Diastereoselective Olefin Amidoacylation via Photoredox PCET/Nickel-Dual Catalysis: Reaction Scope and Mechanistic Insights

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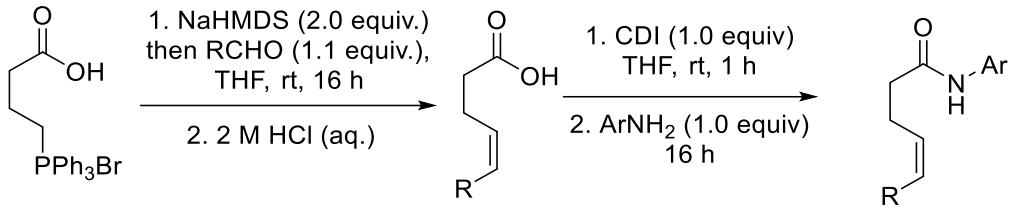
Contents

1. General Considerations

Unless otherwise noted, all reactions were carried out under an inert atmosphere of argon or nitrogen via standard Schlenk techniques or in a glovebox. Reactions were monitored by HPLC, ^{1}H NMR, and/or by TLC on silica gel plates (F_{254}, 60 Å). Thin layer chromatography was performed using hexanes/EtOAc as the eluents and visualized using $KMnO_4$ stain and/or UV light. Reactions were purified by flash chromatography accompanied with an automated system (visualized at 254 nm, monitored with all-wavelength and ELS detector) with silica cartridges (60 Å porosity, 20-40 μm). Unless otherwise mentioned, all acyl chlorides, anhydrides, carboxylic acids, isocyanates, anlines, and alcohols were purchased from commercial sources and used as received. $[Ir\{dF(CF_3)_2ppy\}_2(bpy)][PF_6]$,[1] $[Ir\{dF(CF_3)_2ppy\}_2(dFbpy)][PF_6]$,[2] $[Ir\{dF(CF_3)_2ppy\}_2(dCF_3bpy)][PF_6]$,[2] $(dMeObpy)Ni(H_2O)_2Br_2$,[3] and $Bu_4N[OP(O)(OBu)_2]$[4] were synthesized using literature procedures. Unless otherwise noted, all amides were synthesized according to a previous report.[3] MeCN and 1,2-dichloroethane (extra dry, 99.8%) were purchased and used as received. Other solvents were purified either by distillation over Na or CaH_2 or by passing through alumina cartridges in a solvent purification system. Irradiation of reaction vessels was accomplished using 5W 455 nm blue LED (light emitting diodes) strip about 3 cm from the reaction vessel with a fan above to maintain room temperature. The photoredox reaction equipment was constructed according to a previous report.[5] Reaction optimization was carried out via high throughput experimentation and verified on the benchtop. Factors affecting reaction performance, such as solvents, nickel sources, photoredox catalysts, bases, substrates loadings as well as temperature have been thoroughly examined. Melting points (°C) are uncorrected. NMR spectra (^{1}H, ^{13}C {^{1}H}, ^{19}F) were recorded on a 500 MHz spectrometer at 298 K. All ^{1}H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signal for $CHCl_3$ (7.26 ppm). All ^{13}C NMR spectra were reported in ppm relative to residual $CHCl_3$ (77.2 ppm) and were obtained with ^{1}H decoupling. All ^{19}F and ^{31}P NMR spectra were obtained in $CDCl_3$ solution and are reported unreferenced. Coupling constants (*J*) are reported in Hertz (Hz). HRMS was obtained by either ESI or EI with a TOF spectrometer in CH_3CN or $CHCl_3$. The data were calibrated and reported by neutral atom masses, and the electron mass is not included. IR spectra were obtained with neat samples.

2. Synthesis of Starting Materials

2.1 Procedure for Amide Starting Materials Synthesis (*General Procedure I*)

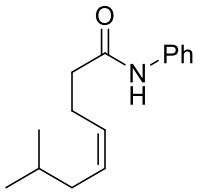


Under an intert atmosphere, (3-carboxypropyl)triphenylphosphonium bromide (1.288 g, 3 mmol, 1.0 equiv, purchased or prepared according to the literature[6]) was charged in a round-bottom flask and suspended in dry THF (1.0 M). The mixture was cooled to 0 °C followed by slow addition of NaHMDS (3 mL, 2.0 M soln in THF). The reaction was then stirred at 0 °C for another 30 min, and the corresponding aldehyde was subsequently added dropwise into the reaction (3.6 mmol, 1.2 equiv, neat if liquid; 1.0 M in THF if solid). The reaction was left to slowly warm to rt overnight before being quenched by satd aq NH_4Cl. The pH was adjusted to 2 by addition of 2 M HCl, and the reaction was extracted with 50 mL EtOAc. After concentrating the organic phase, the residue was directly used in the next step without purification.

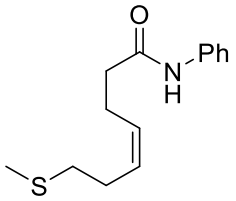
Under an inert atmosphere, CDI (3 mmol, 1.0 equiv) was added to a soln of the corresponding carboxylic acid (1.0 equiv) in dry THF (1.0 M) (*Caution! CO_2 is released violently!*). Upon stirring at rt for 1 h, the corresponding aniline derivative (1.0 equiv) was added. The reaction was stirred at rt overnight. The reaction was subsequently taken to dryness under reduced pressure and the resulting product was purified using an automated system (silica gel, hexanes/EtOAc gradient).

2.2 Characterization Data

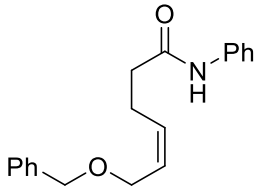
N-Phenylhex-4-enamide (**S1**)[7] was prepared *via* General Procedure I. Other starting materials were synthesized according to the literature.[3,4] All characterization data match previous literature reports.



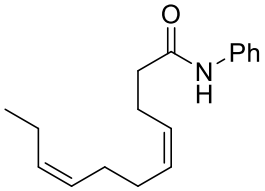
7-Methyl-*N*-phenyloct-4-enamide (S31): Prepared following General Procedure I, starting from commercially available isovaleraldehyde (310 mg, 3.6 mmol, 1.2 equiv). The corresponding product was obtained as a yellow oil (488.2 mg, 2.6 mmol, 86% yield), upon purification using an automated system (silica gel, hexanes/EtOAc, 0 to 20%). ^{1}H NMR (500 MHz, $CDCl_3$) of major stereoisomer δ 7.52 (d, *J* = 7.9 Hz, 2H), 7.43 – 7.29 (m, 3H), 7.10 (t, *J* = 7.4 Hz, 1H), 5.62 – 5.36 (m, 2H), 2.52 – 2.36 (m, 4H), 1.97 (t, *J* = 7.0 Hz, 2H), 1.61 (qt, *J* = 12.9, 6.6 Hz, 1H), 0.90 (d, *J* = 6.6 Hz, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.1, 138.0, 130.8, 129.1, 128.2, 124.3, 120.0, 42.0, 37.7, 36.4, 28.7, 22.5 ppm. IR (neat, cm^{-1}): 3300, 2955, 2926, 1659, 1619, 1599, 1543, 1498, 1465, 1442, 1383, 1309, 1253, 753, 691. HRMS (ES+) calcd for ($C_{15}H_{22}NO$) $[M+H]^+$ 232.1701, found 232.1703.



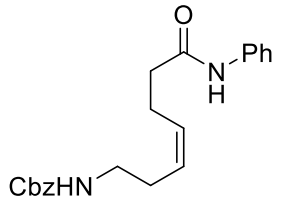
7-(Methylthio)-*N*-Phenylhept-4-enamide (S32): Prepared following General Procedure I, starting from commercially available 3-(methylthio)propanal (375 mg, 3.6 mmol, 1.2 equiv). The corresponding product was obtained as a tan solid (638.4 mg, 2.2 mmol, 74% yield), upon purification using an automated system (silica gel, hexanes/EtOAc, 0 to 20%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.9 Hz, 2H), 7.44 – 7.36 (m, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 5.61 – 5.43 (m, 2H), 2.52 (dt, *J* = 17.0, 7.4 Hz, 4H), 2.47 – 2.36 (m, 4H), 2.10 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.8, 138.0, 130.0, 129.3, 129.1, 124.4, 120.0, 76.9, 37.6, 34.2, 27.1, 23.5, 15.7 ppm. IR (neat, cm^{-1}): 3300, 2914, 1660, 1599, 1543, 1499, 1442, 1309, 1255, 1078, 967, 755. HRMS (ES+) calcd for ($C_{14}H_{20}NOS$) $[M+H]^+$ 250.1266, found 250.1272.



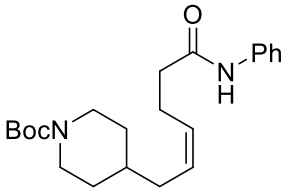
6-(Benzyloxy)-*N*-phenylhex-4-enamide (S33): Prepared following General Procedure I, starting from commercially available 2-(benzyloxy)acetaldehyde (541 mg, 3.6 mmol, 1.2 equiv). The corresponding product was obtained as a yellow oil (752.6 mg, 2.6 mmol, 85% yield), upon purification using an automated system (silica gel, hexanes/EtOAc, 0 to 50%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.46 (m, 3H), 7.35 (d, *J* = 4.4 Hz, 4H), 7.32 – 7.28 (m, 3H), 7.10 (t, *J* = 7.5 Hz, 1H), 5.72 (dt, *J* = 12.6, 6.5 Hz, 1H), 5.68 – 5.60 (m, 1H), 4.52 (s, 2H), 4.13 (d, *J* = 6.4 Hz, 2H), 2.50 (d, *J* = 7.4 Hz, 2H), 2.48 – 2.36 (m, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 138.2, 131.8, 129.0, 128.5, 128.5, 128.0, 127.9, 127.8, 124.4, 120.0, 72.6, 65.8, 37.3, 23.7 ppm. IR (neat, cm^{-1}): 3301, 1660, 1600, 1540, 1498, 1441, 1387, 1363, 1309, 1248, 1167, 1070, 971, 752, 693. HRMS (ES+) calcd for ($C_{19}H_{22}NO_2$) $[M+H]^+$ 296.1652, found 296.1656.



(8*Z*)-*N*-Phenylundeca-4,8-dienamide (S34): Prepared following General Procedure I, starting from commercially available (*Z*)-hept-4-enal (404 mg, 3.6 mmol, 1.2 equiv). The corresponding product was obtained as a tan solid (695.4 mg, 2.7 mmol, 90% yield), upon purification using an automated system (silica gel, hexanes/EtOAc, 0 to 20%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.9 Hz, 2H), 7.41 – 7.29 (m, 3H), 7.10 (t, *J* = 7.4 Hz, 1H), 5.59 – 5.26 (m, 4H), 2.48 (d, *J* = 7.3 Hz, 1H), 2.47 – 2.38 (m, 3H), 2.18 – 2.06 (m, 4H), 2.06 – 2.00 (m, 2H), 0.95 (td, *J* = 7.5, 1.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.0, 138.0, 132.4, 131.5, 129.1, 128.4, 128.0, 124.4, 120.0, 37.7, 32.8, 27.2, 23.5, 20.7, 14.5 ppm. IR (neat, cm^{-1}): 3300, 2914, 1660, 1599, 1543, 1499, 1442, 1309, 1255, 1078, 967, 755. HRMS (ES+) calcd for ($C_{17}H_{23}NO$) $[M+H]^+$ 258.1858, found 258.1848.



Benzyl (7-oxo-7-(phenylamino)hept-3-en-1-yl)carbamateenamide (S35): Prepared following General Procedure I, starting from commercially available benzyl (3-oxopropyl)carbamate (746.0 mg, 3.6 mmol). The corresponding product was obtained as a tan solid (655.0 mg, 1.9 mmol, 62% yield), upon purification using an automated system (silica gel, hexanes/EtOAc, 0 to 20%). mp = 127 – 130 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.52 (dd, *J* = 13.4, 7.9 Hz, 3H), 7.44 – 7.29 (m, 6H), 7.10 (dt, *J* = 14.9, 7.4 Hz, 2H), 5.61 – 5.51 (m, 1H), 5.48 – 5.38 (m, 1H), 5.10 (s, 2H), 3.29 – 3.19 (m, 2H), 2.51 – 2.44 (m, 1H), 2.40 (t, *J* = 8.2 Hz, 2H), 2.37 – 2.27 (m, 1H), 2.18 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.8, 156.8, 138.2, 136.8, 130.8, 129.1, 129.1, 128.7, 128.3, 128.2, 128.1, 127.8, 124.4, 124.3, 120.0, 119.9, 66.8, 41.0, 37.7, 27.9, 23.6 ppm. IR (neat, cm^{-1}):3309, 3064, 1696, 1667, 1599, 1540, 1499, 1442, 1314, 1255, 1137, 1028, 754, 694. HRMS (ES+) calcd for ($C_{21}H_{25}N_2O_3$) $[M+H]^+$ 353.1865, found 353.1849.



***tert*-Butyl 4-(6-oxo-6-(phenylamino)hex-2-en-1-yl)piperidine-1-carboxylate (S36):** Prepared following General Procedure I, starting from commercially available *N*-Boc-4-piperidineacetaldehyde (818 mg, 3.60 mmol). The corresponding product was obtained as a sticky yellow oil (1.018 g, 2.7 mmol, 91% yield), upon purification using an automated system (silica gel, hexanes/EtOAc, 0 to 40%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.52 (t, *J* = 6.5 Hz, 2H), 7.29 (t, *J* = 7.7 Hz, 2H), 7.08 (t, *J* = 7.4 Hz, 1H), 5.50 – 5.39 (m, 2H), 4.19 – 3.89 (m, 2H), 2.62 (s, 2H), 2.50 – 2.30 (m, 4H), 2.00 (t, *J* = 6.5 Hz, 2H), 1.60 (t, *J* = 13.7 Hz, 2H), 1.45 (s, 9H), 1.38 (dtt, *J* = 14.7, 7.6, 3.9 Hz, 1H), 1.12 – 0.97 (m, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.0, 155.0, 138.2, 130.1, 129.1, 129.0, 124.2, 119.9, 79.4, 39.7, 37.5, 36.5, 34.1, 32.0, 28.6, 23.5 ppm. IR (neat, cm^{-1}): 3310, 2925, 1660, 1600, 1543, 1499, 1441, 1425, 1392, 1365, 1278, 1244, 1158, 1125, 909, 755, 730, 693. HRMS (ES+) calcd for ($C_{22}H_{33}N_2O_3$) $[M+H]^+$ 373.2491, found 373.2482.

3. Photoredox PCET/Nickel-Catalyzed Amidoacylation Reaction

3.1 General Procedure

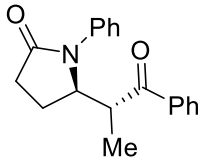
General Procedure II

An 8.0 mL screw-cap vial containing a stirring bar was charged with [Ni(dMeObpy)Cl_2] (6.3 mg, 0.018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), amide (0.36 mmol, 1.2 equiv), acyl (pseudo)halide (if solid) (0.3 mmol, 1.0 equiv) and Bu_4N[OP(O)(OBu)$_2$] (338.8 mg, 0.75 mmol, 2.5 equiv). Next, the vial was closed, and three vacuum/argon cycles were carried out. Under an inert atmosphere, MeCN was added (6.0 mL, 0.05 M), followed by addition of the acyl (pseudo)halide (if liquid). After further sealing with Parafilm®, the reaction was placed in the blue LED bay and stirred at rt until completion (a fan was added to disperse any heat coming from the blue LEDs). When completed, the reactions were taken to dryness and purified by column chromatography using an automated system (hexanes/EtOAc gradient), delivering the corresponding pure product.

General Procedure III

Under an inert atmosphere, an 8.0 mL screw-cap vial containing a stirring bar was charged with carboxylic acid (0.3 mmol, 1.0 equiv), $(COCl)_2$ (0.33 mmol, 1.1 equiv) and CH_2Cl_2 (2 mL). The reaction was cooled to 0 °C, followed by addition of DMF (10 µL). The mixture was stirred for 30 min before removal of the solvent under vacuum. It was subsequently charged with [Ni(dMeObpy)(H_2O)$_2$(Br_2)] (8.5 mg, 0.018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), amide (0.36 mmol, 1.2 equiv), and Bu_4N[OP(O)(OBu)$_2$] (338.8 mg, 0.75 mmol, 2.5 equiv). Next, the vial was closed, and three vacuum/argon cycles were carried out. Under inert atmosphere, MeCN was added (6.0 mL, 0.05 M). After further sealing with Parafilm®, the reaction was placed in the blue LED bay and stirred at rt until completion (a fan was added to disperse any heat coming from the blue LEDs). When completed, the reactions were taken to dryness and purified by column chromatography using an automated system (hexanes/EtOAc gradient), delivering the corresponding pure product.

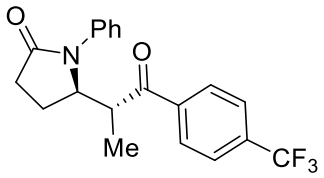
3.2 Characterization Data



(*R)-5-((*R**)-1-Oxo-1-phenylpropan-2-yl)-1-phenylpyrrolidin-2-one (1):**

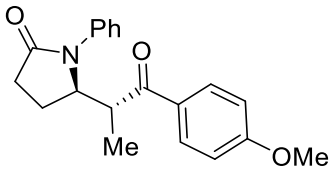
General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), Bu_4N[OP(O)(OBu)$_2$] (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (66.1 mg, 0.23 mmol, 75% yield). mp = 93 – 95 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 – 7.71 (m, 2H), 7.56 (ddt, *J* = 8.8, 7.2, 1.7 Hz, 1H), 7.43 (dd, *J* = 8.7, 7.2 Hz, 4H), 7.38 (dd, *J* = 8.6, 1.5 Hz, 2H), 7.26 (tt, *J* = 7.2, 1.4 Hz, 1H), 4.71 (dt, *J* = 8.5, 4.2 Hz, 1H), 3.78 (qd, *J* = 6.8, 3.8 Hz, 1H), 2.61 (ddd, *J* = 17.5, 10.3, 7.2 Hz, 1H), 2.53 (ddd, *J* = 17.5, 10.3, 6.1 Hz, 1H), 2.20 – 2.12 (m, 1H), 2.12 – 2.03 (m, 1H), 1.12 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.2, 174.4, 137.0, 136.1, 133.4, 129.4, 128.9, 128.0, 126.6, 124.9, 60.3, 42.3, 31.5, 18.9, 9.6 ppm. IR (neat, cm^{-1}): 2975, 1679, 1596, 1498, 1448,

1395, 1365, 1295, 1211, 1158, 908. HRMS (ES+) calcd for ($C_{19}H_{20}NO_2$) $[M+H]^+$ 294.1494, found 294.1499.



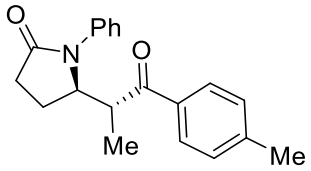
(*R)-5-((*R**)-1-Oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl)-1-phenylpyrrolidin-2-one (2):**

General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), 4-(trifluoromethyl)benzoyl chloride (75.1 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (62.6 mg, 0.21 mmol, 69% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.46 – 7.40 (m, 2H), 7.38 – 7.33 (m, 2H), 7.27 (ddt, *J* = 8.7, 7.2, 1.5 Hz, 1H), 4.71 (dt, *J* = 8.6, 4.4 Hz, 1H), 3.76 (qd, *J* = 6.9, 4.0 Hz, 1H), 2.71 – 2.49 (m, 2H), 2.21 (dddd, *J* = 13.6, 10.2, 8.6, 7.2 Hz, 1H), 2.07 (dddd, *J* = 13.8, 10.7, 6.3, 4.8 Hz, 1H), 1.16 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.6, 174.5, 138.9, 136.9, 134.7 (q, *J* = 33.6 Hz), 129.5, 128.5, 127.0, 126.0 (q, *J* = 3.8 Hz), 123.6 (q, *J* = 272.4 Hz), 60.4, 43.0, 31.4, 19.3, 9.9 ppm. ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.2 ppm. IR (neat, cm^{-1}): 1685, 1498, 1408, 1392, 1321, 1296, 1210, 1166, 1125, 1112, 1065, 972, 759, 694. HRMS (ES+) calcd for ($C_{20}H_{19}F_3NO_2$) $[M+H]^+$ 362.1368, found 362.1364.



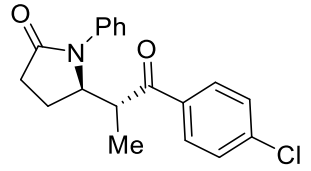
(*R)-5-((*R**)-1-(4-Methoxyphenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (3):**

General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), 4-(methoxy)benzoyl chloride (51.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (50.5 mg, 0.16 mmol, 52% yield). mp = 109 – 112 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.73 (m, 2H), 7.45 (dd, *J* = 8.5, 7.2 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.30 – 7.25 (m, 1H), 6.94 – 6.89 (m, 2H), 4.70 (ddd, *J* = 8.4, 4.8, 3.7 Hz, 1H), 3.87 (s, 3H), 3.74 (qd, *J* = 6.9, 3.7 Hz, 1H), 2.63 (ddd, *J* = 17.6, 10.1, 7.5 Hz, 1H), 2.54 (ddd, *J* = 17.4, 10.0, 6.3 Hz, 1H), 2.21 – 2.07 (m, 2H), 1.12 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.7, 174.6, 163.9, 137.1, 130.5, 129.4, 129.1, 126.7, 125.1, 114.1, 60.7, 55.6, 41.9, 31.6, 19.0, 9.8 ppm. IR (neat, cm^{-1}): 2930, 1693, 1670, 1595, 1572, 1498, 1378, 1365, 1317, 1288, 1250, 1219, 1184, 1151, 1029, 862, 786, 756, 695. HRMS (ES+) calcd for ($C_{20}H_{22}NO_3$) $[M+H]^+$ 324.1600, found 324.1606.



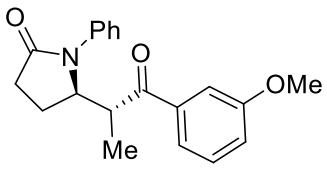
(*R)-5-((*R**)-1-Oxo-1-(*p*-tolyl)propan-2-yl)-1-phenylpyrrolidin-2-one (4&13):**

General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), *p*-toluoyl chloride (46.3 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (52.6 mg, 0.17 mmol, 57% yield for entry **4**; 60.9 mg, 0.20 mmol, 66% yield for entry **13**, following General Procedure III). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.1 Hz, 2H), 7.45 (dd, *J* = 8.4, 7.2 Hz, 2H), 7.42 – 7.37 (m, 2H), 7.29 – 7.22 (m, 3H), 4.70 (dt, *J* = 8.4, 4.2 Hz, 1H), 3.77 (qd, *J* = 6.8, 3.7 Hz, 1H), 2.62 (ddd, *J* = 17.5, 10.2, 7.4 Hz, 1H), 2.53 (ddd, *J* = 17.3, 10.2, 6.1 Hz, 1H), 2.41 (s, 3H), 2.20 – 2.05 (m, 2H), 1.11 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.8, 174.5, 144.4, 137.1, 133.6, 129.6, 129.4, 128.2, 126.6, 125.0, 60.5, 42.2, 31.5, 21.7, 18.8, 9.5 ppm. IR (neat, cm^{-1}): 2975, 1694, 1674, 1605, 1598, 1497, 1364, 1336, 1293, 1218, 1206, 1184, 968, 758, 729, 694. HRMS (ES+) calcd for ($C_{20}H_{22}NO_2$) $[M+H]^+$ 308.1651, found 308.1678.



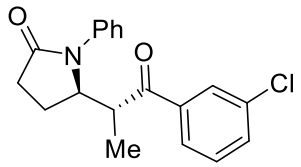
(*R)-5-((*R**)-1-(4-Chlorophenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (5):**

General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), 4-chlorobenzoyl chloride (52.5 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (58.9 mg, 0.18 mmol, 60% yield). mp = 99 – 103 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (dt, *J* = 8.5, 1.9 Hz, 2H), 7.46 – 7.40 (m, 4H), 7.39 – 7.34 (m, 2H), 7.30 – 7.25 (m, 1H), 4.70 (dt, *J* = 8.6, 4.3 Hz, 1H), 3.72 (qd, *J* = 6.8, 3.8 Hz, 1H), 2.70 – 2.51 (m, 2H), 2.20 (dddd, *J* = 14.1, 10.4, 8.5, 7.1 Hz, 1H), 2.14 – 2.03 (m, 1H), 1.14 (dd, *J* = 6.9, 1.3 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.2, 174.5, 140.0, 137.0, 134.5, 129.6, 129.5, 129.3, 126.9, 125.2, 60.5, 42.6, 31.5, 19.2, 9.9 ppm. IR (neat, cm^{-1}): 2975, 1680, 1589, 1498, 1456, 1397, 1333, 1295, 1210, 1091, 1012, 971, 846, 760, 695. HRMS (ES+) calcd for ($C_{19}H_{19}ClNO_2$) $[M+H]^+$ 328.1104, found 328.1107.



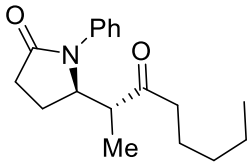
(*R)-5-((*R**)-1-(3-Methoxyphenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (6):**

General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), 3-methoxybenzoyl chloride (51.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (65.0 mg, 0.23 mmol, 78% yield). mp = 92 – 95 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.73 (m, 2H), 7.45 (dd, *J* = 8.5, 7.2 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.30 – 7.25 (m, 1H), 6.94 – 6.89 (m, 2H), 4.70 (ddd, *J* = 8.4, 4.8, 3.7 Hz, 1H), 3.87 (s, 3H), 3.74 (qd, *J* = 6.9, 3.7 Hz, 1H), 2.63 (ddd, *J* = 17.6, 10.1, 7.5 Hz, 1H), 2.54 (ddd, *J* = 17.4, 10.0, 6.3 Hz, 1H), 2.21 – 2.07 (m, 2H), 1.12 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.2, 174.6, 160.2, 137.6, 137.1, 129.9, 129.5, 126.8, 125.1, 120.6, 120.0, 112.6, 60.6, 55.6, 42.6, 31.6, 18.9, 9.6 ppm. IR (neat, cm^{-1}): 1693, 1670, 1595, 1572, 1498, 1378, 1365, 1317, 1288, 1250, 1219, 1184, 1151, 1029, 862, 786, 756, 695. HRMS (ES+) calcd for ($C_{20}H_{22}NO_3$) $[M+H]^+$ 324.1600, found 324.1606.



(*R)-5-((*R**)-1-(3-Chlorophenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (7&12):**

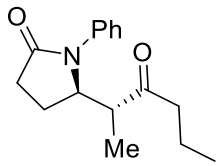
General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), 4-chlorobenzoyl chloride (52.5 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (56.8 mg, 0.17 mmol, 58% yield for entry **7**; 55.7 mg, 0.17 mmol, 57% yield for entry **12**, General Procedure III was followed). mp = 99 – 103 ℃. NMR spectra represent the major diastereoisomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (dt, *J* = 8.5, 1.9 Hz, 2H), 7.46 – 7.40 (m, 4H), 7.39 – 7.34 (m, 2H), 7.30 – 7.25 (m, 1H), 4.70 (dt, *J* = 8.6, 4.3 Hz, 1H), 3.72 (qd, *J* = 6.8, 3.8 Hz, 1H), 2.70 – 2.51 (m, 2H), 2.20 (dddd, *J* = 14.1, 10.4, 8.5, 7.1 Hz, 1H), 2.14 – 2.03 (m, 1H), 1.14 (dd, *J* = 6.9, 1.3 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.2, 174.5, 140.0, 137.0, 134.5, 129.6, 129.5, 129.3, 126.9, 125.2, 60.5, 42.6, 31.5, 19.2, 9.9 ppm. IR (neat, cm^{-1}): 2975, 1680, 1589, 1498, 1456, 1397, 1333, 1295, 1210, 1091, 1012, 971, 846, 760, 695. HRMS (ES+) calcd for ($C_{19}H_{19}ClNO_2$) $[M+H]^+$ 328.1104, found 328.1107.



(*R)-5-((*R**)-3-Oxooctan-2-yl)-1-phenylpyrrolidin-2-one (8):**

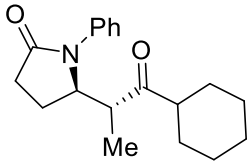
General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), hexanoic anhydride (64.3 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for

24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (37.2 mg, 0.13 mmol, 43% yield). NMR data represent the major diastereoisomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.39 (m, 2H), 7.39 – 7.35 (m, 2H), 7.27 – 7.23 (m, 1H), 4.75 (dt, *J* = 8.7, 4.5 Hz, 1H), 2.83 (qd, *J* = 7.1, 4.0 Hz, 1H), 2.58 (ddd, *J* = 9.5, 7.2, 3.8 Hz, 2H), 2.37 (ddd, *J* = 17.2, 8.4, 6.3 Hz, 1H), 2.32 – 2.21 (m, 2H), 1.91 (dddd, *J* = 14.0, 9.3, 6.9, 4.9 Hz, 1H), 1.55 – 1.42 (m, 2H), 1.32 – 1.24 (m, 2H), 1.24 – 1.16 (m, 2H), 1.03 (d, *J* = 7.1 Hz, 3H), 0.88 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 211.8, 174.6, 137.0, 129.4, 126.5, 124.8, 59.8, 47.4, 41.7, 31.6, 31.4, 23.3, 22.6, 19.5, 14.0, 9.3 ppm. IR (neat, cm^{-1}): 2931, 1700, 1598, 1458, 1392, 1296, 1224, 1045, 760, 695, 555. HRMS (ES+) calcd for ($C_{18}H_{26}NO_2$) $[M+H]^+$ 288.1964, found 288.1989.



(*R)-5-((*R**)-3-Oxohexan-2-yl)-1-phenylpyrrolidin-2-one (9):**

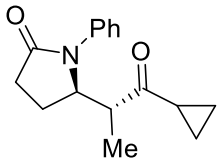
General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), butyryl chloride (32.0 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (38.1 mg, 0.15 mmol, 49% yield). NMR data represent the major diastereoisomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (t, *J* = 7.8 Hz, 2H), 7.38 – 7.34 (m, 2H), 7.26 – 7.20 (m, 1H), 4.74 (dt, *J* = 8.7, 4.4 Hz, 1H), 2.81 (qd, *J* = 7.1, 4.0 Hz, 1H), 2.56 (ddd, *J* = 9.4, 7.3, 4.1 Hz, 2H), 2.35 (ddd, *J* = 17.2, 8.1, 6.4 Hz, 1H), 2.30 – 2.19 (m, 2H), 1.90 (dddd, *J* = 13.9, 9.2, 6.9, 4.9 Hz, 1H), 1.50 (tq, *J* = 14.2, 7.1 Hz, 2H), 1.02 (d, *J* = 7.1 Hz, 3H), 0.85 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 211.6, 174.6, 137.0, 129.4, 126.5, 124.8, 59.7, 47.5, 43.6, 31.6, 19.5, 17.0, 13.8, 9.2 ppm. IR (neat, cm^{-1}): 2963, 2934, 1693, 1597, 1498, 1388, 1295, 1223, 1120, 1029, 900, 834, 760, 695, 555. HRMS (ES+) calcd for ($C_{16}H_{22}NO_2$) $[M+H]^+$ 260.1651, found 260.1671.



(*R)-5-((*R**)-1-Cyclohexyl-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (10):**

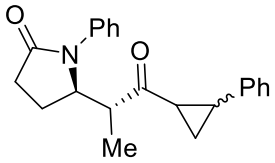
General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), cyclohexanecarbonyl chloride (44.0 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (39.7 mg, 0.13 mmol, 44% yield). NMR data represent the major diastereoisomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (t, *J* = 7.8 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.28 – 7.23 (m, 1H), 4.68 (dt, *J* = 8.5, 4.3 Hz, 1H), 2.98 (qd, *J* = 6.9, 3.6 Hz, 1H), 2.66 – 2.49 (m, 2H), 2.32 (ddt, *J* = 11.3, 7.1, 3.9 Hz,

1H), 2.28 – 2.17 (m, 1H), 1.98 (tt, *J* = 14.2, 6.2 Hz, 1H), 1.81 – 1.69 (m, 3H), 1.65 (d, *J* = 9.5 Hz, 1H), 1.56 (d, *J* = 12.6 Hz, 1H), 1.31 – 1.14 (m, 5H), 1.01 (d, *J* = 7.0 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 214.7, 174.6, 137.0, 129.4, 126.5, 124.6, 59.7, 49.8, 45.5, 31.6, 28.7, 28.5, 25.8, 25.7, 25.6, 19.5, 9.5 ppm. IR (neat, cm^{-1}): 2929, 2854, 1695, 1597, 1498, 1389, 1295, 1251, 1222, 1143, 1055, 988, 759, 695. HRMS (ES+) calcd for ($C_{19}H_{26}NO_2$) $[M+H]^+$ 300.1964, found 300.1960.



(*R)-5-((*R**)-1-Cyclopropyl-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (11):**

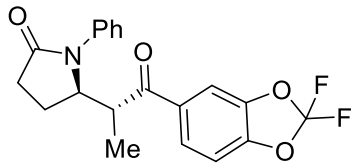
General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), cyclopropanecarbonyl chloride (31.4 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (40.2 mg, 0.16 mmol, 52% yield). NMR data represent the major diastereoisomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.38 (m, 4H), 7.27 – 7.23 (m, 1H), 4.83 (dt, *J* = 8.6, 4.3 Hz, 1H), 3.05 (qd, *J* = 7.0, 3.8 Hz, 1H), 2.66 – 2.45 (m, 2H), 2.31 – 2.18 (m, 1H), 1.97 – 1.86 (m, 2H), 1.07 (d, *J* = 7.0 Hz, 3H), 1.03 – 0.97 (m, 1H), 0.94 (dt, *J* = 9.3, 4.3 Hz, 1H), 0.90 – 0.81 (m, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 211.1, 174.6, 137.1, 129.4, 126.5, 124.7, 59.8, 48.2, 31.6, 19.8, 19.2, 11.4, 11.4, 8.8 ppm. IR (neat, cm^{-1}): 2964, 1689, 1597, 1498, 1456, 1381, 1294, 1247, 1223, 1196, 1101, 1045, 1013, 998, 694, 554. HRMS (ES+) calcd for ($C_{16}H_{20}NO_2$) $[M+H]^+$ 258.1494, found 258.1505.



(5*R)-5-((2*R**)-1-Oxo-1-(2-phenylcyclopropyl)propan-2-yl)-1-phenylpyrrolidin-2-one (14):**

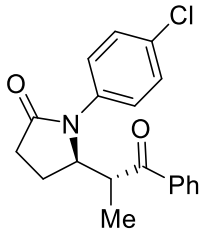
General Procedure III was followed using 2-phenylcyclopropane-1-carboxylic acid (48.7 mg, 0.3 mmol, 1.0 equiv), $(COCl)_2$ (41.9 mg, 0.33 mmol, 1.1 equiv), DMF (10 µL), CH_2Cl_2 (2 mL), *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (54.0 mg, 0.16 mmol, 54% yield). NMR spectra represent a 1:1 mixture of two diastereoisomers originating from the acid coupling partner. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (ddd, *J* = 13.7, 8.6, 6.9 Hz, 4H), 7.37 – 7.32 (m, 1H), 7.32 – 7.28 (m, 1H), 7.24 (tt, *J* = 7.4, 4.5 Hz, 2H), 7.07 (dd, *J* = 7.5, 2.0 Hz, 2H), 4.83 (ddt, *J* = 15.6, 8.6, 4.3 Hz, 1H), 3.07 (qd, *J* = 7.1, 3.7 Hz, 1H), 2.67 – 2.54 (m, 2H), 2.53 – 2.39 (m, 1H), 2.33 – 2.20 (m, 1H), 2.13 (dddd, *J* = 16.5, 8.0, 5.2, 4.0 Hz, 1H), 1.98 – 1.87 (m, 1H), [diastereoisomer 1: 1.67 (dt, *J* = 9.2, 4.7 Hz, 1H), diasteroisomer 2: 1.59 (dt, *J* = 9.3, 4.6 Hz, 1H)], 1.38 (dddd, *J* = 17.4, 8.1, 6.6, 4.2 Hz, 1H), 1.09 (dd, *J* = 7.5 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 209.2, 208.9, 174.5, 174.4, 140.0, 139.9, 137.0, 137.0, 129.4, 128.8, 128.7, 126.9, 126.8, 126.5, 126.5, 126.2, 126.0, 124.8, 124.6, 59.7, 59.5, 48.3, 31.7, 31.5, 29.6, 29.6, 19.4, 19.2, 19.2, 8.9, 8.7 ppm. IR (neat, cm^{-1}):

2975, 1688, 1497, 1456, 1392, 1342, 1294, 1246, 1223, 1120, 1055, 994, 756, 695. HRMS (ES+) calcd for ($C_{22}H_{24}NO_2$) $[M+H]^+$ 334.1807, found 334.1815.



(*R)-5-((*R**)-1-(2,2-Difluorobenzo[*d*][1,3]dioxol-5-yl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (15):**

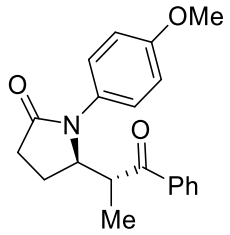
General Procedure III was followed using 2,2-difluorobenzo[*d*][1,3]dioxole-5-carboxylic acid (60.6 mg, 0.3 mmol, 1.0 equiv), $(COCl)_2$ (41.9 mg, 0.33 mmol, 1.1 equiv), DMF (10 µL), CH_2Cl_2 (2 mL), *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (66.0 mg, 0.18 mmol, 59% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.47 (d, *J* = 1.7 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.29 – 7.24 (m, 1H), 7.10 (d, *J* = 8.3 Hz, 1H), 4.69 (dt, *J* = 8.6, 4.3 Hz, 1H), 3.68 (qd, *J* = 6.8, 3.9 Hz, 1H), 2.70 – 2.48 (m, 2H), 2.21 (ddt, *J* = 13.2, 9.9, 7.7 Hz, 1H), 2.15 – 2.02 (m, 1H), 1.14 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.0, 174.4, 147.3, 144.4, 137.0, 132.7, 131.8, 129.5, 126.9, 125.2, 125.1, 109.4, 60.6, 42.6, 31.4, 19.3, 10.2 ppm. ^{19}F NMR (471 MHz, $CDCl_3$) δ 49.8, 49.8 ppm. IR (neat, cm^{-1}): 1708, 1686, 1493, 1440, 1379, 1292, 1242, 1215, 1177, 1149, 1091, 1035, 908, 883, 789, 698. HRMS (ES+) calcd for ($C_{20}H_{18}F_2NO_4$) $[M+H]^+$ 374.1204, found 374.1203. One carbon missing in ^{13}C-NMR due to fluorine substitution.



(*R)-1-(4-Chlorophenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (16):**

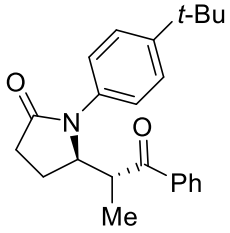
General Procedure II was followed using *N*-(4-chlorophenyl)hex-4-enamide (80.5 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (50.0 mg, 0.15 mmol, 51% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.59 (td, *J* = 7.3, 1.4 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.41 – 7.36 (m, 2H), 7.34 – 7.30 (m, 2H), 4.69 (dt, *J* = 8.7, 4.4 Hz, 1H), 3.76 (qd, *J* = 6.9, 4.0 Hz, 1H), 2.69 – 2.49 (m, 2H), 2.21 (dddd, *J* = 13.6, 10.1, 8.5, 7.2 Hz, 1H), 2.10 (dddd, *J* = 13.6, 10.5, 6.2, 4.6 Hz, 1H), 1.13 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.3, 174.6, 136.2, 135.6, 133.6, 132.1, 129.6, 129.0, 128.1, 126.3, 60.4, 42.5, 31.4, 19.3, 10.1 ppm. IR (neat, cm^{-1}): 2975, 1695, 1679, 1595, 1492, 1448, 1415, 1382, 1364, 1293, 1211, 1091,

1013, 1002, 969, 830, 726, 700, 649. HRMS (ES+) calcd for ($C_{19}H_{19}ClNO_2$) $[M+H]^+$ 328.1104, found 328.1116.



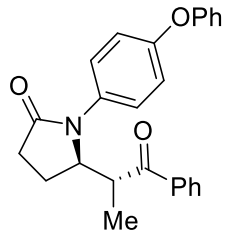
(*R)-1-(4-Methoxyphenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (17):**

General Procedure II was followed using *N*-(4-methoxyphenyl)hex-4-enamide (78.9 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (40.0 mg, 0.12 mmol, 41% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.70 (m, 2H), 7.60 – 7.52 (m, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 4.63 (dt, *J* = 8.7, 4.5 Hz, 1H), 3.82 (s, 3H), 3.75 (qd, *J* = 6.7, 4.0 Hz, 1H), 2.67 – 2.47 (m, 2H), 2.22 – 2.12 (m, 1H), 2.11 – 2.01 (m, 1H), 1.14 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.4, 174.7, 158.3, 136.2, 133.4, 129.7, 128.9, 128.1, 126.9, 114.8, 61.1, 55.6, 42.6, 31.4, 19.3, 9.9 ppm. IR (neat, cm^{-1}): 2976, 1682, 1610, 1596, 1511, 1447, 1424, 1397, 1365, 1336, 1291, 1247, 1212, 1181, 1106, 1032, 832, 700, 650. HRMS (ES+) calcd for ($C_{20}H_{22}NO_3$) $[M+H]^+$ 324.1600, found 324.1609.



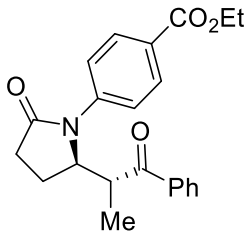
(*R)-1-(4-(*tert*-Butyl)phenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (18):**

General Procedure II was followed using *N*-(4-(*tert*-butyl)phenyl)hex-4-enamide (88.3 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (61.8 mg, 0.18 mmol, 59% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.7 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 – 7.38 (m, 4H), 7.32 – 7.24 (m, 2H), 4.71 (dt, *J* = 8.8, 4.5 Hz, 1H), 3.79 (qd, *J* = 6.9, 3.9 Hz, 1H), 2.69 – 2.47 (m, 2H), 2.21 – 2.11 (m, 1H), 2.06 (ddt, *J* = 14.1, 10.5, 5.5 Hz, 1H), 1.32 (s, 9H), 1.14 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.4, 174.7, 149.7, 136.2, 134.1, 133.4, 128.9, 128.2, 126.3, 124.8, 60.6, 42.7, 31.4, 19.3, 18.7, 13.7, 9.9 ppm. IR (neat, cm^{-1}): 2961, 1680, 1515, 1448, 1393, 1297, 1212, 1159, 1028, 972, 835, 730, 647. HRMS (ES+) calcd for ($C_{23}H_{28}NO_2$) $[M+H]^+$ 350.2120, found 350.2135.



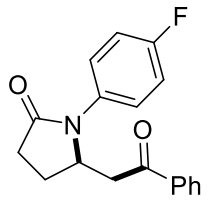
(*R)-5-((*R**)-1-Oxo-1-phenylpropan-2-yl)-1-(4-phenoxyphenyl)pyrrolidin-2-one (19):**

General Procedure II was followed using *N*-(4-phenoxyphenyl)hex-4-enamide (101.3 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (55.6 mg, 0.14 mmol, 48% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 – 7.73 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.9 Hz, 2H), 7.33 – 7.28 (m, 2H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.06 – 7.00 (m, 4H), 4.68 (dt, *J* = 8.7, 4.5 Hz, 1H), 3.78 (qd, *J* = 6.8, 4.1 Hz, 1H), 2.68 – 2.50 (m, 2H), 2.19 (dddd, *J* = 15.5, 10.1, 8.5, 7.0 Hz, 1H), 2.13 – 2.03 (m, 1H), 1.15 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.1, 174.4, 156.5, 155.7, 135.9, 133.3, 131.6, 129.7, 128.7, 127.9, 126.6, 123.6, 119.1, 119.0, 60.6, 42.4, 31.1, 19.2, 9.9 ppm. IR (neat, cm^{-1}): 3050, 2976, 1681, 1589, 1505, 1488, 1422, 1393, 1334, 1291, 1233, 1163, 972, 842, 754, 731, 693. HRMS (ES+) calcd for ($C_{25}H_{24}NO_3$) $[M+H]^+$ 386.1756, found 386.1748.



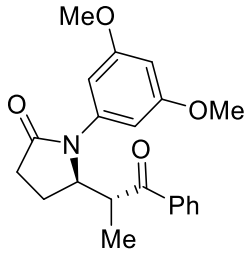
Ethyl 4-((*R)-2-oxo-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-1-yl)benzoate (20):**

General Procedure II was followed using ethyl (*Z*)-4-(hex-4-enamido)benzoate (94.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (30.7 mg, 0.084 mmol, 28% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.6 Hz, 2H), 7.79 – 7.73 (m, 2H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.54 – 7.51 (m, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 4.79 (dt, *J* = 8.5, 4.1 Hz, 1H), 4.40 (q, *J* = 7.2 Hz, 2H), 3.81 (qd, *J* = 6.8, 3.7 Hz, 1H), 2.66 (ddd, *J* = 17.8, 10.3, 7.6 Hz, 1H), 2.56 (ddd, *J* = 17.4, 10.3, 5.8 Hz, 1H), 2.25 – 2.18 (m, 1H), 2.13 (ddt, *J* = 14.4, 9.1, 3.7 Hz, 1H), 1.41 (t, *J* = 7.2 Hz, 3H), 1.11 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.3, 174.7, 166.0, 141.3, 136.3, 133.7, 130.9, 129.1, 128.1, 128.1, 123.7, 61.2, 59.9, 42.3, 31.7, 18.9, 14.5, 9.8 ppm. IR (neat, cm^{-1}): 2980, 1706, 1682, 1605, 1511, 1448, 1421, 1383, 1367, 1274, 1212, 1177, 1108, 1019, 971, 772, 700. HRMS (ES+) calcd for ($C_{22}H_{24}NO_4$) $[M+H]^+$ 366.1705, found 366.1699.



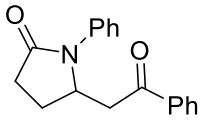
(*R)-1-(4-Fluorophenyl)-5-(2-oxo-2-phenylethyl)pyrrolidin-2-one (21):**

Following general procedure I using *N*-(4-fluorophenyl)pent-4-enamide (69.5 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (51.7 mg, 0.17 mmol, 58% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.6 Hz, 2H), 7.61 – 7.55 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.39 (dd, *J* = 8.8, 4.7 Hz, 2H), 7.08 (t, *J* = 8.5 Hz, 2H), 4.85 (ddt, *J* = 10.0, 7.8, 3.9 Hz, 1H), 3.30 (dd, *J* = 17.3, 3.2 Hz, 1H), 3.10 (dd, *J* = 17.3, 9.6 Hz, 1H), 2.72 – 2.64 (m, 1H), 2.64 – 2.57 (m, 2H), 1.86 (tdd, *J* = 10.8, 5.5, 2.9 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.5, 174.4, 161.6, 160.7 (d, *J* = 246.3 Hz), 159.7, 136.6, 133.8, 133.3, 128.9, 128.1, 125.9 (d, *J* = 8.3 Hz), 116.2 (d, *J* = 22.5 Hz), 56.6, 42.4, 31.0, 25.2 ppm. ^{19}F NMR (471 MHz, $CDCl_3$) δ -115.5 ppm. IR (neat, cm^{-1}): 2925, 1681, 1598, 1507, 1449, 1421, 1385, 1331, 1292, 1216, 1203, 1159, 1003, 835, 812, 756, 690, 647, 543. HRMS (ES+) calcd for ($C_{18}H_{17}FNO_2$) $[M+H]^+$ 298.1243, found 298.1233.



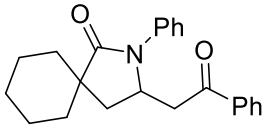
(*R)-1-(3,5-Dimethoxyphenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (22):**

Following general procedure I using *N*-(3,5-dimethoxyphenyl)hex-4-enamide (89.8 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (56.2 mg, 0.16 mmol, 53% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.76 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 6.56 (d, *J* = 2.2 Hz, 2H), 6.36 (t, *J* = 2.3 Hz, 1H), 4.66 (dt, *J* = 8.5, 4.2 Hz, 1H), 3.86 (qd, *J* = 6.7, 3.8 Hz, 1H), 3.79 (s, 6H), 2.68 – 2.49 (m, 2H), 2.19 – 2.11 (m, 1H), 2.07 (ddt, *J* = 14.2, 10.3, 4.9 Hz, 1H), 1.14 (d, *J* = 6.8 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.4, 174.5, 161.4, 138.7, 136.2, 133.5, 128.9, 128.2, 103.5, 99.0, 60.7, 55.6, 42.5, 31.7, 19.0, 9.8 ppm. IR (neat, cm^{-1}): 2940, 1697, 1595, 1448, 1429, 1391, 1341, 1270, 1262, 1206, 1155, 1064, 968, 838, 690. HRMS (ES+) calcd for ($C_{21}H_{24}NO_4$) $[M+H]^+$ 354.1705, found 354.1721.



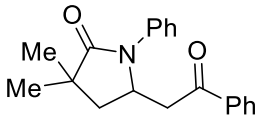
5-(2-Oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (24):

General Procedure II was followed using *N*-phenylpent-4-enamide (63.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (47.2 mg, 0.17 mmol, 56% yield). mp = 104 – 106 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 – 7.81 (m, 2H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.48 – 7.42 (m, 4H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.21 (t, *J* = 7.4 Hz, 1H), 4.91 (dddd, *J* = 10.0, 4.5, 3.1, 2.5 Hz, 1H), 3.34 (dd, *J* = 17.4, 3.0 Hz, 1H), 3.11 (dd, *J* = 17.4, 9.8 Hz, 1H), 2.73 – 2.63 (m, 1H), 2.60 (ddd, *J* = 13.0, 7.1, 4.4 Hz, 2H), 1.86 (ddt, *J* = 11.5, 9.8, 4.8 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.7, 174.3, 137.4, 136.6, 133.7, 129.4, 128.8, 128.1, 126.1, 123.8, 56.3, 42.4, 31.2, 25.1 ppm. IR (neat, cm^{-1}): 3051, 1679, 1596, 1581, 1497, 1449, 1381, 1289, 1181, 1003, 982, 756, 690, 639. HRMS (ES+) calcd for ($C_{18}H_{18}NO_2$) $[M+H]^+$ 280.1338, found 280.1319.



3-(2-Oxo-2-phenylethyl)-2-phenyl-2-azaspiro[4.5]decan-1-one (25):

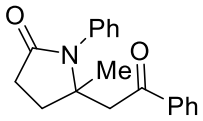
General Procedure II was followed using 1-allyl-*N*-phenylcyclohexane-1-carboxamide (87.6 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (66.8 mg, 0.19 mmol, 64% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 – 7.82 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.42 – 7.36 (m, 4H), 7.21 (dq, *J* = 6.3, 4.0, 3.1 Hz, 1H), 4.87 – 4.74 (m, 1H), 3.44 (dd, *J* = 17.3, 3.2 Hz, 1H), 2.99 (dd, *J* = 17.3, 9.9 Hz, 1H), 2.69 (dd, *J* = 13.2, 7.5 Hz, 1H), 1.94 (td, *J* = 12.8, 3.9 Hz, 1H), 1.80 – 1.71 (m, 2H), 1.71 – 1.57 (m, 4H), 1.56 – 1.51 (m, 1H), 1.50 – 1.40 (m, 1H), 1.32 (dtd, *J* = 21.7, 12.4, 9.2 Hz, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.9, 178.9, 137.6, 136.7, 133.7, 129.2, 128.8, 128.1, 126.1, 124.3, 52.8, 45.7, 44.0, 37.4, 35.0, 32.7, 25.5, 22.3 ppm. IR (neat, cm^{-1}): 2928, 2855, 1681, 1596, 1581, 1495, 1448, 1373, 1307, 1274, 1205, 1001, 917, 757, 722, 690. HRMS (EI+) calcd for ($C_{23}H_{25}NO_2$) $[M]^+$ 347.1885, found 347.1879.



3,3-Dimethyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (26):

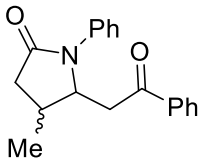
General Procedure II was followed using 2,2-dimethyl-*N*-phenylpent-4-enamide (73.2 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at

rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (78.4 mg, 0.26 mmol, 85% yield). mp = 98 – 101 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 – 7.82 (m, 2H), 7.59 – 7.55 (m, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.42 – 7.38 (m, 4H), 7.24 – 7.19 (m, 1H), 4.88 – 4.75 (m, 1H), 3.44 (dd, *J* = 17.3, 3.2 Hz, 1H), 3.00 (dd, *J* = 17.3, 9.8 Hz, 1H), 2.53 (dd, *J* = 13.0, 7.1 Hz, 1H), 1.67 (dd, *J* = 13.0, 7.3 Hz, 1H), 1.33 (s, 3H), 1.27 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.8, 179.2, 137.6, 136.7, 133.7, 129.3, 128.8, 128.1, 126.1, 124.3, 52.5, 43.6, 41.6, 41.1, 26.2, 25.4 ppm. IR (neat, cm^{-1}): 2964, 2929, 1684, 1597, 1496, 1449, 1390, 1372, 1207, 1180, 1118, 1001, 762, 692, 628. HRMS (EI+) calcd for ($C_{20}H_{21}NO_2$) $[M]^+$ 307.1572, found 307.1596.



5-Methyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (27):

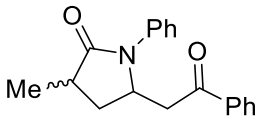
General Procedure II was followed using 4-methyl-*N*-phenylpent-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), Bu_4N[OP(O)(OBu)$_2$] (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (36.2 mg, 0.12 mmol, 41% yield). mp = 104 – 106 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 – 7.80 (m, 2H), 7.61 – 7.53 (m, 1H), 7.48 – 7.41 (m, 4H), 7.40 – 7.35 (m, 1H), 7.19 (dd, *J* = 7.6, 1.7 Hz, 2H), 3.27 – 3.10 (m, 2H), 2.76 – 2.55 (m, 2H), 2.45 (ddd, *J* = 13.2, 9.9, 6.5 Hz, 1H), 2.24 (ddd, *J* = 13.2, 9.6, 6.5 Hz, 1H), 1.47 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.2, 175.5, 137.4, 136.3, 133.5, 129.8, 129.5, 128.8, 128.4, 127.9, 63.8, 46.8, 32.1, 30.2, 27.3 ppm. IR (neat, cm^{-1}): 2965, 1681, 1596, 1580, 1496, 1448, 1374, 1349, 1219, 1126, 1005, 756, 699, 691, 575. HRMS (ES+) calcd for ($C_{19}H_{20}NO_2$) $[M+H]^+$ 294.1494, found 294.1483.



4-Methyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (28):

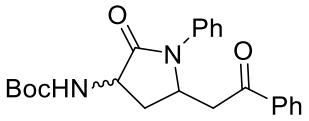
General Procedure II was followed using 3-methyl-*N*-phenylpent-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), Bu_4N[OP(O)(OBu)$_2$] (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (61.6 mg, 0.21 mmol, 70% yield). mp = 130 – 132, 134 – 138 ºC. The two distinguishable melting ranges are likely because that the sample consists two diastereoisomer. ^{1}H NMR for major diastereoisomer (500 MHz, $CDCl_3$) δ 7.86 (t, *J* = 8.7 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (dt, *J* = 15.7, 8.1 Hz, 4H), 7.37 (td, *J* = 8.1, 2.4 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 4.51 (dt, *J* = 9.3, 2.8 Hz, 1H), 3.28 (dd, *J* = 17.2, 3.0 Hz, 1H), 3.16 (dd, *J* = 17.5, 9.4 Hz, 1H), 2.94 – 2.85 (m, 1H), 2.71 (dd, *J* = 16.8, 8.2 Hz, 1H), 2.29 – 2.19 (m, 1H), 1.31 (d, *J* = 6.9 Hz, 3H) ppm. ^{1}H NMR for minor isomer (500 MHz, $CDCl_3$) δ 7.86 (t, *J* = 8.7 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (dt, *J* = 15.7, 8.1 Hz, 4H), 7.37 (td, *J* = 8.1, 2.4 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 5.06 (ddd, *J* = 10.0, 7.1, 3.0 Hz, 1H), 3.37 – 3.31 (m, 1H), 3.03 (dd, *J* = 17.8, 3.1 Hz,

1H), 2.94 – 2.85 (m, 1H), 2.35 (dd, *J* = 16.8, 8.3 Hz, 1H), 2.29 – 2.20 (m, 1H), 1.01 (d, *J* = 7.0 Hz, 3H) ppm. ^{13}C NMR of mixture of two isomers (126 MHz, $CDCl_3$) δ 197.9, 197.7, 173.8, 173.4, 137.6, 137.5, 136.6, 136.5, 133.7, 133.6, 129.3, 129.3, 128.8, 128.0, 128.0, 125.9, 123.6, 123.5, 63.7, 59.2, 41.5, 39.5, 39.2, 36.8, 32.4, 30.1, 20.7, 15.2 ppm. IR (neat, cm^{-1}): 3061, 2960, 1679, 1596, 1581, 1497, 1449, 1387, 1374, 1353, 1289, 1204, 1181, 1119, 1071, 1000, 990, 756, 690, 642. HRMS (ES+) calcd for ($C_{19}H_{19}NaNO_2$) $[M+Na]^+$ 316.1313, found 316.1341.



3-Methyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (29):

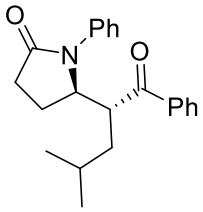
General Procedure II was followed using 2-methyl-*N*-phenylpent-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (42.3 mg, 0.14 mmol for major isomer; 14.1 mg, 0.048 mmol for minor isomer. 64% yield in total). mp (major isomer) = 140 – 142 ºC. ^{1}H NMR for firstly eluted (major) diastereoisomer (500 MHz, $CDCl_3$) δ 7.91 – 7.83 (m, 2H), 7.60 – 7.53 (m, 3H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.39 (ddd, *J* = 8.6, 5.7, 1.9 Hz, 2H), 7.21 – 7.17 (m, 1H), 4.89 (dtd, *J* = 10.3, 5.2, 2.9 Hz, 1H), 3.30 (dd, *J* = 17.4, 2.9 Hz, 1H), 3.16 (dd, *J* = 17.3, 10.1 Hz, 1H), 2.78 (tq, *J* = 9.0, 7.1 Hz, 1H), 2.15 (dd, *J* = 9.1, 5.2 Hz, 2H), 1.30 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.9, 176.6, 137.7, 136.6, 133.7, 129.3, 128.9, 128.1, 125.6, 122.8, 54.0, 41.4, 36.3, 33.5, 16.3 ppm. IR (neat, cm^{-1}): 3061, 2960, 1679, 1596, 1581, 1497, 1449, 1387, 1374, 1353, 1289, 1204, 1181, 1119, 1071, 1000, 990, 756, 690, 642. HRMS (ES+) calcd for ($C_{19}H_{20}NO_2$) $[M+H]^+$ 294.1494, found 294.1500. mp (minor isomer) = 136 – 139 ºC. ^{1}H NMR for secondly eluted (minor) isomer (500 MHz, $CDCl_3$) δ7.84 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.59 – 7.55 (m, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.41 – 7.38 (m, 2H), 7.37 – 7.33 (m, 2H), 7.22 (tt, *J* = 7.5, 1.2 Hz, 1H), 4.83 – 4.74 (m, 1H), 3.44 (dd, *J* = 17.3, 3.2 Hz, 1H), 2.96 (dd, *J* = 17.3, 9.7 Hz, 1H), 2.89 (ddd, *J* = 12.9, 9.1, 6.8 Hz, 1H), 2.70 (td, *J* = 9.5, 7.0 Hz, 1H), 1.48 – 1.37 (m, 1H), 1.34 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.7, 176.9, 137.4, 136.7, 133.7, 129.3, 128.8, 128.1, 126.3, 124.6, 54.0, 43.9, 37.2, 35.2, 17.0 ppm. IR (neat, cm^{-1}): 3062, 2928, 1697, 1597, 1497, 1449, 1372, 1310, 1204, 1115, 1001, 760, 719, 692, 629. HRMS (ES+) calcd for ($C_{19}H_{20}NO_2$) $[M+H]^+$ 294.1494, found 294.1501.



***tert*-Butyl (2-oxo-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-3-yl)carbamate (30):**

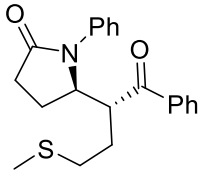
General Procedure II was followed using *tert*-butyl (*R*)-(1-oxo-1-(phenylamino)pent-4-en-2-yl)carbamate (104.5 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil. First eluted isomer (60.4 mg, 0.15 mmol, 51% yield): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 – 7.81 (m, 2H), 7.60 – 7.53 (m, 3H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.42 – 7.37 (m, 2H), 7.23 – 7.19 (m, 1H), 5.15 (s, 1H), 5.02 – 4.91 (m, 1H), 4.56 (s, 1H), 3.35 – 3.20

(m, 2H), 2.65 – 2.57 (m, 1H), 2.30 (d, *J* = 11.1 Hz, 1H), 1.46 (s, 9H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.3, 171.7, 156.1, 137.1, 136.5, 133.8, 129.5, 128.9, 128.1, 126.1, 122.3, 53.1, 52.1, 40.7, 33.7, 28.5 ppm. IR (neat, cm^{-1}): 3347, 2978, 1685, 1597, 1497, 1392, 1367, 1328, 1294, 1248, 1207, 1168, 1053, 1001, 756, 735, 691. HRMS (ES+) calcd for ($C_{23}H_{27}N_2O_4$) $[M+H]^+$ 395.1971, found 395.1943. Second eluted isomer (12.1 mg, 0.03 mmol, 10% yield): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.78 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.46 – 7.38 (m, 4H), 7.38 – 7.33 (m, 2H), 7.25 (dd, *J* = 8.2, 6.6 Hz, 1H), 5.29 (d, *J* = 13.5 Hz, 1H), 4.79 (tdd, *J* = 9.0, 6.4, 3.4 Hz, 1H), 4.33 (td, *J* = 9.6, 5.3 Hz, 1H), 3.38 (dd, *J* = 17.4, 3.4 Hz, 1H), 3.28 – 3.15 (m, 1H), 3.06 (dd, *J* = 17.2, 9.1 Hz, 1H), 1.75 (dt, *J* = 13.0, 9.7 Hz, 1H), 1.47 (s, 9H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.2, 171.7, 155.8, 136.6, 133.7, 129.4, 128.8, 128.1, 126.9, 124.8, 80.2, 61.0, 53.0, 43.1, 35.0, 29.8, 28.5 ppm. IR (neat, cm^{-1}): 3396, 1717, 1690, 1596, 1519, 1496, 1450, 1405, 1377, 1327, 1290, 1210, 1164, 1050, 1001, 731, 693. HRMS (ES+) calcd for ($C_{23}H_{26}NaN_2O_4$) $[M+Na]^+$ 417.1790, found 417.1803.



(*R)-5-((*R**)-4-Methyl-1-oxo-1-phenylpentan-2-yl)-1-phenylpyrrolidin-2-one (31):**

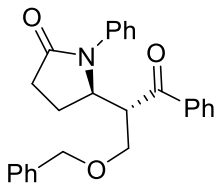
General Procedure II was followed using 7-methyl-*N*-phenyloct-4-enamide (83.3 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (60.4 mg, 0.18 mmol, 60% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.79 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.44 (m, 4H), 7.42 – 7.37 (m, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 4.55 (dt, *J* = 8.4, 4.0 Hz, 1H), 3.83 (ddd, *J* = 11.0, 3.5, 2.1 Hz, 1H), 2.64 (ddd, *J* = 17.4, 10.3, 7.1 Hz, 1H), 2.51 (ddd, *J* = 17.2, 10.5, 5.9 Hz, 1H), 2.21 – 2.11 (m, 1H), 2.11 – 1.94 (m, 2H), 1.26 (tq, *J* = 8.9, 3.3, 2.0 Hz, 1H), 1.15 (ddd, *J* = 13.0, 9.0, 2.0 Hz, 1H), 0.78 (d, *J* = 6.6 Hz, 3H), 0.56 (d, *J* = 6.5 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.5, 174.5, 136.9, 136.8, 133.7, 129.4, 129.1, 128.1, 126.8, 125.2, 60.4, 45.5, 32.5, 31.5, 26.5, 23.8, 21.8, 18.8 ppm. IR (neat, cm^{-1}): 2955, 1697, 1679, 1596, 1498, 1447, 1385, 1292, 1238, 1225, 1206, 1156, 992, 909, 762, 733, 692, 649. HRMS (ES+) calcd for ($C_{22}H_{26}NO_2$) $[M+H]^+$ 358.1783, found 358.1798.



(*R)-5-((*R**)-4-(Methylthio)-1-oxo-1-phenylbutan-2-yl)-1-phenylpyrrolidin-2-one (32):**

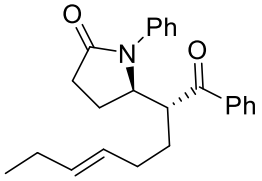
General Procedure II was followed using 7-(methylthio)-*N*-phenylhept-4-enamide (89.8 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product

as a colorless oil (52.0 mg, 0.15 mmol, 49% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.7 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (td, *J* = 7.8, 1.7 Hz, 4H), 7.40 (d, *J* = 7.9 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 4.60 (dt, *J* = 8.6, 4.3 Hz, 1H), 4.03 (dt, *J* = 10.0, 2.9 Hz, 1H), 2.63 (ddd, *J* = 17.2, 10.1, 6.9 Hz, 1H), 2.51 (ddd, *J* = 17.2, 10.3, 6.0 Hz, 1H), 2.35 (dddd, *J* = 16.1, 11.6, 5.5, 4.8 Hz, 2H), 2.21 (dt, *J* = 15.8, 7.9 Hz, 1H), 2.18 – 2.09 (m, 1H), 2.03 – 1.97 (m, 1H), 1.86 (s, 3H), 1.72 – 1.62 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.0, 174.4, 136.8, 136.8, 133.7, 129.5, 129.1, 128.2, 126.9, 124.9, 60.1, 46.6, 32.2, 31.3, 22.7, 19.1, 15.0 ppm. IR (neat, cm^{-1}): 3062, 2918, 1698, 1596, 1498, 1447, 1386, 1295, 1254, 1221, 1118, 1073, 1001, 935, 762, 694. HRMS (ES+) calcd for ($C_{21}H_{24}NO_2S$) $[M+H]^+$ 354.1528, found 354.1529.



(*R)-5-((*S**)-3-(benzyloxy)-1-oxo-1-phenylpropan-2-yl)-1-phenylpyrrolidin-2-one (33):**

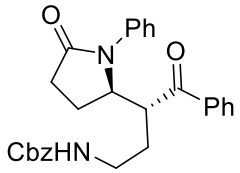
General Procedure II was followed using 6-(benzyloxy)-*N*-phenylhex-4-enamide (106.3 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (61.2 mg, 0.15 mmol, 51% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.46 – 7.36 (m, 4H), 7.33 – 7.22 (m, 6H), 7.14 (dd, *J* = 7.3, 2.0 Hz, 2H), 4.70 (ddd, *J* = 7.4, 5.5, 3.8 Hz, 1H), 4.43 (d, *J* = 12.1 Hz, 1H), 4.35 (d, *J* = 12.1 Hz, 1H), 4.07 – 4.00 (m, 1H), 3.91 (dd, *J* = 9.2, 7.0 Hz, 1H), 3.69 (dd, *J* = 9.2, 4.7 Hz, 1H), 2.61 – 2.46 (m, 2H), 2.28 – 2.19 (m, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.5, 174.5, 137.6, 137.0, 136.6, 133.5, 129.4, 128.8, 128.5, 128.3, 127.8, 127.7, 126.8, 125.4, 73.7, 66.7, 59.6, 48.6, 31.3, 20.5 ppm. IR (neat, cm^{-1}): 3062, 2864, 1698, 1596, 1498, 1448, 1392, 1294, 1209, 1182, 1100, 1028, 954, 758, 695, 552. HRMS (ES+) calcd for ($C_{26}H_{26}NO_3$) $[M+H]^+$ 400.1913, found 400.1927.



(*R)-5-((*R**,*E*)-1-Oxo-1-phenyloct-5-en-2-yl)-1-phenylpyrrolidin-2-one (34):**

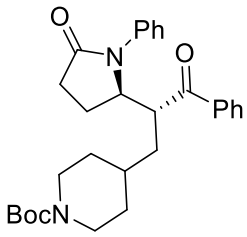
General Procedure II was followed using (8*Z*)-*N*-phenylundeca-4,8-dienamide (92.7 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (95.4 mg, 0.26 mmol, 88% yield). *E* : *Z* = 3:1 likely due to photoisomerization. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 6.8, 6.8 Hz, 2H), 7.59 (dd, *J* = 8.4, 6.4 Hz, 1H), 7.47 (q, *J* = 7.7 Hz, 4H), 7.37 (d, *J* = 7.8 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 5.27 – 5.11 (m, 1H), 5.06 – 4.95 (m, 1H), 4.55 (ddt, *J* = 12.7, 8.4, 4.1 Hz, 1H), 3.77 (ddt, *J* = 19.4, 10.9, 2.8 Hz, 1H), 2.63 (ddd, *J* = 13.5, 9.9, 5.1 Hz, 1H), 2.57 – 2.46 (m, 1H), 2.19 – 2.08 (m, 2H), 2.02 (ddt, *J* = 18.6, 9.5, 7.2 Hz, 1H), 1.95 – 1.84 (m, 1H), 1.82 – 1.61

(m, 3H), 1.48 – 1.35 (m, 1H), 0.77 (td, *J* = 7.5, 2.2 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.5, 174.5, 137.6, 137.0, 136.6, 133.5, 129.4, 128.8, 128.5, 128.3, 127.8, 127.7, 126.8, 125.4, 73.7, 66.7, 59.6, 48.6, 31.3, 20.5 ppm. IR (neat, cm^{-1}): 3062, 2864, 1698, 1596, 1498, 1448, 1392, 1294, 1209, 1182, 1100, 1028, 954, 758, 695, 552. HRMS (ES+) calcd for ($C_{24}H_{28}NO_2$) $[M+H]^+$ 362.2120, found 362.2132.



Benzyl ((*R)-4-oxo-3-((*R**)-5-oxo-1-phenylpyrrolidin-2-yl)-4-phenylbutyl)carbamate (35):**

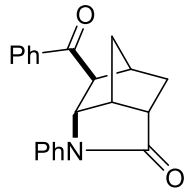
General Procedure II was followed using benzyl (7-oxo-7-(phenylamino)hept-3-en-1-yl)carbamate (126.9 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (67.1 mg, 49% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.7 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.41 (m, 4H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.34 – 7.30 (m, 3H), 7.30 – 7.25 (m, 1H), 7.23 (d, *J* = 6.9 Hz, 2H), 4.93 (d, *J* = 12.2 Hz, 1H), 4.85 (d, *J* = 12.3 Hz, 1H), 4.56 (dt, *J* = 9.3, 4.7 Hz, 2H), 3.81 (d, *J* = 10.8 Hz, 1H), 3.08 – 2.93 (m, 2H), 2.59 (ddd, *J* = 17.3, 9.9, 7.1 Hz, 1H), 2.49 (ddd, *J* = 17.3, 10.2, 6.3 Hz, 1H), 2.25 (dq, *J* = 12.2, 6.3 Hz, 1H), 2.05 – 1.99 (m, 2H), 1.62 (dt, *J* = 13.9, 7.1 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.9, 174.2, 156.1, 136.5, 136.4, 136.3, 133.6, 129.4, 128.9, 128.4, 128.0, 128.0, 127.9, 126.9, 125.0, 66.4, 60.1, 45.5, 39.2, 31.0, 24.2, 18.8 ppm. IR (neat, cm^{-1}): 1681, 1597, 1516, 1498, 1448, 1402, 1294, 1233, 1138, 1002, 983, 906, 759, 725, 693, 647, 552. HRMS (ES+) calcd for ($C_{28}H_{29}N_2O_4$) $[M+H]^+$ 457.2127, found 457.2139.



***tert*-Butyl 4-((*R**)-3-oxo-2-((*R**)-5-oxo-1-phenylpyrrolidin-2-yl)-3-phenylpropyl)piperidine-1-carboxylate (36):**

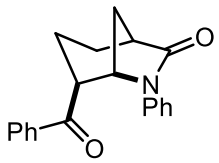
Following general procedure I using *tert*-butyl 4-(6-oxo-6-(phenylamino)hex-2-en-1-yl)piperidine-1-carboxylate (134.1 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (95.4 mg, 0.17 mmol, 55% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.48 (q, *J* = 6.9 Hz, 4H), 7.37 (d, *J* = 7.9 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 4.57 (dt, *J* = 8.2, 4.0 Hz, 1H), 3.92 (d, *J* = 16.4 Hz, 2H), 3.88 – 3.78 (m, 1H), 2.60 (ddd, *J* = 17.4, 10.1, 6.9 Hz, 1H), 2.49 (ddd, *J* = 17.1, 10.4, 6.0 Hz, 2H), 2.41 – 2.30 (m, 1H), 2.08 (ddt, *J* = 14.1, 10.3, 4.5 Hz, 2H), 1.97 (dq, *J* = 12.1, 7.3, 6.2 Hz, 1H), 1.40 (s, 9H), 1.19 (t, *J* = 10.5 Hz, 2H), 1.10 – 0.97 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 1H), 0.76 – 0.64 (m, 1H) ppm. ^{13}C NMR (126

MHz, $CDCl_3$) δ 200.0, 174.4, 154.8, 136.7, 136.4, 133.8, 129.5, 129.2, 128.0, 126.9, 125.0, 79.3, 60.1, 44.7, 34.2, 31.4, 31.3, 29.9, 28.5, 28.5, 18.6 ppm. IR (neat, cm^{-1}): 2974, 2923, 1679, 1597, 1498, 1447, 1423, 1392, 1366, 1289, 1277, 1244, 1165, 1131, 1071, 910, 762, 727, 693. HRMS (ES+) calcd for ($C_{29}H_{36}N_2O_4Na$) $[M+Na]^+$ 499.2573, found 499.2580.



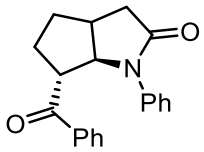
(6*S,6a*R**)-6-Benzoyl-1-phenylhexahydro-3,5-methanocyclopenta[*b*]pyrrol-2(1*H*)-one (37):**

General Procedure II was followed using endo-N-phenylbicyclo[2.2.1]hept-5-ene-2-carboxamide (92.7 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), $[Ni(dMeObpy)Cl_2]$ (6.3 mg, 0.0018 mmol, 6 mol %), $[[Ir\{dF(CF_3)_2ppy\}_2(bpy)]PF_6]$ (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (58.1 mg, 0.18 mmol, 61% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.8 Hz, 2H), 7.67 – 7.55 (m, 1H), 7.55 – 7.41 (m, 4H), 7.39 – 7.22 (m, 2H), 7.08 (t, *J* = 7.4 Hz, 1H), 4.94 (d, *J* = 5.0 Hz, 1H), 3.36 (s, 1H), 3.18 (d, *J* = 5.2 Hz, 1H), 2.76 (d, *J* = 3.5 Hz, 1H), 2.75 – 2.71 (m, 1H), 2.12 (ddt, *J* = 12.8, 10.9, 2.8 Hz, 1H), 1.98 (d, *J* = 13.1 Hz, 1H), 1.79 (dt, *J* = 11.1, 2.0 Hz, 1H), 1.49 (d, *J* = 11.1 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.3, 178.2, 139.0, 135.3, 133.7, 129.2, 129.0, 128.8, 124.1, 118.8, 61.5, 56.0, 44.2, 43.7, 43.2, 35.4, 34.2 ppm. IR (neat, cm^{-1}): 2979, 1701, 1671, 1596, 1581, 1495, 1448, 1385, 1350, 1315, 1278, 1209, 1158, 1013, 1005, 912, 754, 691. HRMS (ES+) calcd for ($C_{21}H_{20}NO_2$) $[M+H]^+$ 318.1494, found 318.1484.



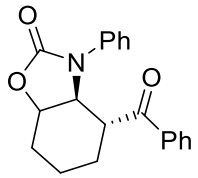
(1*S,4*R**,5*S**)-4-Benzoyl-6-phenyl-6-azabicyclo[3.2.1]octan-7-one (38):**

General Procedure II was followed using *N*-phenylcyclohex-3-ene-1-carboxamide (72.5 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), $[Ni(dMeObpy)Cl_2]$ (6.3 mg, 0.0018 mmol, 6 mol %), $[[Ir\{dF(CF_3)_2ppy\}_2(bpy)]PF_6]$ (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a colorless oil (52.2 mg, 0.17 mmol, 57% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 7.88 – 7.83 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.46 (t, *J* = 7.9 Hz, 2H), 7.22 (t, *J* = 7.4 Hz, 1H), 4.65 (dd, *J* = 5.6, 3.5 Hz, 1H), 3.90 (dd, *J* = 7.1, 3.4 Hz, 1H), 2.71 – 2.62 (m, 1H), 2.24 (dd, *J* = 14.4, 5.9 Hz, 1H), 2.15 (dt, *J* = 11.4, 5.6 Hz, 1H), 2.10 – 1.97 (m, 2H), 1.93 (d, *J* = 11.4 Hz, 1H), 1.91 – 1.82 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.6, 176.9, 138.0, 136.4, 133.5, 129.6, 129.1, 128.2, 125.1, 120.9, 59.5, 42.3, 42.1, 31.2, 23.9, 20.5 ppm. IR (neat, cm^{-1}): 2950, 1701, 1678, 1596, 1493, 1448, 1382, 1303, 1291, 1254, 1204, 1181, 978, 899, 765, 731, 690. HRMS (ES+) calcd for ($C_{20}H_{20}NO_2$) $[M+H]^+$ 306.1494, found 306.1494.



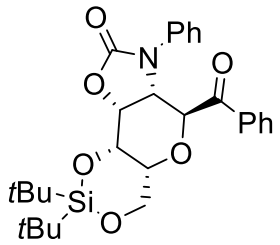
(6*R,6a*R**)-6-Benzoyl-1-phenylhexahydrocyclopenta[*b*]pyrrol-2(1H)-one (39):**

General Procedure II was followed using 2-(cyclopent-2-en-1-yl)-*N*-phenylacetamide (72.5 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (55.9 mg, 0.18 mmol, 61% yield). mp = 110 – 113 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.7 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 5.20 (dd, *J* = 7.9, 2.6 Hz, 1H), 3.76 – 3.67 (m, 1H), 3.11 – 3.00 (m, 1H), 2.92 (dd, *J* = 17.7, 10.0 Hz, 1H), 2.45 (dd, *J* = 17.7, 3.4 Hz, 1H), 2.23 (ddd, *J* = 14.1, 7.3, 7.2 Hz, 1H), 2.12 (ddd, *J* = 14.3, 7.3, 7.2 Hz, 1H), 1.83 (ddd, *J* = 12.7, 6.4, 6.4 Hz, 1H), 1.66 (ddd, *J* = 13.0, 6.4, 6.4 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.2, 173.6, 137.9, 135.7, 133.4, 129.2, 128.7, 128.5, 125.5, 122.7, 66.8, 52.3, 38.6, 35.2, 33.4, 31.3 ppm. IR (neat, cm^{-1}): 2951, 1693, 1673, 1596, 1498, 1448, 1386, 1354, 1310, 1285, 1206, 1180, 1125, 1005, 979, 907, 758, 729, 692. HRMS (ES+) calcd for ($C_{20}H_{20}NO_2$) $[M+H]^+$ 306.1494, found 306.1512.



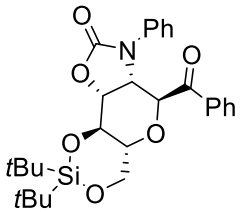
(3a*S*,4*R)-4-benzoyl-3-phenylhexahydrobenzo[d]oxazol-2(3H)-one (40):**

A modified General Procedure II was followed using cyclohex-2-en-1-yl phenylcarbamate (78.2 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), Ni(dMeObpy)Cl_2 (2.1 mg, 0.006 mmol, 2 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (47.2 mg, 0.17 mmol, 56% yield). mp = 145 – 150 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.6 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 2H), 7.28 (d, *J* = 1.3 Hz, 2H), 7.10 (t, *J* = 7.7 Hz, 2H), 6.95 (t, *J* = 7.4 Hz, 1H), 4.97 – 4.93 (m, 1H), 4.91 (dd, *J* = 6.9 Hz, 1H), 3.65 – 3.59 (m, 1H), 2.35 – 2.26 (m, 1H), 1.95 – 1.82 (m, 2H), 1.73 – 1.63 (m, 2H), 1.44 – 1.34 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.4, 156.1, 136.2, 135.7, 133.4, 129.0, 128.6, 128.0, 126.0, 124.1, 73.4, 58.3, 47.2, 27.3, 26.9, 18.6 ppm. IR (neat, cm^{-1}): 2942, 1750, 1674, 1598, 1501, 1448, 1392, 1350, 1337, 1292, 1274, 1226, 1196, 1135, 1087, 1015, 1001, 979, 953, 759, 693. HRMS (ES+) calcd for ($C_{20}H_{20}NO_3$) $[M+H]^+$ 321.1365, found 321.1357.



(4a*R*,8*R*,8a*S*)-6-benzoyl-2,2-di-*tert*-butylhexahydropyrano[3,2-*d*][1,3,2]dioxasilin-8-yl phenylcarbamate (41):

General Procedure II was followed using (4a*R*,8*R*,8a*R*)-2,2-di-*tert*-butyl-4,4a,8,8a-tetrahydropyrano[3,2-*d*][1,3,2]dioxasilin-8-yl phenylcarbamate (145.9 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), Ni(dMeObpy)Cl_2 (6.3 mg, 0.018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a white solid (104.8 mg, 0.21 mmol, 69% yield). mp = 78 – 82 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.7 Hz, 2H), 7.62 (q, *J* = 7.7 Hz, 1H), 7.46 (dt, *J* = 16.0, 7.6 Hz, 4H), 7.29 (dd, *J* = 12.4, 4.6 Hz, 3H), 5.26 (s, 1H), 5.13 (d, *J* = 7.6 Hz, 1H), 4.80 (t, *J* = 7.4 Hz, 1H), 4.22 – 4.04 (m, 1H), 3.82 (d, *J* = 7.5 Hz, 2H), 3.23 (dt, *J* = 10.1, 7.5 Hz, 1H), 1.07 (s, 9H), 0.93 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.8, 156.6, 136.1, 134.6, 134.0, 129.8, 129.6, 129.0, 127.2, 124.6, 76.7, 75.8, 73.8, 69.2, 66.2, 56.5, 27.5, 27.0, 22.8, 20.0. IR (neat, cm^{-1}): 2933, 2859, 1767, 1682, 1501, 1472, 1387, 1106, 1021, 1009, 967, 837, 824, 764, 692, 634. HRMS (ES+) calcd for ($C_{28}H_{36}NO_6Si$) $[M+H]^+$ 510.2320, found 510.2312.

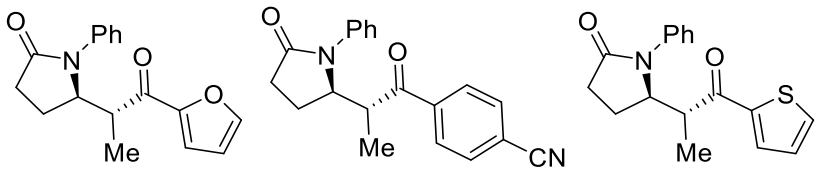


(4a*R*,8*R*,8a*R*)-6-benzoyl-2,2-di-*tert*-butylhexahydropyrano[3,2-*d*][1,3,2]dioxasilin-8-yl phenylcarbamate (42):

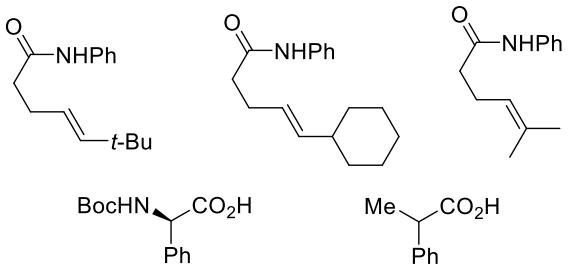
General Procedure II was followed using (4a*R*,8*R*,8a*S*)-2,2-di-*tert*-butyl-4,4a,8,8a-tetrahydropyrano[3,2-*d*][1,3,2]dioxasilin-8-yl phenylcarbamate (145.9 mg, 0.36 mmol, 1.2 equiv), benzoyl chloride (42.2 mg, 0.3 mmol, 1.0 equiv), Ni(dMeObpy)Cl_2 (6.3 mg, 0.018 mmol, 2 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as an off-white solid (63.4 mg, 0.13 mmol, 42% yield). mp = 89 – 92 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 7.98 (m, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.21 (t, *J* = 7.3 Hz, 1H), 5.41 (s, 1H), 5.10 (d, *J* = 7.9 Hz, 1H), 4.98 (dd, *J* = 7.9, 4.6 Hz, 1H), 4.53 (dd, *J* = 4.8, 2.2 Hz, 1H), 4.05 (dd, *J* = 5.3, 3.1 Hz, 2H), 3.40 (q, *J* = 2.9 Hz, 1H), 1.10 (s, 9H), 1.04 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.5, 156.5, 136.7, 134.6, 134.2, 129.7, 129.5, 129.0, 125.5, 121.9, 73.0, 70.8, 69.5, 67.2, 66.7, 52.2, 27.7, 27.2, 23.1, 21.2. IR (neat, cm^{-1}): 2925, 2850, 1761, 1680, 1386, 1197, 1197, 1127, 1068, 914, 796, 752, 693, 639. HRMS (ES+) calcd for ($C_{28}H_{36}NO_6Si$) $[M+H]^+$ 510.2316, found 510.2312.

3.3 Challenging Substrates

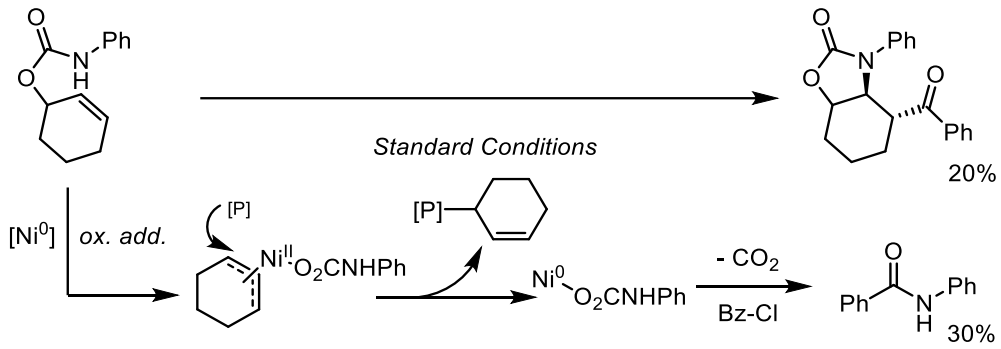
The following contain inseparable decarbonylative byproducts:



The following are proven challenging likely due to their sterically demanding nature:



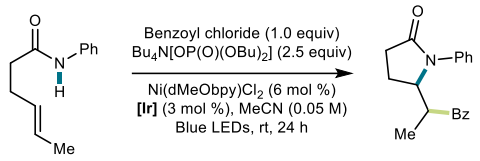
The following example suffered the formation of a significant amount of *N*-phenyl benzamide, therefore a reduced loading of Ni catalyst has to be applied for entry 40 of Section 3.2:



4. Mechanistic Studies

4.1 Control Experiments

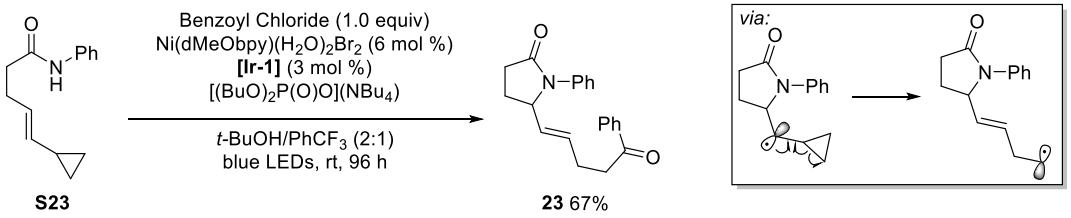
All reactions were done according to General Procedure II on a 0.1 mmol scale and monitored by HPLC. As is seen in Table S1, all components were required for reaction success.



entry	variation from standard conditions[a]	yield (%)[b]
1	none	75
2	no light	0
3	no **[Ir]**	0
4	no nickel	0
5	no base	0

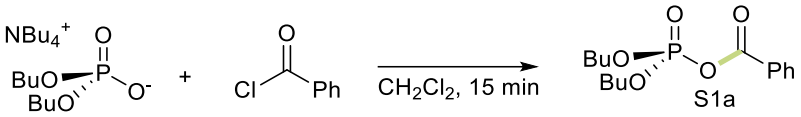
Table S1. Control Reactions

4.2 Radical Probe Experiment

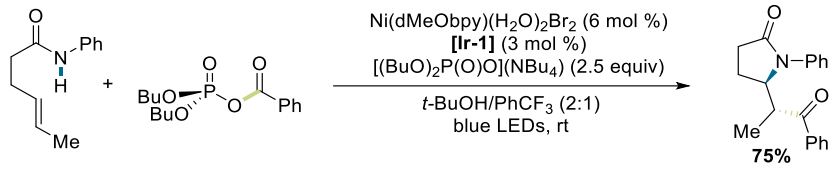


(*E*)-4-(4-(5-Oxo-1-phenylpyrrolidin-2-yl)but-3-en-1-yl)benzonitrile (23): General Procedure II was followed using (*E*)-5-cyclopropyl-*N*-phenylpent-4-enamide (77.5 mg, 0.36 mmol, 1.2 equiv, synthesized according to literature[3]), 4-bromobenzonitrile (54.6 mg, 0.3 mmol, 1.0 equiv), [Ni(dMeObpy)Cl_2] (6.3 mg, 0.0018 mmol, 6 mol %), [[Ir{dF(CF_3)$_2$ppy}$_2$(bpy)]PF_6] (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (338.8 mg, 0.75 mmol, 2.5 equiv) and dry *t*-BuOH/$PhCF_3$ (2:1, 6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 96 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave the product as a yellowish oil (64.2 mg, 0.20 mmol, 67% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.41 – 7.36 (m, 2H), 7.34 (t, *J* = 7.9 Hz, 2H), 7.18 (t, *J* = 7.1 Hz, 1H), 7.10 (d, *J* = 7.9 Hz, 2H), 5.55 (dt, *J* = 14.2, 6.7 Hz, 1H), 5.34 (dd, *J* = 15.3, 7.3 Hz, 1H), 4.60 (td, *J* = 7.4, 4.8 Hz, 1H), 2.64 (t, *J* = 7.3 Hz, 2H), 2.63 – 2.55 (m, 1H), 2.55 – 2.48 (m, 1H), 2.37 – 2.27 (m, 3H), 1.88 – 1.76 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.4, 146.9, 138.2, 132.3, 131.8, 131.0, 129.3, 128.8, 125.4, 123.1, 119.1, 110.0, 61.9, 35.5, 33.2, 31.2, 26.4 ppm. IR (neat, cm^{-1}): 2927, 2225, 1693, 1497, 1379, 1217. HRMS (ES+) calcd for ($C_{21}H_{22}N_2O$) $[M+H]^+$ 320.1651, found 320.1662.

4.3 Reaction with Benzoyl Dibutylphosphonate



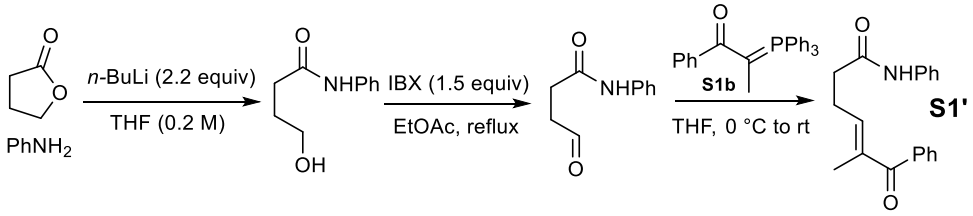
Benzoic (dibutyl phosphoric) anhydride was prepared by charging benzoyl chloride (140.6 mg, 1.0 mmol, 1.0 equiv) in a CH_2Cl_2 solution of $Bu_4N[OP(O)(OBu)_2]$ (451.7 mg, 1.0 mmol, 1.0 equiv) and stirred for 15 min. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 20%) gave the product as a colorless oil (299.0 mg, 95% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ ^{1}H NMR (500 MHz, C_6D_6) δ 8.09 – 8.00 (m, 2H), 7.66 – 7.62 (m, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 4.29 (td, *J* = 6.6, 4.0 Hz, 4H), 1.73 (tt, *J* = 7.0 Hz, 4H), 1.45 (q, *J* = 7.5 Hz, 4H), 0.95 (t, *J* = 7.4 Hz, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.2 (d, *J* = 8.3 Hz), 134.6, 130.8, 128.9, 128.4 (d, *J* = 8.4 Hz), 69.1 (d, *J* = 6.2 Hz), 32.4 (d, *J* = 6.9 Hz), 18.7, 13.7 ppm. IR (neat, cm^{-1}): 2961, 1693, 1465, 1220, 1023, 1003, 713, 526. ^{31}P NMR (203 MHz, $CDCl_3$) δ -7.4 ppm. HRMS (ES+) calcd for ($C_{15}H_{24}O_5P$) $[M+H]^+$ 315.1356, found 315.1367.



General Procedure II was followed using *N*-phenylhex-4-enamide (68.1 mg, 0.36 mmol, 1.2 equiv), benzoic (dibutyl phosphoric) anhydride (94.3 mg, 0.3 mmol, 1.0 equiv), $[Ni(dMeObpy)(H_2O)_2(Br)_2]$ (8.5 mg, 0.0018 mmol, 6 mol %), $[[Ir\{dF(CF_3)_2ppy\}_2(bpy)]PF_6]$ (9.0 mg, 0.009 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (203.3 mg, 0.45 mmol, 1.5 equiv) and dry MeCN (6.0 mL, 0.05 M). The reaction was stirred under blue LED irradiation at rt for 36 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 40%) gave product with 75% yield and > 20:1 diastereoselectivity. ^{1}H and ^{13}C NMR spectra match with those of substrate **1**.

4.4 Experiments toward Insights of Diastereoselectivity

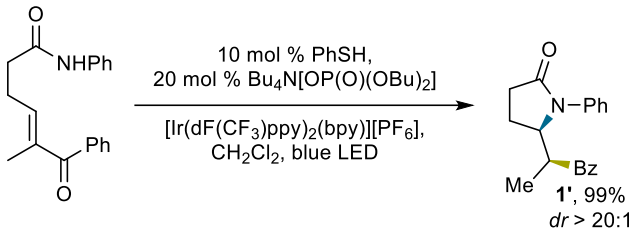
4.4.1 Synthesis of Opposite Diastereoisomer and Tautomerization Study



The synthesis of substrate **S1'** was carried out according to modified procedures from the literature.[8] To a solution of aniline (0.3 mL, 3.3 mmol, 1.1 equiv) in THF (15 mL), *n*-BuLi (2.5 M in hexanes, 2.65 mL, 6.6 mmol, 2.2 equiv) was added at 0 °C and stirred 1 h, which was subsequently cooled −78 °C. γ-Butyrolactone (258.3 mg, 3 mmol, 1 equiv) was added dropwise, and the reaction mixture was stirred for 1 h at −78 °C. The reaction was quenched with saturated NH_4Cl (5 mL) and extracted with EtOAc (20 mL x 3). The organic extracts were combined, dried (Na_2SO_4), and concentrated in vacuo. Silica gel purification using an automated system (CH_2Cl_2/MeOH, 0 to 10%) gave the product 4-hydroxy-*N*-phenylbutanamide as a white solid (925 mg, 2.94 mmol, 98%). Characterization data matched the literature report.[8]

To a microwave tube was charged 4-hydroxy-*N*-phenylbutanamide (358.4 mg, 2.0 mmol, 1.0 equiv) and 2-iodoxybenzoic acid (840 mg, 3.0 mmol, 1.5 equiv) under argon. The tube was sealed under argon and the solid was suspended in EtOAc (0.2 M, 10 mL). The reaction was heated under reflux for 12 h before cooling and filtration, and the resulting solution was concentrated in vacuo. Silica gel purification using an automated system (hexane/EtOAc, 0 to 100%) gave the product 4-oxo-*N*-phenylbutanamide as a colorless oil (336.68 mg, 1.90 mmol, 95%).

Under an argon atmosphere, the Wittig reagent **S1b** (394.5 mg, 1.0 mmol, synthesized according to the literature[9]) was suspended in THF (0.2 M, 5 mL) and cooled to 0 °C. 4-Oxo-*N*-phenylbutanamide (177 mg, 1.0 mmol, dissolved in 5 mL THF) was added dropwise to the mixture via syringe. The reaction mixture was then allowed to warm to rt overnight, followed by concentration in vacuo. Silica gel purification using an automated system (hexane/EtOAc, 0 to 100%) gave the product **S1'** as a yellow oil (242 mg, 0.83 mmol, 83%). ^{1}H NMR (500 MHz, $CDCl_3$) δ δ 7.66 – 7.59 (m, 2H), 7.52 – 7.41 (m, 4H), 7.39 – 7.27 (m, 4H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.33 – 6.19 (m, 1H), 2.69 (dt, *J* = 7.2, 7.3 Hz, 2H), 2.46 (t, *J* = 7.3 Hz, 2H), 1.99 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.1, 170.2, 143.7, 138.3, 137.9, 137.7, 131.8, 129.5, 129.1, 128.2, 124.5, 120.0, 36.1, 25.0, 12.8 ppm. IR (neat, cm^{-1}): 3321, 1638, 1598, 1540, 1498, 1442, 1309, 1280, 1176, 1017, 907, 755, 728, 692, 632. HRMS (ES+) calcd for ($C_{19}H_{20}NO_2$) $[M+H]^+$ 294.1494, found 294.1500.



The reaction was carried out following the literature,[4] using **S1'** (29.3 mg, 0.1 mmol, 1.0 equiv), $[[Ir\{dF(CF_3)_2ppy\}_2(bpy)]PF_6]$ (3.0 mg, 0.003 mmol, 3 mol %), $Bu_4N[OP(O)(OBu)_2]$ (9.0 mg, 0.45 mmol, 20 mol %), PhSH (1 μL, 0.01 mmol, 10 mol%) and dry CH_2Cl_2 (1.0 mL, 0.1 M). The reaction was stirred under blue LED irradiation at rt for 24 h. Silica gel purification using an automated system (hexanes/EtOAc, 0 to 30%) gave the product as a yellow oil (29.0 mg, 0.99 mmol, 99% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (dt, *J* = 8.4, 1.6 Hz, 2H), 7.51 (tt, *J* = 7.3, 1.4 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.32 – 7.28 (m, 2H), 7.25 – 7.21 (m, 2H), 7.17 (tt, *J* = 7.1, 1.3 Hz, 1H), 4.63 (ddd, *J* = 8.7, 5.2, 3.9 Hz, 1H), 3.88 (qd, *J* = 7.1, 5.0 Hz, 1H), 2.66 (dt, *J* = 17.2, 9.3 Hz, 1H), 2.46 (ddd, *J* = 17.3, 9.8, 4.6 Hz, 1H), 2.39 – 2.23 (m, 2H), 1.17 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.8, 174.5, 137.9, 136.9, 133.4, 129.1, 128.8, 128.2, 126.0, 124.1, 62.7, 42.1, 31.2, 20.8, 15.0 ppm. IR (neat, cm^{-1}): 2926, 1678, 1597, 1498, 1447, 1387, 1294, 1220, 973, 758, 694. HRMS (ES+) calcd for ($C_{19}H_{20}NO_2$) $[M+H]^+$ 294.1494, found 294.1498. Overlay of NMR suggested that the opposite (thermodynamically favorable) diastereoisomer was generated highly selectively, likely via a facile Hydrogen Atom Transfer (HAT) event:

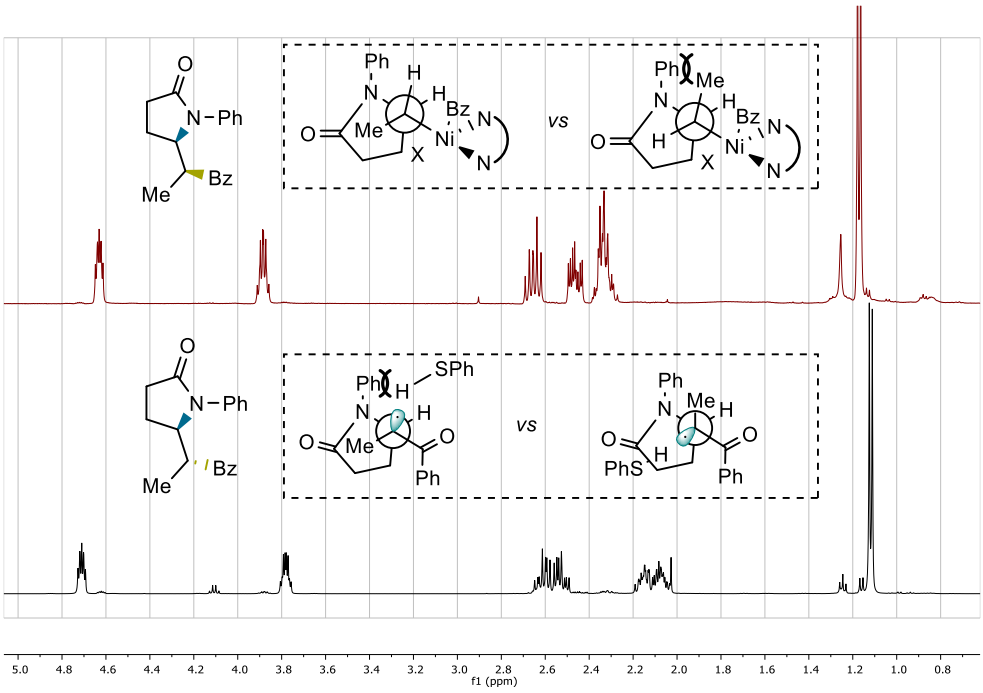
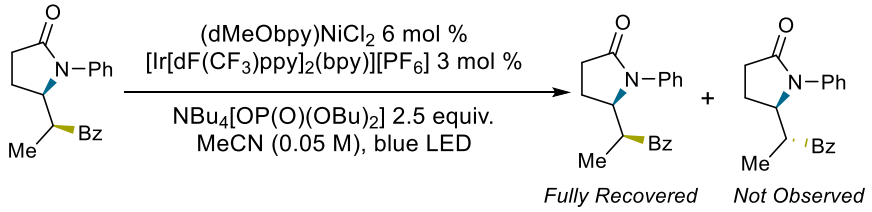


Figure S1. Mechanistic Proposal for Complementary Diastereoselectivity

Subsequently, we subject substrate 1' into the standard reaction conditions for amidoacylation, and unsurprisingly, after 36 h, the same diastereoisomer was fully recovered, with no observation of tautomerization.



4.4.2 Influence of Ligands on Diastereoselectivity

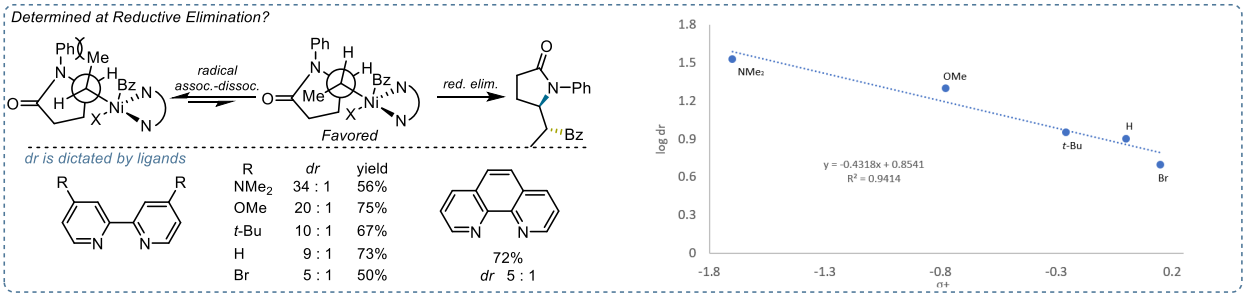


Figure S2. Ligand's Influence on Diastereoselectivity

Reactions were set up following GPII using corresponding Ni(II) precatalysts. Because the crude ^{1}H-NMR was often inconclusive and the corresponding diastereoisomers were inseparable in either automated chromatography or HPLC analysis, the *dr* was analyzed by ^{1}H NMR after purification. As is indicated in the charts, although 1,10-phenanthroline gave a comparable yield, the diastereoselectivity was significantly

compromised. Other bpy-type ligands that gave reasonable yields, such as dBrbpy, dtbpy and bpy, led to an 5:1 to 9:1 ratio of diastereoisomers, while d(NMe_2)bpy gave higher dr value but compromised yield. Together with the observation in 4.4.1, these results strongly supported the hypothesis that the diastereoselectivities were established during the Ni-catalyzed cross-coupling cycle.

4.5 Computation Study

4.5.1 General Information

All DFT calculations were performed with the Gaussian 09 software package[10]. Geometry optimizations of all the minima and transition states were carried out at the B3LYP[11] level of theory with additional Grimme's D3 dispersion correction (Becke-Johnson damping)[12] using the def2-SVP basis set[13]. Vibrational frequencies were computed at the same level to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K, as well as to check whether each optimized structure is a transition state or not. The single-point energies were computed at the same level of theory, combined with def2-TZVPP[12] basis set and SMD solvation model[14] for acetonitrile using the optimized structures. The 3D diagrams of molecules were generated using CYLView[15]. In addition, to correct the Gibbs free energies under pressure of 1 atm to the standard state in solution (1 mol/L), a correction of $RT\ln(c_s/c_g)$ (about 1.89 kcal/mol) is added to Gibbs energies of all the calculated species except acetonitrile. c_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in gas phase (0.0446 mol/L), and R is the gas constant. For acetonitrile, the actual molar concentration of 19.1 mol/L was used to correct the Gibbs free energy, and thus a correction of about 3.64 kcal/mol is added to the Gibbs energy of acetonitrile. The stability of "wavefunction" was checked for each calculated species. The conformation of each calculated species was carefully searched and only the most stable ones were presented. All the absolute configurations were only drawn for clarity. To reduce computational time consumption, bpy was used as model ligands and $BzOP(O)(OBu)_2$ is simplified to $BzOP(O)(OMe)_2$.

4.5.2 Computational Details

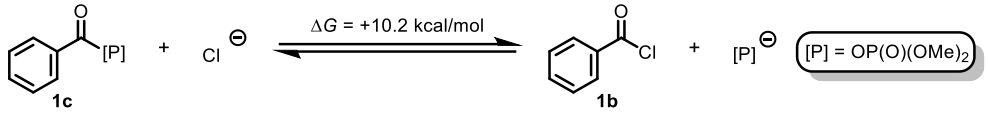


Figure S3. DFT computed relative Gibbs energies in kcal/mol of **1c** and **1b** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

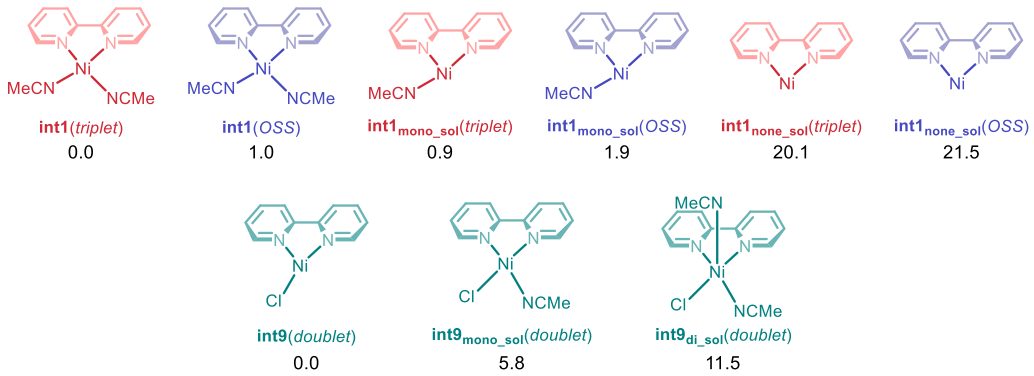


Figure S4. DFT computed relative Gibbs energies in kcal/mol of **int1** with different spin states or ligation of MeCN and DFT computed relative Gibbs energies in kcal/mol of **int9** with ligation of MeCN at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

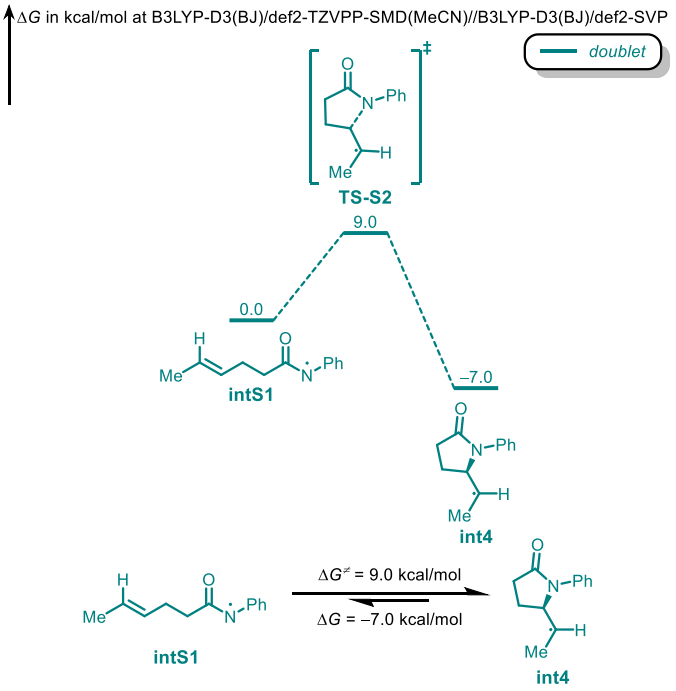


Figure S5. DFT computed free energy diagram of generation of **int4** from the open-chain radical **intS1** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

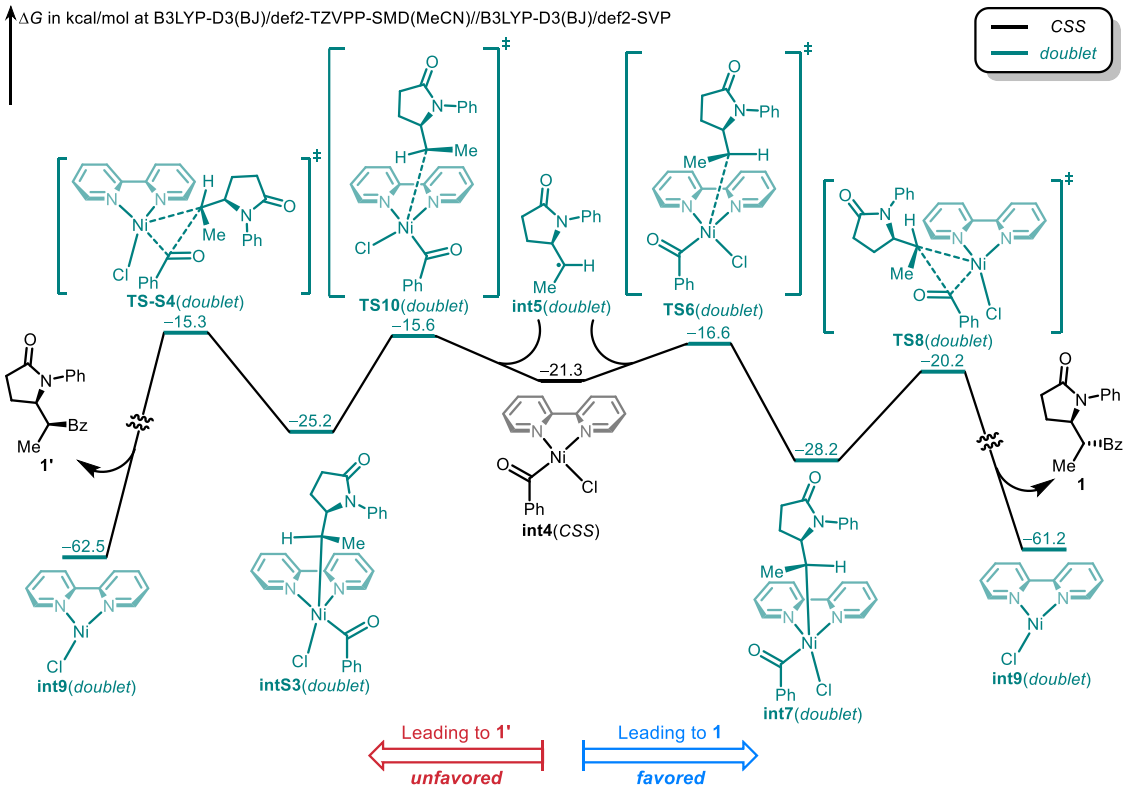


Figure S6. Full reaction pathways for generation of **1** and **1'** from **int3** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

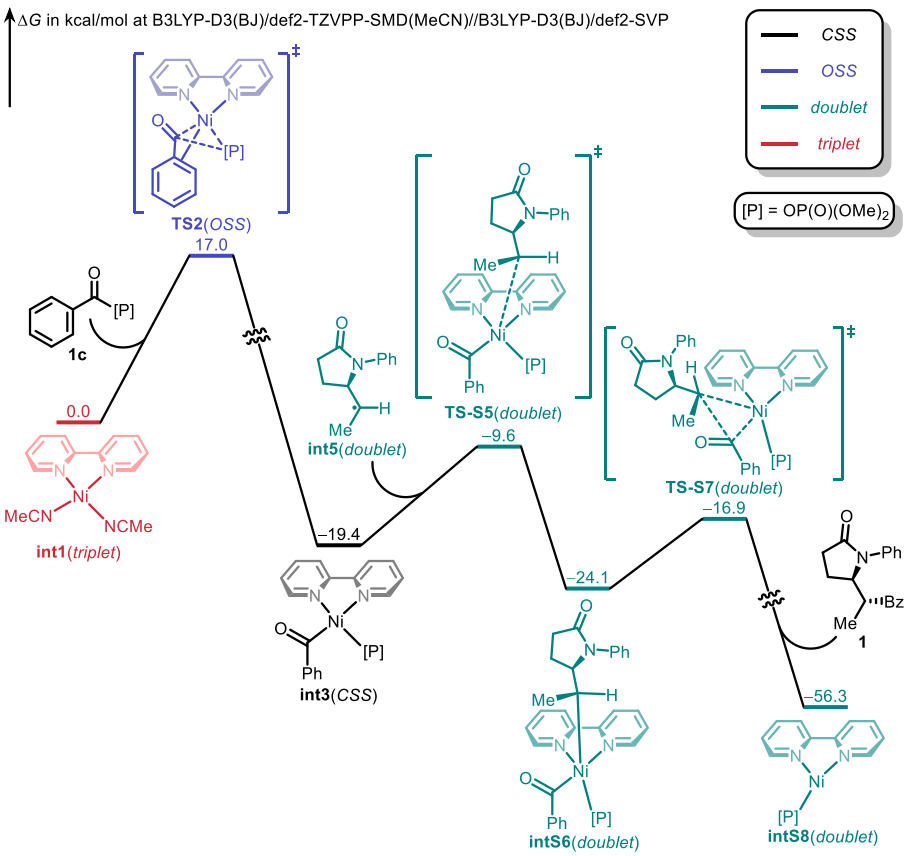


Figure S7. DFT computed free energy diagram between **1a** and **1d** of the thermochemical part (from **C** to **F**) of the catalytic cycle at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

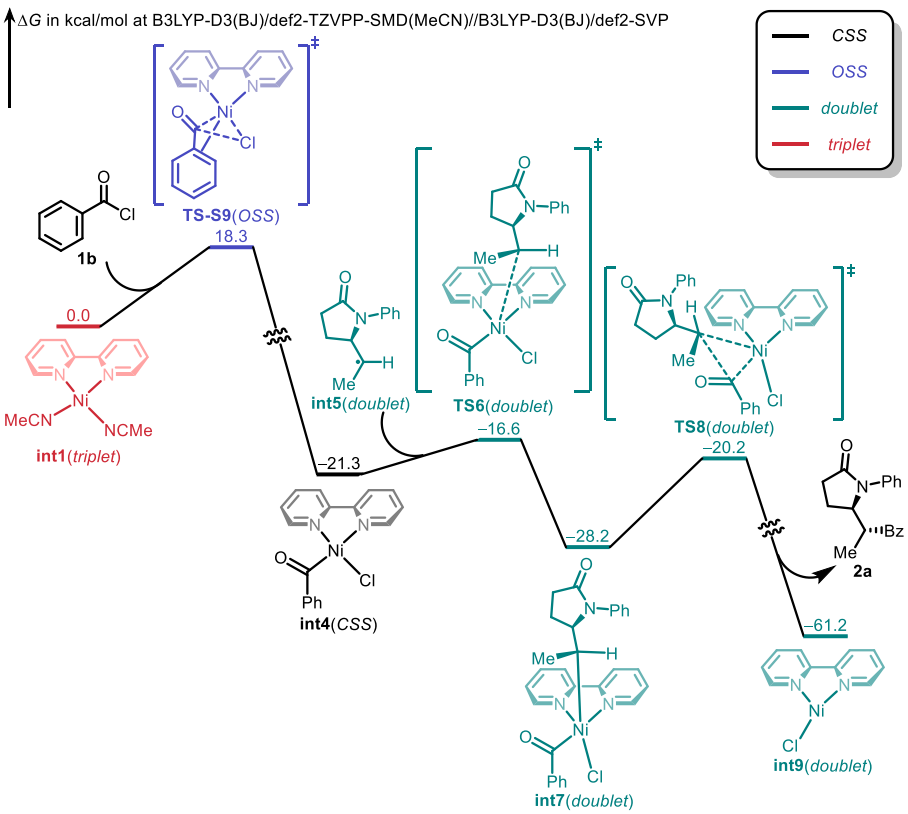


Figure S8. DFT computed free energy diagram between **1a** and **1b** of the thermochemical part (from **C** to **F**) of the catalytic cycle at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP. The oxidative addition of **1b** via **TS-S9** is less favorable than **TS2** by 1.3 kcal/mol. This is the result of the calculated equilibrium between **1b** and **1c** shown in Figure S3.

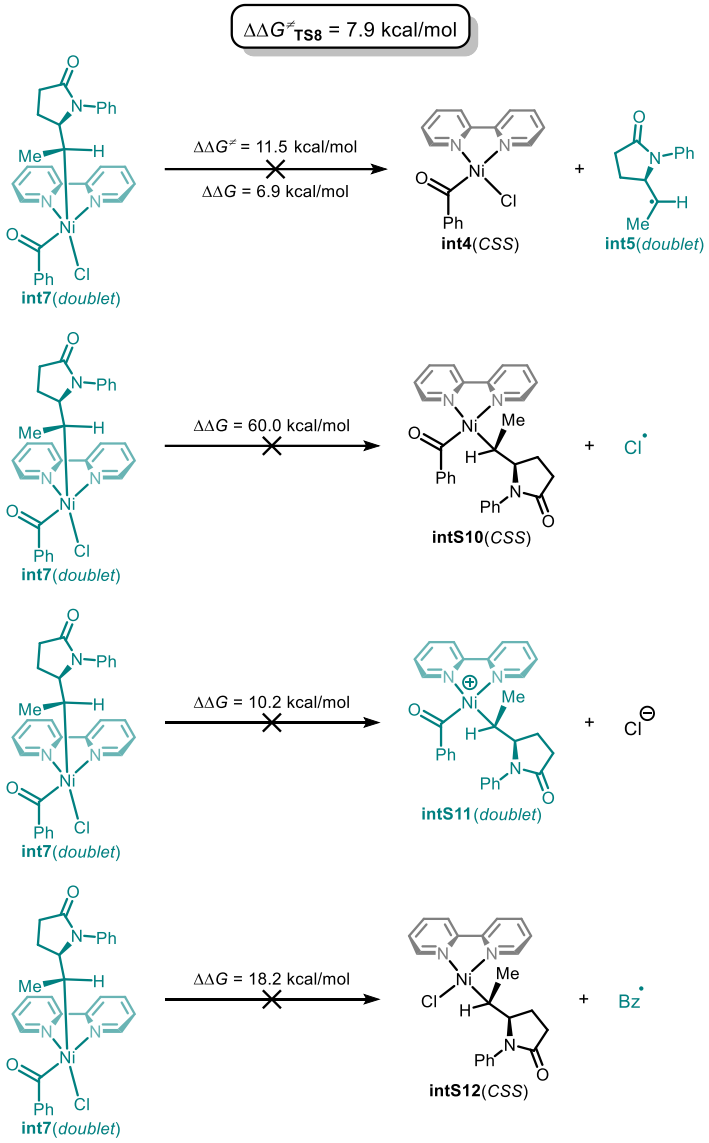


Figure S9. DFT computed relative thermodynamics of the dissociation of ligands from **int6** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP. (**int7** is set to be the new relative zero and thus $\Delta\Delta G$ is used.) These dissociation processes are all unfavorable as **TS8** only requires a barrier of 7.9 kcal/mol.

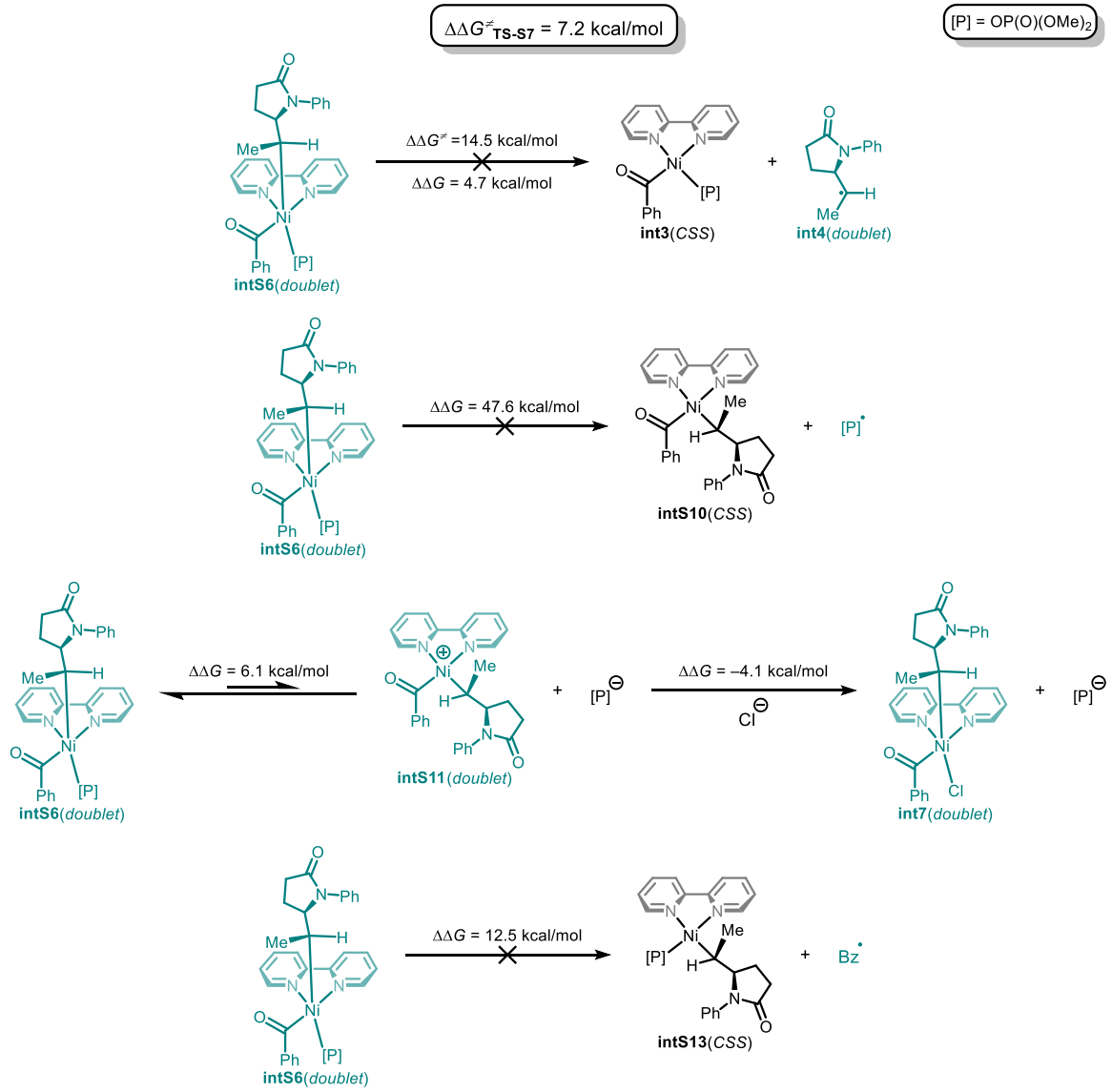


Figure S10. DFT computed relative thermodynamics of the dissociation of ligands from **intS6** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP. (**intS6** is set to be the new relative zero and thus $\Delta\Delta G$ is used.) These dissociation processes are all unfavorable as **TS-S7** only requires a barrier of 7.2 kcal/mol except for the one generating the cationic species **intS11**. However, this dissociation would further give rise to the more stable **int7**.

An alternative reaction pathway featuring the oxidation states sequence of Ni as Ni(0), Ni(I) and Ni(III) could also be operative. **TS-S9** requires 7.8 kcal/mol at standard states and should be diffusion controlled. In this scenario, the dr outcome of the reaction is controlled by **TS-S14** and **TS-S18**, which has a difference of 6.0 kcal/mol, since the oxidation of the radical **int5** is irreversible. However, considering the relative low concentration of **int5**, this pathway might not be operative.

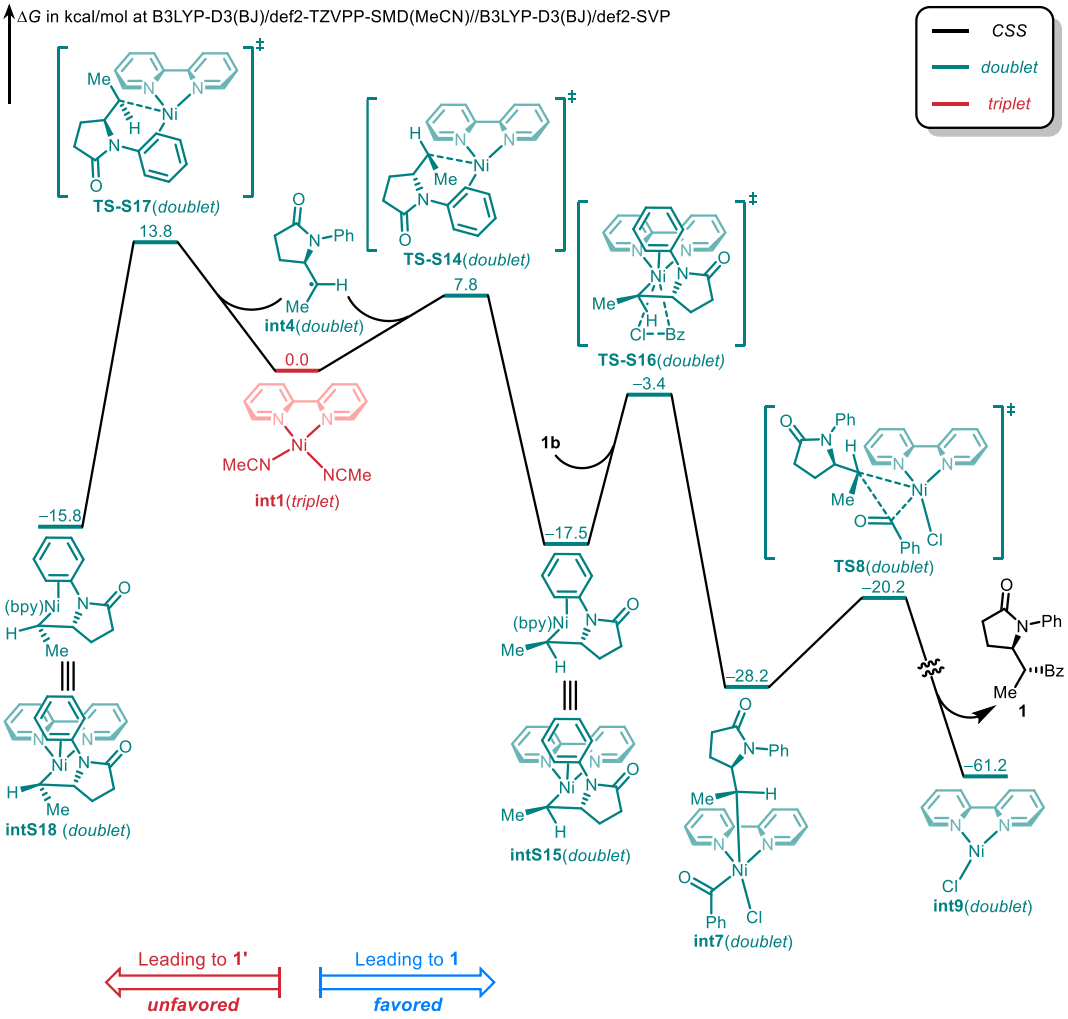


Figure S11. DFT computed free energy diagram of the alternative reaction pathway between **1a** and **1b** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

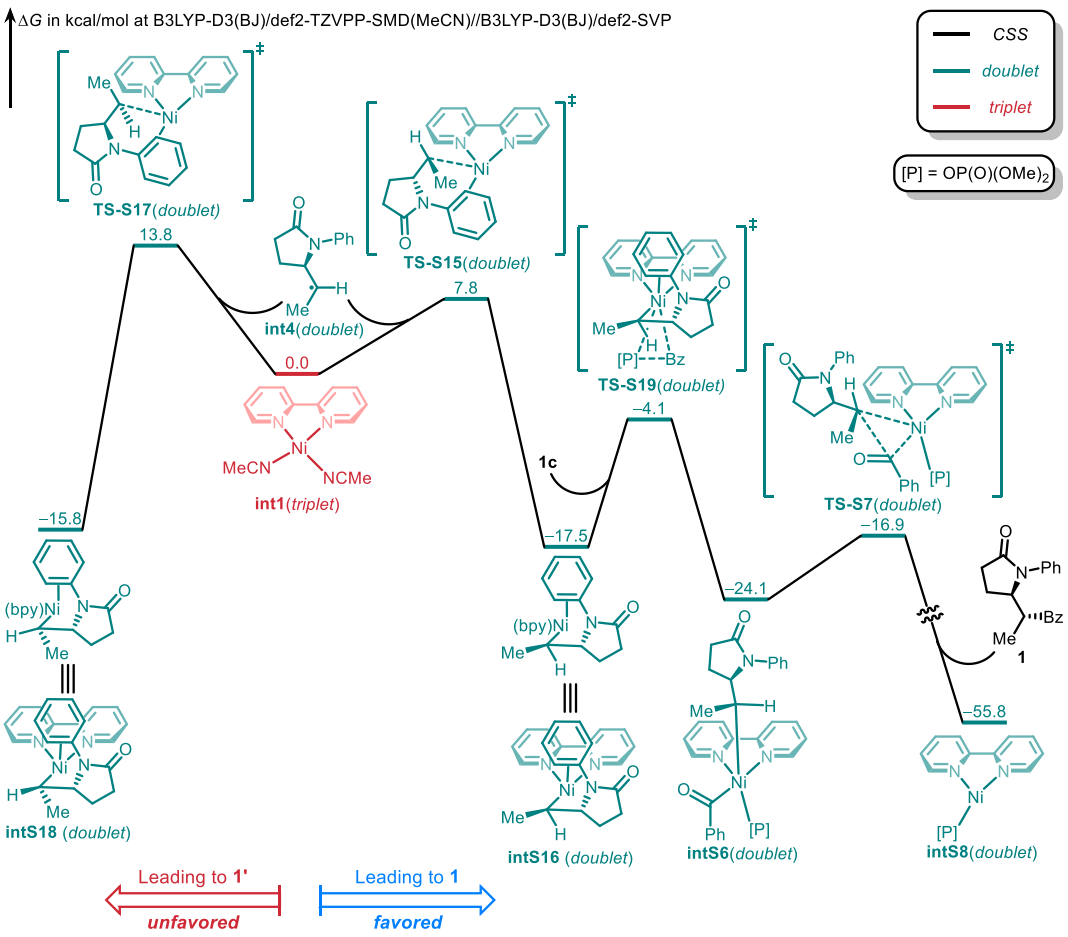


Figure S12. DFT computed free energy diagram of the alternative reaction pathway between **1a** and **1c** at B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP.

Table S2. Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the B3LYP-D3(BJ)/def2-TZVPP-SMD(MeCN)//B3LYP-D3(BJ)/def2-SVP level of theory. [P] = $OP(O)(OMe)_2$.

Structures	*ZPE*	*TCH*	*TCG*	*E*	*H*	*G*	Imaginary Frequency
1b (Bz–Cl)	0.101366	0.109614	0.068306	−805.390781	−805.281167	−805.322475	
1c (Bz–[P])	0.197056	0.213484	0.152091	−1067.572185	−1067.358701	−1067.420094	
MeCN	0.045072	0.049634	0.022077	−132.826335	−132.776701	−132.804258	
Bz•	0.097847	0.105074	0.066635	−345.089566	−344.984492	−345.022931	
Cl•	0.000000	0.002360	−0.014813	−460.169325	−460.166965	−460.184138	
[P]•	0.092702	0.102745	0.057158	−722.335318	−722.232573	−722.278160	
Cl^-	0.000000	0.002360	−0.015023	−460.396980	−460.394620	−460.412003	
$[P]^-$	0.092796	0.102323	0.058775	−722.551540	−722.449217	−722.492765	
int1(*triplet*)	0.250374	0.271906	0.195122	−2269.725625	−2269.453719	−2269.530503	
int1(*OSS*)	0.250540	0.271973	0.196831	−2269.725775	−2269.453802	−2269.528944	
int1$_{mono_sol}$(*triplet*)	0.204681	0.220780	0.158975	−2136.889640	−2136.668860	−2136.730665	
int1$_{mono_sol}$(*OSS*)	0.204603	0.220743	0.159816	−2136.888795	−2136.668052	−2136.728979	

int1$_{none_sol}$(*triplet*)	0.157725	0.169005	0.119752	−2004.021254	−2003.852249	−2003.901502	
int1$_{none_sol}$(*OSS*)	0.157726	0.169008	0.120896	−2004.020297	−2003.851289	−2003.899401	
TS2(*OSS*)	0.354554	0.382380	0.295208	−3071.618743	−3071.236363	−3071.323535	176.1*i*
int3(*CSS*)	0.357526	0.385572	0.296437	−3071.678026	−3071.292454	−3071.381589	
int3(*triplet*)	0.356389	0.384851	0.293522	−3071.666158	−3071.281307	−3071.372636	
int4(*CSS*)	0.263297	0.282901	0.214048	−2809.517831	−2809.234930	−2809.303783	
int4(*triplet*)	0.261368	0.281748	0.209491	−2809.505799	−2809.224051	−2809.296308	
int5	0.233223	0.247092	0.192291	−595.949591	−595.702499	−595.757300	
TS6	0.498852	0.532225	0.431111	−3405.481814	−3404.949589	−3405.050703	37.7*i*
int7	0.501944	0.535148	0.434715	−3405.503804	−3404.968656	−3405.069089	
TS8	0.500785	0.533633	0.433708	−3405.490070	−3404.956437	−3405.056362	213.4*i*
int9	0.160753	0.173720	0.119854	−2464.371011	−2464.197291	−2464.251157	
int9$_{mono-sol}$	0.206713	0.225017	0.158142	−2597.198586	−2596.973569	−2597.040444	
int9$_{di-sol}$	0.252864	0.276305	0.196588	−2730.026341	−2729.750036	−2729.829753	
1	0.340312	0.359666	0.293657	−941.167223	−940.807557	−940.873566	
TS10	0.499245	0.532364	0.432486	−3405.481590	−3404.949226	−3405.049104	13.4*i*
1'	0.339907	0.359429	0.291870	−941.167552	−940.808123	−940.875682	
intS1	0.230757	0.245732	0.186518	−595.932584	−595.686852	−595.746066	
TS-S2	0.231214	0.244870	0.190927	−595.922689	−595.677819	−595.731762	359.7*i*
intS3	0.501838	0.534924	0.436224	−3405.500600	−3404.965676	−3405.064376	
TS-S4	0.501336	0.534013	0.434645	−3405.483230	−3404.949217	−3405.048585	282.0*i*
TS-S5	0.593326	0.635302	0.512856	−3667.633181	−3666.997879	−3667.120325	31.7*i*
intS6	0.596705	0.637908	0.520527	−3667.663871	−3667.025963	−3667.143344	
TS-S7	0.596146	0.636782	0.521003	−3667.652951	−3667.016169	−3667.131948	181.3*i*
intS8	0.254891	0.276102	0.202291	−2726.525657	−2726.249555	−2726.323366	
TS-S9(*OSS*)	0.260473	0.279910	0.212080	−2809.452755	−2809.172845	−2809.240675	92.3*i*
TS-S9 (*triplet*)	0.259137	0.278699	0.209984	−2809.446112	−2809.167413	−2809.236128	51.3*i*
intS10(*CSS*)	0.500709	0.531373	0.440021	−2945.232386	−2944.701013	−2944.792365	
intS10(*triplet*)	0.498730	0.529859	0.436143	−2945.191507	−2944.661648	−2944.755364	
intS11	0.501862	0.532728	0.440064	−2945.083926	−2944.551198	−2944.643862	
intS12(*CSS*)	0.401544	0.426902	0.347393	−3060.367526	−3059.940624	−3060.020133	
intS12(*triplet*)	0.399300	0.425809	0.339215	−3060.351032	−3059.925223	−3060.011817	
intS13(*CSS*)	0.496833	0.530291	0.432763	−3322.536211	−3322.005920	−3322.103448	
intS13(*triplet*)	0.494226	0.528808	0.424999	−3322.520817	−3321.992009	−3322.095818	
TS-S14	0.392535	0.417172	0.337957	−2600.013463	−2599.596291	−2599.675506	70.9*i*
intS15	0.395570	0.420141	0.340119	−2600.055887	−2599.635746	−2599.715768	
TS-S16	0.499314	0.531886	0.435689	−3405.465255	−3404.933369	−3405.029566	40.5*i*
TS-S17	0.393146	0.417513	0.338948	−2600.004787	−2599.587274	−2599.665839	23.5*i*
intS18	0.396111	0.420458	0.341360	−2600.054348	−2599.633890	−2599.712988	
TS-S19	0.591884	0.633609	0.511029	−3667.622540	−3666.988931	−3667.111511	44.0*i*

4.6 Transient Absorption Studies

The nanosecond transient absorption (nsTA) setup was assembled according to previous report.[16] Briefly, it has a frequency-tripled Nd:YAG laser as pump (Quanta-Ray DCR-1A, 355nm, pulse width 10 ns, 10 Hz rep. rate, ~15 mW), a flash lamp (Hamamatsu, pulse width ~2 μs) as a white-light probe source and a monochromator (SPEX) with a diode-array detector (Princeton Instruments, DIDA-512).

The concentrations for [Ir-1] and TEOA are 0.03 and 0.6 mM, respectively, whereas for [**Ir-1**], 1a and $Bu_4N[OP(O)(OBu)_2]$, the concentrations are 0.1, 10 and 20 mM, respectively. Both experiments were measured with a 10-mm quartz cuvette (Starna) in DCM, which was degassed with nitrogen for more than 10 minutes.

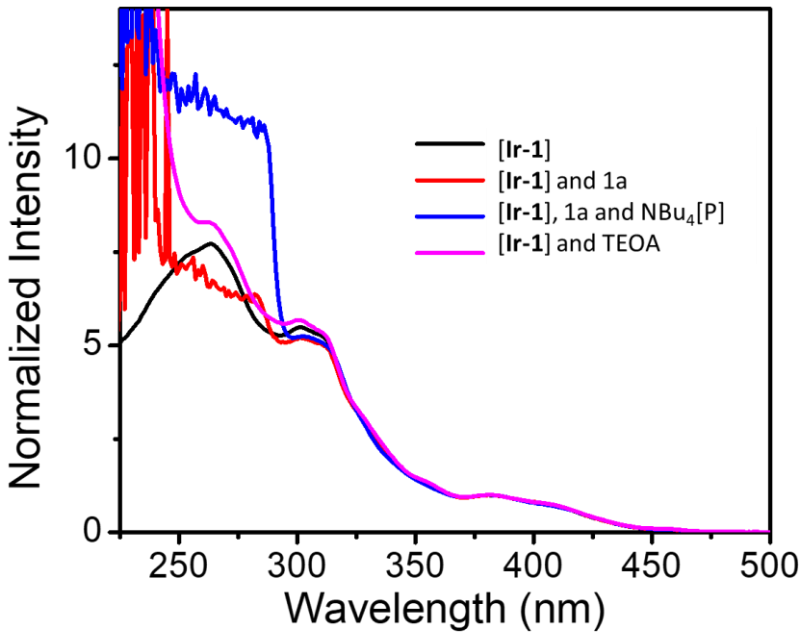


Figure S13. UV-Vis Absorption Traces.

5. References

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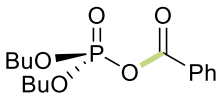
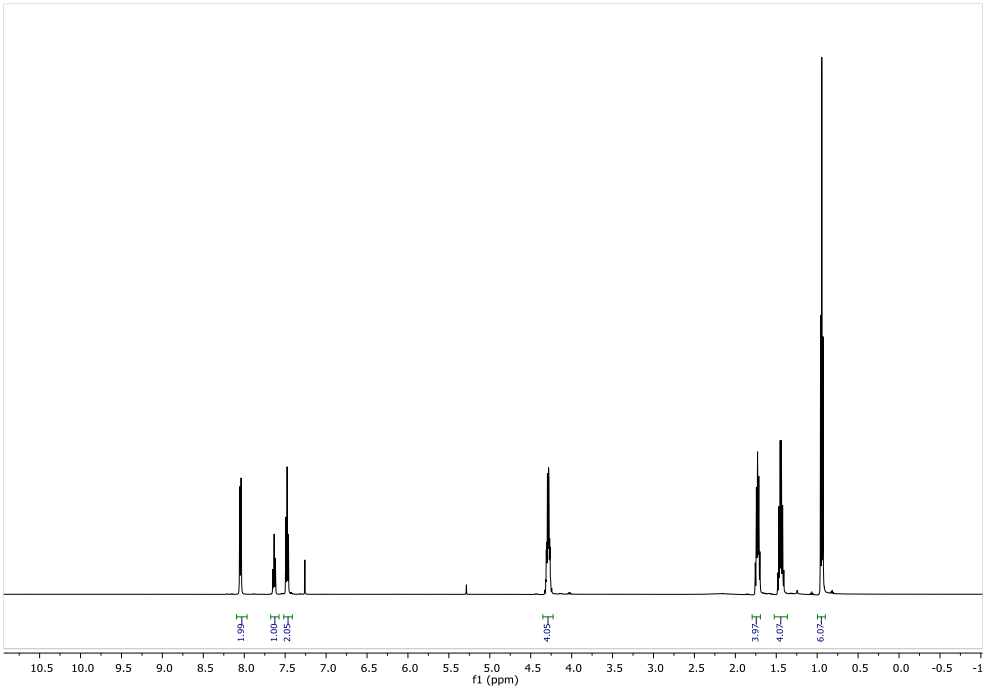
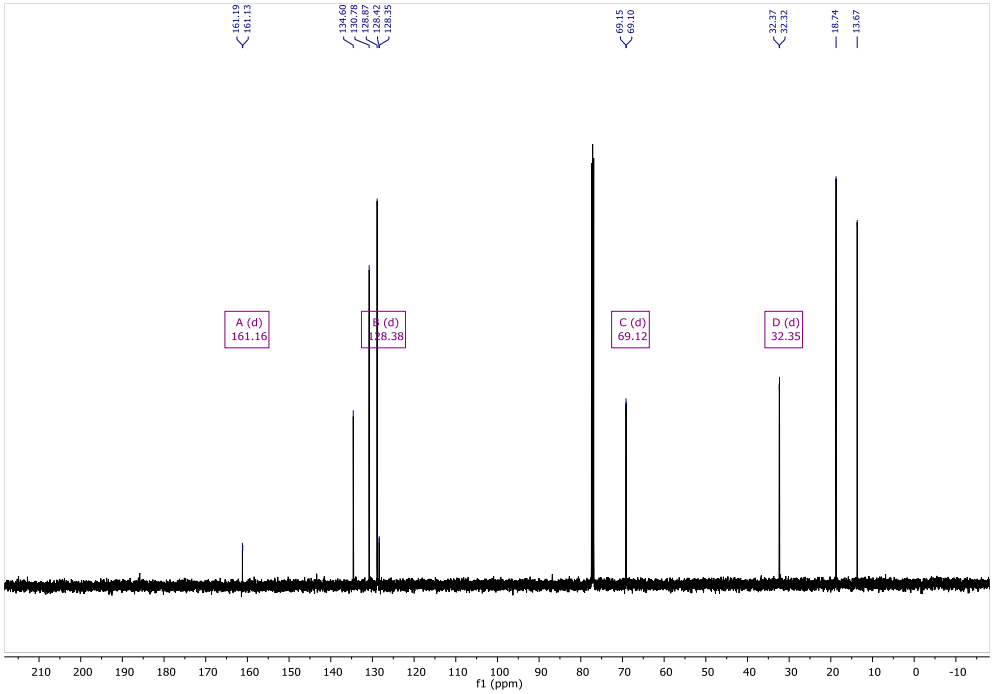
6. Spectra and Structure Data

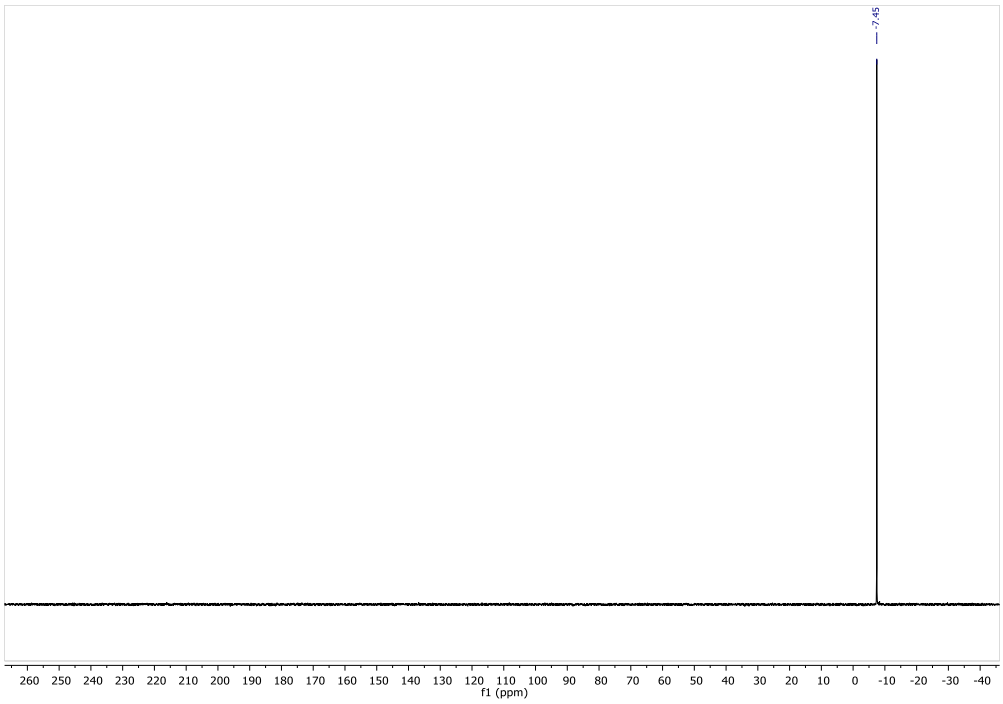
6.1 ^{1}H, ^{13}C and ^{19}F NMR Spectra

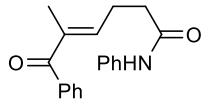


^{1}H NMR ($CDCl_3$, 500 MHz), ^{13}C NMR ($CDCl_3$, 126 MHz) and ^{31}P NMR ($CDCl_3$, 203 MHz) of Benzoic (dibutyl phosphoric) anhydride(S1a):

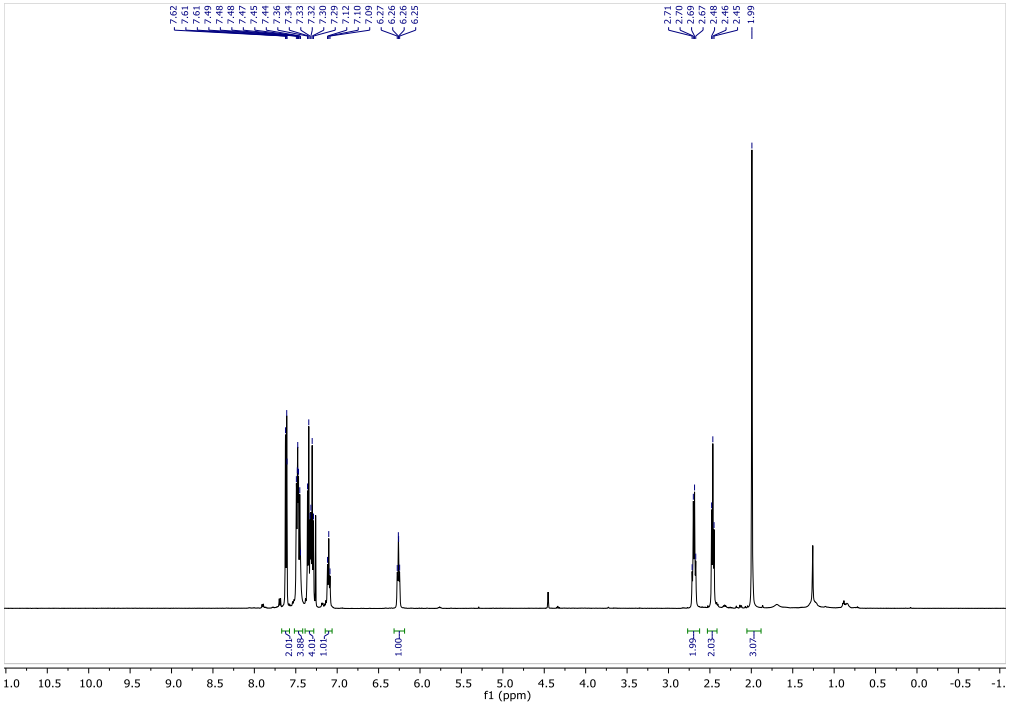


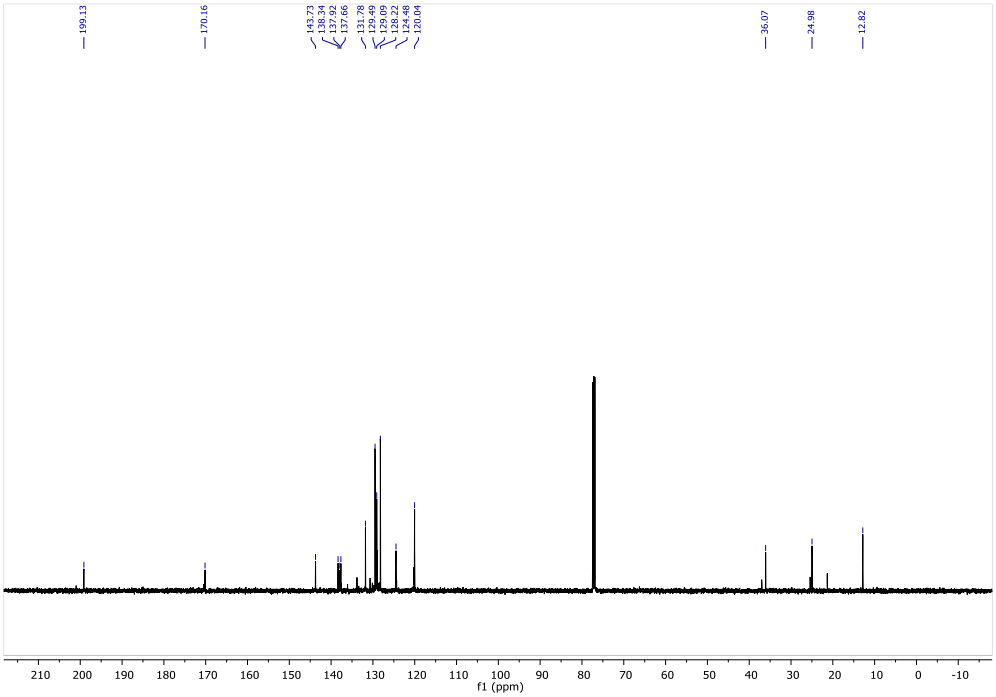


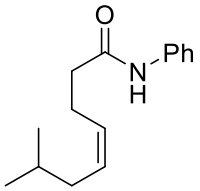

7.45
260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)



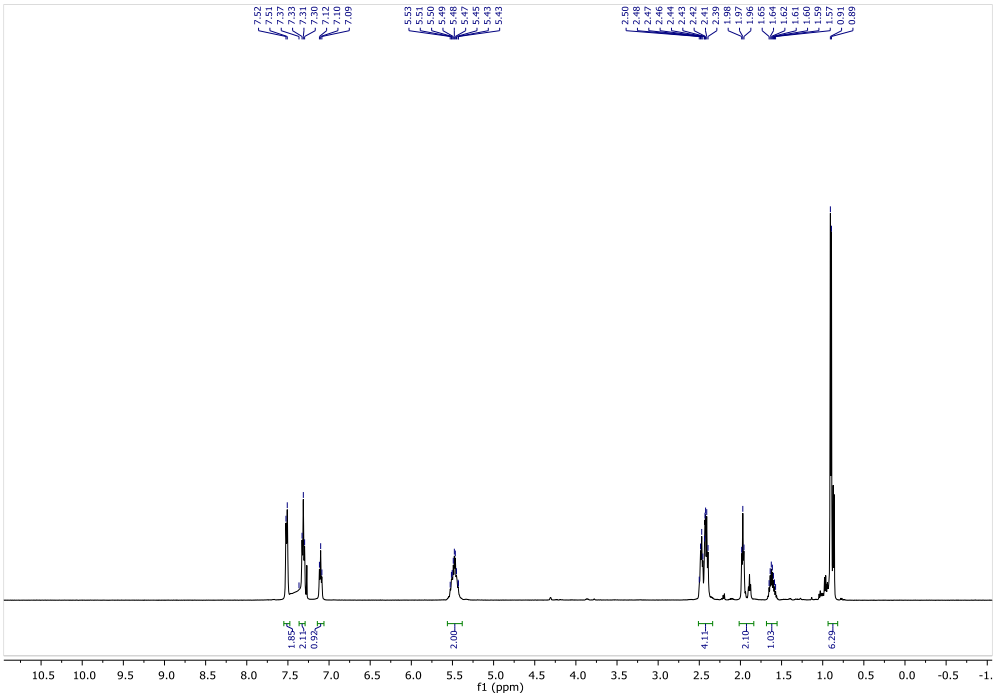
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 5-methyl-6-oxo-N,6-diphenylhex-4-enamide(S1b):

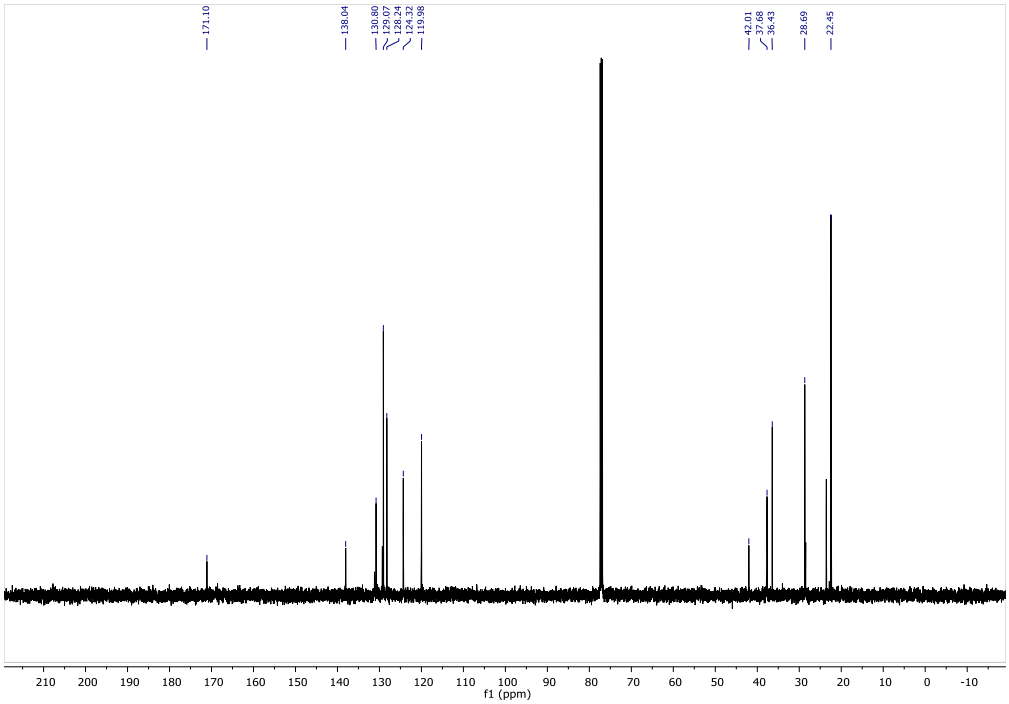


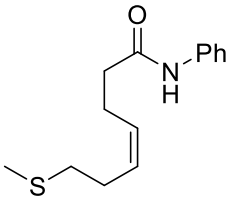




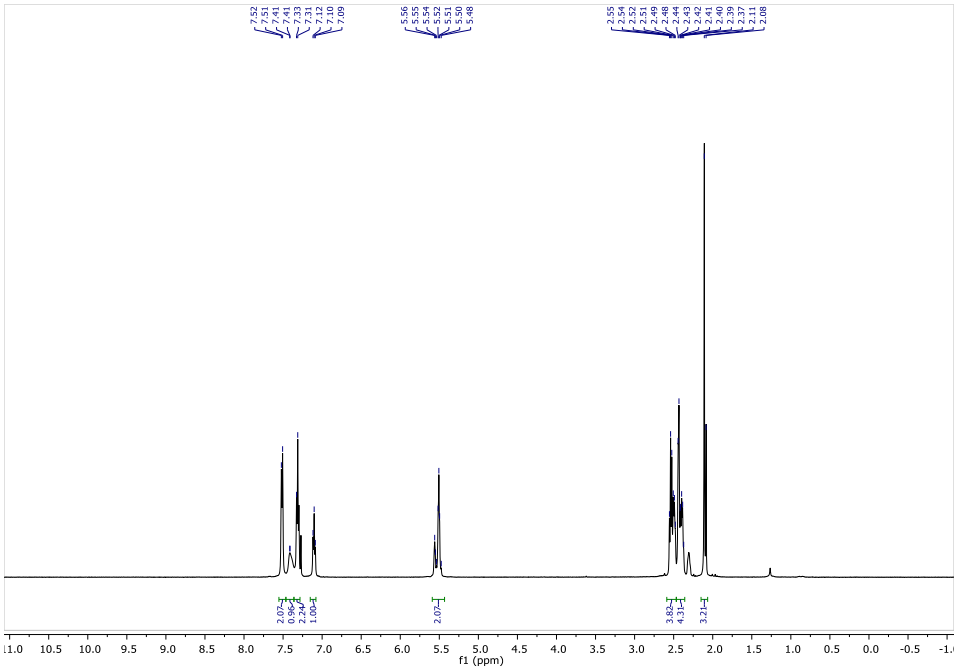
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 7-Methyl-*N*-phenyloct-4-enamide (S31):

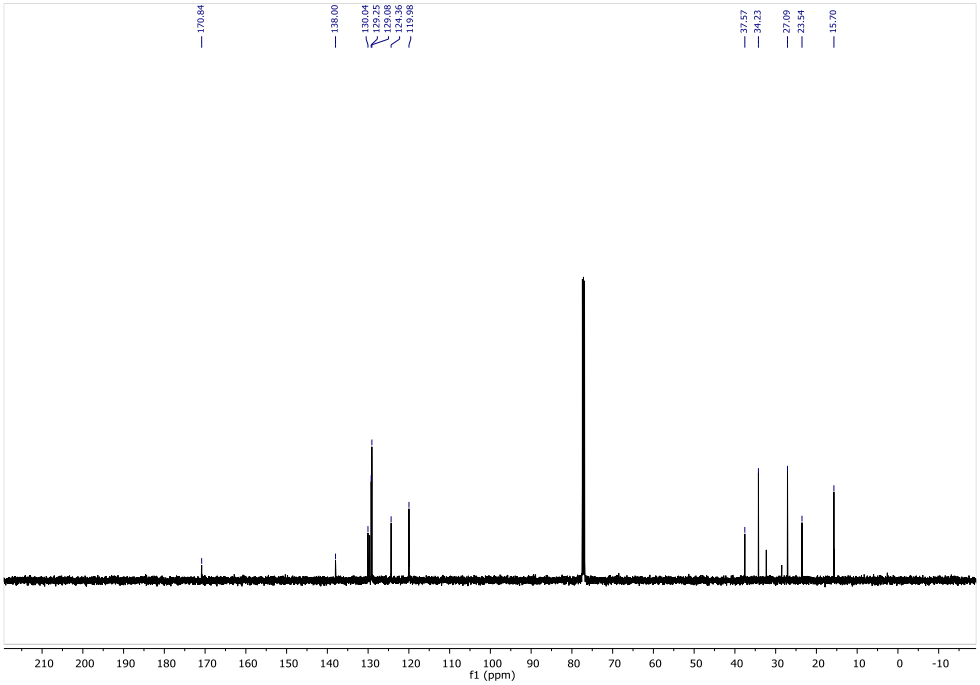


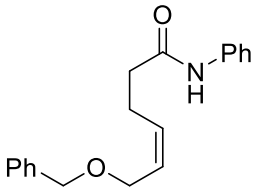




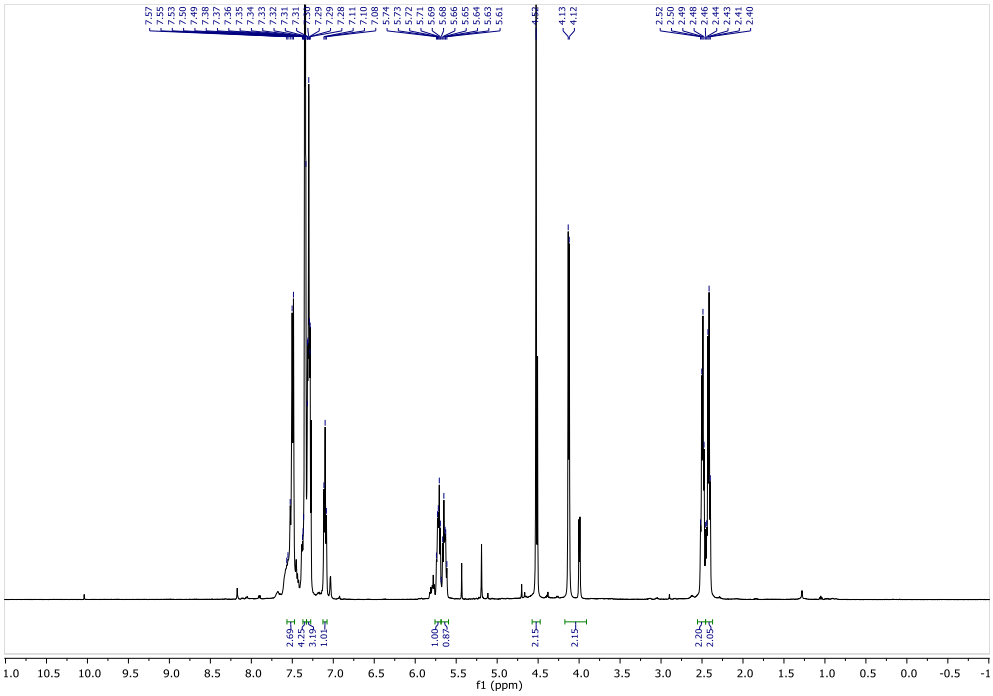
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 7-(methylthio)-*N*-Phenylhept-4-enamide (S32):

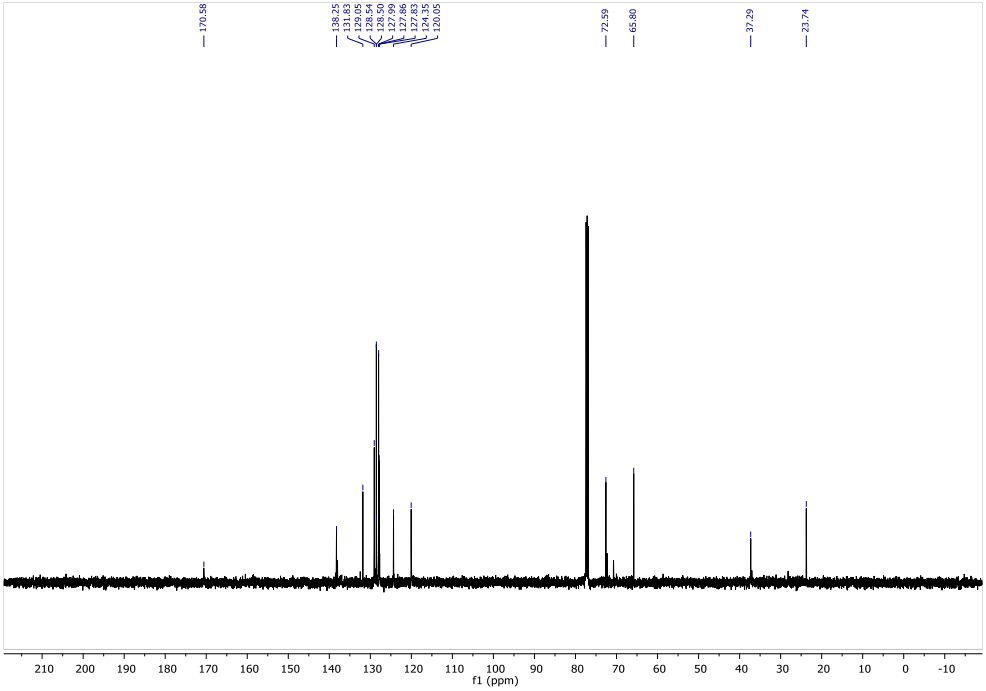


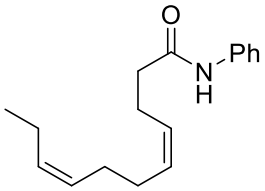




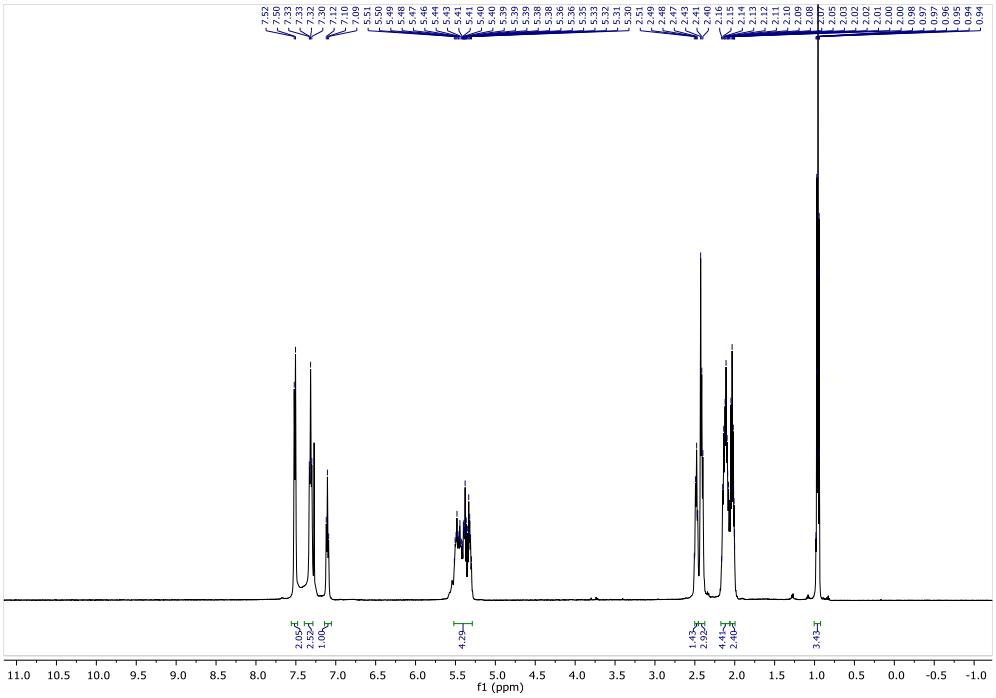
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 6-(Benzyloxy)-*N*-phenylhex-4-enamide (S33):

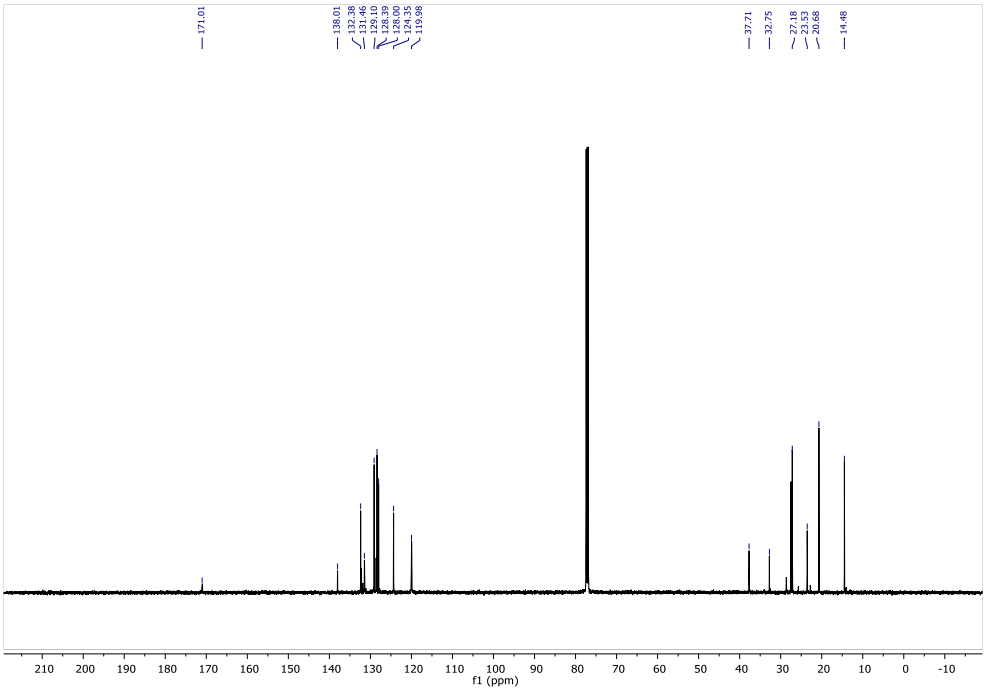


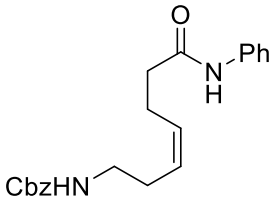




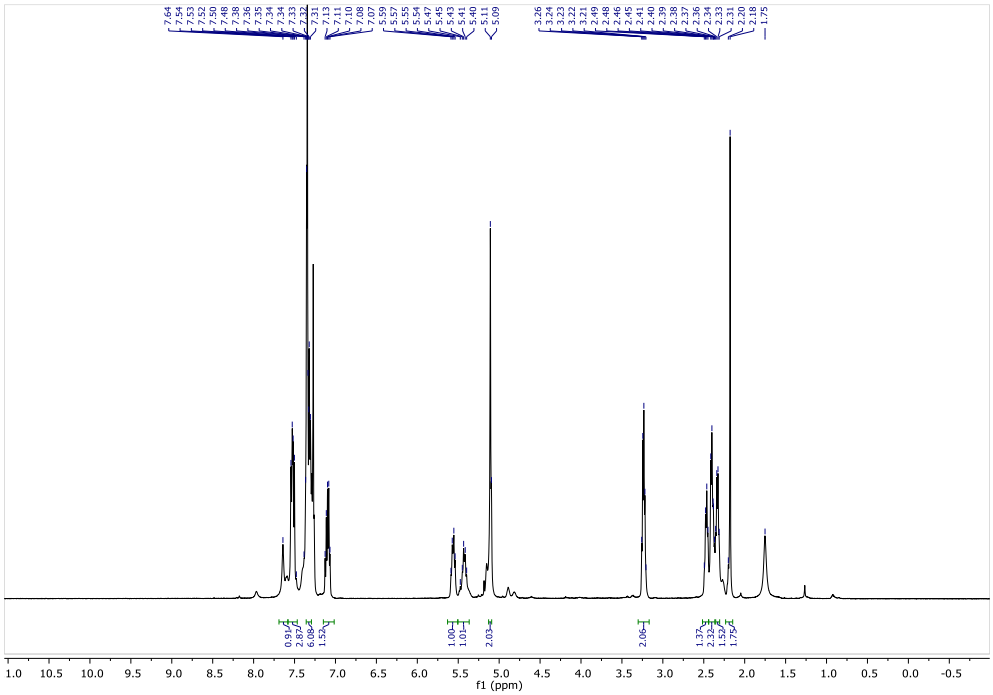
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (8*Z*)-*N*-Phenylundeca-4,8-dienamide (S34):

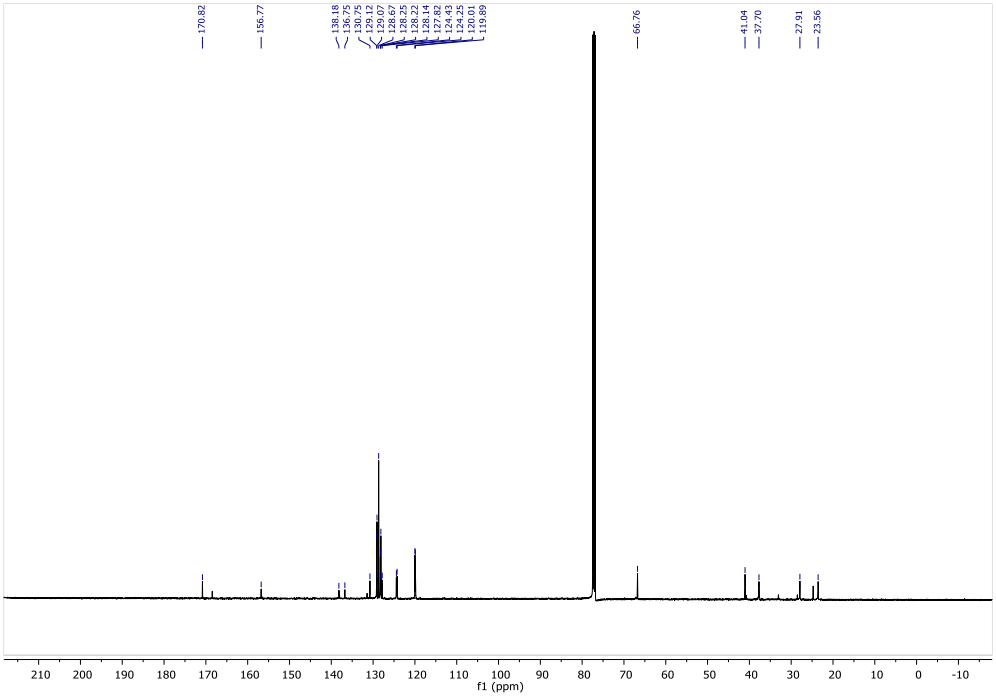


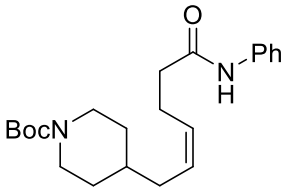




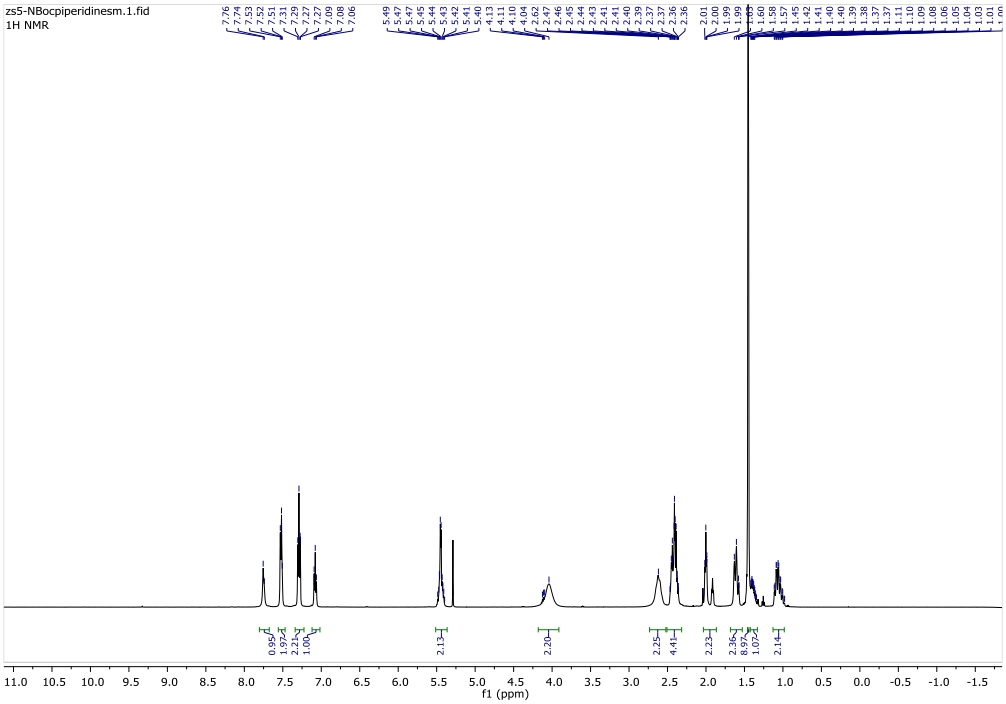
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of Benzyl (7-oxo-7-(phenylamino)hept-3-en-1-yl)carbamateenamide (S35):

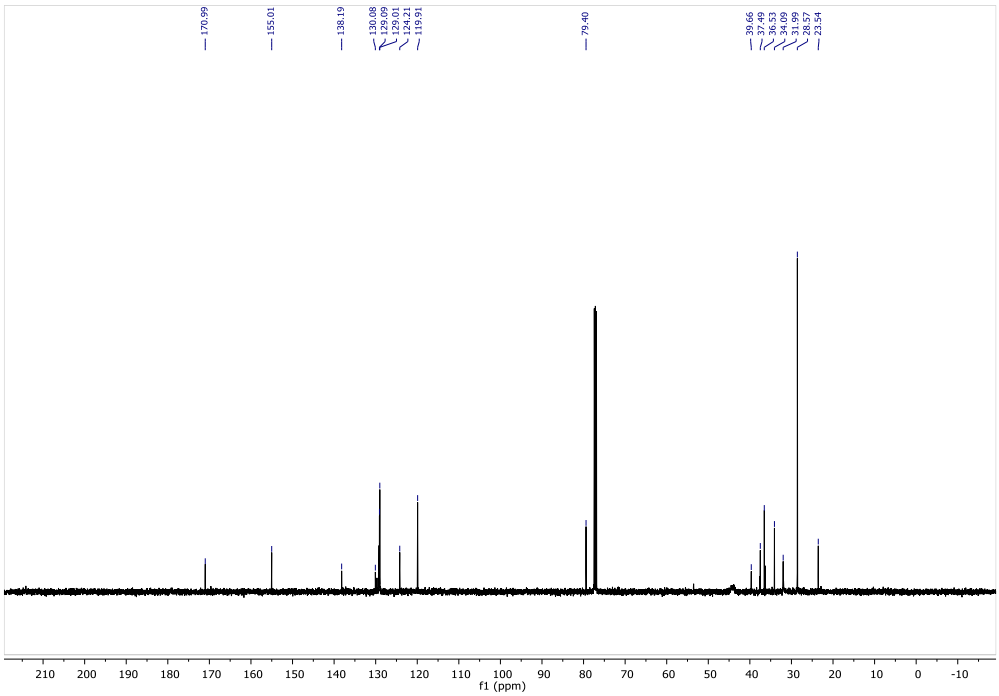


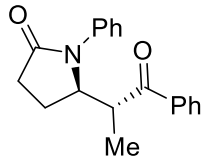




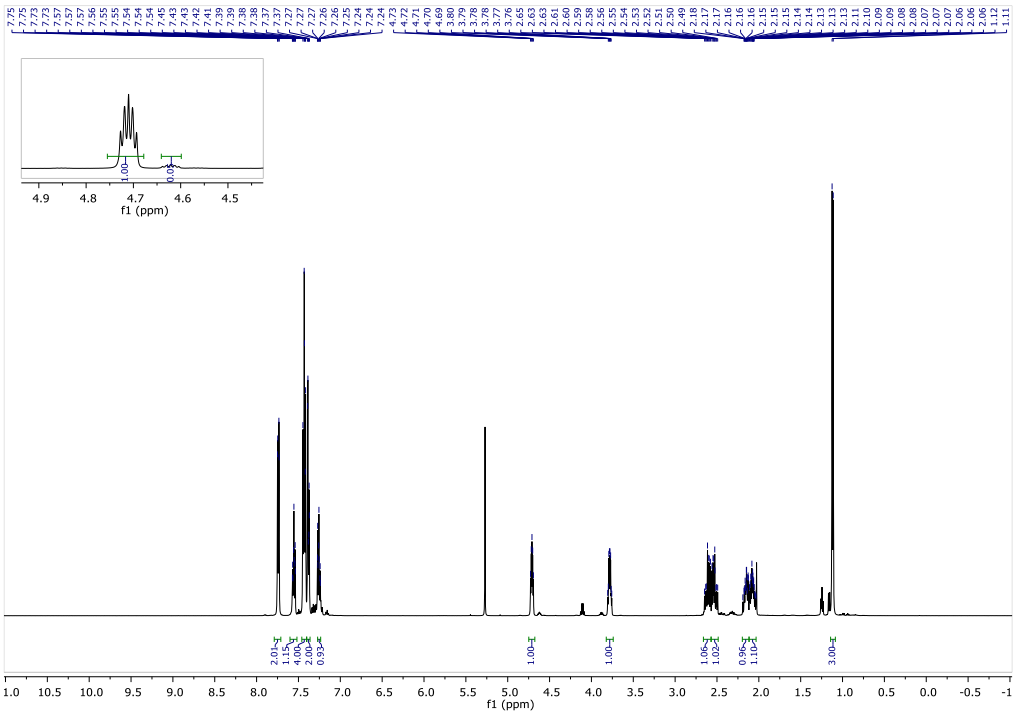
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of *tert*-Butyl 4-(6-oxo-6-(phenylamino)hex-2-en-1-yl)piperidine-1-carboxylate (S36):

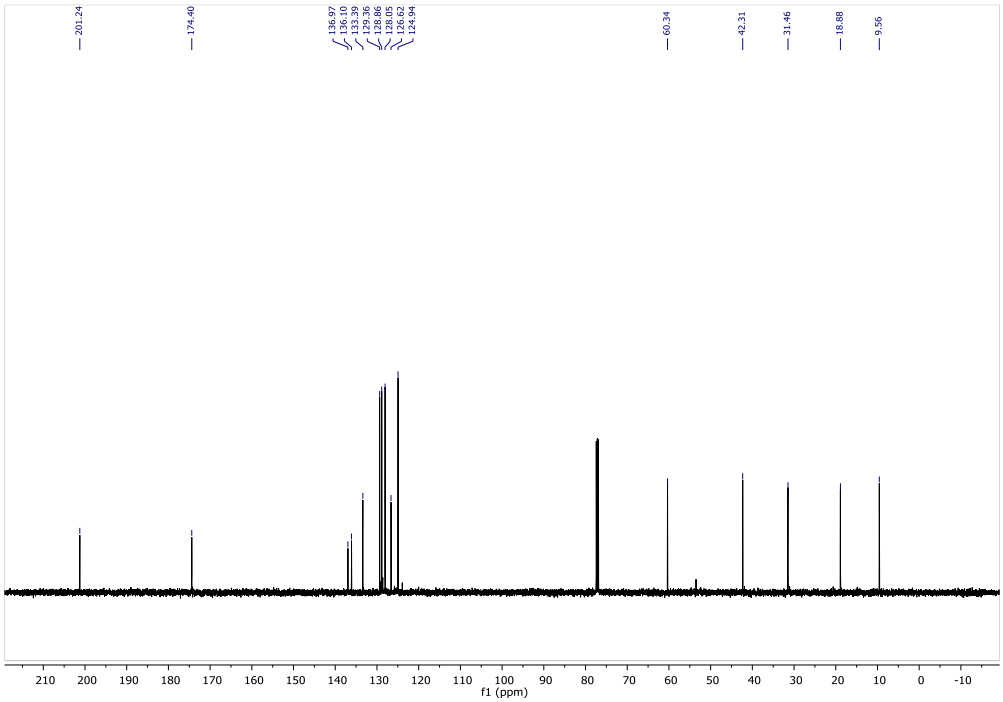


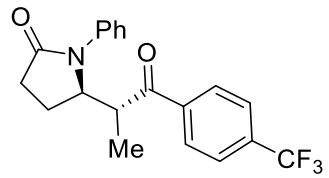




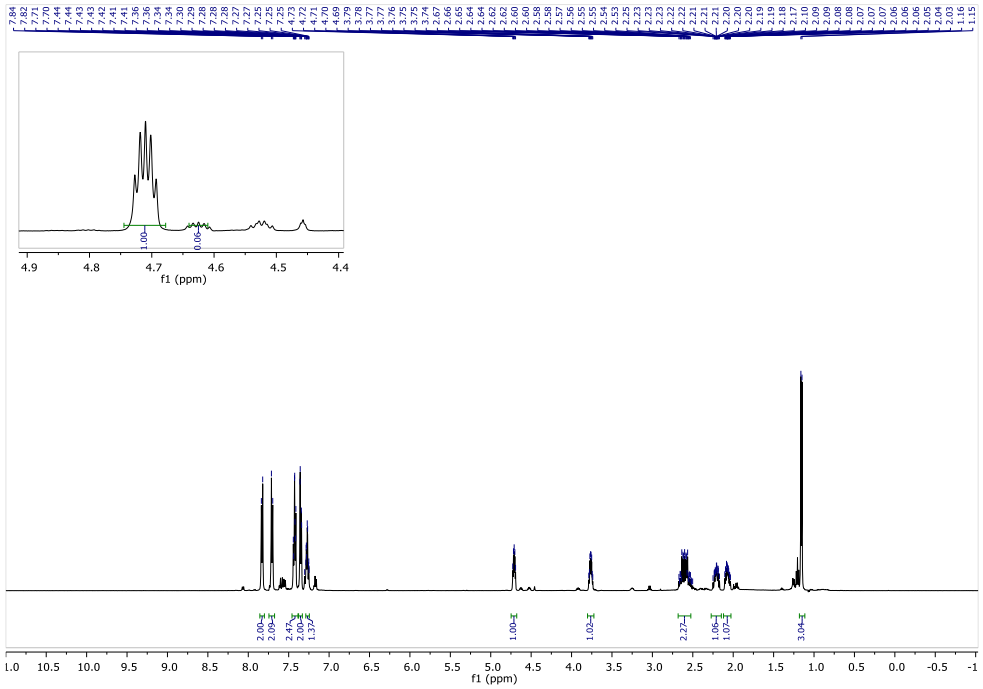
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)-1-phenylpyrrolidin-2-one (1):**

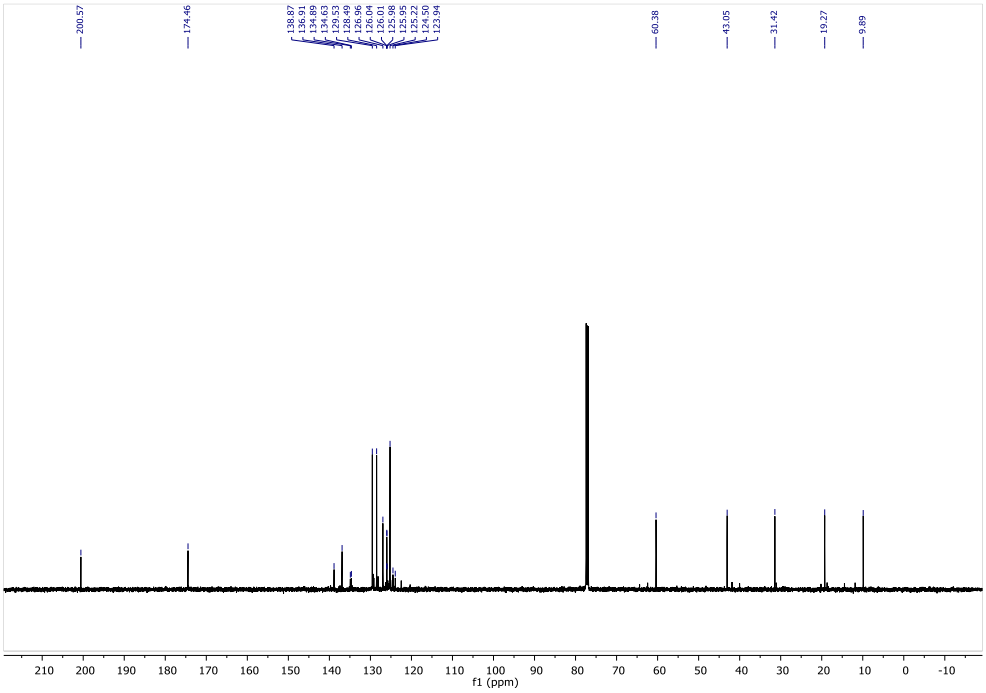


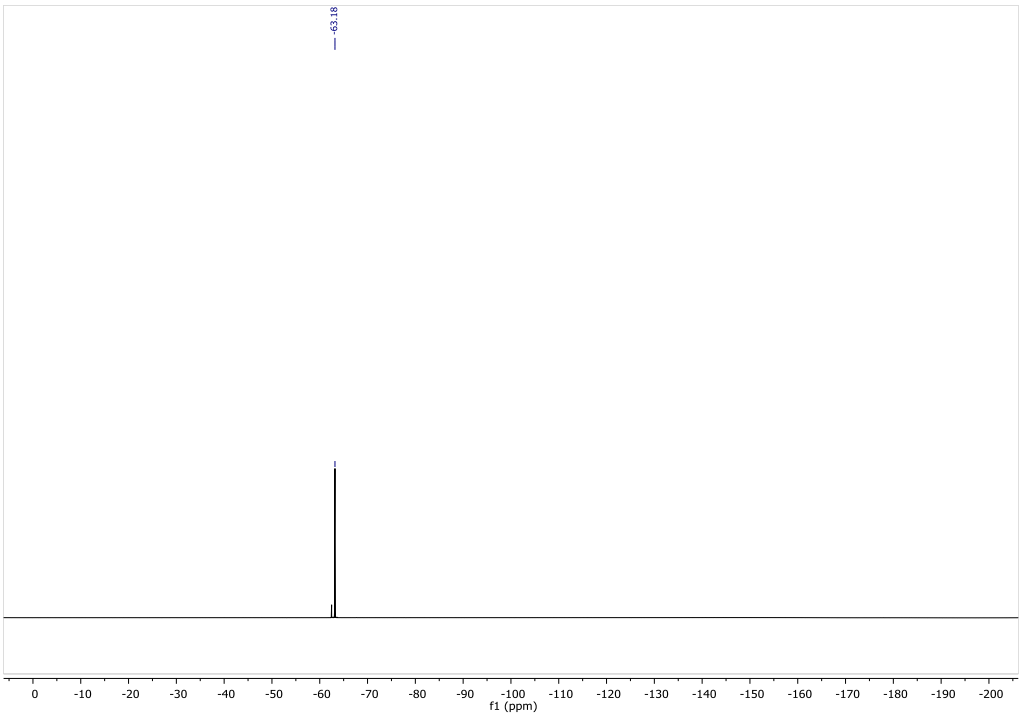


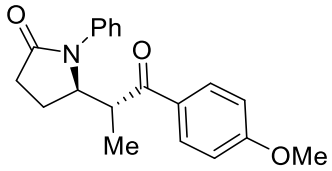


^{1}H NMR ($CDCl_3$, 500 MHz), ^{13}C NMR ($CDCl_3$, 126 MHz) and ^{19}F NMR ($CDCl_3$, 471 MHz) of (*R)-5-((*R**)-1-oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl)-1-phenylpyrrolidin-2-one (2):**

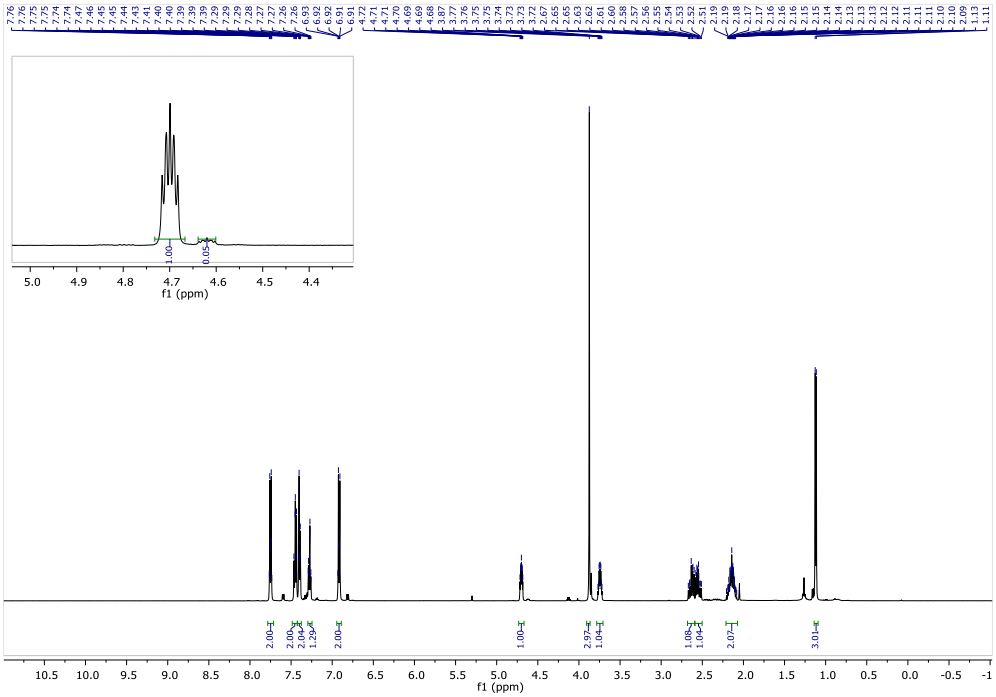


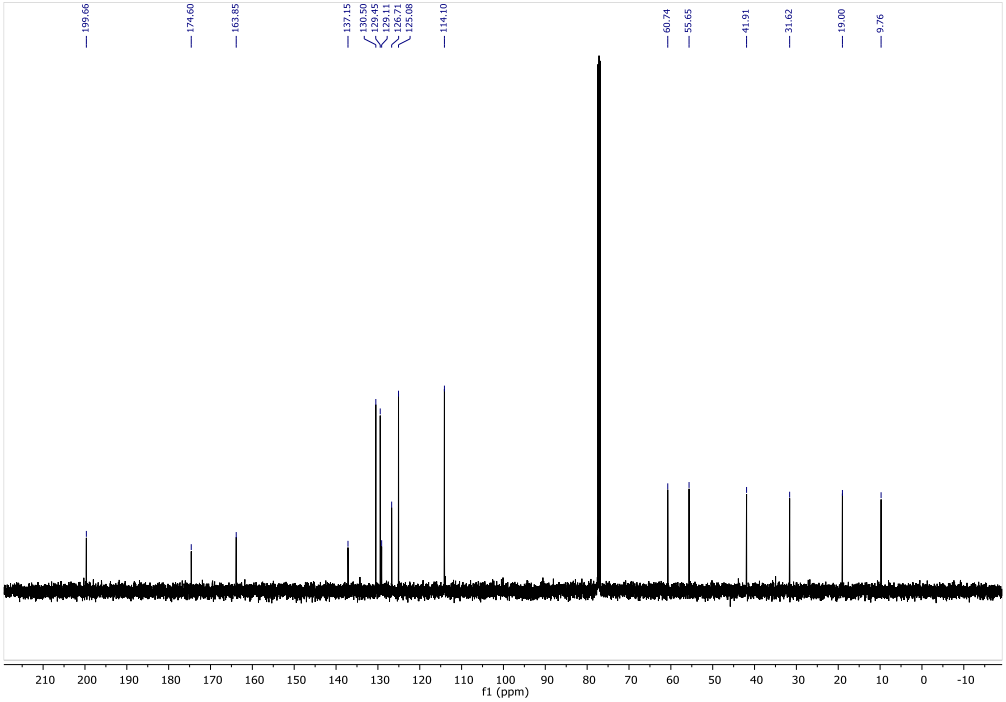


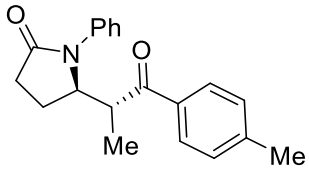

-63.18
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)



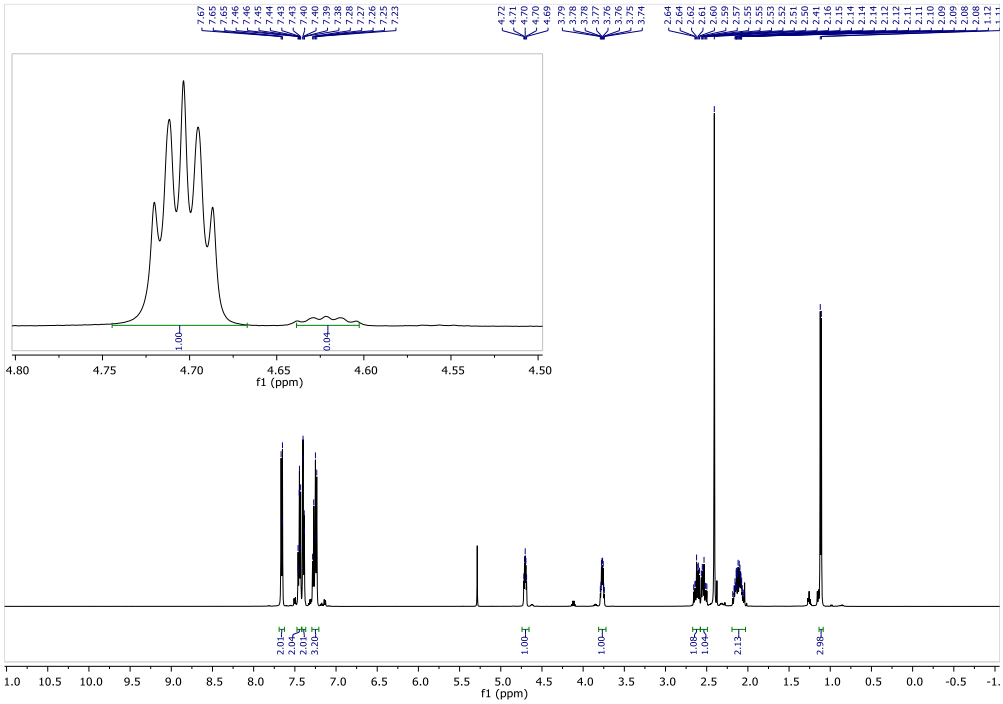
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-(4-methoxyphenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (3)**

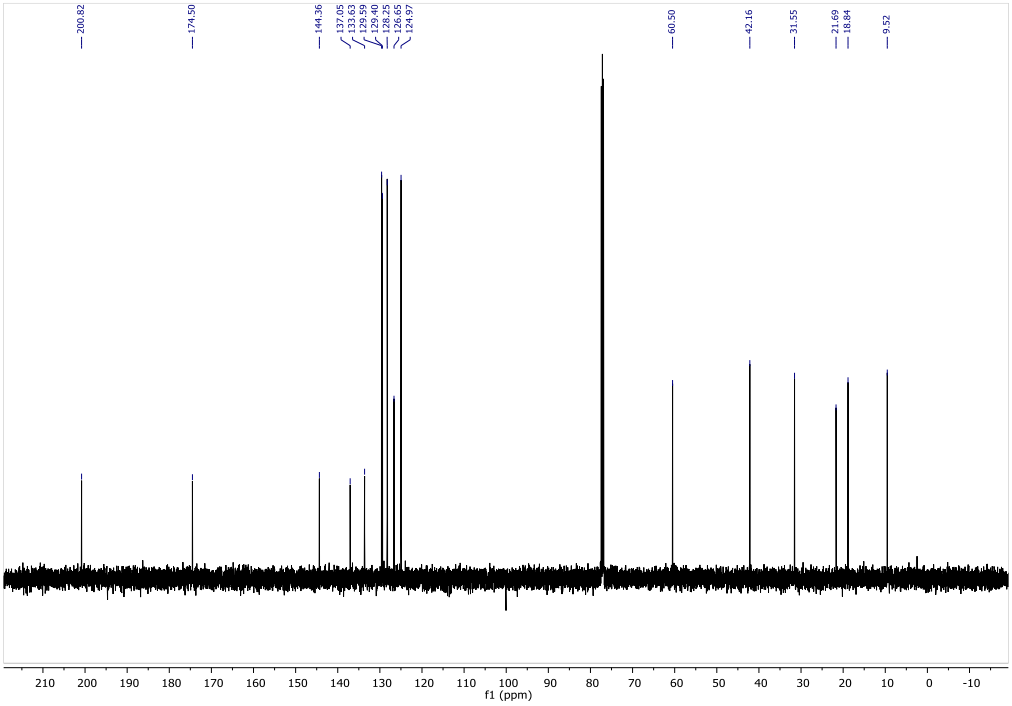


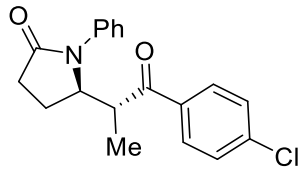




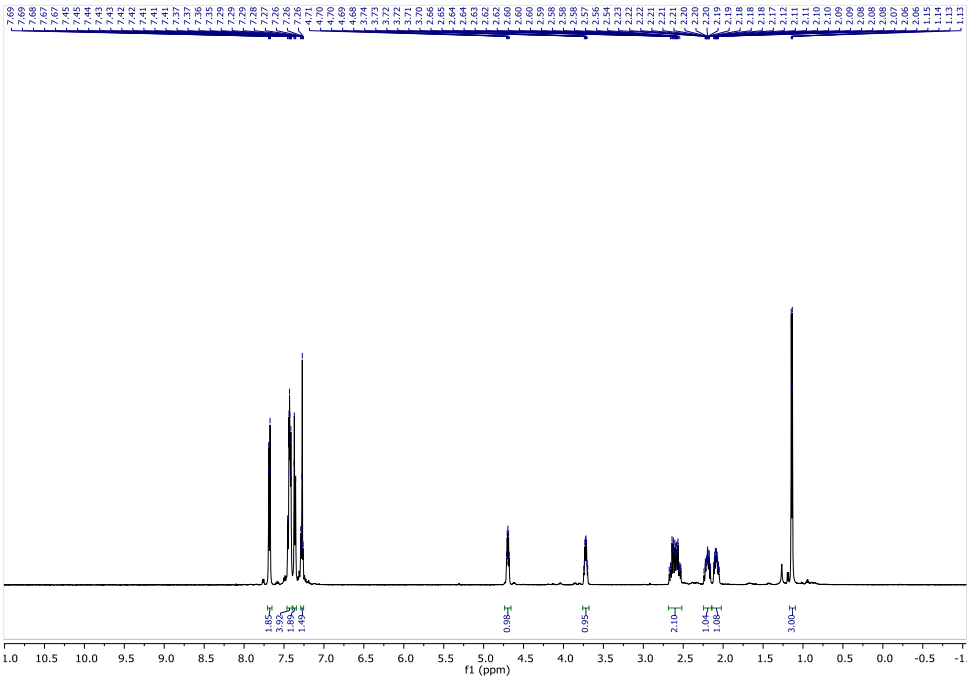
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-oxo-1-(*p*-tolyl)propan-2-yl)-1-phenylpyrrolidin-2-one (4&13):**

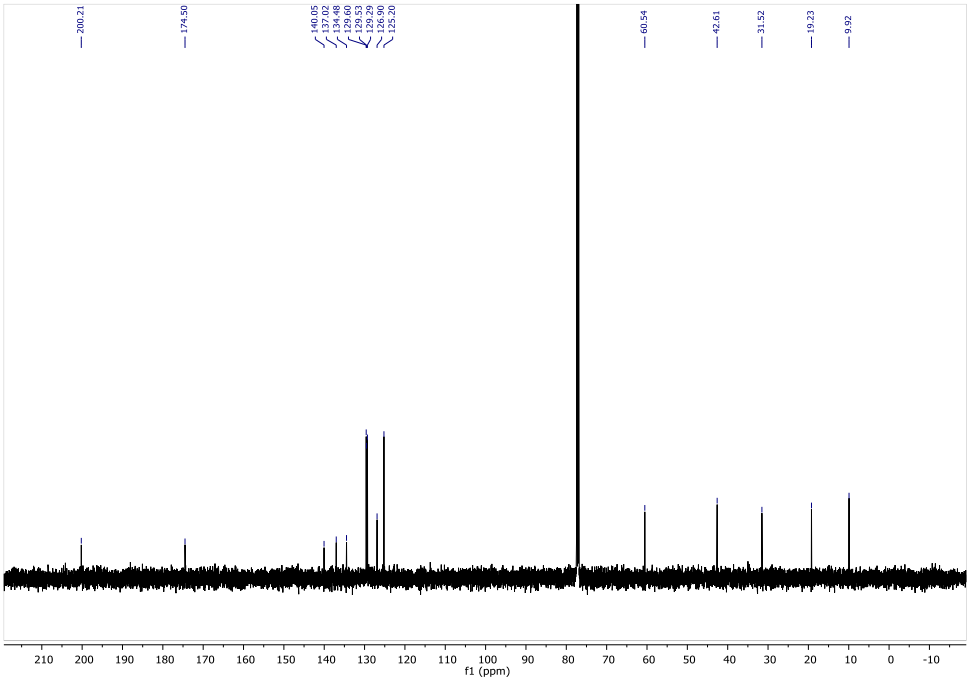


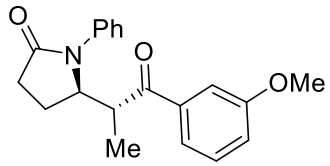




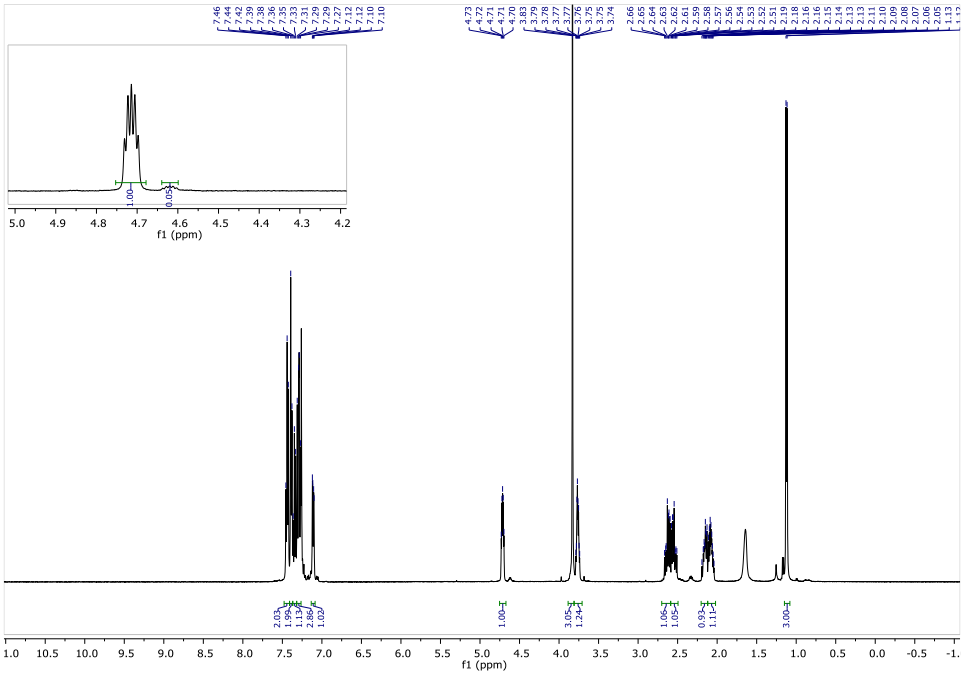
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-(4-chlorophenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (5):**

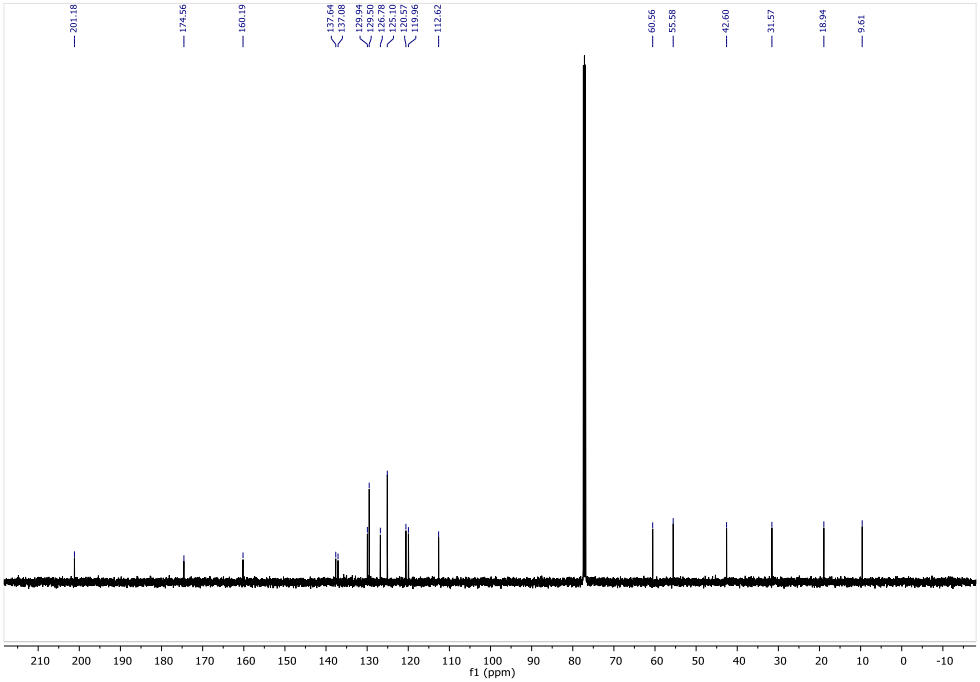


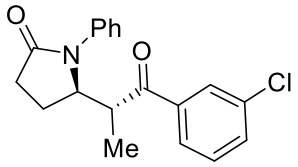




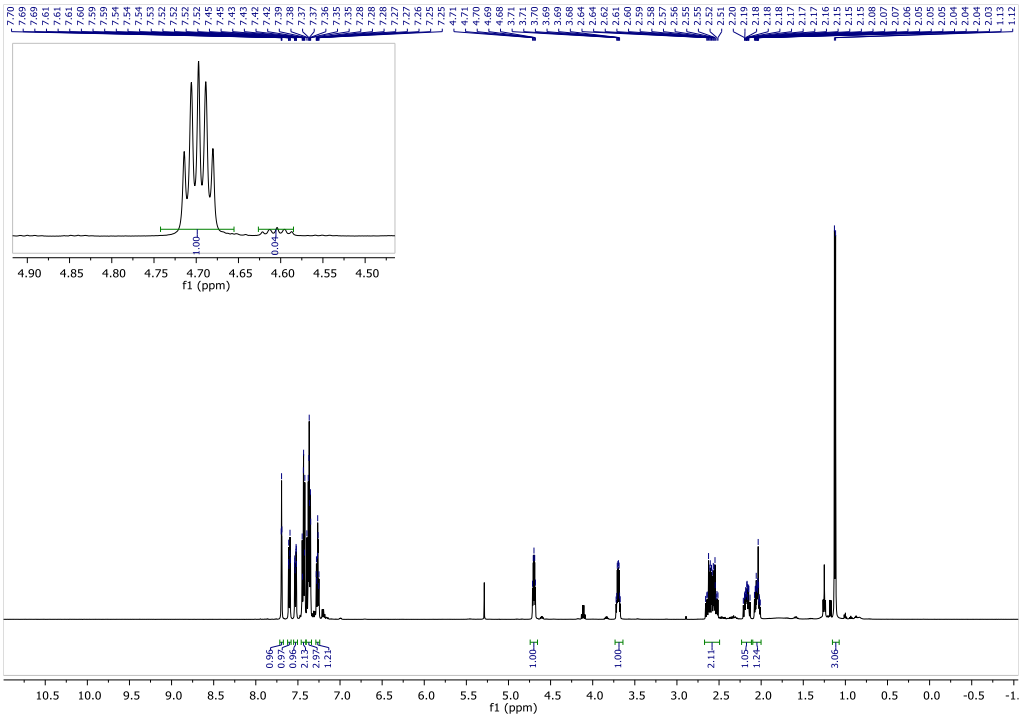
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-(3-methoxyphenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (6):**

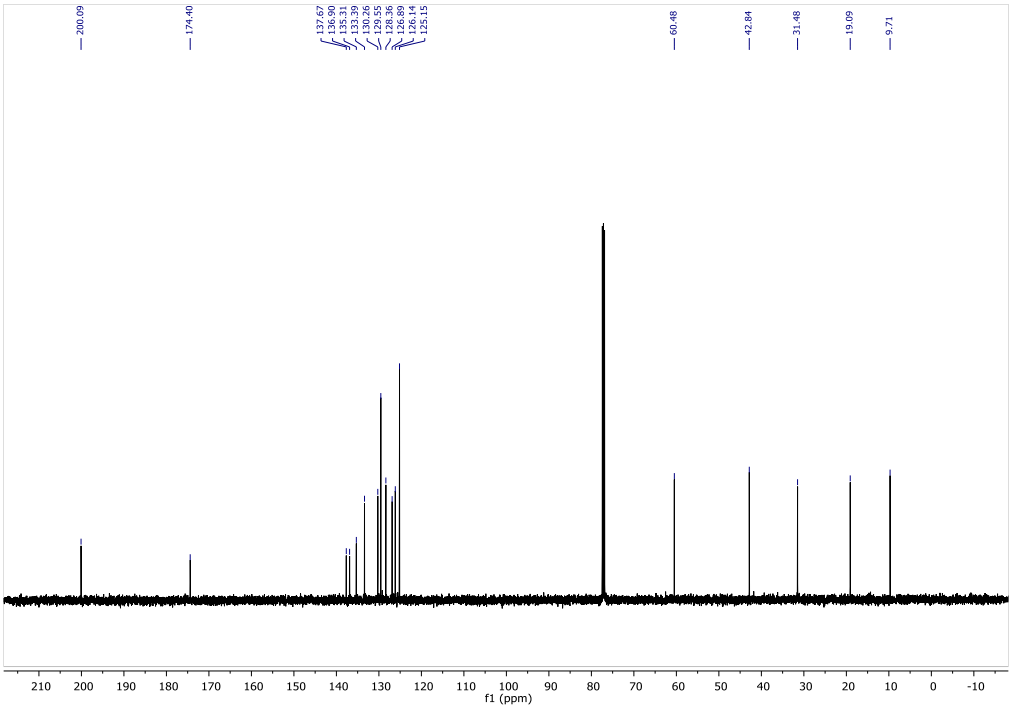


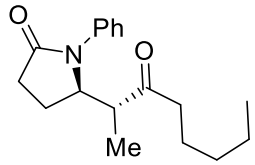




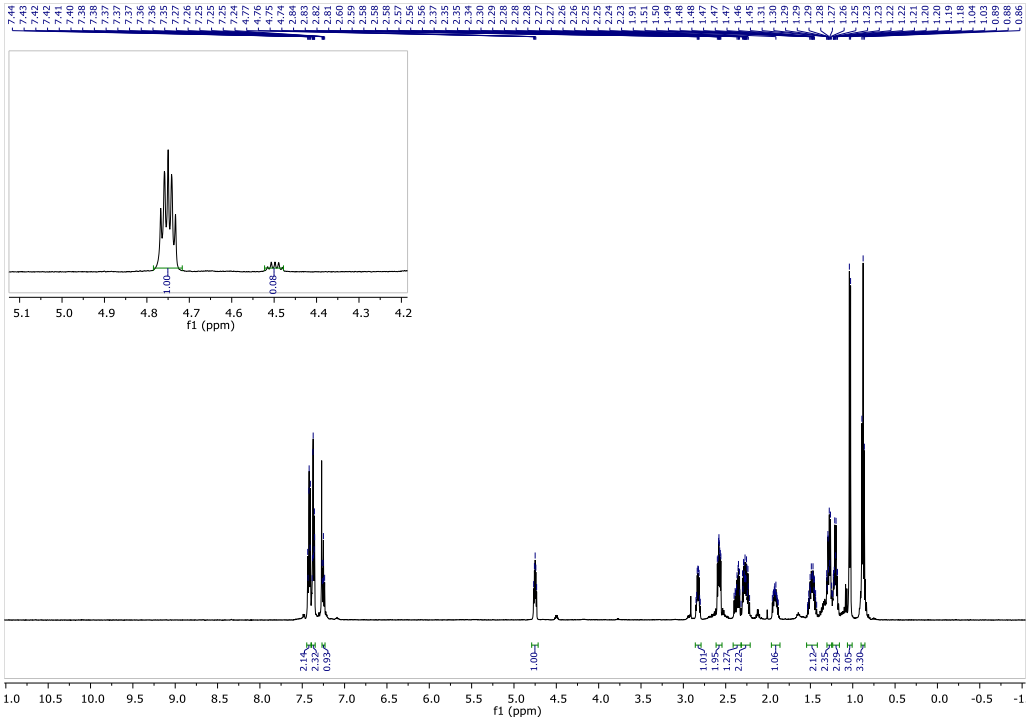
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-(3-chlorophenyl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (7&12):**

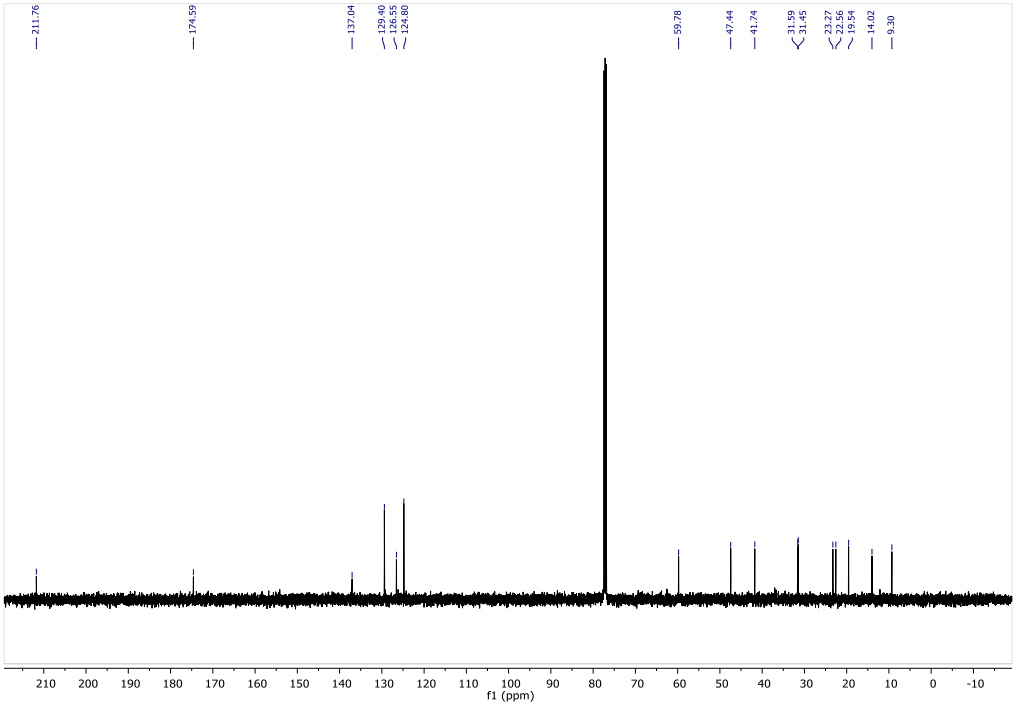


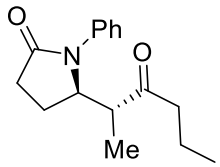




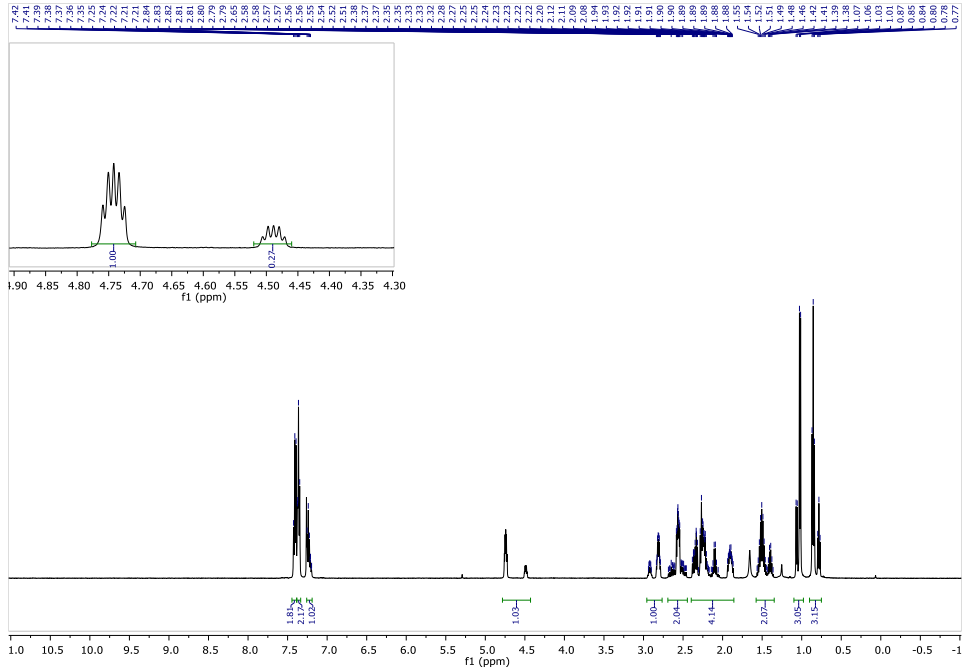
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-3-oxooctan-2-yl)-1-phenylpyrrolidin-2-one (8):**

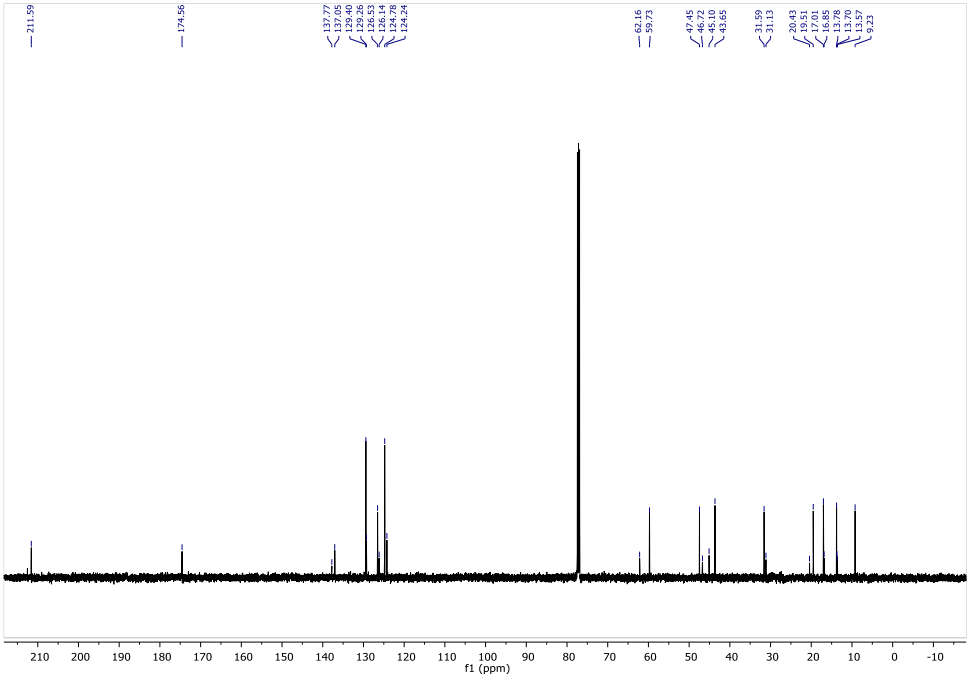


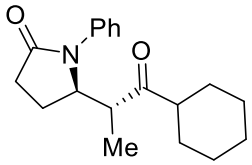




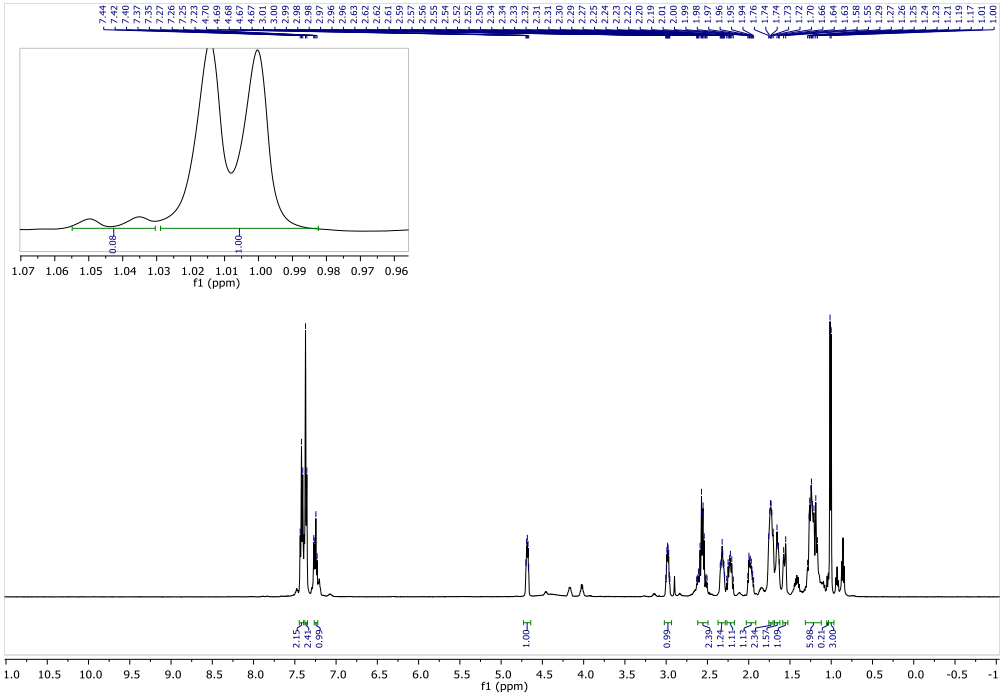
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-oxo-1-(*p*-tolyl)propan-2-yl)-1-phenylpyrrolidin-2-one (9):**

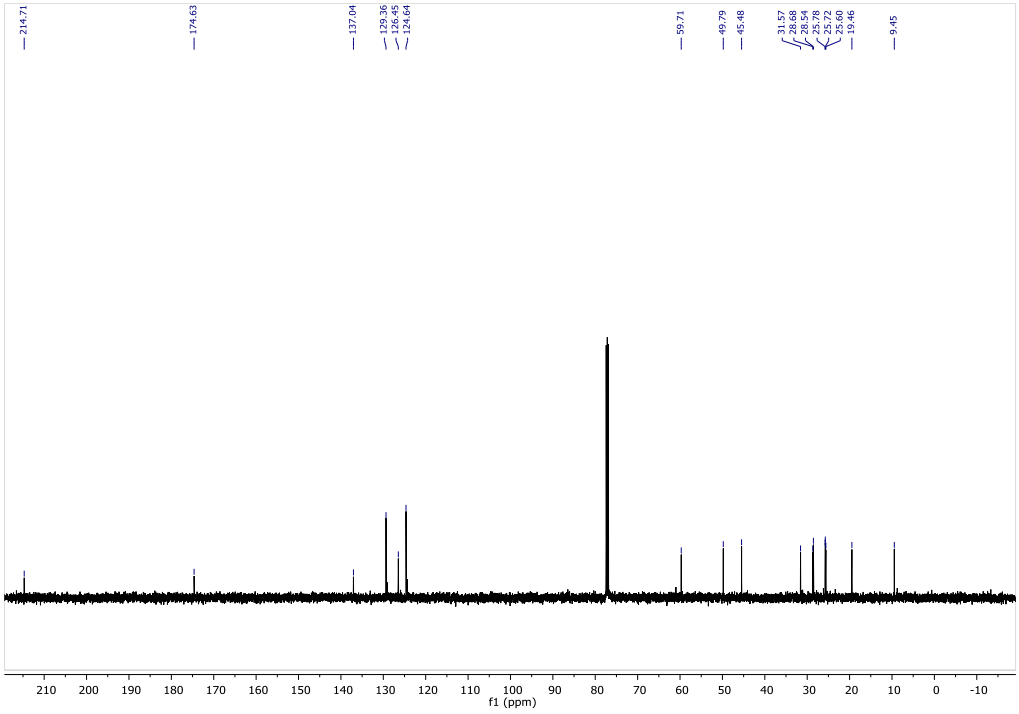


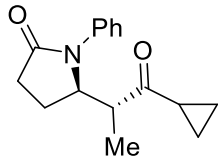




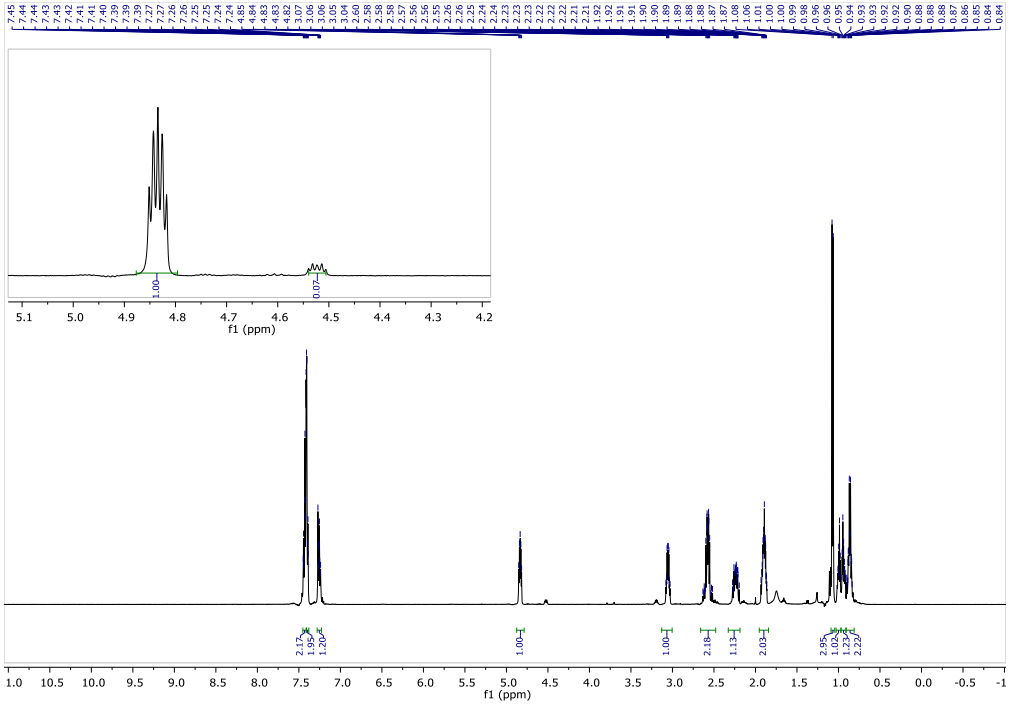
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-cyclohexyl-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (10):**

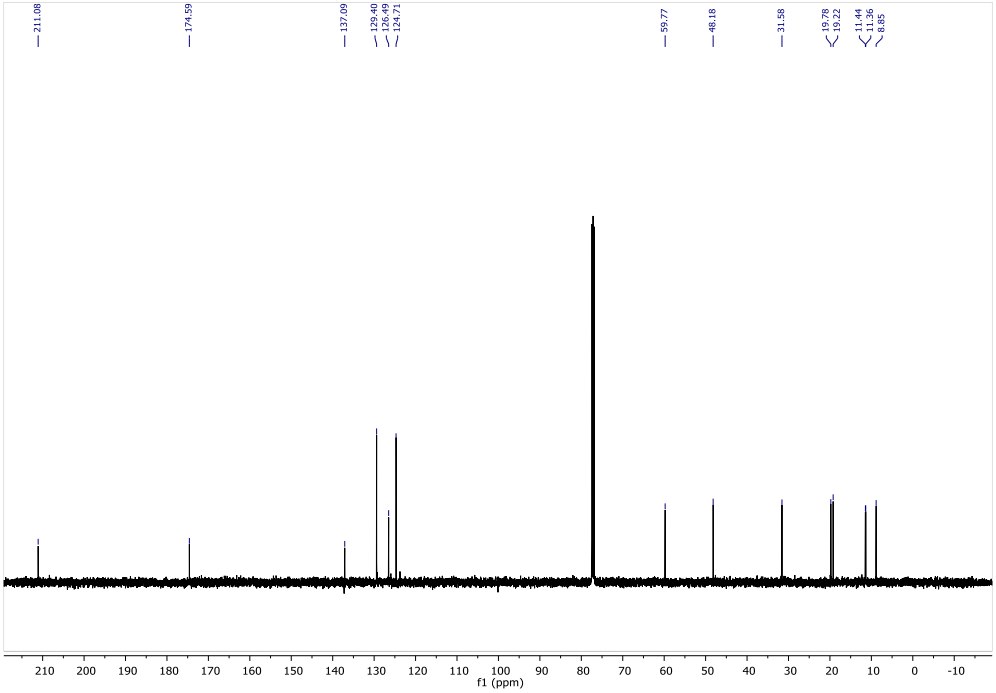


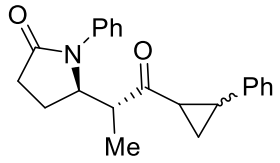




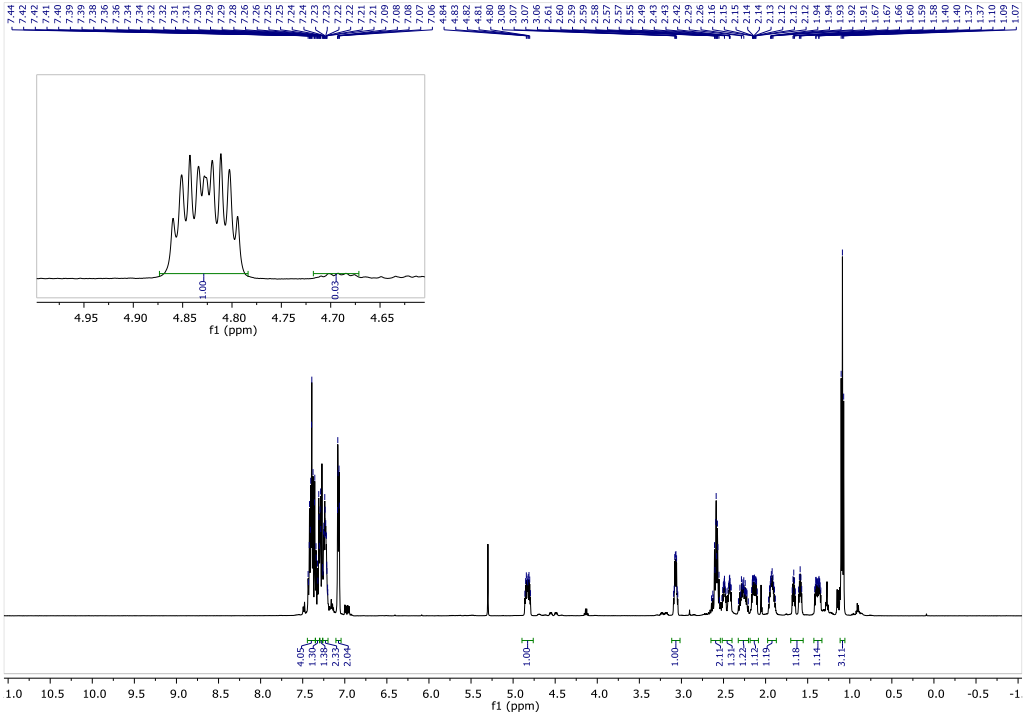
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-cyclopropyl-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (11):**

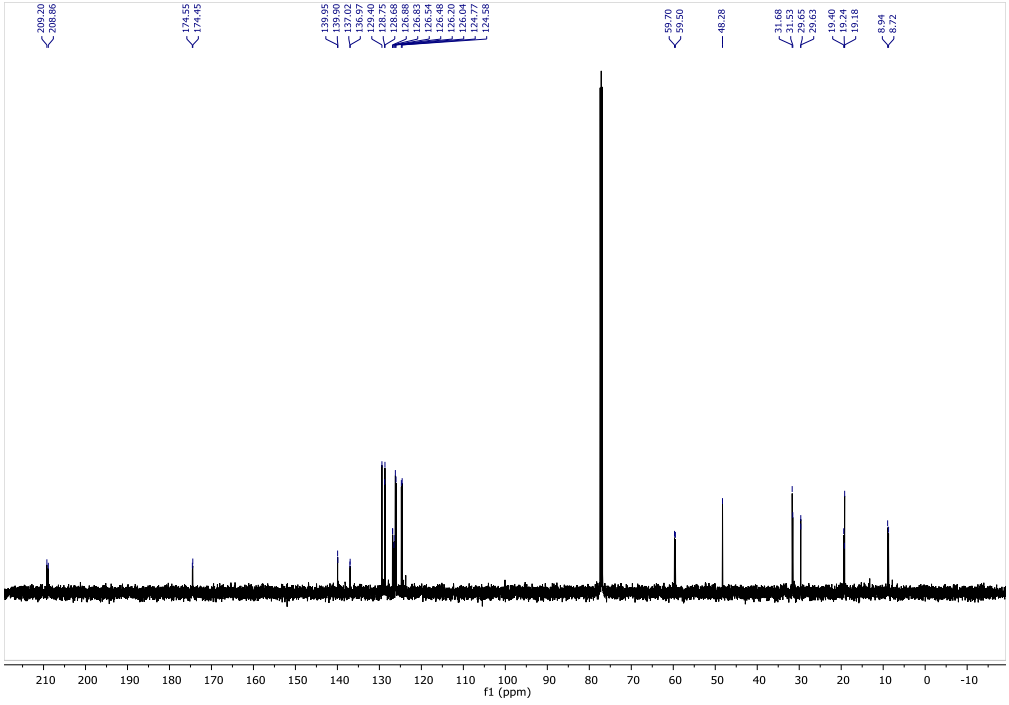


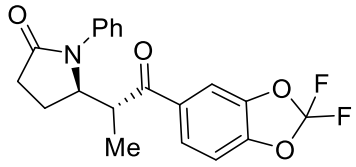




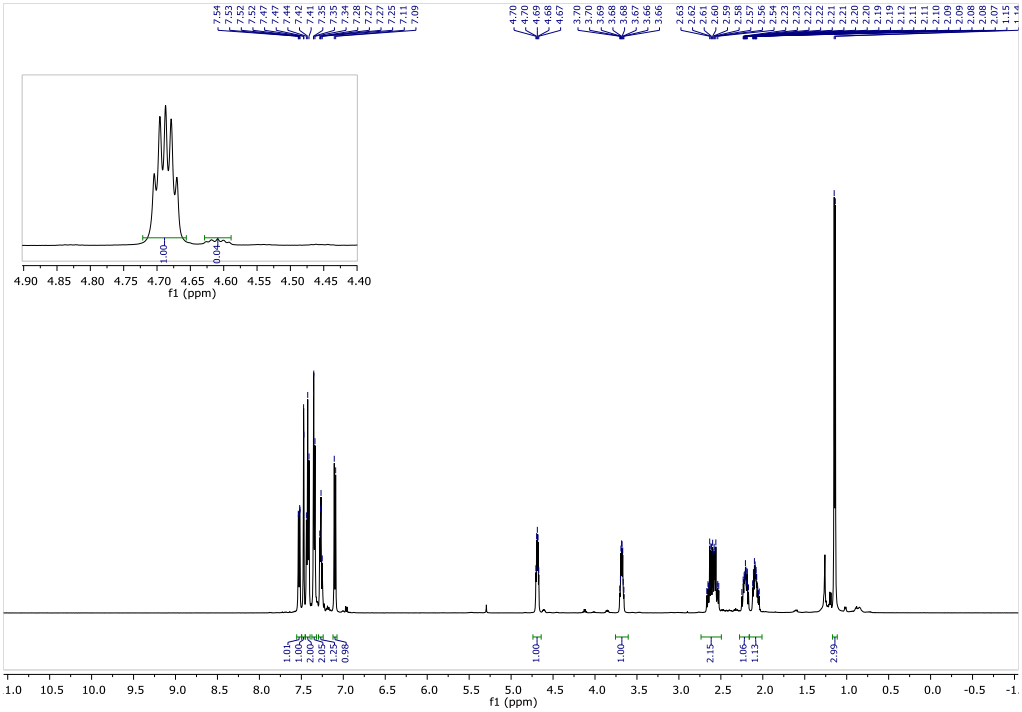
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (5*R)-5-((2*R**)-1-oxo-1-(2-phenylcyclopropyl)propan-2-yl)-1-phenylpyrrolidin-2-one (14):**

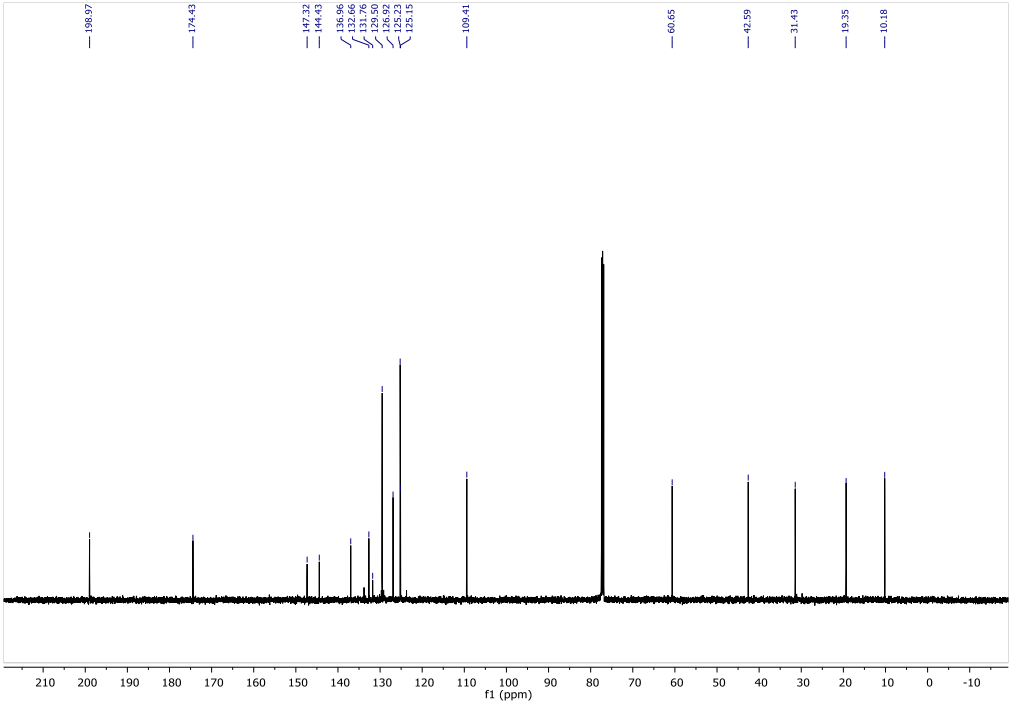


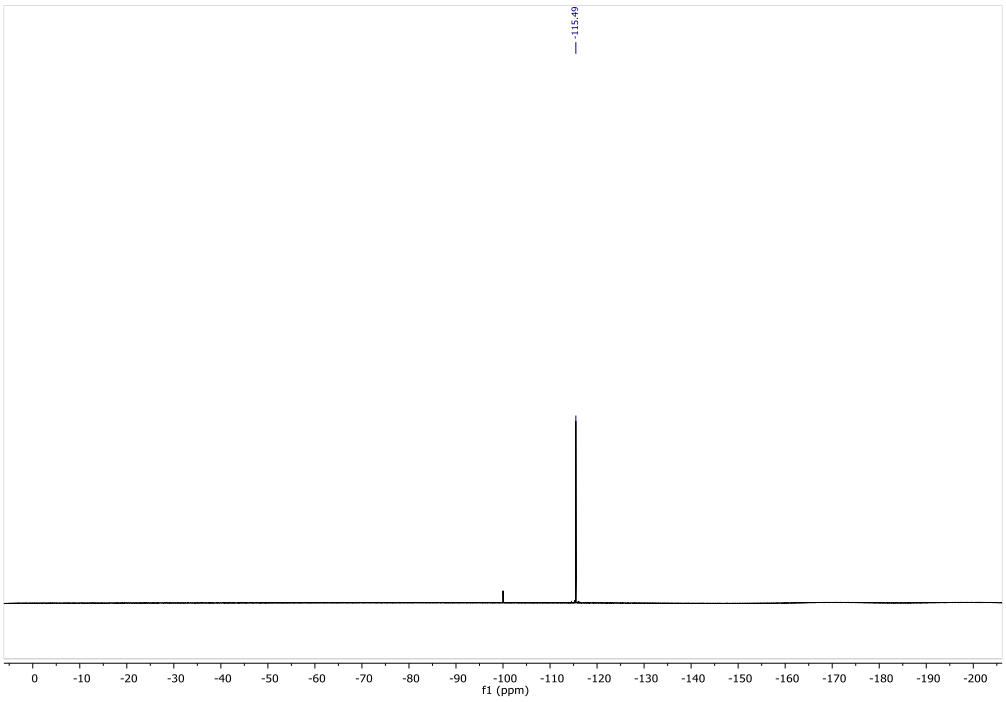




^{1}H NMR ($CDCl_3$, 500 MHz), ^{13}C NMR ($CDCl_3$, 126 MHz) and ^{19}F-NMR ($CDCl_3$, 471 MHz) of (*R)-5-((*R**)-1-(2,2-difluorobenzo[*d*][1,3]dioxol-5-yl)-1-oxopropan-2-yl)-1-phenylpyrrolidin-2-one (15):**



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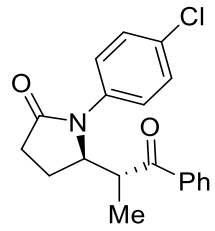
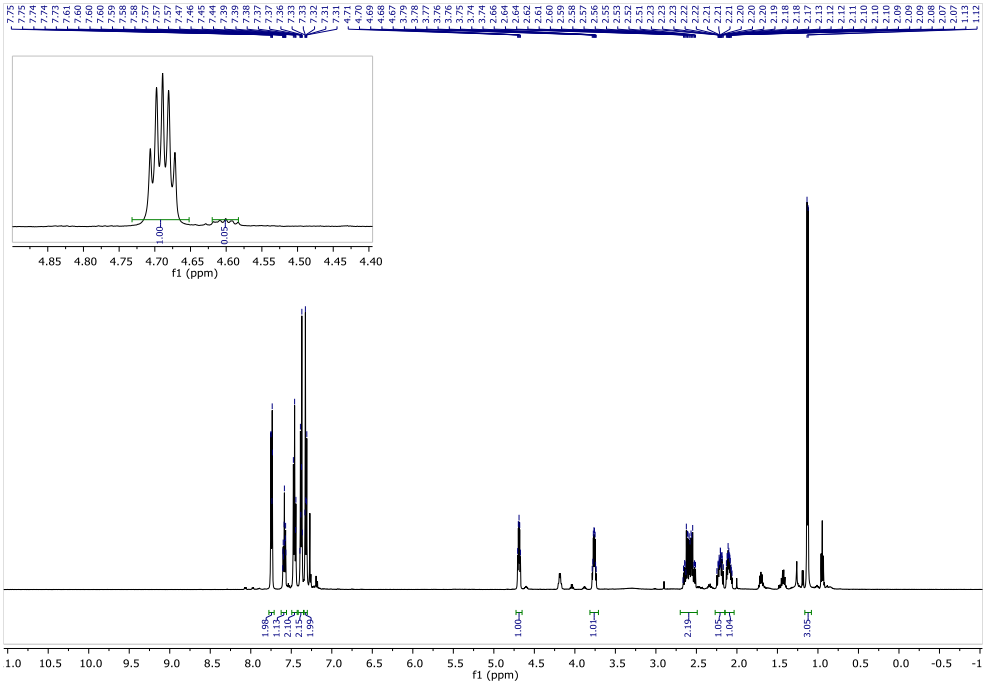
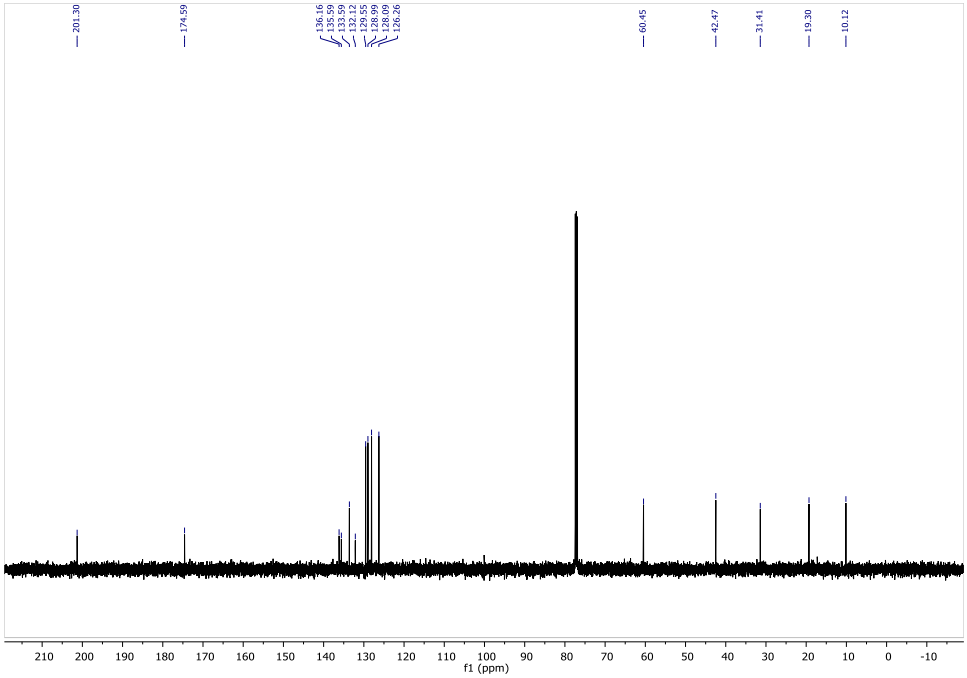
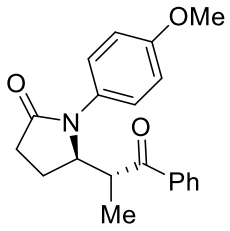
f1 (ppm)



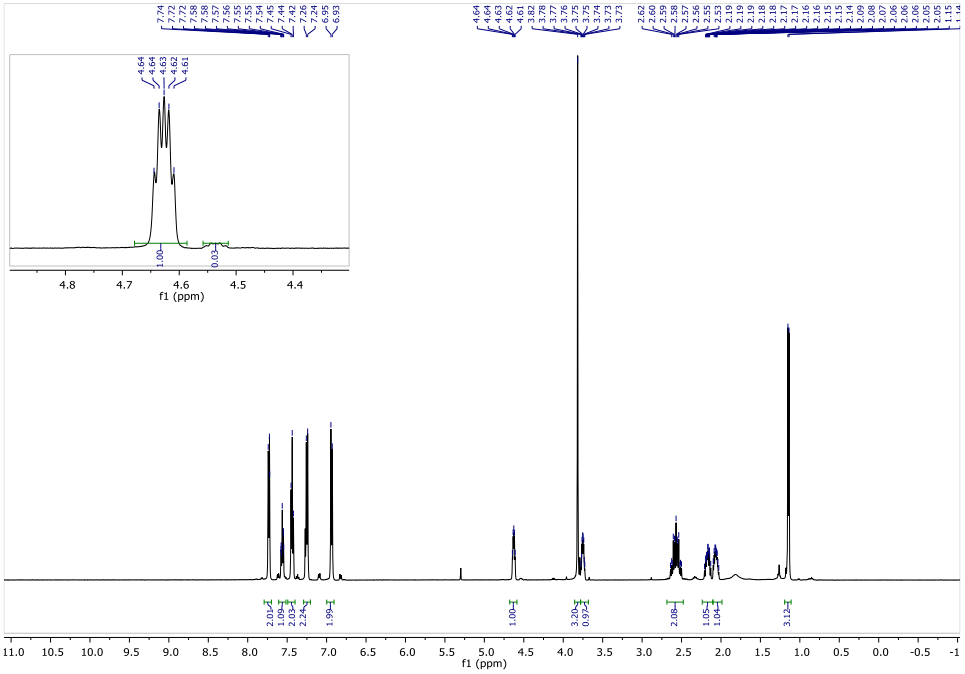
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-1-(4-Chlorophenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (16):**

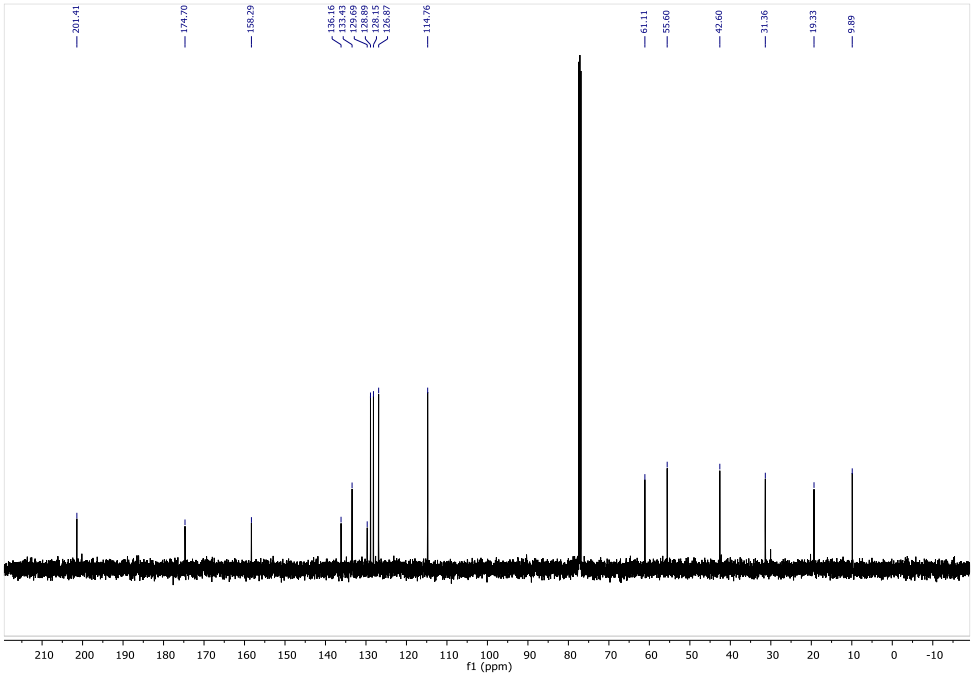


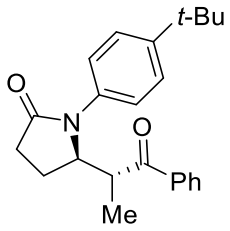




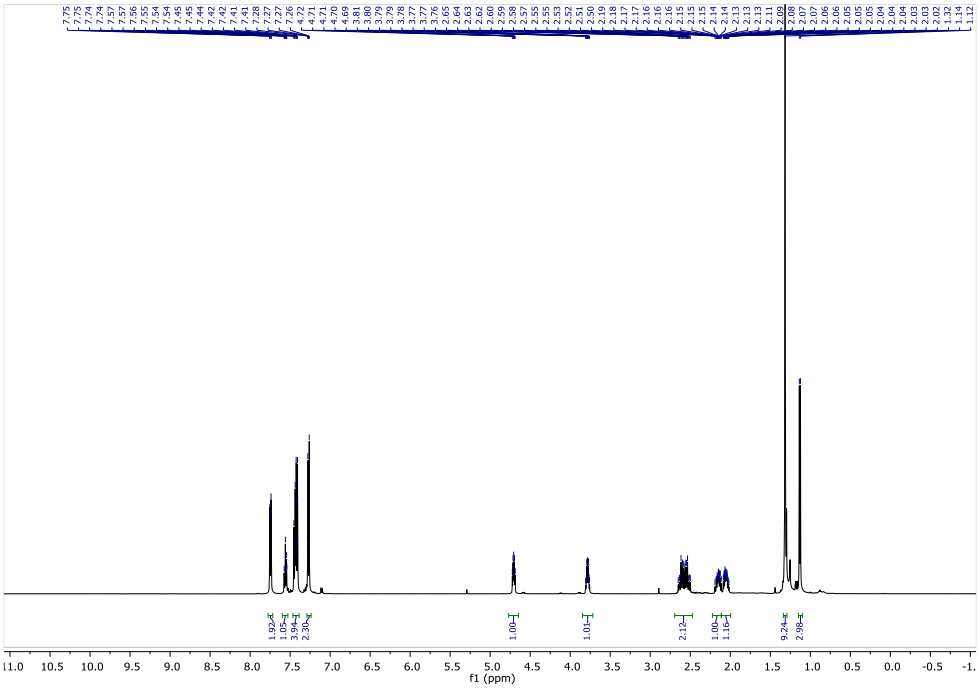
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-1-(4-Methoxyphenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (17):**

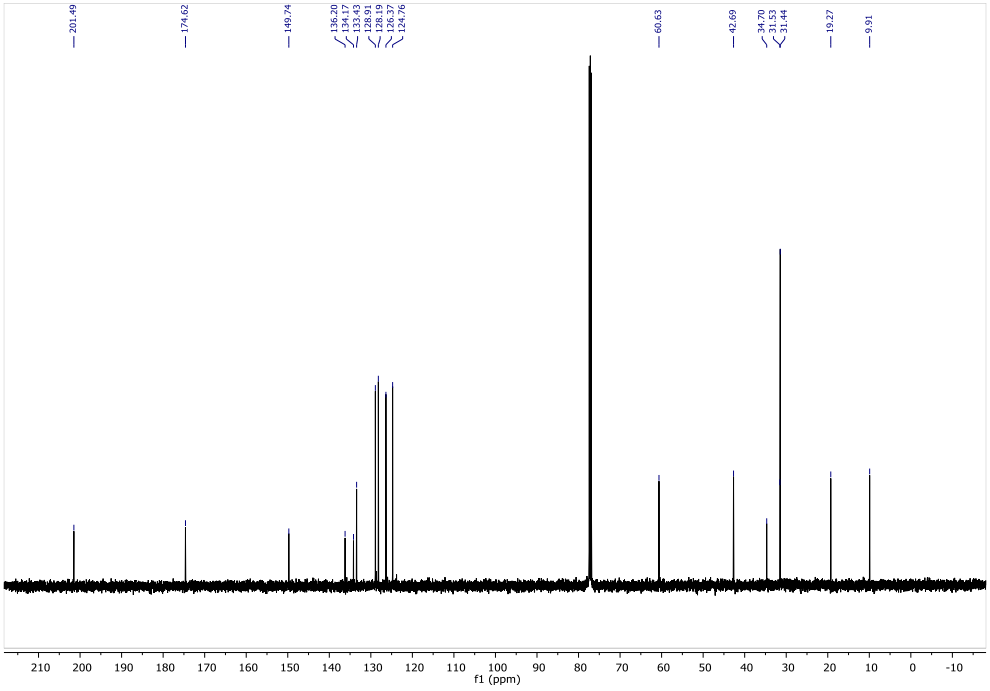


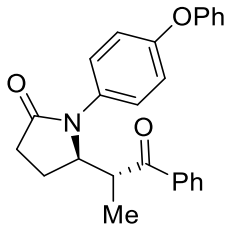




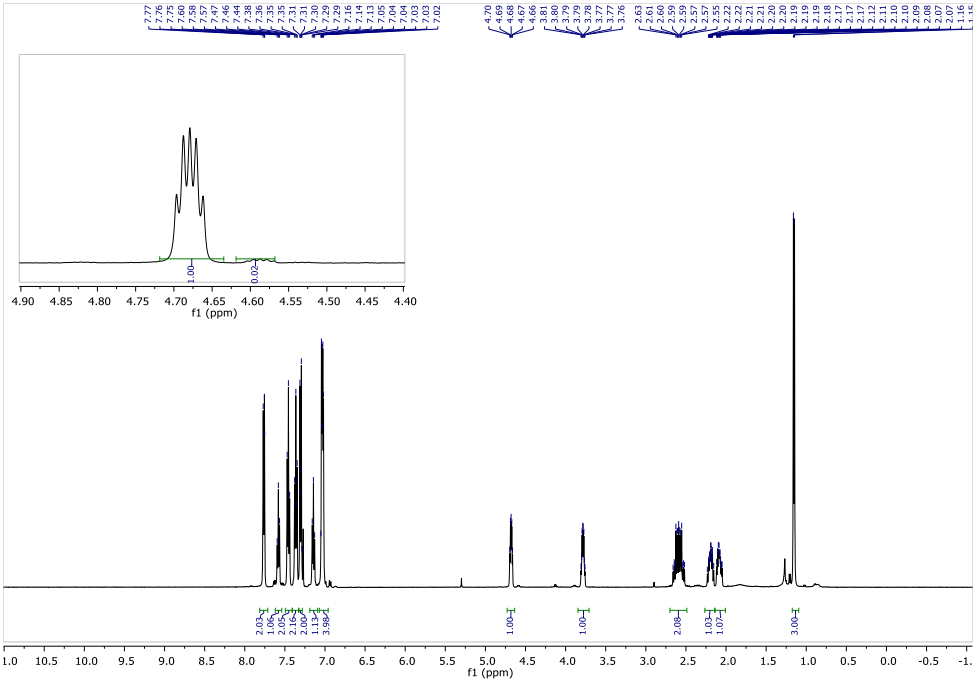
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-1-(4-(*tert*-Butyl)phenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (18):**

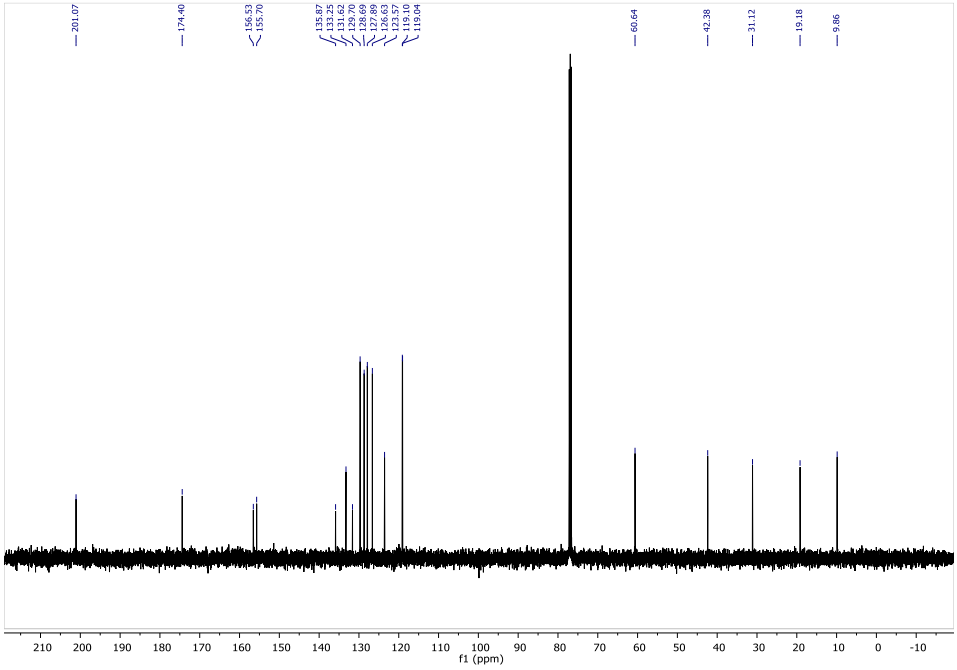


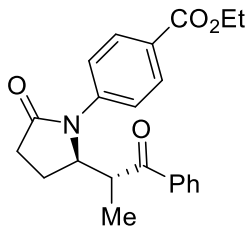




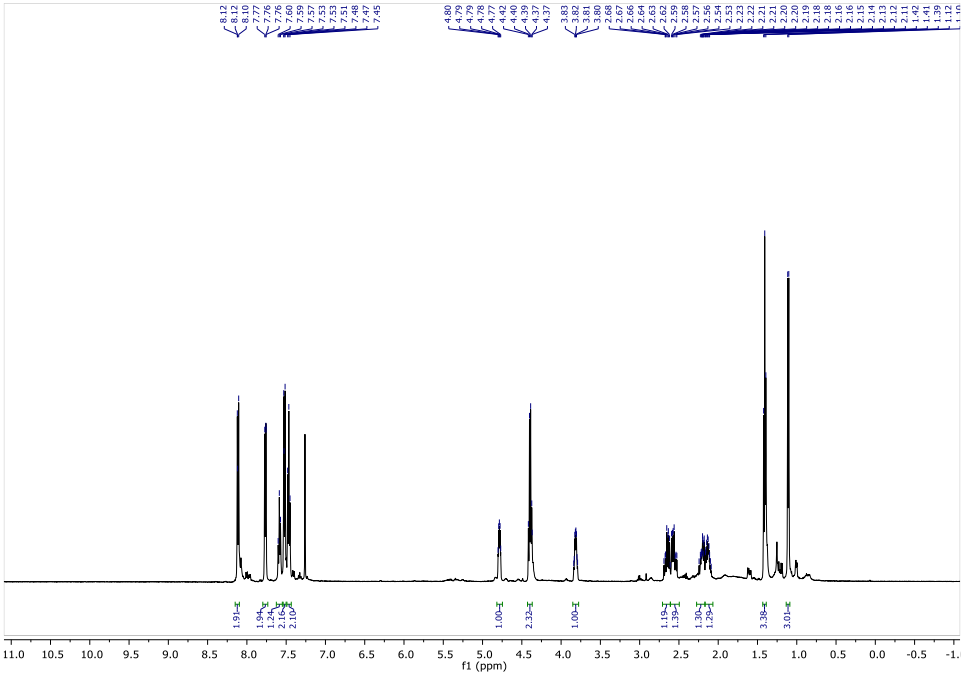
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-1-Oxo-1-phenylpropan-2-yl)-1-(4-phenoxyphenyl)pyrrolidin-2-one (19):**

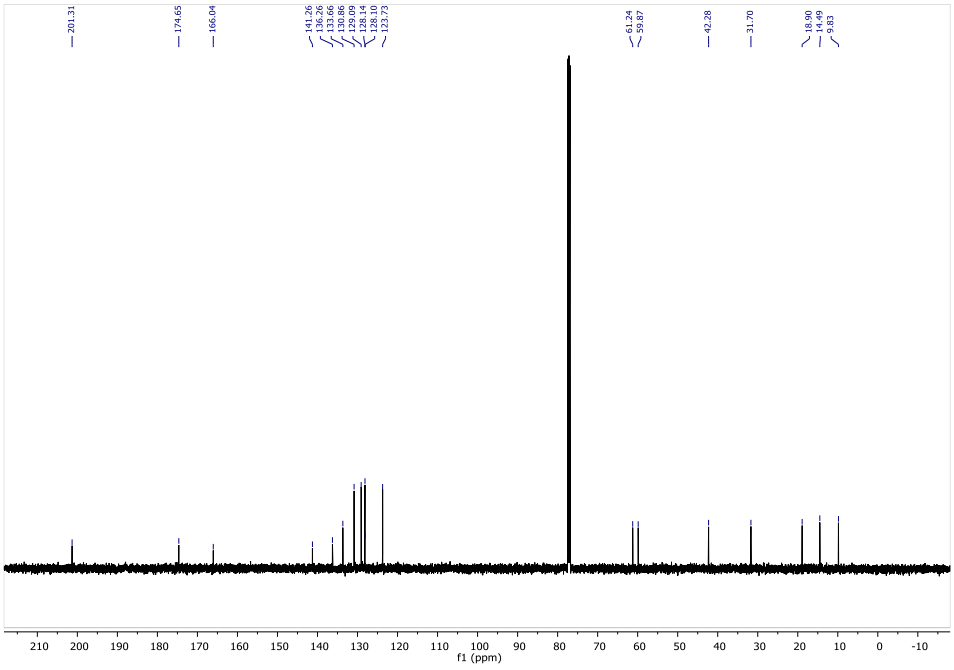


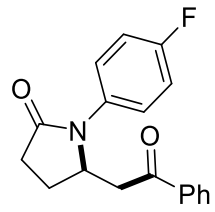




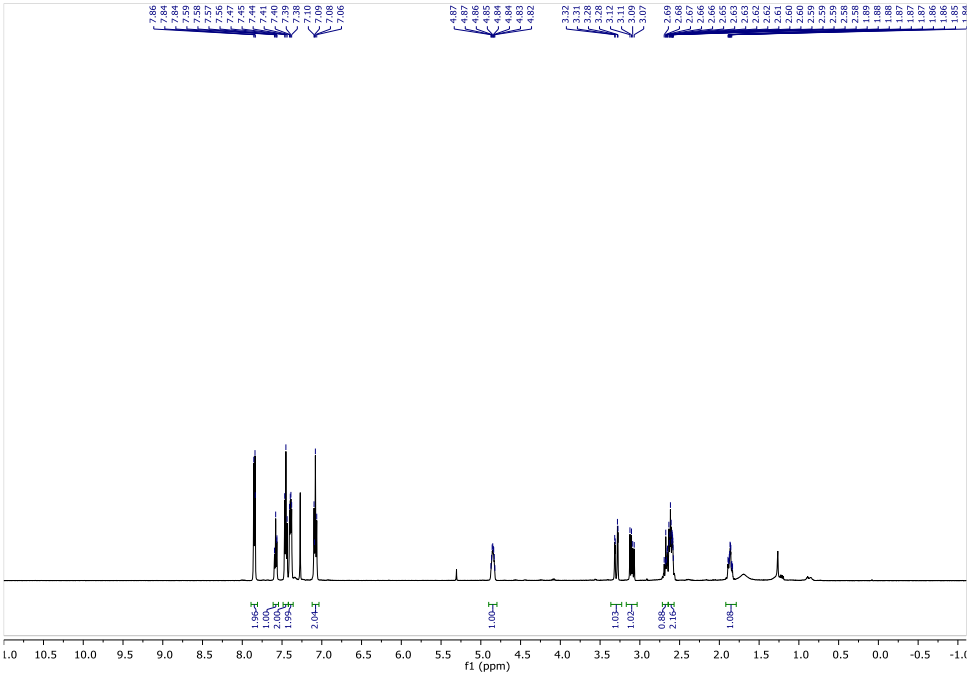
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of Ethyl 4-((*R)-2-oxo-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-1-yl)benzoate (20):**

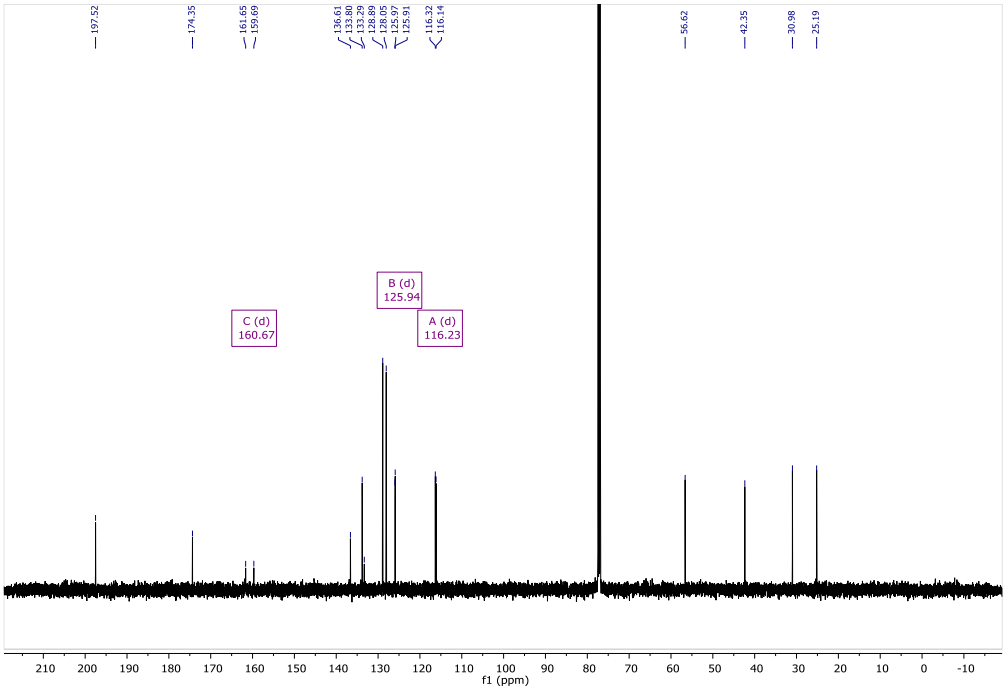


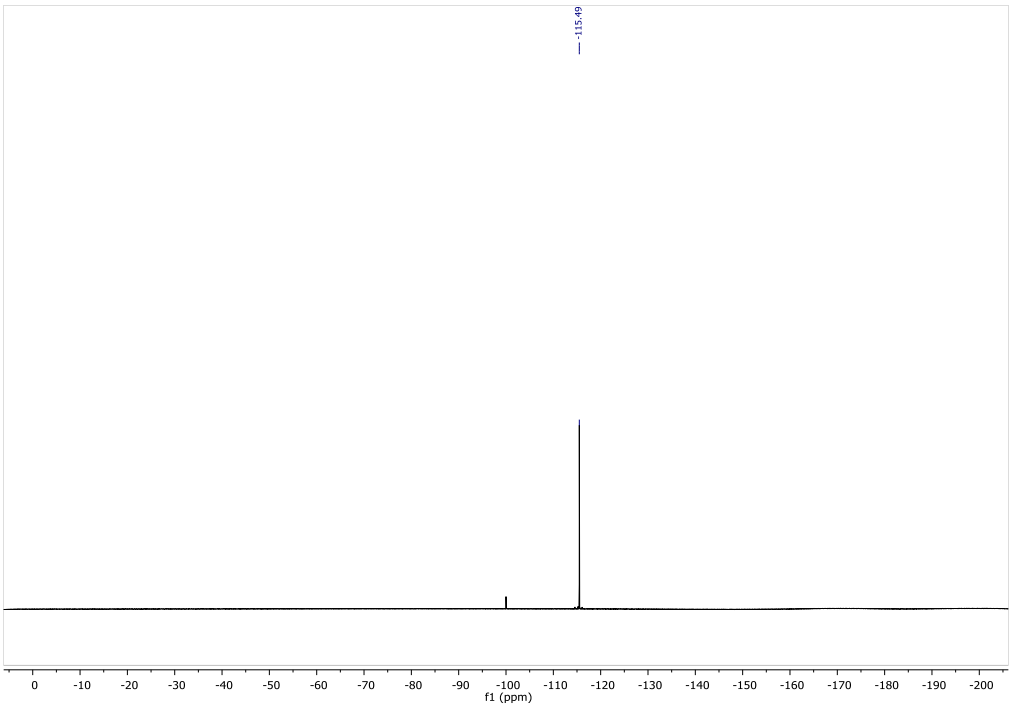




^{1}H NMR ($CDCl_3$, 500 MHz), ^{13}C NMR ($CDCl_3$, 126 MHz) and ^{19}F-NMR ($CDCl_3$, 471 MHz) of (*R)-1-(4-fluorophenyl)-5-(2-oxo-2-phenylethyl)pyrrolidin-2-one (21):**



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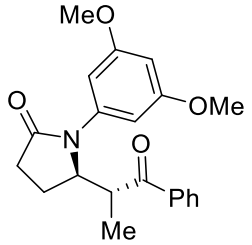
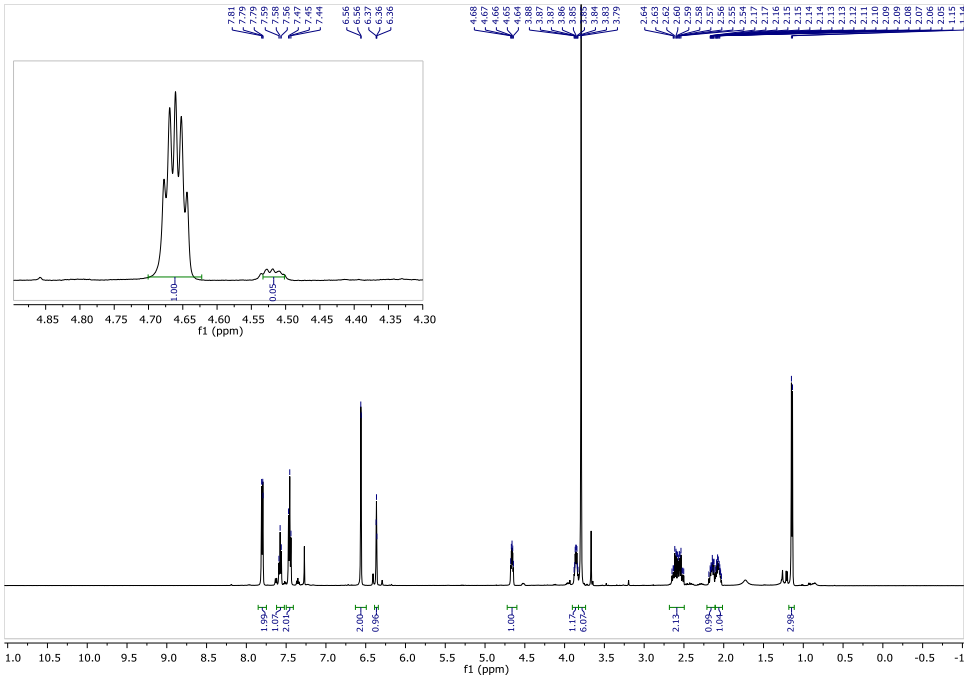
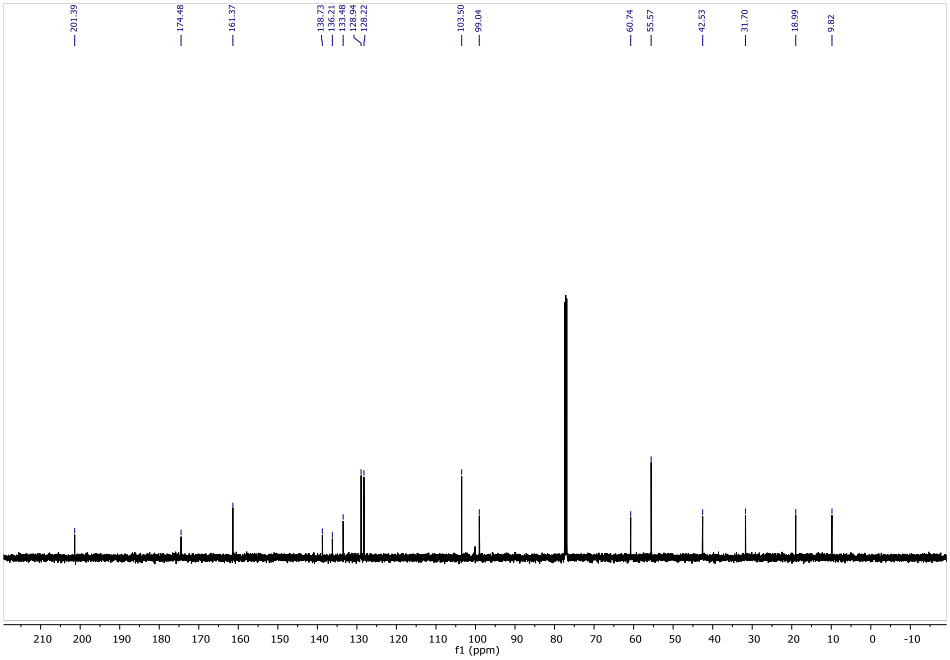
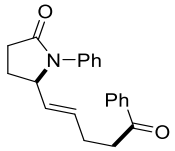


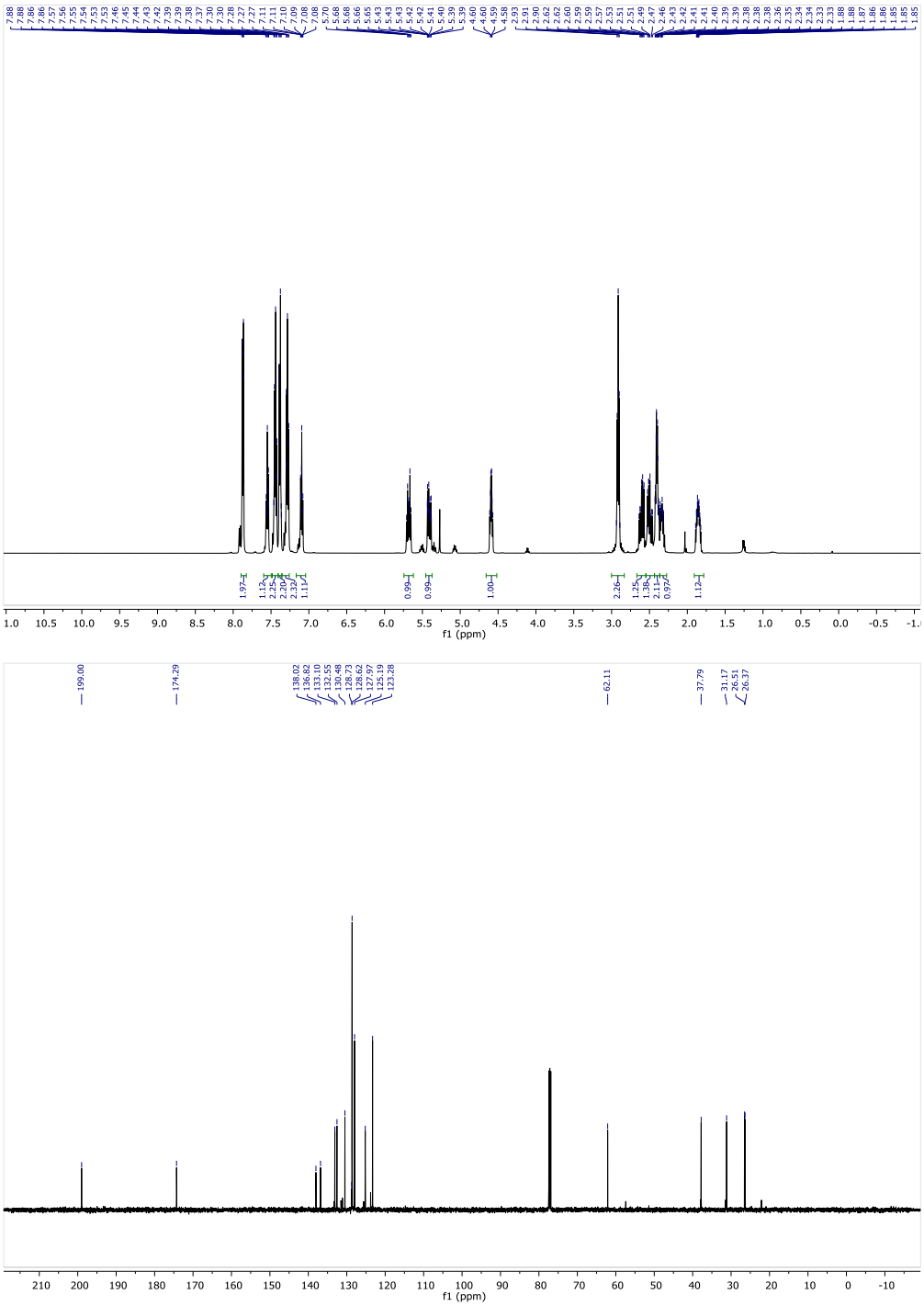
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-1-(3,5-Dimethoxyphenyl)-5-((*R**)-1-oxo-1-phenylpropan-2-yl)pyrrolidin-2-one (22):**

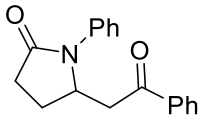




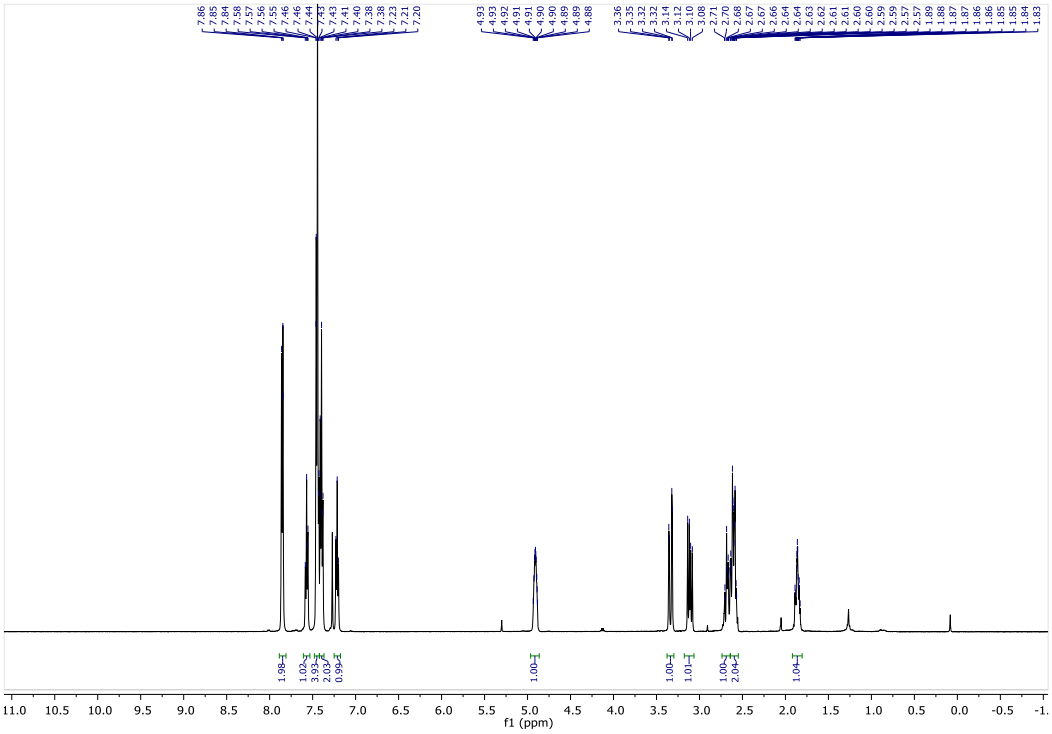


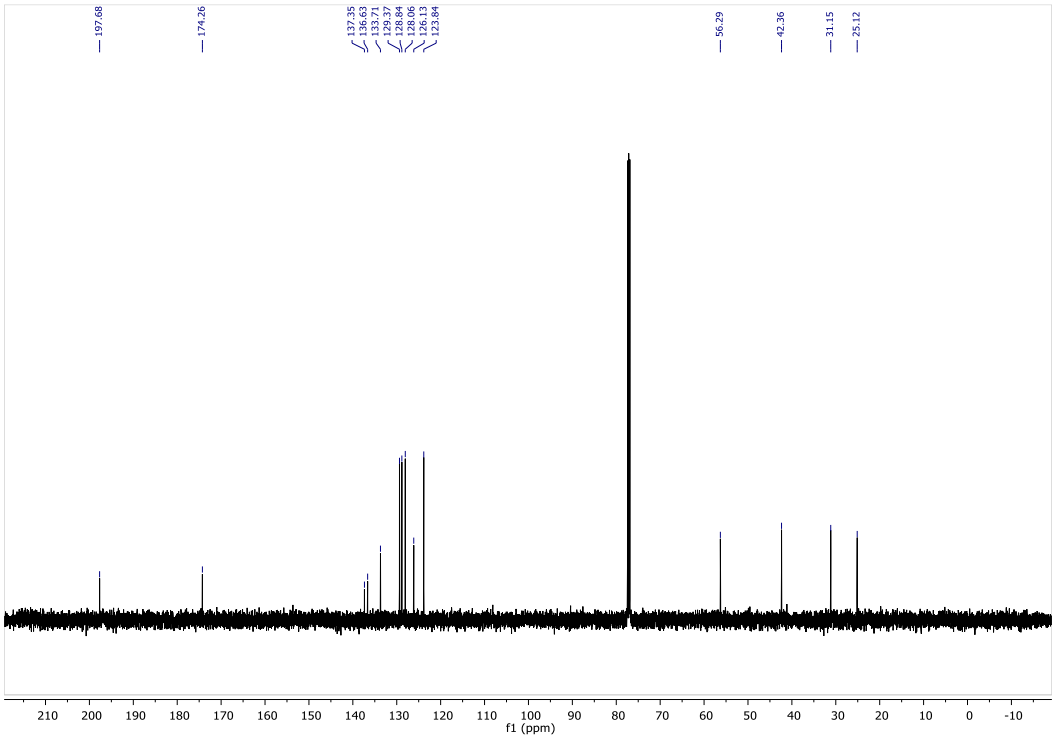
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*E*)-4-(4-(5-Oxo-1-phenylpyrrolidin-2-yl)but-3-en-1-yl)benzonitrile (23):

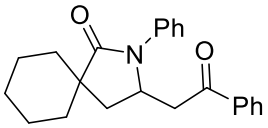




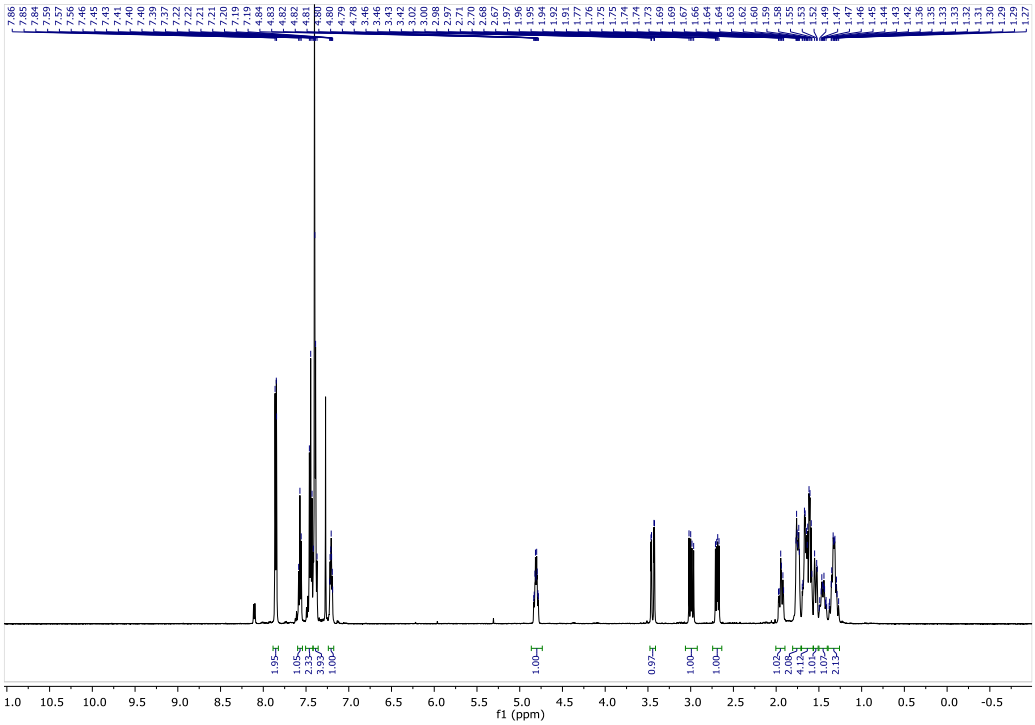
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 5-(2-Oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (24):

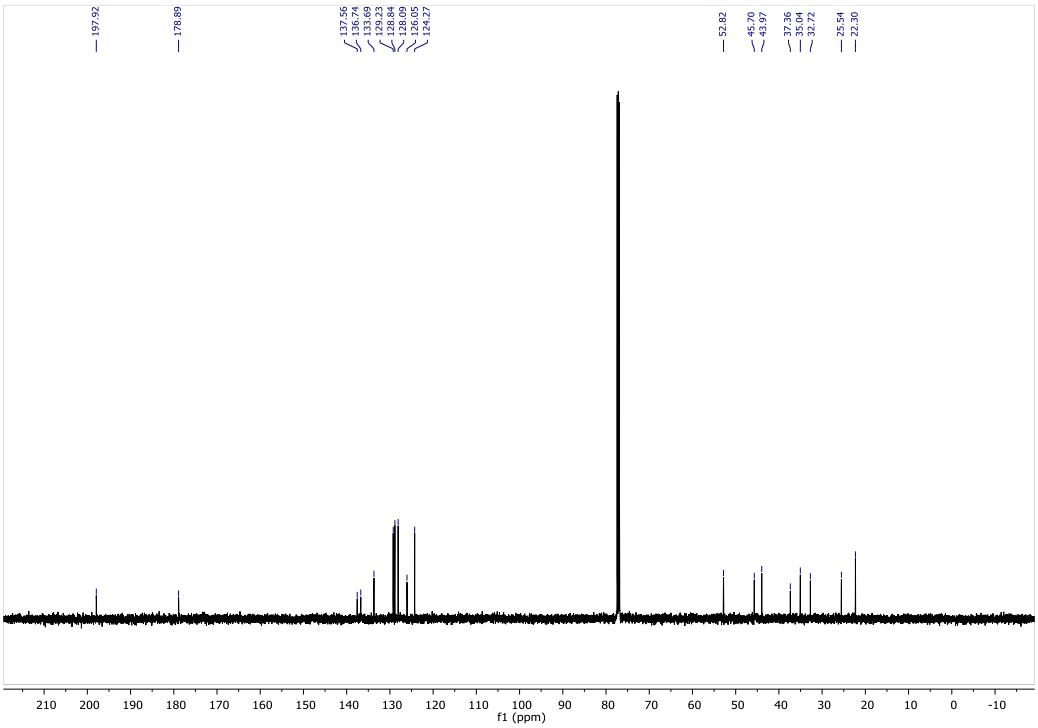


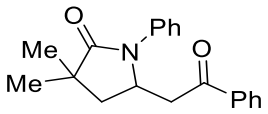




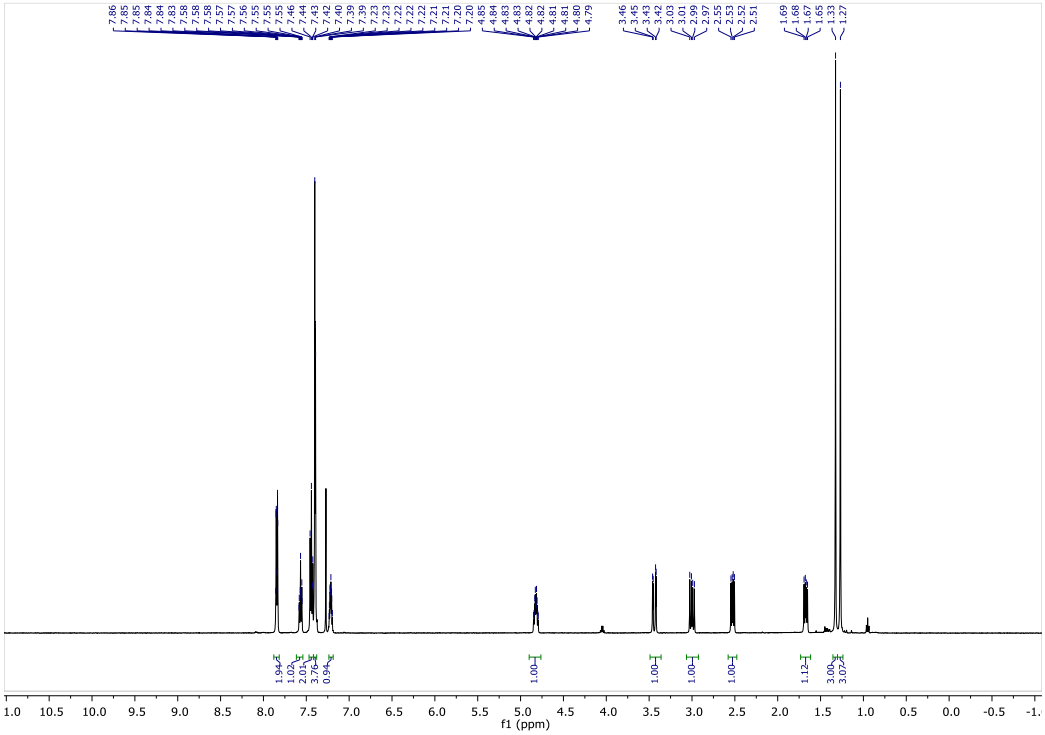
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 3-(2-Oxo-2-phenylethyl)-2-phenyl-2-azaspiro[4.5]decan-1-one (25):

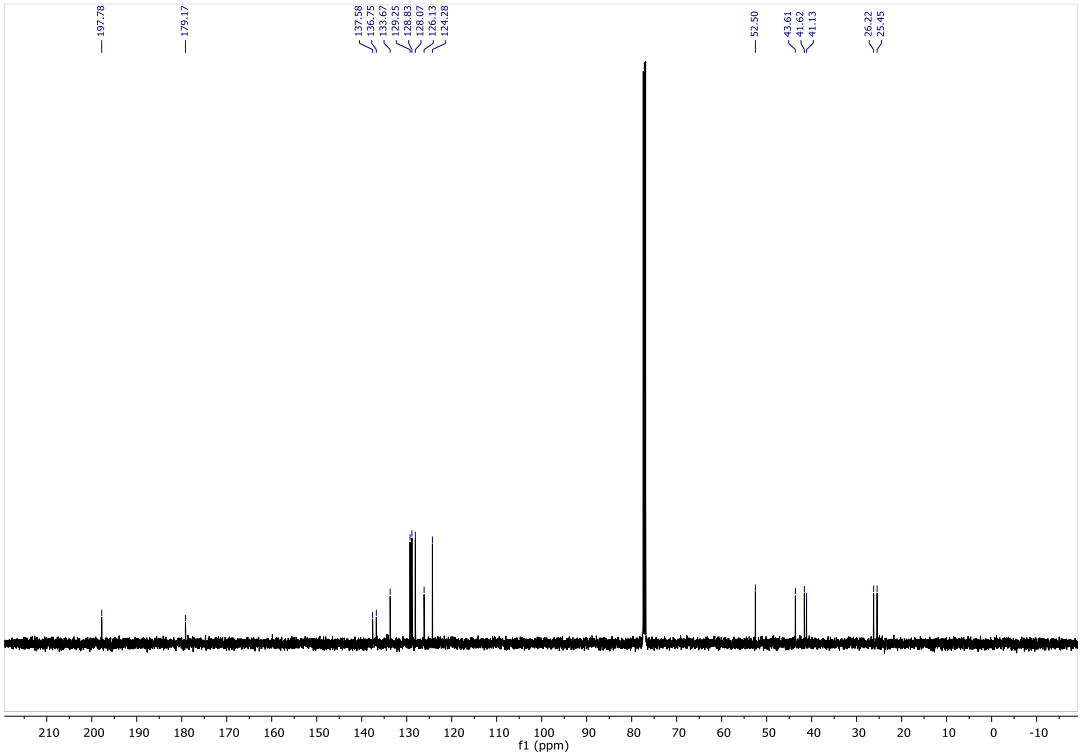


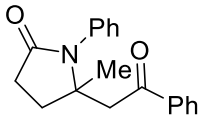




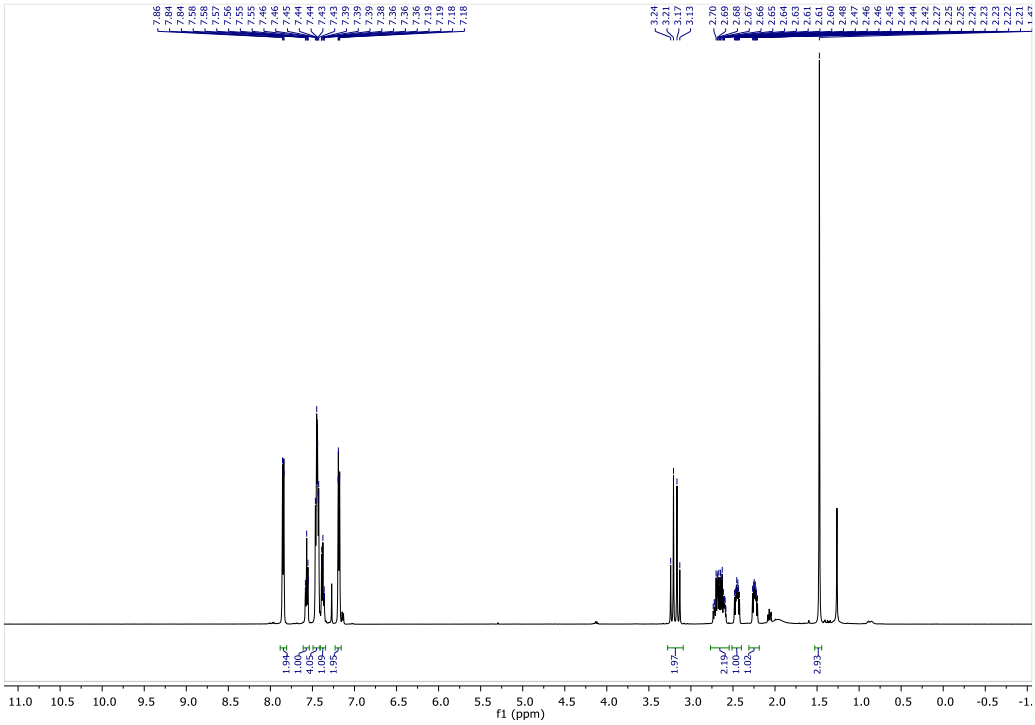
3,3-Dimethyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (26):

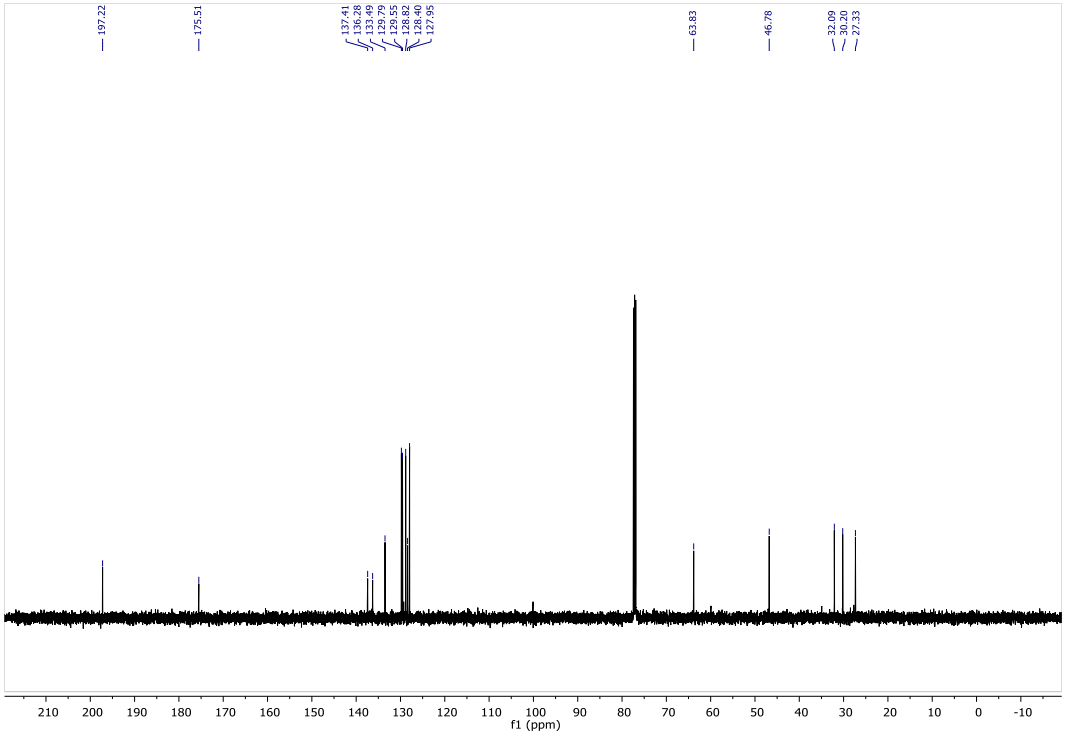


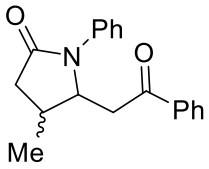




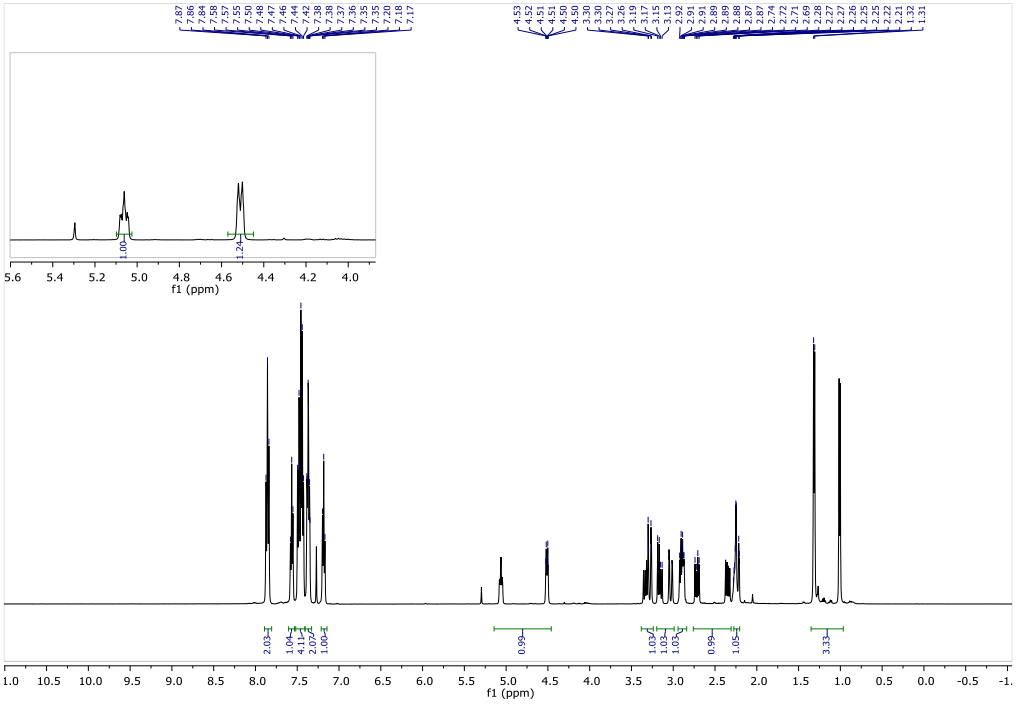
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 5-Methyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (27):

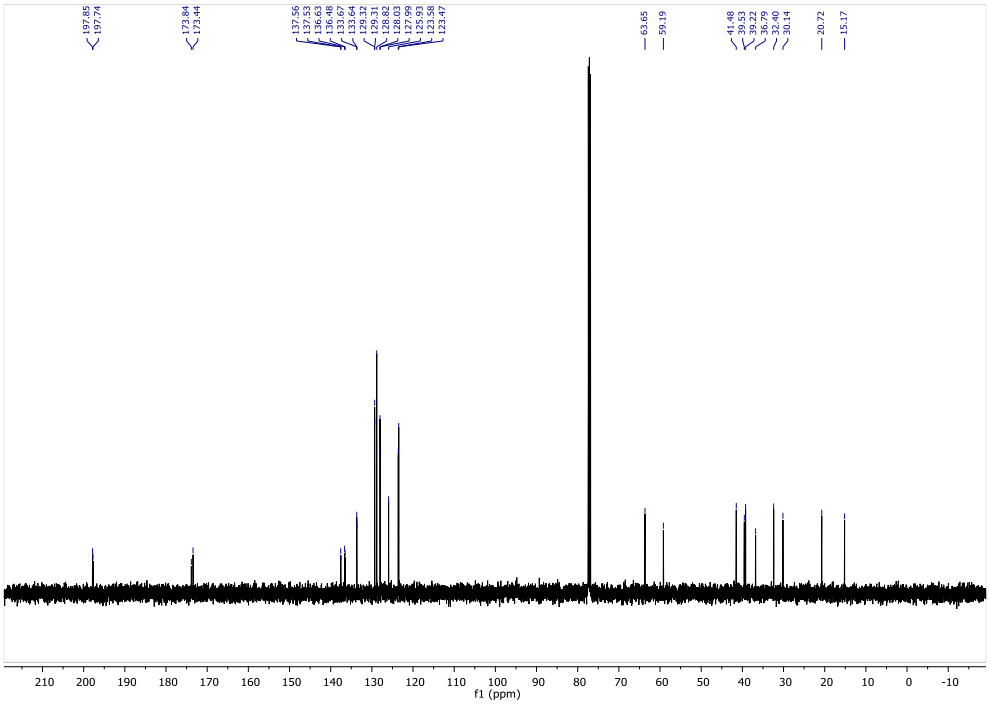


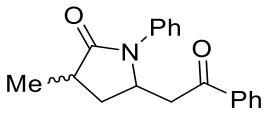




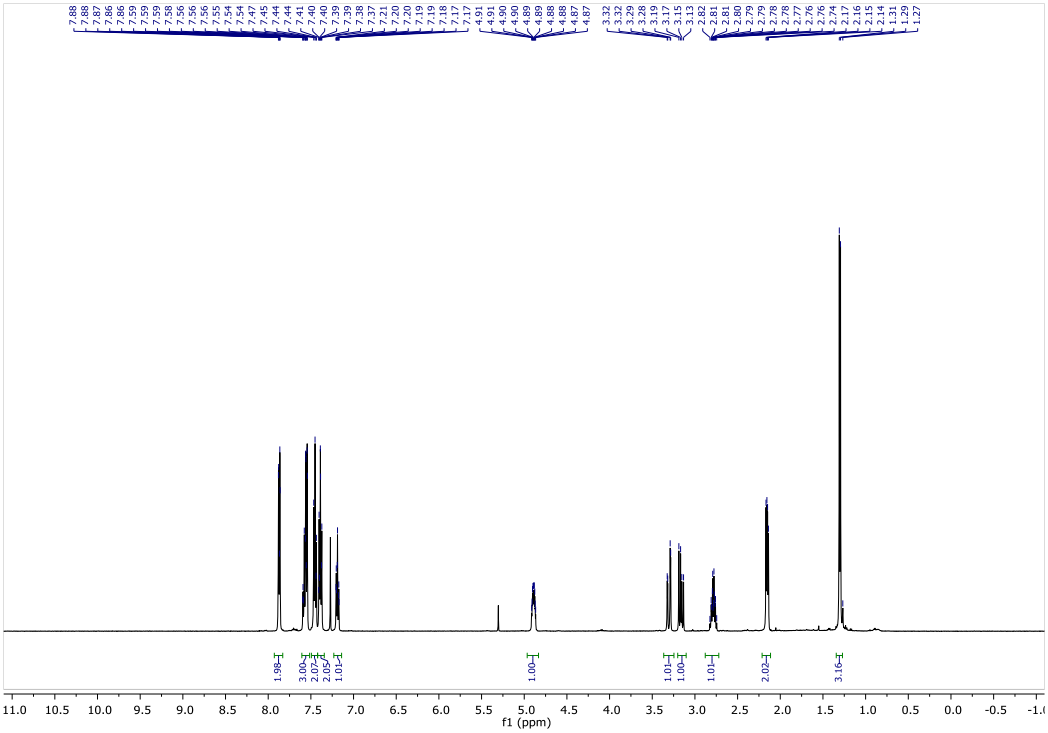
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 4-Methyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (28):

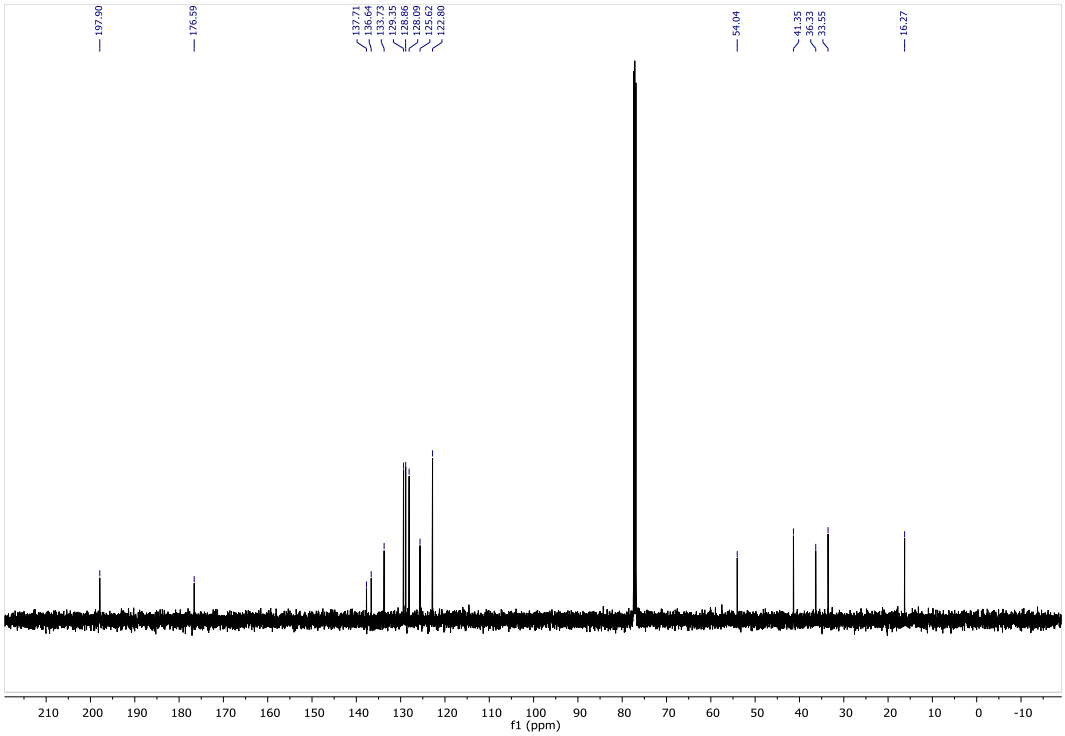




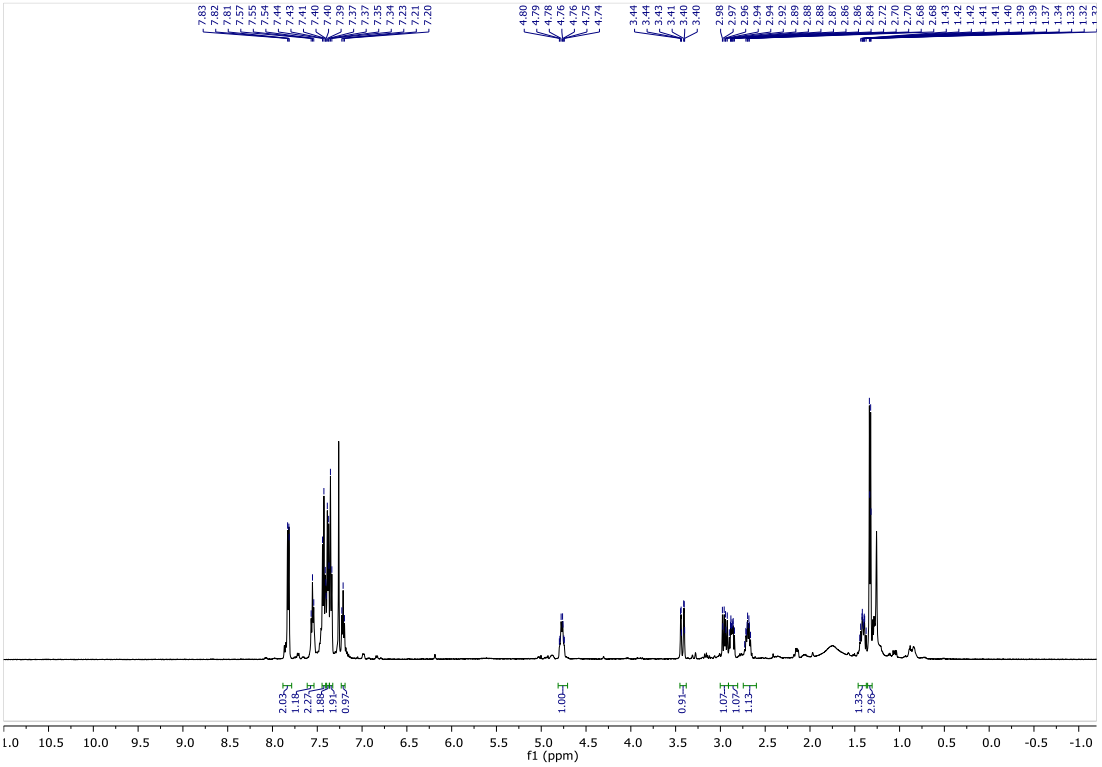


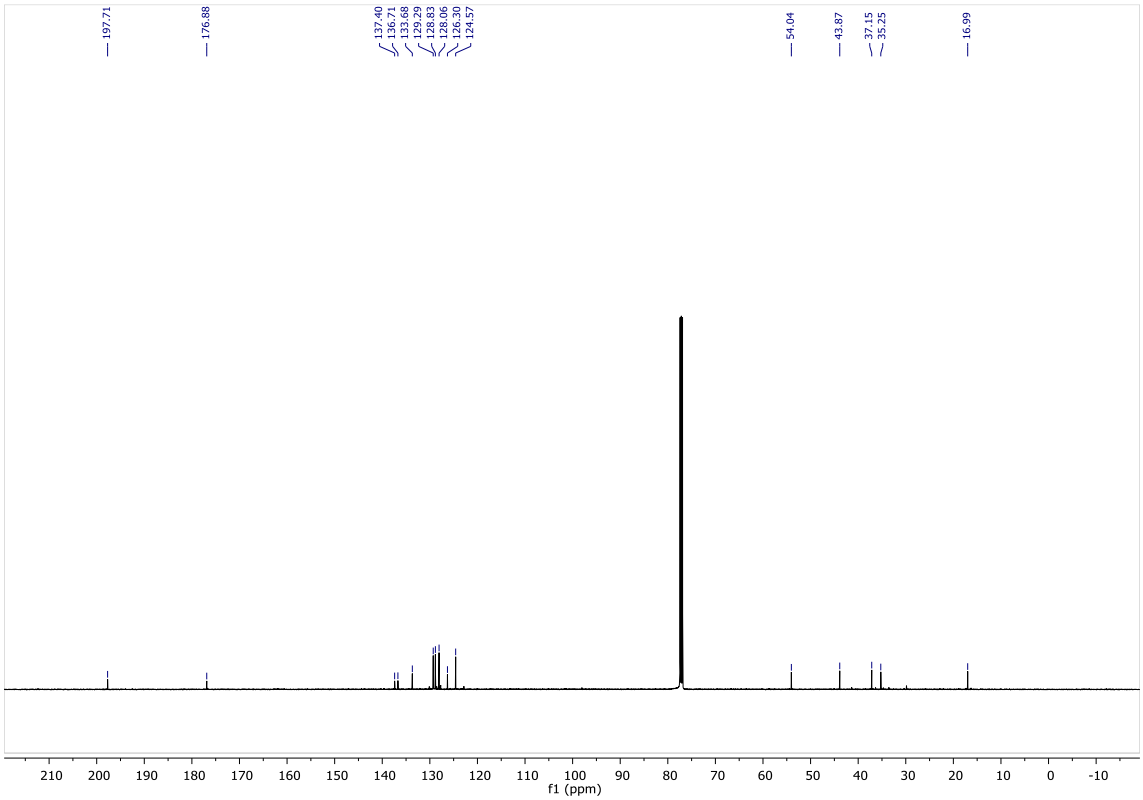
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of 3-Methyl-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-2-one (29): First diastereomer:

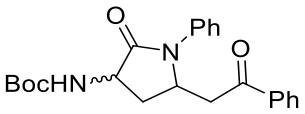




Second diastereomer:

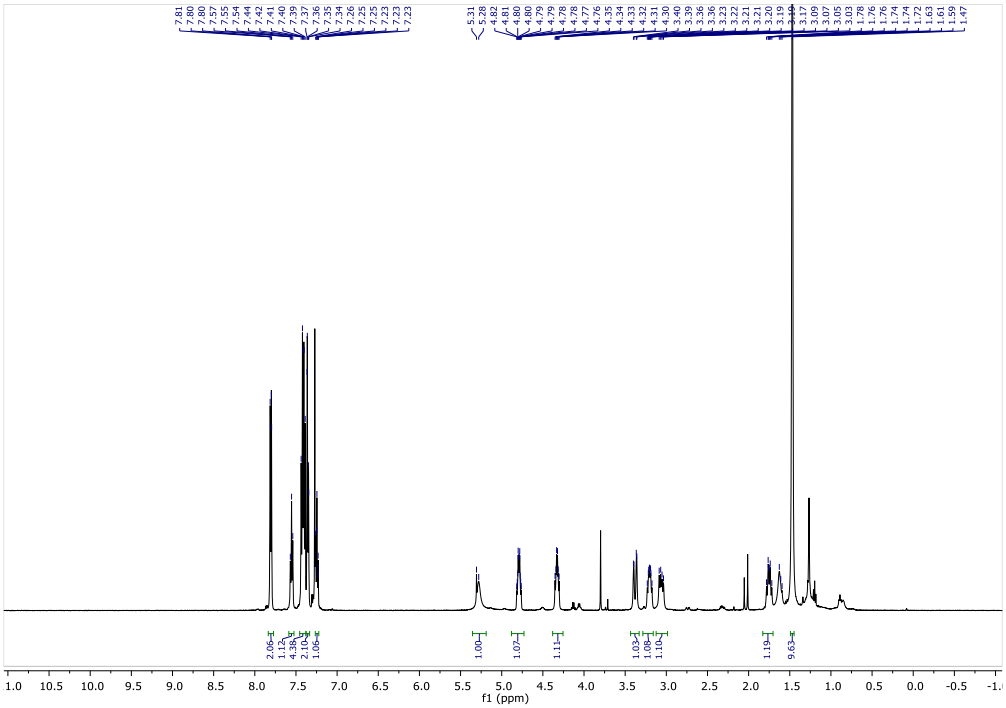


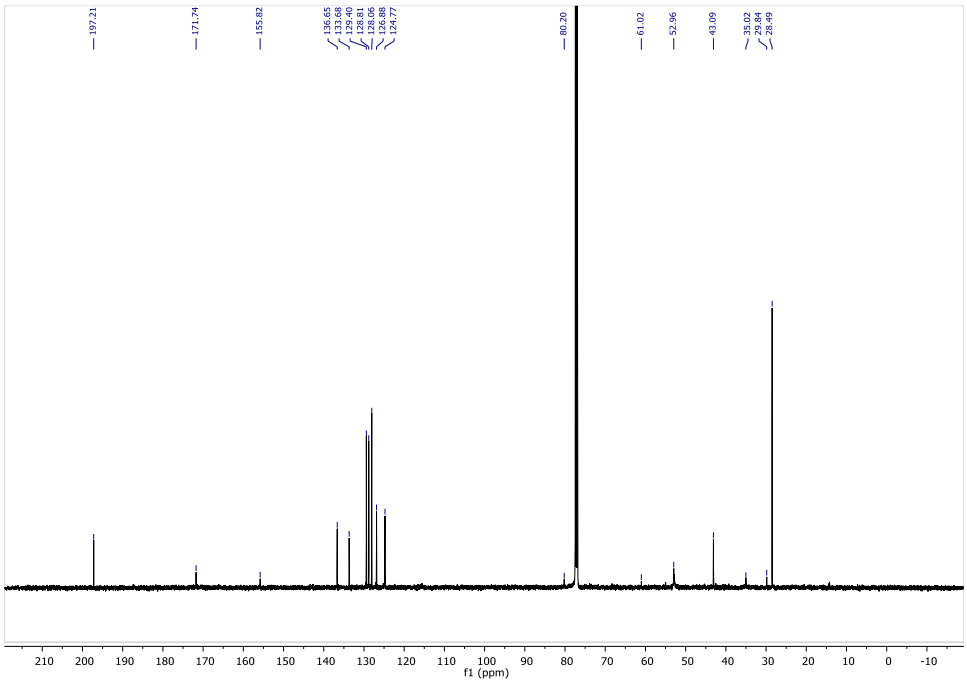




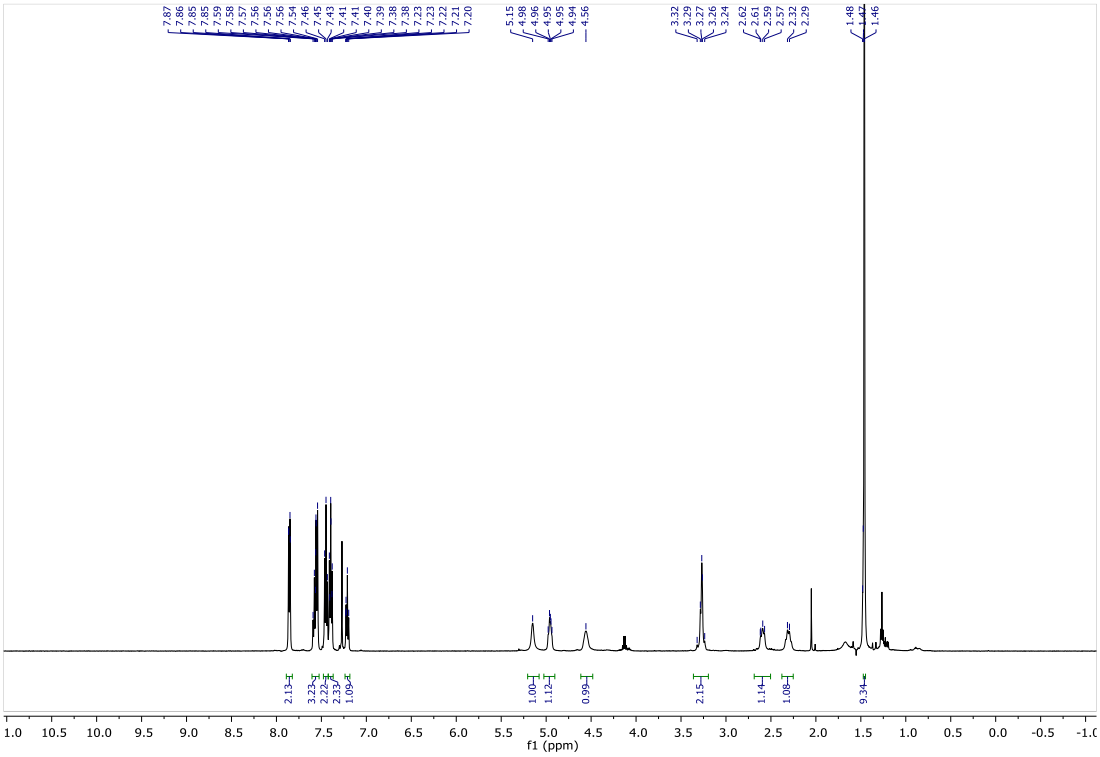
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of *tert*-Butyl (2-oxo-5-(2-oxo-2-phenylethyl)-1-phenylpyrrolidin-3-yl)carbamate (30):

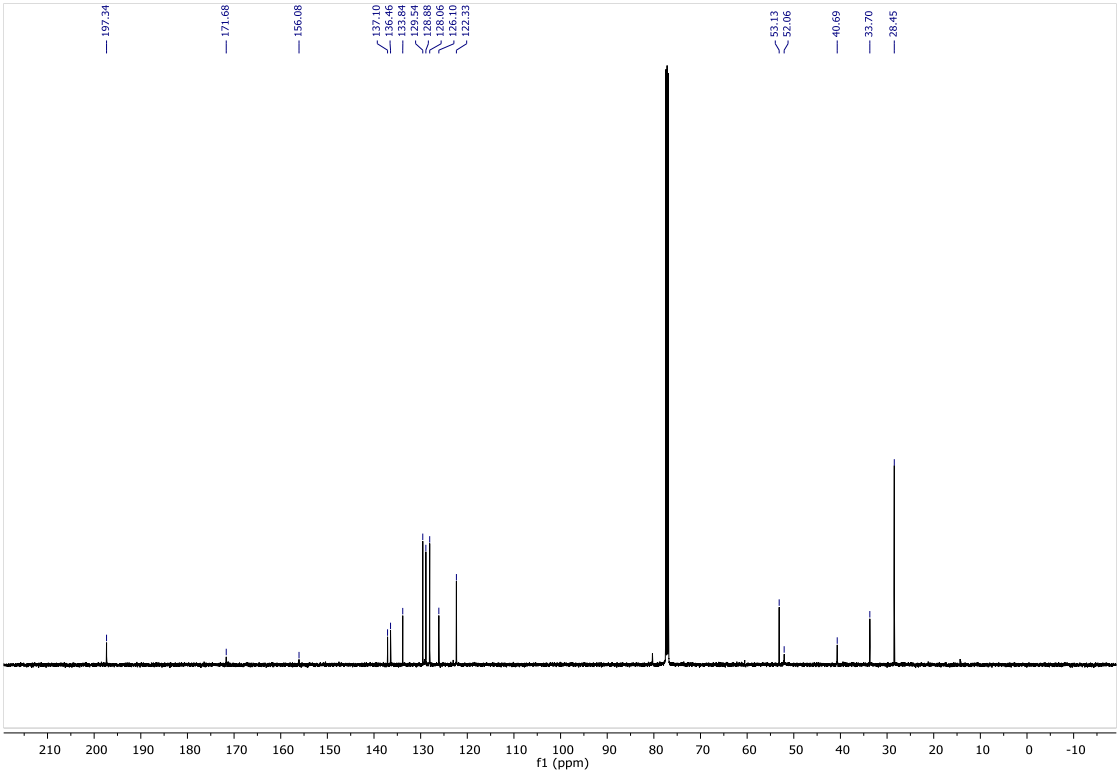
First diastereomer:

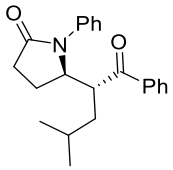




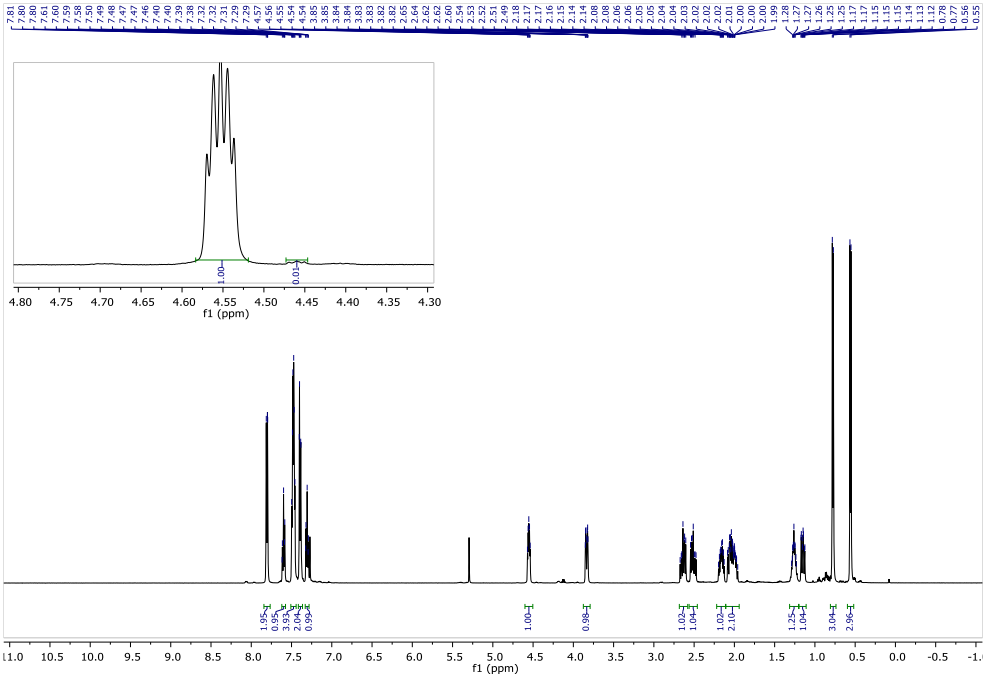
Second Diastereomer:

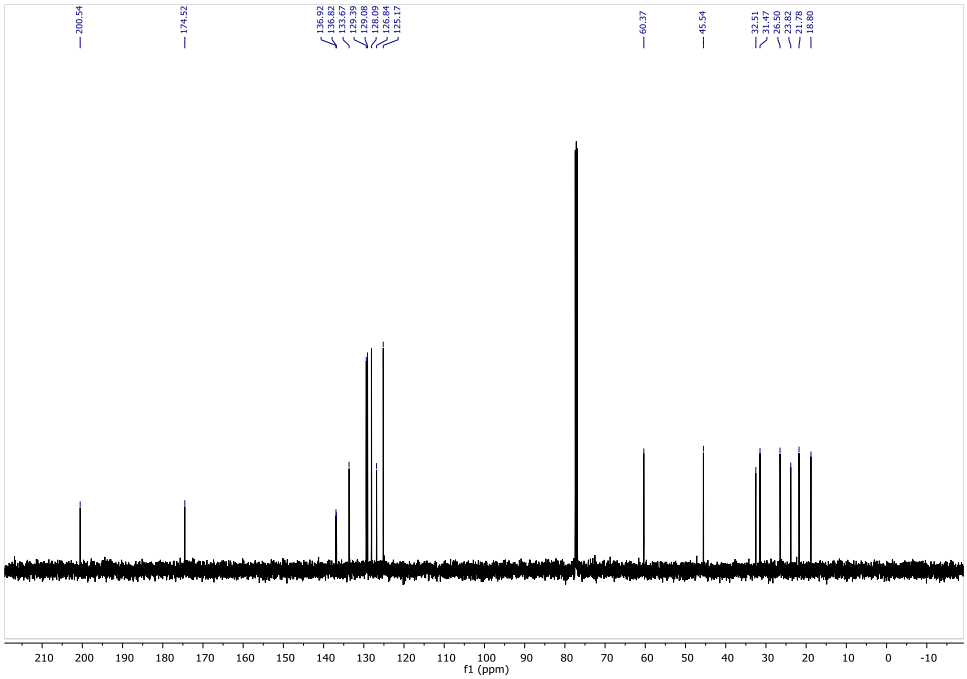


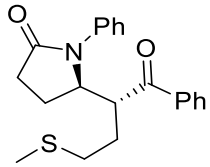




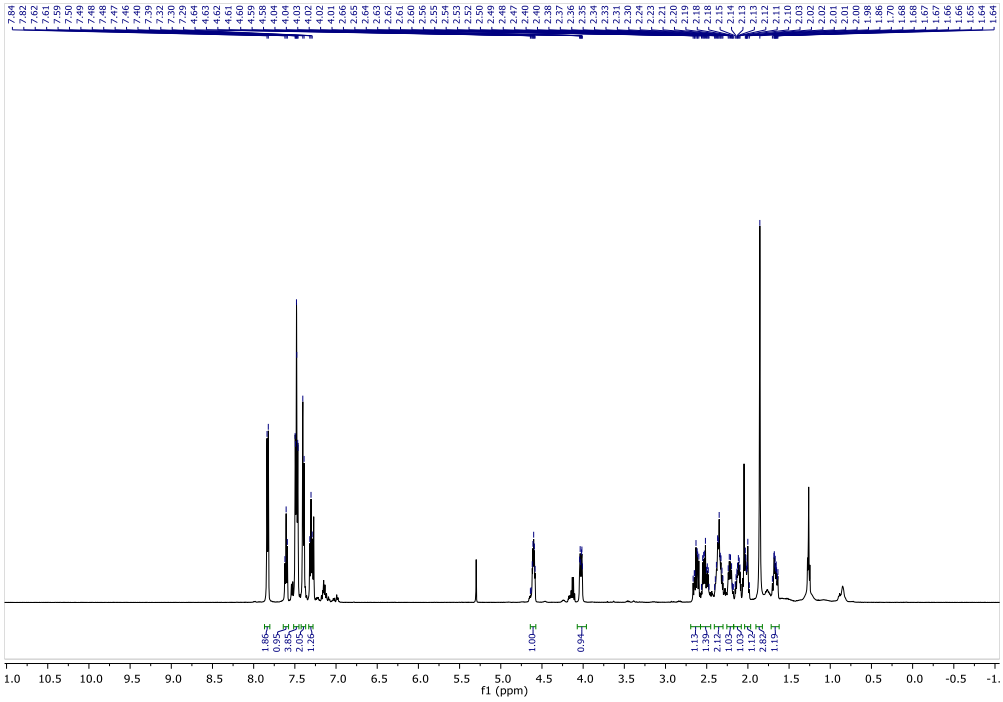
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-4-methyl-1-oxo-1-phenylpentan-2-yl)-1-phenylpyrrolidin-2-one (31):**

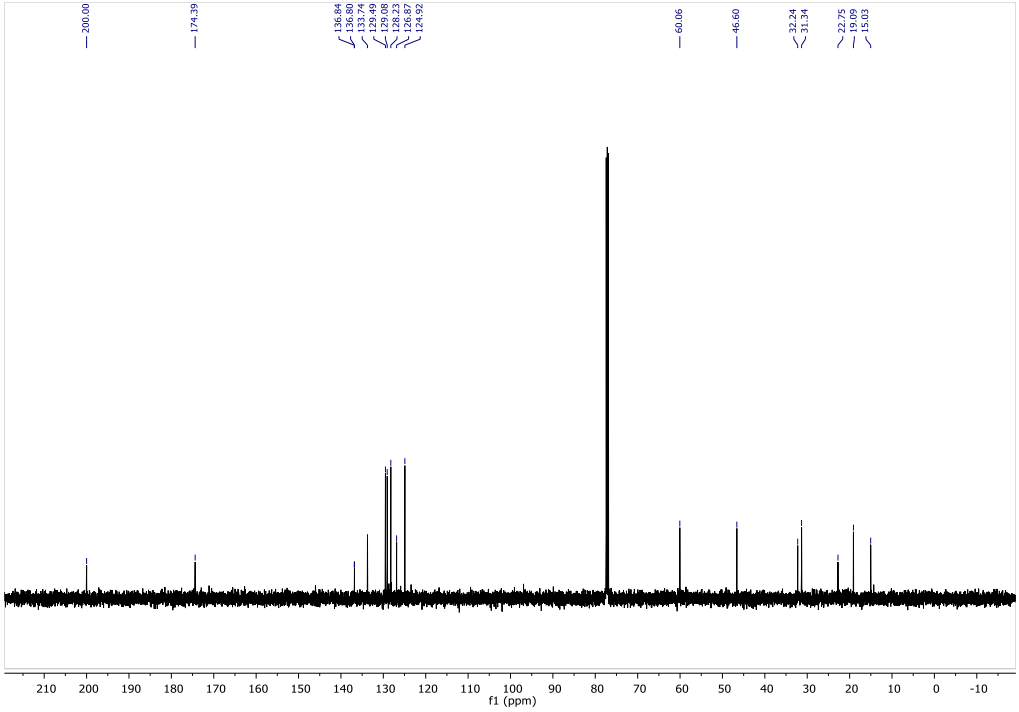


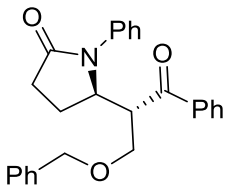




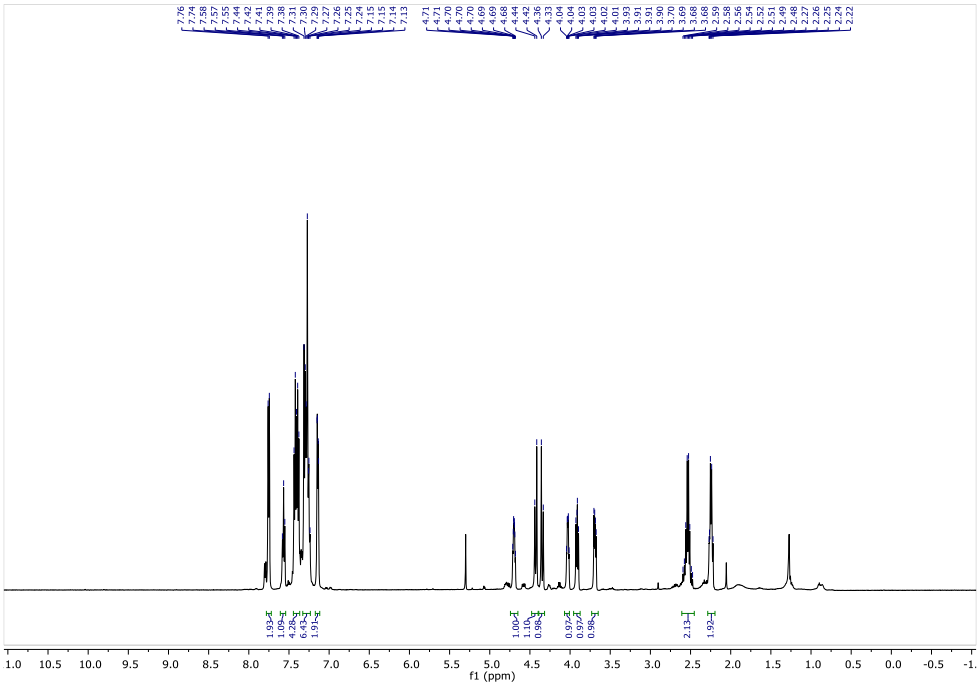
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**)-4-(Methylthio)-1-oxo-1-phenylbutan-2-yl)-1-phenylpyrrolidin-2-one (32):**

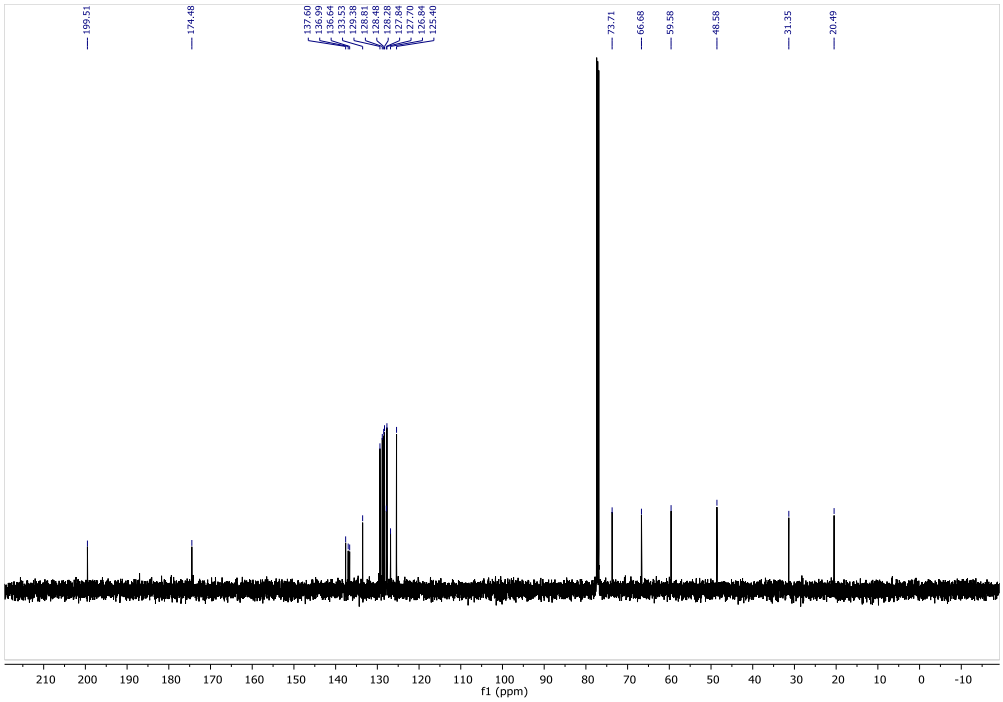


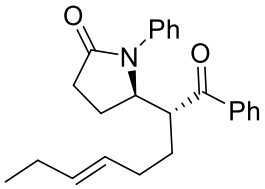




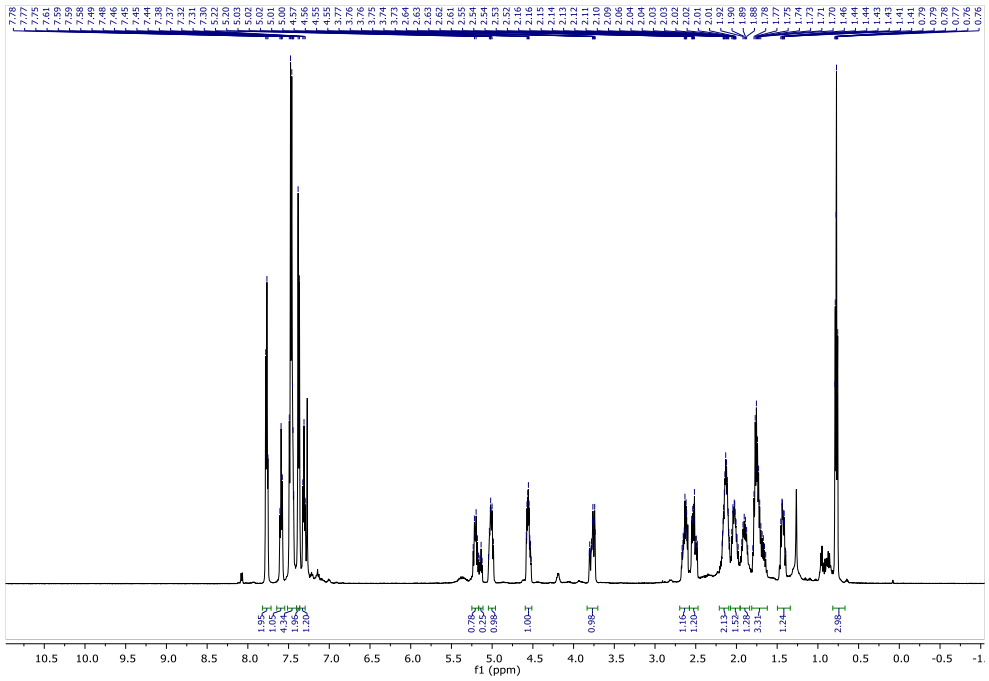
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*S**)-3-(benzyloxy)-1-oxo-1-phenylpropan-2-yl)-1-phenylpyrrolidin-2-one (33):**

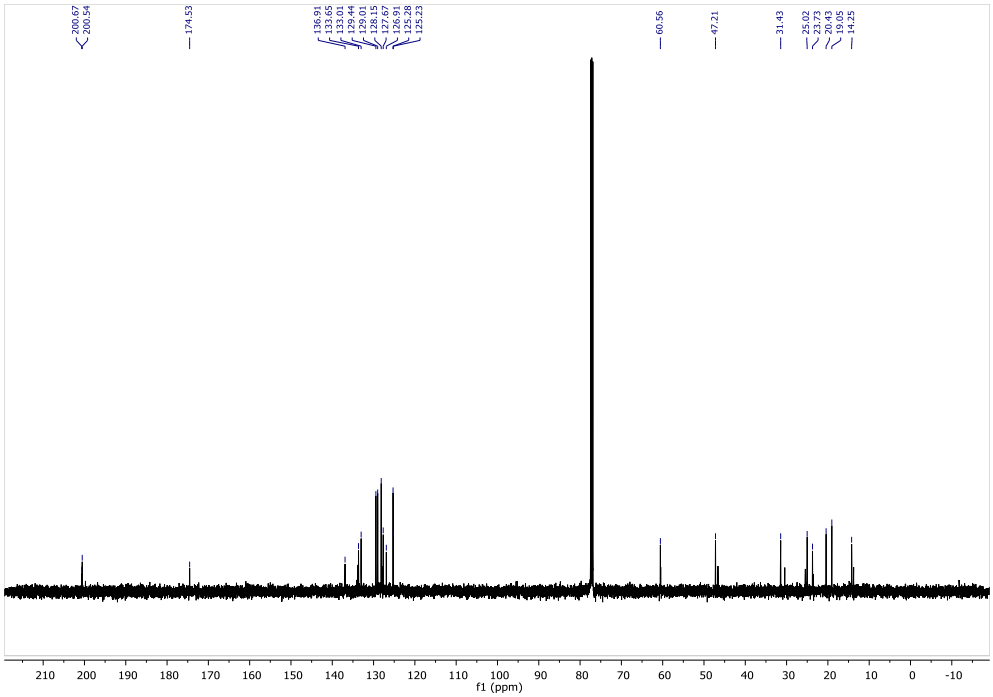


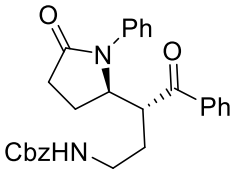




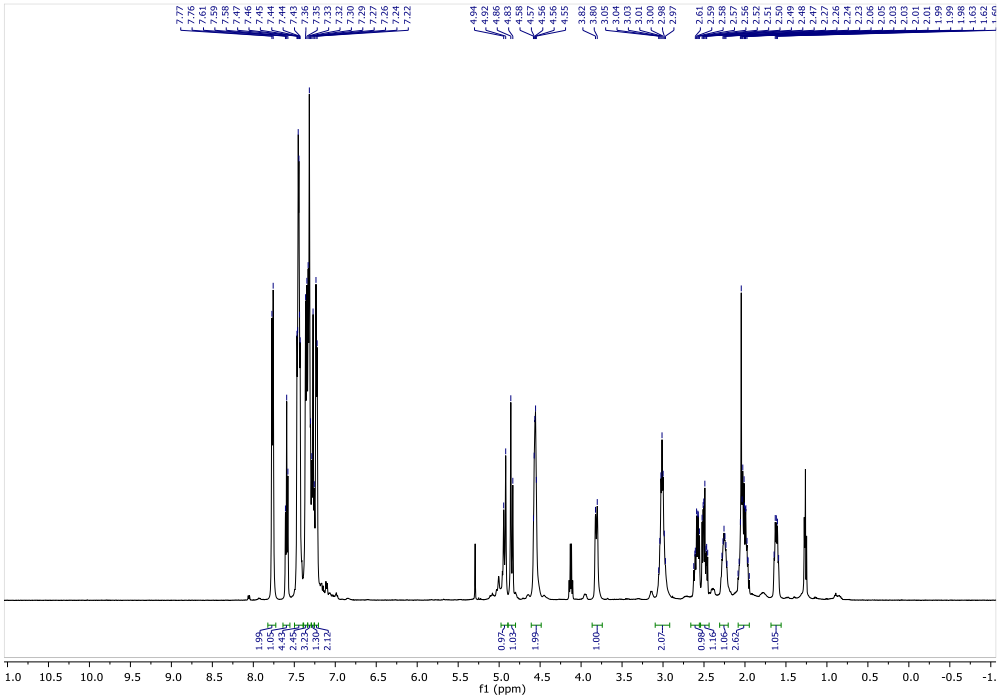
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (*R)-5-((*R**,*Z*)-1-Oxo-1-phenyloct-5-en-2-yl)-1-phenylpyrrolidin-2-one (34):**

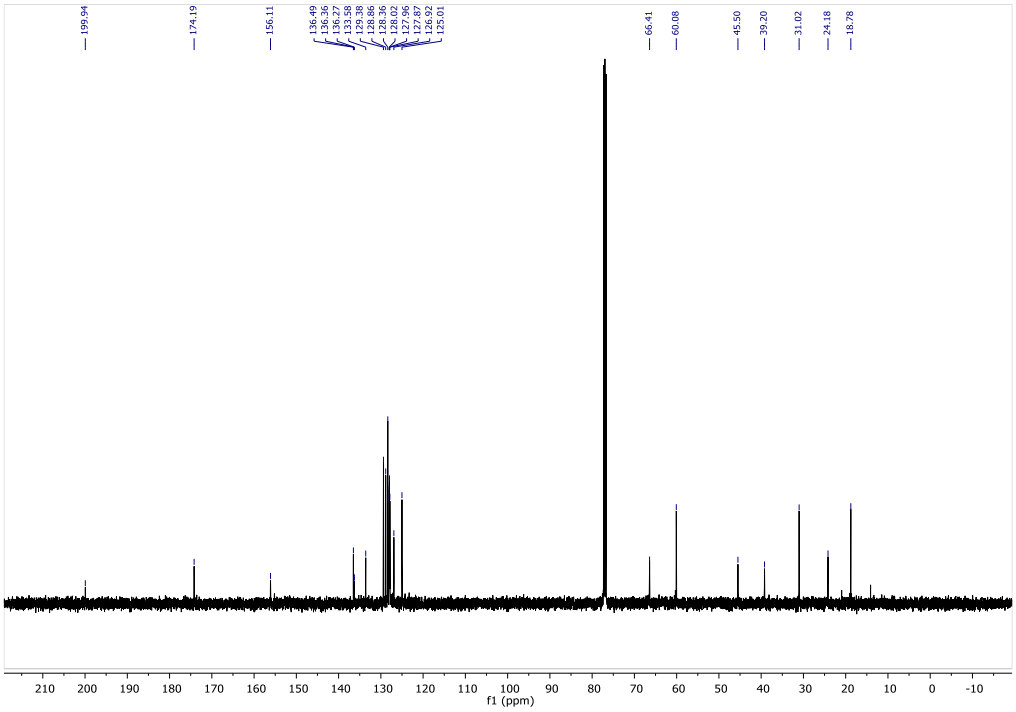


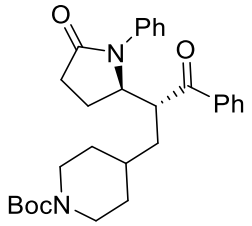




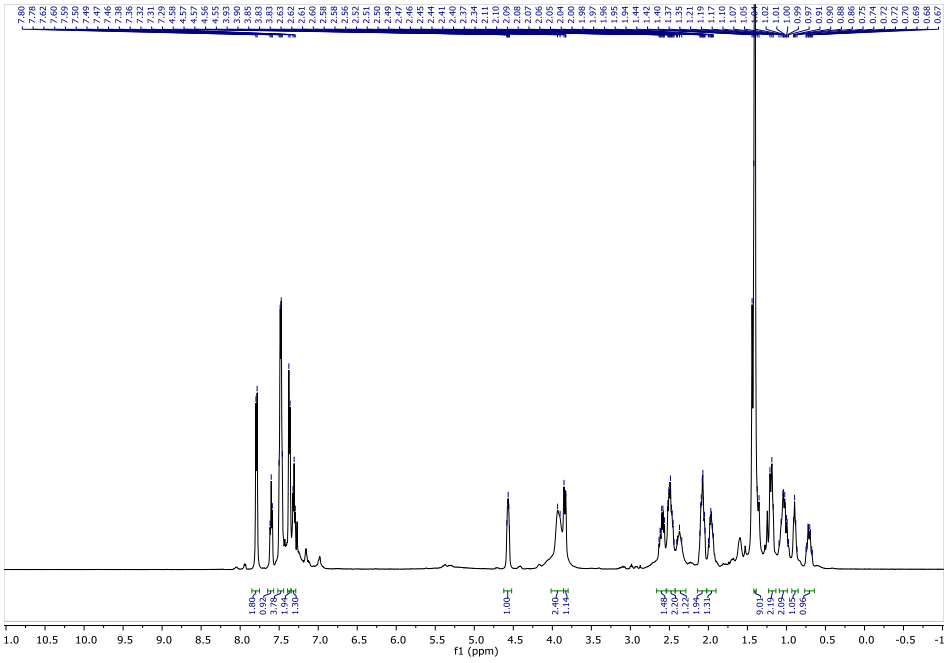
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of Benzyl ((*R)-4-oxo-3-((*R**)-5-oxo-1-phenylpyrrolidin-2-yl)-4-phenylbutyl)carbamate (35):**

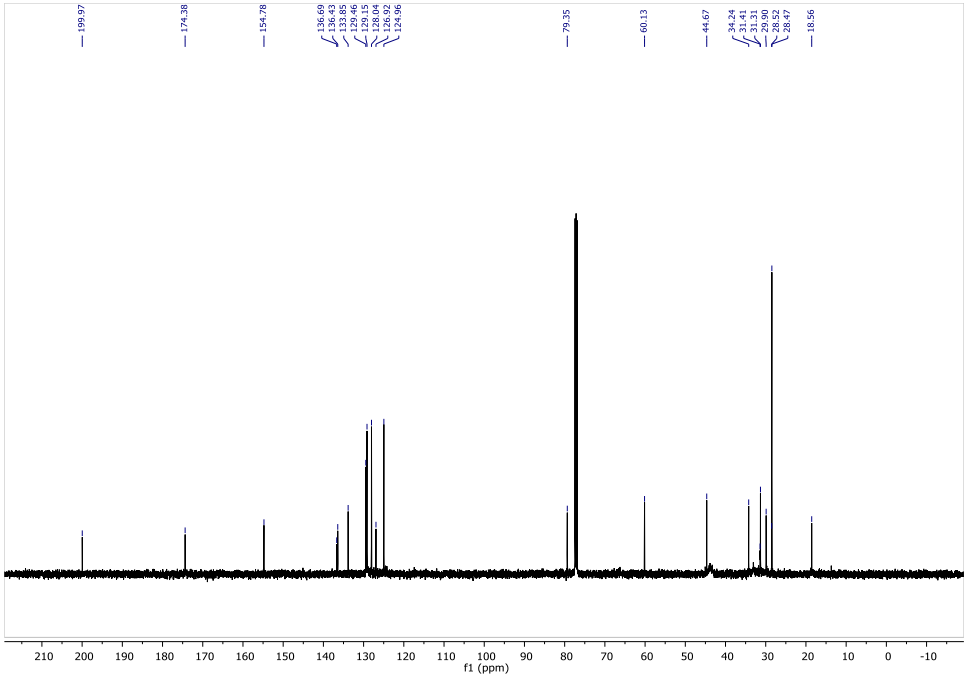


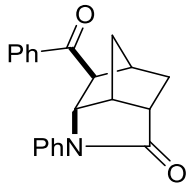




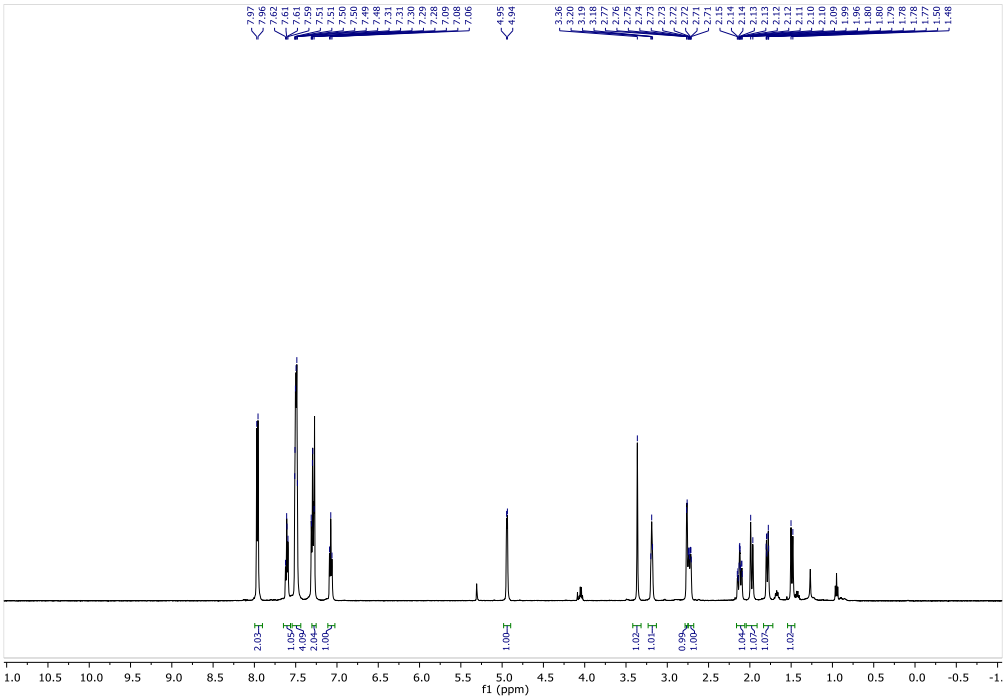
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of *tert*-Butyl 4-((*R)-3-oxo-2-((*R**)-5-oxo-1-phenylpyrrolidin-2-yl)-3-phenylpropyl)piperidine-1-carboxylate (36):**

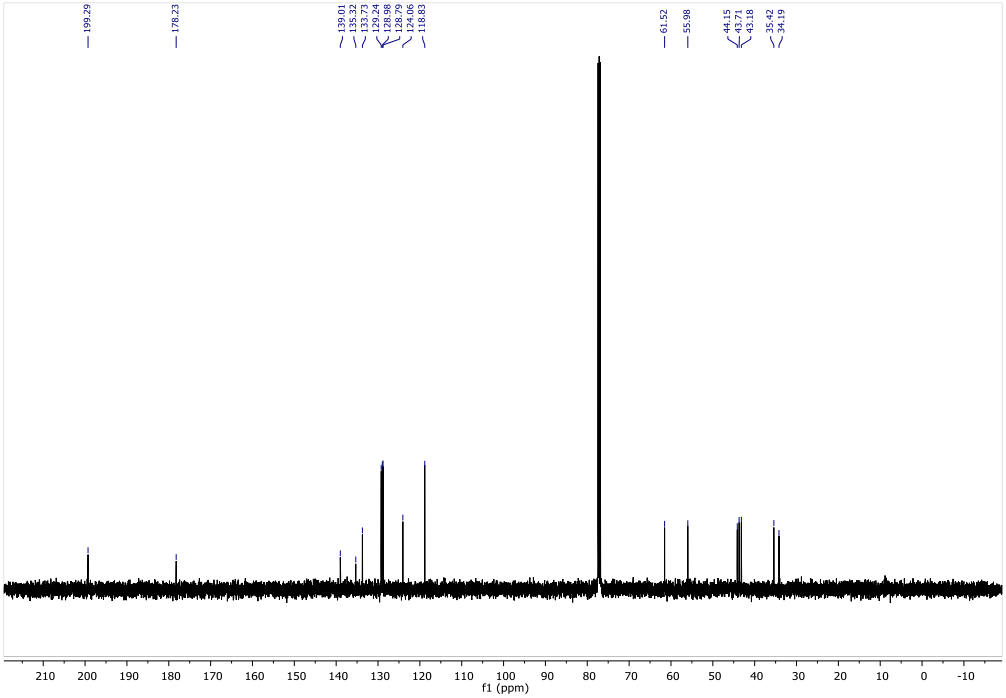


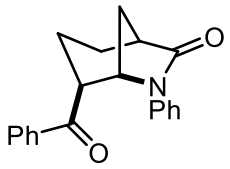




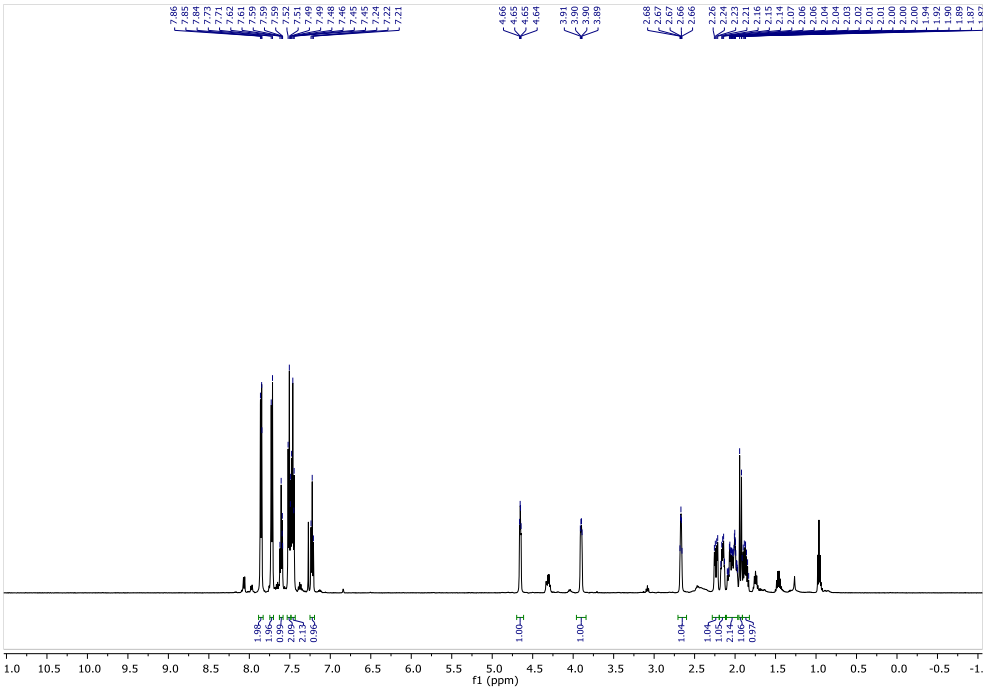
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (6*S,6a*R**)-6-Benzoyl-1-phenylhexahydro-3,5-methanocyclopenta[*b*]pyrrol-2(1*H*)-one (37):**

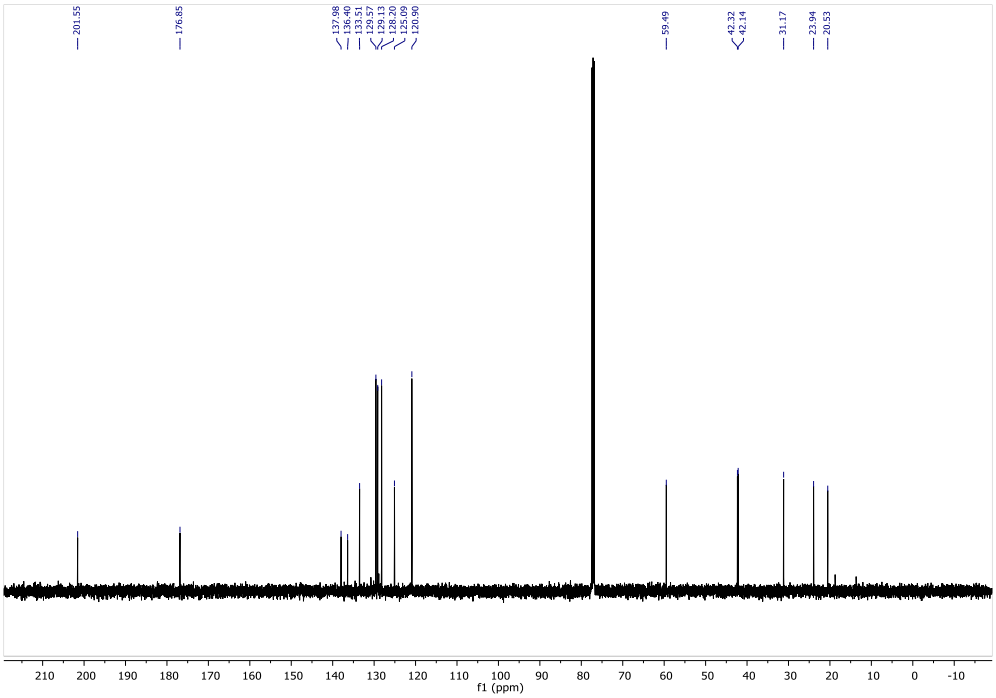


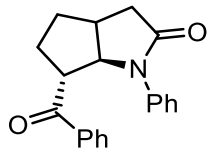




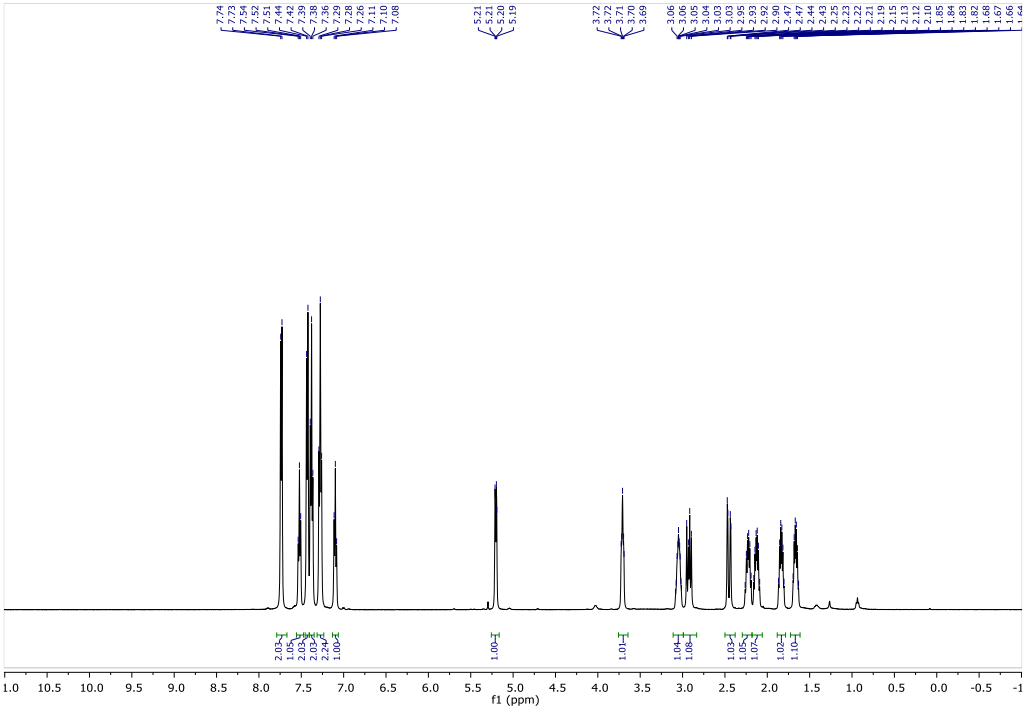
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (1*S,4*R**,5*S**)-4-Benzoyl-6-phenyl-6-azabicyclo[3.2.1]octan-7-one (38):**

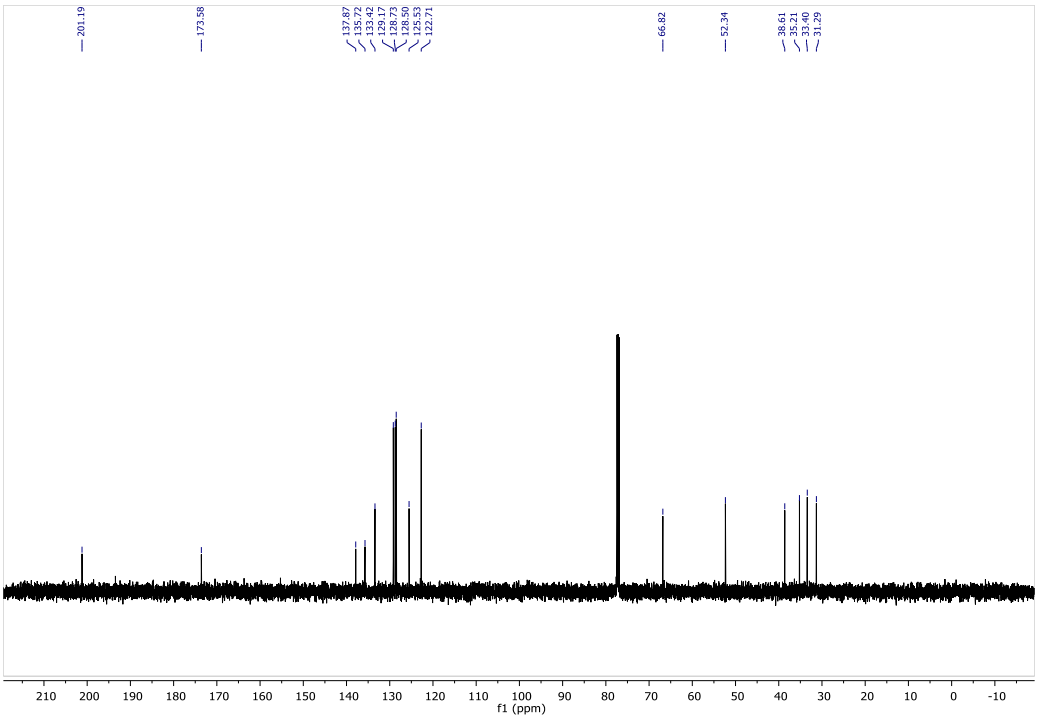


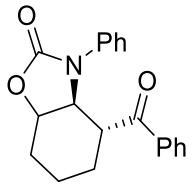




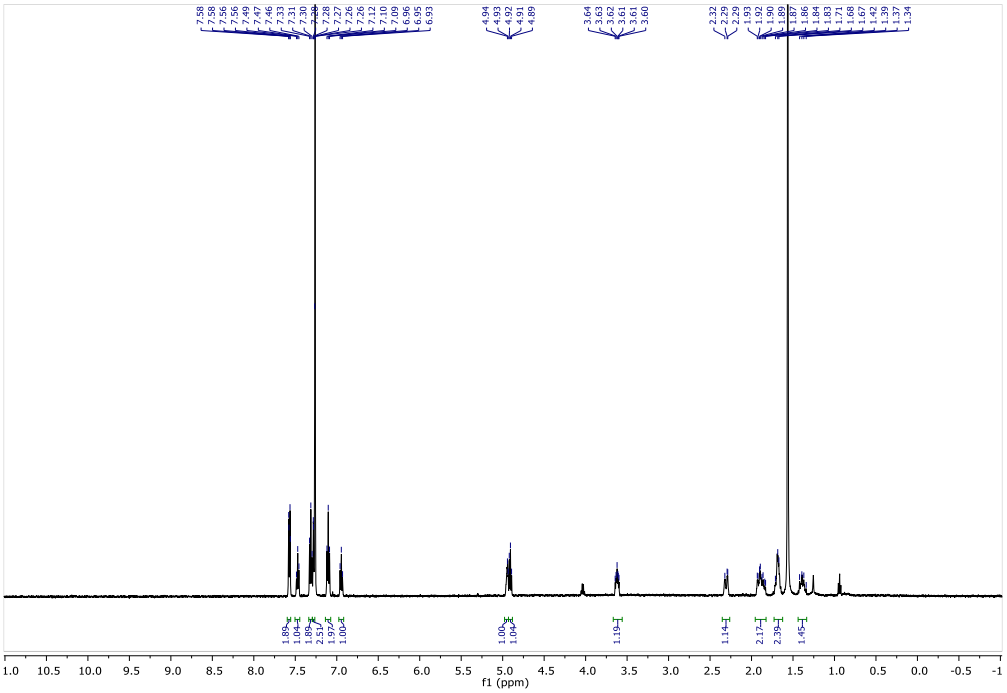
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (6*R,6a*R**)-6-Benzoyl-1-phenylhexahydrocyclopenta[*b*]pyrrol-2(1H)-one (39):**

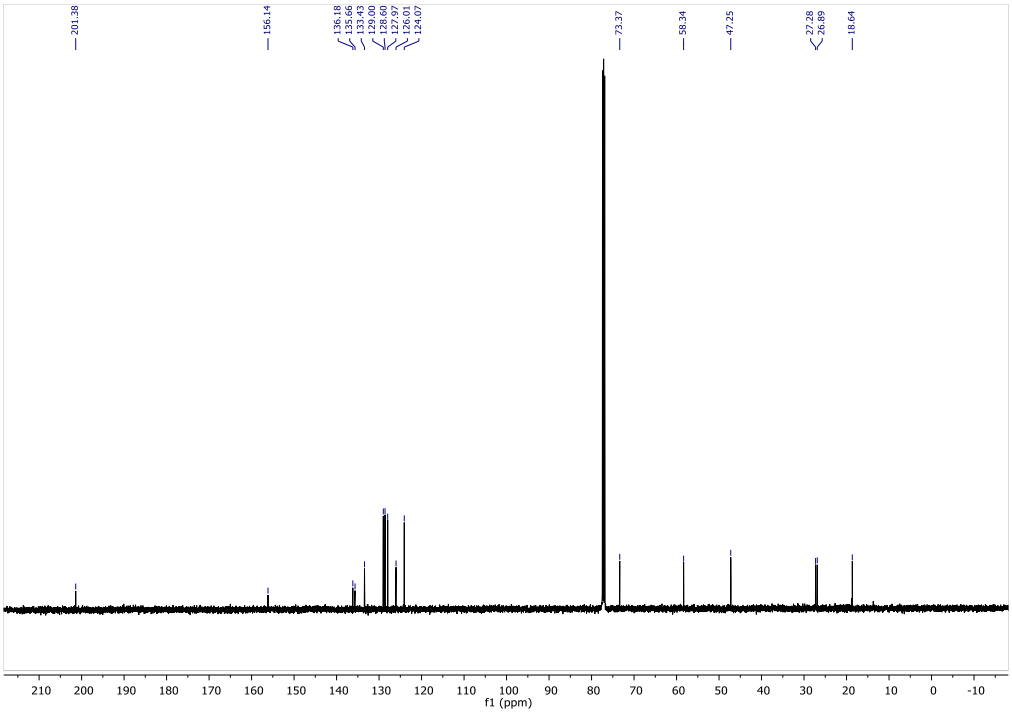


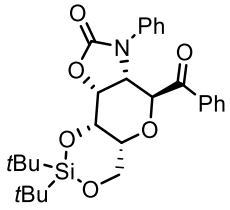




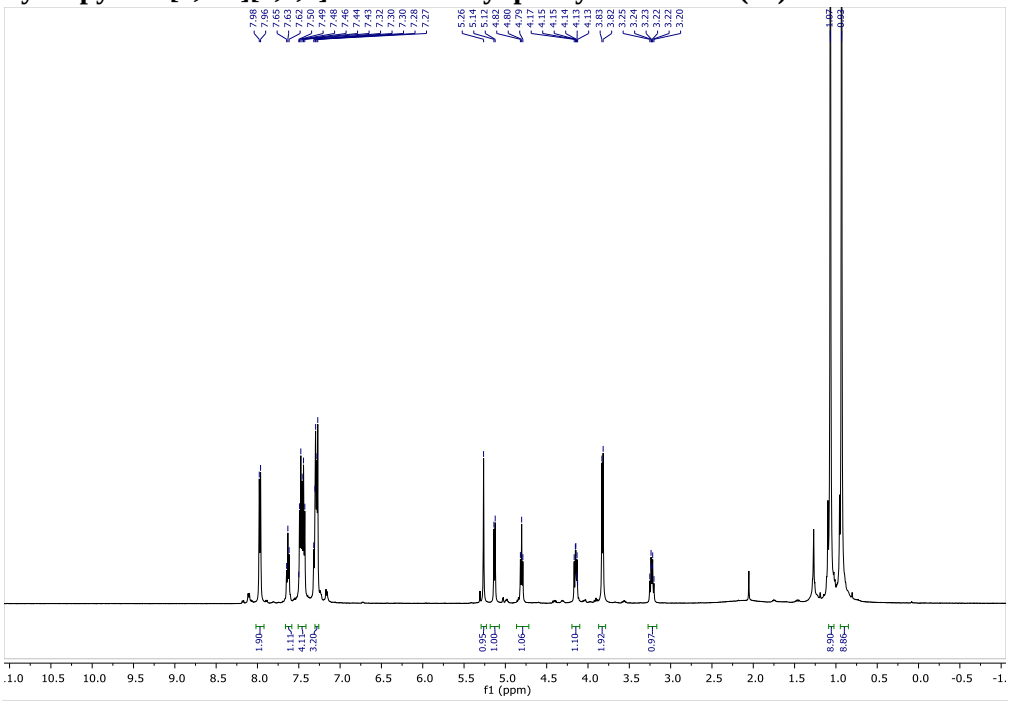
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (3a*S*,4*R)-4-benzoyl-3-phenylhexahydrobenzo[d]oxazol-2(3H)-one (40):**

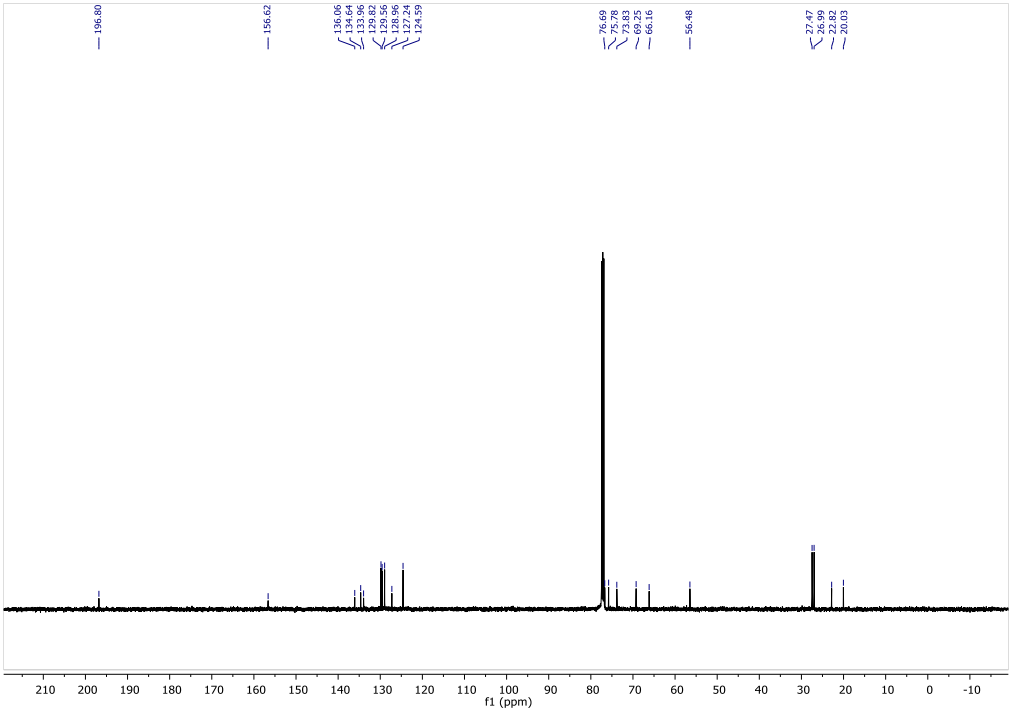


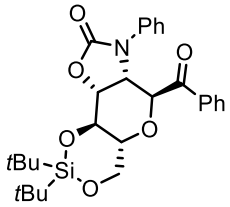




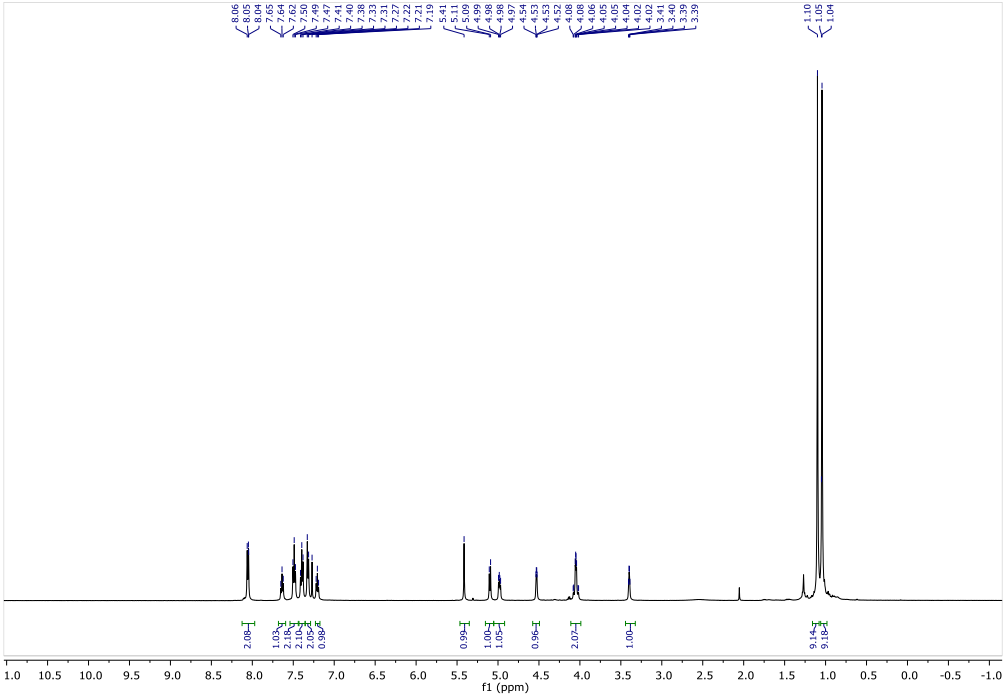
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (4a*R*,8*R*,8a*S*)-6-benzoyl-2,2-di-*tert*-butylhexahydropyrano[3,2-*d*][1,3,2]dioxasilin-8-yl phenylcarbamate (41):

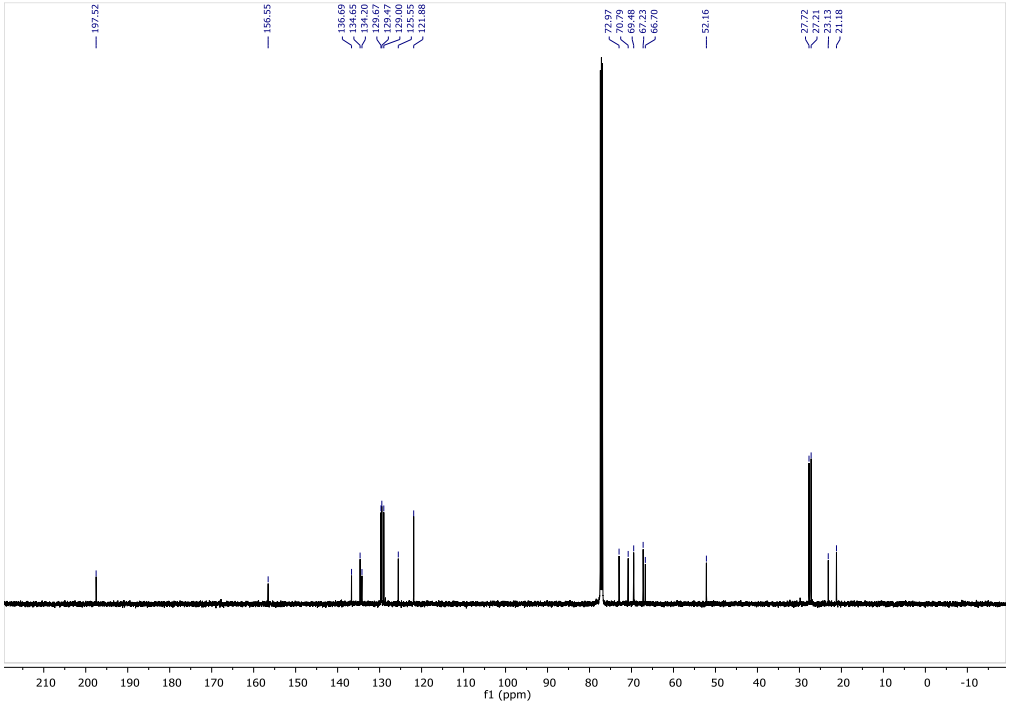




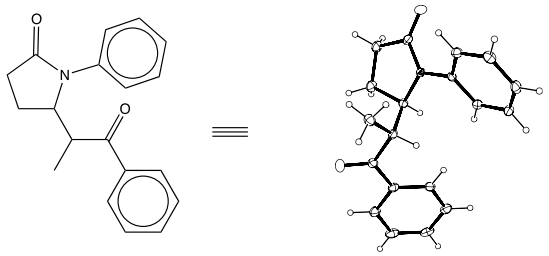


^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 126 MHz) of (4a*R*,8*R*,8a*R*)-6-benzoyl-2,2-di-*tert*-butylhexahydropyrano[3,2-*d*][1,3,2]dioxasilin-8-yl phenylcarbamate (42):





6.2 X-Ray Crystallographic Data of (*R**)-5-((*R**)-1-Oxo-1-phenylpropan-2-yl)-1-phenylpyrrolidin-2-one (**1**)



(*R**)-5-((*R**)-1-Oxo-1-phenylpropan-2-yl)-1-phenylpyrrolidin-2-one (**1**)， $C_{19}H_{19}NO_2$, crystallizes in the monoclinic space group $P2_1/c$ (systematic absences 0k0: k=odd and h0l: l=odd) with a=10.8161(6)Å, b=8.4185(5)Å, c=16.7407(11)Å, β=97.266(2)°, V=1512.09(16)Å^3, Z=4, and d_{calc}=1.289 g/cm$_3$. X-ray intensity data were collected on a Bruker D8QUEST [1] CMOS area detector employing graphite-monochromated Mo-Kα radiation (λ=0.71073Å) at a temperature of 100K. Preliminary indexing was performed from a series of twenty-four 0.5° rotation frames with exposures of 10 seconds. A total of 912 frames were collected with a crystal to detector distance of 33.0 mm, rotation widths of 0.5° and exposures of 5 seconds:

scan type	2θ	ω	φ	χ	Frames
ω	3.18	196.87	0.00	54.72	304
ω	3.18	196.87	288.00	54.72	304
ω	3.18	196.87	144.00	54.72	304

Rotation frames were integrated using SAINT [2], producing a listing of unaveraged F^2 and $\sigma(F^2)$ values. A total of 23261 reflections were measured over the ranges $5.812 \leq 2\theta \leq 50.796°$, $-13 \leq h \leq 13$, $-10 \leq k \leq 10$, $-18 \leq l \leq 20$ yielding 2783 unique reflections (R_{int} = 0.0370). The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABS [3] (minimum and maximum transmission 0.7097, 0.7452). The structure was solved by direct methods - ShelXT [4]. Refinement was by full-matrix least squares based on F^2 using SHELXL-2018 [5]. All reflections were used during refinement. The weighting scheme used was $w=1/[\sigma^2(F_o^2)+ (0.0418P)^2 + 0.7109P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. Refinement converged to R1=0.0379 and wR2=0.0895 for 2437 observed reflections for which $F > 4\sigma(F)$ and R1=0.0450 and wR2=0.0945 and GOF =1.123 for all 2783 unique, non-zero reflections and 200 variables. The maximum Δ/σ in the final cycle of least squares was 0.001 and the two most prominent peaks in the final difference Fourier were +0.24 and -0.30 e/Å^3.

Table 1. lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in Tables 2. and 3. Anisotropic thermal parameters are in Table 4. Tables 5. and 6. list bond distances and bond angles. Figure 1. is an ORTEP representation of the molecule with 50% probability thermal ellipsoids displayed.

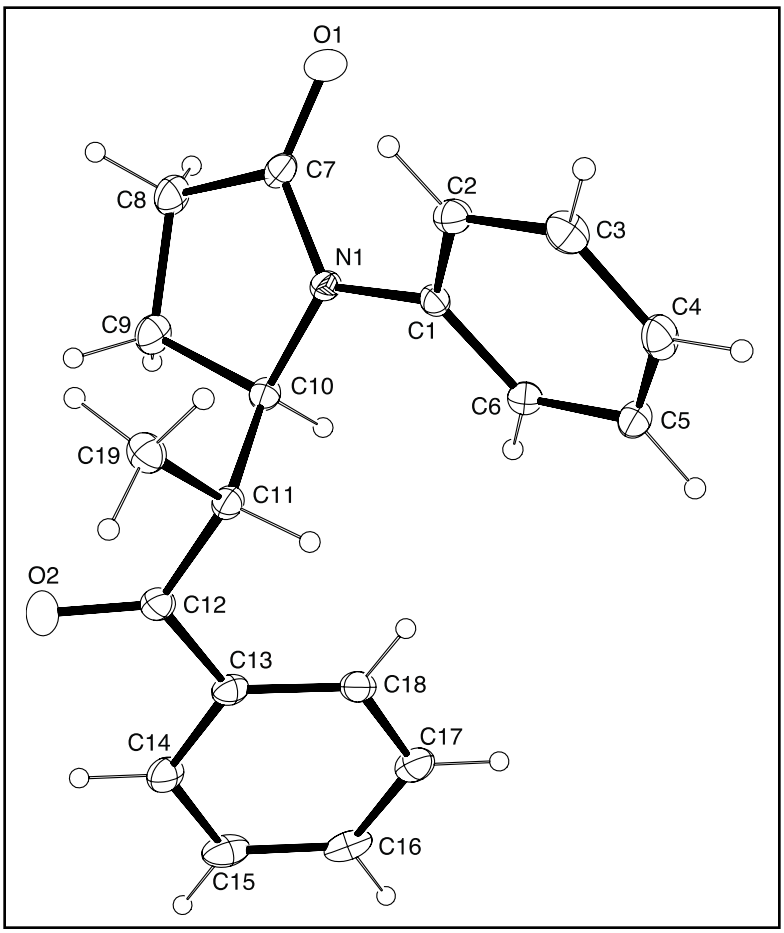


Figure S14. ORTEP drawing of the title compound with 50% thermal ellipsoids.

Table 1. Summary of Structure Determination of Compound 9243

Empirical formula	$C_{19}H_{19}NO_2$
Formula weight	293.35
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a	10.8161(6)Å
b	8.4185(5)Å
c	16.7407(11)Å
β	97.266(2)°
Volume	1512.09(16)Å^3
Z	4
d_{calc}	1.289 g/cm^3
μ	0.083 mm^{-1}
F(000)	624.0
Crystal size, mm	0.41 × 0.14 × 0.12
2θ range for data collection	5.812 - 50.796°
Index ranges	-13 ≤ h ≤ 13, -10 ≤ k ≤ 10, -18 ≤ l ≤ 20
Reflections collected	23261
Independent reflections	2783[R(int) = 0.0370]
Data/restraints/parameters	2783/0/200
Goodness-of-fit on F^2	1.123
Final R indexes [I>=2σ (I)]	R_1 = 0.0379, wR_2 = 0.0895
Final R indexes [all data]	R_1 = 0.0450, wR_2 = 0.0945
Largest diff. peak/hole	0.24/-0.30 eÅ^{-3}

Table 2 . Refined Positional Parameters for Compound 9243

Atom	*x*	*y*	*z*	U(eq)
O1	0.06380(9)	-0.07155(11)	0.60249(6)	0.0194(2)
O2	0.51763(9)	0.22534(12)	0.43126(6)	0.0225(3)
N1	0.16881(10)	0.13864(13)	0.55386(6)	0.0118(2)
C1	0.13631(12)	0.25687(15)	0.60816(8)	0.0115(3)
C2	0.13958(12)	0.22189(17)	0.68976(8)	0.0144(3)
C3	0.11032(13)	0.33855(17)	0.74265(8)	0.0170(3)
C4	0.08092(12)	0.49150(17)	0.71571(9)	0.0178(3)
C5	0.07861(12)	0.52689(17)	0.63457(9)	0.0172(3)
C6	0.10469(12)	0.40954(16)	0.58076(8)	0.0142(3)
C7	0.13106(12)	-0.01683(16)	0.55577(8)	0.0140(3)
C8	0.18365(13)	-0.10607(17)	0.48976(9)	0.0190(3)
C9	0.26135(13)	0.01284(17)	0.44933(8)	0.0173(3)
C10	0.23470(12)	0.17740(16)	0.48448(8)	0.0123(3)
C11	0.35383(12)	0.27696(16)	0.51099(8)	0.0133(3)
C12	0.42437(12)	0.30302(16)	0.43860(8)	0.0148(3)
C13	0.37937(12)	0.42547(16)	0.37645(8)	0.0143(3)
C14	0.44618(14)	0.44601(17)	0.31083(8)	0.0182(3)
C15	0.40956(14)	0.55963(17)	0.25256(9)	0.0207(3)
C16	0.30551(14)	0.65316(17)	0.25853(8)	0.0192(3)
C17	0.23831(13)	0.63350(17)	0.32325(9)	0.0183(3)
C18	0.27543(12)	0.52106(16)	0.38205(8)	0.0149(3)
C19	0.43602(13)	0.19984(17)	0.58123(8)	0.0168(3)

Table 3 . Positional Parameters for Hydrogens in Compound 9243

Atom	*x*	*y*	*z*	U(eq)
H2	0.161806	0.118342	0.709075	0.017
H3	0.110378	0.313565	0.797994	0.02
H4	0.06253	0.571352	0.752532	0.021
H5	0.059158	0.631532	0.615775	0.021
H6	0.100926	0.433558	0.525056	0.017
H8a	0.115607	-0.148742	0.450508	0.023
H8b	0.236117	-0.195636	0.512427	0.023
H9a	0.23741	0.011857	0.39026	0.021
H9b	0.351064	-0.013296	0.460917	0.021
H10	0.177834	0.238695	0.443915	0.015
H11	0.327025	0.383191	0.529271	0.016
H14	0.517095	0.381724	0.306166	0.022
H15	0.45585	0.573398	0.208464	0.025
H16	0.280296	0.730496	0.218438	0.023
H17	0.166822	0.697124	0.327273	0.022
H18	0.229656	0.509061	0.426505	0.018
H19a	0.394895	0.207246	0.63001	0.025
H19b	0.516439	0.254867	0.589974	0.025
H19c	0.449495	0.087882	0.568815	0.025

Table 4 . Refined Thermal Parameters (U's) for Compound 9243

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0227(5)	0.0132(5)	0.0232(6)	0.0019(4)	0.0068(4)	-0.0033(4)
O2	0.0218(5)	0.0226(6)	0.0250(6)	0.0052(4)	0.0108(4)	0.0089(4)
N1	0.0144(5)	0.0095(6)	0.0119(6)	-0.0001(4)	0.0037(4)	0.0002(4)
C1	0.0097(6)	0.0113(6)	0.0137(6)	-0.0014(5)	0.0027(5)	-0.0007(5)
C2	0.0147(6)	0.0140(7)	0.0144(7)	0.0018(5)	0.0018(5)	-0.0005(5)
C3	0.0178(7)	0.0212(7)	0.0122(7)	-0.0020(6)	0.0028(5)	-0.0018(6)
C4	0.0163(7)	0.0167(7)	0.0210(7)	-0.0079(6)	0.0048(6)	-0.0012(6)
C5	0.0152(7)	0.0115(7)	0.0255(8)	-0.0008(6)	0.0047(6)	0.0010(5)
C6	0.0149(6)	0.0134(7)	0.0149(7)	0.0019(5)	0.0040(5)	0.0005(5)
C7	0.0138(6)	0.0103(6)	0.0171(7)	0.0007(5)	-0.0009(5)	0.0011(5)
C8	0.0197(7)	0.0125(7)	0.0252(8)	-0.0046(6)	0.0038(6)	0.0004(6)
C9	0.0221(7)	0.0150(7)	0.0151(7)	-0.0040(6)	0.0041(6)	0.0015(6)
C10	0.0149(7)	0.0123(7)	0.0099(6)	0.0010(5)	0.0024(5)	0.0019(5)
C11	0.0157(7)	0.0111(6)	0.0134(7)	0.0003(5)	0.0034(5)	0.0015(5)
C12	0.0160(7)	0.0124(7)	0.0166(7)	-0.0012(5)	0.0043(5)	-0.0012(5)
C13	0.0183(7)	0.0110(6)	0.0138(7)	-0.0014(5)	0.0027(5)	-0.0023(5)
C14	0.0249(7)	0.0133(7)	0.0179(7)	-0.0018(6)	0.0087(6)	0.0003(6)
C15	0.0338(8)	0.0161(7)	0.0133(7)	-0.0010(6)	0.0078(6)	-0.0064(6)
C16	0.0287(8)	0.0127(7)	0.0145(7)	0.0024(6)	-0.0034(6)	-0.0062(6)
C17	0.0187(7)	0.0138(7)	0.0215(7)	0.0010(6)	-0.0012(6)	-0.0019(5)
C18	0.0165(7)	0.0134(7)	0.0155(7)	0.0001(5)	0.0040(5)	-0.0023(5)
C19	0.0151(7)	0.0199(7)	0.0154(7)	0.0010(6)	0.0019(5)	0.0004(6)

Table 5 . Bond Distances in Compound 9243, Å

O1-C7	1.2236(17)	O2-C12	1.2213(17)	N1-C1	1.4216(17)
N1-C7	1.3726(18)	N1-C10	1.4741(16)	C1-C2	1.3936(19)
C1-C6	1.3927(19)	C2-H2	0.9500	C2-C3	1.385(2)
C3-H3	0.9500	C3-C4	1.388(2)	C4-H4	0.9500
C4-C5	1.388(2)	C5-H5	0.9500	C5-C6	1.3897(19)
C6-H6	0.9500	C7-C8	1.5061(19)	C8-H8a	0.9900
C8-H8b	0.9900	C8-C9	1.520(2)	C9-H9a	0.9900
C9-H9b	0.9900	C9-C10	1.5464(18)	C10-H10	1.0000
C10-C11	1.5541(18)	C11-H11	1.0000	C11-C12	1.5273(18)
C11-C19	1.5266(18)	C12-C13	1.5013(19)	C13-C14	1.3998(19)
C13-C18	1.3953(19)	C14-H14	0.9500	C14-C15	1.388(2)
C15-H15	0.9500	C15-C16	1.387(2)	C16-H16	0.9500
C16-C17	1.389(2)	C17-H17	0.9500	C17-C18	1.388(2)
C18-H18	0.9500	C19-H19a	0.9800	C19-H19b	0.9800
C19-H19c	0.9800				

Table 6 . Bond Angles in Compound 9243, °

C1-N1-C10	122.15(11)	C7-N1-C1	123.66(11)	C7-N1-C10	113.85(11)
C2-C1-N1	120.07(12)	C6-C1-N1	120.39(12)	C6-C1-C2	119.51(12)
C1-C2-H2	120.1	C3-C2-C1	119.81(13)	C3-C2-H2	120.1
C2-C3-H3	119.6	C2-C3-C4	120.76(13)	C4-C3-H3	119.6
C3-C4-H4	120.3	C5-C4-C3	119.49(13)	C5-C4-H4	120.3
C4-C5-H5	119.9	C4-C5-C6	120.12(13)	C6-C5-H5	119.9
C1-C6-H6	119.9	C5-C6-C1	120.27(13)	C5-C6-H6	119.9
O1-C7-N1	125.21(13)	O1-C7-C8	126.26(13)	N1-C7-C8	108.51(11)
C7-C8-H8a	110.5	C7-C8-H8b	110.5	C7-C8-C9	106.24(11)
H8a-C8-H8b	108.7	C9-C8-H8a	110.5	C9-C8-H8b	110.5
C8-C9-H9a	110.5	C8-C9-H9b	110.5	C8-C9-C10	106.29(11)
H9a-C9-H9b	108.7	C10-C9-H9a	110.5	C10-C9-H9b	110.5
N1-C10-C9	103.50(10)	N1-C10-H10	109.4	N1-C10-C11	111.12(10)
C9-C10-H10	109.4	C9-C10-C11	113.84(11)	C11-C10-H10	109.4
C10-C11-H11	107.9	C12-C11-C10	109.28(10)	C12-C11-H11	107.9
C19-C11-C10	111.82(11)	C19-C11-H11	107.9	C19-C11-C12	111.82(11)
O2-C12-C11	120.31(12)	O2-C12-C13	119.83(12)	C13-C12-C11	119.85(11)
C14-C13-C12	118.32(12)	C18-C13-C12	122.87(12)	C18-C13-C14	118.80(13)
C13-C14-H14	119.8	C15-C14-C13	120.47(13)	C15-C14-H14	119.8
C14-C15-H15	119.9	C16-C15-C14	120.16(13)	C16-C15-H15	119.9
C15-C16-H16	120.1	C15-C16-C17	119.87(13)	C17-C16-H16	120.1
C16-C17-H17	119.9	C18-C17-C16	120.10(14)	C18-C17-H17	119.9
C13-C18-H18	119.7	C17-C18-C13	120.60(13)	C17-C18-H18	119.7
C11-C19-H19a	109.5	C11-C19-H19b	109.5	C11-C19-H19c	109.5
H19a-C19-H19b	109.5	H19a-C19-H19c	109.5	H19b-C19-H19c	109.5

This report has been created with Olex2 [6], compiled on 2018.05.29 svn.r3508 for OlexSys.

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6.3 Cartesian Coordinates from Computational Studies

[P] = $OP(O)(OMe)_2$.

1b (Bz–Cl)

C	-1.30636700	0.59815100	-0.00026400
O	-1.71947900	1.71394100	-0.00052900
C	0.12576100	0.20120800	-0.00023200
C	1.06742200	1.24706800	0.00021300
C	0.56542100	-1.13133400	-0.00047900
C	2.42996900	0.95969700	0.00040300
H	0.70835000	2.27730300	0.00040000
C	1.93158500	-1.41271200	-0.00027200
H	-0.16662900	-1.93821400	-0.00086200
C	2.86376000	-0.37085900	0.00016100
H	3.15787000	1.77400700	0.00067700
H	2.27015800	-2.45101700	-0.00052500
H	3.93299800	-0.59591000	0.00039400
Cl	-2.48307200	-0.78382400	0.00041000

1c (Bz–[P])

C	0.49871600	-0.68128600	0.10957700
O	0.14331200	-1.81639200	0.30892900
C	1.91274900	-0.23452400	0.02388700
C	2.91784500	-1.19685800	0.21013900
C	2.26029100	1.10043200	-0.23386300
C	4.25915100	-0.82564700	0.14150500
H	2.62268100	-2.22834300	0.40919700
C	3.60448100	1.46715400	-0.30274500
H	1.47245000	1.83921400	-0.38024200
C	4.60318600	0.50635600	-0.11489400
H	5.04068200	-1.57448100	0.28830500
H	3.87556700	2.50599100	-0.50386100
H	5.65527800	0.79672400	-0.16857400
O	-0.38562800	0.34219000	-0.07082400
P	-2.02732500	0.13395300	0.14869100
O	-2.41159600	-0.08782000	1.55708800
O	-2.45994100	-0.93911900	-0.94294600
O	-2.52952700	1.47563900	-0.56286800
C	-2.41009500	2.72303700	0.12395900
H	-1.37750500	3.10220100	0.05683000
H	-3.08991400	3.42861100	-0.37089300
H	-2.69271300	2.61470100	1.18235900
C	-2.83743700	-2.27247800	-0.56257400
H	-1.94333600	-2.90862700	-0.52692200
H	-3.32018000	-2.26783900	0.42513800
H	-3.53941000	-2.63054700	-1.32668900

MeCN

C	0.00000000	0.00000000	0.28058300
N	0.00000000	0.00000000	1.43863300
C	0.00000000	0.00000000	-1.17865400
H	0.00000000	1.03201200	-1.56066700
H	0.89374800	-0.51600600	-1.56066700
H	-0.89374800	-0.51600600	-1.56066700

Bz•

C	-2.02113800	-0.51908100	0.00001400
O	-2.92116000	0.25631800	-0.00006000
C	-0.56650800	-0.24102300	0.00002400
C	-0.09916600	1.08681200	0.00004400
C	0.34344500	-1.30814600	0.00007200
C	1.27088800	1.33687200	0.00002400
H	-0.82549300	1.90247400	0.00000900
C	1.71529500	-1.05229600	-0.00002900
H	-0.03988200	-2.33092100	0.00003300
C	2.17662600	0.26783400	-0.00003700
H	1.63984800	2.36533500	0.00002600
H	2.42711100	-1.88073900	-0.00011900
H	3.25103800	0.46747400	-0.00013300

Cl•

Cl	0.00000000	0.00000000	0.00000000

[P]•

O	1.48969600	0.15576100	-0.40926300
C	2.21936300	-0.97164200	0.08241600
P	-0.02152600	0.45431200	-0.01139600
H	3.22411100	-0.91207500	-0.35449600
H	1.73359000	-1.90994300	-0.22389100
H	2.29781200	-0.93569800	1.18043200
O	-0.70034400	-0.97839100	-0.28011600
O	-0.24694800	0.93282900	1.42437600
O	-0.59022000	1.57647100	-0.88319600
C	-2.09021700	-1.17146900	0.00628700
H	-2.32190300	-2.21949300	-0.22163700
H	-2.29797100	-0.96259500	1.06674400
H	-2.70509400	-0.50956200	-0.62282800

Cl^-

Cl	0.00000000	0.00000000	0.00000000

$[P]^-$

O	-1.47303800	-0.09346800	-0.51793000
C	-2.01774300	1.10369600	-0.03758700
P	0.01336600	-0.55980100	0.08863800

H	-3.07993800	1.15738600	-0.34118800
H	-1.49280800	1.98857600	-0.45182300
H	-1.95138300	1.16319800	1.06431100
O	0.89567600	0.67216400	-0.67836800
O	0.06274200	-0.27147900	1.56953700
O	0.34653100	-1.87849500	-0.53339800
C	2.08419600	1.07544600	-0.06544600
H	2.42092600	2.02445500	-0.52502300
H	1.94853100	1.22641500	1.02164800
H	2.90018700	0.33235500	-0.19801400

int1(*triplet*)

C	-2.48632100	-0.66744600	-0.30477700
C	-3.64432600	-1.41317800	-0.66819400
C	-2.49973200	0.65155800	0.24744100
C	-3.52076100	-2.67684700	-1.20195400
H	-4.63308400	-0.97442200	-0.52669000
N	-1.23176500	-1.22890500	-0.49190300
C	-3.67397000	1.38807700	0.57590900
N	-1.25577600	1.22262500	0.47244700
C	-2.22485100	-3.23132600	-1.38904800
H	-4.41170300	-3.24481600	-1.48152600
C	-1.13605600	-2.45693400	-1.01738200
C	-3.57634200	2.65217100	1.11398300
H	-4.65459700	0.94187800	0.40429800
C	-1.18548200	2.45097100	1.00124200
H	-2.08096600	-4.22784600	-1.80904700
H	-0.11601400	-2.83773900	-1.14013600
C	-2.29099800	3.21647900	1.34051000
H	-4.47965500	3.21305200	1.36690600
H	-0.17259300	2.83968200	1.15458500
H	-2.16763500	4.21374300	1.76524600
Ni	0.27617400	0.00290000	0.01277000
N	1.53506800	-1.38066800	0.50554900
N	1.53770500	1.39641500	-0.44421600
C	2.13715000	-2.27815300	0.92860300
C	2.14381000	2.29850300	-0.85146200
C	2.86397200	-3.40952100	1.48516000
C	2.87593000	3.43555600	-1.38915300
H	3.34695200	-3.12620200	2.43346000
H	2.17158500	-4.24329000	1.67983200
H	3.64079600	-3.75461100	0.78515700
H	2.17208800	4.21890500	-1.71095000
H	3.47926000	3.12771400	-2.25743800
H	3.54840300	3.85981100	-0.62733100

int1(*OSS*)

Ni	0.85640500	0.00275200	0.00159900
N	-0.66211200	1.23477400	0.45128800
N	-0.65702800	-1.23304500	-0.45526600
C	-1.91058600	0.67818000	0.22285200
C	-0.58077800	2.50450700	0.87433400
C	-1.90786600	-0.68015500	-0.23077700
C	-0.57061800	-2.50254700	-0.87805100
C	-3.07742600	1.46094200	0.44871400
C	-1.67923600	3.31247300	1.12072000
H	0.43519300	2.88531800	1.02607500
C	-3.07164800	-1.46644800	-0.46012300
C	-1.66586600	-3.31389500	-1.12754200
H	0.44695600	-2.88015300	-1.02717100
C	-2.96941300	2.75962300	0.89585800
H	-4.06084300	1.02889200	0.25791900
H	-1.54741900	4.33453300	1.47903600
C	-2.95840500	-2.76490500	-0.90662300
H	-4.05694100	-1.03730600	-0.27246000
H	-1.52991400	-4.33552300	-1.48555700
H	-3.86687100	3.35865600	1.06909300
H	-3.85353600	-3.36665900	-1.08243600
N	2.09538100	1.33601100	-0.60138700
C	2.72176500	2.20399700	-1.05150500
N	2.09331500	-1.32980000	0.61074300
C	2.71549500	-2.20011100	1.06218300
C	3.47180000	-3.29433900	1.65266600
H	4.27750900	-3.62051200	0.97638800
H	3.92182400	-2.98054900	2.60783200
H	2.80749600	-4.15136600	1.84429200
C	3.48378300	3.29492100	-1.64073000
H	2.80728900	3.98874200	-2.16402900
H	4.02600600	3.85565600	-0.86311700
H	4.21546800	2.90574100	-2.36597900

int1$_{mono_sol}$(*triplet*)

Ni	-0.79843000	0.87295700	-0.00006400
N	-0.32239900	-1.03849800	-0.00000900
N	1.09947400	1.17046100	-0.00003800
C	1.05213200	-1.21894000	-0.00000800
C	-1.13009800	-2.10819500	0.00000400
C	1.82814600	-0.01636900	-0.00000500
C	1.75949100	2.34513500	-0.00000600
C	1.57959100	-2.53981100	-0.00000700
C	-0.67418700	-3.41598600	0.00001700
H	-2.20356400	-1.88989700	0.00000300
C	3.24804400	0.04007700	0.00004300
C	3.13749000	2.45365600	0.00004700

H	1.13261600	3.24245500	-0.00003100
C	0.73163900	-3.62610300	0.00000600
H	2.66017400	-2.68860000	-0.00002000
H	-1.37829300	-4.24902300	0.00003100
C	3.90060000	1.25300400	0.00006900
H	3.81986700	-0.88880900	0.00006600
H	3.61274600	3.43521900	0.00006900
H	1.13849400	-4.64014400	0.00000600
H	4.99235200	1.29115800	0.00010900
N	-2.62651000	0.98500900	-0.00003000
C	-3.78893500	0.99877200	0.00003900
C	-5.24289500	1.01337100	0.00009400
H	-5.63243100	0.50178600	0.89442500
H	-5.61348900	2.05037900	0.00035000
H	-5.63250400	0.50219800	-0.89444100

int1$_{mono_sol}$(*OSS*)

Ni	-0.80151700	0.87150100	0.00002700
N	-0.32043700	-1.04218300	-0.00007800
N	1.09792600	1.17296600	0.00009900
C	1.05376800	-1.21793600	0.00003400
C	-1.12543600	-2.11257400	-0.00013800
C	1.82769200	-0.01294700	0.00006500
C	1.75654100	2.34807500	-0.00000900
C	1.58504100	-2.53741400	0.00010100
C	-0.66652900	-3.42013000	-0.00008300
H	-2.19940900	-1.89650800	-0.00022900
C	3.24740100	0.04474600	0.00003400
C	3.13458800	2.45820800	-0.00009900
H	1.12875800	3.24472500	0.00001500
C	0.73934600	-3.62574800	0.00004200
H	2.66588500	-2.68389800	0.00021000
H	-1.36840600	-4.25497400	-0.00013700
C	3.89884100	1.25841000	-0.00005200
H	3.82028100	-0.88346300	0.00006500
H	3.60873500	3.44028700	-0.00019200
H	1.14914400	-4.63866000	0.00010500
H	4.99055800	1.29754800	-0.00008200
N	-2.62833300	0.98244700	-0.00006400
C	-3.79120600	0.99582800	-0.00007700
C	-5.24514900	1.01043100	0.00008300
H	-5.63552900	0.49954200	0.89457000
H	-5.61529700	2.04762900	0.00007500
H	-5.63574000	0.49944900	-0.89425200

int1$_{none_sol}$(*triplet*)

Ni	0.00000000	-1.86982800	-0.00013700

N	1.34833000	-0.53765600	0.00012600
N	-1.34833000	-0.53765500	0.00009300
C	0.71814100	0.70664000	0.00007100
C	2.69255700	-0.60627100	0.00006400
C	-0.71814100	0.70664100	-0.00005000
C	-2.69255700	-0.60627100	0.00029000
C	1.52437200	1.87816700	0.00013100
C	3.51446200	0.50484200	0.00000300
H	3.11829200	-1.61463800	0.00010900
C	-1.52437100	1.87816800	-0.00033600
C	-3.51446200	0.50484300	0.00025100
H	-3.11829200	-1.61463800	0.00044100
C	2.89871000	1.78618300	0.00007800
H	1.04541000	2.85759500	0.00030900
H	4.59866100	0.38871100	-0.00004900
C	-2.89870900	1.78618400	-0.00016100
H	-1.04540900	2.85759500	-0.00077300
H	-4.59866100	0.38871200	0.00046200
H	3.50890100	2.69213200	0.00014300
H	-3.50890000	2.69213200	-0.00039000

int1$_{\text{none_sol}}$(*OSS*)

Ni	-0.00000300	-1.87223700	-0.00006000
N	1.35063600	-0.53705400	-0.00028700
N	-1.35063500	-0.53705100	0.00037700
C	0.71862900	0.70544300	-0.00003100
C	2.69383300	-0.60489700	-0.00014600
C	-0.71862600	0.70544400	0.00002600
C	-2.69383200	-0.60489300	0.00030600
C	1.52326700	1.87821800	0.00012900
C	3.51541500	0.50725700	0.00010700
H	3.12029400	-1.61295100	-0.00018800
C	-1.52326300	1.87822000	-0.00022500
C	-3.51541300	0.50726100	0.00001600
H	-3.12029400	-1.61294700	0.00043800
C	2.89783000	1.78728300	0.00014600
H	1.04369000	2.85730100	0.00037700
H	4.59968700	0.39230500	0.00027100
C	-2.89782600	1.78728700	-0.00017600
H	-1.04368500	2.85730200	-0.00058900
H	-4.59968500	0.39231100	-0.00007000
H	3.50674900	2.69415000	0.00030500
H	-3.50674400	2.69415400	-0.00040000

TS2(*OSS*)

C	0.65221600	-1.36292200	-1.56817000
O	0.84203600	-1.19701500	-2.72388400

C	0.12466000	-2.38077000	-0.69268200
C	-0.78857900	-3.29826100	-1.29484700
C	0.34746000	-2.46293100	0.71181800
C	-1.46195500	-4.22830800	-0.51863100
H	-0.94517800	-3.25077200	-2.37352100
C	-0.35514500	-3.40014400	1.46848600
H	1.11197400	-1.85987000	1.19553400
C	-1.26618000	-4.27944300	0.87320600
H	-2.15016600	-4.92813900	-0.99908800
H	-0.16397500	-3.45796500	2.54249700
H	-1.80242900	-5.01264100	1.47878700
O	1.61030400	-0.22185300	-0.50945800
P	3.06447300	-0.30995500	0.08974000
O	3.96717200	-1.39507700	-0.34194500
O	2.85324400	-0.32509200	1.71060200
O	3.59590600	1.20634200	-0.19809700
C	4.99209700	1.47119700	-0.07560800
H	5.19535400	2.41160800	-0.60612200
H	5.27943500	1.58207200	0.98401000
H	5.58003600	0.65500800	-0.52171500
C	2.09816000	0.69128300	2.35610200
H	2.54538300	1.68506200	2.19150800
H	1.05833600	0.71180100	1.98588400
H	2.09616000	0.46588600	3.43134600
Ni	-0.34270200	-0.00478700	-0.14324700
N	-0.51443300	1.96025600	-0.09940600
N	-2.28175800	0.05278400	0.10127600
C	-1.80968900	2.38943700	-0.04237900
C	0.48002700	2.85243400	-0.26980400
C	-2.79676100	1.32258400	0.10930600
C	-3.11116300	-0.99678900	0.25334800
C	-2.11304700	3.75950400	-0.13675200
C	0.24336700	4.21570400	-0.36262500
H	1.48969700	2.43748900	-0.33551900
C	-4.17889600	1.53050100	0.25864200
C	-4.48149000	-0.85381100	0.40920300
H	-2.64391200	-1.98211500	0.24314900
C	-1.08482000	4.67890200	-0.29133200
H	-3.14931600	4.09627600	-0.09691100
H	1.07866000	4.90530800	-0.49351400
C	-5.02831800	0.44302700	0.40908000
H	-4.57915000	2.54452000	0.26144200
H	-5.11019300	-1.73756600	0.52628500
H	-1.30670900	5.74546300	-0.36566800
H	-6.10305700	0.59504700	0.52743500

int3(*CSS*)

Ni	0.48756400	-0.20626400	0.09034000
N	1.93513900	1.14457600	-0.26952100
N	1.99580700	-1.39219600	0.24910100
C	3.13547900	0.57497200	-0.49851600
C	1.77428300	2.46760000	-0.38986200
C	3.17144500	-0.87171400	-0.19926300
C	1.96441100	-2.67168400	0.65734700
C	4.23186800	1.33258200	-0.92036300
C	2.83352300	3.28860000	-0.78724900
H	0.78848500	2.86633000	-0.12134500
C	4.32301800	-1.65708900	-0.29844500
C	3.07929700	-3.50503300	0.59038800
H	1.01541400	-3.01097900	1.07174400
C	4.07078600	2.71111400	-1.07285000
H	5.19532400	0.86314700	-1.11866800
H	2.67761800	4.36561900	-0.86616100
C	4.27658900	-2.99505500	0.08900700
H	5.25108500	-1.22022700	-0.66579600
H	2.99717600	-4.53814400	0.93108400
H	4.91162300	3.32730200	-1.39902500
H	5.16690200	-3.62279400	0.01421400
C	-0.84363600	-1.43191600	0.59986900
O	-0.75347900	-1.98402800	1.68494100
C	-2.05444200	-1.64117100	-0.25636300
C	-3.23507500	-2.11615700	0.33259500
C	-2.02455700	-1.37990700	-1.63216700
C	-4.37558100	-2.31633400	-0.44376300
H	-3.23540000	-2.30697500	1.40710800
C	-3.15823900	-1.60083800	-2.41430800
H	-1.11025800	-0.98796000	-2.08024100
C	-4.33762300	-2.06171500	-1.81932400
H	-5.29971300	-2.66860500	0.02135200
H	-3.12938200	-1.40141600	-3.48848300
H	-5.23140400	-2.21851800	-2.42877200
O	-0.85033900	0.99837400	-0.37845900
P	-1.63647100	1.89647400	0.62430800
O	-0.90732700	3.12119100	1.08975500
O	-2.17793700	0.97922700	1.84886000
O	-3.06345100	2.17685200	-0.09005700
C	-1.53244100	0.99560000	3.11573300
C	-3.12885800	2.37754500	-1.49093700
H	-0.90891800	0.09306300	3.22334200
H	-0.91429400	1.89997800	3.22552200
H	-2.30868700	0.98814700	3.89592900
H	-2.79482400	1.48025300	-2.03515400
H	-4.17935200	2.58518100	-1.74033300
H	-2.51395600	3.23890300	-1.80701900

int3(*triplet*)

Ni	-0.36765500	-0.16231400	-0.63637100
N	-1.32518800	-1.31067200	0.71296000
N	-2.26498200	0.10418200	-1.29713200
C	-2.65556700	-1.07378300	0.74906300
C	-0.73271200	-2.04830300	1.66219900
C	-3.17684800	-0.25180900	-0.36153400
C	-2.63973700	0.84315400	-2.34928300
C	-3.44833300	-1.60077400	1.77604100
C	-1.46806900	-2.60529200	2.70835200
H	0.35488900	-2.17690500	1.56164400
C	-4.51709600	0.14312800	-0.48403700
C	-3.95212900	1.25795600	-2.54161800
H	-1.85055900	1.11289200	-3.05665900
C	-2.84512000	-2.37450100	2.76495500
H	-4.52056200	-1.40940800	1.80482000
H	-0.95998300	-3.20597500	3.46423200
C	-4.90770600	0.90213700	-1.58133600
H	-5.24384700	-0.13413400	0.27861100
H	-4.21690900	1.85082600	-3.41820300
H	-3.44717000	-2.79338300	3.57443700
H	-5.94720200	1.21916200	-1.68810000
C	-0.52060000	1.51220700	0.46923000
O	-1.53626400	1.69424800	1.11626500
C	0.59789200	2.51273400	0.52529200
C	0.47104300	3.65542600	1.33619500
C	1.76997500	2.31637600	-0.21699100
C	1.50439400	4.58597800	1.40124000
H	-0.45176600	3.78218800	1.90644300
C	2.80859200	3.24815000	-0.14603700
H	1.88240100	1.42467100	-0.83278600
C	2.67711700	4.38164800	0.65962200
H	1.40550300	5.47335100	2.03209700
H	3.72360900	3.07847500	-0.71828200
H	3.49025200	5.11029800	0.71573400
O	1.33764300	-0.81814700	-1.20383300
P	2.50495600	-1.44805500	-0.40855000
O	2.20533600	-2.09464300	0.91205800
O	3.60669100	-0.26321000	-0.31595200
O	3.28207800	-2.47346200	-1.41160200
C	4.75257900	-0.44011300	0.50466400
C	2.81608300	-3.80812300	-1.51777000
H	5.19087300	0.55341200	0.67535700
H	4.47630200	-0.89177800	1.47064200
H	5.49359800	-1.08598400	0.00394400
H	1.87612200	-3.85732500	-2.09618200

H	3.58571000	-4.38922600	-2.04620100
H	2.64350200	-4.24557300	-0.52068800

int4(*CSS*)

Ni	0.03488900	-0.27133700	-0.74500900
N	1.81368100	-1.09883100	-0.15367700
N	0.96287500	1.35440400	-0.22278600
C	2.63034900	-0.21935000	0.46180700
C	2.10916300	-2.40242500	-0.15700400
C	2.18435700	1.18350100	0.35455600
C	0.52700600	2.60498200	-0.45608400
C	3.79483400	-0.64217800	1.11354000
C	3.25761100	-2.89699300	0.46121100
H	1.37925800	-3.03497800	-0.67240400
C	2.95903000	2.27417200	0.76015700
C	1.25265000	3.73298000	-0.07999200
H	-0.42902500	2.67942900	-0.97718800
C	4.11016900	-2.00076600	1.11036900
H	4.44155900	0.07344900	1.62104200
H	3.47270400	-3.96649600	0.43437600
C	2.48517300	3.56787000	0.55255200
H	3.93413300	2.11018800	1.21807100
H	0.84699300	4.72406600	-0.28870900
H	5.01244100	-2.35518500	1.61352900
H	3.07765600	4.43058700	0.86387700
C	-1.65552100	0.51645500	-0.92690200
O	-1.87105600	1.39458200	-1.74349200
C	-2.73784700	0.11803600	0.04530100
C	-3.94443200	0.83664300	0.03552000
C	-2.55742800	-0.90794300	0.98400600
C	-4.95320000	0.53622900	0.94921300
H	-4.06300300	1.62925500	-0.70605800
C	-3.56687400	-1.20860000	1.89941600
H	-1.63537900	-1.48971700	0.96316000
C	-4.76483800	-0.48752700	1.88516200
H	-5.89110800	1.09754300	0.93399900
H	-3.42310600	-2.01513900	2.62277400
H	-5.55535800	-0.72597200	2.60156100
Cl	-0.78784200	-2.12563400	-1.57303300

int4(*triplet*)

Ni	0.22212200	-0.33744600	1.28782200
N	0.44178100	1.39478900	0.28848300
N	1.97821000	-0.70343800	0.35654900
C	1.49449900	1.44460600	-0.55731500
C	-0.38029500	2.44258900	0.41412400
C	2.32006000	0.22060300	-0.57360200

C	2.60796300	-1.88504400	0.38473800
C	1.73262800	2.58305600	-1.33800100
C	-0.20519900	3.60483300	-0.33203300
H	-1.17890800	2.32722300	1.15082600
C	3.35270900	-0.02154700	-1.48600900
C	3.64837400	-2.19146600	-0.48783400
H	2.25544400	-2.60403700	1.12639000
C	0.86921700	3.67099300	-1.22637200
H	2.58556500	2.62225000	-2.01550700
H	-0.89427400	4.44165700	-0.20902300
C	4.03029900	-1.23919500	-1.43728500
H	3.61292900	0.72496100	-2.23640900
H	4.14284500	-3.16194400	-0.42562300
H	1.03784400	4.56806000	-1.82585800
H	4.83806800	-1.44783800	-2.14166400
C	-0.73245000	-1.55799900	0.04971200
O	-0.22847900	-2.60648200	-0.30811300
C	-2.04989000	-1.11298800	-0.52255000
C	-2.45754700	-1.60408200	-1.77414300
C	-2.86317300	-0.19898900	0.16350200
C	-3.65179700	-1.16590000	-2.34443100
H	-1.81681500	-2.32997900	-2.27989900
C	-4.07011200	0.22085500	-0.40022200
H	-2.55568500	0.14359400	1.15491300
C	-4.46041100	-0.25210000	-1.65706100
H	-3.96163200	-1.54027000	-3.32378400
H	-4.71167500	0.91804600	0.14474100
H	-5.39989300	0.08670800	-2.10152400
Cl	-0.84674000	0.17430100	3.15422300

int5

C	1.05754200	-1.75416300	-0.10429600
O	0.45062100	-2.79897900	-0.01030600
N	0.51597000	-0.47562200	-0.04431800
C	2.55400600	-1.60557600	-0.35259500
C	2.85510900	-0.16542000	0.04540600
H	2.72819100	-1.78460500	-1.42798500
H	3.11141400	-2.37119700	0.20373200
H	3.07921600	-0.10762800	1.12205100
H	3.69183000	0.29371800	-0.49876100
C	-0.86951600	-0.19110200	-0.04456200
C	-1.79330600	-1.07672300	0.53891800
C	-1.34048700	0.99680800	-0.63277400
C	-3.15398300	-0.76881100	0.52958200
H	-1.43861300	-2.00491300	0.97907900
C	-2.70417300	1.29427000	-0.62872400
H	-0.64610700	1.69191400	-1.10290300

C	-3.62041500	0.41519400	-0.04805700
H	-3.85840300	-1.46801900	0.98698500
H	-3.04958000	2.22265300	-1.09025400
H	-4.68720300	0.64972000	-0.04647100
C	1.52293700	0.58545700	-0.22704000
C	1.30632200	1.75909000	0.66636100
H	1.51676800	0.92524600	-1.28328100
H	0.97906200	1.54764200	1.68917600
C	1.78357800	3.11867600	0.30124800
H	1.24958700	3.90261200	0.86123500
H	2.86436900	3.26011400	0.51687400
H	1.65702000	3.31773200	-0.77760700

TS6

Ni	-1.52151600	0.34306200	0.05305900
C	0.98097700	-0.10679400	-1.96415600
N	-0.62144800	-1.03391700	1.12299600
N	-0.62301100	1.55244500	1.44837300
C	-2.54371200	-0.83580600	-0.98552100
C	3.82027800	1.65191700	-1.66712800
C	5.25477900	-0.73537700	-0.58919500
C	3.07388400	-1.71675000	-0.19867600
C	2.73345200	2.67606100	-1.96955100
H	0.56322300	2.48816300	-1.50206100
H	1.63920300	2.70021800	-0.10562200
C	1.14865300	0.08218300	-3.42895400
H	0.14518700	-0.71777200	-1.62061500
O	5.00302900	1.78249000	-1.91195200
C	5.84818400	-1.90471100	-0.11430000
H	5.86112000	0.09632300	-0.93633100
C	3.68575600	-2.87871700	0.27245000
H	1.98881200	-1.67727800	-0.25237700
H	3.11342600	3.68639000	-1.76471500
H	2.50617600	2.62515200	-3.04670300
H	0.60637400	0.98430100	-3.78233400
H	2.20636400	0.20490400	-3.71971500
H	0.73328900	-0.76961000	-3.98779200
C	5.07643900	-2.98520200	0.32215500
H	6.93914900	-1.96799000	-0.08905000
H	3.05799900	-3.71351100	0.59376800
H	5.55235600	-3.89813900	0.68715800
C	3.84923300	-0.62248400	-0.63413200
C	-0.57344900	-2.34419300	0.82274100
C	0.10601900	-0.58055700	2.18187700
C	0.16762900	-3.25903500	1.56679900
H	-1.12885300	-2.64988500	-0.06380100
C	0.87648000	-1.44617200	2.96252000

C	0.05067300	0.87821100	2.40210600
C	0.90567600	-2.80478300	2.65882200
H	0.16825000	-4.30980200	1.27389900
H	1.46723500	-1.05512600	3.78980700
C	0.64318800	1.54603100	3.47984000
C	1.55556600	2.24257300	-1.10388600
H	1.51125700	-3.49069800	3.25379300
C	0.52421100	2.93363300	3.55784000
H	1.18415100	0.99538400	4.24883200
C	-0.74536800	2.88116800	1.52033900
C	-0.18180500	3.61501200	2.56383000
H	0.97845100	3.47611400	4.38971700
H	-1.30545100	3.33566200	0.69726100
H	-0.29465900	4.69995500	2.58985600
N	3.21108000	0.55429100	-1.07294800
C	1.73978200	0.70791200	-0.96269500
H	1.44204300	0.39253500	0.04400000
O	-2.02285300	-1.65351600	-1.72623900
C	-4.03852000	-0.81976200	-0.81602200
C	-4.80550200	-1.79385900	-1.47603400
C	-4.67651200	0.11450900	0.01291100
C	-6.18843500	-1.83361900	-1.30795500
H	-4.28774900	-2.50838600	-2.11901300
C	-6.06089500	0.07398000	0.18203100
H	-4.08083100	0.89049600	0.49538000
C	-6.81822800	-0.89959100	-0.47661000
H	-6.78156500	-2.59140500	-1.82620100
H	-6.55350600	0.80883800	0.82338800
H	-7.90302000	-0.92893900	-0.34565100
Cl	-2.16378600	1.98424700	-1.26250700

int7

Ni	-1.01502200	0.40058100	0.20615000
C	0.46893600	-0.97097900	0.05541900
N	2.66676000	-1.55980000	-1.00645000
C	1.54560000	-1.75464800	-3.06788500
C	1.11487300	-0.44685800	-2.40846900
H	0.74564600	-2.51182600	-3.09012600
H	1.91884100	-1.64991800	-4.09636100
H	1.62462000	0.40764000	-2.87685800
H	0.03611400	-0.25710700	-2.47567000
C	3.55568300	-1.73679400	0.07716100
C	4.41469400	-2.85142900	0.15877400
C	3.59954400	-0.77815100	1.11028400
C	5.28380400	-2.98827400	1.24158800
H	4.39889600	-3.58841600	-0.63864400
C	4.47367800	-0.93172300	2.18604400

H	2.95366200	0.09605400	1.08760100
C	5.32374700	-2.03657600	2.26335200
H	5.94149000	-3.86052100	1.28155900
H	4.48318200	-0.17214600	2.97179000
H	6.00662200	-2.15421800	3.10777000
C	1.56621100	-0.56691100	-0.93661800
H	2.00201100	0.38537300	-0.62457700
O	3.40379300	-3.20883100	-2.47833500
C	2.66421700	-2.29044200	-2.18196700
N	-1.96007300	-0.59198300	1.78606300
N	-2.51277600	-0.62529100	-0.79769600
C	-3.00067200	-1.36803400	1.42107100
C	-1.57365600	-0.54916100	3.06387700
C	-3.35149100	-1.32947900	-0.01797700
C	-2.77612000	-0.47108000	-2.09581400
C	-3.68848600	-2.14476800	2.36063700
C	-2.21440200	-1.29349800	4.05633200
H	-0.72609000	0.10896200	3.26972600
C	-4.48776300	-1.94728100	-0.55813600
C	-3.87941700	-1.06033800	-2.70882100
H	-2.08459900	0.15957600	-2.65871700
C	-3.28826200	-2.10630100	3.69568300
H	-4.52057600	-2.77845500	2.05570000
H	-1.86829100	-1.23089500	5.08908600
C	-4.74765800	-1.81838900	-1.92041900
H	-5.16958100	-2.50950100	0.07880200
H	-4.05479600	-0.91781300	-3.77604900
H	-3.81091100	-2.70720400	4.44302700
H	-5.62765200	-2.29325500	-2.35926000
C	0.29314800	1.51642000	1.05350100
O	0.47893700	1.44550800	2.24664200
C	1.11097800	2.45114300	0.20622500
C	2.29789400	2.96189800	0.75699300
C	0.76959600	2.77275400	-1.11490800
C	3.14400100	3.76054800	-0.01127100
H	2.54090300	2.71022300	1.79086400
C	1.61171100	3.58026600	-1.87883300
H	-0.17649500	2.41524900	-1.52195700
C	2.80359300	4.06839000	-1.33256900
H	4.07208300	4.14416700	0.41918900
H	1.33559100	3.83475600	-2.90484000
H	3.46596900	4.69376900	-1.93617500
Cl	-2.31363700	2.25010600	-0.00903600
C	-0.10124000	-2.35820000	-0.23037600
H	-0.81945400	-2.66965700	0.54125400
H	-0.61640100	-2.42385700	-1.20056200
H	0.70019300	-3.11875700	-0.23279800

H	0.91007300	-0.99224200	1.06244400

TS8

C	-4.26660100	1.84579000	-0.60109300
O	-5.41046500	1.92357900	-0.19560200
N	-3.46747800	0.71393800	-0.61073500
C	-3.45137200	3.00195100	-1.16140900
C	-2.21177200	2.35666100	-1.77634100
H	-3.21721300	3.67544900	-0.32044300
H	-4.06816200	3.57641400	-1.86688500
H	-2.36368400	2.19743300	-2.85408200
H	-1.29578000	2.94555200	-1.66601900
C	-3.81439000	-0.53906400	-0.05283700
C	-4.88081300	-0.67595400	0.85790000
C	-3.05484700	-1.67910600	-0.38289800
C	-5.15925700	-1.91942900	1.42779200
H	-5.48972200	0.19172200	1.09586500
C	-3.34557100	-2.91310500	0.20095800
H	-2.22803200	-1.62568500	-1.09345500
C	-4.39538600	-3.04645700	1.11314600
H	-5.99157000	-2.00222100	2.13174300
H	-2.73824200	-3.77840500	-0.07846800
H	-4.62311800	-4.01544600	1.56395600
C	-2.08612500	0.97794500	-1.09213900
H	-1.81609800	0.22339900	-1.83910800
C	-1.10136400	0.87261500	0.08649300
Ni	0.63395000	-0.09235700	-0.76697400
N	1.09799800	-1.58230300	0.61528900
N	2.61741700	-0.33153400	-1.14030800
C	2.33045100	-2.10176800	0.43563800
C	0.20402600	-2.23797700	1.36136600
C	3.21291500	-1.34220100	-0.48004300
C	3.30172600	0.40834500	-2.01433200
C	2.70574600	-3.30175100	1.05198000
C	0.50136600	-3.43980200	2.00093000
H	-0.79286100	-1.79756700	1.43783800
C	4.56680400	-1.63260500	-0.68913200
C	4.64937700	0.17257900	-2.28036800
H	2.74186300	1.21645900	-2.49348700
C	1.78098200	-3.97597700	1.84743200
H	3.70025200	-3.71760900	0.89343900
H	-0.26362200	-3.94058900	2.59582600
C	5.29038000	-0.86603600	-1.60138800
H	5.05231100	-2.44185900	-0.14433200
H	5.18094400	0.79449600	-3.00205300
H	2.05297600	-4.91774100	2.32859600
H	6.34699300	-1.07755900	-1.77840000

C	0.84664300	1.69730000	-0.28450700
O	0.88520900	2.32354600	-1.33518100
C	1.53358900	2.19521300	0.94653700
C	2.00079900	3.51837400	0.95857700
C	1.77459700	1.36925400	2.05272900
C	2.68709800	4.01178100	2.06793000
H	1.81534400	4.14093900	0.08127100
C	2.46663600	1.86046600	3.15965600
H	1.41518600	0.34122900	2.03783000
C	2.92117200	3.18347700	3.17070500
H	3.04233300	5.04512100	2.07498300
H	2.65110800	1.21142700	4.01900700
H	3.45928400	3.56925100	4.04001500
Cl	-0.10311300	-1.57692400	-2.34454900
H	-1.20427200	-0.13980700	0.49750100
C	-1.40602900	1.84355400	1.22351000
H	-0.81258100	1.62931300	2.12049000
H	-1.22271400	2.89543400	0.95574800
H	-2.46677700	1.75240500	1.51101000

int9

C	-1.18120900	1.35279300	0.02785500
N	0.14782200	1.08712600	-0.02016000
C	-1.64632200	2.67656200	0.04511700
C	1.03842600	2.08774200	-0.05190000
Ni	0.59955100	-0.83328700	-0.03575300
C	-2.01963000	0.14894300	0.05775600
C	-0.72334200	3.71772000	0.01211900
H	-2.71539900	2.88716200	0.08395000
C	0.64730900	3.42224400	-0.03738400
H	2.08687200	1.77830300	-0.08983500
N	-1.31185800	-1.02430700	0.03198100
C	-3.41913500	0.15261700	0.10836500
H	-1.06629500	4.75450600	0.02479700
H	1.39797900	4.21358200	-0.06407100
C	-1.99491300	-2.19035800	0.05615100
C	-4.11230500	-1.05327800	0.13279200
H	-3.96021100	1.09924700	0.12847500
C	-3.37855100	-2.25163100	0.10592800
H	-1.38760600	-3.09862300	0.03394600
H	-5.20299400	-1.06572000	0.17201400
H	-3.87739600	-3.22203700	0.12349700
Cl	2.67796500	-1.37272500	-0.10855100

int9$_{\text{mono-sol}}$

C	-1.86150100	0.76282300	-0.18139500
N	-0.65333700	1.37715700	-0.21641300

C	-3.04407100	1.50545200	-0.03591700
C	-0.57532300	2.71114600	-0.10236800
Ni	0.90915400	0.13009400	-0.31017600
C	-1.79192500	-0.69782400	-0.30864400
C	-2.96558400	2.89047800	0.06598400
H	-4.01157400	1.00396300	-0.00077900
C	-1.70660000	3.50856300	0.03288400
H	0.44195600	3.11309100	-0.10036900
N	-0.52460700	-1.19340600	-0.43000700
C	-2.90811300	-1.54632000	-0.31307400
H	-3.87475900	3.48554000	0.17672800
H	-1.60434600	4.59172900	0.11817300
C	-0.36042500	-2.52503900	-0.56357500
C	-2.72926500	-2.91900000	-0.44273600
H	-3.91065600	-1.12856900	-0.21717700
C	-1.42221500	-3.41721700	-0.57249400
H	0.67206700	-2.85950400	-0.68016600
H	-3.58861500	-3.59236500	-0.44683100
H	-1.23135400	-4.48625600	-0.68172000
Cl	2.52429000	1.51268700	0.47224200
N	2.36192100	-1.19345900	-1.38510600
C	3.45210500	-0.81485800	-1.49999800
C	4.76460500	-0.19910300	-1.55134600
H	4.66428000	0.73963700	-0.97784200
H	5.51862400	-0.84439300	-1.07744000
H	5.06131000	0.01308400	-2.58895900

int9$_{\text{di-sol}}$

C	-1.96316000	0.79810500	-0.24255200
N	-0.78913600	1.47983400	-0.35322800
C	-3.18066700	1.48023300	-0.06745100
C	-0.79719000	2.82350300	-0.29043900
Ni	0.85329100	0.32217500	-0.43107900
C	-1.83438700	-0.65580000	-0.33801600
C	-3.18474100	2.86700400	-0.00651800
H	-4.11423600	0.92374800	0.01881300
C	-1.96387800	3.55599700	-0.12161700
H	0.18701300	3.28963300	-0.39482800
N	-0.56279600	-1.10397800	-0.53559400
C	-2.91087300	-1.55683100	-0.24804300
H	-4.12258400	3.41058500	0.12729200
H	-1.92199300	4.64598100	-0.08397100
C	-0.34064400	-2.42512800	-0.62734300
C	-2.67518400	-2.92010100	-0.35633200
H	-3.92385300	-1.18554100	-0.09144500
C	-1.35593400	-3.36771300	-0.54921600
H	0.70240400	-2.71464500	-0.77208000

H	-3.50170600	-3.63073600	-0.28876300
H	-1.12296400	-4.43045600	-0.63405100
Cl	2.39156100	2.13208500	-0.81913800
N	2.42331900	-1.02510200	-1.12255800
C	3.51316800	-0.75944000	-1.40899100
C	4.83257200	-0.25558500	-1.74350300
H	4.77970500	0.83413300	-1.57980600
H	5.60249800	-0.70022800	-1.09604400
H	5.07573800	-0.46182100	-2.79619900
N	1.38762500	-0.09646400	1.76638900
C	1.94941400	0.83101900	2.18213400
C	2.65227500	2.04103800	2.56846300
H	2.88007600	2.56405800	1.61976800
H	2.01630700	2.67330400	3.20547000
H	3.58254300	1.80239100	3.10461400

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C	2.83952700	-0.06072000	1.10395700
O	3.14327900	0.74303800	1.95982700
N	1.91194300	0.12793000	0.08446800
C	3.40575000	-1.47016200	0.95528700
C	3.01074600	-1.87204700	-0.46385100
H	2.94413200	-2.11212200	1.72617500
H	4.48680700	-1.45830800	1.15169000
H	3.77184100	-1.51455800	-1.17533600
H	2.90905100	-2.95331500	-0.61560800
C	1.21368800	1.34933800	-0.13128800
C	0.83667300	2.16535600	0.95122500
C	0.90748700	1.76841000	-1.43777400
C	0.16998300	3.37034700	0.72080500
H	1.08842300	1.86335900	1.96541500
C	0.23182500	2.96994900	-1.65501200
H	1.18568600	1.15169700	-2.29246400
C	-0.13962600	3.78013700	-0.57861300
H	-0.11305200	3.99292100	1.57364400
H	-0.00151400	3.27367200	-2.67870200
H	-0.66575600	4.72211100	-0.75169000
C	1.70221700	-1.09368200	-0.72138000
H	1.60605900	-0.84527000	-1.78726000
C	0.39167900	-1.82684100	-0.30705900
H	0.33061200	-1.80998500	0.78970100
C	-0.82804400	-1.12719200	-0.93216600
O	-0.81070000	-0.88400900	-2.12586500
C	-2.05090000	-0.83017000	-0.11403400
C	-3.14766700	-0.24983900	-0.78001000
C	-2.16022200	-1.10174000	1.26116200
C	-4.31975200	0.05102200	-0.09112500

H	-3.04716000	-0.04242800	-1.84673500
C	-3.33727800	-0.80190500	1.95170000
H	-1.32872100	-1.54751300	1.80845300
C	-4.41747300	-0.22536600	1.27843200
H	-5.16250700	0.50411800	-0.61930900
H	-3.40892400	-1.01727900	3.02060200
H	-5.33665600	0.01078400	1.82093900
C	0.32561100	-3.29257300	-0.78289200
H	-0.66760200	-3.72152100	-0.57598000
H	0.49316000	-3.35459300	-1.86933500
H	1.06653900	-3.92344100	-0.27135500

TS10

Ni	1.28093100	-0.22647100	0.17540400
C	-0.86844000	0.64601800	-2.25508100
N	1.04079200	1.60120900	0.83689200
N	0.01554300	-0.61773700	1.74541400
C	2.63284600	0.18231500	-1.06038000
C	-1.15821700	-0.42388100	-3.24442500
H	0.13846400	1.07489700	-2.25080600
H	-0.60320200	-1.35100400	-2.99578300
H	-2.22730800	-0.67830000	-3.29098000
H	-0.82404000	-0.12719600	-4.25372000
C	1.53795800	2.71009300	0.26077000
C	0.21530900	1.73856600	1.91206400
C	1.27290500	3.99073000	0.73945700
H	2.14596300	2.55252800	-0.62950600
C	-0.08993100	2.99654500	2.44026800
C	-0.34564500	0.47968800	2.44120400
C	0.44984300	4.13933700	1.85526100
H	1.70848100	4.85239000	0.23169700
H	-0.75578200	3.07966000	3.29830700
C	-1.19368100	0.38748300	3.54957200
H	0.21982100	5.12791000	2.25745400
C	-1.66569300	-0.86881500	3.93237700
H	-1.48543400	1.27731300	4.10653200
C	-0.42344600	-1.82294400	2.11507000
C	-1.27409900	-1.99413700	3.20687700
H	-2.33584100	-0.96377300	4.78931100
H	-0.07848500	-2.65077700	1.49055500
H	-1.62994300	-2.99178800	3.46691700
O	2.44865300	0.93743900	-2.00085700
C	4.00701900	-0.37884400	-0.81191900
C	5.05589700	-0.00606100	-1.66841900
C	4.27355300	-1.22522400	0.27403200
C	6.34929000	-0.47348200	-1.44318300
H	4.82523300	0.65274400	-2.50791400

C	5.56906300	-1.69029700	0.50212000
H	3.45152000	-1.53874300	0.91893800
C	6.60818800	-1.31582100	-0.35527300
H	7.16073600	-0.18464000	-2.11606600
H	5.76892700	-2.35439200	1.34652600
H	7.62207200	-1.68389000	-0.17837300
Cl	1.19795600	-2.25496500	-0.67197900
C	-3.99834900	1.48838700	-1.53308500
O	-5.19593500	1.36627400	-1.69202700
N	-3.10724800	0.50884900	-1.11806700
C	-3.19663400	2.76862600	-1.75261500
C	-1.92201200	2.53483400	-0.94752600
H	-2.98439000	2.85946200	-2.83128300
H	-3.79489000	3.63951000	-1.45275800
H	-2.08319100	2.80219500	0.10944000
H	-1.04803700	3.08875000	-1.31366500
C	-3.42456500	-0.81830400	-0.75442500
C	-4.75704900	-1.24171600	-0.57400700
C	-2.38542100	-1.74478300	-0.55144900
C	-5.02266900	-2.55721000	-0.19222000
H	-5.56603300	-0.53829700	-0.74974000
C	-2.67081100	-3.05831700	-0.18008400
H	-1.34398500	-1.47187700	-0.69981700
C	-3.98909300	-3.47714900	0.00827500
H	-6.06256600	-2.86618100	-0.05727400
H	-1.83774100	-3.75520100	-0.05986100
H	-4.21081600	-4.50814900	0.29375600
C	-1.72153700	1.00714700	-1.07364700
H	-1.25368000	0.61978900	-0.15381600

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C	-3.07398900	-0.69390900	-0.52376600
O	-4.05049000	0.01887500	-0.44630600
N	-1.74868400	-0.27965200	-0.44137100
C	-3.08122800	-2.20459100	-0.73106000
C	-1.63116900	-2.55988400	-1.06633400
H	-3.44495800	-2.67583800	0.19620200
H	-3.80344200	-2.45585200	-1.52072000
H	-1.50109900	-2.61690900	-2.15795800
H	-1.30643100	-3.52405100	-0.64980000
C	-1.36845100	1.08905700	-0.34363200
C	-2.09486000	1.97765900	0.46705300
C	-0.27124300	1.57244700	-1.07490400
C	-1.72142500	3.31998100	0.54051500
H	-2.95616200	1.61507200	1.02466000
C	0.10085400	2.91578900	-0.98649200
H	0.29654600	0.90402300	-1.72384100

C	-0.62212400	3.79734900	-0.17967800
H	-2.29543900	3.99887700	1.17635100
H	0.96024500	3.27244400	-1.55998100
H	-0.33208500	4.84873700	-0.11280200
C	-0.78079600	-1.38124300	-0.51932800
H	0.00325600	-1.13376100	-1.24908800
C	-0.07347400	-1.70708100	0.83840900
C	0.95631200	-0.63855200	1.23804300
C	-1.04370200	-1.96558300	1.99257600
H	0.49407500	-2.63208200	0.63830400
O	0.74772600	0.09292500	2.18580500
C	2.24308500	-0.51359700	0.46112100
H	-1.64842400	-1.07383600	2.20731200
H	-1.71516900	-2.80771500	1.77026900
H	-0.49147500	-2.20800900	2.91189800
C	3.04511100	0.61377400	0.71767700
C	2.69305700	-1.46500100	-0.47125000
C	4.25760500	0.79066300	0.05439300
H	2.68661800	1.34079400	1.44851100
C	3.91215900	-1.29058900	-1.13301800
H	2.10630700	-2.36131600	-0.68007200
C	4.69467900	-0.16220000	-0.87411800
H	4.86833100	1.67334600	0.26063100
H	4.25286900	-2.04157500	-1.85017000
H	5.64692600	-0.02612300	-1.39334600

intS1

C	0.13439500	-0.17721400	0.64017100
O	0.05700000	-1.23148600	1.24764200
N	-0.91507100	0.72539600	0.54634300
C	1.41923700	0.32580400	0.00692300
C	2.57625600	-0.67132000	0.10422800
H	1.67755100	1.28316800	0.49038100
H	1.19924900	0.58826700	-1.04432500
H	2.76105200	-0.90775900	1.16343100
H	2.26027700	-1.61964800	-0.36534500
C	-2.15395100	0.37525800	0.17758200
C	-2.52021900	-0.91838200	-0.32723300
C	-3.17607900	1.37588700	0.26624900
C	-3.82613100	-1.17285700	-0.71013700
H	-1.76202100	-1.69901300	-0.38064900
C	-4.47570600	1.10193600	-0.12351300
H	-2.88394000	2.35464000	0.65051700
C	-4.81015300	-0.17240100	-0.61398300
H	-4.09582600	-2.16142000	-1.08939500
H	-5.24353300	1.87551100	-0.04990600
H	-5.83639800	-0.38696300	-0.92080500

C	3.82912500	-0.16285200	-0.54790600
C	4.98575100	0.07082900	0.08274100
H	3.76712200	0.04078000	-1.62652800
H	5.03953200	-0.13099400	1.16131600
C	6.23856900	0.58615400	-0.55942900
H	7.07373600	-0.12603800	-0.43750500
H	6.09913500	0.76625100	-1.63668500
H	6.56699500	1.53228500	-0.09420600

TS-S2

C	1.37194800	1.71977000	-0.80560200
N	0.57032300	-0.48634600	0.58661800
C	2.85535400	-0.87365600	-0.05563700
C	2.95422900	0.44262100	0.71875800
H	3.11544700	-0.74145100	-1.11967400
H	3.52858600	-1.65536600	0.32688600
H	3.01353200	0.23420100	1.79673000
H	3.86037500	1.00710100	0.44337900
C	-0.78761100	-0.40349600	0.36282300
C	-1.42398300	-0.92494300	-0.79035600
C	-1.57130900	0.29325600	1.31127600
C	-2.79359600	-0.75094000	-0.97139400
H	-0.83354900	-1.48640700	-1.51300600
C	-2.93689000	0.47213900	1.11345100
H	-1.07526100	0.68726600	2.20053900
C	-3.55629700	-0.04964400	-0.02912400
H	-3.27512700	-1.16577500	-1.86051400
H	-3.52675600	1.01618400	1.85518600
H	-4.62936300	0.08602500	-0.18250500
C	1.70840200	1.25919800	0.45091100
H	1.22953200	1.74234700	1.30720300
O	1.09554500	-2.49206300	-0.42217400
C	1.41872800	-1.38880300	-0.01268100
C	0.16330000	2.54232500	-1.09012800
H	-0.63833500	1.90833000	-1.51775600
H	-0.24265400	3.00605900	-0.17869900
H	0.36918800	3.33252300	-1.83203000
H	1.93411800	1.34291600	-1.66845300

intS3

Ni	-1.27581000	0.98956800	-0.02348600
C	0.18108200	-0.38766200	0.31296700
N	2.08243400	-1.56330900	-0.80606500
C	0.53109000	-1.72805600	-2.56378900
C	0.73728100	-0.25921900	-2.20535400
H	-0.45155600	-2.11062900	-2.24127300
H	0.64093700	-1.97101500	-3.62958800

H	1.50617800	0.18474200	-2.85579900
H	-0.15878800	0.36626300	-2.28900500
C	3.18786600	-1.78912800	0.04436600
C	3.58847500	-3.09286700	0.39230900
C	3.91859700	-0.69763000	0.55087500
C	4.68726200	-3.28619900	1.23076600
H	3.04392400	-3.94098000	-0.01383100
C	5.01075000	-0.90686500	1.39185500
H	3.63973900	0.32302700	0.29329500
C	5.40441000	-2.20116700	1.74065200
H	4.98243500	-4.30632100	1.48956800
H	5.56013600	-0.04284600	1.77424500
H	6.26065400	-2.36161900	2.39961400
C	1.26977200	-0.31940100	-0.76580400
H	1.92728500	0.52964600	-0.56954400
O	1.99489700	-3.58736700	-1.95433400
C	1.61577600	-2.44900900	-1.76420900
N	-2.44418800	0.20697900	1.56483000
N	-2.56132700	-0.35191200	-1.00364800
C	-3.12670800	-0.91236600	1.24553900
C	-2.37464700	0.59772700	2.84144900
C	-3.24309200	-1.19224500	-0.20526000
C	-2.72077600	-0.40852300	-2.32703100
C	-3.72744300	-1.70445900	2.23109100
C	-2.96878600	-0.12776600	3.87587200
H	-1.79836300	1.50858500	3.01505100
C	-4.06275500	-2.19357700	-0.74361700
C	-3.51901000	-1.37371300	-2.93875100
H	-2.20742000	0.36627000	-2.89986800
C	-3.64422000	-1.30713400	3.56491300
H	-4.25632600	-2.61825000	1.96233000
H	-2.88827100	0.22944800	4.90362600
C	-4.18647600	-2.29397600	-2.12814800
H	-4.61414700	-2.87152300	-0.09312800
H	-3.61514900	-1.39560900	-4.02519600
H	-4.10640300	-1.91138200	4.34851400
H	-4.81713200	-3.06949500	-2.56794700
C	-0.11107700	2.23596600	0.83745300
O	-0.34043500	2.54890400	1.98179100
C	1.09670600	2.76556800	0.12351900
C	2.24799300	2.98515400	0.89901600
C	1.14628400	2.96955100	-1.26245300
C	3.44619700	3.35752300	0.28883400
H	2.18804200	2.84188100	1.97931600
C	2.34080900	3.36480300	-1.86562500
H	0.23642800	2.83421600	-1.84702800
C	3.49570500	3.54343000	-1.09665100

H	4.34343400	3.50572400	0.89465800
H	2.37197800	3.53168700	-2.94494700
H	4.43338900	3.83475100	-1.57607800
C	0.75115000	-0.49562100	1.72019700
H	1.29556100	-1.44427300	1.86279100
H	1.46266300	0.31268500	1.94329200
H	-0.03654600	-0.45855100	2.48552500
H	-0.43093100	-1.28537100	0.11839600
Cl	-2.19979300	2.69515400	-1.19498500

TS-S4

C	-4.04264100	1.83739200	-0.82814800
O	-5.14219700	2.20701400	-0.46616100
N	-3.47684700	0.58276800	-0.63435400
C	-3.03294700	2.68016400	-1.60113400
C	-2.05981600	1.64879600	-2.16393300
H	-2.54662500	3.38180600	-0.90134800
H	-3.56142500	3.28664400	-2.34937900
H	-2.46728900	1.22233400	-3.09395700
H	-1.05571700	2.03168000	-2.36175800
C	-4.13805600	-0.54631500	-0.09391300
C	-5.32289500	-0.40963600	0.65634700
C	-3.61334100	-1.83746000	-0.30233300
C	-5.95611500	-1.53894000	1.17772400
H	-5.74088700	0.58116900	0.80857000
C	-4.25887700	-2.95349100	0.23037300
H	-2.68974400	-1.99054100	-0.86057800
C	-5.43381500	-2.81800300	0.97356000
H	-6.87489900	-1.40865200	1.75566400
H	-3.82802300	-3.94264600	0.05489700
H	-5.93524600	-3.69633600	1.38680400
C	-2.06602700	0.54499800	-1.09349100
H	-1.84445100	-0.42613600	-1.54202200
C	-1.11350500	0.80016800	0.10419100
Ni	0.74154800	-0.27766900	-0.58578000
N	1.78039500	-1.47630100	0.79729900
N	2.61628600	-0.18118200	-1.34052300
C	3.04814500	-1.73574600	0.41212500
C	1.23167200	-2.21597200	1.76777000
C	3.54540000	-0.93887100	-0.73000700
C	2.93775600	0.55838900	-2.40487500
C	3.81088000	-2.73273600	1.03443800
C	1.92518600	-3.22465400	2.43231600
H	0.19719100	-1.99024600	2.02155400
C	4.86909200	-0.95987100	-1.18707800
C	4.23030700	0.57630600	-2.92528100
H	2.13108100	1.16646400	-2.81976900

C	3.24540900	-3.48275100	2.06186100
H	4.82881800	-2.93465300	0.70333400
H	1.43013000	-3.79542400	3.21918200
C	5.21252400	-0.19441600	-2.29995400
H	5.62365500	-1.55870200	-0.67819600
H	4.45758400	1.18951900	-3.79845500
H	3.82286100	-4.26745700	2.55491900
H	6.23899900	-0.19784000	-2.67257700
C	0.67166600	1.59582800	-0.20802900
O	0.75999800	2.19513800	-1.27855300
C	1.17926000	2.24919900	1.04797800
C	1.28290700	3.65081000	1.04822100
C	1.57530900	1.53739000	2.18815400
C	1.74912900	4.32616200	2.17476000
H	0.99164500	4.19014200	0.14500700
C	2.05286500	2.21332200	3.31340300
H	1.53354300	0.45127200	2.18538900
C	2.13433700	3.60808000	3.31249400
H	1.81561000	5.41691400	2.16769600
H	2.36434300	1.64698700	4.19441900
H	2.50148000	4.13629200	4.19579400
H	-1.28795600	1.83560800	0.43387300
C	-1.36812500	-0.08570200	1.32091500
H	-2.36515400	0.11606500	1.74317800
H	-1.34113800	-1.14989500	1.05573400
H	-0.64100200	0.11783300	2.11862100
Cl	-0.09859300	-2.13213600	-1.62204300

TS-S5

C	-4.22548100	2.41574400	-1.07262100
O	-5.42807500	2.58869000	-1.12297800
N	-3.56303200	1.21134800	-0.88166800
C	-3.17706400	3.51235700	-1.19969100
C	-1.87189100	2.76726800	-1.45591700
H	-3.16597000	4.07917600	-0.25407800
H	-3.47610200	4.21216700	-1.99239300
H	-1.71949600	2.62043900	-2.53490200
H	-0.97567300	3.26645200	-1.07249800
C	-4.16674400	-0.05339100	-0.71098000
C	-5.56772700	-0.22090400	-0.75607300
C	-3.36405900	-1.19068000	-0.49179700
C	-6.12891500	-1.48692700	-0.58811500
H	-6.19679800	0.64887200	-0.91938700
C	-3.94505600	-2.44794200	-0.31832600
H	-2.28296500	-1.12777800	-0.40275700
C	-5.33007300	-2.61199800	-0.36597100
H	-7.21678800	-1.58814800	-0.62713500

H	-3.28871000	-3.30020800	-0.12505500
H	-5.78091800	-3.59727700	-0.22626700
C	-2.08002500	1.39130400	-0.79270300
H	-1.59876700	0.60821700	-1.39307400
C	-1.59146200	1.27414400	0.62048400
H	-1.47497300	0.26636300	1.01119900
Ni	1.25280900	-0.62325400	0.09034300
N	1.43112700	-1.25196300	-1.89445900
N	3.29396600	-0.68723700	-0.12317600
C	2.67048300	-1.09190600	-2.39891000
C	0.39461900	-1.48694200	-2.69876500
C	3.72841900	-0.81081500	-1.39558100
C	4.15024700	-0.44734200	0.87433000
C	2.89912900	-1.18117500	-3.77687200
C	0.54420700	-1.59122000	-4.08143100
H	-0.57817000	-1.59558500	-2.21198600
C	5.08863200	-0.67709100	-1.69766000
C	5.51797800	-0.30607900	0.64579300
H	3.70479100	-0.37535300	1.87008500
C	1.82087800	-1.43368100	-4.62496800
H	3.90004600	-1.04565500	-4.18599000
H	-0.32388300	-1.78574000	-4.71292100
C	5.98993900	-0.41935100	-0.66470600
H	5.44228000	-0.77526600	-2.72373700
H	6.19435300	-0.11062700	1.47916200
H	1.97726800	-1.50134600	-5.70366800
H	7.05449100	-0.31047800	-0.88262200
C	-1.64462200	2.39345100	1.59786600
H	-1.20833000	3.32610200	1.20408800
H	-2.69180700	2.62585300	1.88664400
H	-1.10726900	2.13118300	2.51973000
O	1.24501600	-1.07073700	2.34329700
P	-0.06593900	-1.83396400	2.17188500
O	-0.46858500	-1.90723700	0.68681900
O	-1.20627600	-1.16260500	3.08487100
O	-0.02375700	-3.32899200	2.80359400
C	-2.51818200	-1.73398000	3.10229200
C	0.75782500	-4.31630100	2.14600800
H	-3.23233100	-0.91850500	3.27849100
H	-2.74793200	-2.20705400	2.13630900
H	-2.59182300	-2.47900300	3.90953200
H	1.81454800	-4.00450600	2.08300300
H	0.69196600	-5.23852200	2.73960300
H	0.37898700	-4.50408700	1.12795400
C	1.15428700	1.31805000	-0.39231600
O	0.92840700	1.63756500	-1.55094500
C	1.60401100	2.36483400	0.59117100

C	1.90777100	3.65892200	0.13609200
C	1.71594400	2.06591400	1.95712800
C	2.31531700	4.64323600	1.03477000
H	1.81218600	3.86323000	-0.93276200
C	2.12075200	3.05548200	2.85661200
H	1.46550900	1.06254300	2.31232800
C	2.42127500	4.34198500	2.39882900
H	2.54986500	5.64986100	0.67834400
H	2.19522600	2.82256300	3.92183500
H	2.73689200	5.11439900	3.10508900

intS6

C	3.56988800	-3.18258200	0.31021200
O	4.65012300	-3.58837700	0.69497900
N	3.26522800	-1.91310800	-0.15159800
C	2.29767200	-4.02030300	0.25422600
C	1.32898400	-3.19631800	-0.59032400
H	1.94589400	-4.17996900	1.28589100
H	2.53963900	-5.00967100	-0.15890400
H	1.39312600	-3.49508100	-1.64714700
H	0.28247700	-3.31092800	-0.28793500
C	4.19078700	-0.87098900	-0.39302700
C	5.54845800	-0.99150300	-0.02958400
C	3.76787900	0.30716700	-1.04206600
C	6.45032000	0.02686200	-0.33836600
H	5.87998600	-1.89178100	0.47883100
C	4.69001200	1.30541600	-1.35596800
H	2.72399900	0.48607800	-1.29056200
C	6.03678600	1.17898500	-1.01192200
H	7.49784200	-0.09208100	-0.04885700
H	4.33342400	2.19807000	-1.87531400
H	6.75223400	1.96667400	-1.26002900
C	1.81993800	-1.74215500	-0.44532400
H	1.73014700	-1.22259100	-1.40416300
C	1.13499300	-0.89800100	0.63260700
H	1.76164800	-0.00771400	0.76380600
Ni	-0.49237100	0.19768100	0.14749600
N	-1.98372900	1.31120400	-0.79294500
N	-2.24362900	-0.10254900	1.42802700
C	-3.23348800	1.21886500	-0.30939300
C	-1.73580000	1.95512300	-1.93735700
C	-3.36290900	0.49166300	0.97597400
C	-2.25725300	-0.70579400	2.61646800
C	-4.31003400	1.79844500	-0.99307300
C	-2.75717000	2.55970400	-2.66913600
H	-0.68460700	1.97822000	-2.23466800
C	-4.56016000	0.44011500	1.70198700

C	-3.40308700	-0.78911200	3.40760800
H	-1.31666900	-1.14680100	2.94388100
C	-4.06485300	2.47454400	-2.18748600
H	-5.32561700	1.71455000	-0.60844300
H	-2.52575400	3.08042900	-3.59946300
C	-4.58116300	-0.21503000	2.93105900
H	-5.46126400	0.91901400	1.32108000
H	-3.36368700	-1.29536900	4.37322100
H	-4.89146400	2.92823600	-2.73875400
H	-5.50369400	-0.26421000	3.51341300
C	1.00262200	-1.55616000	1.99395900
H	0.29875300	-2.40534900	2.00664100
H	1.97771900	-1.94178100	2.34363200
H	0.67968000	-0.81288100	2.73698200
O	-0.04280900	1.64431300	1.55117700
P	0.91204800	2.47923500	0.69161600
O	0.95489900	1.98765800	-0.74935100
O	2.34268400	2.49375300	1.42825000
O	0.55357000	4.06969400	0.76623100
C	3.38552500	3.35731200	0.98932500
C	-0.57958300	4.55806800	0.07484600
H	4.34036800	2.88323700	1.25141800
H	3.35607100	3.50075600	-0.10078300
H	3.29853900	4.33659600	1.48659900
H	-1.50015200	4.03903500	0.39401900
H	-0.67718700	5.62755400	0.31029600
H	-0.46620300	4.43749000	-1.01547900
C	-0.86173500	-1.01978500	-1.28174800
O	-0.33566400	-0.84781000	-2.35562800
C	-2.06179800	-1.91597500	-1.15116600
C	-2.98301000	-1.93575600	-2.20937400
C	-2.30863100	-2.68659500	-0.00882000
C	-4.15076500	-2.69332000	-2.11012200
H	-2.76820100	-1.34272800	-3.10064800
C	-3.46169000	-3.46633300	0.07984800
H	-1.58763700	-2.67440000	0.80686100
C	-4.39174200	-3.46006200	-0.96521100
H	-4.87273300	-2.69319200	-2.93050400
H	-3.63978400	-4.07581400	0.96887600
H	-5.30267400	-4.05885200	-0.88950600

TS-S7

C	3.68970600	2.96952400	-0.63864000
O	4.81919400	3.10423800	-1.06735600
N	3.20452000	1.92284900	0.12921300
C	2.54827600	3.95379600	-0.86617200
C	1.45900000	3.52033200	0.11185300

H	2.23967900	3.87999700	-1.92088400
H	2.92121100	4.97606500	-0.71170200
H	1.54160700	4.09353800	1.04732500
H	0.44117600	3.66913600	-0.26426200
C	3.95661000	0.83225100	0.62819800
C	5.29407400	0.61802000	0.23483300
C	3.37372800	-0.05861600	1.55335500
C	6.02252800	-0.44161800	0.77601700
H	5.74892700	1.29809500	-0.47920900
C	4.12071000	-1.11068500	2.08361300
H	2.33249300	0.03076300	1.85502900
C	5.44970700	-1.31122800	1.70761900
H	7.05941100	-0.58325800	0.45988600
H	3.63680900	-1.78886200	2.79033300
H	6.02800400	-2.13835600	2.12595500
C	1.75578700	2.03572700	0.41035400
H	1.60904300	1.83604700	1.47425400
C	0.98285700	0.98464100	-0.41806700
H	1.53744800	0.05371000	-0.26286700
Ni	-0.66461400	-0.45852100	-0.23741600
N	-2.07266000	-1.43852800	0.84918800
N	-2.41902600	-0.00775900	-1.31421700
C	-3.35449700	-1.14720900	0.56604600
C	-1.74795100	-2.12865700	1.94561500
C	-3.55090800	-0.41193200	-0.70629500
C	-2.47995400	0.55168300	-2.52314800
C	-4.38709600	-1.55364100	1.41885700
C	-2.72540500	-2.57994400	2.83256000
H	-0.67614500	-2.29995700	2.07803100
C	-4.80573600	-0.18668000	-1.28551500
C	-3.68865000	0.79447000	-3.17427000
H	-1.52585600	0.81956800	-2.97886700
C	-4.06336100	-2.27965800	2.56534600
H	-5.42435900	-1.30160100	1.19947300
H	-2.43749500	-3.14685200	3.71922100
C	-4.87385700	0.43425100	-2.53118400
H	-5.71543000	-0.50977300	-0.78020600
H	-3.69358300	1.25734500	-4.16214300
H	-4.85211300	-2.60542800	3.24701300
H	-5.84206800	0.61786200	-3.00185900
C	0.93497000	1.29441300	-1.91030200
H	0.31009800	2.16807700	-2.15530900
H	1.95099100	1.51159000	-2.28583600
H	0.58037000	0.42327700	-2.47696900
O	-0.15096900	-1.75250900	-1.87975000
P	0.90699600	-2.47461800	-1.04724100
O	0.83659300	-2.06435900	0.42537600

O	2.34567900	-2.18999900	-1.70870400
O	0.82176600	-4.09412700	-1.19683300
C	3.53139400	-2.68360800	-1.08646000
C	-0.25380200	-4.76778200	-0.56625000
H	4.36242100	-2.03866500	-1.40100900
H	3.44863300	-2.63589500	0.00820700
H	3.72156700	-3.72221200	-1.40186900
H	-1.22727900	-4.38167200	-0.91562600
H	-0.17848900	-5.83255000	-0.82888200
H	-0.20334300	-4.65885900	0.53030900
C	-0.57083100	0.89027300	1.09431000
O	-0.07545000	0.57009900	2.16048600
C	-1.63409400	1.95025400	1.04003600
C	-2.38155600	2.16997900	2.20881300
C	-1.95030900	2.67644300	-0.11510000
C	-3.43661700	3.08266300	2.21314200
H	-2.11315600	1.60760400	3.10480000
C	-2.99447000	3.60107700	-0.10891900
H	-1.37081200	2.51526700	-1.02013900
C	-3.74660200	3.80067100	1.05343200
H	-4.01704600	3.24039400	3.12565500
H	-3.22454800	4.16659200	-1.01504100
H	-4.57015700	4.51891900	1.05632900

intS8

C	-1.32606300	1.40422300	-0.03679500
N	0.01418100	1.34145800	-0.22604600
C	-1.97718600	2.64224400	0.06590100
C	0.74167700	2.46285800	-0.31442600
Ni	0.73126600	-0.50041500	-0.36394500
C	-1.97660400	0.08745600	0.04733800
C	-1.22553800	3.81064400	-0.02825300
H	-3.05581700	2.69117900	0.21742300
C	0.16065500	3.72393900	-0.22109300
H	1.81487600	2.31066800	-0.46104700
N	-1.12172900	-0.97141200	-0.09080600
C	-3.34637400	-0.11116100	0.25982000
H	-1.71458300	4.78411700	0.04883000
H	0.77963100	4.61933900	-0.29696800
C	-1.61760600	-2.22321600	-0.00270600
C	-3.85191400	-1.40570600	0.33811900
H	-4.01177900	0.74619700	0.36605800
C	-2.96321000	-2.48532800	0.20682100
H	-0.88656500	-3.02893600	-0.10139400
H	-4.91752100	-1.57530600	0.50295800
H	-3.31229900	-3.51745500	0.26907100
O	2.67380800	-0.12367500	-0.46433200

P	3.23348200	-1.48603000	-0.88683500
O	3.96848700	-1.76640200	-2.14963000
O	1.75277500	-2.34759400	-0.88223100
O	3.97705600	-2.08050500	0.42920900
C	1.47483800	-3.33410000	-1.87046600
C	4.74874200	-3.26673400	0.31839900
H	2.25544000	-3.31451700	-2.64543100
H	1.43776000	-4.33358300	-1.40558400
H	0.49776400	-3.11513900	-2.32927200
H	5.43346000	-3.30100800	1.17808700
H	4.10056200	-4.16145600	0.34736300
H	5.32618700	-3.27569300	-0.61915000

TS-S9(*OSS*)

Ni	-0.25523600	-0.08341800	-0.38358900
C	-2.11432400	-0.87100500	0.76832400
O	-2.16229800	-1.64810900	1.66739100
C	-2.25535700	0.55315000	0.61248900
C	-2.15989400	1.33648500	1.80984200
C	-2.36563300	1.23367200	-0.64385400
C	-2.14702600	2.71387700	1.74304200
H	-2.08510500	0.81691500	2.76630600
C	-2.36750300	2.63658900	-0.66961400
H	-2.59355500	0.66770100	-1.54547500
C	-2.24312800	3.38125300	0.49940800
H	-2.06864800	3.29499800	2.66508200
H	-2.48704600	3.14386300	-1.63040200
H	-2.23883900	4.47242400	0.46193200
N	1.22505400	1.18507200	-0.42446000
C	2.41253400	0.65930700	0.02866900
C	1.17870500	2.49419500	-0.75068900
C	2.36275100	-0.75140500	0.39201300
C	3.56281800	1.46384000	0.12510500
C	2.27629000	3.33297400	-0.67445700
H	0.20684800	2.86423600	-1.08173600
N	1.13617800	-1.33507800	0.25190600
C	3.45726000	-1.50333900	0.86033800
C	3.50525900	2.80258100	-0.22861300
H	4.49704400	1.03126300	0.48398100
H	2.17891200	4.38196300	-0.95827500
C	0.96841300	-2.62935700	0.56808200
C	3.28024200	-2.84022100	1.18540300
H	4.43687700	-1.03697600	0.96659700
H	4.39355900	3.43319200	-0.15770500
C	2.00630300	-3.42024600	1.04044600
H	-0.04178600	-3.02306200	0.43282200
H	4.12188700	-3.43273900	1.55052200

H	1.82469500	-4.46627200	1.29094600
Cl	-1.96920200	-1.75859200	-1.14261400

TS-S9(*triplet*)

Ni	-0.21303800	-0.44550800	-0.27601200
C	-1.63253900	-1.80099100	0.96239500
O	-1.53303700	-2.13250800	2.10535400
C	-2.31208400	-0.69197700	0.32380400
C	-3.01391200	0.21983200	1.18610800
C	-2.34604800	-0.45685400	-1.09233200
C	-3.71857000	1.27929500	0.65862300
H	-2.99708600	0.02995800	2.26068300
C	-3.06380700	0.64799500	-1.59137300
H	-2.02724400	-1.23446100	-1.78671700
C	-3.74375400	1.51239000	-0.74167100
H	-4.27043600	1.94463200	1.32803600
H	-3.11198900	0.79658500	-2.67337400
H	-4.31257800	2.35210600	-1.14713400
N	0.40566600	1.44197600	-0.04206200
C	1.76771300	1.55992600	0.05746000
C	-0.34817100	2.55652200	0.01332300
C	2.50519500	0.30424600	-0.01327400
C	2.36898000	2.82503500	0.21551700
C	0.18280200	3.82777400	0.17256300
H	-1.42414400	2.40825200	-0.07901600
N	1.73790400	-0.81115100	-0.22678900
C	3.90438300	0.19714600	0.12527300
C	1.58096900	3.96413000	0.27669700
H	3.45383600	2.90817200	0.28712300
H	-0.48032400	4.69357000	0.21310900
C	2.34223800	-2.01501000	-0.28804000
C	4.51499100	-1.04453700	0.04645000
H	4.50490000	1.09020900	0.30038100
H	2.03982700	4.94758100	0.40103800
C	3.71245400	-2.18346300	-0.16274700
H	1.67849300	-2.86916900	-0.43617800
H	5.59840800	-1.13547500	0.15195700
H	4.14487400	-3.18356300	-0.22333000
Cl	-0.92807200	-3.04933200	-0.39539800

intS10(*CSS*)

C	-3.03829500	-2.41305900	0.15408900
O	-4.13064600	-1.97064700	-0.15901200
N	-2.01615400	-1.74157100	0.80370200
C	-2.55776100	-3.83019600	-0.13056900
C	-1.32345800	-3.97530000	0.75136400
H	-2.31855000	-3.90621500	-1.20494800

H	-3.37167000	-4.54047100	0.07116000
H	-1.62338200	-4.27876300	1.76729600
H	-0.59348300	-4.70642300	0.38526200
C	-2.09184500	-0.43196500	1.32210900
C	-3.21378000	0.39351100	1.09982800
C	-1.01901300	0.08075800	2.07972700
C	-3.23532900	1.69691500	1.59664400
H	-4.05077000	0.00345500	0.52977600
C	-1.06373600	1.38529100	2.57353000
H	-0.13304600	-0.51628100	2.29005400
C	-2.16190000	2.21098400	2.32969000
H	-4.11287300	2.31920800	1.40116300
H	-0.20991400	1.75523700	3.14644700
H	-2.18543600	3.23443500	2.71106100
C	-0.75537300	-2.54040900	0.79482200
H	-0.20804000	-2.38217900	1.73389600
C	0.16256500	-2.16370600	-0.38742000
H	-0.43237400	-2.25720900	-1.31531800
Ni	0.55254300	-0.23477000	-0.31540500
N	-1.07874900	0.44428100	-1.44961000
N	0.79455500	1.75429400	-0.14699000
C	-1.30575000	1.76744900	-1.29471900
C	-1.98573200	-0.29775800	-2.08984300
C	-0.25040600	2.50500600	-0.57126000
C	1.79341800	2.35478700	0.51935000
C	-2.47180800	2.36846300	-1.78112000
C	-3.18120300	0.22089600	-2.58150600
H	-1.75677000	-1.35806400	-2.19491100
C	-0.30949300	3.88086200	-0.32261900
C	1.80124100	3.71784800	0.80182300
H	2.61500300	1.71656300	0.84348400
C	-3.42679200	1.58373400	-2.42289100
H	-2.64566400	3.43388600	-1.63891400
H	-3.90345300	-0.44241500	-3.05767700
C	0.72610200	4.49761000	0.37332100
H	-1.16369600	4.46390700	-0.66307500
H	2.63934200	4.15062200	1.35001000
H	-4.35389600	2.03138500	-2.78667400
H	0.69200400	5.56926100	0.57986800
C	1.33123500	-3.14483400	-0.52333800
H	1.90276000	-3.23763800	0.41378400
H	1.00460700	-4.16293600	-0.80513300
H	2.03901300	-2.81514800	-1.29791500
C	2.01703300	-0.67156200	0.75315600
O	1.95491600	-0.91019800	1.95363400
C	3.39026100	-0.62154600	0.10753600
C	4.53629000	-0.83930000	0.88712200

C	3.53278300	-0.34189800	-1.25811700
C	5.80410100	-0.77753900	0.30958500
H	4.39690000	-1.05677900	1.94845200
C	4.80033000	-0.27815200	-1.83975800
H	2.63133500	-0.17688400	-1.85564700
C	5.93786800	-0.49661800	-1.05583500
H	6.69429000	-0.94999900	0.92033500
H	4.90422400	-0.06144700	-2.90596100
H	6.93129600	-0.44942900	-1.50943100

intS10(*triplet*)

C	3.21507600	-2.54507700	-0.10548500
O	4.34009800	-2.12608800	0.07407600
N	2.16654800	-1.88055100	-0.73250900
C	2.69770600	-3.90812000	0.33769100
C	1.40723400	-4.08028100	-0.45322400
H	2.52300700	-3.86699900	1.42663400
H	3.46513500	-4.67350000	0.15966400
H	1.63090700	-4.49033400	-1.45045800
H	0.67060500	-4.74046200	0.01893400
C	2.20915700	-0.56574200	-1.23500100
C	3.28135300	0.30691800	-0.95572700
C	1.12851400	-0.08734800	-2.00762700
C	3.24005300	1.62194600	-1.40935100
H	4.12111500	-0.05337200	-0.37091700
C	1.11353300	1.23970400	-2.45936200
H	0.31788100	-0.74791500	-2.31059100
C	2.15739800	2.10535600	-2.15530600
H	4.06823300	2.28867600	-1.15802800
H	0.25715100	1.58833800	-3.03995900
H	2.12951700	3.14518500	-2.48609400
C	0.89443100	-2.63280000	-0.61897600
H	0.31763900	-2.55707600	-1.55129100
C	0.04488000	-2.09929800	0.54747700
H	0.70305000	-1.93285600	1.41334900
Ni	-0.43812700	-0.15627300	0.17817300
N	0.99345800	0.79796600	1.34043900
N	-0.98747200	1.76311800	-0.16415000
C	0.96952800	2.17224600	1.15865600
C	1.99229000	0.24862700	2.05049400
C	-0.09893600	2.69196400	0.36843700
C	-1.98886600	2.19225300	-0.96099200
C	2.00520600	2.96508100	1.72680500
C	3.02066200	0.97031100	2.62525700
H	1.97378600	-0.83921100	2.15105200
C	-0.28429500	4.07159600	0.07768400
C	-2.20143500	3.51746800	-1.27911400

H	-2.64957000	1.42254700	-1.36428300
C	3.01997400	2.37790600	2.44771400
H	1.99866700	4.04434700	1.57588000
H	3.80744700	0.45821700	3.17900100
C	-1.31431000	4.48750300	-0.73313400
H	0.40446100	4.80246800	0.50119000
H	-3.03092800	3.79795900	-1.92865500
H	3.81827900	2.99048700	2.87273000
H	-1.44743400	5.54847700	-0.95540500
C	-1.07154300	-3.04423900	0.97993800
H	-1.69610400	-3.37609300	0.13604600
H	-0.66619400	-3.95068900	1.46265600
H	-1.74054900	-2.57164500	1.71396500
C	-1.90168500	-0.92661700	-0.79764400
O	-1.80049700	-1.35122000	-1.92631300
C	-3.22530000	-0.88407100	-0.09001500
C	-4.34258400	-1.47882700	-0.69685700
C	-3.36198500	-0.26712100	1.16186800
C	-5.57898200	-1.46067100	-0.05412600
H	-4.21355600	-1.94955700	-1.67342200
C	-4.60009700	-0.24591000	1.80373800
H	-2.50213500	0.22211500	1.62899000
C	-5.70842500	-0.84511100	1.19667800
H	-6.44755300	-1.92589900	-0.52633200
H	-4.70262600	0.24144600	2.77568600
H	-6.67855300	-0.83014100	1.69926800

intS11

C	3.32922200	-1.88671400	-0.06434900
O	4.24440700	-1.15952900	0.26000100
N	2.22596600	-1.53000200	-0.83954800
C	3.15446100	-3.33824500	0.34843600
C	2.01377700	-3.85169700	-0.52478300
H	2.91597700	-3.36088900	1.42563600
H	4.10564500	-3.87422600	0.22713900
H	2.41293100	-4.26960300	-1.46092800
H	1.40979800	-4.63228300	-0.04814900
C	1.98803200	-0.26946600	-1.40947900
C	2.83663100	0.83877500	-1.18042800
C	0.85350400	-0.08975000	-2.23532900
C	2.53998200	2.06947600	-1.75613400
H	3.71567300	0.71031100	-0.55630600
C	0.58327200	1.16092800	-2.81319700
H	0.21838200	-0.92522100	-2.51690000
C	1.41287200	2.24850500	-2.57320100
H	3.21041900	2.91133500	-1.56640200
H	-0.29279500	1.25677500	-3.45771700

H	1.20241400	3.22077200	-3.02233300
C	1.18900500	-2.58479600	-0.85559000
H	0.76856800	-2.68048300	-1.86634800
C	0.04048800	-2.29539200	0.12983200
H	0.44647100	-2.26720700	1.15683100
Ni	-0.42866400	-0.34050800	0.00971700
N	0.97234900	0.47072300	1.43489000
N	-0.88274800	1.67754200	-0.05821500
C	1.03487400	1.81983400	1.38994900
C	1.86547200	-0.20542300	2.15929400
C	-0.00787000	2.48905700	0.57581400
C	-1.85716700	2.20898800	-0.80883600
C	2.03322800	2.51673200	2.07650500
C	2.89879600	0.41518400	2.85869500
H	1.76276800	-1.29099300	2.17324000
C	-0.10722800	3.88050000	0.45968100
C	-2.01822900	3.58264000	-0.96505400
H	-2.53017200	1.51218500	-1.30929400
C	2.98330700	1.80475400	2.80960500
H	2.08460100	3.60337800	2.03356900
H	3.62203500	-0.18559000	3.41029100
C	-1.12205300	4.43349200	-0.31777100
H	0.60011700	4.53023600	0.97196900
H	-2.82949500	3.96843100	-1.58357800
H	3.78044800	2.33410600	3.33524200
H	-1.21076000	5.51732700	-0.41554100
C	-1.02931000	-3.37894200	0.06994100
H	-1.44132800	-3.49480900	-0.94378700
H	-0.61852500	-4.35889300	0.36585000
H	-1.86522300	-3.17294900	0.75158700
C	-1.99974600	-0.90485000	-0.91450500
O	-2.05181300	-1.07101400	-2.10338100
C	-3.18695400	-0.89958000	-0.01332500
C	-4.46475400	-1.09202800	-0.56457600
C	-3.04570100	-0.68705400	1.36764600
C	-5.58629600	-1.06961000	0.26235100
H	-4.55445100	-1.26017100	-1.63943600
C	-4.16793300	-0.66424900	2.19282200
H	-2.05275500	-0.54752400	1.81089100
C	-5.43881100	-0.85555600	1.63799400
H	-6.58043500	-1.22279300	-0.16294200
H	-4.05692200	-0.50275500	3.26682300
H	-6.31974000	-0.84083300	2.28362900

intS12(*CSS*)

C	-3.16272200	1.15269700	0.55062600
O	-3.13797300	2.37061300	0.58376600

N	-2.15823500	0.28351300	0.94455000
C	-4.32751300	0.31697300	0.03439700
C	-3.99937200	-1.09697700	0.50013300
H	-4.35569700	0.40524200	-1.06504000
H	-5.27182400	0.73171400	0.41381200
H	-4.37544600	-1.25108400	1.52410000
H	-4.41768200	-1.88794400	-0.13357300
C	-0.93029000	0.65933700	1.53033600
C	-0.51665900	2.00615600	1.59350100
C	-0.07494500	-0.32914000	2.05608400
C	0.72923700	2.33281100	2.12914100
H	-1.17654700	2.77837700	1.21130400
C	1.16750700	0.01607600	2.58790500
H	-0.34923600	-1.37986900	2.03099700
C	1.58859600	1.34605000	2.62058400
H	1.03065700	3.38343900	2.15550400
H	1.81431500	-0.78012400	2.96361200
H	2.56648100	1.61055700	3.02921400
C	-2.45638200	-1.11394900	0.51651500
H	-2.09652100	-1.82554300	1.27049600
C	-1.80187100	-1.44630100	-0.83688300
H	-2.14711800	-0.69430800	-1.56420400
Ni	0.13206800	-1.20011400	-0.71474700
N	0.17515000	0.68507800	-1.35715800
N	2.13278000	-0.82859100	-0.52003800
C	1.35362600	1.32609300	-1.12989400
C	-0.86090700	1.41739400	-1.79326200
C	2.46018900	0.46990200	-0.66995500
C	3.05961500	-1.70302700	-0.11066400
C	1.48828400	2.70496600	-1.31594500
C	-0.80566700	2.79435100	-1.98121800
H	-1.78808300	0.88408600	-1.98516500
C	3.75297600	0.93351100	-0.39928600
C	4.36947600	-1.31729000	0.16935100
H	2.70121700	-2.72750200	0.01592800
C	0.39483400	3.45638500	-1.73442700
H	2.44168500	3.18952500	-1.11230000
H	-1.70250500	3.32588700	-2.29991700
C	4.72030400	0.02608900	0.02549700
H	4.00050300	1.98803300	-0.51167700
H	5.09486200	-2.06265400	0.49932200
H	0.47916800	4.53743700	-1.86085200
H	5.73481000	0.36619900	0.24445700
C	-2.24287000	-2.80346700	-1.38564900
H	-2.12371800	-3.60435000	-0.64393000
H	-3.29851700	-2.78722000	-1.71646200
H	-1.63927900	-3.08981200	-2.26045000

Cl	0.34140200	-3.19668400	0.23087000

intS12(*triplet*)

C	-3.69042900	-1.56145500	-1.49780900
O	-4.79857500	-1.45923600	-1.99119000
N	-3.17788900	-0.84533400	-0.43237000
C	-2.60850200	-2.52205600	-1.98158100
C	-1.54761100	-2.50224600	-0.88313200
H	-2.23689500	-2.14546300	-2.94799300
H	-3.05842200	-3.50699600	-2.17094700
H	-1.71661300	-3.32849100	-0.17609800
H	-0.51907300	-2.60121100	-1.26023100
C	-3.85478700	0.14493300	0.31066200
C	-5.10848500	0.64887900	-0.09272200
C	-3.27333800	0.65121200	1.49347300
C	-5.74967100	1.62604500	0.66920900
H	-5.56726800	0.25467200	-0.99496300
C	-3.93074300	1.62886400	2.24083300
H	-2.30655500	0.29019700	1.84288100
C	-5.17190300	2.12689600	1.83829700
H	-6.72205500	1.99936100	0.33670200
H	-3.45855300	2.00043300	3.15403900
H	-5.68181100	2.89229800	2.42806000
C	-1.75016700	-1.15583200	-0.15524600
H	-1.63050200	-1.31116100	0.92234000
C	-0.80360400	-0.03311500	-0.58441800
H	-1.14589000	0.88951400	-0.08298400
Ni	0.99793600	-0.34414800	0.20721200
N	1.98114800	1.41002500	-0.24154000
N	2.99155500	-0.95535600	0.27957300
C	3.30979900	1.28859300	-0.46149100
C	1.36269400	2.56756400	-0.49831600
C	3.89250800	-0.01865700	-0.07484000
C	3.39378800	-2.14372700	0.73657200
C	4.05199000	2.35215100	-0.98932100
C	2.04052800	3.67517300	-1.00369900
H	0.29030200	2.59421500	-0.29275400
C	5.26675400	-0.28411300	-0.01922700
C	4.74332200	-2.48286400	0.81843800
H	2.59841900	-2.81700000	1.06683800
C	3.40868000	3.55831200	-1.26271900
H	5.11791200	2.23958800	-1.18667900
H	1.50175900	4.60464200	-1.19313300
C	5.69264700	-1.53586500	0.42389900
H	5.99440500	0.47894500	-0.29498800
H	5.04026100	-3.46407000	1.19176200
H	3.97075900	4.39931200	-1.67408700

H	6.75938000	-1.76340100	0.47827100
C	-0.77267400	0.22247300	-2.09280500
H	-0.36793500	-0.63197300	-2.66232200
H	-1.77722500	0.43656400	-2.50764100
H	-0.14296000	1.09235300	-2.34481000
Cl	0.56097000	-0.94497800	2.33249200

intS13(*CSS*)

C	-2.47092000	-2.67258200	0.80788400
O	-3.57968900	-2.33024900	1.18038400
N	-1.29028400	-1.96691900	0.94243200
C	-2.15587000	-3.96952500	0.07179200
C	-0.63451700	-4.06919500	0.12488000
H	-2.54051300	-3.88211000	-0.95884800
H	-2.69754200	-4.80103500	0.54369400
H	-0.32487000	-4.58650800	1.04690500
H	-0.19175300	-4.60538700	-0.72377800
C	-1.14375000	-0.71966800	1.58960800
C	-2.25007700	0.07650800	1.94658300
C	0.14912500	-0.23611500	1.86697700
C	-2.04640000	1.33049500	2.52430000
H	-3.25273400	-0.29565400	1.75863200
C	0.33845100	1.02369600	2.43592800
H	1.02308800	-0.83691900	1.63632900
C	-0.75865100	1.82163700	2.76290200
H	-2.91859800	1.93689600	2.78389400
H	1.36336600	1.37400200	2.57498800
H	-0.61438500	2.81370200	3.19653000
C	-0.17446000	-2.59565100	0.18204900
H	0.75776600	-2.51698100	0.75286800
C	0.04939400	-1.95087000	-1.19981300
H	-0.83345300	-2.16263000	-1.82582000
Ni	0.11721800	0.00013800	-1.04507700
N	-1.83573800	0.32800300	-1.25403300
N	0.07039500	2.03451100	-0.67518100
C	-2.24567300	1.58591400	-0.93321100
C	-2.77412800	-0.57872300	-1.56309300
C	-1.17480000	2.54219400	-0.59810500
C	1.11983700	2.79415600	-0.34155100
C	-3.60051700	1.92859400	-0.90644400
C	-4.13957900	-0.31486100	-1.53182000
H	-2.42078100	-1.57017500	-1.83218200
C	-1.40197200	3.86634100	-0.20838000
C	0.96980500	4.12207600	0.05983600
H	2.09705300	2.31236300	-0.34339100
C	-4.56473300	0.96747400	-1.19449100
H	-3.89838900	2.94154800	-0.64141000

H	-4.84484600	-1.11485600	-1.75747000
C	-0.31110800	4.66893700	0.11903300
H	-2.41391400	4.26393200	-0.14619100
H	1.85290300	4.70244700	0.33077400
H	-5.62677700	1.21682000	-1.15337600
H	-0.46484000	5.70425900	0.43107800
C	1.25168100	-2.56744100	-1.91248200
H	2.14809200	-2.56775400	-1.27991900
H	1.04989500	-3.61353900	-2.21176300
H	1.50058800	-2.01050400	-2.82734100
O	2.02109300	-0.02004500	-1.01801600
P	3.17744700	-0.08667100	-0.01137800
O	3.41045400	1.08108800	0.90345000
O	4.52553200	-0.46424200	-0.85078900
O	2.98150800	-1.49322900	0.80172300
C	5.32423000	0.58110300	-1.37971500
C	3.92727200	-1.82540800	1.81138900
H	5.50768800	1.35915000	-0.62098500
H	6.28108900	0.14082200	-1.69573100
H	4.84068200	1.04407200	-2.25816100
H	3.51973500	-2.67418500	2.37836100
H	4.88883300	-2.11492400	1.35715400
H	4.09117200	-0.97095700	2.48709700

intS13(*triplet*)

C	4.22487800	-1.91019000	0.09350600
O	5.43023500	-1.91378400	0.26234000
N	3.39569000	-0.80695500	0.04778400
C	3.35608600	-3.15053300	-0.10189800
C	1.99914600	-2.61338200	-0.55852800
H	3.30939800	-3.68135900	0.86234100
H	3.84770500	-3.82640300	-0.81623100
H	1.94201100	-2.61300800	-1.65763500
H	1.13989500	-3.19214300	-0.19435900
C	3.79849500	0.53933300	0.16670000
C	5.01728500	0.89529600	0.77585800
C	2.96146400	1.56101000	-0.33041500
C	5.37473200	2.23936900	0.89354200
H	5.67808000	0.11008100	1.13395700
C	3.33579300	2.89941300	-0.19925000
H	2.02640700	1.32616400	-0.84178500
C	4.53966400	3.25284800	0.41598500
H	6.32501000	2.49412300	1.37035000
H	2.67494500	3.67236300	-0.60210200
H	4.82812700	4.30223800	0.51337000
C	1.95502700	-1.15973500	-0.04786400
H	1.49718000	-0.51999900	-0.80575800

C	1.21526200	-0.94475700	1.27583500
H	1.44847100	0.08342400	1.60495700
Ni	-0.74718100	-0.92211100	0.95095800
N	-1.30604500	1.05978700	1.08861400
N	-2.82899600	-1.09901300	1.22989700
C	-2.63413500	1.28724100	1.10455500
C	-0.44855900	2.07554500	0.97617300
C	-3.48633000	0.07257900	1.13317100
C	-3.50485400	-2.24951400	1.20370500
C	-3.14027900	2.58914000	1.05199200
C	-0.87902100	3.40062100	0.90911000
H	0.60993200	1.82139300	0.92522600
C	-4.88216900	0.10669500	1.03295700
C	-4.89398200	-2.29843400	1.10338900
H	-2.90985800	-3.16512300	1.25858600
C	-2.24780900	3.65791300	0.95424400
H	-4.21389600	2.77141400	1.07627900
H	-0.14546100	4.20180000	0.81242000
C	-5.59179400	-1.09232100	1.02056600
H	-5.40962600	1.05573800	0.94715300
H	-5.41009700	-3.25932800	1.08483200
H	-2.62416700	4.68201300	0.90476300
H	-6.68055900	-1.08443500	0.93609200
C	1.64136000	-1.88679300	2.40684400
H	1.38499700	-2.94109600	2.20512000
H	2.73192900	-1.85266400	2.59893000
H	1.15180300	-1.61613600	3.35768500
O	-1.01671100	-1.24911200	-0.97284500
P	-1.03390500	-0.05037500	-1.93673100
O	0.00847200	1.02256400	-1.79083700
O	-2.54914100	0.55411700	-1.80449600
O	-1.10106700	-0.62504900	-3.45902000
C	-2.85964100	1.75996800	-2.48324700
C	0.11558400	-0.96812800	-4.10696700
H	-2.08166200	2.52047400	-2.30801800
H	-2.95118000	1.58637300	-3.56863600
H	-3.82311400	2.12273100	-2.09492200
H	0.55725600	-1.87757700	-3.66349200
H	-0.11617600	-1.16604300	-5.16312500
H	0.84622600	-0.14603400	-4.03684300

TS-S14

Ni	0.29530000	-0.82319000	0.48065600
C	-0.47506200	0.32800200	-1.92915900
N	-2.54910800	-0.21830500	-0.70507000
C	-3.33503100	1.80892900	-1.60468400
C	-2.82828500	0.93259000	-2.74639600

H	-2.65310700	2.64748600	-1.38340800
H	-4.33811200	2.23207000	-1.75012300
H	-3.66864400	0.40500700	-3.22461400
H	-2.28590800	1.48323000	-3.52677000
C	-2.06968800	-1.16929200	0.21346900
C	-2.47797400	-1.20485500	1.56181500
C	-1.10840100	-2.13557500	-0.23844500
C	-1.94253900	-2.15102300	2.44898000
H	-3.21647500	-0.48320100	1.89865800
C	-0.53038900	-3.02731300	0.69685800
H	-0.91208800	-2.27636000	-1.29904600
C	-0.95446700	-3.04198400	2.03757900
H	-2.28967600	-2.15581900	3.48409800
H	0.18804700	-3.77016400	0.34394900
H	-0.51436900	-3.75199100	2.74012600
C	-1.91000000	-0.09645700	-2.03761400
H	-1.97255100	-1.06343000	-2.56077500
O	-3.85610600	1.12133700	0.67729700
C	-3.32041400	0.89484800	-0.38852800
N	2.17434800	-0.77263000	-0.07143300
N	0.58773300	1.03903900	1.01611900
C	2.72707200	0.48908000	0.10526200
C	2.91274400	-1.75193800	-0.61293200
C	1.86454800	1.47263000	0.68823800
C	-0.29964000	1.90339900	1.53614100
C	4.07348600	0.71423300	-0.29773200
C	4.22430200	-1.58824600	-1.02600600
H	2.41026100	-2.71908800	-0.72286300
C	2.21881500	2.82735400	0.94007900
C	-0.01054900	3.23482000	1.78618200
H	-1.29383000	1.49977900	1.75199600
C	4.81322300	-0.30488700	-0.85668900
H	4.51772400	1.70075300	-0.16047200
H	4.77585100	-2.42024300	-1.46469000
C	1.29783100	3.69814300	1.48072500
H	3.22352500	3.17579500	0.69760700
H	-0.77024300	3.89341600	2.20803500
H	5.84598300	-0.12697900	-1.16551900
H	1.57305000	4.73846900	1.66982100
H	-0.28982900	1.26820500	-1.40338100
C	0.52559000	-0.12812600	-2.93191400
H	1.54950800	0.11555300	-2.61599000
H	0.47250300	-1.21938700	-3.09623100
H	0.36698100	0.34281800	-3.92583000

intS15

C	-3.86074300	0.63219700	-0.26648800

O	-4.11341500	1.82112500	-0.31150800
N	-2.83112600	0.02747500	0.44020500
C	-4.60955000	-0.45984500	-1.01675500
C	-4.13512100	-1.75927900	-0.37252200
H	-4.31464900	-0.38595300	-2.07711900
H	-5.69173800	-0.27626900	-0.96692500
H	-4.78993100	-2.01962200	0.47518400
H	-4.12147900	-2.61554000	-1.06038900
C	-1.79228600	0.69495000	1.10993000
C	-1.68202500	2.10185800	1.13664200
C	-0.79430500	-0.07191100	1.76803500
C	-0.59161300	2.70917400	1.76074000
H	-2.45429500	2.69433300	0.65471700
C	0.28714500	0.56387500	2.39546900
H	-0.90964300	-1.14814400	1.87703500
C	0.40675900	1.95141200	2.38275100
H	-0.52368000	3.79985300	1.75652000
H	1.04267600	-0.05056900	2.89030000
H	1.26086500	2.43914600	2.85694700
C	-2.71358500	-1.42428600	0.12995700
H	-2.52819700	-1.96984500	1.07011000
C	-1.56011000	-1.69499300	-0.84565100
H	-1.89374700	-1.33522800	-1.84225800
Ni	0.04067000	-0.54004500	-0.43280800
N	1.18992600	1.01300500	-0.87009300
N	1.82623000	-1.34049900	-0.02249100
C	2.52797600	0.83113300	-0.67697100
C	0.74310500	2.21962500	-1.26264000
C	2.88916600	-0.50612700	-0.21110700
C	2.04559600	-2.58670900	0.43307900
C	3.43953300	1.87375000	-0.90846400
C	1.58839400	3.29402500	-1.49803300
H	-0.33783000	2.31130200	-1.38785400
C	4.20131600	-0.93967600	0.04236800
C	3.31408700	-3.07432400	0.71208600
H	1.15709700	-3.20903400	0.56022800
C	2.97119100	3.11472600	-1.32184600
H	4.50717600	1.71177500	-0.75740300
H	1.17494200	4.25259300	-1.81526700
C	4.42001100	-2.23027500	0.50655000
H	5.04174600	-0.26502100	-0.12280100
H	3.43851400	-4.09536600	1.07629200
H	3.66752900	3.93620700	-1.50185600
H	5.43428200	-2.58092700	0.70762300
C	-1.27880900	-3.19353400	-0.94899800
H	-0.97967700	-3.61319500	0.03053000
H	-2.14725000	-3.79957300	-1.28383400

H	-0.45617500	-3.40312600	-1.65122500

TS-S16

C	3.53586700	0.86986800	0.81398300
O	3.88438400	0.17836900	1.75588800
N	2.86824600	0.45670300	-0.32536500
C	3.74094500	2.37385200	0.70402500
C	3.53738400	2.66177800	-0.77986600
H	2.97602300	2.86704800	1.32822300
H	4.72319500	2.64727700	1.11297100
H	4.48549600	2.51184600	-1.32222100
H	3.18129100	3.67817000	-0.99253400
C	2.50994700	-0.86105200	-0.64903600
C	2.84740500	-1.95180500	0.17903800
C	1.79748600	-1.12033900	-1.84019900
C	2.47096500	-3.24637600	-0.17618800
H	3.39294400	-1.76209600	1.09826300
C	1.43894500	-2.42415600	-2.18407700
H	1.52134800	-0.30649800	-2.50582300
C	1.76260600	-3.49820900	-1.35438600
H	2.74117000	-4.07286000	0.48639100
H	0.88384400	-2.59341100	-3.10977600
H	1.47050600	-4.51539500	-1.62413900
C	2.49865700	1.59958900	-1.20345900
H	2.68953400	1.29495600	-2.24334600
C	1.04110800	2.07767500	-1.07517200
H	0.98845100	2.75174800	-0.19747500
Ni	-0.34806400	0.68774300	-0.70756700
N	0.01220900	-0.31038400	1.04496200
N	-1.34845800	-1.06624900	-1.06102300
C	-0.37509000	-1.60130900	1.05512000
C	0.71771500	0.17805500	2.06483900
C	-1.12544600	-2.03260600	-0.14220800
C	-1.99937700	-1.36993700	-2.19134600
C	-0.04915800	-2.44516400	2.12268000
C	1.10073200	-0.60172800	3.15272100
H	0.99599500	1.23018400	1.99317400
C	-1.57446500	-3.34263200	-0.34503600
C	-2.46690700	-2.65240100	-2.46636800
H	-2.15854500	-0.54174200	-2.88516300
C	0.70315400	-1.93901900	3.17995100
H	-0.36123400	-3.48867800	2.12039600
H	1.71444800	-0.16882200	3.94244600
C	-2.25292800	-3.65789900	-1.51926100
H	-1.38407400	-4.11152300	0.40253400
H	-2.99202400	-2.85251600	-3.40163600
H	0.98597700	-2.58651300	4.01250200

H	-2.60576100	-4.67608300	-1.69599700
C	0.71201500	2.90844200	-2.32173400
H	0.68061600	2.27906600	-3.23080800
H	1.46166600	3.70195400	-2.52094600
H	-0.25897700	3.41126700	-2.23378200
C	-1.93741500	2.50354200	-0.22281700
O	-1.47574300	3.60406900	-0.14771700
C	-2.38387100	1.64612900	0.89637300
C	-1.93097000	2.01249900	2.17998600
C	-3.19869000	0.51072300	0.75481700
C	-2.22454200	1.21472600	3.28114900
H	-1.32676900	2.91499900	2.28169600
C	-3.48777000	-0.28345500	1.86186700
H	-3.59025500	0.25786600	-0.22763000
C	-2.98889400	0.05223500	3.12478200
H	-1.85205000	1.49564800	4.26898600
H	-4.10883600	-1.17363500	1.73747300
H	-3.20748900	-0.58057700	3.98794800
Cl	-2.69472000	1.98972700	-1.92037100

TS-S17

Ni	0.35536100	0.30848900	0.96989500
C	-0.62776100	-0.97509600	-1.46161800
N	-2.73608100	-0.61985100	-0.23071400
C	-3.85233900	-1.12708500	-2.23906100
C	-2.82677400	-2.22500700	-1.96761900
H	-3.56901400	-0.47671500	-3.08305300
H	-4.87051700	-1.48868300	-2.43853400
H	-3.31976500	-3.10975300	-1.53633100
H	-2.27637600	-2.55182500	-2.86019800
C	-2.26048300	0.07398300	0.89715700
C	-2.62238000	1.39609700	1.18251800
C	-1.32856500	-0.59519700	1.75171300
C	-2.05735400	2.06284900	2.28772100
H	-3.35074100	1.89426800	0.54852900
C	-0.73484400	0.10734500	2.83183600
H	-1.19657700	-1.67308600	1.66745900
C	-1.11322500	1.44500000	3.09834900
H	-2.35869200	3.09294600	2.49004700
H	-0.09653300	-0.42782100	3.53760400
H	-0.67032000	1.97561800	3.94307100
C	-1.86706000	-1.61202000	-0.90583800
H	-1.57418100	-2.39972700	-0.19853500
O	-4.65102600	0.60129900	-0.71081600
C	-3.84608700	-0.26339800	-0.98503400
N	1.77752300	-1.05258600	0.76437600
N	1.50092700	1.41372300	-0.15715500

C	2.76293600	-0.61861100	-0.11075900
C	1.84667200	-2.28562400	1.28320000
C	2.61132700	0.71481900	-0.61241600
C	1.29036900	2.67443200	-0.57361200
C	3.83102600	-1.50022800	-0.43919500
C	2.85927200	-3.18686200	0.99683100
H	1.03701400	-2.56108100	1.96857400
C	3.50021200	1.35020700	-1.52324900
C	2.12292600	3.33762800	-1.45710600
H	0.39617800	3.16313500	-0.17305500
C	3.88095800	-2.76598900	0.10287800
H	4.61272700	-1.16803100	-1.12321200
H	2.86408500	-4.17892000	1.44929000
C	3.26301400	2.64068000	-1.94361100
H	4.37309800	0.80844000	-1.88909900
H	1.90196800	4.36049400	-1.76335100
H	4.70237700	-3.43956300	-0.15232100
H	3.94783500	3.12410600	-2.64412800
C	-0.69835900	0.23765800	-2.32304400
H	-1.11325000	0.00623800	-3.32740600
H	-1.34659700	1.01711000	-1.88847600
H	0.29610600	0.67636400	-2.47853600
H	0.27180900	-1.59405600	-1.49465300

intS18

Ni	0.21432600	-0.98366400	-0.43691100
C	-1.54437200	-1.65088300	-1.15740700
N	-2.65078600	-0.30893100	0.64698900
C	-4.58474100	-0.26035400	-0.69328400
C	-4.12038600	-1.70883000	-0.55632500
H	-4.45238800	0.13812100	-1.71136400
H	-5.63182100	-0.08107700	-0.40964900
H	-4.71755900	-2.22349800	0.21285400
H	-4.20463800	-2.28822300	-1.48559200
C	-1.55008800	0.05458000	1.43863200
C	-1.31259700	1.38308700	1.84684900
C	-0.61044200	-0.94251000	1.81174800
C	-0.14914200	1.70726300	2.54377600
H	-2.04076400	2.14588700	1.58881600
C	0.54740800	-0.59234000	2.52270100
H	-0.83113600	-1.99574300	1.64734900
C	0.80036900	0.73270100	2.86971400
H	0.01960600	2.74879700	2.82842100
H	1.25634800	-1.37719700	2.79563900
H	1.71513600	1.00141700	3.40182500
C	-2.64822800	-1.60744400	-0.08958200
H	-2.46085500	-2.41144900	0.63722200

O	-3.81259700	1.70527200	0.52323200
C	-3.67026200	0.53169700	0.23110400
N	2.17711100	-1.14777100	-0.27179300
N	0.72034900	0.93371900	-0.78345400
C	2.88112200	0.01350200	-0.43490000
C	2.84913400	-2.27674800	0.03579400
C	2.05767900	1.18269100	-0.72982000
C	-0.12636500	1.94805500	-1.01912800
C	4.28122200	0.03135500	-0.31326400
C	4.22460800	-2.32282300	0.18215000
H	2.23791900	-3.17532200	0.16081600
C	2.56071000	2.47808500	-0.95218400
C	0.29999700	3.25035500	-1.23861900
H	-1.18827700	1.69920000	-1.02486800
C	4.96311600	-1.13690500	-0.00353200
H	4.82827400	0.96359700	-0.45623600
H	4.71582400	-3.26480300	0.43132700
C	1.67908900	3.51797400	-1.20948700
H	3.63450900	2.66263100	-0.91763600
H	-0.43149900	4.03768100	-1.42534500
H	6.05027600	-1.13484400	0.09523200
H	2.05406700	4.52917600	-1.38133600
C	-1.89982400	-0.92197500	-2.45717700
H	-2.81804200	-1.29736500	-2.95422300
H	-2.04783400	0.16055000	-2.30402000
H	-1.08467100	-1.01629300	-3.19200500
H	-1.39759600	-2.72313400	-1.39832900

TS-S19

C	-2.30033000	-0.75991400	0.81510300
O	-2.44422000	-0.46658500	2.00037600
C	-2.73031400	-2.04838700	0.20530400
C	-2.93233600	-3.13143300	1.08211300
C	-2.93147600	-2.24024100	-1.17476800
C	-3.31775500	-4.37817200	0.59081100
H	-2.79178300	-2.96697700	2.15169300
C	-3.32488400	-3.49024400	-1.65784800
H	-2.81660400	-1.40839400	-1.87162700
C	-3.51392900	-4.56439700	-0.78220600
H	-3.47289200	-5.20934300	1.28391300
H	-3.49267600	-3.62152300	-2.72993700
H	-3.81969800	-5.54067200	-1.16710800
O	-2.31778500	0.37522400	-0.18319200
P	-3.48027600	1.20347800	-0.94207700
O	-3.66741000	0.88394000	-2.37540500
O	-4.81516600	1.00196200	-0.07770600
O	-2.97293900	2.71472900	-0.63917300

C	-3.27816300	3.76798200	-1.55637900
H	-2.50038100	4.53629000	-1.44292900
H	-3.28796400	3.39327000	-2.59083100
H	-4.26000000	4.21286900	-1.32393800
C	-4.98819900	1.45416900	1.27229500
H	-4.34483700	0.88166500	1.95566900
H	-4.75616000	2.52773200	1.35429200
H	-6.04481100	1.28793400	1.52162400
Ni	-0.29869000	-0.27945900	0.01996700
N	0.78553500	0.86705500	-1.40614600
N	0.18251000	1.42160800	1.11480200
C	1.38302800	1.96305000	-0.89380800
C	0.99760300	0.53275800	-2.68353500
C	1.04405700	2.27497800	0.51902600
C	-0.24703300	1.67276300	2.35870100
C	2.23447000	2.75384100	-1.67942100
C	1.81944400	1.27491200	-3.53034300
H	0.48395000	-0.36342300	-3.04191300
C	1.54800000	3.38859100	1.20398400
C	0.19859700	2.77168800	3.09350000
H	-0.98887700	0.96858800	2.74750100
C	2.45250500	2.40600500	-3.01099300
H	2.72402900	3.63185700	-1.25880000
H	1.95800300	0.96734700	-4.56815600
C	1.12623600	3.63490800	2.50848200
H	2.26435000	4.05726800	0.72817800
H	-0.17498700	2.93676100	4.10573200
H	3.11230100	3.01211200	-3.63608300
H	1.51459000	4.49554200	3.05776300
C	3.07534300	-0.14023600	2.20311900
O	3.77943900	0.85347800	2.20247400
N	2.85746100	-0.99986200	1.13448800
C	2.33296800	-0.68936500	3.41013300
C	1.31868300	-1.67515600	2.83862100
H	1.90436400	0.13177300	4.00193700
H	3.09353100	-1.17758300	4.04483400
H	1.21985300	-2.58867500	3.44227000
H	0.32126000	-1.21737800	2.78216800
C	3.74850000	-1.07432400	0.03271300
C	4.40653600	0.07129900	-0.45794200
C	4.04429100	-2.31691900	-0.56155800
C	5.31940700	-0.03332400	-1.51001300
H	4.21679300	1.03192300	0.01136400
C	4.95355000	-2.40764500	-1.61607200
H	3.56668100	-3.22421000	-0.19680000
C	5.59876100	-1.26723200	-2.10204500
H	5.81955200	0.87067100	-1.86895600

H	5.16202700	-3.38660400	-2.05610900
H	6.31268800	-1.34140400	-2.92606800
C	1.79446400	-2.01374100	1.39952300
H	2.28519300	-3.00875200	1.41344600
C	0.59717300	-2.04679300	0.43508800
C	0.83387200	-2.76850100	-0.89852800
H	1.27451600	-3.77896600	-0.76598700
H	-0.12069500	-2.92174000	-1.43010100
H	1.50747600	-2.22284000	-1.57843300
H	-0.15364200	-2.64156800	0.98415300