STUDIES ON THE INTRAMOLECULAR CYCLIZATIONS OF BICYCLIC δ -HYDROXYNITRILES PROMOTED BY TRIFLIC ANHYDRIDE

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Supporting Information

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Experimental Section

General Methods

Melting points were determined on a capillary melting point apparatus and are uncorrected. IR spectra were determined on an FT-IR spectrometer. ^1H and ^{13}C NMR spectra were recorded at 200 and 50.0 MHz or 300 and 75.5 MHz, respectively in CDCl_3 solutions with Me_4Si as internal standard. High-resolution mass spectra were recorded using DEI unless otherwise noted.

Column chromatography was performed on silica gel 60 H, slurry packed, run under low pressure of nitrogen and employing increasing amounts of EtOAc in hexane as solvent. Analytical TLC was carried out using GF₂₅₄ silica gel plates with thickness 0.20 mm and visualization was effected with short wavelength UV light (254 nm) and a p-anisaldehyde solution (2.5 mL of p-anisaldehyde + 2.5 mL of H_2SO_4 + 0.25 mL of AcOH + 95 mL of EtOH). Reactions were routinely run under a dry nitrogen atmosphere with magnetic stirring. All reagents were used directly as purchased or purified according to standard procedures. Freshly distilled triflic anhydride was used in all reactions studied.

6-Oxo-5-phenyl-6,7,8,8a-tetrahydro-fluorene-8a-carboxylic acid methyl ester (16).

Alcohol **12** was prepared following the procedure used for **11** by replacing ethyl bromide with benzyl bromide and changing the reaction conditions to $-30\text{ }^\circ\text{C}$ to rt, further stirring at rt for 24 h. Alcohol **12** was obtained as a foam (213.4 mg, 78%). **12**: ^1H NMR (200 MHz) δ : 7.30-7.10 (m, 6 H), 6.80-6.70 (m, 2 H), 6.37 (d, $J = 7.5$ Hz, 1 H), 3.87 (s, 3 H), 3.48 (d, $J = 16.7$ Hz, 1 H), 3.00-2.70 (m, 3 H), 2.65-2.00 (m, 4 H), 1.90-1.70 (m, 1 H); ^{13}C NMR (50 MHz) δ : 173.8 (CO), 142.4 (C), 136.8 (C), 135.1 (C), 130.6 (d x 2), 128.2 (CH), 127.2 (d x 2), 126.4 (CH), 126.0 (CH), 124.7 (CH), 124.4 (CH), 119.0 (CN), 85.8 (C), 62.4 (C), 52.0 (CH_3), 43.9 (CH_2), 35.1 (CH_2), 28.6 (CH_2), 13.2 (CH_2). Enone **16** was obtained following the procedure used for **15** by changing the reaction conditions from 24 h at room temperature to 3 h at room temperature and then 24 h at $40\text{ }^\circ\text{C}$ and using a 2:1 molar ratio for Tf_2O to **12**. Enone **16** (77.8 mg, 65%) was obtained as a crystalline solid. **16**: mp $151.2\text{-}151.9^\circ\text{C}$; IR (film) ν_{max} : 1662 cm^{-1} ; ^1H NMR (300

MHz) δ : 7.50-7.35 (m, 3 H), 7.30-7.10 (m, 4 H), 6.95-6.85 (m, 1 H), 6.41 (d, $J = 7.9$ Hz, 1 H), 3.68 (s, 3 H), 3.59 (d, $J = 16.5$ Hz, 1 H), 3.12 (d, $J = 16.5$ Hz, 1 H), 2.87-2.73 (m, 1 H), 2.70-2.60 (m, 2 H), 2.42-2.28 (m, 1 H); ^{13}C NMR (75.5 MHz) δ : 197.3 (s, CO), 174.4 (CO), 158.4 (C), 145.9 (C), 138.1 (C), 134.7 (C), 133.9 (C), 130.8 (CH), 128.6 (d x 4), 127.8 (CH), 126.9 (CH), 126.5 (CH), 124.8 (CH), 55.3 (C), 52.8 (CH₃), 42.9 (CH₂), 35.1 (CH₂), 32.6 (CH₂); HRMS calcd for C₂₁H₁₈O₃ (M⁺): 318.1256, found: 318.1255.

6-Oxo-6,7,8,8a,9,10-hexahydro-phenanthrene-8a-carboxylic acid methyl ester (17). To a stirred suspension of NaH (684 mg, 42% in mineral oil, 11.97 mmol) in 1.2 mL dimethyl carbonate was added dropwise a solution of 1-tetralone (500 mg, 3.42 mmol) in 8 mL of dimethyl carbonate. The mixture was refluxed at 80 °C for 3.5 h. After cooling to rt, H₂O (15 mL) was added. The mixture was then acidified with an aqueous solution of HCl 6N. The aqueous phase was separated and extracted with Et₂O. The combined organic extracts were washed with brine, dried (Na₂SO₄) and concentrated under reduced pressure. The crude oil (684 mg) thus obtained was subjected to chromatography to yield **6** (645g, 92 %). **6**: ^1H NMR (200 MHz) δ : 12.38 (s, 1 H, OH enol), 8.04 (d, $J = 8.6$ Hz, 0.6 H, ketone), 7.80 (dd, $J = 6.7, 2.2$ Hz, 1 H, enol), 7.53-7.45 (m, 0.6 H, ketone), 7.36-7.14 (m, 4.2 H, enol and ketone), 3.82 (s, 3 H, CO₂CH₃ enol), 3.78 (s, 1.8 H, CO₂CH₃ ketone), 3.62 (dd, $J = 10, 5.1$ Hz, 0.6 H, ketone), 3.1-2.95 (m, 1.2 H ketone), 2.90-2.75 (m, 2 H enol), 2.65-2.30 (m, 3.2 H, enol and ketone); ^{13}C NMR (50 MHz) δ : 192.8 (CO, ketone), 172.8 (CO, ester enol), 170.4 (CO ester ketone), 164.8 (C, enol), 143.4 (C, ketone), 139.1 (C, enol), 133.6 (CH, ketone), 131.5 (C, ketone), 130.3 (CH, enol), 129.7 (C, enol), 128.6 (CH, ketone), 127.4 (CH, ketone), 127.2 (CH, enol), 126.6 (CH, ketone), 126.3 (CH, enol), 124.1 (CH, enol), 96.6 (C, enol), 54.2 (CH, ketone), 52.0 (CH₃, ketone), 51.3 (CH₃, enol), 27.5 (CH₂, enol), 27.4 (CH₂, ketone), 26.1 (CH₂, ketone), 20.3 (CH₂, enol). To a solution of **6** (300 mg, 1.46 mmol) in EtOH (3 mL) an aqueous solution of NaOH 1 N (0.15 mL) was added followed by the slow addition (30 min) of a solution of acrylonitrile (0.16 mL, 2.47 mmol) in EtOH (0.5 mL). After 4 h part of the EtOH was evaporated and the

mixture was poured into brine and extracted with Et₂O. The combined organic extracts were washed with 0.6 N aqueous HCl and brine, dried (Na₂SO₄) and concentrated. The residue (374 mg) was chromatographed yielding **9** (298 mg, 79 %) as a crystalline solid. **9**: mp 76.7-77.3°C; ¹H NMR (200 MHz) δ: 8.05 (d, *J* = 7.9 Hz, 1 H), 7.60-7.45 (m, 1 H), 7.40-7.15 (m, 2 H), 3.70 (s, 3 H), 3.15-2.85 (m, 2 H), 2.80-2.05 (m, 6 H); ¹³C NMR (50 MHz) δ: 194.4 (CO), 171.2 (CO), 142.5 (C), 133.8 (CH), 131.5 (C), 128.7 (CH), 128.0 (CH), 126.9 (CH), 119.2 (CN), 56.2 (C), 52.6 (CH₃), 31.5 (CH₂), 30.1 (CH₂), 25.7 (CH₂), 13.2 (CH₂). Alcohol **13** was prepared following the procedure used for **11** by replacing ethyl bromide with methyl iodide and by changing the reaction conditions to 1 h to prepare the Grignard reagent, then -30 °C to rt and further stirring for 3h at rt. The starting ketone had to be dissolved in THF because its solubility in Et₂O was low. Alcohol **13** (116 mg, 54%) was obtained as an oil. **13**: ¹H NMR (200 MHz) δ: 7.66 (dd, *J* = 7.1, 1.9 Hz, 1 H), 7.30-7.00 (m, 3 H), 3.85 (s, 3 H), 3.44 (s, 1 H, OH), 3.00-2.70 (m, 2 H), 2.68-2.45 (m, 1 H), 2.40-2.10 (m, 4 H), 1.90-1.70 (m, 1 H), 1.44 (s, 3 H); ¹³C NMR (50 MHz) δ: 175.8 (CO), 140.5 (C), 132.3 (C), 128.0 (CH), 127.0 (CH), 126.6 (CH), 126.3 (CH), 118.8 (CN), 74.4 (C), 52.3 (CH₃), 52.1 (C), 31.0 (CH₃), 26.0 (CH₂), 24.2 (CH₂), 23.3 (CH₂), 13.2 (CH₂). Enone **17** was obtained following the procedure used for **15** by changing the reaction conditions from 24 h to 4.5 h at room temperature. **17** (53 mg, 79 %) was obtained as a crystalline solid. **17**: mp 141.0-141.4°C; IR (film) ν_{max}: 1654 cm⁻¹; ¹H NMR (300 MHz) δ: 7.78 (dd, *J* = 7.9, 0.9 Hz, 1 H), 7.40-7.12 (m, 3 H), 6.69 (s, 1 H), 3.65 (s, 3 H), 2.88 (dd, *J* = 8.8, 3.2 Hz, 2 H), 2.60-2.40 (m, 4 H), 2.20-2.00 (m, 1 H), 1.95-1.80 (m, 1 H); ¹³C NMR (75.5 MHz) δ: 198.9 (CO), 173.6 (CO), 154.6 (C), 138.1 (C), 131.2 (C), 130.5 (CH), 129.4 (CH), 126.7 (CH), 125.5 (CH), 122.1 (CH), 52.5 (CH₃), 47.7 (C), 34.8 (CH₂), 34.6 (CH₂), 34.4 (CH₂), 26.9 (CH₂); HRMS calcd for C₁₆H₁₆O₃ (M⁺): 256.1099, found: 256.1092.

2-Imino-11b-methyl-2,3,4,4a,5,6,7,11b-octahydro-1-oxa-dibenzo[a,c]cycloheptene-4a-carboxylic acid methyl ester (18), 11b-Methyl-2-trifluoromethanesulfonylimino-2,3,4,4a,5,6,7,11b-octahydro-1-oxa-dibenzo[a,c]cycloheptene-4a-carboxylic acid methyl

ester (20), 11b-Methyl-2-oxo-2,3,4,4a,5,6,7,11b-octahydro-1-oxa-dibenzo[a,c]cycloheptene-4a-carboxylic acid methyl ester (19) and 6-(2-Cyano-ethyl)-5-methylene-6,7,8,9-tetrahydro-5H-benzocycloheptene-6-carboxylic acid methyl ester (21). To a stirred suspension of NaH (1.2 g, 42% in mineral oil, 21.84 mmol) in 3 mL dimethyl carbonate was added dropwise a solution of 1-benzosuberone (1 g, 6.24 mmol) in 6 mL of dimethyl carbonate. The mixture was refluxed at 80 °C for 3 h. After cooling to rt, H₂O (20 mL) was added. The mixture was then acidified with an aqueous solution of HCl 6N. The aqueous phase was separated and extracted with Et₂O. The combined organic extracts were washed with brine, dried (Na₂SO₄) and concentrated under reduced pressure. The crude oil (1.5 g) thus obtained was subjected to chromatography to yield **7** (1.125g, 82 %). **7**: ¹H NMR (200 MHz) δ: 12.59 (s, 1 H, enol), 7.75 (dd, *J* = 7.5, 1.3 Hz, 0.26 H, ketone), 7.70-7.55 (m, 1 H, enol), 7.45-7.15 (m, 3.78 H, enol and ketone), 3.83 (s, 3 H, enol), 3.75 (s, 0.78 H, ketone), 2.75-2.55 (m, 2.26 H, enol and ketone), 2.25-1.90 (m, 5.56 H, enol and ketone); ¹³C NMR (50 MHz) δ: 200.2 (CO, ketone), 173.2 (CO, enol), 170.5 (CO, ketone), 170.3 (CO enol), 141.0 (C, ketone), 140.9 (C, enol), 137.8 (C, ketone), 135.5 (C, enol), 132.2 (CH, ketone), 129.9 (CH, enol), 129.7 (CH, ketone), 128.9 (CH, ketone), 128.7 (CH, enol), 127.0 (CH, enol), 126.5 (CH, ketone), 126.1 (CH, enol), 100.0 (C, enol), 56.4 (CH, ketone), 52.0 (CH₃, ketone), 51.4 (CH₃, enol), 33.3 (CH₂, enol), 32.6 (CH₂, ketone), 31.6 (CH₂, enol), 25.2 (CH₂, ketone), 24.1 (CH₂, ketone), 21.6 (CH₂, enol). To a solution of **7** (1.125g, 5.13 mmol) in EtOH (10 mL) an aqueous solution of NaOH 1N (0.53 mL) was added followed by the slow addition (30 min) of a solution of acrylonitrile (0.56 mL, 8.69 mmol) in EtOH (1.7 mL). After 7 h part of the EtOH was evaporated and the mixture was poured into brine and extracted with Et₂O. The combined organic extracts were washed with 0.6 N aqueous HCl and brine, dried (Na₂SO₄) and evaporated. The residue (1.165 mg) was chromatographed yielding **10** (1.075 mg, 77 %) as an oil. **10**: ¹H NMR (200 MHz) δ: 7.50-7.20 (m, 3 H), 7.14 (d, *J* = 7.5 Hz, 1 H), 3.61 (s, 3 H), 3.05-2.70 (m, 2 H), 2.60-1.70 (m, 8 H); ¹³C NMR (50 MHz) δ: 203.3 (CO), 171.4 (CO), 139.3 (C), 138.2 (C), 131.3 (CH), 129.0 (CH), 128.8

(CH), 126.4 (CH), 119.0 (CN), 60.6 (C), 52.3 (CH₃), 32.7 (CH₂), 32.6 (CH₂), 31.7 (CH₂), 23.4 (CH₂), 12.9 (CH₂). Alcohol **14** was prepared following the procedure used for **11** by replacing ethyl bromide with methyl iodide and by changing the reaction conditions to 1 h to prepare the Grignard reagent, then -40 °C to rt and further stirring for 5.5 h at rt. Alcohol **14** (420 mg, 61%) was obtained as a crystalline solid. **14**: mp 103.3-103.8 °C; ¹H NMR (300 MHz) δ: 7.79 (dd, *J* = 7.5, 1.5 Hz, 1 H), 7.30-7.05 (m, 3 H), 3.80 (s, 3 H), 3.43 (s, 1 H, OH), 3.13 (dt, *J* = 14.3, 1.9 Hz, 1 H), 2.77 (dd, *J* = 14.9, 4.7 Hz, 1 H), 2.50-2.15 (m, 3 H), 2.10-1.85 (m, 3 H), 1.78 (s, 3 H), 1.70-1.50 (m, 2 H); ¹³C NMR (50 MHz) δ: 175.6 (CO), 144.0 (C), 137.3 (C), 130.9 (CH), 127.2 (CH), 126.5 (CH), 125.4 (CH), 119.6 (CN), 78.5 (C), 54.8 (C), 52.0 (CH₃), 36.4 (CH₂), 32.6 (CH₂), 27.6 (CH₂), 25.7 (CH₃), 22.4 (CH₂), 13.2 (CH₂). To a solution of Tf₂O (0.12 mL, 0.71 mmol) in CH₂Cl₂ (2.5 mL) at room temperature a solution of **14** (205 mg, 0.71 mmol) in CH₂Cl₂ (3 mL) was added dropwise. After 3 h a saturated aqueous solution of NaHCO₃ (6 mL) added and the stirring was continued for further 30 min. The mixture was then extracted with Et₂O. The combined organic extracts were washed with brine, dried (Na₂SO₄) and evaporated. The residue (199 mg) was chromatographed to yield alkene **21** (25 mg, 13%). **21**: IR (film) ν_{max}: 2247, 1729 cm⁻¹; ¹H NMR (200 MHz) δ: 7.30-7.15 (m, 2 H), 7.15-7.00 (m, 2 H), 5.20 (s, 1 H), 5.16 (s, 1 H), 3.69 (s, 3 H), 2.90-2.60 (m, 2 H), 2.45-1.55 (m, 8 H); ¹³C NMR (75.5 MHz) δ: 174.3 (CO), 151.7 (C), 141.1 (C), 138.6 (C), 129.3 (CH), 128.11 (CH), 128.08 (CH), 126.5 (CH), 119.6 (CN), 116.0 (CH₂), 52.5 (C), 52.1 (CH₃), 34.4 (CH₂), 33.4 (CH₂), 32.3 (CH₂), 22.9 (CH₂), 13.2 (CH₂); N-((trifluoromethyl)sulfonyl)imidate **20** (47.5 mg, 16 %). **20**: IR (film) ν_{max}: 1733 and 1596 cm⁻¹; ¹H NMR (300 MHz) δ: 7.35-7.15 (m, 4 H), 3.80 (s, 3 H), 3.10-2.80 (m, 3 H), 2.69 (dt, *J* = 14.2, 3.1 Hz, 1 H), 2.45-2.30 (m, 1 H), 1.95-1.85 (m, 3 H), 1.94 (s, 3 H), 1.80-1.55 (m, 2 H); ¹³C NMR (75.5 MHz) δ: 177.6 (CO), 173.6 (C=N), 140.4 (C), 137.3 (C), 132.0 (CH), 128.7 (CH), 127.8 (CH), 124.5 (CH), 118.9 (*J*_{C-F} = 319.3 Hz, q, CF₃), 93.9 (C), 52.9 (CH₃), 51.4 (C), 36.9 (CH₂), 34.3 (CH₂), 27.8 (CH₂), 23.6 (CH₃), 22.5 (CH₂), 21.8 (CH₂); FABHRMS calcd for C₁₈H₂₀F₃NO₅SN⁺: 442.09119, found: 442.091341; lactone **19** (22.4 mg, 11%). **19**: IR

(film) ν_{max} : 1742, 1729 cm^{-1} ; ^1H NMR (300 MHz) δ : 7.45-7.35 (m, 1 H), 7.30-7.10 (m, 3 H), 3.77 (s, 3 H), 3.15-2.55 (m, 4 H), 2.30-2.10 (m, 1 H), 2.00-1.75 (m, 5 H), 1.84 (s, 3 H); ^{13}C NMR (75.5 MHz) δ : 174.6 (CO), 172.9 (CO), 142.9 (C), 137.5 (C), 131.7 (CH), 128.0 (CH), 127.3 (CH), 125.0 (CH), 88.6 (C), 52.3 (CH_3), 51.7 (C), 37.1 (CH_2), 34.6 (CH_2), 28.2 (CH_2), 23.9 (CH_3), 22.9 (CH_2), 22.6 (CH_2); HRMS calcd for $\text{C}_{17}\text{H}_{20}\text{O}_4$ (M^+): 288.1362, found: 288.1360; imidate **18** (77 mg, 40%). **18**: IR (film) ν_{max} : 1725 and 1660 cm^{-1} ; ^1H NMR (300 MHz) δ : 7.50-7.35 (m, 1 H), 7.25-7.05 (m, 3 H), 3.74 (s, 3H), 3.10-2.95 (m, 1 H), 2.88-2.70 (m, 2 H), 2.57 (dt, $J = 14.1, 3.3$ Hz, 1 H), 2.26 (ddd, $J = 8.1, 7.5, 2.5$ Hz, 1 H), 2.00-1.55 (m, 5 H), 1.81 (s, 3 H); ^{13}C NMR (75.5 MHz) δ : 175.0 (CO), 167.9 (C=N), 143.9 (C), 137.5 (C), 131.4 (CH), 127.7 (CH), 127.1 (CH), 125.4 (CH), 86.9 (C), 52.0 (C), 51.9 (CH_3), 37.1 (CH_2), 35.0 (CH_2), 25.8 (CH_2), 24.0 (CH_3), 22.7 ($\text{CH}_2 \times 2$).

Table S1. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of protonated triflates **22**, **23** and **24** (step 1, path a, Scheme 3 and Figure 3).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
22	87.70	87.14	89.51	9.99
23	91.82	91.30	93.65	14.13
24	96.31	95.94	98.10	17.66

Table S2. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of triflates **25**, **26** and **27** (step 2, path a, Scheme 3 and Figure 3).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
25	-95.81	-94.96	-97.89	-23.03
26	-97.97	-97.24	-99.51	-26.62
27	-101.75	-101.21	-102.87	-29.37

Table S3. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of carbocations **28**, **29** and **30** (step 3, path a, Scheme 3 and Figure 3).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
28	96.25	96.33	82.70	14.44
29	96.58	96.62	83.14	15.94
30	99.12	99.17	85.63	19.06

Table S4. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of alkenes **4**, **31** and **21** (step 4, path a, Scheme 3 and Figure 3).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
4	-86.81	-86.81	-86.95	-11.18
31	-86.12	-85.95	-86.63	-11.28
21	-90.99	-90.70	-91.87	-16.18

Table S5. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of compounds **35**, **36** and **37** (step 6, path a, Scheme 3 and Figure 6).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
35	-21.02	-21.97	-19.95	-18.02
36	-18.50	-19.43	-17.49	-16.25
37	-18.36	-19.14	-17.54	-13.52

Table S6. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the cyclization of compounds **39**, **40** and **41** (step 2', path b, Scheme 3 and Figure 7).

Compnd	ΔE_0	ΔH	ΔG	ΔG_{Sol}
39	-4.14	-5.17	-2.57	1.82
40	-8.82	-9.74	-7.38	-3.53
41	-11.39	-12.38	-9.89	-7.85

Table S7. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of protonated alcohols **49**, **50** and **51** (Figure 8).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
49	96.80	96.23	98.06	18.31
50	92.82	92.33	93.90	14.50
51	91.43	90.90	92.55	13.22

Table S8. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of protonated nitriles **39**, **40** and **41** from protonated alcohols **49**, **50** and **51** (Figure 8).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
49	5.72	6.20	4.81	2.89
50	9.10	9.43	8.58	7.05
51	12.87	13.21	12.17	11.16

Table S9. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of intermediates **52**, **53** and **54** (Figure 10).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
52	-38.88	-38.72	-39.63	-45.08
53	-30.94	-30.62	-31.92	-37.03
54	-30.59	-30.33	-31.18	-34.13

Table S10. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of carbocations **55**, **56** and **57** (Figure 10).

	ΔE_0	ΔH	ΔG	ΔG_{Sol}
55	6.76	7.76	4.15	14.14
56	8.10	8.96	6.15	13.44
57	15.29	16.03	14.14	19.98

Table S11. B3LYP/6-31G* $\Delta E_0^{\#}$, $\Delta H^{\#}$, $\Delta G^{\#}$ and $\Delta G_{\text{Sol}}^{\#}$ (in kcal mol⁻¹) for the formation of protonated lactams **58**, **59** and **60** (Figure 10).

	$\Delta E_0^{\#}$	$\Delta H^{\#}$	$\Delta G^{\#}$	$\Delta G_{\text{Sol}}^{\#}$
58	18.11	18.10	17.85	20.47
59	17.50	17.40	17.51	19.18
60	26.15	26.27	25.46	27.78

Table S12. B3LYP/6-31G* ΔE_0 , ΔH , ΔG and ΔG_{Sol} (in kcal mol⁻¹) for the formation of protonated lactams **58**, **59** and **60** (Figure 10).

Compnd	ΔE_0	ΔH	ΔG	ΔG_{Sol}
58	7.99	7.78	8.59	9.20
59	3.45	3.05	4.30	4.76
60	5.64	5.37	6.16	6.99

δ-Hydroxynitrile 1

B3LYP/6-31G* Geometry

C	-3.614578	-0.462067	-1.075226
C	-2.322617	-0.389587	-1.608017
C	-3.813110	-0.792526	0.268921
C	-1.235962	-0.655533	-0.778519
C	-2.722366	-1.065857	1.100845
C	-1.441620	-0.995117	0.563110
C	0.246674	-0.627075	-1.094391
C	0.890686	-0.485062	0.313065
C	-0.119446	-1.303619	1.238281
C	0.894974	0.998489	0.787415
C	2.296219	-1.032623	0.498444
C	0.132736	-2.826263	1.195633
O	-0.119415	-0.865921	2.586884
C	1.705154	2.002609	-0.065353
O	2.788345	-1.190964	1.602753
O	2.932800	-1.307983	-0.649048
C	3.162064	1.831741	-0.021866
C	4.307785	-1.729156	-0.517624
N	4.316345	1.710327	0.008209
H	-4.470810	-0.249664	-1.710022
H	-2.173828	-0.119400	-2.651000
H	-4.822006	-0.832077	0.670990
H	-2.865250	-1.314362	2.148575
H	0.525482	0.175110	-1.785294
H	0.571823	-1.560333	-1.569870
H	-0.140457	1.351913	0.798996
H	1.249786	1.036774	1.818542
H	0.151016	-3.211624	0.170380
H	1.080795	-3.081284	1.679504
H	-0.676285	-3.329971	1.732788
H	0.768051	-1.071991	2.932190
H	1.393219	1.978485	-1.115814
H	1.484436	3.014984	0.295105
H	4.626953	-1.986938	-1.527390
H	4.903610	-0.903885	-0.121811
H	4.378738	-2.593170	0.146576

B3LYP/6-31G* Energy = -861.954038

B3LYP/6-31G* Free energy in solution = -862.252803

Number of imaginary frequencies = 0

δ-Hydroxynitrile 13

B3LYP/6-31G* Geometry

C	-4.080276	0.348068	-0.170029
C	-2.999481	0.912491	-0.839935
C	-3.8544	-0.647614	0.783539
C	-1.684433	0.495346	-0.585663
C	-2.555481	-1.074158	1.042465
C	-1.462204	-0.518753	0.360275
C	-0.539276	1.203247	-1.285904
C	-0.069382	-1.097092	0.62291
C	0.824646	0.517303	-1.131073
C	1.049973	-0.022263	0.296722
C	0.092209	-2.3824	-0.226105

O	-0.014465	-1.458435	2.000916
C	0.973389	1.101837	1.375961
C	2.408768	-0.715942	0.457703
C	1.885757	2.334106	1.174011
O	2.705475	-1.378586	1.440643
O	3.241608	-0.52832	-0.571762
C	3.323547	2.073074	1.310303
C	4.569916	-1.074356	-0.418411
N	4.461823	1.8732	1.422134
H	-5.090866	0.684906	-0.385513
H	-3.169113	1.698273	-1.573761
H	-4.68779	-1.089996	1.322876
H	-2.367493	-1.839798	1.787323
H	-0.481644	2.231125	-0.896759
H	-0.7668	1.314392	-2.353638
H	1.623672	1.211197	-1.408981
H	0.905624	-0.312195	-1.839569
H	1.061356	-2.859589	-0.0437
H	-0.689713	-3.08699	0.069839
H	-0.012741	-2.196548	-1.299057
H	0.909637	-1.733627	2.16272
H	-0.055878	1.470413	1.411865
H	1.172745	0.660309	2.353622
H	1.715942	2.801422	0.197037
H	1.617798	3.08699	1.925644
H	5.059555	-0.907898	-1.377716
H	5.090881	-0.541061	0.379623
H	4.517532	-2.139847	-0.185272

B3LYP/6-31G* Energy = -901.239611

B3LYP/6-31G* Free energy in solution = -901.566610

Number of imaginary frequencies = 0

δ-Hydroxynitrile 14

B3LYP/6-31G* Geometry

C	-3.966858	-0.262054	-1.803192
C	-2.976242	0.42952	-2.496017
C	-3.590271	-1.166	-0.815979
C	-1.609665	0.250031	-2.234238
C	-2.238007	-1.357635	-0.535294
C	-1.228882	-0.661835	-1.219391
C	-0.641479	1.064911	-3.074585
C	0.237732	-0.981766	-0.851868
C	0.316452	1.973297	-2.291763
C	1.044296	0.304855	-0.370193
C	0.915283	-1.724319	-2.028244
C	1.446335	1.258102	-1.541107
O	0.17955	-1.902481	0.244858
C	0.258469	1.133194	0.694
C	2.376312	-0.13649	0.279541
C	0.040314	0.453354	2.065857
O	2.772858	-1.280106	0.440628
O	3.102844	0.918472	0.689835
C	-0.611313	1.367142	3.009033
C	4.363937	0.614334	1.317337
N	-1.125488	2.10257	3.745819
H	-5.014923	-0.093719	-2.035858

H	-3.26561	1.135239	-3.271332
H	-4.339233	-1.724045	-0.260452
H	-1.9476	-2.070908	0.224213
H	-1.2341	1.6967	-3.745819
H	-0.054138	0.412735	-3.735153
H	-0.260361	2.60585	-1.606384
H	0.79483	2.658707	-3.00383
H	1.954025	-1.969147	-1.787857
H	0.369186	-2.658722	-2.185654
H	0.903595	-1.165771	-2.965012
H	2.0504	0.69458	-2.26358
H	2.109543	2.021591	-1.124786
H	1.106857	-2.150497	0.419144
H	0.798141	2.071335	0.857147
H	-0.71933	1.393448	0.283081
H	-0.563858	-0.450073	1.955612
H	0.994476	0.138092	2.506622
H	4.792679	1.5802	1.583267
H	4.209595	0.000839	2.20813
H	5.014923	0.079086	0.622086

B3LYP/6-31G* Energy = -940.513169
 B3LYP/6-31G* Free energy in solution = -940.868863
 Number of imaginary frequencies = 0

Protonated triflate 22
 B3LYP/6-31G* Geometry

C	-2.636765	1.359818	-3.625778
C	-1.295471	1.472794	-3.250534
C	-3.526108	0.57399	-2.882858
C	-0.860352	0.789368	-2.117203
C	-3.089127	-0.114212	-1.749725
C	-1.750229	0.009995	-1.380615
C	0.527969	0.705811	-1.536377
C	-1.050659	-0.675797	-0.228226
C	0.285034	0.212585	-0.071838
C	-0.803223	-2.16069	-0.508575
O	-1.982437	-0.495163	0.924835
C	0.000198	1.41777	0.890823
C	1.471252	-0.581711	0.454559
S	-1.993973	-1.403458	2.261612
C	1.075089	2.526627	0.983154
O	1.508667	-1.177139	1.586838
O	2.512268	-0.65242	-0.288025
O	-2.579971	-2.711655	2.058182
O	-0.669525	-1.284607	2.921982
C	-3.172943	-0.2977	3.233932
C	2.372192	2.036224	1.456741
C	3.741516	-1.298676	0.211884
F	-3.323898	-0.851563	4.423355
F	-2.630051	0.908676	3.3416
F	-4.32341	-0.237671	2.587387
N	3.378082	1.579834	1.813644
H	-2.994339	1.891006	-4.502655
H	-0.610413	2.083206	-3.832306
H	-4.565842	0.502884	-3.186752
H	-3.779556	-0.714752	-1.165359

H	1.134293	-0.018967	-2.090271
H	1.080231	1.648331	-1.568741
H	-0.190933	-2.253708	-1.411407
H	-0.296555	-2.685379	0.307434
H	-1.753265	-2.66507	-0.6976
H	-0.923279	1.883636	0.536987
H	-0.202789	1.048721	1.898193
H	1.220581	3.037064	0.025513
H	0.713364	3.288239	1.683807
H	0.647705	-1.162384	2.135132
H	4.405731	-1.29921	-0.64859
H	4.126831	-0.680283	1.023651
H	3.506454	-2.308762	0.545929

B3LYP/6-31G* Energy = -1747.85721
 B3LYP/6-31G* Free energy in solution = -1748.225107
 Number of imaginary frequencies = 0

Protonated triflate 23
 B3LYP/6-31G* Geometry

C	-1.884323	-0.056717	-3.636581
C	-0.848541	0.73999	-3.163803
C	-2.275665	-1.183456	-2.908127
C	-0.185867	0.439468	-1.965225
C	-1.626785	-1.4955	-1.720581
C	-0.578445	-0.692291	-1.234238
C	0.929932	1.336227	-1.488266
C	0.100342	-1.132843	0.066895
C	1.839935	0.637329	-0.482925
C	1.045258	-0.006912	0.68837
C	0.81955	-2.473343	-0.123444
O	-1.107361	-1.294785	0.976334
C	0.19223	1.056534	1.460388
C	2.061066	-0.627548	1.664093
S	-1.334671	-2.307388	2.200531
C	0.919891	2.355087	1.886765
O	1.792892	-1.153549	2.797943
O	3.291397	-0.607346	1.3078
C	-3.151947	-1.883286	2.470398
O	-1.191711	-3.704834	1.841354
O	-0.601227	-1.775177	3.379578
C	2.099075	2.102844	2.719269
C	4.342758	-1.061829	2.235992
F	-3.5533	-2.571457	3.524414
F	-3.823807	-2.239456	1.38797
F	-3.26207	-0.5813	2.686554
N	3.037674	1.827042	3.344376
H	-2.381836	0.194168	-4.568405
H	-0.535721	1.613541	-3.730209
H	-3.0831	-1.815826	-3.263763
H	-1.951309	-2.362854	-1.154938
H	0.510727	2.258377	-1.061905
H	1.537735	1.659958	-2.340317
H	2.577316	1.3376	-0.08197
H	2.414581	-0.138794	-0.997467
H	1.225067	-2.887375	0.804764
H	0.141586	-3.213837	-0.548584

H	1.641464	-2.332413	-0.831238
H	-0.642319	1.338043	0.813446
H	-0.257523	0.604294	2.346359
H	1.228607	2.950729	1.021469
H	0.214218	2.973328	2.453476
H	0.809448	-1.285416	3.056351
H	5.255219	-1.003235	1.648117
H	4.355957	-0.369019	3.078339
H	4.127396	-2.081833	2.553146

B3LYP/6-31G* Energy = -1787.136217
 B3LYP/6-31G* Free energy in solution = -1787.532323
 Number of imaginary frequencies = 0

Protonated triflate 24

B3LYP/6-31G* Geometry

C	0.53743	4.0934	0.43663
C	1.58757	3.556229	-0.303207
C	-0.540878	3.280212	0.763977
C	1.591644	2.22821	-0.752197
C	-0.564911	1.957169	0.327713
C	0.472046	1.411926	-0.445923
C	2.839645	1.759674	-1.478104
C	0.326202	-0.0269	-0.981918
C	3.530411	0.553436	-0.826355
C	1.452881	-1.036728	-0.41655
C	0.231461	-0.06842	-2.512421
C	2.84729	-0.798004	-1.064911
O	-0.932175	-0.608612	-0.395157
C	1.501495	-0.90802	1.145462
C	1.0383	-2.472961	-0.76062
S	-2.403549	-0.67569	-1.190613
C	2.621536	-1.676605	1.887543
O	-0.022659	-3.041122	-0.294769
O	1.784042	-3.16684	-1.527161
O	-2.835144	0.644073	-1.604782
O	-2.388321	-1.827271	-2.078583
C	-3.328156	-1.178726	0.371643
C	2.60025	-3.119675	1.63353
C	1.480606	-4.590088	-1.787613
F	-4.538895	-1.562363	0.018448
F	-2.667984	-2.204514	0.936493
F	-3.38179	-0.161591	1.21756
N	2.540222	-4.246628	1.361435
H	0.571976	5.129105	0.760132
H	2.442429	4.18306	-0.541046
H	-1.368744	3.663742	1.35199
H	-1.414246	1.350845	0.600891
H	2.644104	1.543198	-2.536667
H	3.550476	2.591202	-1.486847
H	3.666245	0.748962	0.244705
H	4.538879	0.462296	-1.246231
H	1.141876	0.320587	-2.963379
H	0.065826	-1.081635	-2.89119
H	-0.587021	0.570648	-2.850143
H	2.768066	-0.964111	-2.14325
H	3.511169	-1.590286	-0.705658

H	1.629929	0.153168	1.367615
H	0.535767	-1.187363	1.57695
H	3.611908	-1.291138	1.623962
H	2.498779	-1.506866	2.963394
H	-0.615662	-2.361954	0.108047
H	2.201202	-4.875076	-2.549591
H	1.640289	-5.129089	-0.852905
H	0.453934	-4.676651	-2.141815

B3LYP/6-31G* Energy = -1826.402625
 B3LYP/6-31G* Free energy in solution = -1826.828946
 Number of imaginary frequencies = 0

Triflate 25

B3LYP/6-31G* Geometry

C	-3.694672	0.112549	-2.476944
C	-2.342072	0.277756	-2.7883
C	-4.086365	-0.333206	-1.210907
C	-1.388184	-0.005951	-1.815491
C	-3.130356	-0.613998	-0.2321
C	-1.782104	-0.441803	-0.546326
C	0.114807	0.074112	-1.915176
C	0.625931	-0.75853	-0.700424
C	-0.575851	-0.660843	0.340149
C	1.967041	-0.251831	-0.124649
C	0.791885	-2.249741	-1.062744
C	-0.662064	-1.783798	1.364548
O	-0.249832	0.609085	1.092651
C	3.133575	-0.328888	-1.136169
O	1.620056	-2.97995	-0.55864
O	-0.087006	-2.667831	-1.990723
S	-1.344345	1.494476	1.888611
C	4.362656	0.24881	-0.584747
C	0.00502	-4.058487	-2.356094
O	-1.801056	2.607452	1.071838
O	-2.286789	0.655945	2.623245
C	-0.107468	2.172943	3.119202
N	5.328568	0.711823	-0.13768
F	-0.740417	3.063339	3.881226
F	0.897079	2.764771	2.476196
F	0.363327	1.186752	3.879166
H	-4.449265	0.327225	-3.228806
H	-2.043167	0.613403	-3.777985
H	-5.140915	-0.461533	-0.984772
H	-3.438248	-0.945404	0.75412
H	0.454575	1.113541	-1.812225
H	0.494293	-0.301376	-2.870071
H	1.841553	0.783463	0.195648
H	2.235107	-0.838928	0.757645
H	-0.915619	-2.726028	0.870361
H	0.291046	-1.910797	1.884964
H	-1.435837	-1.562622	2.101791
H	3.33432	-1.370102	-1.408432
H	2.889664	0.212967	-2.058426
H	-0.777878	-4.213882	-3.097961
H	0.989105	-4.276733	-2.778137
H	-0.157104	-4.693558	-1.481903

B3LYP/6-31G* Energy = -1747.52002
 B3LYP/6-31G* Free energy in solution = -1747.82811
 Number of imaginary frequencies = 0

Triflate 26

B3LYP/6-31G* Geometry

C	-3.715042	-0.065308	-2.222031
C	-2.534195	0.224091	-2.897141
C	-3.667252	-0.800735	-1.035721
C	-1.29039	-0.2063	-2.412964
C	-2.442719	-1.240509	-0.543594
C	-1.248108	-0.948883	-1.220245
C	-0.0325	0.183563	-3.164505
C	0.067261	-1.534668	-0.700378
C	1.226791	-0.553482	-2.699448
C	1.305588	-0.670959	-1.15657
C	0.142334	-3.018555	-1.097092
O	0.008377	-1.38446	0.791992
C	1.260269	0.719376	-0.46312
C	2.605637	-1.422623	-0.808121
S	0.156403	-2.557083	1.888657
C	2.380035	1.684204	-0.914276
O	3.141617	-2.226166	-1.542023
O	3.080231	-1.097168	0.407364
O	-1.111496	-3.25354	2.074387
O	1.399231	-3.307053	1.744461
C	0.375748	-1.366623	3.31813
C	2.306259	2.961243	-0.198059
C	4.234589	-1.839981	0.850143
F	1.45285	-0.60878	3.11763
F	-0.7005	-0.597992	3.444672
F	0.54213	-2.096878	4.420044
N	2.235229	3.968994	0.373459
H	-4.666473	0.279831	-2.617142
H	-2.565826	0.799728	-3.819778
H	-4.580093	-1.033142	-0.494843
H	-2.411224	-1.81308	0.377533
H	0.109329	1.269287	-3.061035
H	-0.175674	0.011658	-4.238419
H	1.271698	-1.555328	-3.131775
H	2.120285	-0.042313	-3.072464
H	0.089722	-3.102661	-2.184418
H	1.055893	-3.50618	-0.756912
H	-0.724152	-3.546082	-0.689468
H	0.290741	1.188004	-0.653824
H	1.336472	0.582703	0.614746
H	3.365784	1.244171	-0.724991
H	2.322296	1.897003	-1.987854
H	4.502289	-1.405396	1.812897
H	3.971619	-2.89296	0.964127
H	5.051987	-1.736298	0.133072

B3LYP/6-31G* Energy = -1786.802471
 B3LYP/6-31G* Free energy in solution = -1787.141055
 Number of imaginary frequencies = 0

Triflate 27

B3LYP/6-31G* Geometry

C	3.048746	3.529819	0.475491
C	3.538391	2.516847	-0.345155
C	1.725159	3.474513	0.895447
C	2.744314	1.442806	-0.772381
C	0.913896	2.416621	0.487588
C	1.393001	1.39545	-0.345026
C	3.419981	0.407127	-1.657433
C	0.425582	0.28558	-0.810648
C	3.384015	-1.041875	-1.145519
C	0.870904	-1.180257	-0.369202
C	0.120374	0.456634	-2.306056
C	2.021757	-1.735841	-1.254099
O	-0.833766	0.461753	-0.016078
C	1.246054	-1.149516	1.138798
C	-0.349	-2.124842	-0.522656
S	-2.289862	0.886404	-0.573137
C	1.713587	-2.500835	1.726194
O	-1.017309	-2.537978	0.400538
O	-0.580955	-2.469124	-1.803925
O	-2.310951	2.273189	-1.020833
O	-2.88323	-0.168902	-1.386775
C	-3.077463	0.817236	1.125918
C	2.070228	-2.366413	3.141893
C	-1.738559	-3.303777	-2.022107
F	-4.371593	1.095478	0.971951
F	-2.934027	-0.390286	1.65359
F	-2.515451	1.731206	1.917482
N	2.356724	-2.246165	4.260409
H	3.697987	4.344632	0.783319
H	4.575228	2.552686	-0.670404
H	1.313963	4.245406	1.540762
H	-0.108707	2.386242	0.834968
H	3.011298	0.434116	-2.677046
H	4.469688	0.701404	-1.763398
H	3.759595	-1.070683	-0.115197
H	4.093668	-1.628463	-1.74314
H	1.034156	0.360484	-2.890682
H	-0.591886	-0.285369	-2.664837
H	-0.273173	1.461206	-2.479406
H	1.697763	-1.73484	-2.298613
H	2.151222	-2.794861	-0.999541
H	2.03405	-0.410518	1.296572
H	0.37497	-0.815183	1.705512
H	0.918703	-3.247537	1.638523
H	2.592696	-2.887492	1.19756
H	-1.744394	-3.511848	-3.092055
H	-1.652429	-4.228238	-1.446701
H	-2.640157	-2.765198	-1.725777

B3LYP/6-31G* Energy = -1826.074908
 B3LYP/6-31G* Free energy in solution = -1826.442059
 Number of imaginary frequencies = 0

Carbocation 28

B3LYP/6-31G* Geometry

C	-2.442078	1.265350	-1.224472
C	-1.107758	1.457825	-1.597961
C	-2.804886	0.609467	-0.024704
C	-0.115311	0.990219	-0.748535
C	-1.830917	0.127686	0.824249
C	-0.470291	0.318695	0.459793
C	1.376343	1.068314	-0.888123
C	1.926315	0.360809	0.394287
C	0.688965	-0.063019	1.147079
C	2.926468	1.211685	1.233139
C	2.696671	-0.927521	-0.047226
C	0.728424	-0.790268	2.437607
C	2.471222	2.624603	1.660538
O	3.894852	-0.994751	-0.138275
O	1.832275	-1.905289	-0.344269
C	1.269012	2.613327	2.497620
C	2.413086	-3.146194	-0.836227
N	0.302734	2.528809	3.135773
H	-3.229538	1.633652	-1.876175
H	-0.865982	1.966858	-2.525742
H	-3.854919	0.490509	0.220551
H	-2.093689	-0.373367	1.750137
H	1.720078	2.105698	-0.961060
H	1.713913	0.576935	-1.808441
H	3.211456	0.642441	2.123200
H	3.834290	1.305542	0.631119
H	1.716141	-1.198959	2.660965
H	0.458176	-0.089066	3.241013
H	-0.009430	-1.598984	2.457413
H	3.287766	3.089355	2.225342
H	2.291000	3.275391	0.797318
H	1.566086	-3.810806	-0.997437
H	2.947128	-2.959213	-1.769500
H	3.099136	-3.555176	-0.092606

B3LYP/6-31G* Energy = -785.89593

B3LYP/6-31G* Free energy in solution = -786.229188

Number of imaginary frequencies = 0

Carbocation 29

B3LYP/6-31G* Geometry

C	2.462463	-1.800613	-0.495636
C	2.462418	-0.403290	-0.496277
C	1.258240	-2.527359	-0.495560
C	1.268555	0.308228	-0.510345
C	0.059662	-1.849030	-0.477432
C	0.025925	-0.417404	-0.491913
C	1.253036	1.810364	-0.496155
C	-1.208862	0.268921	-0.475800
C	0.049591	2.332184	-1.279221
C	-1.286194	1.757492	-0.742905
C	-2.478958	-0.456818	-0.161133
C	-2.470642	2.169128	-1.679962
C	-1.567795	2.472748	0.626480

C	-2.328049	1.829971	-3.182495
O	-1.949753	3.611800	0.702362
O	-1.283264	1.678650	1.667175
C	-2.069489	0.408844	-3.424057
C	-1.475189	2.259384	2.989456
N	-1.844559	-0.725952	-3.526703
H	3.409393	-2.333267	-0.502518
H	3.405548	0.134964	-0.496338
H	1.275269	-3.611800	-0.512833
H	-0.867386	-2.408737	-0.498810
H	2.184464	2.200317	-0.917969
H	1.218048	2.158524	0.546906
H	0.167511	2.040115	-2.327805
H	0.001358	3.424500	-1.245758
H	-2.333542	-1.202057	0.623138
H	-3.273010	0.222458	0.150925
H	-2.826385	-0.981079	-1.062714
H	-3.409378	1.749649	-1.309616
H	-2.562714	3.254547	-1.584579
H	-3.259338	2.111786	-3.687469
H	-1.534515	2.417557	-3.655900
H	-1.197617	1.471466	3.687485
H	-0.831711	3.132919	3.106216
H	-2.519500	2.548767	3.117538

B3LYP/6-31G* Energy = -825.177856

B3LYP/6-31G* Free energy in solution = -825.539733

Number of imaginary frequencies = 0

Carbocation 30

B3LYP/6-31G* Geometry

C	-3.328506	0.384140	-1.552139
C	-2.138733	0.647156	-2.237366
C	-3.302368	-0.140488	-0.252716
C	-0.894058	0.444534	-1.650162
C	-2.087540	-0.392822	0.349243
C	-0.848892	-0.062500	-0.296677
C	0.350296	0.599900	-2.482437
C	0.335938	-0.221893	0.471375
C	1.263809	1.765533	-2.045914
C	1.572388	0.649277	0.320740
C	0.358124	-1.262161	1.553070
C	1.362411	1.937531	-0.528000
C	2.140381	1.089400	1.727600
C	2.736816	-0.173386	-0.322708
C	1.372192	2.202362	2.479111
O	3.845947	0.276016	-0.456589
O	2.346664	-1.396988	-0.708481
C	-0.019455	1.857025	2.777573
C	3.371384	-2.234329	-1.318542
N	-1.116241	1.525009	2.965012
H	-4.280121	0.572830	-2.040878
H	-2.182922	0.998520	-3.263900
H	-4.225998	-0.341721	0.279297
H	-2.076431	-0.750793	1.370500
H	0.067993	0.734741	-3.530441
H	0.912277	-0.339035	-2.435303

H	2.257736	1.606323	-2.477203
H	0.888107	2.705109	-2.464844
H	-0.263184	-2.120605	1.295273
H	1.374863	-1.612350	1.737778
H	-0.017776	-0.841125	2.495682
H	2.202072	2.606247	-0.314850
H	0.457245	2.430847	-0.157730
H	2.258926	0.227371	2.387527
H	3.146300	1.466888	1.525300
H	1.894882	2.395889	3.423279
H	1.386246	3.143997	1.920944
H	4.189682	-2.388809	-0.613480
H	2.869125	-3.172424	-1.548172
H	3.748245	-1.757309	-2.224747

B3LYP/6-31G* Energy = -864.446247
 B3LYP/6-31G* Free energy in solution = -864.835767
 Number of imaginary frequencies = 0

Alkene 4

B3LYP/6-31G* Geometry

C	-4.051025	0.833649	0.111343
C	-4.095200	-0.563843	0.205460
C	-2.826721	1.499725	0.025558
C	-1.648254	0.755463	0.033661
C	-2.918381	-1.308945	0.216354
C	-1.690170	-0.641891	0.130844
C	-0.226807	1.257492	-0.065857
C	0.669800	-0.009445	0.143600
C	-0.330551	-1.197220	0.130859
C	0.031113	-2.485840	0.130859
C	1.400726	0.014069	1.508942
C	1.673264	-0.254013	-0.985016
C	2.474548	1.117859	1.641006
O	2.776459	-0.739502	-0.829956
O	1.175674	0.070129	-2.194382
C	3.034470	1.172058	2.993988
C	2.024338	-0.232697	-3.315842
N	3.465286	1.205582	4.071472
H	-4.976669	1.402939	0.106750
H	-5.054443	-1.069305	0.274124
H	-2.796936	2.584229	-0.047592
H	-2.956848	-2.392014	0.296387
H	-0.017654	2.021957	0.692000
H	-0.041290	1.718964	-1.040497
H	-0.706192	-3.283569	0.136856
H	1.074524	-2.786438	0.115540
H	0.644745	0.141327	2.291641
H	1.877258	-0.954849	1.675171
H	3.286972	0.926315	0.932800
H	2.061005	2.106583	1.406708
H	1.469238	0.092041	-4.196030
H	2.972198	0.305435	-3.236053
H	2.225845	-1.305908	-3.360703

B3LYP/6-31G* Energy = -785.544407
 B3LYP/6-31G* Free energy in solution = -785.813316

Number of imaginary frequencies = 0

Alkene 31

B3LYP/6-31G* Geometry

C	-4.278259	0.344620	-0.163803
C	-3.281876	1.219100	-0.583008
C	-3.924011	-0.924881	0.301239
C	-1.929474	0.852463	-0.562881
C	-2.587753	-1.302307	0.325104
C	-1.567810	-0.438644	-0.122300
C	-0.888351	1.870102	-0.981827
C	-0.144531	-0.882462	-0.122300
C	0.499634	1.269745	-1.211838
C	0.902878	0.240189	-0.112335
C	0.198700	-2.179794	-0.122314
C	0.951187	0.939407	1.276321
C	2.308075	-0.274979	-0.465240
C	1.224670	0.004410	2.474625
O	3.264435	-0.274429	0.283386
O	2.388153	-0.704163	-1.741043
C	1.153564	0.729095	3.746094
C	3.681152	-1.175735	-2.157959
N	1.092102	1.316223	4.745956
H	-5.320206	0.651657	-0.187256
H	-3.549286	2.213654	-0.934113
H	-4.686615	-1.613083	0.655106
H	-2.322937	-2.277832	0.720215
H	-0.837082	2.658142	-0.217300
H	-1.214218	2.376587	-1.899094
H	0.523087	0.752304	-2.174789
H	1.248886	2.069870	-1.259079
H	-0.542374	-2.970978	-0.166595
H	1.233170	-2.505325	-0.101868
H	1.722092	1.716553	1.249557
H	-0.006287	1.438705	1.447357
H	0.493118	-0.811371	2.498520
H	2.216675	-0.445175	2.378296
H	3.559296	-1.472321	-3.199783
H	4.426636	-0.381836	-2.066040
H	3.993835	-2.028000	-1.548920

B3LYP/6-31G* Energy = -824.825225
 B3LYP/6-31G* Free energy in solution = -825.124012
 Number of imaginary frequencies = 0

Alkene 21

B3LYP/6-31G* Geometry

C	-2.501251	0.613297	-2.591843
C	-1.326874	0.170929	-3.203033
C	-2.751800	0.283981	-1.261520
C	-0.381287	-0.592957	-2.509598
C	-1.819107	-0.474823	-0.553909
C	-0.632813	-0.914520	-1.157898
C	0.852921	-1.100754	-3.228073
C	0.333206	-1.730133	-0.358170
C	2.204117	-0.638580	-2.646240

C	1.739258	-1.132202	-0.103333
C	-0.039505	-2.933548	0.095154
C	2.640472	-1.343460	-1.353973
C	1.594208	0.368210	0.281525
C	2.383194	-1.912842	1.057877
C	2.928925	1.071700	0.613602
O	3.159958	-2.834946	0.930161
O	1.966751	-1.470139	2.265427
C	2.720505	2.469620	1.003067
C	2.477478	-2.191467	3.400208
N	2.542084	3.575012	1.309479
H	-3.215073	1.208054	-3.155365
H	-1.142059	0.414337	-4.246979
H	-3.662766	0.618164	-0.772537
H	-2.000595	-0.727905	0.486954
H	0.797852	-0.780563	-4.274872
H	0.839111	-2.200729	-3.242386
H	2.189346	0.451645	-2.515579
H	2.980118	-0.840378	-3.395737
H	-1.025848	-3.327713	-0.131866
H	0.614304	-3.575012	0.678619
H	2.701309	-2.421783	-1.531540
H	3.662750	-1.031052	-1.107788
H	1.109879	0.902679	-0.538620
H	0.929382	0.450150	1.144730
H	3.441208	0.562683	1.438324
H	3.609512	1.057236	-0.245331
H	2.073166	-1.681686	4.274857
H	2.142822	-3.231903	3.372864
H	3.570084	-2.170410	3.409698

B3LYP/6-31G* Energy = -864.101385
 B3LYP/6-31G* Free energy in solution = -864.427866
 Number of imaginary frequencies = 0

Triflic anhydride

B3LYP/6-31G* Geometry

C	2.542598	0.414008	-0.007909
S	1.208442	-0.915131	0.015057
F	3.571598	-0.074105	-0.690973
F	2.068540	1.501205	-0.602484
F	2.903582	0.689359	1.236349
O	-0.000098	0.000139	0.773850
O	0.838898	-1.228567	-1.349130
O	1.567869	-1.909965	1.002261
S	-1.208531	0.915195	0.015067
C	-2.542526	-0.414034	-0.007894
O	-1.567888	1.910079	1.002219
O	-0.839124	1.228610	-1.349166
F	-3.571928	0.074117	-0.690301
F	-2.068422	-1.500881	-0.603146
F	-2.902955	-0.690055	1.236392

B3LYP/6-31G* Energy = -1847.513642
 B3LYP/6-31G* Free energy in solution = -1847.564142
 Number of imaginary frequencies = 0

Triflate anion

B3LYP/6-31G* Geometry

S	0.926198	-0.000006	-0.000008
O	1.244184	1.322015	-0.586670
O	1.243951	-1.169211	-0.851490
O	1.244101	-0.152899	1.438208
C	-0.941124	0.000006	0.000007
F	-1.445599	-1.146465	0.508876
F	-1.445617	1.013951	0.738437
F	-1.445486	0.132605	-1.247347

B3LYP/6-31G* Energy = -961.470711
 B3LYP/6-31G* Free energy in solution = -961.575914
 Number of imaginary frequencies = 0

Triflic acid

B3LYP/6-31G* Geometry

C	1.008529	0.009414	-0.001930
S	-0.852889	-0.148445	0.075910
O	-1.256919	1.097587	-0.898373
O	-1.216039	-1.372622	-0.605503
O	-1.260738	0.173918	1.435866
F	1.542841	-0.924068	0.780345
F	1.424878	-0.154460	-1.252631
F	1.361169	1.219768	0.435825
H	-1.495372	1.856417	-0.330748

B3LYP/6-31G* Energy = -961.960579
 B3LYP/6-31G* Free energy in solution = -962.009607
 Number of imaginary frequencies = 0

Cyclization leading to the enones

Cyclization of 32

Starting material 32

B3LYP/6-31G* Geometry

C	-3.150055	0.860733	-2.670471
C	-3.472656	0.392197	-1.389343
C	-1.817856	0.972839	-3.076416
C	-0.810837	0.615723	-2.182892
C	-2.467194	0.035355	-0.493317
C	-1.131546	0.155762	-0.8954
C	0.684311	0.585434	-2.406189
C	1.269562	0.446884	-0.965439
C	0.099594	-0.152802	-0.151886
C	0.225998	-0.832031	1.000229
C	1.600296	1.881042	-0.46254
C	2.509064	-0.44162	-0.8367
C	1.97641	2.008163	1.045547
O	3.304153	-0.33844	0.086716
O	2.603714	-1.361145	-1.790161
C	0.853836	2.093277	1.943466
C	3.709793	-2.292603	-1.683212
N	-0.044754	2.161713	2.661453
H	-3.945648	1.136353	-3.356415

H	-4.514236	0.307343	-1.094238
H	-1.576889	1.325974	-4.075424
H	-2.722397	-0.330017	0.49826
H	1.067261	1.474609	-2.920578
H	0.967712	-0.280457	-3.011459
H	-0.643295	-1.239105	1.509674
H	1.194672	-1.070313	1.429123
H	2.469116	2.2612	-1.008408
H	0.7594	2.540161	-0.69751
H	2.571747	2.916473	1.215652
H	2.595428	1.141281	1.328751
H	3.609924	-2.951019	-2.544327
H	4.657471	-1.751678	-1.711334
H	3.633865	-2.854309	-0.750168
H	-0.834625	2.206177	3.284332

B3LYP/6-31G* Energy = -785.865641
 B3LYP/6-31G* Free energy in solution = -786.210652
 Number of imaginary frequencies = 0

Transition structure 32-TS
 RHF/3-21G Geometry

C	3.793177	-1.567405	0.211919
C	3.885027	-0.449755	-0.615458
C	2.572784	-1.997174	0.705982
C	1.437665	-1.288616	0.370841
C	2.752768	0.258690	-0.952036
C	1.528110	-0.159864	-0.441242
C	-0.004596	-1.592469	0.719701
C	-0.743033	-0.295547	0.303038
C	0.211412	0.415286	-0.641394
C	-0.130257	1.509831	-1.375158
C	-0.875092	0.660237	1.539626
C	-2.127209	-0.499676	-0.272514
C	-1.246108	2.096839	1.141687
O	-2.771219	0.381853	-0.799039
O	-2.590188	-1.726862	-0.077637
C	-0.169353	2.732627	0.330542
C	-3.942590	-2.067378	-0.542182
N	0.569680	3.642482	0.279491
H	4.683706	-2.107960	0.462240
H	4.840062	-0.147190	-0.992927
H	2.515349	-2.867552	1.327828
H	2.821804	1.109969	-1.599677
H	-0.147385	-1.822093	1.766993
H	-0.364658	-2.426226	0.134924
H	0.601179	1.966683	-2.014825
H	-1.163479	1.675263	-1.613155
H	-1.641004	0.272607	2.199472
H	0.066601	0.651737	2.072814
H	-1.351830	2.713984	2.026928
H	-2.166481	2.107499	0.576187
H	-4.076303	-3.096130	-0.262646
H	-4.663260	-1.429918	-0.056260
H	-3.999454	-1.938980	-1.610780
H	1.292421	4.067249	-0.260260

RHF/3-21G Energy = -776.609079
 B3LYP/6-31G* Energy = -786.146055982
 B3LYP/6-31G* Free energy in solution = -786.202105
 Number of imaginary frequencies = 1 (-559.2638)

Cyclization product 35
 B3LYP/6-31G* Geometry

C	-3.262817	-0.298676	-2.209778
C	-3.606522	-0.495087	-0.852234
C	-1.935074	-0.191208	-2.634644
C	-0.928421	-0.286057	-1.682861
C	-2.620132	-0.585434	0.1082
C	-1.266113	-0.481918	-0.309464
C	0.560516	-0.210205	-1.855865
C	1.122742	-0.341354	-0.412445
C	-0.089233	-0.540268	0.454483
C	0.047058	-0.602142	1.90802
C	1.816803	0.985092	0.09697
C	2.163132	-1.479706	-0.241379
C	2.075104	0.979874	1.610336
O	2.318497	-2.118378	0.777191
O	2.905609	-1.602722	-1.339645
C	0.820847	0.675964	2.40004
C	3.981293	-2.580368	-1.280075
N	0.455231	1.38623	3.37442
H	-4.059433	-0.229431	-2.945343
H	-4.652069	-0.574188	-0.573532
H	-1.705902	-0.038239	-3.684708
H	-2.872452	-0.739609	1.152435
H	0.866135	0.733017	-2.324203
H	0.928329	-1.006668	-2.510056
H	-0.904068	-0.709015	2.433731
H	0.716141	-1.444519	2.148438
H	2.750854	1.111526	-0.4588
H	1.161728	1.823471	-0.168228
H	2.44989	1.954453	1.931992
H	2.836411	0.230896	1.862534
H	4.46582	-2.525146	-2.253143
H	4.675644	-2.318726	-0.47963
H	3.568039	-3.574463	-1.101608
H	-0.407379	1.074081	3.829636

B3LYP/6-31G* Energy = -785.899144
 B3LYP/6-31G* Free energy in solution = -786.239369
 Number of imaginary frequencies = 0

Cyclization of 33

Starting material 33
 B3LYP/6-31G* Geometry

C	-3.600189	0.217957	-1.566208
C	-2.410675	0.267105	-2.257523
C	-3.605469	-0.1922	-0.240402
C	-1.207275	-0.087662	-1.654343
C	-2.4218	-0.539505	0.369415
C	-1.207077	-0.495895	-0.322739
C	0.06723	-0.013794	-2.481308

C	0.066711	-0.885254	0.35582
C	1.279846	-0.650848	-1.790558
C	1.329926	-0.30835	-0.280869
C	0.101105	-1.685043	1.411102
C	1.425339	1.217331	-0.076263
C	2.579742	-0.943832	0.310287
C	1.383804	1.661392	1.418594
O	3.325562	-0.391998	1.090225
O	2.775375	-2.185898	-0.118683
C	0.027237	1.694534	1.942657
C	3.952515	-2.927322	0.341782
N	-1.025177	1.772461	2.348953
H	-4.516296	0.487259	-2.051666
H	-2.405975	0.572906	-3.285812
H	-4.527481	-0.247925	0.302963
H	-2.438324	-0.863419	1.391296
H	0.270187	1.024536	-2.724533
H	-0.099457	-0.525543	-3.422104
H	1.233749	-1.725632	-1.869736
H	2.193344	-0.322098	-2.273788
H	-0.784302	-2.140167	1.806549
H	1.016266	-1.97258	1.888077
H	2.375671	1.56311	-0.459488
H	0.642319	1.716736	-0.625214
H	1.994781	0.990997	2.008057
H	1.777603	2.669052	1.518753
H	3.889542	-3.878448	-0.154312
H	4.849503	-2.398178	0.063019
H	3.916367	-3.042572	1.413361
H	-1.968979	1.814194	2.659744

B3LYP/6-31G* Energy = -825.149262
 B3LYP/6-31G* Free energy in solution = -825.515527
 Number of imaginary frequencies = 0

Transition structure 33-TS

RHF/3-21G Geometry

C	4.109267	-0.852366	-0.250083
C	3.248550	-1.195746	0.770776
C	3.631142	-0.185797	-1.371443
C	1.901027	-0.872729	0.709351
C	2.302126	0.146985	-1.445028
C	1.416523	-0.166447	-0.400433
C	0.982101	-1.296926	1.836844
C	0.011557	0.225686	-0.477607
C	-0.448668	-1.493498	1.329405
C	-0.961451	-0.236987	0.599726
C	-0.461740	1.152175	-1.371898
C	-1.170415	0.934735	1.600198
C	-2.290423	-0.559816	-0.068287
C	-1.459351	2.290815	0.937775
O	-3.278138	0.131468	-0.005784
O	-2.224488	-1.692016	-0.764460
C	-0.346794	2.679794	0.026902
C	-3.417623	-2.165029	-1.475449
N	0.480212	3.487091	-0.182029
H	5.145007	-1.118703	-0.186981

H	3.619061	-1.732116	1.621402
H	4.290875	0.051081	-2.180621
H	1.941764	0.621623	-2.333240
H	1.020532	-0.564830	2.636084
H	1.342194	-2.231145	2.248908
H	-0.475722	-2.320556	0.636669
H	-1.115104	-1.720255	2.153633
H	0.154467	1.518722	-2.166638
H	-1.517780	1.248980	-1.537463
H	-2.016577	0.688598	2.226765
H	-0.297786	1.028949	2.229053
H	-2.389646	2.246617	0.394004
H	-1.514571	3.066736	1.693439
H	-3.117294	-3.090363	-1.931812
H	-4.222640	-2.316076	-0.774578
H	-3.710320	-1.439350	-2.217377
H	1.248092	3.707749	-0.779586

RHF/3-21G Energy = -815.396170
 B3LYP/6-31G* Energy = -825.458134714
 B3LYP/6-31G* Free energy in solution = -825.513607
 Number of imaginary frequencies = 1 (-554.9124)

Cyclization product 36

B3LYP/6-31G* Geometry

C	-3.283875	-0.609863	0.536682
C	-2.8862	0.292542	-0.433624
C	-2.376419	-1.117615	1.46875
C	-1.574387	0.70874	-0.509933
C	-1.078674	-0.703812	1.429337
C	-0.632004	0.220261	0.442261
C	-1.153992	1.719727	-1.548996
C	0.698288	0.649551	0.397507
C	0.298691	1.481155	-1.960556
C	1.230728	1.494202	-0.728348
C	1.64444	0.512802	1.543854
C	1.475388	2.925888	-0.171982
C	2.550919	0.910477	-1.204773
C	1.837143	1.954559	2.110428
C	2.372574	2.915314	1.07988
O	3.500793	1.544235	-1.567535
O	2.476105	-0.43045	-1.228134
N	1.603378	2.295792	3.286453
C	3.59906	-1.193649	-1.79097
H	-4.306641	-0.92865	0.570389
H	-3.602112	0.668503	-1.135315
H	-2.699203	-1.826431	2.201874
H	-0.386551	-1.111832	2.13298
H	-1.282166	2.716415	-1.138733
H	-1.801147	1.639267	-2.412354
H	0.377914	0.513351	-2.440552
H	0.631165	2.239197	-2.657242
H	1.292053	-0.142654	2.3201
H	2.602005	0.158112	1.187988
H	1.954941	3.489883	-0.959854
H	0.527054	3.391312	0.061584
H	3.377121	2.625778	0.79483

H	2.408142	3.899445	1.522614
H	1.247116	1.593109	3.922592
H	3.309113	-2.224472	-1.697174
H	3.738831	-0.919464	-2.824081
H	4.497772	-0.985504	-1.233078

B3LYP/6-31G* Energy = -825.178749
 B3LYP/6-31G* Free energy in solution = -825.541422
 Number of imaginary frequencies = 0

Cyclization of 34

Starting material 34

B3LYP/6-31G* Geometry

C	-3.245392	0.807495	-2.716034
C	-1.87973	0.894119	-2.986069
C	-3.674103	0.56662	-1.41185
C	-0.923706	0.752777	-1.975906
C	-2.73497	0.423904	-0.393585
C	-1.35376	0.525269	-0.647369
C	0.545456	0.836502	-2.31131
C	-0.421387	0.385361	0.511078
C	1.270813	-0.519836	-2.169556
C	0.841064	-0.523895	0.42421
C	-0.748672	0.949997	1.691483
C	0.900635	-1.325974	-0.91037
C	2.192505	0.232819	0.574463
C	0.719772	-1.516724	1.599106
C	2.422714	1.106415	1.84494
O	1.326309	-1.401978	2.653229
O	-0.144608	-2.494949	1.347076
C	1.845184	2.426285	1.793945
C	-0.368362	-3.450287	2.412552
N	1.383438	3.481339	1.753616
H	-3.966156	0.917938	-3.520874
H	-1.544128	1.079102	-4.003464
H	-4.732758	0.477112	-1.187195
H	-3.070892	0.198029	0.613678
H	1.022873	1.589981	-1.668076
H	0.674683	1.202362	-3.335052
H	1.025177	-1.1456	-3.035049
H	2.354126	-0.352829	-2.221832
H	-1.619598	1.591888	1.78096
H	-0.22522	0.728241	2.61705
H	-0.073318	-1.800079	-1.047913
H	1.620941	-2.14476	-0.794922
H	2.382843	0.842346	-0.309128
H	2.990402	-0.514923	0.6167
H	2.044388	0.575897	2.730347
H	3.501938	1.259521	1.991898
H	0.567474	-3.948395	2.673019
H	-0.770462	-2.941788	3.291351
H	-1.088791	-4.160583	2.010284
H	0.953766	4.391403	1.714981

B3LYP/6-31G* Energy = -864.418503
 B3LYP/6-31G* Free energy in solution = -864.821932

Number of imaginary frequencies = 0

Transition structure 34-TS

RHF/3-21G Geometry

C	4.021692	-0.966986	-0.441302
C	3.483065	-0.264520	0.622964
C	3.235301	-1.283394	-1.534182
C	2.156312	0.127876	0.625478
C	1.915130	-0.887436	-1.556516
C	1.358551	-0.180090	-0.485449
C	1.597293	0.904241	1.794649
C	-0.072678	0.149691	-0.567391
C	0.619417	0.053132	2.638478
C	-1.030747	-0.007298	0.617661
C	-0.602247	0.614115	-1.745275
C	-0.396660	-0.760254	1.811093
C	-1.623846	1.363538	1.054656
C	-2.177156	-0.860011	0.077173
C	-1.977457	2.309778	-0.103300
O	-3.274517	-0.440194	-0.197887
O	-1.801065	-2.124949	-0.092467
C	-0.801023	2.512745	-0.997839
C	-2.778891	-3.100948	-0.586118
N	-0.054303	3.319348	-1.420537
H	5.049607	-1.267553	-0.414177
H	4.103040	-0.016177	1.460908
H	3.641947	-1.839406	-2.353662
H	1.298076	-1.163878	-2.386891
H	1.110649	1.801503	1.432184
H	2.409068	1.233396	2.430238
H	1.195021	-0.651162	3.226912
H	0.106844	0.701134	3.339732
H	0.034078	0.723109	-2.602154
H	-1.651782	0.522552	-1.952196
H	0.066647	-1.653398	1.422232
H	-1.195723	-1.081460	2.470030
H	-0.937257	1.862929	1.716043
H	-2.533446	1.165485	1.603625
H	-2.809177	1.917055	-0.666961
H	-2.233450	3.288852	0.286229
H	-3.622239	-3.141969	0.084145
H	-3.109954	-2.817379	-1.572450
H	-2.249533	-4.035936	-0.605266
H	0.756012	3.392947	-2.000618

RHF/3-21G Energy = -854.170526
 B3LYP/6-31G* Energy = -864.758854693
 B3LYP/6-31G* Free energy in solution = -864.813014
 Number of imaginary frequencies = 1 (-519.0885)

Cyclization product 37

B3LYP/6-31G* Geometry

C	-3.055542	0.668091	-1.738129
C	-1.816467	0.89386	-2.346298
C	-3.153183	0.537186	-0.347473
C	-0.638519	0.954193	-1.607819

C	-2.008621	0.629395	0.422073
C	-0.722031	0.788879	-0.17984
C	0.651184	1.356018	-2.280563
C	0.416168	0.724121	0.679504
C	1.730606	0.25235	-2.322235
C	1.747375	0.12619	0.303955
C	0.365067	1.326736	2.031555
C	1.781311	-0.616882	-1.061768
C	2.867508	1.211441	0.425415
C	2.06485	-1.00296	1.34169
C	2.828857	1.995804	1.744568
O	3.164459	-1.219727	1.784988
O	0.969833	-1.734283	1.595413
C	1.436127	2.489319	2.04628
C	1.162766	-2.898972	2.444809
N	1.168427	3.69426	2.294281
H	-3.950378	0.612991	-2.351395
H	-1.771515	1.0495	-3.420151
H	-4.11528	0.364258	0.12323
H	-2.08136	0.484863	1.494064
H	1.046814	2.236649	-1.760056
H	0.435776	1.687225	-3.300659
H	1.542053	-0.413528	-3.171448
H	2.699783	0.724976	-2.513168
H	-0.611908	1.734512	2.288742
H	0.686325	0.626053	2.811127
H	2.698929	-1.215332	-1.086502
H	0.948471	-1.328629	-1.072067
H	3.821457	0.683655	0.336456
H	2.786331	1.905136	-0.415741
H	3.500595	2.856094	1.700073
H	3.164063	1.349243	2.565475
H	1.565704	-2.594833	3.412628
H	0.172806	-3.33931	2.552231
H	1.849686	-3.596985	1.963028
H	0.177368	3.889709	2.461777

B3LYP/6-31G* Energy = -864.447766
 B3LYP/6-31G* Free energy in solution = -864.843483
 Number of imaginary frequencies = 0

Cyclization leading to the imidates

Cyclization of 39

Starting material 39

B3LYP/6-31G* Geometry

C	-3.594818	0.352188	-2.701096
C	-2.308289	0.677353	-3.14444
C	-3.783615	-0.355881	-1.509445
C	-1.214798	0.283096	-2.377136
C	-2.685989	-0.756744	-0.741394
C	-1.409378	-0.426926	-1.187561
C	0.264465	0.504333	-2.625565
C	0.876266	0.300705	-1.207565
C	-0.073196	-0.806061	-0.5802
C	0.748108	1.671921	-0.478867

C	2.329575	-0.145615	-1.132416
O	-0.118912	-0.734955	0.853363
C	0.31929	-2.234879	-0.992493
C	1.195068	1.749634	1.017319
O	2.879639	-0.373093	-0.061142
O	2.928986	-0.271927	-2.311981
C	0.113434	1.568115	1.954895
C	4.310593	-0.713745	-2.292969
N	-0.749985	1.4236	2.702194
H	-4.456848	0.656204	-3.287582
H	-2.170578	1.2312	-4.069412
H	-4.79007	-0.597778	-1.180542
H	-2.824997	-1.313019	0.181564
H	0.496536	1.489395	-3.04541
H	0.671097	-0.234161	-3.32515
H	-0.280106	2.02832	-0.585052
H	1.381348	2.390976	-1.007568
H	0.613174	-1.28476	1.182526
H	1.289124	-2.522812	-0.568207
H	-0.440338	-2.933807	-0.630859
H	0.378281	-2.3376	-2.079727
H	1.6353	2.731995	1.237488
H	1.956604	0.982346	1.222168
H	4.379807	-1.701569	-1.833496
H	4.61232	-0.747482	-3.338364
H	4.921829	-0.004623	-1.731522
H	-1.5244	1.240677	3.318237

B3LYP/6-31G* Energy = -862.280522
 B3LYP/6-31G* Free energy in solution = -862.652705
 Number of imaginary frequencies = 0

Transition structure 39-TS

RHF/3-21G Geometry

C	-3.744123	-1.556882	-0.495479
C	-2.491855	-2.063965	-0.822843
C	-3.868969	-0.421363	0.287405
C	-1.370974	-1.412271	-0.359728
C	-2.739033	0.230247	0.764334
C	-1.505317	-0.272652	0.424464
C	0.103858	-1.746907	-0.578753
C	0.756999	-0.378707	-0.273003
C	-0.133991	0.168794	0.866088
C	0.630338	0.488715	-1.557302
C	2.199901	-0.353670	0.131008
O	0.017551	1.645109	0.948393
C	0.171930	-0.382376	2.265508
C	0.905650	1.996801	-1.360781
O	2.658702	0.574307	0.775425
O	2.912183	-1.362745	-0.332853
C	-0.160824	2.621256	-0.552671
C	4.354241	-1.432360	-0.050612
N	-1.007499	3.426423	-0.481811
H	-4.624240	-2.051249	-0.853934
H	-2.406875	-2.944120	-1.428535
H	-4.842791	-0.047728	0.530935
H	-2.830790	1.096863	1.389164

H	0.320683	-2.087768	-1.581186
H	0.444047	-2.502906	0.118066
H	-0.359743	0.352386	-1.968258
H	1.342580	0.113449	-2.282340
H	0.865363	1.836210	1.395348
H	1.173484	-0.131637	2.585073
H	-0.542223	0.032919	2.964049
H	0.056031	-1.456923	2.267081
H	0.910484	2.501942	-2.317862
H	1.855821	2.153223	-0.869375
H	4.511315	-1.469895	1.015055
H	4.682298	-2.337295	-0.527650
H	4.845995	-0.567492	-0.465518
H	-1.703420	3.763739	0.149023

RHF/3-21G Energy = -852.228282
 B3LYP/6-31G* Energy = -862.582205225
 B3LYP/6-31G* Free energy in solution = -862.640216
 Number of imaginary frequencies = 1 (-365.2877)

Cyclization product 39-P

B3LYP/6-31G* Geometry

C	-3.638748	-0.460205	-0.376434
C	-2.715347	0.038071	-1.302231
C	-3.213959	-1.052002	0.81781
C	-1.357483	-0.050568	-1.011292
C	-1.851761	-1.163788	1.108475
C	-0.939529	-0.641434	0.195129
C	-0.165665	0.399185	-1.847977
C	0.942657	0.47406	-0.76532
C	0.557571	-0.730881	0.14563
C	0.764389	1.844009	-0.017792
C	2.409683	0.355972	-1.125656
O	1.323257	-0.516769	1.490814
C	1.027252	-2.124008	-0.275238
C	1.407227	1.946777	1.379059
O	3.223724	0.022476	-0.254654
O	2.729324	0.676163	-2.356873
C	1.02301	0.792648	2.238663
C	4.142624	0.635132	-2.717575
N	0.551163	0.740829	3.379974
H	-4.70105	-0.386063	-0.588348
H	-3.057098	0.491333	-2.228485
H	-3.94696	-1.432571	1.522186
H	-1.523422	-1.641266	2.027649
H	-0.319931	1.359024	-2.349548
H	0.084473	-0.334061	-2.62442
H	-0.308212	2.03067	0.076981
H	1.169937	2.635483	-0.656433
H	2.26828	-0.425293	1.101395
H	2.114731	-2.212463	-0.335922
H	0.648529	-2.861633	0.437271
H	0.602005	-2.363327	-1.254379
H	1.088394	2.861633	1.884369
H	2.502121	1.973984	1.307022
H	4.701035	1.332977	-2.091766
H	4.52504	-0.377777	-2.583954

H	4.172012	0.932892	-3.763504
H	0.392685	-0.192139	3.763504

B3LYP/6-31G* Energy = -862.287125
 B3LYP/6-31G* Free energy in solution = -862.649805
 Number of imaginary frequencies = 0

Cyclization of 40

Starting material 40

B3LYP/6-31G* Geometry

C	-3.753586	-0.152924	1.001221
C	-3.228287	0.346008	-0.18605
C	-2.924454	-0.849609	1.885345
C	-1.87674	0.16655	-0.520844
C	-1.581436	-1.033386	1.569763
C	-1.044357	-0.524902	0.374908
C	-1.3593	0.75502	-1.822357
C	0.418213	-0.811325	0.042389
C	0.103485	0.412766	-2.159973
C	0.997726	0.307327	-0.90181
C	0.539841	-2.222946	-0.56897
O	1.150223	-0.801941	1.286087
C	1.026688	1.713593	-0.224319
C	2.453217	-0.048981	-1.239838
C	1.851959	1.893875	1.088776
O	3.275818	-0.352341	-0.379974
O	2.748764	0.030045	-2.53038
C	1.116562	1.531616	2.283249
C	4.115494	-0.281097	-2.908127
N	0.532059	1.24411	3.23114
H	-4.804764	-0.008743	1.233093
H	-3.874542	0.882874	-0.876785
H	-3.328552	-1.260605	2.806366
H	-0.934906	-1.592941	2.238861
H	-1.995926	0.423035	-2.65097
H	-1.488937	1.845871	-1.788895
H	0.509903	1.162628	-2.844971
H	0.154037	-0.536758	-2.698639
H	1.57988	-2.472839	-0.809128
H	0.179077	-2.949097	0.164154
H	-0.064163	-2.335526	-1.472336
H	2.071	-1.029587	1.045929
H	0.003204	2.050232	-0.047028
H	1.46611	2.420151	-0.936508
H	2.136383	2.949097	1.205383
H	2.7695	1.293015	1.073074
H	4.1445	-0.158966	-3.989349
H	4.804749	0.407959	-2.416534
H	4.355423	-1.306885	-2.622742
H	-0.0215	0.881058	3.989365

B3LYP/6-31G* Energy = -901.56706
 B3LYP/6-31G* Free energy in solution = -901.965966
 Number of imaginary frequencies = 0

Transition structure 40-TS

RHF/3-21G Geometry

C	-4.148033	-0.820708	-0.154581
C	-3.134613	-1.628414	-0.621951
C	-3.844675	0.292804	0.615683
C	-1.800422	-1.347189	-0.339723
C	-2.529393	0.583672	0.901014
C	-1.503504	-0.223551	0.418272
C	-0.724667	-2.272130	-0.898090
C	-0.075589	0.076401	0.819219
C	0.701092	-1.973287	-0.391042
C	0.929247	-0.464577	-0.215216
C	0.160121	-0.405851	2.260757
O	0.099531	1.559379	0.835204
C	0.765803	0.255225	-1.582855
C	2.339661	-0.151577	0.246633
C	0.930184	1.794224	-1.534960
O	2.618366	0.844399	0.898586
O	3.248344	-0.999051	-0.192636
C	-0.156591	2.441246	-0.774198
C	4.666958	-0.795165	0.144272
N	-1.026785	3.211547	-0.729312
H	-5.168255	-1.057887	-0.378862
H	-3.372291	-2.493956	-1.209439
H	-4.629174	0.915441	0.995880
H	-2.286044	1.428358	1.513147
H	-0.975290	-3.294548	-0.641091
H	-0.748683	-2.210561	-1.981062
H	1.430554	-2.365927	-1.083340
H	0.868439	-2.466900	0.556702
H	1.172257	-0.217150	2.589023
H	-0.522187	0.121714	2.912532
H	-0.055728	-1.460961	2.337510
H	0.995357	1.731991	1.201531
H	-0.202101	0.017202	-1.996170
H	1.521235	-0.130134	-2.256839
H	0.888107	2.199029	-2.538254
H	1.871705	2.075359	-1.084304
H	4.785608	-0.799635	1.215286
H	5.176270	-1.623752	-0.311610
H	5.002001	0.145833	-0.260512
H	-1.747695	3.601107	-0.163578

RHF/3-21G Energy = -891.025879

B3LYP/6-31G* Energy = -901.901644039

B3LYP/6-31G* Free energy in solution = -901.956159

Number of imaginary frequencies = 1 (-380.4695)

Cyclization product 40-P

B3LYP/6-31G* Geometry

C	-4.134415	0.207489	-0.719833
C	-3.151321	0.428329	-1.679153
C	-3.788803	-0.334503	0.521179
C	-1.804077	0.132294	-1.427551
C	-2.46051	-0.645065	0.787247
C	-1.461441	-0.395432	-0.167816

C	-0.7751	0.398315	-2.514145
C	-0.037674	-0.82486	0.090698
C	0.639938	-0.130997	-2.216232
C	0.996841	0.007629	-0.720169
C	0.097412	-2.347015	0.003448
O	0.33667	-0.541656	1.598587
C	0.947693	1.514023	-0.294327
C	2.400986	-0.494965	-0.373383
C	1.123566	1.774246	1.214462
O	2.693329	-0.85173	0.779007
O	3.268616	-0.459015	-1.352982
C	0.240463	0.905075	2.048325
C	4.641693	-0.858795	-1.058975
N	-0.470047	1.200394	3.019928
H	-5.170013	0.447067	-0.941071
H	-3.427475	0.835358	-2.648682
H	-4.550827	-0.522079	1.271103
H	-2.195007	-1.089279	1.742233
H	-1.122131	-0.040634	-3.456421
H	-0.73407	1.4796	-2.70047
H	1.376373	0.410751	-2.815598
H	0.723221	-1.183044	-2.508408
H	1.106674	-2.707397	0.218018
H	-0.600464	-2.813492	0.703018
H	-0.186249	-2.67099	-1.001221
H	1.359207	-0.771606	1.547668
H	-0.014526	1.923508	-0.607254
H	1.721527	2.058533	-0.845123
H	0.891129	2.813492	1.458496
H	2.16156	1.594559	1.523682
H	4.654327	-1.893707	-0.7146
H	5.170013	-0.750061	-2.003647
H	5.057907	-0.20195	-0.293884
H	-0.966583	0.422104	3.456436

B3LYP/6-31G* Energy = -901.581109

B3LYP/6-31G* Free energy in solution = -901.971599

Number of imaginary frequencies = 0

Cyclization of 41**Starting material 41**

B3LYP/6-31G* Geometry

C	-4.258331	0.209763	-0.601624
C	-3.381317	0.417648	-1.659866
C	-3.754837	-0.291183	0.596054
C	-2.002411	0.163239	-1.564926
C	-2.388275	-0.527206	0.720551
C	-1.478271	-0.274429	-0.325562
C	-1.198318	0.330307	-2.838577
C	0.006271	-0.640549	-0.05484
C	-0.003693	1.28418	-2.755936
C	1.093018	0.44899	-0.490189
C	0.308075	-2.02153	-0.669571
C	1.20575	0.706284	-2.021423
O	0.097839	-0.75264	1.380829
C	0.820206	1.825623	0.191452

C	2.479813	-0.046692	0.015076
C	0.935684	1.932175	1.746292
O	2.695343	-0.409332	1.171051
O	3.439194	-0.024445	-0.898575
C	-0.291794	1.628235	2.443954
C	4.755966	-0.465164	-0.47702
N	-1.269089	1.387238	2.999512
H	-5.319839	0.408859	-0.722565
H	-3.774292	0.771683	-2.610428
H	-4.423477	-0.52121	1.422409
H	-2.008591	-0.9588	1.637604
H	-1.876434	0.6866	-3.620148
H	-0.841568	-0.650345	-3.186783
H	-0.319229	2.245193	-2.331451
H	0.329147	1.507034	-3.776581
H	1.331757	-2.348083	-0.445038
H	-0.380676	-2.752579	-0.238907
H	0.178543	-2.031815	-1.754105
H	1.492752	-0.231598	-2.508179
H	2.054733	1.3797	-2.173019
H	1.0224	-1.002213	1.582596
H	1.549286	2.545105	-0.194275
H	-0.162888	2.18129	-0.124619
H	1.708038	1.257278	2.137283
H	1.204727	2.959335	2.0307
H	5.382431	-0.366531	-1.361816
H	5.120026	0.168488	0.333786
H	4.711563	-1.502487	-0.14093
H	-2.162796	1.127029	3.383224

B3LYP/6-31G* Energy = -940.836828
 B3LYP/6-31G* Free energy in solution = -941.2637
 Number of imaginary frequencies = 0

Transition structure 41-TS
 RHF/3-21G Geometry

C	-4.293300	-0.022525	-0.242908
C	-3.538924	-1.170671	-0.363319
C	-3.700981	1.119940	0.253415
C	-2.188174	-1.211307	-0.029906
C	-2.358386	1.105891	0.570313
C	-1.570503	-0.029488	0.394994
C	-1.520634	-2.577291	-0.071492
C	-0.097719	0.065319	0.820200
C	-0.275665	-2.671664	-0.959918
C	0.965202	-0.511240	-0.161842
C	0.033457	-0.424329	2.272143
C	0.966549	-2.050263	-0.316434
O	0.228218	1.533160	0.834460
C	0.817348	0.168742	-1.547328
C	2.364829	-0.118147	0.334820
C	0.225506	2.507001	-0.750282
C	1.142891	1.679859	-1.560912
O	2.605363	0.753913	1.155259
O	3.332274	-0.765022	-0.292270
N	-0.410174	3.477271	-0.670688
C	4.736620	-0.496583	0.056924

H	-5.331705	-0.030991	-0.505315
H	-4.010110	-2.070616	-0.704256
H	-4.277401	2.010166	0.405853
H	-1.919061	1.978477	0.995475
H	-2.254124	-3.288455	-0.427927
H	-1.263280	-2.887100	0.936703
H	-0.478074	-2.242719	-1.933420
H	-0.052716	-3.720795	-1.122522
H	1.048919	-0.355461	2.632755
H	-0.605652	0.186420	2.894642
H	-0.303199	-1.446766	2.348069
H	1.115170	-2.498657	0.660182
H	1.833205	-2.300741	-0.907522
H	1.091998	1.622651	1.301008
H	1.508333	-0.303549	-2.232664
H	-0.185354	0.013432	-1.915077
H	2.147733	1.871167	-1.204932
H	1.072229	2.061219	-2.572291
H	-1.008775	4.039179	-0.108689
H	5.303588	-1.159903	-0.569504
H	4.970057	0.535574	-0.147524
H	4.893905	-0.709311	1.101389

RHF/3-21G Energy = -929.797093
 B3LYP/6-31G* Energy = -941.200240007
 B3LYP/6-31G* Free energy in solution = -941.25427
 Number of imaginary frequencies = 1 (-384.6174)

Cyclization product 41-P
 B3LYP/6-31G* Geometry

C	-4.174286	0.83783	0.467194
C	-3.58287	0.7312	-0.7883
C	-3.444992	0.458939	1.588013
C	-2.268784	0.274887	-0.968735
C	-2.132935	0.015579	1.437195
C	-1.506424	-0.052811	0.180649
C	-1.796432	0.124359	-2.402313
C	-0.074005	-0.627365	0.126205
C	-0.518661	0.882309	-2.76918
C	0.985809	0.201447	-0.712769
C	-0.143097	-2.11441	-0.253067
C	0.766739	0.235016	-2.253525
O	0.488571	-0.646179	1.515549
C	1.023483	1.646988	-0.120041
C	2.380722	-0.396896	-0.491928
C	0.745514	0.584534	2.201965
C	1.368637	1.684418	1.374924
O	2.71846	-1.08754	0.53566
O	3.284332	-0.15834	-1.372009
N	0.60614	0.664459	3.446136
C	4.655197	-0.658997	-1.179611
H	-5.195206	1.195145	0.561203
H	-4.160995	0.995926	-1.669388
H	-3.885315	0.500854	2.579437
H	-1.601135	-0.299545	2.322556
H	-2.602036	0.47084	-3.056473
H	-1.661804	-0.938889	-2.651642

H	-0.593307	1.928146	-2.449341
H	-0.430954	0.908081	-3.86174
H	0.839172	-2.59552	-0.312622
H	-0.737946	-2.64061	0.497192
H	-0.638748	-2.2377	-1.217804
H	0.822678	-0.790787	-2.64
H	1.61702	0.769592	-2.685379
H	1.732513	2.26123	-0.684219
H	0.028915	2.068909	-0.281891
H	2.456238	1.608109	1.517609
H	1.080627	2.64061	1.817886
H	1.891266	-1.138336	1.152756
H	0.235504	-0.194427	3.861755
H	5.19519	-0.296143	-2.050491
H	5.059204	-0.247757	-0.254364
H	4.632446	-1.748383	-1.145767

B3LYP/6-31G* Energy = -940.854984
 B3LYP/6-31G* Free energy in solution = -941.276202
 Number of imaginary frequencies = 0

Protonated alcohol 49

B3LYP/6-31G* Geometry

C	-3.565674	-0.54216	-1.151047
C	-2.256668	-0.473221	-1.641464
C	-3.812851	-0.837433	0.192932
C	-1.2016	-0.707245	-0.765152
C	-2.753769	-1.082	1.07341
C	-1.455673	-1.009628	0.580017
C	0.294617	-0.669952	-1.04126
C	0.856537	-0.464462	0.388885
C	-0.143158	-1.326431	1.271515
C	0.756729	1.0524	0.808044
C	2.245468	-0.938248	0.68959
C	0.10939	-2.847153	1.221649
O	0.049973	-0.866806	2.628357
C	1.652222	2.045776	0.032272
O	2.613632	-1.067398	1.922424
O	3.059509	-1.227127	-0.246658
C	3.080597	1.856216	0.301041
C	4.459488	-1.596237	0.056915
N	4.195496	1.637497	0.539688
H	-4.399033	-0.355545	-1.821487
H	-2.07402	-0.232498	-2.685226
H	-4.834579	-0.875397	0.557861
H	-2.952347	-1.309555	2.117737
H	0.5878	0.124374	-1.732895
H	0.654114	-1.610794	-1.476334
H	-0.28418	1.343948	0.64946
H	0.950333	1.160233	1.876755
H	0.074066	-3.228577	0.197754
H	1.063995	-3.134323	1.675873
H	-0.690384	-3.354919	1.772568
H	-0.412415	-1.46051	3.244736
H	1.487885	1.992416	-1.049622
H	1.375092	3.062103	0.335846
H	1.808792	-0.935028	2.517395

H	4.854965	-1.932144	-0.898087
H	4.958527	-0.692871	0.410431
H	4.467514	-2.389359	0.803787

B3LYP/6-31G* Energy = -862.289644
 B3LYP/6-31G* Free energy in solution = -862.657311
 Number of imaginary frequencies = 0

Protonated alcohol 50

B3LYP/6-31G* Geometry

C	-4.051407	0.8349	-0.584946
C	-2.850861	1.239014	-1.162827
C	-4.051956	-0.166534	0.388062
C	-1.629776	0.662827	-0.787277
C	-2.849915	-0.755722	0.769836
C	-1.636002	-0.342621	0.196915
C	-0.347672	1.177933	-1.421219
C	-0.353424	-1.062393	0.586426
C	0.917648	0.369431	-1.085159
C	0.900864	-0.108292	0.380722
C	-0.237061	-2.388733	-0.18718
O	-0.372055	-1.470383	1.99144
C	0.813889	1.096298	1.388397
C	2.128372	-0.917892	0.744751
C	1.912949	2.180756	1.294846
O	2.162613	-1.610596	1.828766
O	3.139984	-0.916336	-0.033539
C	3.233185	1.685364	1.694885
C	4.383316	-1.616119	0.34935
N	4.250687	1.225723	2.012344
H	-4.983978	1.295807	-0.89592
H	-2.854706	2.017853	-1.921692
H	-4.983032	-0.494797	0.839508
H	-2.8564	-1.556396	1.504684
H	-0.207184	2.225677	-1.1205
H	-0.461655	1.207748	-2.510651
H	1.809479	0.970535	-1.283859
H	0.996506	-0.500458	-1.743027
H	0.6604	-2.956711	0.083176
H	-1.104034	-3.006195	0.057831
H	-0.23967	-2.22287	-1.266037
H	-0.890457	-0.830765	2.510651
H	-0.148682	1.584427	1.21785
H	0.798813	0.719681	2.415237
H	1.980759	2.605881	0.287827
H	1.638138	3.00621	1.961945
H	1.2184	-1.631775	2.220993
H	4.983978	-1.600037	-0.556412
H	4.843948	-1.037933	1.151413
H	4.142944	-2.6317	0.661896

B3LYP/6-31G* Energy = -901.581555
 B3LYP/6-31G* Free energy in solution = -901.977195
 Number of imaginary frequencies = 0

Protonated alcohol 51

B3LYP/6-31G* Geometry

C	-3.811737	0.777435	-1.6053
C	-2.633316	0.420822	-2.25679
C	-3.909134	0.586655	-0.231552
C	-1.5446	-0.148529	-1.582092
C	-2.840271	0.021286	0.46228
C	-1.658997	-0.373489	-0.188217
C	-0.289307	-0.413498	-2.392029
C	-0.578262	-1.101913	0.638458
C	0.962555	0.296677	-1.856567
C	0.819382	-0.325577	0.717148
C	-0.422577	-2.566116	0.194153
C	1.605957	-0.350739	-0.62439
O	-1.024597	-1.139481	2.042236
C	0.52272	1.136597	1.212875
C	1.704041	-1.008362	1.772568
C	1.715149	2.103317	1.392242
O	1.248566	-1.434174	2.891083
O	2.954239	-1.142105	1.528549
C	2.584274	1.747452	2.517609
C	3.856812	-1.682922	2.5625
N	3.241669	1.411011	3.413254
H	-4.634216	1.211868	-2.165405
H	-2.545792	0.593155	-3.32608
H	-4.806	0.875885	0.307587
H	-2.933395	-0.092239	1.535141
H	-0.469559	-0.064514	-3.413269
H	-0.083649	-1.488037	-2.489639
H	0.734406	1.354553	-1.675552
H	1.729019	0.284531	-2.640381
H	0.300995	-3.105392	0.816833
H	-1.390518	-3.072266	0.280289
H	-0.111694	-2.656952	-0.845688
H	1.849365	-1.392151	-0.864716
H	2.570984	0.13205	-0.448471
H	-1.751038	-1.781387	2.127289
H	-0.1485	1.57489	0.471237
H	-0.041718	1.092529	2.148087
H	2.322098	2.180756	0.48381
H	1.311188	3.105392	1.578903
H	0.218018	-1.367508	2.834091
H	4.806	-1.802307	2.046188
H	3.920822	-0.943314	3.361511
H	3.464828	-2.635406	2.917923

B3LYP/6-31G* Energy = -940.857335
 B3LYP/6-31G* Free energy in solution = -941.281489
 Number of imaginary frequencies = 0

Intermediate 52
 B3LYP/6-31G* Geometry

N	0.320435	1.1512	2.884369
C	0.496048	0.923996	1.59584
O	-0.022293	-0.158127	1.14
C	1.279709	1.87941	0.754044
C	0.01268	-0.620911	-0.32312
C	0.942734	1.725571	-0.730804
C	-1.362808	-0.411423	-0.907196

C	0.937317	0.256958	-1.233688
C	0.39798	-2.090317	-0.191147
C	-1.251434	0.052719	-2.220947
C	-2.602722	-0.692459	-0.333618
C	0.198364	0.223358	-2.605927
C	2.365631	-0.28949	-1.366119
C	-2.398087	0.259003	-2.985962
C	-3.749298	-0.475098	-1.099594
O	2.856186	-0.680939	-2.396713
O	3.02327	-0.275208	-0.181717
C	-3.64566	-0.004181	-2.414276
C	4.38443	-0.780273	-0.222534
H	0.695145	1.980423	3.327698
H	-0.18454	0.484283	3.459427
H	1.094055	2.901749	1.100616
H	2.3378	1.655869	0.933273
H	-0.049316	2.149017	-0.919724
H	1.655197	2.309097	-1.321182
H	0.451538	-2.535568	-1.189316
H	1.3658	-2.209579	0.302094
H	-0.365158	-2.628525	0.377029
H	-2.682083	-1.061951	0.68515
H	0.398056	1.129608	-3.187668
H	0.564026	-0.617615	-3.204437
H	-2.326584	0.619095	-4.008453
H	-4.727921	-0.674316	-0.673737
H	-4.547195	0.157639	-2.99762
H	4.389084	-1.814041	-0.572693
H	4.99054	-0.167618	-0.892365
H	4.747879	-0.714828	0.802216

B3LYP/6-31G* Energy = -862.349092
 B3LYP/6-31G* Free energy in solution = -862.721651
 Number of imaginary frequencies = 0

Intermediate 53
 B3LYP/6-31G* Geometry

C	-3.353073	0.075684	-1.834396
C	-2.04866	0.234863	-2.289688
C	-3.589417	-0.133545	-0.473785
C	-0.957962	0.183395	-1.412781
C	-2.517654	-0.194656	0.407852
C	-1.192291	-0.048828	-0.04274
C	0.437714	0.357651	-1.964981
C	1.419174	0.821716	-0.890717
C	-0.061081	-0.126251	0.958603
C	1.374359	-0.096527	0.360794
C	-0.26796	-1.158691	2.064163
O	-0.259232	1.254044	1.771027
C	2.406967	0.370132	1.41864
C	1.744598	-1.520889	-0.118927
C	0.667694	2.002274	2.2312
C	2.122971	1.781418	1.941986
O	0.95311	-2.413971	-0.322067
O	3.062698	-1.616684	-0.342987
N	0.286667	3.038818	2.961029

C	3.524994	-2.88826	-0.86377
H	-4.182236	0.121567	-2.53421
H	-1.863297	0.406464	-3.347
H	-4.60289	-0.250748	-0.102753
H	-2.722473	-0.351929	1.460846
H	0.777985	-0.590179	-2.403915
H	0.423904	1.081909	-2.786652
H	2.442657	0.840927	-1.278366
H	1.162231	1.848145	-0.600891
H	-1.154968	-0.926483	2.654953
H	-0.399246	-2.139114	1.604858
H	0.585175	-1.203934	2.746277
H	3.400421	0.354965	0.968231
H	2.439041	-0.331131	2.257828
H	2.414276	2.539749	1.202896
H	2.707474	1.993195	2.844162
H	-0.699997	3.2117	3.123581
H	0.958572	3.689789	3.347
H	3.281662	-3.689774	-0.163727
H	3.054749	-3.09111	-1.828018
H	4.60289	-2.777588	-0.971436

B3LYP/6-31G* Energy = -901.630418
 B3LYP/6-31G* Free energy in solution = -902.030608
 Number of imaginary frequencies = 0

Intermediate 54

B3LYP/6-31G* Geometry

C	-3.872849	-0.266022	-1.628754
C	-2.822067	-0.128387	-2.533157
C	-3.589096	-0.468109	-0.282654
C	-1.477844	-0.19577	-2.141739
C	-2.26088	-0.528625	0.137253
C	-1.196564	-0.396927	-0.766693
C	-0.427567	-0.071442	-3.238083
C	0.253418	-0.477509	-0.27771
C	0.775955	0.882477	-2.974213
C	0.696381	1.674484	-1.664291
C	0.978302	0.916458	-0.336975
C	1.020157	-1.656906	-0.89119
O	0.198593	-0.95433	1.174728
C	0.40892	1.807495	0.804153
C	2.481125	0.704666	-0.062729
C	0.495667	-0.256485	2.212585
C	0.624741	1.234863	2.207397
O	2.887695	0.1539	0.949539
O	3.2834	1.187836	-1.007217
N	0.609192	-0.932053	3.339493
C	4.708618	1.037781	-0.782654
H	-4.900055	-0.212753	-1.97644
H	-3.046143	0.03447	-3.583878
H	-4.388977	-0.580292	0.442917
H	-2.06459	-0.705887	1.187805
H	-0.947845	0.269455	-4.137711
H	-0.060455	-1.0728	-3.49614
H	1.725845	0.34111	-3.024475
H	0.81842	1.614563	-3.786972

H	-0.29921	2.123749	-1.58609
H	1.405853	2.505203	-1.705612
H	1.227768	-1.490921	-1.946274
H	1.968079	-1.81044	-0.371704
H	0.416855	-2.563538	-0.799759
H	0.854919	2.804749	0.746506
H	-0.662827	1.926315	0.618973
H	1.614456	1.477707	2.604156
H	-0.115494	1.642105	2.90834
H	0.548615	-1.944931	3.337097
H	0.830292	-0.465897	4.210159
H	4.964539	-0.020264	-0.700684
H	5.181732	1.48822	-1.653397
H	4.998489	1.556992	0.132721

B3LYP/6-31G* Energy = -940.903738
 B3LYP/6-31G* Free energy in solution = -941.330591
 Number of imaginary frequencies = 0

Carbocation 55

B3LYP/6-31G* Geometry

C	2.280655	-3.151062	-0.381653
C	2.280655	-1.756134	-0.381653
C	1.083191	-3.911209	-0.381653
C	1.05571	-1.096603	-0.379669
C	-0.13913	-3.278992	-0.37915
C	-0.158432	-1.853607	-0.371216
C	0.760773	0.362122	-0.425446
C	-0.78476	0.459564	-0.309036
C	-1.251617	-0.982391	-0.356873
C	-1.460876	1.291183	-1.459686
C	-1.30484	1.077972	1.031387
C	-2.674576	-1.369186	-0.401291
C	-0.995544	2.755936	-1.5717
O	-2.47876	1.095383	1.326416
O	-0.330078	1.609848	1.768082
C	0.138519	2.956451	-2.586395
C	-0.748093	2.230835	3.01506
N	0.336868	4.235687	-2.984482
O	0.830795	2.025803	-2.993607
H	3.230591	-3.67865	-0.384659
H	3.215454	-1.204758	-0.39061
H	1.141708	-4.994522	-0.383179
H	-1.061707	-3.849991	-0.377975
H	1.074951	0.783127	-1.394089
H	1.28772	0.91922	0.352631
H	-1.257492	0.783493	-2.407532
H	-2.538315	1.270844	-1.280411
H	-3.230591	-0.81398	0.365448
H	-3.106155	-1.049042	-1.3618
H	-2.832474	-2.443222	-0.293518
H	-0.662323	3.15181	-0.603256
H	-1.84993	3.3759	-1.867523
H	-1.219559	1.486237	3.658844
H	0.168716	2.611603	3.461609
H	-1.452194	3.03891	2.809753
H	1.067474	4.422073	-3.658829

H -0.274124 4.994537 -2.72023

B3LYP/6-31G* Energy = -862.338316
B3LYP/6-31G* Free energy in solution = -862.699123
Number of imaginary frequencies = 0

Carbocation 56

B3LYP/6-31G* Geometry

C	2.966858	-3.070511	-0.654907
C	2.945282	-1.677719	-0.661911
C	1.771927	-3.820419	-0.649658
C	1.738831	-0.978592	-0.656937
C	0.565659	-3.162964	-0.661804
C	0.506592	-1.72789	-0.66452
C	1.71965	0.515488	-0.695007
C	0.443146	1.085678	-0.079895
C	-0.733276	-1.0625	-0.709885
C	-0.832703	0.443604	-0.679535
C	-2.013275	-1.828415	-0.867554
C	-1.136093	0.871872	-2.16832
C	-2.034637	0.834229	0.222214
C	-1.171341	2.385513	-2.439514
O	-2.942474	1.563065	-0.099274
O	-1.912827	0.254288	1.428268
C	0.187881	2.9673	-2.836685
C	-2.942276	0.578812	2.398056
N	0.267319	4.322723	-2.794968
O	1.136154	2.26384	-3.177063
H	3.92189	-3.588715	-0.648178
H	3.879105	-1.123703	-0.664642
H	1.809448	-4.90451	-0.637329
H	-0.352188	-3.738663	-0.654816
H	1.803421	0.850891	-1.741104
H	2.600723	0.910446	-0.177521
H	0.410217	2.16951	-0.22
H	0.442917	0.902863	0.999771
H	-1.962143	-2.527832	-1.708344
H	-2.201889	-2.42186	0.036591
H	-2.871536	-1.171478	-1.014908
H	-0.380585	0.43515	-2.828247
H	-2.104309	0.446564	-2.441025
H	-1.615051	2.939514	-1.608475
H	-1.8434	2.54541	-3.29361
H	-2.940964	1.652328	2.596191
H	-3.921875	0.278229	2.020828
H	-2.678345	0.018478	3.293625
H	1.097076	4.762253	-3.171982
H	-0.543243	4.90451	-2.637344

B3LYP/6-31G* Energy = -901.617516
B3LYP/6-31G* Free energy in solution = -902.009191
Number of imaginary frequencies = 0

Carbocation 57

B3LYP/6-31G* Geometry

C	-4.358658	0.344681	-0.495773
C	-3.501785	0.627396	-1.556198
C	-3.858948	-0.2296	0.679733
C	-2.1239	0.394958	-1.492737
C	-2.511993	-0.516006	0.767502
C	-1.595642	-0.166168	-0.278961
C	-1.357758	0.589859	-2.786667
C	-0.2088	-0.38678	0.029846
C	0.167847	0.627274	-2.71524
C	0.635513	1.484177	-1.533783
C	0.871445	0.634979	-0.246796
C	0.17688	-1.61	0.746613
C	0.845993	1.66011	0.966217
C	2.261887	-0.020981	-0.461807
C	1.010208	1.210449	2.434082
O	2.423218	-1.121429	-0.943665
O	3.244522	0.841797	-0.198242
C	2.338684	0.537842	2.774078
C	4.589767	0.337509	-0.395462
N	3.165115	1.221786	3.598602
O	2.632843	-0.568054	2.318054
H	-5.419647	0.556778	-0.59053
H	-3.915466	1.026428	-2.478195
H	-4.519592	-0.4543	1.510544
H	-2.127	-0.93457	1.689468
H	-1.716614	1.527451	-3.230957
H	-1.678955	-0.198669	-3.4823
H	0.542496	1.034149	-3.659683
H	0.590118	-0.38237	-2.637482
H	1.575211	1.999023	-1.751984
H	-0.100281	2.271408	-1.327591
H	0.722626	-2.180588	-0.031738
H	0.960556	-1.448013	1.501572
H	-0.655075	-2.2191	1.094971
H	1.629486	2.383438	0.723358
H	-0.110046	2.189316	0.898056
H	0.860504	2.107437	3.045837
H	0.21582	0.51297	2.722305
H	4.765182	-0.4908	0.293137
H	4.718887	0.002136	-1.42598
H	5.244141	1.179169	-0.173431
H	4.031586	0.783356	3.883667
H	2.911865	2.099091	4.02803

B3LYP/6-31G* Energy = -940.879373
B3LYP/6-31G* Free energy in solution = -941.298744
Number of imaginary frequencies = 0

Transition structure 55-TS

B3LYP/6-31G* Geometry

C	2.433945	-2.115829	-0.909027
C	2.433945	-0.716476	-0.909027
C	1.236298	-2.852707	-0.909027
C	1.212784	-0.053314	-0.908508
C	0.011322	-2.199493	-0.909851

C	0.005737	-0.791656	-0.901093
C	0.924103	1.425278	-0.915329
C	-0.582306	1.506836	-0.502121
C	-1.120392	0.108292	-0.863785
C	-1.359268	2.733749	-1.0542
C	-0.636475	1.618057	1.06015
C	-2.513092	-0.326065	-0.565292
C	-1.502609	2.833176	-2.592712
O	-1.1595	0.820816	1.80455
O	-0.024139	2.737076	1.454651
C	-2.215195	1.60791	-3.105347
C	-0.016891	2.987747	2.886002
N	-1.407288	0.428909	-2.992188
O	-3.381424	1.51973	-3.401077
H	3.381424	-2.646835	-0.904785
H	3.371155	-0.16806	-0.903534
H	1.273865	-3.937164	-0.900467
H	-0.914917	-2.765839	-0.897888
H	1.073059	1.848557	-1.918488
H	1.566177	2.000351	-0.244629
H	-2.362915	2.749008	-0.613358
H	-0.851379	3.631836	-0.694351
H	-2.567856	-0.442337	0.524902
H	-3.263641	0.41217	-0.857422
H	-2.754486	-1.286102	-1.028412
H	-0.521957	2.943954	-3.070831
H	-2.10083	3.7119	-2.842377
H	-1.04126	3.051804	3.257019
H	0.512329	2.18399	3.401077
H	0.502594	3.937164	3.003464
H	-0.455994	0.507492	-3.347595
H	-1.87764	-0.395508	-3.367737

B3LYP/6-31G* Energy = -862.320225
 B3LYP/6-31G* Free energy in solution = -862.689037
 Number of imaginary frequencies = 1 (-165.634)

Transition structure 56-TS
 B3LYP/6-31G* Geometry

C	-2.979568	0.347137	-1.337845
C	-1.706726	0.458725	-1.89357
C	-3.132889	0.124237	0.037506
C	-0.560379	0.356277	-1.1046
C	-2.011795	0.012192	0.838379
C	-0.700867	0.120377	0.296417
C	0.797043	0.439957	-1.754044
C	1.882675	0.862366	-0.768112
C	0.461	-0.035614	1.147797
C	1.865311	-0.013382	0.508942
C	0.327606	-0.732407	2.46759
C	3.028397	0.39328	1.46936
C	2.135071	-1.48967	0.062744
C	2.984604	1.826889	2.053329
O	1.346313	-2.401581	0.179321
O	3.345627	-1.597565	-0.487442
C	1.721268	2.026505	2.856415
C	3.720276	-2.922516	-0.9514
N	0.555923	2.058365	2.0381

O	1.624466	1.978516	4.059891
H	-3.855225	0.43808	-1.973938
H	-1.598923	0.629059	-2.961121
H	-4.123428	0.039688	0.47226
H	-2.151352	-0.156311	1.899048
H	1.042267	-0.544067	-2.180847
H	0.762192	1.131775	-2.602249
H	2.869659	0.788254	-1.231277
H	1.739502	1.915955	-0.500748
H	-0.580963	-0.473785	3.010071
H	0.2874	-1.805328	2.236023
H	1.176743	-0.56459	3.128784
H	3.95369	0.289093	0.898621
H	3.103424	-0.320374	2.295776
H	3.059296	2.572983	1.254013
H	3.83812	1.964355	2.720718
H	3.709198	-3.625092	-0.116302
H	3.0251	-3.257614	-1.723434
H	4.72551	-2.807266	-1.352921
H	-0.293991	2.225922	2.576263
H	0.60173	2.646835	1.209808

B3LYP/6-31G* Energy = -901.602523
 B3LYP/6-31G* Free energy in solution = -902.000044
 Number of imaginary frequencies = 1 (-136.6389)

Transition structure 57-TS
 B3LYP/6-31G* Geometry

C	-3.496628	0.687332	-0.56691
C	-2.526352	1.2769	-1.376556
C	-3.135254	0.176117	0.68045
C	-1.18573	1.375412	-1.00061
C	-1.823807	0.285736	1.098251
C	-0.791031	0.868225	0.290161
C	-0.274353	2.062119	-1.986191
C	0.544525	0.813248	0.846695
C	0.965744	1.252487	-2.371262
C	2.056458	1.343872	-1.313293
C	1.861725	0.612671	0.044083
C	0.652084	0.500412	2.314896
C	3.166061	0.898392	0.875198
C	1.845398	-0.9337	-0.217163
C	3.44693	2.375519	1.265656
O	1.015961	-1.694351	0.234634
O	2.874283	-1.302689	-0.979294
C	2.318832	3.001495	2.065308
C	2.98616	-2.7249	-1.254074
N	1.16008	3.273834	1.312744
O	2.3172	3.120193	3.272324
H	-4.524353	0.625366	-0.912735
H	-2.822525	1.676041	-2.341522
H	-3.868027	-0.3069	1.318115
H	-1.57547	-0.154419	2.052032
H	-0.858551	2.287994	-2.882446
H	0.041595	3.038589	-1.588776
H	0.692703	0.211136	-2.581924
H	1.373016	1.658325	-3.304062
H	2.243057	2.404541	-1.117523

H	2.988434	0.948502	-1.723938
H	0.618683	-0.593231	2.417908
H	1.585068	0.827393	2.76152
H	-0.154648	0.938385	2.899643
H	4.00061	0.562424	0.255341
H	3.199997	0.275787	1.772125
H	3.658707	2.972366	0.372009
H	4.341354	2.39859	1.892441
H	3.101044	-3.275711	-0.318863
H	2.095428	-3.073288	-1.779877
H	3.872986	-2.8226	-1.877762
H	0.445129	3.758362	1.852295
H	1.294571	3.675034	0.390076

B3LYP/6-31G* Energy = -940.862066
 B3LYP/6-31G* Free energy in solution = -941.286321
 Number of imaginary frequencies = 1 (-44.191)

Protonated lactam 58

B3LYP/6-31G* Geometry

C	-3.774139	-0.509811	-0.771378
C	-2.524109	-0.437271	-1.396698
C	-3.878708	-0.790695	0.593948
C	-1.378189	-0.647354	-0.635849
C	-2.731567	-1.0157	1.36174
C	-1.491119	-0.931061	0.735123
C	0.079437	-0.613632	-1.066544
C	0.800598	-0.398315	0.292694
C	-0.104767	-1.2352	1.26358
C	0.728638	1.133987	0.61145
C	2.253723	-0.821411	0.440308
N	0.1922	-0.773453	2.703705
C	0.154678	-2.753281	1.259552
C	0.923325	1.527466	2.092041
O	2.741745	-1.023193	1.5504
O	2.921417	-0.887695	-0.696564
C	0.015091	0.732025	2.972641
C	4.335617	-1.223083	-0.614624
O	-0.77327	1.050949	3.804245
H	-4.674561	-0.339325	-1.353516
H	-2.453873	-0.212326	-2.457245
H	-4.856171	-0.835403	1.063782
H	-2.827057	-1.237991	2.42218
H	0.306793	0.18428	-1.779495
H	0.389526	-1.555328	-1.535172
H	1.482819	1.649933	0.008926
H	-0.246368	1.501144	0.280411
H	1.198334	-1.013016	2.824203
H	-0.377686	-1.28212	3.389526
H	-0.582855	-3.257828	1.893234
H	0.022629	-3.145645	0.248138
H	1.159897	-3.01152	1.60495
H	0.716339	2.58812	2.250977
H	1.954987	1.326431	2.411392
H	4.684738	-1.222839	-1.645248

H	4.859665	-0.472061	-0.021133
H	4.455124	-2.207153	-0.158646

B3LYP/6-31G* Energy = -862.336352
 B3LYP/6-31G* Free energy in solution = -862.706985
 Number of imaginary frequencies = 0

Protonated lactam 59

B3LYP/6-31G* Geometry

C	-3.890732	-0.283356	-1.545654
C	-2.588455	-0.243057	-2.031815
C	-4.113419	-0.505737	-0.185516
C	-1.483215	-0.417435	-1.186661
C	-3.029205	-0.68634	0.666626
C	-1.709641	-0.633865	0.185913
C	1.05423	-0.697144	-0.82959
C	0.785507	-0.24057	0.62291
C	-0.532455	-0.93605	1.114105
C	0.630447	1.314087	0.668228
C	1.95311	-0.596146	1.562439
C	0.177536	1.890732	2.027283
O	1.819641	-0.72821	2.779419
O	3.119431	-0.677429	0.952164
C	-1.003967	1.161957	2.59021
C	4.287186	-0.938583	1.781708
N	-0.79895	-0.35257	2.528732
C	-0.405457	-2.458435	1.320648
O	-2.005524	1.566849	3.091461
C	-0.091324	-0.326828	-1.784164
H	-4.728455	-0.145462	-2.222305
H	-2.414642	-0.072906	-3.091476
H	-5.123322	-0.542725	0.210251
H	-3.239075	-0.871017	1.717392
H	1.987	-0.248291	-1.178558
H	1.221161	-1.778885	-0.835693
H	-0.098114	1.60936	-0.089523
H	1.583664	1.774323	0.389893
H	0.982025	1.804108	2.77153
H	-0.08316	2.94838	1.945313
H	4.168076	-1.894241	2.294525
H	5.123337	-0.967178	1.086
H	4.408447	-0.136658	2.511703
H	0.083084	-0.585144	3.049271
H	-1.606598	-0.795486	2.977203
H	-1.341843	-2.859146	1.722885
H	-0.245651	-2.948364	0.35817
H	0.412781	-2.728546	1.99472
H	0.057632	0.693161	-2.163071
H	-0.032089	-0.97	-2.669662

B3LYP/6-31G* Energy = -901.624915
 B3LYP/6-31G* Free energy in solution = -902.023028
 Number of imaginary frequencies = 0

Protonated lactam 60

B3LYP/6-31G* Geometry

C	-3.856903	0.868561	-1.860016
C	-2.606369	0.693665	-2.445511

C	-4.00029	0.611084	-0.5036
C	-1.481949	0.268356	-1.723831
C	-2.896469	0.1911	0.238327
C	-1.620209	0.019836	-0.332779
C	1.655685	0.380142	-0.739456
C	0.862595	0.320862	0.599686
C	-0.465073	-0.552475	0.529144
C	0.481476	1.747711	1.086166
C	1.847702	-0.263687	1.660263
C	-0.156097	1.772537	2.489883
O	1.540878	-1.042542	2.563553
O	3.071045	0.21666	1.54071
C	-1.213242	0.731323	2.72229
C	4.060715	-0.230316	2.511002
N	-0.939377	-0.593658	2.005264
C	-0.218048	-2.029022	0.159622
O	-2.165344	0.7742	3.439117
C	-0.193573	0.126892	-2.509827
C	0.972275	0.963959	-1.975891
H	-4.700928	1.197205	-2.458313
H	-2.489166	0.889008	-3.50766
H	-4.959778	0.729568	-0.010086
H	-3.089523	0.003036	1.286041
H	2.5551	0.964783	-0.536118
H	2.007538	-0.631485	-0.979111
H	-0.214752	2.183105	0.365295
H	1.374359	2.378967	1.09761
H	-0.602768	2.74408	2.717636
H	0.606659	1.595566	3.263382
H	4.975464	0.290222	2.234772
H	3.741638	0.039368	3.519119
H	4.184647	-1.311676	2.436874
H	-0.116257	-1.034683	2.499359
H	-1.764206	-1.189957	2.124985
H	0.096619	-2.112183	-0.880569
H	0.548126	-2.491211	0.787552
H	-1.148544	-2.598145	0.256393
H	0.118576	-0.924866	-2.577728
H	-0.397751	0.430374	-3.540771
H	1.742218	1.023285	-2.754166
H	0.642395	1.995224	-1.800705

B3LYP/6-31G* Energy = -940.894753
 B3LYP/6-31G* Free energy in solution = -941.319451
 Number of imaginary frequencies = 0