Supporting Information

Oxidative functionalization of alkylidenecyclopropanes and alkylidenecyclobutanes: a versatile platform to access nitrated cyclopropanes and cyclobutanes

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1. General Information

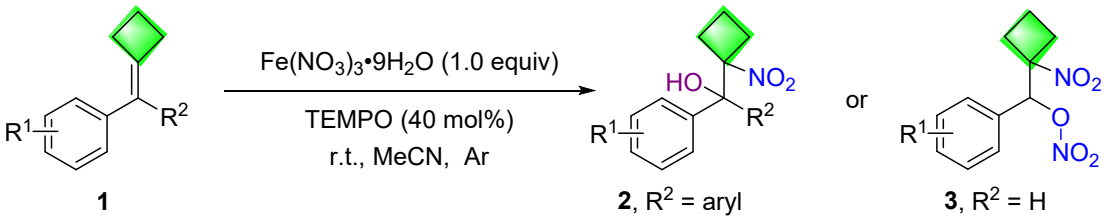
All reagents were obtained commercially and used without further purification. All solvents were dried and distilled according to standard procedures. Column chromatography was performed on silica gel (200-300 mesh). ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker Ascend 500 spectrometer operating at 500 MHz and 126 MHz, respectively. The chemical shifts (δ) were expressed in ppm and coupling constants (J) were in Hz. High-resolution mass spectra (HRMS) were obtained on a mass spectrometer by the ESI method.

2. Experimental Section

2.1 General procedure for the synthesis of ACBs (1) and ACPs (4):

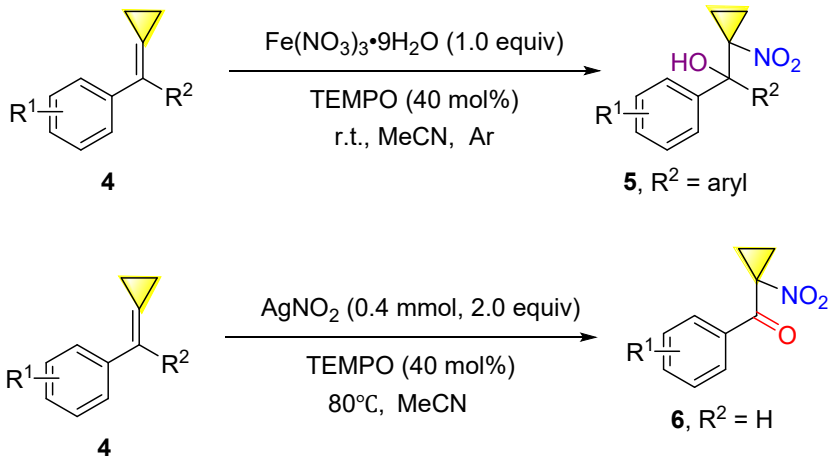
All of the ACBs **(1)**[1] and ACPs **(4)**[2] were synthesized according to the known methods.

2.2 General procedure for the reaction of ACBs.



To a Schlenk tube were added **1** (0.2 mmol, 1.0 equiv.), $Fe(NO_3)_3 \cdot 9H_2O$ (0.2 mmol, 1.0 equiv.), TEMPO (0.08 mmol, 0.4 equiv.), CH_3CN (2.0 mL). Then the mixture was stirred at room temperature under argon atmosphere for 3-6 h. After the reaction was finished, the reaction mixture was washed with NH_4Cl solution. The aqueous phase was extracted with EtOAc for three times. The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by flash column chromatography over silica gel using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **2** or **3**.

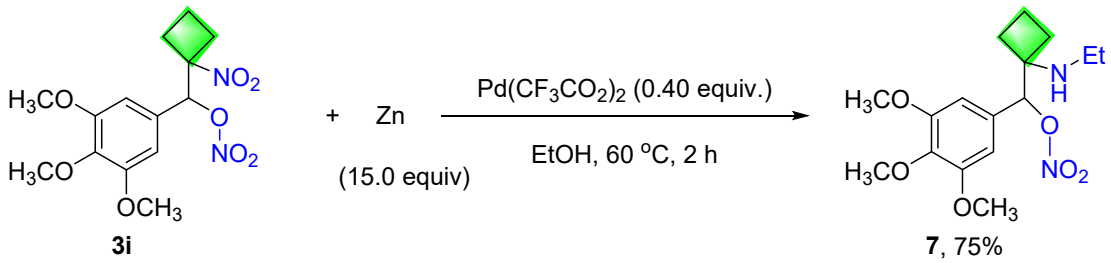
2.3 General procedure for the reaction of ACPs.



When R^2= aryl group, to a Schlenk tube were added **4** (0.2 mmol, 1.0 equiv.), $Fe(NO_3)_3 \cdot 9H_2O$ (0.2 mmol, 1.0 equiv.), TEMPO (0.08 mmol, 0.4 equiv.), CH_3CN (2.0 mL). Then the mixture was stirred at room temperature under argon atmosphere for 3-6 h. After the reaction was finished, the reaction mixture was washed with NH_4Cl solution. The aqueous phase was extracted with EtOAc for three times. The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by flash column chromatography over silica gel using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **5**.

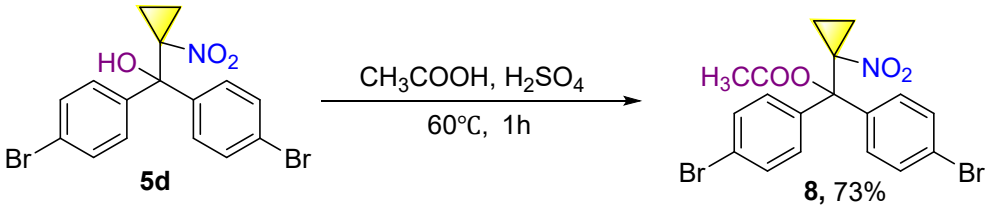
When R^2= H group, to a Schlenk tube were added **4** (0.2 mmol, 1.0 equiv.), $AgNO_2$ (0.4 mmol, 2.0 equiv.), TEMPO (0.08 mmol, 0.4 equiv.), CH_3CN (2.0 mL). Then the mixture was stirred at 80 ℃ under air atmosphere for 12 h. Upon completion as indicated by TLC, the solution was concentrated under reduced pressure. The residue was purified by flash column chromatography over silica gel using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **6**.

2.4 The experimental procedure for the synthesis of product 7



To a stirred mixture of the (1-nitrocyclobutyl) (3,4,5-trimethoxyphenyl) methyl nitrate **3i** (0.1 mmol, 1 equiv.) in EtOH (2.0 mL) was added Zn (1.5 mmol, 15.0 equiv.) and $Pd(CF_3CO_2)_2$ (0.04 mmol, 0.4 equiv.). The mixture was stirred at 60 ℃ for 2 h. Upon completion as monitored by TLC, the mixture was filtered and evaporated under reduced pressure. The residue was purified by flash column chromatography over silica gel using petroleum ether/ethyl acetate as eluent to afford the desired product **7**.

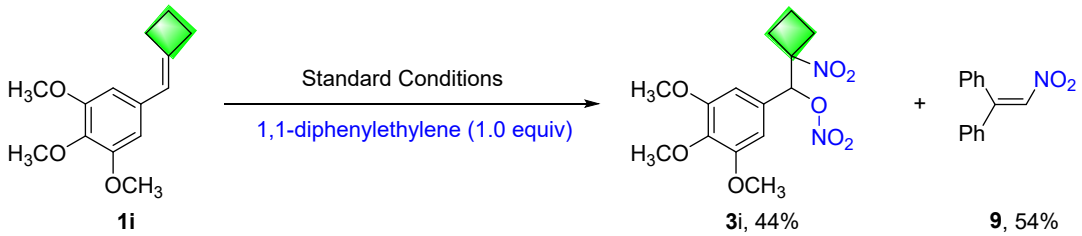
2.5 The experimental procedure for the synthesis of product 8



To a Schlenk tube were added **5d** (0.1 mmol, 1.0 equiv), CH_3COOH (1.0 ml), two drops of H_2SO_4. The mixture was stirred at 60 ℃ for 1 h. Upon completion as monitored by TLC, adjusting the pH of the reaction mixture to 7 with $NaHCO_3$ solution. The aqueous phase was extracted with EtOAc for three times. The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. The residue

was purified by flash column chromatography over silica gel using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **8**.

2.6 Control experiments



1i **3i**, 44% **9**, 54%

To a Schlenk tube were added **1i** (0.2 mmol, 1.0 equiv.), $Fe(NO_3)_3 \cdot 9H_2O$ (0.2 mmol, 1.0 equiv.), TEMPO (0.08 mmol, 0.4 equiv.), 1,1-diphenylethylene (0.2 mmol, 1.0 equiv.), CH_3CN (2.0 mL). Then the mixture was stirred at room temperature under argon atmosphere for 3 h. After the reaction was finished, the reaction mixture was washed with NH_4Cl solution. The aqueous phase was extracted with EtOAc for three times. The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. Then the reaction mixture was concentrated under reduced pressure and purified by flash column chromatography over silica gel using a mixture of petroleum ether and ethyl acetate as eluent.

3. Single crystal X-ray structure of compound 3i and 5a

X-ray crystallographic data for compound **3i** (CCDC: 2174132)

Crystal Data for $C_{14}H_{18}N_2O_8$ (M =342.30 g/mol): triclinic, space group P-1 (no. 2), a = 6.309(9) Å, b = 9.725(14) Å, c = 13.99(2) Å, α = 72.28(3)°, β = 86.43(3)°, γ = 86.25(3)°, V = 815(2) Å^3, Z = 2, T = 296.15 K, μ(Mo Kα) = 0.116 mm^{-1}, *Dcalc* = 1.394 g/cm^3, 13836 reflections measured (6.072° ≤ 2Θ ≤ 50.084°), 2867 unique (R_{int} = 0.0551, R_{sigma} = 0.0528) which were used in all calculations. The final R_1 was 0.0504 (I > 2σ(I)) and wR_2 was 0.1307 (all data).

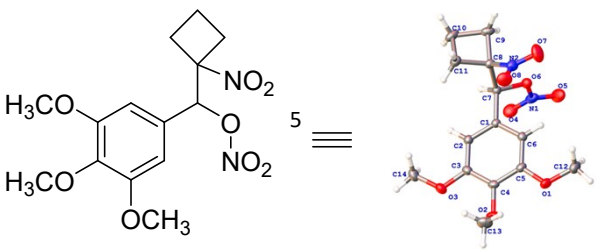


Table 1 Crystal data and structure refinement for 3i .

Identification code	**3i**
Empirical formula	$C_{14}H_{18}N_2O_8$
Formula weight	342.30
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	6.309(9)
b/Å	9.725(14)
c/Å	13.99(2)
α/°	72.28(3)
β/°	86.43(3)
γ/°	86.25(3)
Volume/Å^3	815(2)
Z	2
ρ_{calc}g/cm^3	1.394
μ/mm^{-1}	0.116
F(000)	360.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.072 to 50.084
Index ranges	-7 ≤ h ≤ 7, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16
Reflections collected	13836
Independent reflections	2867 [R_{int} = 0.0551, R_{sigma} = 0.0528]
Data/restraints/parameters	2867/0/220
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0504, wR_2 = 0.1020
Final R indexes [all data]	R_1 = 0.1103, wR_2 = 0.1307
Largest diff. peak/hole / e Å^{-3}	0.16/-0.16

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3i. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	9208(3)	7521.9(18)	2229.3(15)	65.9(5)
O2	6342(3)	8516.9(18)	827.2(14)	68.2(6)
O3	3579(3)	6771.2(19)	464.3(13)	65.0(5)
O4	3221(4)	3603(2)	4460.2(18)	83.3(7)
O5	5455(4)	3332(2)	5617.1(17)	98.8(8)
O6	6503(3)	2617.5(17)	4329.3(12)	54.5(5)
O7	10671(4)	1530(3)	3721(2)	107.1(9)
O8	10470(3)	2510(2)	2143.3(18)	85.2(7)
N1	4884(5)	3256(2)	4841(2)	65.1(7)
N2	9693(4)	1882(3)	2960(2)	59.6(6)
C1	6213(4)	4251(2)	2623.3(17)	39.4(6)
C2	4788(4)	4763(3)	1869.8(17)	45.5(6)
C3	4896(4)	6172(3)	1239.8(18)	46.9(6)
C4	6382(4)	7075(3)	1383.3(18)	48.4(6)
C5	7812(4)	6551(3)	2146.6(19)	47.4(6)
C6	7729(4)	5133(3)	2767.8(18)	45.6(6)
C7	6002(4)	2721(2)	3312.0(16)	43.0(6)
C8	7384(4)	1527(2)	3044.2(17)	43.2(6)
C9	6909(5)	-9(3)	3709(2)	63.6(8)
C10	5494(5)	-122(3)	2888(2)	73.4(9)
C11	6615(4)	1145(3)	2144(2)	58.4(7)
C12	10695(5)	7053(3)	3007(2)	73.1(9)
C13	7618(5)	8861(3)	-78(2)	84.6(10)
C14	2019(4)	5879(3)	305(2)	66.9(8)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3i. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	65.1(12)	45.8(11)	88.8(14)	-19.5(10)	-11.5(11)	-12.8(9)
O2	85.9(14)	36.2(10)	73.9(13)	-6.8(9)	4.2(11)	4.6(9)
O3	65.9(13)	60.6(12)	60.9(12)	-5.5(9)	-18.5(10)	3.1(10)
O4	73.8(15)	87.6(16)	96.1(17)	-44.4(13)	17.8(14)	2.7(13)
O5	164(2)	84.6(16)	54.5(13)	-33.3(12)	0.7(15)	0.5(15)
O6	66.6(12)	51.7(10)	45.5(10)	-16.0(8)	-1.8(9)	-0.5(9)
O7	56.3(14)	166(3)	102.5(19)	-43.4(17)	-21.9(13)	-0.3(14)
O8	61.9(13)	86.1(15)	96.6(17)	-13.6(13)	26.4(12)	-20.7(11)
N1	95(2)	45.5(14)	55.4(17)	-18.9(12)	16.4(16)	-7.7(14)
N2	45.0(14)	60.5(15)	76.0(18)	-26.0(14)	0.4(14)	1.0(12)
C1	38.4(13)	37.4(13)	43.4(14)	-14.3(11)	1.0(11)	-0.8(11)
C2	43.5(14)	45.2(15)	50.1(15)	-18.2(12)	-2.3(12)	-0.9(11)
C3	49.0(15)	44.9(15)	44.4(15)	-11.9(12)	-2.1(13)	6.9(13)
C4	56.3(16)	35.0(14)	51.0(16)	-11.5(12)	3.3(13)	4.7(12)
C5	47.1(15)	40.1(15)	58.9(17)	-21.4(13)	2.6(13)	-4.0(12)
C6	44.4(14)	44.7(15)	48.7(15)	-16.1(12)	-4.7(12)	1.5(12)
C7	43.3(14)	44.4(14)	42.4(14)	-14.7(11)	-1.8(11)	-1.8(11)
C8	38.1(14)	39.6(14)	52.1(15)	-14.5(12)	3.9(12)	-4.6(11)
C9	75(2)	36.8(15)	71.5(19)	-9.9(13)	17.4(16)	-0.8(13)
C10	64.9(19)	54.0(18)	112(3)	-42.6(18)	15.6(18)	-15.3(15)
C11	61.1(17)	54.6(17)	66.3(18)	-29.2(14)	2.4(14)	-4.1(14)
C12	58.1(18)	68(2)	104(2)	-39.6(18)	-16.3(18)	-5.8(15)
C13	88(2)	62(2)	84(2)	4.3(17)	15(2)	-9.3(17)
C14	53.6(17)	85(2)	61.7(18)	-20.8(16)	-12.6(14)	5.5(16)

Table 4 Bond Lengths for 3i.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C5	1.367(3)	C1	C2	1.381(3)
O1	C12	1.429(3)	C1	C6	1.388(3)
O2	C4	1.380(3)	C1	C7	1.516(4)
O2	C13	1.419(4)	C2	C3	1.388(4)
O3	C3	1.368(3)	C3	C4	1.389(4)
O3	C14	1.425(4)	C4	C5	1.394(4)
O4	N1	1.188(3)	C5	C6	1.390(4)
O5	N1	1.191(3)	C7	C8	1.530(3)
O6	N1	1.427(3)	C8	C9	1.538(4)
O6	C7	1.450(3)	C8	C11	1.532(4)
O7	N2	1.211(3)	C9	C10	1.532(4)
O8	N2	1.210(3)	C10	C11	1.531(4)
N2	C8	1.508(4)			

Table 5 Bond Angles for 3i.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	O1	C12	118.0(2)	O2	C4	C5	119.7(2)
C4	O2	C13	115.8(2)	C3	C4	C5	119.8(2)
C3	O3	C14	117.1(2)	O1	C5	C4	115.4(2)
N1	O6	C7	113.5(2)	O1	C5	C6	124.7(2)
O4	N1	O5	130.1(3)	C6	C5	C4	119.9(2)
O4	N1	O6	117.9(3)	C1	C6	C5	119.6(2)
O5	N1	O6	111.9(3)	O6	C7	C1	110.89(19)
O7	N2	C8	117.8(3)	O6	C7	C8	105.50(18)
O8	N2	O7	123.3(3)	C1	C7	C8	117.2(2)
O8	N2	C8	118.9(2)	N2	C8	C7	109.8(2)
C2	C1	C6	120.9(2)	N2	C8	C9	114.8(2)
C2	C1	C7	117.8(2)	N2	C8	C11	114.6(2)
C6	C1	C7	121.3(2)	C7	C8	C9	114.1(2)
C1	C2	C3	119.5(2)	C7	C8	C11	113.3(2)
O3	C3	C2	123.9(2)	C11	C8	C9	88.9(2)
O3	C3	C4	115.7(2)	C10	C9	C8	87.9(2)

Table 5 Bond Angles for 3i.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C3	C4	120.4(2)	C11	C10	C9	89.2(2)
O2	C4	C3	120.3(2)	C10	C11	C8	88.1(2)

Table 6 Torsion Angles for 3i.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C5	C6	C1	178.8(2)	C2	C1	C7	C8	94.8(3)
O2	C4	C5	O1	-4.9(3)	C2	C3	C4	O2	-173.1(2)
O2	C4	C5	C6	174.2(2)	C2	C3	C4	C5	1.8(4)
O3	C3	C4	O2	6.0(3)	C3	C4	C5	O1	-179.9(2)
O3	C3	C4	C5	-179.0(2)	C3	C4	C5	C6	-0.8(4)
O6	C7	C8	N2	-68.3(2)	C4	C5	C6	C1	-0.2(3)
O6	C7	C8	C9	62.3(3)	C6	C1	C2	C3	1.0(3)
O6	C7	C8	C11	162.10(19)	C6	C1	C7	O6	33.4(3)
O7	N2	C8	C7	85.6(3)	C6	C1	C7	C8	-87.8(3)
O7	N2	C8	C9	-44.6(3)	C7	O6	N1	O4	10.7(3)
O7	N2	C8	C11	-145.5(3)	C7	O6	N1	O5	-170.4(2)
O8	N2	C8	C7	-93.8(3)	C7	C1	C2	C3	178.4(2)
O8	N2	C8	C9	136.0(2)	C7	C1	C6	C5	-177.2(2)
O8	N2	C8	C11	35.1(3)	C7	C8	C9	C10	96.8(2)
N1	O6	C7	C1	73.7(2)	C7	C8	C11	C10	-97.6(2)
N1	O6	C7	C8	-158.44(18)	C8	C9	C10	C11	18.34(19)
N2	C8	C9	C10	-135.1(2)	C9	C8	C11	C10	18.3(2)
N2	C8	C11	C10	135.3(2)	C9	C10	C11	C8	-18.41(19)
C1	C2	C3	O3	179.0(2)	C11	C8	C9	C10	-18.33(19)
C1	C2	C3	C4	-1.9(3)	C12	O1	C5	C4	179.2(2)
C1	C7	C8	N2	55.7(3)	C12	O1	C5	C6	0.1(3)
C1	C7	C8	C9	-173.7(2)	C13	O2	C4	C3	-91.8(3)
C1	C7	C8	C11	-73.9(3)	C13	O2	C4	C5	93.3(3)
C2	C1	C6	C5	0.1(3)	C14	O3	C3	C2	-0.2(3)
C2	C1	C7	O6	-144.0(2)	C14	O3	C3	C4	-179.2(2)

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3i.

Atom	*x*	*y*	*z*	U(eq)
H2	3764.67	4169.03	1785.07	55
H6	8681.95	4778.01	3276.81	55
H7	4513.61	2481.77	3325.15	52
H9A	8141.67	-679.45	3816.75	76
H9B	6144.08	-43.06	4338.41	76
H10A	5716.5	-1022.83	2725.32	88
H10B	3995.15	84.83	3012.37	88
H11A	5654.93	1876	1732.83	70
H11B	7751.07	855.08	1734.81	70
H12A	11576.46	6258.36	2912.06	110
H12B	9939.89	6750.35	3647.78	110
H12C	11567.74	7836.02	2984.49	110
H13A	7251.12	8278.36	-480.98	127
H13B	9090.56	8674.13	76.57	127
H13C	7376.1	9864.45	-440.85	127
H14A	1265.91	6390.49	-284.76	100
H14B	1035.93	5631.54	875.55	100
H14C	2703.34	5012.22	215.3	100

X-ray crystallographic data for compound **5a** (CCDC: 2174133).

Crystal Data for $C_{16}H_{15}NO_3$ (M =269.29 g/mol): triclinic, space group P-1 (no. 2), a =9.438(3) Å, b =11.990(3) Å, c =12.647(4) Å, α =74.614(7)°, β =89.797(7)°, γ = 77.565(7)°, V = 1345.4(7) Å^3, Z = 4, T = 296.15 K, μ(Mo Kα) = 0.092 mm^{-1}, *Dcalc* = 1.329 g/cm^3, 44711 reflections measured (3.346° ≤ 2Θ ≤ 50.634°), 4868 unique (R_{int} = 0.0972, R_{sigma} = 0.0712) which were used in all calculations. The final R_1 was 0.0557 (I > 2σ(I)) and wR_2 was 0.1587 (all data).

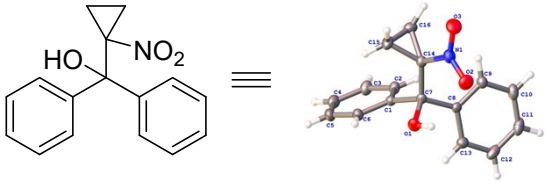


Table 1 Crystal data and structure refinement for 5a.

Identification code	**5a**
Empirical formula	$C_{16}H_{15}NO_3$
Formula weight	269.29
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	9.438(3)
b/Å	11.990(3)
c/Å	12.647(4)
α/°	74.614(7)
β/°	89.797(7)
γ/°	77.565(7)
Volume/Å^3	1345.4(7)
Z	4
ρ_{calc}g/cm^3	1.329
μ/mm^{-1}	0.092
F(000)	568.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.346 to 50.634
Index ranges	-11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	44711
Independent reflections	4868 [R_{int} = 0.0972, R_{sigma} = 0.0712]
Data/restraints/parameters	4868/0/364
Goodness-of-fit on F^2	0.987
Final R indexes [I>=2σ (I)]	R_1 = 0.0557, wR_2 = 0.1203
Final R indexes [all data]	R_1 = 0.1332, wR_2 = 0.1587
Largest diff. peak/hole / e Å^{-3}	0.20/-0.18

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	4080(2)	6881.0(16)	7801.2(14)	59.0(6)
O2	5103(2)	5397.4(19)	6511(2)	74.9(7)
O3	6244(3)	6136(2)	5124(2)	87.9(8)
N1	5390(3)	6240(2)	5837(2)	56.3(7)
C1	2913(3)	8799(2)	6741(2)	41.7(7)
C2	1864(3)	9565(2)	5969(2)	50.8(8)
C3	1409(3)	10743(3)	5952(3)	61.6(9)
C4	1978(4)	11168(3)	6728(3)	67.0(9)
C5	2997(4)	10417(3)	7510(3)	66.4(9)
C6	3470(3)	9238(3)	7526(2)	55.4(8)
C7	3475(3)	7511(2)	6719(2)	41.3(7)
C8	2212(3)	7005(2)	6438(2)	40.5(7)
C9	2007(3)	6795(2)	5434(2)	50.1(7)
C10	840(4)	6338(3)	5231(3)	64.4(9)
C11	-141(4)	6113(3)	6013(4)	72.0(10)
C12	37(3)	6331(3)	7011(3)	71.1(10)
C13	1208(3)	6772(2)	7225(3)	56.1(8)
C14	4696(3)	7457(2)	5912(2)	44.5(7)
C15	5798(3)	8213(3)	5814(3)	63.3(9)
C16	4756(3)	8405(3)	4882(3)	60.8(9)
O4	2792(2)	7012.9(16)	2879.5(14)	52.4(5)
O5	2512(3)	5363(2)	1781(2)	72.8(7)
O6	914(3)	5975(2)	437(2)	92.6(8)
N2	1718(3)	6161(2)	1094(2)	60.0(7)
C17	2778(3)	8894(2)	1681(2)	39.6(7)
C18	2038(3)	9369(2)	2471(2)	49.6(7)
C19	1865(3)	10564(3)	2396(3)	58.9(8)
C20	2415(3)	11293(3)	1550(3)	58.8(8)
C21	3145(3)	10830(3)	765(3)	55.7(8)
C22	3330(3)	9642(2)	836(2)	46.8(7)
C23	2949(3)	7573(2)	1750(2)	39.0(7)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 5a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C24	4448(3)	7056(2)	1404(2)	37.6(6)
C25	4680(3)	6767(2)	416(2)	42.1(7)
C26	6058(3)	6262(2)	169(2)	50.3(7)
C27	7218(3)	6044(2)	897(3)	53.1(8)
C28	7018(3)	6347(2)	1872(3)	55.9(8)
C29	5648(3)	6857(2)	2118(2)	46.8(7)
C30	1712(3)	7419(2)	1049(2)	45.6(7)
C31	186(3)	8158(3)	971(3)	64.6(9)
C32	1057(3)	8290(3)	-5(3)	61.7(9)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 5a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	79.9(15)	49.1(12)	41.0(12)	-2.6(10)	-13.2(10)	-11.0(11)
O2	86.0(17)	39.8(13)	84.1(17)	-3.5(12)	1.8(13)	0.7(12)
O3	80.5(17)	78.5(17)	111(2)	-45.9(15)	33.0(16)	-5.8(13)
N1	50.0(16)	48.9(17)	68.0(19)	-20.3(15)	-2.5(14)	-1.2(13)
C1	46.0(17)	40.8(16)	41.2(16)	-13.4(13)	6.0(13)	-12.7(13)
C2	45.6(17)	44.1(18)	65(2)	-17.9(15)	0.1(15)	-9.9(14)
C3	52.9(19)	44.3(19)	86(2)	-19.1(17)	1.1(17)	-4.6(15)
C4	75(2)	47.2(19)	85(3)	-29(2)	25(2)	-14.9(18)
C5	94(3)	62(2)	60(2)	-32.2(19)	16(2)	-32(2)
C6	70(2)	52.3(19)	48.8(19)	-17.3(15)	3.3(15)	-19.6(16)
C7	48.0(16)	39.1(16)	33.1(16)	-3.3(12)	-5.2(13)	-9.6(12)
C8	46.3(16)	31.6(15)	41.8(17)	-7.5(13)	3.9(14)	-8.1(12)
C9	50.8(18)	46.3(17)	53.4(19)	-15.9(14)	-1.1(14)	-8.4(14)
C10	58(2)	54(2)	86(3)	-31.8(18)	-12.5(19)	-7.4(16)
C11	51(2)	46(2)	124(3)	-33(2)	-4(2)	-9.2(16)
C12	51(2)	49(2)	112(3)	-17(2)	24(2)	-15.2(16)
C13	63(2)	50.7(18)	57(2)	-17.4(15)	13.5(17)	-15.0(16)
C14	45.1(16)	39.1(16)	48.8(18)	-13.0(14)	1.7(13)	-7.0(13)
C15	53.2(19)	61(2)	87(2)	-30.7(18)	16.7(18)	-22.6(16)
C16	69(2)	52.1(19)	59(2)	-12.0(16)	21.2(18)	-12.2(16)
O4	68.3(13)	44.2(11)	38.5(12)	-6.0(9)	15.2(10)	-6.1(10)
O5	79.7(17)	51.8(14)	90.5(18)	-19.2(13)	9.9(14)	-22.2(12)
O6	75.8(17)	93.5(19)	134(2)	-66.8(17)	-6.2(16)	-27.2(14)
N2	49.8(17)	62.6(19)	80(2)	-33.3(17)	13.3(15)	-21.0(14)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 5a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17	36.9(15)	39.8(16)	39.8(16)	-10.7(13)	-0.6(13)	-3.5(12)
C18	54.1(18)	47.8(18)	47.3(18)	-17.2(14)	7.4(14)	-7.2(14)
C19	67(2)	53(2)	60(2)	-28.2(17)	3.9(17)	-2.2(16)
C20	61(2)	38.6(17)	77(2)	-19.6(18)	-3.0(18)	-5.9(15)
C21	50.3(18)	40.9(18)	72(2)	-9.3(16)	4.7(16)	-8.5(14)
C22	44.0(16)	44.6(18)	49.9(18)	-12.3(14)	7.1(14)	-6.6(13)
C23	44.7(16)	39.8(16)	32.2(16)	-11.0(12)	5.4(12)	-7.2(12)
C24	42.4(16)	31.6(14)	37.8(16)	-7.2(12)	3.5(13)	-8.5(12)
C25	42.4(16)	42.9(16)	42.0(17)	-13.8(13)	3.5(13)	-8.4(13)
C26	51.9(19)	49.8(18)	53.3(19)	-21.3(15)	13.6(16)	-11.1(14)
C27	41.9(17)	45.8(18)	70(2)	-16.6(16)	9.9(16)	-5.7(13)
C28	48.2(19)	52.3(19)	64(2)	-13.8(16)	-8.8(16)	-7.5(15)
C29	51.2(18)	44.6(17)	45.9(17)	-16.0(13)	0.2(15)	-8.4(14)
C30	41.8(16)	44.7(17)	55.1(19)	-20.6(15)	9.0(14)	-10.8(13)
C31	41.8(18)	70(2)	86(2)	-32.2(19)	0.9(17)	-6.0(16)
C32	55.5(19)	74(2)	56(2)	-17.9(17)	-8.6(16)	-13.9(16)

Table 4 Bond Lengths for 5a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C7	1.429(3)	O4	C23	1.430(3)
O2	N1	1.217(3)	O5	N2	1.220(3)
O3	N1	1.221(3)	O6	N2	1.222(3)
N1	C14	1.492(3)	N2	C30	1.492(4)
C1	C2	1.384(4)	C17	C18	1.391(4)
C1	C6	1.393(4)	C17	C22	1.381(4)
C1	C7	1.528(4)	C17	C23	1.535(4)
C2	C3	1.379(4)	C18	C19	1.385(4)
C3	C4	1.378(4)	C19	C20	1.368(4)
C4	C5	1.368(4)	C20	C21	1.376(4)
C5	C6	1.383(4)	C21	C22	1.376(4)
C7	C8	1.531(4)	C23	C24	1.530(4)
C7	C14	1.539(4)	C23	C30	1.540(4)
C8	C9	1.380(4)	C24	C25	1.387(3)
C8	C13	1.388(4)	C24	C29	1.390(4)
C9	C10	1.384(4)	C25	C26	1.384(4)
C10	C11	1.367(5)	C26	C27	1.368(4)
C11	C12	1.373(5)	C27	C28	1.375(4)

Table 4 Bond Lengths for 5a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C12	C13	1.380(4)	C28	C29	1.379(4)
C14	C15	1.504(4)	C30	C31	1.508(4)
C14	C16	1.494(4)	C30	C32	1.496(4)
C15	C16	1.475(4)	C31	C32	1.473(4)

Table 5 Bond Angles for 5a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	N1	O3	123.1(3)	O5	N2	O6	122.5(3)
O2	N1	C14	118.1(3)	O5	N2	C30	119.3(3)
O3	N1	C14	118.7(3)	O6	N2	C30	118.2(3)
C2	C1	C6	118.3(3)	C18	C17	C23	120.3(2)
C2	C1	C7	121.1(2)	C22	C17	C18	118.3(2)
C6	C1	C7	120.6(2)	C22	C17	C23	121.4(2)
C3	C2	C1	121.2(3)	C19	C18	C17	120.1(3)
C4	C3	C2	119.9(3)	C20	C19	C18	120.8(3)
C5	C4	C3	119.7(3)	C19	C20	C21	119.5(3)
C4	C5	C6	120.8(3)	C22	C21	C20	120.2(3)
C5	C6	C1	120.1(3)	C21	C22	C17	121.2(3)
O1	C7	C1	106.0(2)	O4	C23	C17	105.23(19)
O1	C7	C8	109.9(2)	O4	C23	C24	110.1(2)
O1	C7	C14	108.6(2)	O4	C23	C30	108.9(2)
C1	C7	C8	109.7(2)	C17	C23	C30	109.4(2)
C1	C7	C14	109.0(2)	C24	C23	C17	110.9(2)
C8	C7	C14	113.3(2)	C24	C23	C30	112.1(2)
C9	C8	C7	123.2(2)	C25	C24	C23	123.7(2)
C9	C8	C13	118.5(3)	C25	C24	C29	117.9(2)
C13	C8	C7	118.2(2)	C29	C24	C23	118.4(2)
C8	C9	C10	120.4(3)	C26	C25	C24	120.8(3)
C11	C10	C9	120.4(3)	C27	C26	C25	120.3(3)
C10	C11	C12	119.9(3)	C26	C27	C28	119.9(3)
C11	C12	C13	120.0(3)	C27	C28	C29	120.0(3)
C12	C13	C8	120.7(3)	C28	C29	C24	121.1(3)
N1	C14	C7	115.0(2)	N2	C30	C23	114.5(2)
N1	C14	C15	111.0(2)	N2	C30	C31	111.6(2)
N1	C14	C16	113.4(2)	N2	C30	C32	113.9(2)
C15	C14	C7	122.0(2)	C31	C30	C23	122.3(2)
C16	C14	C7	124.7(2)	C32	C30	C23	124.3(2)

Table 5 Bond Angles for 5a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C16	C14	C15	58.91(19)	C32	C30	C31	58.72(19)
C16	C15	C14	60.20(19)	C32	C31	C30	60.23(19)
C15	C16	C14	60.89(19)	C31	C32	C30	61.04(19)

Table 6 Torsion Angles for 5a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C7	C8	C9	-136.8(3)	O4	C23	C24	C25	136.9(2)
O1	C7	C8	C13	44.7(3)	O4	C23	C24	C29	-42.6(3)
O1	C7	C14	N1	62.7(3)	O4	C23	C30	N2	-62.7(3)
O1	C7	C14	C15	-76.5(3)	O4	C23	C30	C31	77.4(3)
O1	C7	C14	C16	-148.6(3)	O4	C23	C30	C32	149.2(2)
O2	N1	C14	C7	-10.4(3)	O5	N2	C30	C23	11.3(4)
O2	N1	C14	C15	133.2(3)	O5	N2	C30	C31	-133.0(3)
O2	N1	C14	C16	-162.7(3)	O5	N2	C30	C32	162.8(3)
O3	N1	C14	C7	171.4(2)	O6	N2	C30	C23	-169.0(2)
O3	N1	C14	C15	-45.0(3)	O6	N2	C30	C31	46.7(3)
O3	N1	C14	C16	19.1(4)	O6	N2	C30	C32	-17.5(4)
N1	C14	C15	C16	105.3(3)	N2	C30	C31	C32	-105.6(3)
N1	C14	C16	C15	-101.3(3)	N2	C30	C32	C31	101.7(3)
C1	C2	C3	C4	-1.5(4)	C17	C18	C19	C20	0.0(4)
C1	C7	C8	C9	107.0(3)	C17	C23	C24	C25	-107.0(3)
C1	C7	C8	C13	-71.5(3)	C17	C23	C24	C29	73.4(3)
C1	C7	C14	N1	177.8(2)	C17	C23	C30	N2	-177.2(2)
C1	C7	C14	C15	38.6(3)	C17	C23	C30	C31	-37.1(3)
C1	C7	C14	C16	-33.5(3)	C17	C23	C30	C32	34.7(3)
C2	C1	C6	C5	-1.3(4)	C18	C17	C22	C21	-0.6(4)
C2	C1	C7	O1	-158.7(2)	C18	C17	C23	O4	-23.0(3)
C2	C1	C7	C8	-40.1(3)	C18	C17	C23	C24	-142.0(2)
C2	C1	C7	C14	84.6(3)	C18	C17	C23	C30	93.9(3)
C2	C3	C4	C5	0.2(5)	C18	C19	C20	C21	0.1(5)
C3	C4	C5	C6	0.4(5)	C19	C20	C21	C22	-0.5(4)
C4	C5	C6	C1	0.1(5)	C20	C21	C22	C17	0.7(4)
C6	C1	C2	C3	2.0(4)	C22	C17	C18	C19	0.2(4)

Table 6 Torsion Angles for 5a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C6	C1	C7	O1	22.8(3)	C22	C17	C23	O4	157.9(2)
C6	C1	C7	C8	141.4(2)	C22	C17	C23	C24	38.8(3)
C6	C1	C7	C14	-94.0(3)	C22	C17	C23	C30	-85.3(3)
C7	C1	C2	C3	-176.6(2)	C23	C17	C18	C19	-178.9(2)
C7	C1	C6	C5	177.3(3)	C23	C17	C22	C21	178.6(2)
C7	C8	C9	C10	-179.8(2)	C23	C24	C25	C26	-177.7(2)
C7	C8	C13	C12	179.1(3)	C23	C24	C29	C28	177.2(2)
C7	C14	C15	C16	-114.1(3)	C23	C30	C31	C32	113.4(3)
C7	C14	C16	C15	109.6(3)	C23	C30	C32	C31	-110.0(3)
C8	C7	C14	N1	-59.7(3)	C24	C23	C30	N2	59.4(3)
C8	C7	C14	C15	161.1(2)	C24	C23	C30	C31	-160.5(2)
C8	C7	C14	C16	89.1(3)	C24	C23	C30	C32	-88.7(3)
C8	C9	C10	C11	1.4(4)	C24	C25	C26	C27	-0.2(4)
C9	C8	C13	C12	0.5(4)	C25	C24	C29	C28	-2.4(4)
C9	C10	C11	C12	-0.5(5)	C25	C26	C27	C28	-1.1(4)
C10	C11	C12	C13	-0.3(5)	C26	C27	C28	C29	0.7(4)
C11	C12	C13	C8	0.3(4)	C27	C28	C29	C24	1.1(4)
C13	C8	C9	C10	-1.3(4)	C29	C24	C25	C26	1.9(4)
C14	C7	C8	C9	-15.1(3)	C30	C23	C24	C25	15.6(3)
C14	C7	C8	C13	166.4(2)	C30	C23	C24	C29	-164.0(2)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5a.

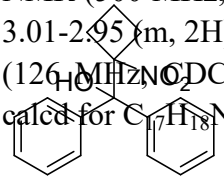
Atom	*x*	*y*	*z*	U(eq)
H1	4301.96	6168.45	7850.73	89
H2	1458.88	9280.85	5453.18	61
H3	719.15	11250.1	5417.71	74
H4	1671.84	11960.54	6721.54	80
H5	3375.59	10704.03	8035.99	80
H6	4161.73	8736.46	8062.29	66
H9	2656.84	6961.41	4891.22	60
H10	722.52	6183.79	4557.22	77
H11	-927.31	5812.02	5869.23	86
H12	-631.66	6180.76	7542.74	85
H13	1325.33	6914.04	7903.61	67
H15A	5659.72	8803.44	6223.46	76
H15B	6803.36	7846.3	5747.31	76
H16A	5125.64	8158.52	4244.14	73

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5a.

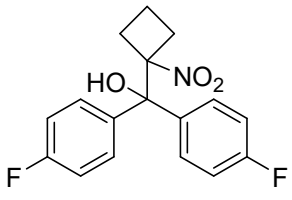
Atom	*x*	*y*	*z*	U(eq)
H16B	3982.54	9115.21	4720.06	73
H4A	3113.94	6295.62	3005.35	79
H18	1658.97	8883.41	3049.79	59
H19	1369.62	10875.88	2927.01	71
H20	2295.96	12094.23	1506.46	71
H21	3515.34	11320.87	184.98	67
H22	3835.2	9336.79	304.78	56
H25	3899.28	6913.22	-86.35	51
H26	6197.04	6070.17	-495.48	60
H27	8139.99	5692.47	733.9	64
H28	7806.48	6206.78	2364.54	67
H29	5524.22	7071.22	2772.98	56
H31A	-610.94	7761.68	985.22	78
H31B	15.14	8795.58	1326.41	78
H32A	1416.41	9010.49	-248.86	74
H32B	790.67	7977.16	-589.86	74

4. Characterization data of products

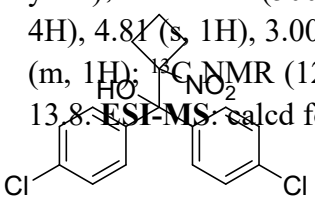
(1-nitrocyclobutyl)diphenylmethanol (2a): White solid (50.9 mg, 90% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.5 Hz, 4H), 7.34-7.27 (m, 6H), 4.79 (s, 1H), 3.01-2.95 (m, 2H), 2.90-2.84 (m, 2H), 1.81-1.70 (m, 1H), 0.93-0.79 (m, 1H).^{13}C NMR (126 MHz, $CDCl_3$) δ 142.4, 128.1, 127.9, 127.1, 96.1, 80.2, 30.7, 13.8. **ESI-MS**: calcd for $C_{17}H_{18}NO_3$ $[M + H]^+$: 284.1287, Found: 284.1290.



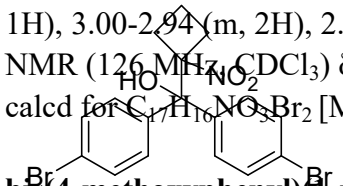
bis(4-fluorophenyl)(1-nitrocyclobutyl)methanol (2b): Brown oil (47.2 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47-7.39 (m, 4H), 7.02 (t, *J* = 8.7 Hz, 4H), 4.81 (s, 1H), 3.01-2.95 (m, 2H), 2.83-2.77 (m, 2H), 1.84-1.72 (m, 1H), 0.97-0.83 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.4 (d, *J* = 248.2Hz), 138.0 (d, *J* = 3.0 Hz), 128.9 (d, *J* = 8.1 Hz), 115.1(d, *J* = 21.4Hz), 95.8, 79.6, 30.6, 13.7; ^{19}F NMR (471 MHz, $CDCl_3$) δ -113.86. **ESI-MS**: calcd for $C_{17}H_{16}NO_3F_2$ $[M + H]^+$: 320.1098, Found: 320.1104.



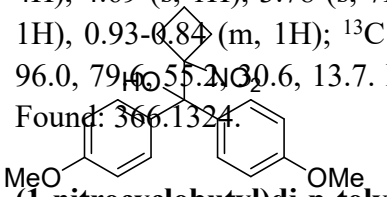
bis(4-chlorophenyl)(1-nitrocyclobutyl)methanol (2c): White solid (42.1 mg, 60% yield)；^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.5 Hz, 4H), 7.30 (d, *J* = 8.5 Hz, 4H), 4.81 (s, 1H), 3.00-2.94 (m, 2H), 2.80-2.75 (m, 2H), 1.85-1.73 (m, 1H), 0.99-0.86 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.5, 134.3, 128.5, 128.4, 95.6, 79.6, 30.5, 13.8. **ESI-MS**: calcd for $C_{17}H_{16}NO_3Cl_2$ $[M + H]^+$: 352.0507, Found: 352.0514.



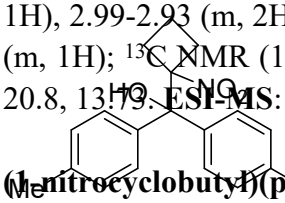
bis(4-bromophenyl)(1-nitrocyclobutyl)methanol (2d): White solid (63.3 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.37 (m, 4H), 7.26-7.21 (m, 4H), 4.74 (s, 1H), 3.00-2.94 (m, 2H), 2.80-2.74 (m, 2H), 1.79-1.67 (m, 1H), 0.92-0.82 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.9, 131.4, 128.8, 122.5, 95.5, 79.6, 30.5, 13.9. **ESI-MS**: calcd for $C_{17}H_{16}NO_3Br_2$ $[M + H]^+$: 439.9497, Found: 439.9482.



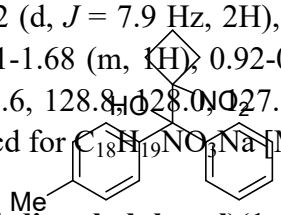
bis(4-methoxyphenyl)(1-nitrocyclobutyl)methanol (2e): Yellow oil (28.8 mg, 42% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.8 Hz, 4H), 6.83 (d, *J* = 8.8 Hz, 4H), 4.69 (s, 1H), 3.78 (s, 7H), 2.98-2.89 (m, 2H), 2.85-2.79 (m, 2H), 1.76-1.69 (m, 1H), 0.93-0.84 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.9, 134.6, 128.3, 113.3, 96.0, 79.6, 55.2, 30.6, 13.7. **ESI-MS**: calcd for $C_{19}H_{21}NO_5Na$ $[M + Na]^+$: 366.1317, Found: 366.1324.



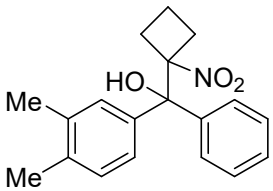
(1-nitrocyclobutyl)di-p-tolylmethanol (2f): Yellow solid (49.8 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.2 Hz, 4H), 7.12 (d, *J* = 8.2 Hz, 4H), 4.71 (s, 1H), 2.99-2.93 (m, 2H), 2.92-2.81 (m, 2H), 2.33 (s, 6H), 1.81-1.69 (m, 1H), 0.99-0.82 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.5, 137.4, 128.6, 126.8, 96.1, 79.8, 30.5, 20.8, 13.79. **ESI-MS**: calcd for $C_{19}H_{22}NO_3$ $[M +H]^+$:312.1600, Found: 312.1604.



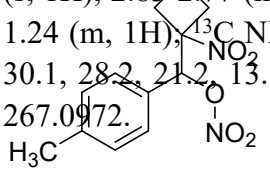
(1-nitrocyclobutyl)(phenyl)(p-tolyl)methanol (2g): White solid (47.5 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.1 Hz, 2H), 7.36-7.27 (m, 5H), 7.12 (d, *J* = 7.9 Hz, 2H), 4.74 (s, 1H), 2.96 (s, 2H), 2.88-2.83 (m, 2H), 2.32 (s, 3H), 1.81-1.68 (m, 1H), 0.92-0.83 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.5, 139.4, 137.6, 128.8, 128.0, 127.8, 127.1, 127.0, 96.1, 80.1, 30.7, 30.6, 21.0, 13.8. **ESI-MS**: calcd for $C_{18}H_{19}NO_3Na$ $[M + Na]^+$: 320.1263, Found: 320.1266.



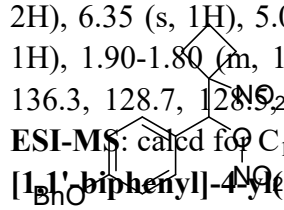
(3,4-dimethylphenyl)(1-nitrocyclobutyl)(phenyl)methanol (2h): white solid **(**37.3 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.6 Hz, 2H), 7.34-7.27 (m, 3H), 7.25 (s, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 4.73 (s, 1H), 3.04-2.94 (m, 1H), 2.93-2.86 (m, 2H), 2.85-2.79 (m, 1H), 2.22 (s, 6H), 1.83-1.69 (m, 1H), 0.95-0.82 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.4, 139.8, 136.4, 136.3, 129.2, 128.2, 128.0, 127.8, 127.1, 124.3, 96.2, 80.0, 30.7, 30.6, 20.1, 19.4, 13.9.



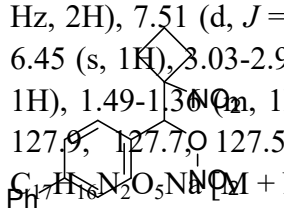
(1-nitrocyclobutyl)(p-tolyl)methyl nitrate (3a): Colorless oil (21.3 mg, 40% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (d, *J* = 7.1 Hz, 2H), 7.15 (d, *J* = 7.7 Hz, 2H), 5.14 (s, 1H), 2.83-2.77 (m, 1H), 2.62-2.54 (m, 3H), 2.33 (s, 3H), 1.78-1.68 (m, 1H), 1.36-1.24 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.8, 134.6, 129.2, 126.7, 91.5, 75.7, 30.1, 28.2, 21.2, 13.1. **ESI-MS**: calcd for $C_{12}H_{15}N_2O_5$ $[M + H]^+$: 267.0981, Found: 267.0972.



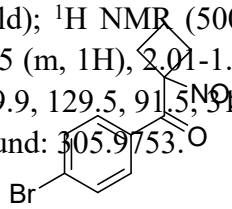
(4-(benzyloxy)phenyl)(1-nitrocyclobutyl)methyl nitrate (3b): White solid (53.7 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47-7.33 (m, 7H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.35 (s, 1H), 5.07 (s, 2H), 3.00-2.94 (m, 1H), 2.72-2.61 (m, 2H), 2.52-2.50 (m, 1H), 1.90-1.80 (m, 1H), 1.42-1.32 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.0, 136.3, 128.7, 128.2, 128.2, 127.5, 124.2, 115.2, 89.0, 83.5, 70.1, 30.3, 27.8, 13.6. **ESI-MS**: calcd for $C_{18}H_{18}N_2O_6Na$ $[M + Na]^+$: 381.1063, Found: 381.1058.



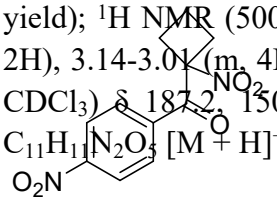
[1,1'-biphenyl]-4-yl(1-nitrocyclobutyl) methyl nitrate (3c): White solid (15.7 mg, 24% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 6.45 (s, 1H), 3.03-2.97 (m, 1H), 2.75-2.69 (m, 2H), 2.62-2.53 (m, 1H), 1.94-1.82 (m, 1H), 1.49-1.36 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.0, 139.8, 131.1, 128.9, 127.9, 127.7, 127.5, 127.1, 89.1, 83.5, 30.3, 28.0, 13.7. **ESI-MS**: calcd for $C_{17}H_{16}N_2O_5Na$ $[M + Na]^+$:351.0957, Found: 351.0956.



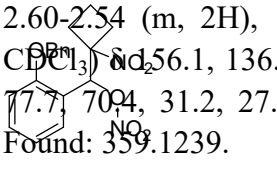
(4-bromophenyl) (1-nitrocyclobutyl) methanone (3d): Yellow solid (17.0 mg, 30% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64-7.57 (m, 4H), 3.10-2.97 (m, 4H), 2.24-2.15 (m, 1H), 2.01-1.91 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.6, 132.4, 131.0, 129.9, 129.5, 91.5, 31.0, 14.1. **ESI-MS**: calcd for $C_{11}H_{10}NO_3Na$ $[M + Na]^+$: 305.9742, Found: 305.9753.



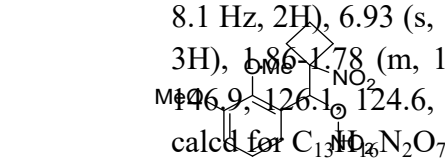
(1-nitrocyclobutyl)(4-nitrophenyl)methanone (3e): Yellow solid (7.5 mg,15% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.7 Hz, 2H), 7.92 (d, *J* = 8.7 Hz, 2H), 3.14-3.01 (m, 4H), 2.31-2.21 (m, 1H), 2.08-1.96 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.2, 150.6, 137.0, 129.5, 124.2, 91.6, 30.9, 14.1. **ESI-MS**: calcd for $C_{11}H_{11}N_2O_5$ $[M + H]^+$: 251.0668, Found: 251.0663.



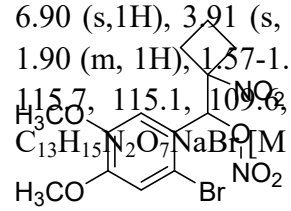
(2-(benzyloxy)phenyl)(1-nitrocyclobutyl)methyl nitrate (3f): Yellow solid (42.9 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.33 (m, 7H), 7.13 (s, 1H), 7.06 (t, *J* = 7.4 Hz, 2H), 5.21 (q, *J* = 12.0 Hz, 2H), 3.02-2.95 (m, 1H), 2.68-2.62 (m, 1H), 2.60-2.54 (m, 2H), 1.90-1.79 (m, 1H), 1.42-1.30 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 136.1, 131.1, 128.7, 128.2, 127.0 , 126.8, 121.5, 121.4, 112.4, 89.1, 77.7, 70.4, 31.2, 27.1, 14.1. **ESI-MS**: calcd for $C_{18}H_{19}N_2O_6$ $[M + H]^+$:359.1243, Found: 359.1239.



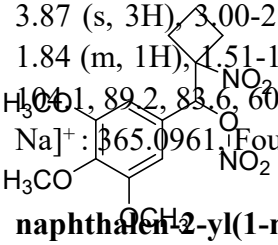
(2,3-dimethoxyphenyl)(1-nitrocyclobutyl)methyl nitrate (3g): White solid (41.2 mg, 66 % yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.1 Hz, 2H), 6.93 (s, 1H), 3.99 (s, 3H), 3.91 (s, 3H), 3.03-2.97 (m, 1H), 2.64 -2.53 (m, 3H), 1.86-1.78 (m, 1H), 1.35-1.21 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5, 146.9, 126.1, 124.6, 117.9, 113.6, 88.9, 78.3, 60.6, 55.7, 31.2, 26.7, 13.9. **ESI-MS**: calcd for $C_{13}H_{16}N_2O_7Na$ $[M + Na]^+$: 335.0855, Found: 335.0860.



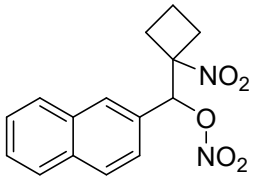
(2-bromo-4,5-dimethoxyphenyl)(1-nitrocyclobutyl)methyl nitrate (3h): Yellow solid (70.2 mg, 90% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.10 (s, 1H), 6.91 (s, 1H), 6.90 (s,1H), 3.91 (s, 3H), 3.88 (s, 3H), 3.05-2.96 (m, 1H), 2.70-2.52 (m, 3H), 2.02-1.90 (m, 1H), 1.57-1.50 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.7, 149.1, 123.7, 115.7, 115.1, 109.6, 89.5, 81.8, 56.3, 56.2, 31.6, 27.3, 14.4. **ESI-MS**: calcd for $C_{13}H_{15}N_2O_7NaBr$ [M + Na]$^+$: 412.9960, Found: 412.9966.



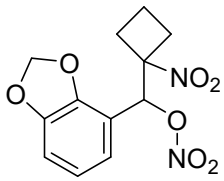
(1-nitrocyclobutyl)(3,4,5-trimethoxyphenyl)methyl nitrate (3i): White solid (60.2 mg, 88% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.61 (s, 2H), 6.33 (s, 1H), 3.88 (s, 6H), 3.87 (s, 3H), 3.00-2.93 (m, 1H), 2.72-2.66 (m, 2H), 2.56 (d, *J* = 6.3 Hz, 1H), 1.95-1.84 (m, 1H), 1.51-1.42 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.6, 139.2, 127.5, 104.1, 89.2, 83.6, 60.8, 56.2, 30.3, 28.0, 13.7. **ESI-MS**: calcd for $C_{14}H_{18}N_2O_8Na$ [M + Na]$^+$: 365.0961, Found: 365.0961.



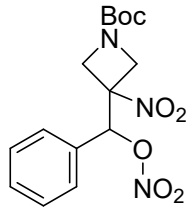
naphthalen-2-yl(1-nitrocyclobutyl)methyl nitrate (3j): White solid (18.1 mg, 30% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97-7.86 (m, 4H), 7.59-7.56 (m, 2H), 7.54-7.52 (m, 1H), 6.58 (s, 1H), 3.07-2.98 (m, 1H), 2.78-2.65 (m, 2H), 2.63-2.55 (m, 1H), 1.91-1.80 (m, 1H), 1.38-1.26 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 133.8, 132.8, 129.6, 129.1), 128.3, 127.8, 127.3, 127.1, 123.7, 89.2, 83.8, 30.5, 27.9, 13.8. **ESI-MS**: calcd for $C_{15}H_{15}N_2O_5$ [M + H]$^+$: 303.0981, Found: 303.0976.



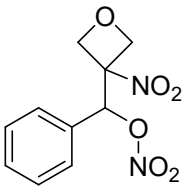
benzo[d][1,3]dioxol-4-yl(1-nitrocyclobutyl)methyl nitrate (3k): White oil (23.7 mg, 40% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.90 (s, 3H), 6.62 (s, 1H), 6.07 (s, 1H), 6.02 (s, 1H), 3.05-2.99(m, 1H), 2.72-2.62 (m, 2H), 2.60-2.56 (m, 1H), 1.93-1.84 (m, 1H), 1.50-1.38 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.7, 145.8, 122.6, 119.0, 114.0, 110.0, 101.6, 88.6, 78.6, 30.7, 27.4, 13.8.



tert-butyl3-nitro-3-((nitrooxy)(phenyl)methyl)azetidine-1-carboxylate (3l):Yellow soild (28.2 mg, 40% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.45 (m, 3H), 7.43-7.38 (m, 2H), 6.47 (s, 1H), 4.56 (d, *J* = 10.8 Hz, 1H), 4.56 (d, *J* = 10.8 Hz, 1H), 4.41 (d, *J* = 10.8 Hz, 1H),4.20 (d, *J* = 10.6 Hz, 1H), 1.37 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 131.0, 130.7, 129.5, 126.9, 83.4, 81.7, 81.2, 28.1.

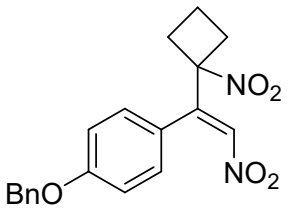


(3-nitrooxetan-3-yl)(phenyl)methyl nitrate (3m): Yellow solid (22.8 mg，45% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48-7.45 (m, 3H), 7.40 (d, *J* = 5.5 Hz, 2H), 6.47 (s, 1H), 5.16 (d, *J* = 8.5 Hz, 1H), 5.03-4.98 (m, 2H),

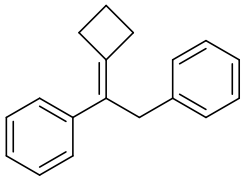


4.82 (d, J = 8.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 131.1, 130.7, 129.5, 126.8, 87.7, 81.5, 74.9, 74.0.

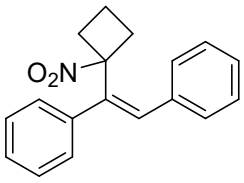
1-(benzyloxy)-4-(2-nitro-1-(1-nitrocyclobutyl)vinyl)benzene (3aa): Yellow solid (31.8 mg, 45% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45-7.38 (m, 4H), 7.35 (t, J = 6.9 Hz, 1H), 7.29 (s, 1H), 7.04 (d, J = 8.8 Hz, 2H), 6.98 (d, J = 8.8 Hz, 2H), 5.05 (s, 2H), 2.96-2.90 (m, 2H), 2.72-2.67 (m, 2H), 2.19-2.10 (m, 1H), 1.96-1.88 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 144.5, 139.2, 136.4, 128.9, 128.6, 128.2, 127.6, 122.8, 115.1, 91.8, 70.1, 33.0, 14.5. **ESI-MS**: calcd for $C_{19}H_{19}N_2O_5$ $[M + H]^+$: 355.1294 , Found: 355.1289.



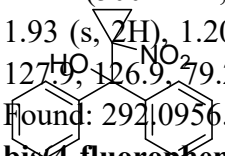
(1-cyclobutylideneethane-1,2-diyl)dibenzene: White solid (329 mg, 56% yield).^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, J = 7.9 Hz, 2H), 7.23-7.19 (m, 4H), 7.16 (t, J = 7.6 Hz, 2H), 7.13-7.06 (m, 2H), 6.39 (t, J = 3.9 Hz, 1H), 4.01 (s, 1H), 2.36-2.28 (m, 2H), 2.12-2.02 (m, 1H), 1.88-1.81 (m, 1H), 1.59-1.54 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.2, 141.9, 137.9, 128.5, 128.1, 128.0, 127.8, 126.3, 125.8, 125.7, 42.6, 32.7, 26.1, 17.4. **ESI-MS**: calcd for $C_{18}H_{19}$ $[M + H]^+$:235.1487, Found: 235.1492 .



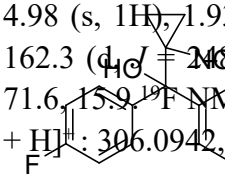
(2-(cyclohexa-2,4-dien-1-yl)-1-(1-nitrocyclobutyl)vinyl)benzene (3ab): White solid (34.8 mg, 62% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13-7.09 (m, 6H), 7.03 (d, J = 6.7 Hz, 2H), 6.99 (d, J = 6.7 Hz, 2H), 5.58 (s, 1H), 2.79 (d, J = 18.6 Hz, 1H), 2.56 (d, J = 14.2 Hz, 1H), 2.47-2.35 (m, 1H), 2.29-2.24(m, 1H), 2.10-1.99 (m, 1H), 1.94 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.8, 141.5, 138.9, 129.5, 128.6, 128.5, 128.0, 127.8, 127.0, 126.9, 86.7, 31.8, 28.9, 18.3. **ESI-MS**: calcd for $C_{18}H_{18}NO_2$ $[M + H]^+$: 280.1338, Found: 280.1338.



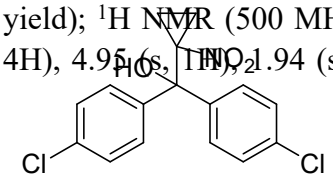
(1-nitrocyclopropyl)diphenylmethanol (5a): White solid (26.9 mg, 50% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, J = 7.3 Hz, 4H), 7.34-7.26 (m, 6H), 4.95 (s, 1H), 1.93 (s, 2H), 1.20 (d, J = 2.1 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.9, 128.2, 127.9, 126.9, 79.2, 71.8, 16.1. **ESI-MS**: calcd for $C_{16}HNO_3Na$ $[M + Na]^+$: 292.0950, Found: 292.0956.



bis(4-fluorophenyl)(1-nitrocyclopropyl)methanol (5b): Yellow oil (41.4 mg, 68% yield).^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (q, J = 5.0 Hz, 4H), 7.00 (t, J = 8.6 Hz, 4H), 4.98 (s, 1H), 1.93 (s, 2H), 1.14 (d, J = 2.2 Hz, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 162.3 (d, J = 248.2 Hz), 138.6, 128.8 (d, J = 8.0 Hz), 115.2 (d, J = 21.4 Hz), 78.6, 71.6, 15.9.^{19}F NMR (471MHz, $CDCl_3$) δ-113.94. **ESI-MS**: calcd for $C_{16}H_{14}NO_3F_2$ $[M + H]^+$: 306.0942, Found: 306.0935.

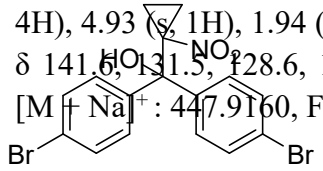


bis(4-chlorophenyl)(1-nitrocyclopropyl)methanol (5c): White solid (40.4 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, J = 7.8 Hz, 4H), 7.29 (d, J = 8.4 Hz, 4H), 4.95 (s, 1H), 1.94 (s, 2H), 1.14 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.1,

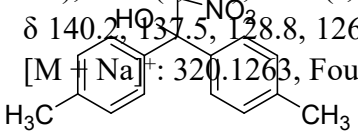


134.2, 128.5, 128.3, 78.6, 71.4, 15.9. **ESI-MS**: calcd for $C_{16}H_{13}NO_3NaCl_2$ $[M + Na]^+$: 360.0170 , Found: 360.0167.

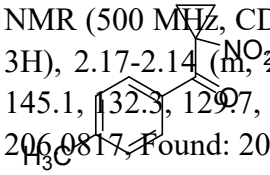
bis(4-bromophenyl)(1-nitrocyclopropyl)methanol (5d): Yellow solid (69.5 mg, 82% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.5 Hz, 4H), 7.28 (d, *J* = 8.0 Hz, 4H), 4.93 (s, 1H), 1.94 (s, 2H), 1.14 (d, *J* = 1.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.6, 131.5, 128.6, 122.4, 78.7, 71.3, 15.9. **ESI-MS**: calcd for $C_{16}H_{13}NO_3NaBr_2$ $[M + Na]^+$: 447.9160, Found: 447.9152.



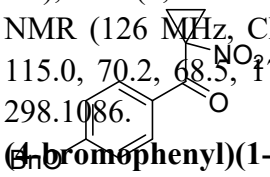
(1-nitrocyclopropyl)di-p-tolylmethanol (5f): White solid (47.5 mg, 80% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.6 Hz, 4H), 7.11 (d, *J* = 8.0 Hz, 4H), 4.88 (s, 1H), 2.31 (s, 6H), 1.90 (s, 2H), 1.19 (d, *J* = 2.1 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.2, 137.5, 128.8, 126.8, 79.0, 71.8, 21.0, 16.1. **ESI-MS**: calcd for $C_{18}H_{19}NO_3Na$ $[M + Na]^+$: 320.1263, Found: 320.1260.



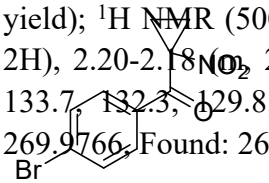
(1-nitrocyclopropyl)(p-tolyl)methanone (6a):White solid (8.2 mg, 20% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 2.43 (s, 3H), 2.17-2.14 (m, 2H), 1.82-1.79 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.6, 145.1, 132.3, 129.7, 128.6, 68.7, 21.8, 17.9. **ESI-MS**: calcd for $C_{11}H_{12}NO_3$ $[M + H]^+$: 206.0817, Found: 206.0822.



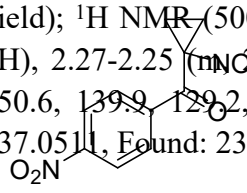
(4-(benzyloxy)phenyl)(1-nitrocyclopropyl)methanone (6b):Yellow solid (35.6 mg, 60% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.7 Hz, 2H), 7.45-7.33 (m, 5H), 7.03 (d, *J* = 8.7 Hz, 2H), 5.14 (s, 2H), 2.16-2.13 (m, 2H), 1.79-1.76 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.2, 163.3, 135.8, 130.9, 128.7, 128.3, 127.7, 127.5, 115.0, 70.2, 68.5, 17.7. **ESI-MS**: calcd for $C_{17}H_{16}NO_4$ $[M+H]^+$: 298.1079, Found: 298.1086.



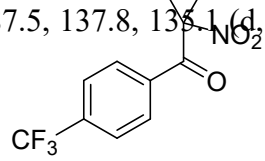
(4-bromophenyl)(1-nitrocyclopropyl)methanone (6c): Yellow solid (26.9 mg, 50% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 2.20-2.18 (m, 2H), 1.84-1.82 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.2, 133.7, 132.3, 129.8, 129.3, 68.7, 18.0. **ESI-MS**: calcd for $C_{10}H_9NO_3$ $[M + H]^+$: 269.9766, Found: 269.9763.



(1-nitrocyclopropyl)(4-nitrophenyl)methanone (6d): Yellow solid (11.8 mg, 25% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.6 Hz, 2H), 8.02 (d, *J* = 8.6 Hz, 2H), 2.27-2.25 (m, 2H), 1.93-1.90 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.2, 150.6, 139.9, 129.2, 124.2, 68.9, 18.6. **ESI-MS**: calcd for $C_{10}H_9N_2O_5$ $[M + H]^+$: 237.0511, Found: 237.0518.

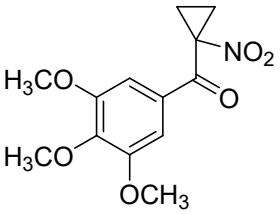


(1-nitrocyclopropyl)(4-(trifluoromethyl)phenyl)methanone (6e): Yellow solid (7.8 mg, 15% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 2.24-2.21 (m, 2H), 1.89-1.86 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.5, 137.8, 135.1 (d, *J* = 32.7 Hz), 128.5, 126.2 (q, *J* = 277.2 Hz), 126.0 (q, *J* = 3.7

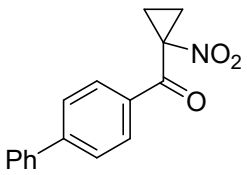


Hz), 68.8, 18.2. **ESI-MS**: calcd for $C_{11}H_8NO_3F_3Na$ $[M + Na]^+$: 282.0354, Found: 282.0363.

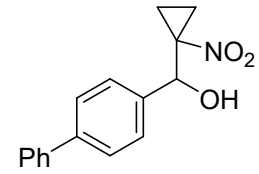
(1-nitrocyclopropyl)(3,4,5-trimethoxyphenyl)methanone (6f): White solid (17.4 mg, 31% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.13 (s, 2H), 3.93 (s, 3H), 3.89 (s, 6H), 2.17-2.15 (m, 2H), 1.83-1.80(m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.8, 153.3, 143.5, 129.7, 105.9, 68.8, 61.0, 56.3, 17.7. **ESI-MS**: calcd for $C_{13}H_{16}NO_6$ $[M + H]^+$: 282.0978, Found: 282.0978.



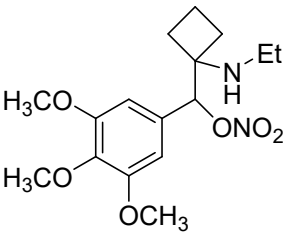
[1,1'-biphenyl]-4-yl(1-nitrocyclopropyl)methanone (6g): White solid (32.0 mg, 60% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, J = 8.3 Hz, 2H), 7.70 (d, J = 8.3 Hz, 2H), 7.62 (d, J = 7.4 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.42 (t, J = 7.2 Hz, 1H), 2.21-2.19 (m, 2H), 1.87-1.84 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.6, 146.8, 139.5, 133.5, 129.1, 129.0, 128.5, 127.6, 127.3, 68.8, 17.9. **ESI-MS**: calcd for $C_{16}H_{14}NO_3$ $[M + H]^+$: 268.0974, Found: 268.0966.



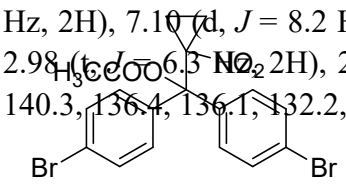
[1,1'-biphenyl]-4-yl(1-nitrocyclopropyl)methanol (6g'): Yellow solid (26.9 mg, 50% yield).^1H NMR (500 MHz, $CDCl_3$) δ 7.60-7.57 (m, 4H), 7.48-7.43 (m, 4H), 7.37 (t, J = 7.3 Hz, 1H), 5.73 (s, 1H), 3.25 (s, 1H), 1.93-1.88 (m, 1H), 1.85-1.79 (m, 1H), 1.40-1.35 (m, 1H), 1.09-1.04 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.3, 140.3, 137.2, 128.8, 127.6, 127.2, 127.1, 127.0, 71.6, 69.3, 17.2, 14.6. **ESI-MS**: calcd for $C_{16}H_{16}NO_3$ $[M + H]^+$: 270.1130, Found: 270.1125.



(1-(ethylamino)cyclobutyl)(3,4,5-trimethoxyphenyl)methyl nitrate (7): Colorless oil(51.0 mg, 75% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 6.60 (s, 2H), 4.77 (s, 1H), 3.86 (s, 9H), 3.53-3.47 (m, 1H), 3.37-3.31 (m, 1H), 2.87-2.80 (m, 1H), 2.68-2.60 (m, 1H), 2.56-2.47 (m, 2H), 1.73-1.66 (m,1H), 1.26-1.20 (m, 1H), 1.18-1.12 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.2, 138.2, 131.4, 104.6, 91.5, 82.7, 65.27, 60.8, 56.1, 29.7, 28.1, 14.9, 13.3. **ESI-MS**: calcd for $C_{16}H_{25}N_2O_6$ $[M + H]^+$: 341.1713, Found: 341.1705.



bis(4-bromophenyl)(1-nitrocyclopropyl)methyl acetate (8) : Yellow solid (34.0 mg, 73% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, J = 8.2 Hz, 2H), 7.45 (d, J = 8.3 Hz, 2H), 7.10 (d, J = 8.2 Hz, 2H), 7.00 (d, J = 8.3 Hz, 2H), 4.23 (t, J = 6.3 Hz, 2H), 2.98 (t, J = 6.3 Hz, 2H), 2.04 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 147.6, 140.3, 136.4, 136.1, 132.2, 132.1, 130.6, 129.6, 123.8, 123.6, 61.3, 30.8, 20.7.



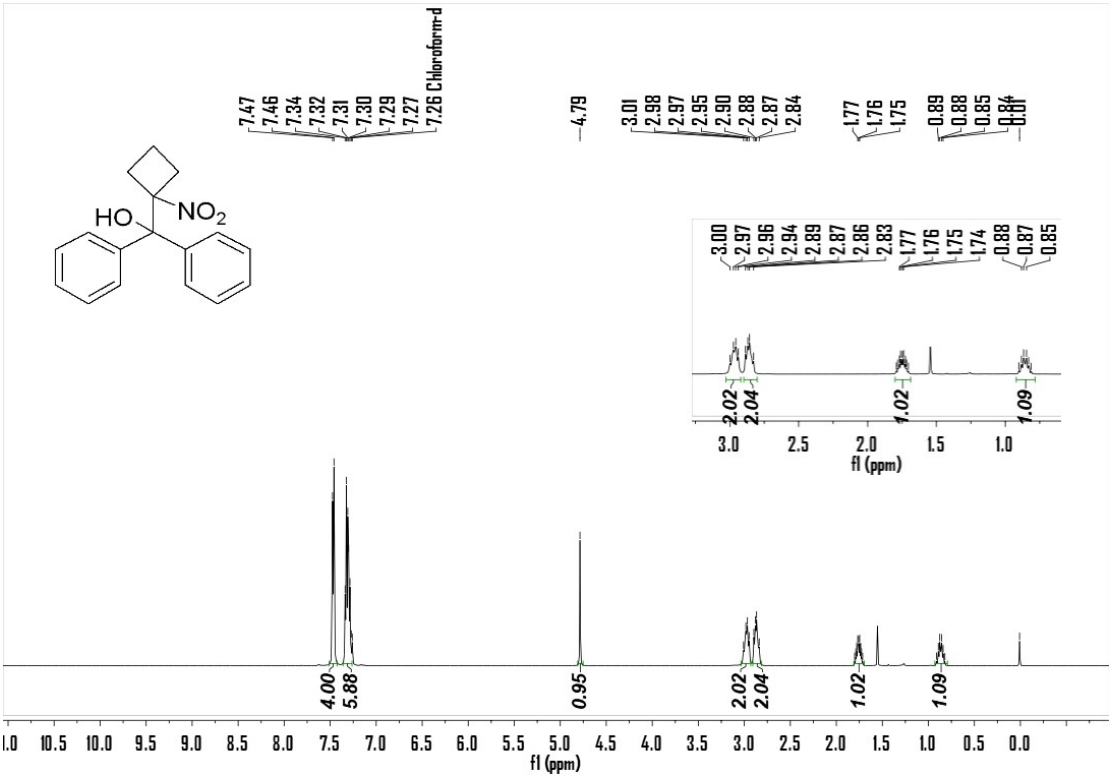
5.Reference

[1] T. Kang, T.-G. Erbay, K.-L. Xu, G.-M. Gallego, A.-Burtea, S.-K. Nair, R.-L. Patman, R. Zhou, S.-C. Sutton, I.- J. Mc Alpine, P. Liu, and K.-M. Engle, *ACS Catal.* 2020, 10, 13075−13083.

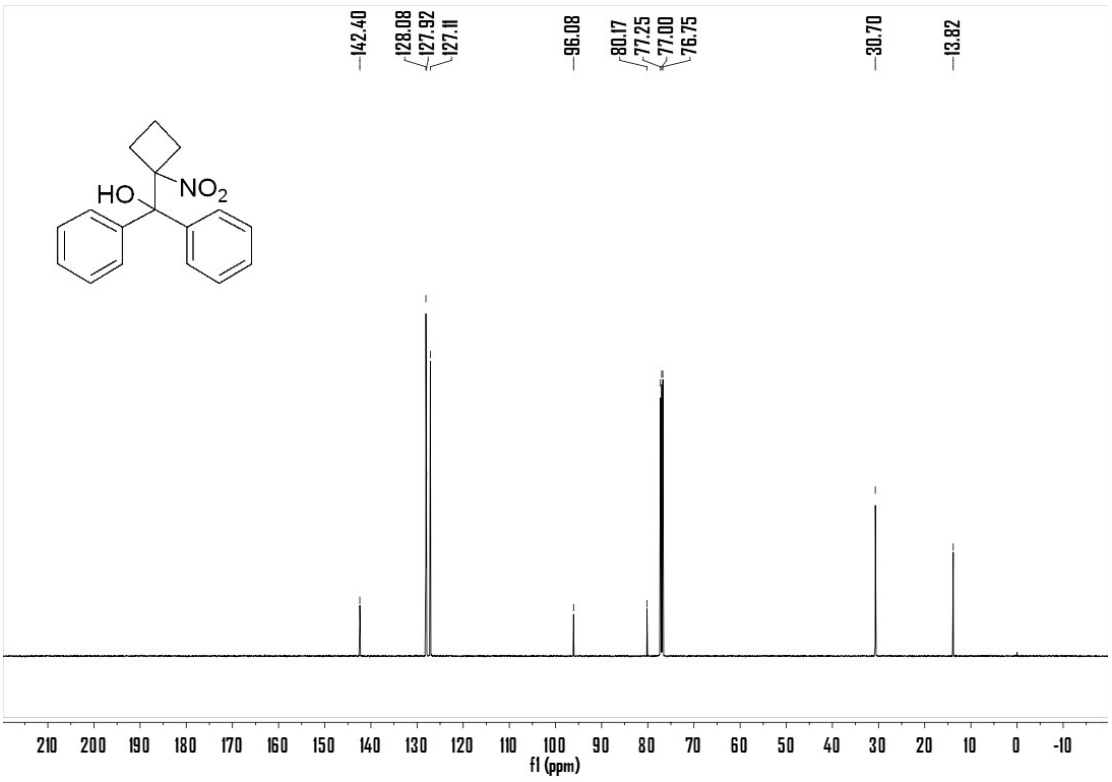
[2] Z.-Z. Zhu, K. Chen, L.-Z. Yu, X.-Y. Tang, and M. Shi, *Org. Lett.* 2015, **17**, 5994.

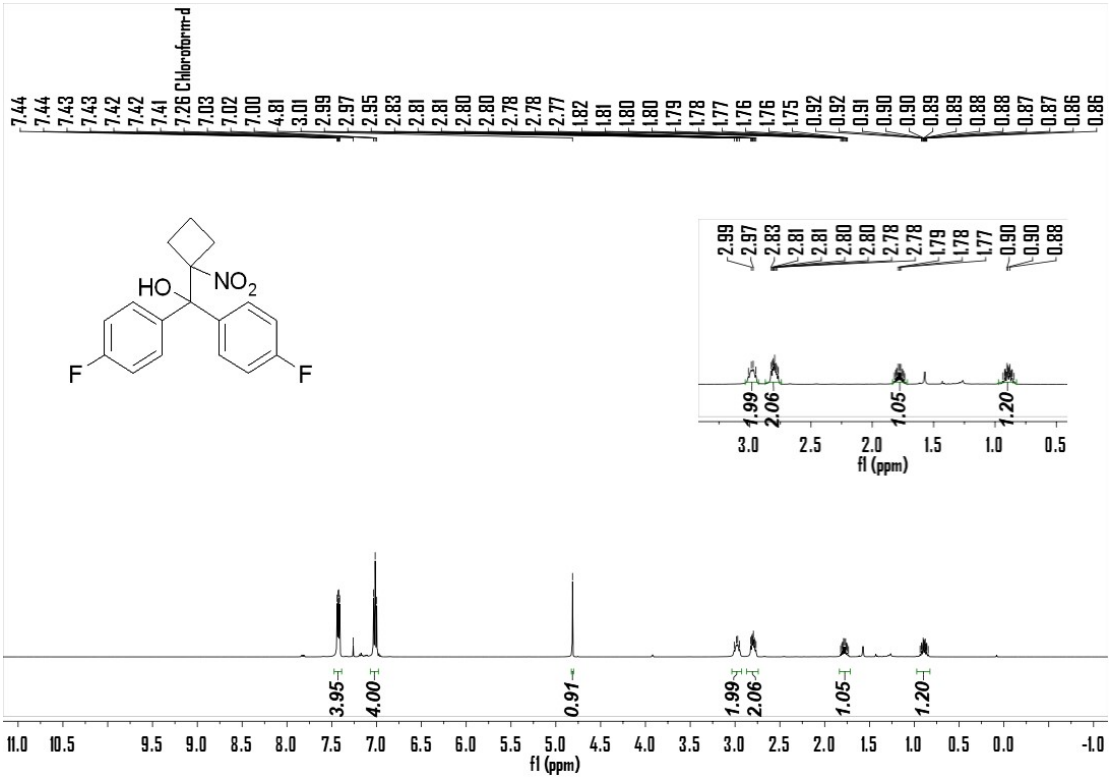
6. NMR spectra of products

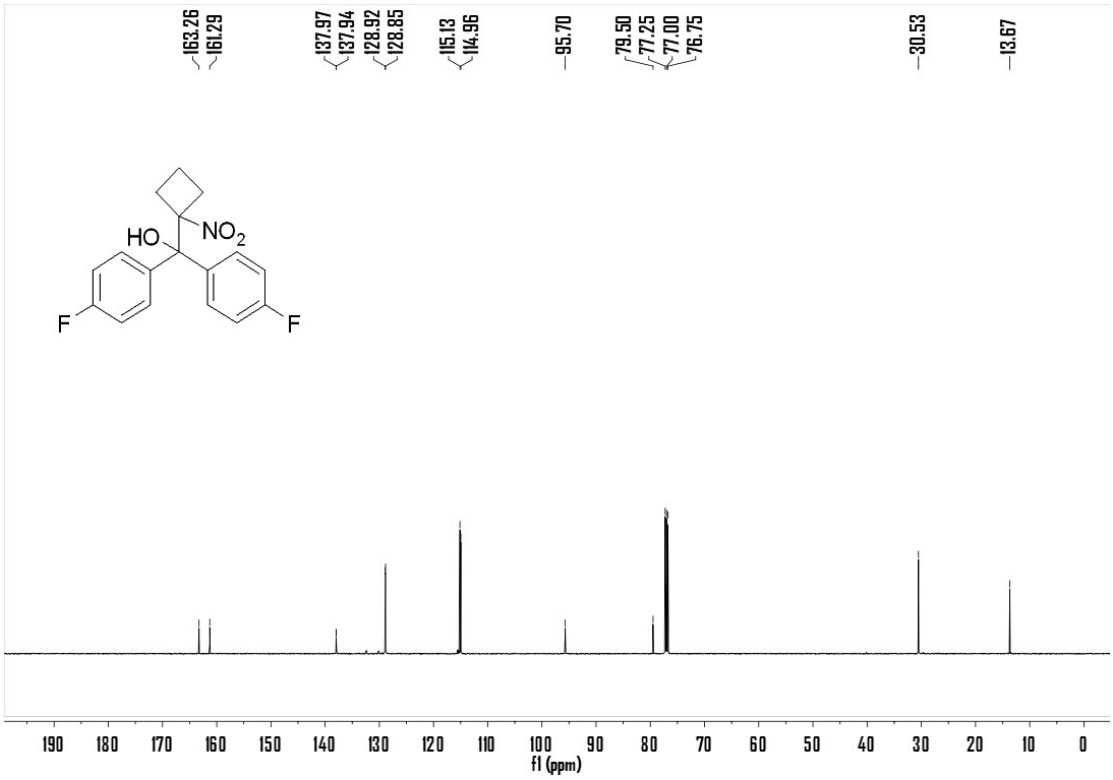
(1-nitrocyclobutyl)diphenylmethanol (2a)

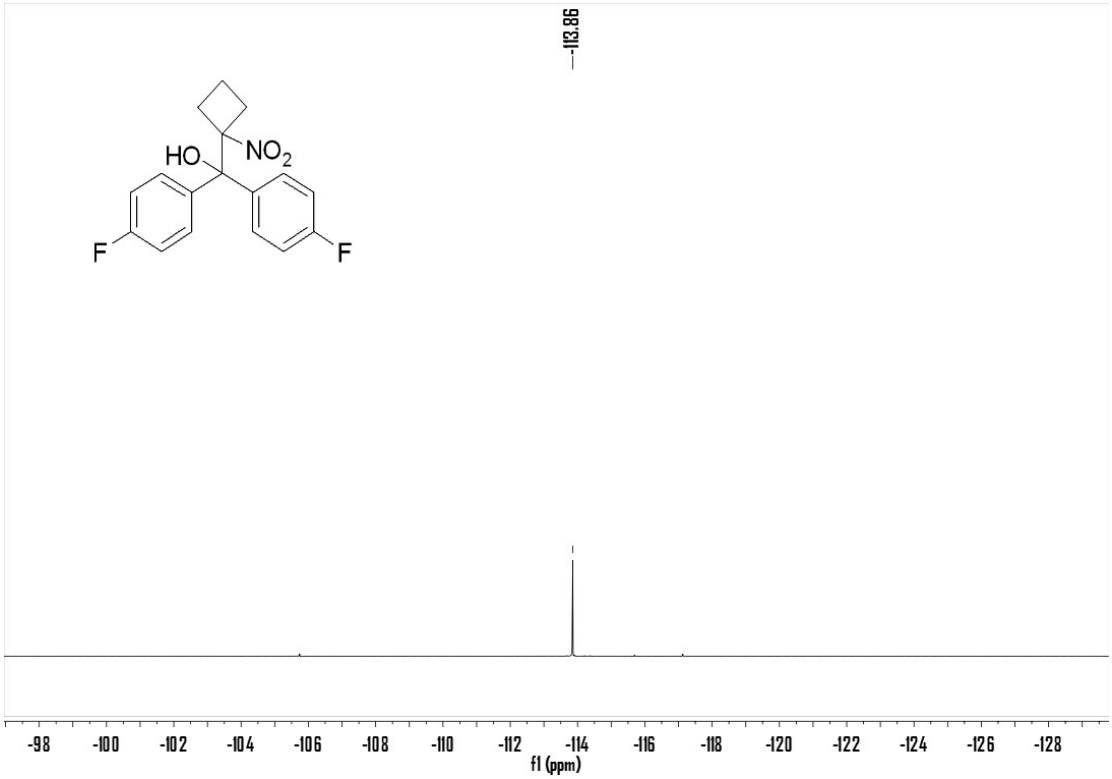


bis(4-fluorophenyl)(1-nitrocyclobutyl) methanol (2b)

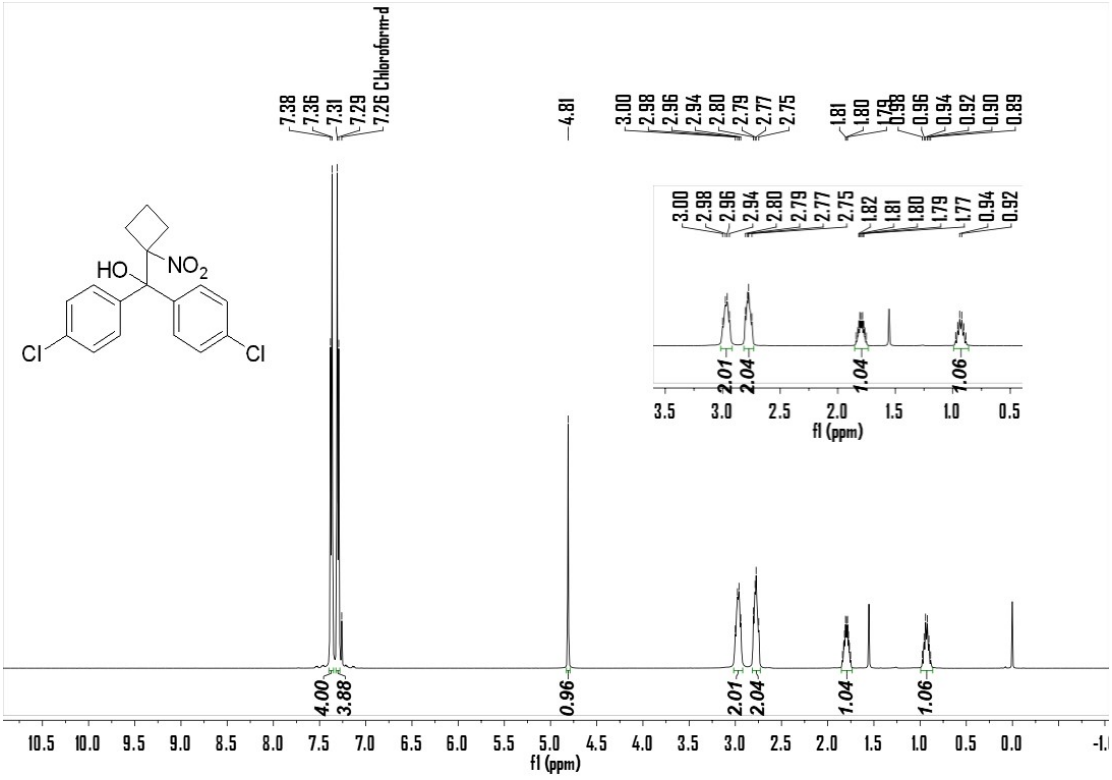


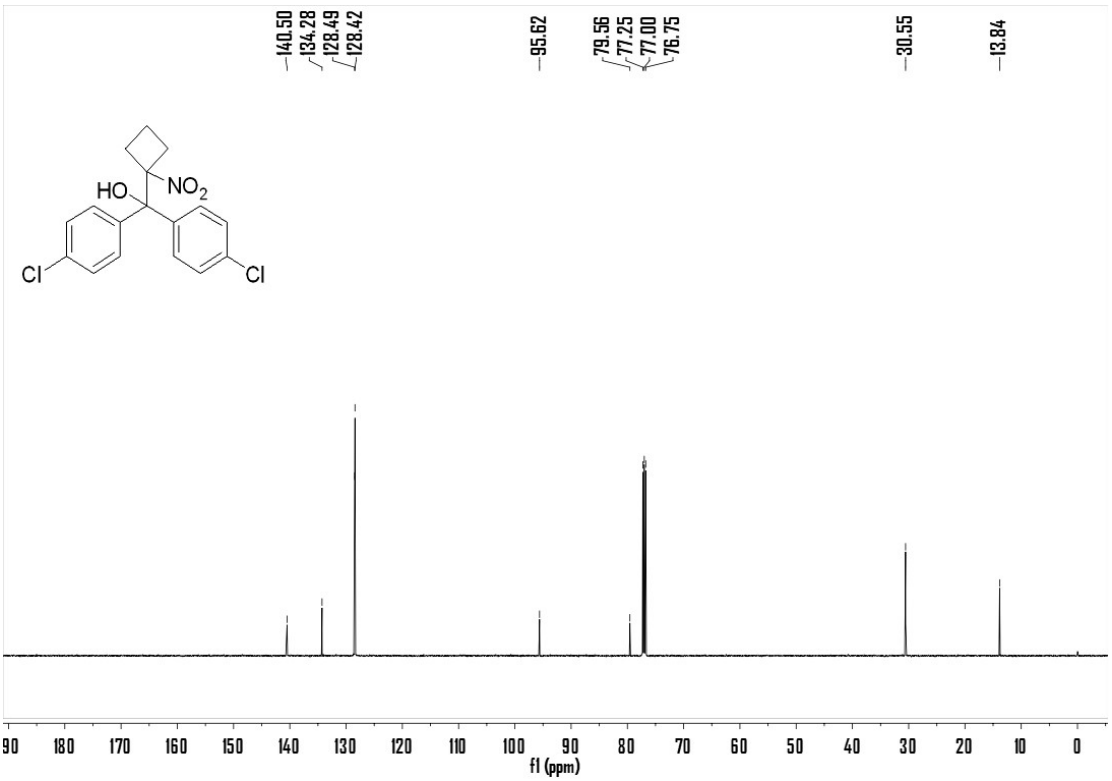

Chloroform-d
HO
NO2
F
F
f1 (ppm)


HO
NO2
F
F
f1 (ppm)

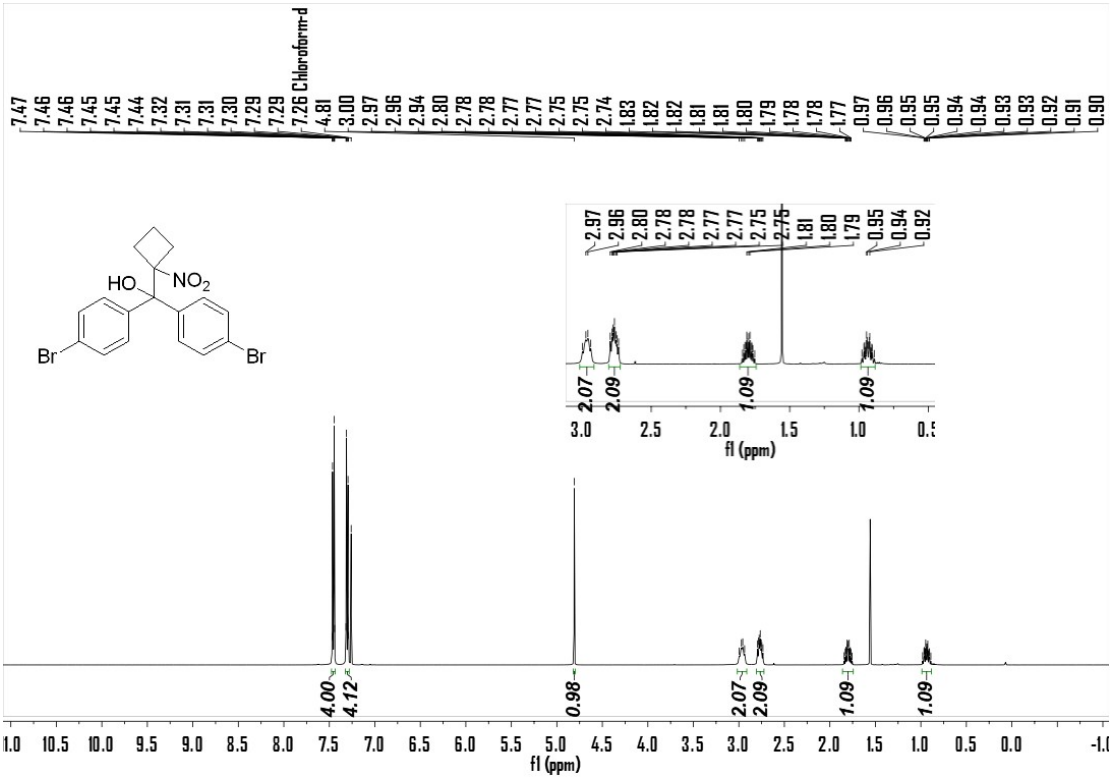


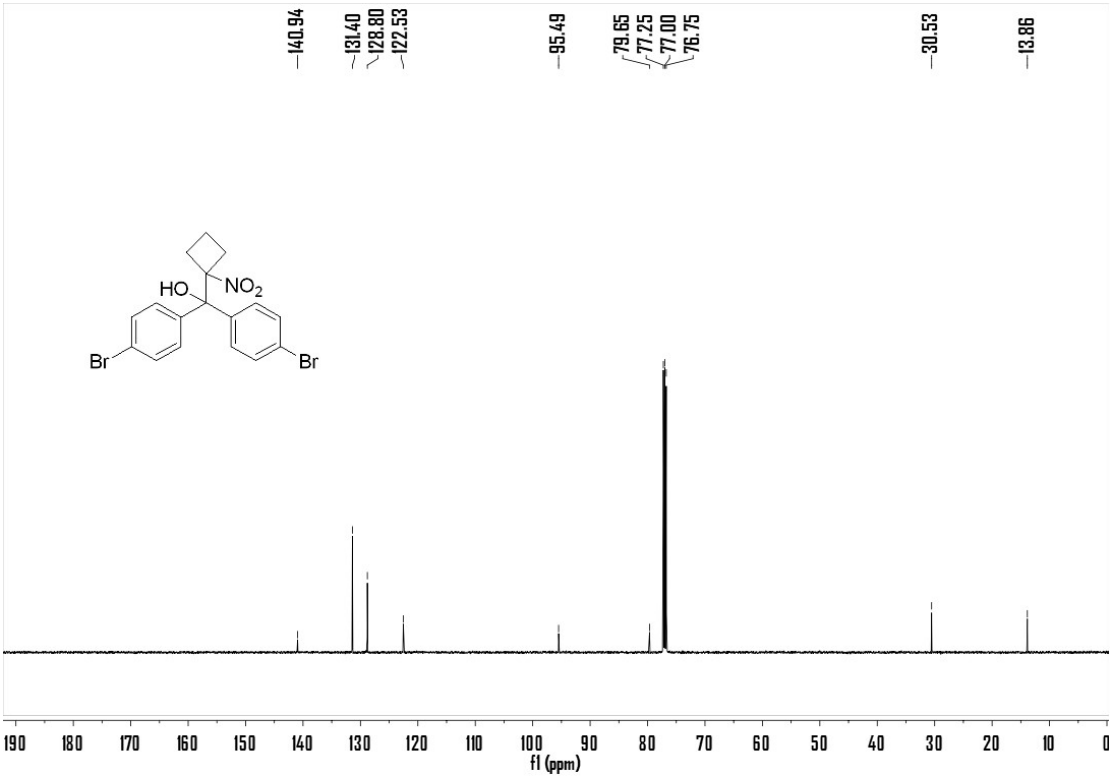
bis(4-chlorophenyl)(1-nitrocyclobutyl)methanol (2c)



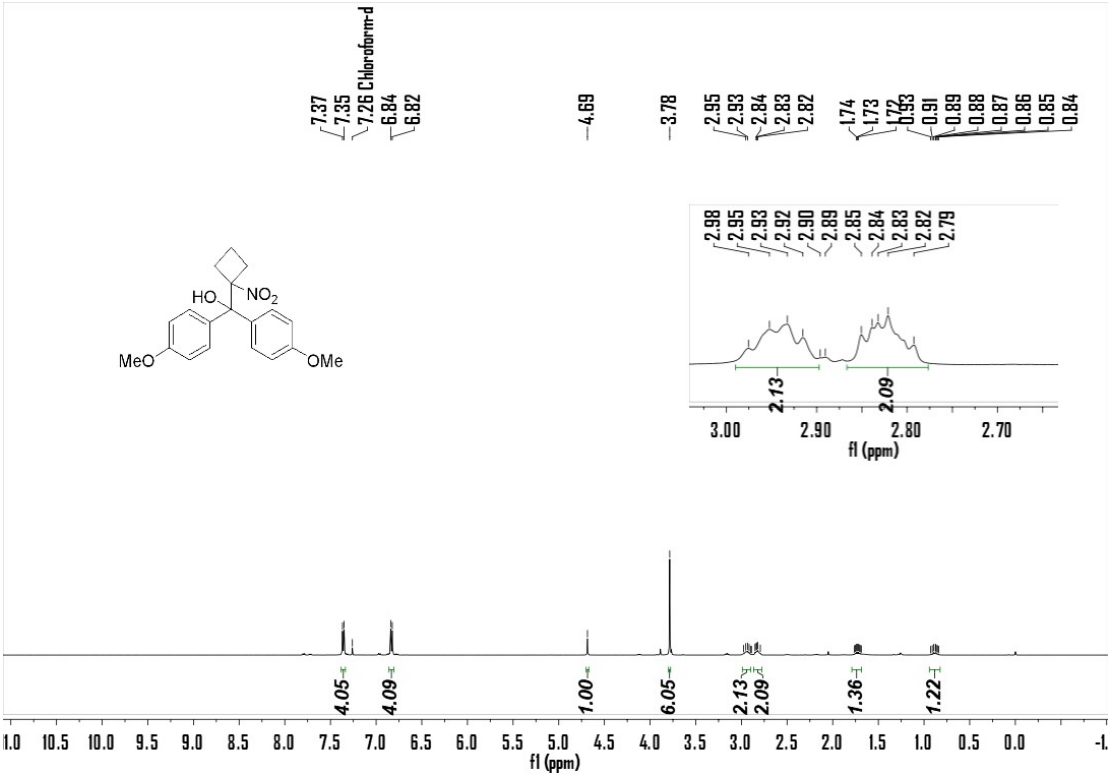


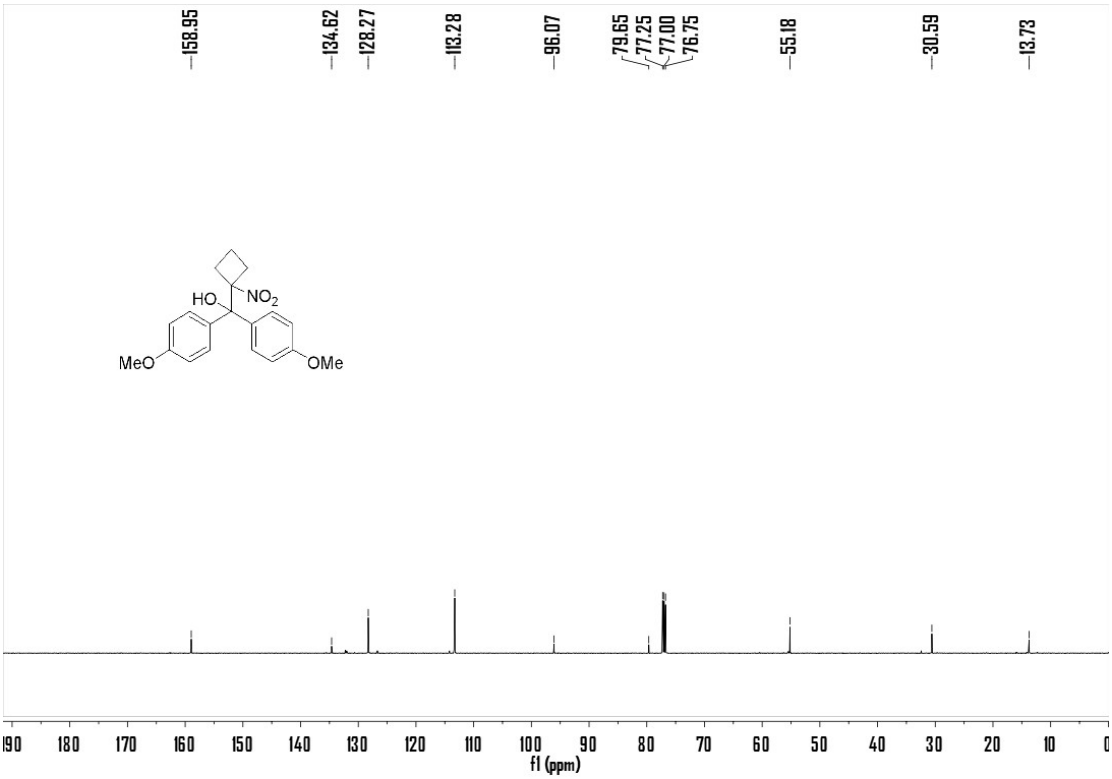
bis(4-bromophenyl)(1-nitrocyclobutyl)methanol (2d)



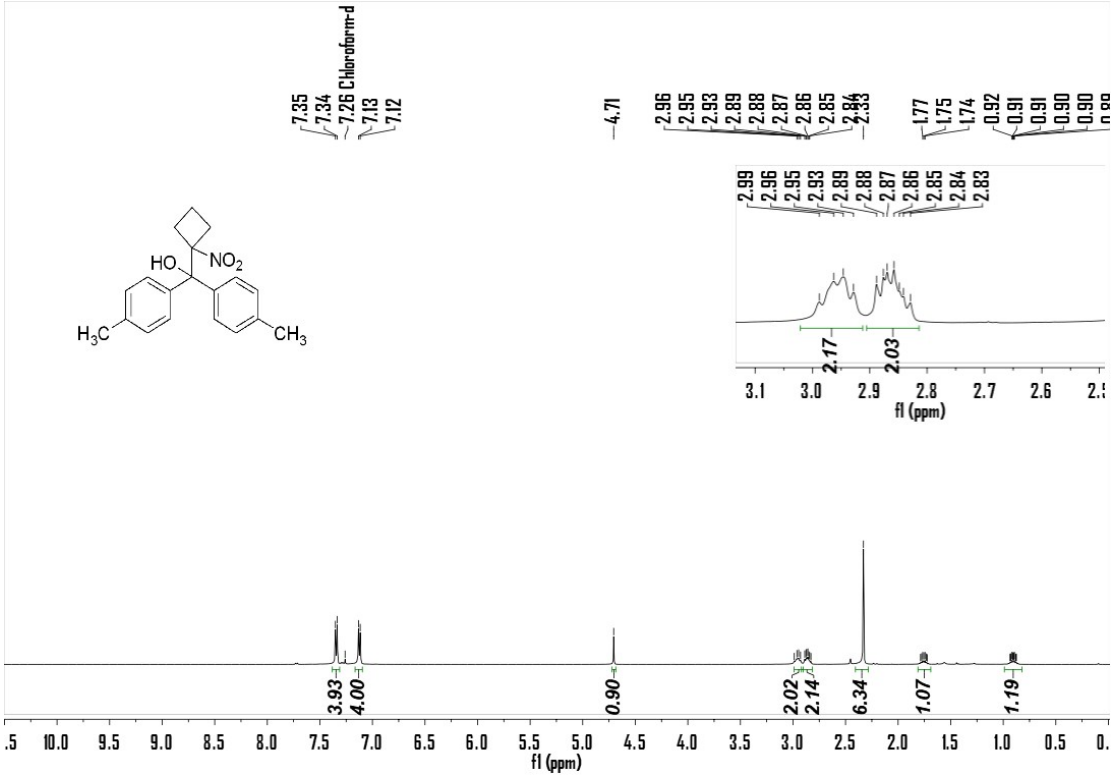


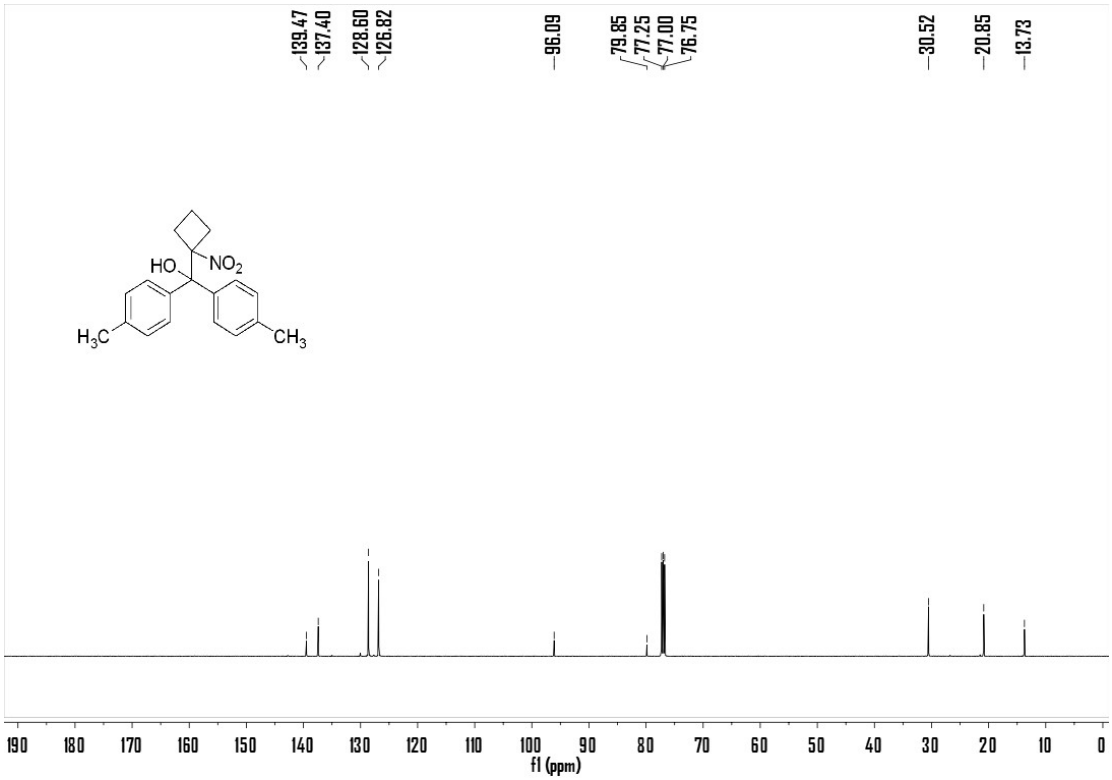
bis(4-methoxyphenyl)(1-nitrocyclobutyl)methanol (2e)



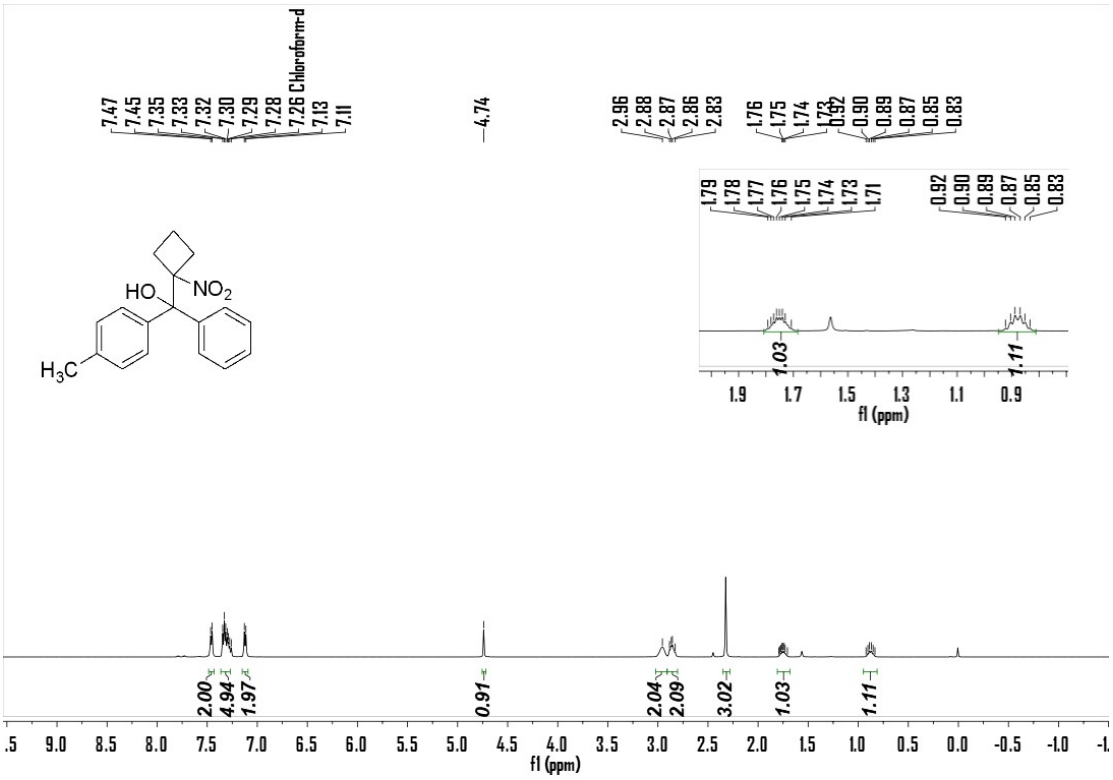


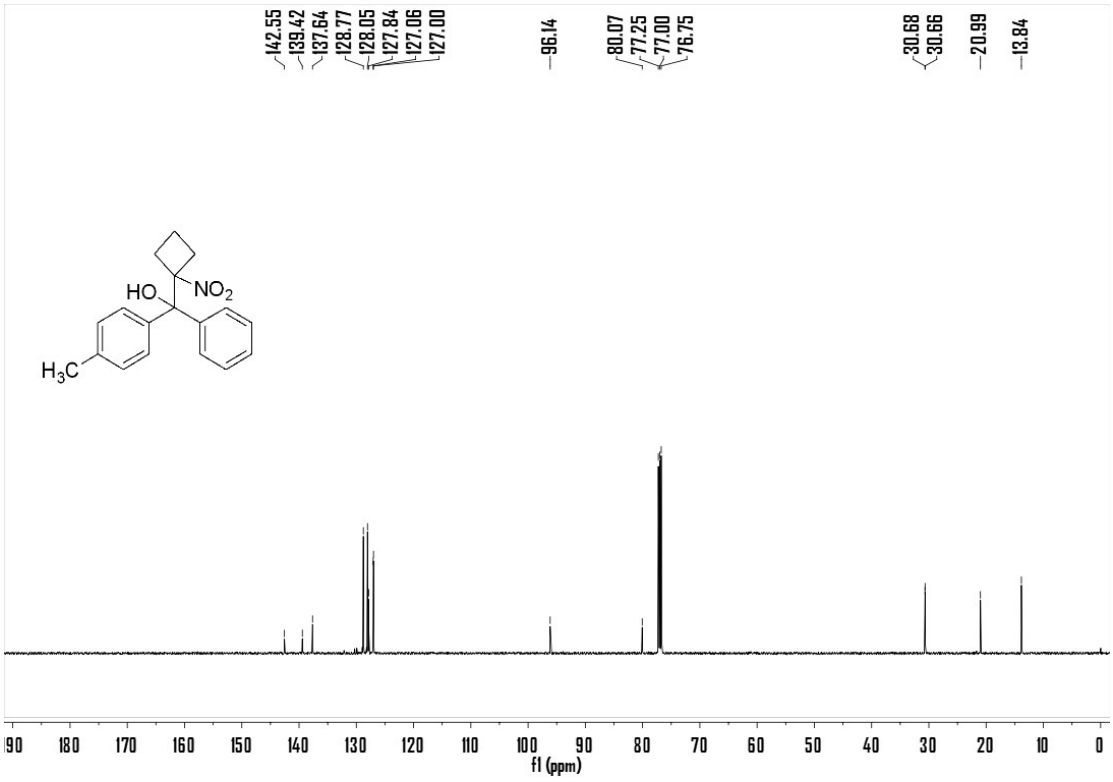
(1-nitrocyclobutyl)di-p-tolylmethanol (2f)



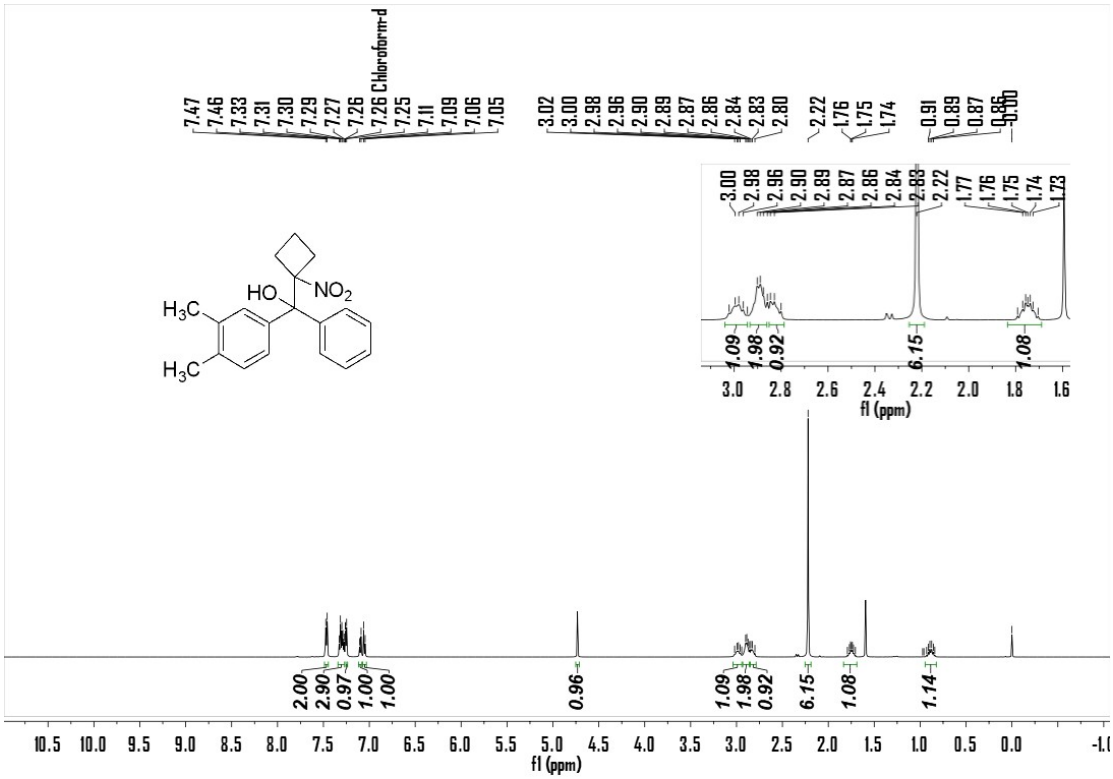


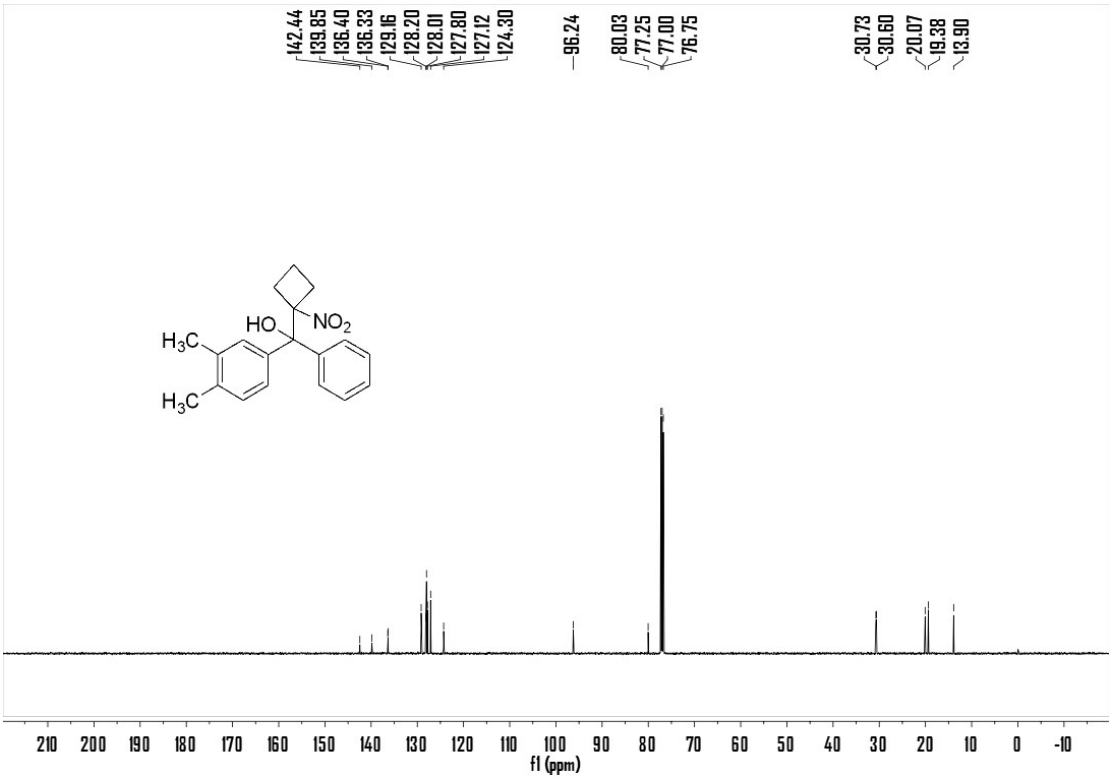
(1-nitrocyclobutyl)(phenyl)(p-tolyl)methanol (2g)



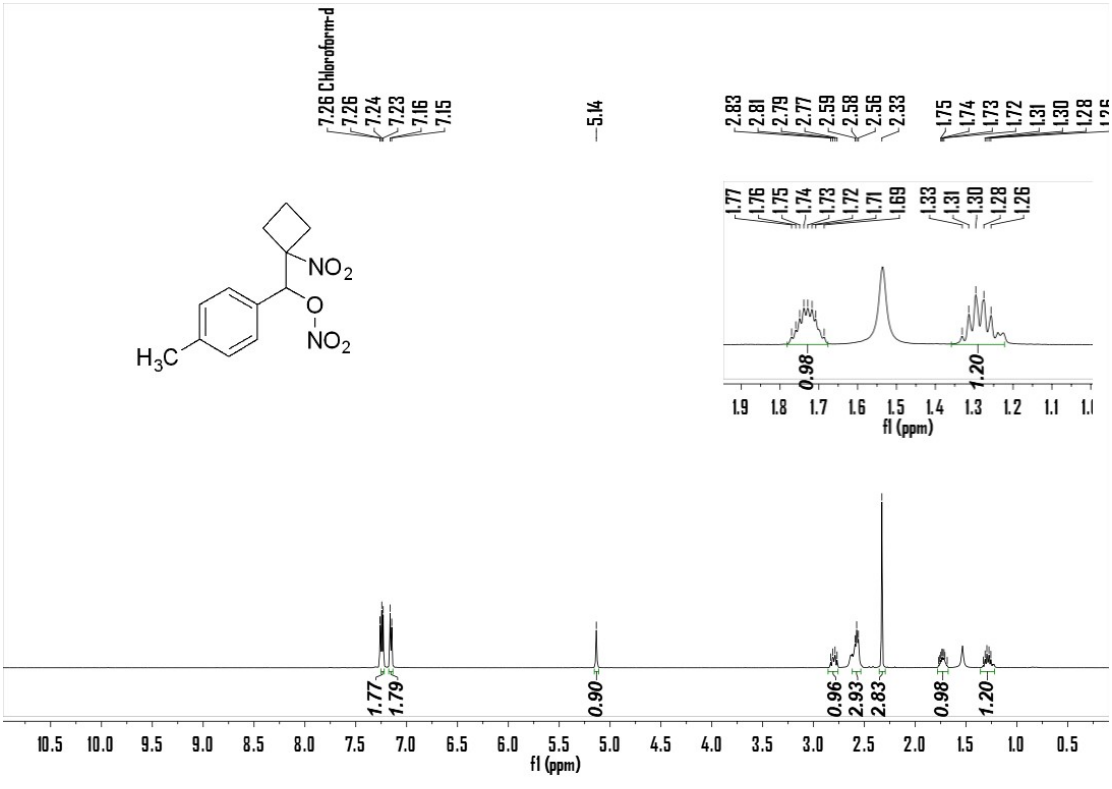


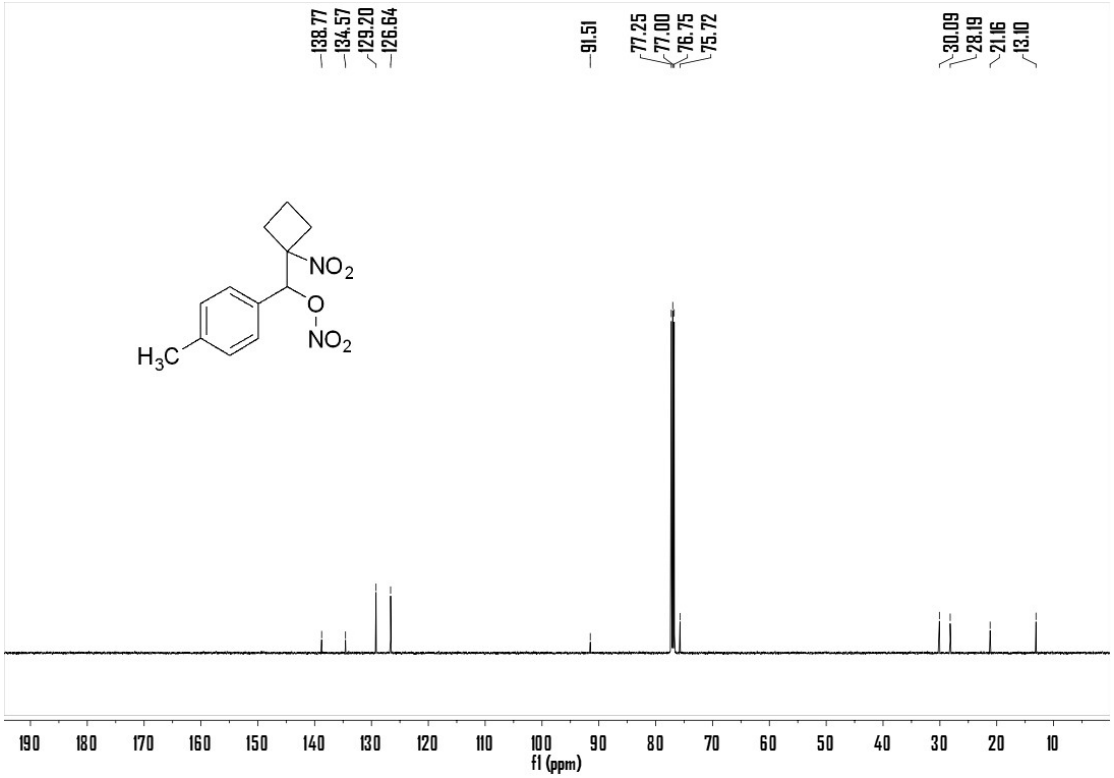
(3,4-dimethylphenyl)(1-nitrocyclobutyl)(phenyl)methano (2h)



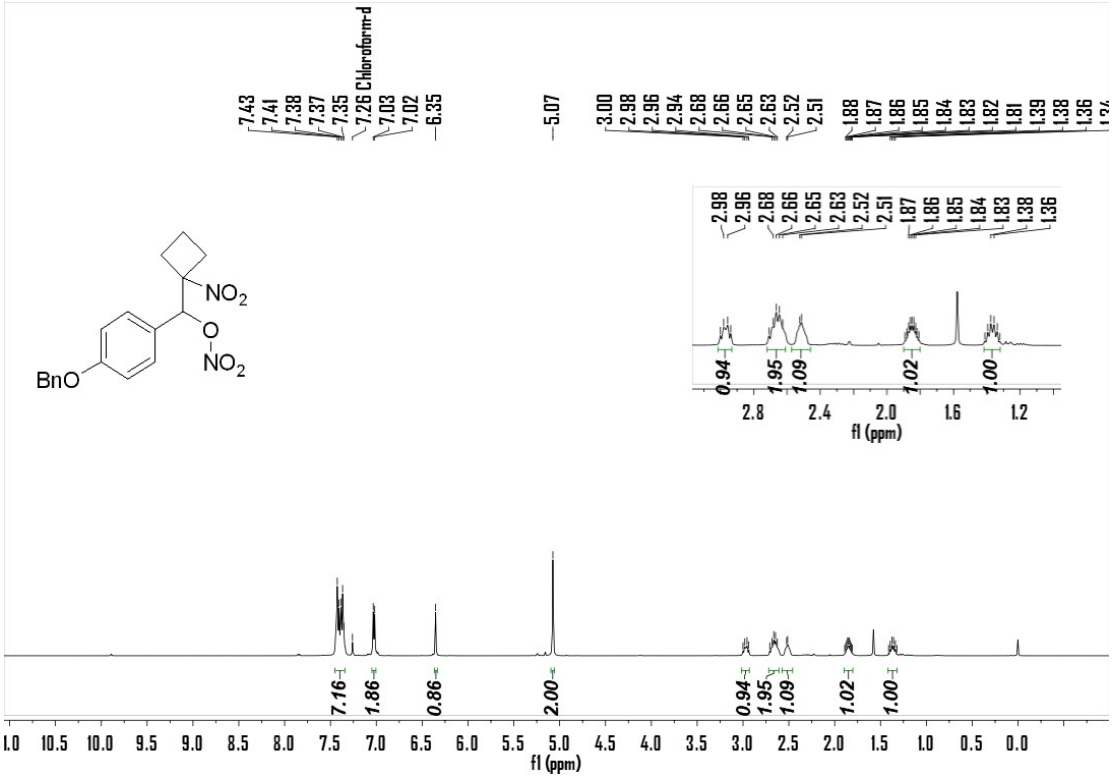


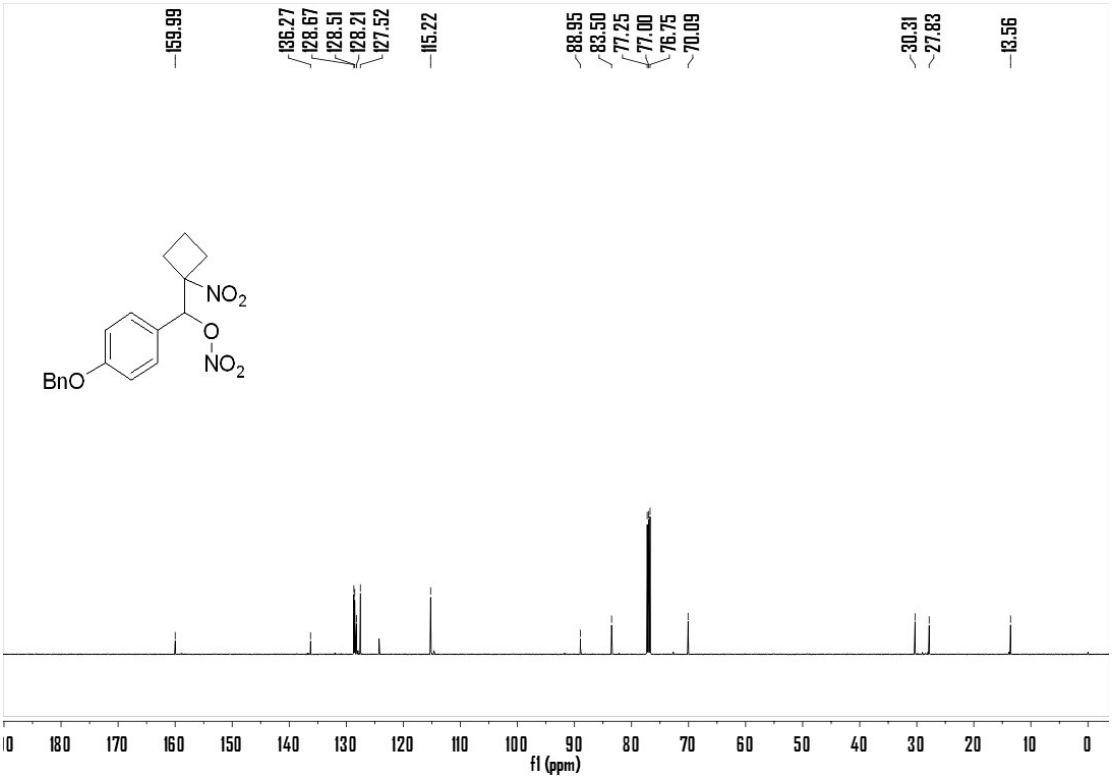
(1-nitrocyclobutyl)(p-tolyl)methyl nitrate (3a)



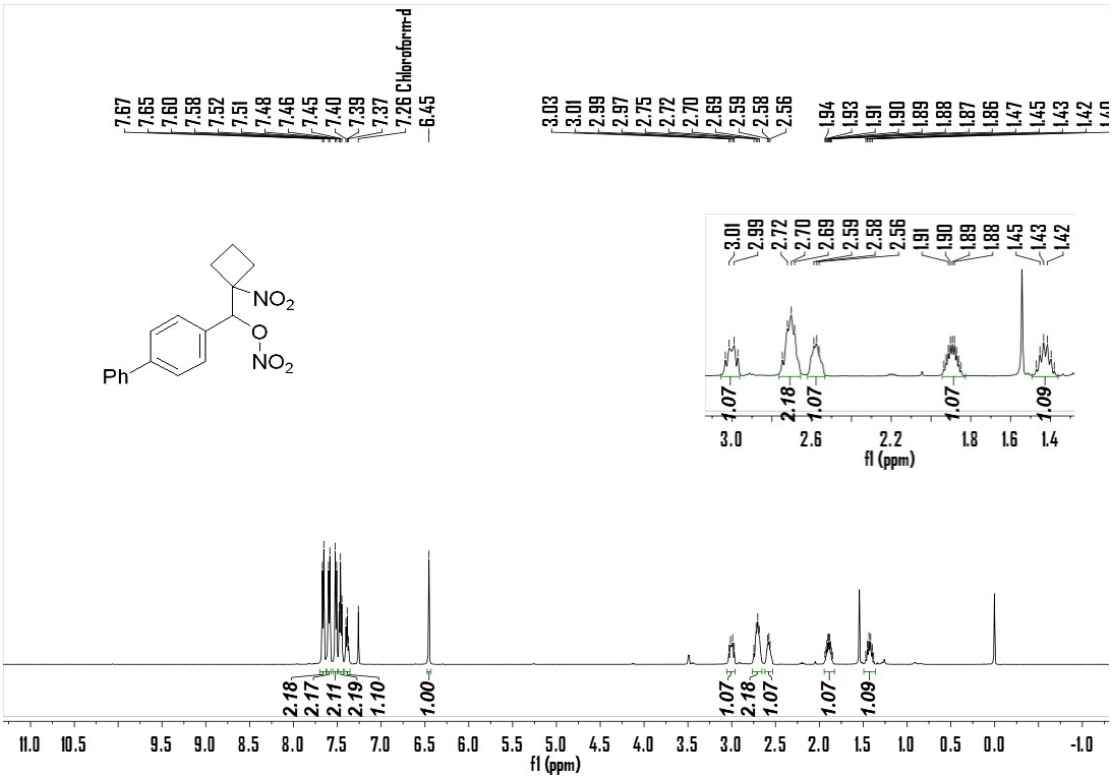


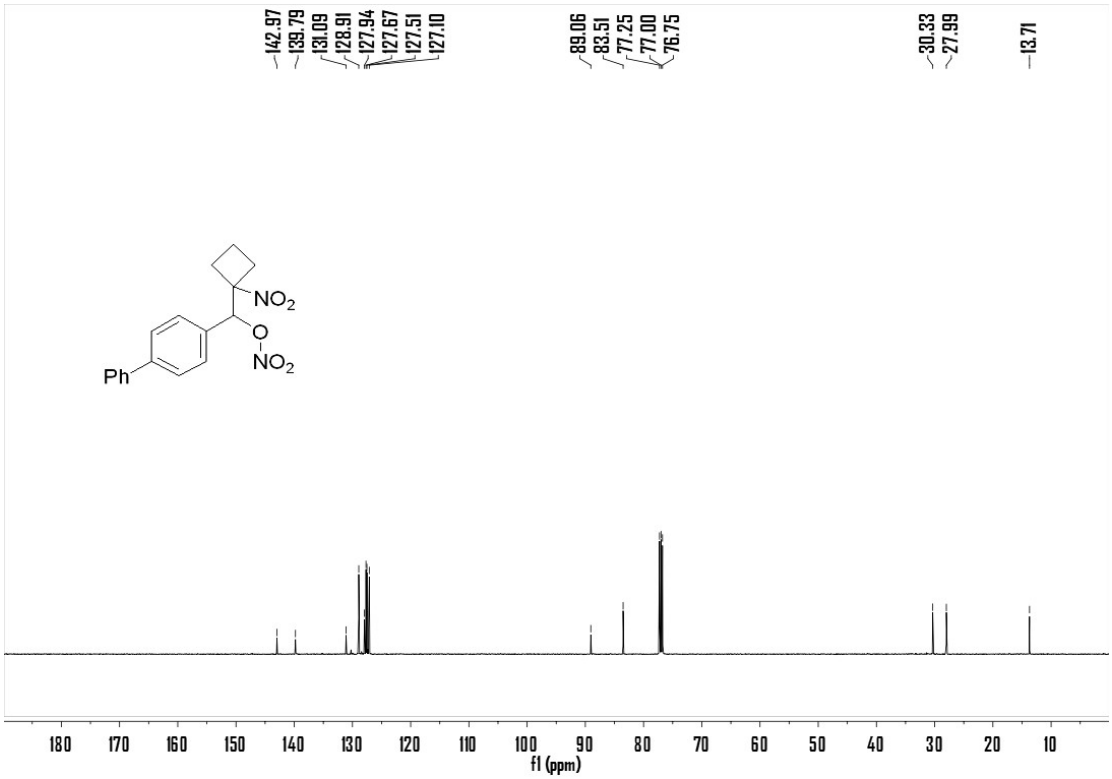
(4-(benzyloxy)phenyl)(1-nitrocyclobutyl)methyl nitrate (3b)



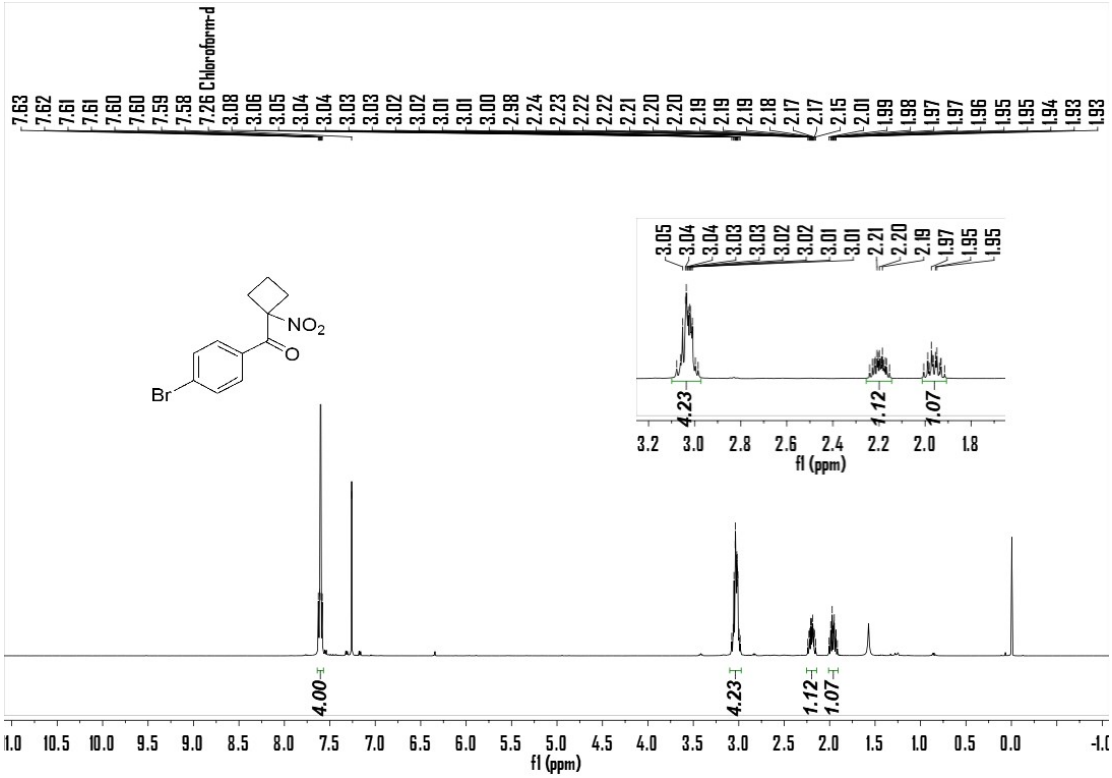


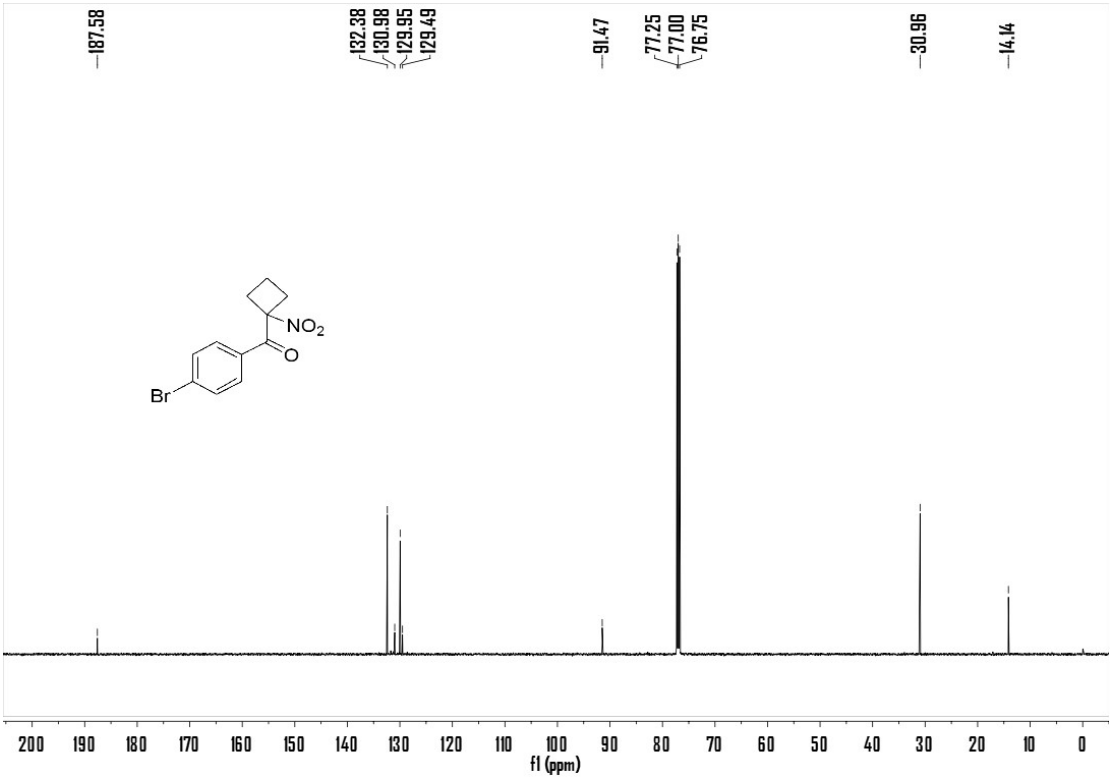
[1,1'-biphenyl]-4-yl(1-nitrocyclobutyl)methyl nitrate (3c)



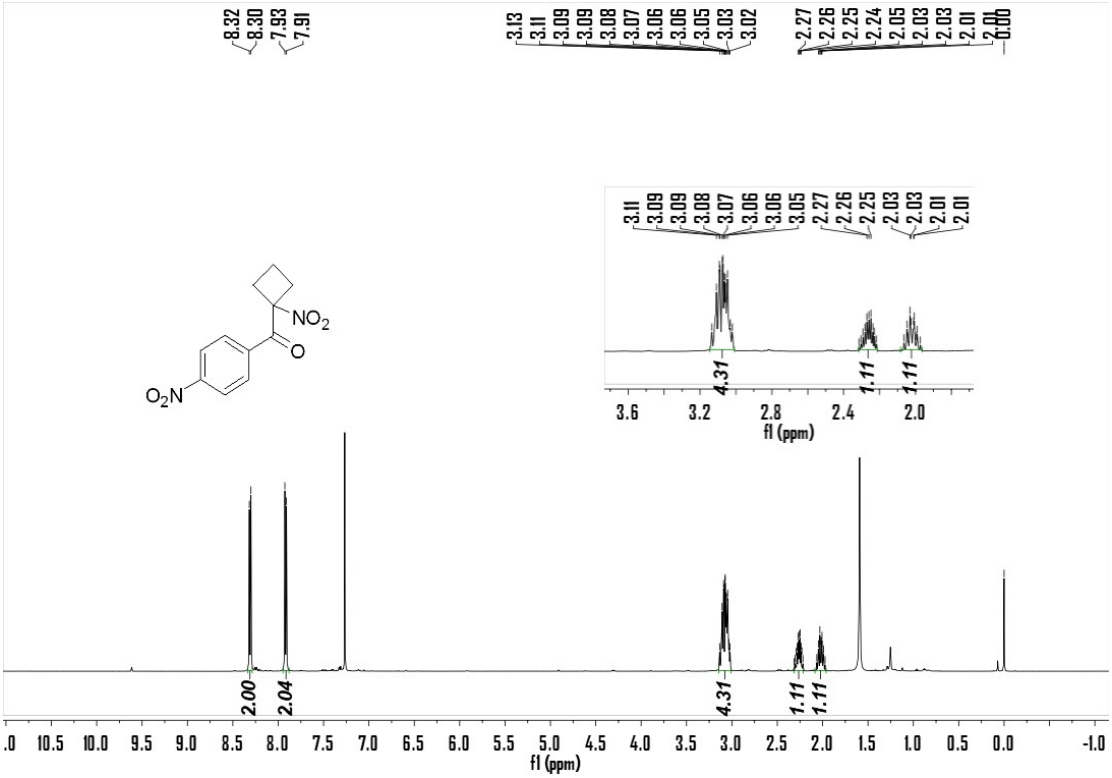


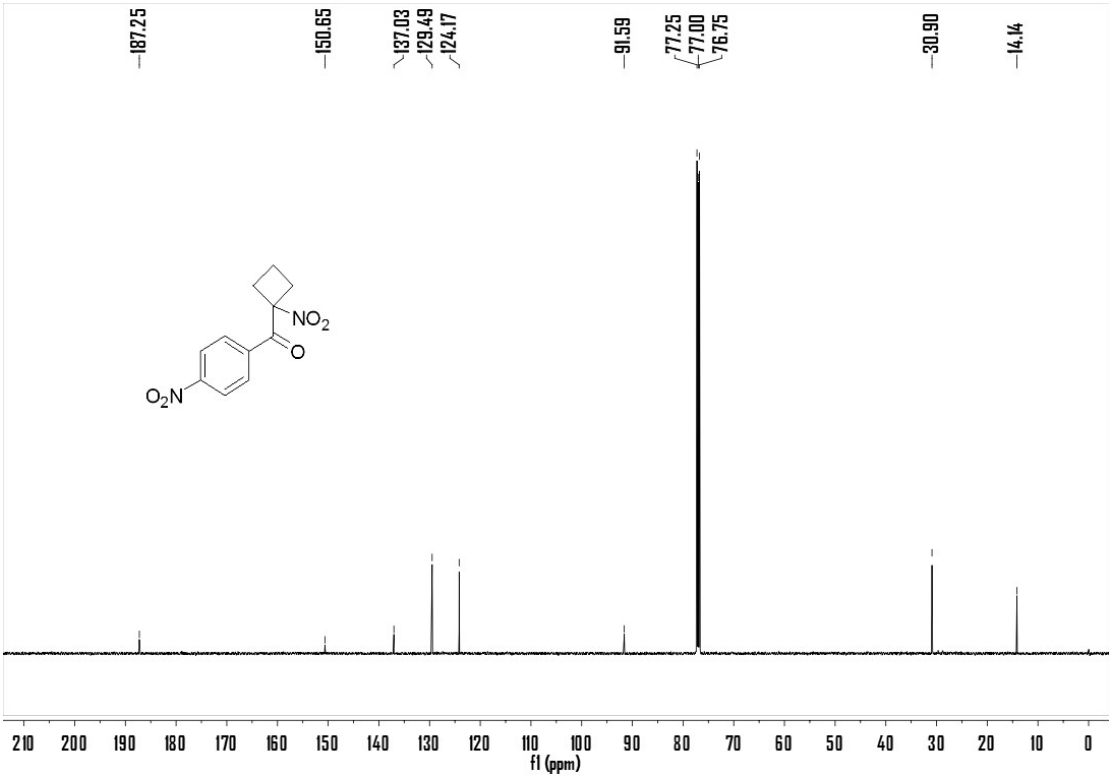
(4-bromophenyl)(1-nitrocyclobutyl)methanone (3d)



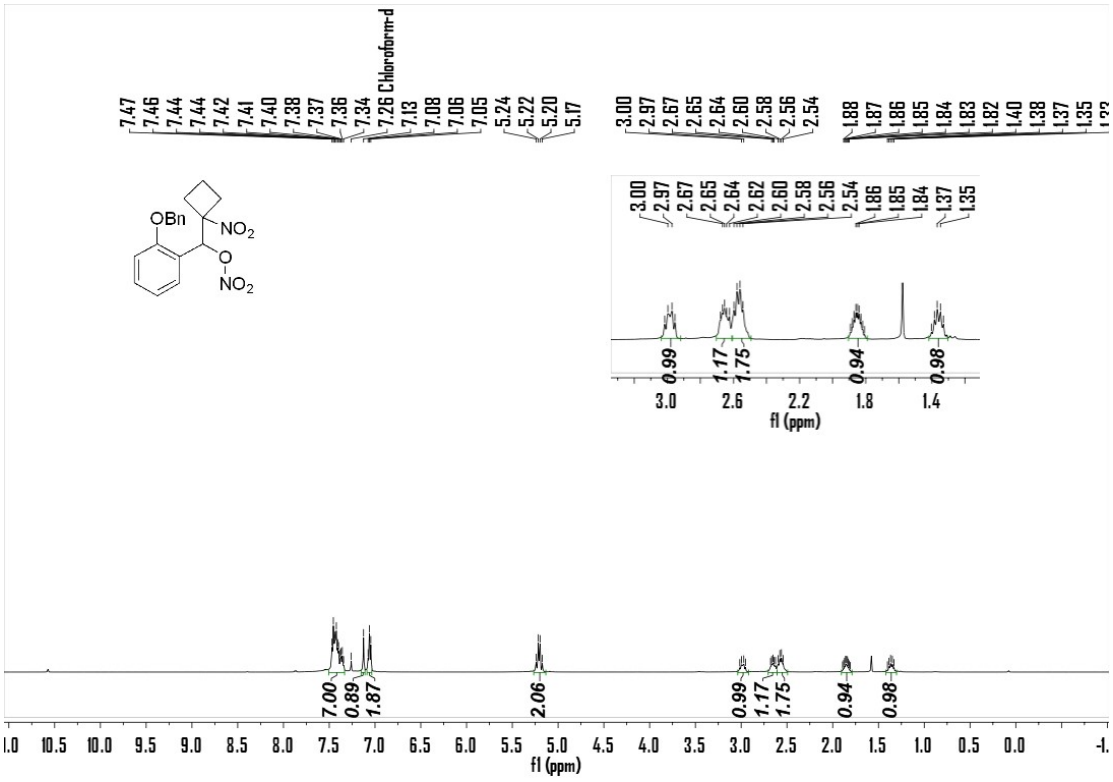


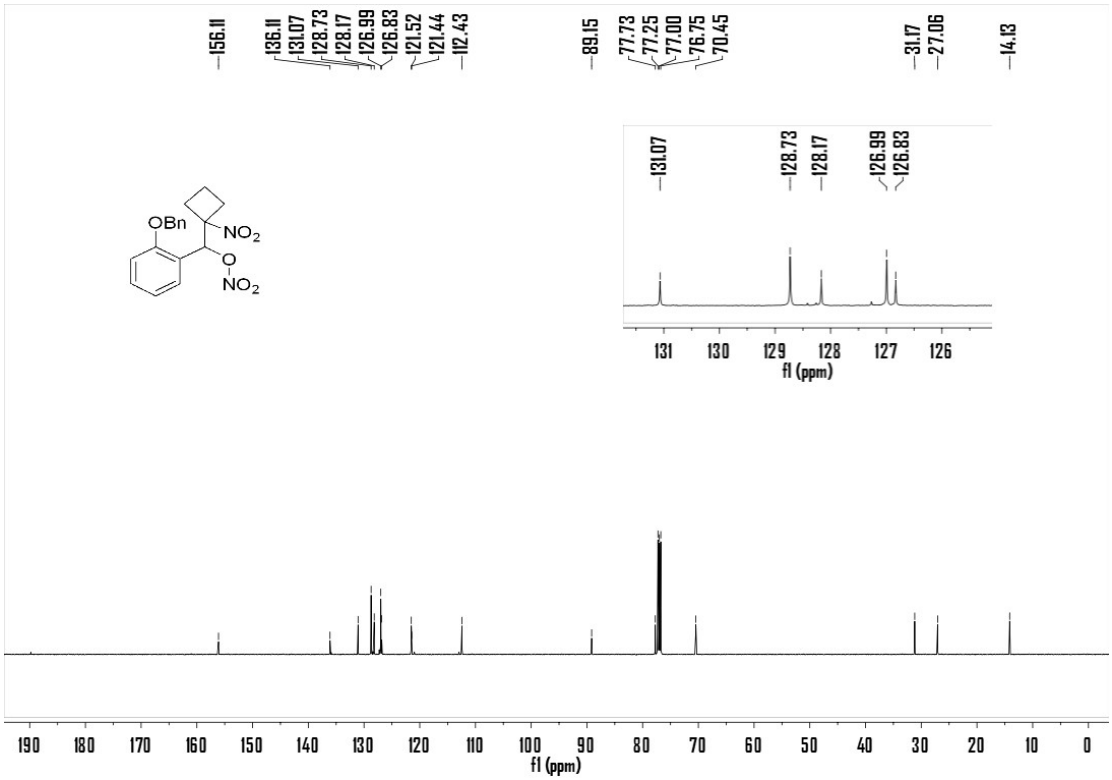
(1-nitrocyclobutyl)(4-nitrophenyl)methanone (3e)



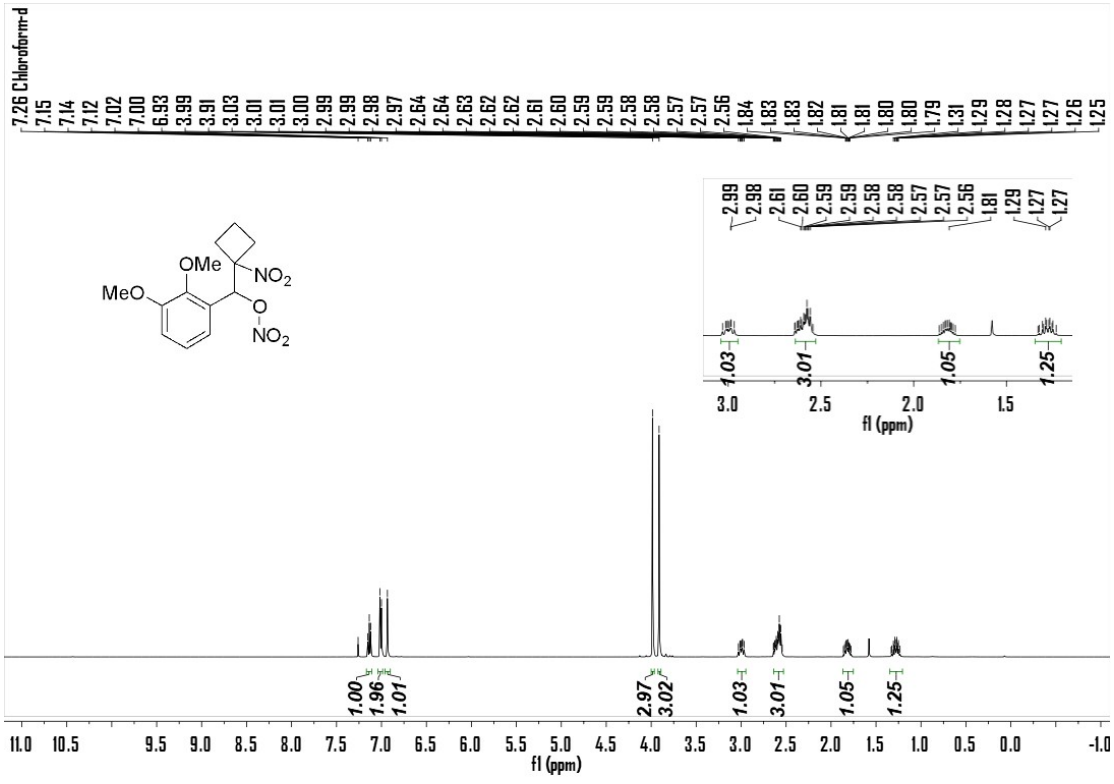


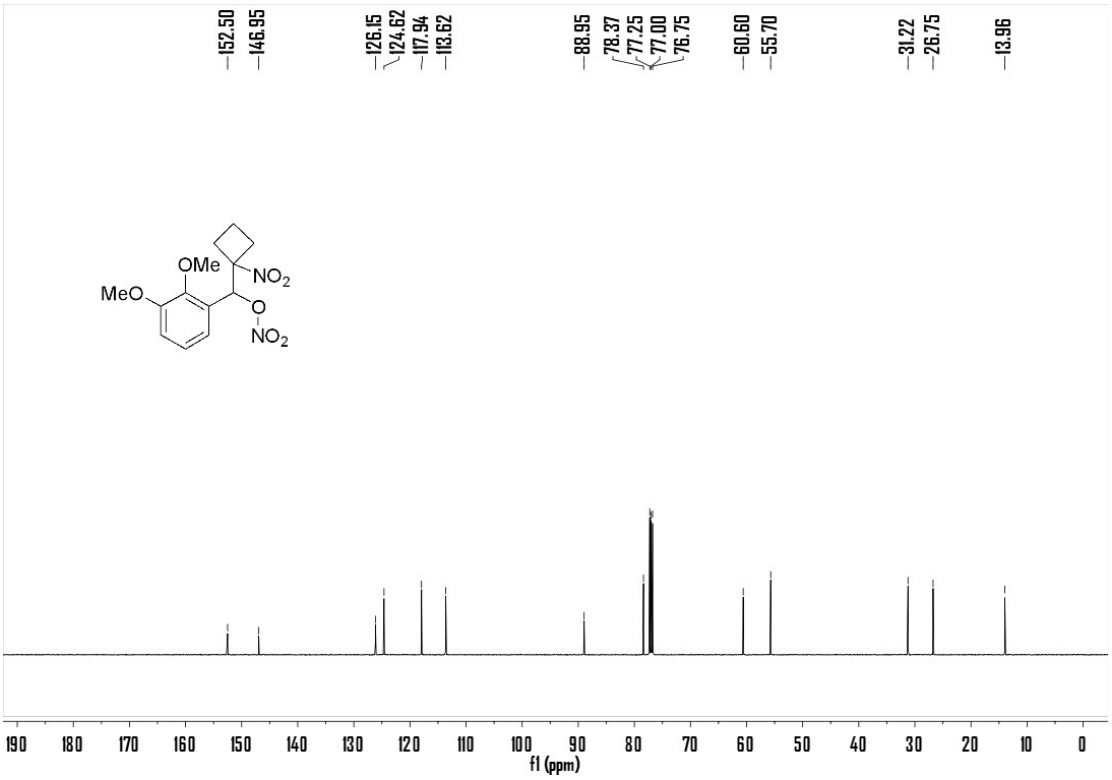
(2-(benzyloxy)phenyl)(1-nitrocyclobutyl)methyl nitrate (3f)



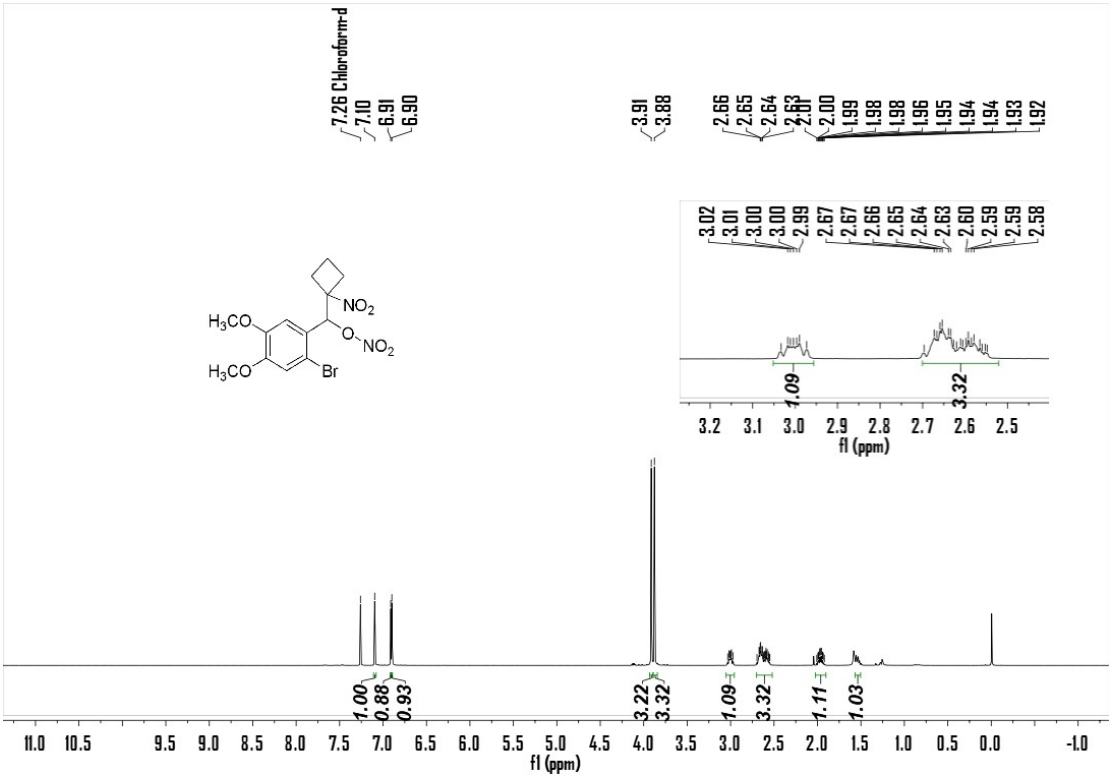


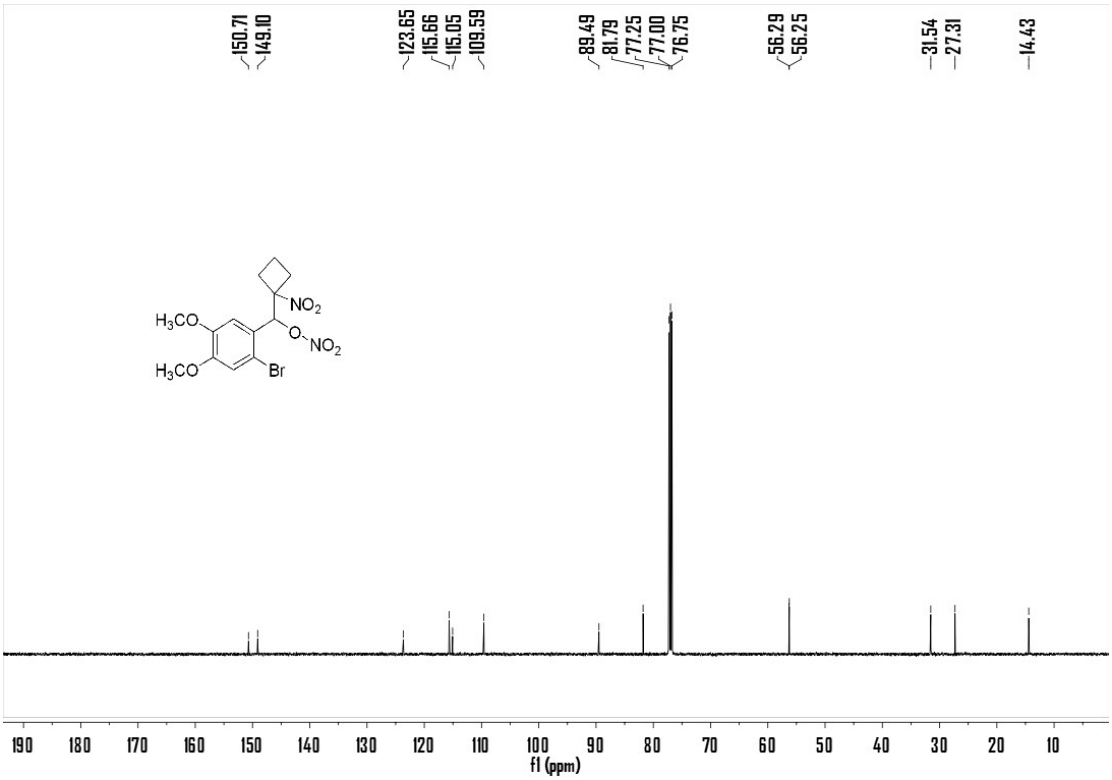
(2,3-dimethoxyphenyl)(1-nitrocyclobutyl)methyl nitrate (3g)



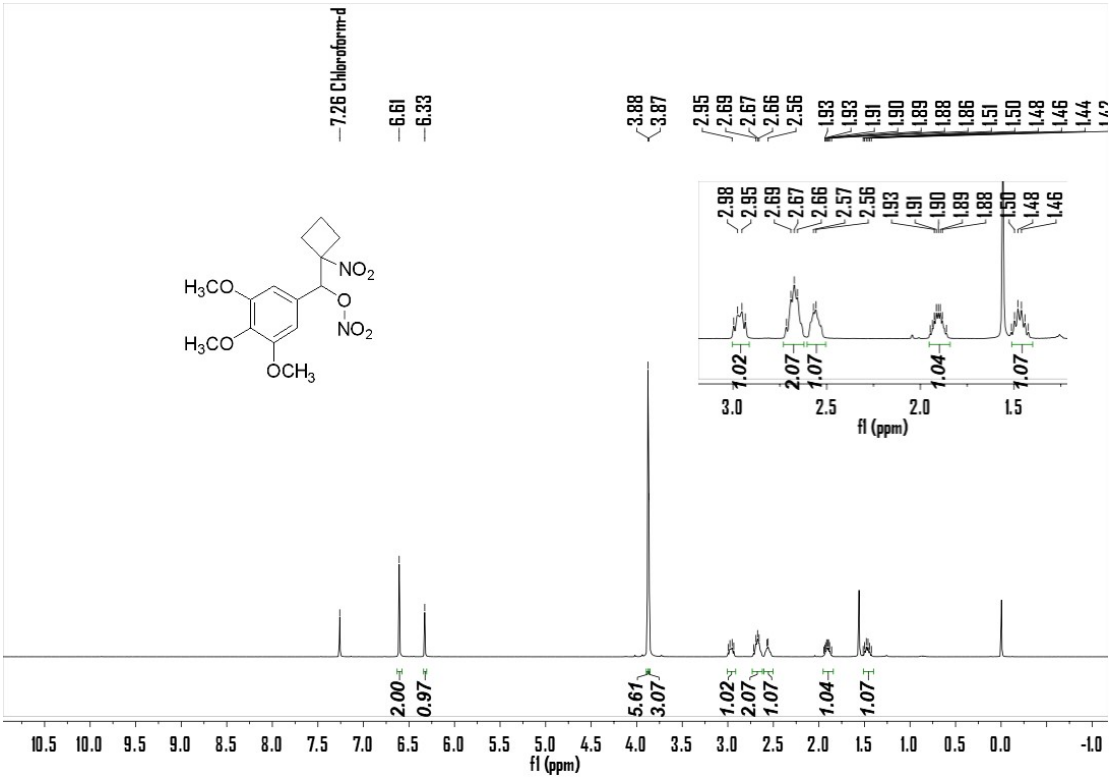


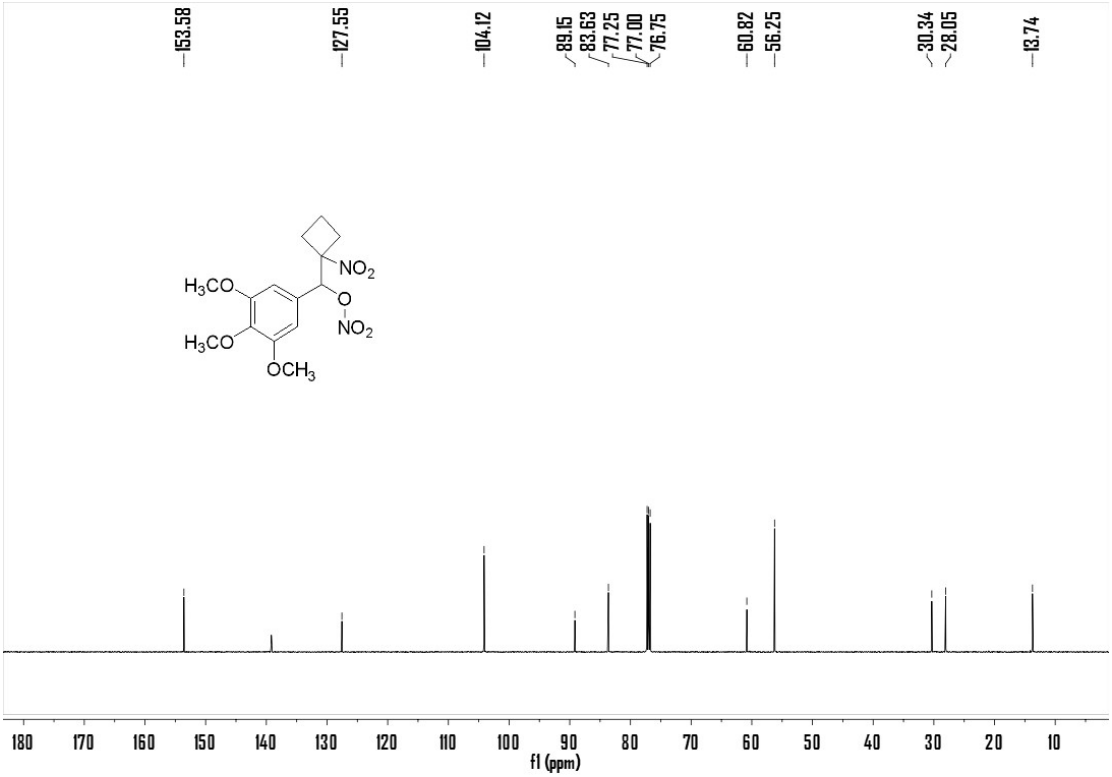
(2-bromo-4,5-dimethoxyphenyl)(1-nitrocyclobutyl)methyl nitrate (3h)



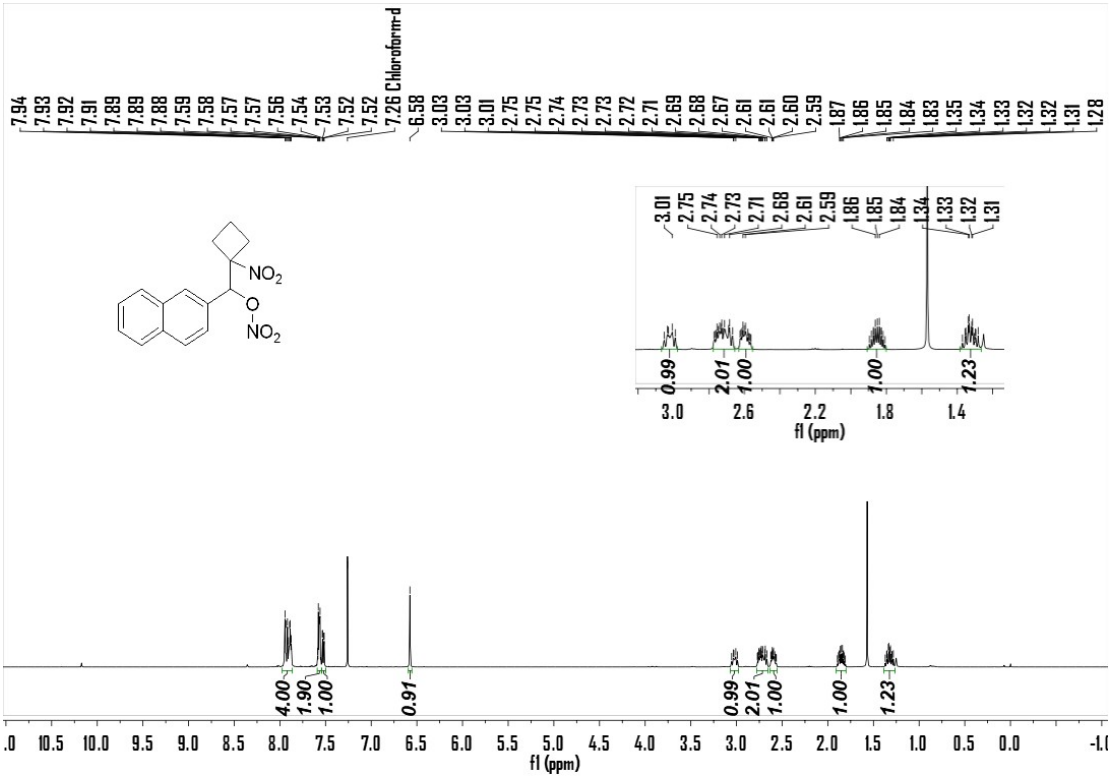


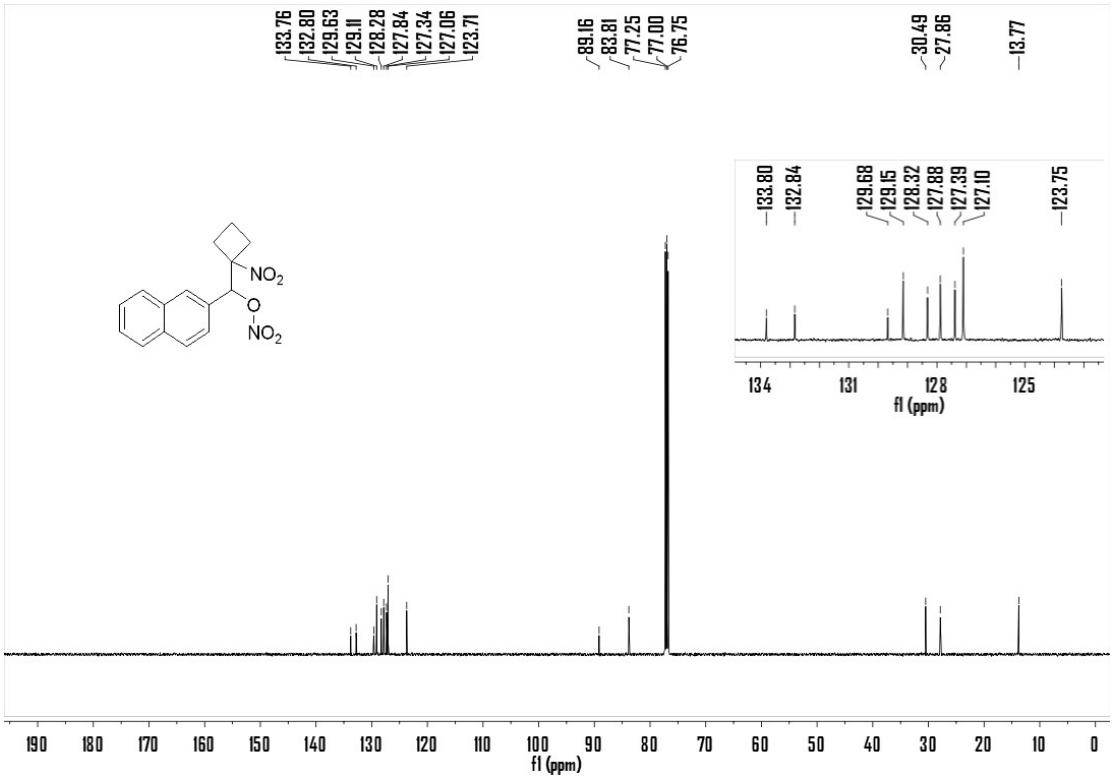
(1-nitrocyclobutyl)(3,4,5-trimethoxyphenyl)methyl nitrate (3i)



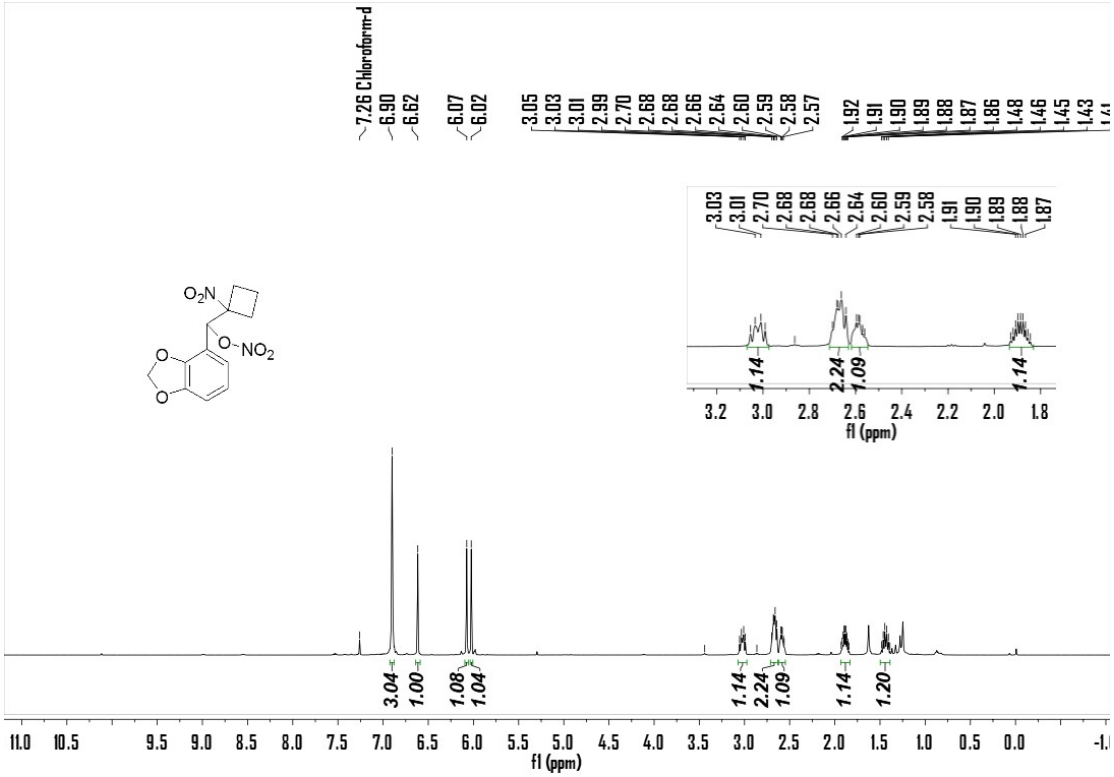


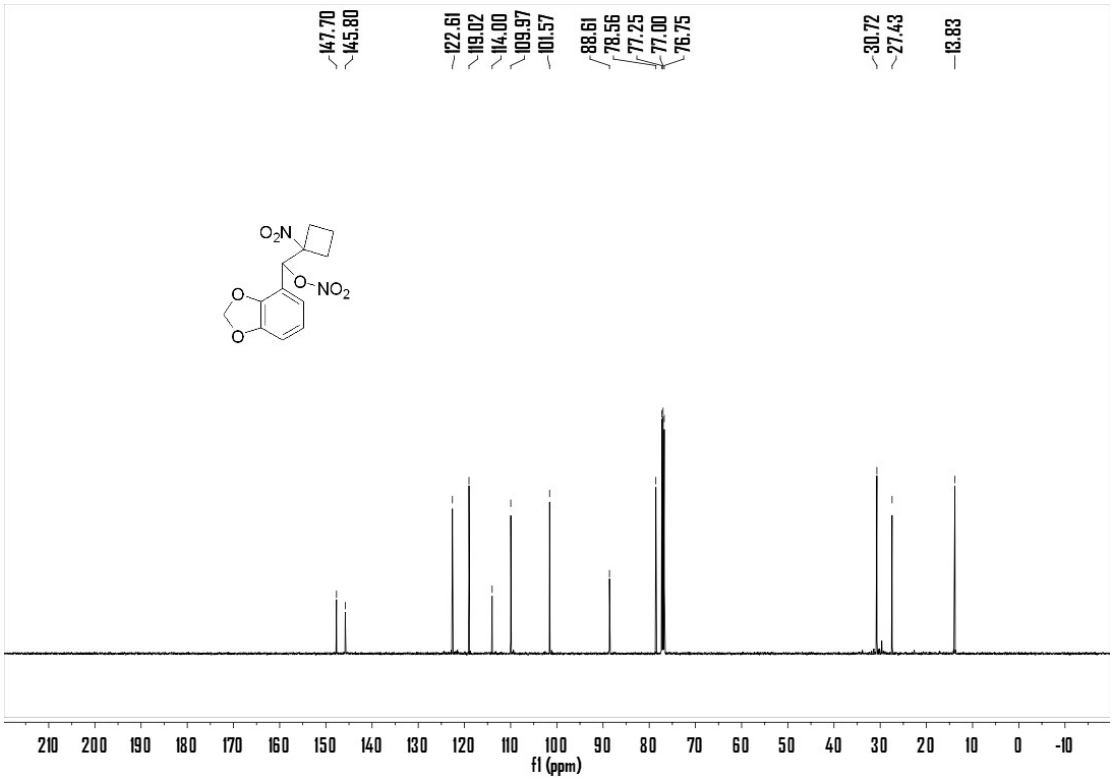
naphthalen-2-yl(1-nitrocyclobutyl)methyl nitrate (3j)



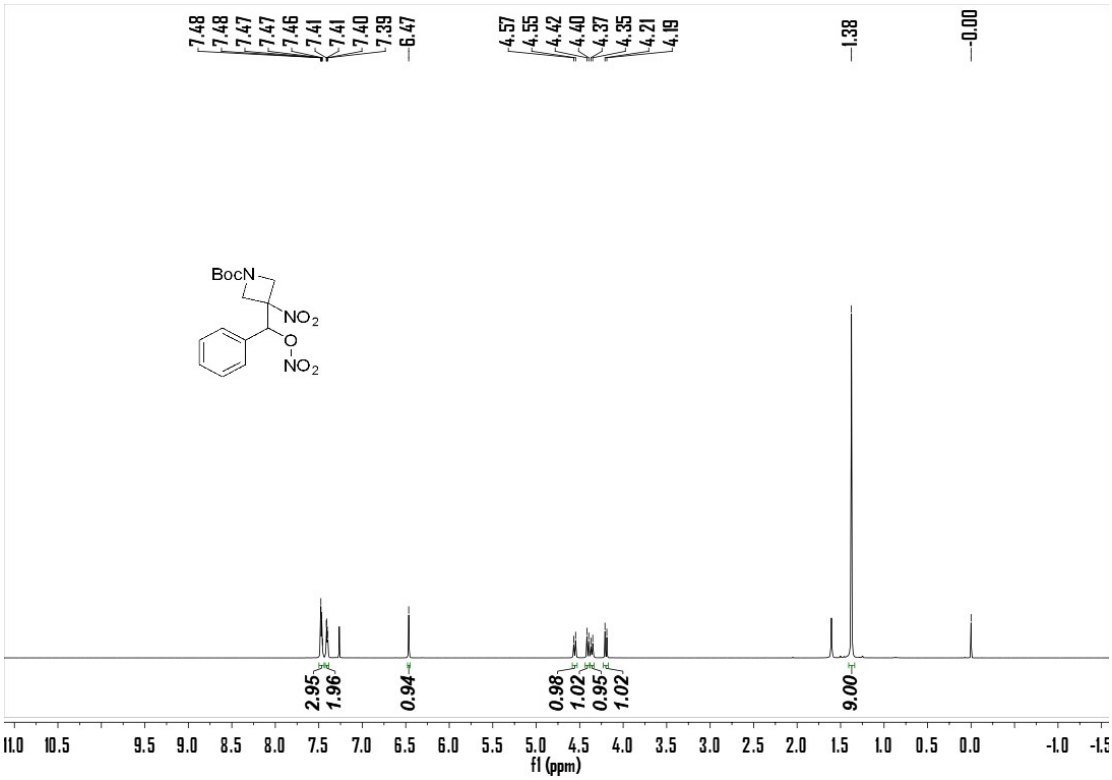


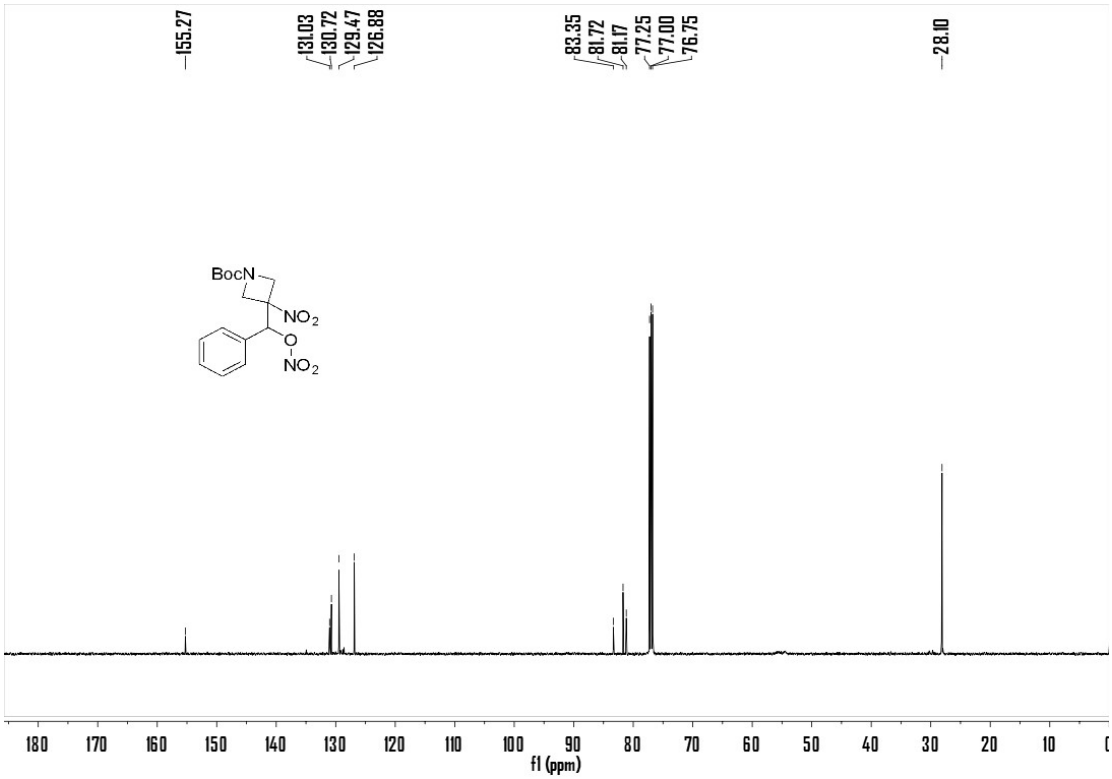
benzo[d][1,3]dioxol-4-yl(1-nitrocyclobutyl)methyl nitrat (3k)



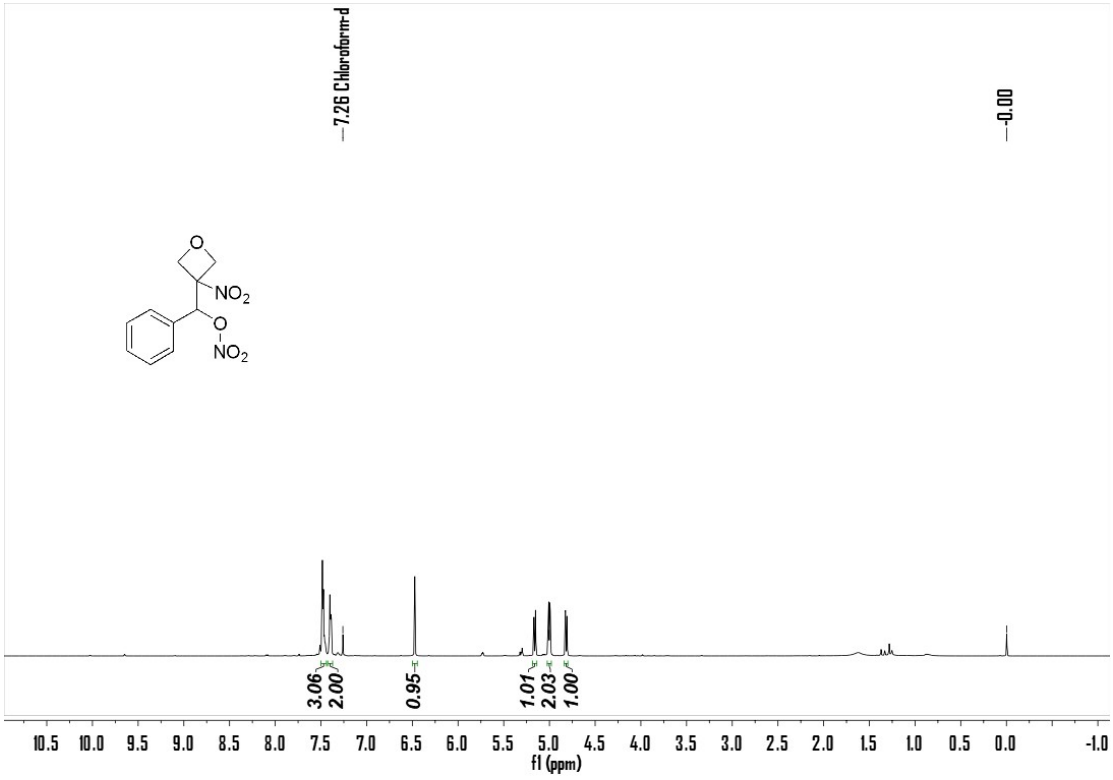


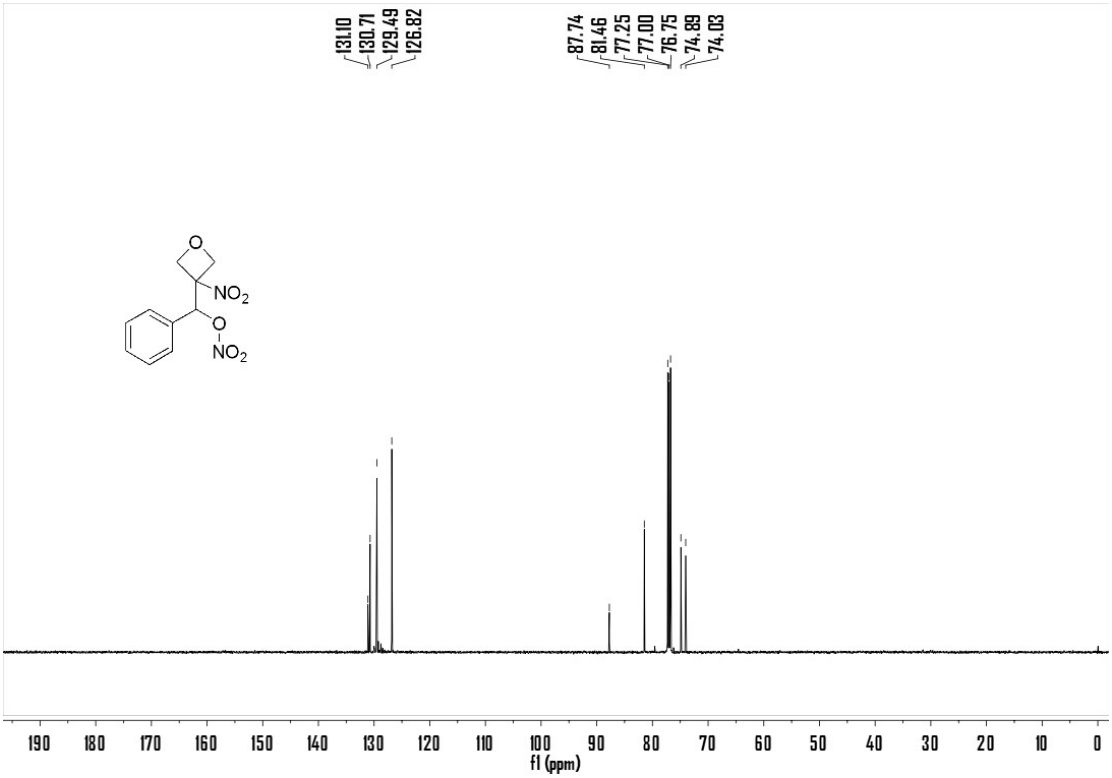
tert-butyl 3-nitro-3-((nitrooxy)(phenyl)methyl)azetidine-1-carboxylate (3l)



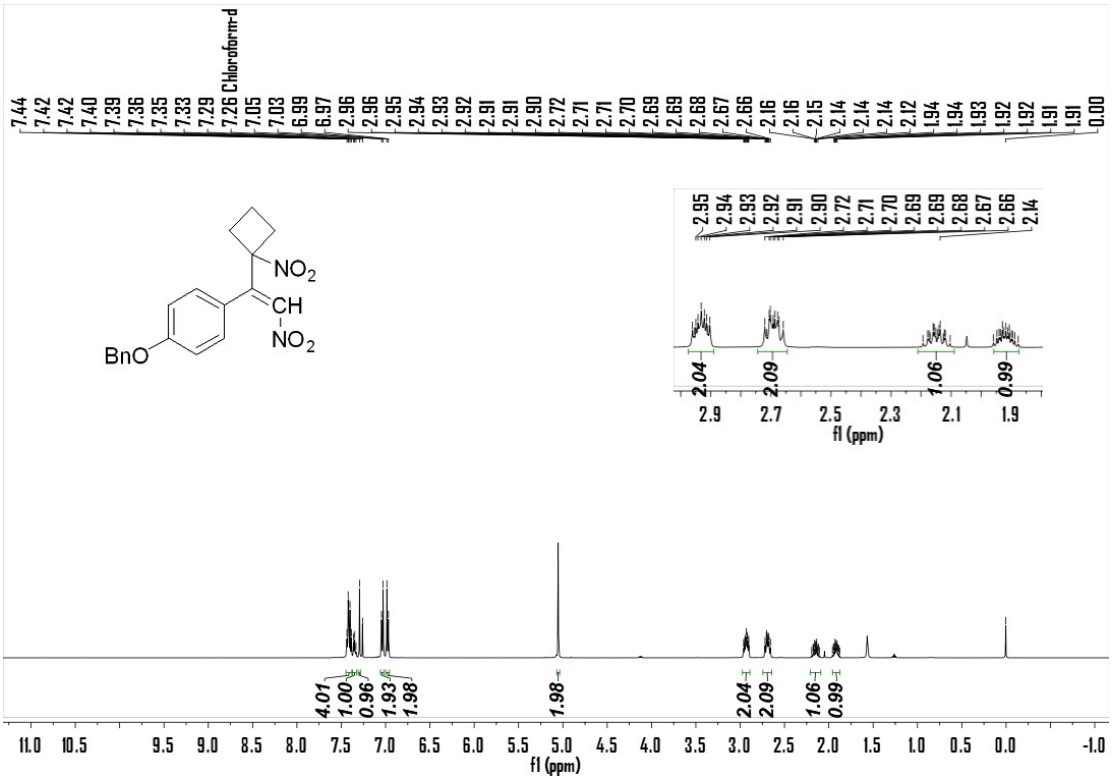


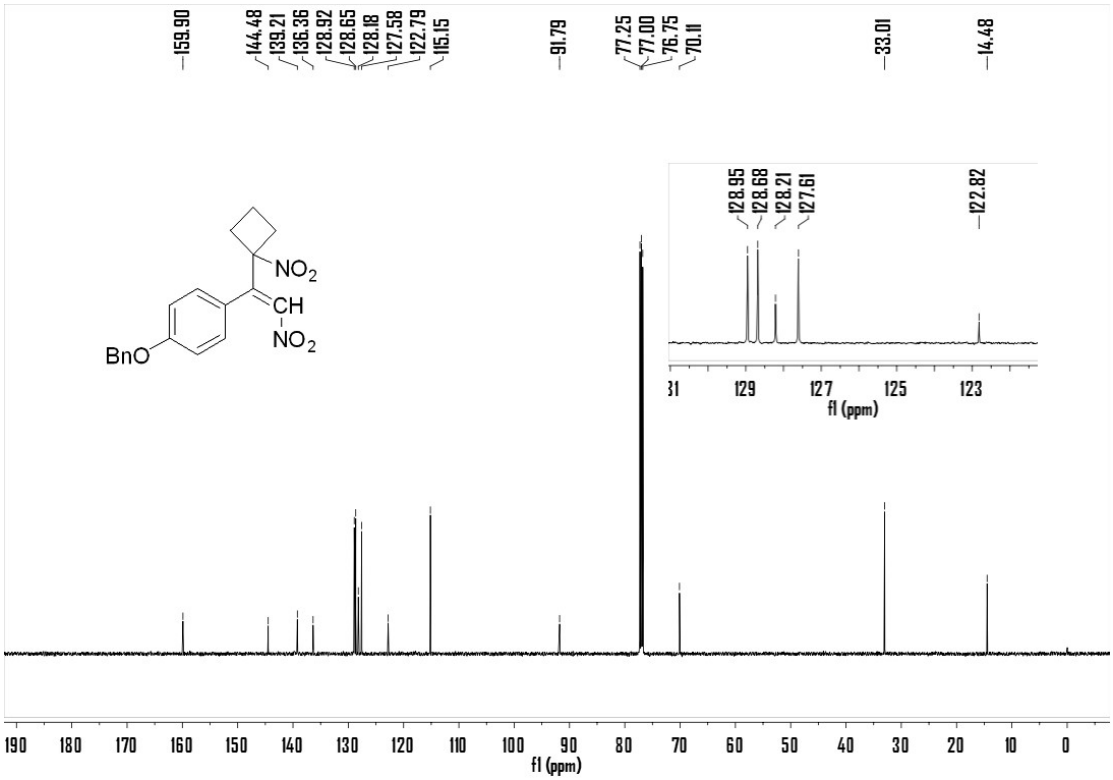
(3-nitrooxetan-3-yl)(phenyl)methyl nitrate (3m)



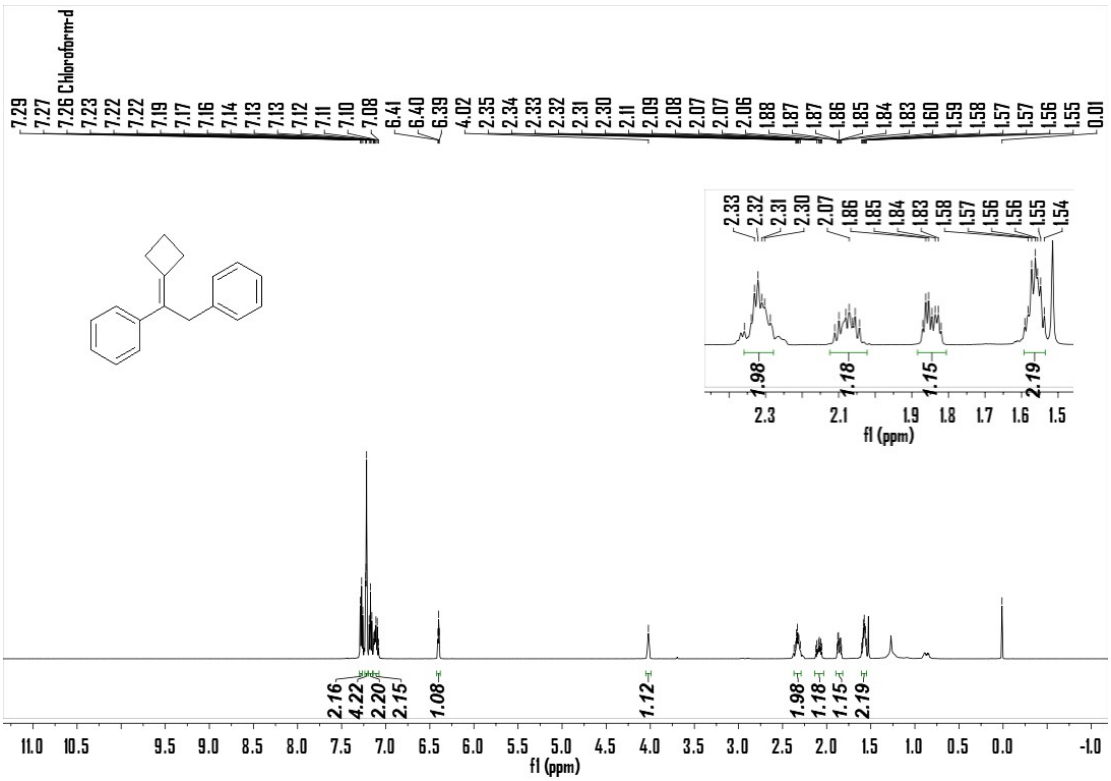


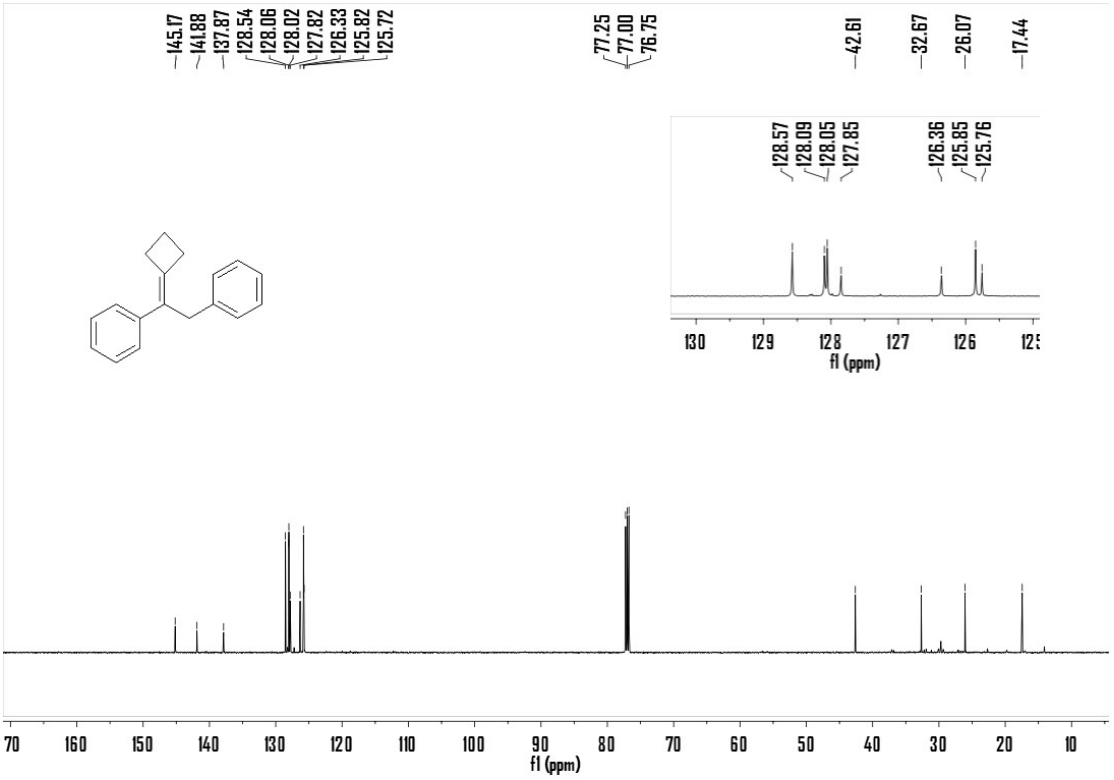
1-(benzyloxy)-4-(2-nitro-1-(1-nitrocyclobutyl)vinyl)benzene (3aa)



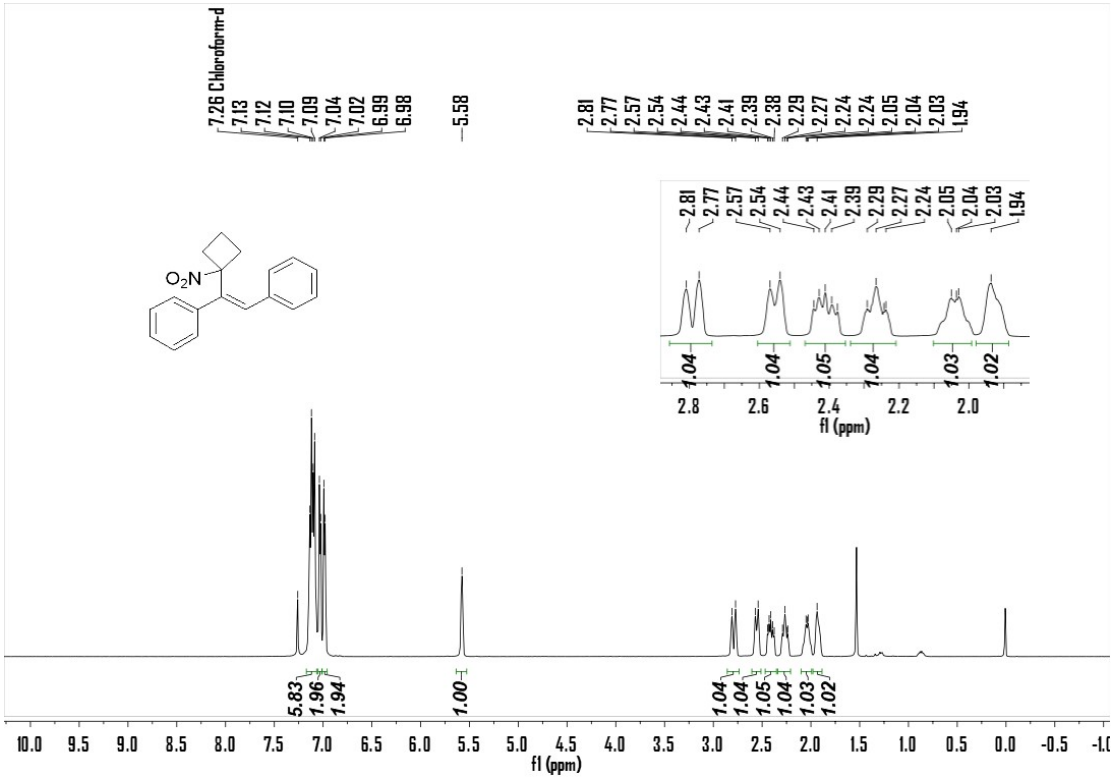


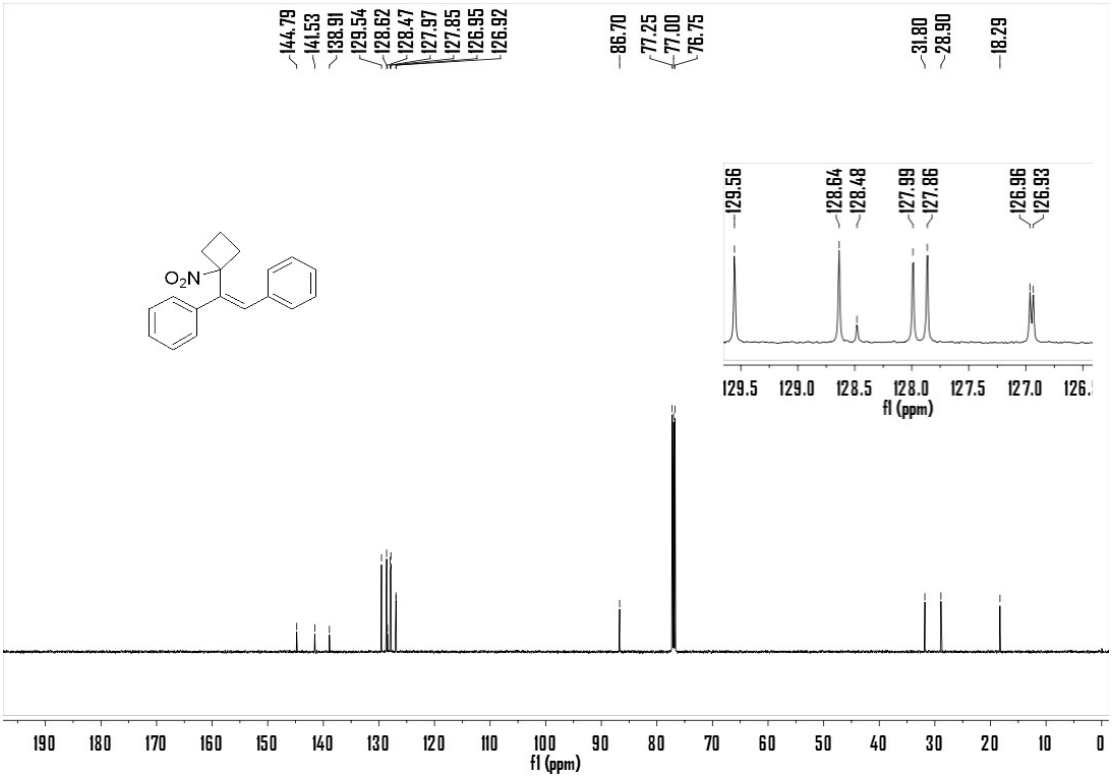
(1-cyclobutylideneethane-1,2-diyl)dibenzene



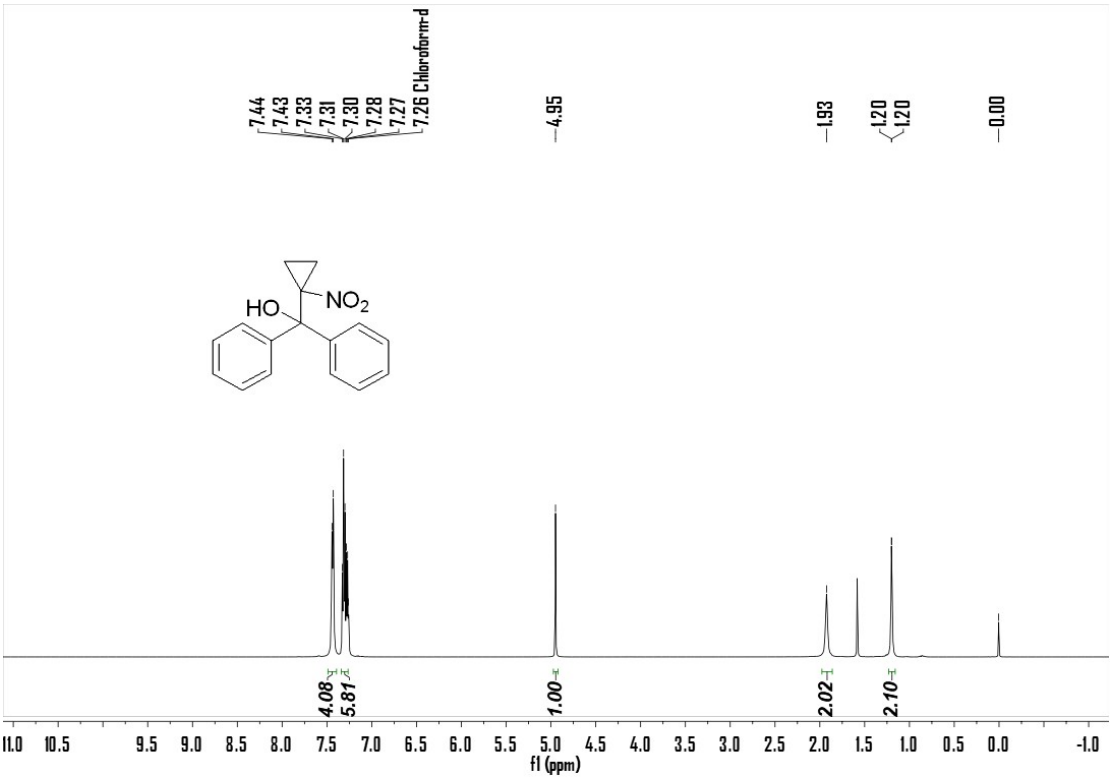


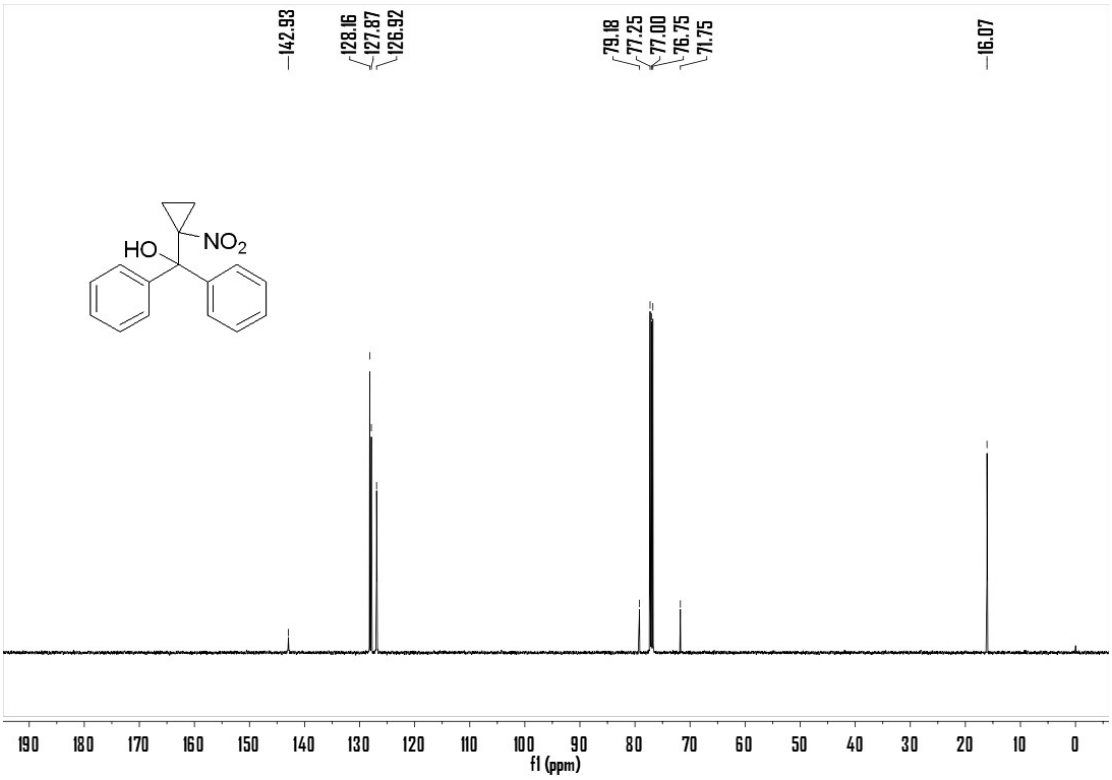
(2-(cyclohexa-2,4-dien-1-yl)-1-(1-nitrocyclobutyl)vinyl)benzene (3ab)



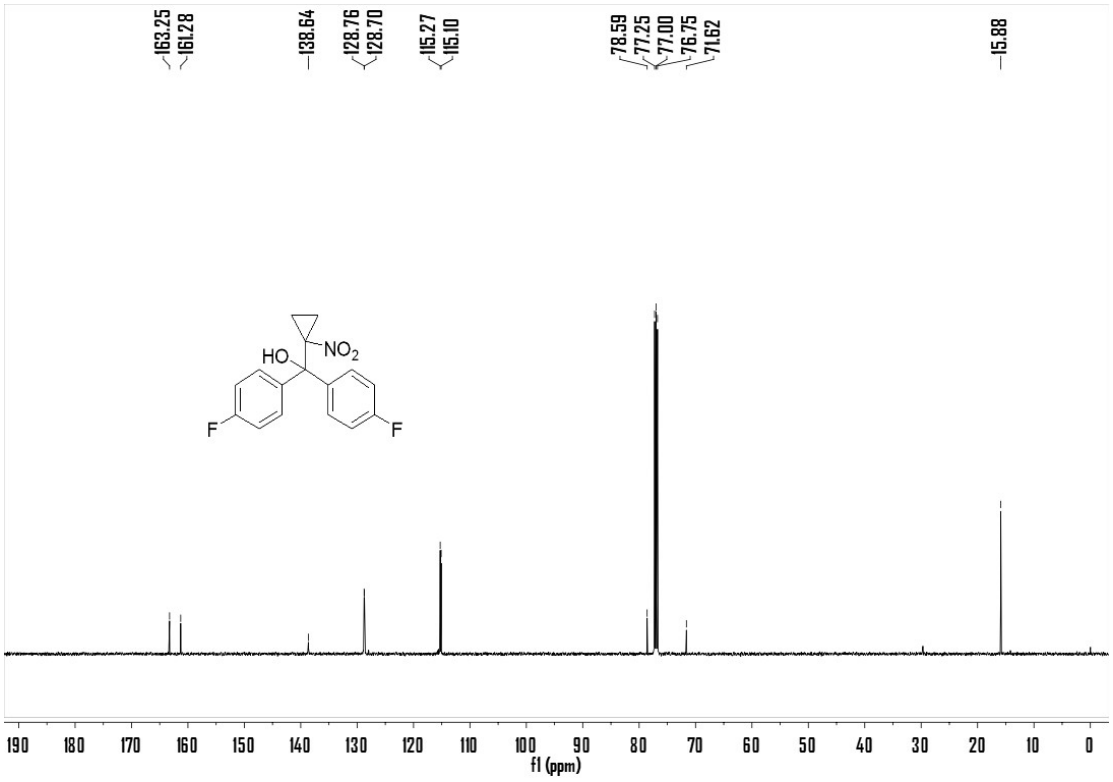


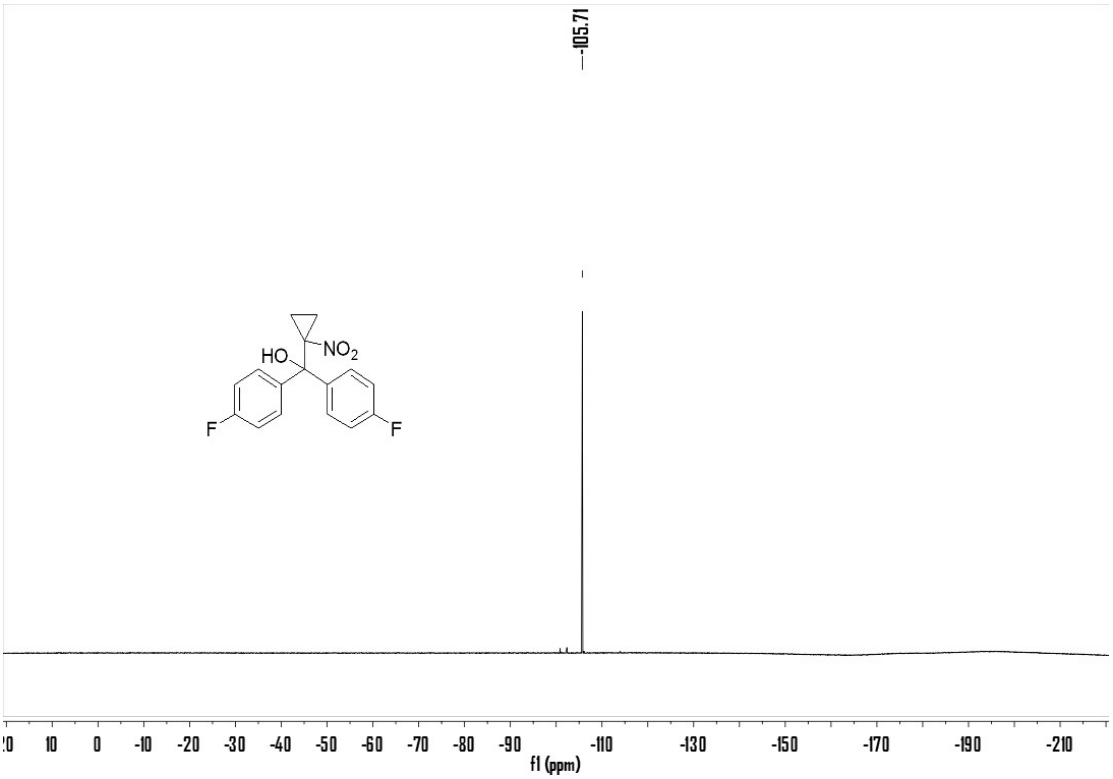
(1-nitrocyclopropyl)diphenylmethanol (5a)



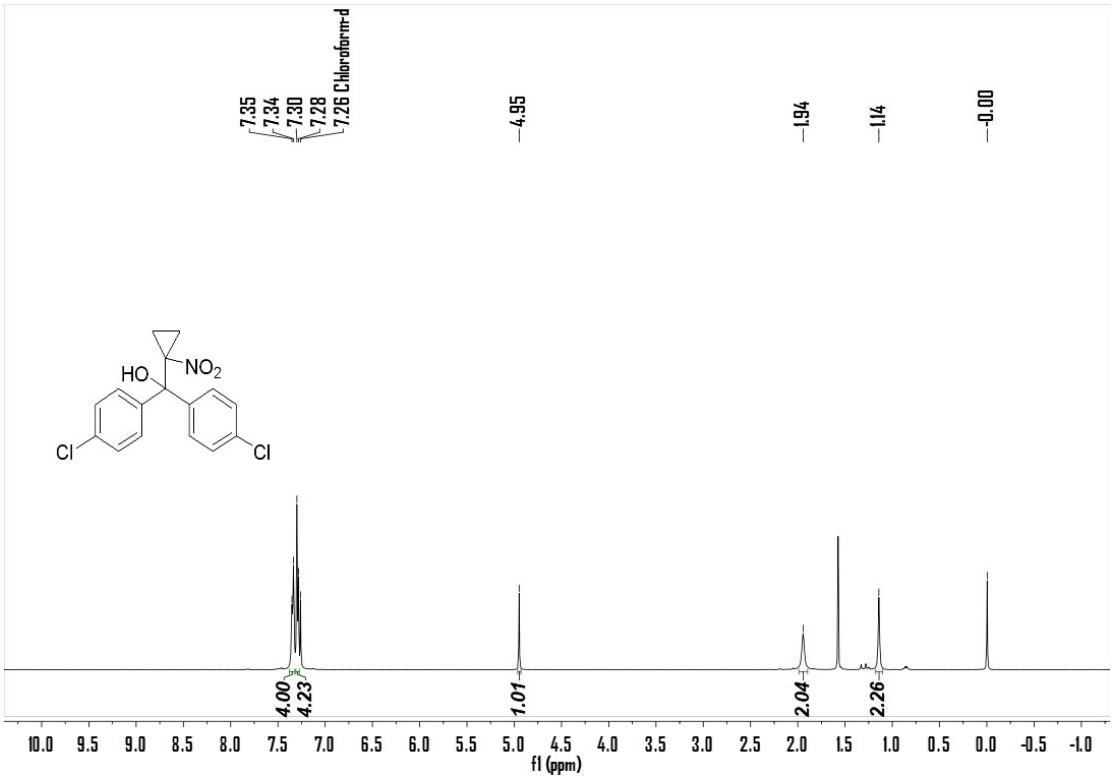


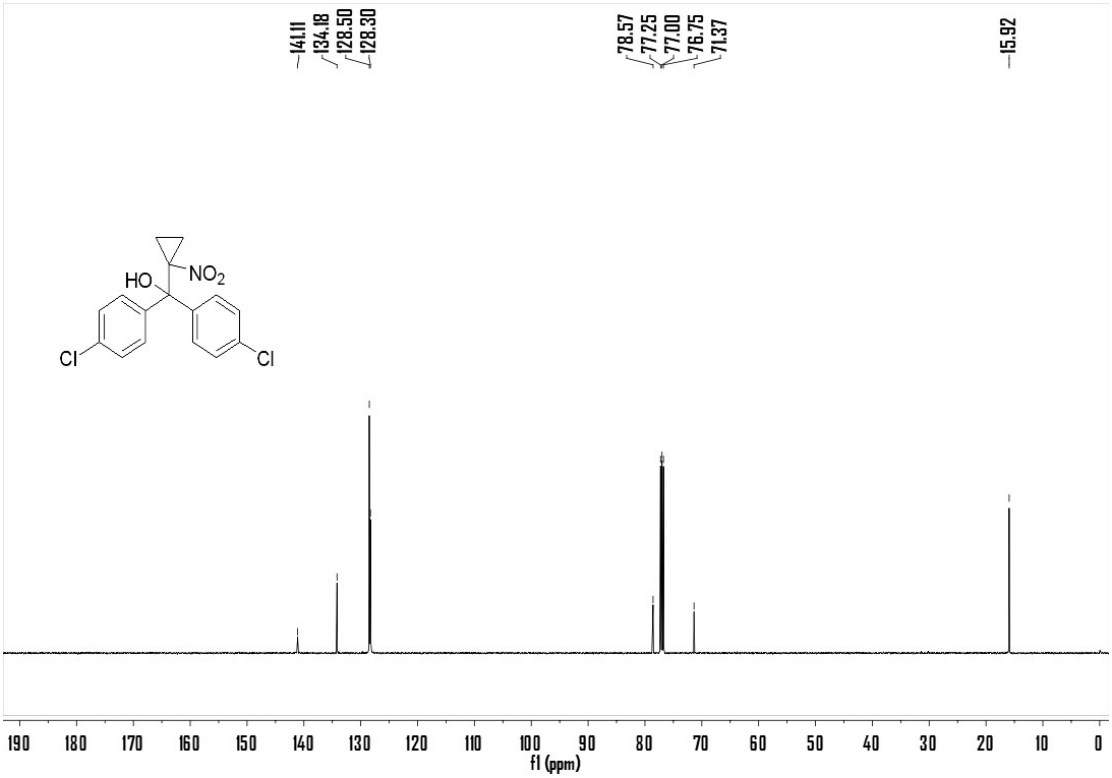
bis(4-fluorophenyl)(1-nitrocyclopropyl)methanol (5b)


163.25
161.28
138.64
128.76
128.70
115.27
115.10
78.59
77.25
77.00
76.75
71.62
15.88
HO
NO2
F
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

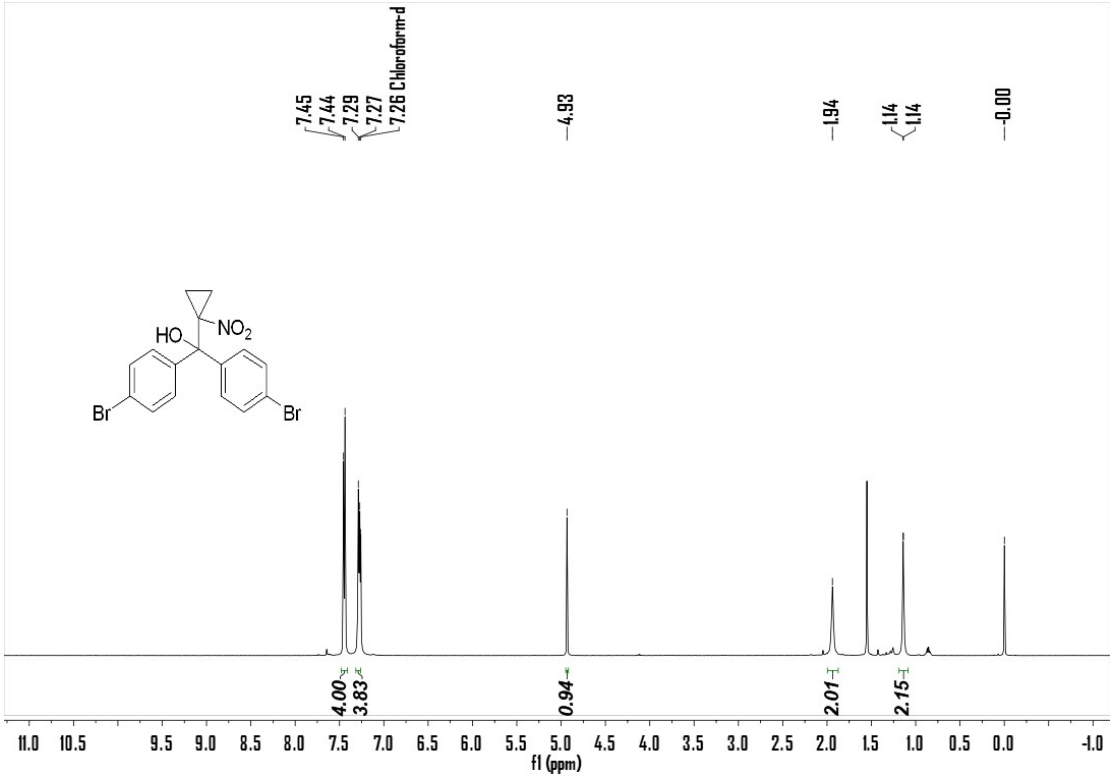

-105.71
HO
NO2
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

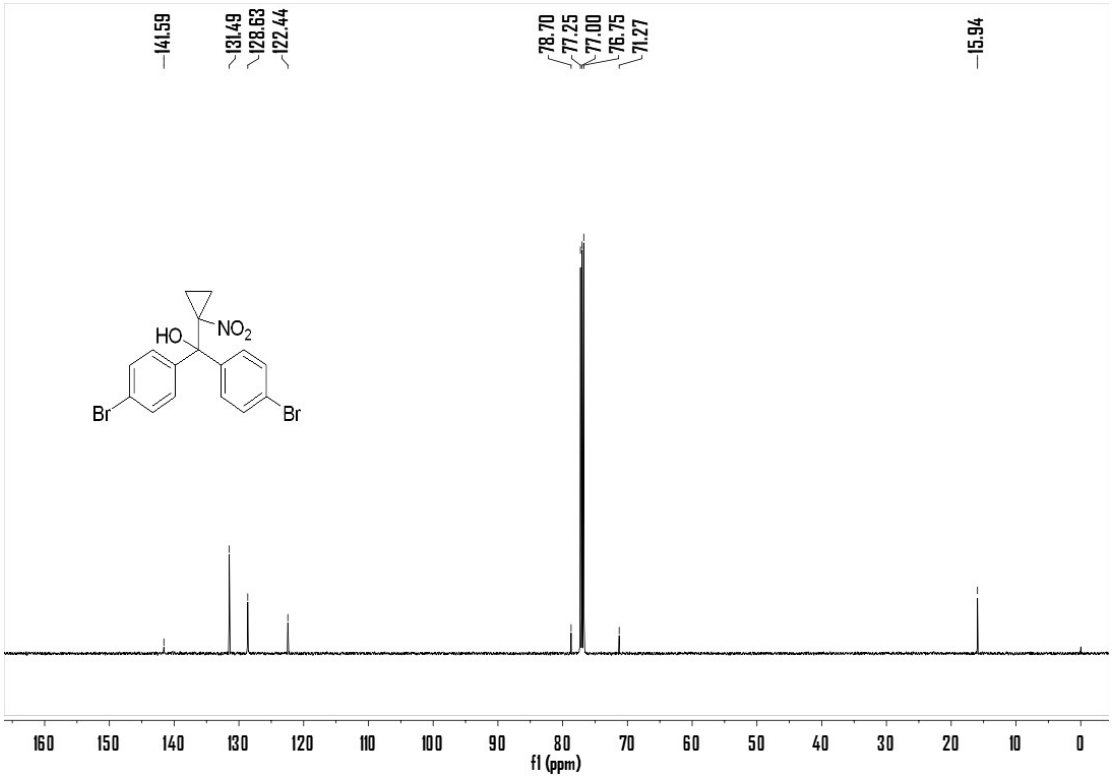
bis(4-chlorophenyl)(1-nitrocyclopropyl)methanol (5c)



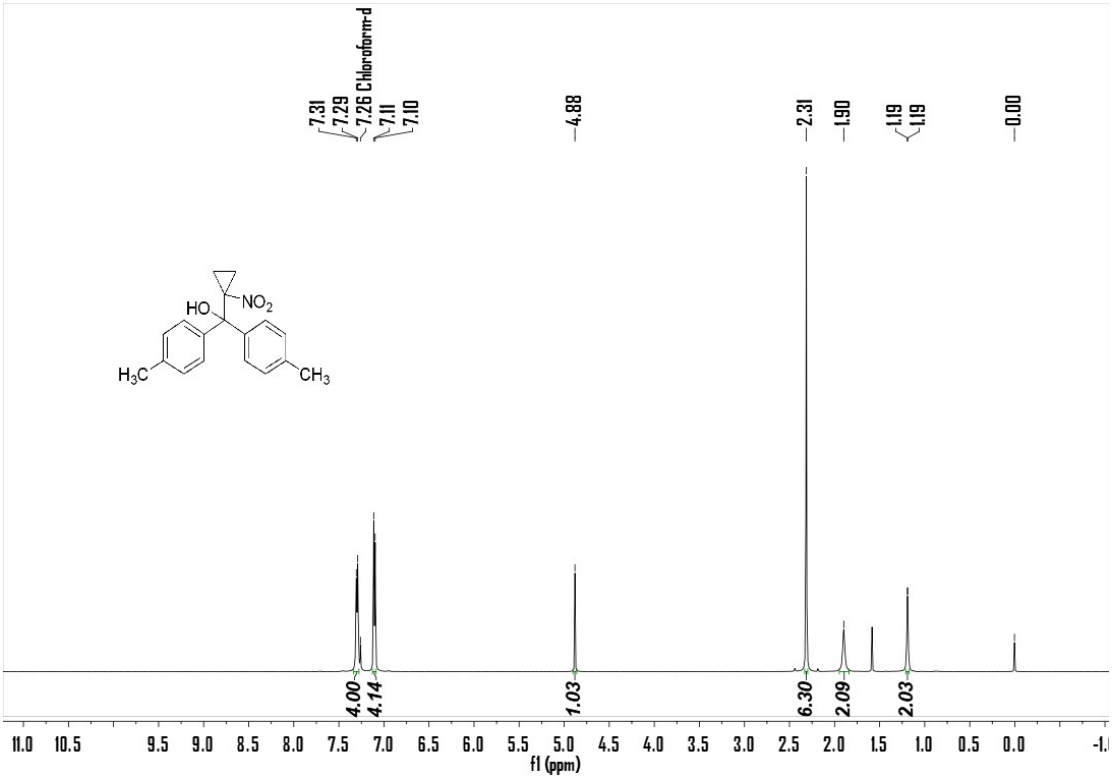


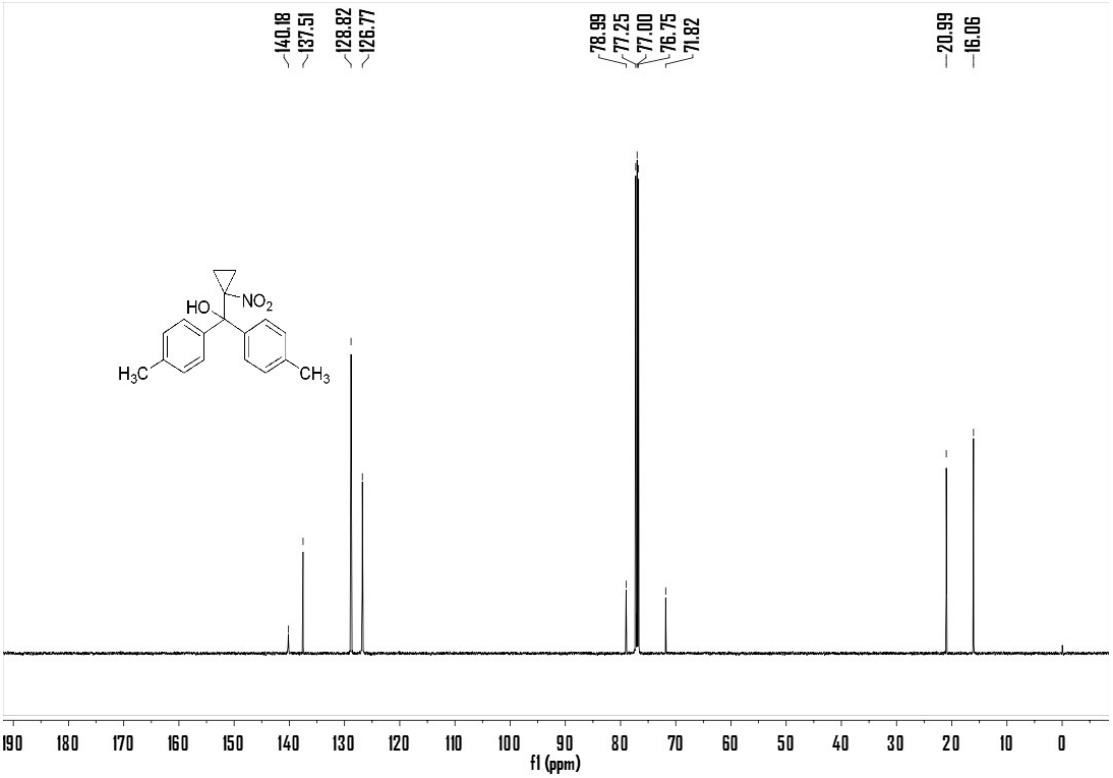
bis(4-bromophenyl)(1-nitrocyclopropyl)methanol (5d)



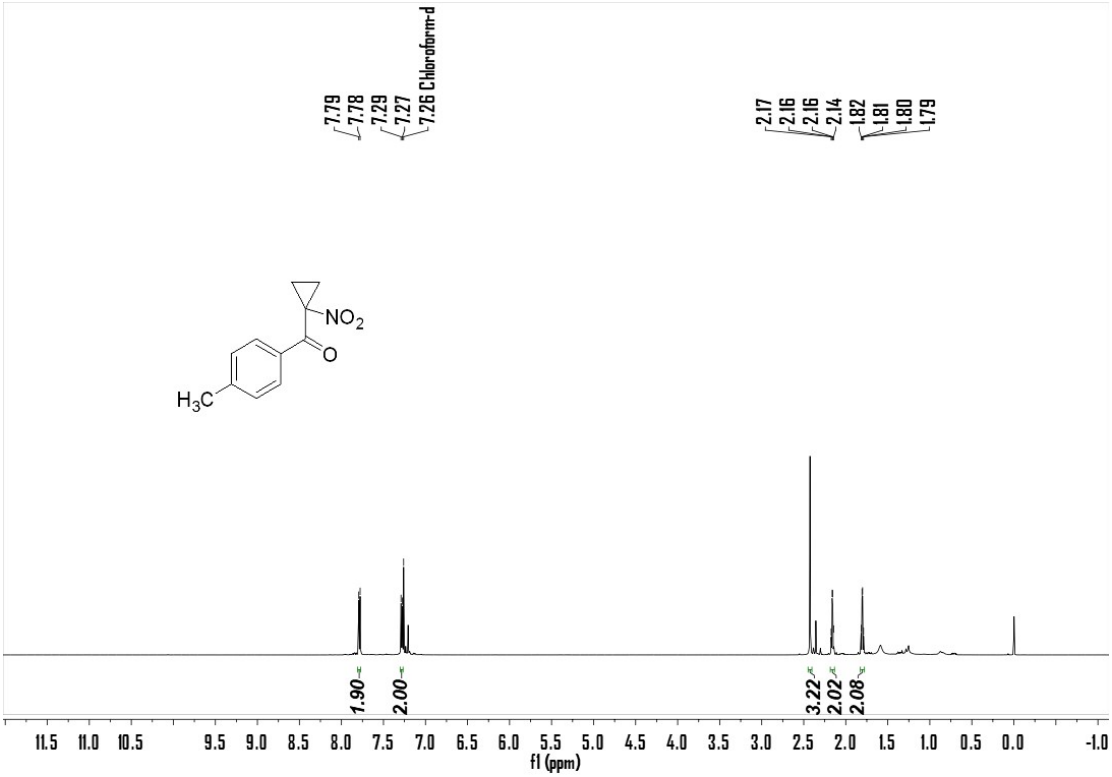


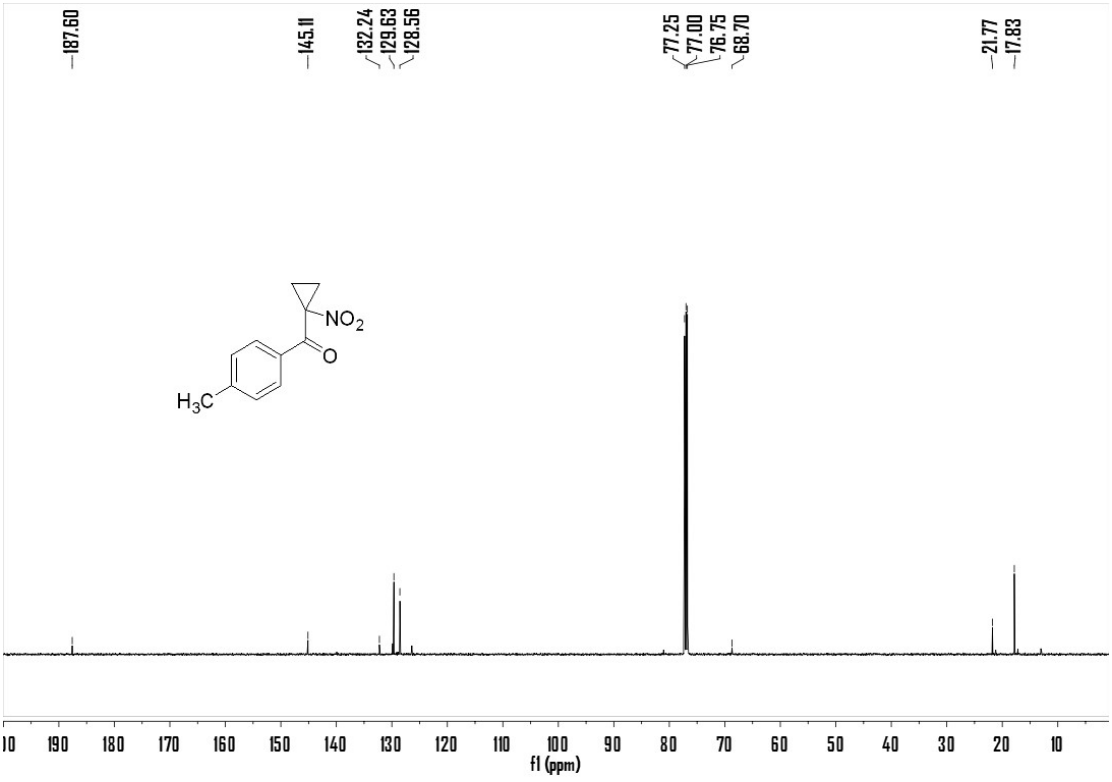
(1-nitrocyclopropyl)di-p-tolylmethanol (5f)



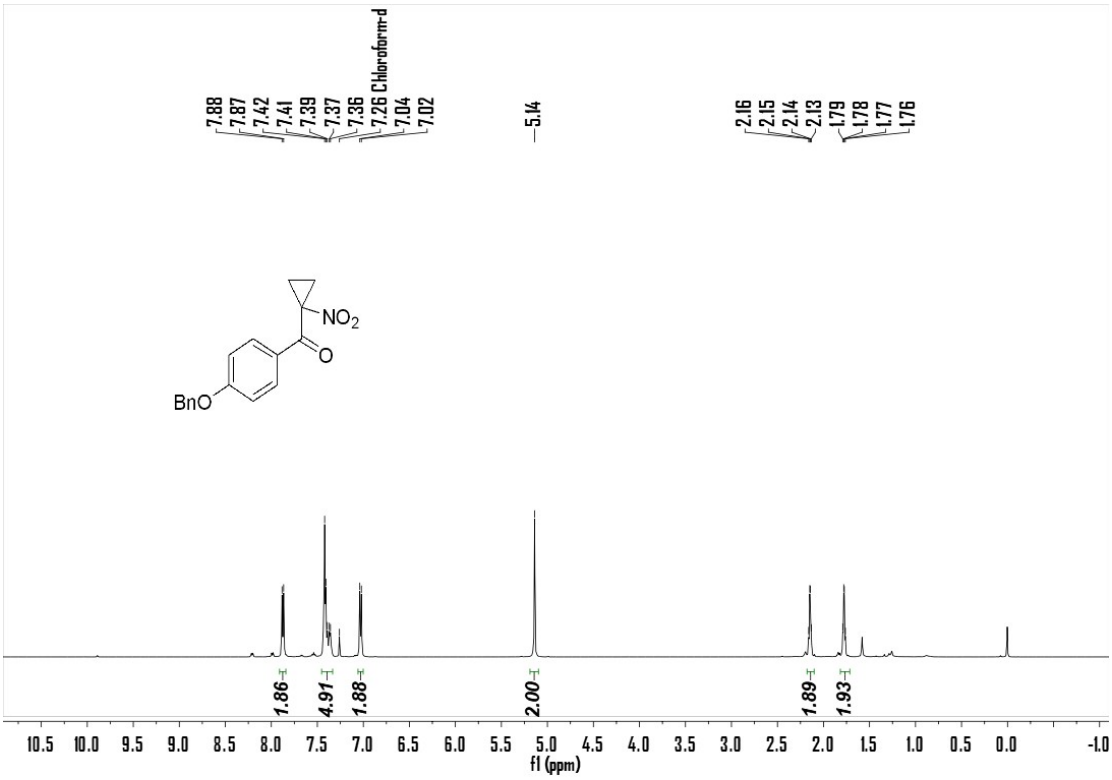


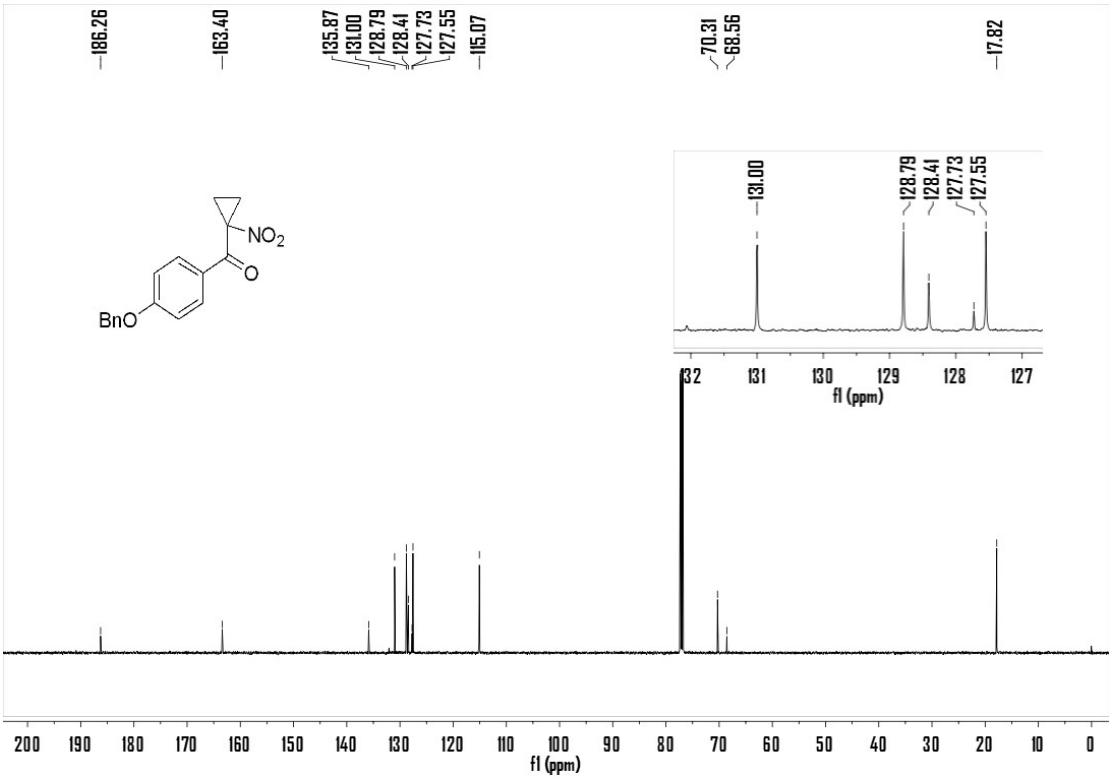
(1-nitrocyclopropyl)(p-tolyl)methanone (6a)



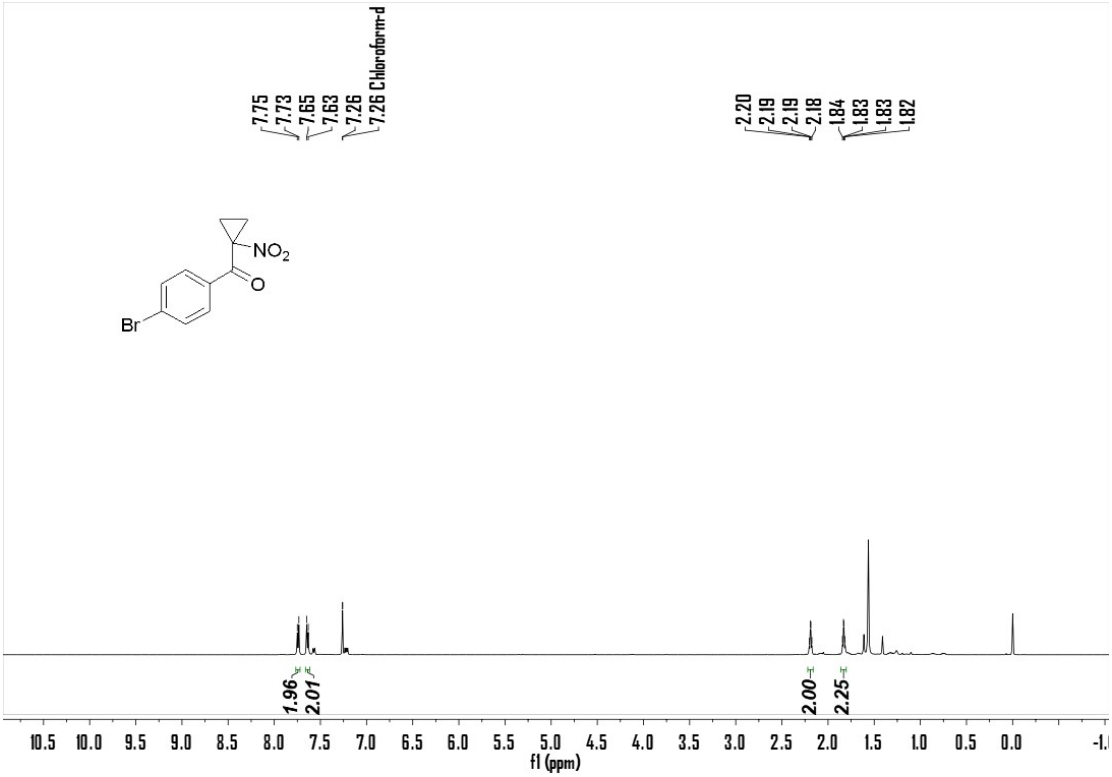


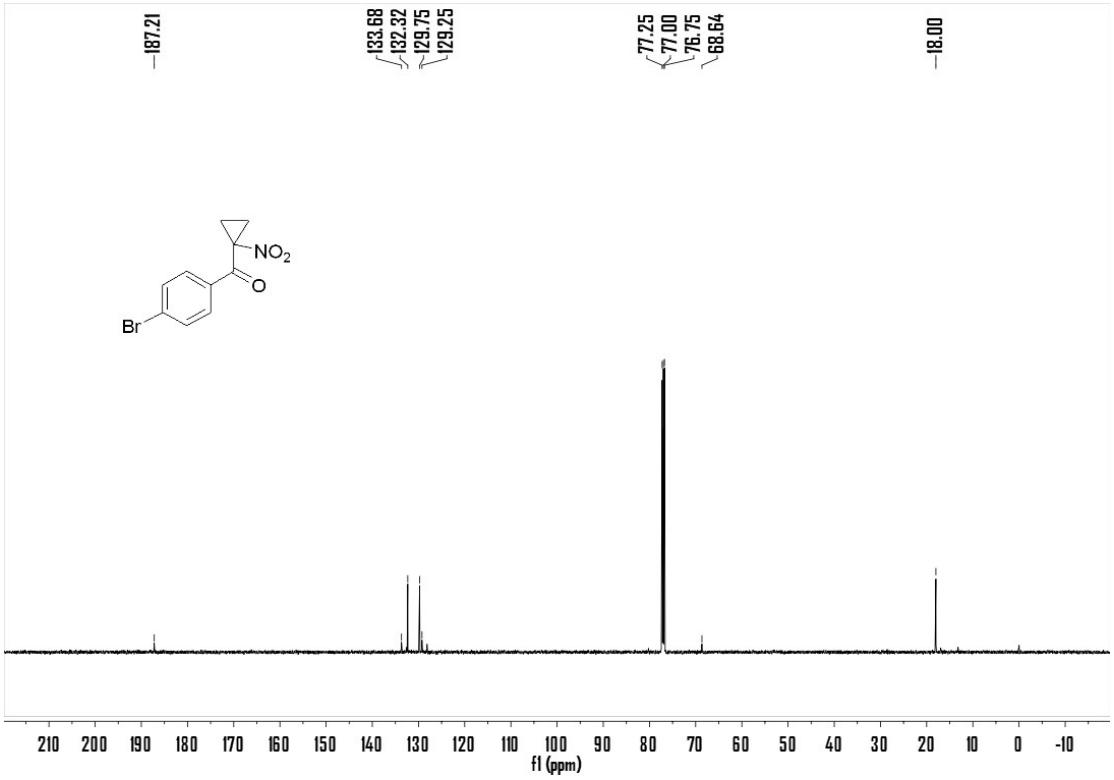
(4-(benzyloxy)phenyl)(1-nitrocyclopropyl)methanone (6b)



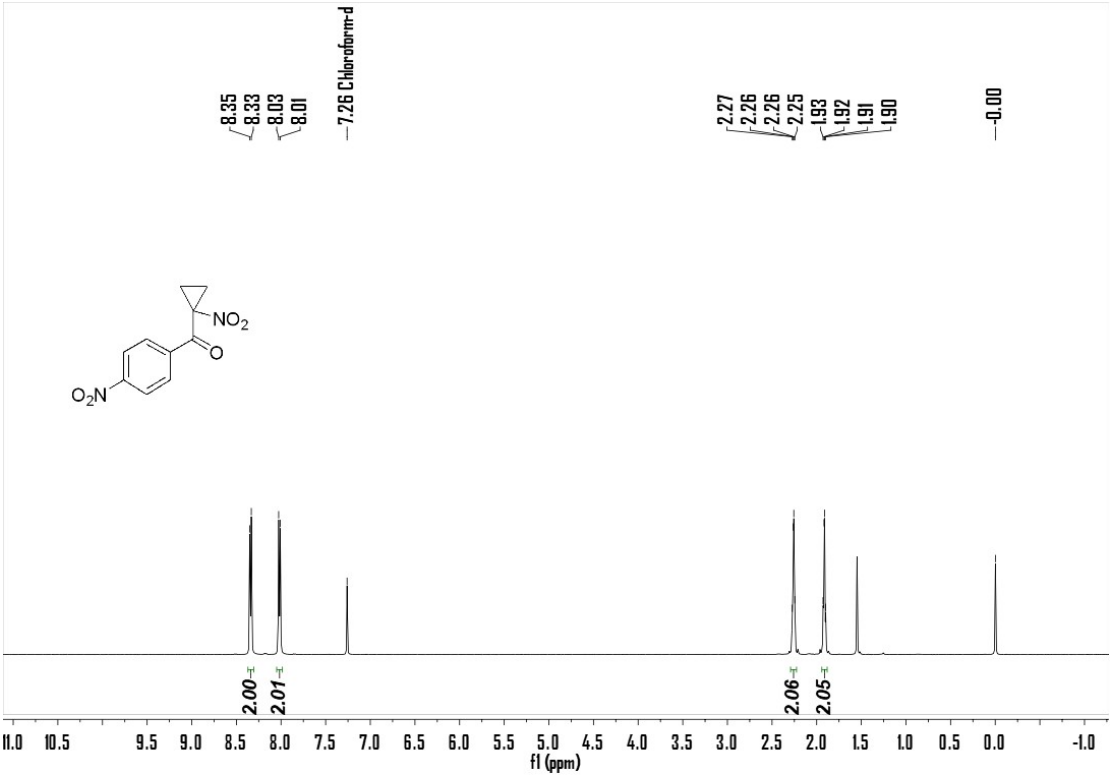


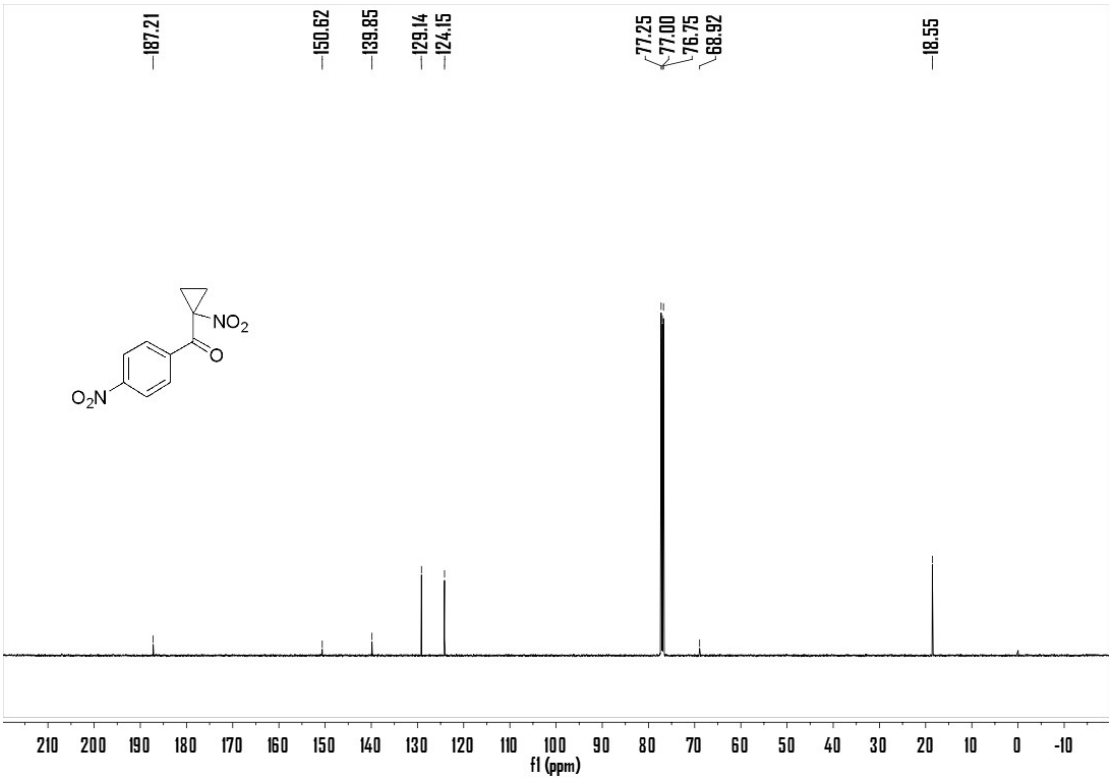
(4-bromophenyl)(1-nitrocyclopropyl)methanone (6c)



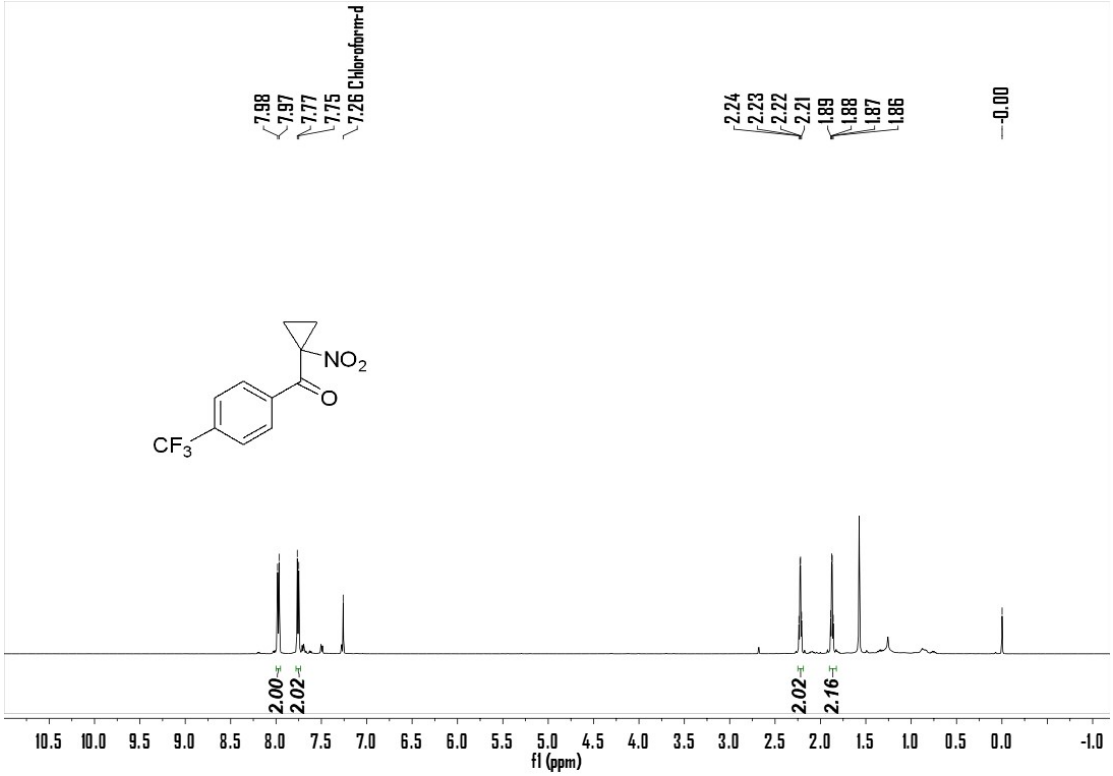


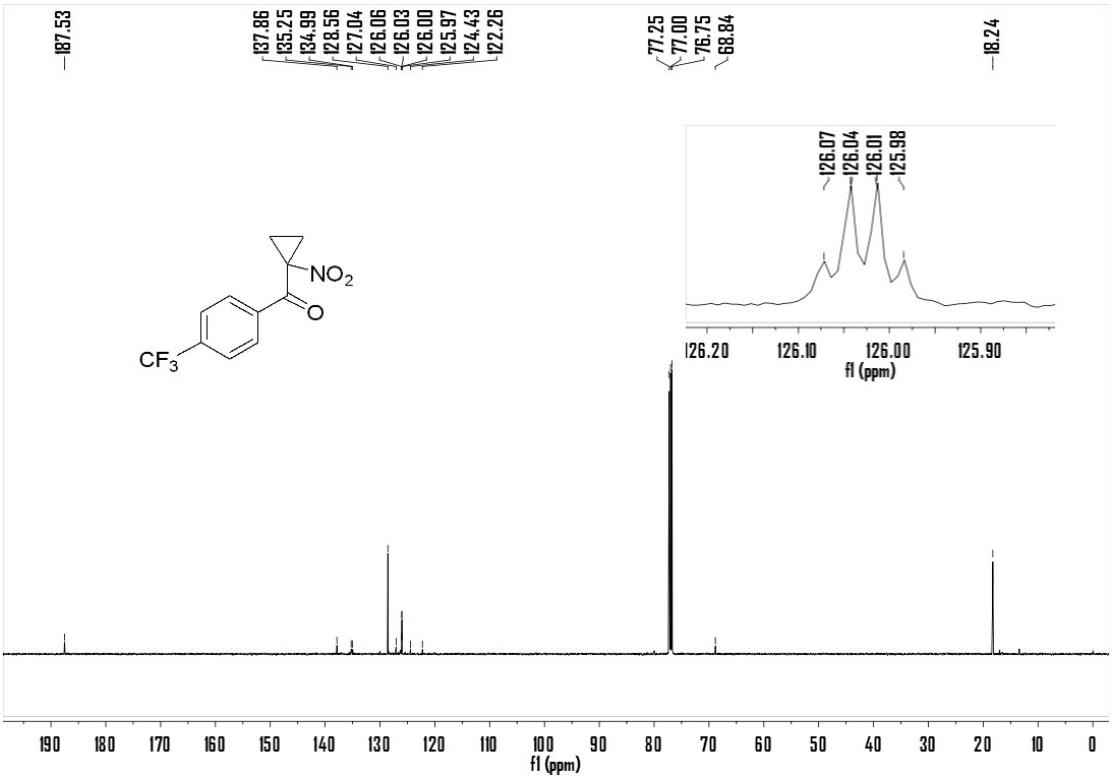
(1-nitrocyclopropyl)(4-nitrophenyl)methanone (6d)

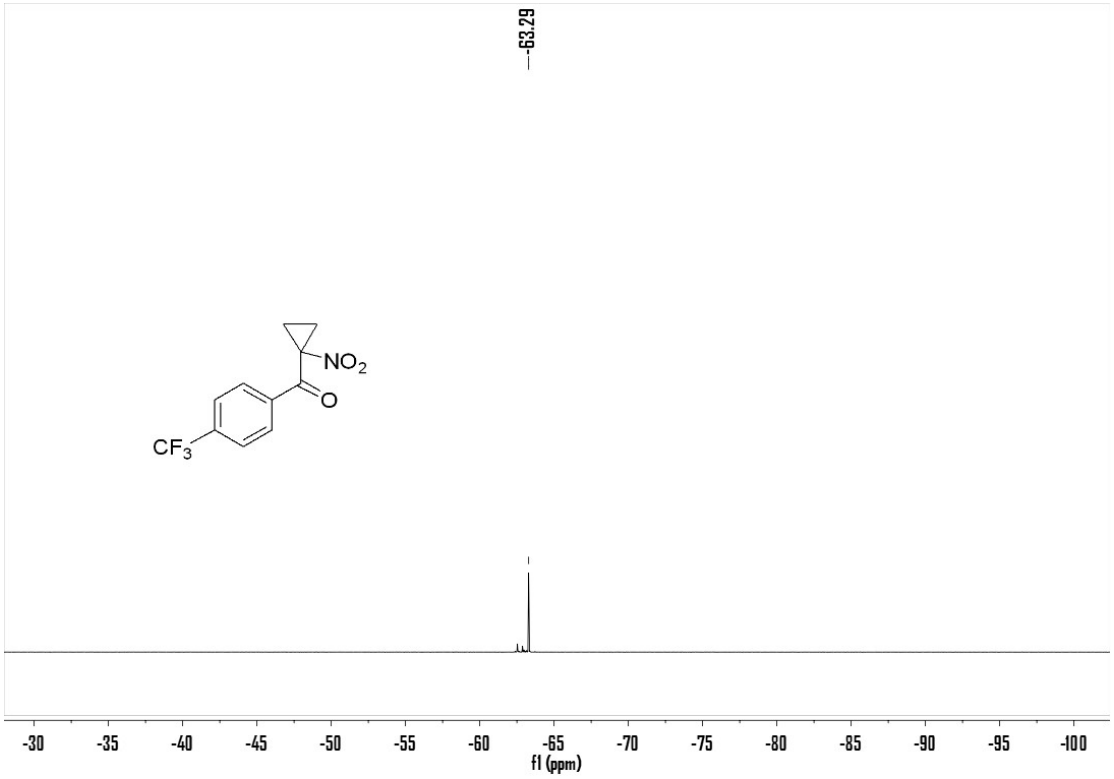




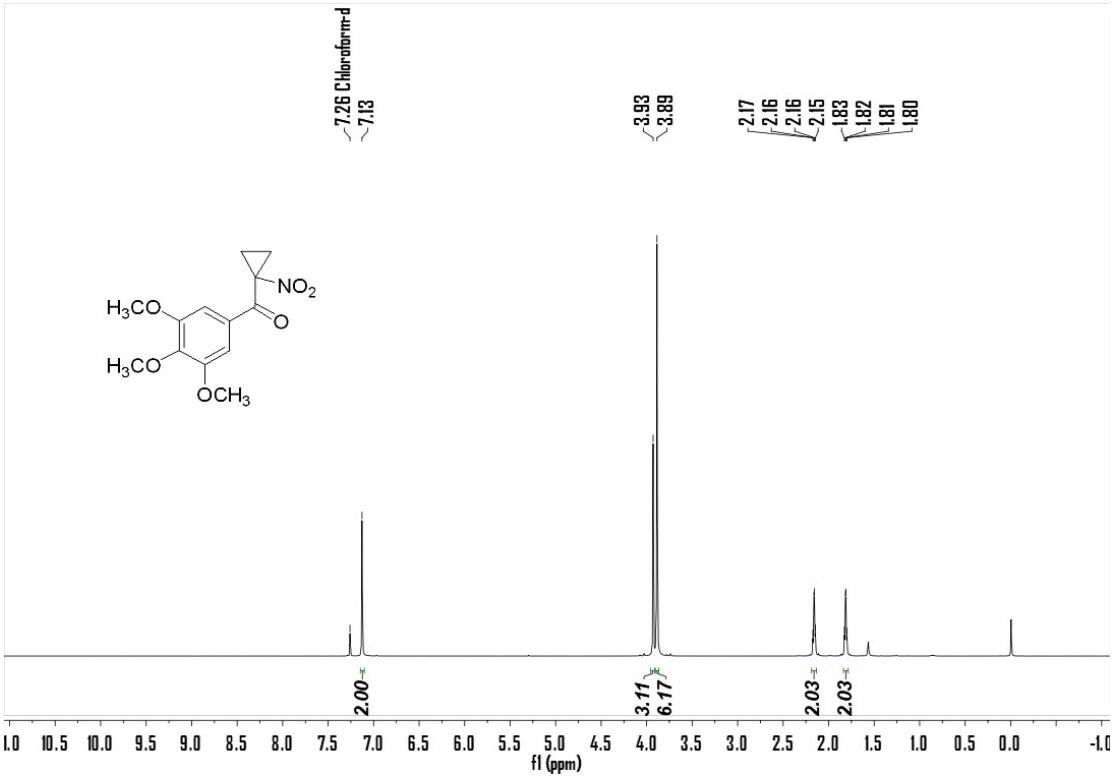
(1-nitrocyclopropyl)(4-(trifluoromethyl)phenyl)methanone (6e)

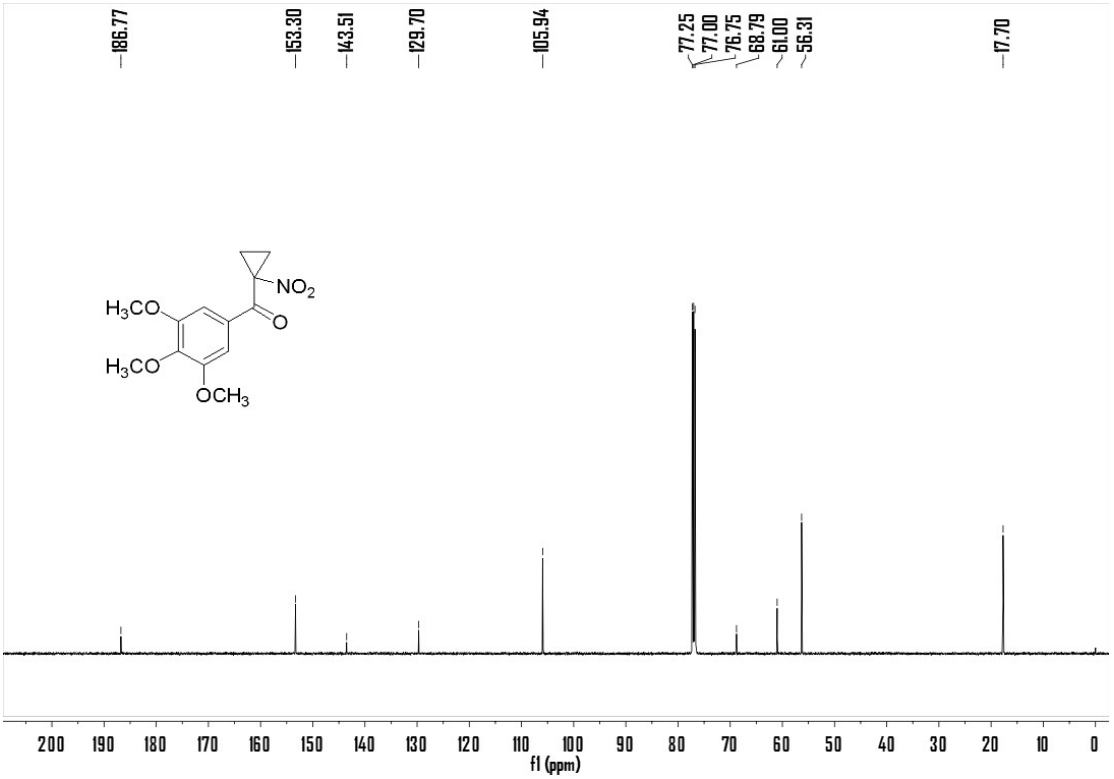




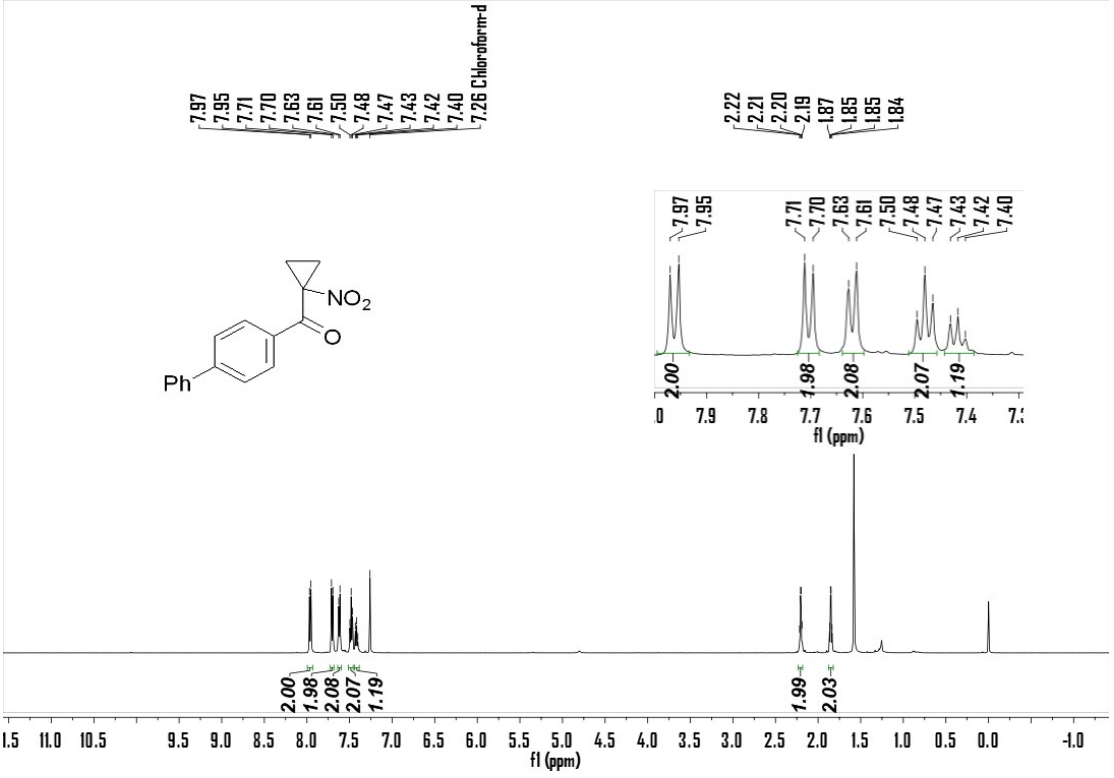


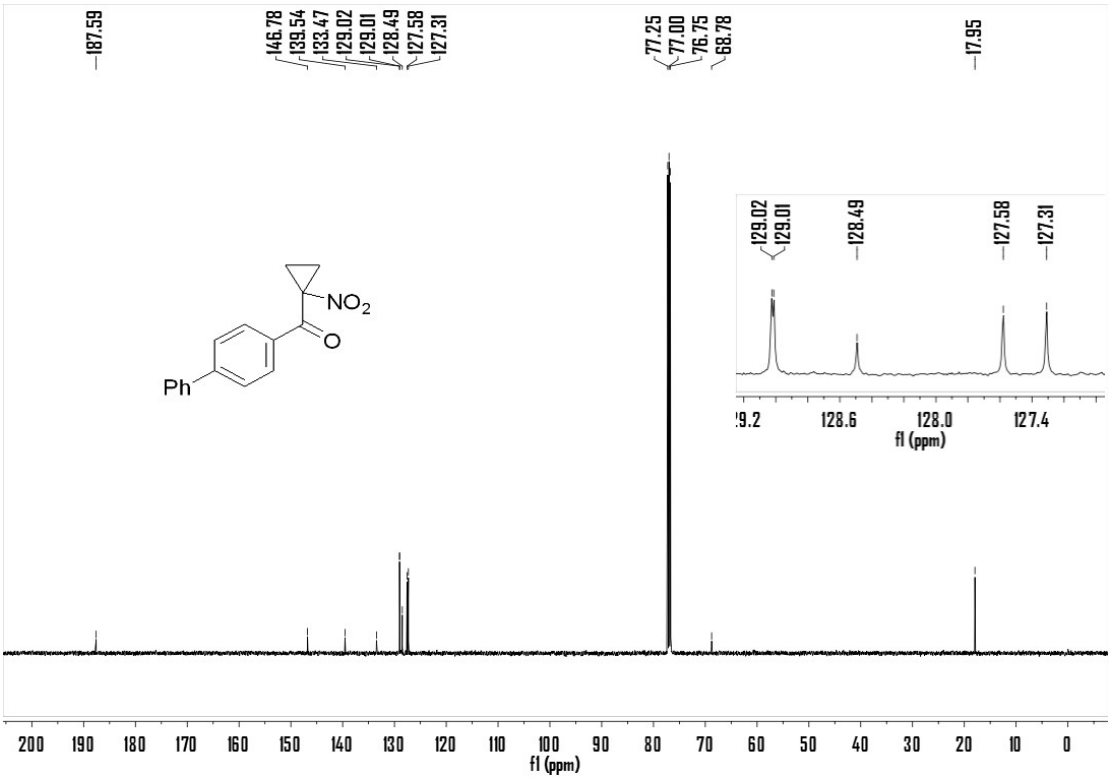
(1-nitrocyclopropyl)(3,4,5-trimethoxyphenyl)methanone (6f)



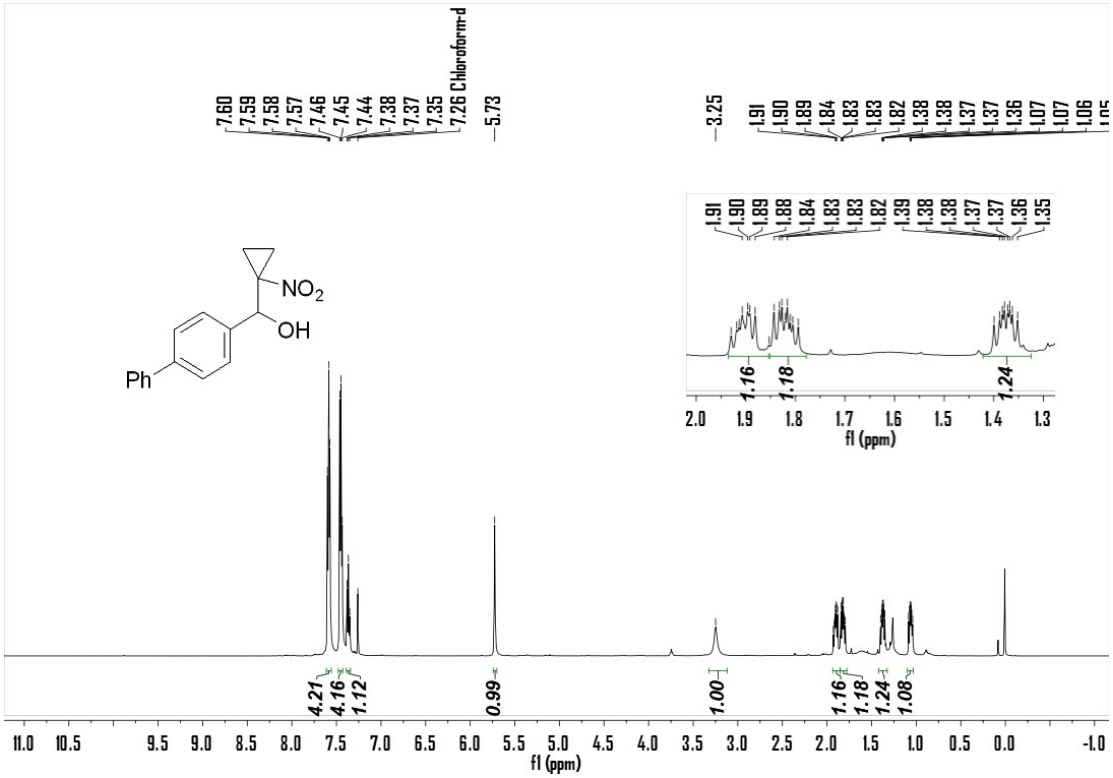


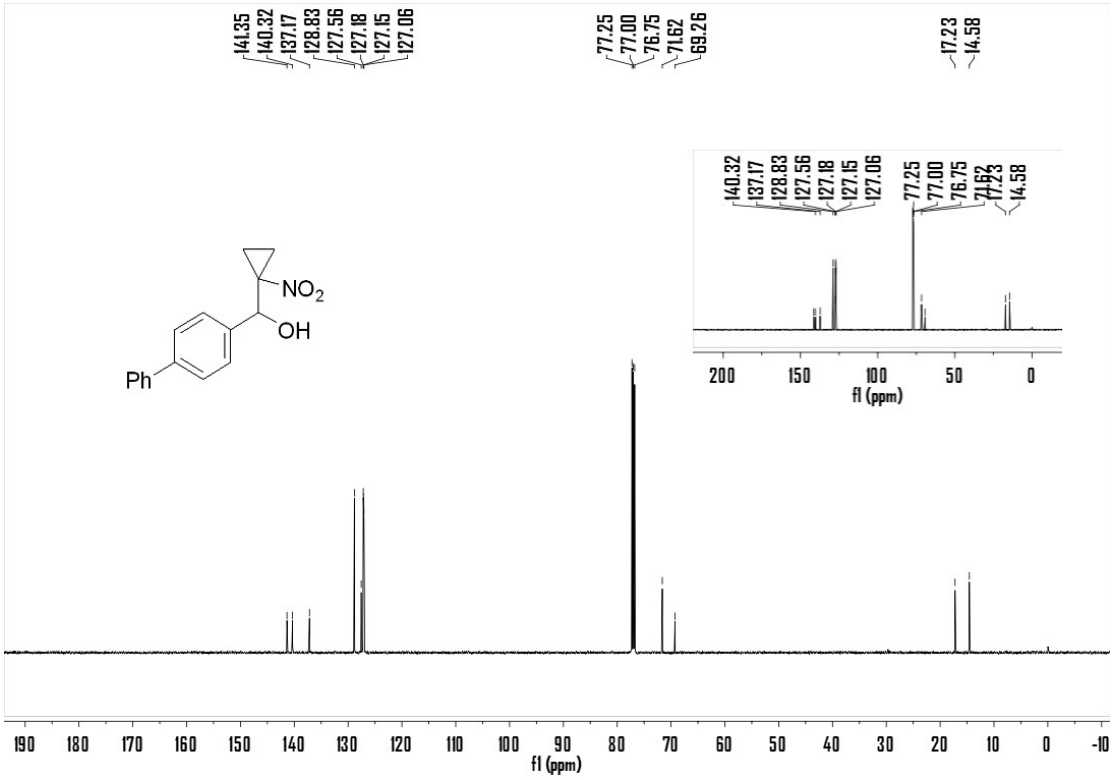
[1,1'-biphenyl]-4-yl(1-nitrocyclopropyl)methanone (6g)



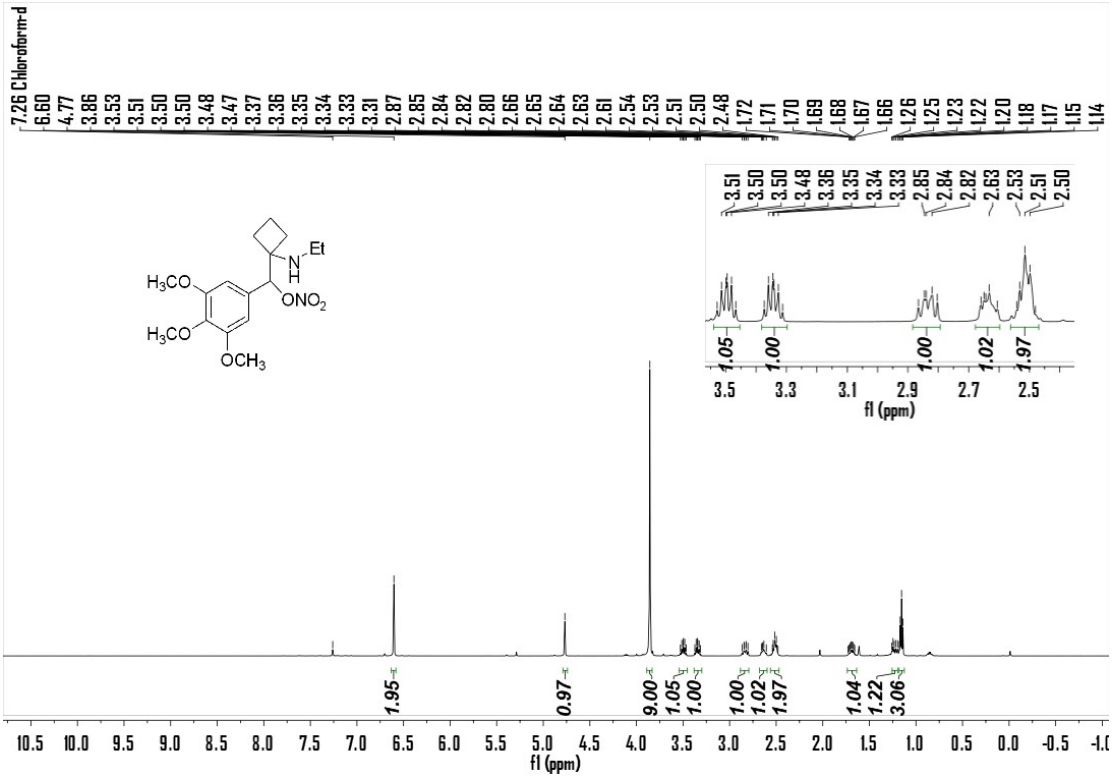


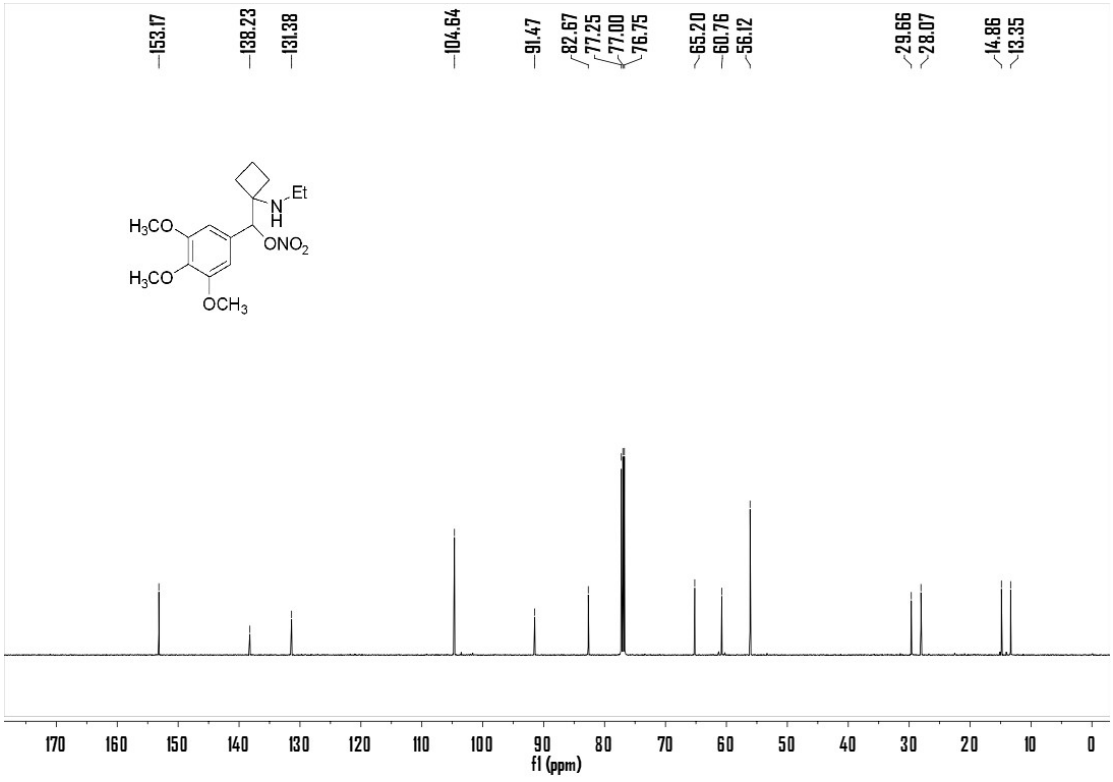
[1,1'-biphenyl]-4-yl(1-nitrocyclopropyl)methanol (6g')



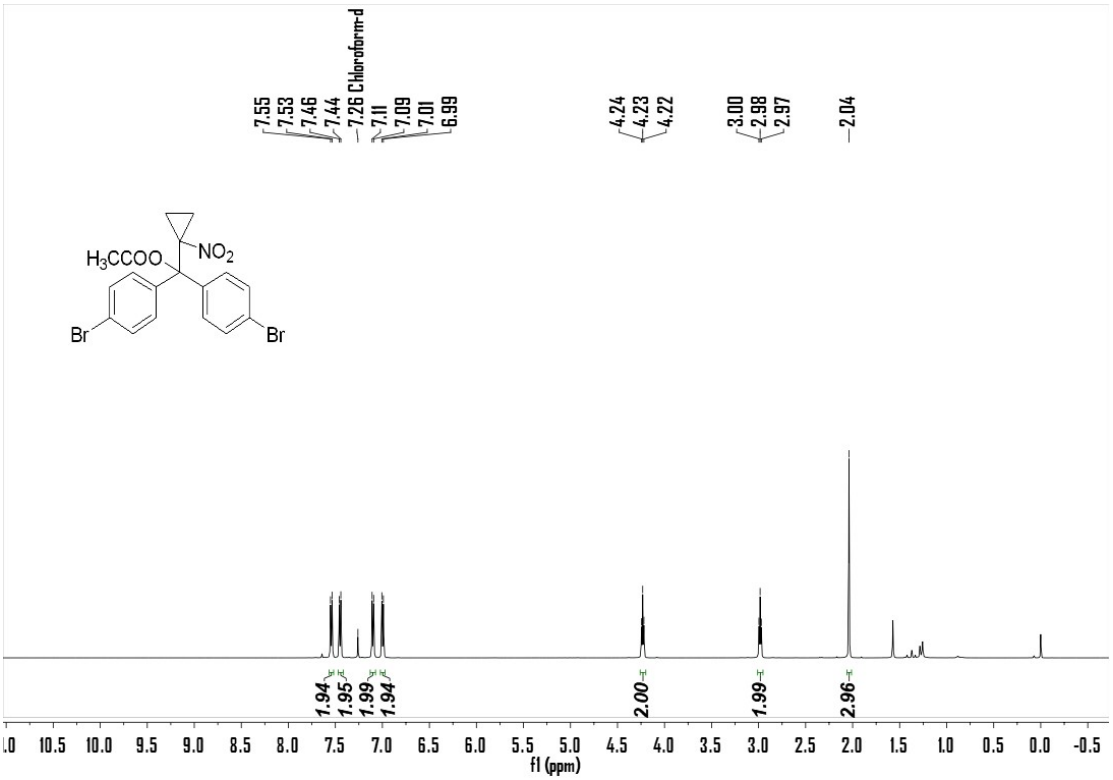


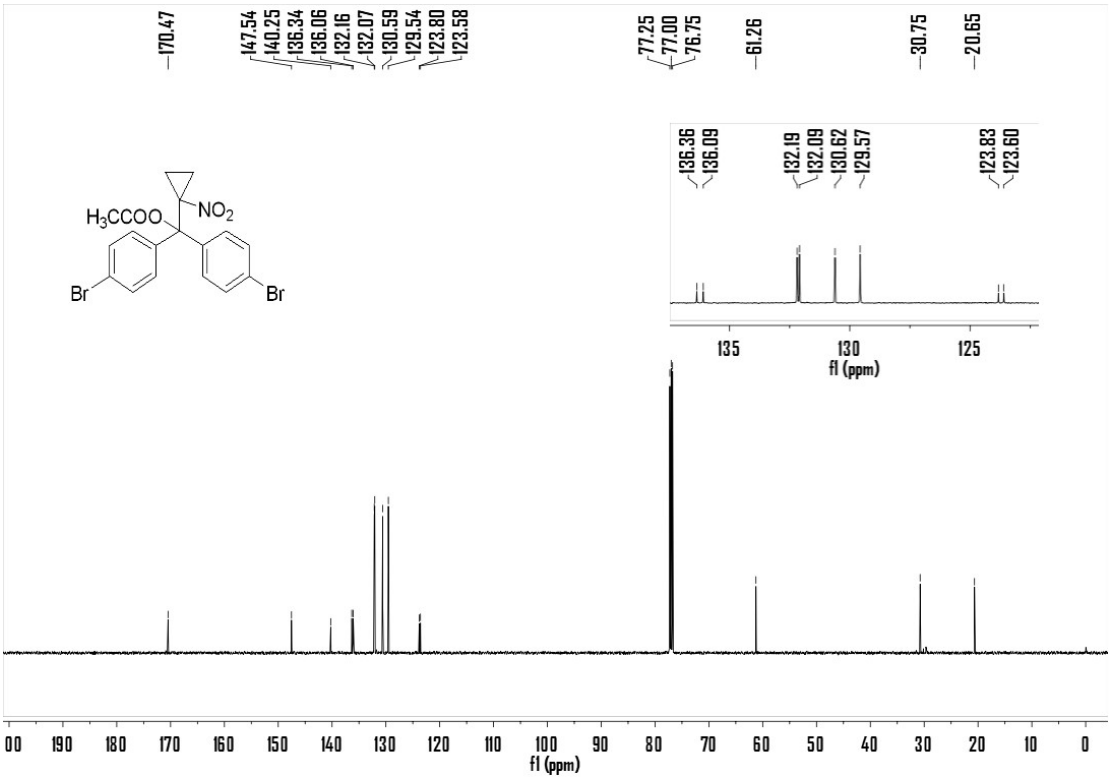
(1-(ethylamino)cyclobutyl)(3,4,5-trimethoxyphenyl)methyl nitrate (7)





bis(4-bromophenyl)(1-nitrocyclopropyl)methyl acetate (8)

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132.09
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NO2
Br
Br
135
130
125
f1 (ppm)
f1 (ppm)