Supporting Information

Tunable Regiodivergent Phosphine-Catalyzed [3+2] Cycloaddition of Alkynones and Trifluoroacetyl Phenylamides

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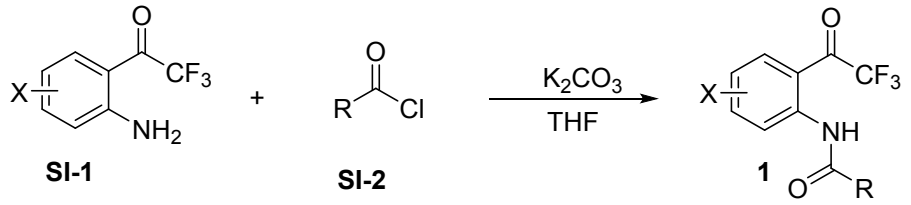
CONTENTS

General Remarks. ^{1}H NMR spectra were recorded on a Varian Mercury-300 and 400 spectrometer for solution in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard; coupling constants (*J*) are given in Hz. ^{13}C NMR spectra were recorded on a Varian Mercury-300 and 400 spectrophotometers (75 or 100 MHz) with complete proton decoupling spectrophotometers ($CDCl_3$: 77.0 ppm). Mass and HRMS spectra were recorded by EI or ESI method. Organic solvents used were dried by standard methods when necessary. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1}. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. Commercially obtained reagents were used without further purification. All these reactions were monitored by TLC with silica gel coated plates. Flash column chromatography was carried out using silica gel at increased pressure.

General Procedure for Synthesis of ortho-Amino trifluoroacetophenone derivatives 1 and Spectroscopic Data of Substrates 1

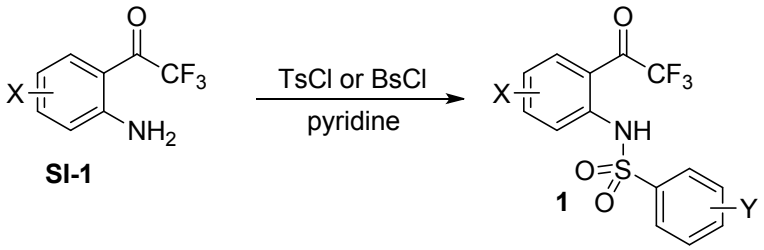
ortho-Amino trifluoroacetophenone derivatives **1a-1o** were prepared according to a previous procedure reported in the literature with slight modification.[1] Among them, **1a**, **1b**, **1d** and **1f** are known compounds.



To a solution of aniline derivative **SI-1** (1.0 mmol, 1.0 equiv) in dry THF (20 mL) was added the corresponding benzyl chloride **SI-2** (1.5 mmol, 1.5 equiv) and K_2CO_3 (1.5 mmol, 1.5 equiv). Then, the resulting reaction mixture was stirred at room temperature overnight. After that, K_2CO_3 was removed by filtration. The reaction mixture was concentrated under high vacuum and purified by a column chromatography on silica gel to give the desired products **1** (PE:EA = 4:1).

Compound **1p** is a known compound and was prepared according to a previous procedure reported in the literature.[2]

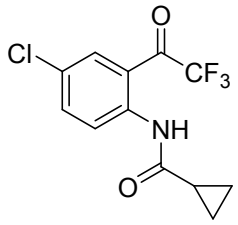
ortho-Amino trifluoroacetophenone derivatives **1q-1s** were prepared to a previous procedure reported in the literature with slight modification.



To a solution of aniline derivative **SI-1** (1.0 mmol, 1.0 equiv) in dry pyridine (20 mL) was added TsCl or BsCl (1.5 mmol, 1.5 equiv). Then, the resulting reaction mixture was stirred at room temperature overnight. The reaction mixture was concentrated under high vacuum and purified by a column chromatography on silica gel to give the desired products **1** (PE:EA = 4:1). Among them, **1q** is a known compound.

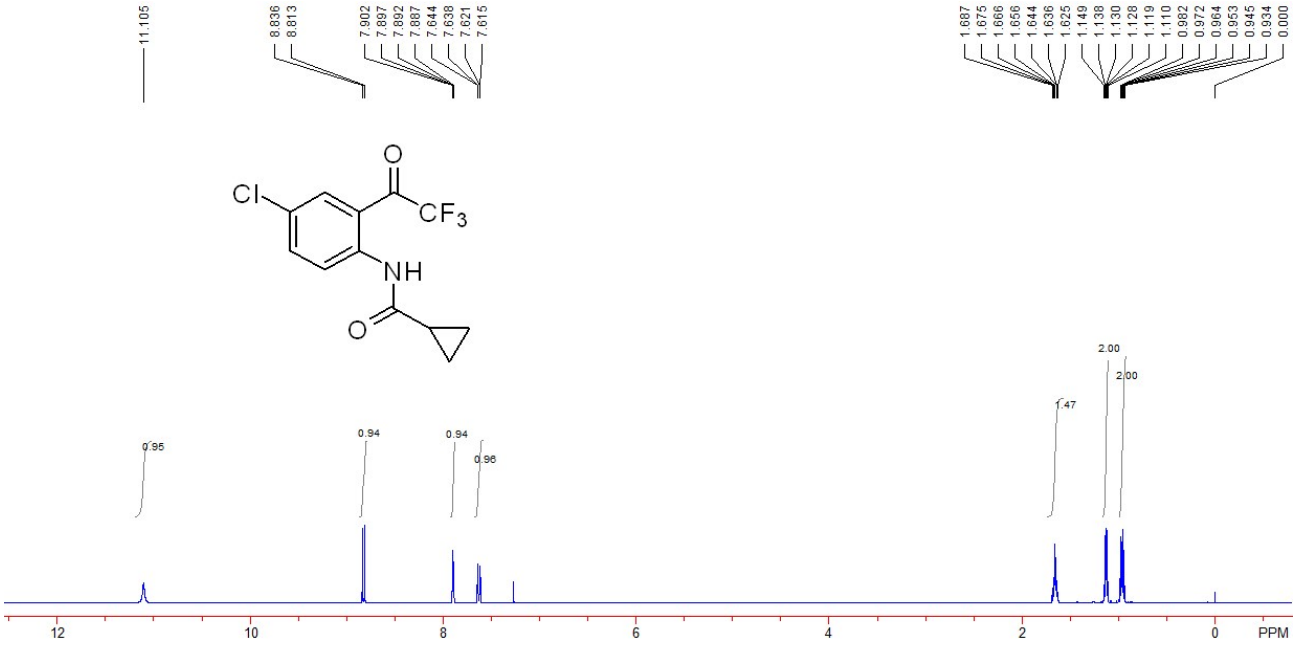
ortho-Hydroxy trifluoroacetophenone derivatives **1t-1v** were prepared based on a previous procedure reported in the literature with slight modification.[3] Among them, **1t** and **1u** are known compounds.

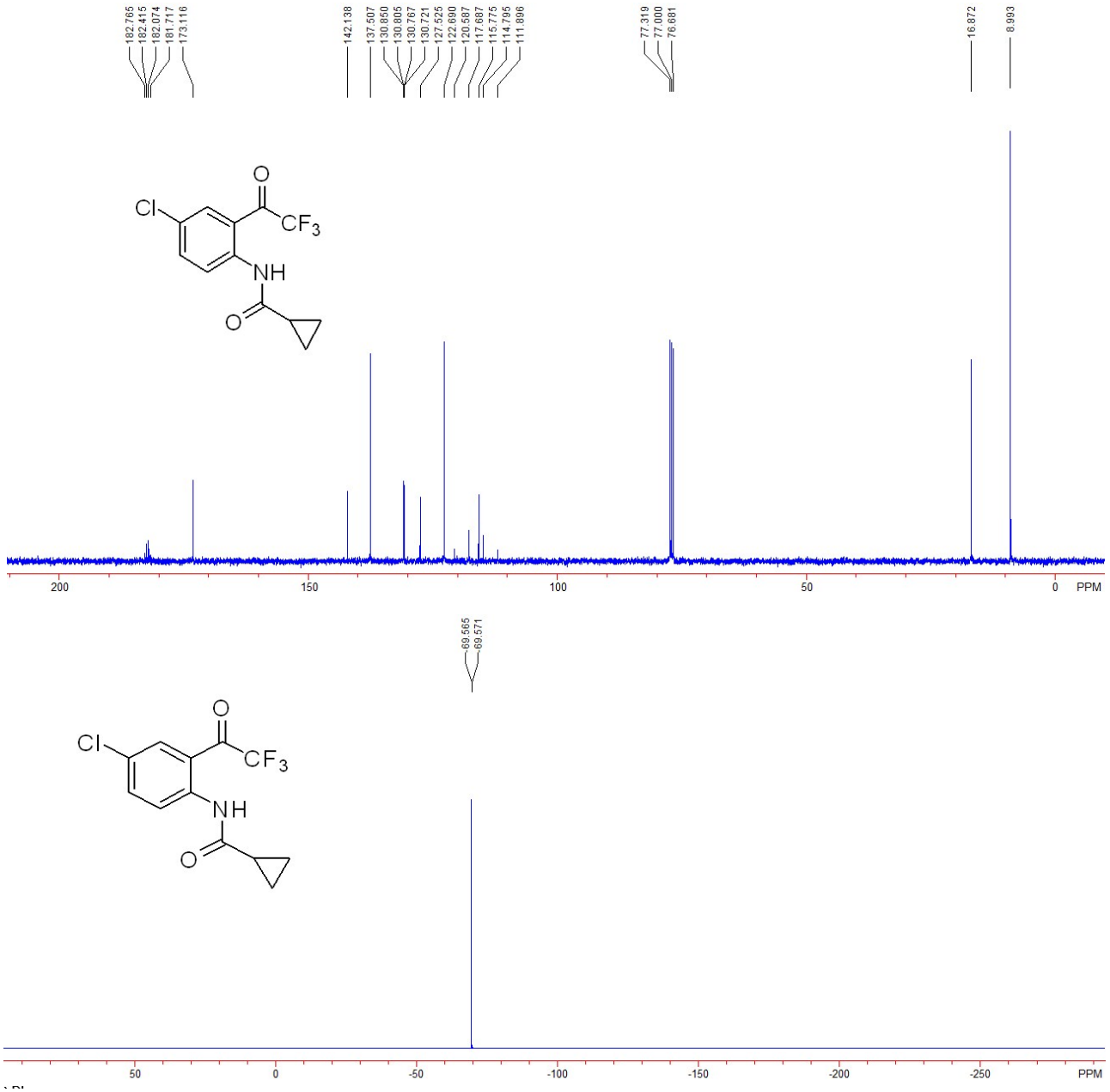
Compounds **1w**, **1y**, **1z** are from commercially available resource. Compound **1x** is a known compound and was prepared according to a previous procedure reported in the literature.[4]

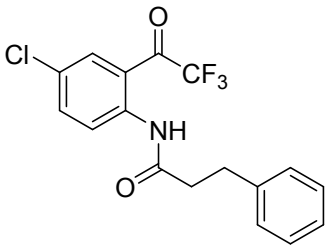


N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)cyclopropanecarboxamide (1c)

A yellow solid, 67% yield (196 mg). M.p.: 131-133 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 0.93~0.99 (m, 2H, CH_2), 1.11~1.15 (m, 2H, CH_2), 1.62~1.69 (m, 1H, CH), 7.63 (dd, *J* = 2.4, 9.2 Hz, 1H, ArH), 7.88~7.91 (m, 1H, ArH), 8.82 (d, *J* = 9.2 Hz, 1H, ArH), 11.11 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 9.0, 16.9, 115.8, 116.2 (q, *J* = 289.2 Hz), 122.7, 127.5, 130.8 (q, *J* = 3.8 Hz), 137.5, 142.1, 173.1, 182.2 (q, *J* = 34.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.57 (d, *J* = 2.25 Hz). IR (CH_2Cl_2) ν 3675, 2988, 2901, 2360, 2343, 1507, 1405, 1075, 1066, 879, 681 cm^{-1}. HRMS (ESI) Calcd. For $C_{12}H_{10}ClF_3NO_2^{+1}(M+H)^+$ requires 292.0347, Found: 292.0347.



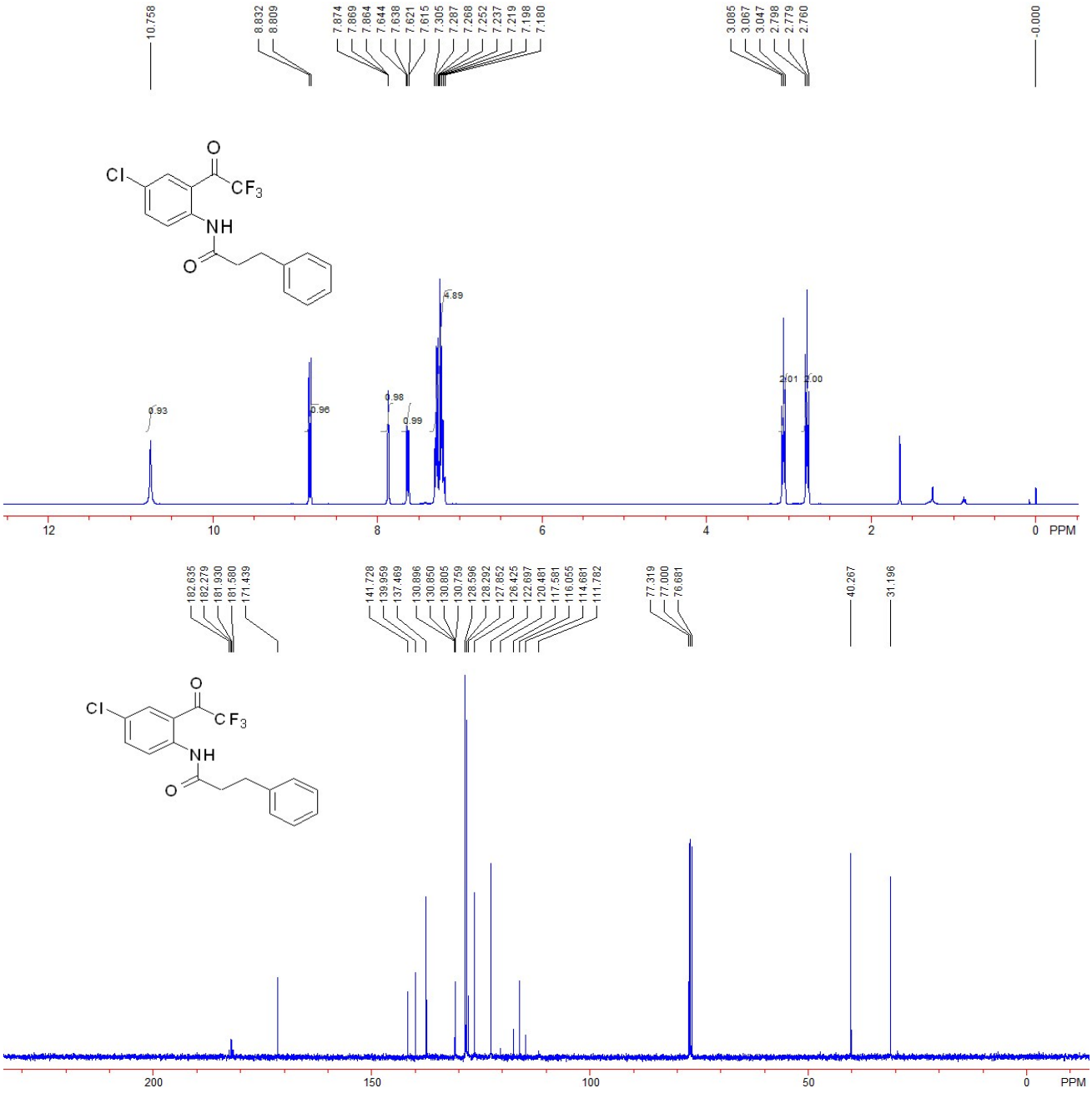


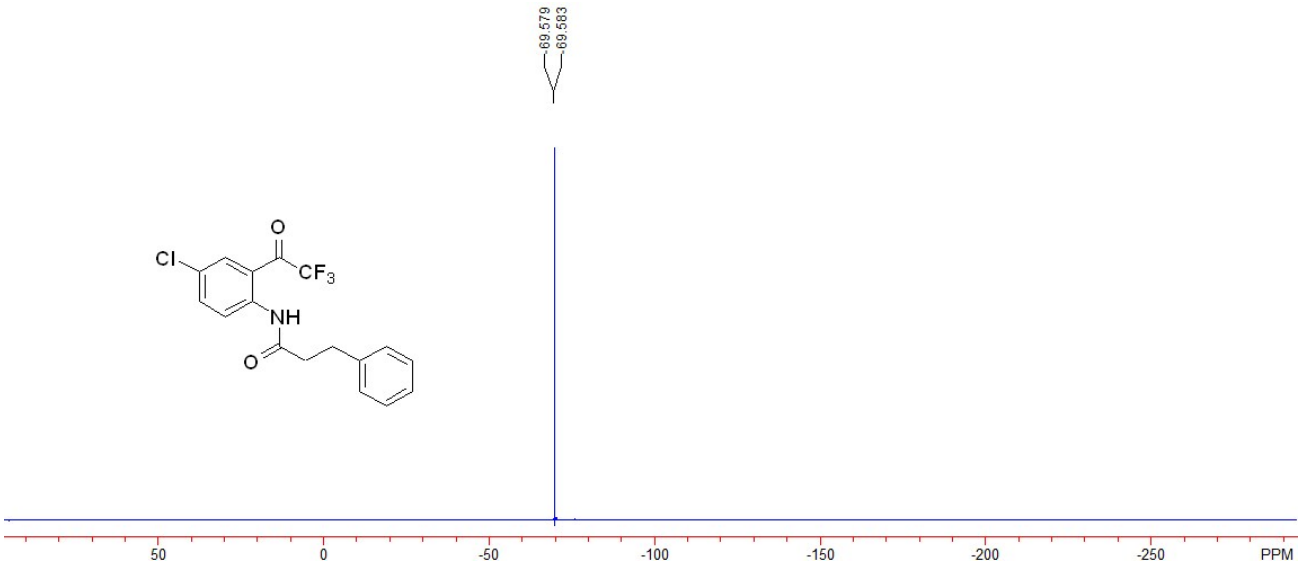


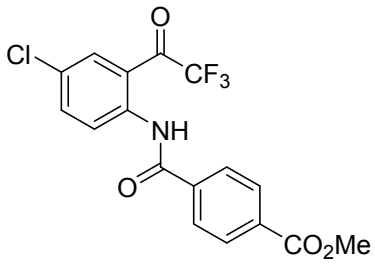
N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)-3-phenylpropanamide (1e)

A yellow solid, 53% yield (189 mg). M.p.: 117-1119 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.78 (t, J = 7.6 Hz, 2H, CH_2), 3.07 (t, J = 7.6 Hz, 2H, CH_2), 7.18~7.31 (m, 5H, ArH), 7.63 (dd, J = 2.4,

9.2 Hz, 1H, ArH), 7.87 (s, 1H, ArH), 8.82 (d, J = 9.2 Hz, 1H, ArH), 10.76 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 31.2, 40.3, 116.06, 116.13 (q, J = 290.0 Hz), 122.7, 126.4, 127.9, 128.3, 128.6, 130.8 (q, J = 4.5 Hz), 137.5, 140.0, 141.7, 171.4, 182.1 (q, J = 34.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.58 (d, J = 1.5 Hz). IR (CH_2Cl_2) ν 3675, 2969, 2920, 2358, 2343, 1683, 1516, 1172, 1076, 668 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{14}ClF_3NO_2^{+1}(M+H)^+$ requires 356.0660, Found: 356.0661.

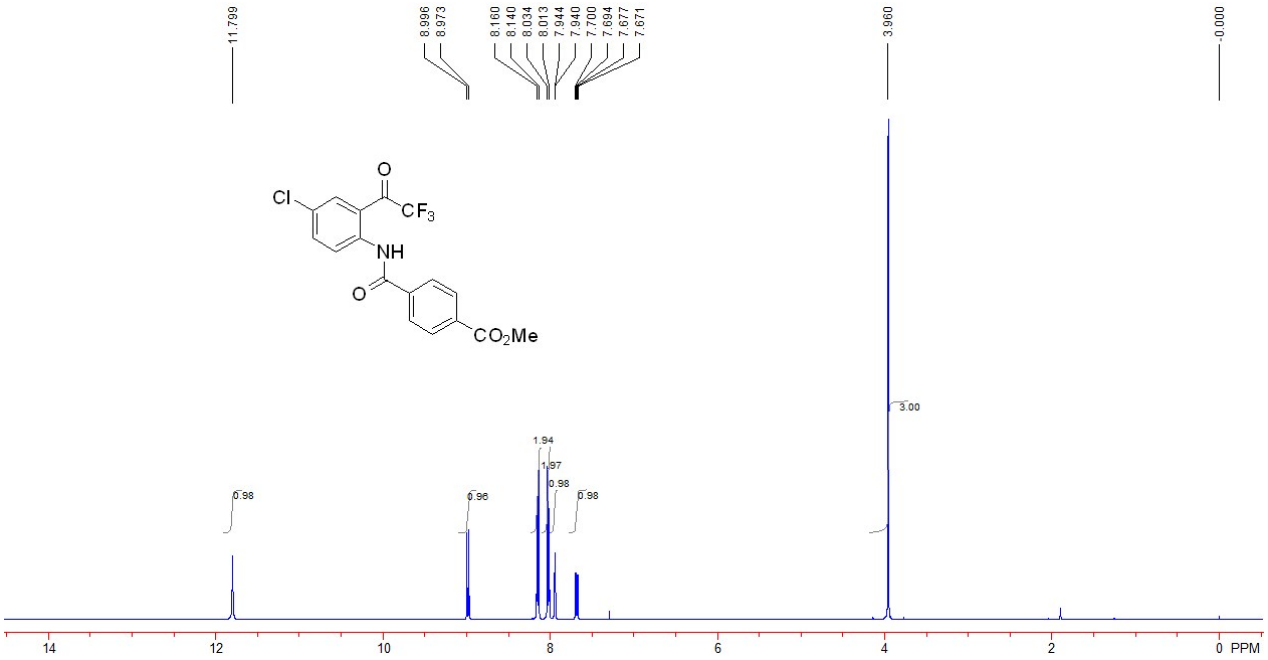






methyl 4-((4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)carbamoyl)benzoate (1g)

A yellow solid, 73% yield (282 mg). M.p.: 116-118 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 3.96 (s, 3H, CH_3), 7.69 (dd, *J* = 2.4, 9.2 Hz, 1H, ArH), 7.94 (s, 1H, ArH), 8.02 (d, *J* = 8.4 Hz, 2H, ArH), 8.15 (d, *J* = 8.4 Hz, 2H, ArH), 8.98 (d, *J* = 9.2 Hz, 1H, ArH), 11.80 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 52.5, 116.2 (q, *J* = 290.0 Hz), 116.4, 122.6, 127.4, 128.4, 130.1, 131.2 (q, *J* = 4.3 Hz), 133.6, 137.3, 137.7, 142.0, 164.8, 165.9, 182.7 (q, *J* = 35.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.43 (d, *J* = 1.875 Hz). IR (CH_2Cl_2) ν 3345, 2976, 1667, 1526, 1283, 1172, 1130, 1107, 1077, 960, 722 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{12}ClF_3NO_4^{+1}(M+H)^+$ requires 386.0401, Found: 386.0408.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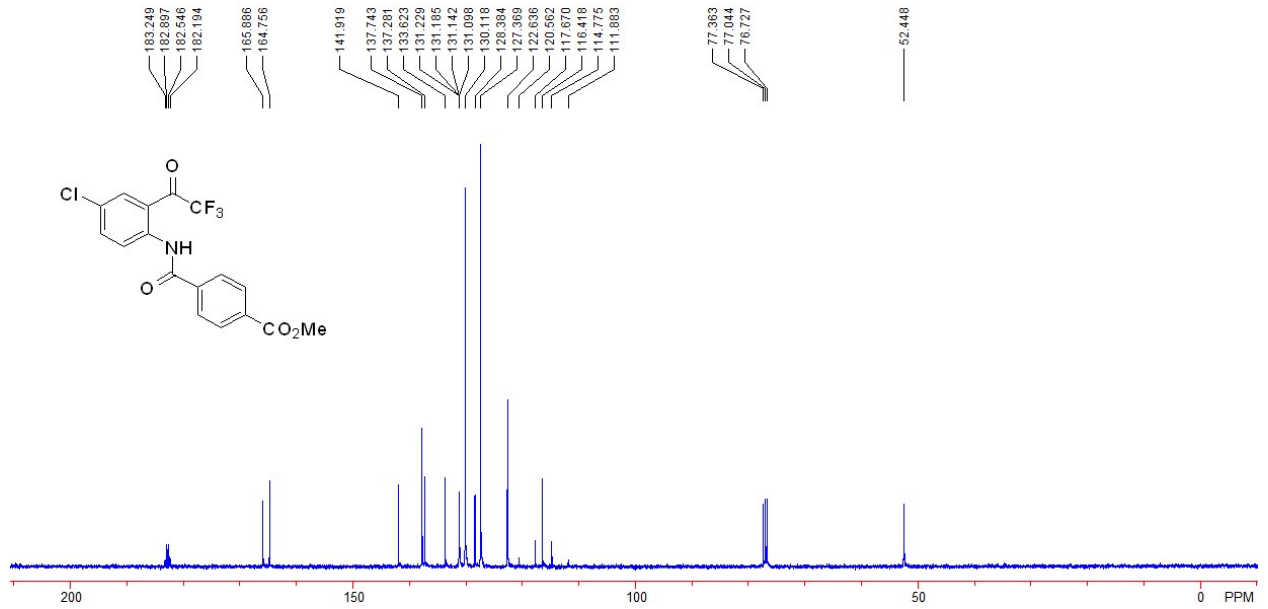
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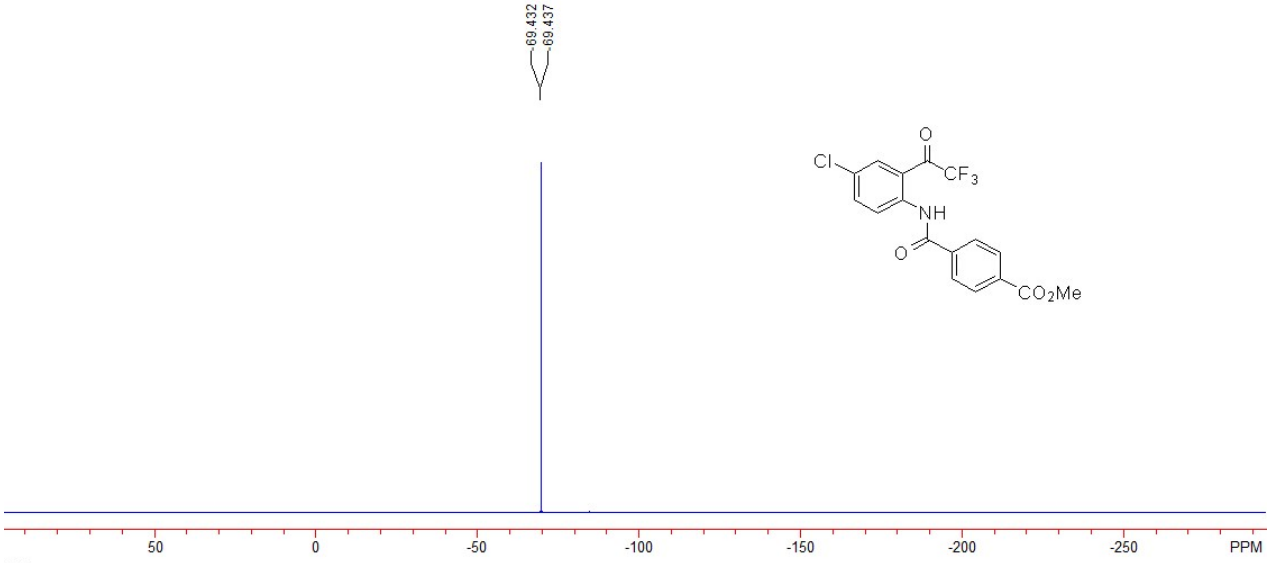
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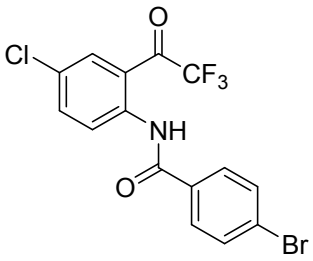
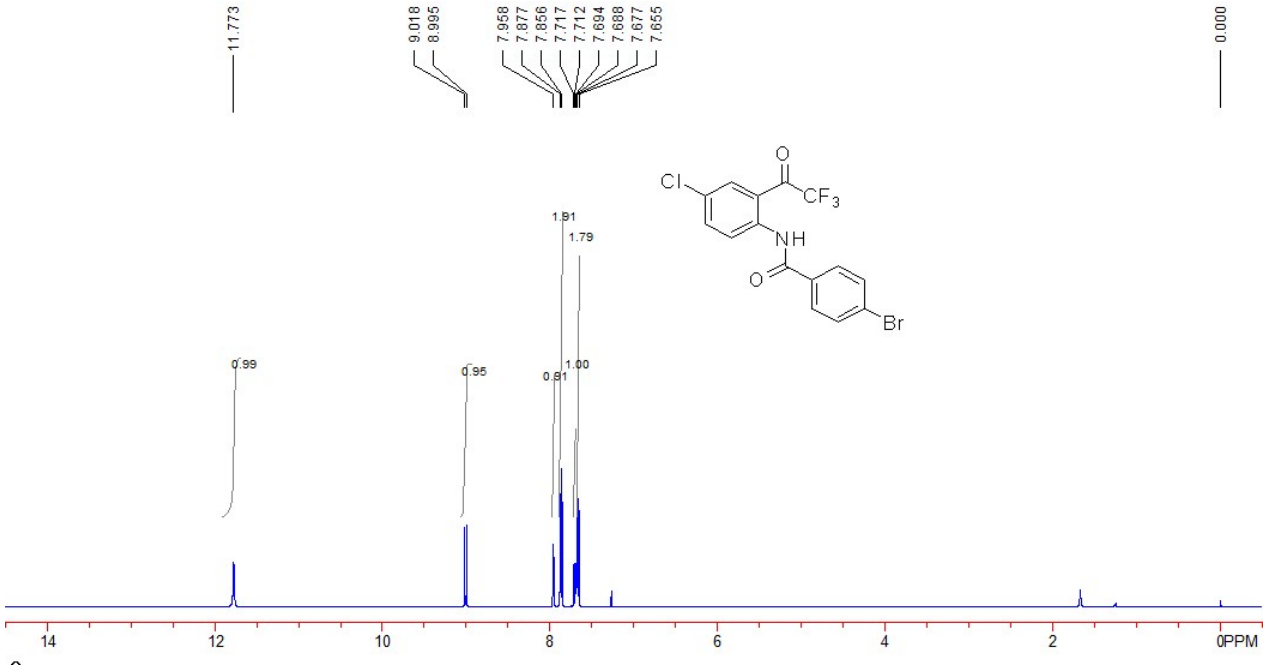
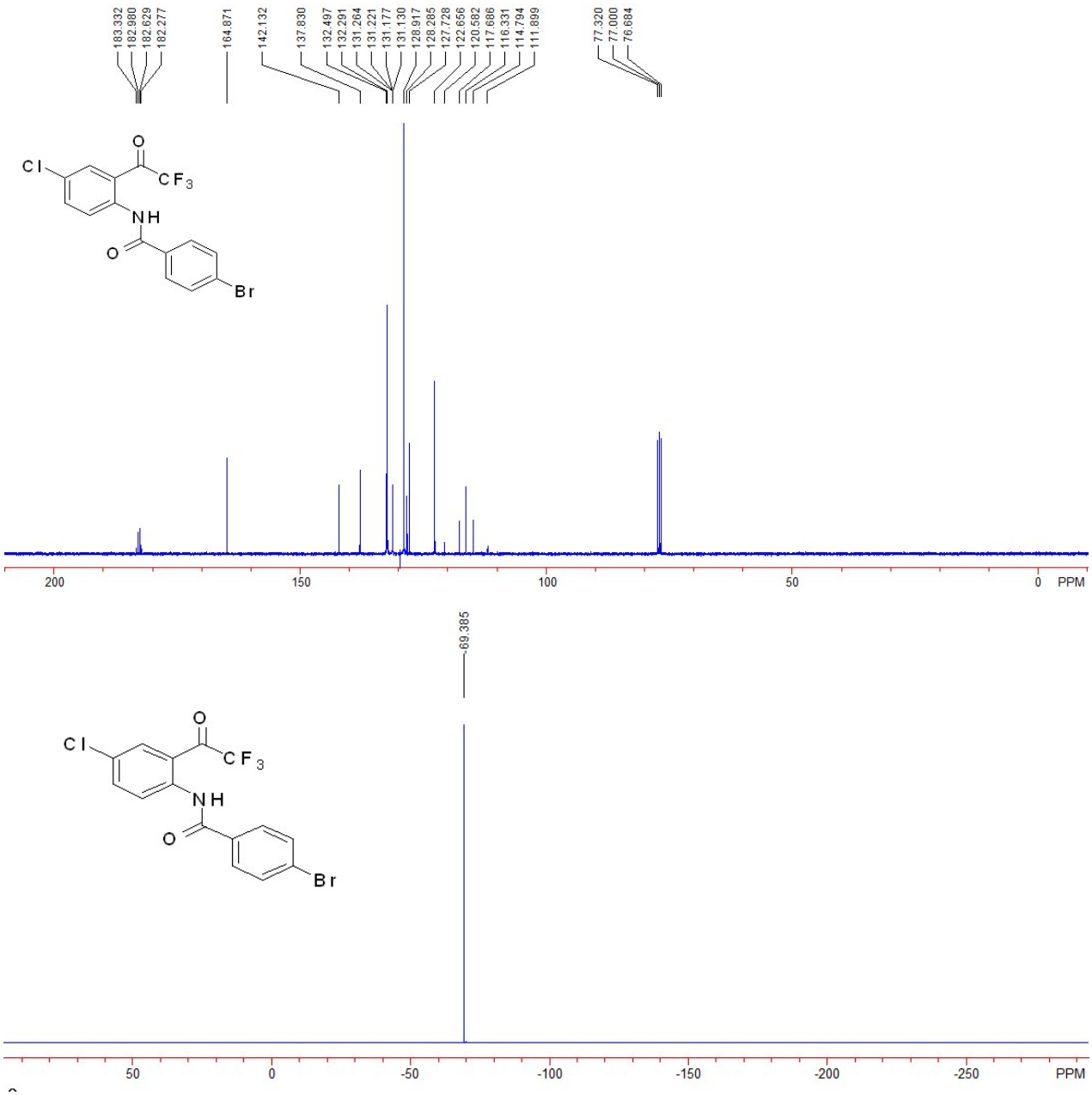
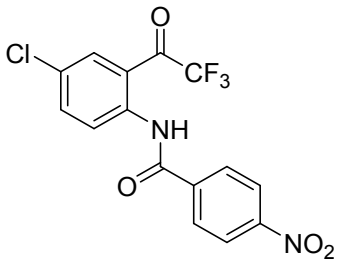


4-bromo-N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)benzamide (1h)

A yellow solid, 53% yield (215 mg). M.p.: 156-158 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 7.66 (d, *J* = 8.8 Hz, 2H, ArH), 7.70 (dd, *J* = 2.0, 9.2 Hz, 1H, ArH), 7.87 (d, *J* = 8.4 Hz, 2H, ArH), 7.96 (s, 1H, ArH), 9.00 (d, *J* = 9.2 Hz, 1H, ArH), 11.77 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 116.2 (q, *J* = 289.2 Hz), 116.3, 122.7, 127.7, 128.3, 128.9, 131.2 (q, *J* = 4.4 Hz), 132.3, 132.5, 137.8, 142.1, 164.9, 182.8 (q, *J* = 35.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.39. IR (CH_2Cl_2) ν 3328, 2924, 2853, 1683, 1606, 1517, 1297, 1202, 1170, 959 cm^{-1}. HRMS (ESI) Calcd. For $C_{15}H_9BrClF_3NO_2^{+1}(M+H)^+$ requires 405.9452, Found: 405.9446.



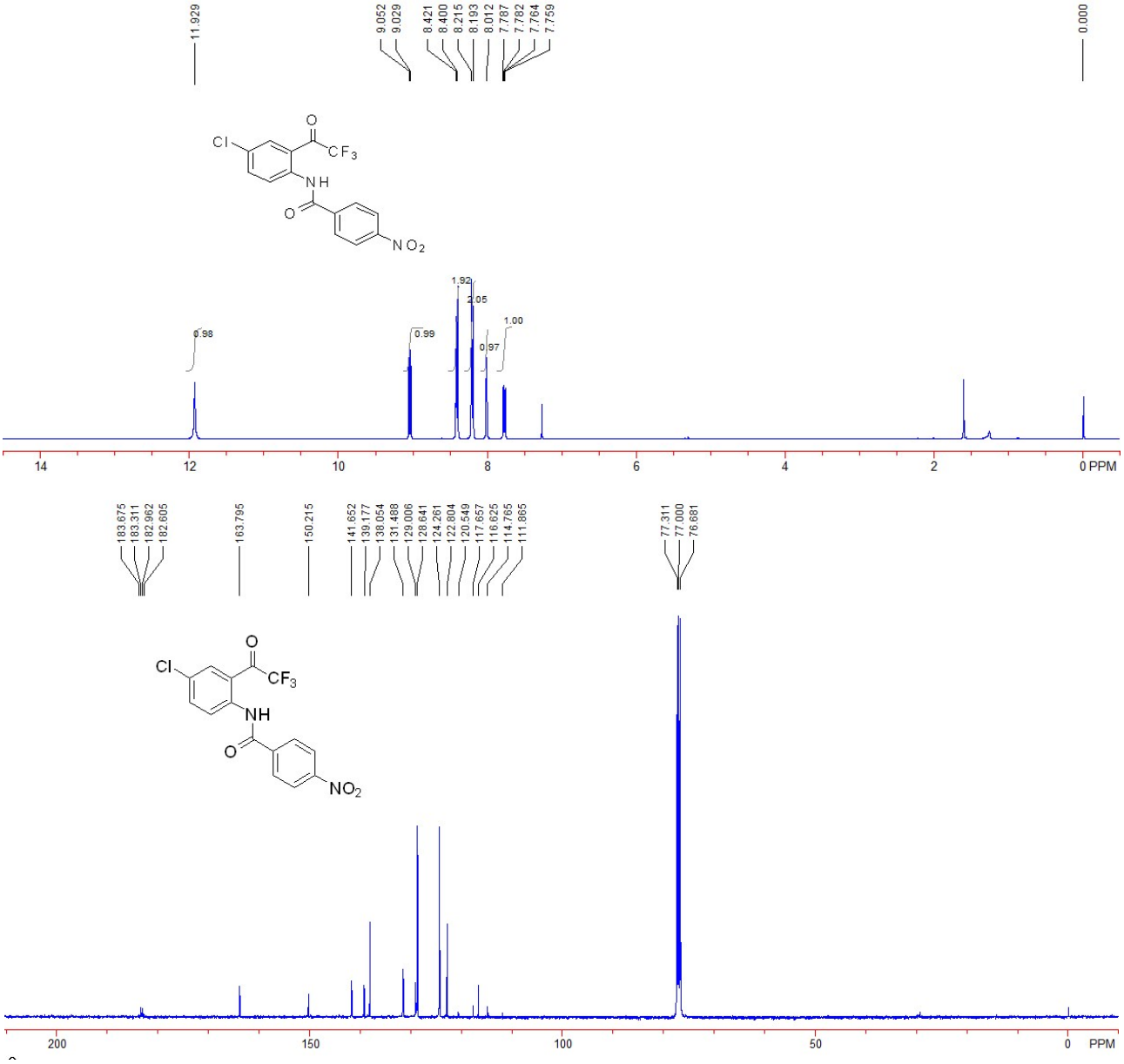


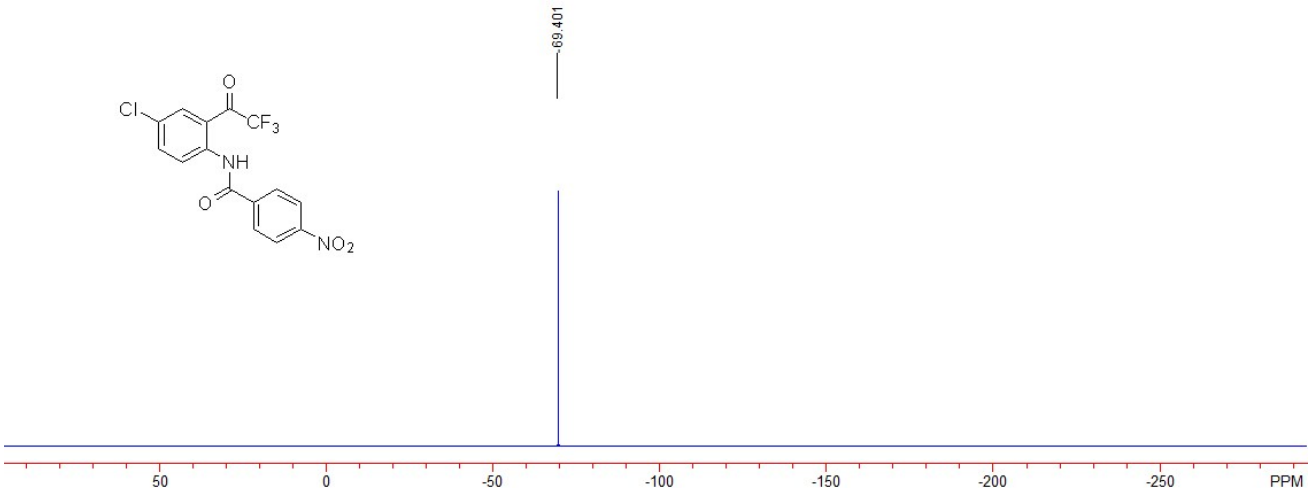


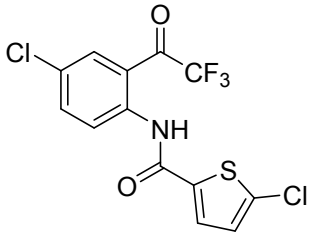
N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)-4-nitrobenzamide (1i)

A yellow solid, 89% yield (332 mg). M.p.: 205-207 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 7.77 (dd, J = 2.0, 9.2 Hz, 1H, ArH), 8.01 (s, 1H, ArH), 8.20 (d, J = 8.8 Hz, 2H, ArH), 8.41 (d, J = 8.8 Hz,

2H, ArH), 9.04 (d, J = 9.2 Hz, 1H, ArH), 11.93 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 116.2 (q, J = 289.2 Hz), 116.6, 122.8, 124.3, 128.6, 129.0, 131.5, 138.1, 139.2, 141.7, 150.2, 163.8, 183.1 (q, J = 34.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.40. IR (CH_2Cl_2) ν 3355, 2970, 2916, 1673, 1530, 1349, 1147, 1136, 869, 723 cm^{-1}. HRMS (ESI) Calcd. For $C_{15}H_9F_3O_4N_2Cl^{+1}(M+H)^+$ requires 373.0196, Found: 373.0197.

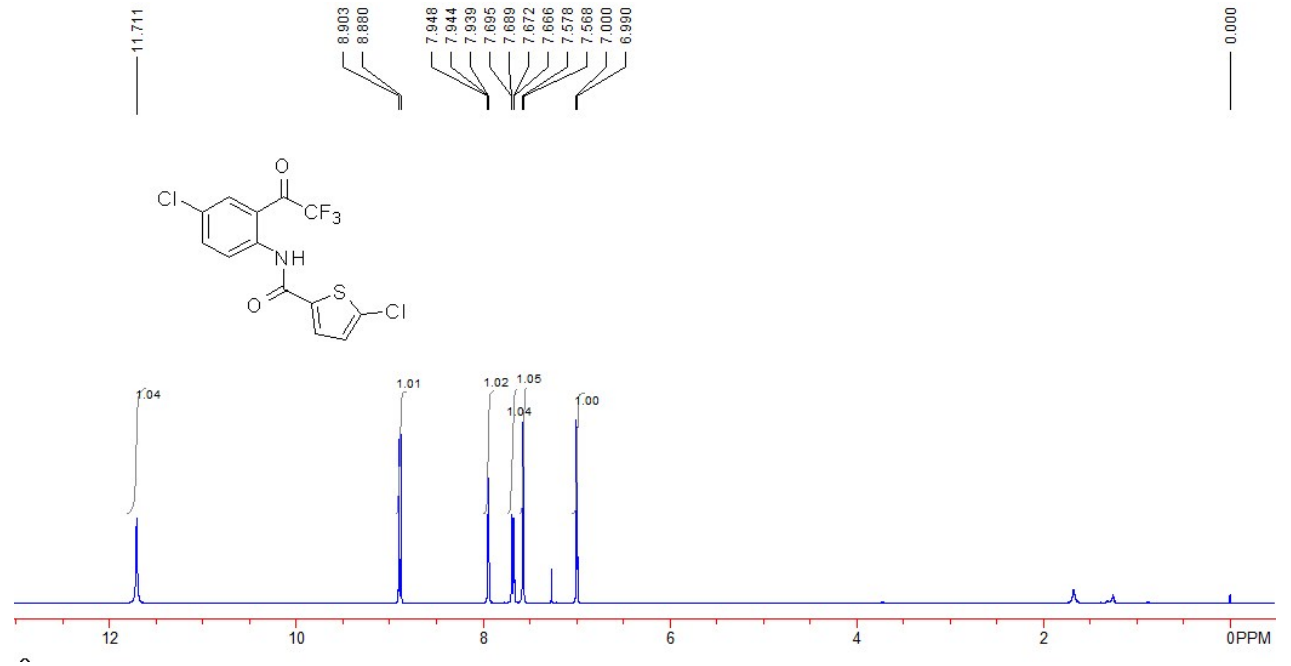






5-chloro-N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)thiophene-2-carboxamide (1j)

A yellow solid, 31% yield (114 mg). M.p.: 121-123 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 7.00 (d, *J* = 4.0 Hz, 1H, ArH), 7.57 (d, *J* = 4.0 Hz, 1H, ArH), 7.68 (dd, *J* = 2.4, 9.2 Hz, 1H, ArH), 7.94 (t, *J* = 1.6 Hz, 1H, ArH), 8.89 (d, *J* = 9.2 Hz, 1H, ArH), 11.71 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 115.9, 116.2 (q, *J* = 289.5 Hz), 122.4, 127.5, 128.2, 128.5, 131.2 (q, *J* = 44.0 Hz), 137.4, 137.9, 138.0, 142.0, 159.3, 183.3 (q, *J* = 35.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.39 (d, *J* = 1.88 Hz). IR (CH_2Cl_2) ν 3311, 2972, 2900, 2360, 2337, 1541, 1510, 1423, 1168, 1084, 880 cm^{-1}. HRMS (ESI) Calcd. For $C_{13}H_7Cl_2F_3NO_2S^{+1}(M+H)^+$ requires 367.9521, Found: 367.9528.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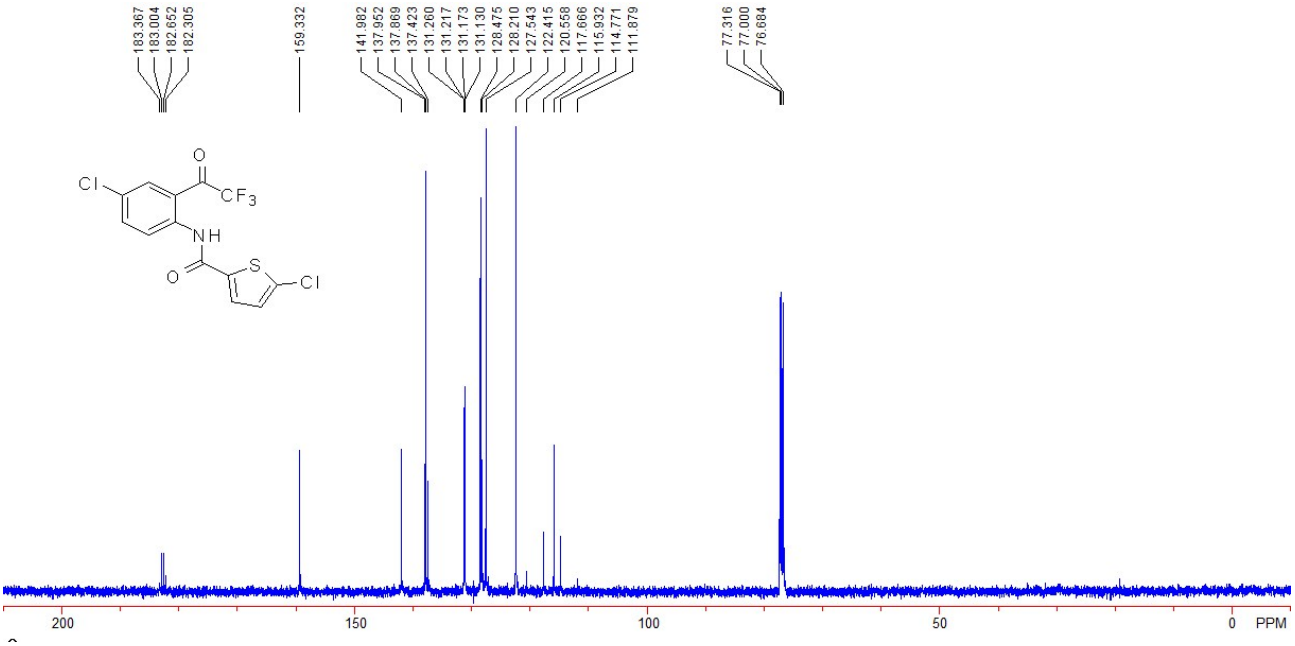
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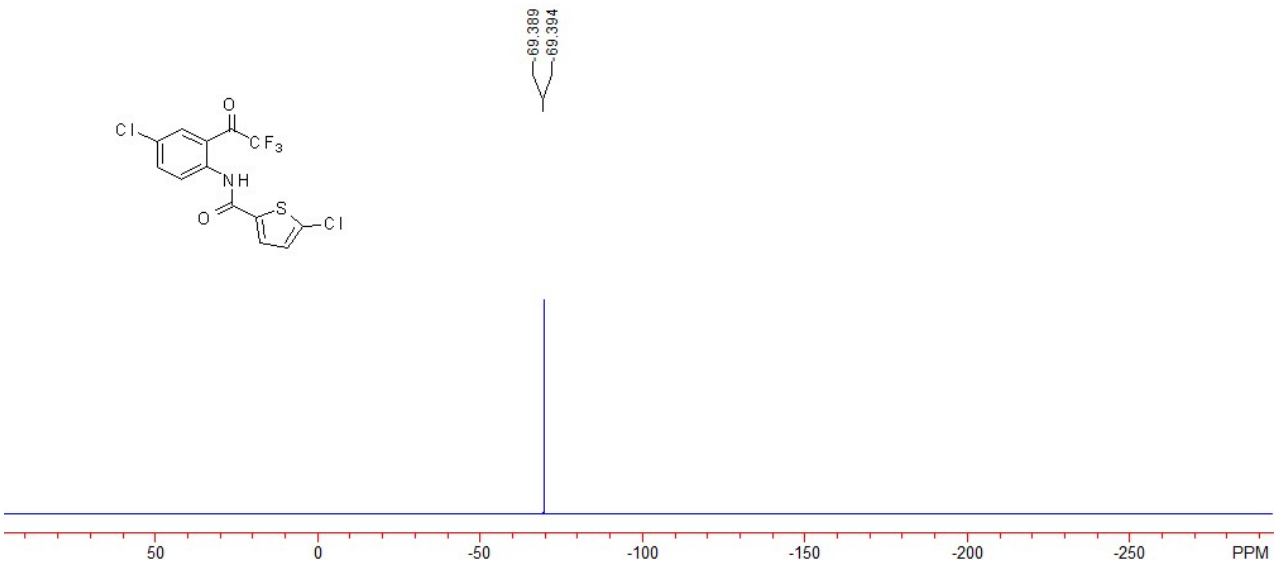
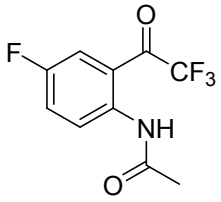
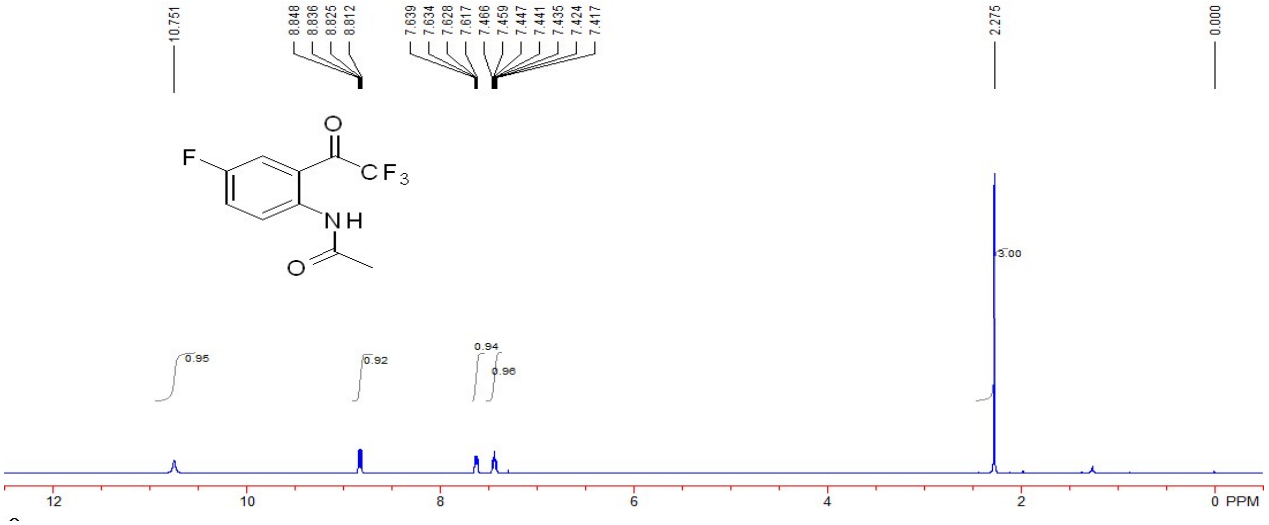




N-(4-fluoro-2-(2,2,2-trifluoroacetyl)phenyl)acetamide (1k)

A yellow solid, 74% yield (185 mg). M.p.: 130-132 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.28 (s, 3H, CH_3), 7.41~7.47 (m, 1H, ArH), 7.61~7.64 (m, 1H, ArH), 8.83 (dd, *J* = 4.8, 9.2 Hz, 1H, ArH), 10.75 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 25.3, 115.8 (d, *J* = 5.0 Hz), 116.2 (q, *J* = 290.0 Hz), 117.2 (qd, *J* = 4.6, 24.3 Hz), 123.2 (d, *J* = 6.8 Hz), 125.0 (d, *J* = 22.0 Hz), 139.8 (d, *J* = 1.6 Hz), 156.8 (d, *J* = 243.7 Hz), 169.2, 182.1 (dq, *J* = 2.3, 34.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -117.51 ~ (-117.44), -70.00 (d, *J* = 1.88 Hz). IR (CH_2Cl_2) ν 3340, 2926, 2854, 1677, 1529, 1414, 1195, 1152, 989, 870 cm^{-1}. HRMS (ESI) Calcd. For $C_{10}H_8F_4NO_2^{+1}(M+H)^+$ requires 250.0486, Found: 250.0486.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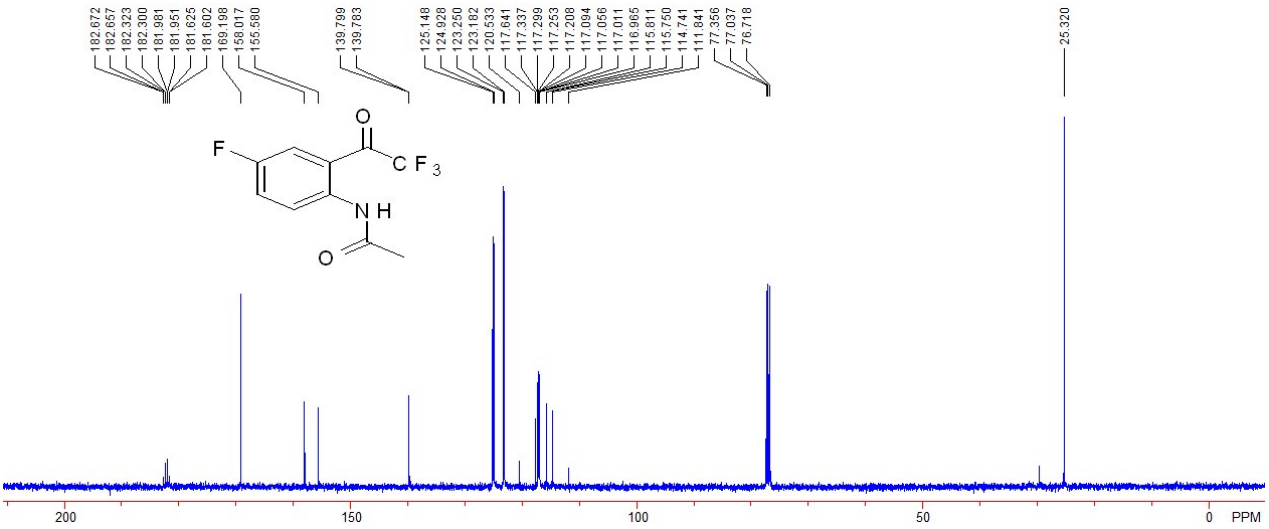
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117.056
117.011
116.965
115.811
115.750
114.741
111.841
77.356
77.037
76.718
25.320
F
O
CF3
NH
O
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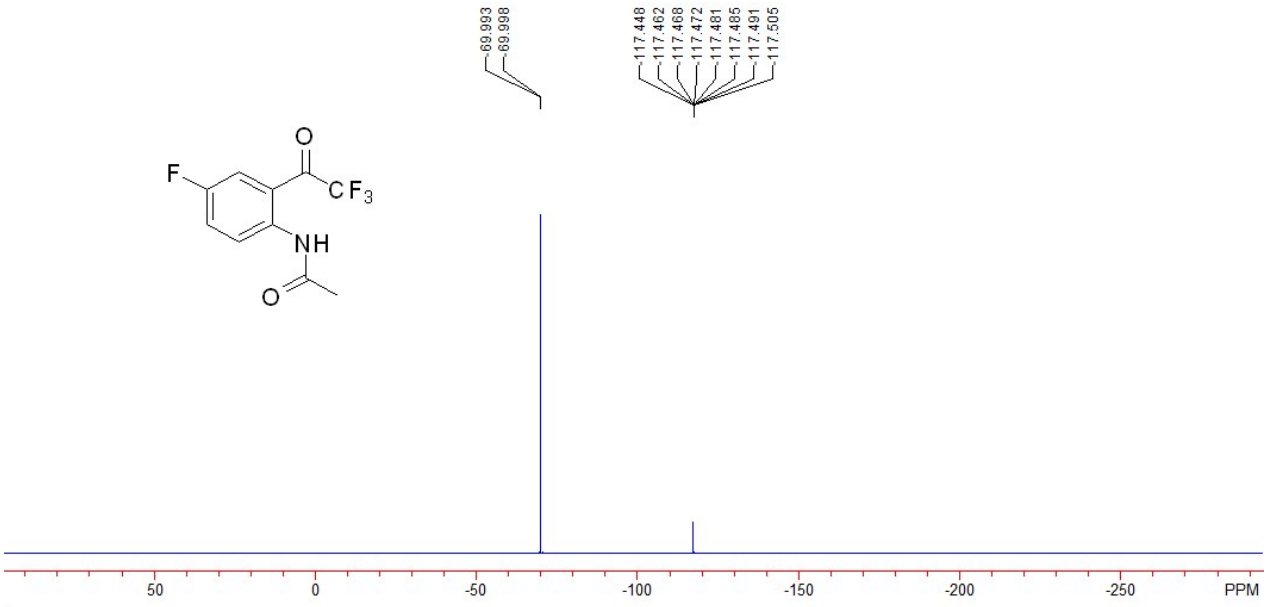
150
100
50
0 PPM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117.485
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O
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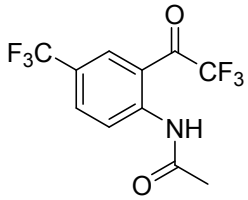
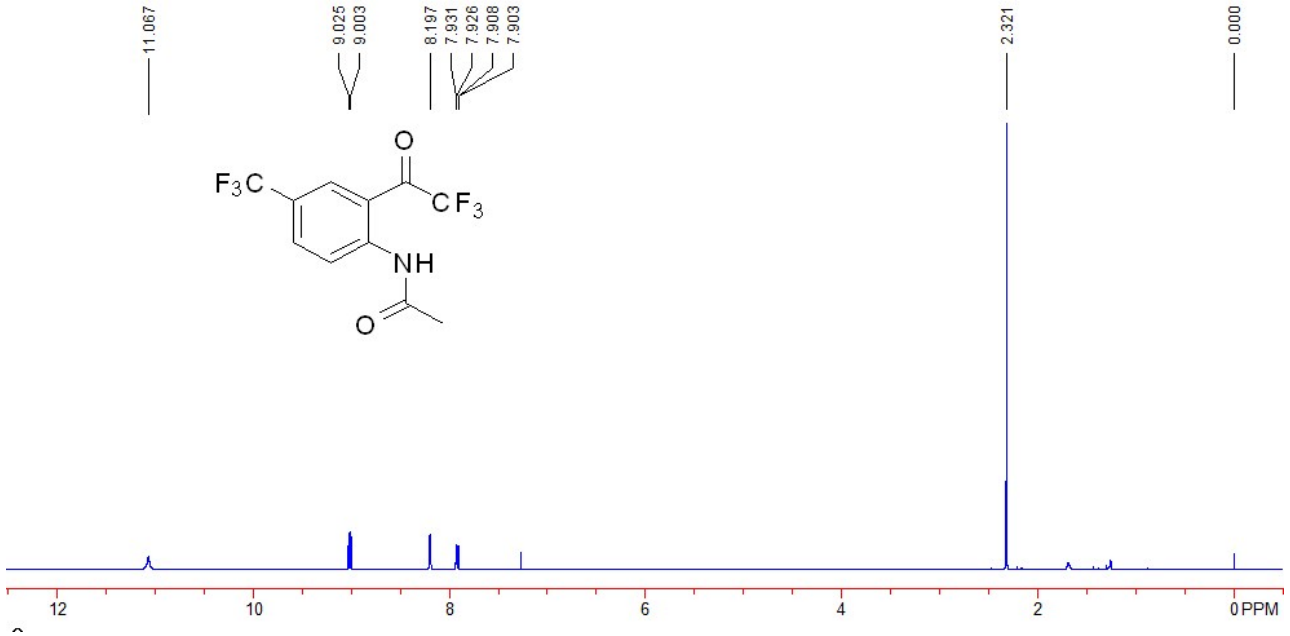
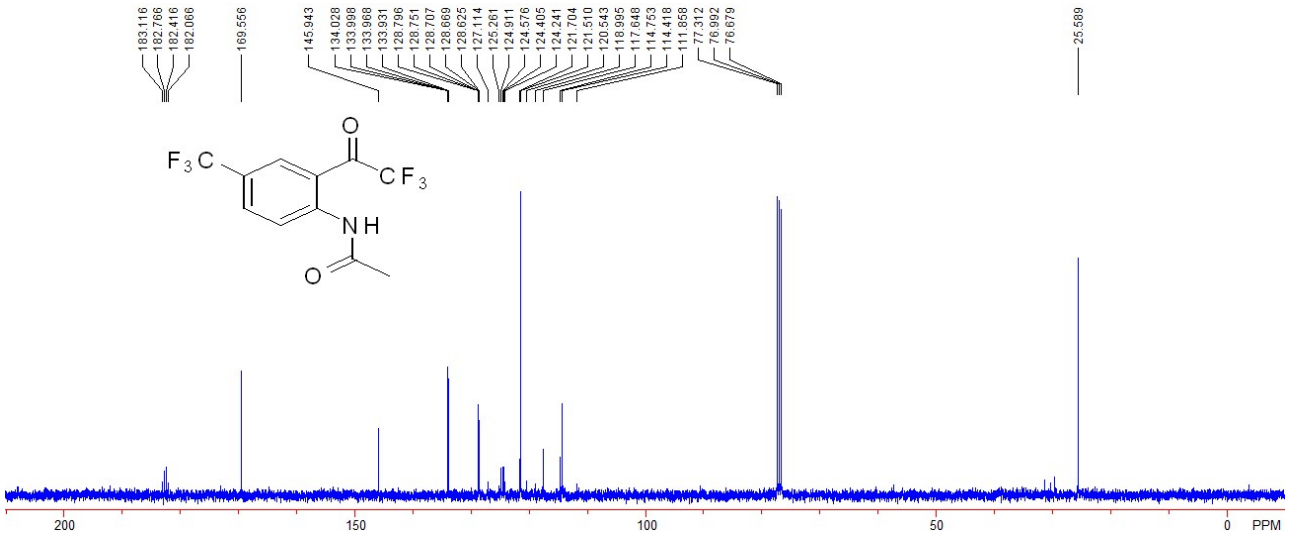
PPM

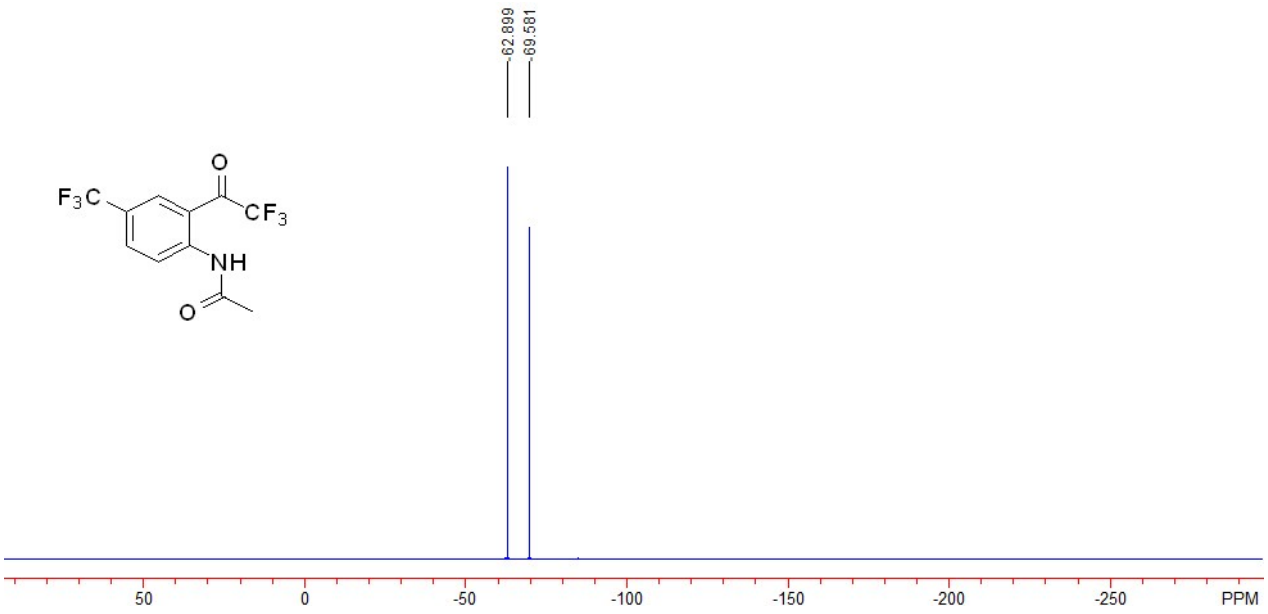


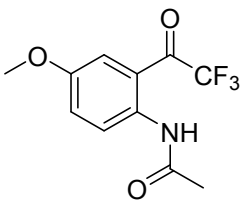
N-(2-(2,2,2-trifluoroacetyl)-4-(trifluoromethyl)phenyl)acetamide (1l)

A yellow solid, 69% yield (207 mg). M.p.: 101-103 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.32 (s, 3H, CH_3), 7.92 (dd, *J* = 2.0, 9.2 Hz, 1H, ArH), 8.20 (s, 1H, ArH), 9.01 (d, *J* = 8.8 Hz, 1H, ArH), 10.07 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 25.6, 114.4, 116.2 (q, *J* = 289.5 Hz), 121.5, 123.1 (q, *J* = 270.1 Hz), 124.7 (q, *J* = 33.5 Hz), 128.6~128.8 (m), 134.0 (q, *J* = 3.0 Hz), 145.9, 169.6, 182.6 (q, *J* = 35.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.58, -62.90. IR (CH_2Cl_2) ν 3345, 2924, 2852, 1684, 1601, 1532, 1330, 1304, 1165, 1124, 1086 cm^{-1}. HRMS (ESI) Calcd. For $C_{11}H_8F_6NO_2^{+1}(M+H)^+$ requires 300.0454, Found: 300.0447.





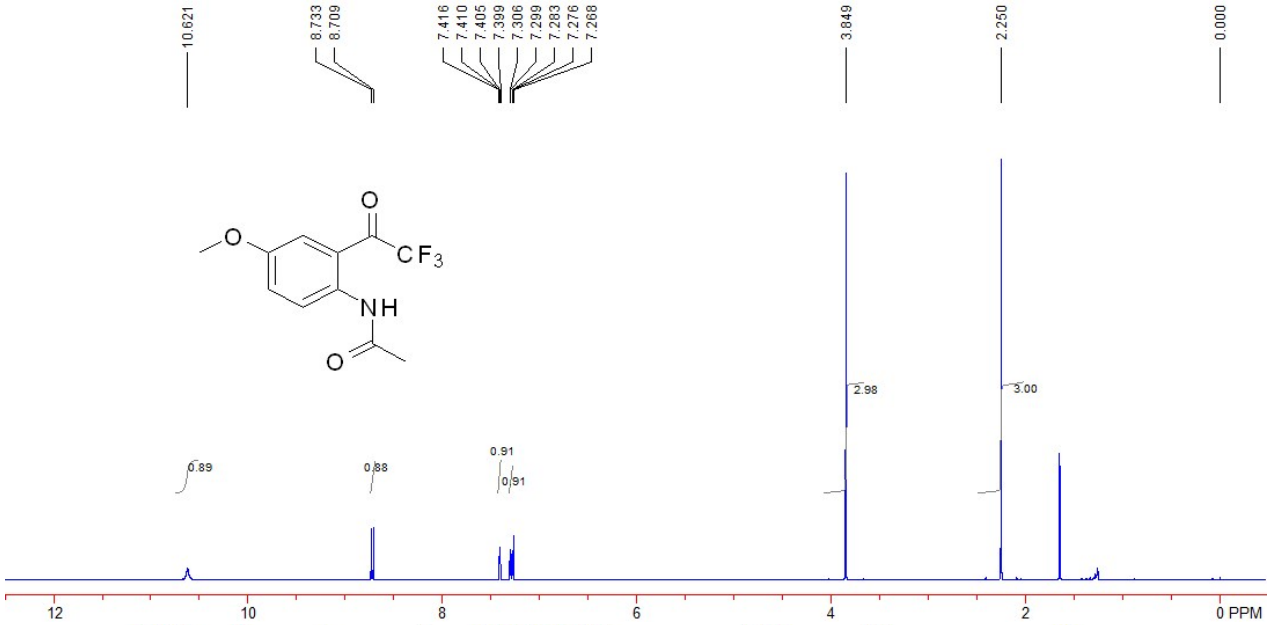


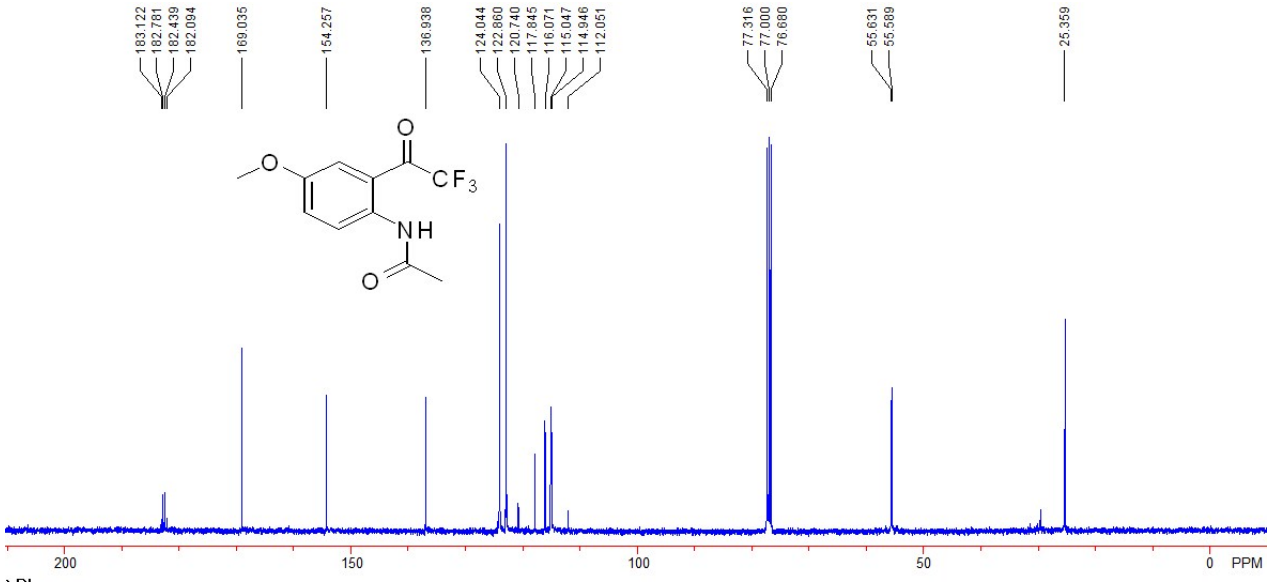


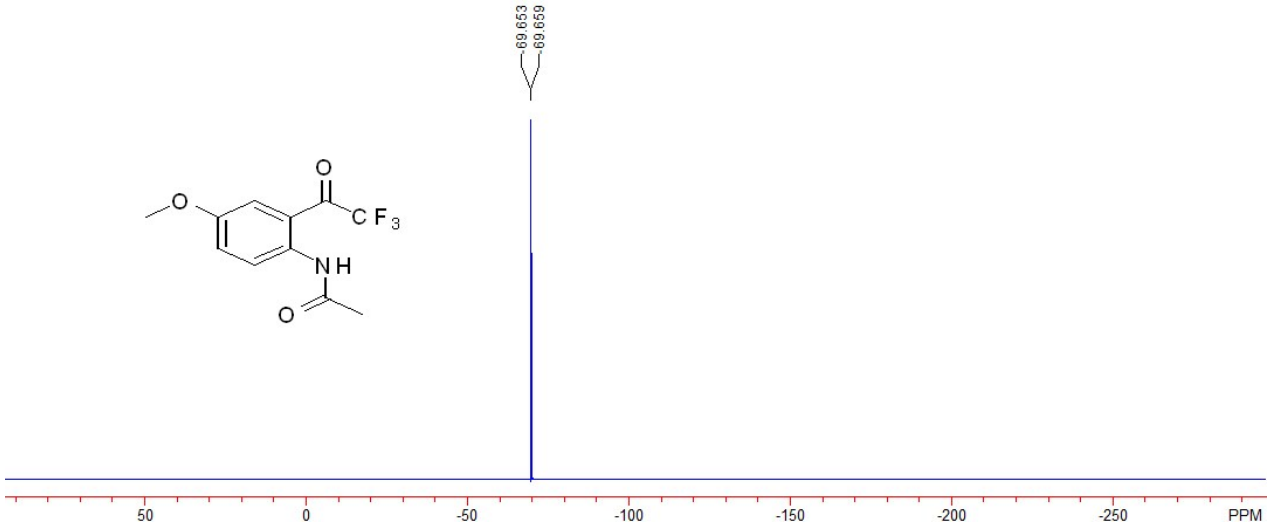
N-(4-methoxy-2-(2,2,2-trifluoroacetyl)phenyl)acetamide (1m)

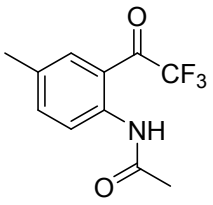
A yellow solid, 78% yield (204 mg). M.p.: 107-109 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.25 (s, 3H, CH_3), 3.85 (s, 3H, CH_3), 7.29 (dd, J = 2.8, 9.2 Hz, 1H, ArH), 7.39~7.42 (m, 1H, ArH), 8.72 (d, J = 9.2 Hz, 1H, ArH), 10.62 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 25.4, 55.6 (d, J = 4.2 Hz), 115.0, 116.1, 116.4 (q, J = 289.9 Hz), 122.9, 124.0, 136.9, 154.3, 169.0, 182.6 (q, J = 34.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.66 (d, J = 2.26 Hz). IR (CH_2Cl_2) ν 3348, 2926, 2852, 1673, 1523, 1371, 1184, 1160, 1041, 974, 863 cm^{-1}. HRMS (ESI) Calcd. For

$C_{11}H_{11}F_3NO_3^{+1}(M+H)^+$ requires 262.0686, Found: 262.0680.



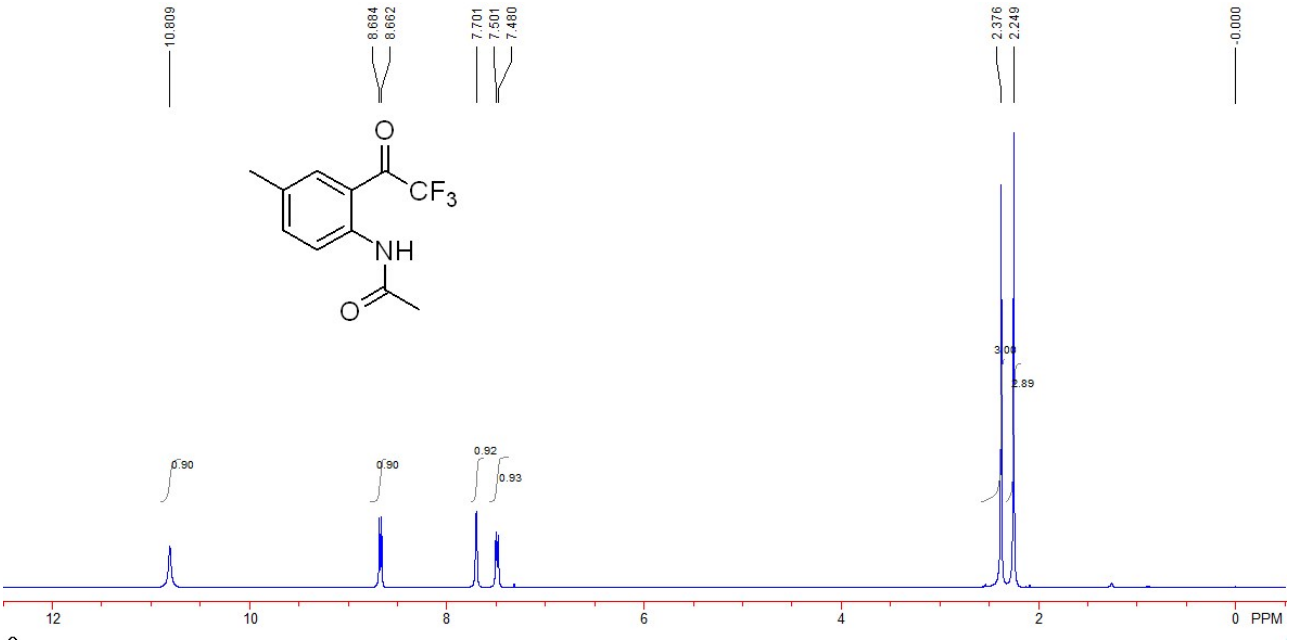


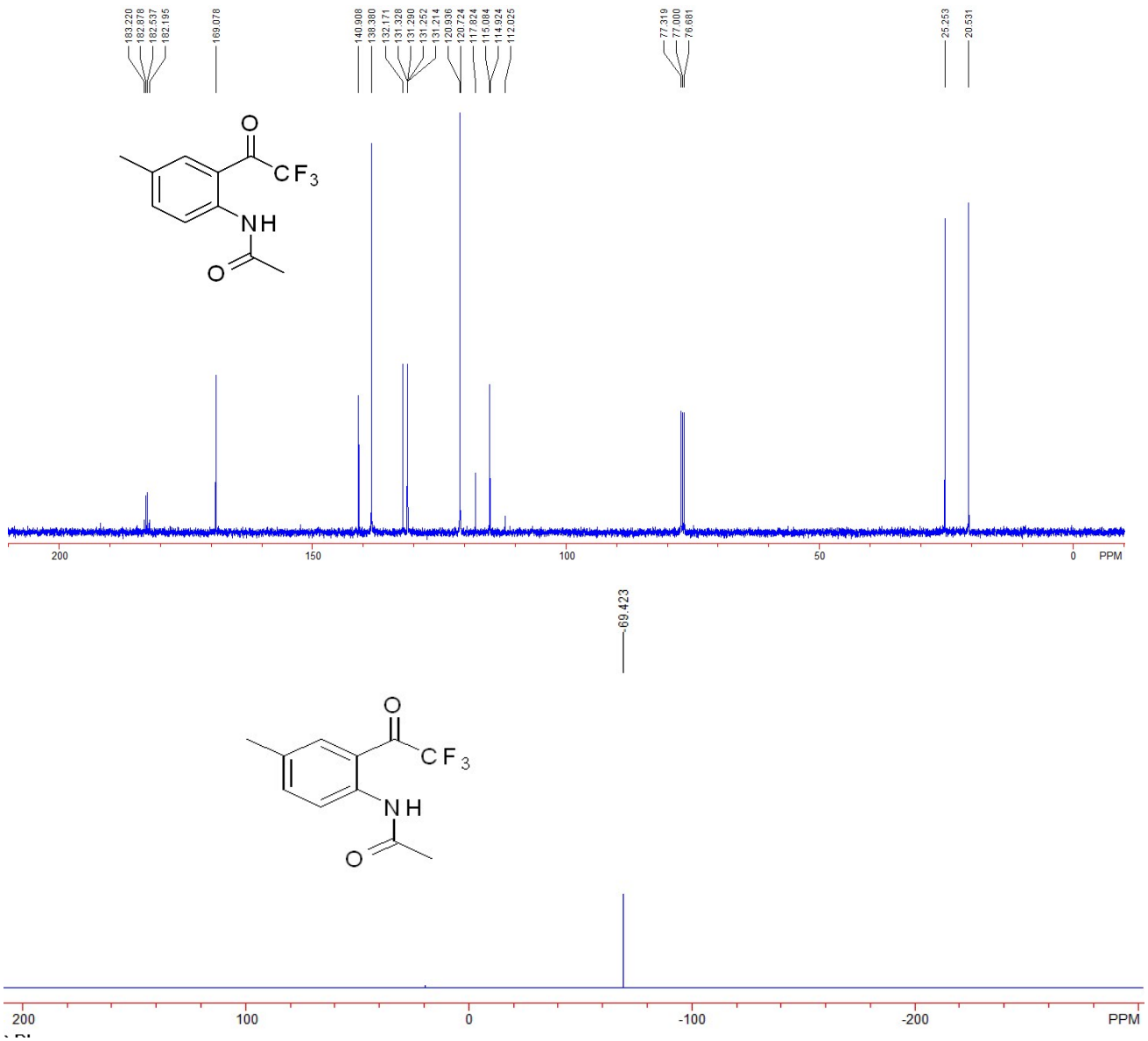


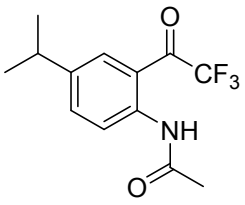


N-(4-methyl-2-(2,2,2-trifluoroacetyl)phenyl)acetamide (1n)

A yellow oil, 63% yield (155 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.25 (s, 3H, CH_3), 2.38 (s, 3H, CH_3), 7.49 (d, J = 8.4 Hz, 1H, ArH), 7.70 (s, 1H, ArH), 8.67 (d, J = 8.8 Hz, 1H, ArH), 11.81 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 20.5, 25.3, 115.1, 116.4 (q, J = 290.0 Hz), 120.9, 131.3 (q, J = 3.8 Hz), 132.2, 138.4, 140.9, 169.1, 182.7 (q, J = 34.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.42. IR (CH_2Cl_2) ν 3338, 2955, 2926, 1675, 1522, 1199, 1158, 977, 943, 737 cm^{-1}. HRMS (ESI) Calcd. For $C_{11}H_{11}F_3NO_2^{+1}(M+H)^+$ requires 246.0736, Found: 246.0737.



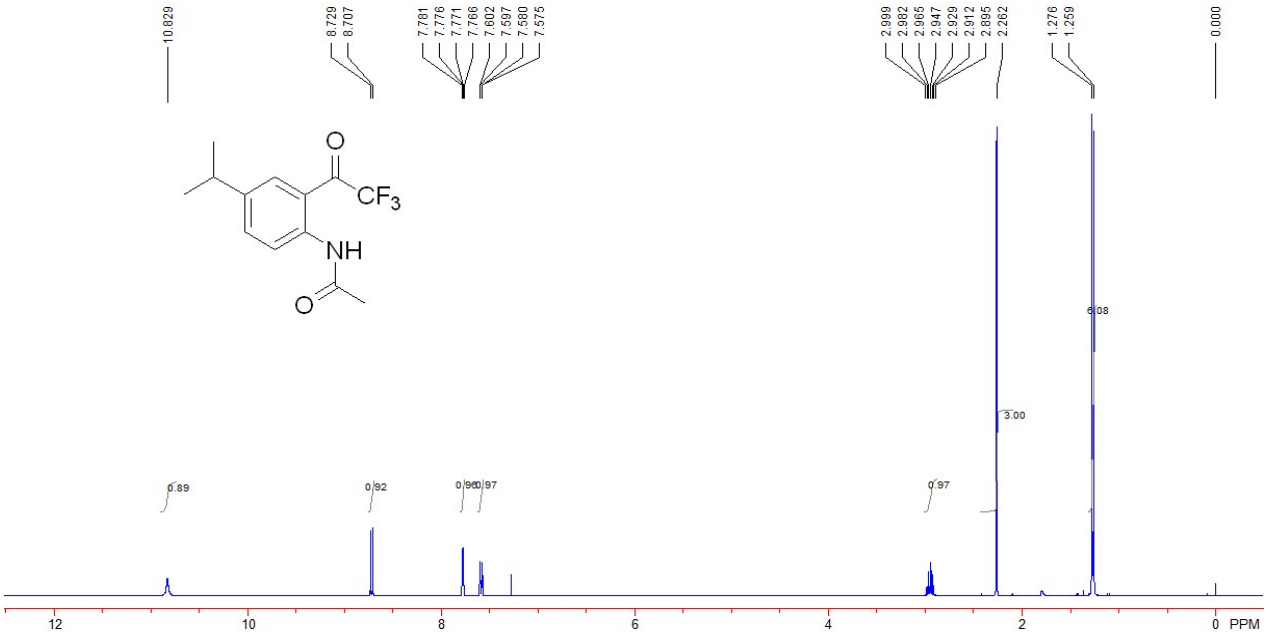


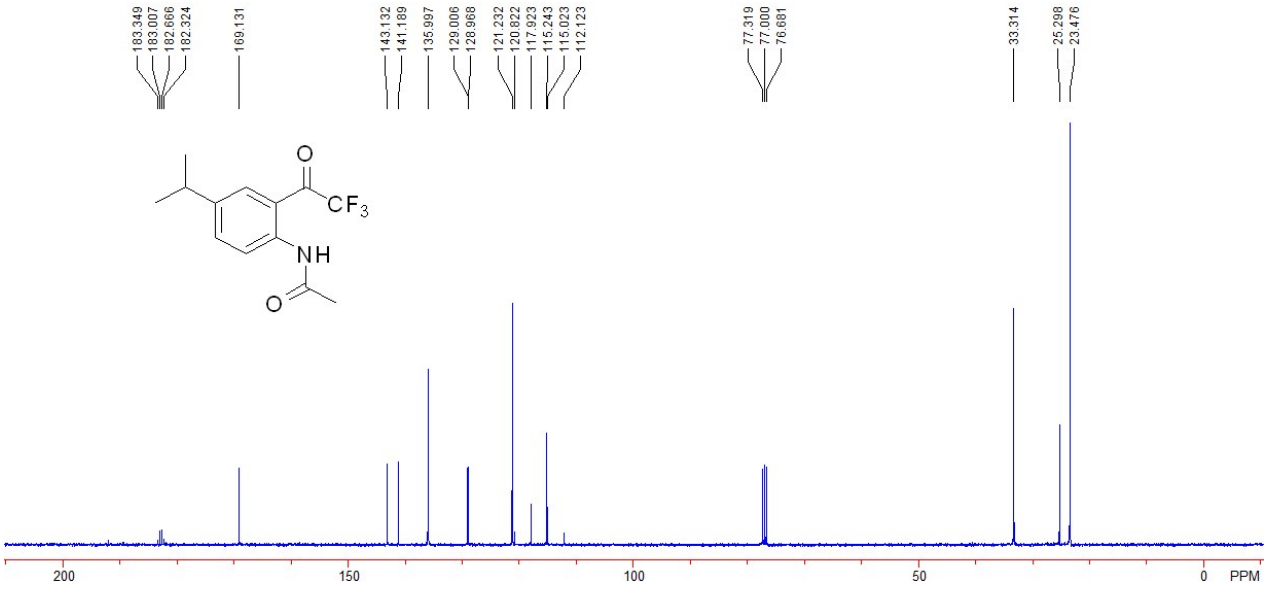


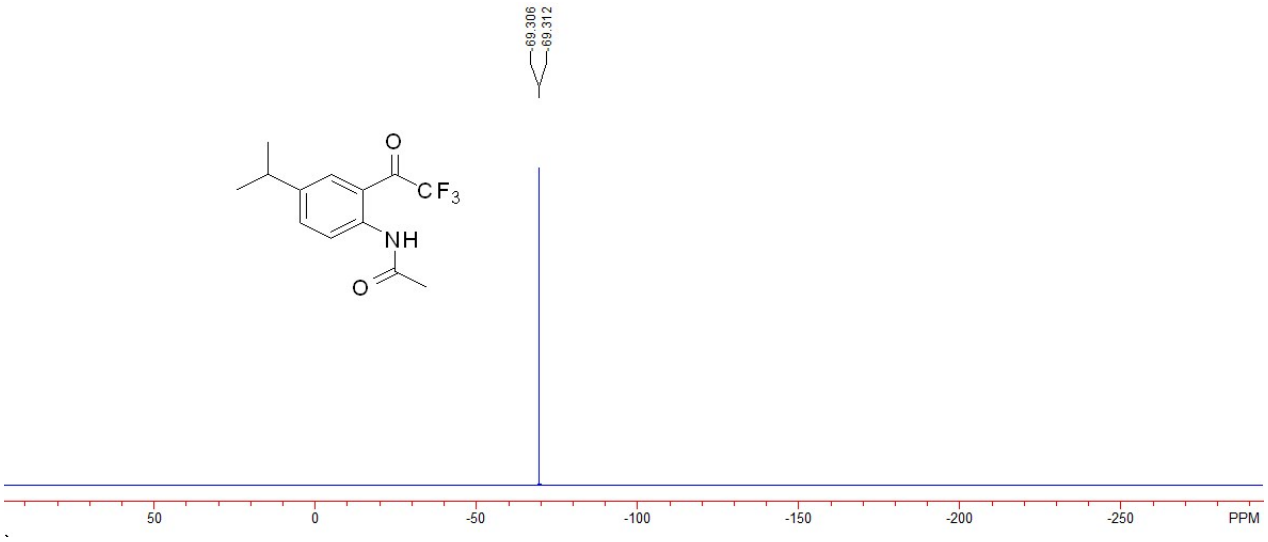
N-(4-isopropyl-2-(2,2,2-trifluoroacetyl)phenyl)acetamide (1o)

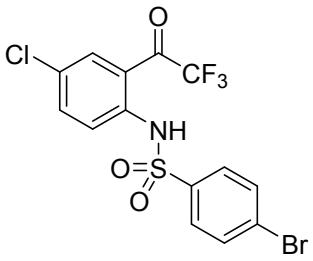
A yellow oil, 59% yield (162 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.27 (d, J = 6.8 Hz, 6H, CH_3), 2.26 (s, 3H, CH_3), 2.89~3.00 (m, 1H, CH), 7.59 (dd, J = 2.0, 8.8 Hz, 1H, ArH), 7.76~7.79 (m, 1H, ArH), 8.72 (d, J = 8.8 Hz, 1H, ArH), 10.8 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 23.5, 25.3, 33.3, 115.2, 116.5 (q, J = 290.0 Hz), 120.8, 121.2, 129.0 (q, J = 3.8 Hz), 136.0, 141.2, 143.1, 169.1, 182.8 (q, J = 34.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.31 (d, J = 2.26 Hz).

IR (CH_2Cl_2) ν 3340, 2964, 2932, 1674, 1596, 1522, 1305, 1170, 1149, 1080, 978 cm^{-1}. HRMS (ESI) Calcd. For $C_{13}H_{15}F_3NO_2^{+1}(M+H)^+$ requires 274.1049, Found: 274.1043.



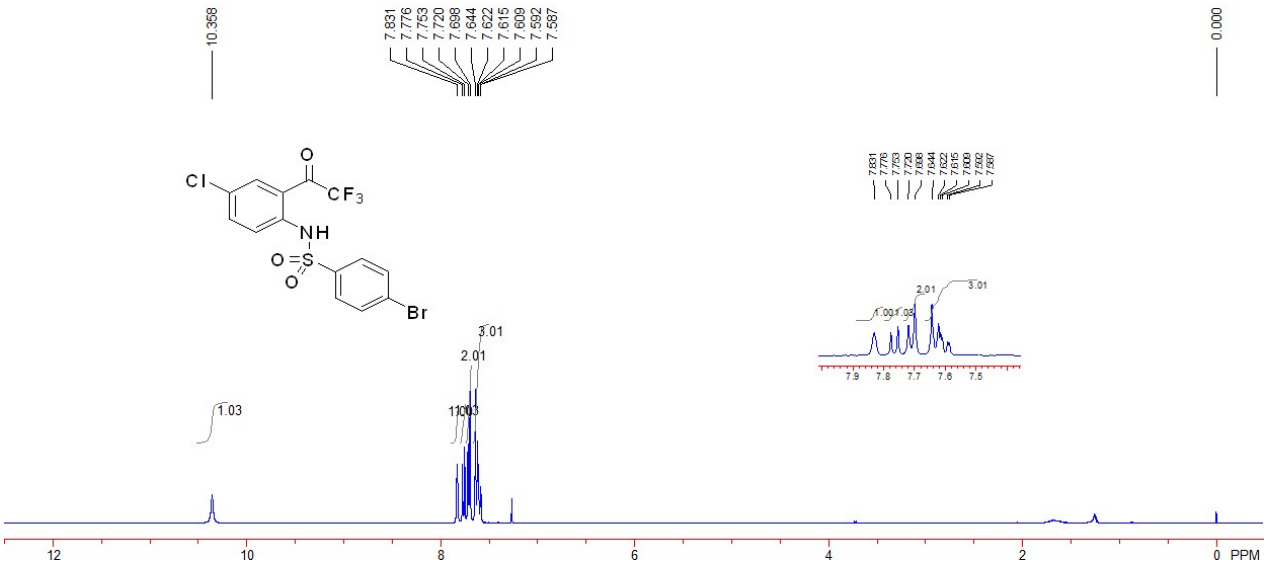






4-bromo-N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)benzenesulfonamide (1r)

A yellow solid, 31% yield (142 mg). M.p.: 141-143 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) 7.58~7.65 (m, 3H, ArH), 7.71 (d, J = 8.8 Hz, 2H, ArH), 7.76 (d, J = 9.2 Hz, 1H, ArH), 7.83 (s, 1H, ArH), 10.36 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 115.9 (q, J = 290.0 Hz), 117.1, 121.1, 128.7, 129.0, 131.5 (q, J = 4.6 Hz), 132.7, 137.4, 137.5, 140.3, 182.1 (q, J = 34.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -69.92. IR (CH_2Cl_2) ν 3229, 2964, 2903, 2359, 1690, 1204, 1178, 1164, 739, 702 cm^{-1}. HRMS (ESI) Calcd. For $C_{14}H_{12}O_3N_2BrClF_3S^{+1}(M+NH_4)^+$ requires 458.9387, Found: 458.9387.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CF3
NH
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Br
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2.01
1.03
1.00
1.03
12
10
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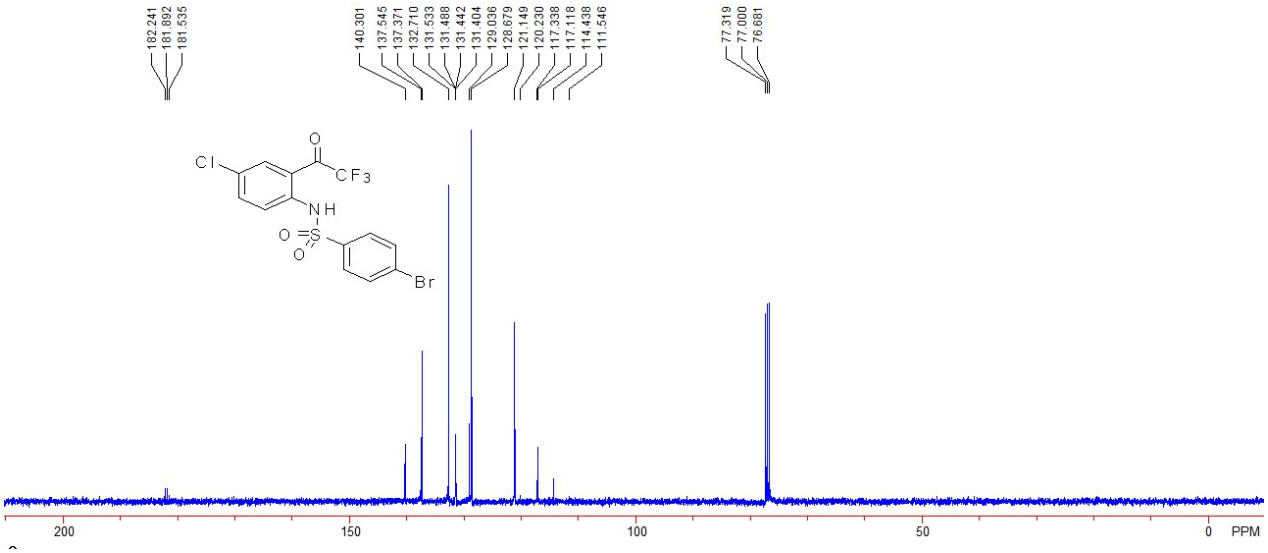
6
4
2
0
PPM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132.710
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114.438
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Cl
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CF3
NH
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Br
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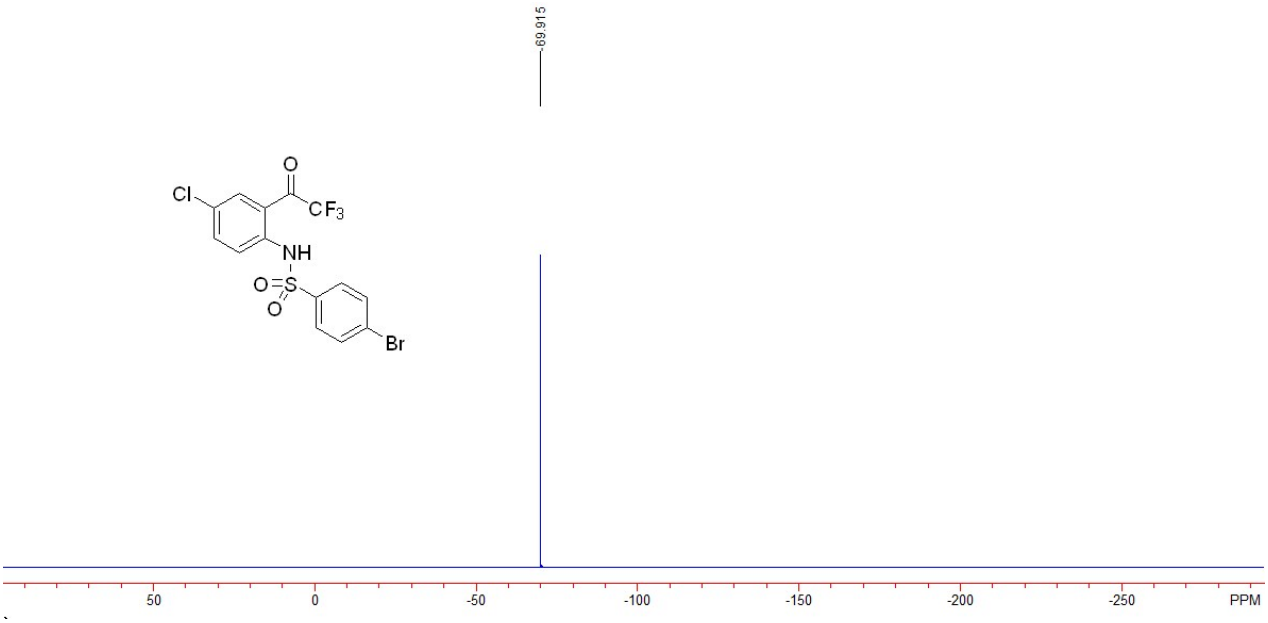
PPM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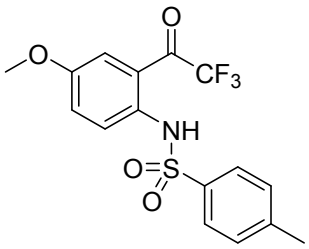
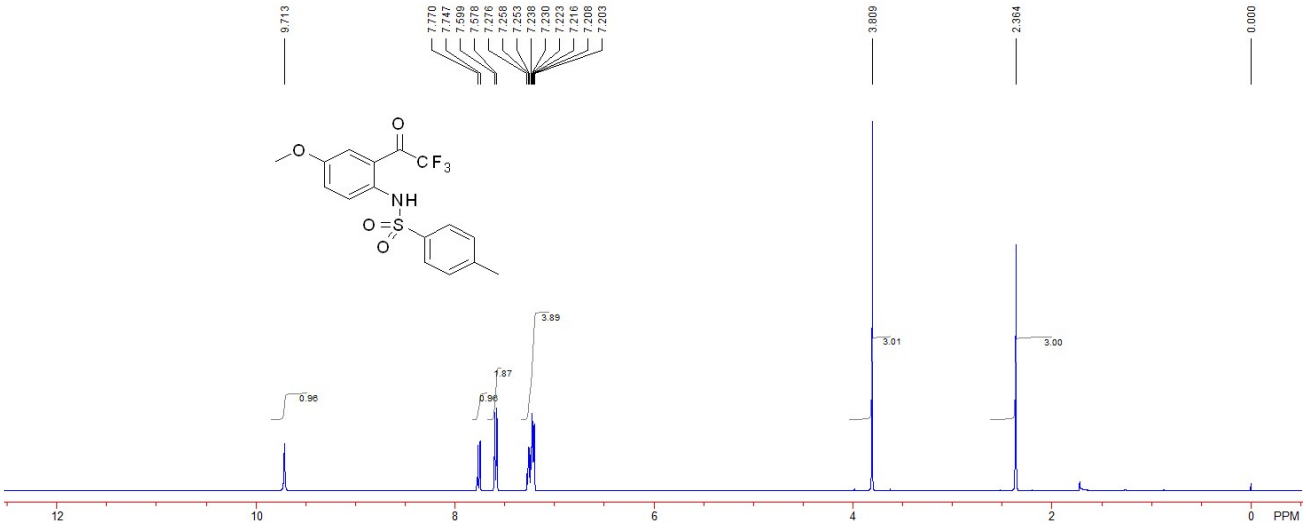
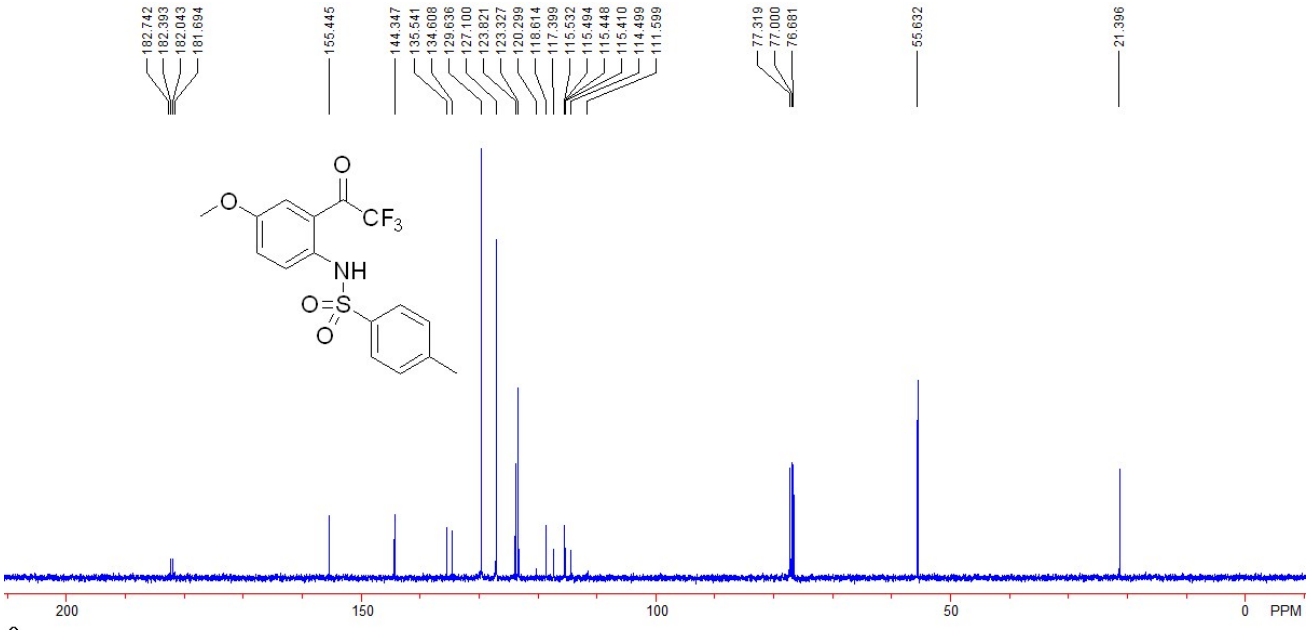
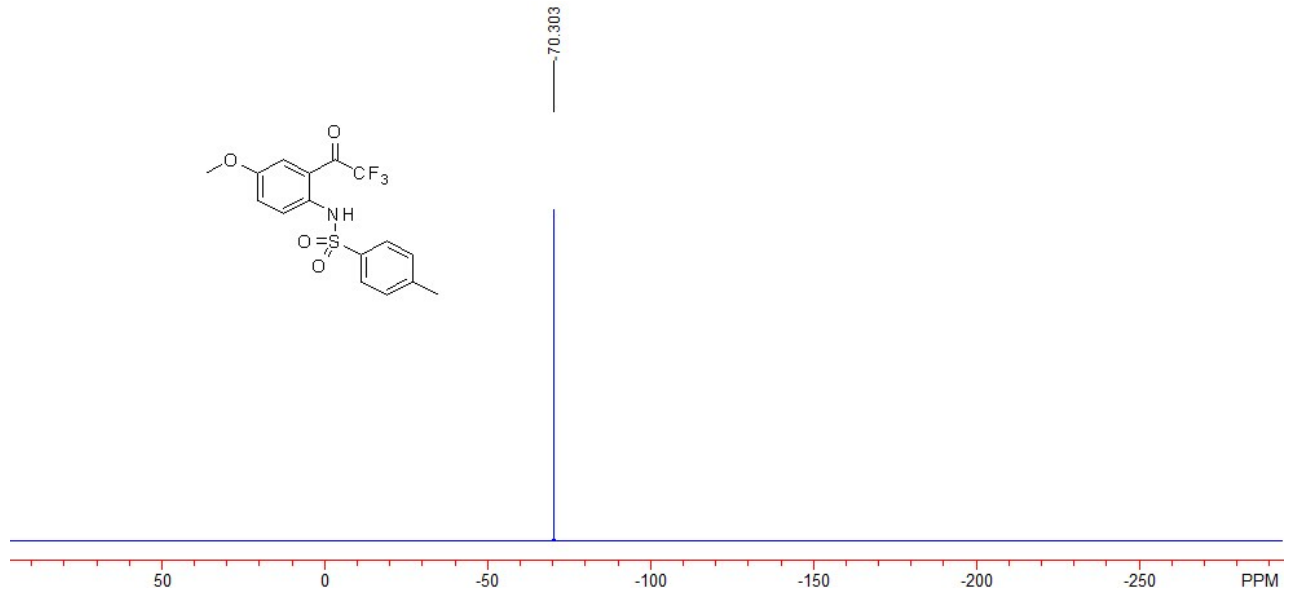


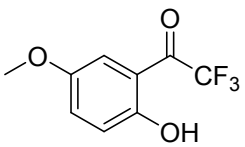
N-(4-methoxy-2-(2,2,2-trifluoroacetyl)phenyl)-4-methylbenzenesulfonamide (1s)

A yellow solid, 42% yield (157 mg). M.p.: 122-124 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) 2.36 (s, 3H, CH_3), 3.81 (s, 3H, CH_3), 7.20~7.28 (m, 4H, ArH), 7.59 (d, J = 8.4 Hz, 2H, ArH), 7.76 (d, J = 9.2 Hz, 1H, ArH), 9.71 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 21.4, 55.6, 115.5 (q, J = 4.6 Hz), 115.9 (q, J = 290.0 Hz), 118.6, 123.3, 123.8, 127.1, 129.6, 134.6, 135.5, 144.3, 155.4, 182.2 (q, J = 35.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -70.30. IR (CH_2Cl_2) ν 3675, 2970, 2900, 2361, 2342, 1506, 1394, 1158, 1075, 1066, 668 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{15}F_3NO_4S^{+1}(M+H)^+$ requires 374.0668, Found: 374.0669.





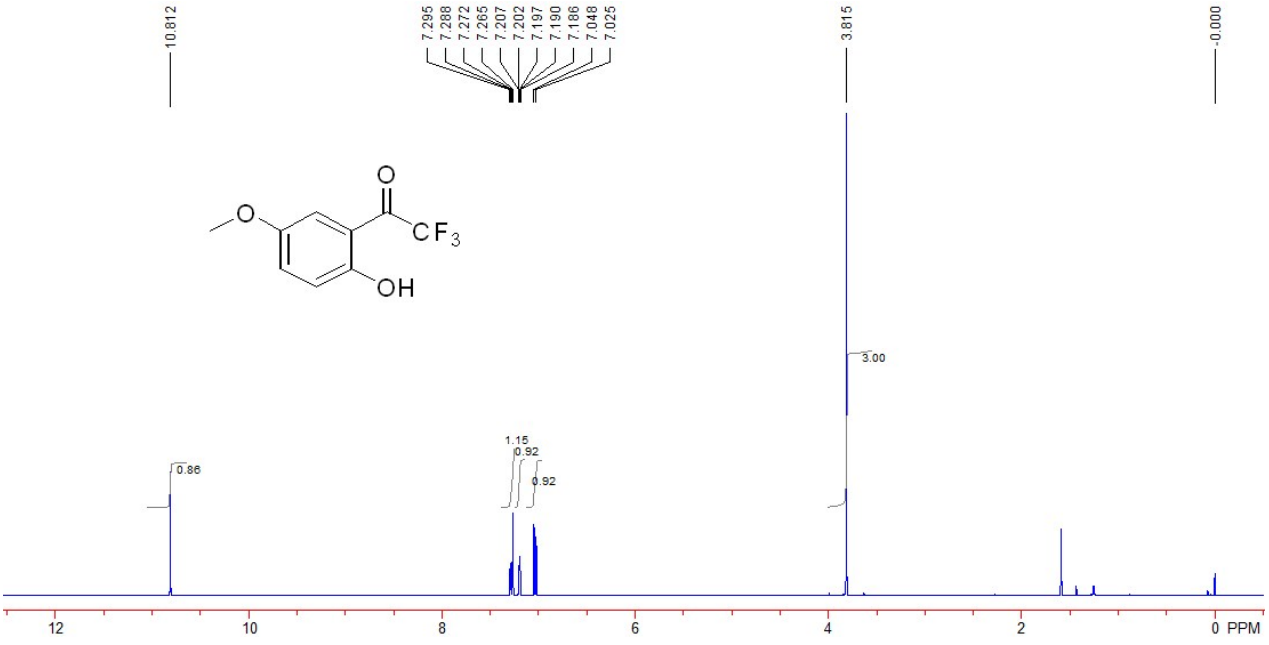


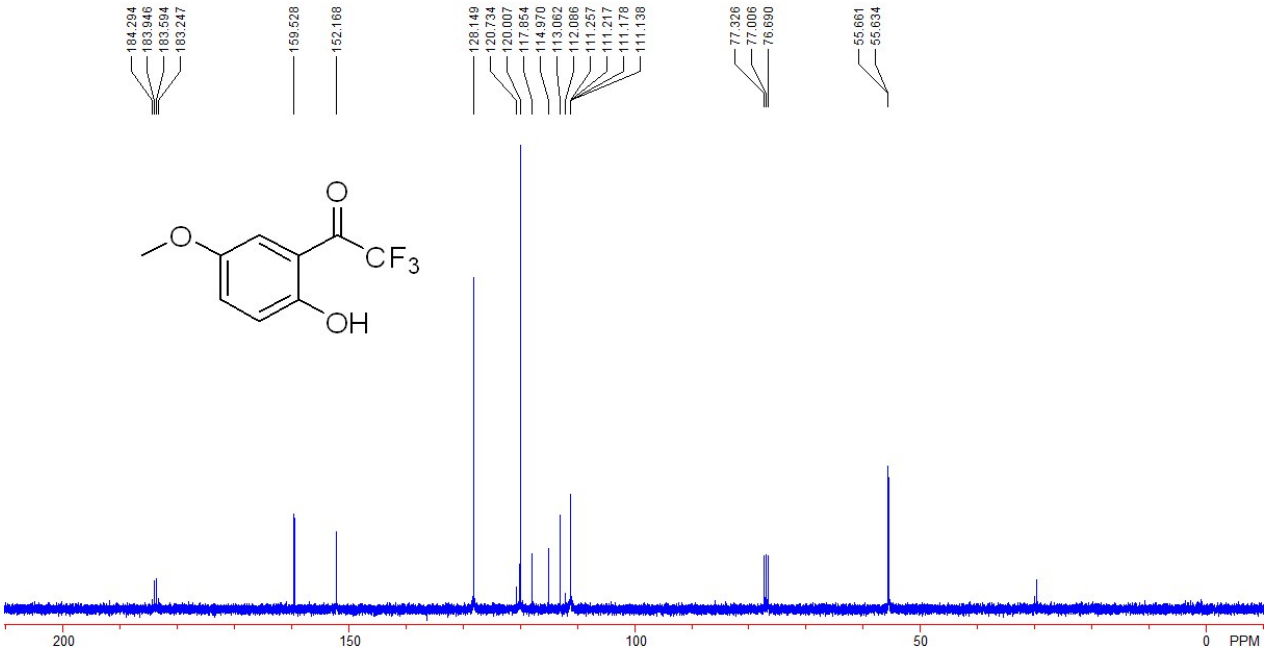


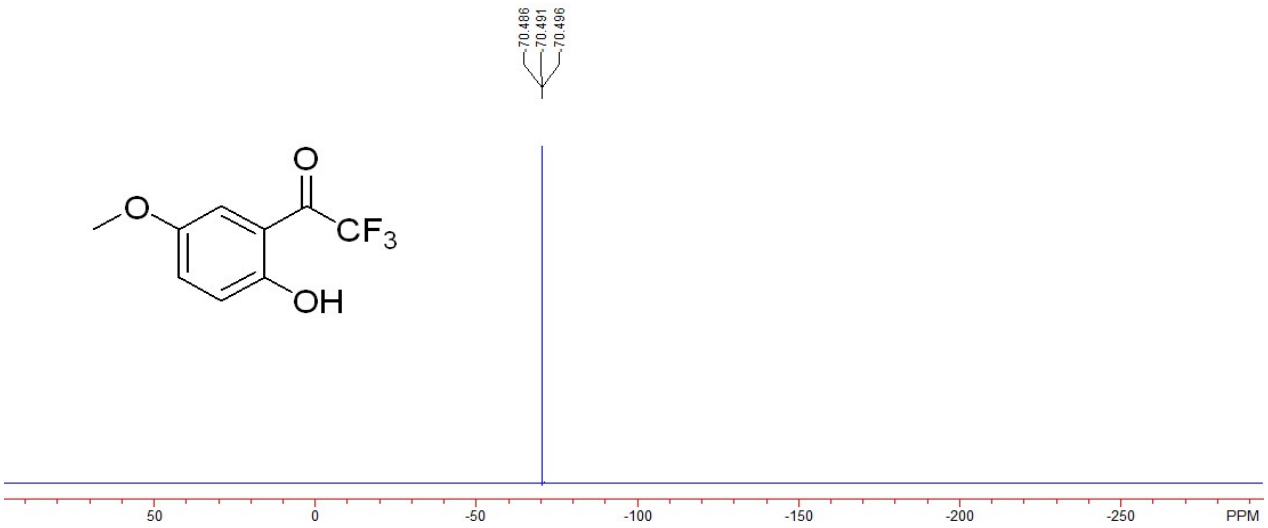
2,2,2-trifluoro-1-(2-hydroxy-5-methoxyphenyl)ethan-1-one (1v)

A yellow oil, 58% yield (128 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 3.82 (s, 3H, CH_3), 7.04 (d, J = 9.2 Hz, 1H, ArH), 7.18~7.21 (m, 1H, ArH), 7.28 (dd, J = 2.8, 9.2 Hz, 1H, ArH), 10.81 (s, 1H, OH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 55.6 (d, J = 2.7 Hz), 111.2 (q, J = 3.9 Hz), 113.1, 116.4 (q, J = 288.4 Hz), 120.0, 128.1, 152.2, 159.5, 183.8 (q, J = 35.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$,

$CFCl_3$) δ -70.49 (t, *J* =1.88 Hz). IR (CH_2Cl_2) ν 3675, 2988, 2900, 2360, 2342, 1394, 1065, 1056, 1027, 668 cm^{-1}. MS (%) m/e 151 (M+, 100.00), 220 (55.09), 95 (21.25), 108 (18.74), 53 (14.88), 123 (14.53), 52 (10.28), 135 (10.22). HRMS (EI) calcd. for $C_9H_7O_3F_3$: 220.0347, Found: 220.0346.



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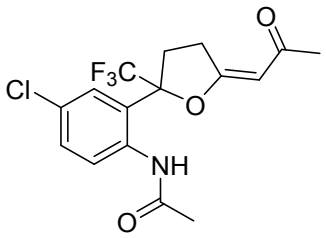
O
CF3
OH
50
0
-50
-100
-150
-200
-250
PPM

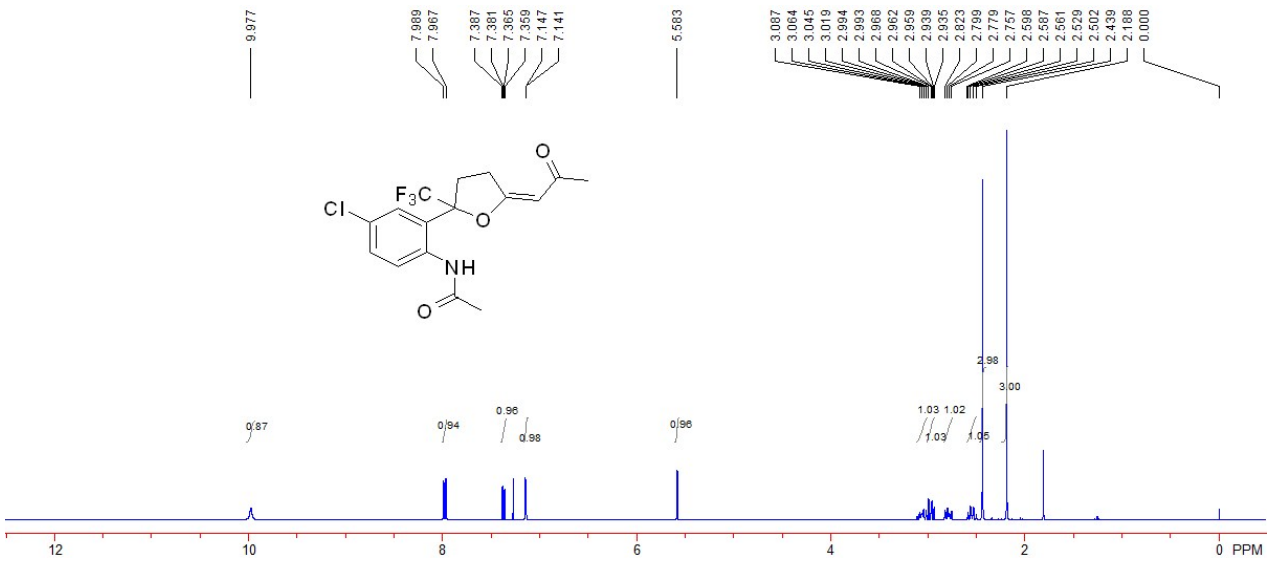
General Procedure for Hex-3-yn-2-one 2a to Trifluoroacetyl Compounds 1 at 65 °C and Spectroscopic Data of the Products 3

General procedure: Under argon atmosphere, to a solution of trifluoroacetyl compound **1** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the hex-3-yn-2-one **1a** (0.6 mmol) at room temperature. Then the resulting mixture was heated to 65 °C and continued stirring at 65 °C until the reaction completed (monitoring by TLC). Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the desired products **3a**-**3o**.



(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (3a)

A white solid, 68% yield (49 mg). M.p.: 139-141 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.19 (s, 3H, CH_3), 2.44 (s, 3H, CH_3), 2.50~2.60 (m, 1H, CH_2), 2.75~2.83 (m, 1H, CH_2), 2.93~3.00 (m, 1H, CH_2), 3.01~3.09 (m, 1H, CH_2), 5.58 (s, 1H, =CH), 7.14 (d, *J* = 2.4 Hz, 1H, ArH), 7.37 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 7.98 (d, *J* = 8.8 Hz, 1H, ArH), 9.98 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 24.1, 29.7 (d, *J* = 1.5 Hz), 31.1, 31.4, 91.9 (q, *J* = 30.3 Hz), 100.4, 124.2 (q, *J* = 285.4 Hz), 126.7, 128.0, 128.1, 129.2, 130.1, 136.3, 166.8, 170.2, 195.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.22. IR (CH_2Cl_2) ν 3750, 3710, 3549, 2918, 2363, 1967, 1275, 1260, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{16}ClF_3NO_3^{+1}$(M+H)$^+$ requires 362.0765, Found: 362.0766.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F3C
Cl
O
NH
O
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3.00
0.96
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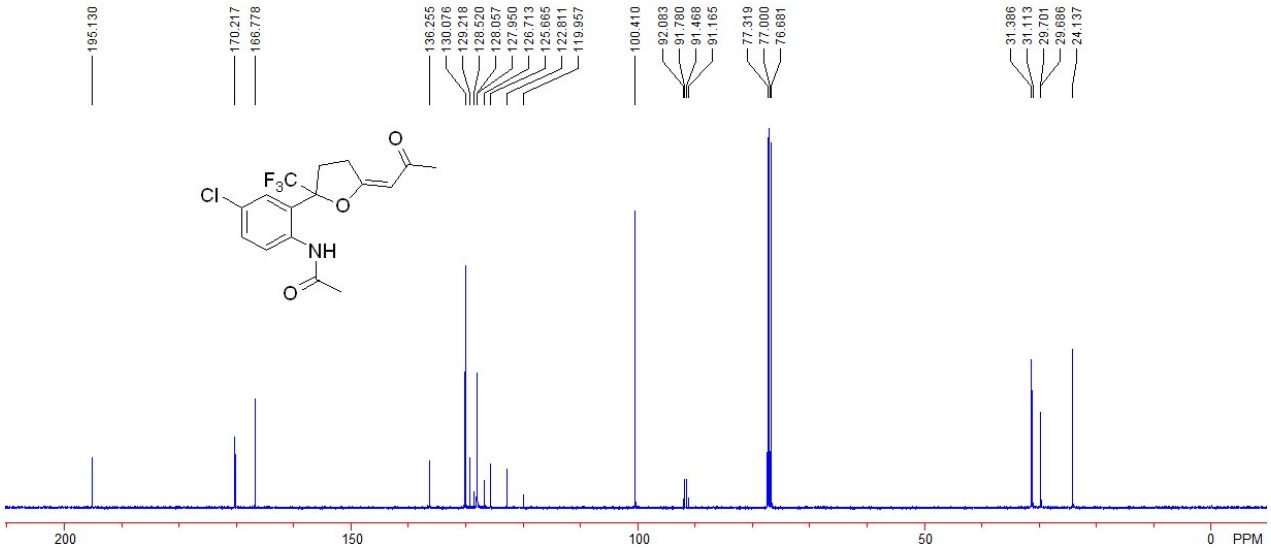
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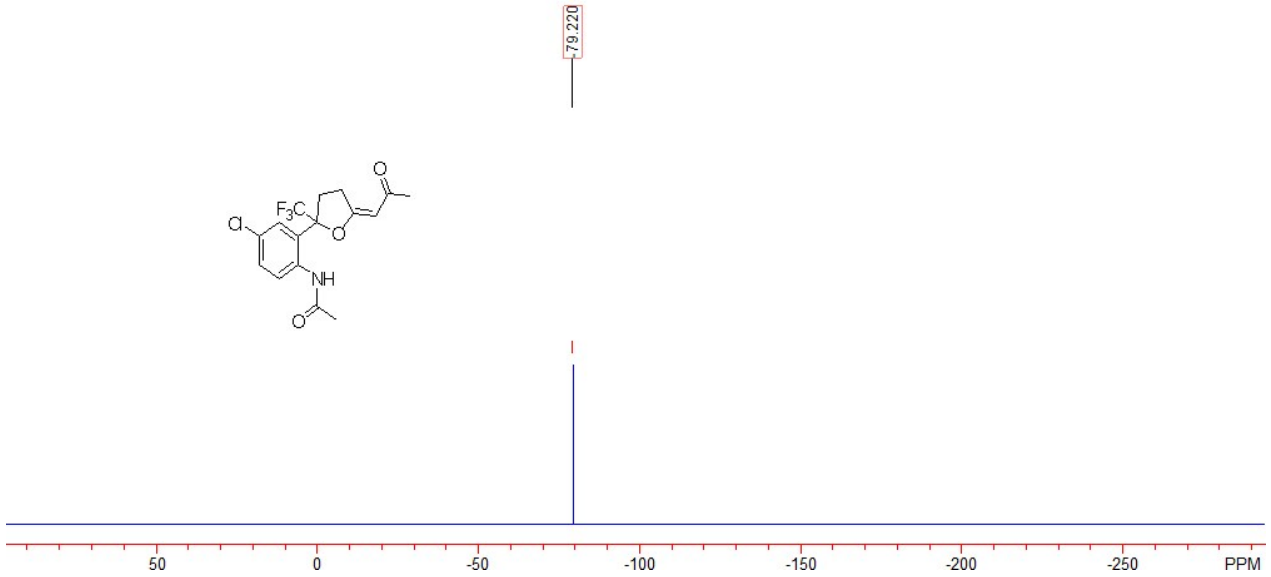
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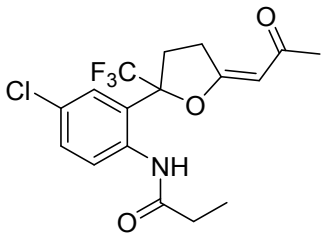
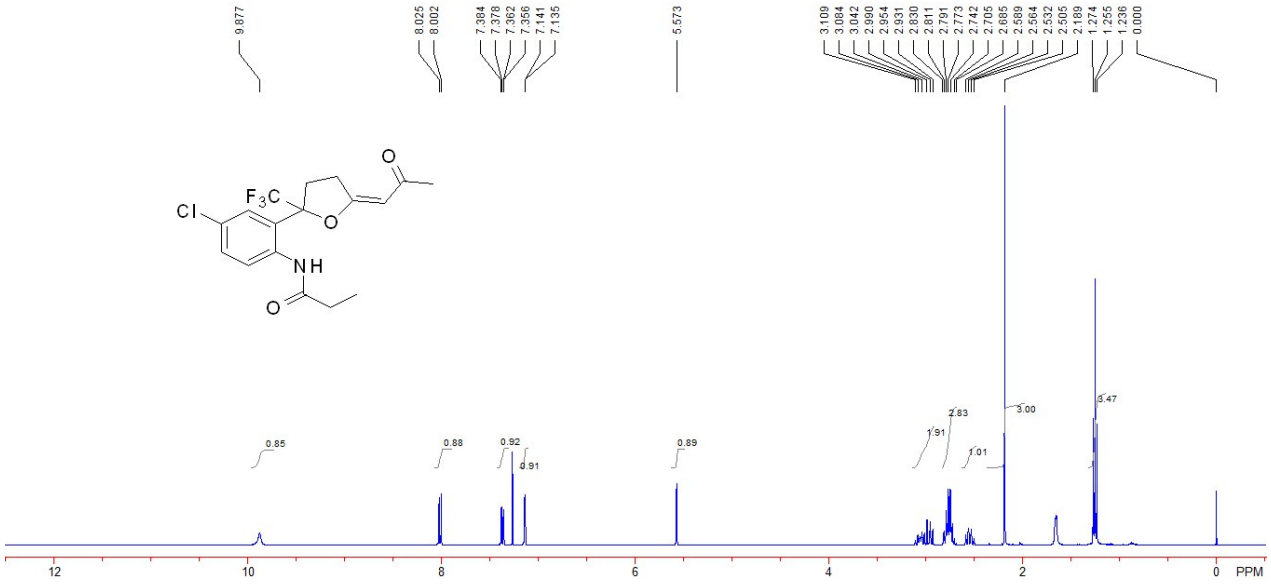
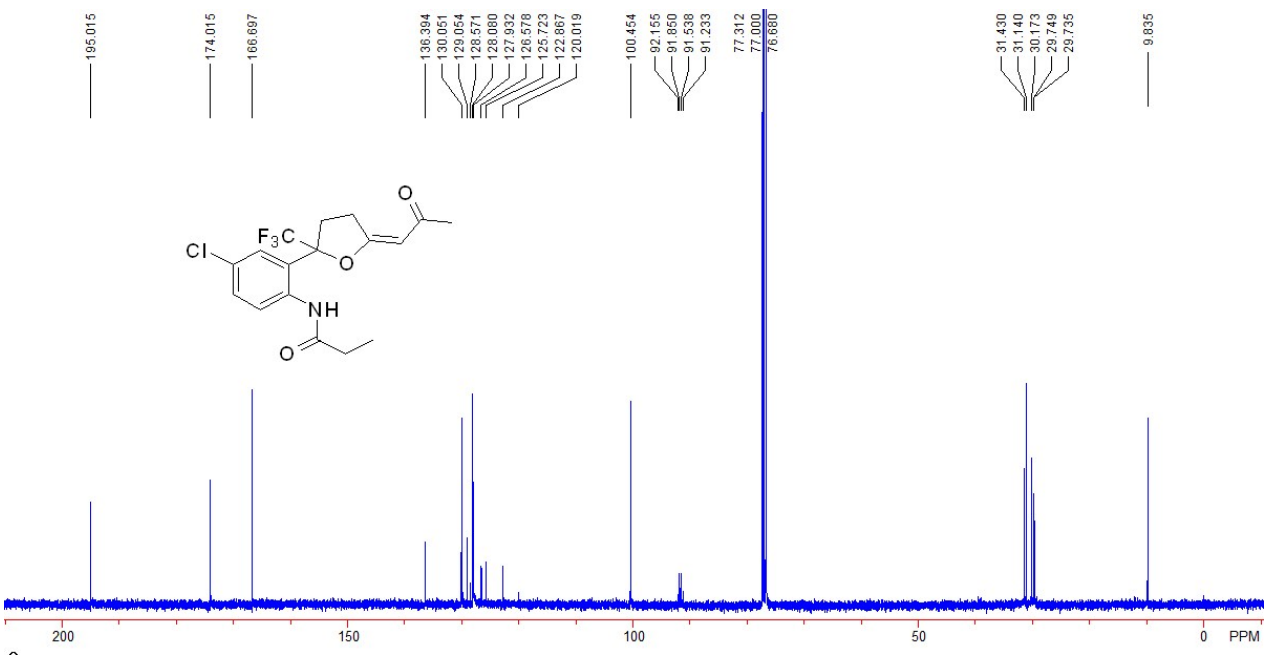
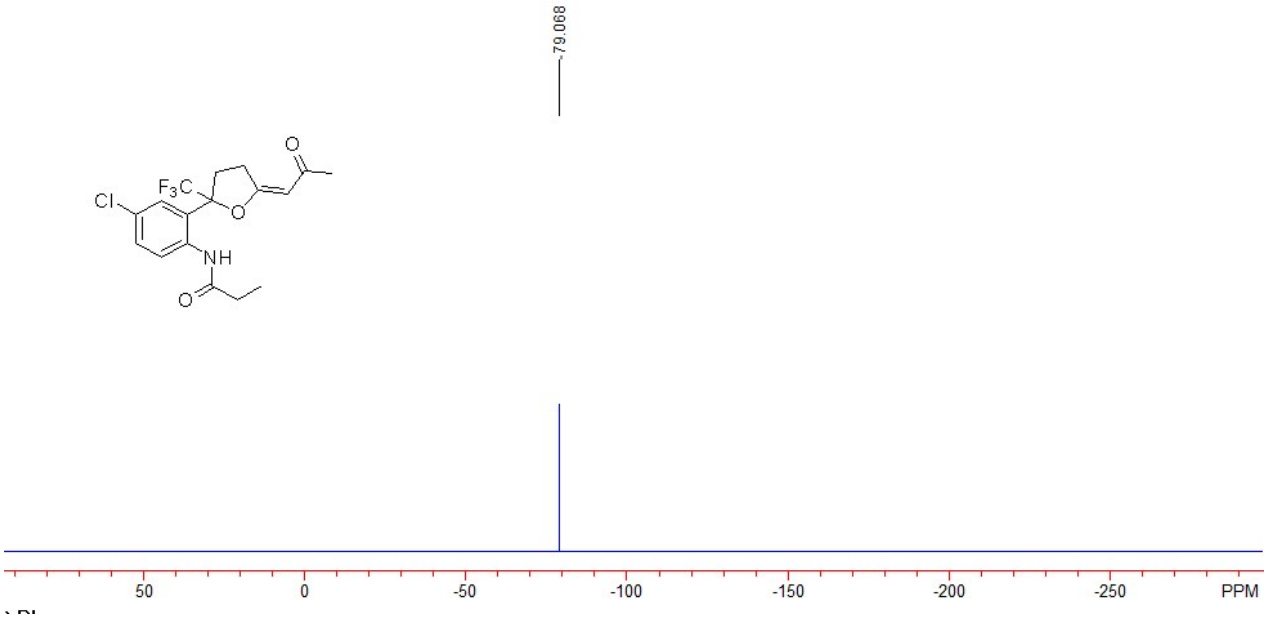


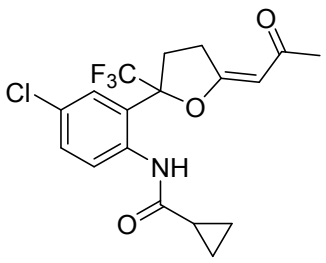
(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)propionamide (3b)

A white solid, 51% yield (38 mg). M.p.: 146-148 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.26 (t, *J* = 7.6 Hz, 3H, CH_3), 2.19 (s, 3H, CH_3), 2.50~2.59 (m, 1H, CH_2), 2.68~2.83 (m, 3H, CH_2), 2.93~3.11 (m, 2H, CH_2), 5.57 (s, 1H, =CH), 7.14 (d, *J* = 2.4 Hz, 1H, ArH), 7.37 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 8.01 (d, *J* = 8.8 Hz, 1H, ArH), 9.88 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 9.8, 29.7 (d, *J* = 1.4 Hz), 30.2, 31.1, 31.4, 91.7 (q, *J* = 31.2 Hz), 100.5, 124.3 (q, *J* = 285.6 Hz), 126.6, 128.0, 128.1, 128.6, 129.1, 130.1, 136.4, 166.7, 174.0, 195.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.07. IR (CH_2Cl_2) ν 3341, 2924, 2852, 1688, 1620, 1507, 1188, 1174, 1077, 924 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{18}ClF_3NO_3^{+1}$(M+H)$^+$ requires 376.0922, Found: 376.0923.





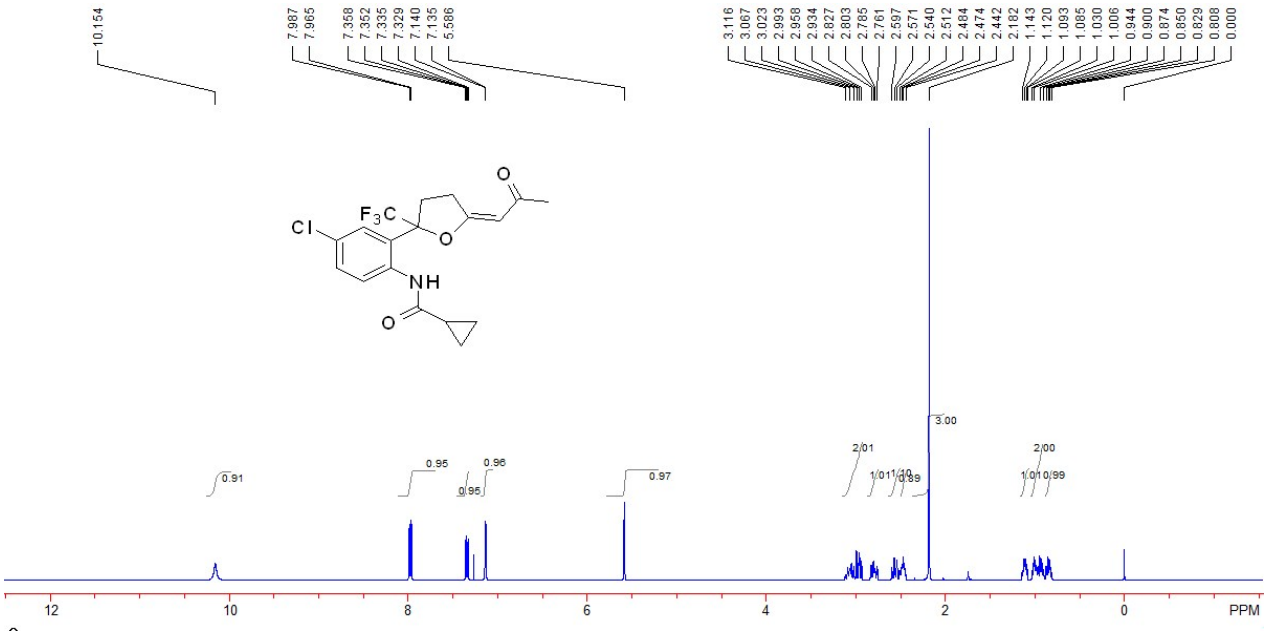


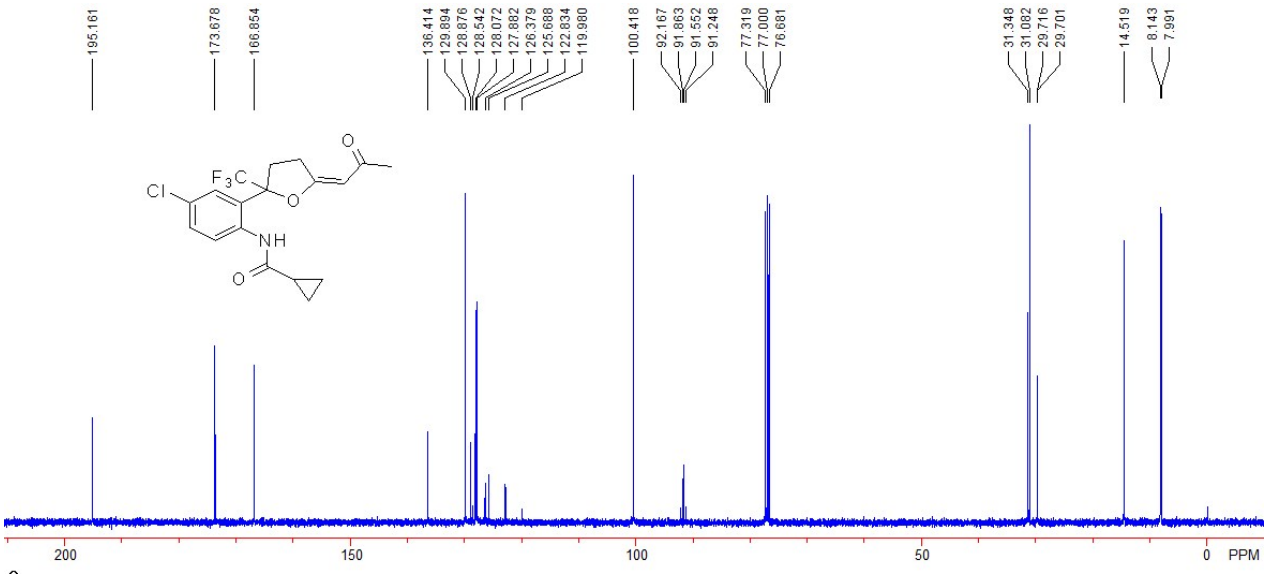


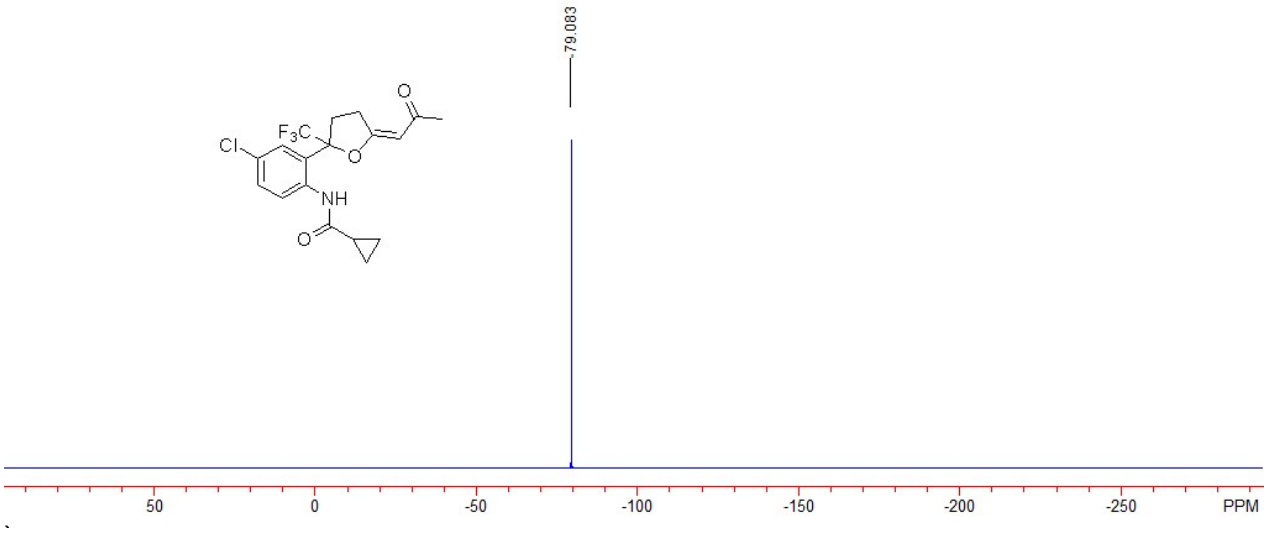
(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)cyclopropanecarboxamide (3c)

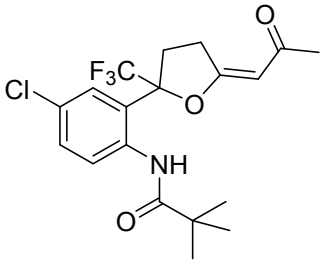
A white solid, 61% yield (47 mg). M.p.: 151-153 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 0.80~0.88 (m, 1H, CH_2), 0.90~1.03 (m, 2H, CH_2), 1.08~1.15 (m, 1H, CH_2), 2.18 (s, 3H, CH_3),

2.44~2.505 (m, 1H, CH), 2.512~2.60 (m, 1H, CH_2), 2.76~2.83 (m, 1H, CH_2), 2.93~3.12 (m, 2H, CH_2), 5.59 (s, 1H, =CH), 7.14 (d, J = 2.0 Hz, 1H, ArH), 7.34 (dd, J = 2.0, 8.8 Hz, 1H, ArH), 7.98 (d, J = 8.8 Hz, 1H, ArH), 10.15 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 8.0, 8.14, 14.5, 29.7 (d, J = 1.5 Hz), 31.1, 31.3, 91.7 (q, J = 31.1 Hz), 100.4, 124.3 (q, J = 285.4 Hz), 126.4, 127.9, 128.1, 128.9, 129.9, 136.4, 166.9, 173.7, 195.2. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.08. IR (CH_2Cl_2) ν 3675, 3345, 2968, 2923, 1686, 1620, 1507, 1401, 1285, 1191, 1173, 1076, 1051, 923, 706 cm^{-1}. HRMS (ESI) Calcd. For $C_{18}H_{18}ClF_3NO_3{}^{+1}(M+H)^+$ requires 388.0922, Found: 388.0921.



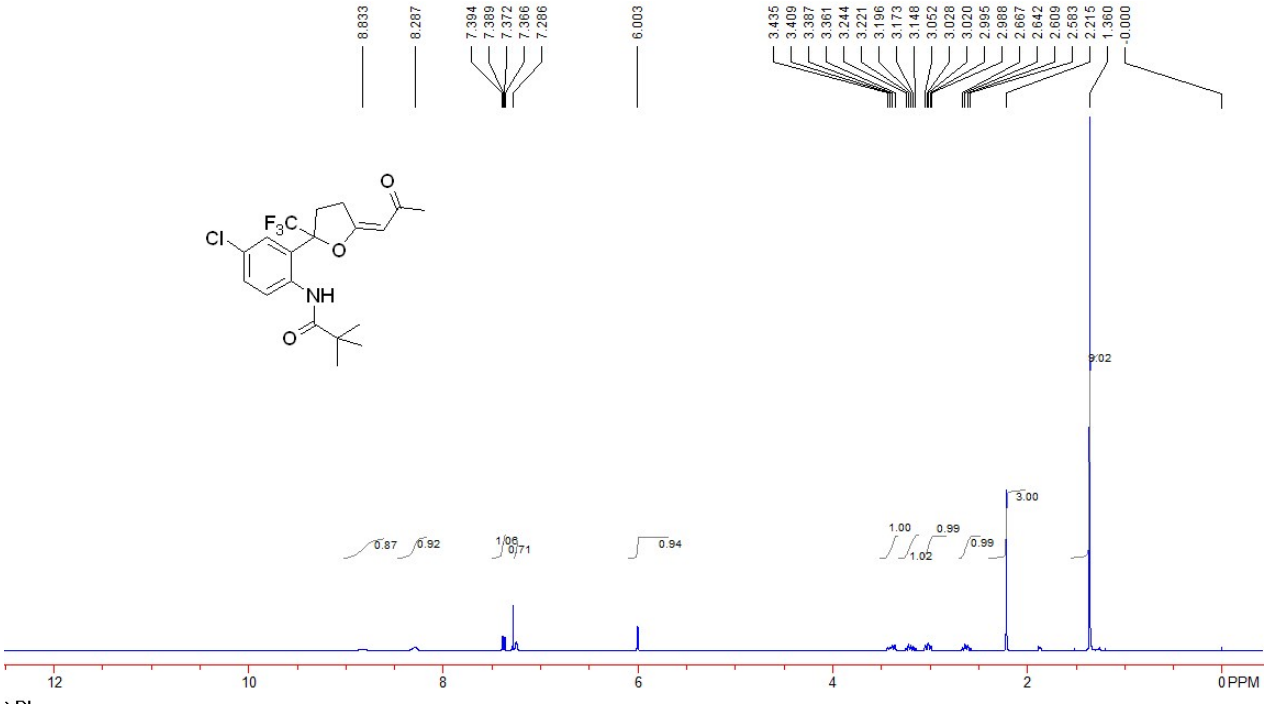






(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)pivalamide (3d)

A white oil, 79% yield (64 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.36 (s, 9H, CH_3), 2.22 (s, 3H, CH_3), 2.58~2.67 (m, 1H, CH_2), 2.98~3.06 (m, 1H, CH_2), 3.14~3.25 (m, 1H, CH_2), 3.36~3.44 (m, 1H, CH_2), 6.00 (s, 1H, =CH), 7.29 (s, 1H, ArH), 7.38 (dd, *J* = 2.0, 8.8 Hz, 1H, ArH), 8.29 (br, 1H, ArH), 8.83 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 27.4, 29.2, 31.4, 32.5, 40.0, 89.6 (q, *J* = 30.4 Hz), 124.5 (q, *J* = 285.4 Hz), 125.2, 128.6, 129.1, 130.4, 136.1, 172.2, 176.6, 197.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.93. IR (CH_2Cl_2) ν 3446, 2965, 2926, 2870, 2362, 2341, 1693, 1614, 1172, 1137, 1047, 1015, 945 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{22}ClF_3NO_3^{+1}(M+H)^+$ requires 404.1235, Found: 404.1235.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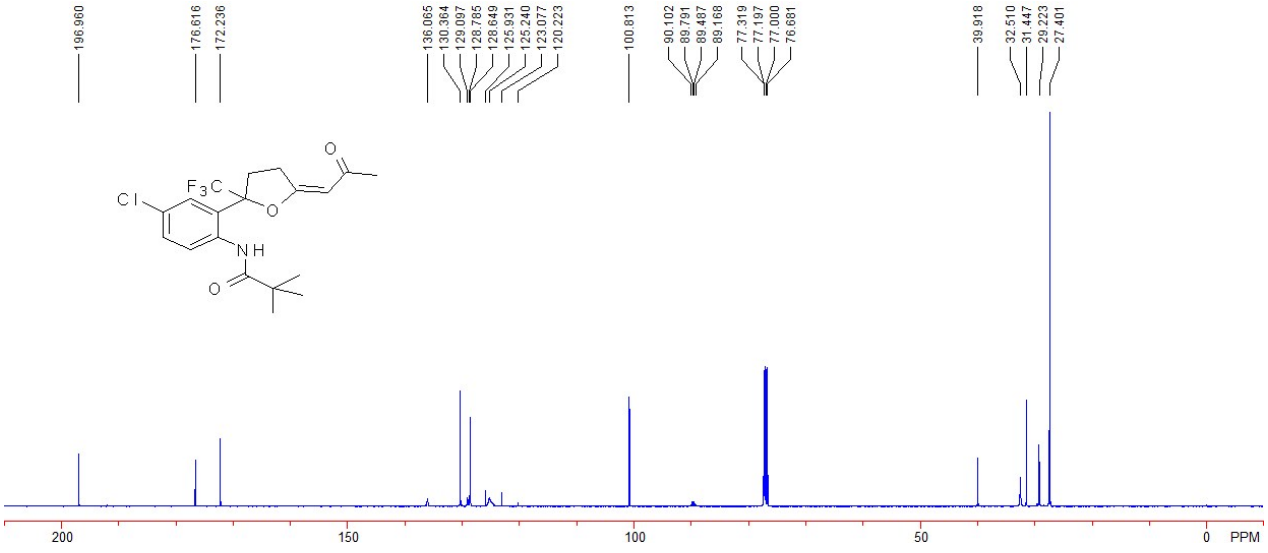
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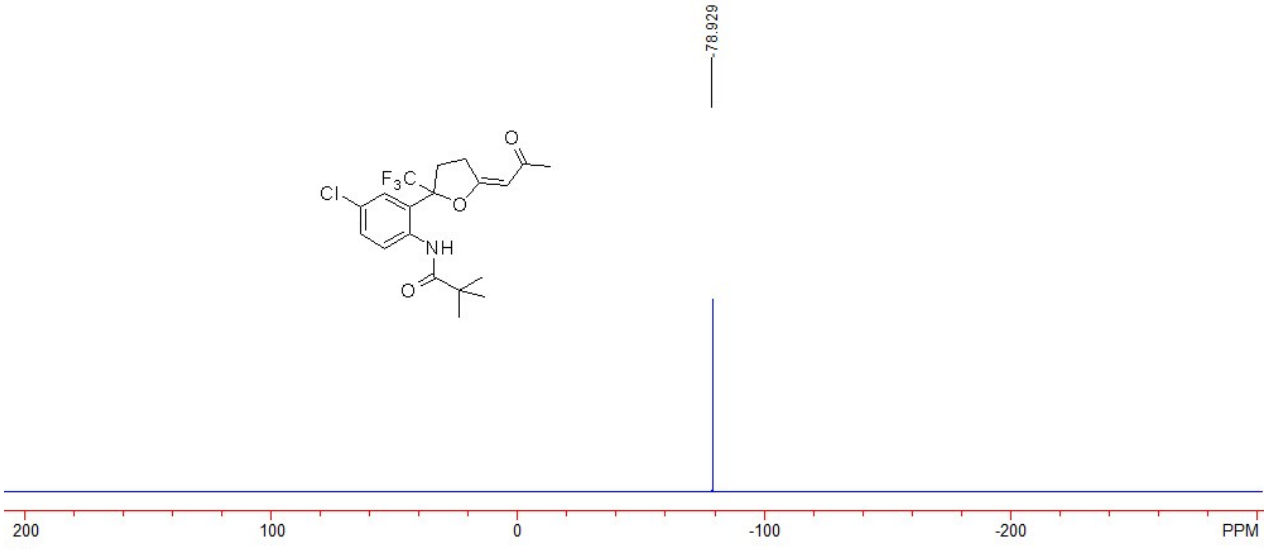
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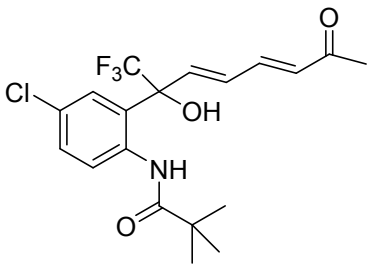
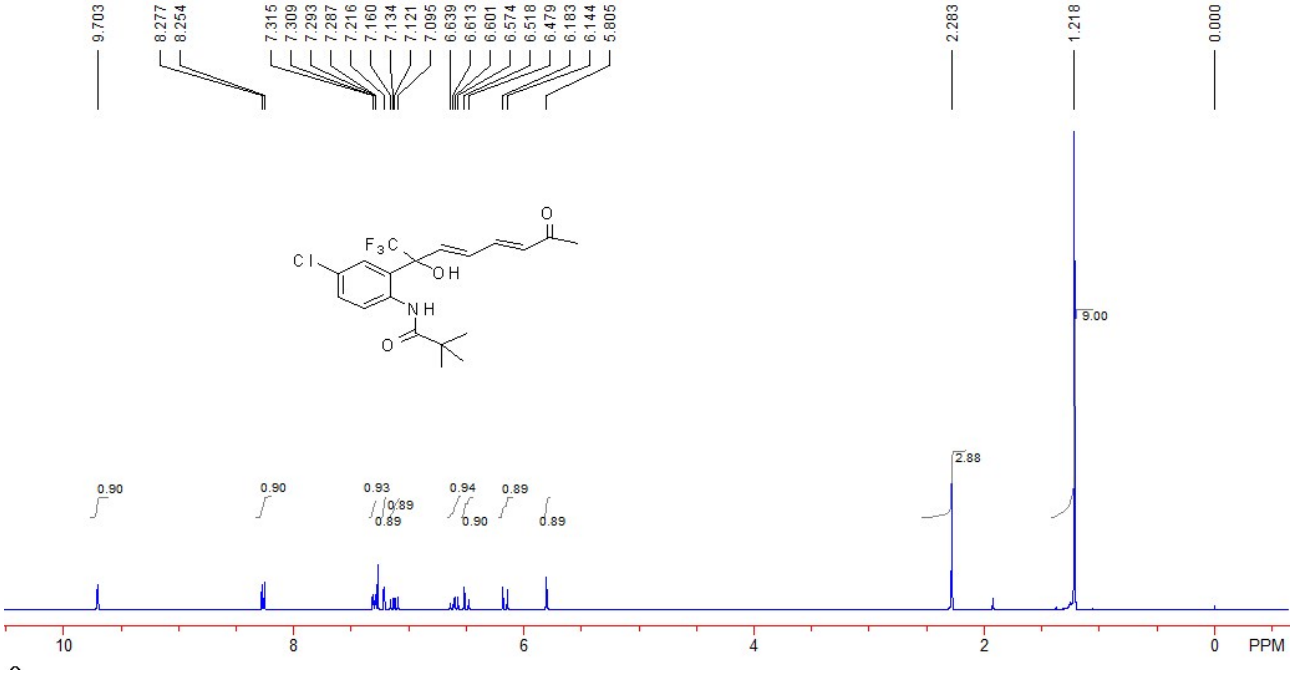
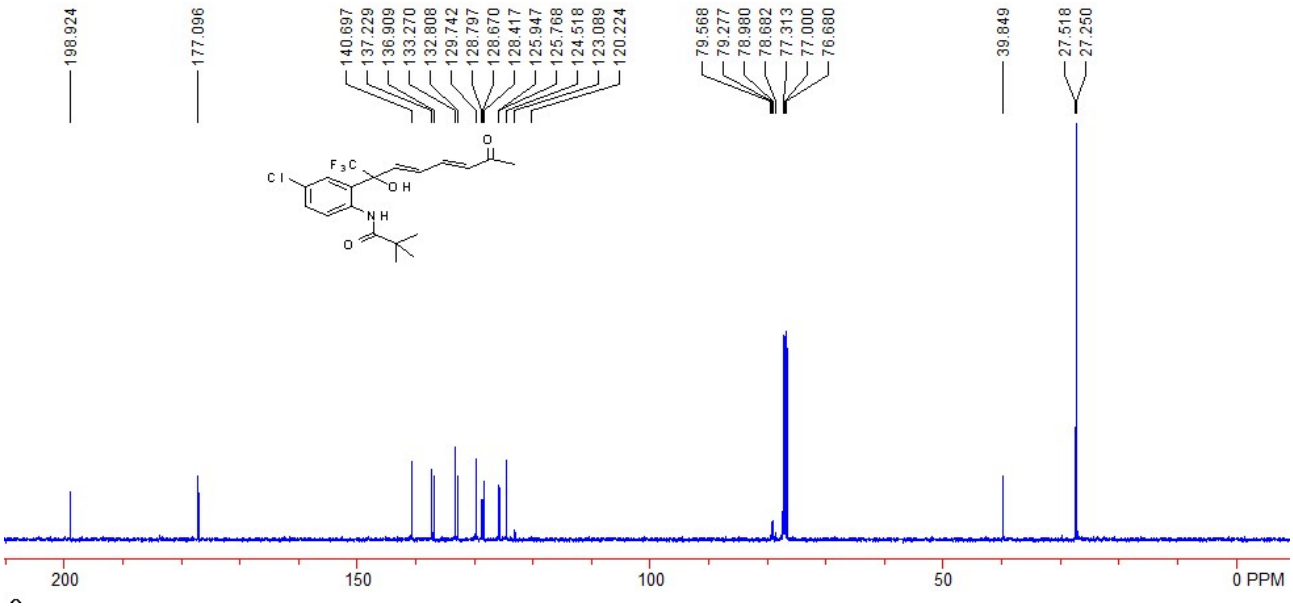
PPM

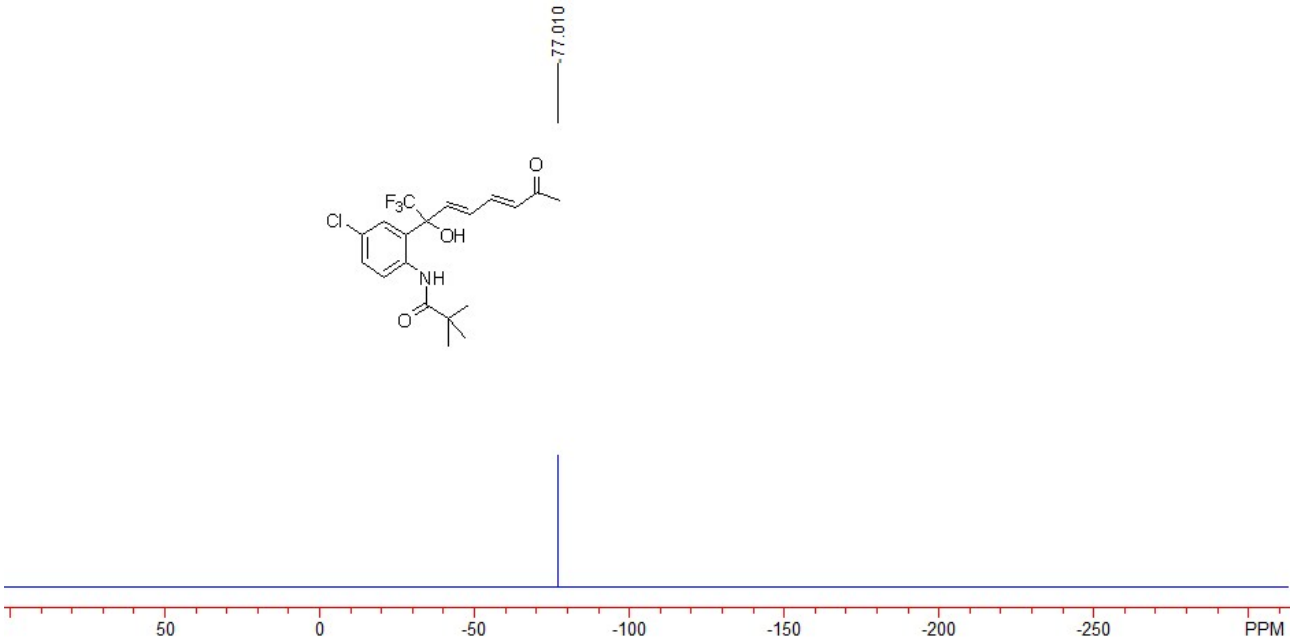


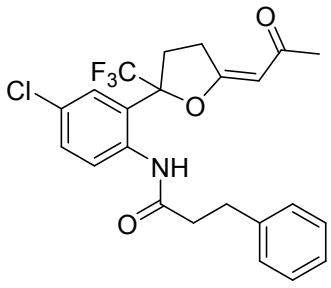
N-(4-chloro-2-((3E,5E)-1,1,1-trifluoro-2-hydroxy-7-oxoocta-3,5-dien-2-yl)phenyl)pivalamide (5d)

A white oil, 17% yield (14 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.22 (s, 9H, CH_3), 2.28 (s, 3H, CH_3), 5.81 (s, 1H, OH), 6.16 (d, *J* = 15.6 Hz, 1H, =CH), 6.50 (d, *J* = 15.6 Hz, 1H, =CH), 6.20 (d, *J* = 15.6 Hz, 1H, =CH), 6.61 (dd, *J* = 10.4, 15.6 Hz, 1H, =CH), 7.13 (dd, *J* = 10.4, 15.6 Hz, 1H, =CH), 7.22 (s, 1H, ArH), 7.30 (dd, *J* = 2.4, 8.8 Hz, 1H, =CH), 8.27 (d, *J* = 9.2 Hz, 1H, ArH), 9.70 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 27.3, 27.5, 39.8, 79.1 (q, *J* = 29.7 Hz), 124.51 (q, *J* = 285.8 Hz), 124.52, 125.8, 128.4, 128.7, 129.7, 132.8, 133.3, 136.9, 137.2, 140.7, 177.1, 198.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -77.01. IR (CH_2Cl_2) ν 3675, 2970, 2916, 2361, 2341, 1676, 1574, 1515, 1385, 1254, 1163, 1066, 668 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{22}ClF_3NO_3$ $^{+1}$(M+H)$^{+}$ requires 404.1235, Found: 404.1238.





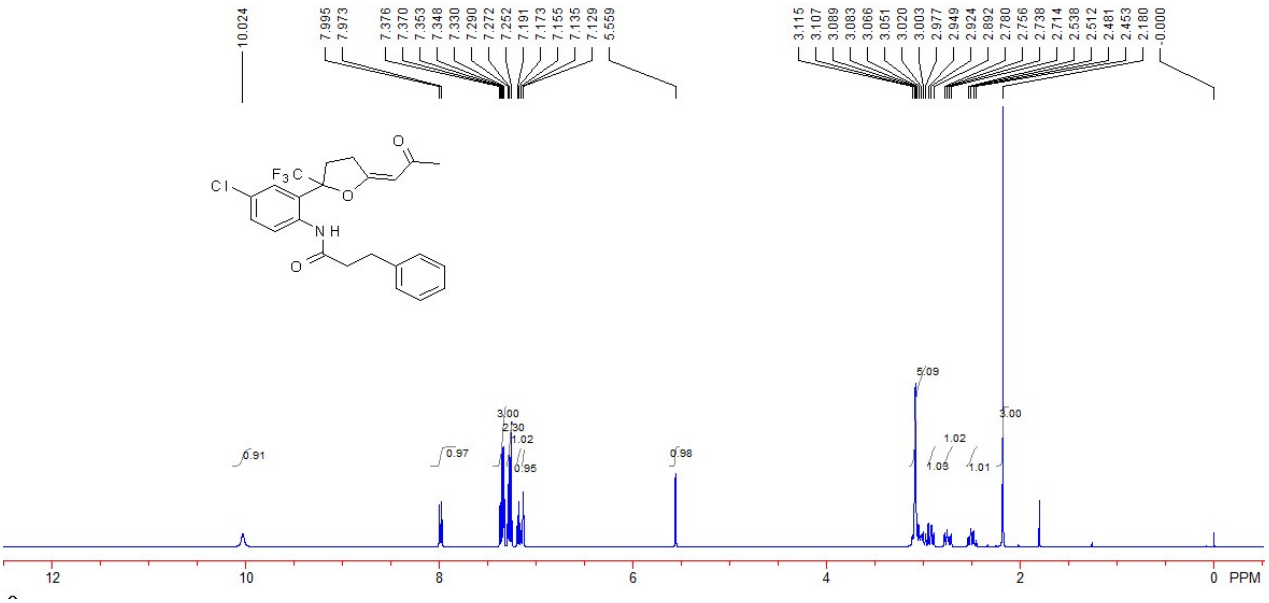


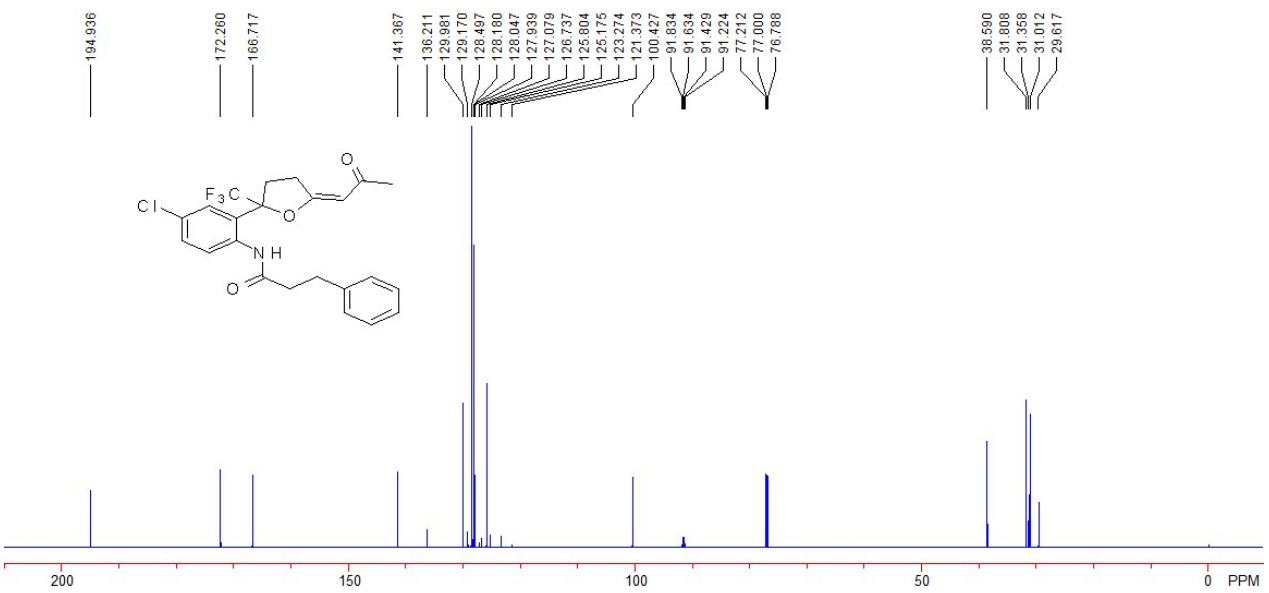


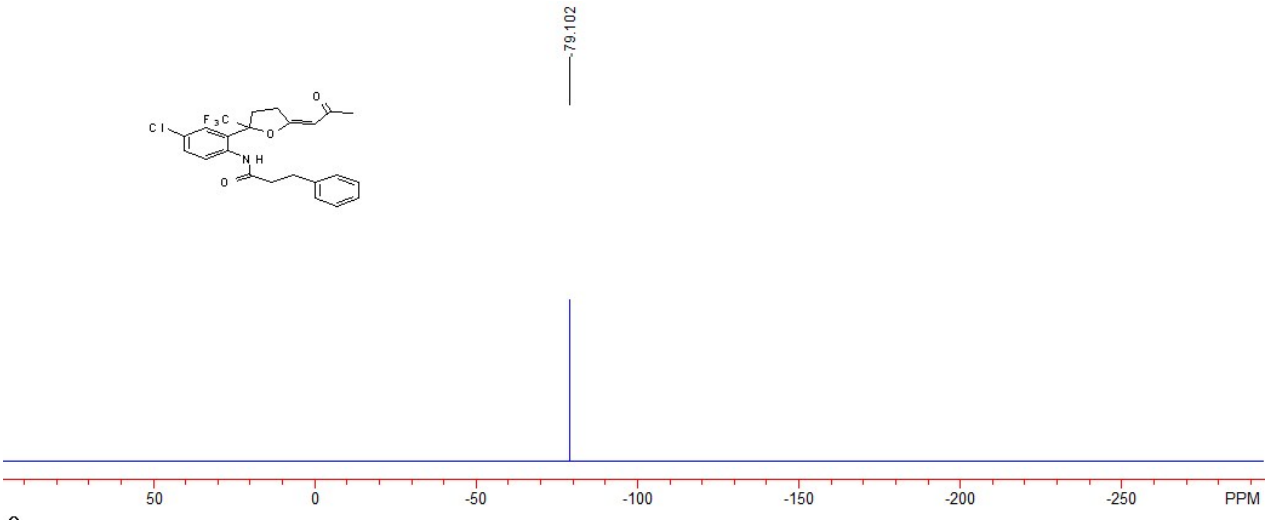
(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-3-phenylpropanamide (3e)

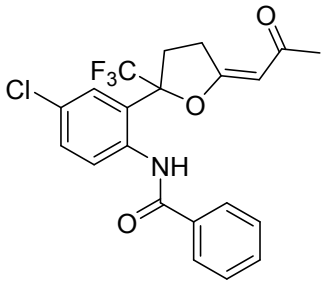
A white solid, 46% yield (42 mg). M.p.: 132-134 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.18 (s,

3H, CH_3), 2.45~2.54 (m, 1H, CH), 2.71~2.78 (m, 1H, CH_2), 2.89~2.95 (m, 1H, CH_2), 2.97~3.12 (m, 5H, CH_2), 5.56 (s, 1H, =CH), 7.13 (d, *J* = 2.4 Hz, 1H, ArH), 7.15~7.19 (m, 1H, ArH), 7.25~7.29 (m, 2H, ArH), 7.33~7.38 (m, 3H, ArH), 7.98 (d, *J* = 8.8 Hz, 1H, ArH), 10.02 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 150 MHz) δ 29.6, 31.0, 31.4, 31.8, 38.6, 91.7 (q, *J* = 30.75 Hz), 100.4, 125.2 (q, *J* = 285.15 Hz), 125.8, 126.7, 127.9, 128.1, 128.2, 128.5, 129.2, 130.0, 136.2, 141.4, 166.7, 172.3, 194.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.10. IR (CH_2Cl_2) ν 3338, 2922, 2359, 2342, 1686, 1619, 1507, 1304, 1189, 1173, 923 cm^{-1}. HRMS (ESI) Calcd. For $C_{23}H_{22}ClF_3NO_3{}^{+1}(M+H)^+$ requires 452.1235, Found: 452.1232.



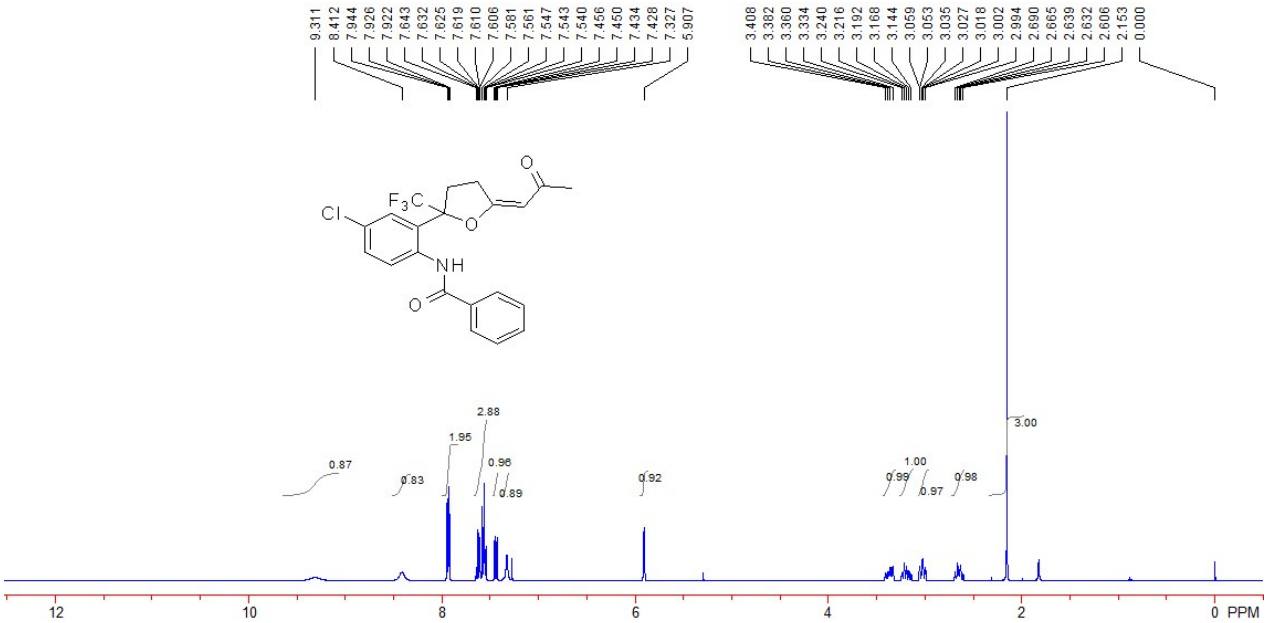






(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)benzamide (3f)

A white solid, 81% yield (69 mg). M.p.: 180-182 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.15 (s, 3H, CH_3), 2.60~2.69 (m, 1H, CH_2), 2.99~3.06 (m, 1H, CH_2), 3.14~3.24 (m, 1H, CH_2), 3.33~3.41 (m, 1H, CH_2), 5.91 (s, 1H, =CH), 7.33 (br, 1H, ArH), 7.44 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 7.54~7.64 (m, 3H, ArH), 7.92~7.94 (m, 2H, ArH), 8.41 (br, 1H, ArH), 9.31 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 29.2, 31.4, 32.5, 89.6 (q, *J* = 30.5 Hz), 101.0, 124.5 (q, *J* = 284.8 Hz), 125.5, 126.9, 128.8, 128.9, 129.7, 130.6, 132.2, 134.6, 135.7, 165.3, 171.9, 196.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.96. IR (CH_2Cl_2) ν 2920, 1688, 1614, 1519, 1398, 1299, 1173, 1141, 1047, 946, 708 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{18}ClF_3NO_3^{+1}(M+H)^+$ requires 424.0922, Found: 424.0923.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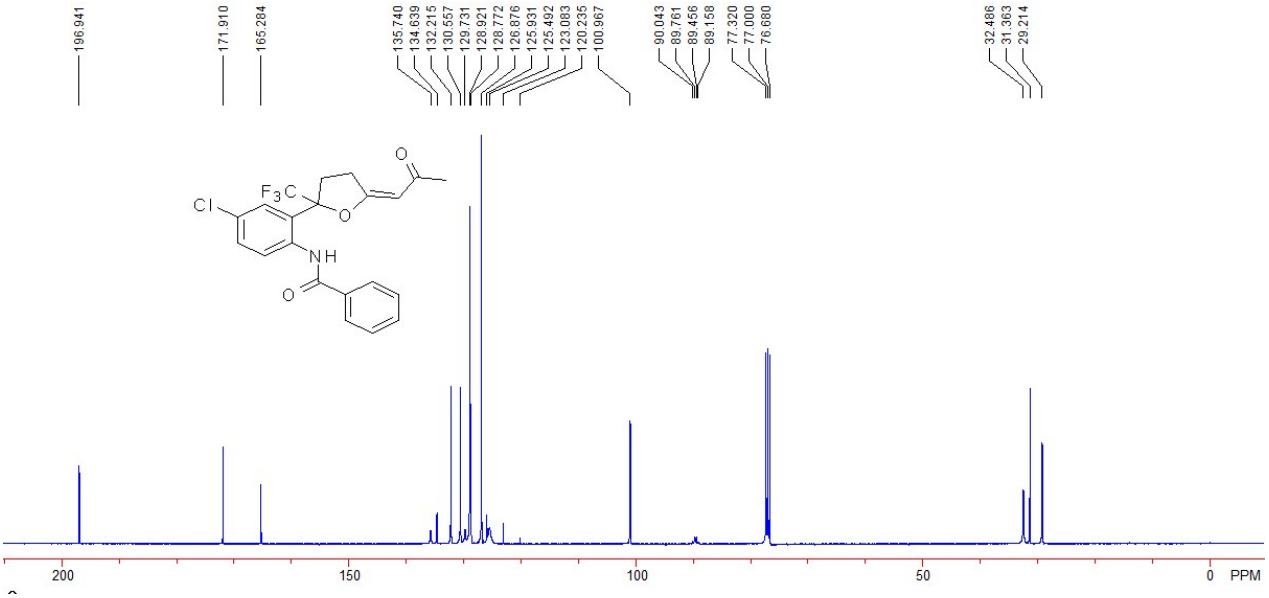
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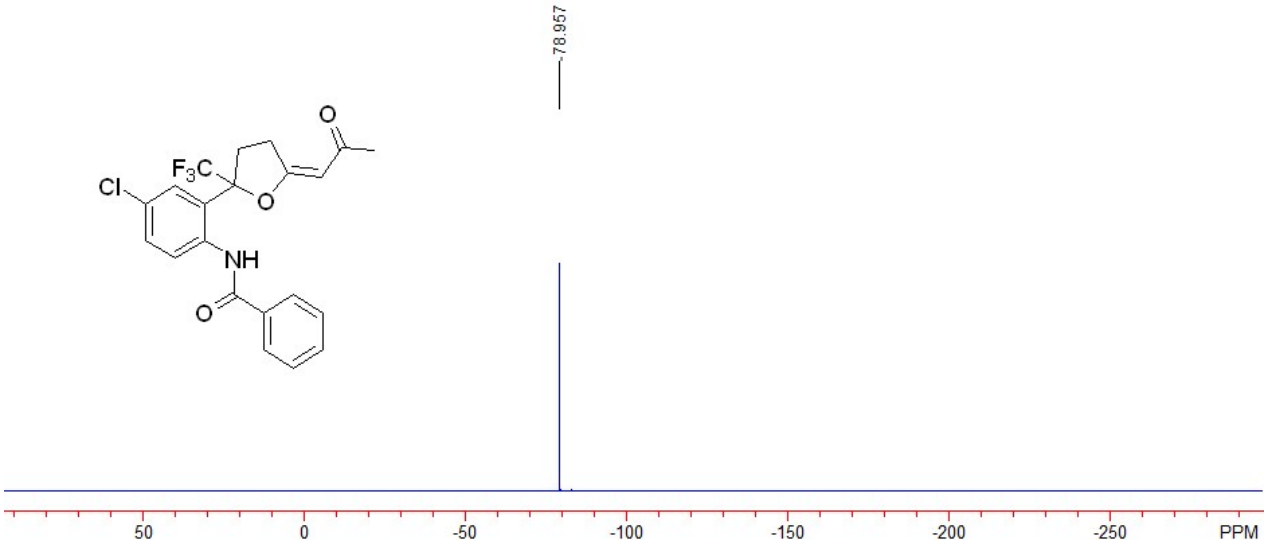
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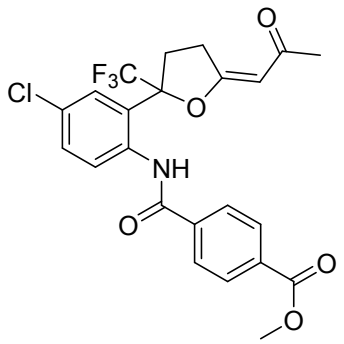
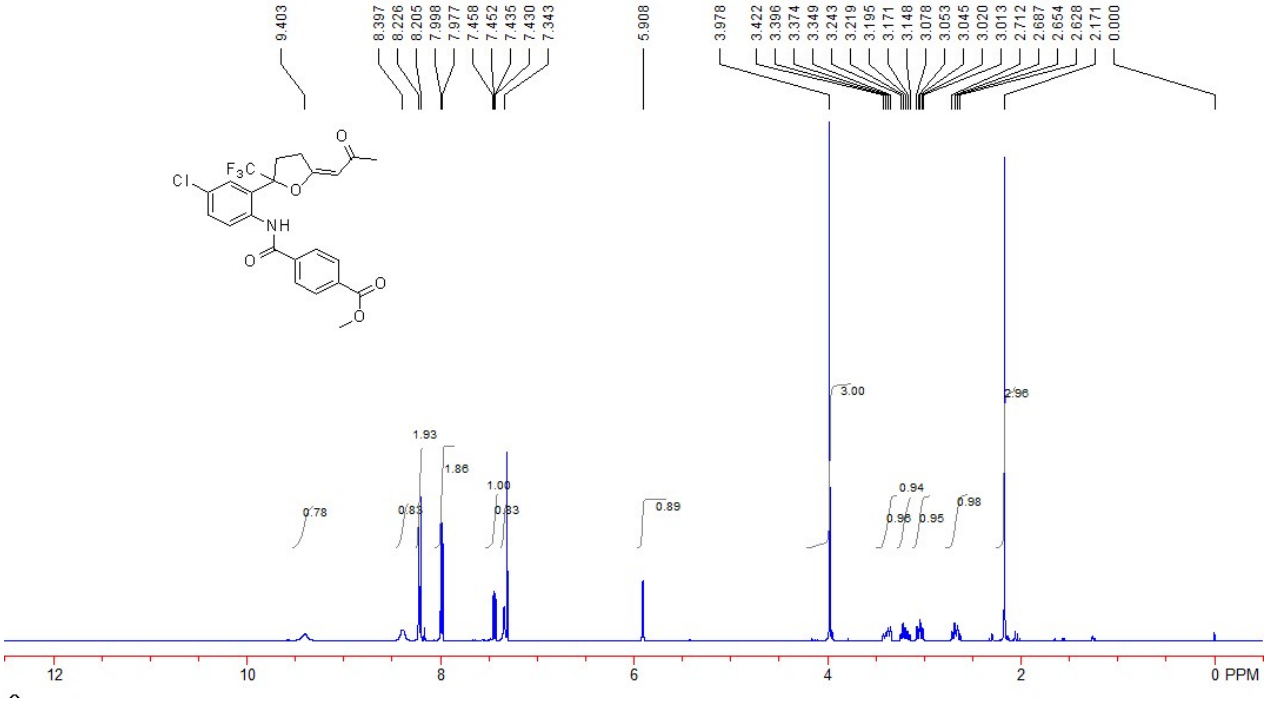
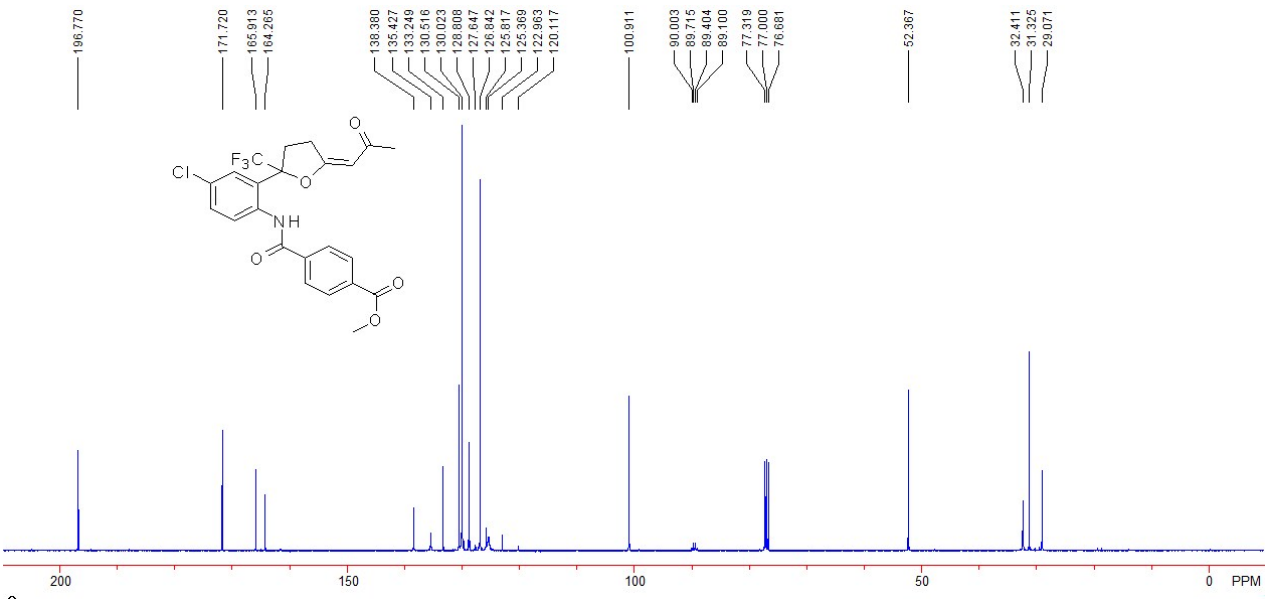
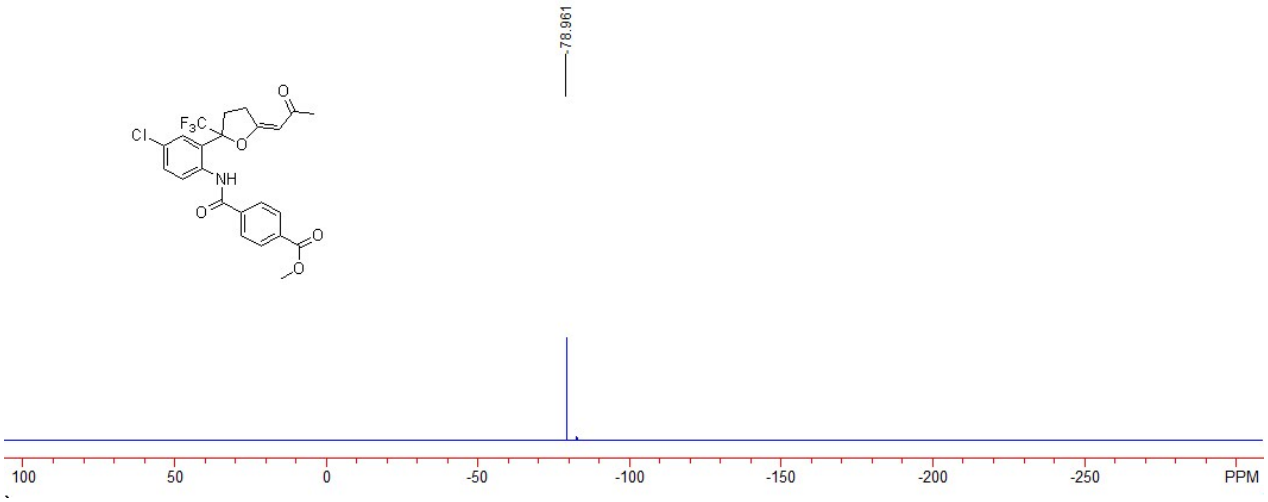


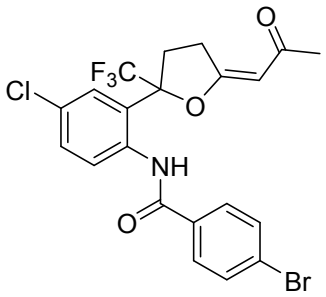
methyl (E)-4-((4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)carbamoyl)benzoate (3g)

A white solid, 76% yield (74 mg). M.p.: 178-180 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.17 (s, 3H, CH_3), 2.62~2.72 (m, 1H, CH_2), 3.01~3.08 (m, 1H, CH_2), 3.14~3.25 (m, 1H, CH_2), 3.34~3.43 (m, 1H, CH_2), 3.98 (s, 3H,CH_3), 5.91 (s, 1H, =CH), 7.34 (br, 1H, ArH), 7.44 (dd, *J* = 2.4, 9.2 Hz, 1H, ArH), 7.99 (d, *J* = 8.4 Hz, 2H, ArH), 8.22 (d, *J* = 8.4 Hz, 2H, ArH), 8.40 (br, 1H, ArH), 9.40 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 29.1, 31.3, 32.4, 52.4, 89.6 (q, *J* = 31.1 Hz), 100.9, 124.4 (q, *J* = 285.4 Hz), 125.4, 126.8, 128.8, 130.0, 130.5, 133.2, 135.4, 138.4, 164.3, 165.9, 171.7, 196.8. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.96. IR (CH_2Cl_2) ν 3675, 3422, 2987, 2901, 2360, 1724, 1280, 1172, 1073, 945 cm^{-1}. HRMS (ESI) Calcd. For $C_{23}H_{20}ClF_3NO_5^{+1}(M+H)^+$ requires 482.0977, Found: 482.0975.





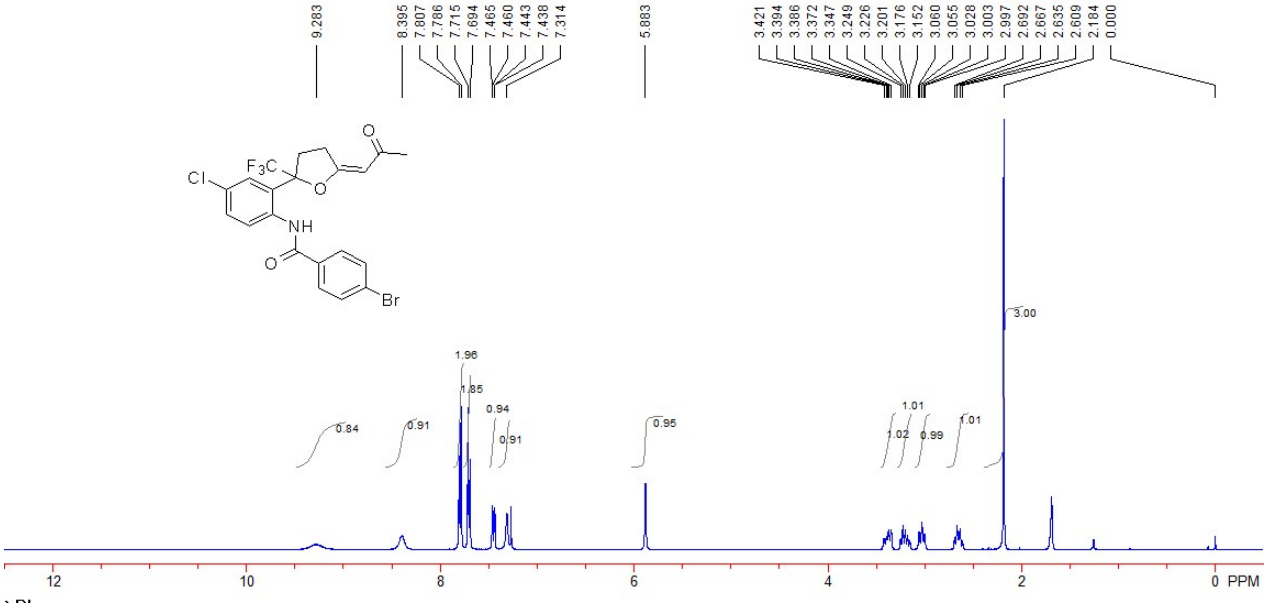


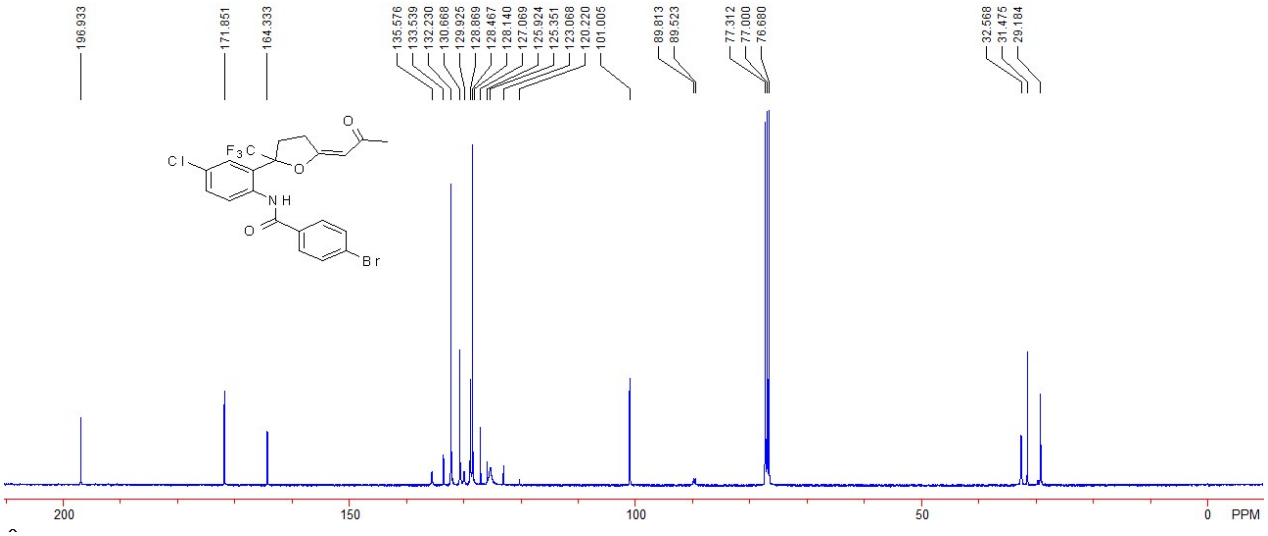


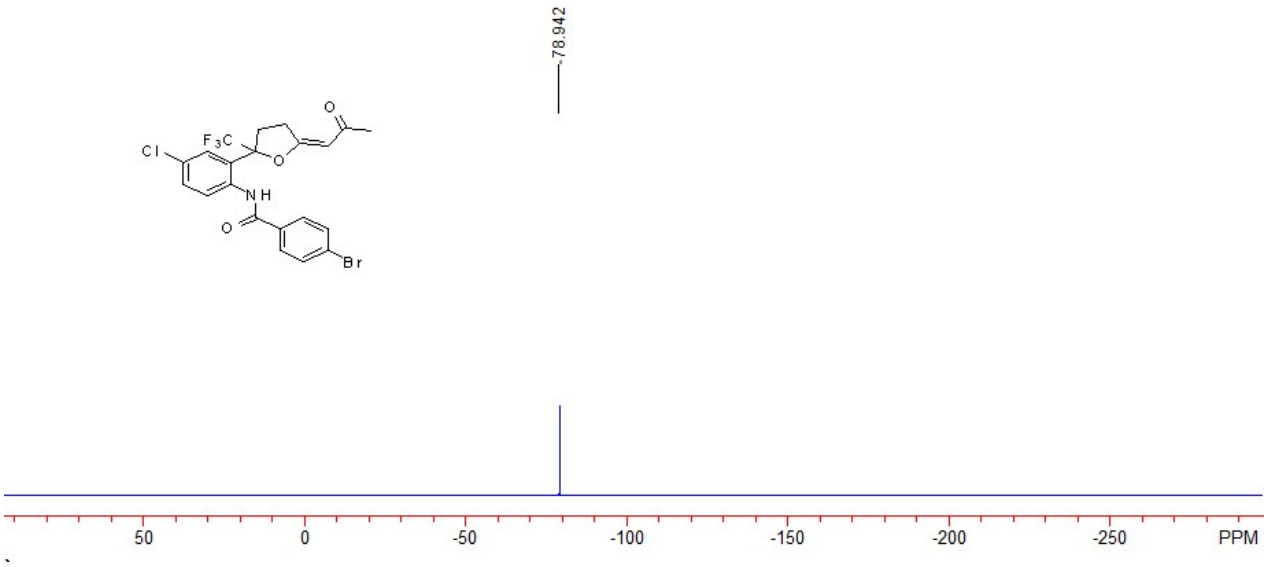
(E)-4-bromo-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)benzamide (3h)

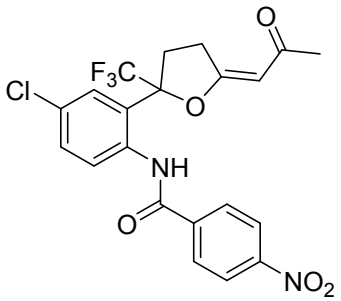
A white solid, 45% yield (45 mg). M.p.: 178-180 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.18 (s, 3H, CH_3), 2.60~2.70 (m, 1H, CH_2), 2.99~3.06 (m, 1H, CH_2), 3.15~3.25 (m, 1H, CH_2), 3.34~3.43 (m, 1H, CH_2), 5.88 (s, 1H, =CH), 7.31 (br, 1H, ArH), 7.45 (dd, J = 2.0, 8.8 Hz, 1H, ArH), 7.70 (d, J = 8.4 Hz, 2H, ArH), 7.80 (d, J = 8.4 Hz, 2H, ArH), 8.40 (br, 1H, ArH), 9.28 (br, 1H, NH). ^{13}C

NMR ($CDCl_3$, TMS, 100 MHz) δ 29.2, 31.5, 32.6, 89.7 (q, J = 29.0 Hz), 101.0, 124.5 (q, J = 285.6 Hz), 125.4, 127.1, 128.5, 128.9, 129.9, 130.7, 132.2, 133.5, 135.6, 164.3, 171.9, 196.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.94. IR (CH_2Cl_2) ν 3015, 2924, 2849, 2398, 1699, 1397, 1242, 1093, 1062, 1030, 1021, 886 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{17}BrClF_3NO_3{}^{+1}(M+H)^+$ requires 502.0027, Found: 502.0027.



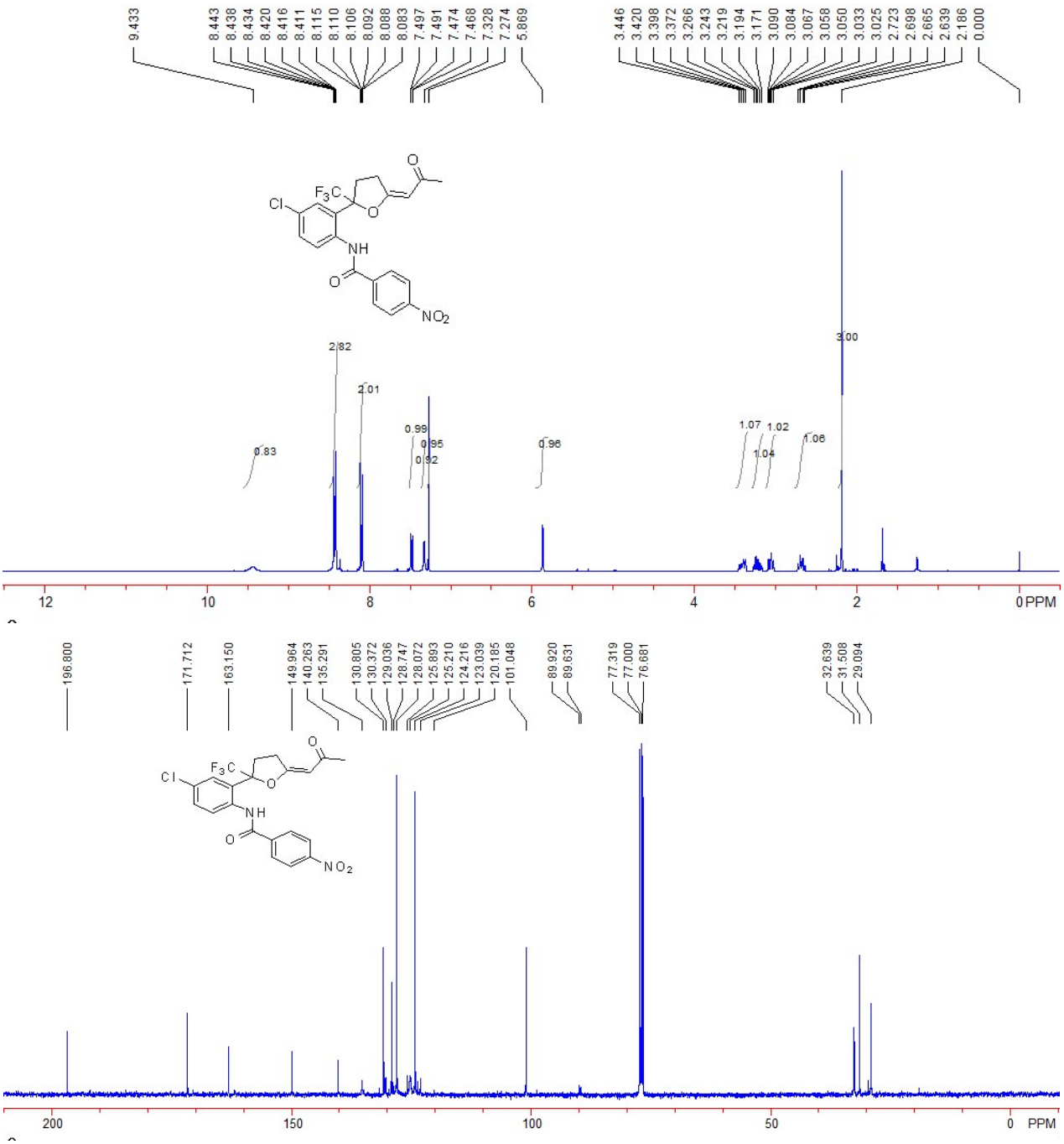






(E)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-4-nitrobenzamide (3ia)

A white solid, 25% yield (24 mg). M.p.: 204-206 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.19 (s, 3H, CH_3), 2.63~2.73 (m, 1H, CH_2), 3.02~3.09 (m, 1H, CH_2), 3.17~3.27 (m, 1H, CH_2), 3.37~3.45 (m, 1H, CH_2), 5.87 (s, 1H, =CH), 7.33 (s, 1H, ArH), 7.48 (dd, J = 2.4, 9.2 Hz, 1H, ArH), 8.08~8.12 (m, 2H, ArH), 8.41~8.45 (m, 3H, ArH), 9.43 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 29.1, 31.5, 32.6, 89.8 (q, J = 28.9 Hz), 101.0, 124.2, 124.5 (q, J = 285.4 Hz), 125.2, 128.1, 129.0, 130.4, 130.8, 135.3, 140.3, 150.0, 163.2, 171.7, 196.8. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.91. IR (CH_2Cl_2) ν 3416, 2920, 2850, 1689, 1605, 1525, 1348, 1173, 1142, 1097, 868, 764 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{17}ClF_3N_2O_5^{+1}(M+H)^+$ requires 469.0773, Found: 469.0773.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2.665
2.639
2.186
0.000
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F3C
Cl
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NH
O
NO2
2.82
2.01
0.99
0.95
0.92
0.83
0.96
1.07
1.02
1.04
1.06
3.00
12
10
8
6
4
2
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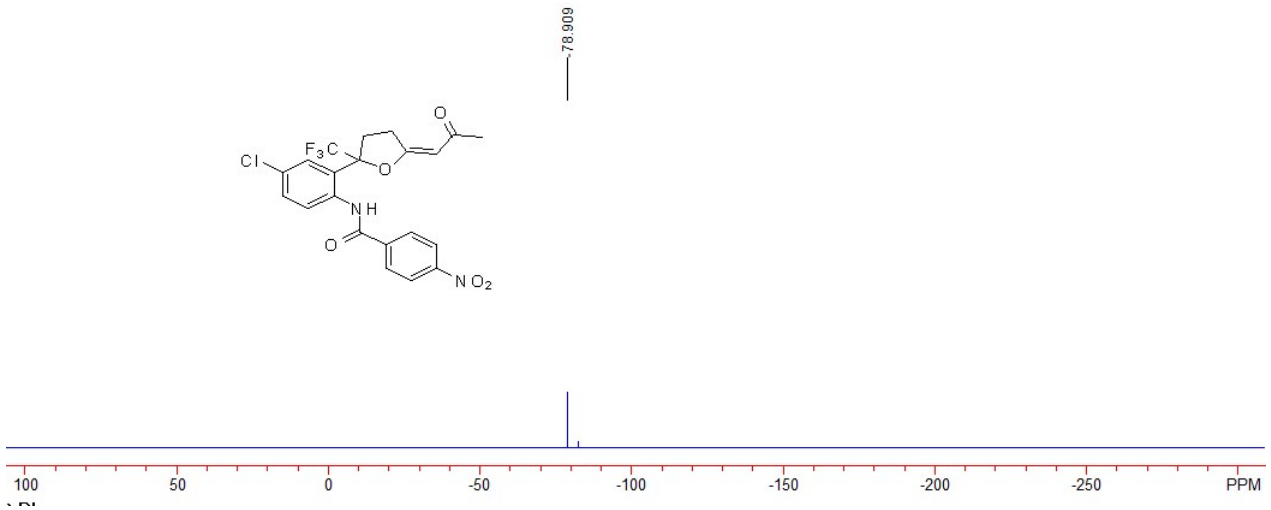
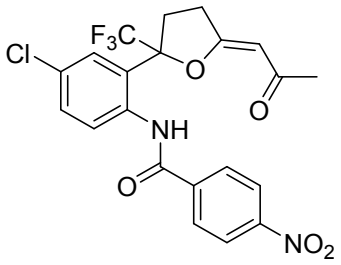
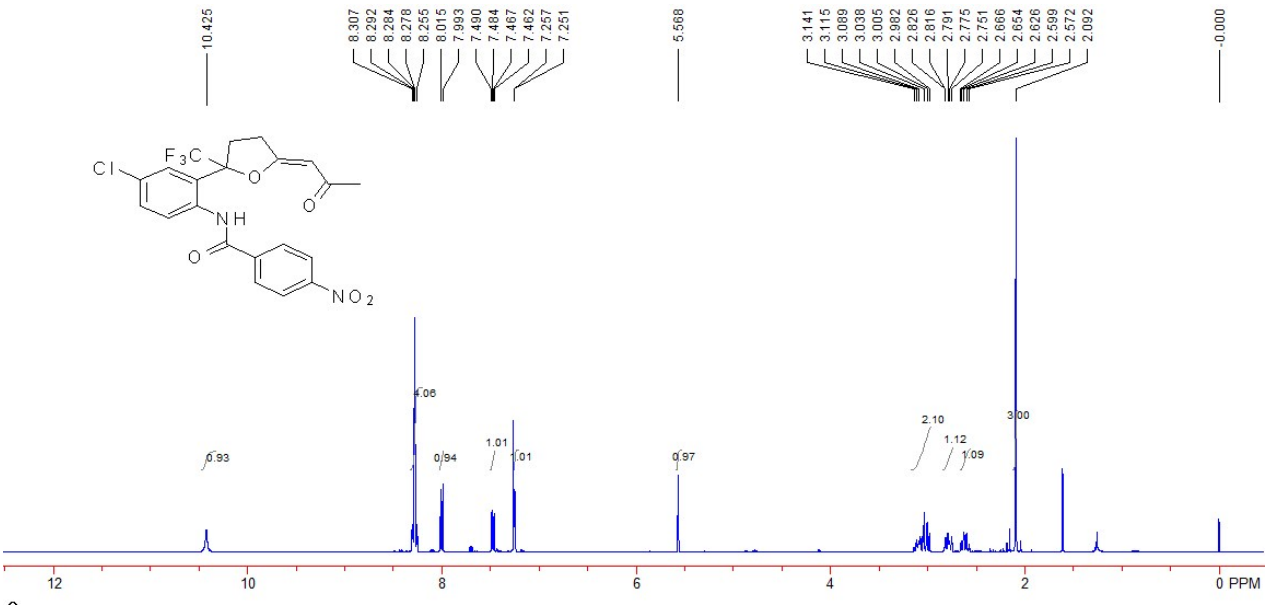




(Z)-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-4-nitrobenzamide (3ib)

A white solid, 25% yield (24 mg). M.p.: 201-203 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.09 (s, 3H, CH_3), 2.57~2.67 (m, 1H, CH_2), 2.75~2.83 (m, 1H, CH_2), 2.98~3.14 (m, 2H, CH_2), 5.57 (s, 1H, =CH), 7.25 (d, *J* = 2.4 Hz, 1H, ArH), 7.48 (dd, *J* = 2.4, 9.2 Hz, 1H, ArH), 8.00 (d, *J* = 9.2 Hz, 1H, ArH), 8.25~8.31 (m, 4H, ArH), 10.43 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 30.0 (d, *J* = 1.7 Hz), 31.1, 31.5, 91.4 (q, *J* = 31.0 Hz), 100.7, 123.3, 124.3 (q, *J* = 285.1 Hz), 128.2, 128.8, 129.6, 129.7, 130.3, 130.8, 135.6, 140.3, 149.5, 165.7, 166.6, 195.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.45. IR (CH_2Cl_2) ν 3326, 2920, 2850, 2363, 1684, 1524, 1348, 1275, 1260, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{17}ClF_3N_2O_5$ $(M+H)^+$ requires 469.0773, Found: 469.0770.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7.251
5.568
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3.115
3.089
3.038
3.005
2.982
2.826
2.816
2.791
2.775
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2.666
2.654
2.626
2.599
2.572
2.092
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F3C
Cl
O
NH
NO2
4.06
0.93
0.94
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0.97
2.10
1.12
1.09
3.00
12
10
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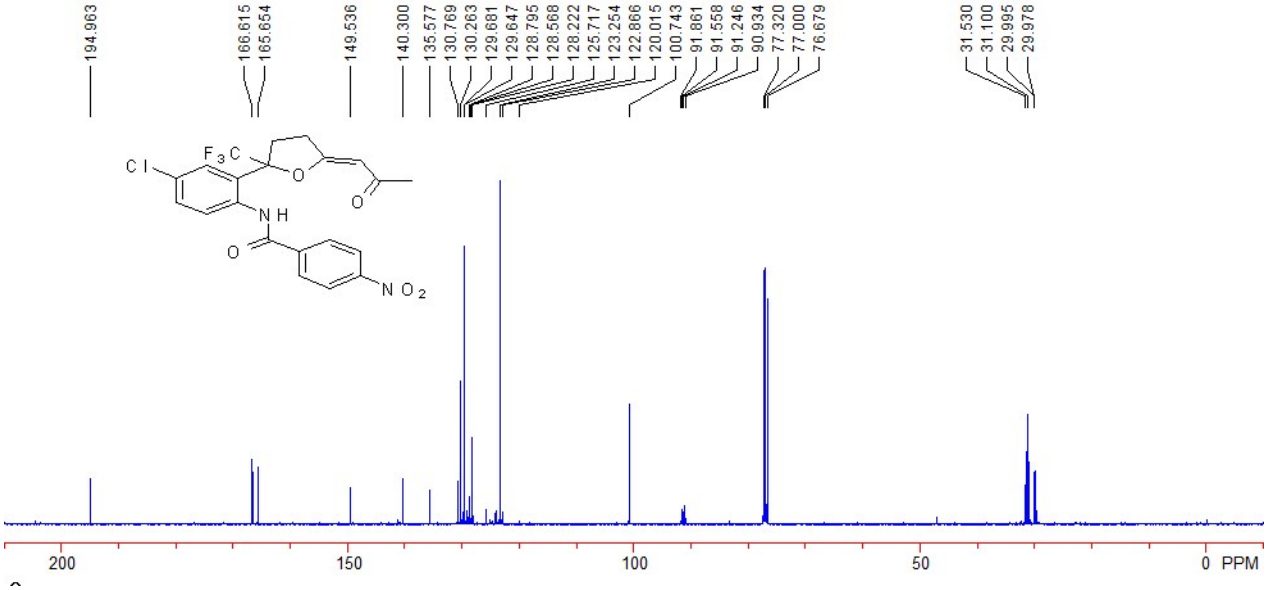
4
2
0 PPM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165.654
149.536
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130.769
130.263
129.681
129.647
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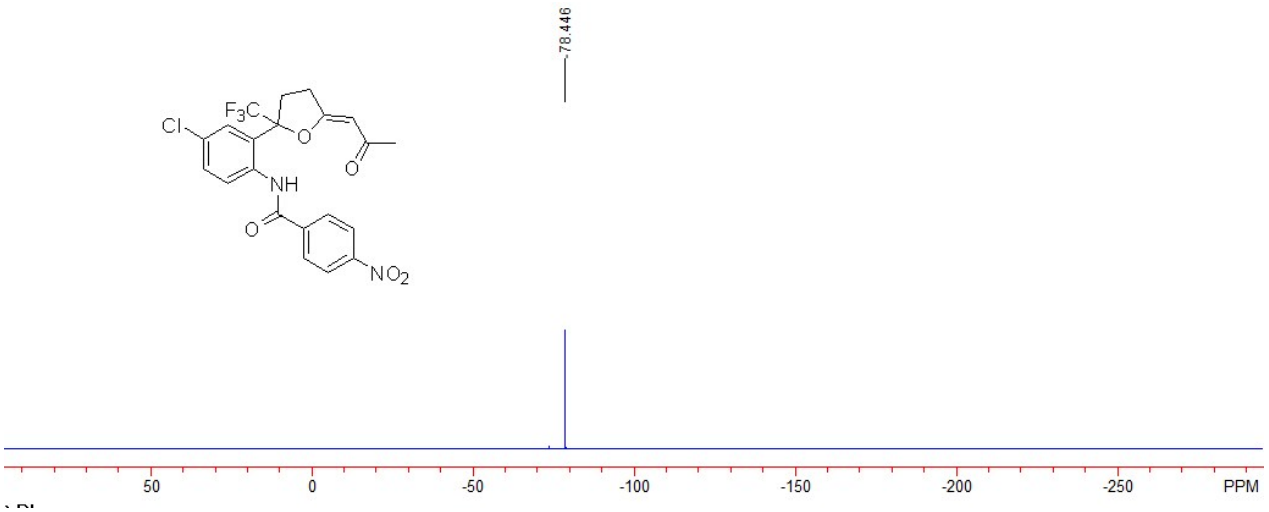
128.568
128.222
125.717
123.254
122.866
120.015
100.743
91.861
91.558
91.246
90.934
77.320
77.000
76.679
31.530
31.100
29.995
29.978
F3C
Cl
O
NH
NO2
200
150
100
50
0 PPM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O
NH
NO2
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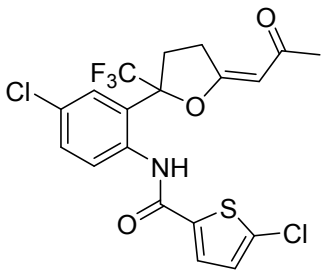
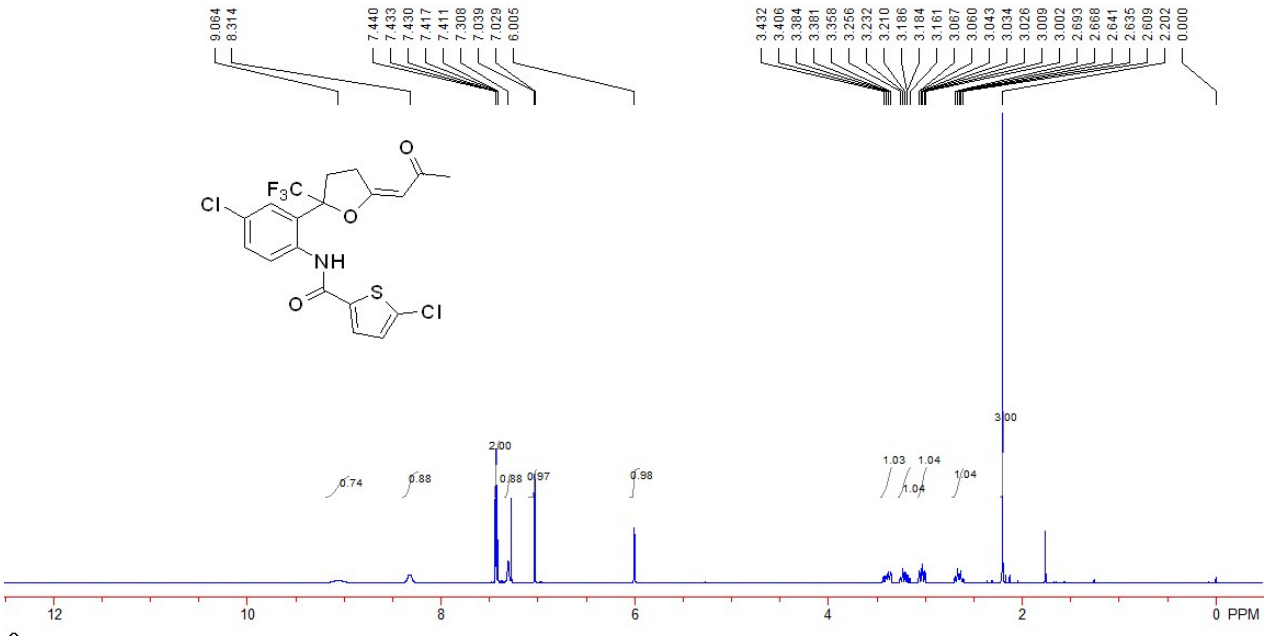
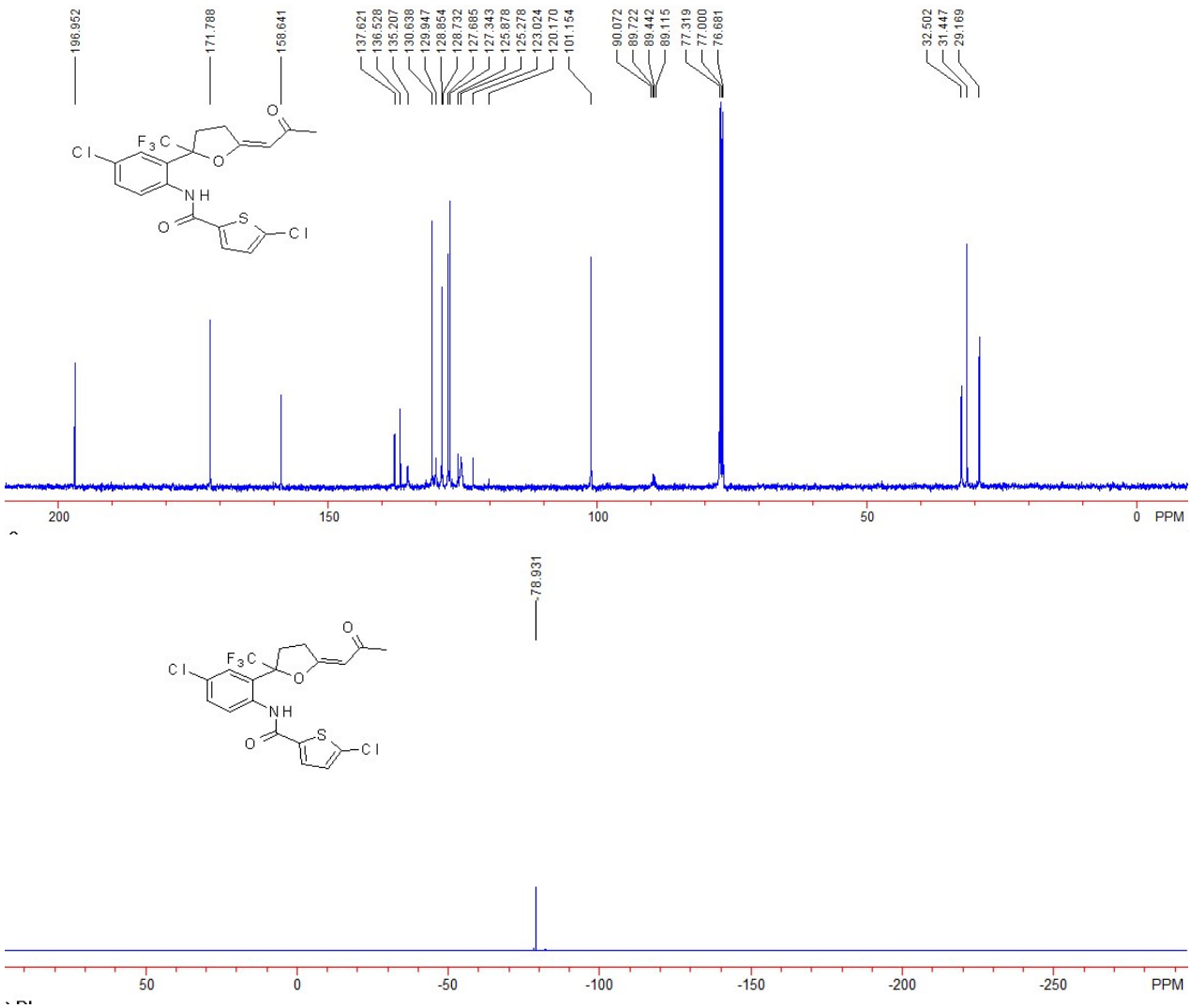
-50
-100
-150
-200
-250
PPM

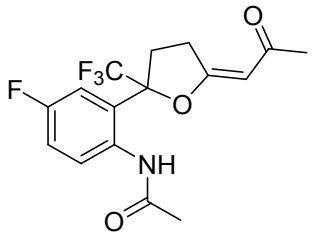


(E)-5-chloro-N-(4-chloro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)thiophene-2-carboxamide (3j)

A white solid, 66% yield (61 mg). M.p.: 177-179 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.20 (s, 3H, CH_3), 2.60~2.70 (m, 1H, CH_2), 3.00~3.07 (m, 1H, CH_2), 3.16~3.26 (m, 1H, CH_2), 3.35~3.44 (m, 1H, CH_2), 6.01 (s, 1H, =CH), 7.03 (d, *J* = 4.0 Hz, 1H, ArH), 7.31 (s, 1H, ArH), 7.14~7.44 (m, 2H, ArH), 8.31 (br, 1H, ArH), 9.06 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 29.2, 31.4, 32.5, 89.6 (q, *J* = 28.0 Hz), 101.2, 124.5 (q, *J* = 285.4 Hz), 125.3, 127.3, 127.7, 128.9, 129.9, 130.6, 135.2, 136.5, 137.6, 158.6, 171.8, 197.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.96. IR (CH_2Cl_2) ν 3675, 2987, 2971, 2900, 2359, 2342, 1404, 1393, 1250, 1074, 1065, 1056, 891 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{15}Cl_2F_3NO_3S^{+1}(M+H)^+$ requires 464.0096, Found: 464.0094.



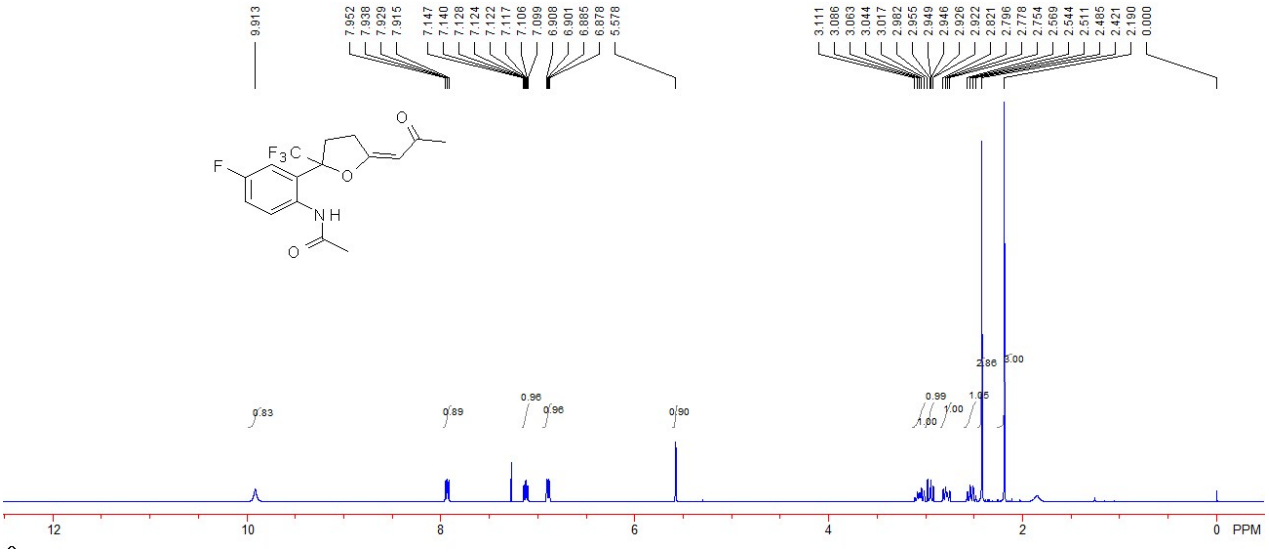


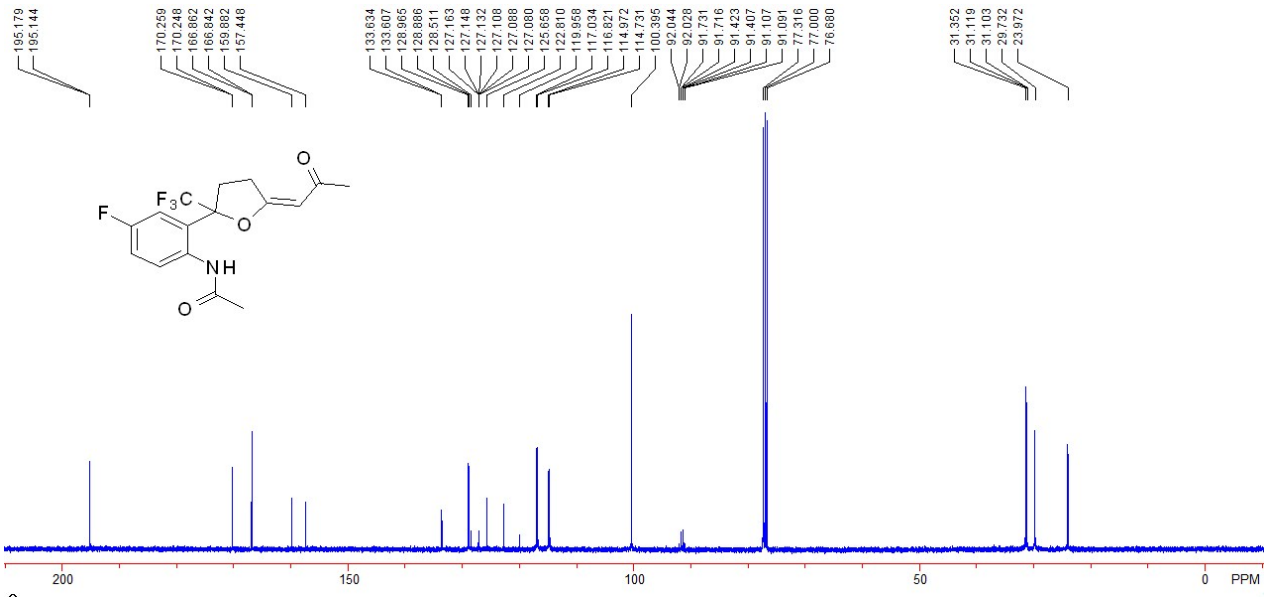


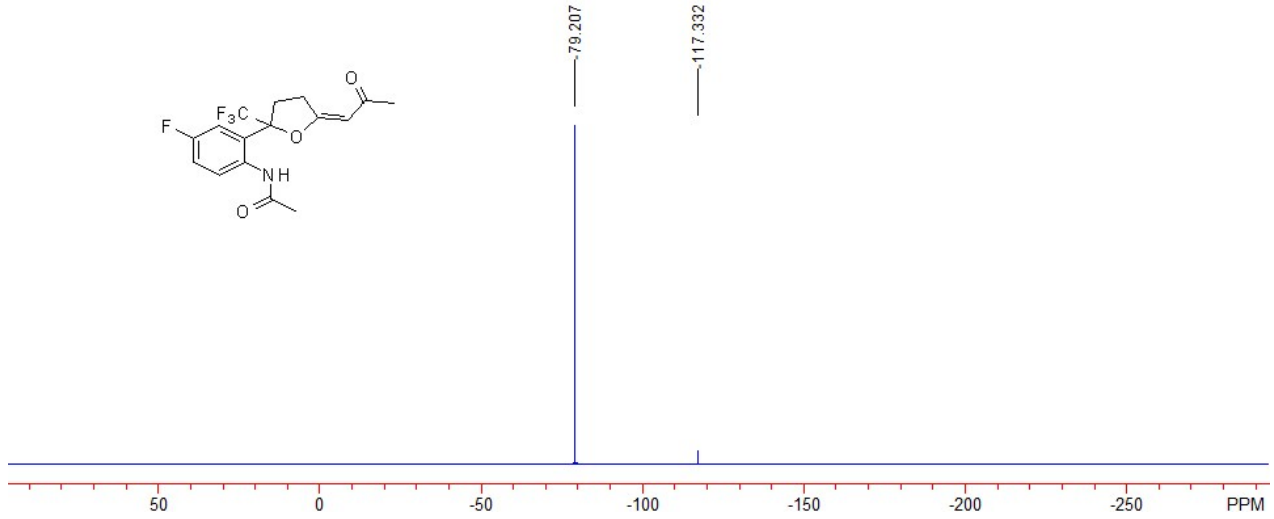
(E)-N-(4-fluoro-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (3k)

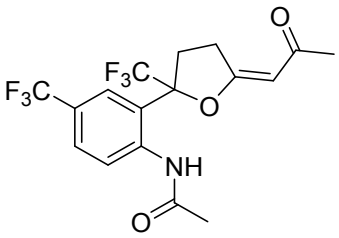
A white solid, 85% yield (59 mg). M.p.: 141-143 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.19 (s, 3H, CH_3), 2.42 (s, 3H, CH_3), 2.48~2.57 (m, 1H, CH_2), 2.75~2.83 (m, 1H, CH_2), 2.92~2.99 (m, 1H, CH_2), 3.01~3.12 (m, 1H, CH_2), 5.58 (s, 1H, =CH), 6.89 (dd, J = 2.8, 9.2 Hz, 1H, ArH), 7.09~7.15 (m, 1H, ArH), 7.93 (dd, J = 5.6, 9.2 Hz, 1H, ArH), 9.91 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 24.0, 29.7, 31.1 (d, J = 1.6 Hz), 31.4, 91.6 (dq, J = 1.5, 30.8 Hz), 100.4, 114.9 (d, J = 24.1 Hz), 116.9 (d, J = 21.3 Hz), 124.2 (q, J = 284.8 Hz), 127.0~127.2, 128.9 (d, J = 7.9 Hz), 133.6 (d, J

= 2.7 Hz), 158.7 (d, *J* = 243.4 Hz), 166.8 (d, *J* = 2.0 Hz), 170.3 (d, *J* = 1.1 Hz), 195.2 (d, *J* = 3.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.21, -117.33. IR (CH_2Cl_2) ν 3675, 3338, 2987, 2959, 2922, 2359, 2343, 1686, 1621, 1411, 1189, 1077, 1051, 937, 858 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{16}F_4NO_3^{+1}(M+H)^+$ requires 346.1061, Found: 346.1060.



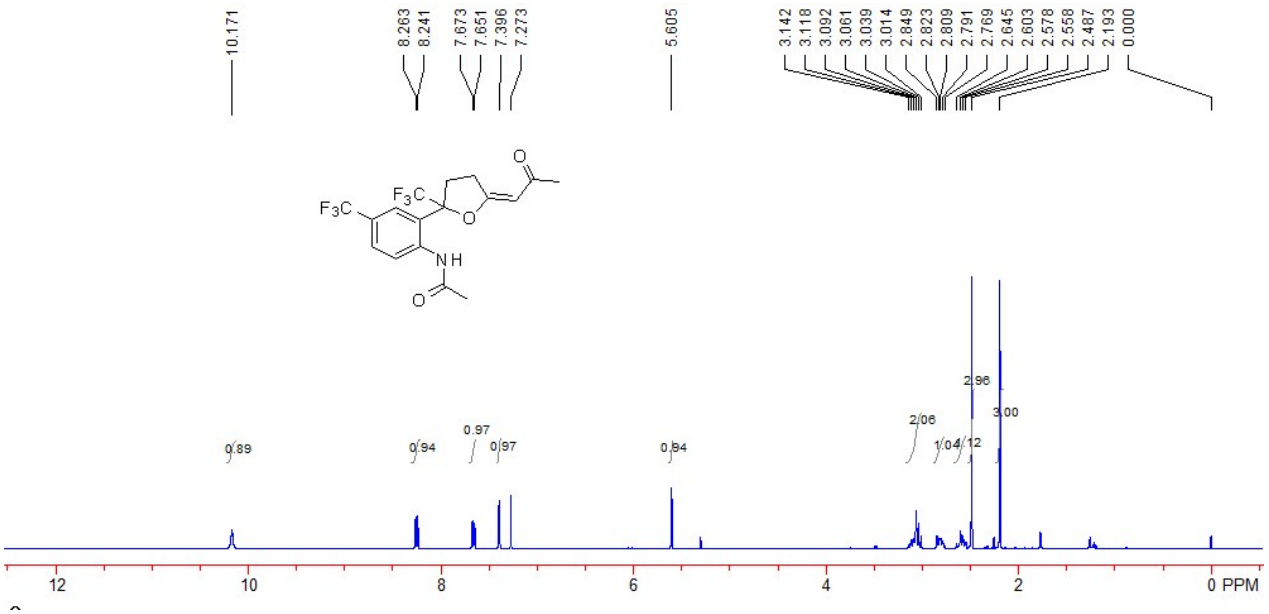






(E)-N-(2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)-4-(trifluoromethyl)phenyl)acetamide (3l)

A white solid, 87% yield (69 mg). M.p.: 133-135 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.19 (s, 3H, CH_3), 2.49 (s, 3H, CH_3), 2.55~2.65 (m, 1H, CH_2), 2.76~2.85 (m, 1H, CH_2), 3.01~3.15 (m, 2H, CH_2), 5.61 (s, 1H, =CH), 7.40 (s, 1H, ArH), 7.66 (d, J = 8.8 Hz, 1H, ArH), 8.25 (d, J = 8.8, 1H, ArH), 10.17 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 24.3, 29.6 (d, J = 1.5 Hz), 31.1, 31.5, 91.8 (q, J = 31.1 Hz), 100.5, 123.6 (q, J = 271.0 Hz), 124.2 (q, J = 285.4 Hz), 125.1, 125.2 (q, J = 3.8 Hz), 125.8 (q, J = 32.6 Hz), 126.5, 127.1 (q, J = 3.8 Hz), 141.0, 166.6, 170.4, 195.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -62.32, -79.33. IR (CH_2Cl_2) ν 3678, 3641, 3016, 2937, 2854, 1691, 1622, 1422, 1289, 1192, 1031, 1023 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{16}F_6NO_3^{+1}(M+H)^+$ requires 396.1029, Found: 396.1028.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3.014
2.849
2.823
2.809
2.791
2.769
2.645
2.603
2.578
2.558
2.487
2.193
0.000
F3C
F3C
O
NH
O
O
2.96
3.00
2.06
1.04
1.12
0.97
0.89
0.94
0.97
0.94
12
10
8
6
4
2
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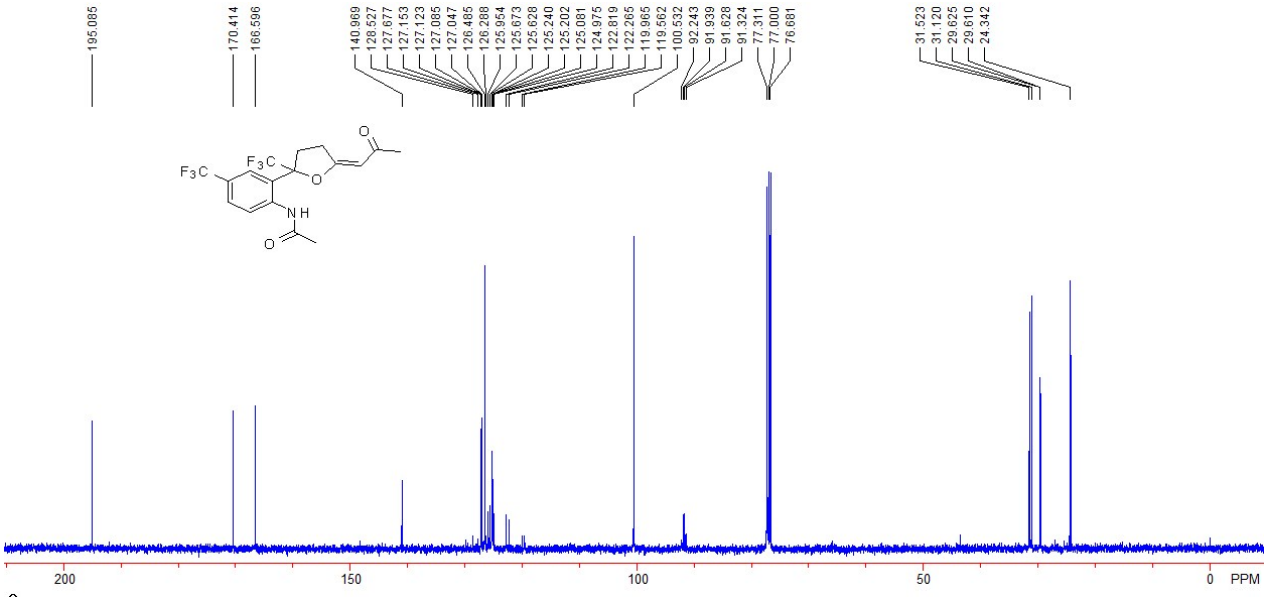
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125.954
125.673
125.628
125.240
125.202
125.081
124.975
122.819
122.265
119.965
119.562
100.532
92.243
91.939
91.628
91.324
77.311
77.000
76.681
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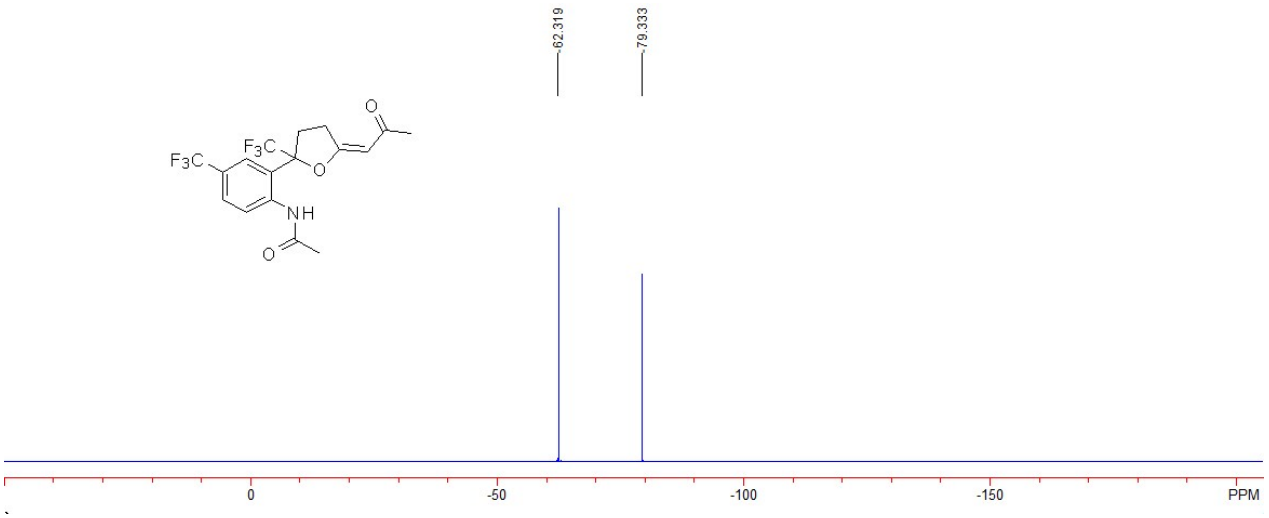
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79.333
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F3C
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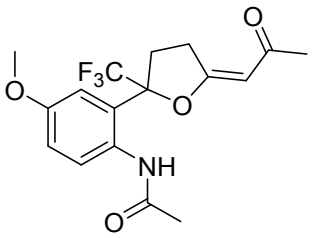
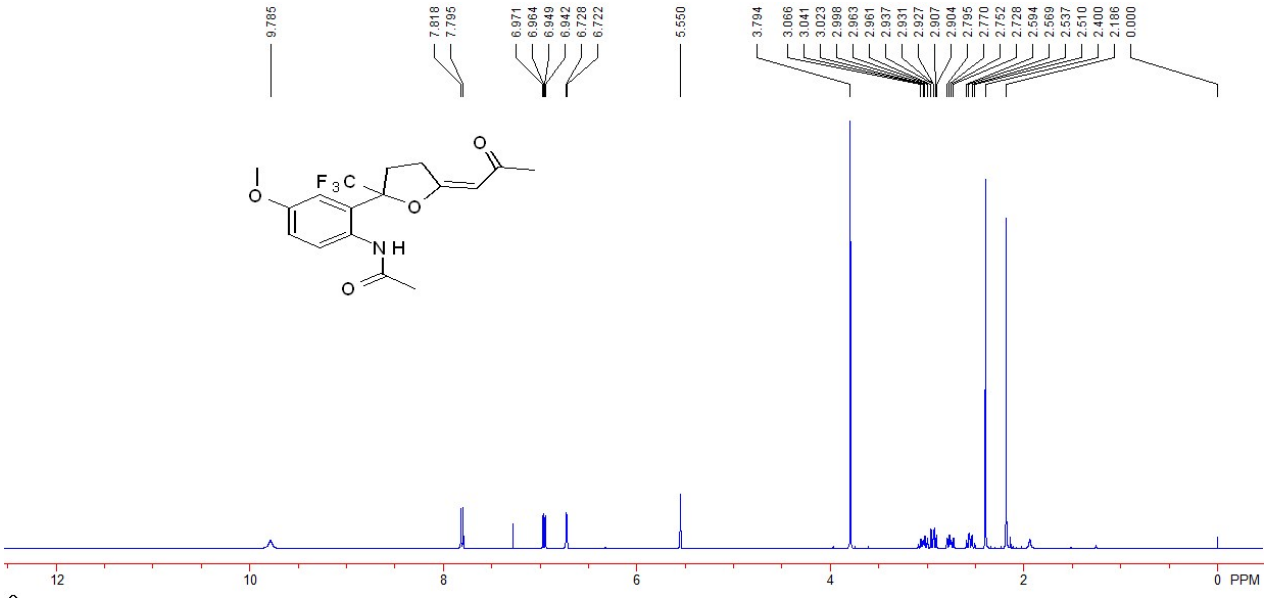
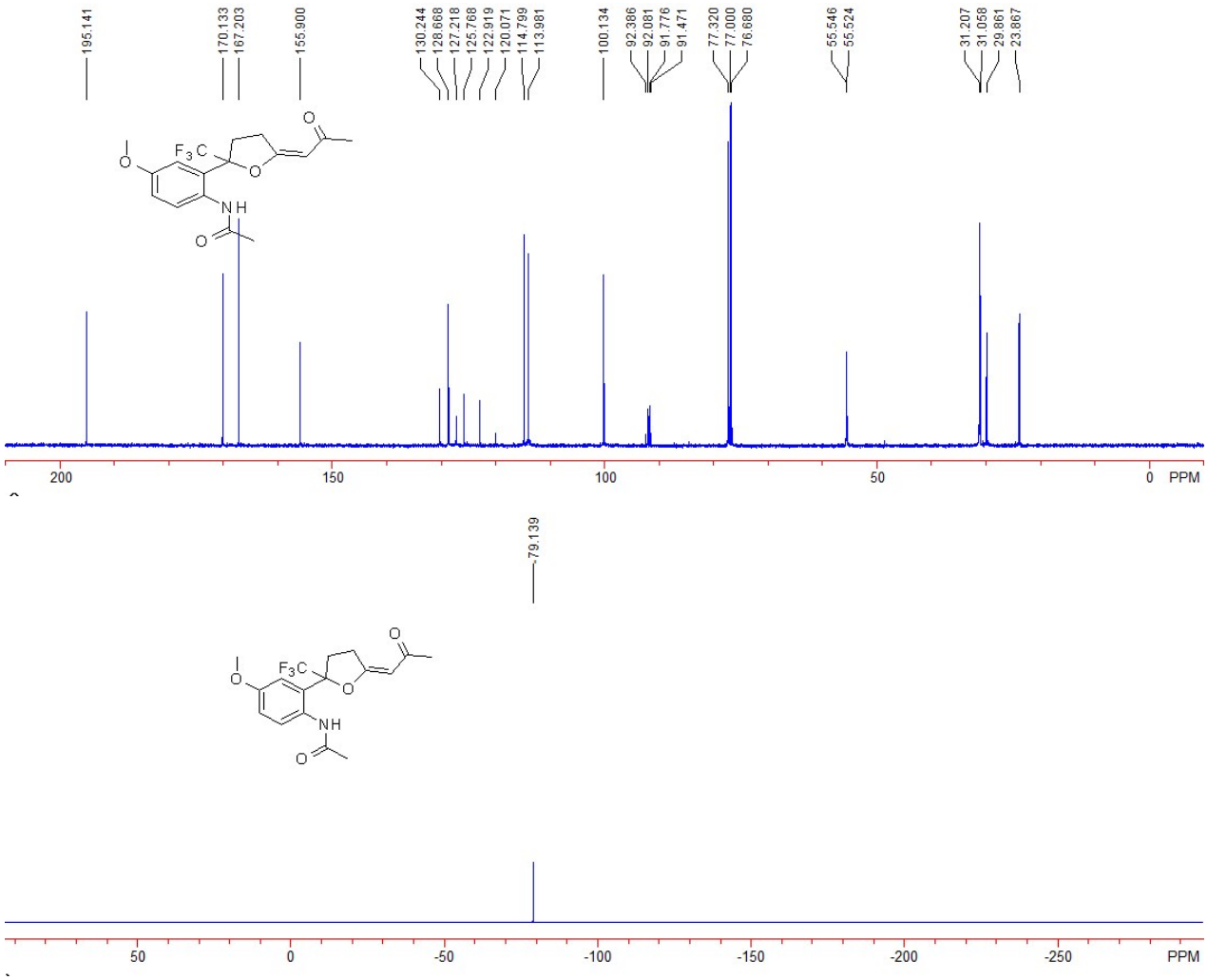
O
0
-50
-100
-150
PPM

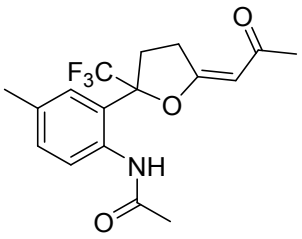


(E)-N-(4-methoxy-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (3m)

A white solid, 63% yield (45 mg). M.p.: 134-136 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.19 (s, 3H, CH_3), 2.40 (s, 3H, CH_3), 2.51~2.59 (m, 1H, CH_2), 2.73~2.80 (m, 1H, CH_2), 2.90~2.97 (m, 1H, CH_2), 2.99~3.07 (m, 1H, CH_2), 3.80 (s, 3H, CH_3), 5.50 (s, 1H, =CH), 6.73 (d, J = 2.4, 1H, ArH), 6.96 (dd, J = 2.8, 8.8 Hz, 1H, ArH), 7.81 (d, J = 9.2, 1H, ArH), 9.79 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 23.9, 29.9, 31.1, 31.2, 55.5 (d, J = 2.2 Hz), 91.9 (q, J = 30.5 Hz), 100.1, 114.0, 114.8, 124.3 (q, J = 284.9 Hz), 127.2, 128.9, 130.2, 155.9, 167.2, 170.1, 195.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.14. IR (CH_2Cl_2) ν 3346, 2925, 2359, 2341, 1684, 1617, 1517, 1287, 1217, 1169, 853 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{19}F_3NO_4^{+1}(M+H)^+$ requires 358.1261, Found: 358.1260.



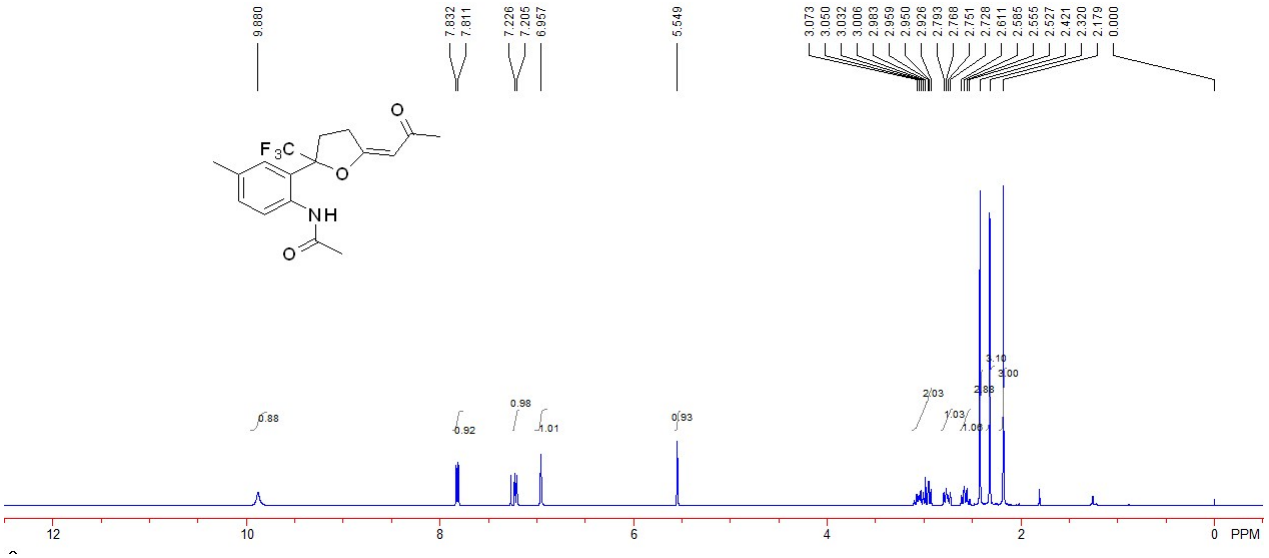


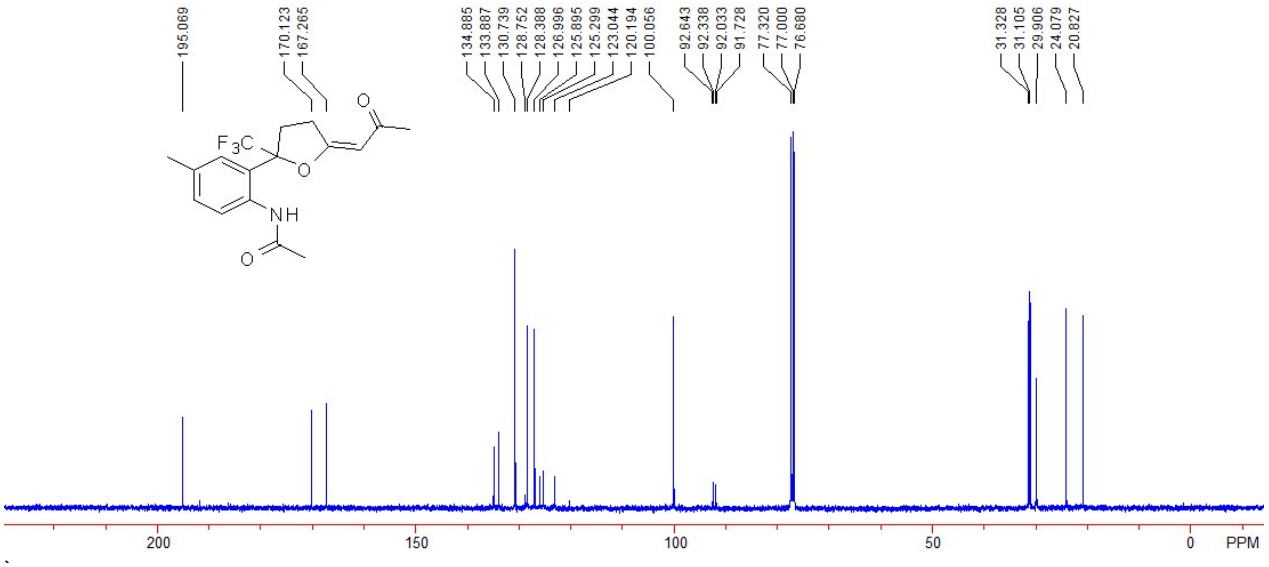


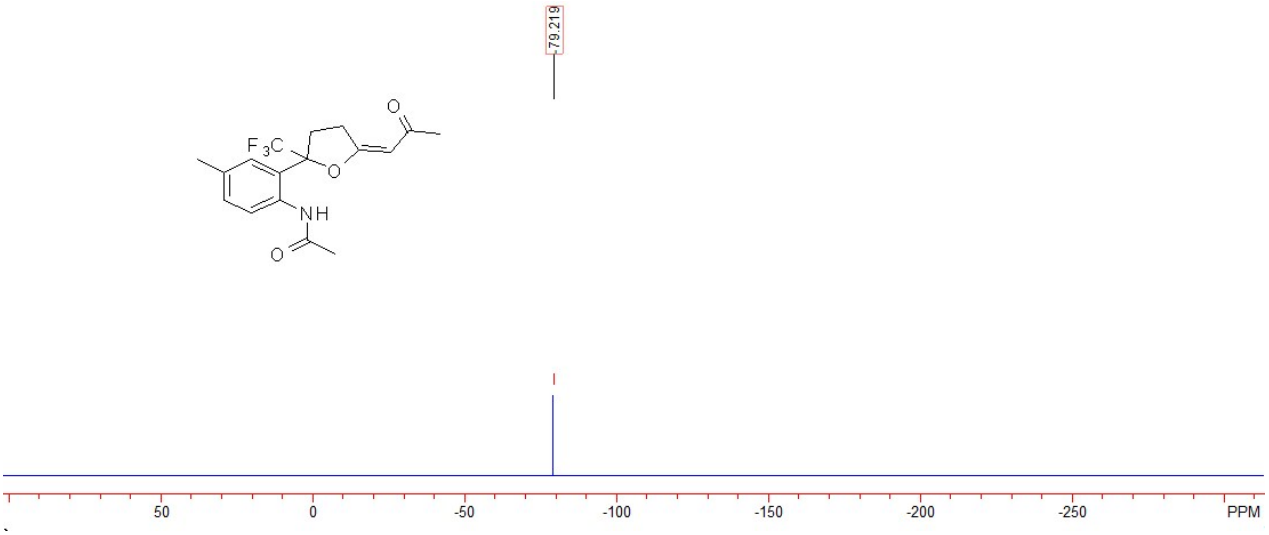
(E)-N-(4-methyl-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (3n)

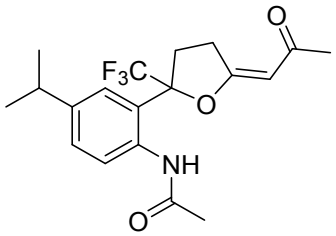
A white solid, 67% yield (46 mg). M.p.: 148-150 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.18 (s, 3H, CH_3), 2.32 (s, 3H, CH_3), 2.42 (s, 3H, CH_3), 2.52~2.62 (m, 1H, CH_2), 2.72~2.80 (m, 1H, CH_2), 2.92~3.10 (m, 2H, CH_2), 5.50 (s, 1H, =CH), 6.96 (s, 1H, ArH), 7.22 (d, J = 8.4 Hz, 1H, ArH), 7.82 (d, J = 8.4 Hz, 1H, ArH), 9.88 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 20.8, 24.1, 29.9, 31.1, 31.3, 92.2 (q, J = 30.5 Hz), 100.1, 124.5 (q, J = 285.1 Hz), 125.3, 127.0, 128.4, 130.7, 133.9, 134.9, 155.9, 167.3, 170.1, 195.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.22. IR (CH_2Cl_2) ν

3347, 2957, 2923, 2359, 2341, 1685, 1618, 1516, 1296, 1189, 1168, 1080, 930 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{19}F_3NO_3^{+1}(M+H)^+$ requires 342.1312, Found: 342.1313.



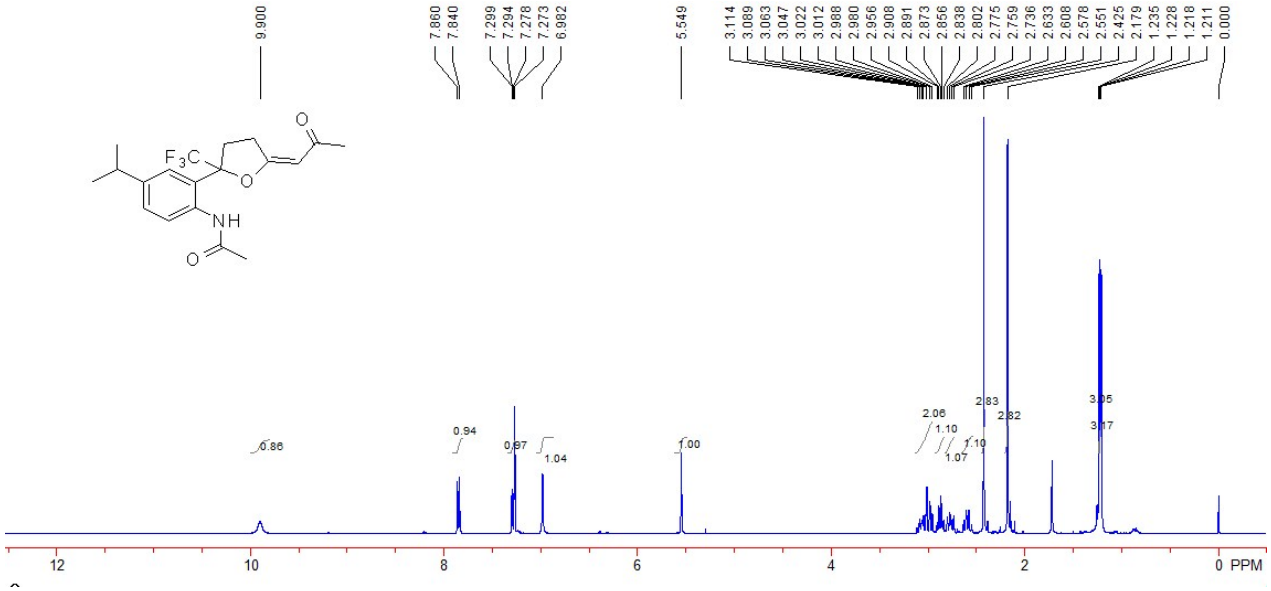


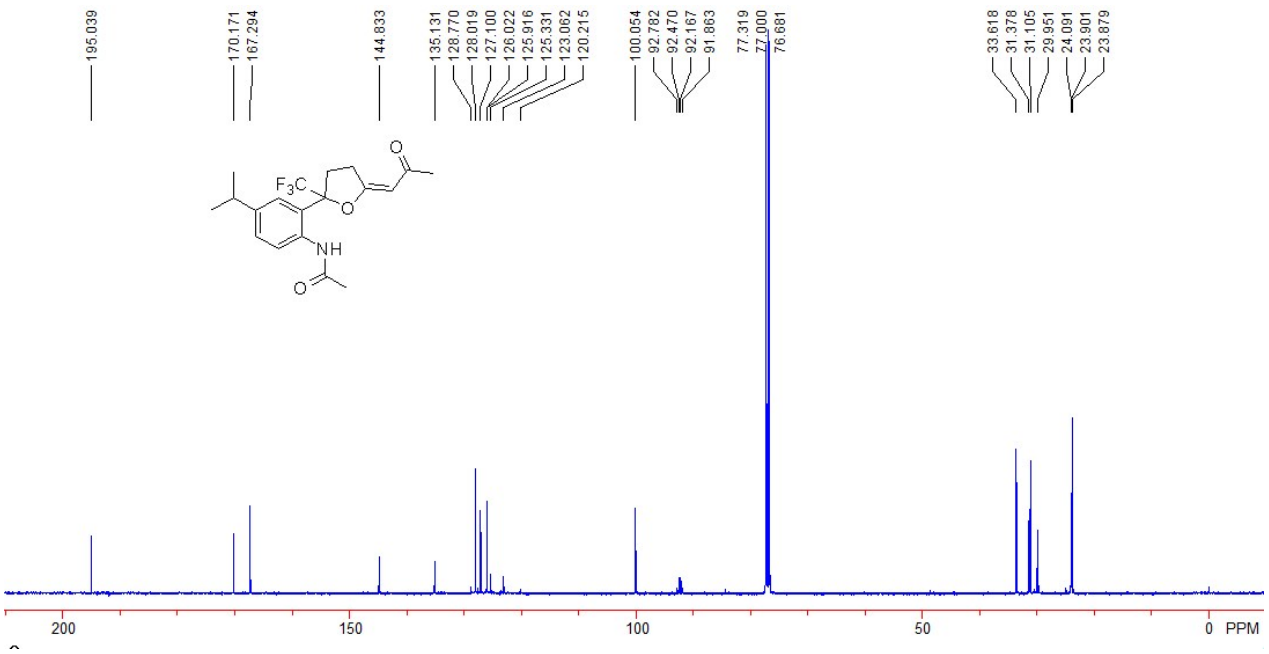




(E)-N-(4-isopropyl-2-(5-(2-oxopropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (3o)

A white oil, 47% yield (35 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.21 (d, J = 2.8 Hz, 3H, CH_3), 1.24 (d, J = 2.8 Hz, 3H, CH_3), 2.18 (s, 3H, CH_3), 2.43 (s, 3H, CH_3), 2.55~2.64 (m, 1H, CH_2), 2.73~2.81 (m, 1H, CH_2), 2.83~2.91 (m, 1H, CH), 2.95~3.12 (m, 2H, CH_2), 5.50 (s, 1H, =CH), 6.98 (s, 1H, ArH), 7.29 (dd, J = 2.0, 8.4 Hz, 1H, ArH), 7.85 (d, J = 8.0 Hz, 1H, ArH), 9.90 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 23.88, 23.90, 24.1, 30.0, 31.1, 31.4, 33.6, 92.3 (q, J = 30.3 Hz), 100.1, 124.5 (q, J = 285.4 Hz), 125.3, 126.0, 127.1, 128.0, 135.1, 144.8, 167.3, 170.2, 195.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.27. IR (CH_2Cl_2) ν 3350, 2958, 2922, 2851, 1687, 1619, 1517, 1325, 1299, 1189, 1050, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{23}NF_3O_3^{+1}(M+H)^+$ requires 370.1625, Found: 370.1624.

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33.618
31.378
31.105
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24.091
23.901
23.879
F3C
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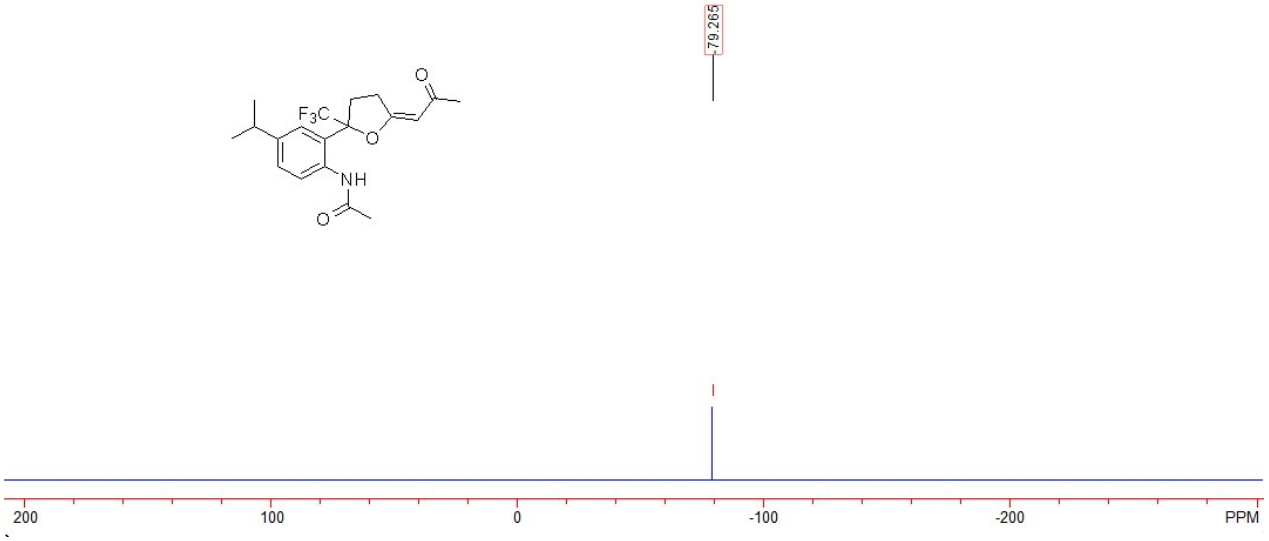
NH
O
200
150
100
50
0
PPM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F3C
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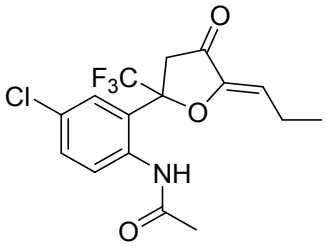
NH
O
200
100
0
-100
-200
PPM

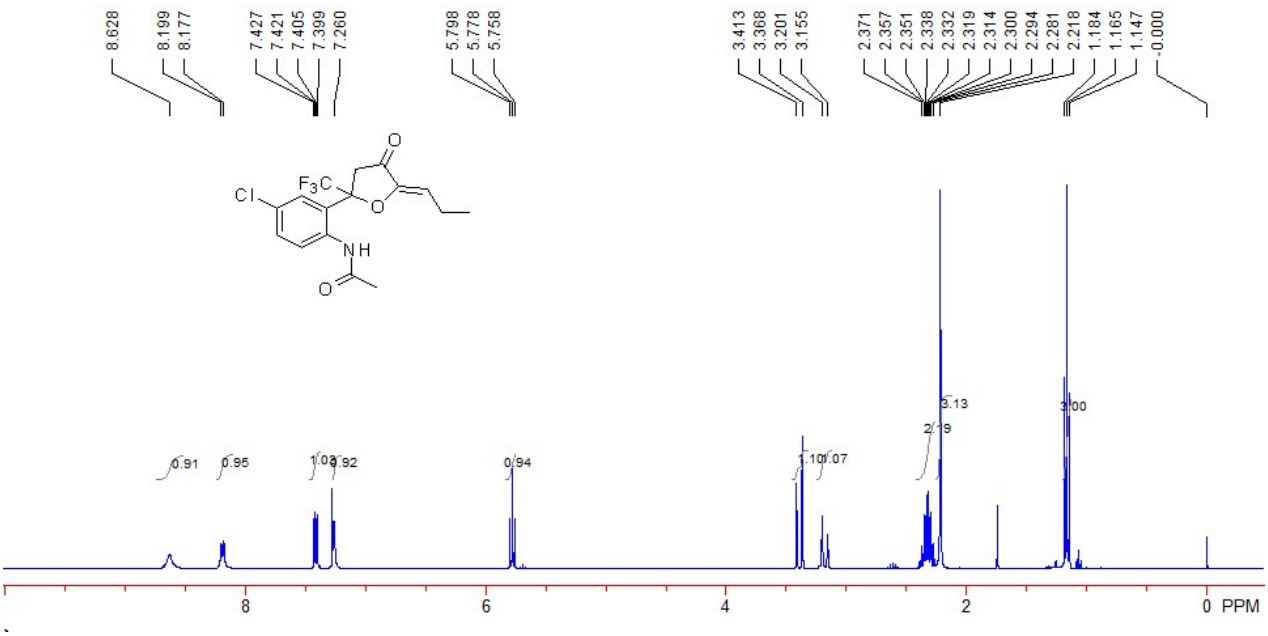
General Procedure for Hex-3-yn-2-one 2a to Trifluoroacetyl Compounds 1 at 10 °C and Spectroscopic Data of the Products 4

General procedure: Under argon atmosphere, to a solution of trifluoroacetyl compound **2** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the hex-3-yn-2-one **2a** (0.6 mmol) at room temperature. Then the resulting mixture was stirred at 10 °C until the reaction completed (monitoring by TLC). Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the desired products **4a**-**4e**, and **4g**-**4o**.



(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (4a)

A white solid, 87% yield (63 mg). M.p.: 137-139 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.17 (t, *J* = 7.6 Hz, 3H, CH_3), 2.22 (s, 3H, CH_3), 2.26~2.41 (m, 2H, CH_2), 3.18 (d, *J* = 18.4 Hz, 1H, CH_2), 3.39 (d, *J* = 18.4 Hz, 1H, CH_2), 5.78 (t, *J* = 8.0 Hz, 1H, =CH), 7.26 (s, 1H, ArH), 7.41 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 8.19 (d, *J* = 8.8 Hz, 1H, ArH), 8.63 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.2, 24.8, 43.1, 84.6 (q, *J* = 29.7 Hz), 112.9, 124.4 (q, *J* = 285.5 Hz), 125.1, 126.1, 128.6, 129.9, 130.7, 135.8, 145.5, 168.2, 191.5. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.06. IR (CH_2Cl_2) ν 3411, 3234, 2982, 2938, 1769, 1641, 1538, 1189, 1265, 1120, 996, 772 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{16}ClF_3NO_3{}^{+1}(M+H)^+$ requires 362.0765, Found: 362.0764.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2.338
2.332
2.319
2.314
2.300
2.294
2.281
2.218
1.184
1.165
1.147
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0.91
0.95
1.00
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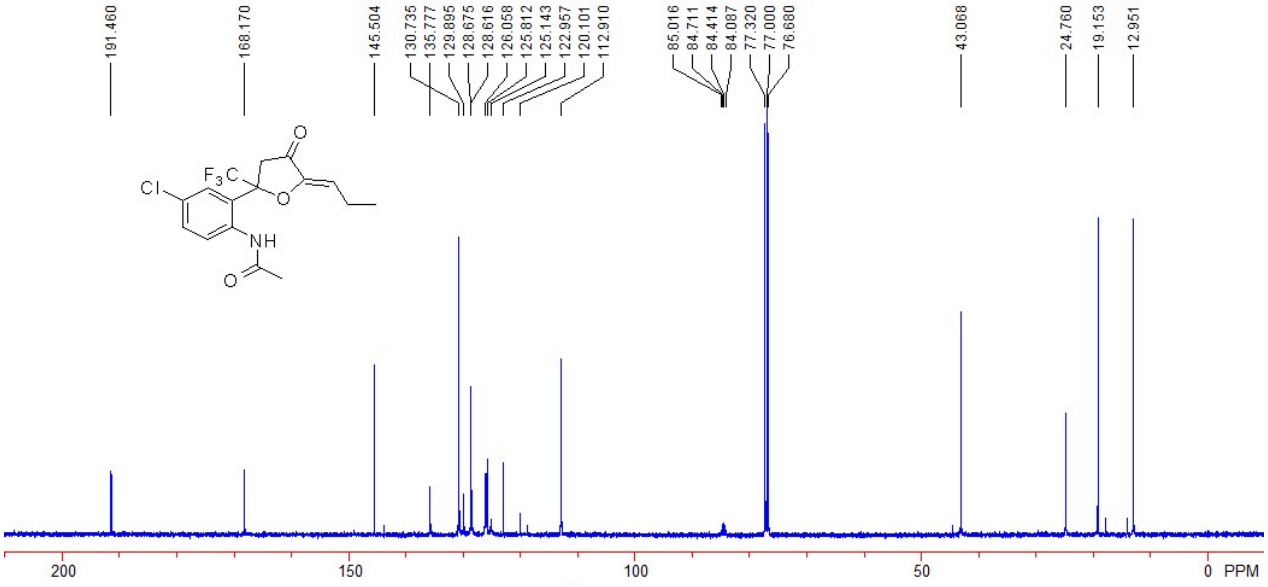
0.94
1.10
1.07
3.13
2.19
3.00
8
6
4
2
0 PPM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125.812
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85.016
84.711
84.414
84.087
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77.000
76.680
43.068
24.760
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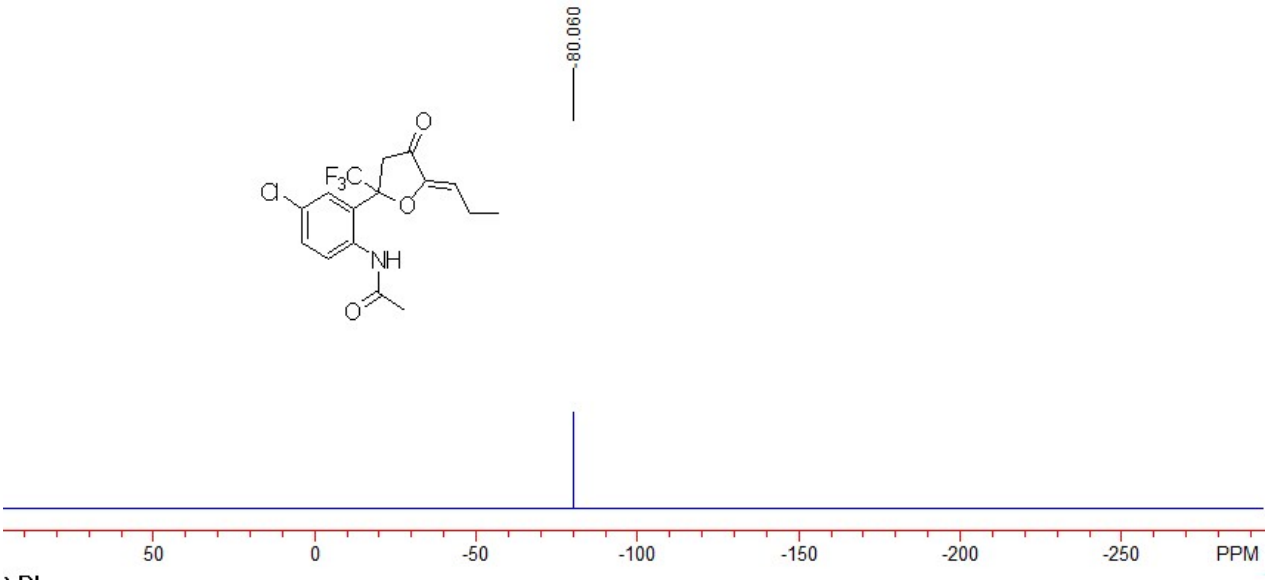
12.951
200
150
100
50
0 PPM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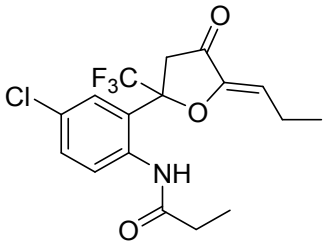
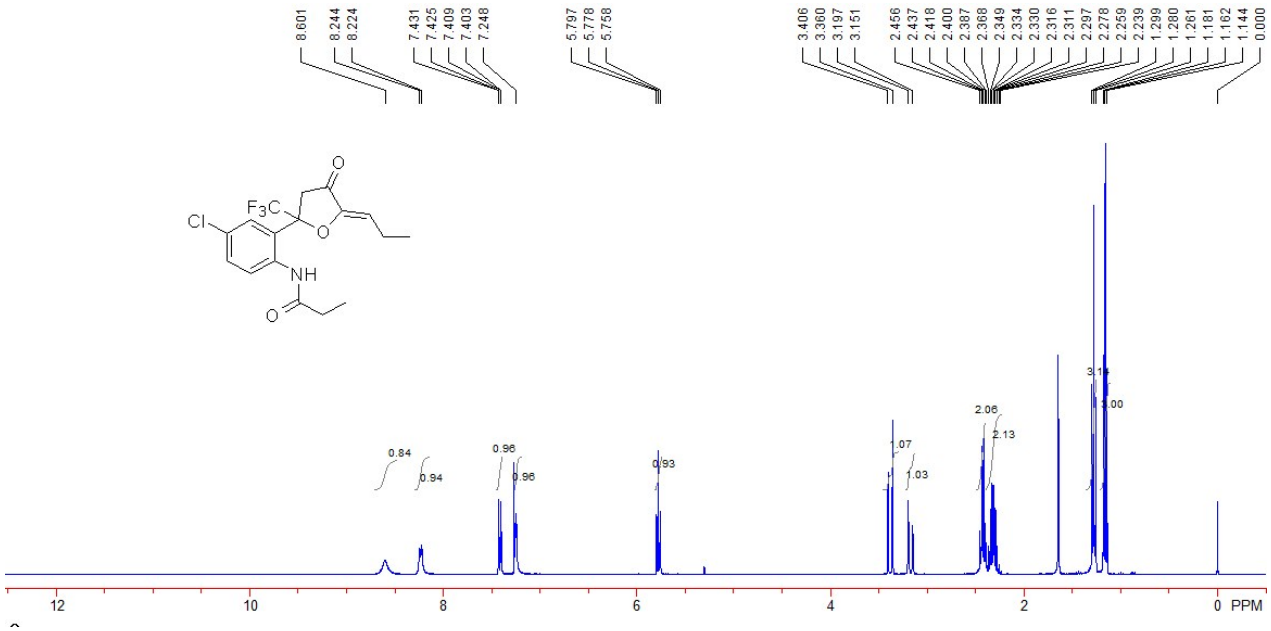
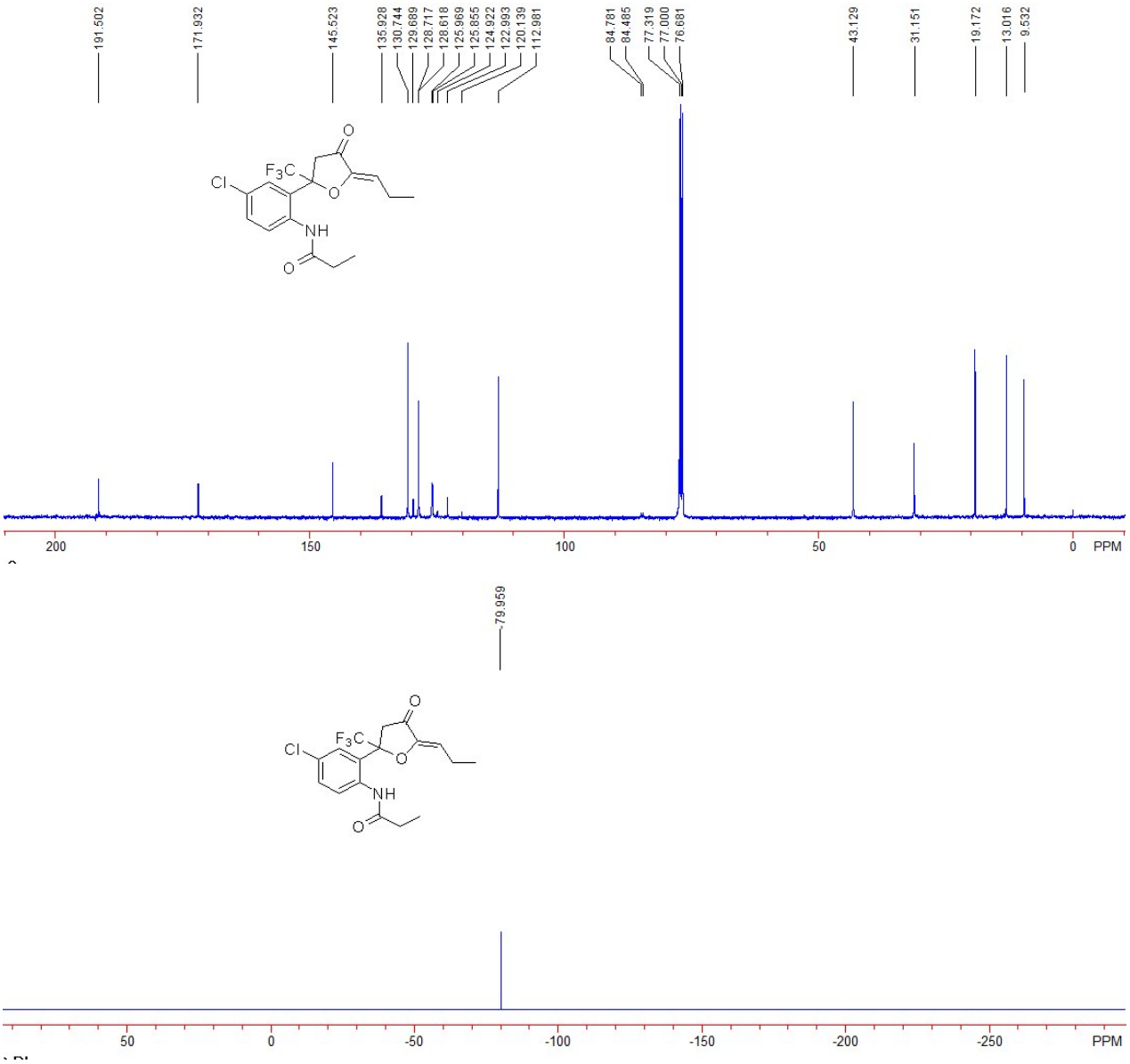
-50
-100
-150
-200
-250
PPM

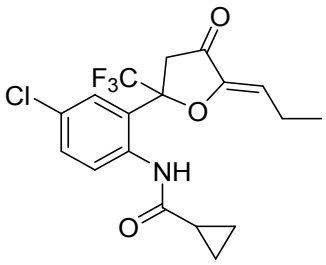


(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)propionamide (4b)

A white solid, 96% yield (72 mg). M.p.: 132-134 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.16 (t, *J* = 7.6 Hz, 3H, CH_3), 1.28 (t, *J* = 7.6 Hz, 3H, CH_3), 2.23~2.39 (m, 2H, CH_2), 2.40~2.46 (m, 2H, CH_2), 2.43 (q, *J* = 7.6 Hz, 1H, CH_2), 3.17 (d, *J* = 18.4 Hz, 1H, CH_2), 3.38 (d, *J* = 18.4 Hz, 1H, CH_2), 5.78 (t, *J* = 7.6 Hz, 1H, =CH), 7.25 (s, 1H, ArH), 7.42 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 8.23 (d, *J* = 8.0 Hz, 1H, ArH), 8.60 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 9.5, 13.0, 19.2, 31.2, 43.1, 84.6 (q, *J* = 29.6 Hz), 113.0, 124.4 (q, *J* = 286.2 Hz), 124.9, 126.0, 128.6, 129.7, 130.7, 135.9, 145.5, 171.9, 191.5. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.96. IR (CH_2Cl_2) ν 3427, 3281, 2974, 2938, 1745, 1670, 1508, 1289, 1175, 1120, 996 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{18}ClF_3NO_3$ $^{+1}$(M+H)$^+$ requires 376.0922, Found: 376.0922.



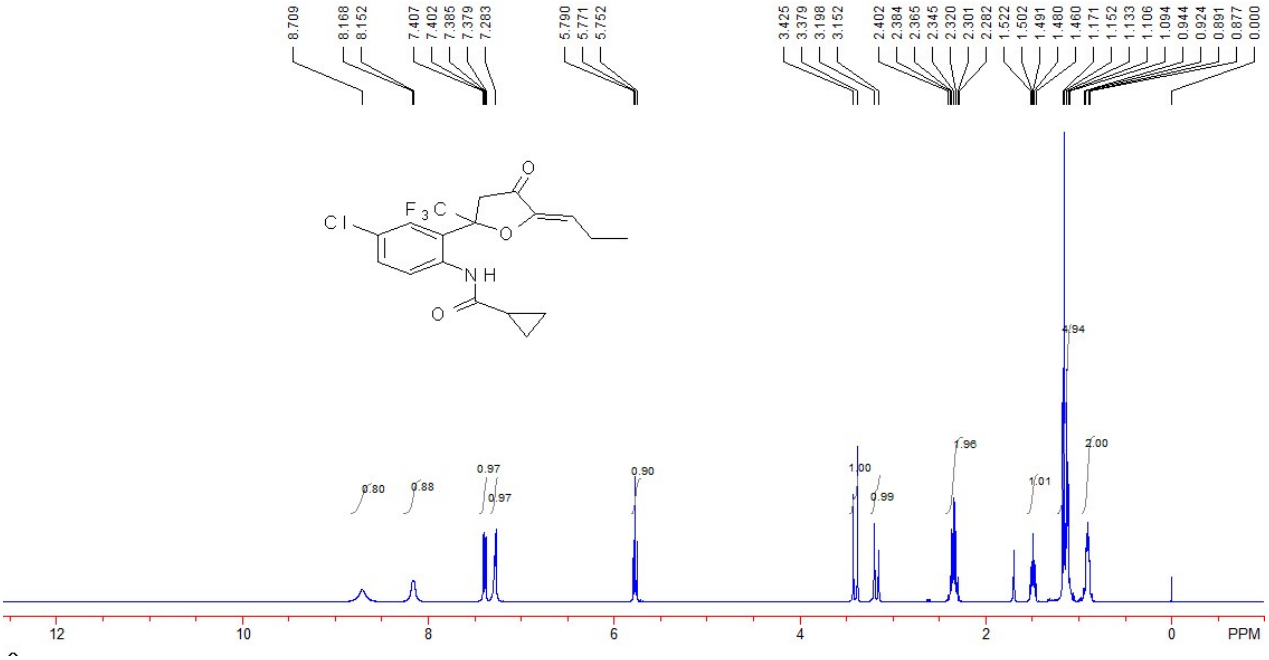


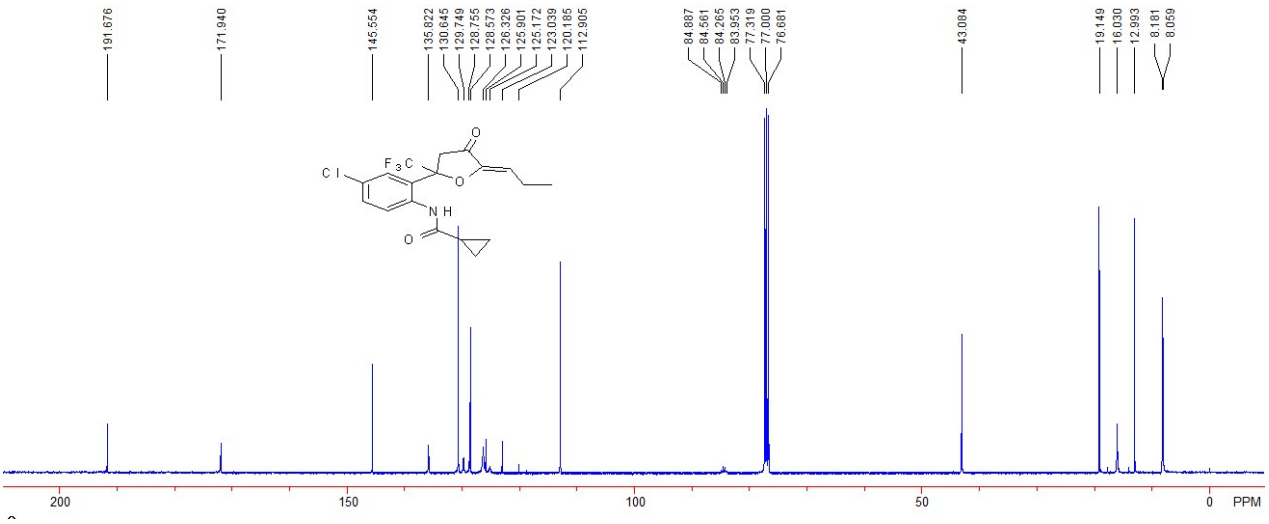


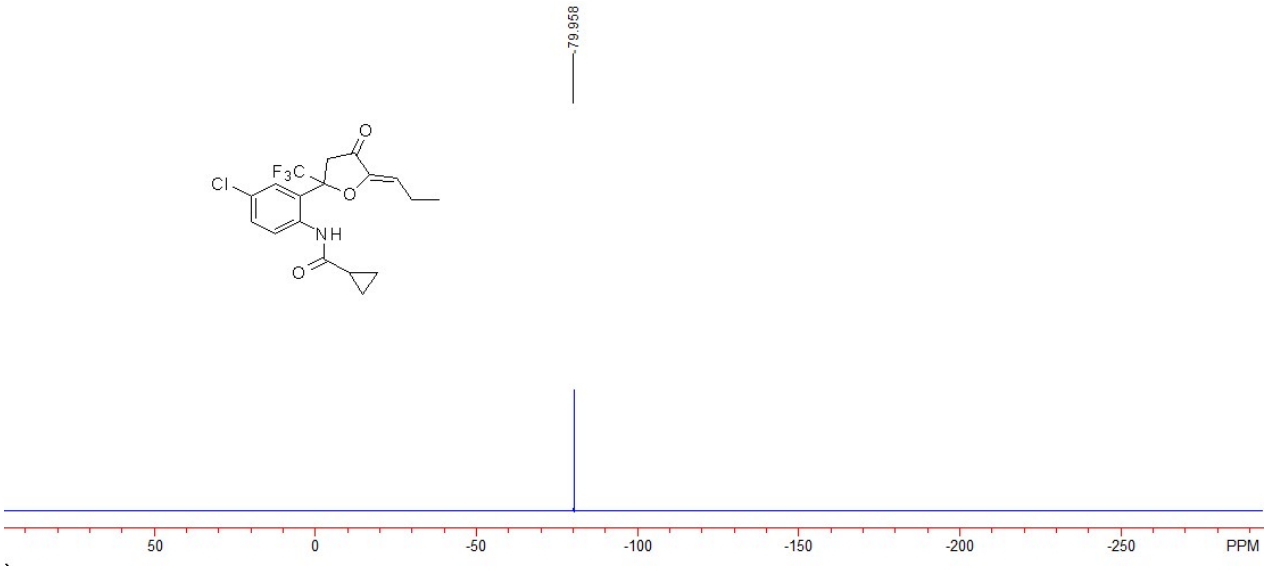
(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)cyclopropanecarboxamide (4c)

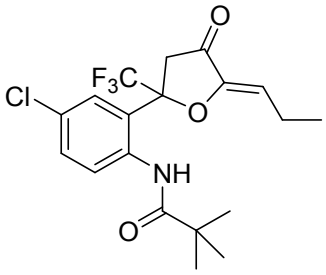
A white solid, 91% yield (71 mg). M.p.: 150-152 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 0.87~0.95 (m, 2H, CH_2), 1.09~1.18 (m, 5H, CH_2, CH_3), 1.46~1.53 (m, 1H, CH), 2.28~2.41 (m, 2H, CH_2), 3.18 (d, J = 18.4 Hz, 1H, CH_2), 3.40 (d, J = 18.4 Hz, 1H, CH_2), 5.77 (t, J = 7.6 Hz, 1H, =CH),

7.28 (s, 1H, ArH), 7.39 (dd, J = 2.0, 8.8 Hz, 1H, ArH), 8.16 (d, J = 6.4 Hz, 1H, ArH), 8.71 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 8.1, 8.2, 13.0, 16.0, 19.1, 43.1, 84.4 (q, J = 29.6 Hz), 112.9, 124.5 (q, J = 286.2 Hz), 125.2, 126.3, 128.6, 129.7, 130.6, 135.8, 145.6, 171.9, 191.7. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.96. IR (CH_2Cl_2) ν 3338, 2957, 2922, 2852, 1686, 1619, 1507, 1284, 1190, 1173, 923 cm^{-1}. HRMS (ESI) Calcd. For $C_{18}H_{18}ClF_3NO_3^{+1}(M+H)^+$ requires 388.0922, Found: 388.0921.



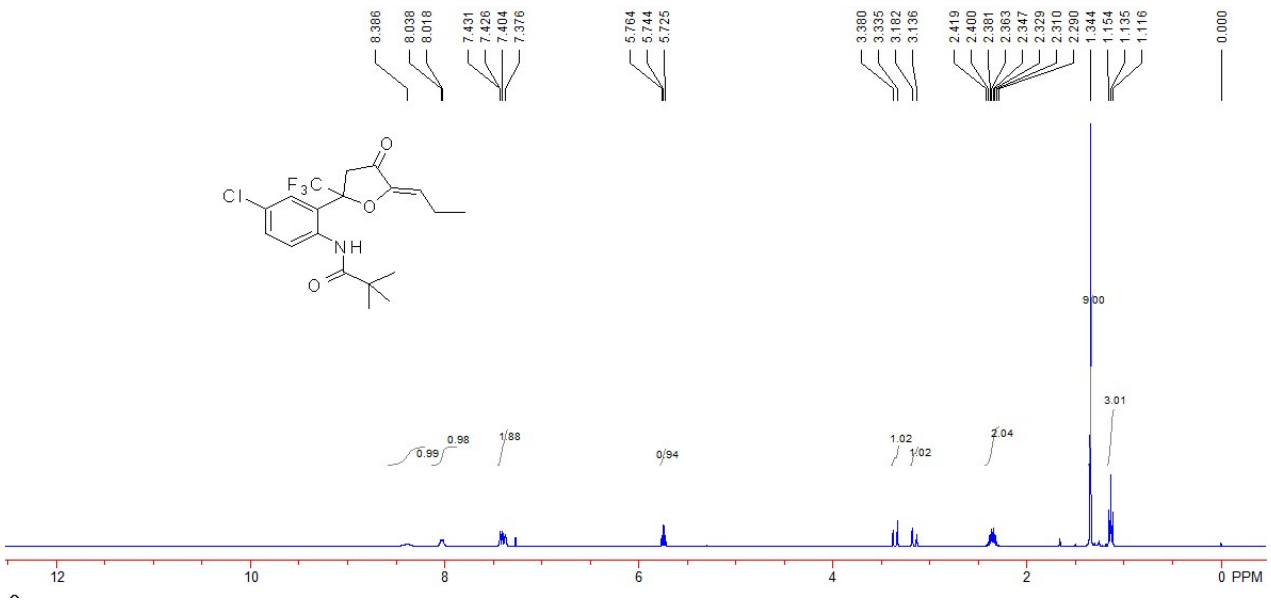






(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)pivalamide (4d)

A white oil, 79% yield (64 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.14 (t, *J* = 7.6 Hz, 3H, CH_3), 1.34 (s, 9H, CH_3), 2.29~2.42 (m, 2H, CH_2), 3.16 (d, *J* = 18.4 Hz, 1H, CH_2), 3.36 (d, *J* = 18.4 Hz, 1H, CH_2), 5.74 (t, *J* = 8.0 Hz, 1H, =CH), 7.37~7.44 (m, 2H, ArH), 8.03 (d, *J* = 8.0 Hz, 1H, ArH), 8.39 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.1, 19.1, 27.4, 39.6, 42.8, 84.0 (q, *J* = 28.1 Hz), 113.0, 124.6 (q, *J* = 286.2 Hz), 126.6, 127.5, 128.6, 130.2, 130.6, 135.6, 145.6, 177.0, 191.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.34. IR (CH_2Cl_2) ν 3443, 3435, 2955, 2924, 2852, 1745, 1691, 1511, 1501, 1398, 1292, 1175, 1033, 997 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{22}ClF_3NO_3$ $^{+1}(M+H)^+$ requires 404.1235, Found: 404.1234.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3.136
2.419
2.400
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2.347
2.329
2.310
2.290
1.344
1.154
1.135
1.116
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9.00
3.01
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0.98
1.88
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1.02
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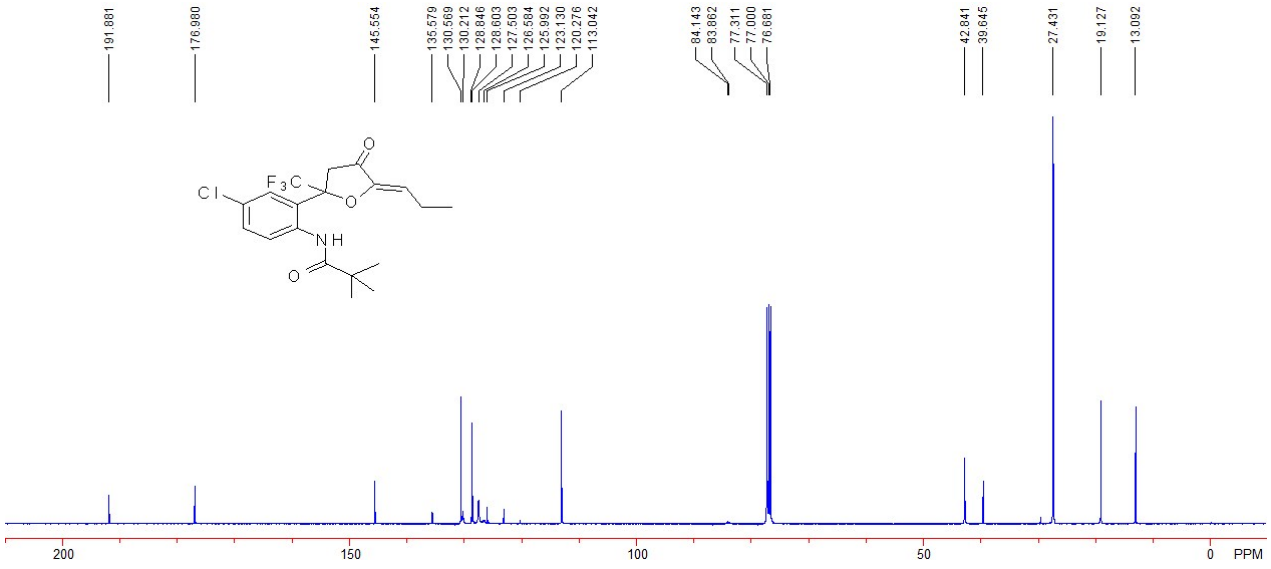
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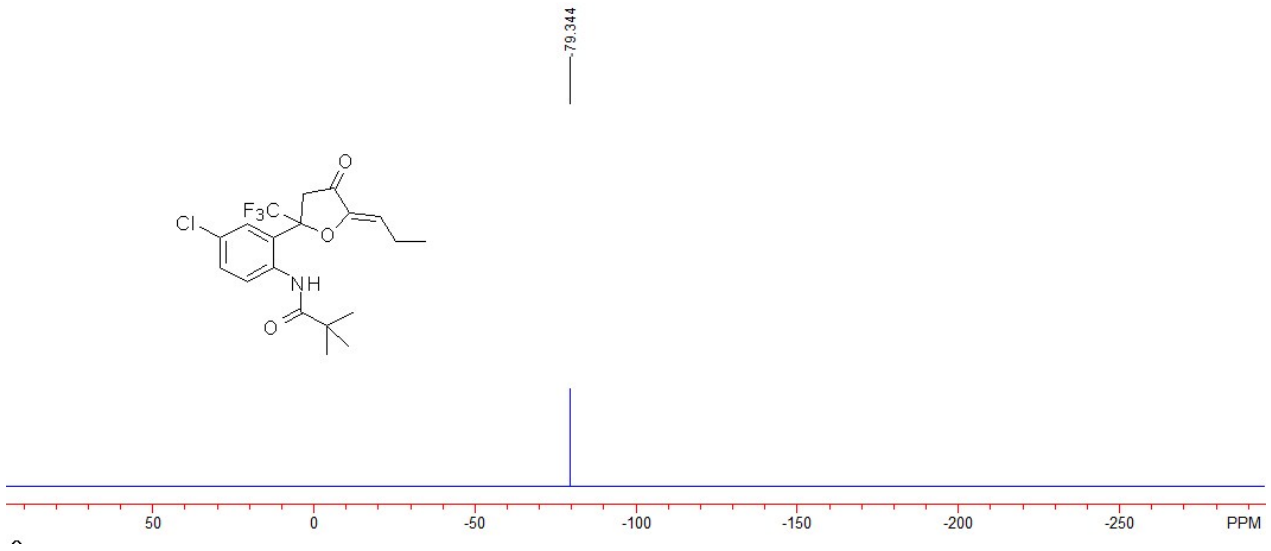
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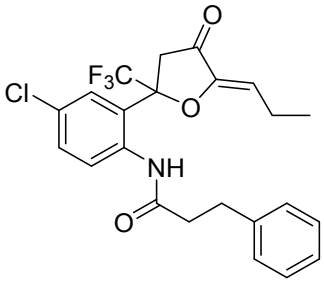
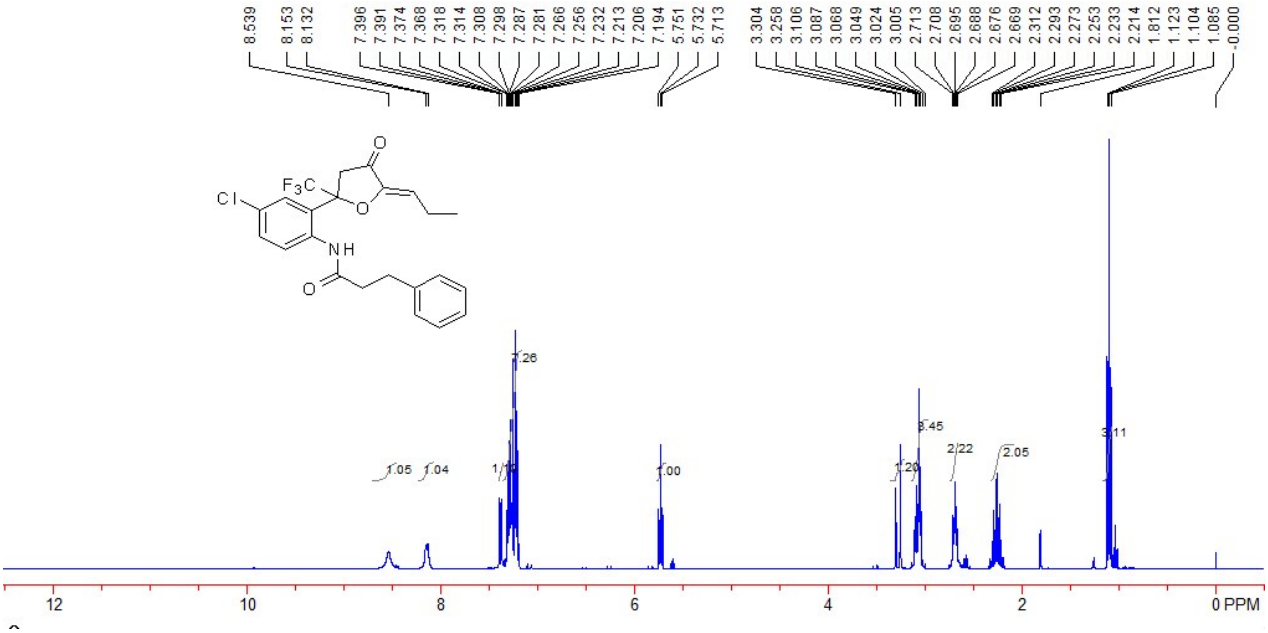
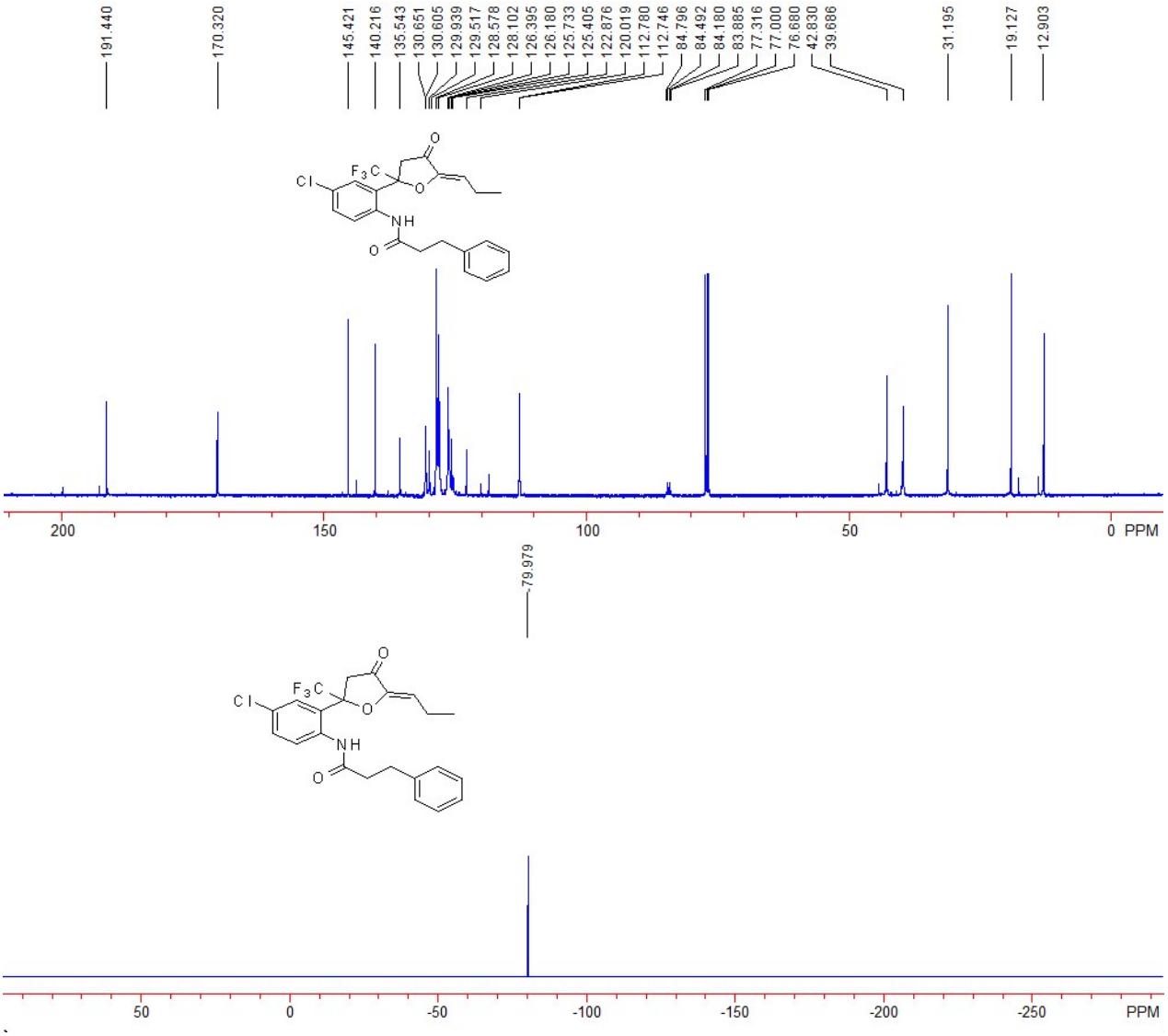
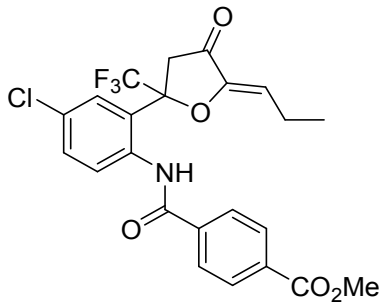


(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-3-phenylpropanamide (4e)

A white solid, 79% yield (71 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.10 (t, *J* = 7.6 Hz, 3H, CH_3), 2.21~2.32 (m, 2H, CH_2), 2.66~2.72 (m, 2H, CH_2), 3.00~3.11 (m, 3H, CH_2), 3.28 (d, *J* = 18.4 Hz, 1H, CH_2), 5.73 (t, *J* = 7.6 Hz, 1H, =CH), 7.19~7.32 (m, 6H, ArH), 7.38 (dd, *J* = 2.0, 8.8 Hz, 1H, ArH), 8.14 (d, *J* = 8.0 Hz, 1H, ArH), 8.54 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 12.9, 19.1, 31.2, 39.7, 42.8, 84.3 (q, *J* = 31.2 Hz), 112.7 (d, *J* = 3.4 Hz), 124.3 (q, *J* = 285.7 Hz), 125.4, 126.2, 126.4, 128.1, 128.6, 129.5, 129.9, 130.6 (d, *J* = 4.6 Hz), 135.5, 140.2, 145.4, 170.3, 191.4. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.98. IR (CH_2Cl_2) ν 3416, 2968, 2937, 1744, 1668, 1509, 1455, 1275, 1233, 1174, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{23}H_{22}ClF_3NO_3$ $^{+1}$(M+H)$^{+}$ requires 452.1235, Found: 452.1233.



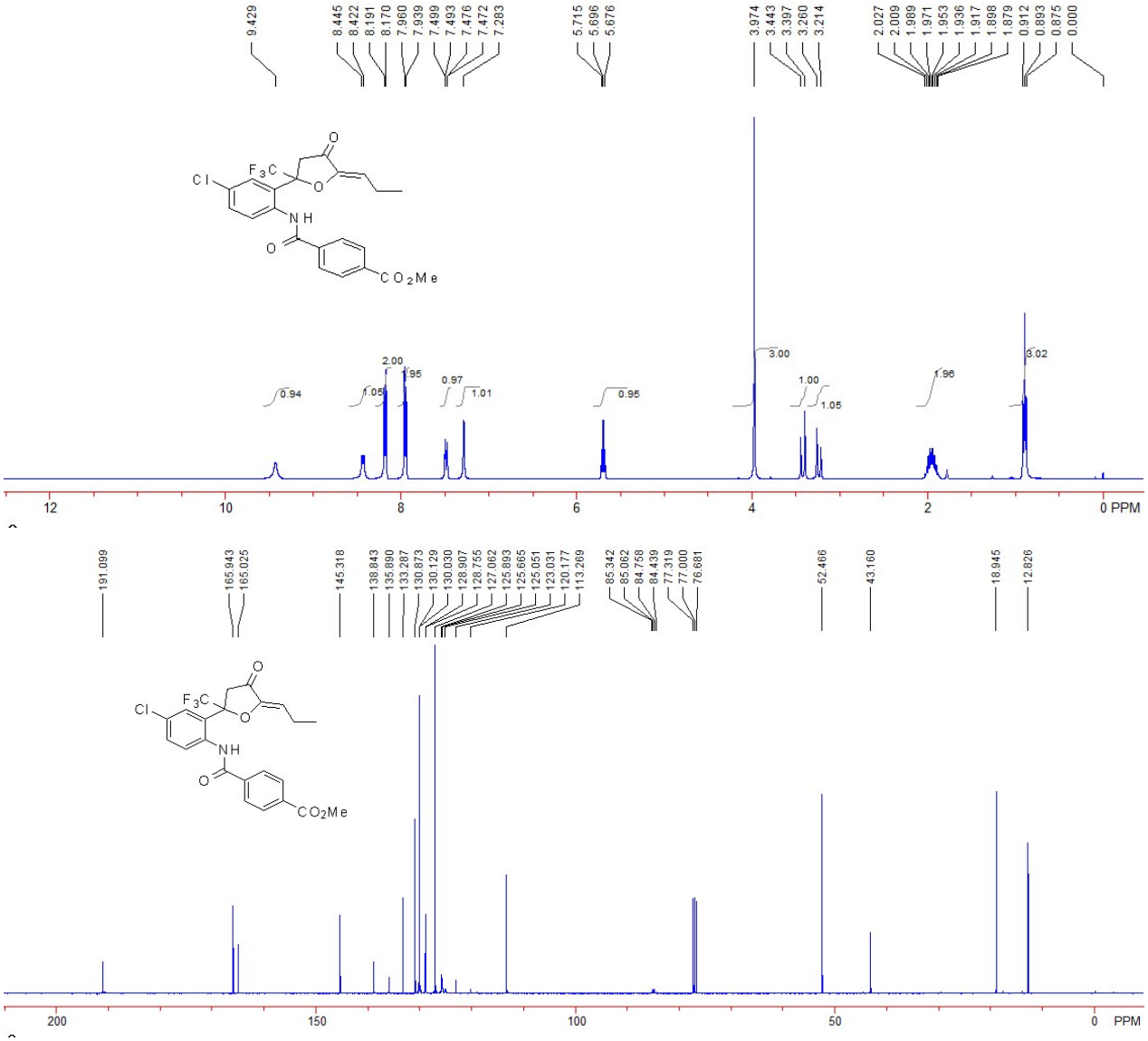


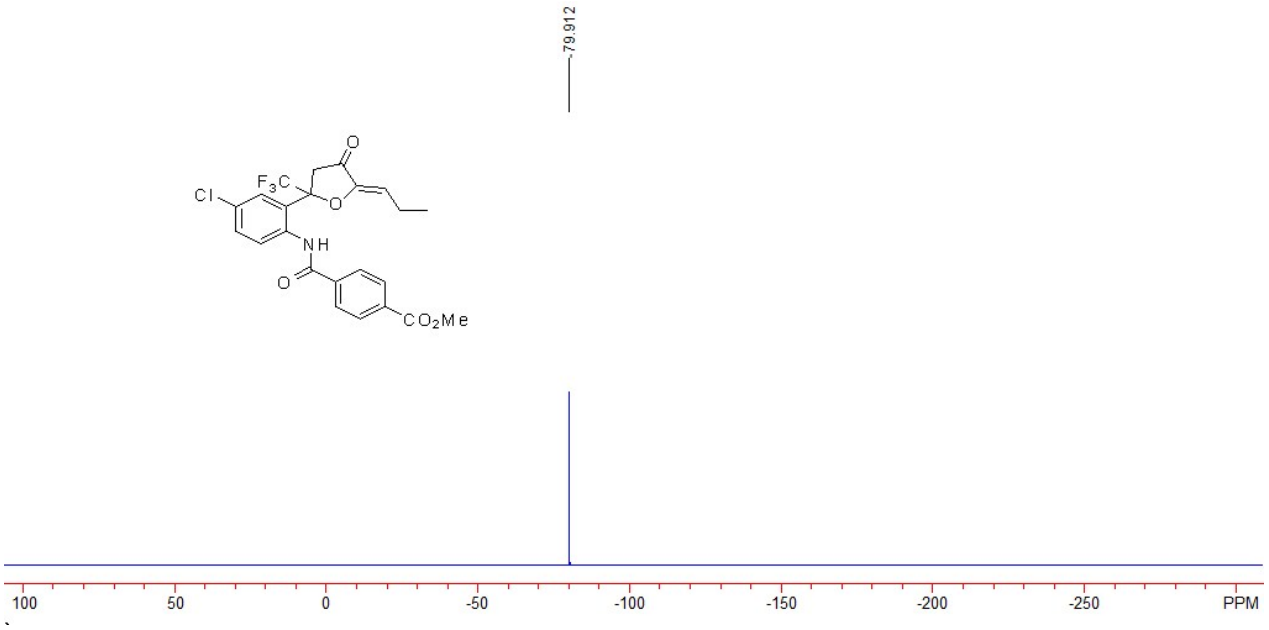


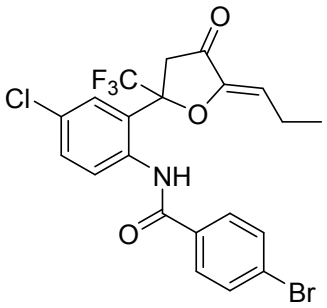
methyl (Z)-4-((4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)carbamoyl)benzoate (4g)

A white solid, 84% yield (81 mg). M.p.: 174-176 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 0.89 (t, J = 7.2 Hz, 3H, CH_3), 1.87~2.03 (m, 2H, CH_2), 3.24 (d, J = 18.4 Hz, 1H, CH_2), 3.42 (d, J = 18.4 Hz, 1H, CH_2), 3.97 (s, 3H, CH_3), 5.70 (t, J = 7.6 Hz, 1H, =CH), 7.28 (s, 1H, ArH), 7.49 (dd, J = 2.4, 9.2

Hz, 1H, ArH), 7.95 (d, J = 8.4 Hz, 2H, ArH), 8.18 (d, J = 8.4 Hz, 2H, ArH), 8.43 (d, J = 9.2 Hz, 1H, ArH), 9.43 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 12.8, 18.9, 43.2, 52.5, 84.9 (q, J = 30.4 Hz), 113.3, 124.5 (q, J = 286.2 Hz), 125.1, 125.7, 127.1, 128.9, 130.0, 130.1, 130.9, 133.3, 135.9, 138.8, 145.3, 165.0, 165.9, 191.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.91. IR (CH_2Cl_2) ν 2985, 2363, 2337, 2032, 1971, 1733, 1522, 1260, 1185, 1109 cm^{-1}. HRMS (ESI) Calcd. For $C_{23}H_{20}ClF_3NO_5^{+1}(M+H)^+$ requires 482.0977, Found: 482.0975.

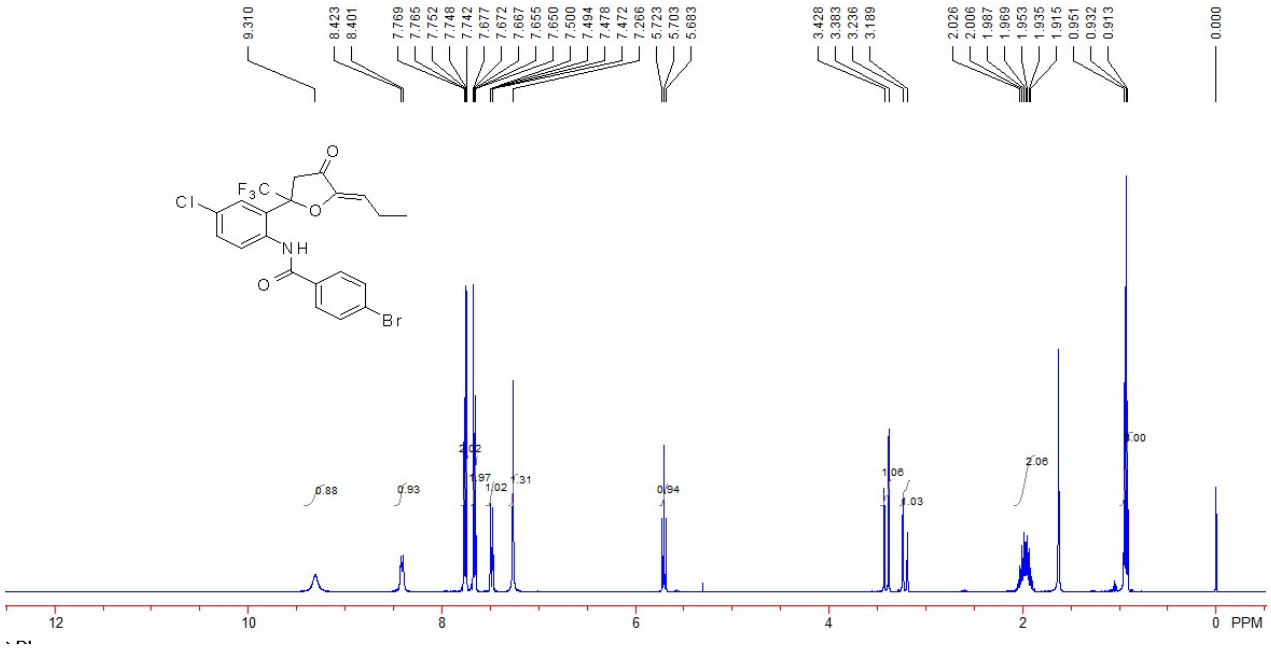






(Z)-4-bromo-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)benzamide (4h)

A white solid, 81% yield (81 mg). M.p.: 174-176 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 0.93 (t, *J* = 7.6 Hz, 3H, CH_3), 1.91~2.03 (m, 2H, CH_2), 3.26 (d, *J* = 18.8 Hz, 1H, CH_2), 3.41 (d, *J* = 18.8 Hz, 1H, CH_2), 5.70 (t, *J* = 8.0 Hz, 1H, =CH), 7.27 (s, 1H, ArH), 7.49 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 7.65~7.68 (m, 2H, ArH), 7.74~7.70 (m, 2H, ArH), 8.41 (d, *J* = 8.8 Hz, 1H, ArH), 9.31 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 12.9, 19.0, 43.2, 84.9 (q, *J* = 34.0 Hz), 113.3, 124.5 (q, *J* = 285.6 Hz), 125.0, 125.7, 127.0, 128.6, 128.9, 130.1, 130.9, 132.1, 133.9, 136.0, 145.3, 165.0, 191.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.91. IR (CH_2Cl_2) ν 3420, 2920, 2850, 1746, 1671, 1519, 1299, 1233, 1176, 1100, 1033, 764, 750 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{17}BrClF_3NO_3{}^{+1}(M+H)^+$ requires 502.0027, Found: 502.0024.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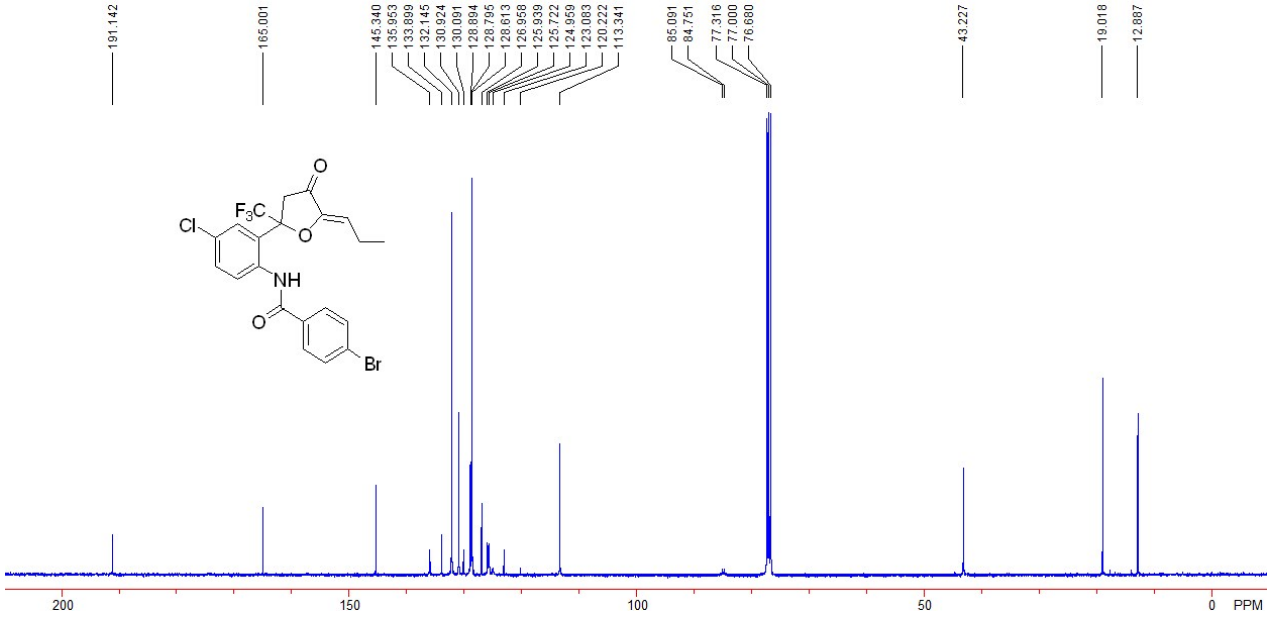
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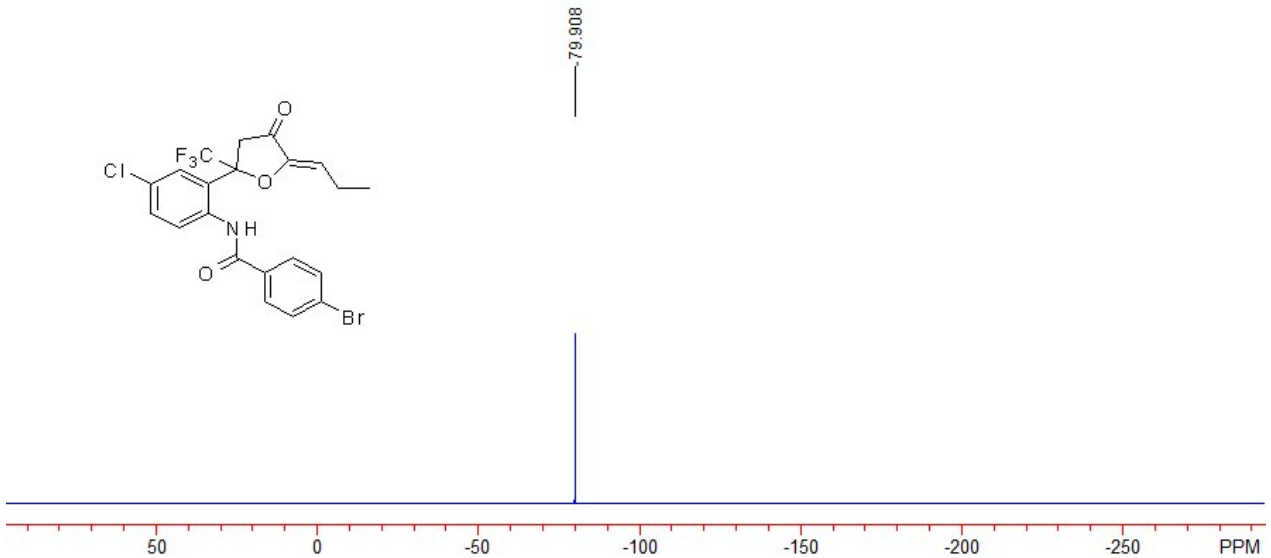
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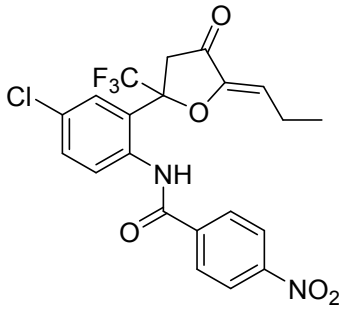
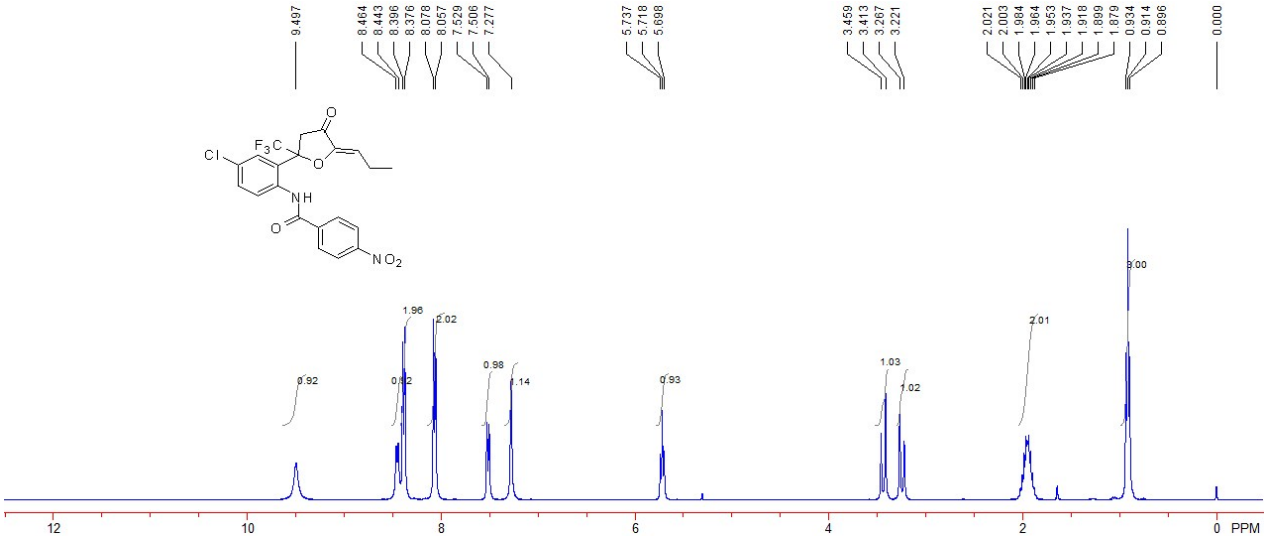
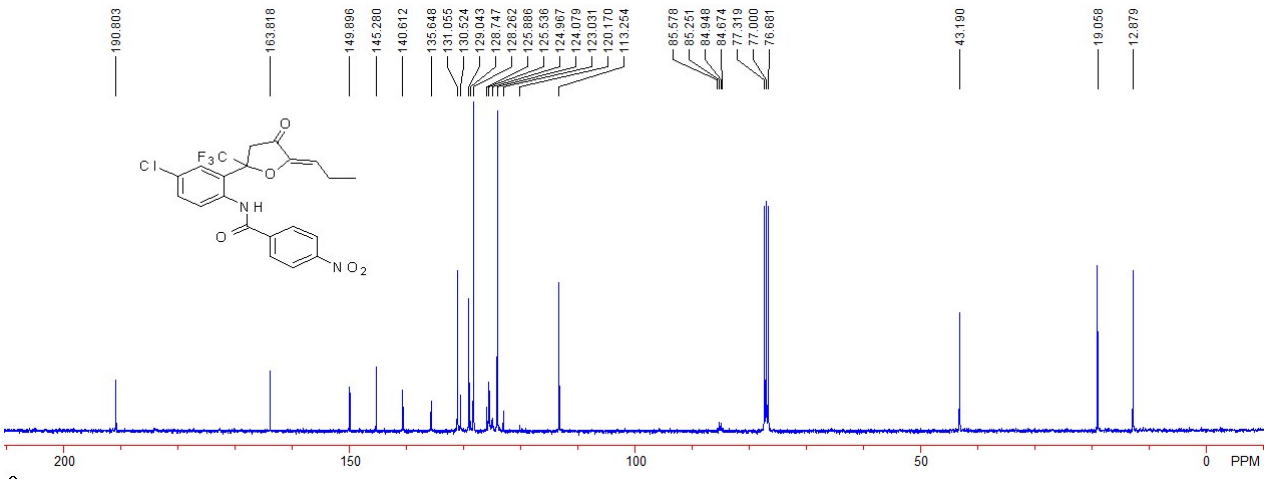
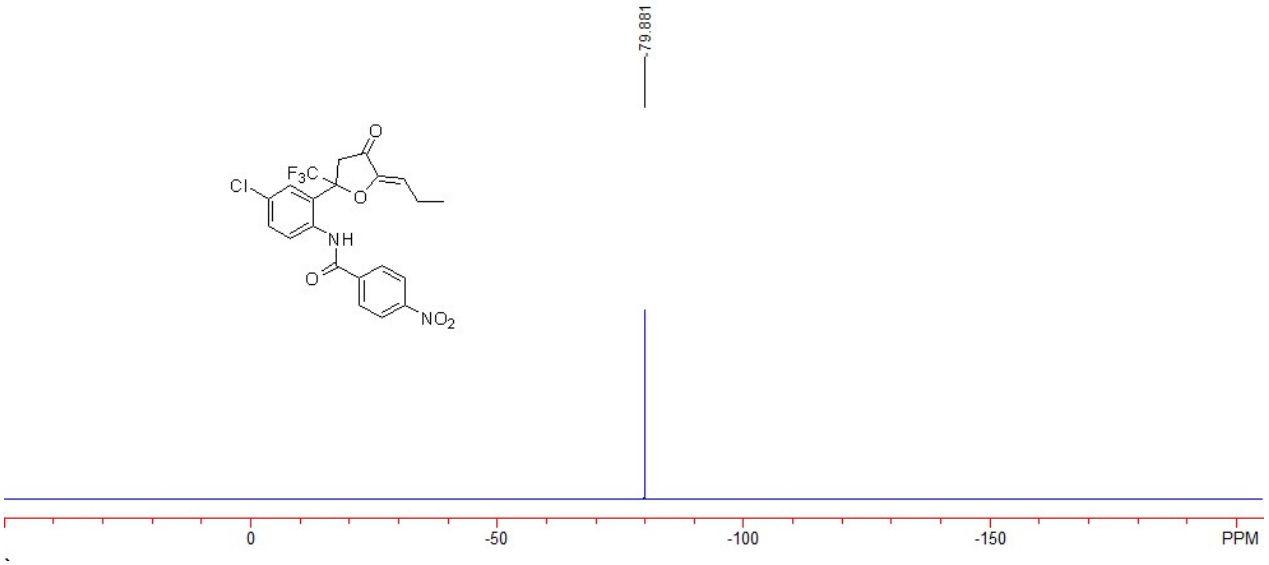


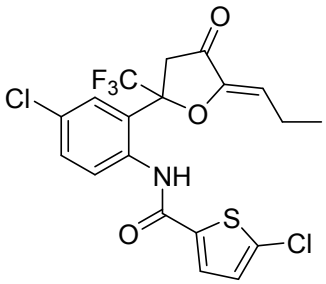
(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-4-nitrobenzamide (4i)

A white solid, 93% yield (87 mg). M.p.: 184-186 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 0.91 (t, *J* = 8.0 Hz, 3H, CH_3), 1.87~2.03 (m, 2H, CH_2), 3.24 (d, *J* = 18.4 Hz, 1H, CH_2), 3.44 (d, *J* = 18.4 Hz, 1H, CH_2), 5.72 (t, *J* = 8.0 Hz, 1H, =CH), 7.28 (s, 1H, ArH), 7.52 (d, *J* = 9.2 Hz, 1H, ArH), 8.07 (d, *J* = 8.4 Hz, 2H, ArH), 8.39 (d, *J* = 8.4 Hz, 2H, ArH), 8.45 (d, *J* = 8.4 Hz, 1H, ArH), 9.50 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 12.9, 19.1, 43.2, 85.1 (q, *J* = 30.3 Hz), 113.3, 124.1, 124.5 (q, *J* = 285.5 Hz), 125.0, 125.5, 128.3, 129.0, 130.5, 131.1, 135.6, 140.6, 145.3, 149.9, 163.8, 190.8. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.88. IR (CH_2Cl_2) ν 3660, 3348, 2971, 1745, 1669, 1491, 1393, 1291, 1231, 1161, 1089, 1034, 874, 662 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{17}ClF_3NO_5$[+1](M+H)$^+$ requires 469.0773, Found: 469.0768.





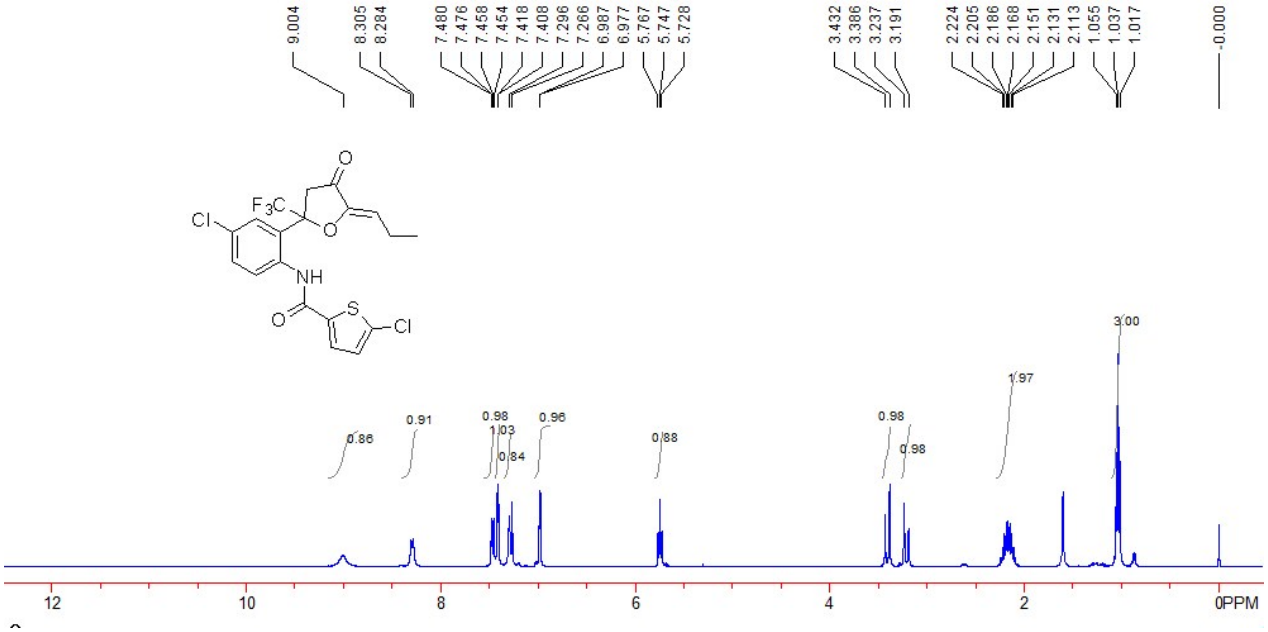


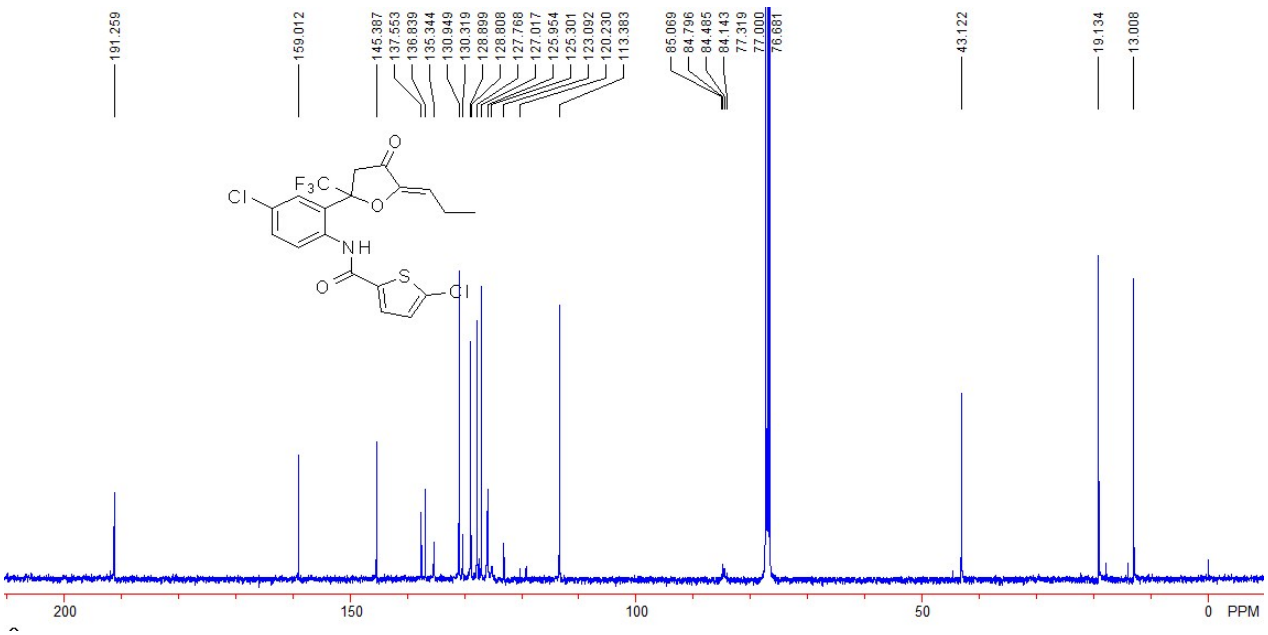


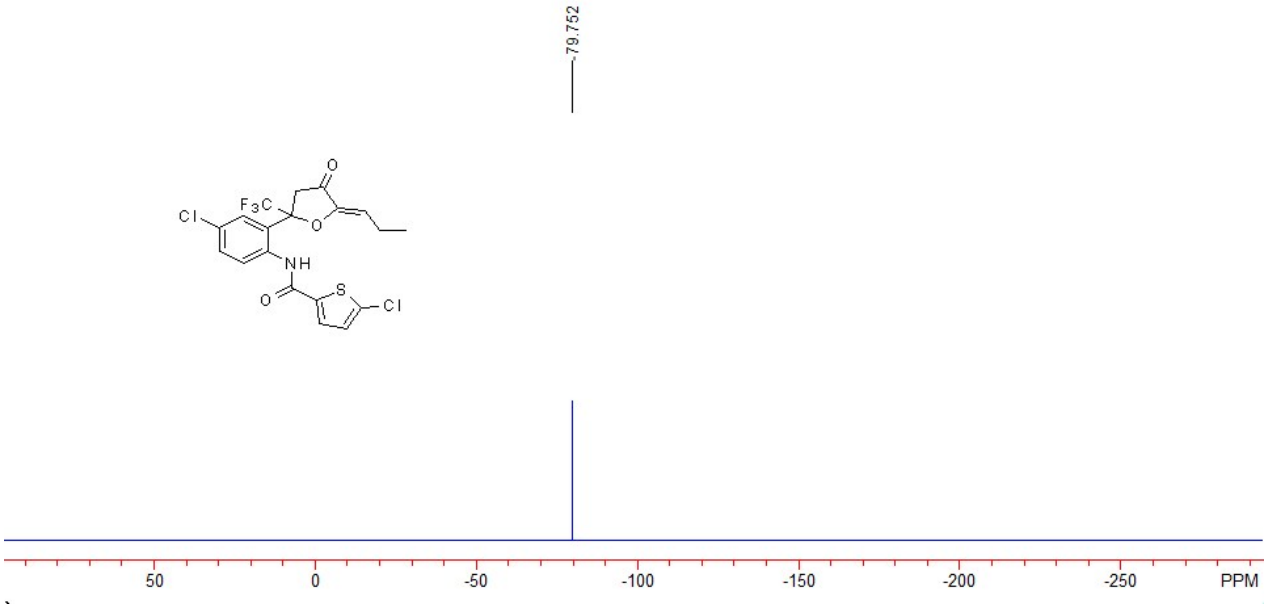
(Z)-5-chloro-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)thiophene-2-carboxamide (4j)

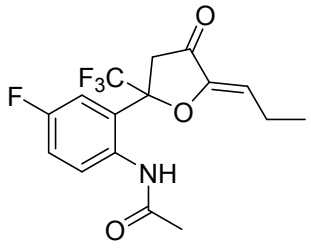
A white solid, 85% yield (79 mg). M.p.: 201-203 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.04 (t, J = 7.2 Hz, 3H, CH_3), 2.11~2.23 (m, 2H, CH_2), 3.21 (d, J = 18.4 Hz, 1H, CH_2), 3.41 (d, J = 18.4 Hz, 1H, CH_2), 5.75 (t, J = 8.0z Hz, 1H, =CH), 6.99 (d, J = 8.0 Hz, 1H, ArH), 7.30 (s, 1H, ArH), 7.41 (d, J = 4.0 Hz, 1H, ArH), 7.47 (dd, J = 1.6, 8.8 Hz, 1H, ArH), 8.29 (d, J = 8.4 Hz, 1H, ArH), 9.00 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.1, 43.1, 84.6 (q, J = 31.1 Hz), 113.4, 124.5

(q, J = 286.2 Hz), 125.3, 126.0, 127.0, 127.8, 128.9, 130.3, 130.9, 135.3, 136.8, 137.6, 145.4, 159.0, 191.3. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.75. IR (CH_2Cl_2) ν 3414, 2921, 2851, 1745, 1670, 1534, 1507, 1424, 1326, 1275, 1260, 1188, 1033, 1001, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{15}Cl_2F_3NO_3S^{+1}(M+H)^+$ requires 464.0096, Found: 464.0096.



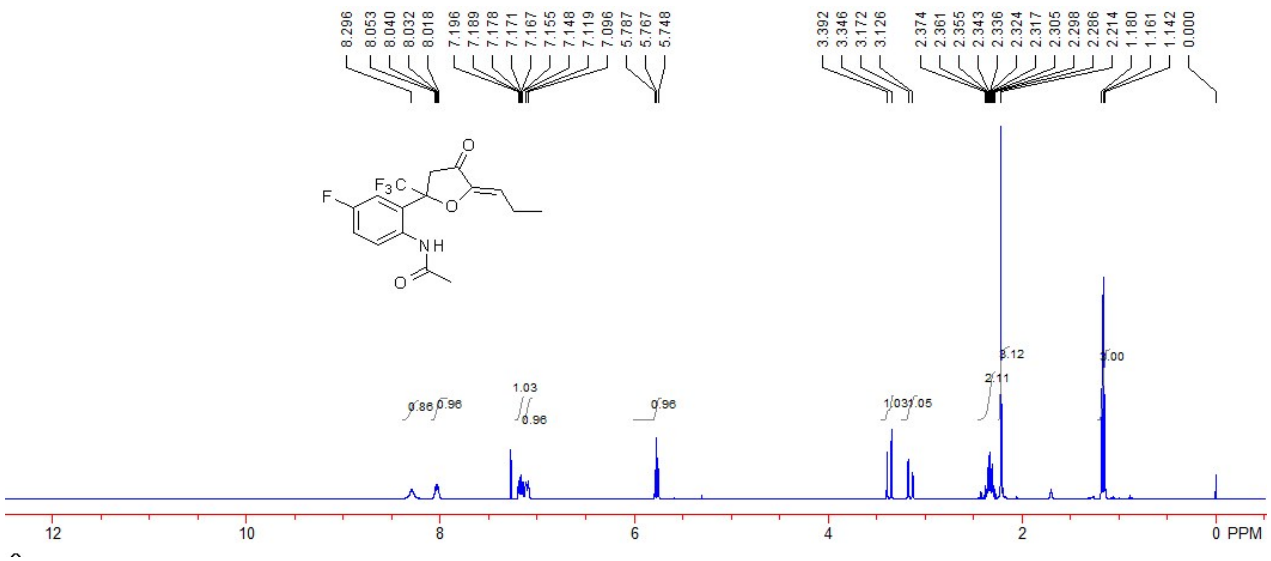






(Z)-N-(4-fluoro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (4k)

A white oil, 69% yield (48 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.16 (t, *J* = 7.6 Hz, 3H, CH_3), 2.21 (s, 3H, CH_3), 2.28~2.38 (m, 2H, CH_2), 3.15 (d, *J* = 18.4 Hz, 1H, CH_2), 3.37 (d, *J* = 18.4 Hz, 1H, CH_2), 5.77 (t, *J* = 8.0 Hz, 1H, =CH), 7.11 (d, *J* = 9.2 Hz, 1H, ArH), 7.14~7.20 (m, 1H, ArH), 8.04 (dd, *J* = 5.2, 8.4 Hz, 1H, ArH), 8.30 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.1, 24.5, 42.8, 83.9 (q, *J* = 30.5 Hz), 112.9, 115.6 (d, *J* = 24.6 Hz), 117.6 (d, *J* = 21.6 Hz), 124.4 (q, *J* = 285.8 Hz), 126.8, 127.8 (d, *J* = 5.2 Hz), 132.7, 145.6, 159.2 (d, *J* = 244.9 Hz), 168.5, 191.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.01, -115.51. IR (CH_2Cl_2) ν 3282, 2932, 2359, 2342, 1745, 1668, 1518, 1412, 1295, 1267, 1197, 1164, 1034, 1009, 997, 823 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{16}F_4NO_3^{+1}(M+H)^+$ requires 346.1061, Found: 346.1062.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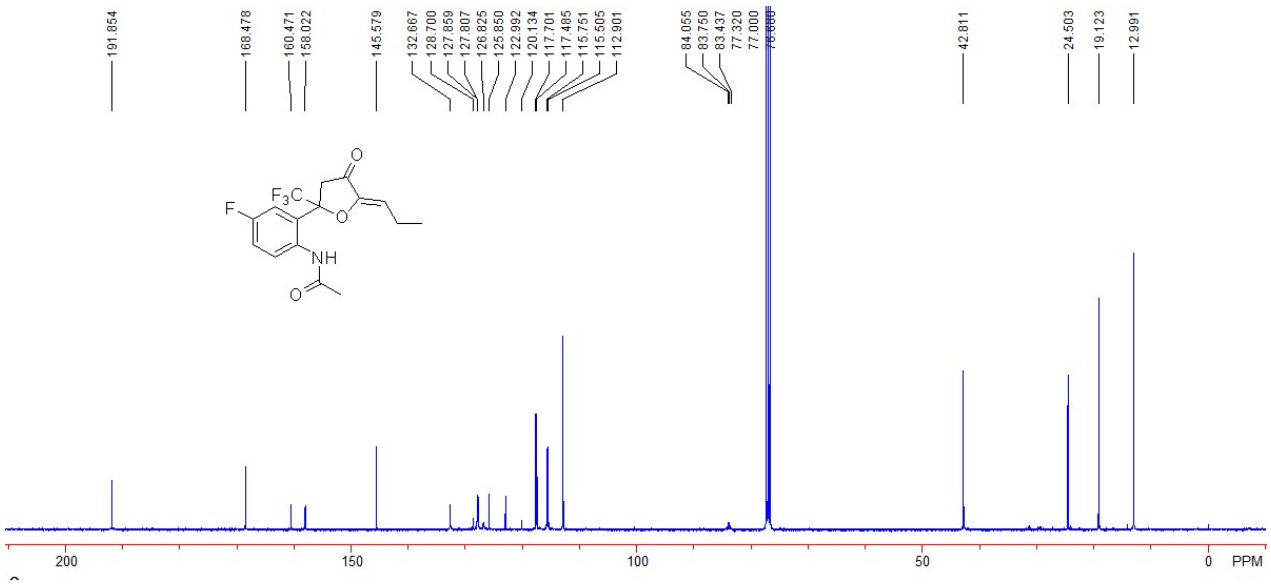
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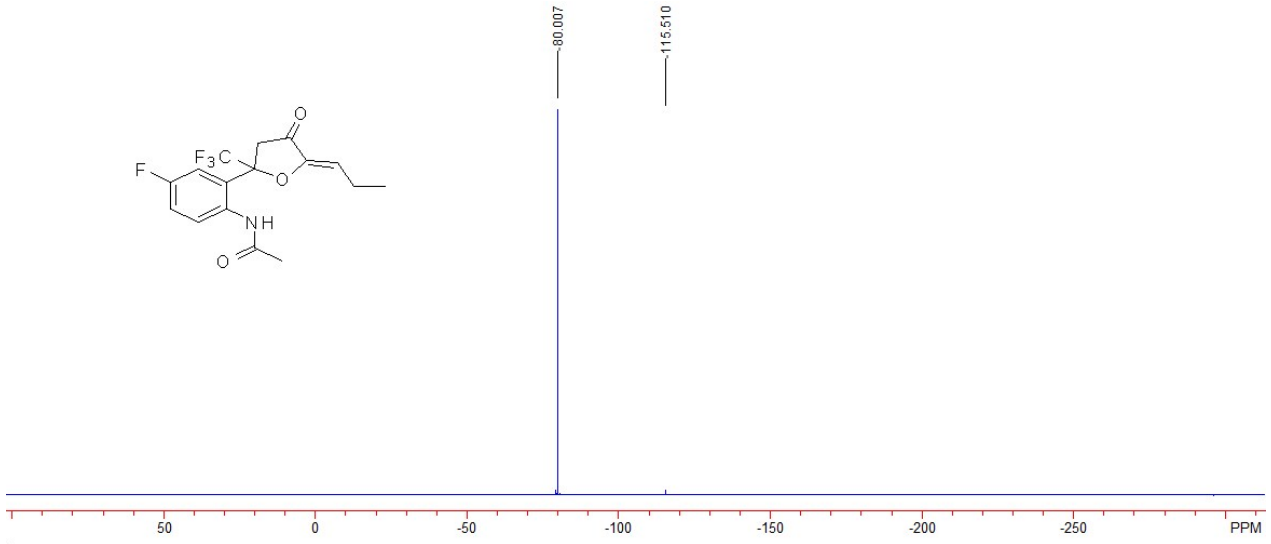
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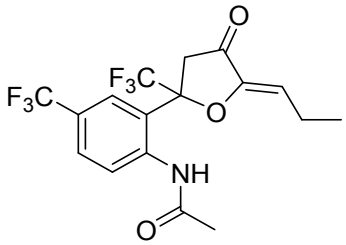
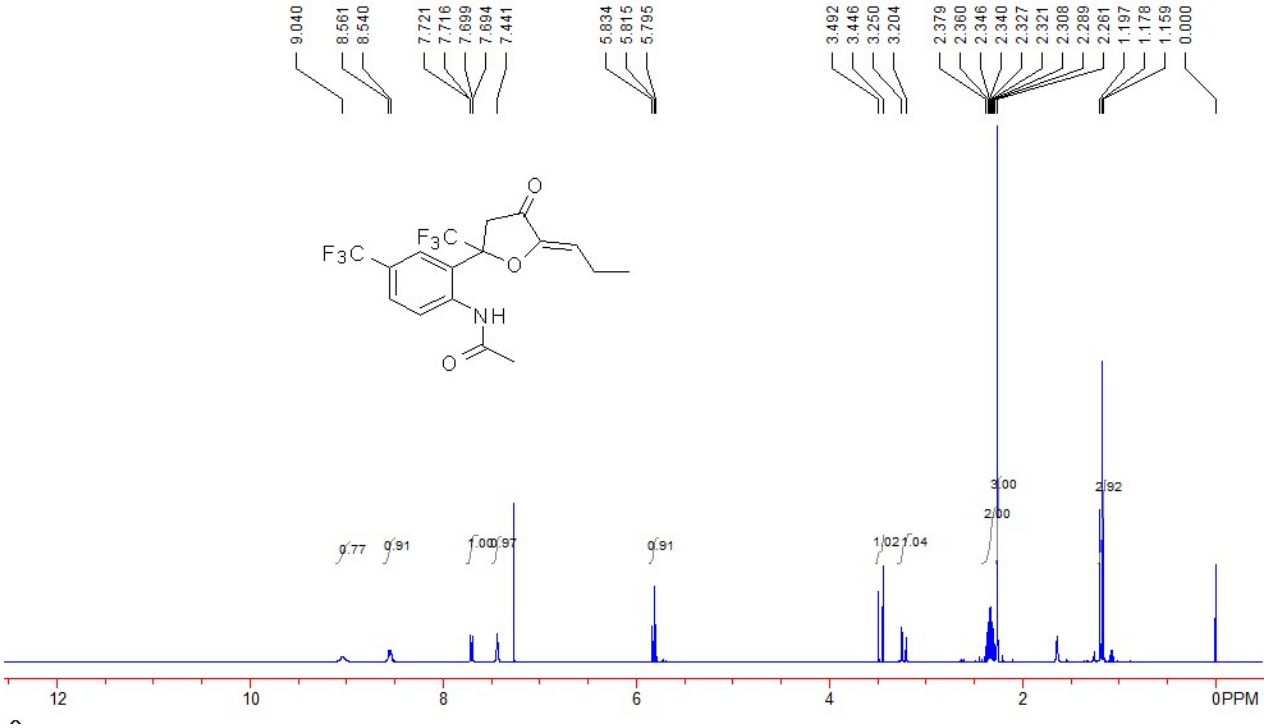
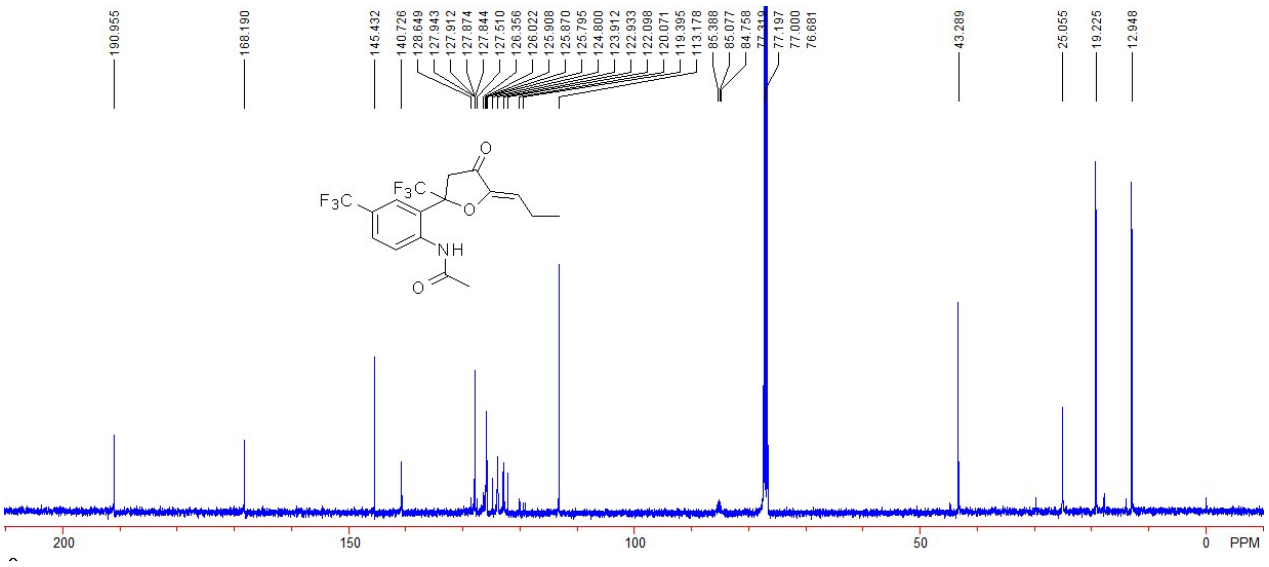
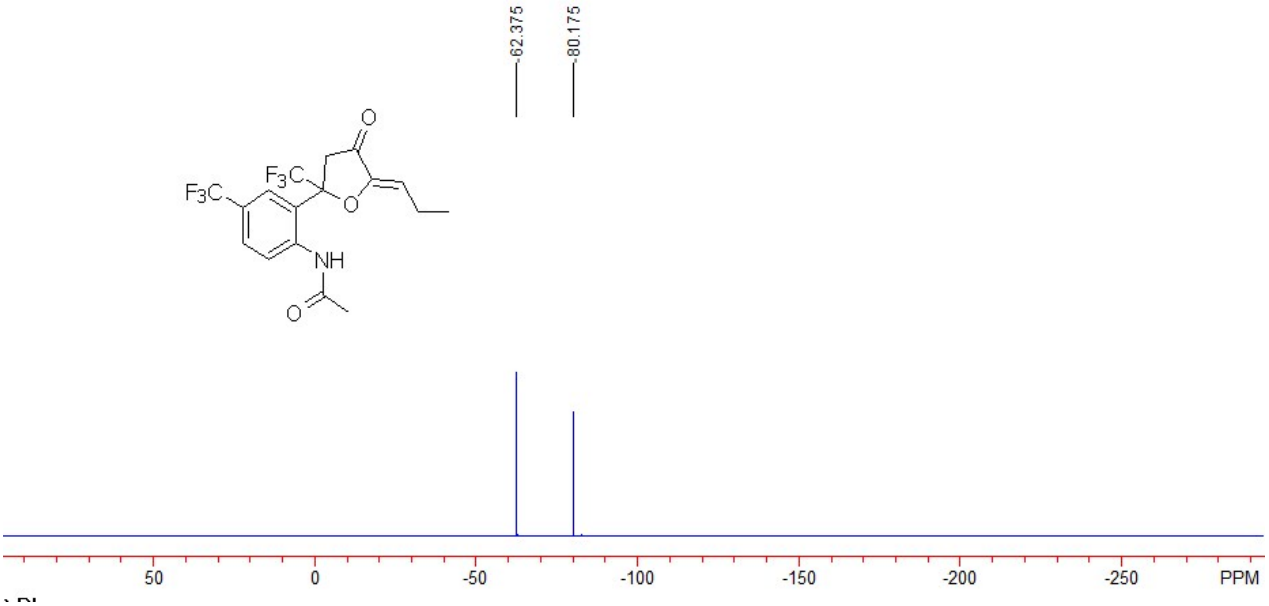


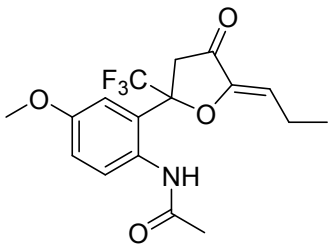
(Z)-N-(2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)-4-(trifluoromethyl)phenyl)acetamide (4l)

A white solid, 73% yield (58 mg). M.p.: 101-103 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.18 (t, *J* = 7.6 Hz, 3H, CH_3), 2.26 (s, 3H, CH_3), 2.28~2.38 (m, 2H, CH_2), 3.23 (d, *J* = 18.4 Hz, 1H, CH_2), 3.47 (d, *J* = 18.4 Hz, 1H, CH_2), 5.82 (t, *J* = 8.0 Hz, 1H, =CH), 7.44 (s, 1H, ArH), 7.71 (dd, *J* = 2.0, 8.8 Hz, 1H, ArH), 8.55 (d, *J* = 8.4 Hz, 1H, ArH), 9.04 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 12.9, 19.2, 25.1, 43.3, 85.2 (q, *J* = 31.1 Hz), 113.2, 123.4 (q, *J* = 270.2 Hz), 123.9, 124.4 (q, *J* = 286.2 Hz), 125.9 (d, *J* = 3.8 Hz), 126.0, 126.4, 127.9 (q, *J* = 38.0 Hz), 140.7, 145.4, 168.2, 191.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -62.38, -80.06. IR (CH_2Cl_2) ν 3423, 2919, 2850, 1748, 1528, 1335, 1297, 1275, 1261, 1170, 1130, 764, 747 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{16}F_6NO^{+1}(M+H)^+$ requires 396.1029, Found: 396.1030.





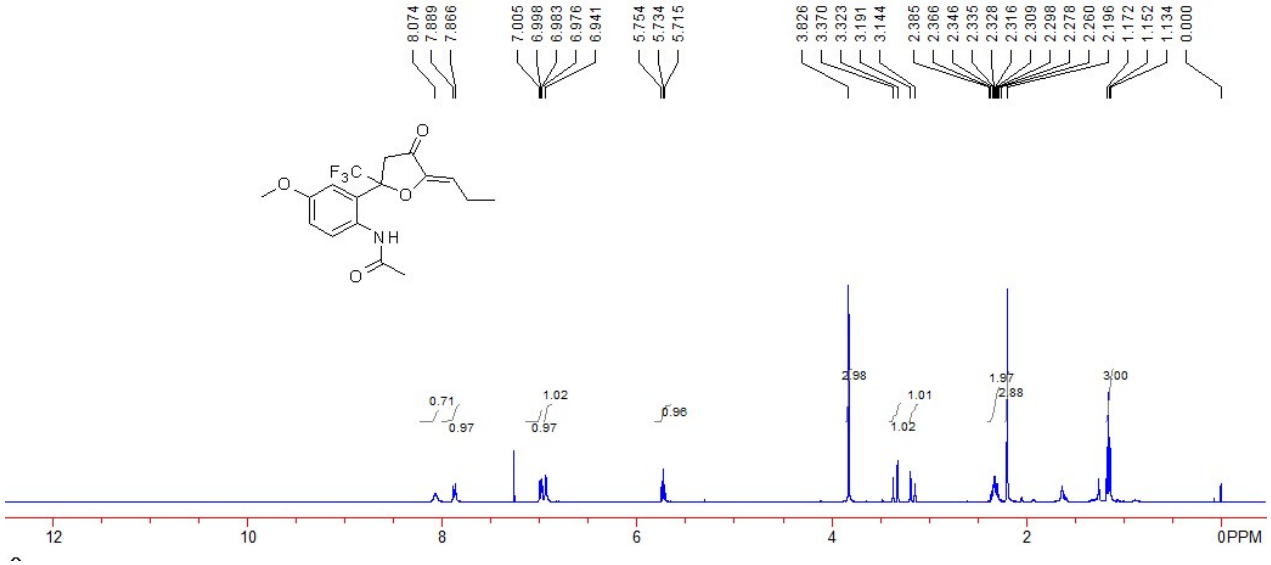


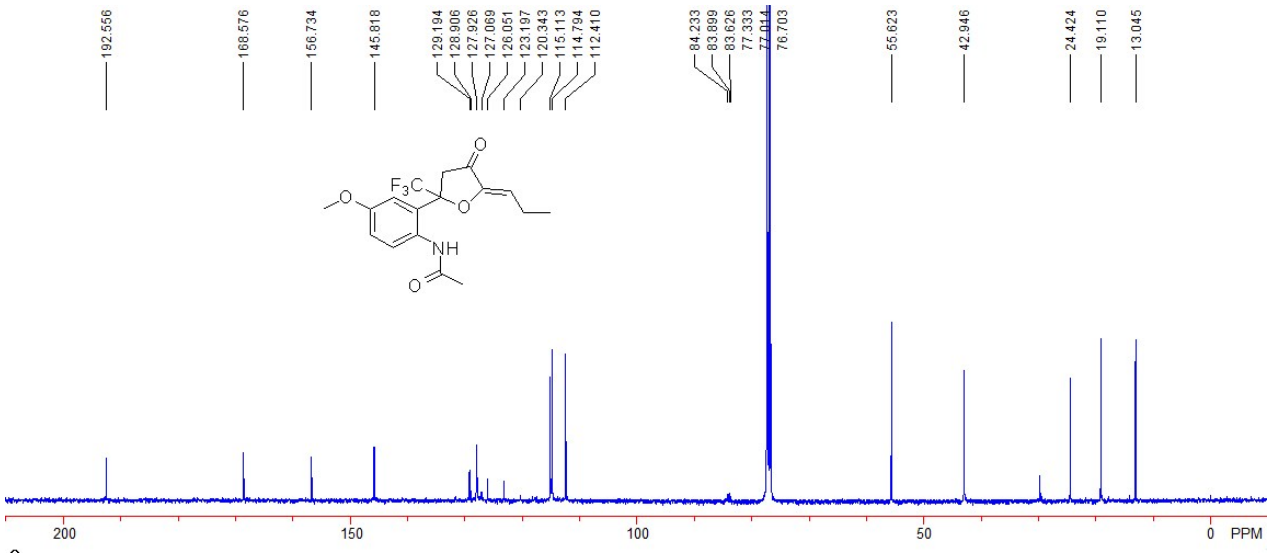


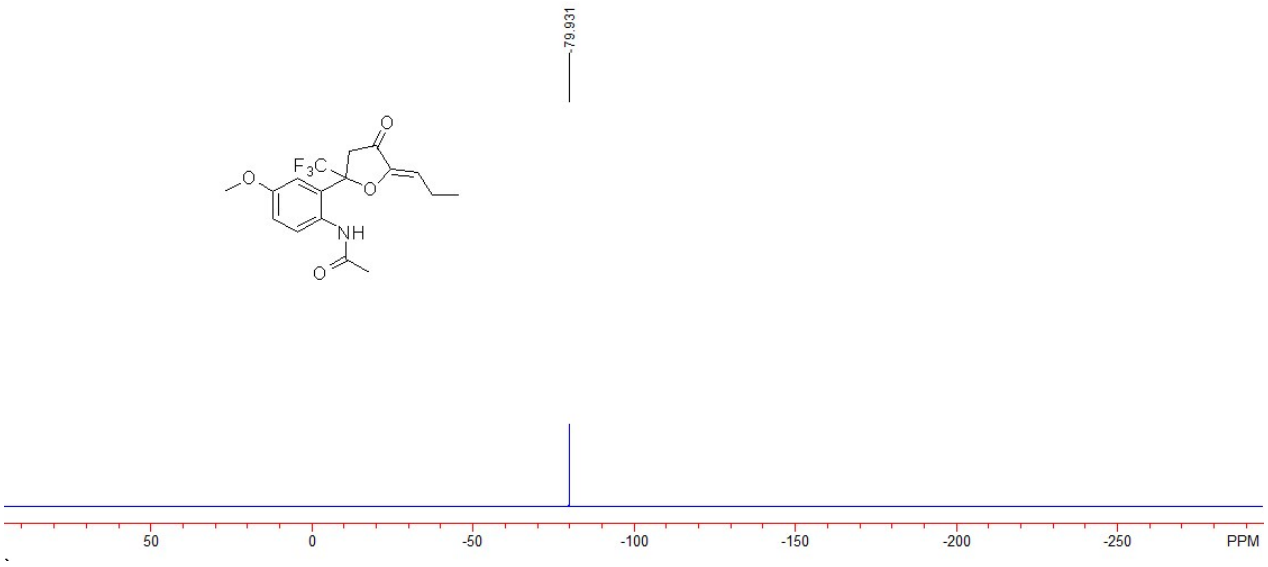
(Z)-N-(4-methoxy-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (4m)

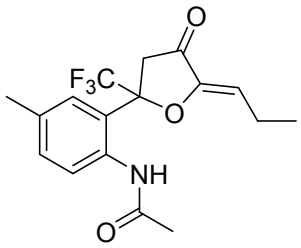
A white oil, 50% yield (36 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.15 (t, J = 8.0 Hz, 3H, CH_3), 2.20 (s, 3H, CH_3), 2.26~2.39 (m, 2H, CH_2), 3.17 (d, J = 18.8 Hz, 1H, CH_2), 3.35 (d, J = 18.8 Hz, 1H, CH_2), 3.83 (s, 3H, CH_3), 5.73 (t, J = 8.0 Hz, 1H, =CH), 6.94 (s, 1H, ArH), 7.34 (dd, J = 2.8, 8.8

Hz, 1H, ArH), 7.88 (d, J = 8.8 Hz, 1H, ArH), 8.07 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.1, 24.4, 42.9, 55.6, 84.1 (q, J = 33.4 Hz), 112.4, 114.8, 115.1, 124.6 (q, J = 285.4 Hz), 127.1, 127.9, 129.2, 145.8, 156.7, 168.6, 192.6. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.93. IR (CH_2Cl_2) ν 3688, 3675, 2987, 2971, 2900, 2359, 2341, 1744, 1407, 1232, 1205, 1066, 1046, 891 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{19}F_3NO_4^{+1}(M+H)^+$ requires 358.1261, Found: 358.1259.



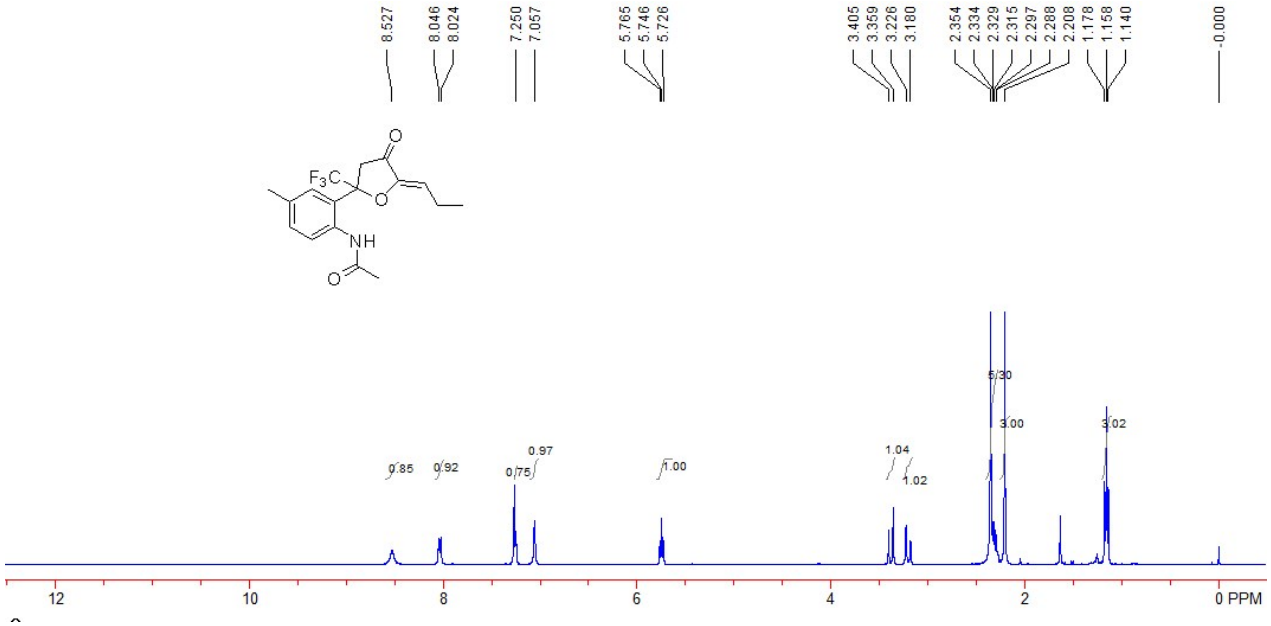






(Z)-N-(4-methyl-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (4n)

A white solid, 39% yield (27 mg). M.p.: 123-125 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.16 (t, *J* = 7.6 Hz, 3H, CH_3), 2.21 (s, 3H, CH_3), 2.28~2.36 (m, 5H, CH_2, CH_3), 3.20 (d, *J* = 18.4 Hz, 1H, CH_2), 3.38 (d, *J* = 18.4 Hz, 1H, CH_2), 5.75 (t, *J* = 8.0 Hz, 1H, =CH), 7.06 (s, 1H, ArH), 7.25 (s, 1H, ArH), 8.04 (d, *J* = 8.8 Hz, 1H, ArH), 8.53 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.1, 20.9, 24.8, 43.4, 85.0 (q, *J* = 31.1 Hz), 112.4, 123.7, 124.6 (q, *J* = 285.4 Hz), 125.1, 129.0, 131.4, 134.5, 145.8, 168.2, 192.4. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.06. IR (CH_2Cl_2) ν 3424, 2921, 2851, 1745, 1669, 1520, 1299, 1275, 1261, 1227, 1183, 1033, 996, 766 cm^{-1}. HRMS (ESI) Calcd. For $C_{17}H_{19}F_3NO_3^{+1}(M+H)^+$ requires 342.1312, Found: 342.1312.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8.024
7.250
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5.746
5.726
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3.226
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2.334
2.329
2.315
2.297
2.288
2.208
1.178
1.158
1.140
-0.000
F3C
O
NH
O
0.85
0.92
0.75
0.97
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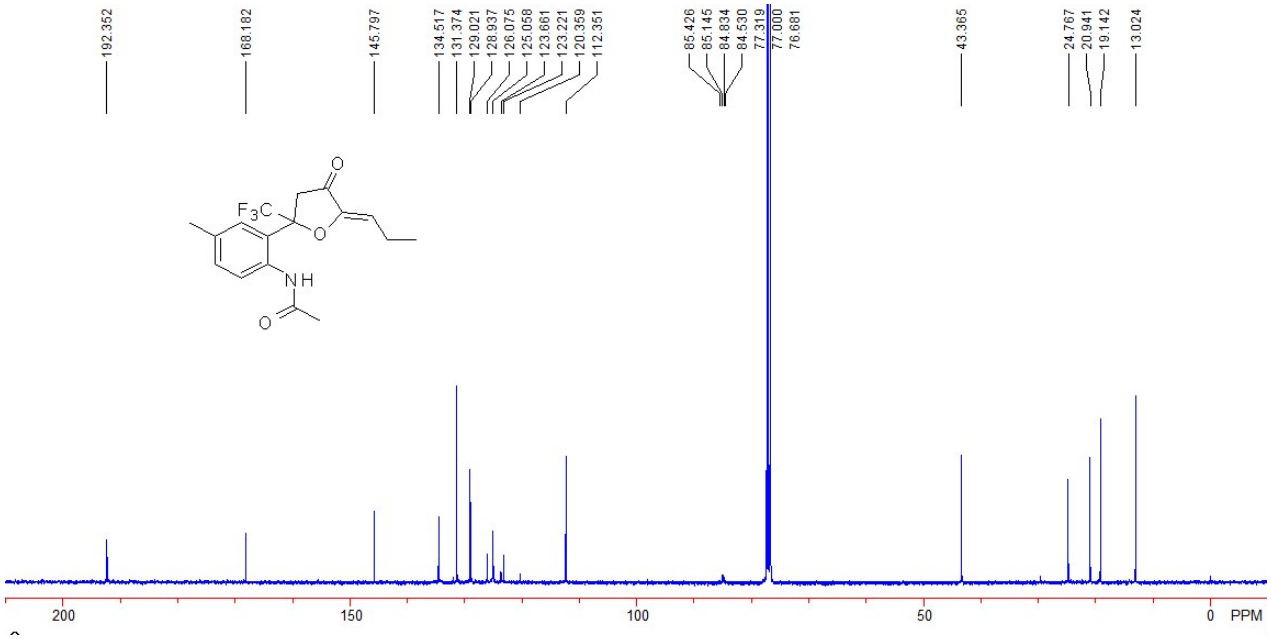
1.04
1.02
5.30
3.00
3.02
12
10
8
6
4
2
0 PPM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145.797
134.517
131.374
129.021
128.937
126.075
125.058
123.661
123.221
120.359
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85.426
85.145
84.834
84.530
77.319
77.000
76.681
43.365
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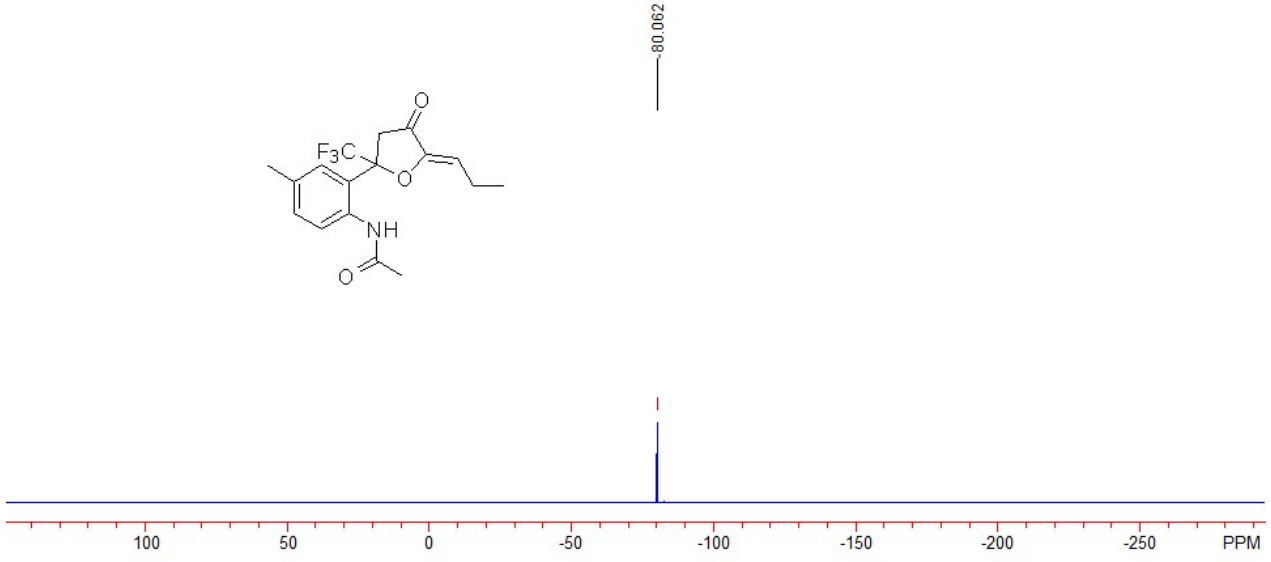
20.941
19.142
13.024
F3C
O
NH
O
200
150
100
50
0 PPM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F3C
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NH
O
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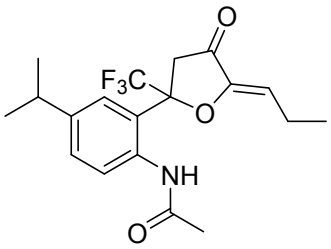
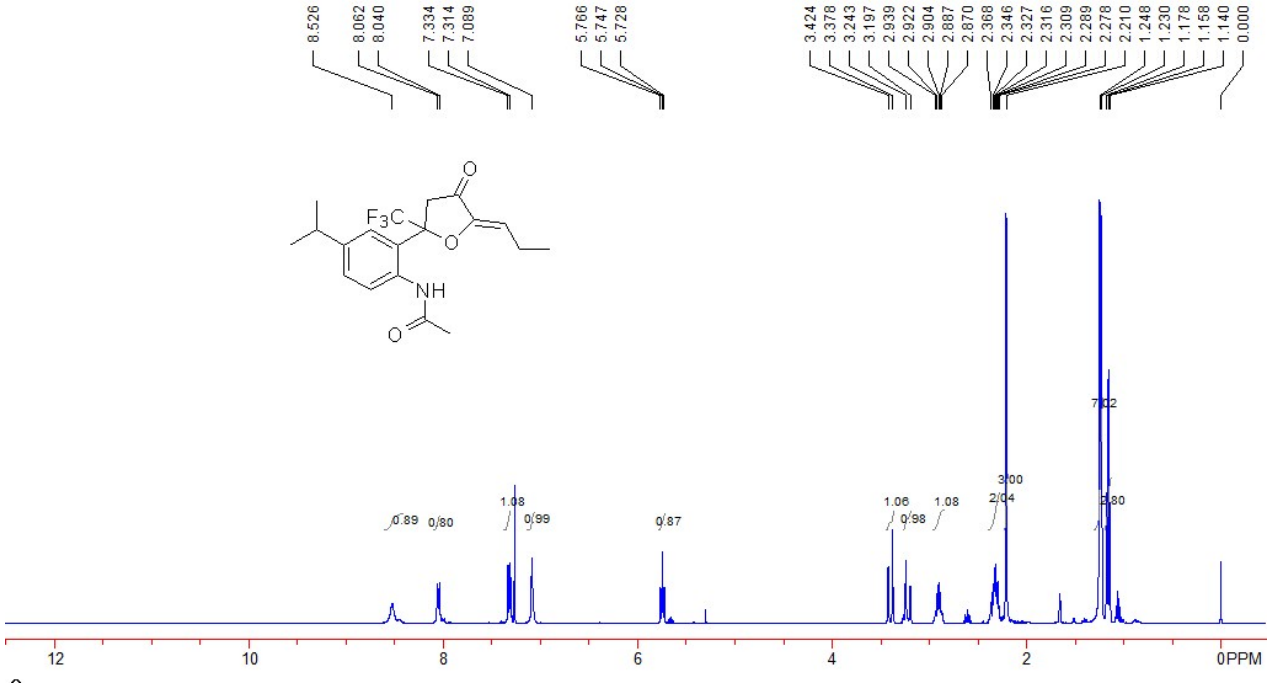
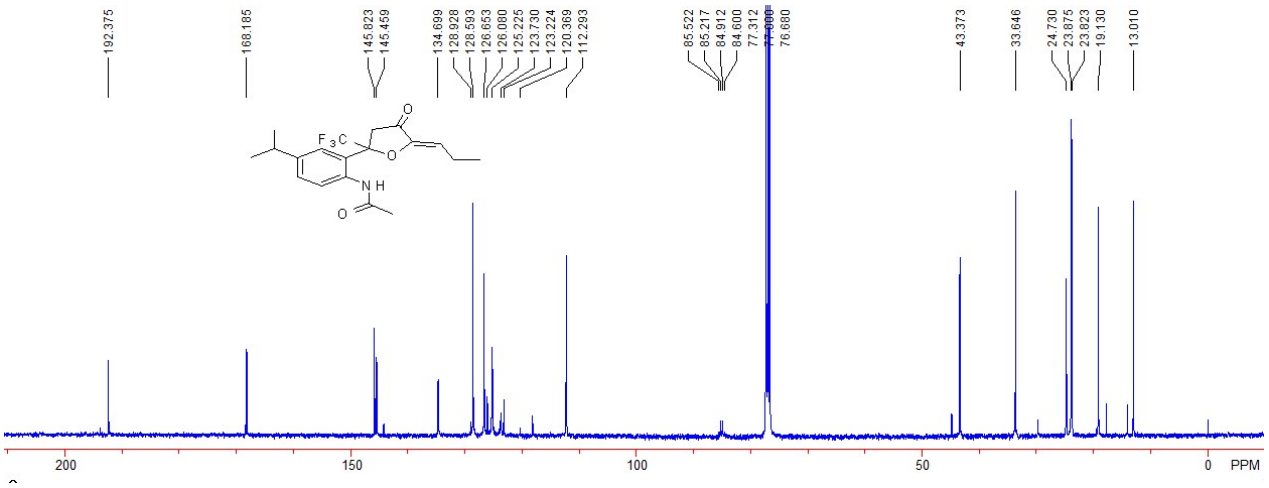
50
0
-50
-100
-150
-200
-250
PPM



(Z)-N-(4-isopropyl-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (4o)

A white oil, 56% yield (41 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.16 (t, *J* = 7.6 Hz, 3H, CH_3), 1.24 (d, *J* = 7.2 Hz, 6H, CH_3), 2.21 (s, 3H, CH_3), 2.27~2.37 (m, 2H, CH_2), 2.87~2.94 (m, 1H, CH), 3.22 (d, *J* = 18.4 Hz, 1H, CH_2), 3.40 (d, *J* = 18.4 Hz, 1H, CH_2), 5.75 (t, *J* = 7.6 Hz, 1H, =CH), 7.10 (s, 1H, ArH), 7.32 (d, *J* = 8.0 Hz, 1H, ArH), 8.05 (d, *J* = 8.4 Hz, 1H, ArH), 8.53 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.1, 23.8, 23.9, 24.7, 33.6, 43.4, 85.1 (q, *J* = 30.5 Hz), 112.3, 123.7, 124.7 (q, *J* = 285.6 Hz), 125.2, 126.7, 128.6, 134.7, 145.5, 145.8, 168.2, 191.4. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.08. IR (CH_2Cl_2) ν 3425, 2964, 1744, 1669, 1519, 1417, 1275, 1225, 1185, 1172, 1034, 1003, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{23}F_3NO_3^{+1}$(M+H)$^+$ requires 370.1625, Found: 370.1623.

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112.293
85.522
85.217
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33.646
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23.875
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13.010
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NH
O
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100
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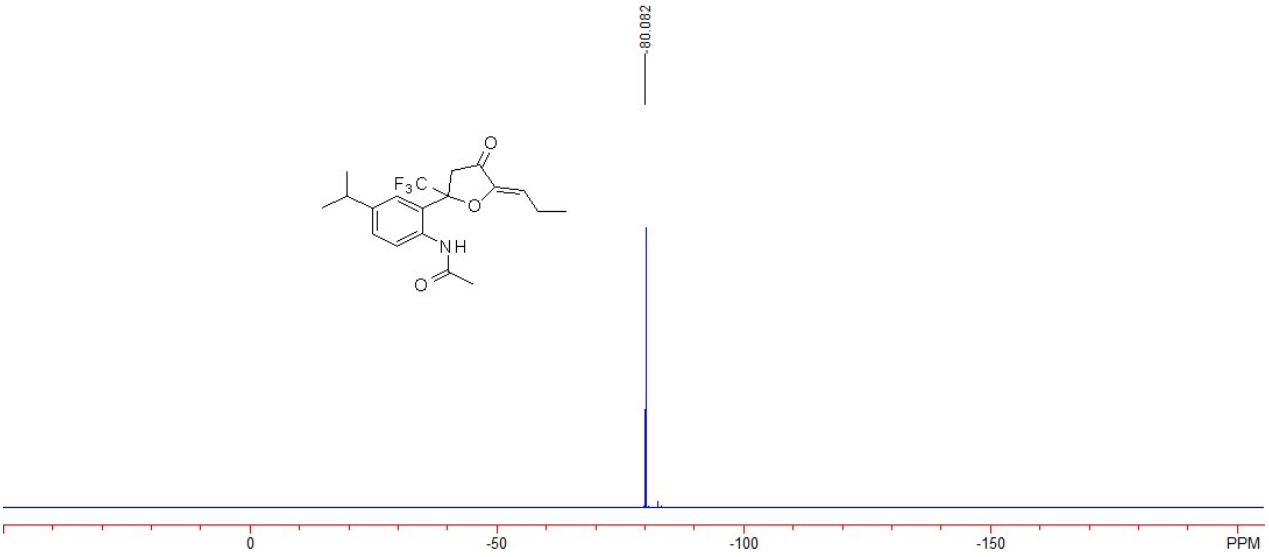
PPM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NH
O
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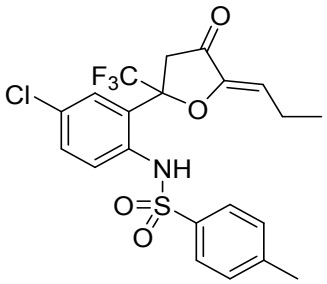
-50
-100
-150
PPM

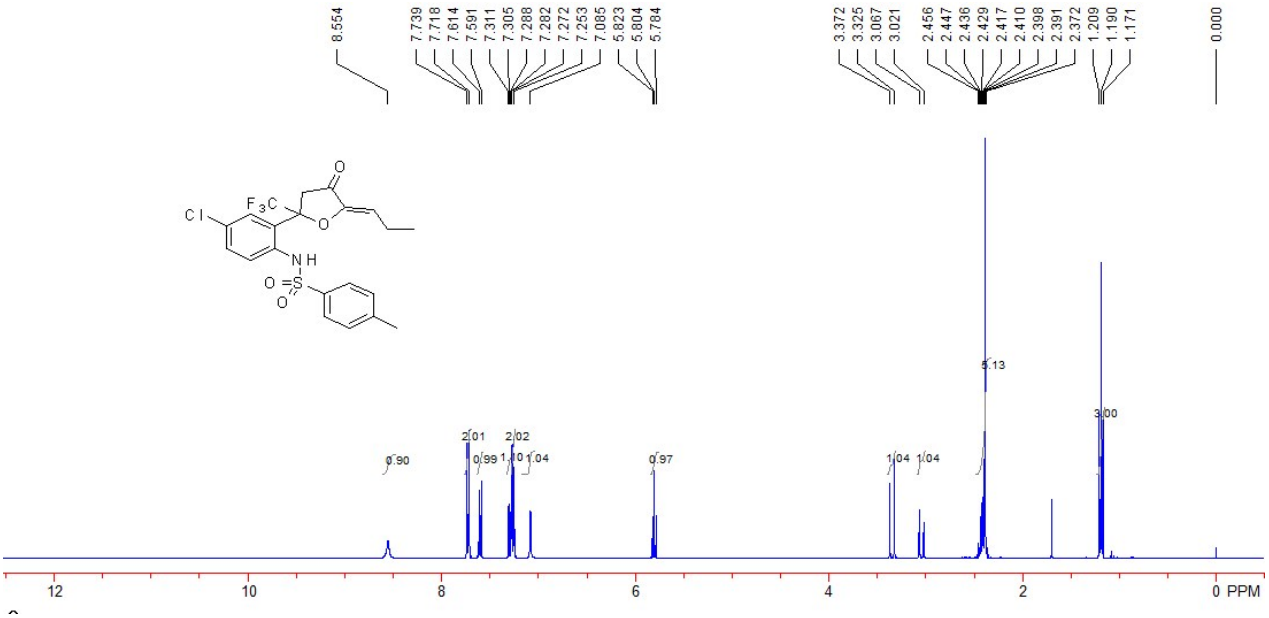
General Procedure for Hex-3-yn-2-one 2a to Trifluoroacetyl Compounds 1q-1v at 10 °C and Spectroscopic Data of the Products 4q-4v

General procedure: Under argon atmosphere, to a solution of trifluoroacetyl compounds **1q-1v** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the hex-3-yn-2-one **2a** (0.4 mmol) at room temperature. Then the resulting mixture was stirred at 10 °C until the reaction completed (monitoring by TLC). Then the solvent was removed under reduced pressure and the residue was directly subjected to flash column chromatography on silica gel to afford the desired products **4q-4v**.



(Z)-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-4-methylbenzenesulfonamide (4q)

A white solid, 89 % yield (87 mg). M.p.: 154-156 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.19 (t, *J* = 7.6 Hz, 3H, CH_3), 2.37~2.46 (m, 5H, CH_3, CH_2), 3.04 (d, *J* = 18.4 Hz, 1H, CH_2), 3.35 (d, *J* = 18.4 Hz, 1H, CH_2), 5.80 (t, *J* = 7.6 Hz, 1H, =CH), 7.09 (s, 1H, ArH), 7.26 (d, *J* = 7.6 Hz, 2H, ArH), 7.30 (dd, *J* = 2.4, 9.2 Hz, 1H, ArH), 7.60 (d, *J* = 9.2 Hz, 1H, ArH), 7.73 (d, *J* = 7.6 Hz, 2H, ArH), 8.55 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.2, 21.5, 43.4, 84.9 (q, *J* = 30.5 Hz), 114.2, 121.4, 123.6, 123.9 (q, *J* = 285.5 Hz), 127.4, 129.2, 129.2, 129.7, 130.9, 135.6, 135.9, 144.4, 145.1, 191.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.53. IR (CH_2Cl_2) ν 3660, 3348, 2971, 1745, 1669, 1491, 1393, 1291, 1161, 1089, 1034, 874, 813, 662 cm^{-1}. HRMS (ESI) Calcd. For $C_{21}H_{23}ClF_3N_2O_4S^{+1}(M+NH_4)^+$ requires 491.1014, Found: 491.1010.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5.804
5.784
3.372
3.325
3.067
3.021
2.456
2.447
2.436
2.429
2.417
2.410
2.398
2.391
2.372
1.209
1.190
1.171
0.000
5.13
3.00
2.01
2.02
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1.10
1.04
0.97
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1.04
12
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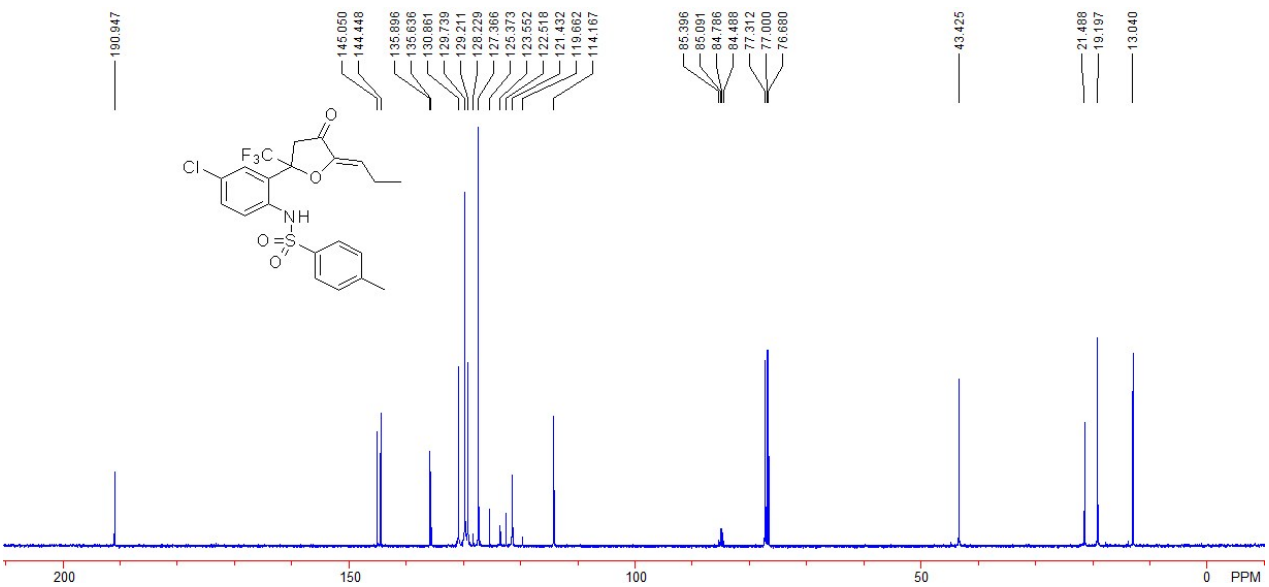
0 PPM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121.432
119.662
114.167
85.396
85.091
84.786
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77.000
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19.197
13.040
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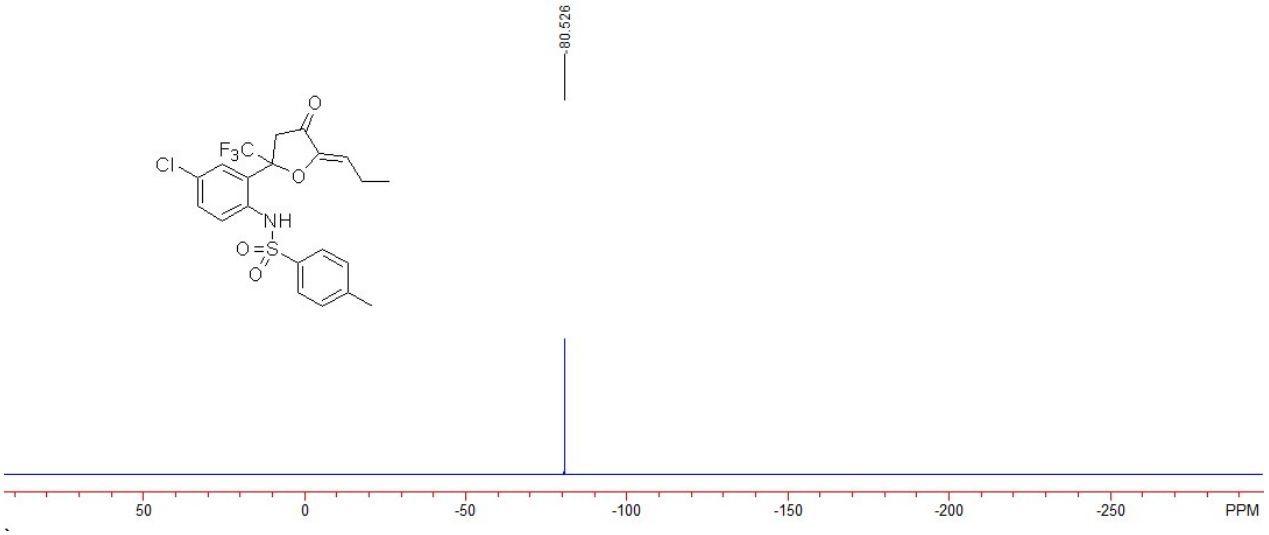
100
50
0 PPM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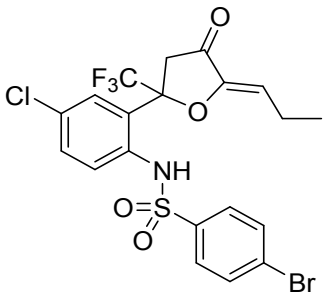
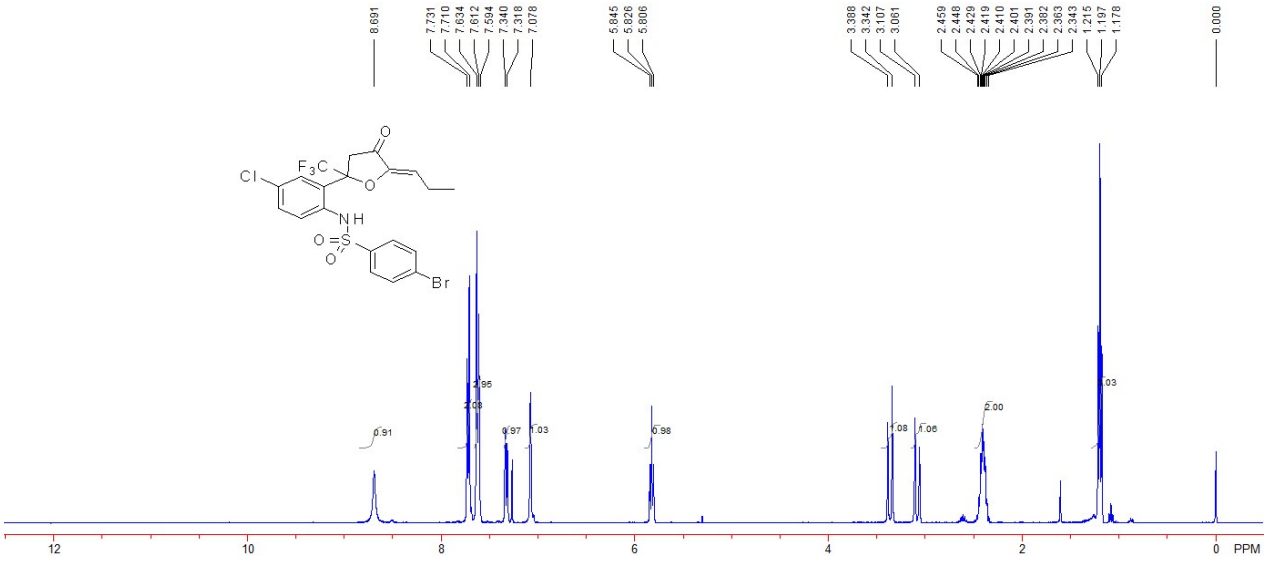
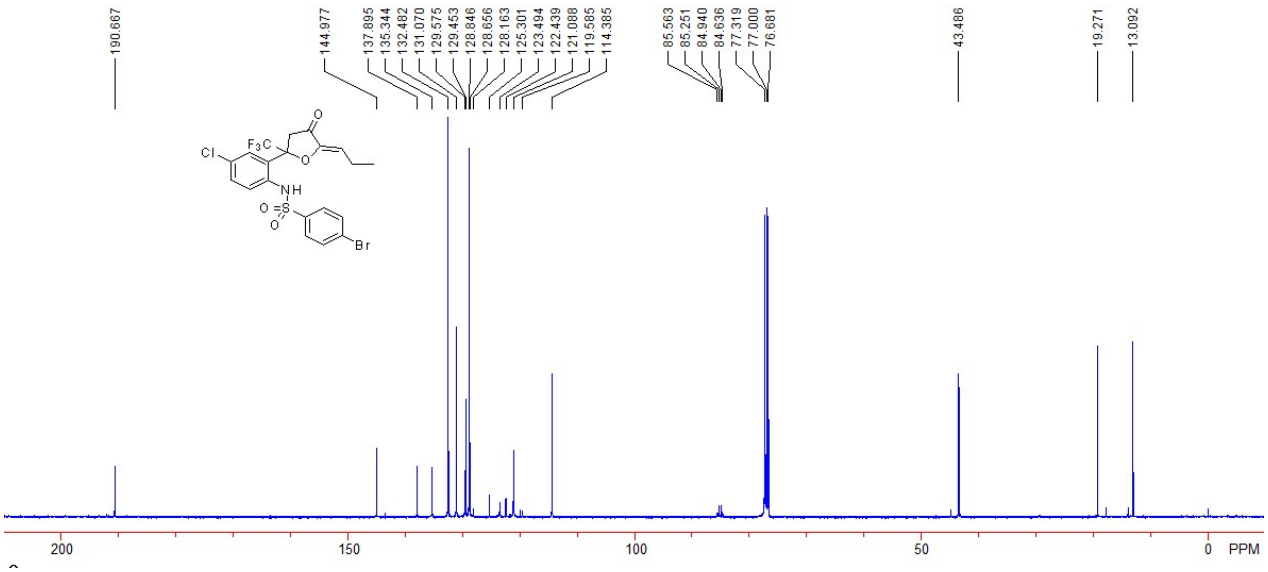
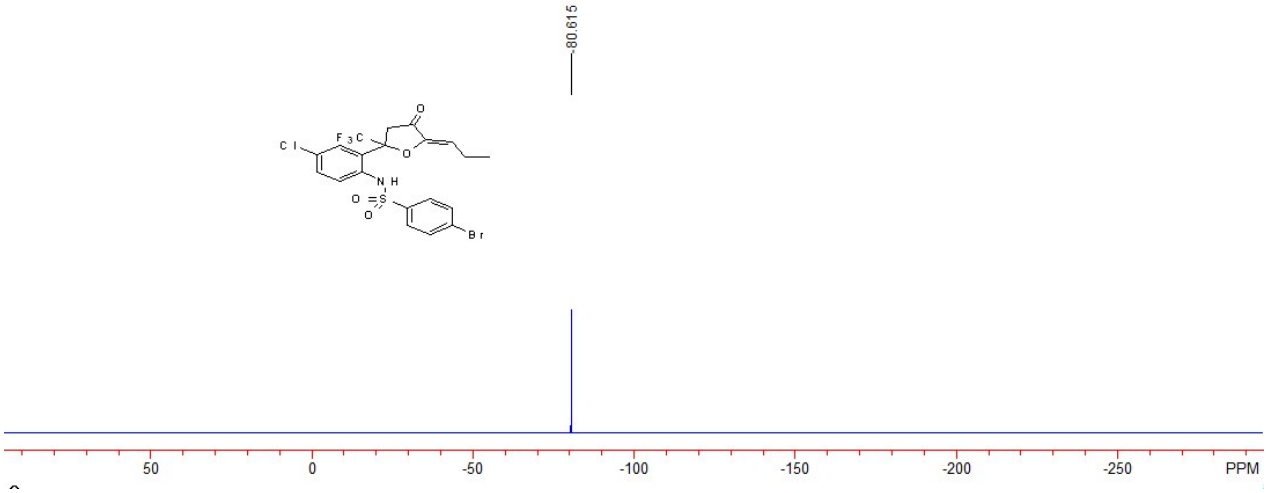


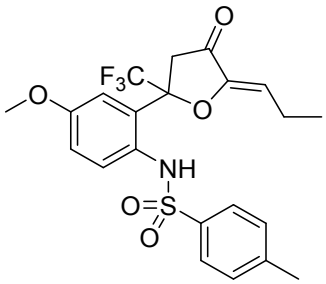
(Z)-4-bromo-N-(4-chloro-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)benzenesulfonamide (4r)

A white solid, 85% yield (94 mg). M.p.: 168-170 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.20 (t, *J* = 7.2 Hz, 3H, CH_3), 2.34~2.46 (m, 2H, CH_2), 3.08 (d, *J* = 18.4 Hz, 1H, CH_2), 3.37 (d, *J* = 18.4 Hz, 1H, CH_2), 5.83 (t, *J* = 7.6 Hz, 1H, =CH), 7.08 (s, 1H, ArH), 7.33 (d, *J* = 8.8 Hz, 1H, ArH), 7.59~7.64 (m, 3H, ArH), 7.72 (d, *J* = 8.4 Hz, 2H, ArH), 8.70 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.1, 19.3, 43.5, 85.1 (q, *J* = 31.1 Hz), 114.4, 121.1, 123.5, 123.9 (q, *J* = 286.2 Hz), 128.7, 128.8, 129.5, 129.6, 131.1, 132.5, 135.3, 137.9, 145.0, 190.7. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.62. IR (CH_2Cl_2) ν 3341, 2922, 2852, 1744, 1668, 1490, 1392, 1290, 1168, 1068, 1034, 740 cm^{-1}. HRMS (ESI) Calcd. For $C_{20}H_{20}BrClF_3N_2O_4S^{+1}(M+NH_4)^+$ requires 554.9962, Found: 554.9959.





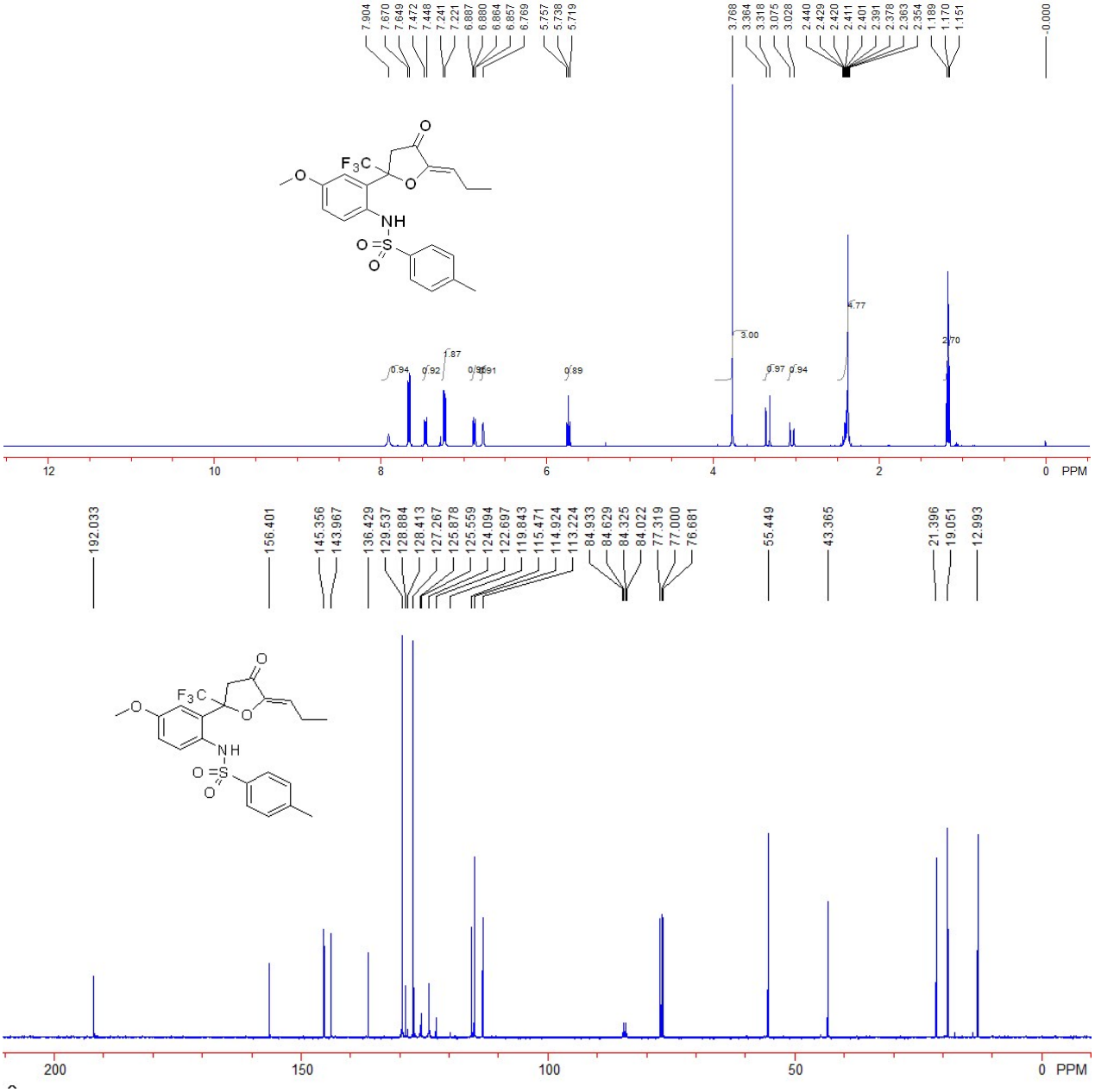


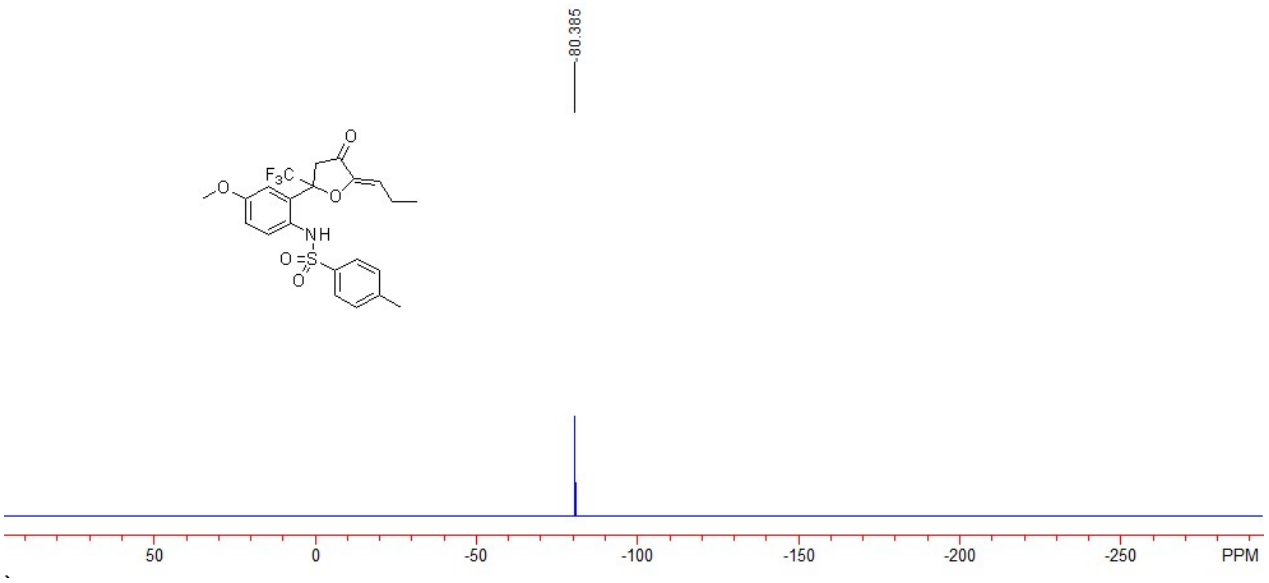


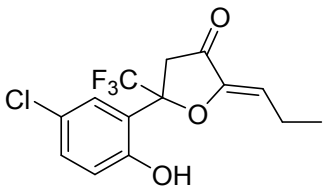
(Z)-N-(4-methoxy-2-(4-oxo-5-propylidene-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)-4-methylbenzenesulfonamide (4s)

A white oil, 69% yield (67 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.17 (t, J = 7.6 Hz, 3H, CH_3), 2.35~2.44 (m, 5H, CH_3, CH_2), 3.05 (d, J = 18.8 Hz, 1H, CH_2), 3.34 (d, J = 18.8 Hz, 1H, CH_2), 3.77 (s, 3H, CH_3), 5.74 (t, J = 7.6 Hz, 1H, =CH), 6.77 (br, 1H, ArH), 6.87 (dd, J = 2.8, 9.2 Hz, 1H, ArH), 7.23 (d, J = 7.6 Hz, 2H, ArH), 7.46 (d, J = 9.2 Hz, 1H, ArH), 7.66 (d, J = 7.6 Hz, 2H, ArH), 7.90 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.1, 21.4, 43.4, 55.4, 84.5 (q, J = 30.3 Hz),

113.2, 114.9, 115.5, 124.09, 124.13 (q, J = 286.2 Hz), 125.9, 127.3, 128.9, 129.5, 136.4, 144.0, 145.4, 156.4, 192.0. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.39. IR (CH_2Cl_2) ν 3357, 2937, 1744, 1505, 1401, 1290, 1204, 1157, 1034, 996, 706 cm^{-1}. HRMS (ESI) Calcd. For $C_{22}H_{26}F_3N_2O_5S^{+1}(M+NH_4)^+$ requires 487.1509, Found: 487.1507.

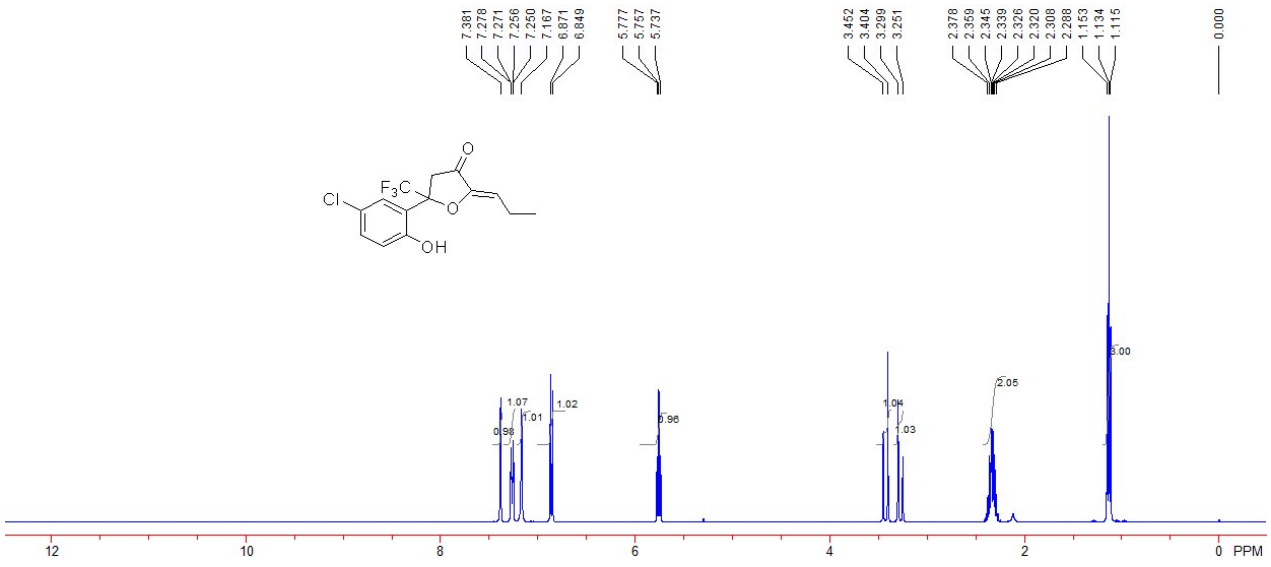






(Z)-5-(5-chloro-2-hydroxyphenyl)-2-propylidene-5-(trifluoromethyl)dihydrofuran-3(2H)-one (4u)

A white solid, 85% yield (54 mg). M.p.: 146-148 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.13 (t, *J* = 7.6 Hz, 3H, CH_3), 2.28~2.38 (m, 2H, CH_2), 3.28 (d, *J* = 19.2 Hz, 1H, CH_2), 3.43 (d, *J* = 19.2 Hz, 1H, CH_2), 5.76 (t, *J* = 8.0 Hz, 1H, =CH), 6.86 (d, *J* = 8.8 Hz, 1H, ArH), 7.17 (s, 1H, ArH), 7.26 (dd, *J* = 2.8, 8.8 Hz, 1H, ArH), 7.38 (s, 1H, OH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 12.9, 19.1, 42.5, 83.0 (q, *J* = 31.1 Hz), 113.6, 118.9, 121.0, 124.2 (q, *J* = 284.7 Hz), 125.5, 128.4, 131.2, 145.6, 153.2, 194.4. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.82. IR (CH_2Cl_2) ν 3351, 2972, 1728, 1658, 1495, 1414, 1289, 1186, 1169, 995, 764 cm^{-1}. MS (%) m/e 251 (M+, 100.00), 202 (86.40), 222 (43.05), 320 (38.77), 253 (36.46), 183 (32.78), 55 (30.02), 204 (28.87). HRMS (EI) calcd. for $C_{14}H_{12}O_3F_3Cl$: 320.0427, Found: 320.0426.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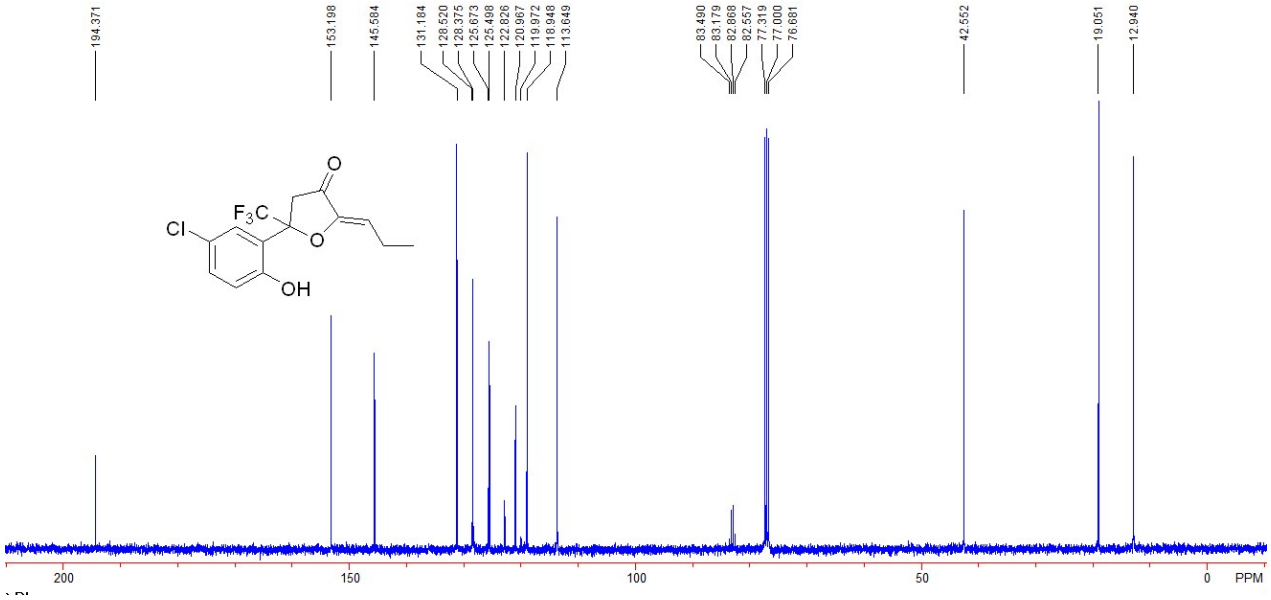
7.271
7.256
7.250
7.167
6.871
6.849
5.777
5.757
5.737
3.452
3.404
3.299
3.251
2.378
2.359
2.345
2.339
2.326
2.320
2.308
2.288
1.153
1.134
1.115
0.000
F3C
Cl
O
OH
0.98
1.07
1.01
1.02
0.96
1.04
1.03
2.05
3.00
12
10
8
6
4
2
0 PPM


194.371
153.198
145.584
131.184
128.520
128.375
125.673
125.498
122.826
120.967
119.972
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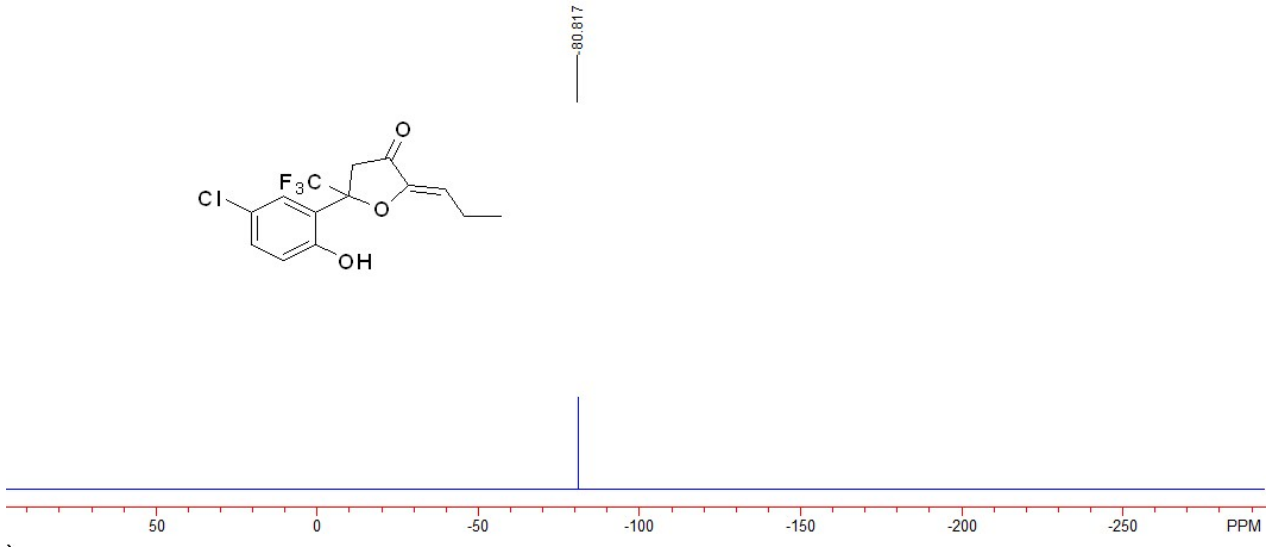
113.649
83.490
83.179
82.868
82.557
77.319
77.000
76.681
42.552
19.051
12.940
F3C
Cl
O
OH
200
150
100
50
0 PPM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O
OH
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-100
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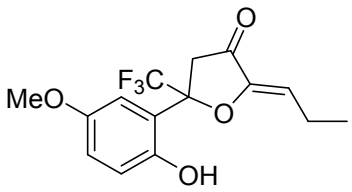
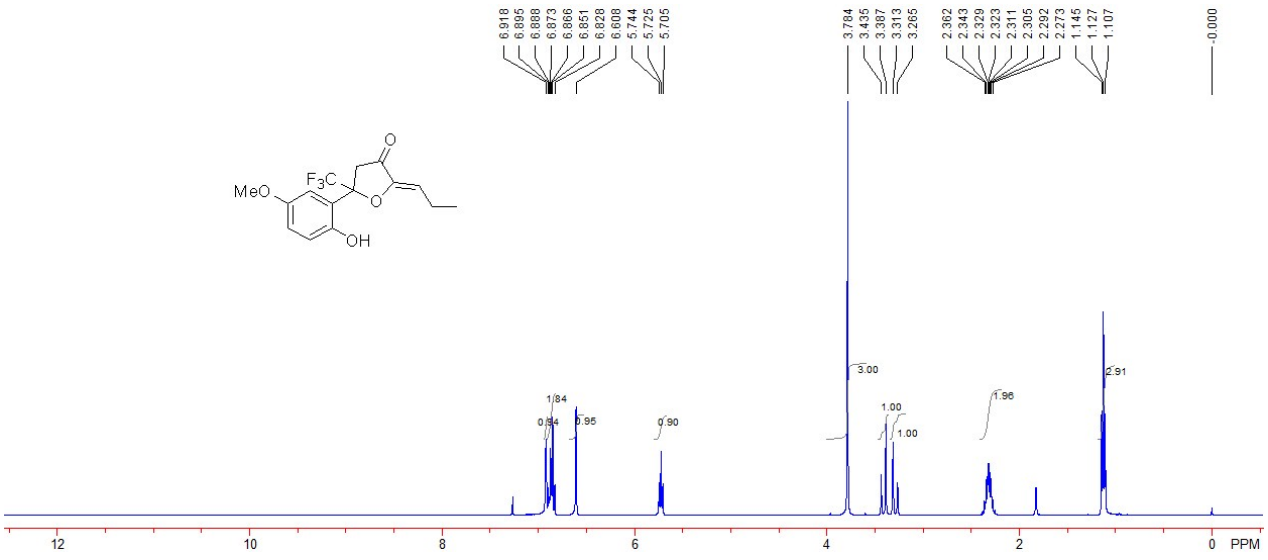
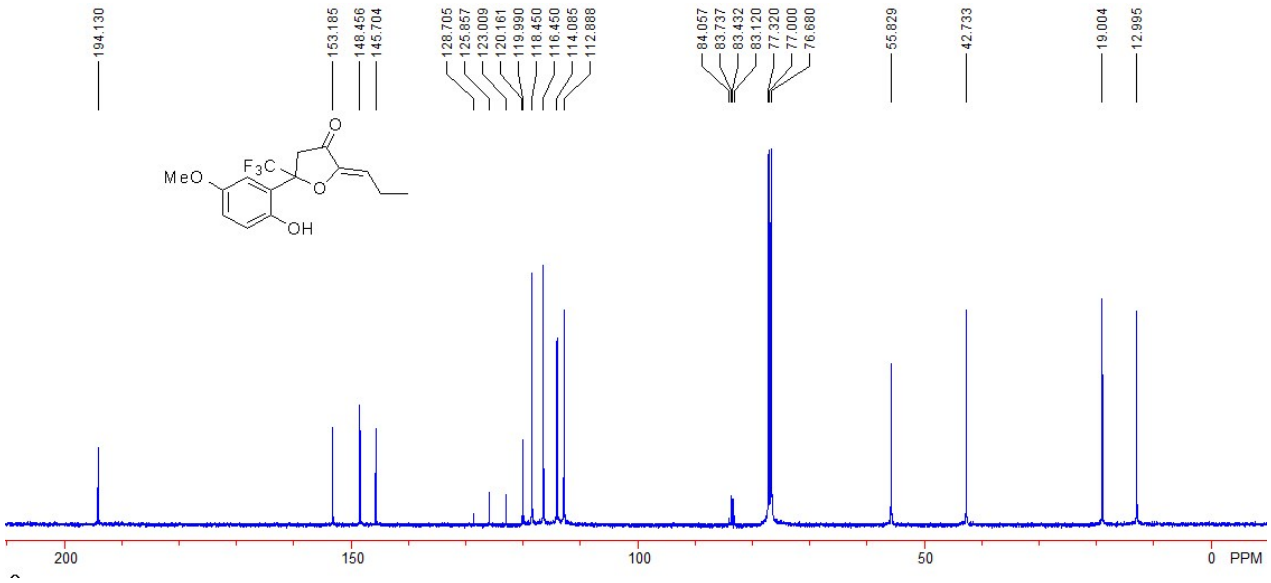
-200
-250
PPM



(Z)-5-(2-hydroxy-5-methoxyphenyl)-2-propylidene-5-(trifluoromethyl)dihydrofuran-3(2H)-one (4v)

A white solid, 73% yield (49 mg). M.p.: 121-123 °C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.13 (t, *J* = 7.6 Hz, 3H, CH_3), 2.27~2.37 (m, 2H, CH_2), 3.29 (d, *J* = 19.2 Hz, 1H, CH_2), 3.41 (d, *J* = 19.2 Hz, 1H, CH_2), 3.78 (s, 3H, CH_3), 5.73 (t, *J* = 8.0 Hz, 1H, =CH), 6.61 (s, 1H, ArH), 6.82~6.90 (m, 2H, ArH), 6.92 (s, 1H, OH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 13.0, 19.0, 42.7, 55.8, 83.6 (q, *J* = 30.5 Hz), 112.9, 114.1, 116.5, 118.5, 120.0, 124.4 (q, *J* = 284.8 Hz), 145.7, 148.5, 153.2, 194.1. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.76. IR (CH_2Cl_2) ν 3346, 2922, 2851, 1741, 1458, 1275, 1260, 1214, 1033, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{15}H_{19}F_3NO_4^{+1}(M+H)^+$ requires 334.1261, Found: 334.1263.

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118.450
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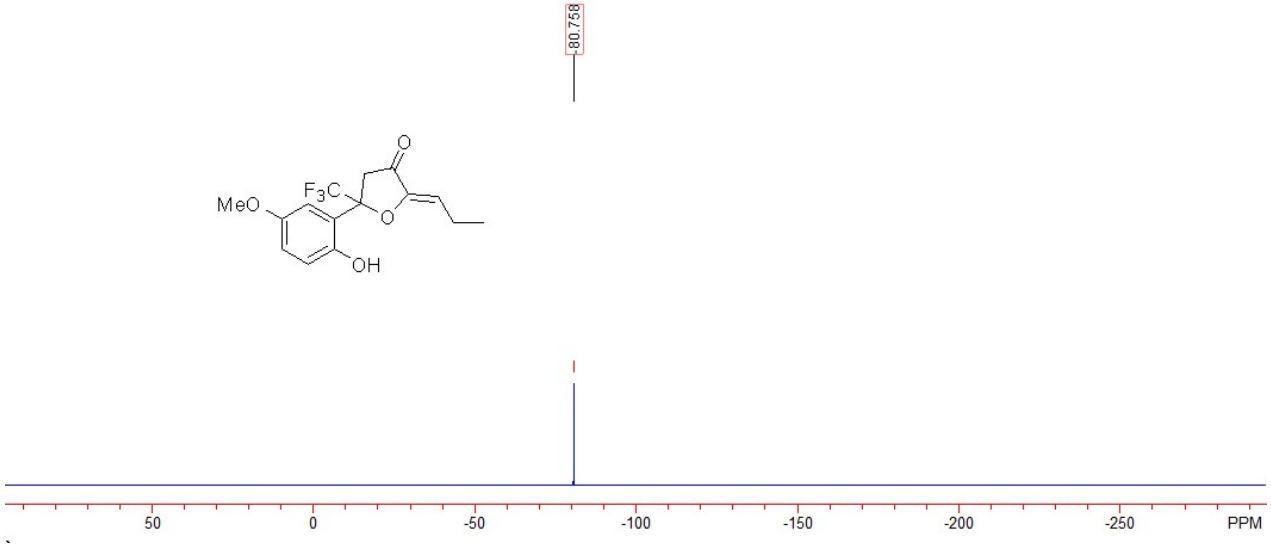
83.737
83.432
83.120
77.320
77.000
76.680
55.829
42.733
19.004
12.995
MeO
F3C
O
OH
200
150
100
50
0
PPM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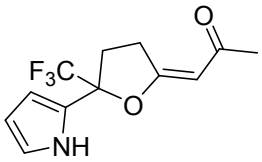
MeO
F3C
O
OH
50
0
-50
-100
-150
-200
-250
PPM

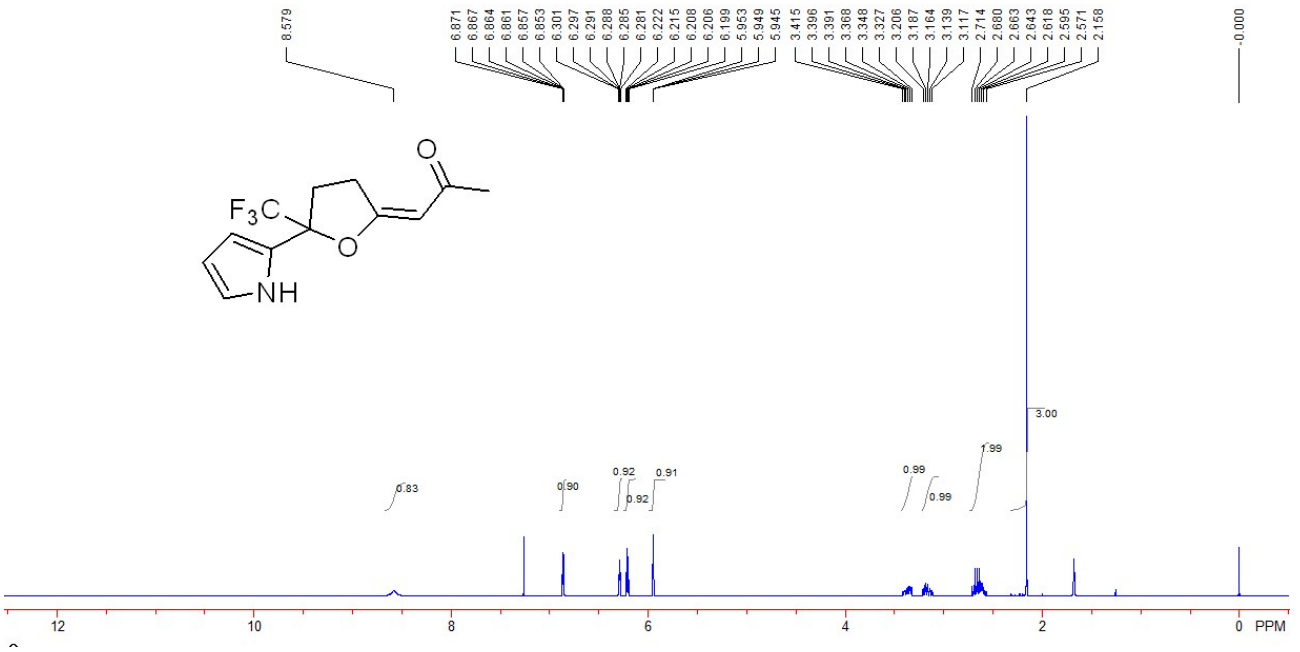
General Procedure for Investigation of Heterocyclic compounds or Phenyl Substitutied Alkynone in 10 ^{o}C or 65 ^{o}C and Spectroscopic Data of the Products 3w, 3x, 4aa, 5w, 5x, 5z and 5aa

General procedure A: Under argon atmosphere, to a solution of heterocyclic compounds (0.2 mmol) and P(4-FC_6H_4)$_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the hex-3-yn-2-one **2a** (0.4 mmol) at room temperature. Then the resulting mixture was heated to 65 ^{o}C and continued stirring at 65 ^{o}C until the reaction completed (monitoring by TLC). Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the desired products **3w**, **3x**, **4aa** and **5z**.



(E)-1-(5-(1H-pyrrol-2-yl)-5-(trifluoromethyl)dihydrofuran-2(3H)-ylidene)propan-2-one (3w)

A white solid, 43% yield (22 mg). M.p.: 102-104 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.16 (s, 3H, CH_3), 2.57~2.72 (m, 2H, CH_2), 3.11~3.21 (m, 1H, CH_2), 3.32~3.42 (m, 1H, CH_2), 5.95 (t, *J* = 1.6 Hz, 1H, =CH), 6.19~6.23 (m, 1H, ArH), 6.28~6.31 (m, 1H, ArH), 6.85~6.88 (m, 1H, ArH), 8.58 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 30.1, 30.3, 31.3, 85.3 (q, *J* = 30.3 Hz), 100.3 (d, *J* = 2.9 Hz), 120.0, 124.06 (q, *J* = 282.5 Hz), 124.07, 173.5, 197.5. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.41. IR (CH_2Cl_2) ν 3296, 2957, 2924, 2366, 1683, 1599, 1376, 1176, 1103, 953, 868 cm^{-1}. HRMS (ESI) Calcd. For $C_{12}H_{13}F_3NO_2^{+1}(M+H)^+$ requires 260.0893, Found: 260.0895.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6.867
6.864
6.861
6.857
6.853
6.301
6.297
6.291
6.288
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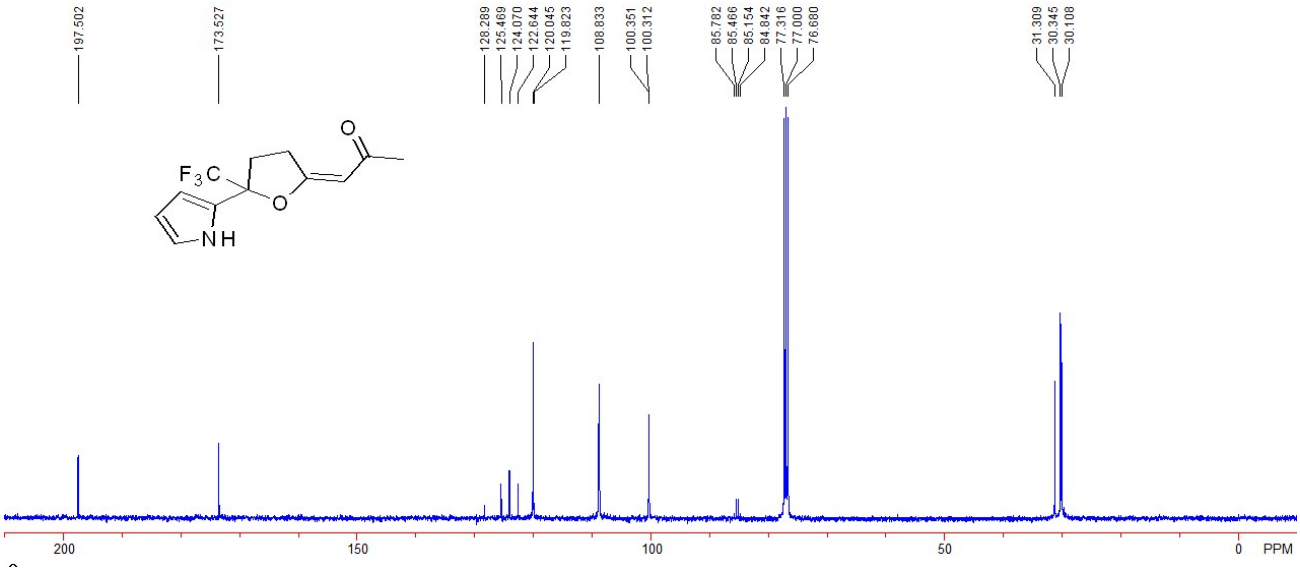
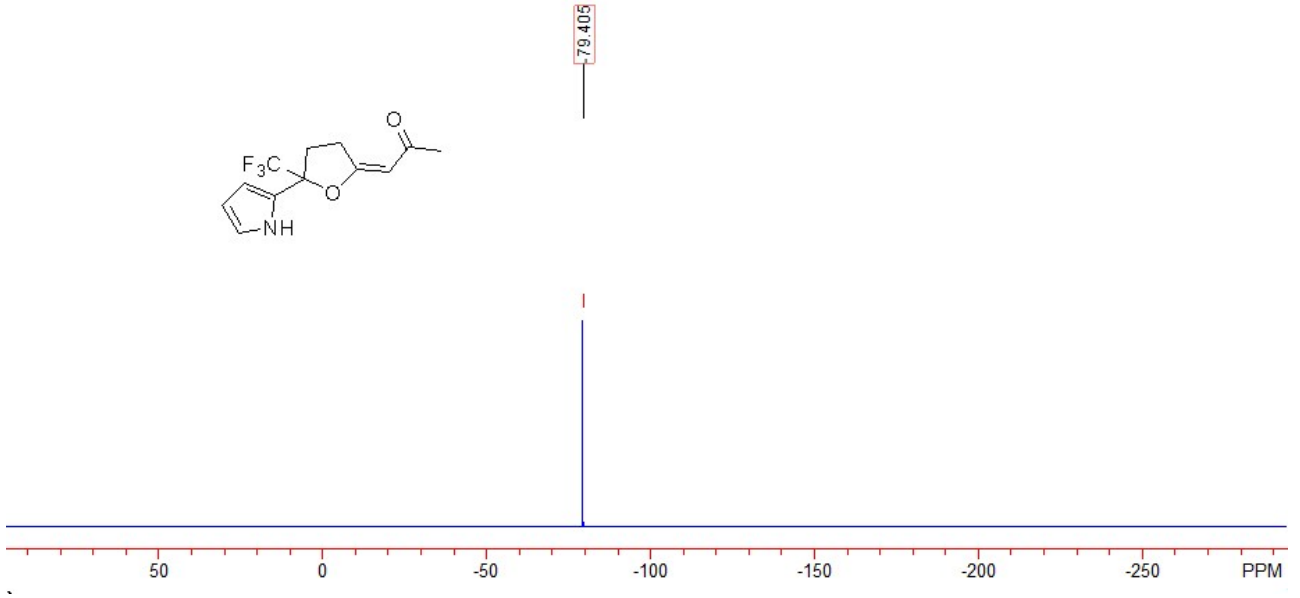
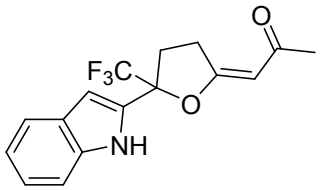
6.222
6.215
6.208
6.206
6.199
5.953
5.949
5.945
3.415
3.396
3.391
3.368
3.348
3.327
3.206
3.187
3.164
3.139
3.117
2.714
2.680
2.663
2.643
2.618
2.595
2.571
2.158
-0.000
O
F3C
O
NH
3.00
1.99
0.99
0.99
0.92
0.92
0.91
0.90
0.83
12
10
8
6
4
2
0 PPM

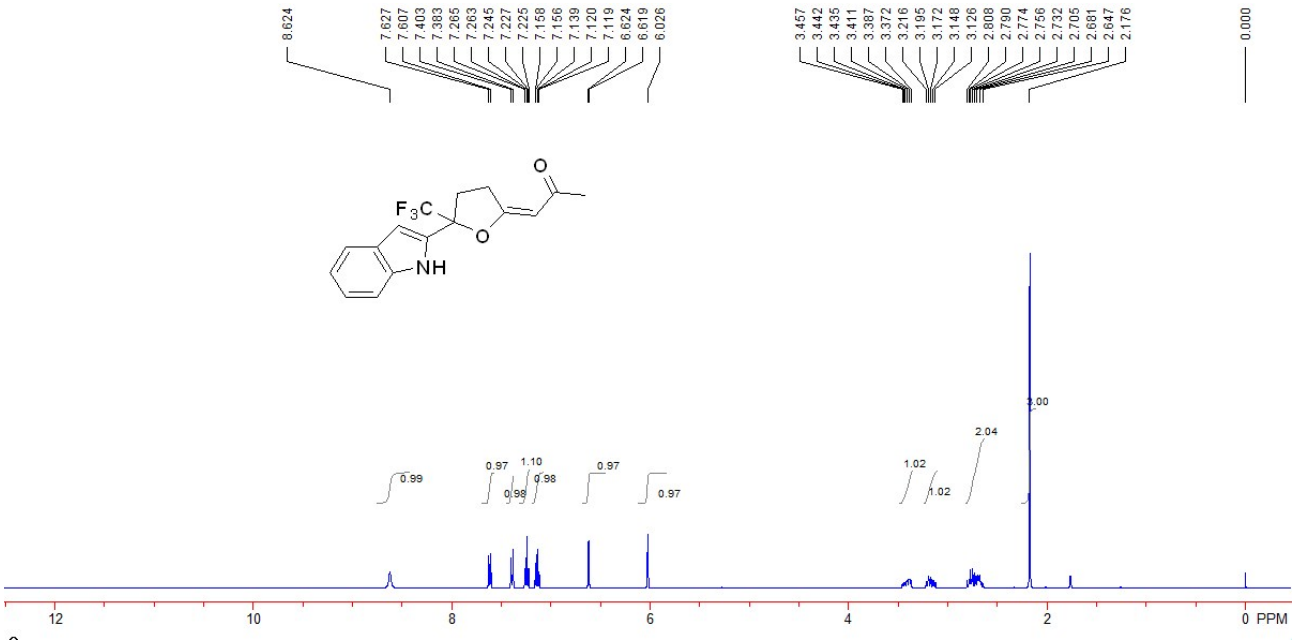

197.502
173.527
128.289
125.469
124.070
122.644
120.045
119.823
108.833
100.351
100.312
85.782
85.466
85.154
84.842
77.316
77.000
76.680
31.309
30.345
30.108
O
F3C
O
NH
200
150
100
50
0 PPM

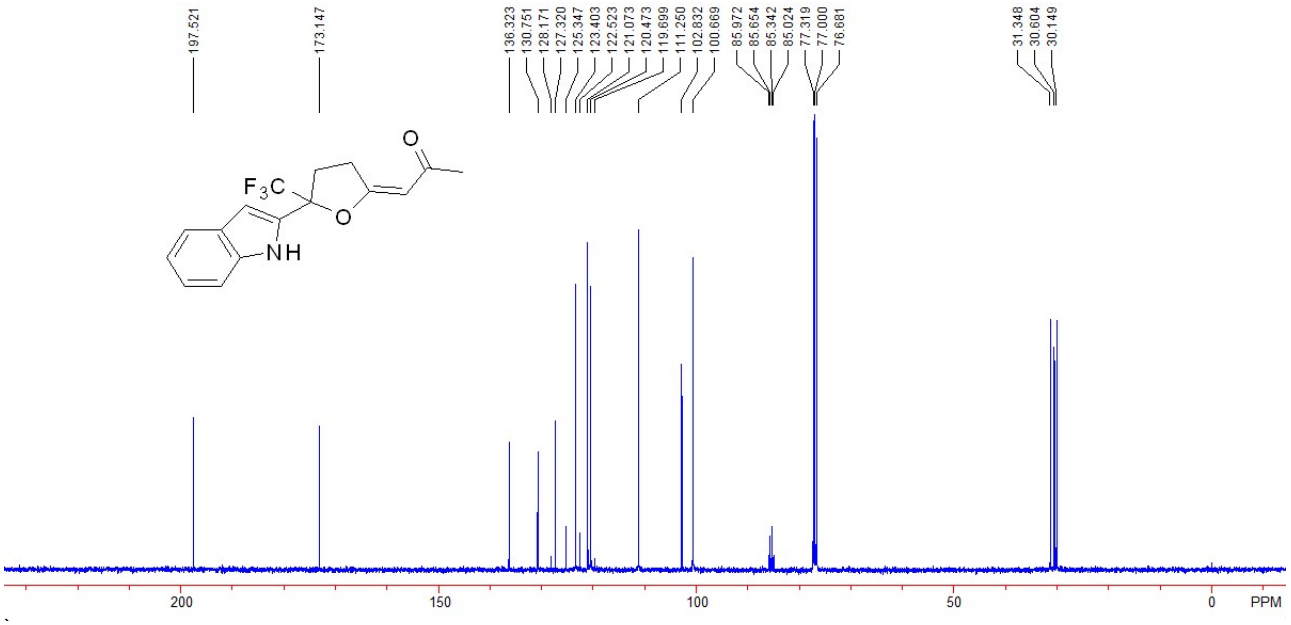

79.405
O
F3C
O
NH
50
0
-50
-100
-150
-200
-250
PPM

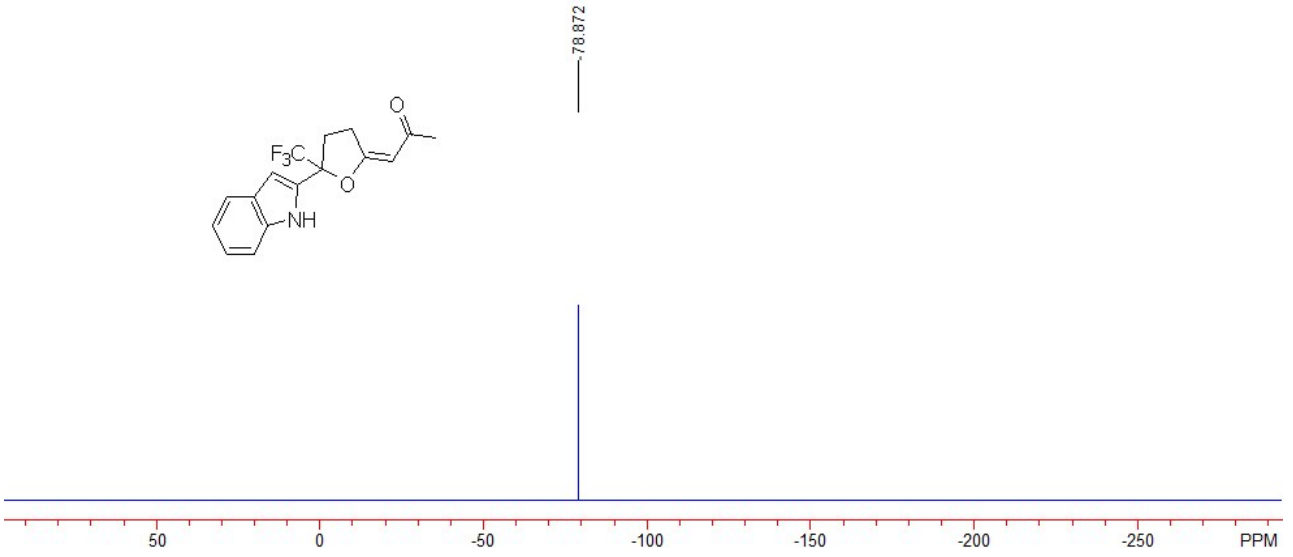


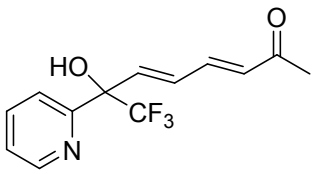
(E)-1-(5-(1H-indol-2-yl)-5-(trifluoromethyl)dihydrofuran-2(3H)-ylidene)propan-2-one (3x)

A white solid, 61 % yield (38 mg). M.p.: 142-144 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.18 (s, 3H, CH_3), 2.64~2.81 (m, 2H, CH_2), 3.12~3.22 (m, 1H, CH_2), 3.37~3.46 (m, 1H, CH_2), 6.03 (s, 1H, =CH), 6.62 (d, *J* = 2.0, 1H, ArH), 7.11~7.16 (m, 1H, ArH), 7.22~7.27 (m, 1H, ArH), 7.39 (d, *J* = 8.0, 1H, ArH), 7.62 (d, *J* = 8.0, 1H, ArH), 8.62 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 30.1, 30.6, 31.3, 85.5 (q, *J* = 31.9 Hz), 100.7, 102.8, 111.3, 120.5, 121.1, 123.4, 123.9 (q, *J* = 282.4 Hz), 127.3, 130.8, 136.3, 173.1, 197.5. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.87. IR (CH_2Cl_2) ν 3313, 2922, 2851, 1684, 1601, 1275, 1162, 1019, 958 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{15}F_3NO_2^{+1}$(M+H)$^+$ requires 310.1049, Found: 310.1052.





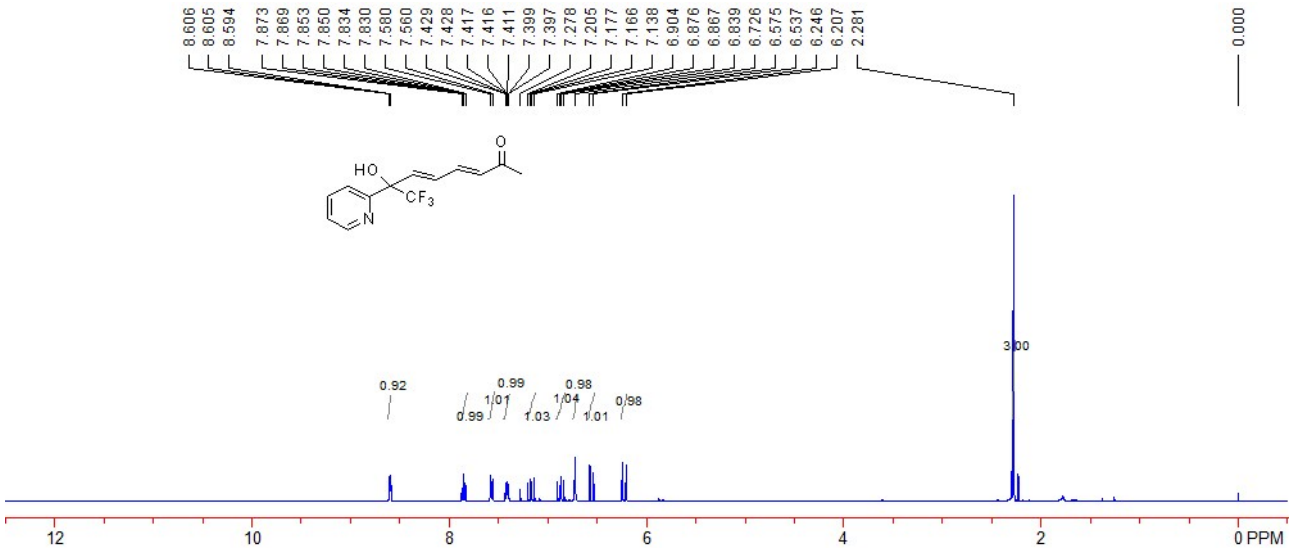


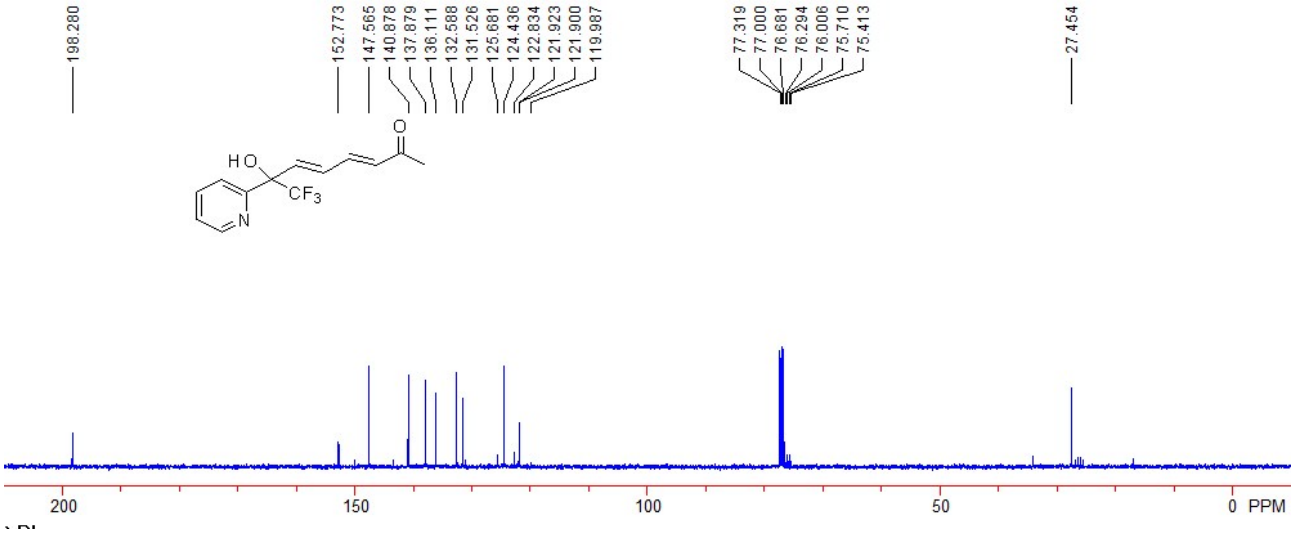


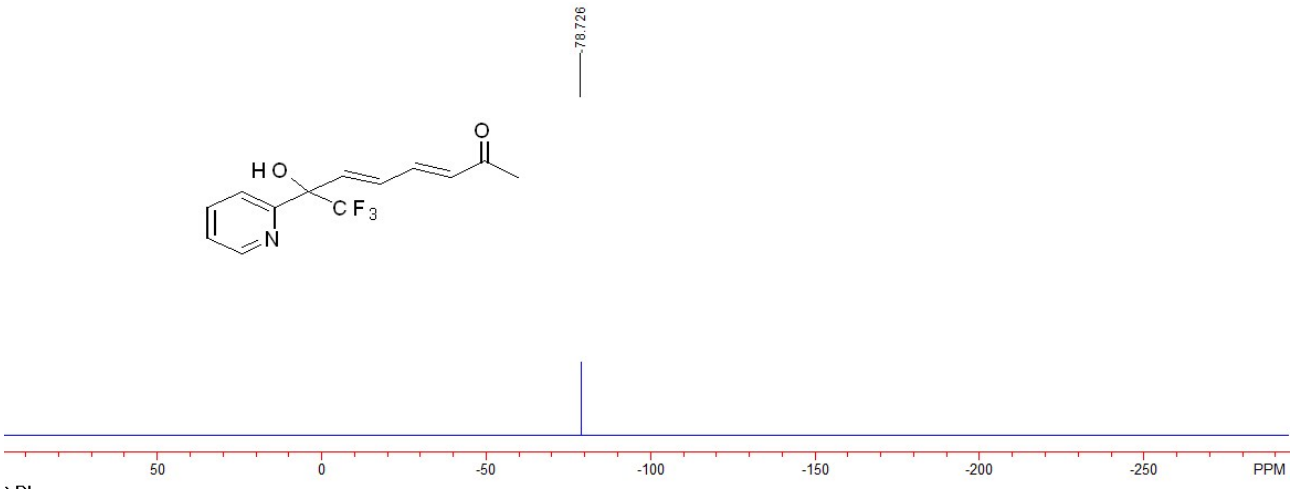
(3E,5E)-8,8,8-trifluoro-7-hydroxy-7-(pyridin-2-yl)octa-3,5-dien-2-one (5z)

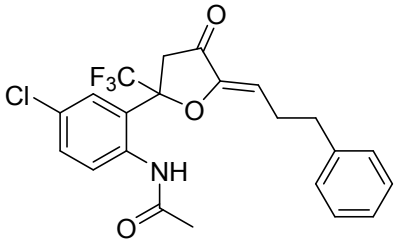
A white solid, 63% yield (34 mg). M.p.: 81-83 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.28 (s, 3H, CH_3), 6.23 (d, J = 15.6 Hz, 1H, =CH), 6.56 (d, J = 15.2 Hz, 1H, =CH), 6.73 (s, 1H, OH), 6.87 (dd, J = 11.2, 14.8 Hz, 1H, =CH), 7.17 (dd, J = 11.2, 15.6 Hz, 1H, =CH), 7.39~7.43 (m, 1H, ArH), 7.57 (d, J = 8.0 Hz, 1H, ArH), 7.83~7.88 (m, 1H, ArH), 8.59~8.61 (m, 1H, ArH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 27.5, 75.9 (q, J = 29.6 Hz), 121.9 (q, J = 2.3 Hz), 124.3 (q, J = 284.7 Hz), 124.4, 131.5,

132.6, 136.1, 137.9, 140.9, 147.6, 152.8, 198.3. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.09. IR (CH_2Cl_2) ν 3283, 2955, 2924, 2850, 1671, 1256, 1150, 1099, 998, 945 cm^{-1}. HRMS (ESI) Calcd. For $C_{13}H_{13}F_3NO_2^{+1}(M+H)^+$ requires 272.0893, Found: 272.0895.



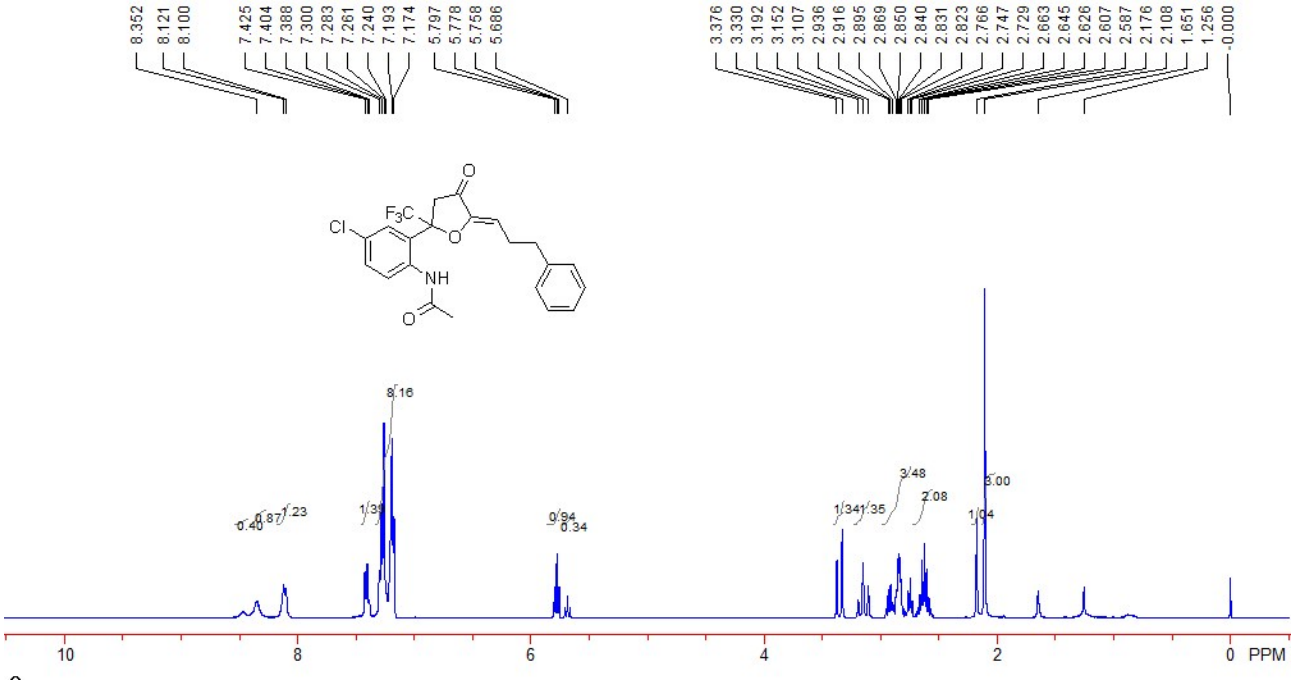


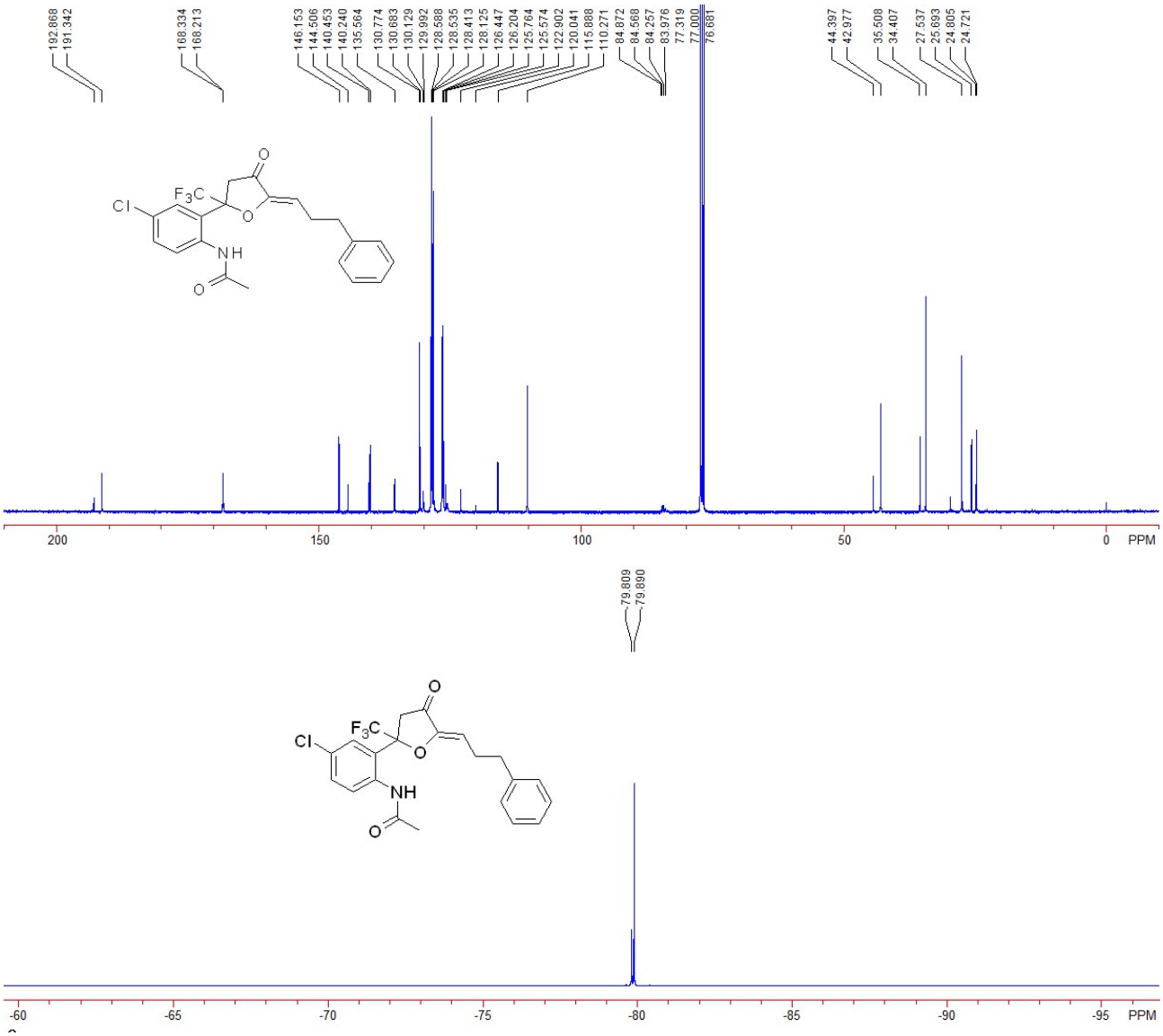




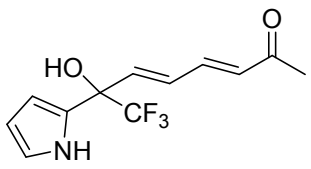
(Z)-N-(4-chloro-2-(4-oxo-5-(3-phenylpropylidene)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (4aa)

This product is a cis-trans-isomer (Z:E = 3:1). A white oil, 59% yield (52 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.11 (s, 3H, CH_3), 2.18 (s, 1H, CH_3), 2.54~2.70 (m, 2H, CH_2), 2.72~2.96 (m, 3.48H, CH_2), 3.10~3.20 (m, 1.35H, CH_2), 3.35 (d, *J* = 18.4 Hz, 1.34H, CH_2), 5.69 (t, *J* = 7.6 Hz, 0.34H, =CH), 5.78 (t, *J* = 8.0 Hz, 1H, =CH), 7.17~7.30 (m, 8.16H, ArH), 7.38~7.43 (m, 1.39H, CH_2), 8.11 (d, *J* = 8.4 Hz, 1.23H, ArH), 8.35 (s, 0.87H, NH), 8.47 (s, 0.40H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 24.7, 24.8, 25.7, 27.5, 34.4, 35.5, 43.0, 44.4, 84.4 (q, *J* = 31.1 Hz), 110.3, 115.9, 124.3 (q, *J* = 286.4 Hz), 125.6, 126.2, 126.4, 128.1, 128.4, 128.5, 128.6, 130.0, 130.1, 130.7, 130.8, 135.6, 140.2, 140.5, 144.5, 146.2, 168.2, 168.3, 191.3, 192.9. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.81, -79.89. IR (CH_2Cl_2) ν 3428, 2929, 1743, 1669, 1497, 1292, 1173, 1000, 749, 699 cm^{-1}. HRMS (ESI) Calcd. For $C_{22}H_{20}ClF_3NO_3^{+1}$(M+H)$^+$ requires 438.1078, Found: 438.1077.



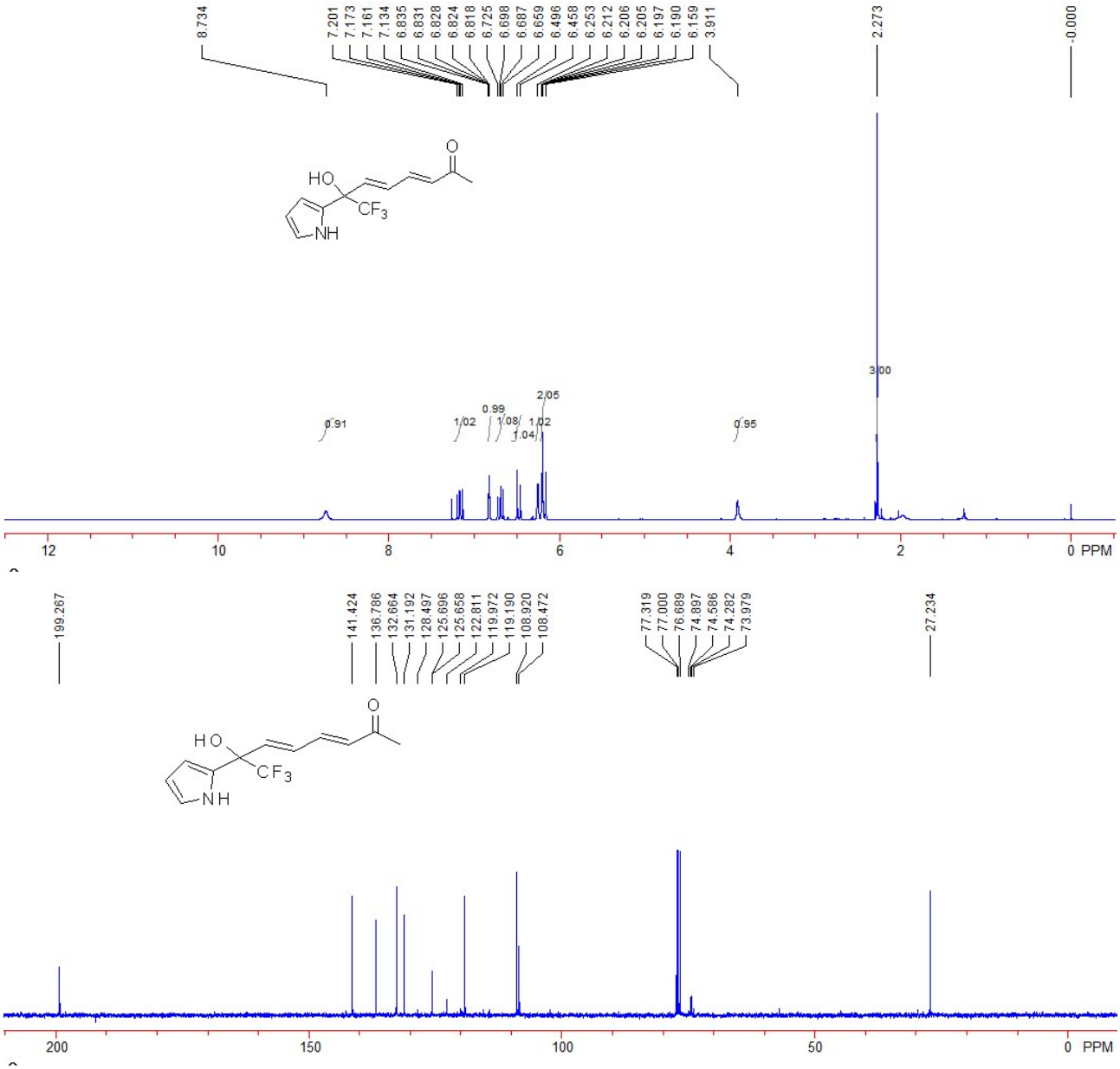


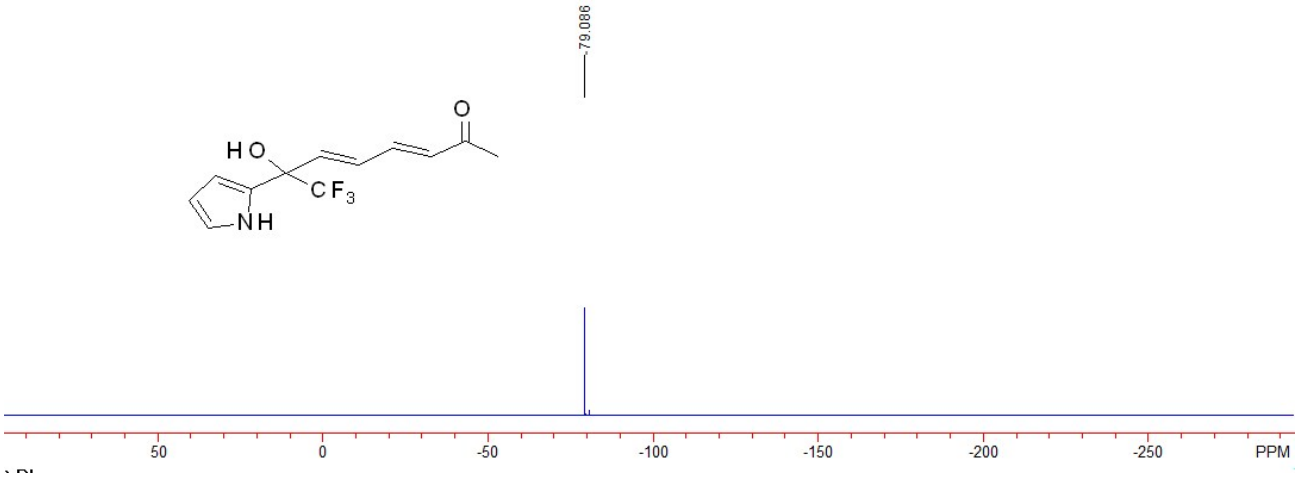
General procedure B: Under argon atmosphere, to a solution of heterocyclic compound (0.2 mmol) and P(4-FC_6H_4)$_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the hex-3-yn-2-one **2a** (0.4 mmol) at room temperature. Then the resulting mixture was cooled to 10 ^oC and continued stirring at 10 ^oC until the reaction completed (monitoring by TLC). Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the desired products **5w**, **5x** and **5aa**.

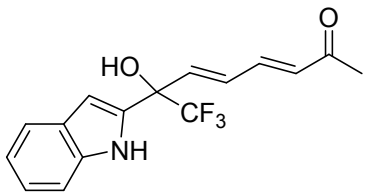


(3E,5E)-8,8,8-trifluoro-7-hydroxy-7-(1H-pyrrol-2-yl)octa-3,5-dien-2-one (5w)

A yellow oil, 67% yield (35 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.27 (s, 3H, CH_3), 3.91 (s, 1H, OH), 6.15~6.26 (m, 2H, =CH, ArH), 6.25 (s, 1H, ArH), 6.48 (d, *J* = 15.2 Hz, 1H, =CH), 6.69 (dd, *J* = 10.8, 15.2 Hz, 1H, =CH), 6.81-6.84 (m, 1H, ArH), 7.17 (dd, *J* = 11.2, 16.0 Hz, 1H, =CH), 8.73 (br, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 27.2, 74.4 (q, *J* = 30.4 Hz), 108.5, 108.9, 119.2, 124.2 (q, *J* = 284.7 Hz), 125.7, 131.2, 132.7, 136.8, 141.4, 199.3. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.09. IR (CH_2Cl_2) ν 3367, 2923, 2851, 1669, 1275, 1260, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{12}H_{13}F_3NO_2^{+1}(M+H)^+$ requires 260.0893, Found: 260.0898.

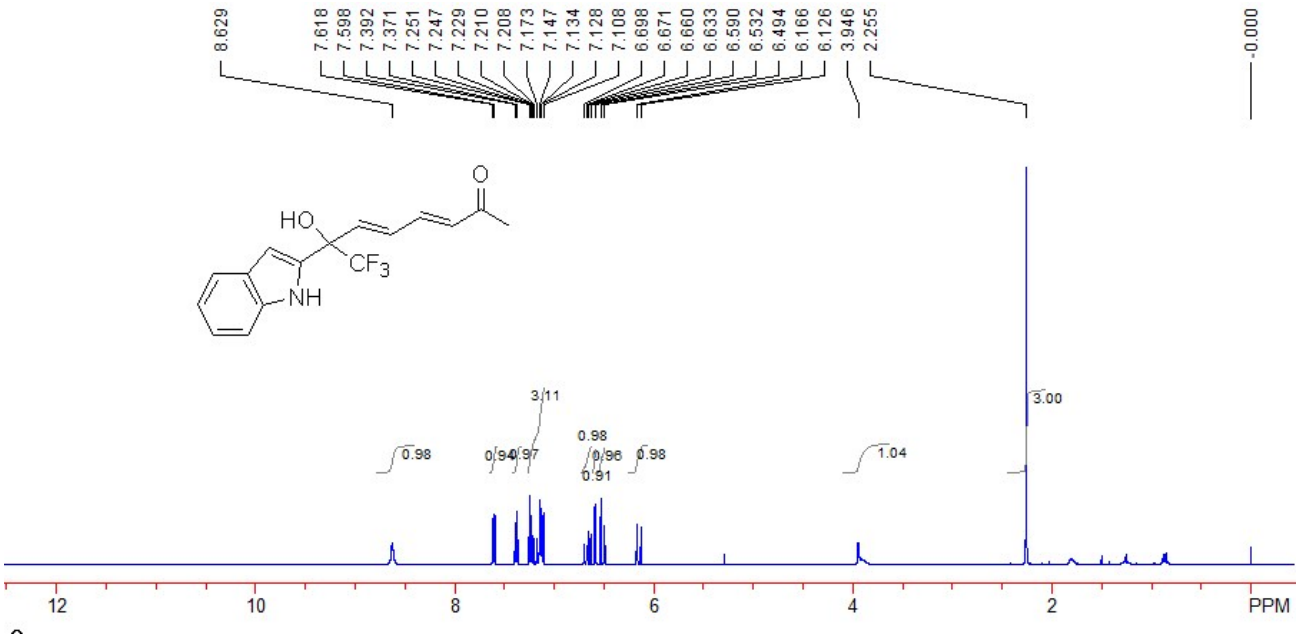






(3E,5E)-8,8,8-trifluoro-7-hydroxy-7-(1H-indol-2-yl)octa-3,5-dien-2-one (5x)

A yellow oil, 74% yield (46 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.26 (s, 3H, CH_3), 3.95 (s, 1H, OH), 6.15 (d, *J* = 16.0 Hz, 1H, =CH), 6.51 (d, *J* = 15.2 Hz, 1H, =CH), 6.59 (s, 1H, ArH), 6.62 (dd, *J* = 10.8, 15.2 Hz, 1H, =CH), 7.10~7.26 (m, 3H, =CH, ArH), 7.38 (d, *J* = 8.4 Hz, 1H, ArH), 7.61 (d, *J* = 8.0 Hz, 1H, ArH), 8.63 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 27.4, 74.9 (q, *J* = 30.4 Hz), 102.5, 111.3, 120.4, 121.1, 123.2, 124.1 (q, *J* = 284.6 Hz), 127.6, 131.6, 132.1, 132.9, 135.7, 136.2, 141.1, 199.2. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -78.80. IR (CH_2Cl_2) ν 3366, 2923, 2851, 1669, 1638, 1596, 1275, 1260, 1159, 996, 764, 749 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{15}F_3NO_2^{+1}(M+H)^+$ requires 310.1049, Found: 310.1052.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7.598
7.392
7.371
7.251
7.247
7.229
7.210
7.208
7.173
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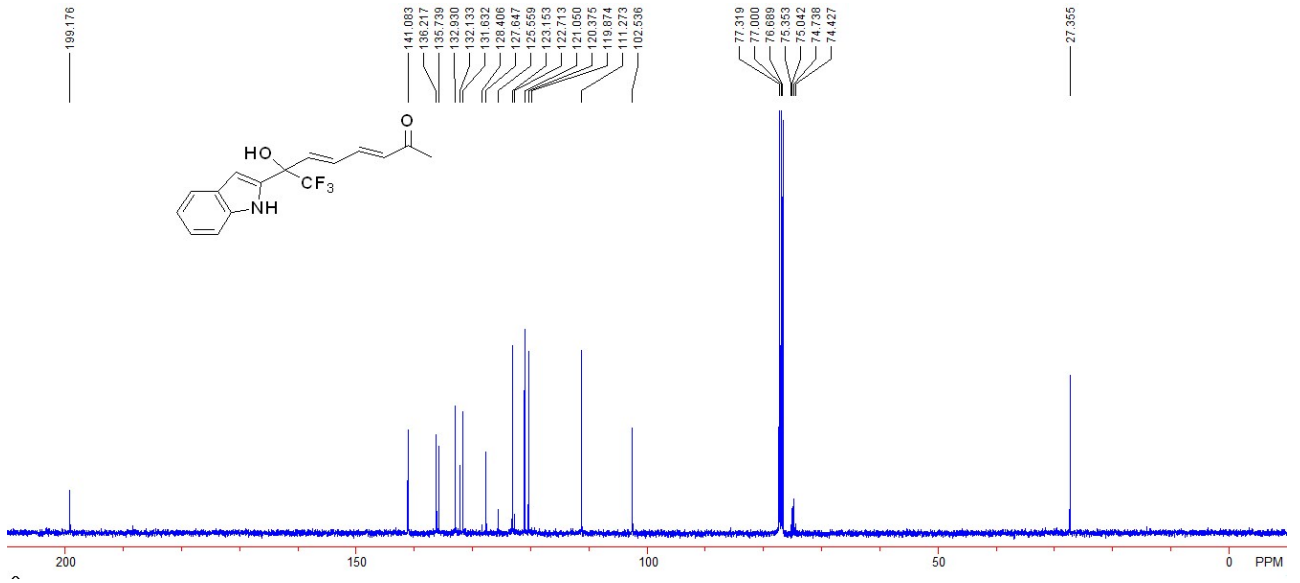
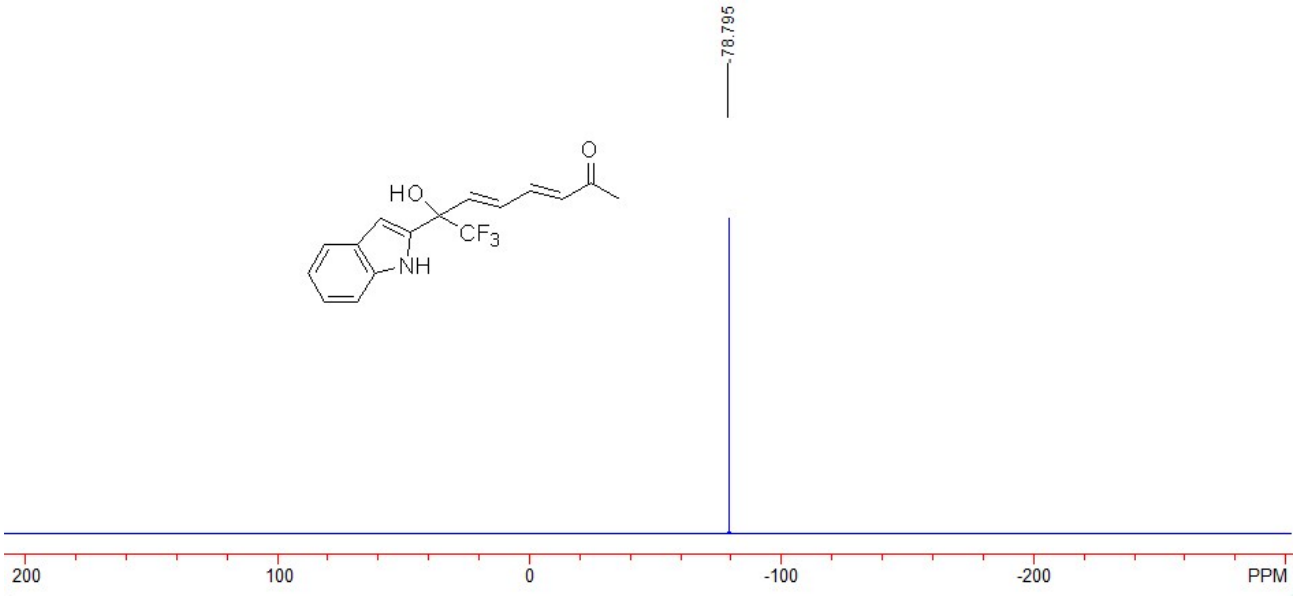
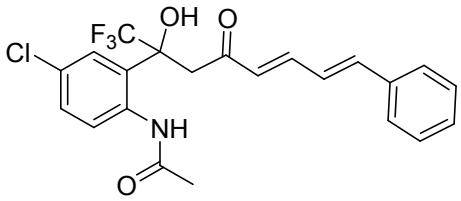
7.134
7.128
7.108
6.698
6.671
6.660
6.633
6.590
6.532
6.494
6.166
6.126
3.946
2.255
-0.000
HO
CF3
NH
O
3.11
3.00
0.98
0.94
0.97
0.98
0.96
0.91
0.98
1.04
12
10
8
6
4
2
PPM

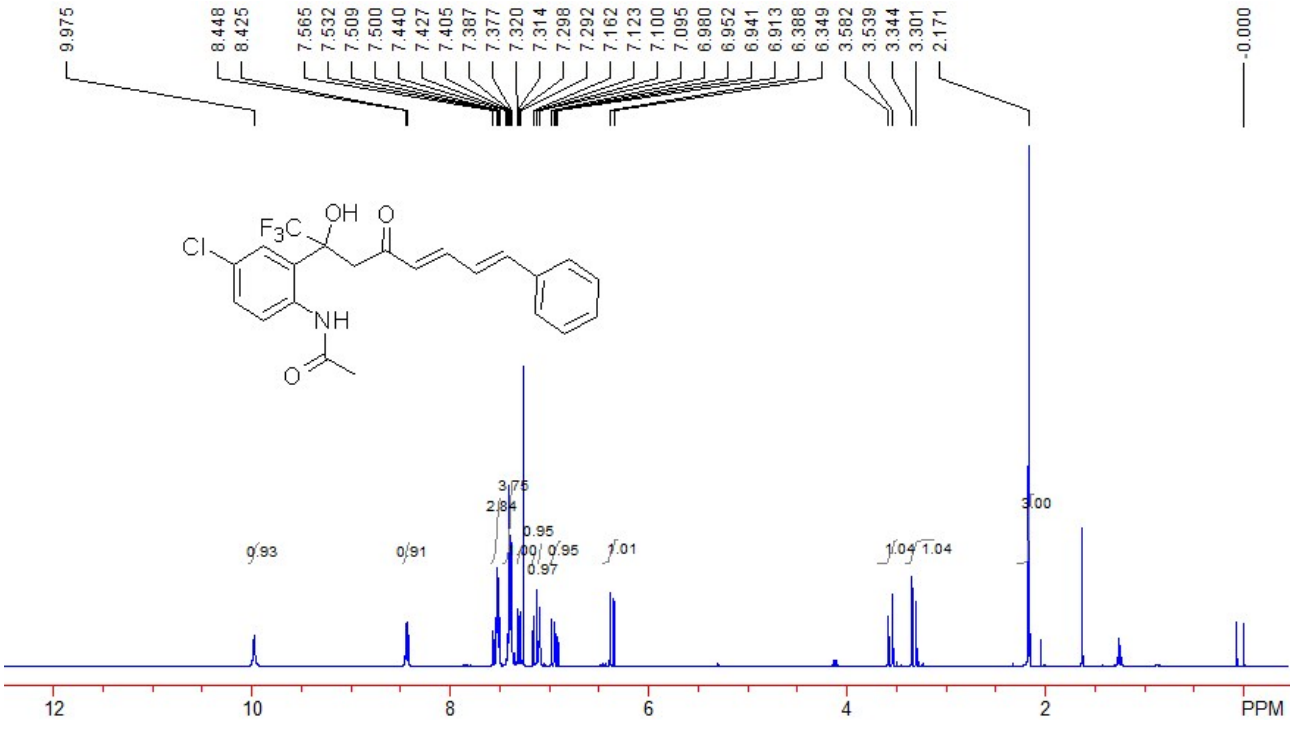

199.176
141.083
136.217
135.739
132.930
132.133
131.632
128.406
127.647
125.559
123.153
122.713
121.050
120.375
119.874
111.273
102.536
77.319
77.000
76.689
75.353
75.042
74.738
74.427
27.355
HO
CF3
NH
O
200
150
100
50
0
PPM

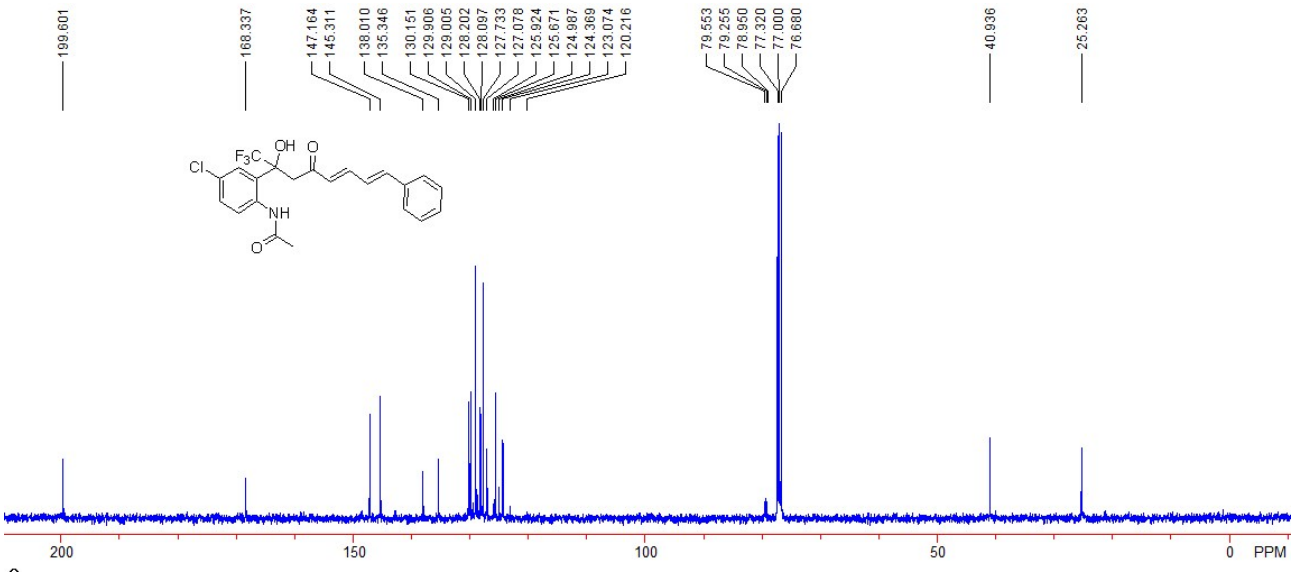

-78.795
HO
CF3
NH
O
200
100
0
-100
-200
PPM



N-(4-chloro-2-((5E,7E)-1,1,1-trifluoro-2-hydroxy-4-oxo-8-phenylocta-5,7-dien-2-yl)phenyl)acetamide (5aa)

A white solid, 34% yield (30 mg). M.p.: 79-81 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 2.17 (s, 3H, CH_3), 3.32 (d, *J* = 17.2 Hz, 1H, CH_2), 3.56 (d, *J* = 17.2 Hz, 1H, CH_2), 6.37 (d, *J* = 15.6 Hz, 1H, CH_2), 6.95 (dd, *J* = 11.2, 15.6 Hz, 1H, CH_2), 7.10 (d, *J* = 2.0 Hz, 1H, ArH), 7.17 (d, *J* = 15.6 Hz, 1H, CH_2), 7.31 (dd, *J* = 2.4, 8.8 Hz, 1H, ArH), 7.37~7.44 (m, 4H, ArH, OH), 7.50~7.57 (m, 3H, ArH, OH), 8.44 (d, *J* = 9.2 Hz, 1H, ArH), 9.98 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 25.3, 40.9, 79.4 (q, *J* = 29.8 Hz), 124.4, 124.5 (q, *J* = 285.0 Hz), 125.0, 125.7, 127.1, 127.7, 128.1, 128.2, 129.0, 130.2, 135.3, 138.0, 145.3, 147.2, 168.3, 199.6. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.72. IR (CH_2Cl_2) ν 3351, 2923, 2852, 1688, 1580, 1519, 1397, 1163, 1027, 749, 689 cm^{-1}. HRMS (ESI) Calcd. For $C_{22}H_{20}ClF_3NO_3^{+1}(M+H)^+$ requires 438.1078, Found: 438.1077.




199.601
168.337
147.164
145.311
138.010
135.346
130.151
129.906
129.005
128.202
128.097
127.733
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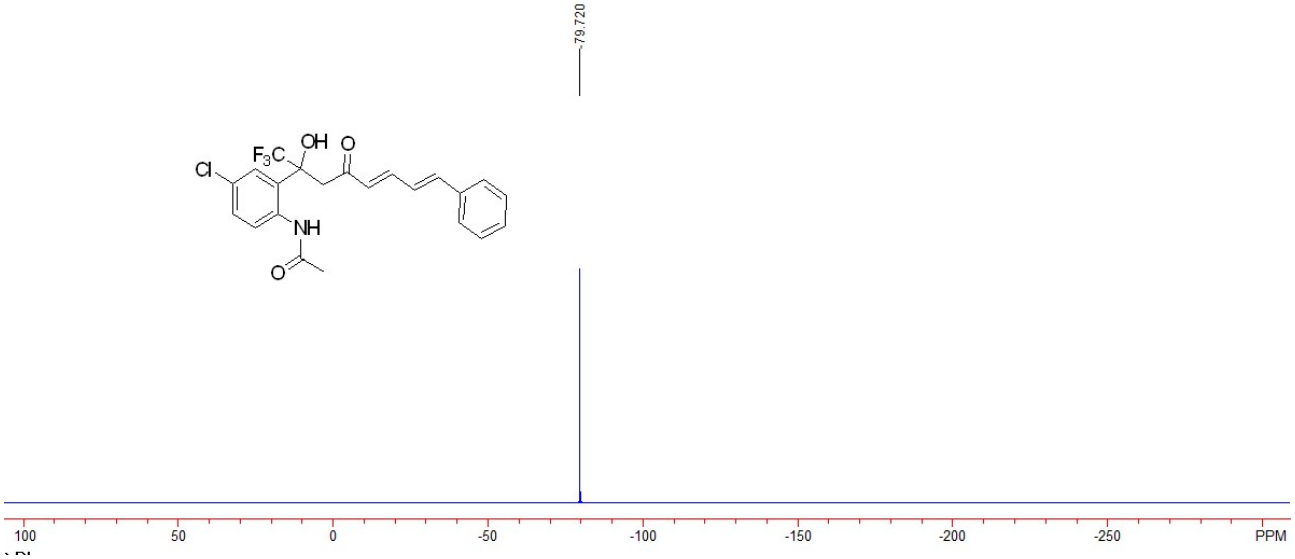
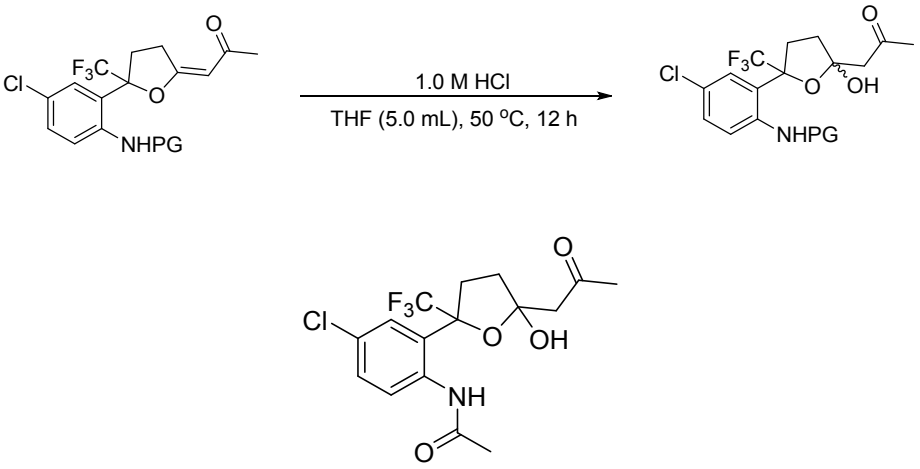
125.924
125.671
124.987
124.369
123.074
120.216
79.553
79.255
78.950
77.320
77.000
76.680
40.936
25.263
Cl
F3C
OH
O
NH
O
200
150
100
50
0
PPM


79.720
Cl
F3C
OH
O
NH
O
100
50
0
-50
-100
-150
-200
-250
PPM

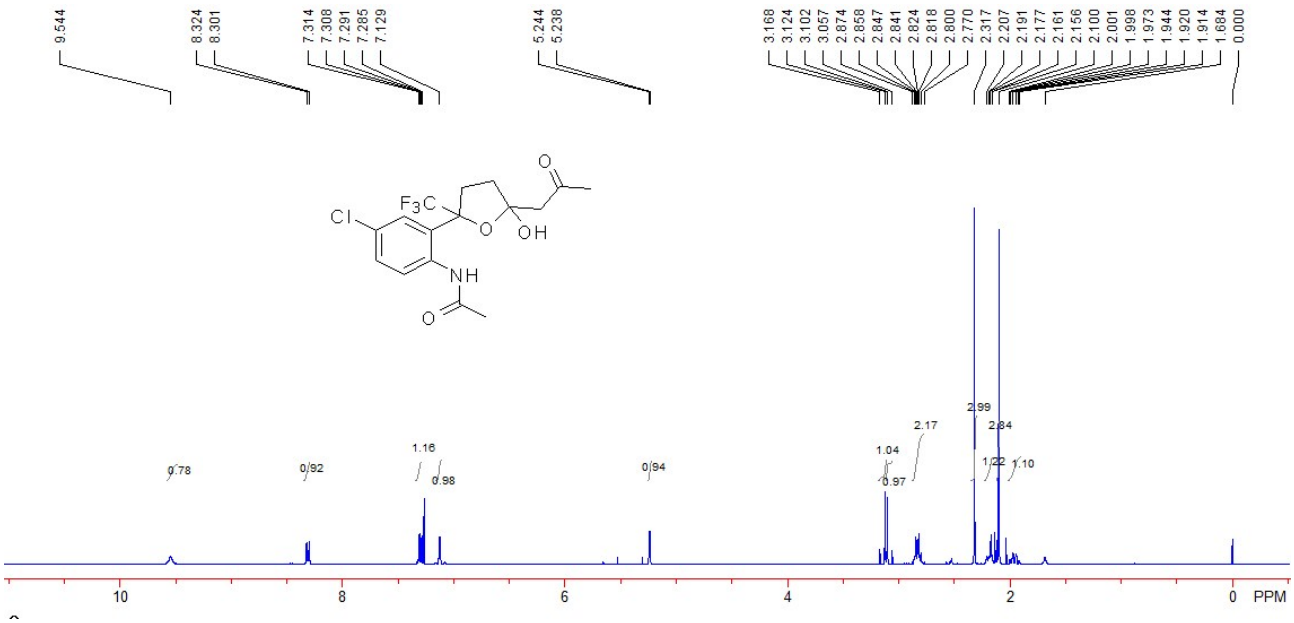
General Procedure for Hydration of 3a and 3d and Spectroscopic Data of the Products 3a' and 3d'

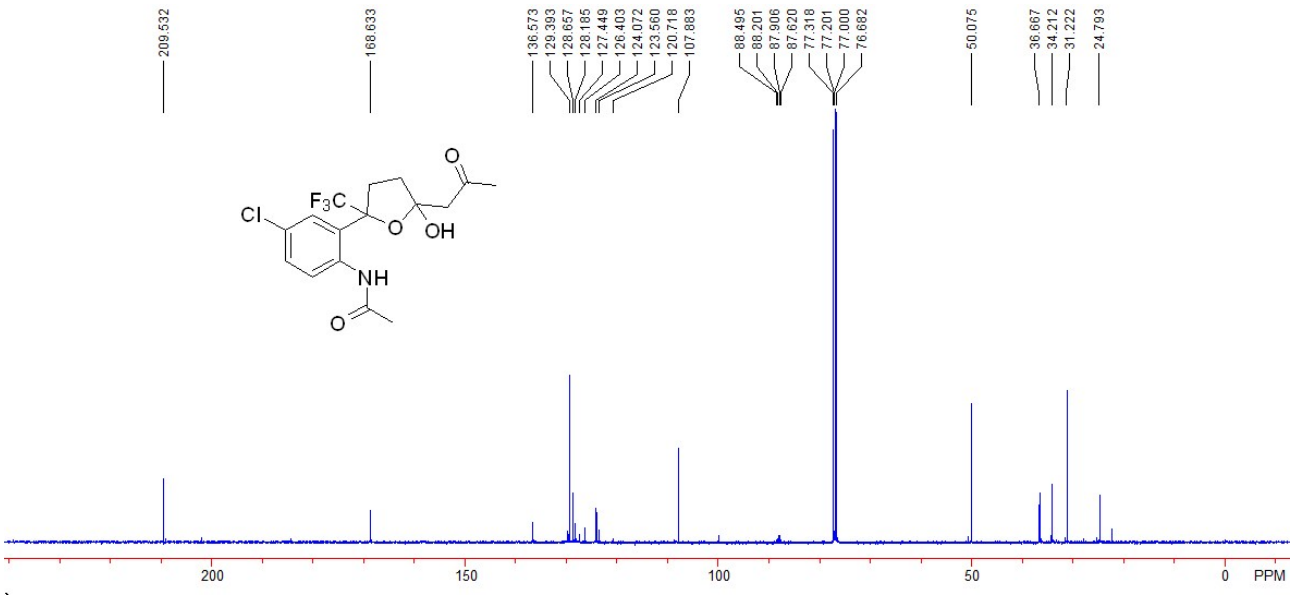
To a solution of compounds **3** (0.1 mmol) in THF (5.0 mL) was added 1.0 M aqueous HCl solution (1.0 mL) at room temperature. Then the resulting mixture was heated to 50 ^{o}C and continued stirring at 50 ^{o}C until the reaction completed (monitoring by TLC). Then the reaction mixture was washed by water and extracted by EA (5.0 mL, three times), the organic phases was combined and concentrated under reduced pressure, then the residue was directly subjected to a flash column chromatography on silica gel to afford the desired products **3a'** and **3d'**.



N-(4-chloro-2-(5-hydroxy-5-(2-oxopropyl)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)acetamide (3a')

These products are a pair of diastereoisomers (dr > 20:1). A white solid, 99% yield (37 mg). M.p.: 109-111 ^{o}C. ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.91~2.01 (m, 1H, CH_2), 2.10 (s, 3H, CH_3), 2.15~2.21 (m, 1H, CH_2), 2.32 (s, 3H, CH_3), 2.77~2.87 (m, 2H, CH_2), 3.08 (d, J = 18.0 Hz, 1H, CH_2), 3.15 (d, J = 18.0 Hz, 1H, CH_2), 5.24 (d, J = 2.4 Hz, 1H, OH), 7.13 (s, 1H, ArH), 7.30 (dd, J = 2.4, 9.2 Hz, 1H, ArH), 8.31 (d, J = 9.2 Hz, 1H, ArH), 9.54 (s, 1H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 24.8, 31.2, 34.2, 36.7, 50.1, 88.1 (q, J = 29.5 Hz), 107.9, 124.1, 124.8 (q, J = 284.3 Hz), 127.4, 128.2, 128.7, 129.4, 136.5, 168.6, 209.5. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -80.35. IR (CH_2Cl_2) ν 3356, 2971, 2900, 1693, 1605, 1519, 1396, 1170, 1066, 1057, 1026, 882 cm^{-1}. HRMS (ESI) Calcd. For $C_{16}H_{18}ClF_3NO_4^{+1}(M+H)^+$ requires 380.0871, Found: 380.0871.


9.544
8.324
8.301
7.314
7.308
7.291
7.285
7.129
5.244
5.238
3.168
3.124
3.102
3.057
2.874
2.858
2.847
2.841
2.824
2.818
2.800
2.770
2.317
2.207
2.191
2.177
2.161
2.156
2.100
2.001
1.998
1.973
1.944
1.920
1.914
1.684
0.000
F3C
Cl
O
OH
NH
O
O
0.78
0.92
1.16
0.98
0.94
1.04
0.97
2.17
2.99
2.84
1.22
1.10
10
8
6
4
2
0
PPM


209.532
168.633
136.573
129.393
128.657
128.185
127.449
126.403
124.072
123.560
120.718
107.883
88.495
88.201
87.906
87.620
77.318
77.201
77.000
76.682
50.075
36.667
34.212
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24.793
F3C
Cl
O
OH
NH
O
O
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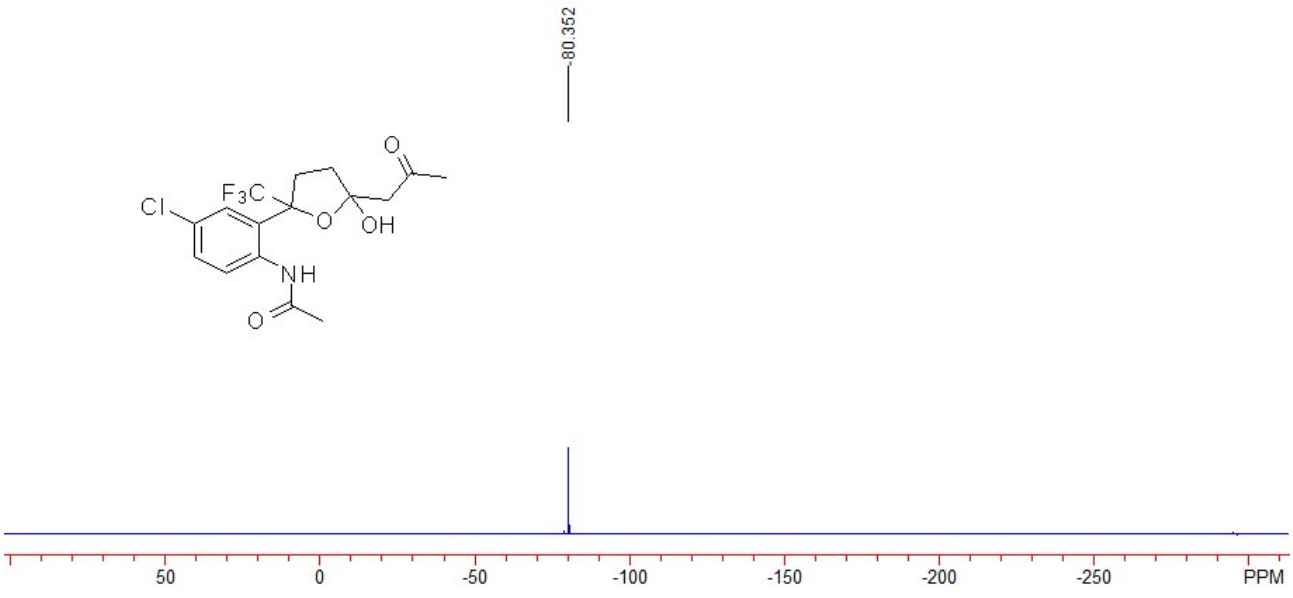
100
50
0
PPM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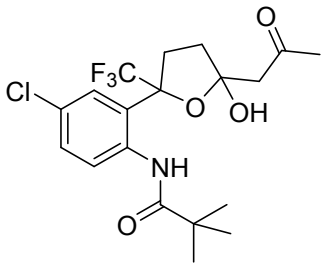
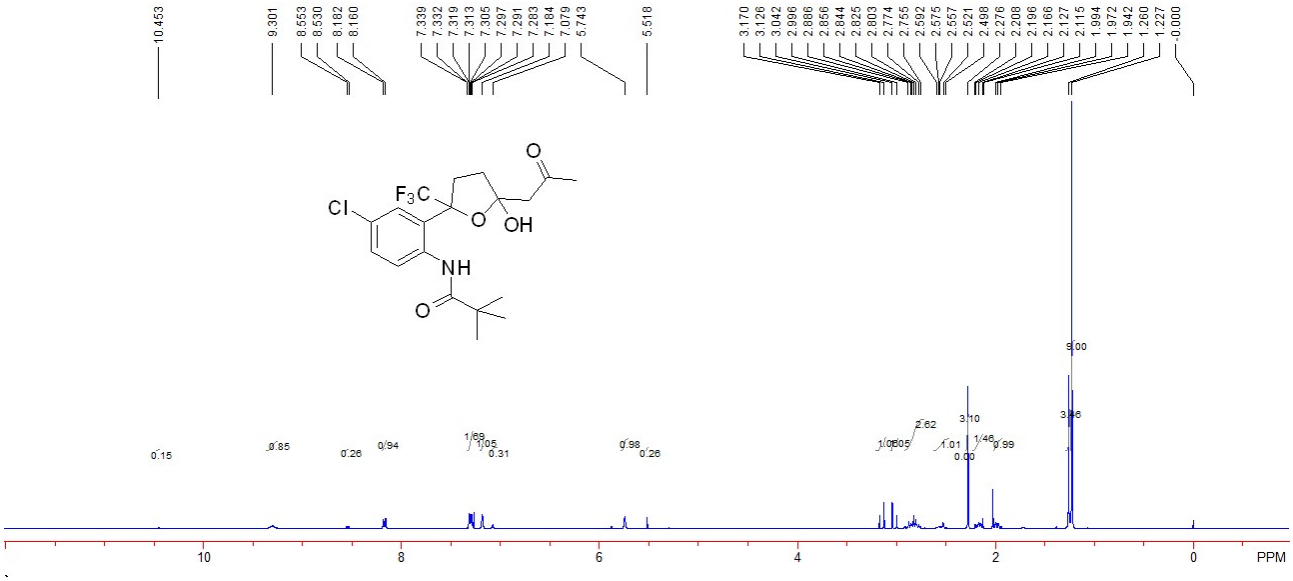
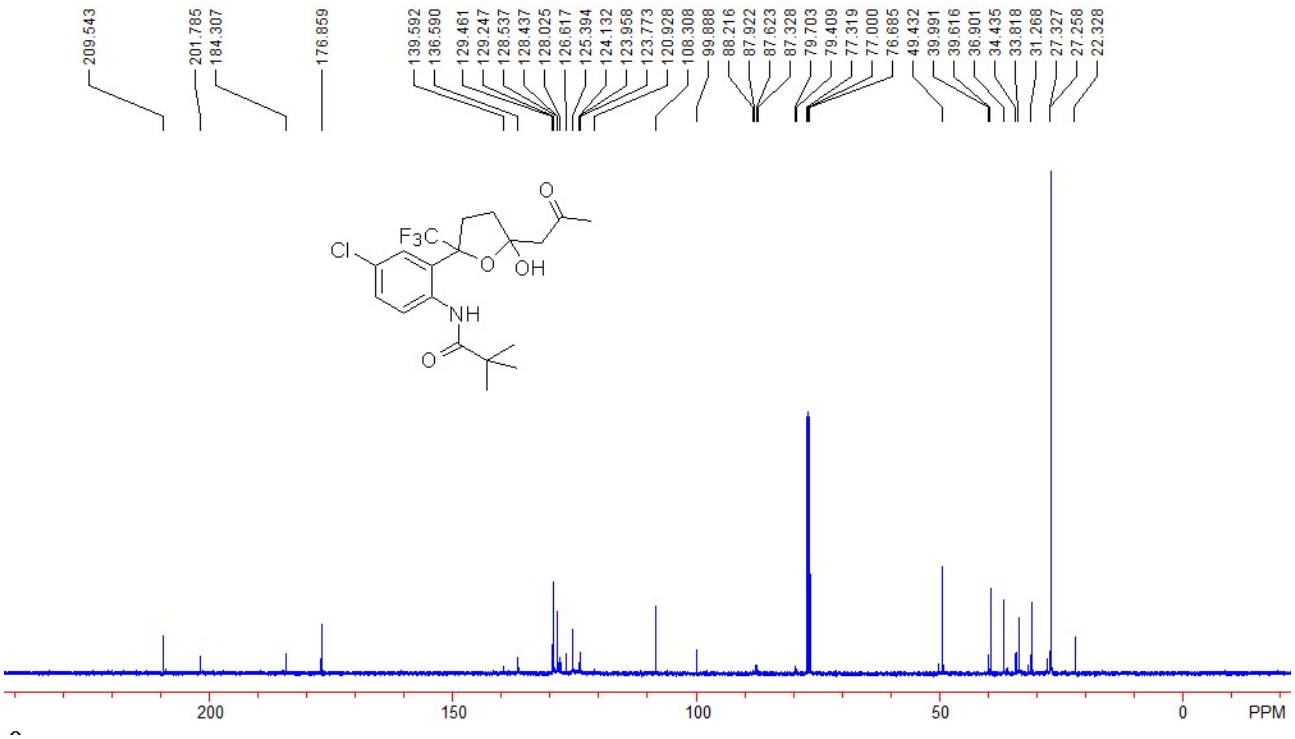
OH
NH
O
O
50
0
-50
-100
-150
-200
-250
PPM



N-(4-chloro-2-(5-hydroxy-5-(2-oxopropyl)-2-(trifluoromethyl)tetrahydrofuran-2-yl)phenyl)pivalamide (3d')

These products are a pair of diastereoisomers (dr = 4:1). A white oil, 79% yield (33 mg). ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) δ 1.23 (s, 9H, CH_3), 1.26 (s, 3.5H, CH_3), 1.94~2.00 (m, 1H, CH_2), 2.11~2.21 (m, 1.5H, CH_2), 2.28 (s, 3.0H, CH_3), 2.49~2.59 (m, 1H, CH_2), 2.75~2.89 (m, 2.6H, CH_2), 3.02 (d, *J* = 18.4 Hz, 1H, CH_2), 3.15 (d, *J* = 18.4 Hz, 1H, CH_2), 5.52 (s, 0.26H, OH), 5.74 (s, 1H, OH), 7.08 (s, 0.31H, ArH), 7.18 (s, 1H, ArH), 7.28~7.34 (m, 1.5H, ArH), 8.17 (d, *J* = 8.8 Hz, 1H, CH_2), 8.54 (d, *J* = 9.2 Hz, 0.26H, CH_2), 9.30 (s, 1H, NH), 10.45 (s, 0.15H, NH). ^{13}C NMR ($CDCl_3$, TMS, 100 MHz) δ 22.3, 27.26, 27.33, 31.3, 33.8, 34.44, 36.9, 39.6, 40.0, 49.4, 79.6 (q, *J* = 29.4 Hz), 87.8 (q, *J* = 29.9 Hz), 99.9, 108.3, 123.9, 124.1, 125.2 (q, *J* = 284.4 Hz), 125.4, 128.0, 128.4, 128.5, 129.2, 129.5, 136.6, 139.6, 176.9, 184.3, 201.8, 209.5. ^{19}F NMR (376 MHz, $CDCl_3$, $CFCl_3$) δ -79.39, -80.48. IR (CH_2Cl_2) ν 3375, 2968, 2358, 2341, 1516, 1398, 1297, 1167, 1024 cm^{-1}. HRMS (ESI) Calcd. For $C_{19}H_{24}ClF_3NO_4^{+1}$(M+H)$^+$ requires 422.1340, Found: 422.1342.

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124.132
123.958
123.773
120.928
108.308
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87.922
87.623
87.328
79.703
79.409
77.319
77.000
76.685
49.432
39.991
39.616
36.901
34.435
33.818
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27.258
22.328
Cl
F3C
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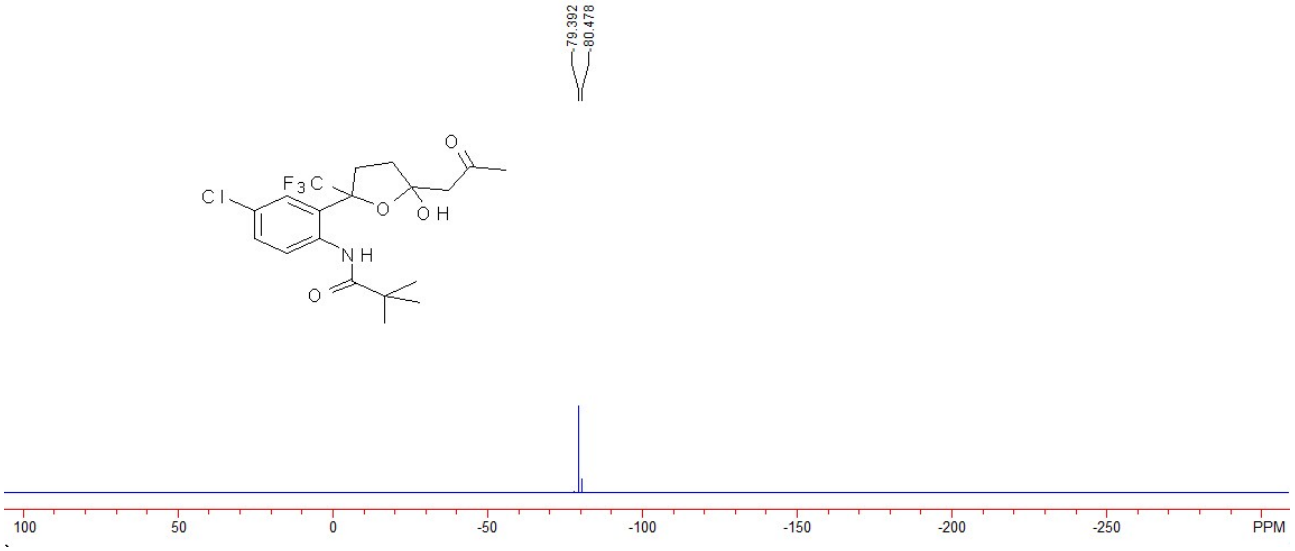
OH
NH
O
200
150
100
50
0
PPM


79.392
80.478
Cl
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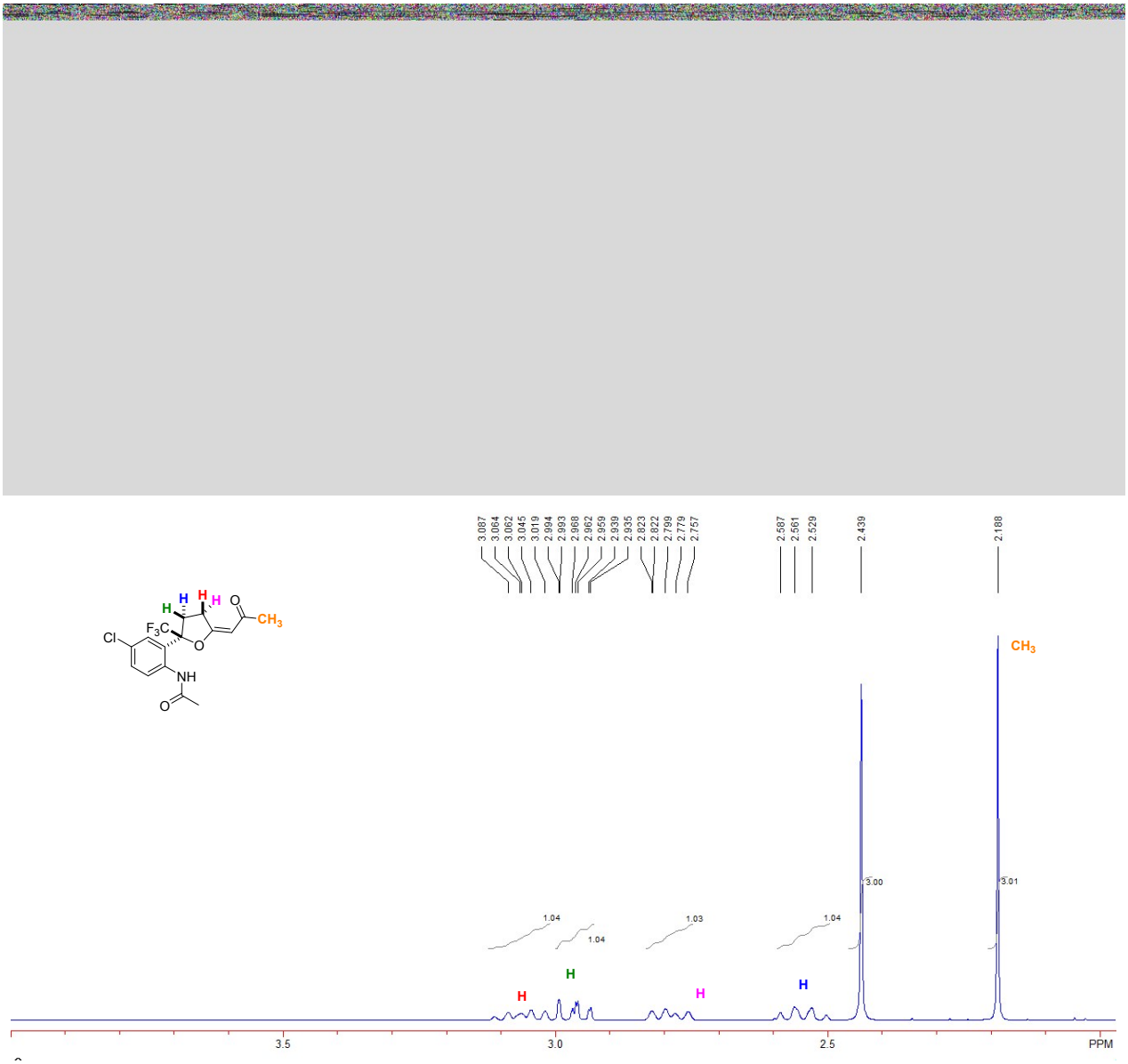
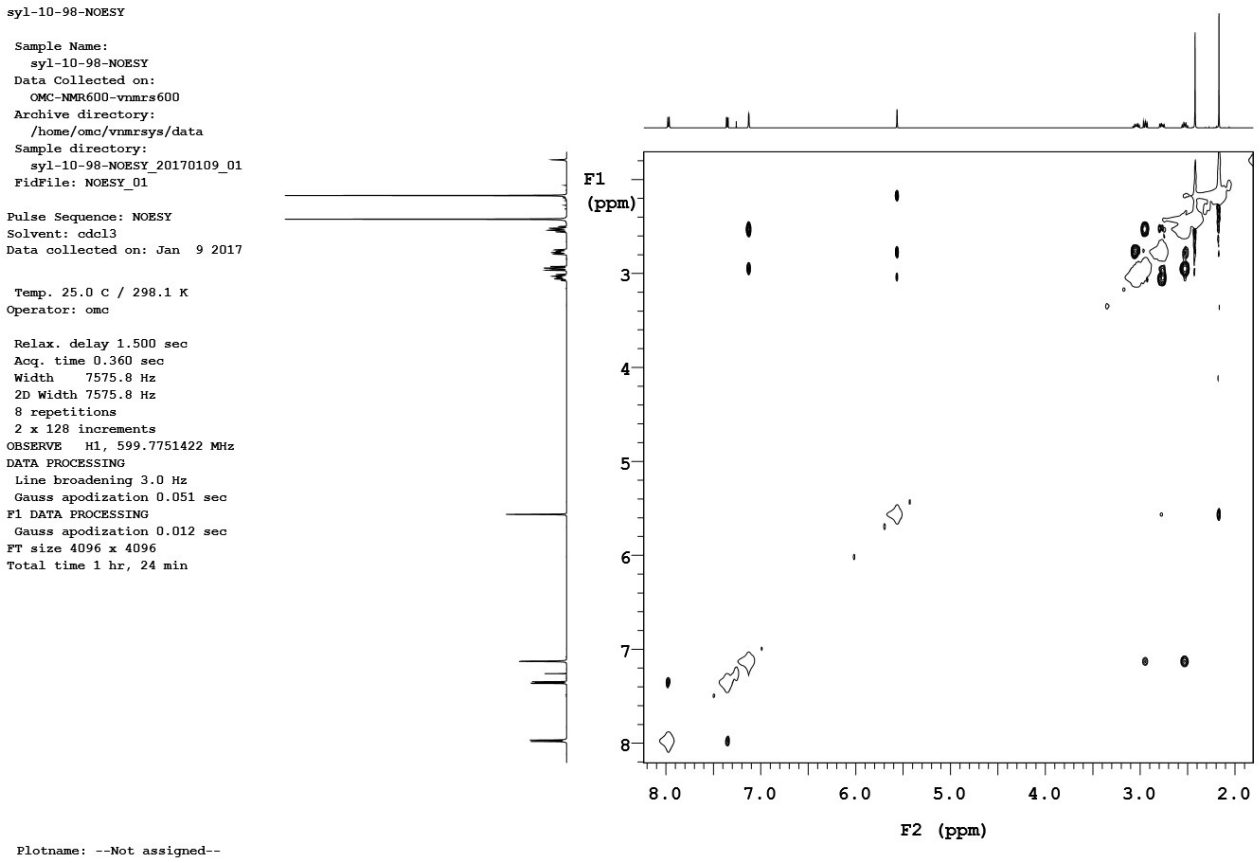
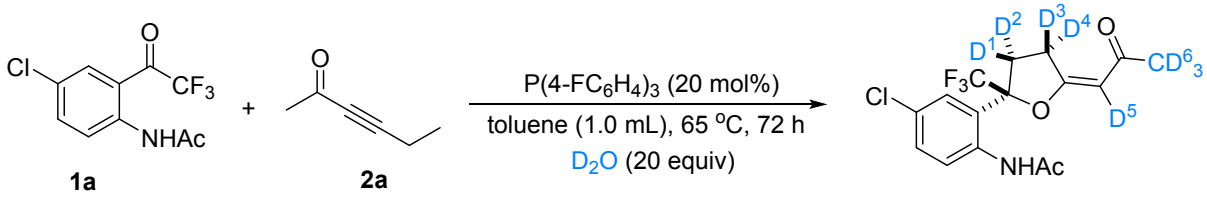
O
OH
NH
O
100
50
0
-50
-100
-150
-200
-250
PPM

Deuterium Labeling Experiment

First, NOESY was used to assign the H peaks in ^{1}H NMR spectrum.

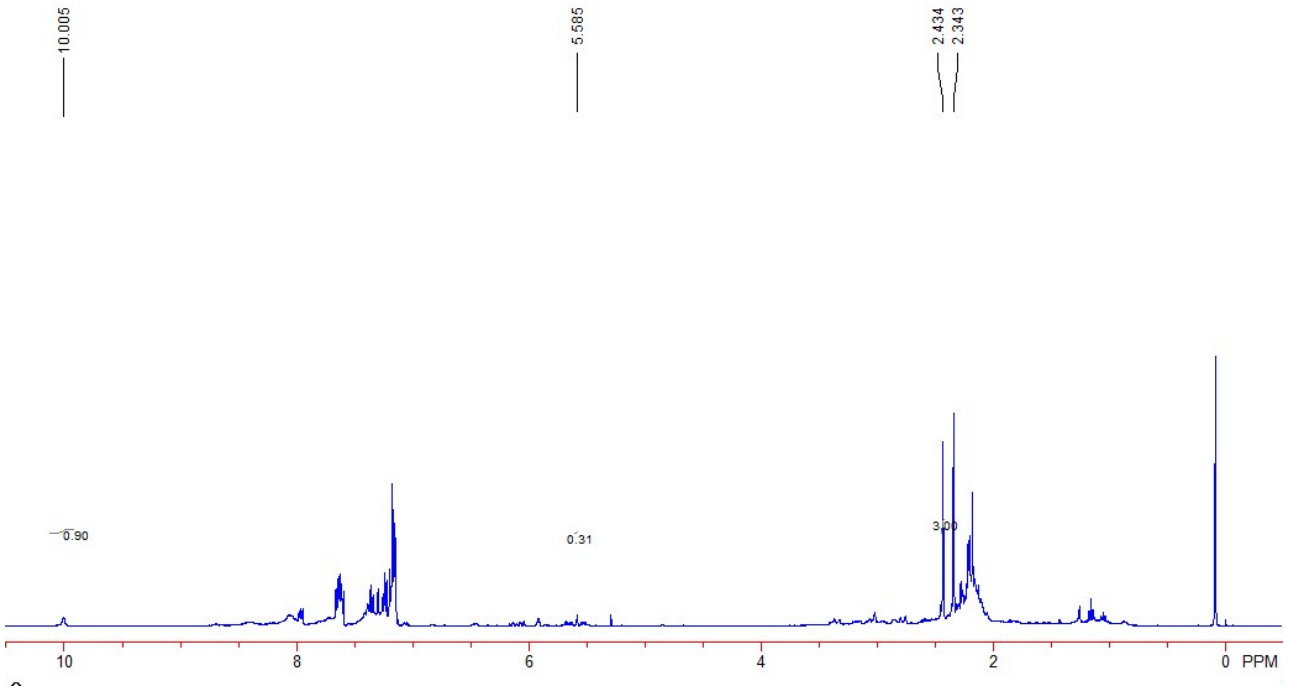


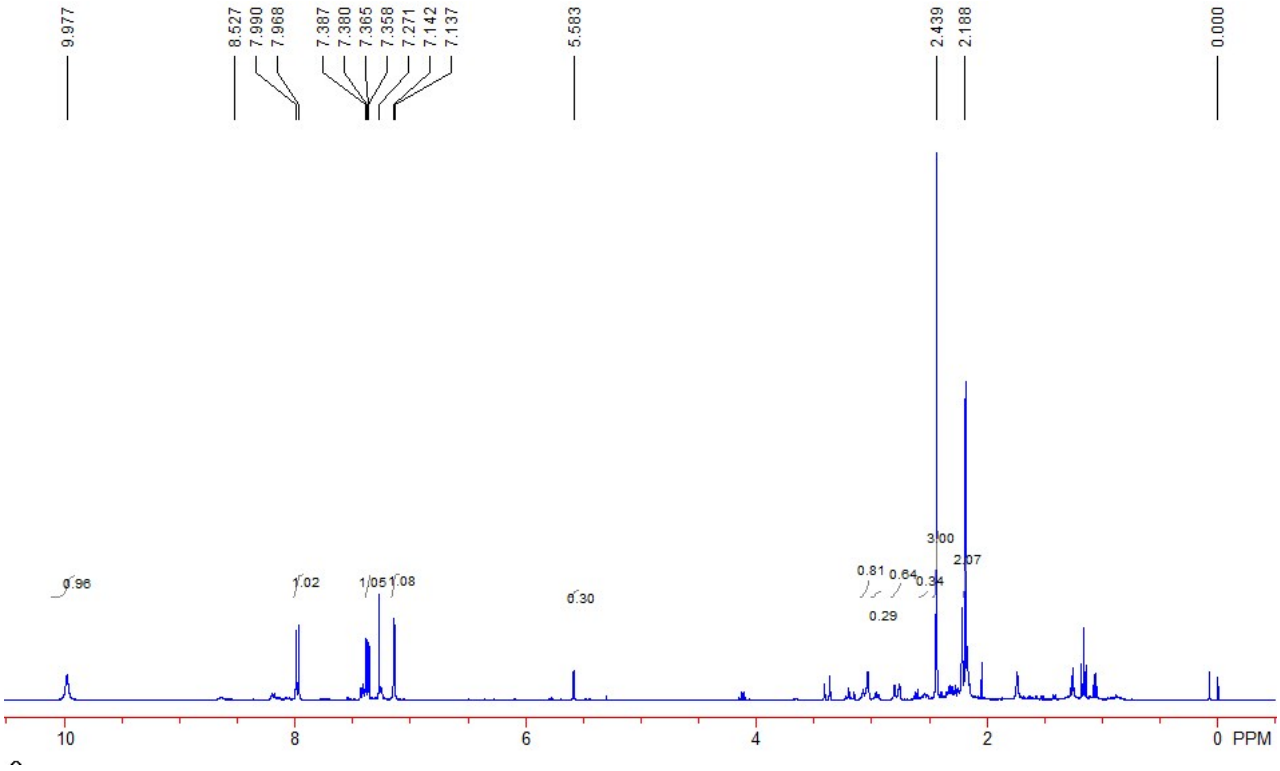


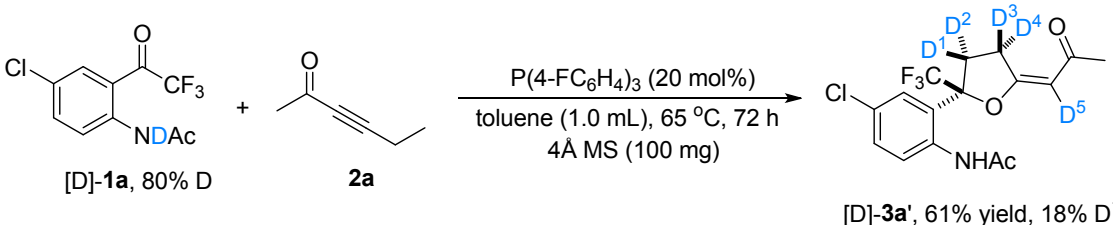


[D]-**3a**, 58% yield
71% D^1, 66% D^2, 19% D^3, 26% D^4
70% D^5, 33% D^6

Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the corresponding hex-3-yn-2-one **2a** (0.6 mmol) and D_2O (80 μL) at room temperature. Then the resulting mixture was heated to 65 °C and continued stirring at 65 °C until the reaction completed (monitoring by TLC). The crude ^1H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that the product was barely deuterated. Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**3a**.





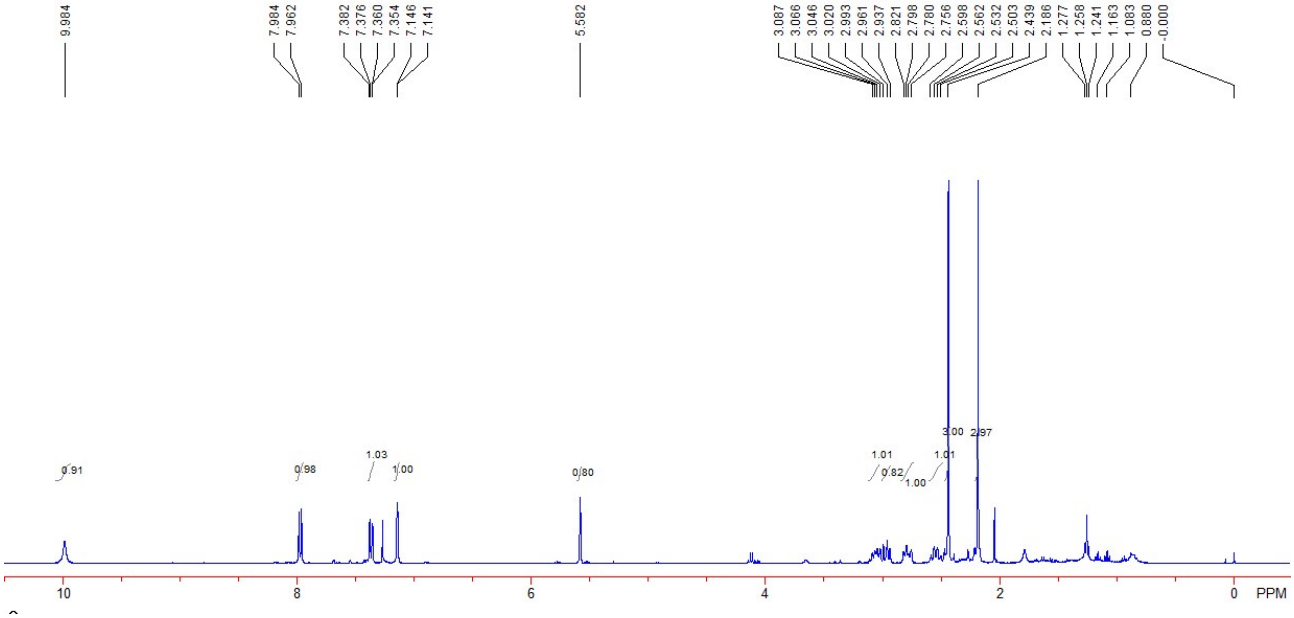


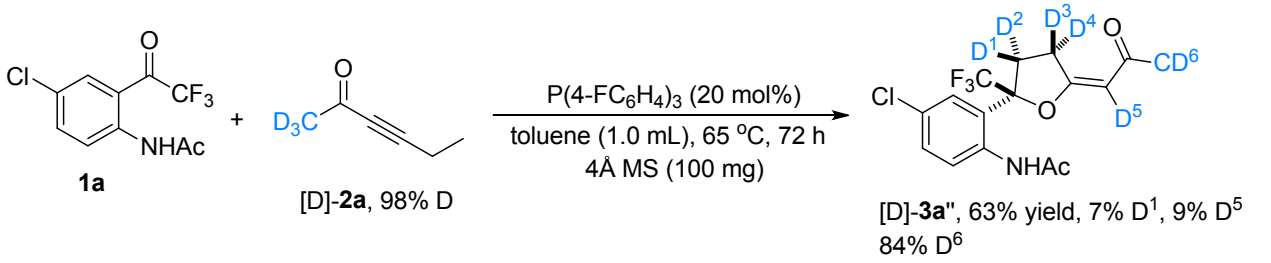
[D]-**1a**, 80% D

2a

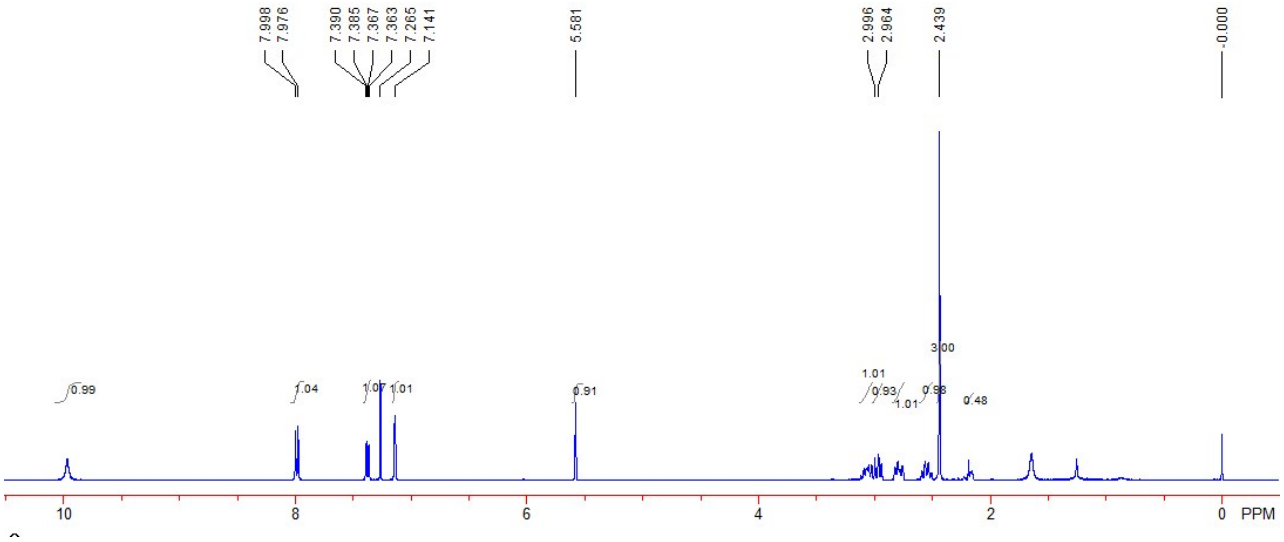
[D]-**3a'**, 61% yield, 18% D^1, 20% D^5

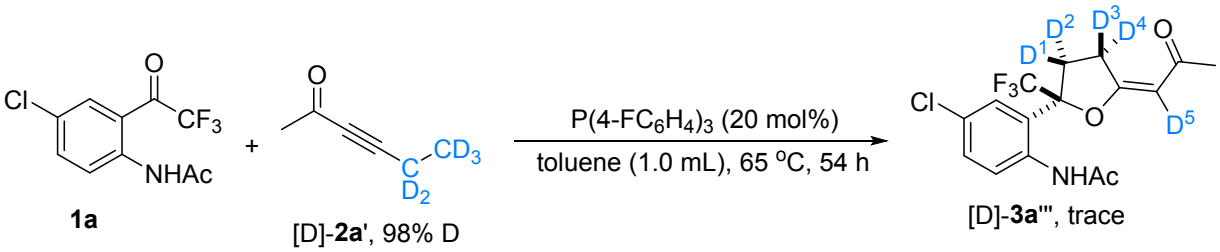
Under argon atmosphere, to a solution of trifluoroacetyl compound [D]-**1a** (0.2 mmol) and P(4-$FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the corresponding hex-3-yn-2-one **2a** (0.6 mmol) at room temperature. Then, 4Å molecular sieve (100 mg) was used to remove the trace water in the solvent. Next, the resulting mixture was heated to 65 °C and continued stirring at 65 °C until the reaction completed (monitoring by TLC). Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**3a'**.



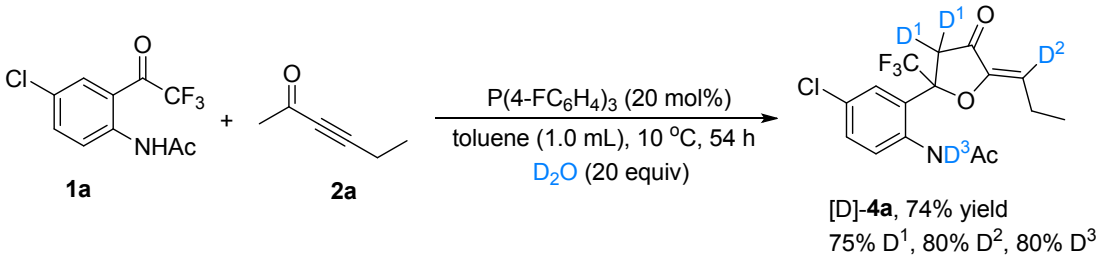


Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and P(4-$FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added the deuterated hex-3-yn-2-one [D]-**2a** (0.6 mmol) at room temperature. 4Å molecular sieve (100 mg) was used to remove the trace water in solvent. Then, the resulting mixture was heated to 65 °C and continued stirring at 65 °C until the reaction completed (monitoring by TLC). Then, the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**3a"**.



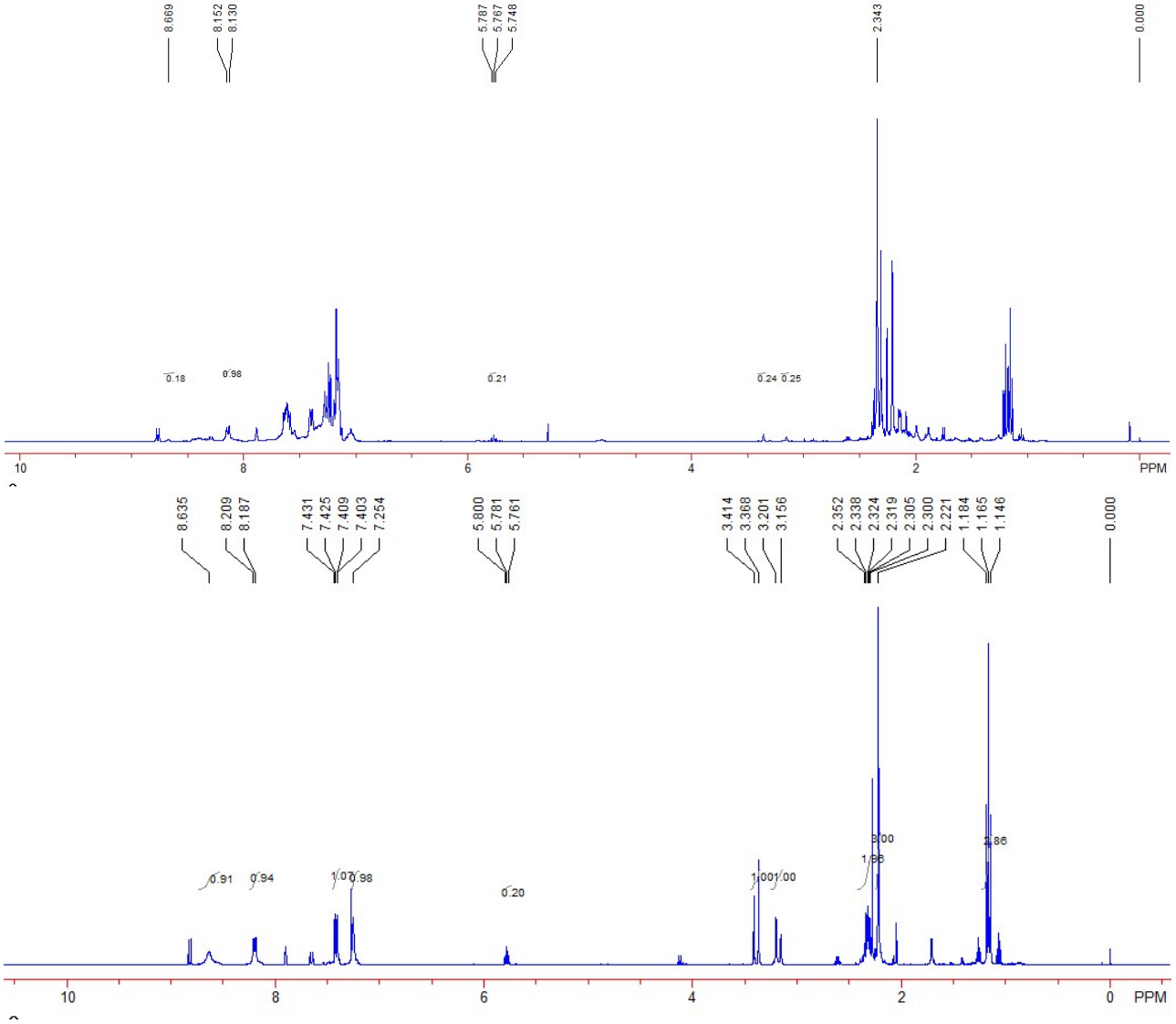


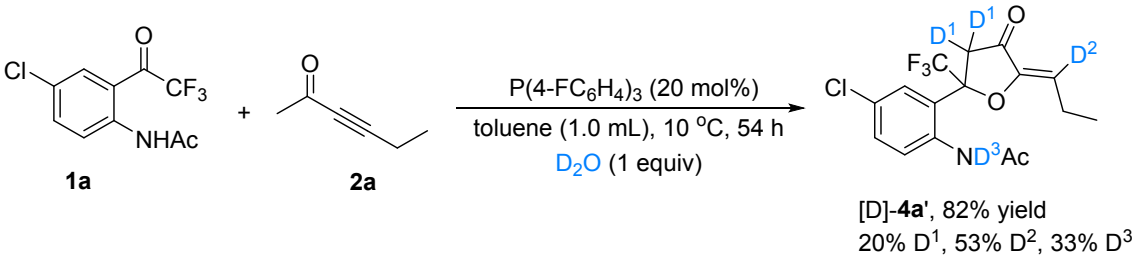
Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one [D]-**2a'** (0.6 mmol) at room temperature. Then, 4Å molecular sieve (100 mg) was used to remove the trace water in solvent. The resulting mixture was heated to 65 °C and continued stirring at 65 °C until the reaction completed (monitoring by TLC).



Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one **2a** (0.6 mmol) and D_2O (80 μL) at room temperature. Then, the resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^1H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that the NHAc group of the product was deuterated largely. The solvent was

removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**4a**.

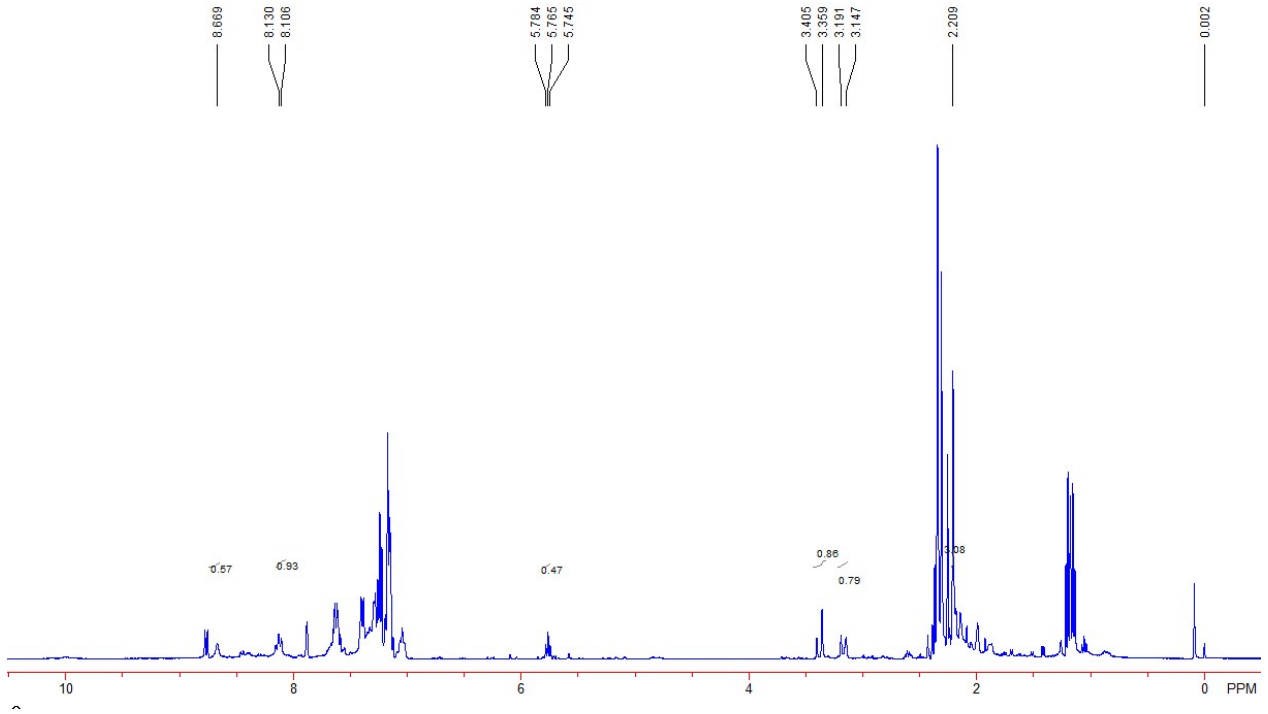


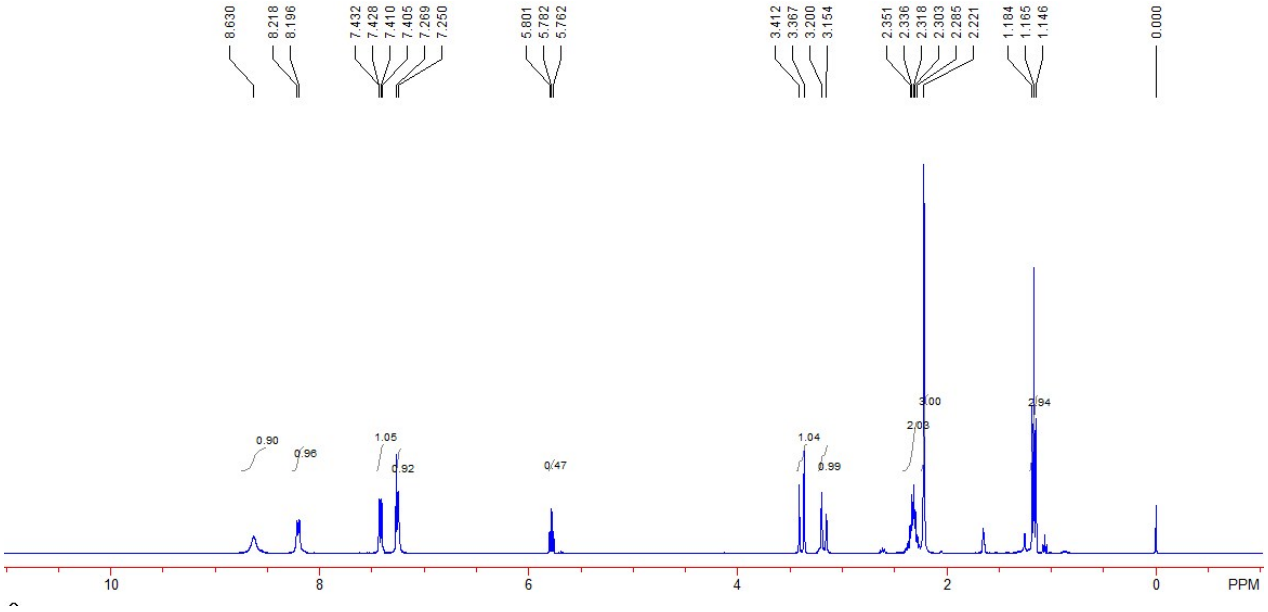


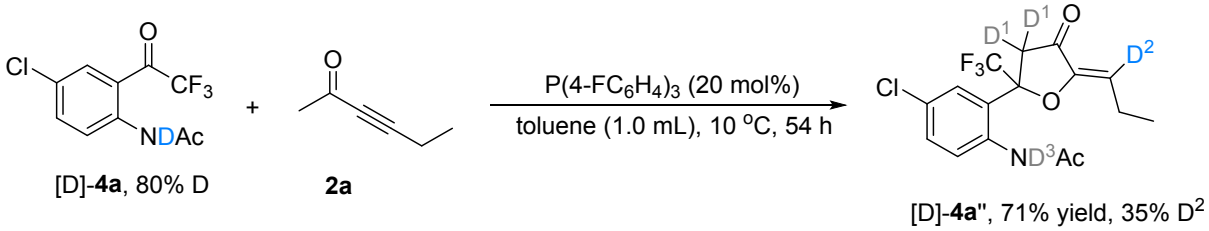
[D]-**4a'**, 82% yield
20% D^1, 53% D^2, 33% D^3

Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and P(4-FC_6H_4)$_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one **2a** (0.6 mmol) and D_2O (4 μL) at room temperature. Then, the resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^{1}H NMR ($CDCl_3$, TMS, 400 MHz)

spectrogram showed that the NHAc group of the product was partially deuterated. Then the solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**4a'**.

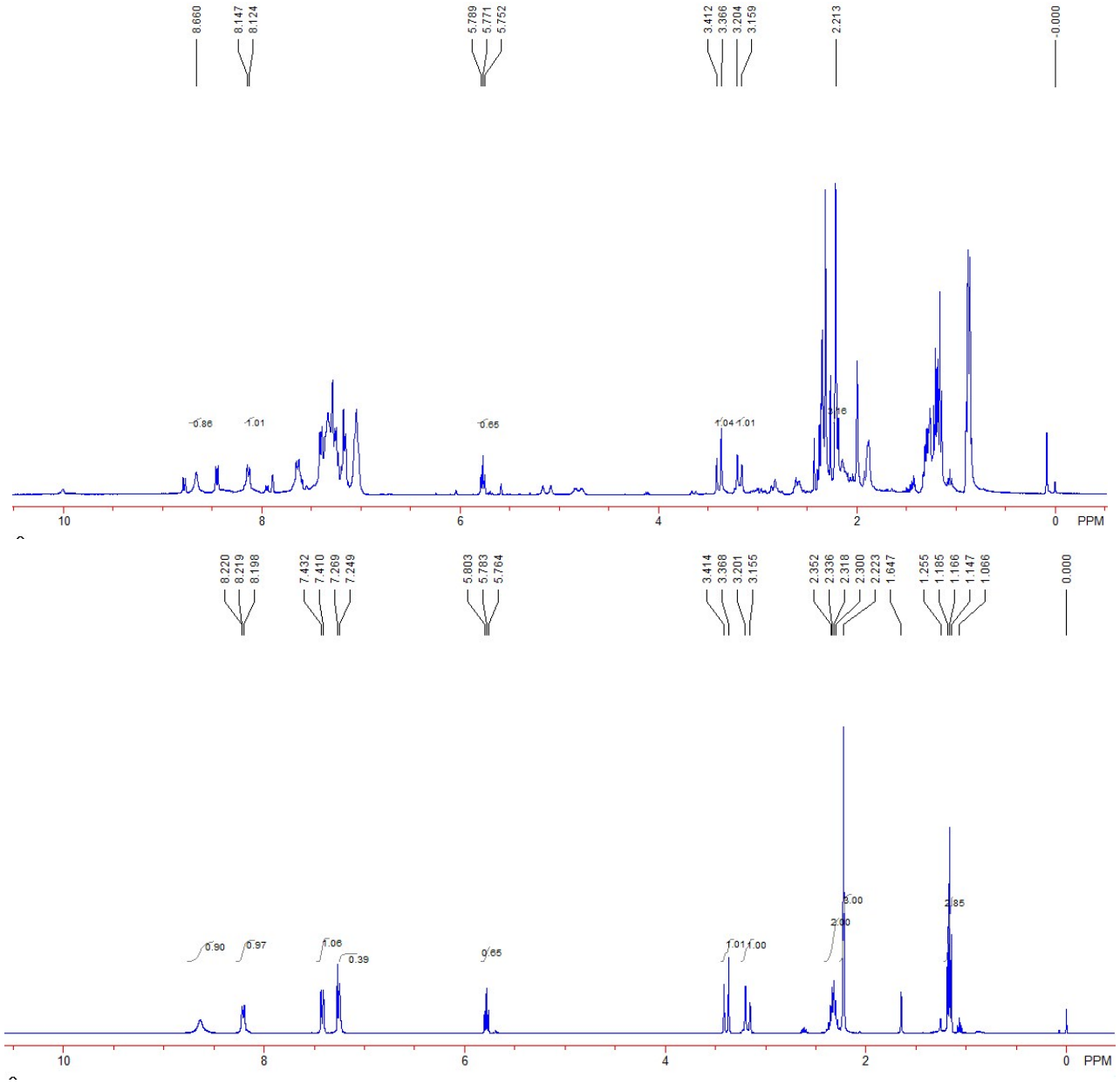


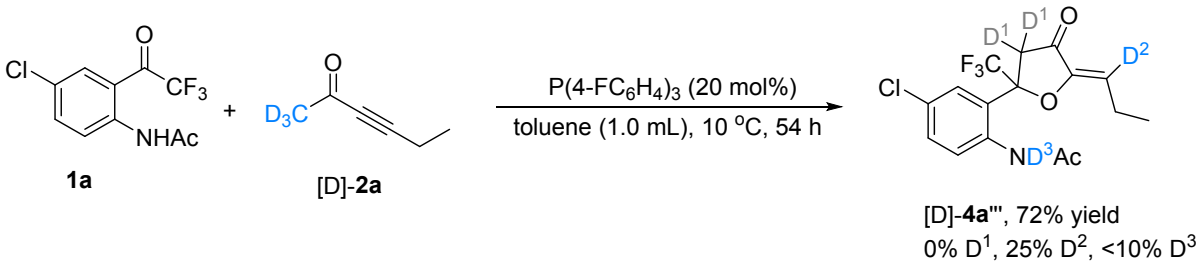




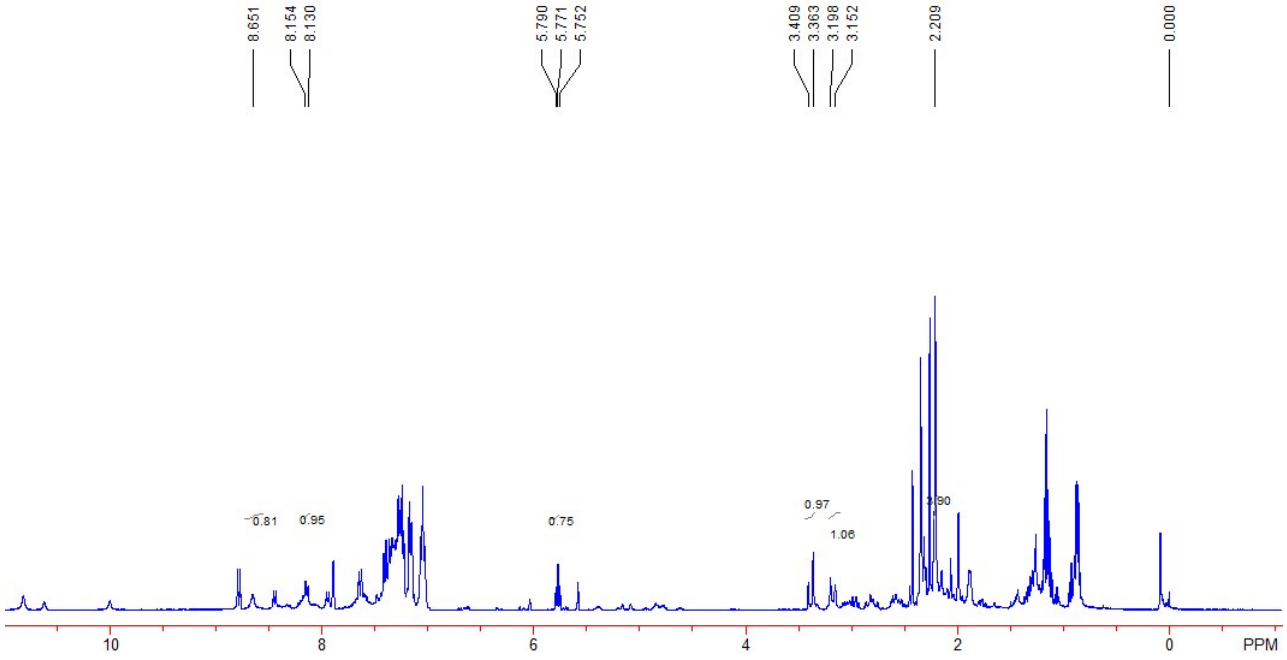
[D]-**4a**, 80% D **2a** [D]-**4a''**, 71% yield, 35% D^2

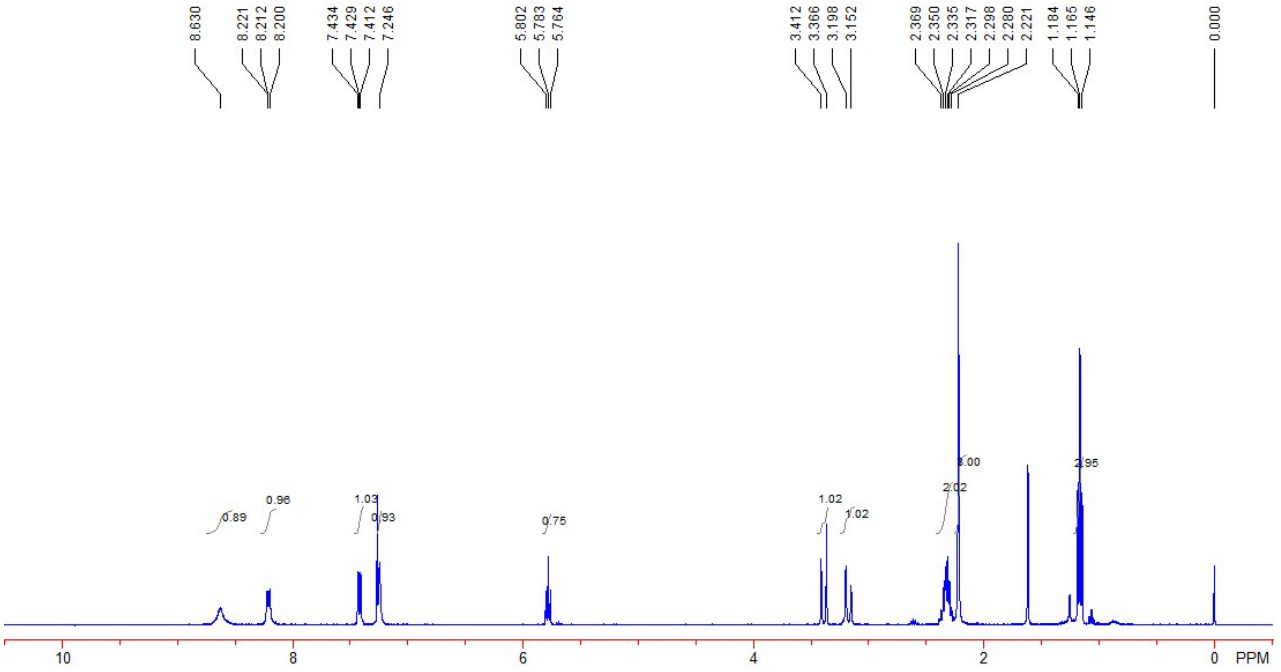
Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one **2a** (0.6 mmol) and D_2O (80 μL) at room temperature. Then, the resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^1H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that the NHAc group of the product was not deuterated. The solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**4a"**.

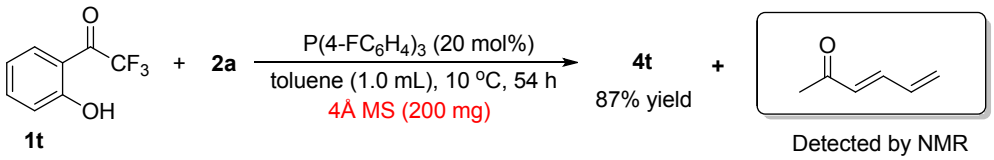




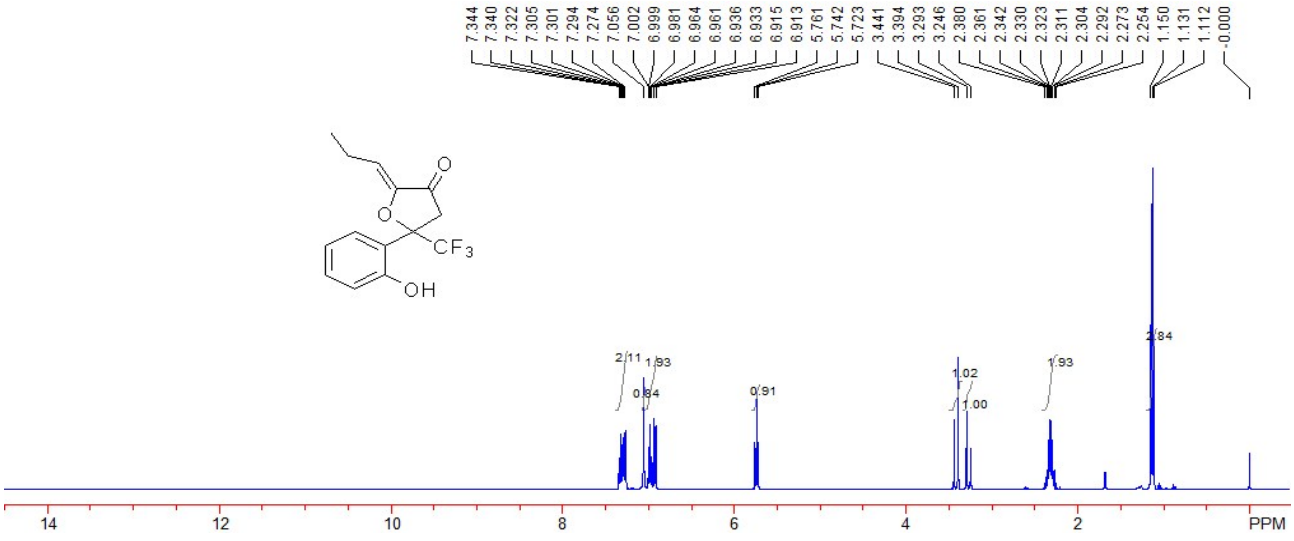
Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one **2a** (0.6 mmol) and D_2O (80 μL) at room temperature. Then, the resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^1H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that the NHAc group of the product was deuterated in < 10% D content. The solvent was removed under reduced pressure and the residue was directly subjected to a flash column chromatography on silica gel to afford the product [D]-**4a'''**.

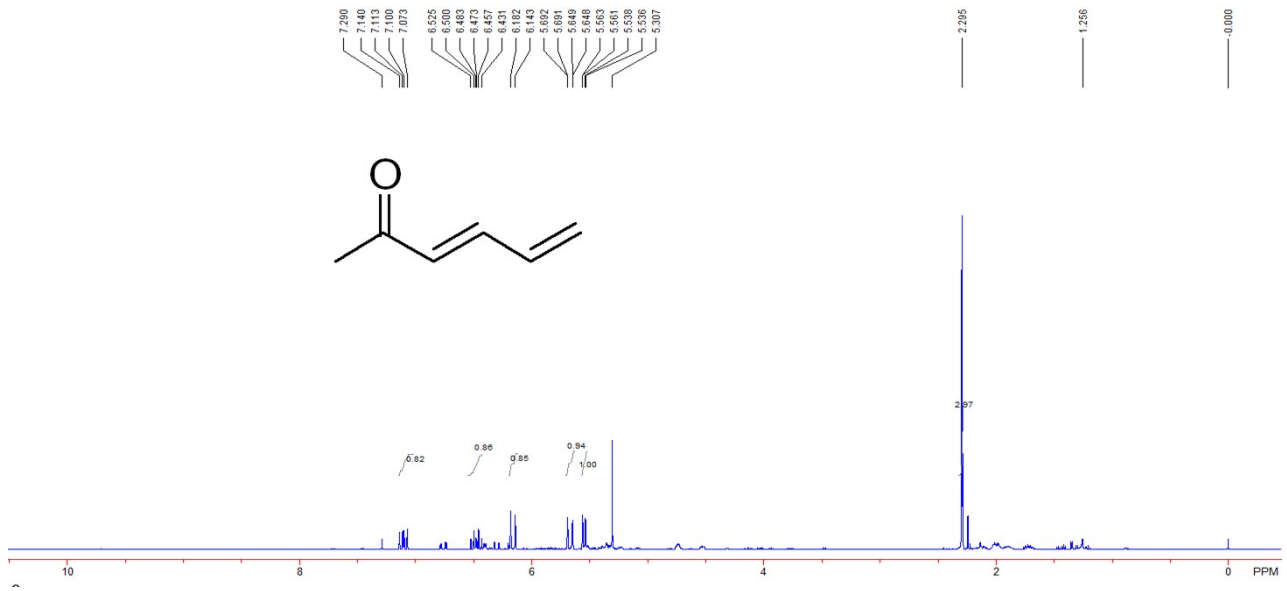




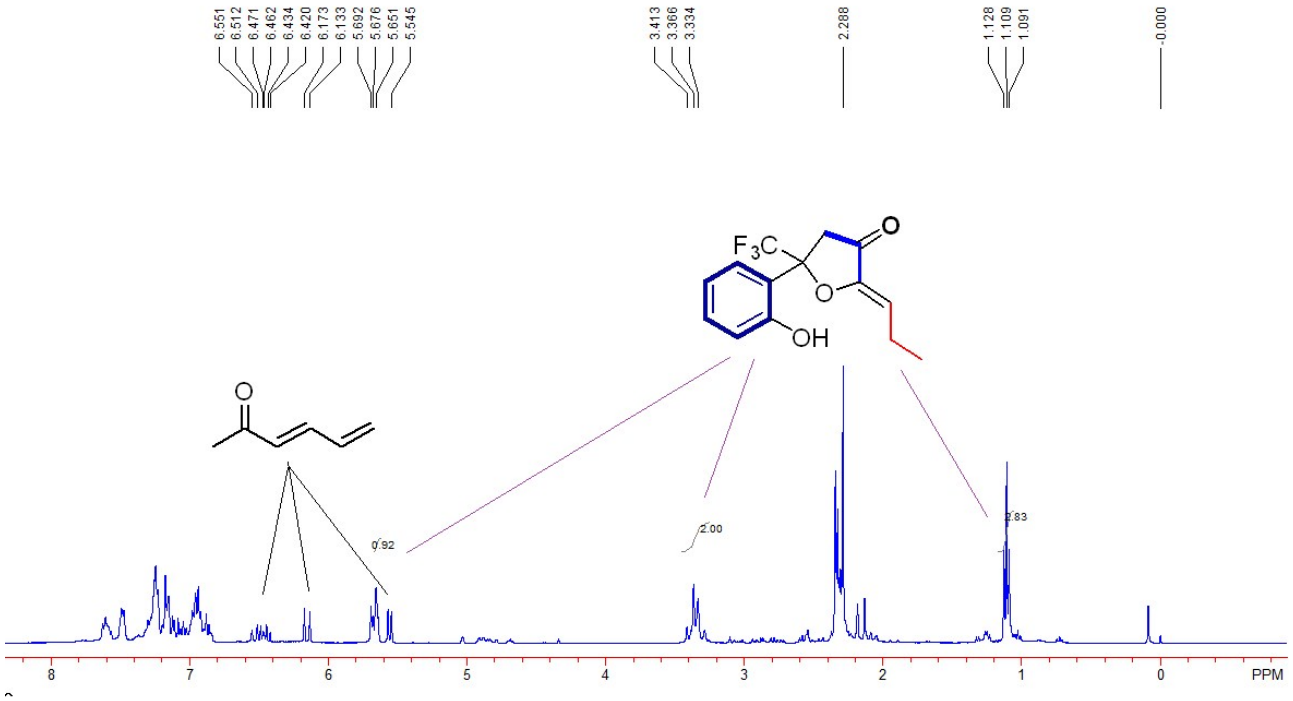


Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one **2a** (0.4 mmol) at room temperature. Then, 4Å molecular sieve (200 mg) was used to remove the trace water in solvent. The resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^1H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that **4t** and (E)-hexa-3,5-dien-2-one were generated in the absence of water.

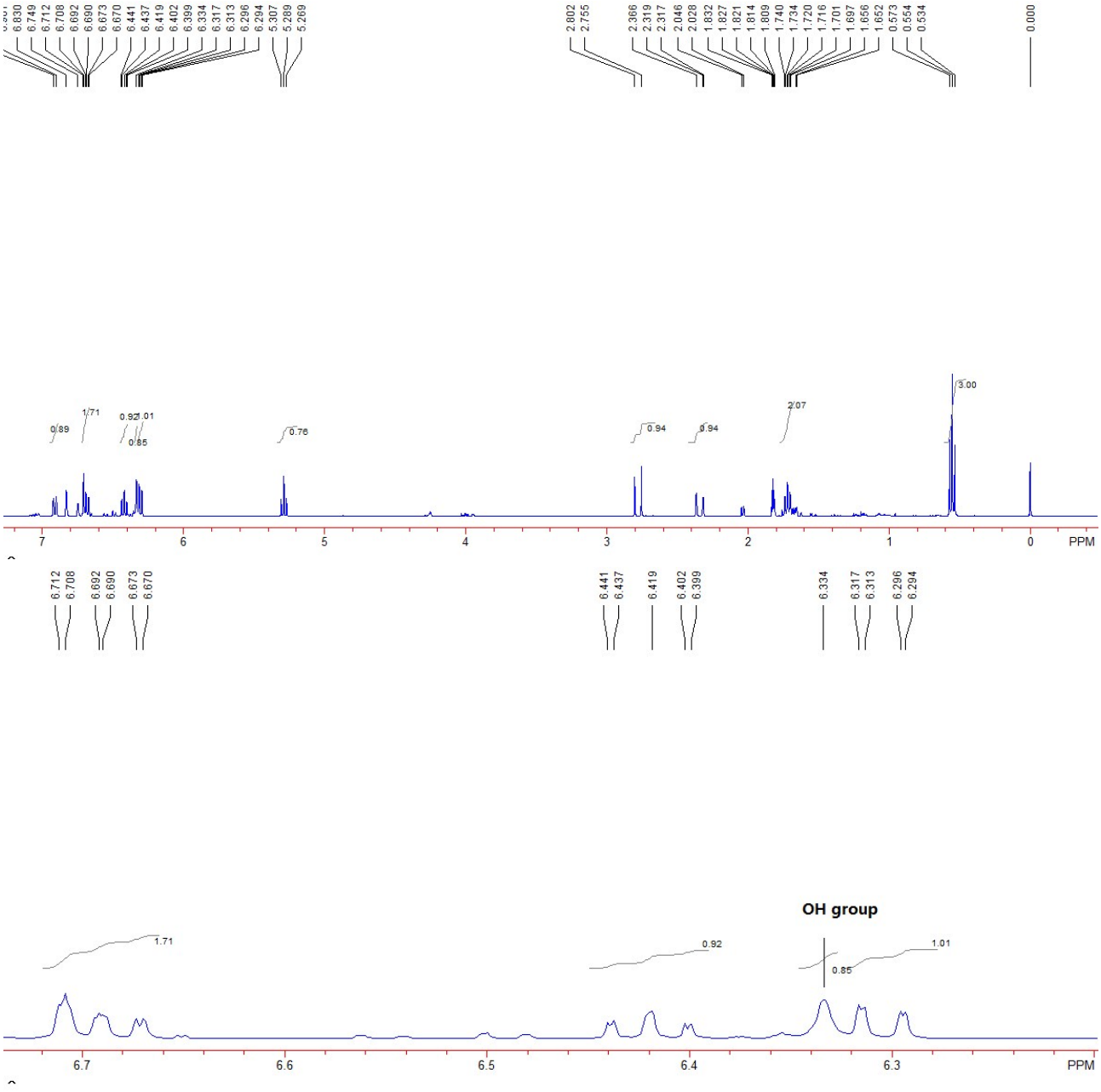


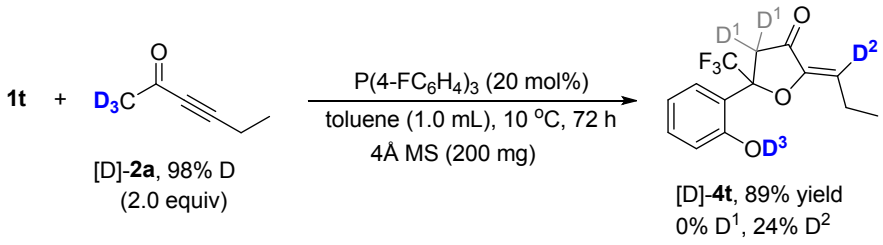


Crude reaction mixture in $CDCl_3$:



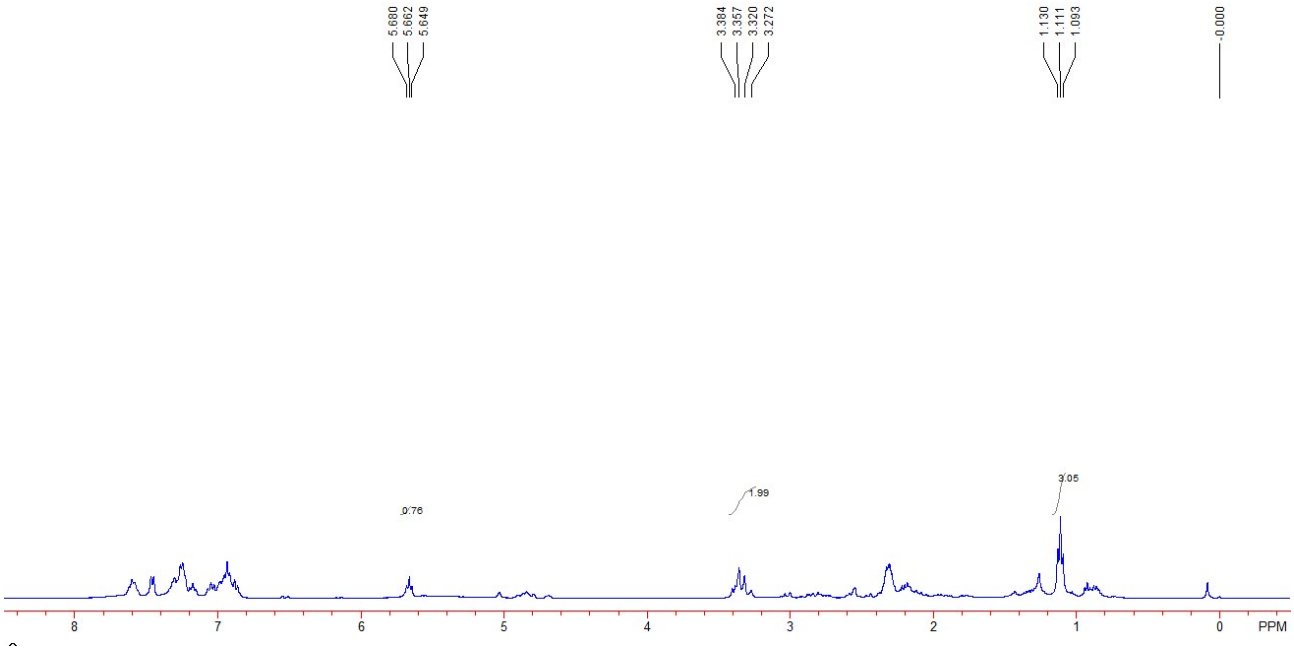
Product **4t** in d_8-toluene:

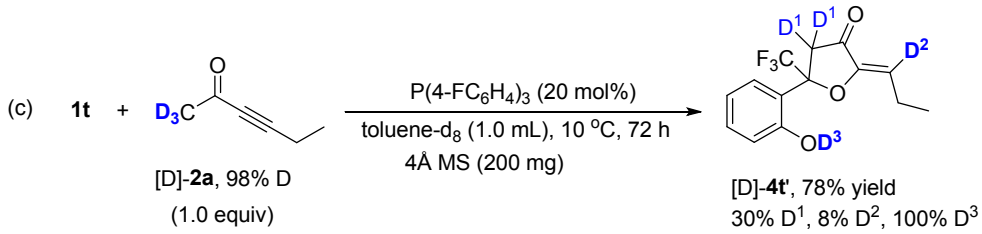




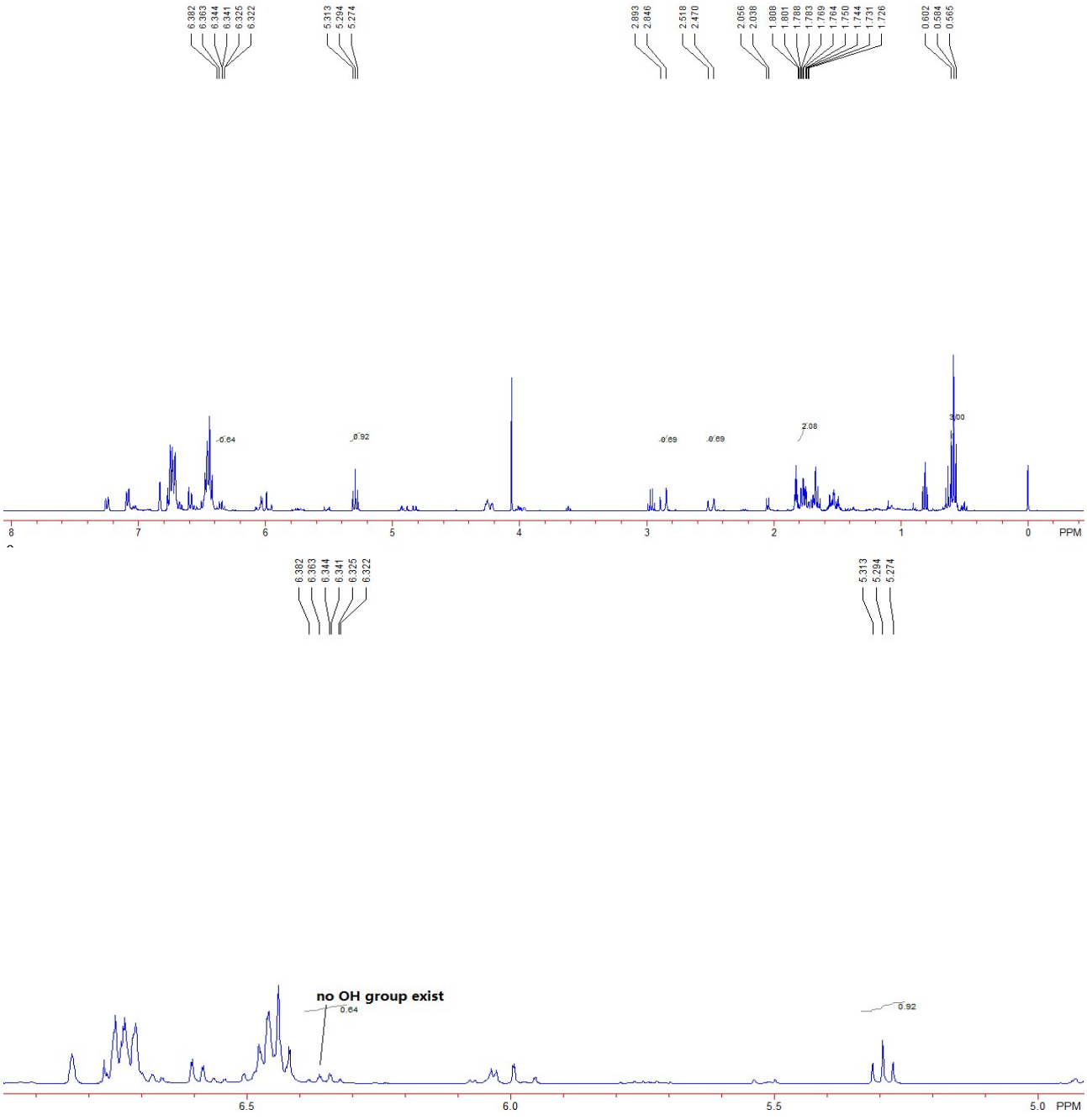
Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and P(4-FC_6H_4)$_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one [D]-**2a** (0.4 mmol) at room temperature. Then, 4Å molecular sieve (200 mg) was used to remove the trace water in solvent. Then the resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction

completed (monitoring by TLC). The crude ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that the deuterium incorporated at D^1 was totally lost.

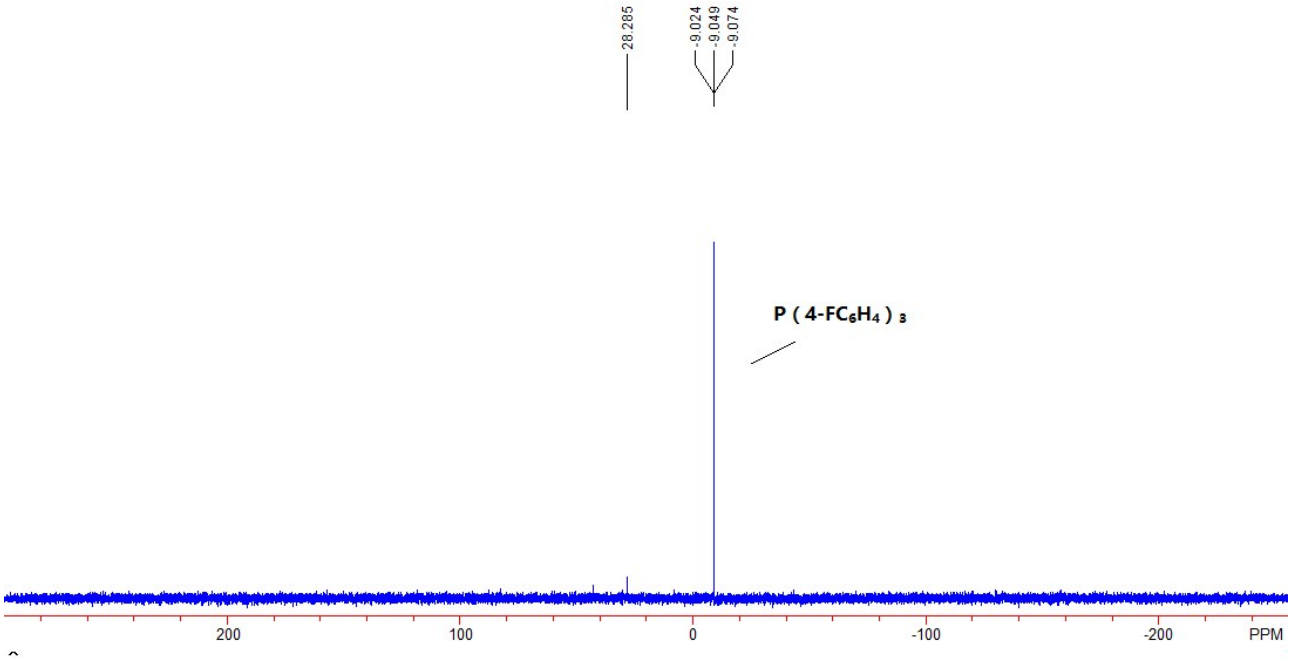


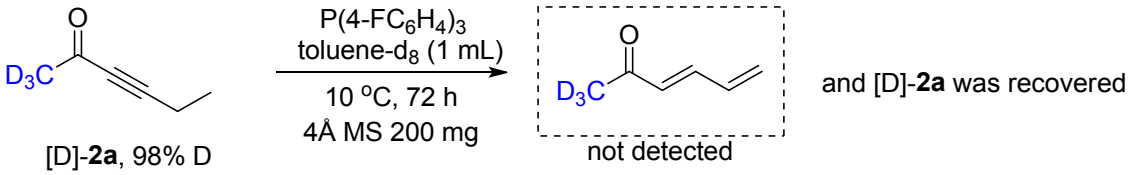


Under argon atmosphere, to a solution of trifluoroacetyl compound **1a** (0.2 mmol) and $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in d_8-toluene (1.0 mL) was added hex-3-yn-2-one [D]-**2a** (0.2 mmol) at room temperature. Then, 4Å molecular sieve (200 mg) was added to remove the trace water in solvent. Then the resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^{1}H NMR (d_8-toluene, TMS, 400 MHz) spectrogram showed that the deuterium incorporated at D^1 was partially lost and phenol group was totally replaced by deuterium.



The crude ^{31}P NMR (d_8-toluene, 85% H_3PO_4, 162 MHz) spectrogram:

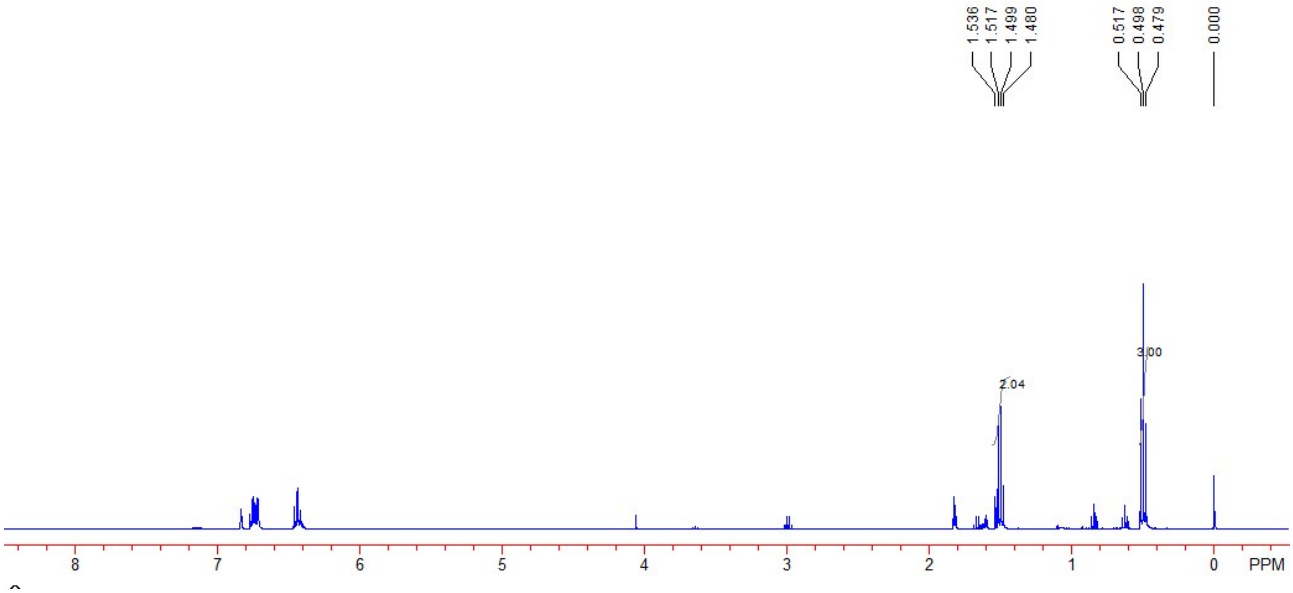




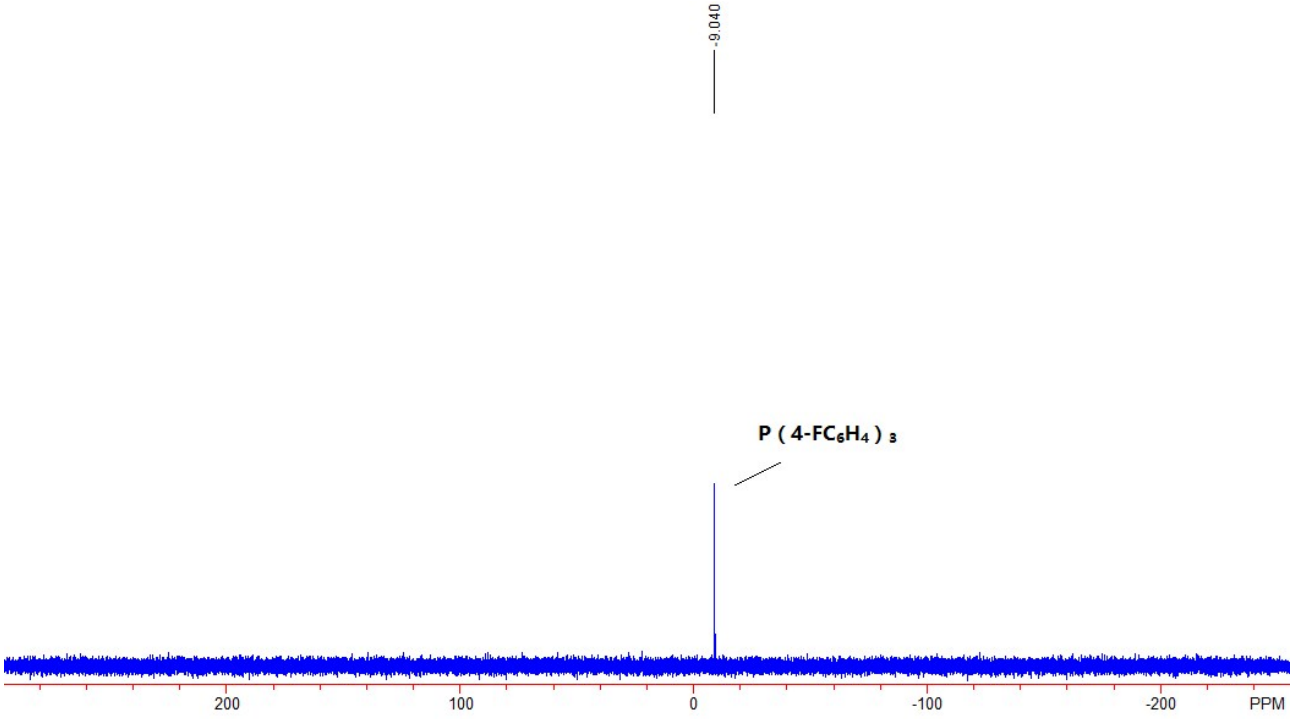
[D]-**2a**, 98% D

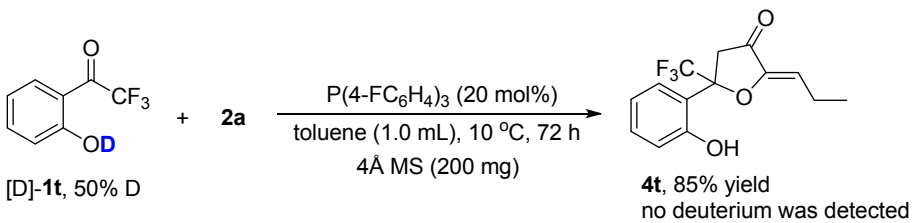
not detected

Under argon atmosphere, to a solution of $P(4\text{-}FC_6H_4)_3$ (13 mg, 0.04 mmol) in d_8-toluene (1.0 mL) was added hex-3-yn-2-one [D]-**2a** (0.2 mmol) at room temperature. Then, 4Å molecular sieve (200 mg) was used to remove the trace water in solvent. The resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^1H NMR (d_8-toluene, TMS, 400 MHz) spectrogram showed that none of (E)-hexa-3,5-dien-2-one was generated without the existence of **1t**. The crude ^{31}P NMR (d_8-toluene, 85% H_3PO_4, 162 MHz) spectrogram indicated that none of phosphonium was generated basically.



The crude ^{31}P NMR (d_8-toluene, 85% H_3PO_4, 162 MHz) spectrogram:

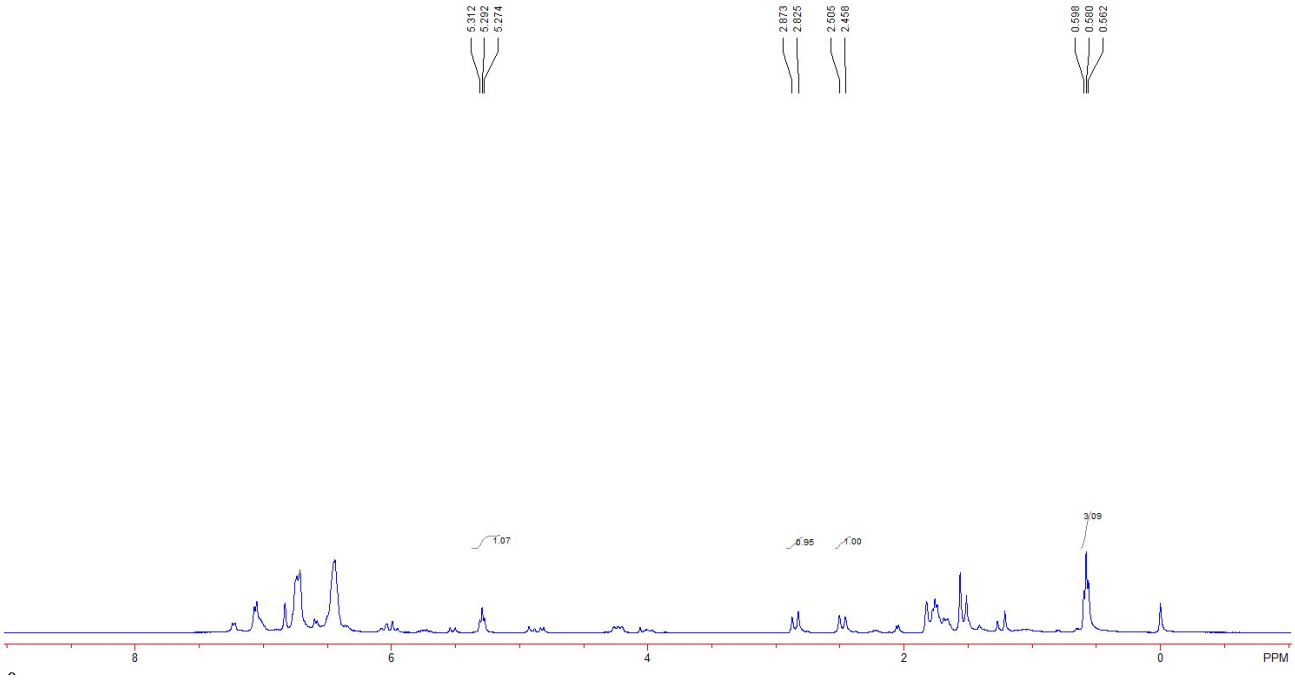




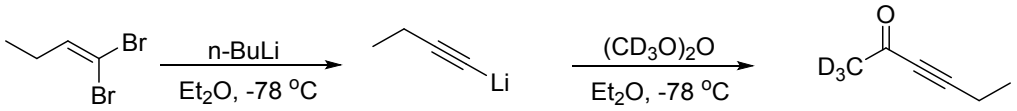
[D]-**1t**, 50% D

4t, 85% yield
no deuterium was detected

Under argon atmosphere, to a solution of trifluoroacetyl compound [D]-**1t** (0.2 mmol) and P(4-$FC_6H_4)_3$ (13 mg, 0.04 mmol) in toluene (1.0 mL) was added hex-3-yn-2-one **2a** (0.4 mmol) at room temperature. Then, 4Å molecular sieve (200 mg) was used to remove the trace water in solvent. The resulting mixture was cooled to 10 °C and continued stirring at 10 °C until the reaction completed (monitoring by TLC). The crude ^{1}H NMR ($CDCl_3$, TMS, 400 MHz) spectrogram showed that **4t** was obtained without any deuterium incorporation.



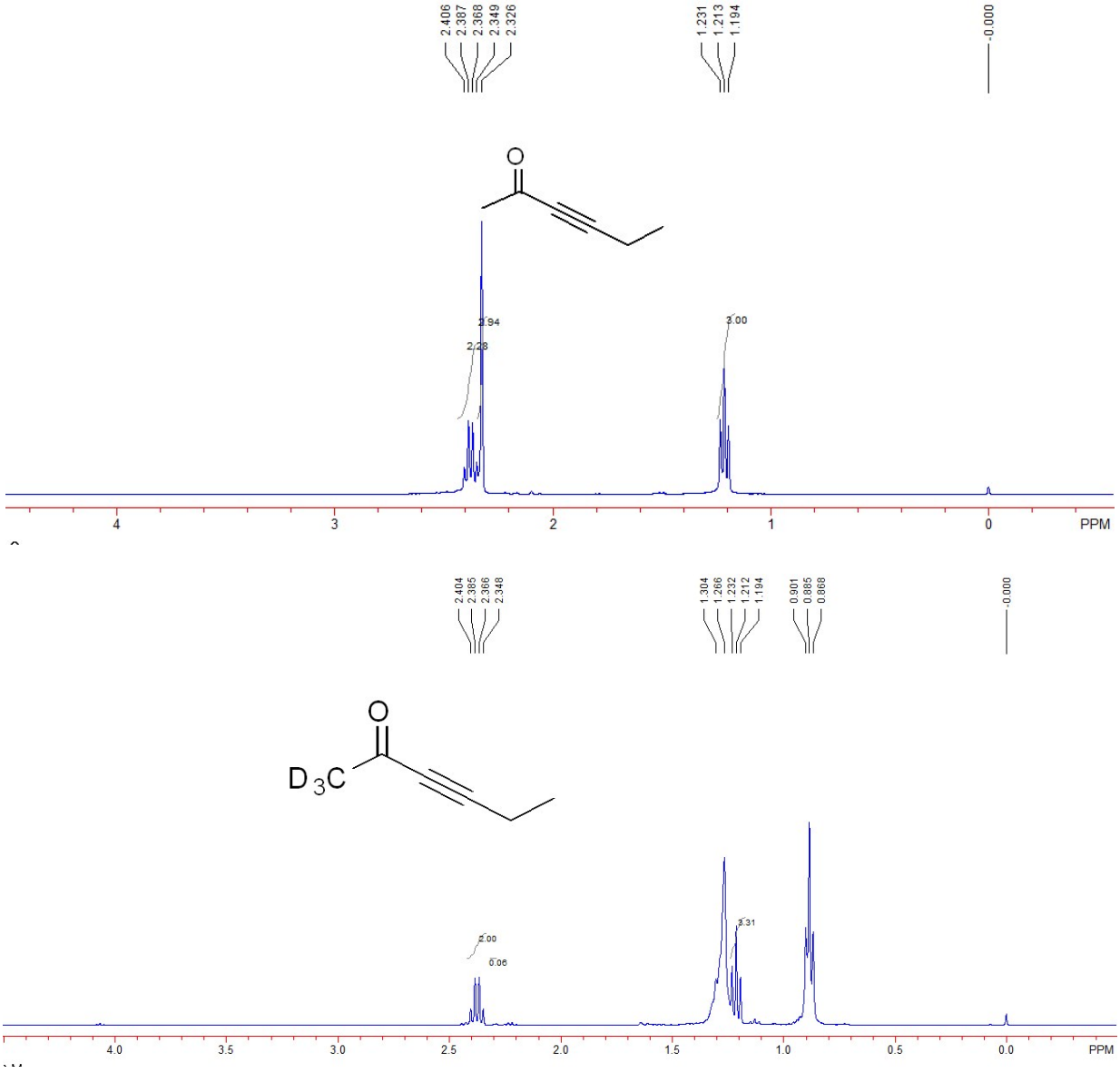
Synthesis of deuterated hex-3-yn-2-one [D]-**2a**



1,1-Dibromobut-1-ene is a known compound and prepared according to the previous literature.

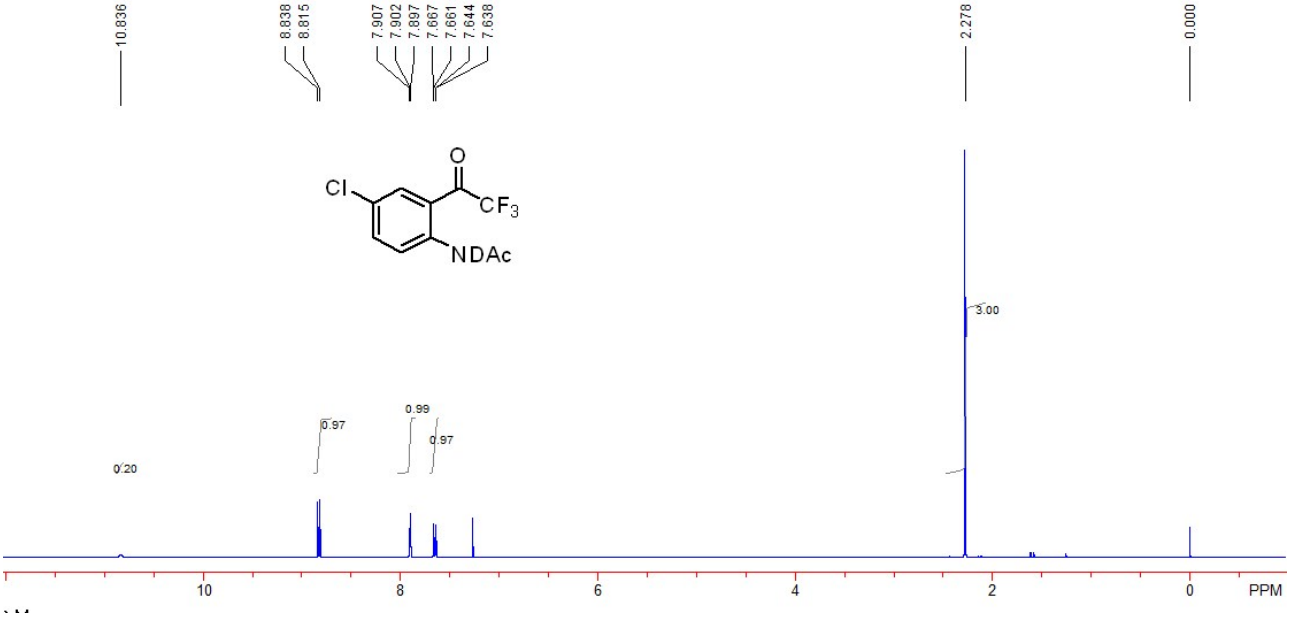
Synthesis of hex-3-yn-2-one-1,1,1-d_3 [D]-**2a**: Under argon atmosphere, to a solution of 1,1-dibromobut-1-ene (5 mmol, 1.06 g) in Et_2O (20 mL) was added n-BuLi (2.5 mL, 2.4 mol/L in hexane) at -78 °C. The reaction mixture was stirred at the same temperature for 0.5 hour. Then acetic-2,2,2-d_3 anhydride (6 mmol, 0.7 mL) was added to the mixture and stirred for another 20 minutes. The reaction solution was allowed to warm to room temperature and was stirred for 2 hours. After that, the resulting dark mixture was quenched with water (5 mL) and extracted with ether (45 mL) for three times. The organic phase was concentrated under reduced pressure and the

residue was purified by a silica gel flash column chromatography with petroleum ether and Et_2O (50:1) as an eluent. Since the boiling point of hex-3-yn-2-one **1a** was 95 °C under 760 Torr, the solvent contained in the product was difficult to be removed. Thus, the crude product mixed with some PE and ether was used for the next reaction without further purification.

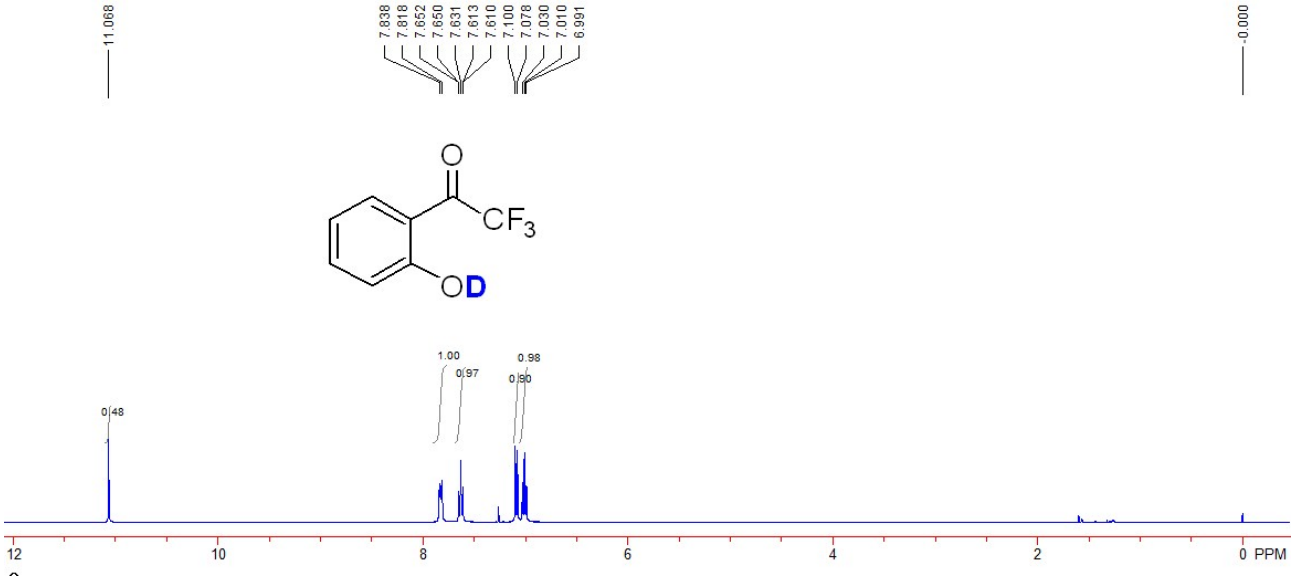


Synthesis of N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)acetamide-N-d [D]-**1a**: Under argon atmosphere, to a solution of N-(4-chloro-2-(2,2,2-trifluoroacetyl)phenyl)acetamide (300 mg) in $CDCl_3$ (10 mL) was added D_2O (5 mL) at room temperature. The resulting mixture was stirred at the 50 ^oC overnight. Then the reaction mixture was cooled to room temperature and the solvent was removed under reduced pressure. The crude product was used for the next reaction without future

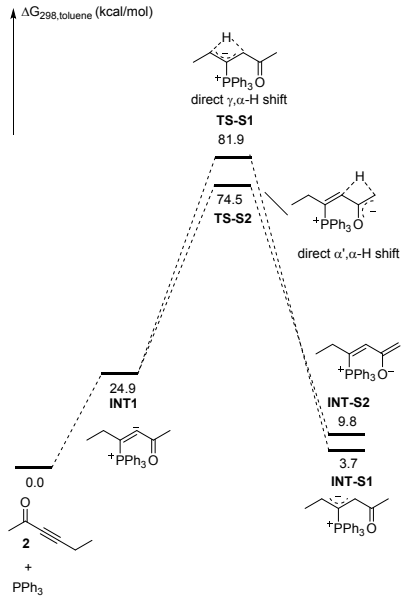
purification.



Synthesis of 2,2,2-trifluoro-1-(2-(hydroxy-d)phenyl)ethan-1-one [D]-**1t**: Under argon atmosphere, to a solution of **1t** (100 mg) in $CDCl_3$ (5.0 mL) was added D_2O (2 mL) at room temperature. The resulting mixture was stirred at the 50 °C overnight. Then the reaction mixture was cooled to room temperature and the solvent was removed under reduced pressure. The crude product was used for the measurement without future purification.

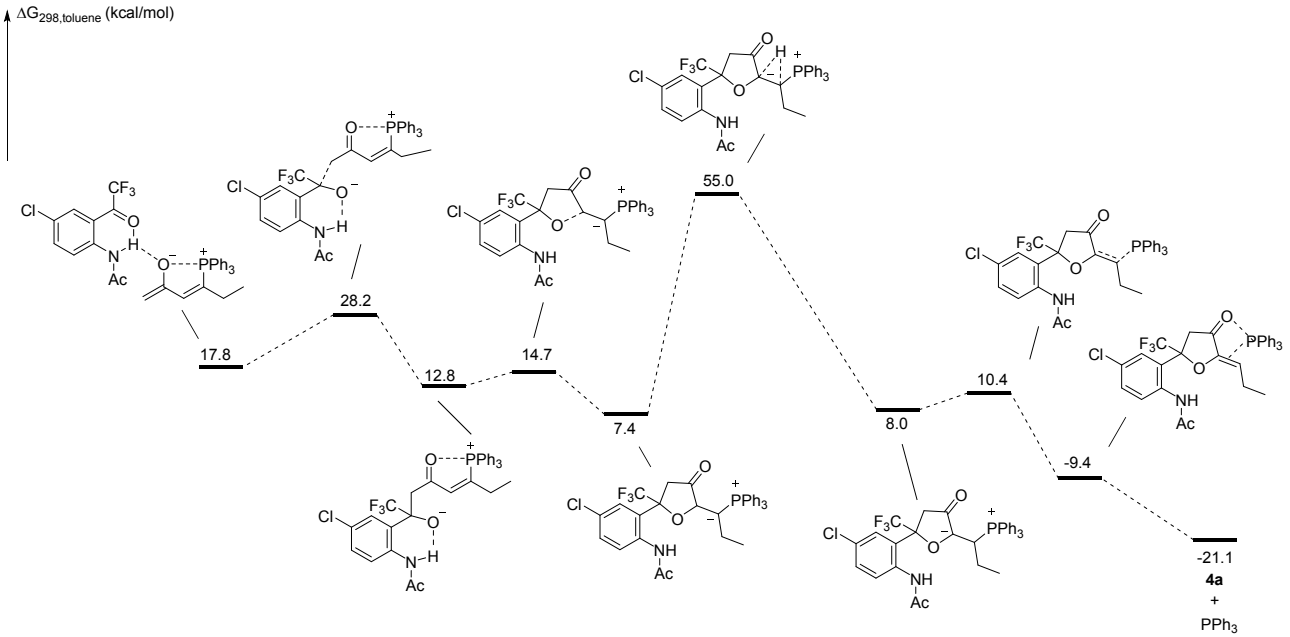


Computational Details and Archive Entries



Scheme S1. Solvation Gibbs free energy profiles for intramolecular proton transfer processes.

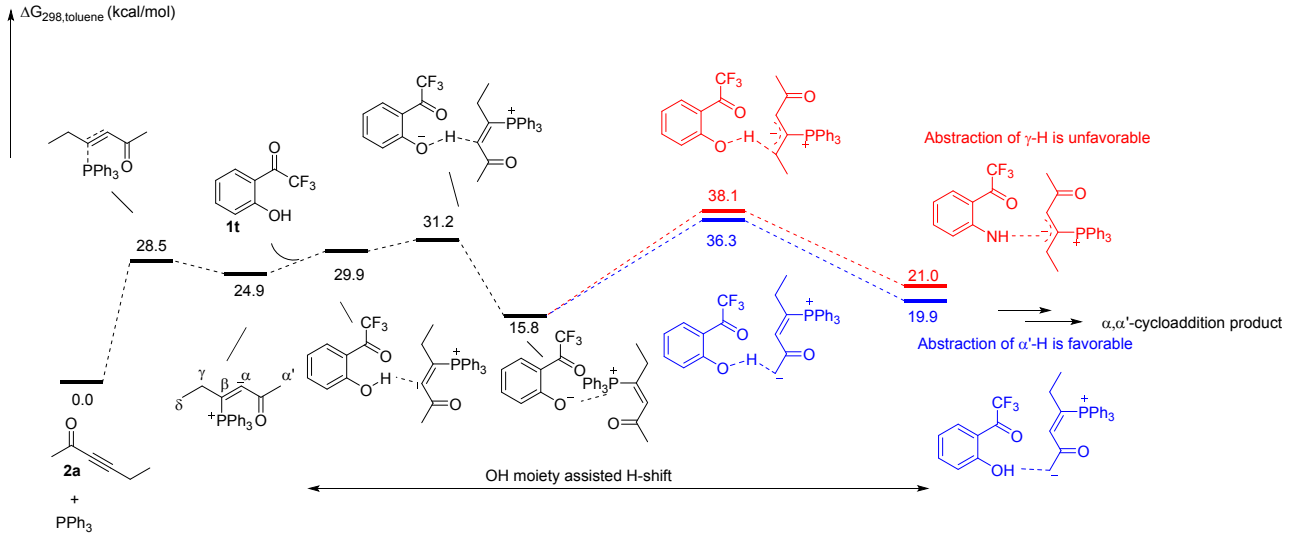
The intramolecular γ,α-H shift and α',α-H shift processes were also investigated by DFT calculations. The calculation results show that the activation free energy of 49.6 kcal/mol is required for direct α',α-H shift and 57.0 kcal/mol is required for direct γ,α-H shift, which are extremely high energy barriers, thus we rules out these pathways.



Scheme S2. Solvation Gibbs free energy profiles for generation of **4a** without assistant of water.

The reaction pathway for generation of product **4a** without assistant of water is shown in Scheme S2. This reaction pathway involves the proton transfer processes with extremely high-energy barriers, which is contrast to the experiment undergoing at low temperature and accounts for why the reaction cannot proceed without addition

of water. Based on the calculation results, we ruled out the reaction pathway without assistant of water.



Scheme S3. Using **1t** and **2a** as substrates, the generation of key zwitterionic intermediates.

In contrast to using **1a** having NHAc moiety, the α',α-cycloaddition product was always obtained when **1t** having OH moiety was employed as a substrate. The calculation results show that the abstraction of α'-H is kinetically and thermodynamically favored over the abstraction of γ-H using **1t** as a substrate, which leads to the α',α-cycloaddition product and may account for the experimental observation.

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 8 (Table S1) and archive entries

Table S1[a]

	E_{tot} (E_h)	$H_{298,toluene}$	$G_{298,toluene}$
1a	-1350.175807	-1349.996158	-1350.05763
2a	-308.570694	-308.4364021	-308.4796811
PPh_3	-1036.185567	-1035.891749	-1035.955583
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INT2	-2694.934437	-2694.32265	-2694.441953
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INT3	-2694.943863	-2694.332816	-2694.449692
TS2	-2694.930808	-2694.32438	-2694.438038
TS2-1	-2694.925984	-2694.320799	-2694.434608
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INT4-1	-2694.963805	-2694.350924	-2694.464504
TS3	-2694.940459	-2694.334469	-2694.450757
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TS4	-2694.924878	-2694.317949	-2694.432884
INT6	-2694.956301	-2694.344052	-2694.461471
TS5	-2694.953136	-2694.342427	-2694.457281
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INT10	-2694.981178	-2694.369024	-2694.48396
TS9	-2694.942077	-2694.333597	-2694.448777
INT11	-2694.980143	-2694.364635	-2694.474558
TS10	-2694.969698	-2694.358482	-2694.471344
INT12	-2695.019837	-2694.405649	-2694.522130
3a	-1658.822356	-1658.503979	-1658.582367

a. SMD/M06-2X/6-311+G(d,p)//M06-2X/6-31G(d)

1a

```
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2a

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PPh_3

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INT2

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843222832\H,0,-3.1089774507,-3.8207942104,0.0345936353\H,0,-5.26288362
92,-2.758880694,-0.6103530366\C,0,-2.0393176151,1.7912429942,2.7305018
5\C,0,-1.6816430711,2.7674687729,1.7953378117\C,0,-2.8991772547,2.1074
0418,3.7922840006\C,0,-2.1818214882,4.0605055655,1.9378973595\H,0,-1.0
623641572,2.5162505393,0.9369178115\C,0,-3.3862904307,3.4019928611,3.9
245080058\H,0,-3.1838625234,1.3461513929,4.513220626\C,0,-3.0235111033
,4.3798214462,2.998531658\H,0,-1.910983089,4.8161817144,1.2077790912\H
,0,-4.0490563036,3.6468188828,4.7484967882\H,0,-3.4047437941,5.3911158
165,3.1036330527\H,0,1.6708125417,-0.1768807488,-1.1456785476\N,0,2.02
4346263,-0.1900369704,-2.110364813\C,0,1.9230547999,-1.3912605991,-2.7
957664859\C,0,1.9894319241,-1.4625887117,-4.200218889\C,0,1.6660836461
,-2.5915082419,-2.0818823346\C,0,1.7766490581,-2.6598341765,-4.8625619
762\H,0,2.2042729372,-0.5631431613,-4.7575098882\C,0,1.4247509208,-3.7
890186785,-2.7721589665\C,0,1.4823387274,-3.8203066599,-4.15071344\H,0
,1.8302741627,-2.6937179172,-5.9457862204\H,0,1.2243200072,-4.70684589
56,-2.2319180597\C,0,1.7490228599,-2.6502416007,-0.6080407054\O,0,2.42
77969337,-1.9372951515,0.0915147851\C,0,2.280265328,1.0643078002,-2.64

76744078\O,0,2.6423597594,1.2480389791,-3.7933979402\C,0,0.9352321666,
-3.7517355815,0.1214306085\C,0,2.0508891209,2.1921415708,-1.6680404081
\H,0,0.9733997774,2.3102327796,-1.4948409867\H,0,2.5232064732,1.986129
2557,-0.7039565872\H,0,2.4596457455,3.1045846147,-2.1014312358\Cl,0,1.
2001360104,-5.3173939573,-4.9986155998\F,0,0.789653963,-3.4445373469,1
.4098192131\F,0,1.5507682945,-4.9392149429,0.0484368018\F,0,-0.2931972
854,-3.9001504327,-0.4017036812\\Version=ES64L-G09RevE.01\State=1-A\HF
=-2694.9344372\RMSD=6.154e-09\Dipole=-2.7405128,-0.5902722,4.3043985\Q
uadrupole=-3.8627655,-2.8015667,6.6643321,-1.4983708,0.715983,13.29785
85\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

TS1

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\27-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.1144568153,1.076345246,-0.07895098
46\C,0,0.9233091505,0.5373425191,-0.7367824509\C,0,1.0576126116,0.4432
205554,-2.2491396712\H,0,2.1189225247,0.416082893,-2.527138344\H,0,0.6
293315572,-0.5088881296,-2.5842040002\C,0,0.3891543798,1.6048454355,-2
.9781676015\H,0,0.8565068673,2.5531842629,-2.6924263593\H,0,0.50014554
19,1.4775817285,-4.0591198059\H,0,-0.6775685214,1.6551157578,-2.749705
5239\C,0,-0.1200750945,1.3131456877,1.3790021099\O,0,0.7796165389,1.93
77323901,1.9271881525\C,0,-1.3518624557,0.8700661788,2.1310368258\H,0,
-1.7123435713,-0.0976357298,1.7674464309\H,0,-1.1338676693,0.825965389
,3.1997495671\H,0,-2.1539222192,1.5972808705,1.9514665528\P,0,2.388458
1468,-0.0870730138,0.1643997274\C,0,3.187007403,-1.3948254815,-0.82446
21653\C,0,4.1860242006,-1.0662212117,-1.7491288014\C,0,2.7476245639,-2
.7185844878,-0.7262077898\C,0,4.7418649937,-2.0524049249,-2.5565827103
\H,0,4.5319185825,-0.0405859226,-1.8392317791\C,0,3.304908689,-3.70008
11218,-1.5404534528\H,0,1.974986897,-2.9923958114,-0.0156622647\C,0,4.
30184978,-3.3696682098,-2.4534365158\H,0,5.5171535831,-1.7884358572,-3
.268666005\H,0,2.9575799746,-4.7246965785,-1.4575662065\H,0,4.73479014
21,-4.1376642682,-3.0865804767\C,0,1.9599151499,-0.8092240708,1.765855
415\C,0,2.6920911971,-0.5248905455,2.9195262811\C,0,0.8376191343,-1.63
92162556,1.8303470905\C,0,2.308702391,-1.0936045677,4.1298272474\H,0,3
.5355199306,0.1571295671,2.8816379688\C,0,0.4586525316,-2.2019183398,3
.0442354829\H,0,0.2434456774,-1.8210989112,0.9418952512\C,0,1.19660551
8,-1.9312890995,4.1933197841\H,0,2.8706834025,-0.8666989577,5.03001196
58\H,0,-0.4224747675,-2.8343285395,3.0868748693\H,0,0.8975038419,-2.36
20824739,5.14376306\C,0,3.6304831687,1.211565037,0.3746563216\C,0,3.25
62280737,2.5492536552,0.2326136289\C,0,4.9528538002,0.8750018216,0.694
8271847\C,0,4.2107228914,3.5487486597,0.4041513777\H,0,2.2230364936,2.
7984873646,0.0140496143\C,0,5.8952933415,1.8802383764,0.874749247\H,0,
5.2442395281,-0.1680932007,0.7939579986\C,0,5.5231732458,3.2160715387,
0.7250423195\H,0,3.9228480846,4.5888509898,0.2926288062\H,0,6.91901854

29,1.6228241417,1.1265913413\H,0,6.2625043846,3.9995428424,0.859618812
\H,0,-1.2867225603,1.5603603598,-0.6492048145\N,0,-2.4774399558,2.0491
360129,-0.9538091825\C,0,-3.5418607439,1.2610619575,-0.577940593\C,0,-
4.7256127948,1.7587806478,0.0231516887\C,0,-3.4117690049,-0.153816387,
-0.654461451\C,0,-5.6837790411,0.9107877263,0.5435941662\H,0,-4.870232
4843,2.8284734005,0.0658814169\C,0,-4.3820758505,-1.0045993005,-0.0951
654836\C,0,-5.5076966965,-0.4739612476,0.4951352678\H,0,-6.5785645098,
1.3196562436,1.002545164\H,0,-4.2755768658,-2.0823447589,-0.1590557048
\C,0,-2.3237572739,-0.7922984226,-1.4162345963\O,0,-1.8147857993,-0.39
5442501,-2.4375066798\C,0,-2.5901154618,3.4027229455,-1.1305345748\O,0
,-3.6316637572,4.0445803552,-1.1853803426\C,0,-1.8174769828,-2.1700070
155,-0.9039926468\C,0,-1.2602724354,4.1178810673,-1.31586012\H,0,-0.43
15759636,3.6029708885,-0.8212903707\H,0,-1.0329607,4.1838235072,-2.384
8018163\H,0,-1.3613518654,5.1319788024,-0.9263464466\Cl,0,-6.722777598
3,-1.5316118561,1.1707115885\F,0,-0.5405713185,-2.3627035922,-1.258773
0984\F,0,-2.5397620677,-3.1729054951,-1.4156304817\F,0,-1.8724106123,-
2.282709536,0.4374155861\\Version=ES64L-G09RevE.01\State=1-A\HF=-2694.
9259814\RMSD=1.012e-09\Dipole=6.0428435,-2.2622083,1.249695\Quadrupole
=4.7276356,-5.4358546,0.708219,11.81472,-11.5473418,2.4570414\PG=C01 [
X(C34H30Cl1F3N1O3P1)]\\@

INT3

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\25-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-1.163329092,-0.6457469455,0.15621863
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60842,1.4378070401\H,0,0.3957752943,1.5444521893,1.9143124744\C,0,1.28
0485012,0.8362439066,0.0918660612\H,0,1.6246164211,-0.094627842,-0.369
2045407\H,0,0.5805748126,1.3215113878,-0.5967490554\H,0,2.1509578144,1
.4825053115,0.2281162148\C,0,-2.5360393741,-1.2025226034,-0.0724281806
\O,0,-3.4294452195,-0.9514084005,0.7124201114\C,0,-2.6995645785,-2.088
9581452,-1.2700880166\H,0,-2.4339958493,-1.5106121276,-2.1597889422\P,
0,-1.6993883789,-0.2565181898,2.8431040491\C,0,-0.5465348451,0.0024822
032,4.2340702537\C,0,-0.2089167075,1.3100386367,4.6071392107\C,0,0.036
3113101,-1.0778911938,4.9027382553\C,0,0.7113523973,1.52887678,5.62584
59805\H,0,-0.6761709075,2.1562279959,4.1107954734\C,0,0.9570656472,-0.
8519644741,5.9223656995\H,0,-0.2366422866,-2.0960434565,4.6447835606\C
,0,1.2974409351,0.4484672267,6.2817209334\H,0,0.965021208,2.5447345343
,5.9110381072\H,0,1.4022094809,-1.6955398955,6.4400666403\H,0,2.013240
6132,0.6217302791,7.0792650847\C,0,-2.4519460105,-1.8802405587,3.09810
38298\C,0,-3.7578168659,-1.9758445483,3.5795871177\C,0,-1.7206864285,-
3.0319072402,2.7915615388\C,0,-4.318861296,-3.2327198259,3.7828453572\
H,0,-4.3483189205,-1.0806336714,3.7477298169\C,0,-2.2914474228,-4.2835
324738,2.9980948837\H,0,-0.7198070748,-2.9526306212,2.3732927122\C,0,-

3.5876668838,-4.3828129484,3.4991644346\H,0,-5.3390308494,-3.310294460
4,4.1440640682\H,0,-1.7289207366,-5.1795006406,2.7558498593\H,0,-4.034
6491539,-5.3599876006,3.6521657539\C,0,-2.8572794914,1.1116420234,2.91
63521383\C,0,-3.1200507519,1.8286518827,1.7491700529\C,0,-3.4613058509
,1.4617468531,4.1310290829\C,0,-3.9932696789,2.9109962036,1.7926364745
\H,0,-2.6620651666,1.5318265949,0.8110345129\C,0,-4.3538783605,2.52558
79827,4.1574989009\H,0,-3.2377846267,0.9100997922,5.0415843744\C,0,-4.
6173134291,3.2461037962,2.991138305\H,0,-4.2197949411,3.4325304868,0.8
679499826\H,0,-4.8477310627,2.7915012693,5.0866760556\H,0,-5.331736014
,4.0629851405,3.0110904678\H,0,-0.5435893783,-0.5674606635,-0.73001879
73\H,0,1.292411818,0.0597543739,2.1246458578\H,0,-2.0146352198,-2.9420
6501,-1.1864023209\C,0,-6.4308313561,1.4849543174,0.3197919281\O,0,-6.
5153281797,2.6883582785,0.2897957623\C,0,-6.780329181,0.8073225501,1.6
757373439\F,0,-7.8097698483,-0.0534864044,1.5871718699\F,0,-5.72363008
18,0.1222119177,2.1399550871\F,0,-7.1137982347,1.7159829709,2.59055902
54\C,0,-5.9895225962,0.6142828909,-0.7939391704\C,0,-4.8754341148,0.98
4135226,-1.5999449781\C,0,-6.7199787305,-0.5530677886,-1.0647797549\C,
0,-4.6124540748,0.1603449995,-2.7229334855\C,0,-6.4136718213,-1.324030
404,-2.1688127903\H,0,-7.5522434366,-0.8425684635,-0.4356045883\C,0,-5
.3696670406,-0.9555549706,-3.0178781294\H,0,-3.7804114978,0.432743429,
-3.362399977\H,0,-5.1496011018,-1.55808762,-3.8943813434\Cl,0,-7.34724
99985,-2.7655951516,-2.5150815911\N,0,-4.1394413519,2.1093887777,-1.33
62141518\C,0,-2.8190445662,2.0525301439,-1.4695743783\O,0,-2.091018757
8,1.0302730326,-1.6089816503\C,0,-2.10738518,3.389504006,-1.314762377\
H,0,-2.8037339792,4.2262599281,-1.3867180605\H,0,-1.6087557154,3.42259
79375,-0.3365452253\H,0,-1.3284540111,3.4773364095,-2.0771999813\H,0,-
3.7311068088,-2.4339543455,-1.3400057604\\Version=ES64L-G09RevE.01\Sta
te=1-A\HF=-2694.9438629\RMSD=1.706e-09\Dipole=4.8008079,-2.2422578,4.8
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6.4664118\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

TS2 -2694.930808

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\17-Apr-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,2.4542861456,-0.9502777365,-2.1568843
74\C,0,1.4621889122,-0.2622039727,-1.510304564\C,0,0.1162515785,-0.135
9192048,-2.0249665551\H,0,-0.5663443845,-1.154243644,-1.471520715\C,0,
-0.0302345147,-0.3151920366,-3.5300394959\H,0,0.7270493887,0.260385655
1,-4.0799946179\H,0,0.0704964367,-1.3644069006,-3.8307115469\H,0,-1.01
80093751,0.0082882228,-3.8581752625\C,0,3.7841275306,-1.2263076908,-1.
630489086\O,0,4.2043444108,-0.69898865,-0.6044242212\C,0,4.6390497841,
-2.1998837804,-2.4101962189\P,0,1.785705883,0.4206053927,0.1697500346\
C,0,0.2860223896,1.2312607428,0.8094776531\C,0,-0.3776858026,0.7608679
12,1.9455978356\C,0,-0.1212942846,2.4345215015,0.2162083311\C,0,-1.444

0553845,1.4846165334,2.4736876483\H,0,-0.0665561113,-0.1575887526,2.42
96894739\C,0,-1.1976749473,3.1399105708,0.7384237696\H,0,0.406407255,2
.821903942,-0.6523222008\C,0,-1.8597655755,2.6653134054,1.869048745\H,
0,-1.9591345941,1.114356035,3.3543234291\H,0,-1.5212400071,4.058297891
4,0.259637727\H,0,-2.7032684336,3.2124699236,2.2791546192\C,0,2.976246
9212,1.7868317278,0.1498088209\C,0,3.1291214822,2.5354417859,1.3210198
695\C,0,3.6743926713,2.1356122036,-1.0060185415\C,0,4.0061206402,3.614
8902271,1.339903777\H,0,2.5596814131,2.2822237052,2.2124616629\C,0,4.5
324694055,3.2299803111,-0.9851266834\H,0,3.546231825,1.5522885235,-1.9
124266576\C,0,4.7046410621,3.9633042732,0.1864222603\H,0,4.1338810365,
4.1885367542,2.2521019137\H,0,5.0726870195,3.5051447672,-1.885171265\H
,0,5.3818594628,4.8116325649,0.1991640356\C,0,2.209335303,-0.883456313
1,1.3463368657\C,0,1.3203690232,-1.955869623,1.4407829985\C,0,3.371794
0853,-0.8522199531,2.1177272501\C,0,1.592958575,-3.0129303296,2.303067
3903\H,0,0.4107820345,-1.9626822152,0.8491800001\C,0,3.6263721967,-1.8
999007729,2.9963049451\H,0,4.0819674332,-0.0390761431,2.0053147398\C,0
,2.7455868234,-2.977936026,3.0848640363\H,0,0.9027973081,-3.8504853572
,2.3352297563\H,0,4.5285092723,-1.8841542506,3.5993319374\H,0,2.966094
1936,-3.7981209602,3.7611851118\H,0,2.2130295903,-1.3781582498,-3.1259
389726\H,0,-0.4267282965,0.7306360998,-1.639881869\H,0,5.6155827237,-2
.292641814,-1.9349513809\C,0,-3.0673117349,-0.212886105,-1.8793828783\
O,0,-2.9279280731,-1.0058355133,-2.7778965552\C,0,-3.3763692014,1.2501
713511,-2.2967010857\F,0,-4.6798267428,1.5378469599,-2.1511420231\F,0,
-2.684060757,2.1295768603,-1.5546922587\F,0,-3.0565069244,1.4511055471
,-3.5708195394\C,0,-3.0085127933,-0.5153014384,-0.4301430804\C,0,-2.22
95374328,-1.6066835756,0.0498607106\C,0,-3.8493786201,0.2024464774,0.4
303136952\C,0,-2.4217820063,-1.9921324573,1.3983695602\C,0,-3.98690960
76,-0.1945166855,1.7462675708\H,0,-4.4235030056,1.0482349884,0.0688389
693\C,0,-3.2947034594,-1.3042832326,2.2247908132\H,0,-1.886300058,-2.8
548782092,1.7685918443\H,0,-3.4313226868,-1.6190991889,3.2551528876\Cl
,0,-5.0081066587,0.7276081057,2.8280324512\N,0,-1.2882543409,-2.146396
0688,-0.7991301614\C,0,-0.6902779771,-3.3501087544,-0.5864953655\O,0,-
0.9045635042,-4.1278702389,0.3450135128\C,0,0.3854271469,-3.694592489,
-1.6037286758\H,0,0.2963074531,-3.1097619184,-2.5207547541\H,0,1.36726
20073,-3.5046548632,-1.1524660873\H,0,0.3223364417,-4.7608670303,-1.83
03005352\H,0,4.15079532,-3.1798808167,-2.4451605447\H,0,4.7587437105,-
1.859667,-3.4440348804\\Version=ES64L-G09RevE.01\State=1-A\HF=-2694.93
08078\RMSD=9.502e-09\Dipole=3.6880257,2.5412903,1.0645672\Quadrupole=-
3.1668474,-1.9199836,5.086831,-2.7184968,-7.4368624,0.0935073\PG=C01 [
X(C34H30Cl1F3N1O3P1)]\\@

TS2-1

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\18-Apr-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen

e)\\Title Card Required\\0,1\C,0,-0.5101235539,-1.4110620141,1.0311265
624\C,0,-1.5896640206,-1.5443975282,0.2511843866\C,0,-1.9286607295,-2.
8061663356,-0.5101899287\H,0,-2.953859367,-3.1148122797,-0.2628422983\
C,0,-0.9520098523,-3.9509019005,-0.2679194178\H,0,0.0590716603,-3.6685
695755,-0.5715853359\H,0,-0.9227891658,-4.2372455292,0.7882003167\H,0,
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\C,0,-4.8282548875,1.8290956311,2.9639235586\H,0,-3.606737814,2.418282
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.3034291772,0.643089326\C,0,3.9228225681,-0.1713765796,-0.1066760674\C
,0,3.6186340135,1.21804341,-0.0052614759\C,0,5.2501804039,-0.613233066
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INT4

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INT4-1

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TS3 -2694.940459

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\YIN\20-Apr-2017\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluene)\\Title Card Required\\0,1\C,0,0.0542742399,-1.6151965563,-0.2699679415\C,0,0.7358286924,-0.4732348277,-0.926541989\C,0,0.2375370352,0.2240885936,-1.9701555304\H,0,-0.7429993537,-1.189945051,0.6959498325\C,0,-1.034287302,-0.0889059376,-2.6940587363\H,0,-1.3816701936,-1.1106553992,-2.5290350066\H,0,-1.8321054509,0.5891384617,-2.3682733503\H,0,-0.9022529929,0.0615963088,-3.7700562664\C,0,0.8609281369,-2.6154299709,0.4182405866\O,0,2.027091652,-2.4081331936,0.7580085798\C,0,0.1616470086,-3.9078369794,0.7710309596\P,0,2.3120051893,0.1258094296,-0.247939535\C,0,2.6698647512,1.77920589,-0.9478098099\C,0,2.4433429253,2.9582323298,-0.2338673199\C,0,3.1922416595,1.8521094315,-2.2478841175\C,0,2.721898585,4.1924604473,-0.8176379263\H,0,2.0651680806,2.9236689371,0.7816907797\C,0,3.4596434437,3.0858558101,-2.8280708957\H,0,3.3929832475,0.9403737979,-2.80482596\C,0,3.2236950673,4.2587309195,-2.1127562128\H,0,2.5466358151,5.1024896648,-0.2529905796\H,0,3.8593520342,3.1311685745

,-3.8359543307\H,0,3.437987568,5.2223073604,-2.5643981867\C,0,3.7594738046,-0.8138618103,-0.8010430021\C,0,5.035339113,-0.3211132445,-0.5115088345\C,0,3.6085714996,-1.9540472939,-1.5903984236\C,0,6.1588840548,-0.9918167768,-0.9842375946\H,0,5.1515996085,0.58856144,0.0733764088\C,0,4.7356100302,-2.6070974285,-2.0781591056\H,0,2.615077525,-2.3291002331,-1.8149592957\C,0,6.0081559243,-2.1329092129,-1.7683432228\H,0,7.1493080692,-0.6162016923,-0.7486469916\H,0,4.6192615917,-3.4931823801,-2.6937320603\H,0,6.8852821189,-2.6503391437,-2.1444154737\C,0,2.2248908039,0.3298362185,1.5413755263\C,0,1.1400983427,1.0349718187,2.0728595517\C,0,3.206283545,-0.2041240863,2.3794726791\C,0,1.0628131051,1.2426983454,3.4484488481\H,0,0.3434347054,1.3962967126,1.4236429117\C,0,3.1182702638,0.0054965955,3.7505806689\H,0,4.0062798407,-0.8094836417,1.9651688157\C,0,2.054818077,0.7330365904,4.2816963743\H,0,0.2019041131,1.7488620531,3.8703022092\H,0,3.8733004638,-0.4145837901,4.4072804315\H,0,1.983291713,0.8824179293,5.3544637191\H,0,-0.7160073759,-2.0683020692,-0.8936576264\H,0,0.7632416327,1.1034527533,-2.3301220297\H,0,0.2559015009,-4.6027523341,-0.0717913863\C,0,-3.4351280944,-1.3824503543,-0.5314788412\O,0,-2.8842363701,-2.3751240523,-0.1081331048\C,0,-4.4264980213,-1.6385387132,-1.7063347343\F,0,-5.6694675696,-1.2273094397,-1.4254045342\F,0,-4.0257306745,-0.9903972436,-2.8196597666\F,0,-4.4789605847,-2.9314446337,-1.9958222916\C,0,-3.2771129587,0.0068728335,-0.0591627068\C,0,-2.4771229807,0.3175533281,1.0830515497\C,0,-4.0140227639,1.027204219,-0.7018310754\C,0,-2.5219882082,1.6566839344,1.5568920003\C,0,-3.9876711996,2.3178249036,-0.228019058\H,0,-4.6184880521,0.8158727135,-1.5740470406\C,0,-3.2497544213,2.6354656417,0.9171162998\H,0,-1.9729307002,1.8951661687,2.4574279542\H,0,-3.2542165862,3.6538813536,1.2929105807\Cl,0,-4.8956124746,3.5680748473,-1.043728008\N,0,-1.6562039275,-0.632902879,1.6357550577\C,0,-1.3541813519,-0.6259040602,2.9682929837\O,0,-1.8129935149,0.1385281341,3.8155690167\C,0,-0.3940541059,-1.7297692411,3.3810405713\H,0,-0.8528427303,-2.7075195956,3.2038065686\H,0,0.540910447,-1.6859536769,2.8108561768\H,0,-0.1716064902,-1.6212343511,4.443251998\H,0,0.6335960973,-4.3572162389,1.6466840152\H,0,-0.9049726733,-3.7349659582,0.9430942475\\Version=EM64L-G09RevA.01\State=1-A\HF=-2694.9404585\RMSD=4.472e-09\Dipole=5.3195133,1.3732681,-2.0507426\Quadrupole=-3.0826405,5.0887971,-2.0061565,1.802645,-1.3169389,2.5049992\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

INT5

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\YIN\18-Apr-2017\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluene)\\Title Card Required\\0,1\C,0,-0.3994447327,1.0890846114,0.173037068\C,0,-0.2689580989,0.353061492,1.4799344079\C,0,0.8522296962,-0.1577901118,2.010063126\C,0,2.2221749637,-0.1935932916,1.4215458226\H,0,2.2833396854,0.2199272312,0.4129318837\H,0,2.8682288205,0.3775614819,2.097

6970963\H,0,2.591700571,-1.2246361001,1.4108592136\C,0,-1.5536067407,0
.6263155559,-0.698525599\O,0,-2.0946595198,-0.4450334571,-0.5214918991
\C,0,-2.0130759837,1.5879649346,-1.7646995752\P,0,-1.7396633641,0.2328
901274,2.5197348458\C,0,-1.4123906475,0.5665529945,4.2703545495\C,0,-1
.6387574166,1.8288738279,4.8252788339\C,0,-0.9882927621,-0.4917408037,
5.0881526691\C,0,-1.4932564207,2.0124322031,6.196664841\H,0,-1.9204218
714,2.6667898963,4.199169363\C,0,-0.8157251588,-0.2891462002,6.4514874
174\H,0,-0.8116879753,-1.4779699455,4.6677748904\C,0,-1.087103816,0.95
9216166,7.0089130929\H,0,-1.6711200619,2.9923187984,6.6267428692\H,0,-
0.4708729966,-1.105269315,7.0766564295\H,0,-0.9599813354,1.1191195477,
8.0757069444\C,0,-2.3984384358,-1.4595972663,2.5182954071\C,0,-3.43550
14682,-1.7727416782,3.4081246227\C,0,-1.870286332,-2.4442229109,1.6841
432924\C,0,-3.949704678,-3.0624777673,3.4455704218\H,0,-3.8312414842,-
1.0109226485,4.0759091605\C,0,-2.382692004,-3.7384144525,1.7369827112\
H,0,-1.0748720661,-2.1935912654,0.9923880641\C,0,-3.4203431271,-4.0462
452459,2.6105831352\H,0,-4.754552623,-3.3025816749,4.1326794356\H,0,-1
.969144093,-4.5051043049,1.0900224748\H,0,-3.8170481739,-5.0562613349,
2.6462572581\C,0,-3.0226022704,1.3529490598,1.8881582262\C,0,-2.750617
7564,2.7239351395,1.7770525223\C,0,-4.2498840031,0.8408304332,1.452807
5974\C,0,-3.7270005677,3.573095688,1.2602676422\H,0,-1.7776081383,3.11
80085347,2.0678193808\C,0,-5.2123123974,1.7002749879,0.9337579697\H,0,
-4.4458671089,-0.2256359881,1.4926550109\C,0,-4.9550615799,3.066227186
9,0.8427089936\H,0,-3.5171463941,4.634958559,1.1787603158\H,0,-6.16189
79807,1.2991125047,0.5946056634\H,0,-5.709727133,3.7336234334,0.437593
3029\H,0,-0.4795969906,2.1677655661,0.3670896548\H,0,0.8128673766,-0.5
757760422,3.0144917422\H,0,-2.6266447243,1.0685000214,-2.5010648542\C,
0,2.4608685571,0.3535645327,5.5657809224\O,0,2.4645913298,-0.205261226
4,4.4855971334\C,0,3.0086127512,-0.5013547452,6.7442471448\F,0,3.95668
69226,0.1411003738,7.4392098281\F,0,2.02686754,-0.8267622595,7.6129784
137\F,0,3.5308896371,-1.6379442093,6.2982562574\C,0,1.9887735066,1.702
0967574,5.862932443\C,0,1.6572799998,2.6064399601,4.801911525\C,0,1.81
7143763,2.0939519252,7.2107843307\C,0,1.103069481,3.8693590147,5.19361
88784\C,0,1.2963815445,3.3231712209,7.5243641765\H,0,2.0697687659,1.42
05652044,8.0204855871\C,0,0.9393398476,4.2248455933,6.5073298715\H,0,0
.8252166256,4.5600210081,4.4059249709\H,0,0.5344578605,5.1977560388,6.
7715098216\Cl,0,1.0259450358,3.7618353053,9.1994646944\N,0,2.000401541
2,2.3609894438,3.522317908\C,0,1.35436557,2.920070837,2.4988570716\O,0
,0.1473484566,3.2537261832,2.455388271\C,0,2.2077721169,3.1436716757,1
.2572235714\H,0,3.1979648293,2.6996630115,1.3618846289\H,0,1.717573407
4,2.760732934,0.3576369006\H,0,2.3171415557,4.2251937269,1.1201333575\
H,0,-2.6180632307,2.3609264232,-1.2723699622\H,0,-1.1690646119,2.08973
35355,-2.2467595259\H,0,0.5146041807,0.9556330998,-0.420118409\\Versio
n=EM64L-G09RevA.01\State=1-A\HF=-2694.9603582\RMSD=2.596e-09\Dipole=-3
.8785492,-0.9403769,-2.9571478\Quadrupole=-5.1431214,6.3352684,-1.1921

47,-0.5609364,-7.2464413,-8.4513917\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

TS4

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\19-Apr-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,2.5197341725,-0.476743975,-2.18533783
2\C,0,1.6250017083,0.4639775718,-1.4086887378\C,0,0.4583941063,0.91814
33356,-1.9976766042\C,0,-0.0583072689,0.5085718035,-3.2432653711\H,0,0
.628641652,0.0639620914,-3.962184862\H,0,-0.80587596,-0.576030321,-2.6
690611907\H,0,-0.8349086755,1.128399518,-3.6797658652\C,0,3.9294126753
,-0.6902763247,-1.6776897874\O,0,4.4601158942,0.073407168,-0.897859735
6\C,0,4.6328676662,-1.9213521053,-2.1929756089\P,0,1.8715817113,0.7412
848844,0.3082667168\C,0,0.3057900891,1.151604125,1.1437586204\C,0,-0.3
22533259,0.2262010885,1.9796225206\C,0,-0.2524267598,2.426253099,0.970
9721794\C,0,-1.4971938534,0.5770266072,2.6429401569\H,0,0.098209998,-0
.7648883978,2.1202941743\C,0,-1.4492620711,2.7515691987,1.5976022245\H
,0,0.2503230947,3.1623391341,0.3482360795\C,0,-2.0687146076,1.82814517
56,2.4397087327\H,0,-1.9716360637,-0.1391141105,3.3069035087\H,0,-1.89
14972268,3.730189189,1.4415229455\H,0,-2.9977195117,2.0874036983,2.937
9631011\C,0,2.9403953331,2.1444271463,0.7613527491\C,0,2.9681899754,2.
6030075238,2.0833882177\C,0,3.6680221822,2.8103813046,-0.2248182433\C,
0,3.7494270871,3.7046067243,2.4181094204\H,0,2.3712934059,2.1089360453
,2.8469006197\C,0,4.4366654805,3.9197743797,0.1126422507\H,0,3.6310614
894,2.4490276155,-1.247042869\C,0,4.4829350634,4.3620925704,1.43231939
05\H,0,3.7764571949,4.055933481,3.4446055968\H,0,5.0007308499,4.437808
9524,-0.6562131664\H,0,5.0853483431,5.2268843232,1.6928913753\C,0,2.46
66168803,-0.7986446725,1.0565681509\C,0,1.9104163233,-1.9803640989,0.5
551493039\C,0,3.4369147921,-0.8453538799,2.0587726419\C,0,2.3171285824
,-3.2090804477,1.066150063\H,0,1.1691330686,-1.9550074631,-0.240153463
9\C,0,3.8339888845,-2.0782826853,2.5686583119\H,0,3.8964830463,0.06933
67193,2.4215517008\C,0,3.2766287342,-3.2571282148,2.0747351439\H,0,1.8
867480528,-4.117853686,0.6562428802\H,0,4.5913509787,-2.1195361621,3.3
450309515\H,0,3.5996740571,-4.2147186166,2.4715332236\H,0,2.054494001,
-1.4674909853,-2.3102081348\H,0,-0.2179667431,1.5269165867,-1.39988790
32\H,0,4.1860442534,-2.7949576966,-1.7023399711\C,0,-3.1662598692,0.19
3121416,-1.1347785317\O,0,-2.560459437,0.7731700236,-2.0047058675\C,0,
-4.5755025571,0.7684901716,-0.8115726956\F,0,-5.5032532571,-0.18822398
31,-0.6947509114\F,0,-4.5531496113,1.4584075644,0.3467614158\F,0,-4.96
07699403,1.6040658452,-1.7661796313\C,0,-2.6962643648,-0.9691922416,-0
.3608686777\C,0,-1.6633949509,-1.8468122853,-0.8249342849\C,0,-3.32683
38409,-1.1975076435,0.8751331164\C,0,-1.3303981835,-2.9222802107,0.045
8012857\C,0,-2.9546284462,-2.2485033069,1.6820593754\H,0,-4.1046855619
,-0.5310652566,1.2252314067\C,0,-1.9516124651,-3.1180419215,1.26359624
89\H,0,-0.5767808728,-3.6244878449,-0.2739870832\H,0,-1.6631264268,-3.

9555592143,1.8915338506\Cl,0,-3.7207572026,-2.4718422262,3.2378194598\
N,0,-1.1292715929,-1.722085822,-2.0951748598\C,0,-0.2291978474,-2.6226
926426,-2.6107377665\O,0,0.475785491,-3.4238028315,-1.9947508632\C,0,-
0.1071248973,-2.572206404,-4.1249666745\H,0,-0.3749062662,-3.563497990
5,-4.5027211731\H,0,-0.7560273048,-1.8245935132,-4.5799101601\H,0,0.93
44851703,-2.3895409803,-4.4075569705\H,0,4.4818183545,-2.0440475221,-3
.2698863159\H,0,5.6958462044,-1.8735001836,-1.956006679\H,0,2.63896184
9,-0.088473214,-3.2104696192\\Version=ES64L-G09RevE.01\State=1-A\HF=-2
694.9248784\RMSD=2.333e-09\Dipole=2.7064293,0.8243602,1.4294239\Quadru
pole=-9.3148942,6.3125506,3.0023436,-0.0485016,-2.536606,4.8279517\PG=
C01 [X(C34H30Cl1F3N1O3P1)]\\@

INT6

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\YIN\20-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,0.0092476214,-0.0330041283,0.03635194
75\C,0,0.0313904608,-0.0038160279,1.5423206474\C,0,1.2672523617,-0.249
671162,2.2325654549\H,0,1.2262627239,-0.1829468675,3.3240666422\C,0,2.
4821023002,-0.512002374,1.6930748396\H,0,2.6373509368,-0.5826332505,0.
6208169862\H,0,3.3707728343,-0.5305551825,2.3139501533\C,0,-0.14923446
27,-1.4308940058,-0.5605856742\O,0,-1.0381265023,-2.1641132944,-0.1783
805768\C,0,0.8040427896,-1.8420590057,-1.6577131214\H,0,0.7799278077,-
1.106124692,-2.4691613303\H,0,1.8260966344,-1.8612813059,-1.2652330363
\H,0,0.5377241705,-2.8300624442,-2.0349822821\P,0,-1.433650405,-0.0654
388174,2.4213821442\C,0,-1.2391122574,0.8495269666,3.998403291\C,0,-0.
4365574014,1.9976406977,3.997123298\C,0,-1.8869132556,0.46596525,5.176
2235602\C,0,-0.2952806485,2.7558937145,5.1559021771\H,0,0.0861537165,2
.2749932771,3.0855390464\C,0,-1.7427694456,1.2275837605,6.3339675703\H
,0,-2.4919028329,-0.4348145004,5.1977299119\C,0,-0.9508475343,2.372700
2652,6.3249519951\H,0,0.3323950336,3.6415404314,5.1476944514\H,0,-2.24
63821651,0.9202043334,7.2452118578\H,0,-0.837056157,2.9623618846,7.229
5388722\C,0,-2.1081251397,-1.6958517144,2.9122660469\C,0,-3.4305679891
,-1.8750790634,3.3348237837\C,0,-1.2392466731,-2.7843820082,2.86270590
09\C,0,-3.8634635459,-3.1346543185,3.7368847633\H,0,-4.1212463559,-1.0
339965959,3.343997137\C,0,-1.6727263185,-4.0419825037,3.2742993472\H,0
,-0.2332162066,-2.6568094083,2.4755608332\C,0,-2.9816708156,-4.2159480
982,3.71356585\H,0,-4.8896565576,-3.2762144131,4.0624867584\H,0,-0.983
8615372,-4.8798672032,3.234634505\H,0,-3.3242401687,-5.1975848403,4.02
73282377\C,0,-2.7906827301,0.7127588168,1.4939145954\C,0,-3.4693423659
,-0.0346416588,0.5237936355\C,0,-3.1246990228,2.051923161,1.7068035312
\C,0,-4.4744881485,0.5659489097,-0.228784681\H,0,-3.1948699999,-1.0732
723886,0.3568077661\C,0,-4.1358675308,2.6432432316,0.9548078866\H,0,-2
.6005272312,2.6306510136,2.4619528489\C,0,-4.8095955149,1.9011577334,-
0.0117898973\H,0,-4.9976900899,-0.0113045015,-0.9846162879\H,0,-4.3981

166704,3.6823992679,1.1267919658\H,0,-5.5976974717,2.364504626,-0.5976
358955\H,0,-0.8369786914,0.5490838454,-0.3571596691\H,0,0.9213224294,0
.4432310144,-0.3451192523\C,0,2.7483188504,-3.4331819001,2.5748539566\
C,0,4.0502870667,-3.0512154569,3.1573401287\C,0,5.2285598372,-3.474972
4096,2.5307459643\C,0,4.1145720994,-2.2819013217,4.347270359\C,0,6.456
8527391,-3.1463255487,3.073329132\H,0,5.1887438974,-4.0727604765,1.627
6740918\C,0,5.3741410302,-1.9453969472,4.8634644333\C,0,6.5304118676,-
2.3792774766,4.2323627164\H,0,5.4317044885,-1.3426849145,5.7579270813\
H,0,7.5002319241,-2.1229225176,4.645796948\C,0,2.6839915291,-3.8101288
956,1.0761033474\O,0,1.7180532215,-3.5646377635,3.2064618836\F,0,1.435
3994853,-3.7265762029,0.6354707809\F,0,3.1026150792,-5.0786544869,0.92
48735747\F,0,3.4602478229,-3.0419893191,0.3048940285\Cl,0,7.9193507835
,-3.6902559598,2.2971511055\N,0,2.9280092495,-1.8557751376,4.938347842
7\H,0,2.0868093792,-2.2682087118,4.552454643\C,0,2.7613331972,-0.91129
71569,5.932340213\O,0,3.6756061885,-0.3591272045,6.5109367799\C,0,1.31
07161273,-0.5864445988,6.2221472594\H,0,1.1792390453,-0.4992333907,7.3
021444721\H,0,1.0799337159,0.3887539413,5.7789976898\H,0,0.6082509289,
-1.3225018604,5.8215620118\\Version=EM64L-G09RevA.01\State=1-A\HF=-269
4.9563007\RMSD=6.131e-09\Dipole=-2.4585471,1.3106346,0.4923825\Quadrup
ole=-0.3084507,0.0160573,0.2923934,-8.5330085,-5.3660687,-3.8645534\PG
=C01 [X(C34H30Cl1F3N1O3P1)]\\@

TS5

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\20-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,1.4013663176,-2.3843212051,0.25313534
91\C,0,1.0664296557,-0.9282797729,0.4530564389\C,0,-0.2044890369,-0.49
93656922,0.8217640845\H,0,-0.312969546,0.5733146767,1.0051062562\C,0,-
1.3927257102,-1.2222525207,0.9090449318\H,0,-1.3829704017,-2.304755468
1,0.8367282534\H,0,-2.1713925995,-0.8118924094,1.5421838363\C,0,1.6474
487783,-2.8057632849,-1.1893370679\O,0,2.1801478198,-2.0495196681,-1.9
729855021\C,0,1.2523529694,-4.2128551167,-1.5625154275\H,0,1.697710341
2,-4.9288532316,-0.8629656202\H,0,0.1645187448,-4.3074012574,-1.482258
2306\H,0,1.5696769449,-4.4351970746,-2.581590623\P,0,2.295046394,0.282
7118125,0.1593771761\C,0,2.062648195,1.6573189273,1.3435130509\C,0,1.7
287042241,1.3611830132,2.6724995253\C,0,2.2330072424,2.9897851425,0.95
87386856\C,0,1.5942912193,2.3839369368,3.6053305316\H,0,1.5490010773,0
.3299930886,2.9650152276\C,0,2.0898598751,4.0113237079,1.8958825963\H,
0,2.4625341365,3.2361239733,-0.0730435914\C,0,1.7781395111,3.710748413
9,3.2179261265\H,0,1.3310416817,2.1458336007,4.6310612173\H,0,2.215941
2338,5.0438810582,1.5860786484\H,0,1.6629430199,4.5087527651,3.9448151
121\C,0,2.3493037403,1.0479894168,-1.486322848\C,0,3.4821668244,1.7573
701717,-1.9050014894\C,0,1.2265936732,0.9543131355,-2.3079500731\C,0,3
.4828483961,2.3826443903,-3.1466513227\H,0,4.3609479024,1.8161261035,-

1.2664263605\C,0,1.2362491802,1.5895174212,-3.5483039748\H,0,0.3499586
615,0.3929890759,-1.992393662\C,0,2.3575471662,2.2988215628,-3.9670294
736\H,0,4.3605357732,2.930610427,-3.4749371014\H,0,0.3607265833,1.5187
255664,-4.1856681515\H,0,2.3610637467,2.7857074076,-4.9376554044\C,0,3
.9556396732,-0.4149139708,0.4403210751\C,0,4.6553269194,-0.9880367481,
-0.6282702119\C,0,4.507305627,-0.4357513728,1.7249224998\C,0,5.8948551
305,-1.5793110407,-0.4043750189\H,0,4.2230275515,-0.9826868636,-1.6233
562645\C,0,5.7471856401,-1.030566048,1.9402706301\H,0,3.9777795798,0.0
205058983,2.5559795711\C,0,6.4404064267,-1.6025321838,0.8765412508\H,0
,6.4333793869,-2.0233627513,-1.2354788601\H,0,6.1733921537,-1.04065966
37,2.9383412007\H,0,7.4087457525,-2.0634306644,1.0457633605\H,0,2.3303
759423,-2.6515851292,0.783732652\H,0,0.6137639478,-2.9999731289,0.6984
794031\C,0,-2.3529249405,-0.5578904702,-1.0271893905\C,0,-3.7152133048
,-0.3781731596,-0.4207904234\C,0,-4.732180204,-1.3100041996,-0.6224739
516\C,0,-3.9769519856,0.7788499969,0.3498837409\C,0,-5.9808550339,-1.1
070877385,-0.0496368121\H,0,-4.567055366,-2.1944034598,-1.2254604932\C
,0,-5.2340429539,0.9551139647,0.9315338143\C,0,-6.2355142093,0.0107484
979,0.7316041063\H,0,-5.4152440863,1.829646813,1.5405707028\H,0,-7.215
0466002,0.1500106758,1.1760810498\C,0,-2.0507220092,-1.8863741101,-1.7
393555781\O,0,-1.7370321939,0.4122809619,-1.5141694377\F,0,-0.73725206
4,-1.9809458405,-1.9822196757\F,0,-2.6830689794,-1.9076252835,-2.92415
53477\F,0,-2.4165046329,-3.0063598904,-1.0927620835\Cl,0,-7.2447382976
,-2.2818990812,-0.3196771223\N,0,-2.9306041715,1.6967494433,0.51070484
01\H,0,-2.1989545998,1.5963297551,-0.1918985999\C,0,-2.7895452746,2.65
62579053,1.4785232246\O,0,-3.6189935581,2.9044099771,2.3344880391\C,0,
-1.4473833909,3.3644445709,1.4275135728\H,0,-1.5843119206,4.4061482258
,1.7216618885\H,0,-0.7769804771,2.8942706117,2.1563264705\H,0,-0.97343
52124,3.3144644075,0.4430050545\\Version=ES64L-G09RevE.01\State=1-A\HF
=-2694.9531359\RMSD=9.807e-09\Dipole=5.3697708,0.5340749,1.1913821\Qua
drupole=-6.2098478,8.4141338,-2.2042861,0.4419162,8.0282679,-5.3429865
\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

INT7

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\18-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.1326024499,0.4851130614,0.09594203
66\C,0,-0.0061067962,0.1805406236,1.569489093\C,0,1.161083154,-0.00512
05622,2.2103859249\H,0,1.1465410802,-0.1789739502,3.2833029485\C,0,2.4
758318151,-0.1878548887,1.5475195872\H,0,2.6006480489,0.4502716526,0.6
710029511\H,0,3.3031148635,0.0129572867,2.2315816868\C,0,-0.8634191165
,-0.6034353681,-0.6744185786\O,0,-1.8370490109,-1.1374683581,-0.179282
6174\C,0,-0.3608015393,-0.9143005726,-2.0533035041\H,0,-0.2977446465,0
.0045232958,-2.6476257281\H,0,0.6517846793,-1.3166237485,-1.9340610693
\H,0,-1.021111261,-1.6318006145,-2.5419916247\P,0,-1.4951545297,-0.124

24051,2.5423349319\C,0,-1.2045103835,0.3605965406,4.2755881354\C,0,-1.
6449666393,1.5802573914,4.7951795158\C,0,-0.4960565706,-0.5304447287,5
.0965436068\C,0,-1.3633331487,1.91322356,6.1177111614\H,0,-2.223278499
8,2.2651747813,4.1838132932\C,0,-0.2037603816,-0.1828539654,6.41055783
64\H,0,-0.1724539764,-1.4964254727,4.7130186485\C,0,-0.6375397529,1.03
91058505,6.9210347981\H,0,-1.7159893672,2.857922997,6.5191825044\H,0,0
.3588024421,-0.8729461572,7.0310357656\H,0,-0.4160566206,1.305885176,7
.9496859156\C,0,-1.9164620368,-1.8732270256,2.6745981251\C,0,-2.959776
8992,-2.2324534115,3.5390560293\C,0,-1.1541922395,-2.8438553712,2.0225
096346\C,0,-3.2620497026,-3.5749060712,3.7235108154\H,0,-3.5225634309,
-1.4696101166,4.0734726371\C,0,-1.4549168226,-4.1898115245,2.234217198
2\H,0,-0.3383571394,-2.5535233824,1.3596962589\C,0,-2.5065189571,-4.54
94380993,3.0714306463\H,0,-4.072580788,-3.8606430244,4.3863341833\H,0,
-0.8630565982,-4.9619471561,1.7513287095\H,0,-2.7333442495,-5.59975679
2,3.2266563887\C,0,-2.8554317063,0.865441168,1.8822601174\C,0,-4.07181
29256,0.2782531026,1.5318658069\C,0,-2.6518611752,2.236025428,1.681968
0292\C,0,-5.0934197597,1.0696969498,1.01624465\H,0,-4.2058096115,-0.79
39245779,1.6349519597\C,0,-3.6771064145,3.0204659232,1.1641283791\H,0,
-1.6893845533,2.6869761542,1.9172606511\C,0,-4.899621978,2.4370633796,
0.8378410498\H,0,-6.0384055184,0.6129263159,0.7410445063\H,0,-3.517453
3984,4.0823384495,1.0074189261\H,0,-5.698566367,3.0484267038,0.4301999
295\H,0,-0.7080680624,1.411600619,-0.0561771133\H,0,0.8601602714,0.623
875889,-0.329120869\C,0,2.4978791351,-1.668507478,0.9770455787\C,0,2.3
86396744,-2.717289603,2.1241943102\C,0,2.7440918069,-2.4031096091,3.43
3867587\C,0,1.9017443082,-4.0233631361,1.8597447363\C,0,2.5939652962,-
3.3254501908,4.4619081779\H,0,3.1488179737,-1.426775555,3.6770871385\C
,0,1.796919186,-4.9558030671,2.9023248449\C,0,2.1316396426,-4.60574614
86,4.2043655068\H,0,1.4368497152,-5.9499658458,2.6768216869\H,0,2.0300
144566,-5.3241434833,5.0108446094\C,0,3.8981674575,-1.8244931087,0.350
0567253\O,0,1.5485440632,-1.8066341165,0.028983878\F,0,4.0912171285,-0
.9367460376,-0.6385225355\F,0,4.0707133296,-3.0454843261,-0.1709989513
\F,0,4.8874270151,-1.630663085,1.2475053066\Cl,0,2.986415867,-2.849260
7388,6.1045379951\N,0,1.5105402894,-4.3104920824,0.5488400607\H,0,1.51
99026157,-3.4366214923,-0.0292477486\C,0,0.975867312,-5.4587955619,0.0
514038527\O,0,0.7384618719,-6.4696827293,0.702415237\C,0,0.6961319248,
-5.3879429145,-1.4385365606\H,0,-0.0723217712,-6.1199310171,-1.6873537
204\H,0,0.3781954927,-4.3871132401,-1.7435623544\H,0,1.609407086,-5.63
66398907,-1.9880273226\\Version=ES64L-G09RevE.01\State=1-A\HF=-2694.98
86243\RMSD=6.936e-09\Dipole=-4.3017446,4.6023228,1.6087743\Quadrupole=
-7.2383991,2.7378935,4.5005055,-3.8644343,1.7739754,-2.4290369\PG=C01
[X(C34H30Cl1F3N1O3P1)]\\@

TS6

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\16-May-20

17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
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2466\C,0,-1.0195905696,-0.5868766801,-1.3063660083\C,0,-0.1203574362,0
.2777453335,-1.8022839179\H,0,-0.1804600806,1.3217746579,-1.5088413195
\C,0,1.082178474,-0.0869842205,-2.6046523204\H,0,0.9006812701,-0.91756
01175,-3.2894976694\H,0,1.4330600889,0.7631440935,-3.193801957\C,0,-0.
9000223562,-2.9853873728,-0.4944315378\O,0,-1.4096585594,-2.7127930139
,0.5739894147\C,0,-0.1175011888,-4.242665223,-0.7387684161\H,0,-0.5499
819477,-4.793995389,-1.5816946355\H,0,0.9011496134,-3.9524114622,-1.01
78984064\H,0,-0.1155915168,-4.8657656256,0.1558631925\P,0,-2.134778473
6,0.0644675512,-0.0376952427\C,0,-2.4021150334,1.8421407892,-0.3289841
515\C,0,-3.5484143001,2.3393011017,-0.9531999164\C,0,-1.391367056,2.72
51625114,0.0832595662\C,0,-3.6734006733,3.7073821089,-1.1816314416\H,0
,-4.3528376677,1.6720860647,-1.244519909\C,0,-1.5154357054,4.086878624
,-0.1669310229\H,0,-0.5050516778,2.3526486389,0.5946941508\C,0,-2.6566
297629,4.577288764,-0.7990816712\H,0,-4.5696988724,4.0914802606,-1.658
0106824\H,0,-0.7178826609,4.7575491999,0.1358055426\H,0,-2.7560017526,
5.6418553506,-0.9866304204\C,0,-1.4404160055,0.0246511557,1.6242886393
\C,0,-2.1826165357,0.6083749798,2.6599866994\C,0,-0.1465821177,-0.4469
745619,1.8454493823\C,0,-1.6319352103,0.6836519293,3.9323399435\H,0,-3
.1755676622,1.011916759,2.4716332798\C,0,0.4065229284,-0.3446249583,3.
1217755006\H,0,0.4306241438,-0.885945145,1.0350278142\C,0,-0.339507471
7,0.2091179911,4.157969834\H,0,-2.2027312464,1.1273051001,4.7419322073
\H,0,1.4223255645,-0.687876061,3.3022240545\H,0,0.0952652976,0.2834801
448,5.1499825733\C,0,-3.7134060273,-0.8050117248,-0.1619807451\C,0,-4.
2799843939,-1.4451299129,0.9414260289\C,0,-4.3385393354,-0.8703707696,
-1.4129971457\C,0,-5.4904018121,-2.1170224826,0.7969383689\H,0,-3.7631
602214,-1.4407846331,1.8961029872\C,0,-5.5469023829,-1.5451102844,-1.5
495586776\H,0,-3.8753704344,-0.4048237751,-2.2812787251\C,0,-6.1249957
783,-2.1615666927,-0.441465813\H,0,-5.9316469714,-2.6170475899,1.65281
7591\H,0,-6.0310754536,-1.5963998436,-2.5193800594\H,0,-7.0676756522,-
2.6890077865,-0.5481207279\H,0,-2.0825033023,-2.2839680312,-2.09597135
19\H,0,-0.342370727,-2.2659116715,-2.4397596018\C,0,2.1750271063,-0.58
01512643,-1.606431913\C,0,2.4961689041,0.4644014037,-0.5166832915\C,0,
2.3857883022,1.8259160514,-0.7886963113\C,0,2.9183369971,0.0345585751,
0.7726817736\C,0,2.6472673727,2.7671520934,0.1977469818\H,0,2.09520894
52,2.1744800269,-1.775089622\C,0,3.2181652512,1.0179921118,1.739028233
5\C,0,3.0734676206,2.3693942477,1.4575080482\H,0,3.556882464,0.6926543
16,2.7125832122\H,0,3.2916118474,3.1141523917,2.2163023346\C,0,3.44462
25365,-0.826718305,-2.4368726746\O,0,1.7500885171,-1.7850650658,-1.073
8921875\F,0,3.2188711318,-1.7222829602,-3.4126696236\F,0,4.4415867128,
-1.2904777652,-1.6837456779\F,0,3.8721486486,0.3031201356,-3.035291079
1\Cl,0,2.4283762652,4.4730384816,-0.1589250939\C,0,3.2564187063,-1.942
1437803,2.1454038457\O,0,3.5827961481,-1.3996528264,3.205714556\C,0,3.

0901320498,-3.4534069341,2.0844847993\H,0,3.6340429518,-3.912966014,2.
9104395308\H,0,2.0257184165,-3.6976832666,2.1871496752\H,0,3.438083873
8,-3.8541274325,1.1292265585\H,0,2.3389809831,-1.829198468,-0.08368654
36\N,0,2.9518641443,-1.3346572867,0.9768914384\\Version=ES64L-G09RevE.
01\State=1-A\HF=-2694.98079\RMSD=3.018e-09\Dipole=-7.2536426,0.7101841
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864,5.9390729\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

INT8

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\27-Apr-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.0301752548,-0.1009176863,-0.050345
5327\C,0,-0.0160158491,-0.0868980845,1.4602534236\C,0,1.097797957,-0.0
373452484,2.2073090226\H,0,1.0009687323,0.0184100006,3.2875143097\C,0,
2.4921235538,-0.2176515985,1.7059346568\H,0,2.6481060242,0.2177749639,
0.7169371112\H,0,3.2147492951,0.2349657103,2.3882492871\C,0,-0.6914632
166,-1.3393652535,-0.6388203671\O,0,-1.6937003292,-1.7878161309,-0.120
1072499\C,0,-0.0784264535,-1.9151090343,-1.8824348938\H,0,0.0023644928
,-1.1392842732,-2.6525224767\H,0,0.9365743587,-2.2455497199,-1.6371730
067\H,0,-0.6804200025,-2.746818825,-2.2489184525\P,0,-1.5760166665,-0.
2433827935,2.3680857227\C,0,-1.4068458599,0.5594782017,3.9936670806\C,
0,-1.9034322753,1.8382434542,4.2567584901\C,0,-0.7324494666,-0.1501775
582,5.0001756279\C,0,-1.7088373227,2.4111711428,5.5110271087\H,0,-2.45
78138914,2.3827843376,3.4996470145\C,0,-0.5257708098,0.4374574068,6.24
29267389\H,0,-0.3636505937,-1.158256251,4.8159697604\C,0,-1.0142100776
,1.7176782018,6.4976435989\H,0,-2.104453403,3.4008989597,5.7153285697\
H,0,0.0159942865,-0.1112021834,7.006403946\H,0,-0.8591081453,2.1719947
796,7.4712461165\C,0,-1.995993816,-1.9426695735,2.7928447133\C,0,-3.12
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,0,-1.7095835568,2.4058244081,1.2503343013\C,0,-4.8026067976,1.9253880
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\C,0,2.4618843336,-2.5311354722,2.8500818718\C,0,2.6825909053,-1.92514

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1472919633\C,0,1.7787286788,-4.551613765,4.014217535\C,0,1.9745818204,
-3.9210887267,5.2339523785\H,0,1.4432103135,-5.5782641908,3.9763157373
\H,0,1.7850957475,-4.4512781609,6.1619935591\C,0,4.2177479901,-1.92111
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3\C,0,1.2549202815,-5.6220655482,1.2897713377\O,0,0.9232677279,-6.4794
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TS7 -2694.930281

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,0,-1.4392982492,-1.8121892043,-0.1716071074\H,0,-1.2677056328,-2.8418
200094,0.1559564204\C,0,1.22945214,-3.3022052828,-0.7491001167\O,0,0.9
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.7938626383\H,0,2.9536297009,-4.0061998563,-1.8196507096\H,0,1.7126652
141,-5.2455105409,-1.5280333594\H,0,1.4811376927,-3.998038085,-2.79458
43136\P,0,2.0121906278,0.2089027004,0.3663144203\C,0,1.3457534859,1.61
62469286,1.2907743467\C,0,1.8585173473,1.9488342686,2.5484169795\C,0,0
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2636575543\H,0,2.6778512866,1.3796038772,2.9760841577\C,0,-0.278740888
7,3.390607712,1.4836636531\H,0,-0.1442680136,2.0847809864,-0.218801388
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5170824\C,0,2.6148704062,1.9933793794,-1.705800798\C,0,3.8750110045,-0
.0769437862,-1.672592039\C,0,3.2466637778,2.3500499277,-2.8940893381\H
,0,1.8697340536,2.6531869244,-1.277310258\C,0,4.5018532291,0.287061919
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,0,3.4782758429,-3.4576707218,3.2826163717\H,0,5.7080524857,-2.4697258
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,-2.3847971039,2.8788138187,-1.9458582858\H,0,-3.7005797351,3.88681125
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\O,0,-0.2708975837,1.9687427356,-2.441597658\C,0,0.0277488905,0.032899
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2513747882,-1.022284239,-3.7801241044\H,0,-0.1977861837,0.4387467757,-
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INT9

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\H,0,0.7418237572,-0.7975151248,-0.3564486145\C,0,3.7832290253,-0.0498
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TS8

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25978\H,0,-1.6707644361,4.6404359766,1.9970438157\H,0,-2.0344669599,5.
4186036612,0.4249842559\P,0,-2.0713866024,-0.4753987472,0.242551812\C,
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78153,0.9079615061\C,0,-0.5950711771,-2.1388119405,-1.3697378918\C,0,-
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INT10 -2694.981178

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\YIN\17-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.3137280803,0.1138029509,-0.3467004
971\C,0,-0.0568092382,0.2049265698,1.0856143107\C,0,1.1332000524,-0.15
3369352,1.6089201773\C,0,1.4434144275,-0.6617508351,2.9769685619\H,0,2
.5062965518,-0.5262922987,3.1946841943\H,0,0.8762246919,-0.1388081732,
3.7467944244\C,0,-0.1373375256,-1.1394317401,-0.9220221147\O,0,0.15133
35188,-2.212095029,-0.2864423977\C,0,-0.3875714018,-1.3036561045,-2.40
65971801\H,0,-0.5881225007,-0.3545642128,-2.909059913\H,0,0.4855454448
,-1.7790109151,-2.8631386782\H,0,-1.2361558868,-1.979851673,-2.5567780
075\P,0,-1.5705043521,0.5505843342,2.0193183607\C,0,-1.4156405063,0.72
05421895,3.8200339115\C,0,-1.0207449524,1.9293227028,4.4009988667\C,0,
-1.5779679267,-0.4227465662,4.613110021\C,0,-0.7737329504,1.9863207208
,5.7695498479\H,0,-0.9047544817,2.8203063473,3.7906892122\C,0,-1.33131
11065,-0.3555177313,5.9794202157\H,0,-1.8587294085,-1.3695969779,4.157
9405413\C,0,-0.9217855088,0.8453531308,6.55588957\H,0,-0.4633337335,2.
9231385237,6.2211963738\H,0,-1.4306039642,-1.2524257404,6.584126952\H,
0,-0.7118561792,0.8897690746,7.6201574134\C,0,-2.9066834784,-0.6553908
599,1.7913806413\C,0,-4.083809578,-0.4558947327,2.5271640055\C,0,-2.78
06125444,-1.7712519638,0.9605437747\C,0,-5.1430583744,-1.347828983,2.4
053122682\H,0,-4.1672562952,0.3849328973,3.2120072717\C,0,-3.848865034
7,-2.6594935883,0.8493942628\H,0,-1.8571393099,-1.9757412842,0.4286150
448\C,0,-5.0268681874,-2.4494771624,1.5602000558\H,0,-6.0505841967,-1.
1881079731,2.9784118722\H,0,-3.7496175383,-3.5251292506,0.2016053061\H
,0,-5.8508782187,-3.150270345,1.4669880937\C,0,-2.0973016806,2.1657688
919,1.3642843609\C,0,-3.4347059417,2.4800645465,1.115371319\C,0,-1.101
5843647,3.1224457125,1.1281276604\C,0,-3.7743273756,3.7493510621,0.654
2916323\H,0,-4.2100956511,1.7349878606,1.2582582185\C,0,-1.4486482376,
4.3902256726,0.6742005743\H,0,-0.056220593,2.864141258,1.2797641365\C,
0,-2.7853909181,4.7052408646,0.4408243924\H,0,-4.813986215,3.987191677
1,0.4538742719\H,0,-0.6735008637,5.1275298013,0.492144576\H,0,-3.05396
6188,5.6932435752,0.0801263628\H,0,-0.7007633587,0.948366734,-0.919737
9252\C,0,1.0733388286,-2.1883710481,3.0754973539\C,0,0.8283761115,-2.6
056077034,4.5350267434\C,0,1.5686167443,-1.950638284,5.5204231541\C,0,
-0.0581027195,-3.6383364753,4.9302553621\C,0,1.416132479,-2.2570252892
,6.8627078583\H,0,2.2714181535,-1.1729774911,5.2472032237\C,0,-0.19893
48386,-3.9325773759,6.2976679059\C,0,0.5308826701,-3.2480487157,7.2591
226218\H,0,-0.8832538005,-4.716486574,6.5888289596\H,0,0.4139086117,-3
.4896828223,8.3103022485\C,0,2.2567187784,-3.0176388572,2.5512800326\O

,0,-0.0444281954,-2.4739652112,2.2842924318\F,0,2.5372601012,-2.709627
4492,1.2802017792\F,0,1.9840882289,-4.3258909907,2.6058993969\F,0,3.36
89753307,-2.8011242332,3.2726949048\Cl,0,2.3318756656,-1.3702087136,8.
0581197924\N,0,-0.783738671,-4.342072649,3.9633680748\H,0,-0.639365092
4,-3.9993872771,3.0159995378\C,0,-1.6788179564,-5.3696858363,4.1339243
883\O,0,-1.9969838314,-5.8527437604,5.2053275716\C,0,-2.2474591839,-5.
8668715068,2.8175477884\H,0,-3.0139669563,-6.6114538835,3.0281581503\H
,0,-2.6794904559,-5.038947632,2.2465531759\H,0,-1.4569686291,-6.318699
2418,2.2105561267\H,0,1.9145882982,-0.2809763272,0.8612165988\H,0,0.12
89238601,-2.309072966,1.2738848915\\Version=EM64L-G09RevA.01\State=1-A
\HF=-2694.9811783\RMSD=6.522e-09\Dipole=-2.7839578,4.1191056,0.0572519
\Quadrupole=4.6703458,9.2053893,-13.8757351,1.7466342,7.6273881,3.7540
228\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

TS9

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\17-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,1.7104307242,2.2397079183,0.496232652
6\C,0,1.4341316062,1.2234190372,-0.3567584931\C,0,0.2565489418,0.76191
01215,-1.0890646818\H,0,-0.1607474078,-0.2730732338,-0.4460074012\C,0,
-1.1268823977,1.3813486421,-0.9789745413\H,0,-1.1397932289,2.440561552
4,-0.7229983131\H,0,-1.6185722106,1.2703588976,-1.9479318576\C,0,0.894
4597543,3.468543023,0.708161123\O,0,0.208495442,3.9588545563,-0.164491
0567\C,0,1.0160498733,4.1034410902,2.0763270882\H,0,0.5087204537,5.068
3447103,2.0749569227\H,0,0.5476365917,3.4447585274,2.8146124092\H,0,2.
0658315709,4.2314544961,2.3601342966\P,0,2.6824234361,-0.1160588414,-0
.3335209611\C,0,2.8051995168,-0.9503028829,-1.9376766045\C,0,3.8591501
415,-0.676580765,-2.8130887661\C,0,1.8140552099,-1.8763694041,-2.29437
6478\C,0,3.916910055,-1.318457356,-4.0469952559\H,0,4.6389613353,0.025
2118415,-2.5347605859\C,0,1.8807296651,-2.5099132251,-3.5293921359\H,0
,0.9937875064,-2.0917391839,-1.6141466999\C,0,2.9293706438,-2.23085124
83,-4.4049203607\H,0,4.7372005979,-1.1059308359,-4.7246601183\H,0,1.11
15882101,-3.2226848361,-3.8078604139\H,0,2.9775800451,-2.7308686891,-5
.3671919194\C,0,2.2034969269,-1.3807727574,0.8631032869\C,0,2.80918900
87,-2.6455744468,0.8058021034\C,0,1.2272148788,-1.1025230073,1.8208100
532\C,0,2.4490577853,-3.6199064288,1.7265844831\H,0,3.5476357343,-2.86
80357593,0.0389762582\C,0,0.8619369034,-2.0951580414,2.7284546562\H,0,
0.7192273996,-0.1454871483,1.8350978092\C,0,1.4725576877,-3.3433172665
,2.6861650268\H,0,2.9150239159,-4.5991101101,1.6875119999\H,0,0.082895
1881,-1.8862839003,3.4541671213\H,0,1.1806146108,-4.1135308321,3.39350
2664\C,0,4.3184499479,0.5361975731,0.088144484\C,0,5.1349398077,-0.123
0350143,1.0103308063\C,0,4.7678020304,1.7102357463,-0.5339559556\C,0,6
.4000798612,0.3813251008,1.2988789262\H,0,4.7819524886,-1.019835214,1.
5099410613\C,0,6.033166461,2.2055009438,-0.2412301274\H,0,4.1213720957

,2.2422007019,-1.2272912951\C,0,6.8492131537,1.54037672,0.6732284116\H
,0,7.0309885079,-0.1311310268,2.0176933743\H,0,6.3792517333,3.11530675
14,-0.7206440953\H,0,7.8347845166,1.9327439568,0.9033259541\H,0,2.6144
56759,2.1978069594,1.1017607023\C,0,-1.9358214151,0.496872783,0.072474
6271\C,0,-3.3959749034,0.2718150021,-0.3651169746\C,0,-4.0617446685,1.
3021525228,-1.0279395971\C,0,-4.1168535891,-0.9019107718,-0.0428037021
\C,0,-5.3932498564,1.171486868,-1.39559412\H,0,-3.5419804285,2.2277293
244,-1.2526484169\C,0,-5.459375891,-1.0201357039,-0.4293657748\C,0,-6.
0964714202,0.0128829664,-1.1035156694\H,0,-5.9940373657,-1.9259018793,
-0.181069569\H,0,-7.1363851853,-0.0825914251,-1.3973938012\C,0,-1.9925
429218,1.2643542823,1.3987376629\O,0,-1.2183942785,-0.6576704436,0.294
2924285\F,0,-0.7385543835,1.5227147579,1.8630127141\F,0,-2.6095848845,
0.5644094936,2.3578836836\F,0,-2.603131209,2.4545624374,1.3050450106\C
l,0,-6.1904506168,2.4877421139,-2.2309524201\N,0,-3.4527591601,-1.9196
084455,0.6535299393\H,0,-2.4467740801,-1.7233395636,0.746227629\C,0,-3
.9620722447,-3.0717566871,1.1699680423\O,0,-5.125022699,-3.4368772084,
1.0946453992\C,0,-2.9299509051,-3.9098599748,1.9095247259\H,0,-3.14698
5424,-3.8614707924,2.9807019094\H,0,-3.0399617628,-4.9500262714,1.5964
591469\H,0,-1.9029013578,-3.5774742908,1.7380397855\H,0,0.5133141721,0
.4407064935,-2.0994692158\\Version=ES64L-G09RevE.01\State=1-A\HF=-2694
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INT11

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\17-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,0.2249209248,0.3885721061,-0.16124661
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33701,1.9089942232\H,0,1.5057782509,0.1981156526,2.9423045414\C,0,1.82
14634508,-1.650574529,1.9156754267\H,0,1.7520581157,-2.0159535788,0.88
80810559\H,0,2.8283666775,-1.8866850768,2.2636502042\C,0,1.3903221394,
0.393858367,-1.0941025576\O,0,2.4833949177,-0.0455834695,-0.7963315717
\C,0,1.1157616912,0.9793378153,-2.4623234505\H,0,0.7284188568,1.999421
5227,-2.3670297159\H,0,2.0325917191,0.9793179994,-3.0515861858\H,0,0.3
48366153,0.3877627355,-2.9739684377\P,0,-1.296993882,-0.0613039509,2.0
674460885\C,0,-1.2973815587,0.2579902809,3.8666376588\C,0,-0.296125524
1,1.0174473605,4.4825724576\C,0,-2.3289347574,-0.2603618976,4.65336413
47\C,0,-0.2993364486,1.2064933549,5.8613139973\H,0,0.4865803188,1.4859
435275,3.8961576177\C,0,-2.3353050455,-0.0649038786,6.03173808\H,0,-3.
1192386599,-0.8503623857,4.2009066276\C,0,-1.3135130277,0.6570425393,6
.6394522967\H,0,0.4981041965,1.7808135114,6.3219489486\H,0,-3.12223873
14,-0.5143190127,6.6288997323\H,0,-1.3066868721,0.7899450161,7.7166674
959\C,0,-2.7010637954,-1.0942902144,1.4755808634\C,0,-3.9979048357,-0.

6986934947,1.823978001\C,0,-2.5192792078,-2.2250190373,0.6731785858\C,
0,-5.095570463,-1.4541662213,1.4220514358\H,0,-4.15476454,0.2037489858
,2.4084747717\C,0,-3.6248960783,-2.9527072909,0.2394610088\H,0,-1.5163
508569,-2.546819155,0.4226422677\C,0,-4.9104906116,-2.5805172743,0.624
7252148\H,0,-6.0942781879,-1.1518327156,1.720759322\H,0,-3.4747517231,
-3.8254677717,-0.3881504568\H,0,-5.7664819289,-3.1639467633,0.29978269
11\C,0,-2.0625375842,1.5927884848,1.5068092294\C,0,-2.7754268769,1.675
3518205,0.2992806496\C,0,-1.854574852,2.784371179,2.2099638624\C,0,-3.
243684574,2.8912328612,-0.1890690861\H,0,-2.9868591596,0.7735833588,-0
.2706334721\C,0,-2.3275340664,4.004833486,1.7291865728\H,0,-1.33292633
92,2.7761319831,3.1605389941\C,0,-3.0201735631,4.0649535706,0.52575945
2\H,0,-3.7931082587,2.9179392404,-1.1254717589\H,0,-2.1563020644,4.908
7787483,2.3061753159\H,0,-3.3913326661,5.0141144293,0.1517173051\H,0,-
0.7315739303,0.6186331406,-0.6221610527\C,0,0.7313188439,-2.3452599033
,2.7532290128\C,0,0.92755985,-2.2529874636,4.2825536661\C,0,2.13064424
58,-1.8009166374,4.820745525\C,0,-0.1198440006,-2.5966600164,5.1794170
778\C,0,2.3054334775,-1.6788693953,6.1936625247\H,0,2.9561016353,-1.52
28483858,4.1770934761\C,0,0.0848115209,-2.4903425011,6.5609120669\C,0,
1.292384383,-2.0305477176,7.0692372979\H,0,-0.7210078259,-2.7640765185
,7.2271089884\H,0,1.4396094095,-1.9450801908,8.140483669\C,0,0.7963869
927,-3.8280195925,2.3203472178\O,0,-0.5318851967,-1.8775810343,2.38490
39174\F,0,0.5170062283,-3.95946904,1.010656102\F,0,-0.059189237,-4.623
8902605,2.9710359323\F,0,2.0281211384,-4.3197963896,2.5190415406\Cl,0,
3.8253334707,-1.0780358426,6.8131539046\N,0,-1.3515807004,-3.016638745
1,4.660362457\H,0,-1.41645226,-2.9044383802,3.651173171\C,0,-2.5188881
324,-3.2851547333,5.3161118919\O,0,-2.6657971483,-3.2943441382,6.52813
48672\C,0,-3.6812356113,-3.5824440237,4.3816435276\H,0,-4.5316148269,-
2.96431247,4.682100078\H,0,-3.4556928088,-3.4019744083,3.3258145131\H,
0,-3.9740050976,-4.6280780339,4.5105855331\H,0,2.393393925,0.368743758
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Cl1F3N1O3P1)]\\@

TS10

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\WEIY\17-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
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,-0.049902,1.313233\C,-0.420808,-1.153337,1.966577\H,-0.091645,-1.8910
07,1.22656\C,0.787247,-0.45475,2.57371\H,0.433426,0.170385,3.395108\H,
1.511333,-1.1515,2.993058\C,-2.273606,0.737425,3.471537\O,-1.635333,0.
02537,4.247606\C,-3.301211,1.714228,4.030875\H,-4.245611,1.662352,3.47
9972\H,-3.472601,1.48996,5.084355\H,-2.921708,2.738143,3.941737\P,-1.7
74001,-0.344391,-0.42065\C,-0.817546,-1.644372,-1.229598\C,-1.246068,-

2.97516,-1.154485\C,0.405851,-1.329581,-1.828507\C,-0.440822,-3.986433
,-1.666289\H,-2.199232,-3.221474,-0.695578\C,1.20436,-2.348917,-2.3377
49\H,0.729892,-0.295813,-1.894549\C,0.784846,-3.673907,-2.250866\H,-0.
770073,-5.018589,-1.604821\H,2.160986,-2.102627,-2.786544\H,1.416178,-
4.466908,-2.639479\C,-1.717465,1.151589,-1.440569\C,-1.789879,1.025889
,-2.832402\C,-1.680891,2.420089,-0.850726\C,-1.868918,2.164955,-3.6294
19\H,-1.770929,0.042387,-3.295918\C,-1.772107,3.551262,-1.655743\H,-1.
545587,2.51389,0.221748\C,-1.877512,3.426339,-3.039776\H,-1.920064,2.0
63979,-4.708692\H,-1.741528,4.535438,-1.198848\H,-1.94251,4.314331,-3.
661035\C,-3.496562,-0.927322,-0.375675\C,-4.357043,-0.734063,-1.459607
\C,-3.936534,-1.647828,0.742143\C,-5.645942,-1.258069,-1.426721\H,-4.0
3342,-0.162119,-2.323699\C,-5.223071,-2.176018,0.764247\H,-3.28345,-1.
776764,1.600057\C,-6.078141,-1.980026,-0.317775\H,-6.313327,-1.096632,
-2.267189\H,-5.559437,-2.730499,1.634305\H,-7.084956,-2.385273,-0.2933
27\H,-2.856591,1.351468,1.492582\C,1.34112,0.441921,1.439966\C,2.44975
,-0.196884,0.575873\C,3.099344,-1.365586,0.970965\C,2.832507,0.385652,
-0.657636\C,4.096348,-1.93717,0.190322\H,2.845371,-1.856303,1.900887\C
,3.85179,-0.192302,-1.422669\C,4.491711,-1.350125,-1.000081\H,4.140967
,0.28459,-2.349071\H,5.282199,-1.794737,-1.595438\C,1.891042,1.701035,
2.136895\O,0.253505,0.813559,0.650589\F,0.915364,2.356807,2.777131\F,2
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41416,0.728178\N,2.142452,1.50889,-1.148308\H,1.277325,1.708573,-0.647
003\C,2.694168,2.531101,-1.890444\O,3.784816,2.481563,-2.424822\C,1.78
1493,3.735336,-1.999342\H,2.293414,4.513854,-2.563715\H,0.853205,3.458
237,-2.508122\H,1.522782,4.10564,-1.001913\H,-1.006198,-1.640034,2.749
326\\Version=ES64L-G09RevE.01\State=1-A\HF=-2694.9696979\RMSD=8.573e-1
0\Dipole=-4.4171375,-1.2723853,-3.5190941\Quadrupole=-1.7433407,13.631
9048,-11.8885641,-3.5437607,9.1094894,-1.6757913\PG=C01 [X(C34H30Cl1F3
N1O3P1)]\\@

INT12

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H30Cl1F3N1O3P1\YIN\20-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,0.2873201299,0.4123543321,0.243362067
8\C,0,0.1093771725,0.2176229074,1.5570582145\C,0,1.0895029129,0.178046
0049,2.6836483662\H,0,1.1703389214,1.1872547841,3.1102491276\C,0,0.396
8932138,-0.779661969,3.6546478526\H,0,0.5982159948,-1.8158255263,3.368
0549722\H,0,0.7131148635,-0.6360026328,4.6845721339\C,0,1.6116147179,0
.747691171,-0.3077434382\O,0,2.5620152912,1.057147769,0.3968612073\C,0
,1.7352984434,0.6872079139,-1.8110079989\H,0,1.5284967184,-0.329971813
6,-2.1621933373\H,0,0.9955604649,1.3532812314,-2.2676553696\H,0,2.7392
467759,0.9887043002,-2.1102244554\P,0,-0.0776992111,3.6984403574,1.459
4748128\C,0,1.4014244145,4.55030861,2.1524337106\C,0,2.5834814332,3.80
25656379,2.2489805985\C,0,1.3891075965,5.8683083259,2.6166730631\C,0,3

.7346578575,4.3736347743,2.7838015279\H,0,2.6086334929,2.7781856125,1.
8795708371\C,0,2.5392125012,6.4295542599,3.167520175\H,0,0.4798759745,
6.4588049703,2.5510256464\C,0,3.7132104918,5.6865014933,3.2498067611\H
,0,4.6473379056,3.7881534866,2.8417094898\H,0,2.517158924,7.4534187139
,3.5288336696\H,0,4.6083984532,6.1282432593,3.6771896761\C,0,-1.386289
3807,4.9877514607,1.605243694\C,0,-1.6324039726,5.9739681277,0.6416379
199\C,0,-2.1983191093,4.9393262201,2.7440544938\C,0,-2.6820506492,6.87
29865222,0.8073198916\H,0,-1.0077237417,6.0329257866,-0.2450784941\C,0
,-3.249986987,5.8371536477,2.9087576949\H,0,-2.0161993089,4.1783558695
,3.5004573092\C,0,-3.4973510689,6.8010972162,1.9358810558\H,0,-2.86604
11947,7.6302509094,0.0508706254\H,0,-3.8888523871,5.7626891144,3.78298
03702\H,0,-4.3258036393,7.4929542631,2.0535061793\C,0,0.2497265412,3.7
705820827,-0.3594647027\C,0,-0.7985682857,3.3982098918,-1.2133243543\C
,0,1.4638423104,4.164977875,-0.925968237\C,0,-0.6550398572,3.465371691
8,-2.5952535349\H,0,-1.7491173829,3.0826584917,-0.7872457226\C,0,1.615
2799915,4.2142443704,-2.3122838855\H,0,2.2939856484,4.4479069162,-0.28
60178224\C,0,0.5567875861,3.877827932,-3.1500988238\H,0,-1.4866313641,
3.19437291,-3.2391903998\H,0,2.5644759305,4.5301901521,-2.7348233646\H
,0,0.6744755067,3.9289312816,-4.2282057302\H,0,-0.561470437,0.33766618
37,-0.4293899779\C,0,-1.0952367929,-0.4681691016,3.4219044138\C,0,-1.7
059128227,0.526216523,4.4141868219\C,0,-1.3718987717,0.3275442591,5.75
71082051\C,0,-2.6643883894,1.5178985863,4.0962872819\C,0,-1.9161271176
,1.1079645868,6.7636414623\H,0,-0.6989368589,-0.4723621138,6.040641148
2\C,0,-3.1958678535,2.3032133299,5.1332993787\C,0,-2.8253433552,2.1069
322523,6.4542166747\H,0,-3.9311633157,3.055304078,4.8876216644\H,0,-3.
2509842368,2.722497463,7.2391290278\C,0,-1.9327258308,-1.7521238273,3.
421713678\O,0,-1.1412840838,-0.0231239264,2.0535597184\F,0,-1.50270733
66,-2.603751173,2.4845851523\F,0,-3.2183002204,-1.4903906457,3.1808664
341\F,0,-1.8409648966,-2.367989278,4.6067832894\Cl,0,-1.4551728407,0.8
211411714,8.4186514117\N,0,-3.062553791,1.7379301876,2.7703498943\H,0,
-2.4926723227,1.2894416654,2.0666786168\C,0,-4.1142794565,2.5046121862
,2.3192901157\O,0,-4.9203487463,3.0661998175,3.0368926264\C,0,-4.16994
21251,2.640785417,0.8121979473\H,0,-5.2139539093,2.6098980229,0.497065
4737\H,0,-3.7637567776,3.6257209711,0.5522508589\H,0,-3.6026190424,1.8
682068208,0.2856600434\H,0,2.0805183361,-0.1362199607,2.3624371621\\Ve
rsion=EM64L-G09RevA.01\State=1-A\HF=-2695.019837\RMSD=8.366e-09\Dipole
=0.9304482,0.3889708,-1.6778848\Quadrupole=-9.4510996,1.6559155,7.7951
842,-5.6823879,8.3049804,2.0483791\PG=C01 [X(C34H30Cl1F3N1O3P1)]\\@

3a

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C16H15Cl1F3N1O3\WEIY\18-Mar-2017
\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluene)
\\Title Card Required\\0,1\C,0,-0.293179105,-0.0395735535,-0.179812885
3\C,0,-0.1778425251,0.1059704603,1.1481723104\C,0,1.0504729913,0.21993

38463,2.0039028769\H,0,1.758669231,0.9282308864,1.5735695617\C,0,0.490
2166002,0.6557080712,3.3630602502\H,0,1.0214032716,0.2158965225,4.2094
291223\H,0,0.5241538795,1.7430914137,3.4587262359\C,0,0.8959470492,-0.
11253501,-1.0464117127\O,0,2.0333265828,-0.0981379542,-0.6066973728\C,
0,0.6255473101,-0.2109748822,-2.5329066801\H,0,0.0282301396,-1.1033710
765,-2.7487418175\H,0,0.0478397303,0.6562820692,-2.8703110871\H,0,1.57
01886007,-0.2590708079,-3.0744869035\H,0,-1.2817539784,-0.1025807243,-
0.6234331165\C,0,-0.9848897408,0.2177950954,3.32079183\C,0,-1.95409867
9,1.1045767913,4.0911403662\C,0,-1.4479594765,1.7393123005,5.226856376
8\C,0,-3.3276360733,1.2387831295,3.7815541662\C,0,-2.2605547442,2.5228
710401,6.0297656429\H,0,-0.4063362699,1.6172631325,5.5024265197\C,0,-4
.1271672147,2.0536952794,4.5980450186\C,0,-3.6005872179,2.6885587673,5
.7124211236\H,0,-5.1726464243,2.1684860836,4.3528145962\H,0,-4.2345996
441,3.3101860476,6.3352492866\C,0,-1.1165590421,-1.2294130085,3.817310
4891\O,0,-1.3007490492,0.1853353588,1.9208266539\F,0,-0.2924209849,-2.
0440894871,3.1422588836\F,0,-2.3594767573,-1.6922695599,3.6538685456\F
,0,-0.8036776612,-1.3116057173,5.1131093509\Cl,0,-1.5883916552,3.30197
1793,7.4368393124\N,0,-3.8729847411,0.5766236807,2.6735433902\H,0,-3.2
131956403,0.0815475942,2.090905278\C,0,-5.1984871463,0.4478010709,2.31
67129234\O,0,-6.1290974102,0.9626748595,2.90307906\C,0,-5.3926886962,-
0.4385977873,1.1002012015\H,0,-5.1878100283,-1.48121393,1.3634508072\H
,0,-6.426350427,-0.3492450764,0.7692485541\H,0,-4.7193209379,-0.153663
5213,0.2862418735\H,0,1.5583918963,-0.7473571619,2.0413244189\\Version
=ES64L-G09RevE.01\State=1-A\HF=-1658.822356\RMSD=5.033e-09\Dipole=0.45
99855,-0.1655504,-1.2126164\Quadrupole=-11.3948432,2.0120836,9.3827596
,4.8242828,10.8611595,1.4737497\PG=C01 [X(C16H15Cl1F3N1O3)]\\@

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 9 (Table S2) and archive entries

Table S2[a]

	E_{tot} (E_h)	$H_{298,toluene}$	$G_{298,toluene}$
INT13	-2771.391869	-2770.75207	-2770.873009
TS11	-2771.383549	-2770.750353	-2770.867758
INT14	-2771.391786	-2770.750765	-2770.86943
TS12	-2771.359008	-2770.7235	-2770.841925
TS12-1	-2771.342256	-2770.70698	-2770.824925
INT15	-2771.399054	-2770.757567	-2770.879959
INT15-1	-2771.394265	-2770.754015	-2770.875675
TS13	-2771.38391	-2770.744295	-2770.865421
INT16	-2771.417623	-2770.776133	-2770.897006
TS14	-2771.409475	-2770.769534	-2770.886403
INT17	-2771.421525	-2770.778516	-2770.895766
TS15	-2771.387064	-2770.748375	-2770.862388
INT18	-2771.414614	-2770.770288	-2770.882231
TS16	-2771.380442	-2770.74284	-2770.855771
INT19	-2771.422493	-2770.779666	-2770.899048
TS17	-2771.414479	-2770.772504	-2770.890555
INT20	-2771.438304	-2770.795877	-2770.920162
H_2O	-76.4260345	-76.4007154	-76.4221494
4a	-1658.810519	-1658.492371	-1658.570908

a. SMD/M06-2X/6-311+G(d,p)//M06-2X/6-31G(d)

INT13

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\05-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.2493405061,0.2219307079,0.06857768
23\C,0,-0.0949271446,0.2936516249,1.3979160781\C,0,1.2717282771,0.2183
07336,2.053685145\H,0,1.3986119334,1.1274950904,2.6593886532\C,0,2.426
5360248,0.1179052997,1.0600035213\H,0,2.4073007988,-0.8398210335,0.530
4405323\H,0,2.381676233,0.9178404104,0.3130569726\H,0,3.3773989861,0.1

84274143,1.5943304898\C,0,-1.5169452738,0.5097552223,-0.6723212237\O,0
,-2.3742355382,1.189627641,-0.1383723911\C,0,-1.6259320687,-0.03839629
82,-2.0614833598\H,0,-0.8279810339,0.4172501457,-2.6601177474\P,0,-1.5
251229027,0.493468417,2.5210061644\C,0,-0.9961630436,-0.2205332494,4.1
145611814\C,0,-0.165700072,0.5363320484,4.9535292123\C,0,-1.3759302864
,-1.5078400925,4.501367742\C,0,0.2938870082,-0.0006666635,6.1493252255
\H,0,0.1057672297,1.5520970717,4.6795272641\C,0,-0.9133458147,-2.04020
56161,5.7032165551\H,0,-2.0454058163,-2.0934699308,3.8808029268\C,0,-0
.0761226708,-1.2919452747,6.5232825598\H,0,0.9367943822,0.5913545841,6
.7925731209\H,0,-1.2159802962,-3.0399079582,5.9974444658\H,0,0.2820213
785,-1.7087840627,7.459359831\C,0,-2.9360303886,-0.4738920651,1.936161
0426\C,0,-4.189053704,0.1312798424,1.8440389465\C,0,-2.7396018806,-1.7
784651422,1.471400003\C,0,-5.2529283655,-0.5786735377,1.2961012873\H,0
,-4.3186350696,1.1681135713,2.1376875962\C,0,-3.8131665174,-2.48627318
2,0.9416765379\H,0,-1.7511985903,-2.2316232196,1.4987343611\C,0,-5.067
9842788,-1.8851458794,0.8539135473\H,0,-6.2169620473,-0.0929574812,1.1
88964314\H,0,-3.6655970896,-3.4988491044,0.5800066462\H,0,-5.898209499
5,-2.4320951357,0.4184706219\C,0,-1.9631500272,2.198940225,2.888036452
4\C,0,-1.7037817044,3.2290243339,1.9812127497\C,0,-2.5933376946,2.4624
035652,4.1166888305\C,0,-2.0486489049,4.538668382,2.3191577281\H,0,-1.
2735918172,3.0296272365,1.0024820599\C,0,-2.9503516461,3.7646686565,4.
431607546\H,0,-2.795672117,1.658277698,4.819153828\C,0,-2.6662286386,4
.7988190523,3.5370300852\H,0,-1.8354944191,5.3361931458,1.6107552856\H
,0,-3.4430330532,3.9742558792,5.3758377867\H,0,-2.9378824138,5.8186034
33,3.7924827965\H,0,0.6157298259,0.0378019359,-0.5583602798\H,0,1.3052
700172,-0.6154218643,2.7654423275\H,0,-1.4655896724,-1.1229358632,-2.0
433993955\C,0,-3.5777982464,3.315065333,-1.2971049367\O,0,-3.300945963
8,4.0732001275,-0.3995737853\C,0,-4.885032338,2.4937314733,-1.11745252
24\F,0,-5.8980121437,3.0843017388,-1.7792286596\F,0,-4.8006021054,1.23
62459057,-1.5714335138\F,0,-5.2302142996,2.4360516228,0.1709231305\C,0
,-2.8157564845,3.096412603,-2.5423166735\C,0,-1.3992719708,3.213303714
6,-2.5455882674\C,0,-3.511200039,2.7076359501,-3.700199806\C,0,-0.7394
560775,2.9152638954,-3.7643624409\C,0,-2.8231818008,2.4437705663,-4.86
56443967\H,0,-4.5923840362,2.6212748537,-3.6913335996\C,0,-1.429582230
9,2.5463851887,-4.9013230629\H,0,0.341938044,2.9737980287,-3.783281469
6\H,0,-0.8992621108,2.3357885492,-5.8248553222\Cl,0,-3.6959627977,1.97
7057747,-6.3076127313\N,0,-0.7199421121,3.6293483272,-1.4245923086\C,0
,0.4470483596,3.0483888177,-1.1160681662\O,0,0.9446142945,2.0208741053
,-1.6296219856\C,0,1.1771278657,3.6869874718,0.0572161125\H,0,0.707840
7976,4.6223708436,0.3692151323\H,0,1.1687944103,2.9851998305,0.9025568
871\H,0,2.2242048483,3.8503380896,-0.2145137303\H,0,-2.6020346889,0.19
90808818,-2.4847843205\H,0,-1.2596077706,5.2445764954,-0.610293902\O,0
,-1.1638754616,6.1320099018,-0.1877589048\H,0,-0.4346771246,6.53110398
47,-0.6799608965\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771.3918692\
RMSD=5.582e-09\Dipole=1.0640345,-4.5845995,5.1395503\Quadrupole=-5.161

2811,-0.8471974,6.0084785,2.5842078,5.1353008,-3.1637303\PG=C01 [X(C34
H32Cl1F3N1O4P1)]\\@

TS11 -2771.383549

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\15-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.0582328059,0.0121646459,-0.0415702
437\C,0,-0.0395826764,-0.0370279704,1.297260781\C,0,1.2577144119,-0.10
18653725,2.0823668633\H,0,1.2720152724,0.7562409983,2.7702102257\C,0,2
.5098017789,-0.0632570288,1.2098788524\H,0,2.5897964688,-0.9671952712,
0.5978545537\H,0,2.5033738497,0.800635461,0.5365024521\H,0,3.397384578
7,-0.0108454402,1.8450421403\C,0,-1.263017704,0.280055741,-0.887887956
\O,0,-2.2289845891,0.8354612336,-0.3964940227\C,0,-1.169823424,-0.1404
963311,-2.3220166092\H,0,-2.0989674134,0.080078896,-2.8470877077\P,0,-
1.5801686125,-0.0134241039,2.2826307174\C,0,-1.1568822015,-0.804216118
1,3.870537279\C,0,-0.4852407471,-0.0529680573,4.8453232971\C,0,-1.4474
287614,-2.1486452136,4.1151915728\C,0,-0.0965365625,-0.6484091844,6.03
87006041\H,0,-0.2793170248,1.0005074654,4.6769275686\C,0,-1.0560512218
,-2.7394925796,5.314726107\H,0,-1.9936823144,-2.7349082973,3.383911780
8\C,0,-0.3780841329,-1.9937180489,6.2728939254\H,0,0.4225834072,-0.060
0611936,6.7883885653\H,0,-1.2897766443,-3.7830481486,5.4986652579\H,0,
-0.0751416845,-2.4560539399,7.2071144181\C,0,-2.8611158808,-1.02227705
67,1.5023505347\C,0,-4.1518109149,-0.5105105133,1.3747077256\C,0,-2.52
90966247,-2.2634603197,0.9492014961\C,0,-5.1186769584,-1.2534703187,0.
7044896864\H,0,-4.3849050822,0.4836534482,1.7430141249\C,0,-3.50579674
95,-3.0043709179,0.2928303751\H,0,-1.5095856333,-2.6381704648,1.006329
1394\C,0,-4.7992309909,-2.4986650677,0.1715770476\H,0,-6.113918533,-0.
8407548966,0.5771747438\H,0,-3.2525410766,-3.9672320164,-0.1391793265\
H,0,-5.55398973,-3.0699667911,-0.3594269462\C,0,-2.1584708936,1.634734
8079,2.7069776013\C,0,-1.8646234486,2.7337825352,1.8973331956\C,0,-2.9
251611403,1.7853832118,3.8751186152\C,0,-2.3139700372,3.9993020181,2.2
745478507\H,0,-1.3204897923,2.6247923227,0.9620458014\C,0,-3.381657166
6,3.0460086397,4.2299881195\H,0,-3.1534836806,0.9277314903,4.502451782
8\C,0,-3.0645450213,4.1496916453,3.4351849753\H,0,-2.0751353202,4.8446
913291,1.6303832081\H,0,-3.9777233958,3.1691026163,5.1287199767\H,0,-3
.4150761143,5.1360971865,3.7239399963\H,0,0.8768553526,-0.0527141469,-
0.5872247569\H,0,1.2657401355,-0.9910559495,2.7244661508\H,0,-0.333584
8744,0.4054806635,-2.7753796483\C,0,-3.395970523,3.0260697416,-1.53671
00198\O,0,-3.3245217683,3.7841826863,-0.5973742142\C,0,-4.6336285095,2
.0863391738,-1.5506657088\F,0,-5.6336035561,2.6733457293,-2.236184416\
F,0,-4.4143928509,0.8966210035,-2.1212997405\F,0,-5.0714461651,1.86954
42067,-0.3089665614\C,0,-2.4696788847,2.9368511247,-2.6798541633\C,0,-
1.0705555256,3.1175073099,-2.5028267828\C,0,-3.0076841181,2.620662795,
-3.9396452674\C,0,-0.2631490743,2.9712585229,-3.6601097498\C,0,-2.1798
760753,2.5008284058,-5.035040123\H,0,-4.0768198882,2.4827288312,-4.062

6456584\C,0,-0.7996473933,2.6781674454,-4.8972886121\H,0,0.8078965911,
3.0869898771,-3.5499654837\H,0,-0.1576813318,2.5851100704,-5.76778765\
Cl,0,-2.8547551949,2.1282453703,-6.6040841847\N,0,-0.5497495265,3.4427
021785,-1.2737454192\C,0,0.6332030467,2.9316522652,-0.9000126802\O,0,1
.2670184575,2.0040315657,-1.4484184915\C,0,1.185192965,3.5113061316,0.
3947764911\H,0,0.63195694,4.3927542038,0.7267748746\H,0,1.1344050052,2
.7423483968,1.1780228314\H,0,2.240584441,3.760559071,0.2540169249\H,0,
-0.9431937091,-1.212416259,-2.3726140666\H,0,-1.1011820142,5.015064975
4,-0.4901363891\O,0,-1.3826570681,5.8748502217,-0.0904065773\H,0,-2.32
18683397,5.8860720333,-0.3223111638\\Version=ES64L-G09RevE.01\State=1-
A\HF=-2771.3943549\RMSD=5.917e-09\Dipole=-0.0206937,-5.4569198,5.04925
66\Quadrupole=-4.9465294,-4.9672918,9.9138212,-7.0524564,5.4600024,-1.
3392432\PG=C01 [X(C34H32Cl1F3N1O4P1)]\\@

INT14

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\08-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.3009083869,-1.0624193854,0.3428203
039\C,0,-0.8458054234,-1.2648671505,1.556173565\C,0,-0.417309398,-2.47
46962197,2.3587483757\H,0,0.6522654922,-2.6466896568,2.1899673669\C,0,
-1.2105509066,-3.7154711328,1.9240512001\H,0,-2.2845313922,-3.53182492
82,1.9991114053\H,0,-0.9846206344,-3.9632545846,0.8826454124\H,0,-0.95
2458078,-4.5741852155,2.5502827938\C,0,-0.7063862383,0.0476258636,-0.5
204207784\O,0,-1.8260218808,0.5530032807,-0.4046487646\C,0,0.275849759
,0.5729375259,-1.5352080322\H,0,0.3202123941,1.664222009,-1.4478665115
\P,0,-2.1406500573,-0.1012017003,2.3450153716\C,0,-3.3009816002,1.3716
724101,2.1589811605\C,0,-4.2872266754,1.4219412552,1.1724863209\C,0,-3
.2527695681,2.4064300323,3.0997191283\C,0,-5.2015464252,2.4731551022,1
.1243709602\H,0,-4.3585107996,0.6340981839,0.4364308377\C,0,-4.1890824
364,3.4379512929,3.0805085945\H,0,-2.4816885261,2.4119881559,3.8637975
476\C,0,-5.1674946071,3.4762690258,2.0897042869\H,0,-5.9482726037,2.48
76589675,0.3358246395\H,0,-4.1459189016,4.2167426437,3.8362260409\H,0,
-5.8929751464,4.2843009994,2.0676677398\C,0,-0.6062989463,1.0294213274
,2.6794777001\C,0,0.4567417295,0.6209927468,3.4982724637\C,0,-0.384562
1495,2.1293069949,1.8431464982\C,0,1.6689181573,1.3069606002,3.5080166
966\H,0,0.3446100811,-0.2459712991,4.1460978753\C,0,0.8340200427,2.805
5077619,1.8224465085\H,0,-1.1742549415,2.446681279,1.1698082671\C,0,1.
8638484294,2.4000374666,2.6670266229\H,0,2.467256333,0.9780527613,4.16
74626458\H,0,0.9683303785,3.6376602161,1.1357183133\H,0,2.8140581746,2
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C,0,-3.2833905679,-1.8682305763,4.2121862971\C,0,-2.0728031477,-0.0332
037434,5.1881376789\C,0,-3.5993780214,-2.3332909214,5.4856922161\H,0,-
3.6623015979,-2.3814953924,3.3377581\C,0,-2.4006624936,-0.4927549756,6
.4603546296\H,0,-1.473433937,0.865026592,5.0956939808\C,0,-3.157846704
5,-1.649878518,6.6140430388\H,0,-4.2041499488,-3.2286478838,5.59244520

82\H,0,-2.0609266379,0.0578389434,7.3322040901\H,0,-3.4090399818,-2.01
0997387,7.6068646032\H,0,0.5190257324,-1.6926371814,-0.0005514281\H,0,
-0.5549620225,-2.3115007566,3.4309577347\H,0,1.2725291426,0.1523167939
,-1.3912156309\C,0,-3.5594580222,0.8573546893,-2.4661879098\O,0,-4.388
2472196,1.4635832311,-1.8271737715\C,0,-3.633289159,-0.688203224,-2.43
70249089\F,0,-4.3729395222,-1.1226678017,-3.4672803811\F,0,-2.43217708
57,-1.2667565531,-2.5308338434\F,0,-4.2063094406,-1.1022588949,-1.3076
495357\C,0,-2.5031235674,1.4747983141,-3.2910923067\C,0,-1.9053119022,
2.6879934024,-2.890075713\C,0,-2.0807107009,0.8241693887,-4.4571056626
\C,0,-0.8703255843,3.213865666,-3.6773106512\C,0,-1.0667087195,1.37230
22075,-5.2203818949\H,0,-2.5458388196,-0.1053942873,-4.7678040247\C,0,
-0.4559977091,2.5623079878,-4.8275214807\H,0,-0.3876138115,4.131281080
8,-3.3708928571\H,0,0.3410797324,2.9807779566,-5.4329193586\Cl,0,-0.54
59679941,0.5711787301,-6.67594146\N,0,-2.325251182,3.3337511704,-1.728
1237631\C,0,-1.4941232654,4.0311017717,-0.8690765596\O,0,-0.3028522258
,4.1818350548,-1.0713989031\C,0,-2.2163992458,4.6223002624,0.317750339
8\H,0,-2.7505223541,5.5240810473,-0.0004729594\H,0,-2.9463155177,3.923
4192467,0.734929007\H,0,-1.4845224779,4.8902222103,1.0802683695\H,0,-0
.0743191677,0.3298780552,-2.5455590665\O,0,-3.3039255945,-1.1409113806
,1.6024199143\H,0,-3.1589562774,-1.126683446,0.6423917642\H,0,-3.22893
42675,3.0520520708,-1.3619431439\\Version=ES64L-G09RevE.01\State=1-A\H
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drupole=-7.7527388,3.5798426,4.1728962,-8.3533226,1.4329487,-5.1123129
\PG=C01 [X(C34H32Cl1F3N1O4P1)]\\@

TS12

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\11-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0.977769,-0.056969,-2.390834\C,2.184793
,-0.489261,-1.999657\C,3.020331,-1.406491,-2.864343\H,2.832506,-1.1450
05,-3.911123\C,2.652333,-2.877674,-2.63614\H,2.796626,-3.166945,-1.591
116\H,1.602038,-3.050753,-2.887979\H,3.272809,-3.529711,-3.256674\C,0.
140621,0.764173,-1.470416\O,0.676136,0.98687,-0.357026\C,-1.208151,1.0
37282,-1.789308\H,-1.667326,1.851642,-1.226818\P,2.796646,0.036023,-0.
342816\C,2.039389,-0.73786,1.113294\C,0.884527,-1.506914,0.968816\C,2.
606809,-0.542092,2.374551\C,0.243348,-2.021314,2.09201\H,0.451531,-1.6
74556,-0.013638\C,1.965867,-1.063293,3.496892\H,3.534706,0.01443,2.484
282\C,0.781557,-1.783676,3.357101\H,-0.699642,-2.549419,1.97361\H,2.39
2032,-0.897932,4.481373\H,0.272954,-2.165089,4.23686\C,3.132599,1.8183
43,-0.254825\C,3.612582,2.467463,-1.394699\C,2.884483,2.539119,0.91285
7\C,3.868748,3.835146,-1.353802\H,3.775103,1.915027,-2.317639\C,3.1445
1,3.904864,0.945589\H,2.454607,2.047104,1.77925\C,3.640858,4.552329,-0
.182913\H,4.236584,4.339525,-2.241631\H,2.937929,4.466705,1.850732\H,3
.834098,5.619847,-0.155182\C,4.486433,-0.71283,-0.264775\C,4.613501,-2
.050374,0.136681\C,5.639896,-0.007668,-0.624828\C,5.856516,-2.673405,0

.147868\H,3.738054,-2.607669,0.459048\C,6.885176,-0.63155,-0.606261\H,
5.5796,1.037394,-0.908787\C,6.995744,-1.965478,-0.227478\H,5.934828,-3
.709742,0.46086\H,7.770287,-0.067698,-0.883248\H,7.967257,-2.449698,-0
.212954\H,0.588481,-0.323428,-3.371981\H,4.088337,-1.256004,-2.684385\
H,-1.490774,0.962125,-2.83646\C,-3.235387,-1.310363,0.723527\O,-2.8623
77,-1.430552,1.918337\C,-3.586467,-2.634449,0.023914\F,-4.788621,-3.06
7325,0.445047\F,-3.650133,-2.535415,-1.312158\F,-2.690434,-3.576571,0.
322502\C,-4.075329,-0.104462,0.322887\C,-3.649029,1.1678,0.757618\C,-5
.216652,-0.209717,-0.464359\C,-4.340885,2.311088,0.357187\C,-5.906805,
0.939329,-0.835837\H,-5.572179,-1.175225,-0.803548\C,-5.4721,2.196545,
-0.444867\H,-3.985851,3.282529,0.673984\H,-6.019776,3.080606,-0.752811
\Cl,-7.343464,0.791511,-1.82261\N,-2.522758,1.229637,1.598276\C,-1.598
552,2.238622,1.662806\O,-1.673679,3.276874,1.02921\C,-0.431378,1.91107
9,2.574676\H,0.131946,2.825459,2.763541\H,-0.761794,1.468268,3.518566\
H,0.212561,1.190807,2.056799\H,-1.678078,-0.053513,-1.109939\O,-1.8144
5,-1.005747,-0.253743\H,-2.374396,0.36693,2.12725\H,-1.274843,-0.63931
4,0.468098\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771.3590082\RMSD=4
.594e-09\Dipole=7.2953307,0.3150117,-0.7868019\Quadrupole=-2.8997585,-
6.5142946,9.4140531,-6.6698219,-4.1382285,2.353845\PG=C01 [X(C34H32Cl1
F3N1O4P1)]\\@

TS12-1 -2771.342256

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\YIN\12-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,0.3680325714,-2.0494584535,-1.2953597
948\C,0,1.6667193153,-1.9427628155,-0.8944722359\C,0,2.6462885499,-2.9
998046993,-0.9372400852\H,0,3.6359137884,-2.6818478015,-1.2809288789\C
,0,2.1995236928,-4.3376935154,-1.4788504543\H,0,1.3315720148,-4.713564
0395,-0.9247743944\H,0,1.9135104832,-4.2989735556,-2.5407918144\H,0,3.
0008530507,-5.0750666765,-1.3825045297\C,0,-0.6589429441,-1.042339684,
-1.0865784024\O,0,-0.6199946681,-0.2550354144,-0.140494763\C,0,-1.7578
483683,-0.9661132367,-2.1233210347\H,0,-2.3906240587,-0.0969388166,-1.
9368102374\P,0,2.3489417772,-0.3759467168,-0.1328072587\C,0,1.95169159
28,0.4335590785,1.463705994\C,0,0.9088841787,0.0054184853,2.2889033034
\C,0,2.7692522372,1.4891613357,1.8762840873\C,0,0.6969456471,0.6222052
187,3.5183745373\H,0,0.2593164271,-0.8024633549,1.9725323351\C,0,2.550
3504548,2.1045214071,3.1088651199\H,0,3.5833482706,1.8327484432,1.2440
023007\C,0,1.5197980912,1.6685648873,3.9344423754\H,0,-0.1200757171,0.
2781922624,4.1439331329\H,0,3.1936668338,2.922195496,3.4188627694\H,0,
1.3539373699,2.1433703984,4.8966555718\C,0,1.7205863681,0.8594793585,-
1.3799102596\C,0,1.5978920423,0.4893134762,-2.7274038039\C,0,1.3121933
179,2.1438256719,-1.0123372012\C,0,1.0808981704,1.3746548428,-3.669007
1297\H,0,1.8936348615,-0.5057369017,-3.0485164086\C,0,0.7769745747,3.0
265167948,-1.9485688961\H,0,1.3909693497,2.4627393945,0.0199632059\C,0
,0.6578741577,2.6429685389,-3.279664204\H,0,0.9968874312,1.0644397853,

-4.7064458688\H,0,0.4230112895,4.0010505418,-1.6265405269\H,0,0.233273
2909,3.3259291697,-4.0088110247\C,0,4.1679961108,-0.2447292186,-0.3860
240203\C,0,5.0636085527,-0.4744396559,0.6678518067\C,0,4.6732372091,0.
1398085933,-1.6333008048\C,0,6.4313332869,-0.3205174657,0.467392375\H,
0,4.6748747435,-0.8006569364,1.6239872241\C,0,6.0452849901,0.268269546
,-1.8320987726\H,0,4.0059996898,0.3499279975,-2.4602233399\C,0,6.92768
67083,0.0435048958,-0.7814162507\H,0,7.1127422512,-0.4970730439,1.2939
047654\H,0,6.4180380923,0.5580200935,-2.8094640111\H,0,7.9972058745,0.
1540252631,-0.9339143308\H,0,0.105329425,-2.9017161879,-1.9188950089\H
,0,2.8715671094,-2.8203507003,0.379377986\H,0,-1.3098815492,-0.8841313
513,-3.1192237812\C,0,-2.7211456867,-0.6491413499,1.6461562399\O,0,-2.
1196348675,-0.1292397064,2.5623864523\C,0,-2.6491184682,-2.195865093,1
.5776620267\F,0,-3.776205782,-2.729688258,2.0732912644\F,0,-2.50457724
04,-2.6479159771,0.3264345183\F,0,-1.6260356523,-2.6367000908,2.298235
9635\C,0,-3.5068435108,0.0626296307,0.6235391165\C,0,-3.2097568305,1.4
086912134,0.2859821344\C,0,-4.5287088826,-0.6239838256,-0.0458636822\C
,0,-3.9506669451,2.0165871578,-0.7408955613\C,0,-5.2516102145,0.005593
6133,-1.0405134652\H,0,-4.7643929692,-1.6499196125,0.212816356\C,0,-4.
9569725269,1.3207807714,-1.3929923746\H,0,-3.7190336285,3.0332153218,-
1.0223178899\H,0,-5.5233171059,1.8048019797,-2.1818535743\Cl,0,-6.5228
213736,-0.8531346778,-1.8635541846\N,0,-2.1968167421,2.0770638833,0.95
74425305\C,0,-1.5812990675,3.2618150592,0.6059845416\O,0,-1.9155957835
,3.9606898426,-0.3311192688\C,0,-0.4614371366,3.6392077795,1.551991640
3\H,0,-0.8860369233,4.0747086304,2.4629749351\H,0,0.1358436615,2.76975
82338,1.8402752452\H,0,0.1693620739,4.386840201,1.0695654904\H,0,-2.36
56851618,-1.8769795307,-2.1040487704\O,0,2.9634589116,-2.0041354595,1.
3723601862\H,0,2.2205758498,-2.2032972256,1.9631289282\H,0,-1.75739293
63,1.5521097547,1.7057378394\\Version=EM64L-G09RevA.01\State=1-A\HF=-2
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INT15

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\22-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
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066086,1.8685783008\H,0,1.8142379386,0.3625407704,2.4919070256\C,0,2.4
242532182,-0.8280161559,0.798717353\H,0,2.0735903974,-1.6761617933,0.2
02243091\H,0,2.6242204868,0.0064102927,0.1190887607\H,0,3.3687933305,-
1.1153757711,1.2674177675\C,0,-1.5755872589,0.4639037785,-0.3585037496
\O,0,-2.2765404704,0.7888920444,0.7262446844\C,0,-1.989010891,0.550470
5015,-1.6327928038\H,0,-2.9667056361,0.9284071337,-1.9038896504\P,0,-1
.3168915946,0.5593216796,2.3971836129\C,0,-0.3767854472,0.3575112383,4
.0364078496\C,0,0.3706305953,1.4089109415,4.5818620069\C,0,-0.27277404

06,-0.8986468698,4.6510818857\C,0,1.174622962,1.2197287676,5.704727329
\H,0,0.3328271977,2.3951059498,4.1280874271\C,0,0.5284646045,-1.094319
8525,5.7722940768\H,0,-0.8228692386,-1.7455313098,4.2475773379\C,0,1.2
53353329,-0.0319496603,6.3062614209\H,0,1.7377277416,2.0556481322,6.10
9013668\H,0,0.58584778,-2.0781722971,6.2284800631\H,0,1.8755745569,-0.
1798887103,7.183787122\C,0,-2.6698908014,-0.6271717998,2.8091887895\C,
0,-3.3001247256,-0.5929747095,4.0565139455\C,0,-3.0971485123,-1.555993
3047,1.8546726455\C,0,-4.3732776597,-1.4390539119,4.326437838\H,0,-2.9
539285413,0.0902796239,4.8254719953\C,0,-4.138359761,-2.4320747597,2.1
438751687\H,0,-2.6280941331,-1.5859057895,0.8768951018\C,0,-4.79450608
44,-2.3610663755,3.3716487764\H,0,-4.8741722058,-1.3818578814,5.287505
0705\H,0,-4.4510294571,-3.1566509456,1.3981081709\H,0,-5.6276196145,-3
.0232217905,3.5833677219\C,0,-1.6367765981,2.3618051251,2.5764262853\C
,0,-1.1895919292,3.2325799675,1.5798409427\C,0,-2.3005315753,2.8718066
102,3.690998414\C,0,-1.3885048041,4.6031515381,1.7105180111\H,0,-0.695
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89345\H,0,-2.64434224,2.2080336645,4.4779319422\C,0,-2.0643097817,5.10
8183592,2.8190094033\H,0,-1.0276840834,5.2748660488,0.9378343509\H,0,-
3.0650638981,4.6264122215,4.6638530614\H,0,-2.2331759914,6.1765558565,
2.9121394871\H,0,0.4564110917,-0.3097388852,-0.7722705321\H,0,1.262056
2511,-1.2845245558,2.5551428453\H,0,-1.3179554242,0.2551519397,-2.4308
889668\C,0,-6.9218982534,-1.4089952656,0.7476966236\O,0,-6.8144393465,
-0.4001116075,1.411449435\C,0,-7.6729787228,-2.5842709701,1.4361003683
\F,0,-8.7749215264,-2.917916505,0.7556423666\F,0,-6.9023931773,-3.6859
6697,1.5256780895\F,0,-8.0266291876,-2.2452807998,2.6669972759\C,0,-6.
436790949,-1.5926027717,-0.6287694091\C,0,-5.82368409,-0.5299889284,-1
.3553503309\C,0,-6.6142372784,-2.8486706677,-1.2418280745\C,0,-5.41778
63654,-0.7927689515,-2.6806860588\C,0,-6.1980555722,-3.0665723903,-2.5
360652556\H,0,-7.0864213067,-3.6632771141,-0.7093762198\C,0,-5.5984162
747,-2.0353538657,-3.2567291812\H,0,-4.9660000107,0.0006529251,-3.2547
174382\H,0,-5.2690911408,-2.210296231,-4.2756152371\Cl,0,-6.4213289373
,-4.6291672857,-3.2726044103\N,0,-5.6180695883,0.7158799392,-0.7788491
233\H,0,-5.7174762837,0.8026727476,0.2348956493\C,0,-5.2514397952,1.88
39937678,-1.4375758192\O,0,-5.1279989908,1.9688368885,-2.6456575827\C,
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324,0.3365165228\H,0,-3.9429058344,2.9496688656,-0.1403040711\H,0,-5.0
289249539,3.9631239869,-1.1232242373\H,0,-5.044675156,0.6453052166,2.3
834190711\O,0,-4.7788901451,1.4495531122,1.9135575357\H,0,-3.949760111
9,1.2129293124,1.45490704\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771
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le=0.4858112,0.7531602,-1.2389713,2.1220824,-1.1936804,4.6586991\PG=C0
1 [X(C34H32Cl1F3N1O4P1)]\\@

INT15-1

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\24-May-20

17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
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183701,1.5102629844\H,0,1.5115904064,-0.8362355816,0.7798535651\C,0,0.
9292306423,-1.4295861073,2.8158533384\H,0,1.5989576875,-0.8675066322,3
.4799870666\H,0,0.004608334,-1.6161324621,3.3683720279\H,0,1.400640041
3,-2.3987241572,2.623271596\C,0,-1.7302701112,0.5180118466,-0.79115873
08\O,0,-2.6065906682,-0.2393802815,-0.2108134879\C,0,-2.1492237505,1.3
142309029,-1.9985978593\H,0,-2.8089748207,2.1243827136,-1.662030688\P,
0,-1.7895712809,0.283339775,2.1771981333\C,0,-2.8586919209,-1.14038060
89,2.4922660609\C,0,-2.4988661273,-2.3690574491,1.9376990319\C,0,-4.05
17973472,-1.0152040743,3.2118247204\C,0,-3.3254416936,-3.4754979266,2.
1101739465\H,0,-1.5931764515,-2.4425169484,1.3442897372\C,0,-4.8739994
009,-2.1249553981,3.3820581643\H,0,-4.3558245589,-0.0510928913,3.61157
69427\C,0,-4.5103604945,-3.3535525975,2.8340471145\H,0,-3.0568294991,-
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\H,0,-5.1600506262,-4.2144096473,2.9576158927\C,0,-2.7777937864,1.7545
594428,1.7548720426\C,0,-2.186692363,3.0164310789,1.8475233335\C,0,-4.
1031911182,1.6331660248,1.3264591008\C,0,-2.9136057797,4.1535001194,1.
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\C,0,-4.236824188,4.0348058407,1.0932867346\H,0,-2.4431559781,5.129611
7763,1.5673460966\H,0,-5.8573138686,2.6770789633,0.676479922\H,0,-4.80
4884707,4.9224338934,0.8316121885\C,0,-1.0562689455,0.7520054608,3.800
3919094\C,0,-1.6425051272,0.3812963949,5.0132314896\C,0,0.1063684464,1
.5339681111,3.8230240909\C,0,-1.0863985593,0.7933724046,6.2221665415\H
,0,-2.5236683587,-0.2509618574,5.0274069599\C,0,0.6554479023,1.9501465
065,5.0309983664\H,0,0.6027578857,1.7925304578,2.8914333453\C,0,0.0586
144498,1.5823440268,6.234663025\H,0,-1.5501778556,0.48875301,7.1551486
381\H,0,1.5583038532,2.5530513039,5.0304457579\H,0,0.4918312754,1.9011
860446,7.1775535389\H,0,0.3220090734,1.215223465,-0.6552875017\H,0,-1.
2928552898,1.7527306296,-2.5182144822\C,0,-2.4801853134,-2.9026815759,
-1.6325002582\O,0,-3.4547622537,-3.2849723045,-1.019812407\C,0,-1.1197
187615,-3.478914729,-1.1557286061\F,0,-0.4999347695,-4.1437872394,-2.1
380190249\F,0,-0.2960233273,-2.5162059542,-0.7225575441\F,0,-1.3069622
657,-4.3326972382,-0.1480504232\C,0,-2.4781444148,-2.0481238127,-2.831
8253656\C,0,-3.6904336669,-1.6599741294,-3.4663605921\C,0,-1.247220673
3,-1.6555200782,-3.3857477297\C,0,-3.612448948,-0.9842953526,-4.699312
1931\C,0,-1.2079435143,-0.9469641104,-4.5679998554\H,0,-0.3146523186,-
1.8930176335,-2.8912374702\C,0,-2.3879102091,-0.6344160115,-5.23979407
06\H,0,-4.5282152293,-0.7227199826,-5.2082812998\H,0,-2.3454022691,-0.
0951112724,-6.1804453758\Cl,0,0.3256248694,-0.441778152,-5.2260259036\
N,0,-4.9071834807,-1.9158253503,-2.8533147012\C,0,-6.1742418222,-1.746
9499934,-3.3846605816\O,0,-6.4005501141,-1.4434698906,-4.5399776403\C,
0,-7.2676862185,-2.017560975,-2.374046658\H,0,-7.3431247706,-3.0962480

118,-2.2004447558\H,0,-7.0386098689,-1.5372807069,-1.4186920142\H,0,-8
.2116338316,-1.6565752447,-2.7808972911\H,0,-2.7200591625,0.6967970539
,-2.6966137004\H,0,-4.876676494,-2.0913903126,-1.8487621235\H,0,-4.786
7643615,-2.0018949638,0.4643827939\O,0,-5.092245897,-1.2203431955,-0.0
230788883\H,0,-4.24334566,-0.7614307379,-0.2434847181\\Version=ES64L-G
09RevE.01\State=1-A\HF=-2771.3942652\RMSD=1.566e-09\Dipole=0.7836217,1
.0614841,3.8681613\Quadrupole=-2.9045562,3.9976705,-1.0931142,5.339320
9,-3.3850095,-0.4047702\PG=C01 [X(C34H32Cl1F3N1O4P1)]\\@

TS13

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\23-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.2343653564,1.2209639437,-0.1323419
302\C,0,-1.5331004555,1.2923472276,-0.4394125268\C,0,-2.1549307876,2.3
695401894,-1.2878628331\H,0,-2.6022101314,1.8836063182,-2.1633657896\C
,0,-1.1539945471,3.4151055934,-1.7665007917\H,0,-0.6822952896,3.936630
3153,-0.9264507728\H,0,-0.3801439936,2.9339875662,-2.3720358901\H,0,-1
.6605960153,4.1620446956,-2.3830436761\C,0,0.2308361717,0.0223647505,0
.5940041278\O,0,-0.6712470173,-0.874639038,0.7225353221\C,0,1.55847135
23,-0.0558094704,0.9864863546\H,0,1.8833190303,-0.8795511055,1.6103100
685\P,0,-2.5643982491,-0.0504219601,0.3037840157\C,0,-4.26765532,0.643
8788984,-0.0750884483\C,0,-4.7565607129,0.4959840771,-1.3824974065\C,0
,-5.0635864111,1.3226303287,0.85233179\C,0,-5.9862243134,1.0243391005,
-1.7552288917\H,0,-4.1695543748,-0.0478941761,-2.1195262615\C,0,-6.301
904931,1.8492385455,0.4815871036\H,0,-4.7353432053,1.4378018954,1.8797
675517\C,0,-6.7640908394,1.7062441081,-0.8208307466\H,0,-6.3409056439,
0.8973614259,-2.7734906287\H,0,-6.9056128981,2.3682541964,1.2199878615
\H,0,-7.7277950857,2.1158027075,-1.1076841681\C,0,-2.6067852053,-0.044
2795073,2.1258377354\C,0,-2.7474009188,-1.23515505,2.8395616466\C,0,-2
.455591089,1.165204925,2.8076414455\C,0,-2.7698360234,-1.2080229784,4.
22990493\H,0,-2.8075513059,-2.1822966598,2.3124771378\C,0,-2.468752455
3,1.1835795362,4.2001082443\H,0,-2.320239853,2.0924212144,2.2553504985
\C,0,-2.6337662566,-0.0009105156,4.9117671436\H,0,-2.8767150495,-2.136
2320222,4.7824600332\H,0,-2.3455497482,2.1248220028,4.7264933648\H,0,-
2.6439178627,0.0147718312,5.997055827\C,0,-2.8178703233,-1.644295565,-
0.5389172097\C,0,-1.999957661,-1.9880183892,-1.6129748419\C,0,-3.88785
11162,-2.4622750374,-0.1687366273\C,0,-2.2390621667,-3.1754882261,-2.2
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504,-3.6617614939,-0.8416085075\H,0,-4.5610045867,-2.1599201825,0.6299
900568\C,0,-3.2746854239,-4.0186821951,-1.9057150031\H,0,-1.6059195713
,-3.442019947,-3.1396300896\H,0,-4.9195753666,-4.3088966036,-0.5441890
117\H,0,-3.4477285301,-4.9501699368,-2.4361050732\H,0,0.4852865314,1.9
763364801,-0.4344738743\H,0,-2.9839522736,2.8416641568,-0.7465046245\H
,0,2.0950498995,0.8828926608,1.0746514984\C,0,2.6241664966,-0.37972332
21,-0.9854260663\O,0,2.1453998547,0.4101885799,-1.8271606023\C,0,2.161

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087388179\F,0,2.225833255,-2.6004919823,-0.0595475081\F,0,0.9078051437
,-1.8736482256,-1.6056692757\C,0,3.9794757913,-0.1478970601,-0.3866116
227\C,0,4.4625998646,1.1722772927,-0.2092219278\C,0,4.7826775102,-1.22
50553742,-0.0011972124\C,0,5.7218013139,1.3747895561,0.3667185519\C,0,
6.0318909607,-0.9996601522,0.5543902015\H,0,4.449360564,-2.2463386286,
-0.1322004978\C,0,6.5031207955,0.2923309343,0.7464776685\H,0,6.0750786
29,2.3850934467,0.5151115255\H,0,7.4812997217,0.4519835815,1.187161763
5\Cl,0,7.0209582963,-2.3608616905,1.0205441065\N,0,3.6466585159,2.2388
19706,-0.6073163669\H,0,2.8928177775,1.959614687,-1.2312009061\C,0,3.7
739047671,3.5697799002,-0.2893717695\O,0,4.6630178323,4.0372216232,0.3
958378128\C,0,2.6504945844,4.4305111824,-0.8384774312\H,0,3.0604419319
,5.4006997731,-1.1216478089\H,0,2.1411960797,3.9802266212,-1.694760283
9\H,0,1.9166083503,4.5950501488,-0.0425438915\H,0,0.4534013391,0.34947
5803,-2.6235971104\O,0,-0.3842190665,0.4847775774,-3.1103140784\H,0,-0
.160105725,0.2743387118,-4.0267493905\\Version=ES64L-G09RevE.01\State=
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0.4990133\PG=C01 [X(C34H32Cl1F3N1O4P1)]\\@

INT16

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\22-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
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8367669278,1.8595324663\H,0,1.5090730961,0.1001073351,2.3631853316\C,0
,2.3697474753,-1.2324458262,0.9238158538\H,0,2.1468707436,-2.160252343
5,0.3875235849\H,0,2.5492365523,-0.4324490152,0.2004035451\H,0,3.28259
27069,-1.3893412803,1.504064683\C,0,-1.4178003825,-0.1776466673,-0.924
1956924\O,0,-2.4086795028,0.1806033241,-0.3080431508\C,0,-1.3552694065
,-0.1729296341,-2.4284171841\H,0,-2.3567403369,0.058463924,-2.79556190
56\P,0,-1.5050221253,-0.1739740626,2.2266048285\C,0,-0.9457656754,-0.4
145224296,3.9469991298\C,0,-0.1650016754,0.5967525256,4.5229782287\C,0
,-1.2506707213,-1.5596276729,4.6867260226\C,0,0.3192160615,0.451658673
7,5.816999734\H,0,0.0575869095,1.4995979844,3.9595432542\C,0,-0.765750
4634,-1.6966861508,5.9858791641\H,0,-1.8750988448,-2.3395144274,4.2633
00413\C,0,0.0206156121,-0.6967490572,6.5487640287\H,0,0.9253937327,1.2
377039869,6.2553581312\H,0,-1.0089518809,-2.5863365796,6.5577445548\H,
0,0.396499962,-0.8073618722,7.5609778709\C,0,-2.8589662476,-1.34495929
19,1.9546553003\C,0,-4.1813162132,-0.9134702264,1.843257404\C,0,-2.546
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,-3.629222442,1.6304976923\H,0,-1.5124028621,-3.0360863304,1.881156793
7\C,0,-4.8871563229,-3.2016333875,1.541117135\H,0,-6.219881884,-1.5104
332642,1.5472998657\H,0,-3.3223088242,-4.6823523312,1.5319862363\H,0,-

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,2.1940952502\C,0,-1.3791135746,2.4514799322,1.3271426218\C,0,-2.97988
32799,1.9921954674,3.1027013808\C,0,-1.769148044,3.78882846,1.34486309
98\H,0,-0.5733484332,2.128793246,0.6701562909\C,0,-3.3615283479,3.3279
435377,3.1044834737\H,0,-3.4286025747,1.2961605523,3.8082186751\C,0,-2
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15059,-2.7632054405\C,0,-0.2491311358,0.801378216,-2.9716888467\O,0,0.
8764037629,0.7014229161,-2.2135402078\C,0,-0.8026154985,2.2342943041,-
2.85520199\F,0,0.0699747038,3.1309604442,-3.3282521023\F,0,-1.96487053
48,2.4128363643,-3.506751118\F,0,-1.0341704011,2.5586678344,-1.5627418
763\C,0,-0.0239129155,0.5484424357,-4.4878915847\C,0,1.2310806694,0.77
49359306,-5.104595479\C,0,-1.0922282706,0.1482918278,-5.2890624214\C,0
,1.3756672508,0.5707363028,-6.4846694965\C,0,-0.930411006,-0.050779371
8,-6.6531256129\H,0,-2.0755641029,-0.0066177473,-4.8606476441\C,0,0.29
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4.4474638115,1.8857670431,-3.4764251261\H,0,4.8208151846,2.9024294381,
-3.622919229\H,0,3.9323064659,1.8206963337,-2.5146679869\H,0,5.3114063
607,1.2164869897,-3.4706894086\H,0,1.1854716515,1.4669622726,-0.798232
4413\O,0,1.4884242707,1.8221965302,0.0884646047\H,0,1.9457183956,2.644
780923,-0.1316329862\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771.4176
228\RMSD=5.824e-09\Dipole=-2.4536218,-2.0364899,8.1360451\Quadrupole=-
5.0314166,15.8671077,-10.8356911,2.2695716,11.0339076,0.387207\PG=C01
[X(C34H32Cl1F3N1O4P1)]\\@

TS14

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\23-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0.577064,-1.431484,0.354558\C,1.478216,
-1.110237,-0.599982\C,1.476798,-1.656782,-2.013019\H,2.493854,-1.96703
5,-2.279973\C,0.931502,-0.671985,-3.051757\H,-0.080302,-0.349685,-2.78
4417\H,1.556915,0.225688,-3.122688\H,0.900069,-1.133392,-4.043045\C,-0
.375022,-2.579899,0.126513\O,0.057253,-3.71748,0.174699\C,-1.794659,-2
.257649,-0.258673\H,-2.415174,-3.142854,-0.099098\P,2.629469,0.185006,
-0.215938\C,1.977047,1.822065,-0.624519\C,0.597611,1.963875,-0.811536\
C,2.826747,2.93633,-0.696996\C,0.079748,3.228479,-1.092315\H,-0.076009
,1.110229,-0.7061\C,2.294499,4.190194,-0.97103\H,3.897648,2.822878,-0.
541351\C,0.920933,4.333595,-1.173905\H,-0.990685,3.34131,-1.240734\H,2
.949102,5.053992,-1.027548\H,0.507208,5.31395,-1.390686\C,4.131759,-0.

112055,-1.192866\C,4.91523,-1.222188,-0.853821\C,4.444322,0.646336,-2.
324956\C,6.022829,-1.545994,-1.628399\H,4.64041,-1.854359,-0.01488\C,5
.557095,0.314071,-3.094056\H,3.82209,1.488135,-2.612294\C,6.348466,-0.
775467,-2.743083\H,6.627015,-2.40781,-1.364848\H,5.800074,0.905685,-3.
970669\H,7.214413,-1.032617,-3.345022\C,3.031663,0.150037,1.553179\C,3
.096219,1.336036,2.290517\C,3.284423,-1.082584,2.173579\C,3.432406,1.2
92579,3.640425\H,2.869662,2.28885,1.822911\C,3.619485,-1.110448,3.5229
32\H,3.201292,-2.014636,1.615043\C,3.697971,0.07268,4.254876\H,3.47497
7,2.21372,4.212406\H,3.808378,-2.063947,4.005517\H,3.954324,0.042374,5
.309353\H,0.878135,-2.57341,-2.024012\H,-1.767442,-2.035654,-1.335091\
C,-2.251174,-0.953263,0.447621\O,-1.193169,-0.095324,0.45171\C,-2.5852
7,-1.3419,1.898025\F,-2.930074,-0.283085,2.635564\F,-3.58144,-2.241099
,1.981854\F,-1.50532,-1.906629,2.488763\C,-3.528648,-0.36172,-0.185759
\C,-3.79867,1.027106,-0.126862\C,-4.458582,-1.199236,-0.796419\C,-4.97
3407,1.528423,-0.703081\C,-5.617841,-0.685012,-1.362001\H,-4.291068,-2
.270263,-0.830974\C,-5.880617,0.675284,-1.319185\H,-5.168122,2.590341,
-0.650078\H,-6.790325,1.068794,-1.759956\Cl,-6.75431,-1.771362,-2.1302
2\N,-2.867843,1.855258,0.515826\H,-2.014544,1.330522,0.776162\C,-2.984
978,3.173593,0.840106\O,-3.917676,3.901146,0.534809\C,-1.822519,3.6995
18,1.667497\H,-2.193788,3.927189,2.670843\H,-0.9932,2.991675,1.743737\
H,-1.466502,4.63375,1.22642\H,0.645331,-1.064386,1.372028\H,3.233882,-
4.601082,0.279909\O,2.973494,-3.672528,0.204602\H,1.996919,-3.689685,0
.195296\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771.4094749\RMSD=4.58
5e-09\Dipole=6.8086426,0.4554468,-0.8303025\Quadrupole=-8.481694,1.090
1959,7.3914981,6.1116,0.3191774,-0.7665366\PG=C01 [X(C34H32Cl1F3N1O4P1
)]\\@

INT17

1\1\GINC-SHI_02\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\YIN\22-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,0.0833787366,-0.3141996436,-0.2685198
056\C,0,0.0911133549,-0.7674938063,1.1413215029\C,0,1.4292745078,-1.00
57394087,1.831315076\H,0,1.2756594826,-1.6374940093,2.7157296994\C,0,2
.2232063315,0.2396261577,2.2508293921\H,0,2.3325055053,0.9466878265,1.
4192755178\H,0,1.7135799017,0.7714360631,3.0619334538\H,0,3.2238695248
,-0.0295425489,2.6062726242\C,0,1.1690772806,-0.9950247517,-1.10489850
01\O,0,1.225275176,-2.1714077619,-1.3573762353\C,0,2.1792689685,0.0558
955343,-1.5280766008\H,0,2.6156609014,-0.1654396589,-2.5032084688\P,0,
-1.2921427964,-0.4454603769,2.0972813592\C,0,-1.4857276387,1.204245258
,2.8906541334\C,0,-0.621530758,2.2305513789,2.5076297384\C,0,-2.460120
0169,1.4498751419,3.8688007686\C,0,-0.723227546,3.4927273638,3.0963312
859\H,0,0.1337166221,2.0369761416,1.7493650883\C,0,-2.5687210912,2.709
9495905,4.4447649274\H,0,-3.1288170217,0.6505090809,4.182153452\C,0,-1
.6984091446,3.7316651934,4.0589949322\H,0,-0.0471698886,4.2876935711,2
.7938125564\H,0,-3.3268579408,2.8957779183,5.1993664297\H,0,-1.7802097

898,4.7136608678,4.5150679896\C,0,-1.3044094698,-1.5879186206,3.522394
4522\C,0,-1.6545747681,-2.928575332,3.3301366323\C,0,-0.8481507444,-1.
1636695122,4.7747422227\C,0,-1.5732885756,-3.8249447489,4.3911452543\H
,0,-1.9657075113,-3.2855455816,2.3528679278\C,0,-0.7626173748,-2.06708
45433,5.8300207031\H,0,-0.5527466402,-0.1299834743,4.9273051396\C,0,-1
.1321002688,-3.3955248034,5.640622589\H,0,-1.8476608054,-4.8631716867,
4.2357557326\H,0,-0.4033416766,-1.731258065,6.7976616596\H,0,-1.066153
2078,-4.0995761724,6.4644708132\C,0,-2.8037335704,-0.6566431557,1.0910
008856\C,0,-3.824601756,0.2997041651,1.0912065705\C,0,-2.9256607154,-1
.7962614059,0.2815341751\C,0,-4.9600831485,0.1132804343,0.3069514804\H
,0,-3.7370145814,1.1971266812,1.6941155275\C,0,-4.0659972331,-1.974642
0484,-0.4958387155\H,0,-2.1265775531,-2.5354262174,0.2411087837\C,0,-5
.0846255888,-1.0248240753,-0.4833094624\H,0,-5.7444238512,0.8637550112
,0.3125412717\H,0,-4.1523862659,-2.8596577687,-1.1182655575\H,0,-5.970
1212424,-1.1679560796,-1.0952164929\H,0,2.052639092,-1.6188323486,1.16
37952195\H,0,2.973476781,0.0702895642,-0.7712019287\C,0,1.3675971454,1
.3550966639,-1.4540885242\O,0,0.3918117514,1.1199205744,-0.4483830218\
C,0,0.6431549341,1.5186903314,-2.7992880148\F,0,-0.2162332956,2.541781
1955,-2.7926706369\F,0,1.5150525193,1.7145157047,-3.7937642032\F,0,-0.
0596920267,0.4069532469,-3.0854267248\C,0,2.1521519422,2.6211976101,-1
.1308581574\C,0,1.5521431335,3.7743327791,-0.5680245891\C,0,3.50714699
,2.6505360695,-1.45606908\C,0,2.352704011,4.8952318378,-0.3057419719\C
,0,4.2767165941,3.7764072064,-1.2038797812\H,0,3.9760930919,1.78861912
55,-1.918252154\C,0,3.7045194107,4.896606854,-0.6202436624\H,0,1.89628
84685,5.7687510225,0.1364754417\H,0,4.3102294744,5.7726283881,-0.41484
01145\Cl,0,5.9697427786,3.772359282,-1.6216916058\N,0,0.1767080869,3.7
836748746,-0.2948605462\H,0,-0.3026749692,2.9137713837,-0.4865852681\C
,0,-0.6021764347,4.8010822006,0.2003981347\O,0,-0.1809311656,5.8821740
33,0.5711480569\C,0,-2.0815363112,4.4646622648,0.2252242589\H,0,-2.536
7660343,4.8091178392,-0.7087861966\H,0,-2.2681746776,3.3922029445,0.33
38209272\H,0,-2.5422455484,4.999471523,1.0563194687\H,0,-0.8836146536,
-0.4837111795,-0.7553411433\H,0,-0.1328533451,-2.8588055693,0.89060793
95\O,0,-0.3115386747,-3.7677534223,0.5748809048\H,0,0.1127809986,-3.75
22997274,-0.2970573294\\Version=EM64L-G09RevA.01\State=1-A\HF=-2771.42
15248\RMSD=3.538e-09\Dipole=-1.9143027,-0.0653447,1.6377141\Quadrupole
=11.1676123,-21.6562714,10.4886591,-2.3066049,0.2906557,0.8932602\PG=C
01 [X(C34H32Cl1F3N1O4P1)]\\@

TS15

1\1\GINC-LOCALHOST\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\YIN\24-Mar
-2017\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=tol
uene)\\Title Card Required\\0,1\C,0,0.0840703801,-1.8203268419,0.16409
21577\C,0,1.1802608795,-1.499573276,-0.8298006194\C,0,0.8492774013,-1.
5312983997,-2.32869011\H,0,1.8019400187,-1.5192225195,-2.8730273452\C,
0,-0.0958706146,-0.492897688,-2.9380953132\H,0,-1.0357396602,-0.408488

3395,-2.3791999843\H,0,0.3509071243,0.5049046922,-2.9720463369\H,0,-0.
3448764851,-0.7773186966,-3.965343122\C,0,-0.7204737312,-3.0311294233,
-0.3219232659\O,0,-0.285591184,-4.1314102975,-0.5119137028\C,0,-2.1478
835026,-2.5646413567,-0.5626010207\H,0,-2.8745542863,-3.3437569729,-0.
3280087778\P,0,2.3857010387,-0.2399453982,-0.2699550746\C,0,1.75753929
79,1.4843417347,-0.4750251854\C,0,0.4152797567,1.7828443751,-0.7054583
718\C,0,2.6746368925,2.5413709087,-0.3531522945\C,0,-0.0067308621,3.10
76796054,-0.8385962483\H,0,-0.3114946332,0.983975262,-0.780888053\C,0,
2.2514568401,3.8597346613,-0.4618872207\H,0,3.7252580179,2.3290845786,
-0.1703306845\C,0,0.907884225,4.1461434638,-0.7131680753\H,0,-1.057542
5446,3.3200481921,-1.0163163782\H,0,2.9710880079,4.665865966,-0.358439
241\H,0,0.5776601627,5.1762676334,-0.804408416\C,0,3.8871672543,-0.098
4909714,-1.2948709404\C,0,5.1393530782,-0.4813653771,-0.8076741366\C,0
,3.77696713,0.4878358592,-2.5578223845\C,0,6.2713687256,-0.2733168801,
-1.5865819989\H,0,5.2061695423,-0.9724509998,0.1562893274\C,0,4.911465
787,0.6562153558,-3.3493173749\H,0,2.8103260935,0.8250081625,-2.924656
3617\C,0,6.1588467268,0.2835490213,-2.8608028928\H,0,7.2450696947,-0.5
625961542,-1.2038222823\H,0,4.81636105,1.0914466931,-4.3389736791\H,0,
7.045805244,0.4270656994,-3.4703955895\C,0,2.6578318852,-0.3544117416,
1.5413365682\C,0,2.1869472638,0.6928648216,2.347612656\C,0,3.240762250
4,-1.4799941871,2.1454487644\C,0,2.3020468451,0.623997682,3.7322371592
\H,0,1.7347741269,1.5717923415,1.9062478296\C,0,3.3520439683,-1.531359
4976,3.5331748416\H,0,3.5779660742,-2.2914644159,1.4967515715\C,0,2.88
70039652,-0.488754232,4.329166963\H,0,1.937363429,1.446889192,4.340336
7593\H,0,3.8047394795,-2.4047030333,3.9926841804\H,0,2.9781735626,-0.5
428541425,5.4099837664\H,0,0.4429027789,-2.5333958539,-2.5179947197\H,
0,-2.2312341208,-2.3019897241,-1.6235886219\C,0,-2.2464491069,-1.30522
44905,0.3018634046\O,0,-0.9133062274,-0.7929604386,0.3597174189\C,0,-2
.6479678249,-1.7527388491,1.7173513446\F,0,-2.5962428378,-0.7548099125
,2.6042182155\F,0,-3.888729589,-2.2480662804,1.7211364743\F,0,-1.81850
00371,-2.7173743099,2.151145258\C,0,-3.1950490961,-0.2227422579,-0.198
7405013\C,0,-3.1084609984,1.1342685161,0.2011718988\C,0,-4.2245781856,
-0.6147137418,-1.0537168893\C,0,-4.0324730162,2.0522002682,-0.32300523
31\C,0,-5.1351580248,0.3071861107,-1.5475915987\H,0,-4.3296609498,-1.6
552232738,-1.3399949066\C,0,-5.0346883358,1.6431371302,-1.1913747843\H
,0,-3.962731008,3.088475813,-0.0266221364\H,0,-5.7434296995,2.36462432
85,-1.5829758867\Cl,0,-6.4007094801,-0.2212845618,-2.6211840932\N,0,-2
.1230296871,1.5370016004,1.1131099194\H,0,-1.4696128374,0.8175555409,1
.3937669278\C,0,-1.8855212904,2.7930264122,1.6215492816\O,0,-2.5124324
249,3.7918215946,1.3201270218\C,0,-0.7211639011,2.8506130319,2.5897681
108\H,0,-0.4487118168,1.8740197281,2.9983817654\H,0,0.1416688563,3.272
9667352,2.0616396205\H,0,-0.9856066091,3.5296864178,3.401989159\H,0,0.
5254343508,-2.0626859859,1.1383340371\H,0,1.9926166405,-2.3449306329,-
0.6663953671\O,0,3.4302196514,-2.6303181866,-0.2920081122\H,0,3.963416
1109,-2.8248067875,-1.0754970706\\Version=EM64L-G09RevA.01\State=1-A\H

F=-2771.3870643\RMSD=1.759e-09\Dipole=0.9842973,2.1678292,-0.3438623\Q
uadrupole=0.7429697,-17.2173645,16.4743947,18.6136534,0.9979067,-1.784
6947\PG=C01 [X(C34H32Cl1F3N1O4P1)]\\@

INT18

1\1\GINC-LOCALHOST\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\YIN\23-Mar
-2017\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=tol
uene)\\Title Card Required\\0,1\C,0,-0.0368714294,0.9304952688,-1.7436
359331\C,0,-1.1473047501,-0.1019834721,-1.8784440486\C,0,-0.698464085,
-1.5265390529,-2.2765451166\H,0,-1.4288896576,-2.2529196257,-1.9079541
175\C,0,0.7031279026,-1.9913435889,-1.8713374477\H,0,1.4846165032,-1.3
813482067,-2.3373480787\H,0,0.8670095854,-1.9721580692,-0.7936906519\H
,0,0.852510875,-3.0172827369,-2.2198868668\C,0,0.8568918204,1.01516206
6,-2.966856682\O,0,0.4945895002,0.9268233925,-4.10968231\C,0,2.2821627
648,1.2299736737,-2.484055033\H,0,2.6872440449,2.1642172693,-2.8822680
005\P,0,-2.4689453927,0.1378321281,-0.5372325838\C,0,-2.2290911034,-1.
587557556,0.3013694441\C,0,-0.9890337301,-1.8145201734,0.9095548152\C,
0,-3.1953845916,-2.5913610549,0.4213790691\C,0,-0.7027644462,-2.988408
7827,1.5981597272\H,0,-0.2199396797,-1.0481049767,0.8314130568\C,0,-2.
9243894996,-3.7730300245,1.1170254666\H,0,-4.1801186029,-2.4652064958,
-0.0192585038\C,0,-1.6814699998,-3.9767004373,1.704592494\H,0,0.274695
8883,-3.1283804288,2.0545332302\H,0,-3.6950713471,-4.5346104685,1.1970
620769\H,0,-1.4733563486,-4.8964886442,2.2427408697\C,0,-4.1794986753,
-0.2285699436,-1.0891266722\C,0,-5.2819157038,0.2820191705,-0.40119573
39\C,0,-4.3850556687,-1.0238905446,-2.218794714\C,0,-6.5741110618,-0.0
067397531,-0.8336626732\H,0,-5.1374062005,0.9036978478,0.47998762\C,0,
-5.6771346606,-1.3019429498,-2.655315026\H,0,-3.5373127493,-1.44132375
96,-2.7572873037\C,0,-6.7742886105,-0.7975941995,-1.9616251766\H,0,-7.
4248680187,0.3903548061,-0.2882239452\H,0,-5.826431546,-1.9190217642,-
3.5360515541\H,0,-7.7816693974,-1.0206649053,-2.2988316541\C,0,-2.2535
264019,0.9810793455,1.1077266343\C,0,-2.9582786308,0.5244011044,2.2269
016286\C,0,-1.4289680385,2.1065449538,1.2404256075\C,0,-2.8765711641,1
.2039327907,3.4405492837\H,0,-3.5716253599,-0.3695101109,2.1513238203\
C,0,-1.302233448,2.7484070172,2.4706045375\H,0,-0.8878627196,2.4868100
509,0.3813651001\C,0,-2.0413749552,2.3112005166,3.5677389015\H,0,-3.45
2591631,0.853583748,4.2914145138\H,0,-0.6335686088,3.5989397513,2.5632
274244\H,0,-1.9608423342,2.8260230851,4.5202447727\H,0,-0.7522208916,-
1.5666954752,-3.371205774\H,0,2.8955973222,0.4071005127,-2.8561029233\
C,0,2.1658604119,1.207333942,-0.9476020118\O,0,0.8643790907,0.68716737
79,-0.6538061837\C,0,2.1786744242,2.6488964573,-0.41997075\F,0,1.92790
52747,2.6879475439,0.8959245451\F,0,3.3538471433,3.2419485751,-0.63992
49061\F,0,1.2315010242,3.3897752385,-1.0240934565\C,0,3.2633514403,0.4
037272121,-0.2523816981\C,0,3.1186637211,-0.2367507453,0.9992921785\C,
0,4.5089074715,0.3727920857,-0.8856674935\C,0,4.2042151905,-0.96756590
63,1.5117367961\C,0,5.5730389799,-0.3305018521,-0.3476746527\H,0,4.663

5715502,0.9103141039,-1.8142205162\C,0,5.4174524322,-1.0211193782,0.84
49334761\H,0,4.0819756038,-1.491630102,2.4474884959\H,0,6.2441367139,-
1.587091832,1.2606095201\Cl,0,7.1030333385,-0.3512800686,-1.1839382895
\N,0,1.9355453561,-0.1089755858,1.7422391469\H,0,1.2612623977,0.563100
675,1.3976410481\C,0,1.5740686485,-0.8024054847,2.881168058\O,0,2.2101
280271,-1.7301921254,3.3469990593\C,0,0.3169531504,-0.2857426188,3.543
0171114\H,0,0.6037866242,0.4111797418,4.3377989426\H,0,-0.3479368078,0
.2324043108,2.8518328622\H,0,-0.2092903658,-1.1289309054,3.9926347325\
H,0,-0.5064775393,1.9139450951,-1.6335896767\O,0,-2.6144480919,1.75744
71314,-1.2761505722\H,0,-3.2781833038,2.2897608526,-0.8142273497\H,0,-
1.7175249733,0.3051929631,-2.7235779862\\Version=EM64L-G09RevA.01\Stat
e=1-A\HF=-2771.4146137\RMSD=3.312e-09\Dipole=-1.7615918,0.403424,0.536
7171\Quadrupole=7.0987177,-2.3974844,-4.7012333,5.8641566,-7.5907583,1
1.5178763\PG=C01 [X(C34H32Cl1F3N1O4P1)]\\@

TS16

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\23-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.0017542359,-1.8208241325,-0.342498
1729\C,0,1.0982345688,-1.294960067,-1.2285643856\C,0,0.7063092211,-0.7
087769462,-2.6053795697\H,0,1.476393261,-0.020635851,-2.9720291902\C,0
,-0.670460981,-0.0524511206,-2.7199525664\H,0,-1.46422062,-0.765555764
2,-2.47530581\H,0,-0.7986149889,0.8135839605,-2.0681235098\H,0,-0.8287
069772,0.2730165165,-3.7524411741\C,0,-0.8114084057,-2.8766757336,-0.9
100027577\O,0,-0.4526991145,-3.8081400962,-1.6079529659\C,0,-2.2654863
245,-2.6188076502,-0.4924146543\H,0,-2.6710728017,-3.4519383352,0.0876
131548\P,0,2.3444094494,-0.3397694829,-0.1911377574\C,0,2.4332344217,1
.2967453891,-1.0570823886\C,0,1.2595164992,2.0590291268,-1.0338354546\
C,0,3.5661517089,1.8226233408,-1.6796968768\C,0,1.2021883962,3.3139574
275,-1.626041495\H,0,0.3751407503,1.6517691729,-0.5485029073\C,0,3.515
2346771,3.0858159279,-2.2722959412\H,0,4.4943719563,1.2597647097,-1.70
17475168\C,0,2.3396116273,3.8290793793,-2.2489708911\H,0,0.2754738977,
3.8815506339,-1.5926776001\H,0,4.4029085463,3.4876331785,-2.7513715534
\H,0,2.3070286368,4.8102822612,-2.7126012234\C,0,4.0326488248,-0.96705
56985,-0.4030858989\C,0,4.9262760979,-1.0435407473,0.6646607275\C,0,4.
4357451081,-1.3591526775,-1.6812151413\C,0,6.2214125766,-1.5039059174,
0.4509347178\H,0,4.6076226242,-0.7559871341,1.6625769637\C,0,5.7300868
676,-1.8285111545,-1.8880490051\H,0,3.7441807032,-1.2981512208,-2.5192
452907\C,0,6.6238877581,-1.8975194992,-0.8232194865\H,0,6.9144041786,-
1.5653484546,1.2840995489\H,0,6.0370218316,-2.140410575,-2.8811410626\
H,0,7.632976963,-2.2633432793,-0.9848146394\C,0,2.0282760945,0.3294618
264,1.4936259814\C,0,2.835223817,1.3961399504,1.9092568353\C,0,1.03302
78683,-0.1474785271,2.3542228995\C,0,2.6682665105,1.9553348536,3.17379
77412\H,0,3.5932107765,1.7983424471,1.2424582116\C,0,0.8423036608,0.44
44657347,3.6004982456\H,0,0.3955824773,-0.9672232409,2.0539800305\C,0,

1.6658272637,1.4866044679,4.0187109833\H,0,3.3124651015,2.7704499818,3
.4876501182\H,0,0.0449571137,0.079374651,4.240095132\H,0,1.5229549905,
1.9366433166,4.9962346355\H,0,0.7133916953,-1.5692020791,-3.284875304\
H,0,-2.8534635955,-2.5267004966,-1.4081701295\C,0,-2.2048358253,-1.294
8866192,0.2939672453\O,0,-0.8934864904,-0.7718562867,0.1097640489\C,0,
-2.3397808989,-1.599715715,1.7912437521\F,0,-2.1565402587,-0.491000561
8,2.5348599376\F,0,-3.5432925958,-2.0948036899,2.0904280938\F,0,-1.420
557665,-2.4904367341,2.1963124358\C,0,-3.2607618929,-0.2608833627,-0.1
035023708\C,0,-3.0798002494,1.1374329264,0.000376011\C,0,-4.4908047699
,-0.7461920656,-0.5516156106\C,0,-4.1014498023,1.9900744443,-0.4448645
887\C,0,-5.4984391083,0.113794101,-0.9577646083\H,0,-4.6728743234,-1.8
14499663,-0.585005898\C,0,-5.2997925335,1.4859215925,-0.926702221\H,0,
-3.9451010514,3.0579784984,-0.4027739639\H,0,-6.0811845014,2.159457236
3,-1.2616506753\Cl,0,-7.0136749672,-0.5403874843,-1.518890254\N,0,-1.9
246967924,1.6707707687,0.6013120729\H,0,-1.3322070178,1.0044754519,1.0
808145438\C,0,-1.5022144379,2.9805423226,0.6087348362\O,0,-2.001887695
4,3.8697992235,-0.0584831652\C,0,-0.3627738925,3.2532222681,1.56972994
43\H,0,0.2585011537,2.3766708411,1.7606685413\H,0,0.2514661468,4.05946
84442,1.1664691413\H,0,-0.7892309643,3.5857650515,2.5222205524\H,0,0.9
770794643,-2.3245868236,0.5820828889\O,0,2.1304040779,-2.3407910298,0.
873940951\H,0,2.2286613877,-2.3418491394,1.8363190626\H,0,1.6976260271
,-2.1979283677,-1.4144893101\\Version=ES64L-G09RevE.01\State=1-A\HF=-2
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pole=11.9376938,-21.626341,9.6886471,6.3032609,-3.0097275,-0.129979\PG
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INT19

1\1\GINC-OM103\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\22-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.0307131463,-0.0178475501,-0.051737
757\C,0,-0.0060140862,-0.021415405,1.4154025901\C,0,1.4127424014,-0.00
40541208,2.0216907955\H,0,1.3695189799,-0.1823275374,3.1053651986\C,0,
2.0929020285,1.3322928008,1.7381522542\H,0,2.1549029786,1.510124229,0.
6604357726\H,0,1.541166699,2.1669625996,2.1892701932\H,0,3.1060642328,
1.3402637153,2.1486498912\C,0,0.3841845795,-1.0041405245,-0.8987435015
\O,0,0.9617080184,-2.1003578314,-0.6243276551\C,0,-0.0932044341,-0.606
6623625,-2.2994194049\H,0,-0.9555766692,-1.2276935921,-2.5734870624\P,
0,-0.992324324,-1.4945752125,2.1228498171\C,0,-2.1995113252,-0.8017538
721,3.2875950622\C,0,-1.7735905069,0.1764028275,4.1955451138\C,0,-3.52
67880027,-1.2366958005,3.3029338405\C,0,-2.6711394916,0.7108297711,5.1
126490603\H,0,-0.7396429264,0.5161466652,4.1907220655\C,0,-4.422438510
4,-0.6923292055,4.2202443679\H,0,-3.8592502751,-1.991411213,2.59622742
28\C,0,-3.9963587323,0.2777885802,5.1226110847\H,0,-2.3383114787,1.467
334479,5.8159408826\H,0,-5.4547083047,-1.0270690538,4.2270885446\H,0,-
4.6973994864,0.7004765757,5.8353772872\C,0,0.0455200365,-2.6546461185,

3.0326801273\C,0,1.0872046619,-3.2709550685,2.3296553524\C,0,-0.125803
9513,-2.8799005267,4.4034605308\C,0,1.9728830825,-4.1000581653,3.00969
89633\H,0,1.2056466364,-3.0800055576,1.2659819824\C,0,0.7561926356,-3.
7256978377,5.0674921273\H,0,-0.9365333258,-2.4029242556,4.9459317913\C
,0,1.8059638544,-4.327513807,4.3736430973\H,0,2.8015426162,-4.53565014
09,2.4620262705\H,0,0.6270841411,-3.9092599941,6.1294491541\H,0,2.5007
169569,-4.9715574072,4.9042828415\C,0,-1.9091103432,-2.3609477926,0.84
01397571\C,0,-2.6263408585,-1.6075092596,-0.0975498654\C,0,-1.92320077
1,-3.756588581,0.7889942386\C,0,-3.3545437327,-2.2616745026,-1.0863491
782\H,0,-2.6025514239,-0.5209682217,-0.0813619718\C,0,-2.6598833816,-4
.4000237455,-0.2008413198\H,0,-1.353597423,-4.3371198637,1.507962762\C
,0,-3.3706006157,-3.6539748701,-1.136967667\H,0,-3.8968244415,-1.67801
08916,-1.8223104234\H,0,-2.6677688215,-5.4841749695,-0.2458662558\H,0,
-3.9368173782,-4.1588262291,-1.9136997502\H,0,1.9977140278,-0.82248397
6,1.5865356928\H,0,0.6862967593,-0.7478488237,-3.0466250977\C,0,-0.490
3822614,0.8690497322,-2.0870665809\O,0,-0.841458253,0.9555271788,-0.70
27191282\C,0,-1.776526504,1.2453203314,-2.816360484\F,0,-2.1355584357,
2.5040776282,-2.5368693329\F,0,-1.6361304573,1.1348007001,-4.141929250
7\F,0,-2.799890558,0.4509232326,-2.4573321286\C,0,0.6247991648,1.85372
43899,-2.4853954259\C,0,1.0087146029,2.992937654,-1.7384270477\C,0,1.2
408402362,1.6303728046,-3.7184066482\C,0,2.0430517878,3.8118603762,-2.
2180474229\C,0,2.2432751393,2.4647840252,-4.1862088488\H,0,0.928003653
6,0.7984936822,-4.338566727\C,0,2.6605447275,3.5500973339,-3.431218706
\H,0,2.3473085209,4.6625095295,-1.6259362075\H,0,3.4544481661,4.194814
8267,-3.7920904534\Cl,0,2.9844475545,2.1370359482,-5.732183822\N,0,0.3
45103116,3.3052079864,-0.5415152815\H,0,-0.4072302754,2.6662642849,-0.
3137267521\C,0,0.6429530105,4.2741894893,0.379700392\O,0,1.5695102124,
5.0603949435,0.304713567\C,0,-0.3358025275,4.3231812942,1.5413747225\H
,0,-1.0385759301,5.1449010748,1.3736964065\H,0,-0.9069409754,3.3987588
587,1.6662784452\H,0,0.2228460912,4.5399902199,2.4533355857\H,0,-0.571
380962,0.8443643322,1.7879867946\H,0,4.1124822964,-2.0667228497,0.0867
821649\O,0,3.3822775171,-2.5108455097,0.536073224\H,0,2.5960835012,-2.
3356023386,-0.0294939018\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771.
4224934\RMSD=7.299e-09\Dipole=-3.1326581,-1.6122811,4.0480424\Quadrupo
le=0.6876528,-13.3827826,12.6951298,1.0670691,-5.7453831,3.8772739\PG=
C01 [X(C34H32Cl1F3N1O4P1)]\\@

TS17

1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\10-May-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
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18380164,-1.4549665303\H,0,-0.4543243033,2.0321824753,-1.664626441\C,0
,1.4330418648,2.2309294874,-2.6839801443\H,0,2.4748581001,1.8984982056
,-2.5997077511\H,0,1.0207925047,1.7530127738,-3.5775777485\H,0,1.43264

89142,3.3125679837,-2.8487486553\C,0,-0.4887757211,-1.6683035304,-0.39
86976969\O,0,0.1645628809,-2.5485793519,-0.9973420665\C,0,-1.675695841
3,-1.9198446515,0.5364586826\H,0,-1.3068228301,-2.3445468173,1.4774175
468\P,0,2.5830577877,0.1481772001,-0.0771215389\C,0,3.2727974776,1.565
2942901,0.8333131094\C,0,3.5124428318,2.7705482836,0.1563555315\C,0,3.
5359598671,1.4897878704,2.2064364971\C,0,4.0141188459,3.8727882131,0.8
392368463\H,0,3.3169349362,2.8476337184,-0.9092964215\C,0,4.0295328527
,2.5997571775,2.885451848\H,0,3.3597246434,0.5633439997,2.7429743022\C
,0,4.2692370896,3.7908125988,2.2062784034\H,0,4.2004024951,4.797821507
,0.3029367096\H,0,4.2316786116,2.5286152872,3.9494796601\H,0,4.6547993
427,4.6540241635,2.7397452807\C,0,3.7894265804,-0.4132246889,-1.299607
4474\C,0,3.424526471,-1.5309956963,-2.064350547\C,0,5.0060847409,0.235
9206446,-1.5334150612\C,0,4.2924958289,-2.0025381117,-3.0435920775\H,0
,2.4932748379,-2.06084732,-1.8651474804\C,0,5.8528156949,-0.2312460856
,-2.5331892472\H,0,5.2956923275,1.0932120347,-0.9330280703\C,0,5.49796
19963,-1.3489165989,-3.2867936887\H,0,4.0206625056,-2.8871458722,-3.60
99655154\H,0,6.7977646916,0.2710470551,-2.7149323095\H,0,6.1683025933,
-1.7150995059,-4.058299849\C,0,2.3132128771,-1.1794979264,1.1120242628
\C,0,1.3081993637,-0.9961940573,2.0731858015\C,0,3.0036554665,-2.39154
21387,1.0425738747\C,0,1.0307789468,-2.0129448825,2.9817163851\H,0,0.7
346961268,-0.0722943157,2.1084183021\C,0,2.6986284956,-3.4130900573,1.
9363910917\H,0,3.7491847993,-2.5649993929,0.2745457857\C,0,1.722009895
2,-3.2212731922,2.9090289237\H,0,0.258161629,-1.8670873953,3.728985054
\H,0,3.2135959347,-4.3632916178,1.8483439718\H,0,1.4872785083,-4.02020
2178,3.6059445091\H,0,0.8609060349,2.4856693587,-0.5962985904\H,0,-2.3
773132326,-2.6229281807,0.0920138475\C,0,-2.2429465592,-0.4971826553,0
.7393266327\O,0,-1.1320192451,0.3784140153,0.4971746712\C,0,-2.6209992
69,-0.2356594317,2.1953323562\F,0,-3.0223007113,1.0290843482,2.3683460
875\F,0,-3.6097017443,-1.0473729091,2.5839813536\F,0,-1.5852715404,-0.
4399741487,3.0261582534\C,0,-3.45887665,-0.1682298832,-0.145775997\C,0
,-3.7243616498,1.110880423,-0.6927956541\C,0,-4.4108064023,-1.17364671
72,-0.324350597\C,0,-4.8807585567,1.3026579947,-1.4628466323\C,0,-5.55
92114827,-0.9582869819,-1.0697725761\H,0,-4.2755678719,-2.1431195143,0
.1396394302\C,0,-5.7920888662,0.2755664805,-1.6563993956\H,0,-5.060415
0816,2.2767568772,-1.8934537755\H,0,-6.6844672071,0.4408104654,-2.2503
620492\Cl,0,-6.7100924156,-2.254789745,-1.2666339486\N,0,-2.841227745,
2.1762530533,-0.4547719698\H,0,-2.0155262743,1.9193177703,0.0715415053
\C,0,-2.9586972228,3.4938454866,-0.8204358909\O,0,-3.8776817446,3.9687
980734,-1.4617058786\C,0,-1.7877440492,4.3526358131,-0.37291123\H,0,-1
.141279221,4.543243153,-1.2358261702\H,0,-2.1786996366,5.3120683836,-0
.0308720833\H,0,-1.1916655352,3.8948939452,0.4204938793\H,0,1.06928704
04,-0.2395113879,-1.946166224\H,0,1.9261956389,-4.9038171181,-1.750700
0619\O,0,2.2791182373,-4.3410164656,-1.0488980254\H,0,1.5139499025,-3.
7808608737,-0.8092109911\\Version=ES64L-G09RevE.01\State=1-A\HF=-2771.
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-7.238702,1.064384,6.174318,19.3639722,-6.4379441,2.5394521\PG=C01 [X(
C34H32Cl1F3N1O4P1)]\\@

INT20 -2771.438304
1\1\GINC-OM111\SP\RM062X\6-311+G(d,p)\C34H32Cl1F3N1O4P1\WEIY\22-Mar-20
17\0\\#p m062x/6-311+g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluen
e)\\Title Card Required\\0,1\C,0,-0.0980018248,0.0192616503,-0.0523851
225\C,0,-0.1498147876,-0.1425179356,1.2686502256\C,0,1.0085823149,-0.2
679830757,2.2084577582\H,0,1.1951634226,-1.340533052,2.3688541171\C,0,
0.7473597439,0.4053422407,3.5573003817\H,0,0.6512842159,1.4884029638,3
.4458985867\H,0,-0.1795781593,0.034631221,4.0075426673\H,0,1.567441863
7,0.202156899,4.2511821799\C,0,-1.2428241193,0.0148482351,-0.997082150
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4a

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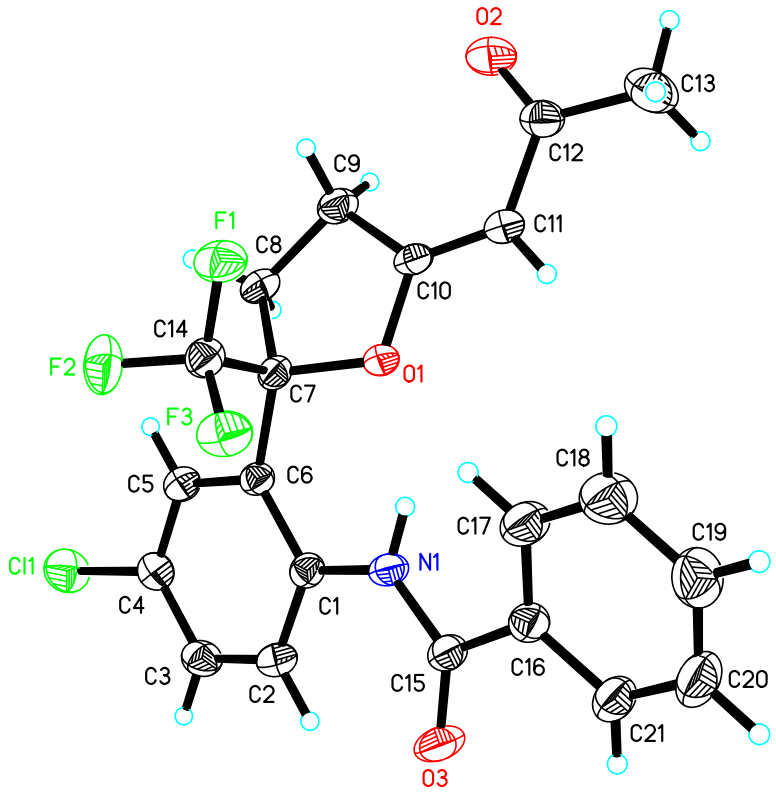
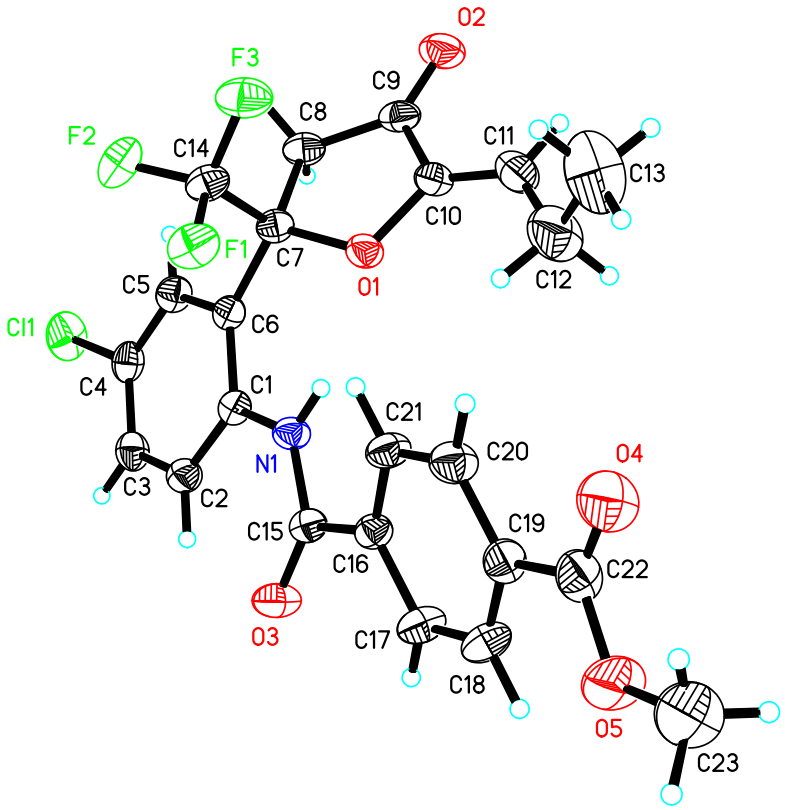
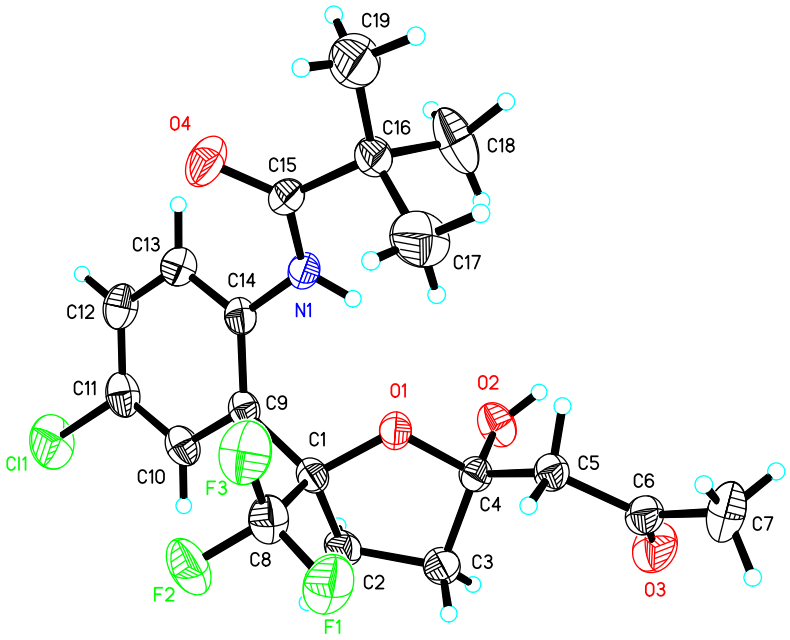
X-ray Crystal Data of 3f, 4g and 3d'.



The crystal data of **3f** have been deposited in CCDC with number 1500323. Empirical Formula: $C_{21}H_{17}ClF_3NO_3$; Formula Weight: 423.81; Crystal Color, Habit: colorless; Crystal Dimensions: 0.200 x 0.140 x 0.120 mm^3; Crystal System: Monoclinic; Lattice Parameters: a = 21.872(3) Å, alpha = 90 deg. b = 7.6040(10) Å, beta = 110.597(3) deg. c = 24.313(3) Å, gamma = 90 deg.; V = 3785.2(8) $Å^3$; Space group: C 2/c; Z = 8; D_{calc} = 1.487 g/cm^3; F_{000} = 1744; Diffractometer: Rigaku AFC7R; Residuals: R; R_w: 0.0487, 0.1124.



The crystal data of **4g** have been deposited in CCDC with number 1521105. Empirical Formula: $C_{23}H_{19}ClF_3NO_5$; Formula Weight: 481.84; Crystal Color, Habit: colorless; Crystal Dimensions: 0.200 x 0.170 x 0.120 mm^3; Crystal System: Triclinic; Lattice Parameters: a = 7.3052(11) Å, alpha = 88.853(3) deg. b = 10.5757(16) Å, beta = 83.694(3) deg. c = 14.449(2) Å, gamma = 77.708(3) deg.; V = 1084.1(3) $Å^3$; Space group: P -1; Z = 2; D_{calc} = 1.476 g/cm^3; F_{000} = 496; Diffractometer: Rigaku AFC7R; Residuals: R; R_w: 0.0465, 0.1114.



The crystal data of **3d'** have been deposited in CCDC with number 1451585. Empirical Formula: $C_{19}H_{23}ClF_3NO_4$; Formula Weight: 421.83; Crystal Color, Habit: colorless; Crystal Dimensions: 0.220 x 0.170 x 0.130 mm^3; Crystal System: Monoclinic; Lattice Parameters: a = 11.287(2) Å, alpha = 90 deg. b = 12.727(2) Å, beta = 103.680(4) deg. c = 14.808(3) Å, gamma = 90 deg.; V = 2066.8(6) $Å^3$; Space group: P 21/n; Z = 4; D_{calc} = 1.356 g/cm^3; F_{000} = 880; Diffractometer: Rigaku AFC7R; Residuals: R; R_w: 0.0568, 0.1427.

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