6	1.302837	0.127028	0.000000
6	0.000000	0.584713	0.000000
6	-0.793994	-0.582846	0.000000
6	-1.245554	-1.856126	0.000000
6	0.093614	-1.684926	0.000000
7	1.343404	-1.251770	0.000000
1	2.182607	-1.811743	0.000000
1	-2.075497	-2.547017	0.000000
1	2.214211	0.704924	0.000000
6	-0.421054	1.938983	0.000000
7	-0.762893	3.036467	0.000000

E = -339.4044376 au
ZPVE = 0.077673 au
(H298 - E0) = 4.3 kcal/mol

5-cyano-2,4-didehydropyridinium cation (20)
+ methane TS (2-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	-1.022543	-2.109500	-0.000368
6	1.377492	0.173253	-0.001096
6	0.720913	1.384958	-0.000696
6	-0.635390	1.227755	-0.000199
6	-1.352384	0.043921	-0.000039
1	1.293074	-1.837448	-0.001030
1	1.236844	2.331557	-0.000748
1	2.881084	0.029180	-0.000221
6	4.073933	-0.141193	0.001474
1	4.306868	-0.644312	0.932942
1	4.491513	0.857666	-0.050837
1	4.298473	-0.734379	-0.877642
7	0.736774	-0.992762	-0.000912
6	-0.601450	-1.115489	-0.000442
6	-2.777262	-0.001624	0.000539
7	0.423390	-0.987572	-0.000569
6	-0.913329	-1.135517	-0.000154
8	-3.007907	-0.121454	0.000592
1	-3.460462	0.723079	0.000785

E = -362.9084277 au
ZPVE = 0.126387 au
(H298 - E0) = 5.9 kcal/mol

1	0.435622	2.687438	-0.000027

E = -362.903507 au
ZPVE = 0.125981 au
(H298 - E0) = 6.0 kcal/mol

5-cyano-2,4-didehydropyridinium cation (20)
+ methane TS (4-position)
MPW1K/6-31+G(d,p)
1A singlet state (C1)

1	1.390759	-2.283305	0.000023
6	-0.014240	-0.613788	-0.000003
6	-0.071653	0.779738	-0.000018
6	1.017472	1.619032	-0.000018
6	2.189263	0.910535	-0.000002
1	0.971229	2.695756	-0.000031
1	3.227432	-0.810477	0.000025
1	-1.440749	1.343556	-0.000007
6	-2.588238	1.733641	0.000019
1	-3.030153	1.333220	-0.904465
1	-2.512549	2.814684	-0.000365
1	-3.029896	1.333844	0.904906
7	2.299765	-0.404688	0.000014
6	1.226334	-1.216427	0.000012
6	-1.197511	-1.412025	-0.000008
7	-2.148999	-2.056959	-0.000011

E = -379.8896362 au

7	-3.925405	-0.053274	0.001006

E = -379.8901795 au
ZPVE = 0.120161 au
(H298 - E0) = 6.3 kcal/mol

ZPVE = 0.119984 au
(H298 - E0) = 6.3 kcal/mol

Dehydrocarbon Atom Surfaces

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.30 A

6	0.000000	0.000000	0.955484
6	0.000000	0.000000	2.349128
6	0.000000	0.650000	-0.236454
6	0.000000	-0.650000	-0.236454
6	0.000000	1.151030	-1.532552
6	0.000000	-1.151030	-1.532552
7	0.000000	0.000000	-2.271605
1	0.000000	2.134631	-1.964569
1	0.000000	-2.134631	-1.964569
1	0.000000	0.000000	-3.287880
7	0.000000	0.000000	3.502664

E = -339.5962675 au
RHF-UCCSD(T)/cc-pVTZ E = -338.8767919 au

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.40 A

6	0.000000	0.000000	0.938841
6	0.000000	0.000000	2.337825
6	0.000000	0.700000	-0.222495
6	0.000000	-0.700000	-0.222495
6	0.000000	1.149815	-1.527951
6	0.000000	-1.149815	-1.527951
7	0.000000	0.000000	-2.265724
1	0.000000	2.128572	-1.973524
1	0.000000	-2.128572	-1.973524
1	0.000000	0.000000	-3.282803
7	0.000000	0.000000	3.490754

E = -339.6129507 au
RHF-UCCSD(T)/cc-pVTZ E = -338.8767919 au

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.50 A

6	0.000000	0.000000	0.919748
6	0.000000	0.000000	2.323167
6	0.000000	0.750000	-0.206962
6	0.000000	-0.750000	-0.206962
6	0.000000	1.147308	-1.521504
6	0.000000	-1.147308	-1.521504
7	0.000000	0.000000	-2.258850
1	0.000000	2.122067	-1.978352
1	0.000000	-2.122067	-1.978352
1	0.000000	0.000000	-3.276796
7	0.000000	0.000000	3.475651

E = -339.6173125 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9007097 au

4-cyano-3,5-didehydropyridinium cation (4)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.60 A

6	0.000000	0.000000	0.898607
6	0.000000	0.000000	2.305503
6	0.000000	0.800000	-0.190364
6	0.000000	-0.800000	-0.190364
6	0.000000	1.144479	-1.513410
6	0.000000	-1.144479	-1.513410
7	0.000000	0.000000	-2.250311
1	0.000000	2.115383	-1.980793
1	0.000000	-2.115383	-1.980793
1	0.000000	0.000000	-3.269102
7	0.000000	0.000000	3.457643

E = -339.6164115 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9007397 au

dehydrocarbon atom separation = 1.70 A

6	0.000000	0.000000	0.876218
6	0.000000	0.000000	2.285677
6	0.000000	0.850000	-0.173463
6	0.000000	-0.850000	-0.173463
6	0.000000	1.142567	-1.504282
6	0.000000	-1.142567	-1.504282
7	0.000000	0.000000	-2.239613
1	0.000000	2.109258	-1.982451
1	0.000000	-2.109258	-1.982451
1	0.000000	0.000000	-3.259137
7	0.000000	0.000000	3.437559

E = -339.6140395 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8994936 au

dehydrocarbon atom separation = 1.80 A

6	0.000000	0.000000	0.853202
6	0.000000	0.000000	2.264419
6	0.000000	0.900000	-0.156942
6	0.000000	-0.900000	-0.156942
6	0.000000	1.142609	-1.494658
6	0.000000	-1.142609	-1.494658
7	0.000000	0.000000	-2.226186
1	0.000000	2.104176	-1.984905
1	0.000000	-2.104176	-1.984905
1	0.000000	0.000000	-3.246259
7	0.000000	0.000000	3.416121

E = -339.6116971 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8987830 au

4-cyano-3,5-didehydropyridinium cation (4)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.90 A

6	0.000000	0.000000	0.829806
6	0.000000	0.000000	2.242309
6	0.000000	0.950000	-0.141177
6	0.000000	-0.950000	-0.141177
6	0.000000	1.145218	-1.484733
6	0.000000	-1.145218	-1.484733
7	0.000000	0.000000	-2.209963
1	0.000000	2.100081	-1.989538

4-cyano-3,5-didehydropyridinium cation (4)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 2.00 A

6	0.000000	0.000000	0.805354
6	0.000000	0.000000	2.218782
6	0.000000	1.000000	-0.125850
6	0.000000	-1.000000	-0.125850
6	0.000000	1.150186	-1.474457
6	0.000000	-1.150186	-1.474457
7	0.000000	0.000000	-2.190257
1	0.000000	2.096965	-1.995572

4-cyano-3,5-didehydropyridinium cation (4)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 2.10 A

6	0.000000	0.000000	0.775148
6	0.000000	0.000000	2.190046
6	0.000000	1.050000	-0.108832
6	0.000000	-1.050000	-0.108832
6	0.000000	1.157797	-1.462400
6	0.000000	-1.157797	-1.462400
7	0.000000	0.000000	-2.163017
1	0.000000	2.094579	-2.001726

1	0.000000	-2.100081	-1.989538
1	0.000000	0.000000	-3.230368
7	0.000000	0.000000	3.393915

E = -339.6094835 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8988740 au

4-cyano-3,5-didehydropyridinium cation (4)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 2.20 A

6	0.000000	0.000000	0.746173
6	0.000000	0.000000	2.162942
6	0.000000	1.100000	-0.093755
6	0.000000	-1.100000	-0.093755
6	0.000000	1.169023	-1.451102
6	0.000000	-1.169023	-1.451102
7	0.000000	0.000000	-2.134074
1	0.000000	2.092539	-2.013160
1	0.000000	-2.092539	-2.013160
1	0.000000	0.000000	-3.152502
7	0.000000	0.000000	3.314419

E = -339.6053173 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8969614 au

4-fluoro-3,5-didehydropyridinium cation (5)

UB3LYP/cc-pVTZ

1	0.000000	-2.096965	-1.995572
1	0.000000	0.000000	-3.210589
7	0.000000	0.000000	3.370343

E = -339.6068654 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8992012 au

4-cyano-3,5-didehydropyridinium cation (4)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 2.30 A

6	0.000000	0.000000	0.719239
6	0.000000	0.000000	2.137846
6	0.000000	1.150000	-0.080644
6	0.000000	-1.150000	-0.080644
6	0.000000	1.182393	-1.440783
6	0.000000	-1.182393	-1.440783
7	0.000000	0.000000	-2.104839
1	0.000000	2.090453	-2.027787
1	0.000000	-2.090453	-2.027787
1	0.000000	0.000000	-3.122540
7	0.000000	0.000000	3.289513

E = -339.6026512 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8927926 au

4-fluoro-3,5-didehydropyridinium cation (5)

UB3LYP/cc-pVTZ

1	0.000000	-2.094579	-2.001726
1	0.000000	0.000000	-3.182276
7	0.000000	0.000000	3.341496

E = -339.6059001 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8988355 au

4-fluoro-3,5-didehydropyridinium cation (5)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.30 A

6	0.000000	0.000000	1.327121
9	0.000000	0.000000	2.589343
6	0.000000	0.650000	0.149031
6	0.000000	-0.650000	0.149031
6	0.000000	1.149463	-1.149331
6	0.000000	-1.149463	-1.149331
7	0.000000	0.000000	-1.886252
1	0.000000	2.133858	-1.578903
1	0.000000	-2.133858	-1.578903
1	0.000000	0.000000	-2.901644

E = -346.6140156 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9332363 au

4-fluoro-3,5-didehydropyridinium cation (5)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.40 A

6	0.000000	0.000000	1.308828
9	0.000000	0.000000	2.575722
6	0.000000	0.700000	0.161797
6	0.000000	-0.700000	0.161797
6	0.000000	1.149210	-1.145014
6	0.000000	-1.149210	-1.145014
7	0.000000	0.000000	-1.880351
1	0.000000	2.128584	-1.588504
1	0.000000	-2.128584	-1.588504
1	0.000000	0.000000	-2.896410

E = -346.6328338 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9533528 au

1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.50 A

6	0.000000	0.000000	1.287309
9	0.000000	0.000000	2.558829
6	0.000000	0.750000	0.175951
6	0.000000	-0.750000	0.175951
6	0.000000	1.147778	-1.139128
6	0.000000	-1.147778	-1.139128
7	0.000000	0.000000	-1.873547
1	0.000000	2.122612	-1.595023
1	0.000000	-2.122612	-1.595023
1	0.000000	0.000000	-2.890319

E = -346.6386831 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9598717 au

1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.60 A

6	0.000000	0.000000	1.263311
9	0.000000	0.000000	2.539018
6	0.000000	0.800000	0.190938
6	0.000000	-0.800000	0.190938
6	0.000000	1.145999	-1.131890
6	0.000000	-1.145999	-1.131890
7	0.000000	0.000000	-1.865405
1	0.000000	2.116427	-1.599444
1	0.000000	-2.116427	-1.599444
1	0.000000	0.000000	-2.882876

E = -346.6387467 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9603414 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.70 A

6	0.000000	0.000000	1.237817
9	0.000000	0.000000	2.517021
6	0.000000	0.850000	0.206110
6	0.000000	-0.850000	0.206110
6	0.000000	1.144965	-1.123746
6	0.000000	-1.144965	-1.123746
7	0.000000	0.000000	-1.855479
1	0.000000	2.110599	-1.603273

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.80 A

6	0.000000	0.000000	1.211486
9	0.000000	0.000000	2.493443
6	0.000000	0.900000	0.220895
6	0.000000	-0.900000	0.220895
6	0.000000	1.145709	-1.115119
6	0.000000	-1.145709	-1.115119
7	0.000000	0.000000	-1.843083
1	0.000000	2.105578	-1.608008

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.90 A

6	0.000000	0.000000	1.184802
9	0.000000	0.000000	2.468925
6	0.000000	0.950000	0.234952
6	0.000000	-0.950000	0.234952
6	0.000000	1.148666	-1.106261
6	0.000000	-1.148666	-1.106261
7	0.000000	0.000000	-1.828204
1	0.000000	2.101410	-1.614498

1	0.000000	-2.110599	-1.603273
1	0.000000	0.000000	-2.873560

E = -346.6369409 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9590635 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.00 A

6	0.000000	0.000000	1.158095
9	0.000000	0.000000	2.443986
6	0.000000	1.000000	0.248133
6	0.000000	-1.000000	0.248133
6	0.000000	1.153918	-1.097370
6	0.000000	-1.153918	-1.097370
7	0.000000	0.000000	-1.811072
1	0.000000	2.097979	-1.623078
1	0.000000	-2.097979	-1.623078
1	0.000000	0.000000	-2.829951

E = -346.6302728 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9575048 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.30 A

1	0.000000	-2.105578	-1.608008
1	0.000000	0.000000	-2.861618

E = -346.6349002 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9580107 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.10 A

6	0.000000	0.000000	1.127356
9	0.000000	0.000000	2.415636
6	0.000000	1.050000	0.262005
6	0.000000	-1.050000	0.262005
6	0.000000	1.160549	-1.088024
6	0.000000	-1.160549	-1.088024
7	0.000000	0.000000	-1.789020
1	0.000000	2.095155	-1.631184
1	0.000000	-2.095155	-1.631184
1	0.000000	0.000000	-2.807130

E = -346.627634 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9568051 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.30 A

1	0.000000	-2.101410	-1.614498
1	0.000000	0.000000	-2.847006

E = -346.6328472 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9576285 au

4-fluoro-3,5-didehydropyridinium cation (5)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.20 A

6	0.000000	0.000000	1.096455
9	0.000000	0.000000	2.387618
6	0.000000	1.100000	0.274815
6	0.000000	-1.100000	0.274815
6	0.000000	1.170240	-1.078976
6	0.000000	-1.170240	-1.078976
7	0.000000	0.000000	-1.764311
1	0.000000	2.092803	-1.642812
1	0.000000	-2.092803	-1.642812
1	0.000000	0.000000	-2.781563

E = -346.6259949 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9546725 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.40 A

6	0.000000	0.000000	1.067974	6	0.000000	0.000000	0.858616	6	0.000000	0.000000	0.841257
9	0.000000	0.000000	2.361849	17	0.000000	0.000000	2.501887	17	0.000000	0.000000	2.492820
6	0.000000	1.150000	0.285849	6	0.000000	0.650000	-0.333610	6	0.000000	0.700000	-0.320065
6	0.000000	-1.150000	0.285849	6	0.000000	-0.650000	-0.333610	6	0.000000	-0.700000	-0.320065
6	0.000000	1.182238	-1.070805	6	0.000000	1.148711	-1.630731	6	0.000000	1.148167	-1.625644
6	0.000000	-1.182238	-1.070805	6	0.000000	-1.148711	-1.630731	6	0.000000	-1.148167	-1.625644
7	0.000000	0.000000	-1.739116	7	0.000000	0.000000	-2.371519	7	0.000000	0.000000	-2.365040
1	0.000000	2.090491	-1.657773	1	0.000000	2.132255	-2.062265	1	0.000000	2.126979	-2.070446
1	0.000000	-2.090491	-1.657773	1	0.000000	-2.132255	-2.062265	1	0.000000	-2.126979	-2.070446
1	0.000000	0.000000	-2.755666	1	0.000000	0.000000	-3.386536	1	0.000000	0.000000	-3.380800

E = -346.6227865 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9503107 au

E = -706.9821807 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9453631 au

E = -706.9990866 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9636051 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.50 A

6	0.000000	0.000000	0.821377	6	0.000000	0.000000	0.799723	6	0.000000	0.000000	0.777201
17	0.000000	0.000000	2.480624	17	0.000000	0.000000	2.465726	17	0.000000	0.000000	2.448453
6	0.000000	0.750000	-0.304491	6	0.000000	0.800000	-0.287637	6	0.000000	0.850000	-0.270003
6	0.000000	-0.750000	-0.304491	6	0.000000	-0.800000	-0.287637	6	0.000000	-0.850000	-0.270003
6	0.000000	1.146406	-1.618386	6	0.000000	1.144452	-1.609424	6	0.000000	1.143274	-1.599126
6	0.000000	-1.146406	-1.618386	6	0.000000	-1.144452	-1.609424	6	0.000000	-1.143274	-1.599126
7	0.000000	0.000000	-2.357235	7	0.000000	0.000000	-2.347403	7	0.000000	0.000000	-2.335350
1	0.000000	2.120965	-2.074946	1	0.000000	2.114804	-2.077181	1	0.000000	2.109082	-2.078261
1	0.000000	-2.120965	-2.074946	1	0.000000	-2.114804	-2.077181	1	0.000000	-2.109082	-2.078261
1	0.000000	0.000000	-3.373809	1	0.000000	0.000000	-3.364762	1	0.000000	0.000000	-3.353394

E = -707.0034328 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9687024 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.80 A

6	0.000000	0.000000	0.754370
17	0.000000	0.000000	2.429511
6	0.000000	0.900000	-0.252445
6	0.000000	-0.900000	-0.252445
6	0.000000	1.143974	-1.588045
6	0.000000	-1.143974	-1.588045
7	0.000000	0.000000	-2.320419
1	0.000000	2.104219	-2.080059
1	0.000000	-2.104219	-2.080059
1	0.000000	0.000000	-3.338967

E = -707.0022524 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9680835 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.90 A

6	0.000000	0.000000	0.731505
17	0.000000	0.000000	2.409420
6	0.000000	0.950000	-0.235383
6	0.000000	-0.950000	-0.235383
6	0.000000	1.146999	-1.576497
6	0.000000	-1.146999	-1.576497
7	0.000000	0.000000	-2.302601
1	0.000000	2.100283	-2.083478
1	0.000000	-2.100283	-2.083478
1	0.000000	0.000000	-3.321440

E = -706.9993381 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9659290 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.00 A

6	0.000000	0.000000	0.708743
17	0.000000	0.000000	2.388788
6	0.000000	1.000000	-0.219158
6	0.000000	-1.000000	-0.219158
6	0.000000	1.152471	-1.564779
6	0.000000	-1.152471	-1.564779
7	0.000000	0.000000	-2.282213
1	0.000000	2.097184	-2.089000
1	0.000000	-2.097184	-2.089000
1	0.000000	0.000000	-3.301121

E = -706.9962432 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9641161 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.10 A

6	0.000000	0.000000	0.680034
17	0.000000	0.000000	2.362773

E = -706.9931582 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9630255 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.20 A

6	0.000000	0.000000	0.651779
17	0.000000	0.000000	2.338513

E = -706.989582 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9622232 au

4-chloro-3,5-didehydropyridinium cation (6)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.30 A

6	0.000000	0.000000	0.625545
17	0.000000	0.000000	2.316155

6	0.000000	1.050000	-0.200212
6	0.000000	-1.050000	-0.200212
6	0.000000	1.159458	-1.550807
6	0.000000	-1.159458	-1.550807
7	0.000000	0.000000	-2.254056
1	0.000000	2.094659	-2.092400
1	0.000000	-2.094659	-2.092400
1	0.000000	0.000000	-3.271927

E = -706.9868664 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9608439 au

4-amino-3,5-didehydropyridinium cation (7)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.30 A

6	0.000000	0.000000	1.321796
7	0.000000	0.000000	2.619766
6	0.000000	0.650000	0.112238
6	0.000000	-0.650000	0.112238
6	0.000000	1.145863	-1.182945
6	0.000000	-1.145863	-1.182945
7	0.000000	0.000000	-1.931193
1	0.000000	2.128641	-1.615731
1	0.000000	-2.128641	-1.615731
1	0.000000	0.867584	3.136577
1	0.000000	-0.867584	3.136577
1	0.000000	0.000000	-2.943989

6	0.000000	1.100000	-0.183301
6	0.000000	-1.100000	-0.183301
6	0.000000	1.170049	-1.537730
6	0.000000	-1.170049	-1.537730
7	0.000000	0.000000	-2.224213
1	0.000000	2.092506	-2.101158
1	0.000000	-2.092506	-2.101158
1	0.000000	0.000000	-3.241224

E = -706.9851065 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9581113 au

4-amino-3,5-didehydropyridinium cation (7)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.40 A

6	0.000000	0.000000	1.303078
7	0.000000	0.000000	2.605828
6	0.000000	0.700000	0.124952
6	0.000000	-0.700000	0.124952
6	0.000000	1.144830	-1.177709
6	0.000000	-1.144830	-1.177709
7	0.000000	0.000000	-1.926242
1	0.000000	2.123473	-1.622452
1	0.000000	-2.123473	-1.622452
1	0.000000	0.867953	3.121031
1	0.000000	-0.867953	3.121031
1	0.000000	0.000000	-2.939639

6	0.000000	1.150000	-0.168531
6	0.000000	-1.150000	-0.168531
6	0.000000	1.182955	-1.525825
6	0.000000	-1.182955	-1.525825
7	0.000000	0.000000	-2.194065
1	0.000000	2.090426	-2.113420
1	0.000000	-2.090426	-2.113420
1	0.000000	0.000000	-3.210341

E = -706.9816387 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9532679 au

4-amino-3,5-didehydropyridinium cation (7)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.50 A

6	0.000000	0.000000	1.281416
7	0.000000	0.000000	2.588365
6	0.000000	0.750000	0.139119
6	0.000000	-0.750000	0.139119
6	0.000000	1.142591	-1.170887
6	0.000000	-1.142591	-1.170887
7	0.000000	0.000000	-1.920361
1	0.000000	2.117407	-1.626547
1	0.000000	-2.117407	-1.626547
1	0.000000	0.868341	3.102108
1	0.000000	-0.868341	3.102108
1	0.000000	0.000000	-2.934428

E = -302.7793373 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1336997 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.60 A

6	0.000000	0.000000	1.257826
7	0.000000	0.000000	2.568220
6	0.000000	0.800000	0.154011
6	0.000000	-0.800000	0.154011
6	0.000000	1.140121	-1.163054
6	0.000000	-1.140121	-1.163054
7	0.000000	0.000000	-1.913142
1	0.000000	2.111337	-1.628707
1	0.000000	-2.111337	-1.628707
1	0.000000	0.868739	3.080645
1	0.000000	-0.868739	3.080645
1	0.000000	0.000000	-2.927850

E = -302.7932908 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1488606 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.70 A

6	0.000000	0.000000	1.233126
7	0.000000	0.000000	2.546247
6	0.000000	0.850000	0.168886
6	0.000000	-0.850000	0.168886
6	0.000000	1.138668	-1.154586
6	0.000000	-1.138668	-1.154586
7	0.000000	0.000000	-1.904092
1	0.000000	2.105812	-1.630736
1	0.000000	-2.105812	-1.630736
1	0.000000	0.869024	3.057678
1	0.000000	-0.869024	3.057678
1	0.000000	0.000000	-2.919325

E = -302.7954143 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1516384 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.80 A

6	0.000000	0.000000	1.208040
7	0.000000	0.000000	2.523213
6	0.000000	0.900000	0.183123
6	0.000000	-0.900000	0.183123
6	0.000000	1.139236	-1.145983
6	0.000000	-1.139236	-1.145983
7	0.000000	0.000000	-1.892587
1	0.000000	2.101379	-1.633979
1	0.000000	-2.101379	-1.633979
1	0.000000	0.869222	3.033907
1	0.000000	-0.869222	3.033907
1	0.000000	0.000000	-2.908167

E = -302.7927276 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1494241 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.90 A

E = -302.7889379 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1462874 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.00 A

E = -302.7854643 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1439442 au

4-amino-3,5-didehydropyridinium cation (7)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.10 A

6	0.000000	0.000000	1.182822
7	0.000000	0.000000	2.499562
6	0.000000	0.950000	0.196405
6	0.000000	-0.950000	0.196405
6	0.000000	1.142372	-1.137305
6	0.000000	-1.142372	-1.137305
7	0.000000	0.000000	-1.878523
1	0.000000	2.097962	-1.639618
1	0.000000	-2.097962	-1.639618
1	0.000000	0.869180	3.010038
1	0.000000	-0.869180	3.010038
1	0.000000	0.000000	-2.894248

E = -302.7823574 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1425928 au

4-amino-3,5-didehydropyridinium cation (7)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 2.20 A

6	0.000000	0.000000	1.099208
7	0.000000	0.000000	2.421540
6	0.000000	1.100000	0.232812
6	0.000000	-1.100000	0.232812
6	0.000000	1.166539	-1.111229
6	0.000000	-1.166539	-1.111229
7	0.000000	0.000000	-1.815417
1	0.000000	2.092419	-1.668856

6	0.000000	0.000000	1.157833
7	0.000000	0.000000	2.475759
6	0.000000	1.000000	0.208561
6	0.000000	-1.000000	0.208561
6	0.000000	1.148085	-1.128784
6	0.000000	-1.148085	-1.128784
7	0.000000	0.000000	-1.861988
1	0.000000	2.095537	-1.647713
1	0.000000	-2.095537	-1.647713
1	0.000000	0.869086	2.986187
1	0.000000	-0.869086	2.986187
1	0.000000	0.000000	-2.877662

E = -302.7790072 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1416580 au

4-amino-3,5-didehydropyridinium cation (7)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 2.30 A

6	0.000000	0.000000	1.073123
7	0.000000	0.000000	2.396603
6	0.000000	1.150000	0.242456
6	0.000000	-1.150000	0.242456
6	0.000000	1.179316	-1.103474
6	0.000000	-1.179316	-1.103474
7	0.000000	0.000000	-1.790623
1	0.000000	2.091149	-1.684224

6	0.000000	0.000000	1.128561
7	0.000000	0.000000	2.448398
6	0.000000	1.050000	0.221301
6	0.000000	-1.050000	0.221301
6	0.000000	1.155606	-1.119801
6	0.000000	-1.155606	-1.119801
7	0.000000	0.000000	-1.840181
1	0.000000	2.093758	-1.656108
1	0.000000	-2.093758	-1.656108
1	0.000000	0.867993	2.960154
1	0.000000	-0.867993	2.960154
1	0.000000	0.000000	-2.854966

E = -302.7758181 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1402594 au

4-hydroxy-3,5-didehydropyridinium cation (8)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.30 A

1	-2.859679	-0.591924	0.000000
7	-1.866605	-0.386719	0.000000
6	-1.371706	0.887708	0.000000
6	0.000000	0.663181	0.000000
6	1.302876	0.258164	0.000000
6	0.261540	-0.610238	0.000000
6	-0.908544	-1.359926	0.000000
1	-1.130872	-2.410569	0.000000

1	0.000000	-2.092419	-1.668856
1	0.000000	0.866722	2.934944
1	0.000000	-0.866722	2.934944
1	0.000000	0.000000	-2.829283

E = -302.7734897 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1375125 au

4-hydroxy-3,5-didehydropyridinium cation (8)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.40 A

1	-2.852538	-0.602283	0.000000
7	-1.859597	-0.393318	0.000000
6	-1.369942	0.882056	0.000000
6	0.000000	0.714618	0.000000
6	1.284058	0.258854	0.000000
6	0.286234	-0.655809	0.000000
6	-0.898580	-1.362585	0.000000
1	-1.130884	-2.412178	0.000000
8	2.550706	0.450497	0.000000
1	-2.007205	1.747735	0.000000
1	2.791542	1.393179	0.000000

E = -322.6402059 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9796445 au

4-hydroxy-3,5-didehydropyridinium cation (8)

1	0.000000	-2.091149	-1.684224
1	0.000000	0.865537	2.911914
1	0.000000	-0.865537	2.911914
1	0.000000	0.000000	-2.803768

E = -302.7696884 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1326184 au

4-hydroxy-3,5-didehydropyridinium cation (8)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.50 A

1	-2.843703	-0.616686	0.000000
7	-1.851199	-0.402290	0.000000
6	-1.367546	0.873558	0.000000
6	0.000000	0.766380	0.000000
6	1.261859	0.260689	0.000000
6	0.313603	-0.700471	0.000000
6	-0.885540	-1.364995	0.000000
1	-1.124507	-2.414199	0.000000
8	2.531342	0.462398	0.000000
1	-2.019713	1.729445	0.000000
1	2.761325	1.407310	0.000000

E = -322.6441084 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9842596 au

4-hydroxy-3,5-didehydropyridinium cation (8)

8	2.566159	0.441358	0.000000
1	-1.993695	1.763068	0.000000
1	2.816222	1.382264	0.000000

E = -322.6238561 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9619951 au

4-hydroxy-3,5-didehydropyridinium cation (8)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.60 A

1	-2.833057	-0.631950	0.000000
7	-1.841270	-0.411046	0.000000
6	-1.364020	0.865201	0.000000
6	0.000000	0.818186	0.000000
6	1.237387	0.262337	0.000000
6	0.342407	-0.744746	0.000000
6	-0.871247	-1.366795	0.000000
1	-1.116595	-2.415555	0.000000
8	2.509184	0.473538	0.000000
1	-2.030996	1.710910	0.000000
1	2.728908	1.420522	0.000000

E = -322.6426826 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9833221 au

4-hydroxy-3,5-didehydropyridinium cation (8)

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	-2.820795	-0.645618	0.000000
7	-1.829780	-0.418670	0.000000
6	-1.359559	0.857932	0.000000
6	0.000000	0.870261	0.000000
6	1.211643	0.263077	0.000000
6	0.371324	-0.788690	0.000000
6	-0.856505	-1.368939	0.000000
1	-1.108719	-2.417061	0.000000
8	2.485191	0.483180	0.000000
1	-2.040104	1.694008	0.000000
1	2.695138	1.432081	0.000000

E = -322.6397611 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9810216 au

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	-2.807324	-0.653009	0.000000
7	-1.816414	-0.423769	0.000000
6	-1.354142	0.854406	0.000000
6	0.000000	0.922509	0.000000
6	1.185780	0.261846	0.000000
6	0.399121	-0.832684	0.000000
6	-0.842790	-1.371913	0.000000
1	-1.103280	-2.418879	0.000000
8	2.460660	0.489256	0.000000
1	-2.049389	1.679407	0.000000
1	2.661799	1.439832	0.000000

E = -322.6368882 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9792190 au

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.90 A

1	-2.798482	-0.627295	0.000000
7	-1.806379	-0.402311	0.000000
6	-0.839997	-1.357552	0.000000
6	0.425163	-0.877107	0.000000
6	1.156785	0.273049	0.000000
6	0.000000	0.974713	0.000000
6	-1.347202	0.876273	0.000000
1	-2.048505	1.697119	0.000000
8	2.406519	0.619981	0.000000
1	-1.126245	-2.398583	0.000000
1	2.997242	-0.151165	0.000000

E = -322.6341864 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9782104 au

4-hydroxy-3,5-didehydropyridinium cation (8)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	-2.774619	-0.656392	0.000000
7	-1.784115	-0.424421	0.000000
6	-1.341497	0.860291	0.000000
6	0.000000	1.026259	0.000000
6	1.134601	0.254801	0.000000
6	0.449643	-0.922541	0.000000

4-hydroxy-3,5-didehydropyridinium cation (8)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	-2.752154	-0.653635	0.000000
7	-1.762636	-0.420966	0.000000
6	-1.335491	0.867988	0.000000
6	0.000000	1.076611	0.000000
6	1.104793	0.250770	0.000000
6	0.475570	-0.968831	0.000000

4-hydroxy-3,5-didehydropyridinium cation (8)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	0.025246	-2.803164	0.000000
7	0.018253	-1.787568	0.000000
6	-1.153693	-1.101039	0.000000
6	-1.098260	0.249972	0.000000
6	0.000000	1.102860	0.000000
6	1.101709	0.261612	0.000000

6	-0.818937	-1.380976	0.000000
1	-1.109406	-2.421564	0.000000
8	2.411823	0.489962	0.000000
1	-2.067882	1.660066	0.000000
1	2.603269	1.442134	0.000000

E = -322.631089 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9775203 au

4-hydroxy-3,5-didehydropyridinium cation (8)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.30 A

1	0.023254	-2.777493	0.000000
7	0.016794	-1.762617	0.000000
6	-1.166994	-1.093032	0.000000
6	-1.147494	0.259885	0.000000
6	0.000000	1.075522	0.000000
6	1.152473	0.272059	0.000000
6	1.194167	-1.077893	0.000000
1	2.108054	-1.655676	0.000000
8	0.056907	2.381249	0.000000
1	-2.072649	-1.683784	0.000000
1	-0.824385	2.786042	0.000000

E = -322.6218688 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9688535 au

6	-0.806796	-1.386545	0.000000
1	-1.116178	-2.422099	0.000000
8	2.384772	0.486315	0.000000
1	-2.077086	1.654235	0.000000
1	2.577239	1.437776	0.000000

E = -322.627919 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9762921 au

3,5-didehydropyridinium cation (9)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.30 A

6	0.000000	0.000000	-1.841894
1	0.000000	0.000000	-2.923065
6	0.000000	0.650000	-0.658526
6	0.000000	-0.650000	-0.658526
6	0.000000	1.149556	0.640030
6	0.000000	-1.149556	0.640030
7	0.000000	0.000000	1.378968
1	0.000000	2.132177	1.074215
1	0.000000	-2.132177	1.074215
1	0.000000	0.000000	2.395170

E = -247.3483561 au

RHF-UCCSD(T)/cc-pVTZ E = -246.8096797 au

6	1.182535	-1.085503	0.000000
1	2.111142	-1.638939	0.000000
8	0.055411	2.406230	0.000000
1	-2.073209	-1.669535	0.000000
1	-0.827989	2.807358	0.000000

E = -322.6256521 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9736543 au

3,5-didehydropyridinium cation (9)

UB3LYP/cc-pVTZ

1A1 singlet state (C2v)

dehydrocarbon atom separation = 1.40 A

6	0.000000	0.000000	-1.823173
1	0.000000	0.000000	-2.905223
6	0.000000	0.700000	-0.668849
6	0.000000	-0.700000	-0.668849
6	0.000000	1.148116	0.638841
6	0.000000	-1.148116	0.638841
7	0.000000	0.000000	1.376897
1	0.000000	2.126092	1.086060
1	0.000000	-2.126092	1.086060
1	0.000000	0.000000	2.393952

E = -247.3653679 au

RHF-UCCSD(T)/cc-pVTZ E = -246.8280940 au

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.50 A

6	0.000000	0.000000	-1.800762
1	0.000000	0.000000	-2.883320
6	0.000000	0.750000	-0.679854
6	0.000000	-0.750000	-0.679854
6	0.000000	1.145479	0.636755
6	0.000000	-1.145479	0.636755
7	0.000000	0.000000	1.374561
1	0.000000	2.119392	1.095307
1	0.000000	-2.119392	1.095307
1	0.000000	0.000000	2.392546

E = -247.3699919 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8336027 au

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.60 A

6	0.000000	0.000000	-1.775366
1	0.000000	0.000000	-2.857974
6	0.000000	0.800000	-0.691104
6	0.000000	-0.800000	-0.691104
6	0.000000	1.142618	0.633984
6	0.000000	-1.142618	0.633984
7	0.000000	0.000000	1.371347
1	0.000000	2.112664	1.102973
1	0.000000	-2.112664	1.102973
1	0.000000	0.000000	2.390244

E = -247.3692948 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8336659 au

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.70 A

6	0.000000	0.000000	-1.747921
1	0.000000	0.000000	-2.830144
6	0.000000	0.850000	-0.702098
6	0.000000	-0.850000	-0.702098
6	0.000000	1.140785	0.630851
6	0.000000	-1.140785	0.630851
7	0.000000	0.000000	1.366472
1	0.000000	2.106559	1.110586
1	0.000000	-2.106559	1.110586
1	0.000000	0.000000	2.386158

E = -247.3670386 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8324252 au

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.80 A

6	0.000000	0.000000	-1.719193
1	0.000000	0.000000	-2.800730
6	0.000000	0.900000	-0.712381
6	0.000000	-0.900000	-0.712381
6	0.000000	1.141024	0.627606
6	0.000000	-1.141024	0.627606

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 1.90 A

6	0.000000	0.000000	-1.689674
1	0.000000	0.000000	-2.770409
6	0.000000	0.950000	-0.721678
6	0.000000	-0.950000	-0.721678
6	0.000000	1.143867	0.624357
6	0.000000	-1.143867	0.624357

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.00 A

6	0.000000	0.000000	-1.657320
1	0.000000	0.000000	-2.737265
6	0.000000	1.000000	-0.730389
6	0.000000	-1.000000	-0.730389
6	0.000000	1.149094	0.620994
6	0.000000	-1.149094	0.620994

7	0.000000	0.000000	1.359210	7	0.000000	0.000000	1.349213	7	0.000000	0.000000	1.335657
1	0.000000	2.101482	1.119620	1	0.000000	2.097473	1.131000	1	0.000000	2.094344	1.144153
1	0.000000	-2.101482	1.119620	1	0.000000	-2.097473	1.131000	1	0.000000	-2.094344	1.144153
1	0.000000	0.000000	2.379480	1	0.000000	0.000000	2.369819	1	0.000000	0.000000	2.356028

E = -247.3646914 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8316431 au

E = -247.3623397 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8315556 au

E = -247.3595547 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8315717 au

3,5-didehydropyridinium cation (9)
UB3LYP/cc-pVTZ
1A1 singlet state (C2v)
dehydrocarbon atom separation = 2.10 A

6	0.000000	0.000000	-1.617158	6	0.000000	0.000000	-1.578604	6	0.000000	0.000000	-1.542660
1	0.000000	0.000000	-2.696835	1	0.000000	0.000000	-2.658699	1	0.000000	0.000000	-2.623575
6	0.000000	1.050000	-0.739234	6	0.000000	1.100000	-0.746663	6	0.000000	1.150000	-0.752857
6	0.000000	-1.050000	-0.739234	6	0.000000	-1.100000	-0.746663	6	0.000000	-1.150000	-0.752857
6	0.000000	1.157530	0.617193	6	0.000000	1.169491	0.613611	6	0.000000	1.183359	0.610384
6	0.000000	-1.157530	0.617193	6	0.000000	-1.169491	0.613611	6	0.000000	-1.183359	0.610384
7	0.000000	0.000000	1.315743	7	0.000000	0.000000	1.293673	7	0.000000	0.000000	1.270941
1	0.000000	2.092064	1.159588	1	0.000000	2.090042	1.179693	1	0.000000	2.087811	1.202156
1	0.000000	-2.092064	1.159588	1	0.000000	-2.090042	1.179693	1	0.000000	-2.087811	1.202156
1	0.000000	0.000000	2.334894	1	0.000000	0.000000	2.311858	1	0.000000	0.000000	2.288316

E = -247.3587002 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8307030 au

E = -247.3580551 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8282769 au

E = -247.3551569 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8235642 au

2-cyano-3,5-didehydropyridinium cation (10)
UB3LYP/cc-pVTZ

2-cyano-3,5-didehydropyridinium cation (10)
UB3LYP/cc-pVTZ

2-cyano-3,5-didehydropyridinium cation (10)
UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.30 A

1	-2.180704	0.169144	0.000000
7	-1.247088	-0.235849	0.000000
6	-0.101614	0.539213	0.000000
6	-0.101614	1.944766	0.000000
6	0.896998	-0.436132	0.000000
6	1.725383	-1.505033	0.000000
6	0.380656	-1.629192	0.000000
6	-1.016179	-1.573245	0.000000
1	2.719357	-1.931880	0.000000
1	-1.799520	-2.309630	0.000000
7	-0.101614	3.097292	0.000000

E = -339.5987211 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8803108 au

2-cyano-3,5-didehydropyridinium cation (10)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.60 A

1	-2.151493	0.245725	0.000000
7	-1.230987	-0.194085	0.000000
6	-0.063923	0.532944	0.000000
6	-0.063923	1.947190	0.000000
6	0.991688	-0.345948	0.000000
6	1.626779	-1.537321	0.000000
6	0.303378	-1.790326	0.000000

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.40 A

1	-2.170541	0.198155	0.000000
7	-1.241825	-0.219832	0.000000
6	-0.087429	0.538280	0.000000
6	-0.087429	1.946973	0.000000
6	0.927165	-0.406927	0.000000
6	1.693926	-1.521025	0.000000
6	0.353570	-1.684029	0.000000
6	-1.029032	-1.559304	0.000000
1	2.682702	-1.961591	0.000000
1	-1.832016	-2.275837	0.000000
7	-0.087429	3.099183	0.000000

E = -339.6144349 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8976081 au

2-cyano-3,5-didehydropyridinium cation (10)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.70 A

1	-2.139846	0.268581	0.000000
7	-1.223717	-0.182011	0.000000
6	-0.050967	0.530837	0.000000
6	-0.050967	1.947256	0.000000
6	1.024801	-0.316941	0.000000
6	1.589596	-1.543418	0.000000
6	0.275880	-1.843085	0.000000

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.50 A

1	-2.161616	0.221627	0.000000
7	-1.236794	-0.206967	0.000000
6	-0.076025	0.535899	0.000000
6	-0.076025	1.947474	0.000000
6	0.958762	-0.376046	0.000000
6	1.661960	-1.529845	0.000000
6	0.329182	-1.737527	0.000000
6	-1.037500	-1.546833	0.000000
1	2.646127	-1.981597	0.000000
1	-1.856907	-2.246110	0.000000
7	-0.076025	3.099444	0.000000

E = -339.6178472 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9020943 au

2-cyano-3,5-didehydropyridinium cation (10)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.80 A

1	-2.125028	0.291936	0.000000
7	-1.213725	-0.169629	0.000000
6	-0.035850	0.529906	0.000000
6	-0.035850	1.948152	0.000000
6	1.058959	-0.290138	0.000000
6	1.549224	-1.551327	0.000000
6	0.244049	-1.895105	0.000000

6	-1.045650	-1.533892	0.000000
1	2.606132	-1.999419	0.000000
1	-1.880363	-2.216411	0.000000
7	-0.063923	3.098973	0.000000

E = -339.6160209 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9012400 au

2-cyano-3,5-didehydropyridinium cation (10)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.90 A

1	-2.106159	0.317128	0.000000
7	-1.201033	-0.157188	0.000000
6	-0.018283	0.530844	0.000000
6	-0.018283	1.950517	0.000000
6	1.092811	-0.266292	0.000000
6	1.506458	-1.560406	0.000000
6	0.207595	-1.947480	0.000000
6	-1.079797	-1.499316	0.000000
1	2.464749	-2.060701	0.000000
1	-1.966376	-2.117027	0.000000
7	-0.018283	3.101959	0.000000

E = -339.6065038 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8971367 au

2-cyano-3,5-didehydropyridinium cation (10)

6	-1.054293	-1.521860	0.000000
1	2.562914	-2.017191	0.000000
1	-1.904579	-2.186330	0.000000
7	-0.050967	3.098898	0.000000

E = -339.6127555 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8991976 au

2-cyano-3,5-didehydropyridinium cation (10)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.00 A

1	-2.081012	0.344988	0.000000
7	-1.184406	-0.144708	0.000000
6	0.002477	0.533184	0.000000
6	0.002477	1.953832	0.000000
6	1.127117	-0.246052	0.000000
6	1.458045	-1.570123	0.000000
6	0.165789	-1.999862	0.000000
6	-1.097237	-1.488689	0.000000
1	2.407168	-2.085966	0.000000
1	-2.004661	-2.076248	0.000000
7	0.002477	3.105206	0.000000

E = -339.603242 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8967751 au

2-cyano-3,5-didehydropyridinium cation (10)

6	-1.065612	-1.510109	0.000000
1	2.515684	-2.037426	0.000000
1	-1.933146	-2.153151	0.000000
7	-0.035850	3.099681	0.000000

E = -339.6095584 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8977442 au

2-cyano-3,5-didehydropyridinium cation (10)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.10 A

1	-2.046630	0.375130	0.000000
7	-1.161152	-0.132263	0.000000
6	0.028117	0.537795	0.000000
6	0.028117	1.958858	0.000000
6	1.161035	-0.231880	0.000000
6	1.399502	-1.579533	0.000000
6	0.116993	-2.053961	0.000000
6	-1.118800	-1.477870	0.000000
1	2.338125	-2.113815	0.000000
1	-2.050027	-2.027186	0.000000
7	0.028117	3.110181	0.000000

E = -339.6023291 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8956682 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-2.006960	0.411028	0.000000
7	-1.134754	-0.117238	0.000000
6	0.060098	0.543824	0.000000
6	0.060098	1.965236	0.000000
6	1.196040	-0.224191	0.000000
6	1.336758	-1.595167	0.000000
6	0.056872	-2.106290	0.000000
6	-1.147641	-1.464698	0.000000
1	2.262149	-2.152923	0.000000
1	-2.105955	-1.965460	0.000000
7	0.060098	3.116534	0.000000

E = -339.6017103 au
RHF-UCCSD(T)/cc-pVTZ E = -338.8931603 au

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-1.963709	0.451189	0.000000
7	-1.107140	-0.100768	0.000000
6	0.096262	0.549857	0.000000
6	0.096262	1.971631	0.000000
6	1.231935	-0.221343	0.000000
6	1.272429	-1.614376	0.000000
6	-0.012029	-2.155911	0.000000
6	-1.181154	-1.448860	0.000000
1	2.183606	-2.196608	0.000000
1	-2.165978	-1.895649	0.000000
7	0.096262	3.122922	0.000000

E = -339.59889 au
RHF-UCCSD(T)/cc-pVTZ E = -338.8885130 au

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	-2.092212	0.811982	0.000000
7	-1.225327	0.280038	0.000000
6	0.000000	0.871047	0.000000
6	0.881416	-0.197806	0.000000
6	1.556310	-1.365890	0.000000
6	0.206528	-1.308899	0.000000
6	-1.160676	-1.096676	0.000000
1	-2.030369	-1.726608	0.000000
1	2.489698	-1.911494	0.000000
9	0.145411	2.161689	0.000000

E = -346.6031478 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9216704 au

2-fluoro-3,5-didehydropyridinium cation (11)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	-2.092389	0.798970	0.000000
7	-1.222454	0.270479	0.000000
6	0.000000	0.867741	0.000000
6	0.922187	-0.153102	0.000000
6	1.550992	-1.348551	0.000000
6	0.201737	-1.353498	0.000000

2-fluoro-3,5-didehydropyridinium cation (11)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	-2.092456	0.788057	0.000000
7	-1.219417	0.262991	0.000000
6	0.000000	0.863266	0.000000
6	0.962529	-0.109695	0.000000
6	1.540971	-1.330020	0.000000
6	0.195601	-1.398812	0.000000

2-fluoro-3,5-didehydropyridinium cation (11)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

1	-2.091987	0.776329	0.000000
7	-1.215750	0.254866	0.000000
6	0.000000	0.858866	0.000000
6	1.002349	-0.066105	0.000000
6	1.528835	-1.309065	0.000000
6	0.190017	-1.444552	0.000000

6	-1.151057	-1.101606	0.000000
1	-2.024687	-1.728226	0.000000
1	2.487627	-1.890134	0.000000
9	0.115941	2.162238	0.000000

E = -346.6213102 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9412786 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.70 A

1	-2.090136	0.764009	0.000000
7	-1.210906	0.246000	0.000000
6	0.000000	0.855053	0.000000
6	1.041719	-0.022300	0.000000
6	1.514655	-1.286887	0.000000
6	0.184290	-1.490228	0.000000
6	-1.121985	-1.112870	0.000000
1	-2.006793	-1.729108	0.000000
1	2.455228	-1.821868	0.000000
9	0.045107	2.156484	0.000000

E = -346.6248402 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9476076 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

6	-1.141787	-1.104441	0.000000
1	-2.019545	-1.727278	0.000000
1	2.479149	-1.869819	0.000000
9	0.091654	2.160701	0.000000

E = -346.6268294 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9477292 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.80 A

1	-2.086415	0.748831	0.000000
7	-1.204109	0.234751	0.000000
6	0.000000	0.852975	0.000000
6	1.080022	0.022789	0.000000
6	1.500856	-1.262201	0.000000
6	0.180075	-1.536087	0.000000
6	-1.111506	-1.121396	0.000000
1	-2.000526	-1.733001	0.000000
1	2.442984	-1.793186	0.000000
9	0.019559	2.155291	0.000000

E = -346.6226653 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9470394 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

6	-1.131750	-1.108039	0.000000
1	-2.013320	-1.727247	0.000000
1	2.467873	-1.847436	0.000000
9	0.067886	2.158630	0.000000

E = -346.6267411 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9484540 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.90 A

1	-2.080740	0.728871	0.000000
7	-1.194817	0.220107	0.000000
6	0.000000	0.853246	0.000000
6	1.116761	0.069787	0.000000
6	1.488358	-1.234946	0.000000
6	0.178115	-1.582164	0.000000
6	-1.100203	-1.134205	0.000000
1	-1.993974	-1.740053	0.000000
1	2.432556	-1.760759	0.000000
9	-0.010256	2.155654	0.000000

E = -346.6203718 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9471035 au

2-fluoro-3,5-didehydropyridinium cation (11)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	-2.073601	0.703032	0.000000
7	-1.183163	0.201687	0.000000
6	0.000000	0.855974	0.000000
6	1.151826	0.119653	0.000000
6	1.477848	-1.205050	0.000000
6	0.179506	-1.628087	0.000000
6	-1.087375	-1.152004	0.000000
1	-1.986439	-1.751103	0.000000
1	2.425269	-1.723614	0.000000
9	-0.045992	2.157440	0.000000

E = -346.6174332 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9473639 au

1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	-2.063848	0.673847	0.000000
7	-1.168875	0.180471	0.000000
6	0.000000	0.860708	0.000000
6	1.184899	0.171931	0.000000
6	1.468868	-1.173202	0.000000
6	0.183668	-1.674021	0.000000
6	-1.073303	-1.173508	0.000000
1	-1.978358	-1.764424	0.000000
1	2.420644	-1.682537	0.000000
9	-0.086789	2.159819	0.000000

E = -346.6131283 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9470909 au

1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-2.052073	0.641565	0.000000
7	-1.152381	0.156992	0.000000
6	0.000000	0.867356	0.000000
6	1.215704	0.226705	0.000000
6	1.461722	-1.139847	0.000000
6	0.190469	-1.719803	0.000000
6	-1.058030	-1.198303	0.000000
1	-1.969788	-1.779698	0.000000
1	2.418470	-1.638874	0.000000
9	-0.132126	2.162379	0.000000

E = -346.6067829 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9454837 au

2-fluoro-3,5-didehydropyridinium cation (11)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-2.022182	0.592261	0.000000
7	-1.115926	0.125085	0.000000
6	0.000000	0.884608	0.000000
6	1.231795	0.278791	0.000000
6	1.428061	-1.090101	0.000000
6	0.210873	-1.782209	0.000000
6	-1.030538	-1.233972	0.000000
1	-1.955329	-1.792917	0.000000

2-chloro-3,5-didehydropyridinium cation (12)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	2.094660	0.557678	0.000000
7	1.272074	-0.039045	0.000000
6	0.000000	0.467075	0.000000
6	-0.773743	-0.694005	0.000000
6	-1.359208	-1.906180	0.000000
6	-0.014346	-1.749143	0.000000
6	1.329009	-1.412248	0.000000
1	2.251121	-1.963103	0.000000

2-chloro-3,5-didehydropyridinium cation (12)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	2.096486	0.515744	0.000000
7	1.262483	-0.066276	0.000000
6	0.000000	0.462947	0.000000
6	-0.830879	-0.644983	0.000000
6	-1.385681	-1.872425	0.000000
6	-0.034821	-1.796629	0.000000
6	1.294510	-1.436567	0.000000
1	2.214038	-1.994088	0.000000

1	2.398459	-1.567313	0.000000
9	-0.183402	2.172185	0.000000

E = -346.6153182 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9410908 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.50 A

1	2.097611	0.478028	0.000000
7	1.253051	-0.090111	0.000000
6	0.000000	0.458335	0.000000
6	-0.884938	-0.595890	0.000000
6	-1.404686	-1.837744	0.000000
6	-0.053381	-1.844294	0.000000
6	1.261258	-1.456976	0.000000
1	2.178409	-2.020695	0.000000
1	-2.309516	-2.431823	0.000000
17	-0.249846	2.133216	0.000000

E = -706.9896792 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9558615 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.80 A

1	-2.243062	-2.528776	0.000000
17	-0.358678	2.116148	0.000000

E = -706.9676377 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9315324 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.60 A

1	2.097182	0.444050	0.000000
7	1.243213	-0.111453	0.000000
6	0.000000	0.453708	0.000000
6	-0.936588	-0.546701	0.000000
6	-1.416254	-1.803783	0.000000
6	-0.069384	-1.891304	0.000000
6	1.230442	-1.474330	0.000000
1	2.145743	-2.043036	0.000000
1	-2.329449	-2.385000	0.000000
17	-0.203839	2.137566	0.000000

E = -706.9889942 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9559579 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.90 A

1	-2.280914	-2.480026	0.000000
17	-0.301516	2.126367	0.000000

E = -706.9849084 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9502003 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.70 A

1	2.095607	0.406791	0.000000
7	1.231768	-0.134701	0.000000
6	0.000000	0.450319	0.000000
6	-0.986464	-0.495332	0.000000
6	-1.427511	-1.766484	0.000000
6	-0.088393	-1.938754	0.000000
6	1.197854	-1.493727	0.000000
1	2.110648	-2.068210	0.000000
1	-2.349401	-2.333089	0.000000
17	-0.156008	2.141252	0.000000

E = -706.986646 au

RHF-UCCSD(T)/cc-pVTZ E = -705.9546554 au

2-chloro-3,5-didehydropyridinium cation (12)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.00 A

1	2.091732	0.365791	0.000000	1	-2.085060	0.316028	0.000000	1	-2.075081	0.256681	0.000000
7	1.217843	-0.160514	0.000000	7	-1.199960	-0.191988	0.000000	7	-1.177465	-0.229213	0.000000
6	0.000000	0.448575	0.000000	6	0.000000	0.448791	0.000000	6	0.000000	0.450942	0.000000
6	-1.034910	-0.441160	0.000000	6	1.083076	-0.381514	0.000000	6	1.130818	-0.315203	0.000000
6	-1.438866	-1.726853	0.000000	6	1.455109	-1.682137	0.000000	6	1.476875	-1.631812	0.000000
6	-0.110759	-1.985810	0.000000	6	0.141543	-2.031822	0.000000	6	0.182411	-2.076033	0.000000
6	1.163950	-1.516327	0.000000	6	-1.125037	-1.545108	0.000000	6	-1.079810	-1.580362	0.000000
1	2.074472	-2.095905	0.000000	1	-2.032714	-2.130361	0.000000	1	-1.983927	-2.172179	0.000000
1	-2.369383	-2.277878	0.000000	1	2.395613	-2.214364	0.000000	1	2.429388	-2.140685	0.000000
17	-0.105777	2.144767	0.000000	17	0.046690	2.148433	0.000000	17	-0.022934	2.151499	0.000000

E = -706.9841525 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9537778 au

2-chloro-3,5-didehydropyridinium cation (12)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	-2.060371	0.189721	0.000000
7	-1.149845	-0.271410	0.000000
6	0.000000	0.455727	0.000000
6	1.175521	-0.242807	0.000000
6	1.504417	-1.575380	0.000000
6	0.233990	-2.119911	0.000000
6	-1.027045	-1.620879	0.000000
1	-1.926340	-2.221057	0.000000
1	2.470535	-2.056576	0.000000
17	-0.103306	2.153370	0.000000

E = -706.9816414 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9536344 au

2-chloro-3,5-didehydropyridinium cation (12)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-2.041359	0.116552	0.000000
7	-1.117305	-0.316346	0.000000
6	0.000000	0.462261	0.000000
6	1.217912	-0.164112	0.000000
6	1.535611	-1.514721	0.000000
6	0.294267	-2.160829	0.000000
6	-0.968350	-1.664611	0.000000
1	-1.862606	-2.273183	0.000000
1	2.515981	-1.965131	0.000000
17	-0.192207	2.152250	0.000000

E = -706.9785544 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9537200 au

2-chloro-3,5-didehydropyridinium cation (12)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-1.999919	0.018508	0.000000
7	-1.060594	-0.374168	0.000000
6	0.000000	0.475046	0.000000
6	1.256512	-0.074747	0.000000
6	1.549404	-1.430052	0.000000
6	0.382660	-2.202277	0.000000
6	-0.889158	-1.721849	0.000000
1	-1.778870	-2.335517	0.000000
1	2.550853	-1.837124	0.000000
17	-0.302613	2.146858	0.000000

E = -706.9741421 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9532133 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	2.091108	0.850542	0.000000
7	1.232696	0.313941	0.000000
6	0.000000	0.870570	0.000000
7	-0.298719	2.175833	0.000000
1	-1.259811	2.469291	0.000000
6	-0.836497	-0.283505	0.000000
6	-1.497086	-1.434285	0.000000
6	-0.120237	-1.368388	0.000000
6	1.208872	-1.110123	0.000000
1	-2.418652	-1.996849	0.000000
1	2.111744	-1.688980	0.000000
1	0.407458	2.891964	0.000000

E = -706.9677059 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9512127 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	2.095443	0.821076	0.000000
7	1.230188	0.293737	0.000000
6	0.000000	0.867788	0.000000
7	-0.257038	2.182906	0.000000
1	-1.208826	2.505306	0.000000
6	-0.880953	-0.234918	0.000000
6	-1.495922	-1.413637	0.000000
6	-0.124302	-1.412831	0.000000
6	1.193681	-1.117680	0.000000
1	-2.420772	-1.973144	0.000000
1	2.096481	-1.699158	0.000000
1	0.470596	2.877091	0.000000

E = -706.975724 au
RHF-UCCSD(T)/cc-pVTZ E = -705.9464448 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	2.098799	0.797906	0.000000
7	1.227575	0.278567	0.000000
6	0.000000	0.864588	0.000000
7	-0.223107	2.186257	0.000000
1	-1.166879	2.531683	0.000000
6	-0.924001	-0.189307	0.000000
6	-1.489569	-1.392897	0.000000
6	-0.124693	-1.458601	0.000000
6	1.179661	-1.122220	0.000000
1	-2.416391	-1.950453	0.000000
1	2.083428	-1.704641	0.000000
1	0.521375	2.862368	0.000000

E = -302.7376009 au
RHF-UCCSD(T)/cc-pVTZ E = -302.0919271 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

E = -302.7559053 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1116136 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

E = -302.7618579 au
RHF-UCCSD(T)/cc-pVTZ E = -302.1184340 au

2-amino-3,5-didehydropyridinium cation (13)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	2.100670	0.777330	0.000000
7	1.223937	0.265437	0.000000
6	0.000000	0.861625	0.000000
7	-0.193443	2.187901	0.000000
1	-1.129753	2.553430	0.000000
6	-0.965903	-0.145358	0.000000
6	-1.479939	-1.371026	0.000000
6	-0.122924	-1.505280	0.000000
6	1.166335	-1.126060	0.000000
1	-2.407451	-1.927697	0.000000
1	2.072078	-1.707588	0.000000
1	0.565584	2.847752	0.000000

E = -302.7623764 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1197220 au

2-amino-3,5-didehydropyridinium cation (13)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.90 A

1	-2.093951	0.706719	0.000000
7	-1.202065	0.217703	0.000000
6	0.000000	0.859396	0.000000
7	0.095217	2.194912	0.000000
1	1.003310	2.627035	0.000000
6	1.088735	-0.008126	0.000000
6	1.449205	-1.293729	0.000000
6	0.121507	-1.643507	0.000000

1	-2.100879	0.756674	0.000000
7	-1.219139	0.251799	0.000000
6	0.000000	0.859038	0.000000
7	0.163453	2.189096	0.000000
1	1.091916	2.574586	0.000000
6	1.008119	-0.100751	0.000000
6	1.468771	-1.347775	0.000000
6	0.121195	-1.551050	0.000000
6	-1.153034	-1.132146	0.000000
1	2.398304	-1.900390	0.000000
1	-2.060158	-1.713460	0.000000
1	-0.609691	2.832422	0.000000

E = -302.7611839 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1195533 au

2-amino-3,5-didehydropyridinium cation (13)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.00 A

1	-2.086859	0.676342	0.000000
7	-1.189596	0.196702	0.000000
6	0.000000	0.862506	0.000000
7	0.054982	2.199535	0.000000
1	0.949874	2.658747	0.000000
6	1.126956	0.041222	0.000000
6	1.441682	-1.263302	0.000000
6	0.124846	-1.689609	0.000000

1	-2.098724	0.733352	0.000000
7	-1.211862	0.236181	0.000000
6	0.000000	0.858331	0.000000
7	0.131342	2.191429	0.000000
1	1.050815	2.598285	0.000000
6	1.048948	-0.055401	0.000000
6	1.458274	-1.322026	0.000000
6	0.120345	-1.597379	0.000000
6	-1.139542	-1.141861	0.000000
1	2.389227	-1.870964	0.000000
1	-2.049296	-1.720684	0.000000
1	-0.656537	2.816750	0.000000

E = -302.7597433 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1196879 au

2-amino-3,5-didehydropyridinium cation (13)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.10 A

1	-2.070223	0.637866	0.000000
7	-1.168003	0.170467	0.000000
6	0.000000	0.869240	0.000000
7	0.010836	2.206671	0.000000
1	0.889669	2.696320	0.000000
6	1.160006	0.091892	0.000000
6	1.422987	-1.225357	0.000000
6	0.134680	-1.740785	0.000000

6	-1.125513	-1.156135	0.000000
1	2.382771	-1.836639	0.000000
1	-2.038363	-1.731359	0.000000
1	-0.709442	2.798547	0.000000

E = -302.7581483 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1203878 au

2-amino-3,5-didehydropyridinium cation (13)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.20 A

1	-2.053100	0.594252	0.000000
7	-1.144671	0.140708	0.000000
6	0.000000	0.878626	0.000000
7	-0.042933	2.214676	0.000000
1	0.815291	2.739852	0.000000
6	1.191457	0.147103	0.000000
6	1.411353	-1.186113	0.000000
6	0.149293	-1.790394	0.000000
6	-1.070137	-1.229954	0.000000
1	2.364851	-1.692478	0.000000
1	-2.000560	-1.778095	0.000000
1	-0.905039	2.733176	0.000000

E = -302.7558923 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1191590 au

6	-1.110877	-1.174984	0.000000
1	2.378786	-1.798544	0.000000
1	-2.028036	-1.744510	0.000000
1	-0.767104	2.779310	0.000000

E = -302.7558305 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1211524 au

2-amino-3,5-didehydropyridinium cation (13)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.30 A

1	-2.035134	0.549541	0.000000
7	-1.120286	0.110590	0.000000
6	0.000000	0.889138	0.000000
7	-0.100243	2.221571	0.000000
1	0.735257	2.782392	0.000000
6	1.221604	0.204780	0.000000
6	1.402594	-1.147058	0.000000
6	0.165604	-1.838469	0.000000
6	-1.048621	-1.262418	0.000000
1	2.365177	-1.638234	0.000000
1	-1.985904	-1.799297	0.000000
1	-0.982775	2.704632	0.000000

E = -302.7537333 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1151931 au

6	-1.091354	-1.199402	0.000000
1	2.367429	-1.747218	0.000000
1	-2.014570	-1.759266	0.000000
1	-0.830048	2.758804	0.000000

E = -302.7558242 au

RHF-UCCSD(T)/cc-pVTZ E = -302.1209087 au

2-hydroxy-3,5-didehydropyridinium cation (14)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.30 A

1	-2.081661	0.836873	0.000000
7	-1.224392	0.292433	0.000000
6	0.000000	0.873549	0.000000
8	0.119885	2.188664	0.000000
1	1.042428	2.475203	0.000000
6	0.862897	-0.236061	0.000000
6	1.526499	-1.400652	0.000000
6	0.168928	-1.335336	0.000000
6	-1.181179	-1.101765	0.000000
1	2.453119	-1.956664	0.000000
1	-2.065090	-1.710169	0.000000

E = -322.5981054 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9362228 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	-2.084144	0.818713	0.000000
7	-1.222466	0.279761	0.000000
6	0.000000	0.870688	0.000000
8	0.088989	2.188449	0.000000
1	1.005191	2.495304	0.000000
6	0.904141	-0.190389	0.000000
6	1.521956	-1.382438	0.000000
6	0.166317	-1.380186	0.000000
6	-1.170790	-1.106348	0.000000
1	2.451920	-1.934620	0.000000
1	-2.057355	-1.713277	0.000000

E = -322.6168474 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9563829 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	-2.085908	0.804313	0.000000
7	-1.220263	0.270120	0.000000
6	0.000000	0.866869	0.000000
8	0.063865	2.186233	0.000000
1	0.974698	2.509491	0.000000
6	0.945084	-0.146537	0.000000
6	1.512335	-1.363708	0.000000
6	0.161486	-1.425590	0.000000
6	-1.160814	-1.108873	0.000000
1	2.444036	-1.913950	0.000000
1	-2.050453	-1.713515	0.000000

E = -322.6230123 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9634499 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

1	-2.086578	0.791006	0.000000
7	-1.217359	0.261034	0.000000
6	0.000000	0.862839	0.000000
8	0.041168	2.183176	0.000000
1	0.947161	2.520697	0.000000
6	0.985740	-0.103209	0.000000
6	1.499670	-1.343401	0.000000
6	0.155808	-1.471131	0.000000
6	-1.150847	-1.111599	0.000000
1	2.432754	-1.891371	0.000000
1	-2.043389	-1.713974	0.000000

E = -322.6236193 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9648408 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	-2.085656	0.776605	0.000000
7	-1.212856	0.251093	0.000000
6	0.000000	0.859691	0.000000
8	0.018354	2.180198	0.000000
1	0.919355	2.531595	0.000000

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	-2.082790	0.758826	0.000000
7	-1.206287	0.238319	0.000000
6	0.000000	0.858215	0.000000
8	-0.008001	2.178363	0.000000
1	0.886812	2.546070	0.000000

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.90 A

1	-2.077641	0.736697	0.000000
7	-1.197145	0.222124	0.000000
6	0.000000	0.858567	0.000000
8	-0.038838	2.177796	0.000000
1	0.846810	2.568010	0.000000

6	1.025783	-0.059750	0.000000	6	1.064944	-0.014737	0.000000	6	1.103166	0.032218	0.000000
6	1.485793	-1.321135	0.000000	6	1.472875	-1.296123	0.000000	6	1.461334	-1.268732	0.000000
6	0.150159	-1.516898	0.000000	6	0.146338	-1.562691	0.000000	6	0.144737	-1.608335	0.000000
6	-1.140780	-1.116129	0.000000	6	-1.129972	-1.124936	0.000000	6	-1.118462	-1.138420	0.000000
1	2.420087	-1.866273	0.000000	1	2.408281	-1.838032	0.000000	1	2.399019	-1.805165	0.000000
1	-2.036351	-1.715831	0.000000	1	-2.029396	-1.720371	0.000000	1	-2.022123	-1.728568	0.000000

E = -322.6224327 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9646821 au

E = -322.6209438 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9647590 au

E = -322.619264 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9653510 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	-2.070613	0.709240	0.000000	1	-2.061458	0.677611	0.000000	1	-2.049968	0.643707	0.000000
7	-1.185367	0.202401	0.000000	7	-1.171030	0.179778	0.000000	7	-1.154447	0.155213	0.000000
6	0.000000	0.861302	0.000000	6	0.000000	0.866115	0.000000	6	0.000000	0.872745	0.000000
8	-0.075746	2.178399	0.000000	8	-0.117950	2.179621	0.000000	8	-0.164340	2.180848	0.000000
1	0.798744	2.593627	0.000000	1	0.742616	2.623407	0.000000	1	0.679632	2.655693	0.000000
6	1.139463	0.081718	0.000000	6	1.173689	0.133677	0.000000	6	1.205561	0.187834	0.000000
6	1.452070	-1.238368	0.000000	6	1.444831	-1.205829	0.000000	6	1.439410	-1.171883	0.000000
6	0.146452	-1.654349	0.000000	6	0.151203	-1.700586	0.000000	6	0.158475	-1.747008	0.000000
6	-1.105292	-1.156784	0.000000	6	-1.090659	-1.179281	0.000000	6	-1.074810	-1.204953	0.000000
1	2.393117	-1.767449	0.000000	1	2.390254	-1.725888	0.000000	1	2.389969	-1.681642	0.000000
1	-2.013874	-1.740535	0.000000	1	-2.004992	-1.755113	0.000000	1	-1.995597	-1.771448	0.000000

E = -322.6168344 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9660112 au

E = -322.6129104 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9660023 au

E = -322.6068133 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9645473 au

2-hydroxy-3,5-didehydropyridinium cation (14)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-2.018942	0.591927	0.000000
7	-1.116698	0.120307	0.000000
6	0.000000	0.889326	0.000000
8	-0.223725	2.187985	0.000000
1	0.595368	2.704461	0.000000
6	1.224306	0.241956	0.000000
6	1.409584	-1.121358	0.000000
6	0.182988	-1.808813	0.000000
6	-1.044747	-1.242301	0.000000
1	2.374945	-1.607808	0.000000
1	-1.977462	-1.787473	0.000000

E = -322.6148171 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9602003 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	2.116982	0.800975	0.000000
7	1.218567	0.339397	0.000000
6	0.985620	-1.048795	0.000000
6	-0.361956	-1.318494	0.000000
6	-0.938757	-0.017342	0.000000
6	-1.286356	1.294351	0.000000
6	0.000000	0.881955	0.000000
1	1.819579	-1.734138	0.000000
1	-0.839357	-2.281696	0.000000
1	-2.018471	2.089035	0.000000

E = -247.3645885 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8267289 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	2.099233	0.852236	0.000000
7	1.206490	0.376440	0.000000
6	1.017817	-1.012884	0.000000
6	-0.320386	-1.326388	0.000000
6	-0.977863	-0.074712	0.000000
6	-1.317917	1.234888	0.000000
6	0.000000	0.927178	0.000000
1	1.873270	-1.672169	0.000000
1	-0.753492	-2.311284	0.000000
1	-2.074340	2.007645	0.000000

E = -247.3763144 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8396177 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	2.079869	0.895665	0.000000
7	1.191666	0.408286	0.000000
6	1.045161	-0.979500	0.000000
6	-0.283200	-1.330317	0.000000

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

1	2.059701	0.931694	0.000000
7	1.174531	0.436094	0.000000
6	1.067561	-0.948089	0.000000
6	-0.250545	-1.332746	0.000000

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	2.039776	0.962408	0.000000
7	1.156499	0.461334	0.000000
6	1.084818	-0.918109	0.000000
6	-0.222536	-1.336112	0.000000

6	-1.012789	-0.130356	0.000000	6	-1.042520	-0.184506	0.000000	6	-1.067681	-0.237666	0.000000
6	-1.340239	1.175171	0.000000	6	-1.354727	1.115804	0.000000	6	-1.362302	1.058758	0.000000
6	0.000000	0.976107	0.000000	6	0.000000	1.029229	0.000000	6	0.000000	1.085232	0.000000
1	1.919259	-1.614860	0.000000	1	1.958041	-1.561218	0.000000	1	1.989712	-1.510568	0.000000
1	-0.676609	-2.332713	0.000000	1	-0.607540	-2.349621	0.000000	1	-0.544114	-2.365636	0.000000
1	-2.117784	1.927268	0.000000	1	-2.150530	1.848338	0.000000	1	-2.174666	1.771837	0.000000

E = -247.3764945 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8404249 au

E = -247.3726758 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8371957 au

E = -247.3688444 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8343397 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	-0.437353	-2.208273	0.000000	1	-0.376721	-2.217462	0.000000	1	-0.319740	-2.228185	0.000000
7	-0.176222	-1.226174	0.000000	7	-0.155884	-1.224886	0.000000	7	-0.138092	-1.227267	0.000000
6	1.141765	-0.831057	0.000000	6	1.148227	-0.801157	0.000000	6	1.150965	-0.770328	0.000000
6	1.245426	0.537430	0.000000	6	1.236895	0.569710	0.000000	6	1.228341	0.602823	0.000000
6	0.000000	1.128438	0.000000	6	0.000000	1.163650	0.000000	6	0.000000	1.205861	0.000000
6	-1.322849	1.059350	0.000000	6	-1.316176	1.018065	0.000000	6	-1.310125	0.971874	0.000000
6	-1.103021	-0.294005	0.000000	6	-1.143245	-0.353910	0.000000	6	-1.175386	-0.412308	0.000000
1	1.931973	-1.570045	0.000000	1	1.953866	-1.523679	0.000000	1	1.971319	-1.476082	0.000000
1	2.177931	1.081067	0.000000	1	2.169537	1.114650	0.000000	1	2.163693	1.144475	0.000000
1	-2.206912	1.679529	0.000000	1	-2.209696	1.622548	0.000000	1	-2.211405	1.563131	0.000000

E = -247.366281 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8333554 au

E = -247.3645736 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8338265 au

E = -247.3627689 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8347762 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	0.040965	2.259511	0.000000
7	0.000000	1.243039	0.000000
6	-1.214740	0.621701	0.000000
6	-1.147491	-0.752756	0.000000
6	0.125673	-1.257394	0.000000
6	1.387090	-0.781451	0.000000
6	1.142269	0.580141	0.000000
1	-2.111774	1.226146	0.000000
1	-2.031872	-1.374883	0.000000
1	2.345872	-1.273491	0.000000

E = -247.3623681 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8351029 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	0.009672	2.271858	0.000000
7	0.000000	1.254554	0.000000
6	-1.198803	0.604904	0.000000
6	-1.142959	-0.772691	0.000000
6	0.117512	-1.312483	0.000000
6	1.363180	-0.750317	0.000000
6	1.162684	0.623393	0.000000
1	-2.101318	1.200629	0.000000
1	-2.042517	-1.373097	0.000000
1	2.324481	-1.238106	0.000000

E = -247.3614521 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8338610 au

2,4-didehydropyridinium cation (15)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-0.025005	2.285316	0.000000
7	0.000000	1.268161	0.000000
6	-1.182577	0.587867	0.000000
6	-1.139061	-0.793818	0.000000
6	0.109623	-1.365830	0.000000
6	1.340493	-0.723602	0.000000
6	1.182312	0.668706	0.000000
1	-2.091091	1.174074	0.000000
1	-2.054030	-1.370904	0.000000
1	2.305388	-1.205554	0.000000

E = -247.3577101 au
RHF-UCCSD(T)/cc-pVTZ E = -246.8305818 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	-1.779715	1.780506	0.000000
7	-1.315246	0.884704	0.000000
6	-1.925999	-0.375084	0.000000
6	-0.986122	-1.377573	0.000000
6	0.243457	-0.653403	0.000000
6	1.294689	0.222931	0.000000

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	-1.801255	1.766373	0.000000
7	-1.316866	0.879369	0.000000
6	-1.917974	-0.379795	0.000000
6	-0.973336	-1.379240	0.000000
6	0.267887	-0.696764	0.000000
6	1.275708	0.221638	0.000000

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	-1.822340	1.746550	0.000000
7	-1.317825	0.869015	0.000000
6	-1.908371	-0.388917	0.000000
6	-0.955533	-1.381050	0.000000
6	0.294855	-0.737710	0.000000
6	1.252481	0.222005	0.000000

6	0.000000	0.623597	0.000000
1	-3.001790	-0.451057	0.000000
1	-1.156797	-2.438485	0.000000
8	2.531872	0.559702	0.000000
1	3.133899	-0.204314	0.000000

E = -322.6342822 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9734254 au

6	0.000000	0.677367	0.000000
1	-2.993800	-0.461415	0.000000
1	-1.154633	-2.439321	0.000000
8	2.516944	0.564786	0.000000
1	3.118490	-0.198749	0.000000

E = -322.6447583 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9851053 au

6	0.000000	0.733025	0.000000
1	-2.983995	-0.478854	0.000000
1	-1.142965	-2.441024	0.000000
8	2.496824	0.574278	0.000000
1	3.098897	-0.188118	0.000000

E = -322.6435024 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9844372 au

3-hydroxy-2,4-didehydropyridinium cation (16)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.60 A

1	-1.843786	1.722022	0.000000
7	-1.317419	0.855734	0.000000
6	-1.896735	-0.400866	0.000000
6	-0.934653	-1.383861	0.000000
6	0.322427	-0.776150	0.000000
6	1.226353	0.223126	0.000000
6	0.000000	0.791027	0.000000
1	-2.971955	-0.500308	0.000000
1	-1.125487	-2.444176	0.000000
8	2.472778	0.585899	0.000000
1	3.076578	-0.174532	0.000000

E = -322.638088 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9794383 au

3-hydroxy-2,4-didehydropyridinium cation (16)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.70 A

1	-1.865312	1.695211	0.000000
7	-1.315054	0.842419	0.000000
6	-1.882572	-0.413441	0.000000
6	-0.912720	-1.388858	0.000000
6	0.348564	-0.812615	0.000000
6	1.198744	0.223617	0.000000
6	0.000000	0.851267	0.000000
1	-2.957187	-0.522397	0.000000
1	-1.107559	-2.449397	0.000000
8	2.446342	0.597526	0.000000
1	3.052592	-0.160375	0.000000

E = -322.632547 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9745778 au

3-hydroxy-2,4-didehydropyridinium cation (16)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.80 A

1	-1.883667	1.671277	0.000000
7	-1.310709	0.832341	0.000000
6	-1.866671	-0.423591	0.000000
6	-0.892570	-1.395537	0.000000
6	0.372985	-0.849181	0.000000
6	1.171183	0.223188	0.000000
6	0.000000	0.911751	0.000000
1	-2.940641	-0.540924	0.000000
1	-1.095604	-2.455497	0.000000
8	2.419647	0.606058	0.000000
1	3.028134	-0.149489	0.000000

E = -322.6282876 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9715764 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.90 A

1	-1.898798	1.652844	0.000000
7	-1.304880	0.827637	0.000000
6	-1.849186	-0.429679	0.000000
6	-0.875322	-1.403594	0.000000
6	0.395755	-0.887465	0.000000
6	1.144354	0.221529	0.000000
6	0.000000	0.970861	0.000000
1	-2.922546	-0.553759	0.000000
1	-1.092130	-2.461762	0.000000
8	2.393726	0.610300	0.000000
1	3.004222	-0.143089	0.000000

E = -322.6250729 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9702997 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	-1.073110	-2.279233	0.000000
7	-0.844248	-1.287861	0.000000
6	-1.846500	-0.356828	0.000000
6	-1.364175	0.935496	0.000000
6	0.000000	1.017128	0.000000
6	1.109729	0.259548	0.000000
6	0.421560	-0.937939	0.000000
1	-2.877987	-0.678769	0.000000
1	-2.012921	1.800252	0.000000
8	2.411076	0.414661	0.000000
1	2.661466	1.351058	0.000000

E = -322.621903 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9697407 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	-1.076157	-2.283828	0.000000
7	-0.829496	-1.296554	0.000000
6	-1.822390	-0.360421	0.000000
6	-1.359057	0.939838	0.000000
6	0.000000	1.071796	0.000000
6	1.080384	0.251033	0.000000
6	0.447143	-0.980048	0.000000
1	-2.852330	-0.685882	0.000000
1	-2.032531	1.786167	0.000000
8	2.383456	0.420855	0.000000
1	2.623360	1.359406	0.000000

E = -322.6193153 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9688699 au

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-1.986633	-1.573121	0.000000
7	-1.090235	-1.091156	0.000000
6	0.053477	-1.832373	0.000000
6	1.229622	-1.104765	0.000000
6	1.097832	0.254268	0.000000

3-hydroxy-2,4-didehydropyridinium cation (16)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-1.988714	-1.589118	0.000000
7	-1.104588	-1.084688	0.000000
6	0.050688	-1.808193	0.000000
6	1.240438	-1.096472	0.000000
6	1.151191	0.267065	0.000000

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	-1.801286	1.745915	0.000000
7	-1.316906	0.859732	0.000000
6	-1.898166	-0.417772	0.000000
6	-0.936662	-1.399061	0.000000
6	0.271038	-0.644047	0.000000

6	0.000000	1.080699	0.000000
6	-1.101993	0.226516	0.000000
1	-0.030634	-2.908946	0.000000
1	2.191973	-1.599204	0.000000
8	-0.119876	2.392520	0.000000
1	0.742322	2.833129	0.000000

E = -322.6170243 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9666103 au

6	0.000000	1.055561	0.000000
6	-1.148581	0.234680	0.000000
1	-0.030780	-2.884767	0.000000
1	2.187674	-1.619892	0.000000
8	-0.117816	2.370029	0.000000
1	0.744048	2.810521	0.000000

E = -322.6125956 au

RHF-UCCSD(T)/cc-pVTZ E = -321.9623431 au

6	1.290374	0.242980	0.000000
6	0.000000	0.627385	0.000000
1	-2.972421	-0.517729	0.000000
1	-1.078094	-2.464406	0.000000
9	2.523404	0.529021	0.000000

E = -346.6272587 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9473998 au

3-fluoro-2,4-didehydropyridinium cation (17)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.40 A

1	-1.821355	1.732364	0.000000
7	-1.317993	0.855034	0.000000
6	-1.889952	-0.421038	0.000000
6	-0.925454	-1.400900	0.000000
6	0.295975	-0.687646	0.000000
6	1.271809	0.240156	0.000000
6	0.000000	0.680711	0.000000
1	-2.964188	-0.526110	0.000000
1	-1.079776	-2.465362	0.000000
9	2.508555	0.534019	0.000000

E = -346.6404597 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9617215 au

3-fluoro-2,4-didehydropyridinium cation (17)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.50 A

1	-1.841829	1.712564	0.000000
7	-1.318485	0.845239	0.000000
6	-1.879890	-0.428966	0.000000
6	-0.909113	-1.403159	0.000000
6	0.323454	-0.728933	0.000000
6	1.248849	0.239624	0.000000
6	0.000000	0.735778	0.000000
1	-2.953849	-0.541736	0.000000
1	-1.071100	-2.467413	0.000000
9	2.488486	0.543761	0.000000

E = -346.6414099 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9631277 au

3-fluoro-2,4-didehydropyridinium cation (17)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.60 A

1	-1.863911	1.687058	0.000000
7	-1.317366	0.832500	0.000000
6	-1.867312	-0.439922	0.000000
6	-0.889020	-1.406539	0.000000
6	0.351413	-0.767670	0.000000
6	1.222589	0.239666	0.000000
6	0.000000	0.793262	0.000000
1	-2.940722	-0.561685	0.000000
1	-1.055977	-2.470992	0.000000
9	2.464016	0.556149	0.000000

E = -346.6377137 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9596665 au

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	-1.884407	1.660631	0.000000
7	-1.314234	0.820135	0.000000
6	-1.852842	-0.450390	0.000000
6	-0.867966	-1.410482	0.000000
6	0.378496	-0.804795	0.000000
6	1.194520	0.239458	0.000000
6	0.000000	0.852534	0.000000
1	-2.925456	-0.581663	0.000000
1	-1.042508	-2.474783	0.000000
9	2.437640	0.566325	0.000000

E = -346.6334787 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9558945 au

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	-1.900953	1.637782	0.000000
7	-1.309374	0.811043	0.000000
6	-1.836285	-0.458870	0.000000
6	-0.848581	-1.417028	0.000000
6	0.403940	-0.842211	0.000000
6	1.166516	0.238985	0.000000
6	0.000000	0.911880	0.000000
1	-2.908258	-0.597719	0.000000
1	-1.032037	-2.480787	0.000000
9	2.410369	0.574097	0.000000

E = -346.6302269 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9537144 au

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.90 A

1	-1.915644	1.619030	0.000000
7	-1.303183	0.806683	0.000000
6	-1.818163	-0.463837	0.000000
6	-0.831296	-1.424738	0.000000
6	0.427831	-0.880561	0.000000
6	1.139018	0.237375	0.000000
6	0.000000	0.970644	0.000000
1	-2.889467	-0.609322	0.000000
1	-1.029334	-2.486864	0.000000
9	2.383597	0.577453	0.000000

E = -346.627819 au
RHF-UCCSD(T)/cc-pVTZ E = -345.9531143 au

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	-1.027885	-2.289574	0.000000
7	-0.809345	-1.295236	0.000000
6	-1.820149	-0.373243	0.000000
6	-1.363140	0.928429	0.000000
6	0.000000	1.024951	0.000000
6	1.102245	0.278133	0.000000

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	-1.941499	1.597349	0.000000
7	-1.290631	0.814262	0.000000
6	-1.776485	-0.460758	0.000000
6	-0.802450	-1.439303	0.000000
6	0.478569	-0.966800	0.000000
6	1.080967	0.235175	0.000000

3-fluoro-2,4-didehydropyridinium cation (17)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-1.978363	-1.566036	0.000000
7	-1.084562	-1.077935	0.000000
6	0.065165	-1.809693	0.000000
6	1.241782	-1.083382	0.000000
6	1.100789	0.275451	0.000000
6	0.000000	1.077203	0.000000

6	0.451656	-0.923384	0.000000
1	-2.848115	-0.708506	0.000000
1	-2.025351	1.783335	0.000000
9	2.371455	0.519120	0.000000

E = -346.6253168 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9532147 au

3-fluoro-2,4-didehydropyridinium cation (17)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.30 A

1	-1.980619	-1.581462	0.000000
7	-1.098962	-1.071480	0.000000
6	0.061894	-1.785360	0.000000
6	1.251812	-1.074887	0.000000
6	1.154680	0.289597	0.000000
6	0.000000	1.051084	0.000000
6	-1.144986	0.250385	0.000000
1	-0.014029	-2.863156	0.000000
1	2.200612	-1.595938	0.000000
9	-0.050403	2.350667	0.000000

E = -346.6174396 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9480189 au

3-cyano-2,4-didehydropyridinium cation (18)

6	0.000000	1.077942	0.000000
1	-2.846468	-0.614101	0.000000
1	-1.045496	-2.493557	0.000000
9	2.331586	0.570326	0.000000

E = -346.6231492 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9530018 au

3-cyano-2,4-didehydropyridinium cation (18)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.30 A

1	2.117143	-1.734579	0.000000
7	1.143078	-1.465537	0.000000
6	0.029039	-2.327997	0.000000
6	-1.146894	-1.612020	0.000000
6	-0.686972	-0.268257	0.000000
6	-0.052259	0.940868	0.000000
6	0.612776	-0.242662	0.000000
1	0.177410	-3.397209	0.000000
1	-2.150865	-1.996486	0.000000
6	-0.052259	2.336784	0.000000
7	-0.052259	3.489533	0.000000

E = -339.6114695 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8929590 au

3-cyano-2,4-didehydropyridinium cation (18)

6	-1.098954	0.241865	0.000000
1	-0.013316	-2.887482	0.000000
1	2.205809	-1.575184	0.000000
9	-0.052765	2.373954	0.000000

E = -346.6213593 au

RHF-UCCSD(T)/cc-pVTZ E = -345.9514873 au

3-cyano-2,4-didehydropyridinium cation (18)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 1.40 A

1	2.114285	-1.748619	0.000000
7	1.143501	-1.462208	0.000000
6	0.033281	-2.320921	0.000000
6	-1.143706	-1.606464	0.000000
6	-0.733746	-0.256172	0.000000
6	-0.057266	0.924150	0.000000
6	0.665933	-0.226170	0.000000
1	0.181492	-3.390711	0.000000
1	-2.142803	-2.005910	0.000000
6	-0.057266	2.325308	0.000000
7	-0.057266	3.477473	0.000000

E = -339.6228297 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9058608 au

3-cyano-2,4-didehydropyridinium cation (18)

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	2.108487	-1.759075	0.000000
7	1.140945	-1.456572	0.000000
6	0.036766	-2.312442	0.000000
6	-1.139560	-1.597821	0.000000
6	-0.778869	-0.243180	0.000000
6	-0.062056	0.903894	0.000000
6	0.720687	-0.206677	0.000000
1	0.184448	-3.382856	0.000000
1	-2.134646	-2.009651	0.000000
6	-0.062056	2.309471	0.000000
7	-0.062056	3.461159	0.000000

E = -339.6226302 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9065703 au

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

1	2.099615	-1.767547	0.000000
7	1.135757	-1.448978	0.000000
6	0.038404	-2.302079	0.000000
6	-1.136553	-1.586671	0.000000
6	-0.821650	-0.230254	0.000000
6	-0.066005	0.880958	0.000000
6	0.777701	-0.184691	0.000000
1	0.185050	-3.373137	0.000000
1	-2.128282	-2.008977	0.000000
6	-0.066005	2.289993	0.000000
7	-0.066005	3.441281	0.000000

E = -339.6184285 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9031534 au

UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	2.088090	-1.777025	0.000000
7	1.129299	-1.440002	0.000000
6	0.037568	-2.289242	0.000000
6	-1.136941	-1.574160	0.000000
6	-0.862214	-0.218160	0.000000
6	-0.068520	0.856699	0.000000
6	0.836838	-0.161401	0.000000
1	0.182521	-3.360955	0.000000
1	-2.125320	-2.006646	0.000000
6	-0.068520	2.268112	0.000000
7	-0.068520	3.419080	0.000000

E = -339.6142535 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9001016 au

3-cyano-2,4-didehydropyridinium cation (18)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	2.075348	-1.788826	0.000000
7	1.123308	-1.430614	0.000000
6	0.034109	-2.273610	0.000000
6	-1.142077	-1.561042	0.000000
6	-0.902339	-0.206437	0.000000
6	-0.068685	0.832269	0.000000

3-cyano-2,4-didehydropyridinium cation (18)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.90 A

1	2.063914	-1.801070	0.000000
7	1.119618	-1.421023	0.000000
6	0.029453	-2.255228	0.000000
6	-1.151457	-1.548284	0.000000
6	-0.943192	-0.195076	0.000000
6	-0.067360	0.808266	0.000000

3-cyano-2,4-didehydropyridinium cation (18)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	2.053255	-1.815778	0.000000
7	1.117793	-1.413146	0.000000
6	0.021744	-2.233942	0.000000
6	-1.164797	-1.533749	0.000000
6	-0.989418	-0.179951	0.000000
6	-0.060915	0.783822	0.000000

6	0.896398	-0.139023	0.000000
1	0.176137	-3.346045	0.000000
1	-2.126183	-2.005475	0.000000
6	-0.068685	2.245120	0.000000
7	-0.068685	3.395855	0.000000

E = -339.6114455 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8990170 au

6	0.955267	-0.118575	0.000000
1	0.167609	-3.328413	0.000000
1	-2.129433	-2.008156	0.000000
6	-0.067360	2.221842	0.000000
7	-0.067360	3.372447	0.000000

E = -339.6096646 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8995891 au

6	1.009099	-0.102965	0.000000
1	0.154699	-3.307797	0.000000
1	-2.134882	-2.011825	0.000000
6	-0.060915	2.198029	0.000000
7	-0.060915	3.348565	0.000000

E = -339.6079255 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9007947 au

3-cyano-2,4-didehydropyridinium cation (18)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.10 A

1	2.042102	-1.837536	0.000000
7	1.117677	-1.409893	0.000000
6	0.008421	-2.206522	0.000000
6	-1.182796	-1.512729	0.000000
6	-1.047824	-0.153924	0.000000
6	-0.043737	0.754991	0.000000
6	1.051350	-0.095018	0.000000
1	0.133491	-3.280898	0.000000
1	-2.143245	-2.010737	0.000000
6	-0.043737	2.171128	0.000000
7	-0.043737	3.321553	0.000000

E = -339.6075584 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9015617 au

3-cyano-2,4-didehydropyridinium cation (18)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.20 A

1	2.039626	-1.856139	0.000000
7	1.127275	-1.403033	0.000000
6	0.003932	-2.178139	0.000000
6	-1.197344	-1.497666	0.000000
6	-1.104687	-0.133868	0.000000
6	-0.036359	0.728060	0.000000
6	1.094770	-0.084982	0.000000
1	0.124022	-3.252812	0.000000
1	-2.143777	-2.022333	0.000000
6	-0.036359	2.146058	0.000000
7	-0.036359	3.296533	0.000000

E = -339.6068588 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9008096 au

3-cyano-2,4-didehydropyridinium cation (18)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation = 2.30 A

1	2.041551	-1.872723	0.000000
7	1.141692	-1.395016	0.000000
6	0.004029	-2.150042	0.000000
6	-1.210351	-1.486494	0.000000
6	-1.160337	-0.118251	0.000000
6	-0.034180	0.703431	0.000000
6	1.139241	-0.074198	0.000000
1	0.120389	-3.224959	0.000000
1	-2.139854	-2.040936	0.000000
6	-0.034180	2.123275	0.000000
7	-0.034180	3.273915	0.000000

E = -339.6035183 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8979710 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	-2.137555	-1.460058	0.000000
7	-1.311973	-0.879224	0.000000
6	0.029221	-1.319995	0.000000
6	0.891125	-0.237129	0.000000
6	0.000000	0.878337	0.000000
6	-1.023363	1.776094	0.000000
6	-1.225513	0.444611	0.000000
1	0.268433	-2.371214	0.000000
8	2.221449	-0.324505	0.000000
1	-1.394906	2.790210	0.000000
1	2.647426	0.540156	0.000000

E = -322.6084558 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9477640 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	-2.052440	-1.573561	0.000000
7	-1.265973	-0.937925	0.000000
6	0.086698	-1.311646	0.000000
6	0.898590	-0.189032	0.000000
6	0.000000	0.908176	0.000000
6	-1.093055	1.714291	0.000000
6	-1.297250	0.381732	0.000000
1	0.376359	-2.350711	0.000000
8	2.231463	-0.235449	0.000000
1	-1.513978	2.709889	0.000000
1	2.630265	0.642329	0.000000

E = -322.6210064 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9614584 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	1.959991	-1.680021	0.000000
7	1.168419	-1.048066	0.000000
6	1.263328	0.343273	0.000000
6	0.000000	0.913787	0.000000
6	-0.926498	-0.148644	0.000000
6	-1.446996	-1.396741	0.000000
6	-0.098481	-1.399398	0.000000
1	2.223410	0.836301	0.000000
8	-0.203913	2.232170	0.000000
1	-2.337791	-2.009835	0.000000
1	-1.141357	2.458991	0.000000

E = -322.6218128 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9628571 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

1	1.956077	-1.673682	0.000000
7	1.156346	-1.049719	0.000000
6	1.260089	0.332168	0.000000
6	0.000000	0.909782	0.000000
6	-0.960920	-0.111306	0.000000

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	1.949627	-1.668963	0.000000
7	1.141964	-1.053423	0.000000
6	1.254980	0.319615	0.000000
6	0.000000	0.907978	0.000000
6	-0.992096	-0.073998	0.000000

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.80 A

1	1.940578	-1.668656	0.000000
7	1.125493	-1.061574	0.000000
6	1.247291	0.303886	0.000000
6	0.000000	0.909133	0.000000
6	-1.021556	-0.035171	0.000000

6	-1.438132	-1.368147	0.000000	6	-1.428089	-1.337577	0.000000	6	-1.418648	-1.305947	0.000000
6	-0.090806	-1.454027	0.000000	6	-0.084713	-1.511585	0.000000	6	-0.081535	-1.570215	0.000000
1	2.223207	0.820525	0.000000	1	2.221437	0.802515	0.000000	1	2.217498	0.780238	0.000000
8	-0.181097	2.231692	0.000000	8	-0.156892	2.232954	0.000000	8	-0.127598	2.237016	0.000000
1	-2.331367	-1.977588	0.000000	1	-2.323623	-1.942583	0.000000	1	-2.317435	-1.904368	0.000000
1	-1.114943	2.474417	0.000000	1	-1.086556	2.492751	0.000000	1	-1.051621	2.517556	0.000000

E = -322.6183108 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9599266 au

E = -322.6144985 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9571311 au

E = -322.6117374 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9561337 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.90 A

1	1.929650	-1.673756	0.000000	1	1.915936	-1.685507	0.000000	1	-1.900924	-1.705697	0.000000
7	1.107234	-1.075531	0.000000	7	1.087633	-1.095126	0.000000	7	-1.067137	-1.123143	0.000000
6	1.236789	0.284000	0.000000	6	1.221993	0.259469	0.000000	6	-1.202813	0.228533	0.000000
6	0.000000	0.913166	0.000000	6	0.000000	0.917918	0.000000	6	0.000000	0.923614	0.000000
6	-1.050819	0.006603	0.000000	6	-1.084910	0.055021	0.000000	6	1.123276	0.111116	0.000000
6	-1.410918	-1.273642	0.000000	6	-1.396469	-1.242935	0.000000	6	1.381780	-1.209327	0.000000
6	-0.082369	-1.628054	0.000000	6	-0.089505	-1.679675	0.000000	6	0.104105	-1.724991	0.000000
1	2.211017	0.752981	0.000000	1	2.201209	0.717844	0.000000	1	-2.187793	0.673858	0.000000
8	-0.090807	2.243699	0.000000	8	-0.046816	2.250265	0.000000	8	-0.008849	2.256172	0.000000
1	-2.314221	-1.863271	0.000000	1	-2.310227	-1.814668	0.000000	1	2.308825	-1.759107	0.000000
1	-1.006724	2.550729	0.000000	1	-0.952474	2.587301	0.000000	1	0.882556	2.629900	0.000000

E = -322.6097517 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9566974 au

E = -322.6083842 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9577455 au

E = -322.6093783 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9580747 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-1.886432	-1.729862	0.000000
7	-1.046436	-1.156163	0.000000
6	-1.181462	0.194494	0.000000
6	0.000000	0.931016	0.000000
6	1.160795	0.170954	0.000000
6	1.373019	-1.172387	0.000000
6	0.122385	-1.768558	0.000000
1	-2.171919	0.627294	0.000000
8	-0.072217	2.261052	0.000000
1	2.312065	-1.702381	0.000000
1	0.800647	2.676555	0.000000

E = -322.6096494 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9569939 au

5-hydroxy-2,4-didehydropyridinium cation (19)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-1.873214	-1.754341	0.000000
7	-1.026432	-1.190468	0.000000
6	-1.159059	0.160659	0.000000
6	0.000000	0.939719	0.000000
6	1.196497	0.232543	0.000000
6	1.367777	-1.135110	0.000000
6	0.141388	-1.811165	0.000000
1	-2.154518	0.581764	0.000000
8	-0.137269	2.263802	0.000000
1	2.317662	-1.647073	0.000000
1	0.713627	2.722638	0.000000

E = -322.606942 au
RHF-UCCSD(T)/cc-pVTZ E = -321.9539188 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.30 A

1	-1.488454	-2.435762	0.000000
7	-0.886161	-1.623439	0.000000
6	-1.296410	-0.287172	0.000000
6	-0.200139	0.561789	0.000000
6	0.899282	-0.351533	0.000000
6	1.787982	-1.377449	0.000000
6	0.449611	-1.571285	0.000000
1	-2.345945	-0.033241	0.000000
1	2.797376	-1.764726	0.000000
6	-0.200139	1.976689	0.000000
7	-0.200139	3.127366	0.000000

E = -339.614329 au
RHF-UCCSD(T)/cc-pVTZ E = -338.8975577 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.40 A

1	-1.533724	-2.401941	0.000000
7	-0.904116	-1.608595	0.000000
6	-1.291395	-0.270593	0.000000
6	-0.182716	0.562381	0.000000

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.50 A

1	-1.568610	-2.370589	0.000000
7	-0.916565	-1.593593	0.000000
6	-1.286727	-0.257045	0.000000
6	-0.167743	0.561038	0.000000

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.60 A

1	-1.597879	-2.339605	0.000000
7	-0.925053	-1.578756	0.000000
6	-1.281196	-0.245168	0.000000
6	-0.153900	0.559671	0.000000

6	0.926912	-0.323658	0.000000	6	0.953856	-0.295106	0.000000	6	0.978847	-0.267487	0.000000
6	1.758171	-1.392655	0.000000	6	1.726698	-1.399045	0.000000	6	1.693144	-1.400422	0.000000
6	0.424594	-1.630439	0.000000	6	0.402333	-1.690034	0.000000	6	0.381415	-1.751763	0.000000
1	-2.337357	-0.000033	0.000000	1	-2.329622	0.027278	0.000000	1	-2.321319	0.051042	0.000000
1	2.761801	-1.796566	0.000000	1	2.724351	-1.818415	0.000000	1	2.685397	-1.832058	0.000000
6	-0.182716	1.979596	0.000000	6	-0.167743	1.980391	0.000000	6	-0.153900	1.980817	0.000000
7	-0.182716	3.130131	0.000000	7	-0.167743	3.130811	0.000000	7	-0.153900	3.131146	0.000000

E = -339.6250232 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9095602 au

E = -339.6241241 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9095602 au

E = -339.6191913 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9054163 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 1.70 A

1	-1.626655	-2.306937	0.000000	1	-1.659827	-2.271011	0.000000	1	-1.700600	-2.230575	0.000000
7	-0.931959	-1.564557	0.000000	7	-0.940951	-1.550909	0.000000	7	-0.954740	-1.537551	0.000000
6	-1.273533	-0.233784	0.000000	6	-1.262629	-0.220784	0.000000	6	-1.248118	-0.205116	0.000000
6	-0.139556	0.560345	0.000000	6	-0.122326	0.564059	0.000000	6	-0.100574	0.570592	0.000000
6	1.001487	-0.242253	0.000000	6	1.023652	-0.220655	0.000000	6	1.047455	-0.203007	0.000000
6	1.657342	-1.401015	0.000000	6	1.618062	-1.406227	0.000000	6	1.574385	-1.418936	0.000000
6	0.359537	-1.816388	0.000000	6	0.332472	-1.882663	0.000000	6	0.297106	-1.948566	0.000000
1	-2.310606	0.074565	0.000000	1	-2.295692	0.101959	0.000000	1	-2.275395	0.136412	0.000000
1	2.643552	-1.844694	0.000000	1	2.597031	-1.863304	0.000000	1	2.545104	-1.890823	0.000000
6	-0.139556	1.982742	0.000000	6	-0.122326	1.987283	0.000000	6	-0.100574	1.994342	0.000000
7	-0.139556	3.133012	0.000000	7	-0.122326	3.137520	0.000000	7	-0.100574	3.144569	0.000000

E = -339.6142507 au

E = -339.6106535 au

E = -339.6080717 au

RHF-UCCSD(T)/cc-pVTZ E = -338.9016691 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.00 A

1	-1.751875	-2.183342	0.000000
7	-0.976823	-1.522656	0.000000
6	-1.228752	-0.185668	0.000000
6	-0.071726	0.577450	0.000000
6	1.080074	-0.186709	0.000000
6	1.517689	-1.445130	0.000000
6	0.251004	-2.006776	0.000000
1	-2.247705	0.179634	0.000000
1	2.480039	-1.932011	0.000000
6	-0.071726	2.001823	0.000000
7	-0.071726	3.152053	0.000000

E = -339.6058798 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9004876 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.30 A

1	-1.960243	-1.999992	0.000000
7	-1.087631	-1.474518	0.000000
6	-1.149622	-0.117845	0.000000

RHF-UCCSD(T)/cc-pVTZ E = -338.8999170 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.10 A

1	-1.816482	-2.128193	0.000000
7	-1.009547	-1.506872	0.000000
6	-1.204092	-0.163063	0.000000
6	-0.035094	0.583149	0.000000
6	1.123256	-0.172775	0.000000
6	1.448109	-1.480234	0.000000
6	0.192814	-2.055400	0.000000
1	-2.211616	0.231488	0.000000
1	2.401193	-1.984623	0.000000
6	-0.035094	2.008278	0.000000
7	-0.035094	3.158530	0.000000

E = -339.6058557 au
RHF-UCCSD(T)/cc-pVTZ E = -338.9005914 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8998487 au

5-cyano-2,4-didehydropyridinium cation (20)
UB3LYP/cc-pVTZ
1A' singlet state (Cs)
dehydrocarbon atom separation = 2.20 A

1	-1.886984	-2.067263	0.000000
7	-1.046844	-1.491522	0.000000
6	-1.177374	-0.140516	0.000000
6	0.004612	0.589522	0.000000
6	1.166255	-0.164747	0.000000
6	1.380737	-1.511633	0.000000
6	0.126742	-2.103668	0.000000
1	-2.171188	0.286729	0.000000
1	2.320292	-2.041451	0.000000
6	0.004612	2.015136	0.000000
7	0.004612	3.165438	0.000000

E = -339.605298 au
RHF-UCCSD(T)/cc-pVTZ E = -338.8994060 au

6	0.047013	0.595681	0.000000
6	1.209309	-0.161706	0.000000
6	1.314935	-1.541826	0.000000
6	0.053655	-2.150289	0.000000
1	-2.127379	0.344630	0.000000
1	2.238124	-2.100855	0.000000
6	0.047013	2.021628	0.000000
7	0.047013	3.171997	0.000000

E = -339.6018843 au

RHF-UCCSD(T)/cc-pVTZ E = -338.8964387 au