

Supporting Information

Enantioselective Hydrogenation of α,β -Disubstituted Nitroalkenes

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1 General remarks

Starting materials, reagents and solvents were purchased from commercial sources (Sigma-Aldrich or TCI) and used without further purification. Unless otherwise noted, all reactions and manipulations that were sensitive to moisture or air were performed in a nitrogen-filled glovebox or using standard Schlenk techniques. Solvents were dried with standard procedures and degassed with N₂.

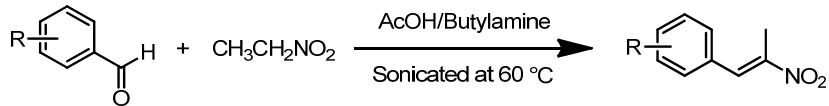
Column chromatography was performed using 200-400 mesh silica gel supplied by Natland International Corp. Thin-layer chromatography (TLC) was performed on EM reagents 0.25 mm silica 60-F plates.

NMR spectra analysis were recorded on Bruker Avance 400 MHz for ¹H NMR, 376.5 MHz for ¹⁹F NMR, and 100 MHz for ¹³C NMR, with CDCl₃ as the solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts were reported are reported in ppm, up field to TMS (0.00 ppm) and relative to CDCl₃ (7.26 ppm, 77.0 ppm) for ¹H NMR and ¹³C NMR.

HPLC analysis was carried out on an Agilent 1200 series chromatograph on a chiral phase, with hexane/2-propanol as eluents and a UV-detector at 222 nm; GC analysis was carried out on Hewlett-Packard 7890 gas chromatography using chiral capillary columns. Optical rotation was obtained on a Perkin-Elmer 341 MC polarimeter.

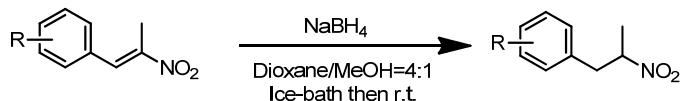
2 Synthesis of (*E*)-α,β-disubstituted nitroalkenes and racemates

2.1 Synthesis of α,β-disubstituted nitroalkenes



To a solution of benzaldehyde (5 mmol) in AcOH (2.5 mL), nitroethane (7.5 mmol) was added, followed by butylamine (10 mmol, 0.75 mL). The mixture was sonicated in a sealed flask (35 KHz frequency) at 60 °C, until TLC showed full conversion of aldehyde. The mixture was poured into ice water, extracted with EtOAc (3×15 mL). The combined organic extracts were washed with brine (2×10 mL) and dried over Na₂SO₄, solvent was evaporated and the product α, β-disubstituted nitroalkenes was purified by flash chromatography (hexane/ EtOAc, 15:1).¹

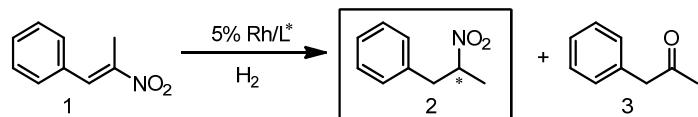
2.2 Synthesis of the racemates



To a stirred solution of nitroalkene (1.00 mmol) in Dioxane :EtOH (4:1, 5mL), NaBH₄ (1.50 mmol, 57 mg) was added step wise with an ice bath. Stirring was continued until gas evolution ceased, stirring is continued until the nitroalkenes was consumed, and the mixture was then quenched with saturated NH₄Cl aqueous solution, the mixture is concentrated under reduced pressure and extracted with CH₂Cl₂(3 × 10mL). The organic layer was dried over Na₂SO₄, the solvent was evaporated in *vacuum* and the product nitroalkane was purified by flash chromatography (Hexane/AcOEt=15:1).²

3 Asymmetric hydrogenation of (*E*)- α,β -disubstituted nitroalkenes

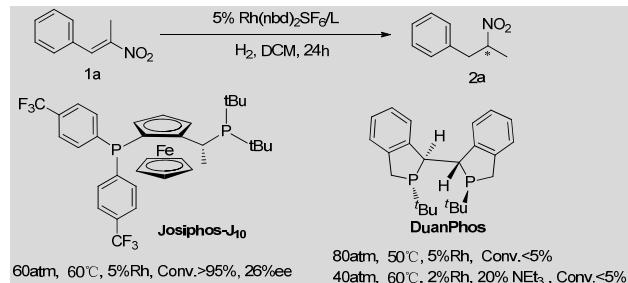
3.1 General procedure for asymmetric hydrogenation optimization



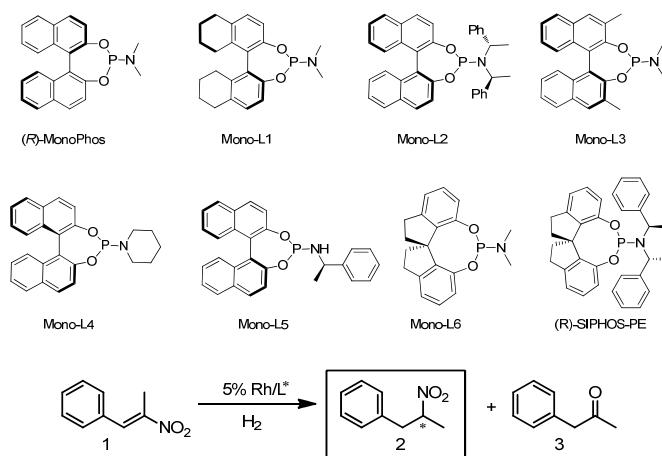
A stock solution was made by mixing Rh(NBD)₂SbF₆ with the chiral ligands in a 1:1:1 molar ratio in DCM at room temperature for 15 min in a nitrogen-filled glovebox. A specified amount of the catalyst solution (0.5 mL, 0.005mmol) was transferred by syringe into a vial containing the substrate (0.1 mmol) in anhydrous DCM (1.5 mL). The resulting vials were transferred to an autoclave, which was pressurized with hydrogen gas(50atm) and depressurized three times before 80 atm of H₂ was set, and the reaction mixtures were stirred at 50°C, for 24 h. The autoclave was cooled to room temperature and the hydrogen gas was released slowly and carefully, the solution was then concentrated and passed through a short column of silica gel (eluent: CH₂Cl₂) to remove the metal complex, the eluate was concentrated under vacuum. The conversion as detected by ¹H NMR of the crude products and the ee values of all systems were determined by HPLC on a chiral stationary phase.

3.2 Results of the optimization of asymmetric hydrogenation

Initial attempts with our previous catalysts³:



Monodentate ligands scanning:

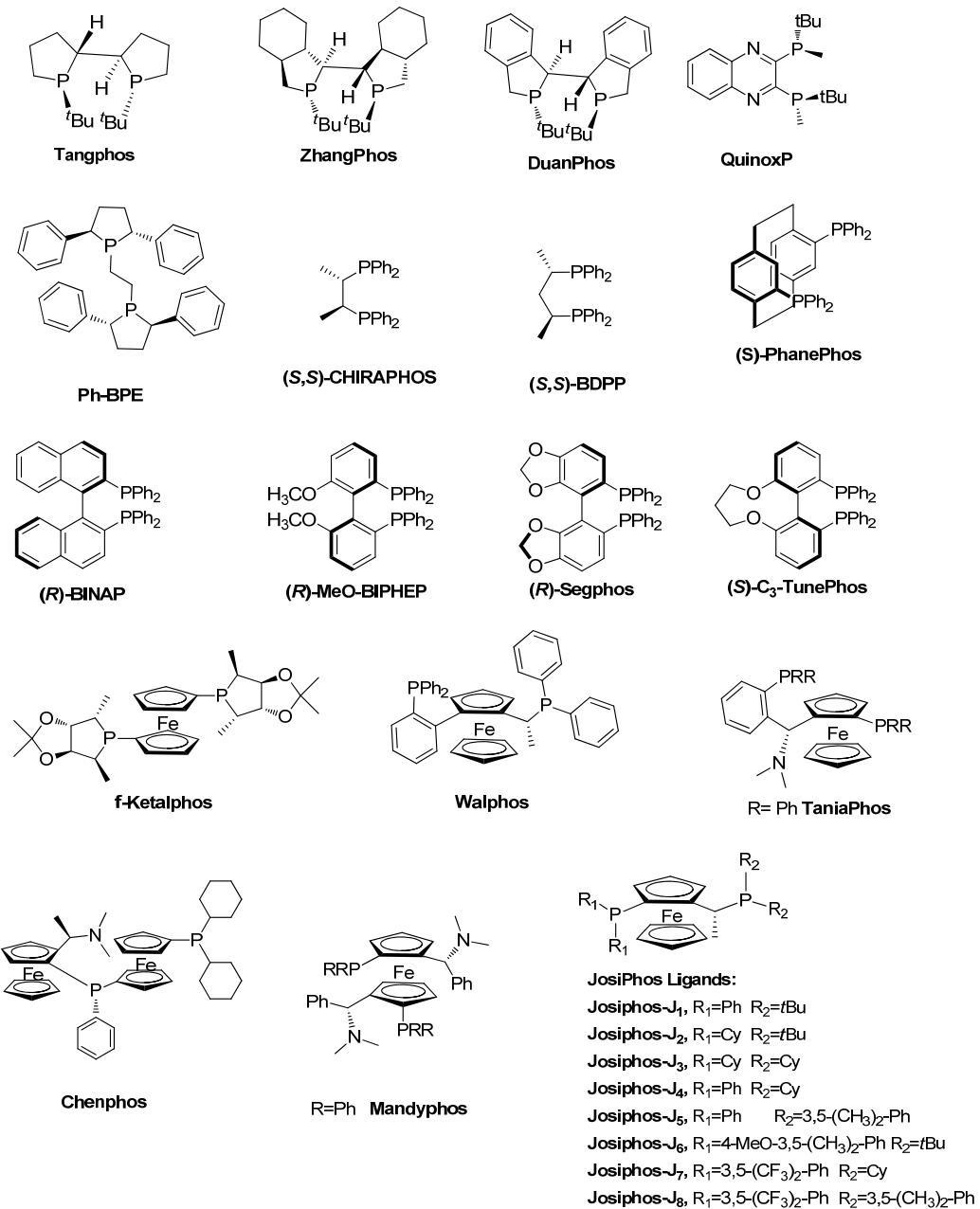


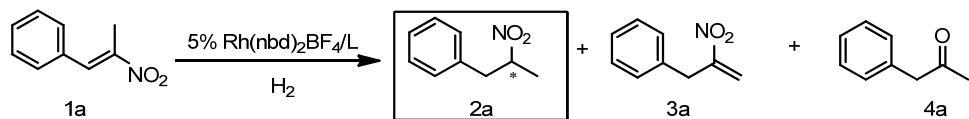
Entry	Ligand	Conv. ^[2]	Ee of 2a ^[3]
1	Mono-L1	<5	N.A.
2	Mono-L2	<5	N.A.
3	Mono-L3	6	50
4	Mono-L4	3.3	N.A.
5	Mono-L5	7.2	N.A.
6	Mono-L6	<5	N.A.
7	(R)-SIPHOS-PE	<5	N.A.
8	(R)-MonoPhos	<5	N.A.

[1]All reactions were carried out with a[Rh(nbd)₂]BF₄/ligand/substrate ratio of 1:1:1:20, under 80atm H₂ in dichloromethane , at 50°C for 24h..

[2]The conversion and molar ratio of products distribution were determined by ¹H NMR of the crude product of hydrogenation. [3]Enantiomeric excess was determined by HPLC on a chiral phase.[4] NA: Not available.

Bidentate ligands scanning:



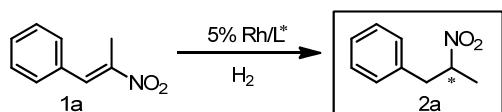


Entry	Ligand	Conv. ^[4]	Prod. Distribution ^[4]				Ee of 2a ^[5]
			1a	2a	3a	4a	
P-chiral ligands:							
1	TangPhos	95	0	100	0	0	6.8
2	ZhangPhos	75	25	75	0	0	4.1
3	QuinoxP*	5					N.A.
ChiralBisphospholane ligands:							
4	(R)-Binaphane	16	83.8	16.2	0	0	39.7
5	(R,R)-Ph-BPE	92	8.5	63.8	0	27.7	35.2
6	(S,S)-Chiraphos	5					NA
7	(S,S)-BDPP	6	94.6	5.4	0	0	40
Planar chiral ligands:							
8	(S)-Phanephos	32	67.7	32.3	0	0	32.8
Chiral axial ligands (AtropisomericBiarylBisphosphine Ligands):							
9	R-Binap	84	15.9	68.2	0	15.9	18
10	(R)-MeO-Biphep	15	84.7	15.3	0	0	7.2
11	S-C ₃ -tunephos	5					NA
Ferrocene-based ligands:							
12	Et-f-ketalphos	95	0	100	0	0	7.5
13	Josiphos-J1	95	0	100	0	0	29.7
14	Walphos	7	92.6	7.4	0	0	42
15	Mandyphos	12	88.1	11.9	0	0	20.8
16	TaniaPhos	59	40.8	59.2	0	0	58.6
17	Chenphos	29	71.2	28.8	0	0	4
18	Josiphos-J1	42	57.7	42.3		0	34.8
19	Josiphos-J2	24	76.2	23.8		0	69.6
20	Josiphos-J3	21	79.5	20.5		0	33
21	Josiphos-J4	<5	95.8	4.2		0	NA

22 ^[2]	Josiphos-J2	38	62.3	37.7	0	87
24 ^[3]	Josiphos-J2	58	41.9	58.1	0	86
25 ^[3]	Josiphos-J1	>95	0.9	99.1	0	27
26	Josiphos-J5	5	94.6	5.4	0	77.2
27	Josiphos-J6	<5				NA
28	Josiphos-J7	57	43.4	56.6	0	3.8
29	Josiphos-J8	14	86.3	2.6	0	11.1
30	Walphos	7	92.9	7.1	0	19.8

[1]Unless otherwise mentioned, all reactions were carried out with a[Rh(nbd)₂]BF₄/ligand/substrate ratio of 1:1.1:20, under 80atm H₂ in dichloromethane , at 50°C for 24h; entries 18~23: 60atm, 40°C,36hrs; entries 26~31:60atm, 40°C,36hrs. [2]Rh(NBD)₂SbF₆ as metal precursor.;[3] 60atm, 60°C, 24hrs. [4] theconversion and molar ratio of products distribution were determined by ¹H NMR of the crude product of hydrogenation. [5]Enantiomeric excess was determined by HPLC on a chiral phase. [6] NA: Not available; Cy: cyclohexyl; tBu:*tert*-butyl.

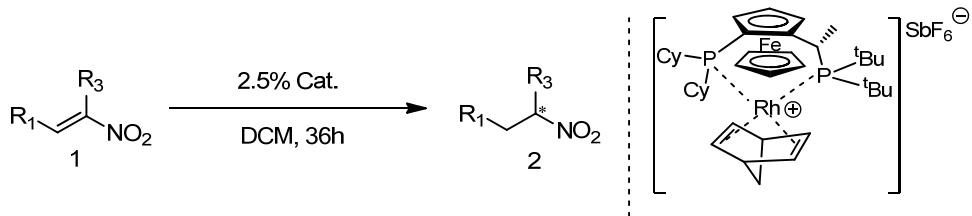
Other parameters optimization(typical results):



Entry	H ₂ (atm)	T (°C)	Rh (%)	Additive	T (h)	Conv. ^[2]	Ee ^[3]
						(%)	(%)
1	60	40	5	10% NEt ₃	36	43	43.6
2	60	40	5	10% PTSA	36	<5	NA
3	60	40	5	10% L-CSA	36	<5	NA
4	60	40	5	50% CH ₃ NO ₂	36	32	49.3
5	80	70	2.5		24	49	83.8
6	80	80	2.5		24	92	85.2
7	80	80	2.5		24	>95	85.1
8	50	70	2.5		36	>95	86

[1]Unless otherwise mentioned, all reactions were carried out with a[Rh(nbd)2]SbF₆/ligand of 1:1.1, in dichloromethane. [2]theconversion and molar ratio of products distribution were determined by ¹H NMR of the crude product of hydrogenation. [3]Enantiomeric excess was determined by HPLC on a chiral phase.[d]Not available.

3.3 Application of asymmetric hydrogenation

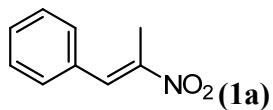


A stock solution was made by mixing Rh(nbd)₂SbF₆ with JosiPhos in a 1:1.1 molar ratio in anhydrous DCM at room temperature for 15 min in a nitrogen-filled glovebox. To a vial containing the substrate (0.1 mmol) and a stir bar in anhydrous DCM (1 mL) was added an aliquot of the catalyst solution (0.25 mL, 0.0025 mmol) by syringe. The resulting vials were transferred to an autoclave, which then underwent three cycles of flushing with hydrogen gas by pressurizing to 50 atm and then depressurizing. The reaction was then stirred under H₂ (50 atm) at 70°C, for 36 h. The autoclave was cooled to room temperature and the hydrogen gas was released slowly and carefully. The solution was concentrated and passed through a short column of silica gel (eluent: CH₂Cl₂). The *ee* values of all compounds were determined by HPLC analysis or GC analysis on a chiral stationary phase.

4 Representative characterization data

Note: In ¹³C NMR spectrum, *C* in parentheses (*C*) stands for **quaternary carbon**, (*CH*) stands for **tertiary carbon**, (*CH*₂) stands for **secondary carbon**, (*CH*₃) stands for **primary carbon**. Spectral data were compared with the literature values^{1a,4}.

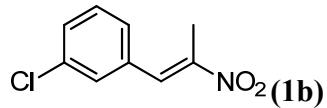
4.1 NMR data of (*E*)- α,β -disubstituted nitroalkenes



(*E*)-(2-nitroprop-1-en-1-yl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.45(s, 3H, *CH*₃), 7.39~7.48(m, 5H, aromatic *H*), 8.08(s, 1H, *CHCNO*₂);

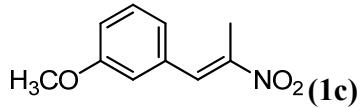
¹³C-NMR (CDCl₃, 100 MHz) δ: 14.0(CH₃), 128.9(2×CH), 129.9(CH), 130.0(2×CH), 132.5(C), 133.5(CH), 147.8(C).



(E)-1-chloro-3-(2-nitroprop-1-en-1-yl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.44(s, 3H, CH₃), 7.29~7.31(m, 1H, aromatic H), 7.39~7.40(m, 3H, aromatic H), 7.99(s, 1H, CHCNO₂);

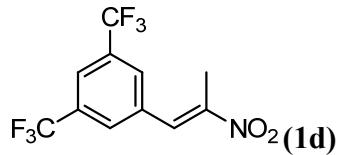
¹³C-NMR (CDCl₃, 100 MHz) δ: 13.9(CH₃), 127.9(CH), 129.6(CH), 129.8(CH), 130.2(CH), 131.9(CH), 134.3(C), 134.9(C), 148.8(C).



(E)-1-methoxy-3-(2-nitroprop-1-en-1-yl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.43(s, 3H, CH₃), 3.83(s, 3H, OCH₃), 6.93~7.01(m, 3H, aromatic H), 7.36(dd, J₁=J₂=8.0Hz, 1H, aromatic H), 8.02(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 14.0(CH₃), 55.3(CH₃), 115.4(CH), 115.5(CH), 122.3(CH), 129.9(CH), 133.4(CH), 133.7(C), 147.9(C), 159.8(C).

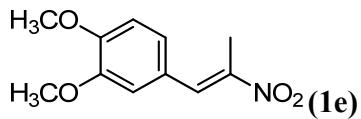


(E)-1-(2-nitroprop-1-en-1-yl)-3,5-bis(trifluoromethyl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.46 (s, 3H, CH₃), 7.86(s, 2H, aromatic H), 7.94(s, 1H, aromatic H), 8.09(s, 1H, CHCNO₂);

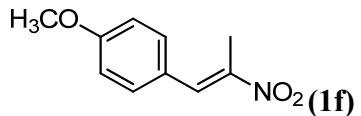
¹³C-NMR (CDCl₃, 100 MHz) δ: 13.8(CH₃), 123.2(m, CH), 123.9(q, J_{CF}=271Hz, 2×CF₃), 129.4(m, 2×CH), 129.9(CH), 132.5(q, J_{CF}=34Hz, 2×C), 134.7(C), 150.5(C).

¹⁹F-NMR (CDCl₃, 376.5 MHz) δ: -63.2.



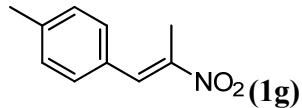
¹H-NMR (CDCl₃, 400 MHz) δ: 2.49(s, 3H, CH₃), 3.92(s, 3H, OCH₃), 3.94(s, 3H, OCH₃), 6.93~6.96(m, 2H, aromatic H), 7.08 (dd, J₁=8.4Hz,J₂=2Hz, 1H, aromatic H), 8.06(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 14.1(CH₃), 56.01(CH₃), 56.02(CH₃), 111.3(CH), 113.2(CH), 124.0(CH), 125.1(C), 133.8(CH), 145.9(C), 149.2(C), 150.9(C).



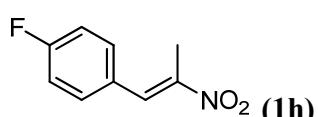
¹H-NMR (CDCl₃, 400 MHz) δ: 2.46(s, 3H, CH₃), 3.86(s, 3H, OCH₃), 6.96~6.99 (m, 2H, aromatic H), 7.39~7.43(m, 2H, aromatic H), 8.06(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 14.1(CH₃), 55.4(CH₃), 114.5(2×CH), 124.8(C), 132.1(2×CH), 133.6(CH), 145.8(C), 161.1(C).



¹H-NMR (CDCl₃, 400 MHz) δ: 2.39(s, 3H, PhCH₃), 2.43(s, 3H, NO₂CCH₃), 7.25(d, J=8.0Hz, 2H, aromatic H), 7.32(d, J=8.0Hz, 2H, aromatic H), 8.04(s, 1H, CHCNO₂);

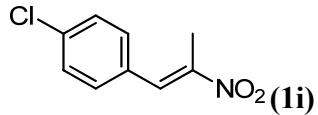
¹³C-NMR (CDCl₃, 100 MHz) δ: 13.0(CH₃), 20.4(CH₃), 128.5(C), 128.7(2×CH), 129.1(2×CH), 132.6(CH), 139.5(C), 145.9(C).



¹H-NMR (CDCl₃, 400 MHz) δ: 2.44(s, 3H, CH₃), 7.13~7.18(m, 2H, aromatic H), 7.42~7.45(m, 2H, aromatic H), 8.05(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 13.9(CH₃), 116.1(d, J_{CF}=21Hz, 2×CH), 128.6(d, J_{CF}=3Hz, C), 131.9(d, J_{CF}=9Hz, 2×CH), 132.4(CH), 147.6(C), 163.5(d, J_{CF}=251Hz, C).

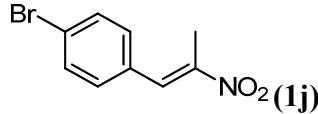
¹⁹F-NMR (CDCl₃, 376.5 MHz) δ: -109.4.



(E)-1-chloro-4-(2-nitroprop-1-en-1-yl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.43(s, 3H, CH₃), 7.36~7.38(m, 2H, aromatic H), 7.42~7.44(m, 2H, aromatic H), 8.02(s, 1H, CHCNO₂);

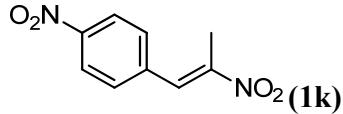
¹³C-NMR (CDCl₃, 100 MHz) δ: 13.9(CH₃), 129.2(2×CH), 130.9(C), 131.2(2×CH), 132.1(CH), 136.1(C), 148.1(C).



(E)-1-bromo-4-(2-nitroprop-1-en-1-yl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.43(s, 3H, NO₂CCH₃), 7.31(dd, J₁=8.4Hz, J₂=2.0Hz, 2H, aromatic H), 7.59(d, J₁=8.4Hz, J₂=2.0Hz, 2H, aromatic H), 8.00(s, 1H, CHCNO₂);

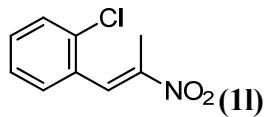
¹³C-NMR (CDCl₃, 100 MHz) δ: 14.0(CH₃), 124.4(C), 131.4(2×CH), 132.2(2×CH), 132.3(CH), 139.5(C), 148.2(C).



(E)-1-nitro-4-(2-nitroprop-1-en-1-yl)benzene

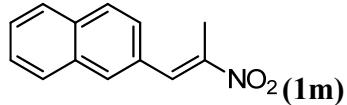
¹H-NMR (CDCl₃, 400 MHz) δ: 2.47(s, 3H, NO₂CCH₃), 7.61(d, J=8.4Hz, 2H, aromatic H), 8.09(s, 1H, CHCNO₂), 8.32(d, J=8.4Hz, 2H, aromatic H);

¹³C-NMR (CDCl₃, 100 MHz) δ: 14.1(CH₃), 124.1(2×CH), 130.6(2×CH), 130.7(CH), 138.9(C), 148.2(C), 150.3(C).



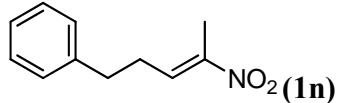
¹H-NMR (CDCl₃, 400 MHz) δ: 2.34(s, 3H, CH₃), 7.33~7.38(m, 3H, aromatic H), 7.46~7.49(m, 1H, aromatic H), 8.17(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 13.9(CH₃), 126.9(CH), 129.9(CH), 130.2(CH), 130.6(CH), 130.9(CH), 131.3 (C), 134.8(C), 149.3(C).



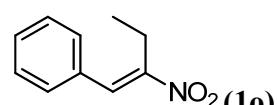
¹H-NMR (CDCl₃, 400 MHz) δ: 2.48(s, 3H, NO₂CCH₃), 7.44 (dd, J₁=8.4Hz, J₁=1.2Hz, 1H, aromatic H), 7.49~7.55(m, 2H, aromatic H), 7.82~7.86(m, 4H, aromatic H), 8.17(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 14.2(CH₃), 126.4(CH), 126.9(CH), 127.7(CH), 127.8(CH), 128.5(CH), 128.7(CH), 129.9(C), 130.6(CH), 133.1(C), 133.6(C), 133.7(CH), 147.8(C).



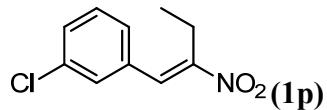
¹H-NMR (CDCl₃, 400 MHz) δ: 2.03(d, J= 0.8Hz, 3H, NO₂CCH₃), 2.54(m, 2H, PhCH₂CH₂), 2.80(t, J= 7.6Hz, 3H, PhCH₂CH₂), 7.12(td, J₁= 7.6Hz, J₂=0.8Hz, 1H, NO₂CCH), 7.14~7.19(m, 2H, aromatic H), 7.21~7.23(m, 1H, aromatic H), 7.27~7.31(m, 2H, aromatic H),

¹³C-NMR (CDCl₃, 100 MHz) δ: 12.4(CH₃), 29.9(CH₂), 34.4(CH₂), 126.5(CH), 128.4(2×CH), 128.7(2×CH), 134.8(CH), 140.1(C), 148.2(C).



¹H-NMR (CDCl₃, 400 MHz) δ: 1.27(t, *J*= 7.6Hz, 3H, CH₃), 2.86(q, *J*= 7.6Hz, 2H, CH₂), 7.39~7.47(m, 5H, aromatic *H*), 8.01(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 12.5(CH₃), 20.7(CH₂), 129.0(2 × CH), 129.6(2 × CH), 129.9(CH), 132.4(C), 133.1(CH), 153.4(C).

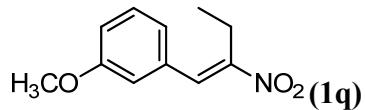


(*E*)-1-chloro-3-(2-nitrobut-1-en-1-yl)benzene

¹H-NMR (CDCl₃, 400 MHz) δ: 1.27(t, *J*= 7.2Hz, 3H, CH₃), 2.84(q, *J*= 7.6Hz, 2H, CH₂),

7.29(m, 1H, aromatic *H*), 7.37~7.41(m, 3H, aromatic *H*), 7.92(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 12.4(CH₃), 20.7(CH₂), 127.5(CH), 129.3(CH), 129.9(CH), 130.2(CH), 131.4(CH), 134.2(C), 135.0(C), 154.4(C).



(*E*)-1-methoxy-3-(2-nitrobut-1-en-1-yl)benzene

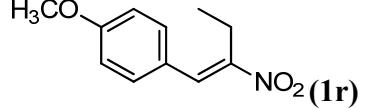
¹H-NMR (CDCl₃, 400 MHz) δ: 1.27(t, *J*= 7.2Hz, 3H, CH₃), 2.87(q, *J*= 7.2Hz, 2H, CH₂), 3.84(s,

3H, OCH₃), 6.94~7.01(m, 3H, aromatic *H*), 7.36(dd, *J*₁=*J*₂= 8.0Hz, 1H, aromatic *H*), 7.98(s, 1H,

CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 12.5(CH₃), 20.8(CH₂), 55.3(OCH₃), 115.1(CH), 115.5(CH),

121.9(CH), 130.0(CH), 132.9(CH), 133.7(C), 153.6(C), 159.9(C).



(*E*)-1-methoxy-4-(2-nitrobut-1-en-1-yl)benzene

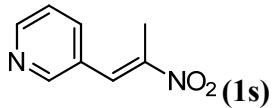
¹H-NMR (CDCl₃, 400 MHz) δ: 1.28(t, *J*= 7.6Hz, 3H, CH₃), 2.88(q, *J*= 7.6Hz, 2H, CH₂), 3.86(s,

3H, OCH₃), 6.98(d, *J*= 8.8Hz, 2H, aromatic *H*), 7.40(d, *J*= 8.8Hz, 2H, aromatic *H*), 7.99(s, 1H,

CHCNO₂);

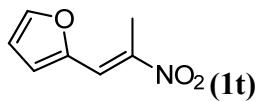
¹³C-NMR (CDCl₃, 100 MHz) δ: 12.3(CH₃), 20.8(CH₂), 55.4(OCH₃), 114.6(2 × CH), 124.6(C),

131.8(2 × CH), 133.2(CH), 151.3(C), 161.2(C).



¹H-NMR (CDCl₃, 400 MHz) δ: 2.47(s, 3H, NO₂CCH₃), 7.45 (m, 1H, aromatic H), 7.81(d, J=6.4Hz, 1H, aromatic H), 8.04(s, 1H, CHCNO₂), 8.66(m, 1H, aromatic H), 8.71(s, 1H, aromatic H);

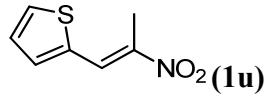
¹³C-NMR (CDCl₃, 100 MHz) δ: 13.9(CH₃), 123.6(CH), 128.5(C), 129.8(CH), 136.6(CH), 149.2(C), 150.5(CH), 150.6(CH).



(E)-2-(2-nitroprop-1-en-1-yl)furan

¹H-NMR (CDCl₃, 400 MHz) δ: 2.57(s, 3H, NO₂CCH₃), 6.59 (m, 1H, aromatic H), 6.83(d, J=3.2Hz, 1H, aromatic H), 7.65(d, J= 1.6Hz, 1H, aromatic H), 7.83(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 13.9(CH₃), 112.9(CH), 119.2(CH), 120.6(CH), 144.4(C), 146.3(CH), 147.9(C).

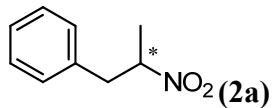


(E)-2-(2-nitroprop-1-en-1-yl)thiophene

¹H-NMR (CDCl₃, 400 MHz) δ: 2.56(s, 3H, NO₂CCH₃), 7.19(dd, J₁= 5.2Hz, J₂= 3.6Hz, 1H, aromatic H), 7.43(d, J= 3.6Hz, 1H, aromatic H), 7.64(d, J= 5.2Hz, 1H, aromatic H), 8.29(s, 1H, CHCNO₂);

¹³C-NMR (CDCl₃, 100 MHz) δ: 14.2(CH₃), 127.2(CH), 128.2(CH), 131.7(CH), 134.7(CH), 135.3(C), 144.5(C).

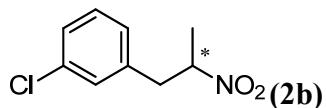
4.2 Analytic data of α -chiral nitroalkanes



$[\alpha]_D^{25} = +44.8^\circ$ (C 0.4, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.52(d, *J*= 6.8Hz, 3H, CH₃), 2.97~3.02(m, 1H, PhCH), 3.28~3.33(m, 1H, PhCH), 4.78(m, 1H, CHNO₂), 7.13~7.16(m, 2H, aromatic H), 7.22~7.32(m, 3H, aromatic H).

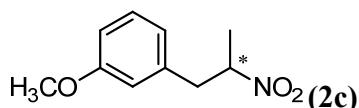
¹³C-NMR (CDCl₃, 100 MHz) δ: 18.8(CH₃), 41.2(CH₂), 84.4(CH), 127.4(CH), 128.8(2×CH), 129.0(2×CH), 135.6(C).



$[\alpha]_D^{25} = +64.2^\circ$ (C 0.5, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.55(d, *J*= 6.4Hz, 3H, CH₃), 2.99(dd, *J*₁=14.1Hz, *J*₂=6.5Hz, 1H, PhCH), 3.29(dd, *J*₁= 14.1Hz, *J*₂=7.6Hz, 1H, PhCH), 4.76 (m, 1H, CHNO₂), 7.03~7.05(m, 1H, aromatic H), 7.17(s, 1H, aromatic H), 7.21~7.26(m, 2H, aromatic H).

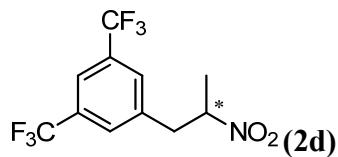
¹³C-NMR (CDCl₃, 100 MHz) δ: 18.9(CH₃), 40.6(CH₂), 84.0(CH), 127.2(CH), 127.7(CH), 129.1(CH), 130.1(CH), 134.6(C), 137.5(C).



$[\alpha]_D^{25} = +44.5^\circ$ (C 0.5, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.53 (d, *J*= 6.8Hz, 3H, CH₃), 2.96(dd, *J*₁=14.0Hz, *J*₂=6.8Hz, 1H, PhCH), 3.29(dd, *J*₁=14.0Hz, *J*₂=7.6Hz, 1H, PhCH), 3.78(s, 3H, OCH₃), 4.76(m, 1H, CHNO₂), 6.69(d, *J*=2.0Hz, 1H, aromatic H), 6.74(d, *J*=8.0Hz, 1H, aromatic H), 6.79(dd, *J*₁=8.0Hz, *J*₂=2.0Hz, 1H, aromatic H), 7.22(dd, *J*₁=*J*₂=8.0Hz, 1H, aromatic H);

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.8(CH₃), 41.2(CH₂), 55.2(CH₃), 84.3(CH), 112.7(CH), 114.8(CH), 121.3(CH), 129.8(C), 137.1(C), 159.9 (C).



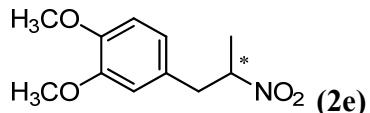
1-(2-nitropropyl)-3,5-bis(trifluoromethyl)benzene

[α]_D²⁵ = +31.7° (C 0.75, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.63(d, *J*= 6.8Hz, 3H, CH₃), 3.17(dd, *J*₁=14.4Hz, *J*₂=5.6Hz, 1H, Ph-CH), 3.46(dd, *J*₁=14.4Hz, *J*₂=8.4Hz, 1H, Ph-CH), 4.84(m, 1H, CHNO₂), 7.64(s, 2H, aromatic H), 7.81(s, 1H, aromatic H);

¹³C-NMR (CDCl₃, 100 MHz) δ: 19.1(CH₃), 40.3(CH₂), 83.6(CH), 121.7(m, CH), 123.1(q, *J*_{CF}=271Hz, 2×CF₃), 129.2(m, 2×CH), 132.3(q, *J*_{CF}=33Hz, 2×C), 138.1(C).

¹⁹F-NMR (CDCl₃, 376.5 MHz) δ: -63.0.

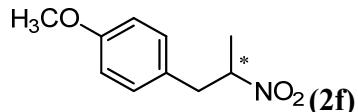


1,2-dimethoxy-4-(2-nitropropyl)benzene

[α]_D²⁵ = +56.2° (C 0.3, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.54(d, *J*= 6.4Hz, 3H, CH₃), 2.95(dd, *J*₁=14.0Hz, *J*₂=6.8Hz, 1H, PhCH), 3.26(dd, *J*₁=14.0Hz, *J*₂=7.6Hz, 1H, PhCH), 3.85(s, 3H, OCH₃), 3.86(s, 3H, OCH₃), 4.75(m, 1H, CHNO₂), 6.66(d, *J*=2.0Hz, 1H, aromatic H), 6.71(dd, *J*₁=8.0Hz, *J*₂=2.0Hz, 1H, aromatic H), 6.80(d, *J*=8.0Hz, 1H, aromatic H).

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.8(CH₃), 40.9(CH₂), 55.90(CH₃), 55.91(CH₃), 84.6(CH), 111.5(CH), 112.1(CH), 121.2(CH), 128.0(C), 148.5(C), 149.2 (C).

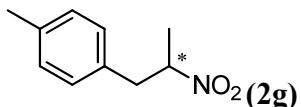


1-methoxy-4-(2-nitropropyl)benzene

$[\alpha]_D^{25} = +52.5^\circ$ (C 0.5, CHCl_3).

$^1\text{H-NMR}$ (CDCl_3 , 400 MHz) δ : 1.53(d, $J= 6.4\text{Hz}$, 3H, CH_3), 2.96(dd, $J_1=14.0\text{Hz}, J_2=6.4\text{Hz}$, 1H, PhCH), 3.26(dd, $J_1=14.0\text{Hz}, J_2=7.2\text{Hz}$, 1H, PhCH), 3.78(s, 3H, OCH_3), 4.74(m, 1H, CHNO_2), 6.85(d, $J=8.4\text{Hz}$, 2H, aromatic H), 7.07(d, $J=8.4\text{Hz}$, 2H, aromatic H).

$^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz) δ : 18.7(CH_3), 40.4(CH_2), 55.2(CH_3), 84.6(CH), 114.2(2 \times CH), 130.1(2 \times CH), 127.5(C), 158.9(C).

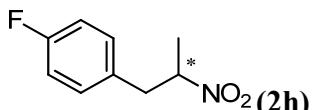


1-methyl-4-(2-nitropropyl)benzene

$[\alpha]_D^{25} = +20.6^\circ$ (C 0.45, CHCl_3).

$^1\text{H-NMR}$ (CDCl_3 , 400 MHz) δ : 1.52(d, $J= 6.4\text{Hz}$, 3H, CH_3), 2.31(s, 3H, PhCH_3) 2.96(dd, $J_1=14.0\text{Hz}, J_2=6.8\text{Hz}$, 1H, PhCH), 3.27(dd, $J_1=14.0\text{Hz}, J_2=7.2\text{Hz}$, 1H, PhCH), 4.75 (m, 1H, CHNO_2), 7.03(d, $J=8.0\text{Hz}$, 2H, aromatic H), 7.11(d, $J=8.0\text{Hz}$, 2H, aromatic H).

$^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz) δ : 18.7(CH_3), 21.0(CH_3), 40.8(CH_2), 84.6(CH), 128.9(2 \times CH), 129.5 (2 \times CH), 132.5(C), 137.1(C).



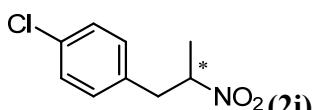
1-fluoro-4-(2-nitropropyl)benzene

$[\alpha]_D^{25} = +37.7^\circ$ (C 0.45, CHCl_3).

$^1\text{H-NMR}$ (CDCl_3 , 400 MHz) δ : 1.55(d, $J= 6.4\text{Hz}$, 3H, CH_3), 3.01(dd, $J_1=14.0\text{Hz}, J_2=6.4\text{Hz}$, 1H, PhCH), 3.28(dd, $J_1=14.0\text{Hz}, J_2=8.0\text{Hz}$, 1H, PhCH), 4.74(m, 1H, CHNO_2), 6.98~7.03(m, 2H, aromatic H), 7.11~7.15(m, 2H, aromatic H).

$^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz) δ : 18.8(CH_3), 40.3(CH_2), 84.4(CH), 115.7(d, $J_{\text{CF}}=21\text{Hz}$, 2 \times CH), 130.5(d, $J_{\text{CF}}=8\text{Hz}$, 2 \times CH), 131.2(d, $J_{\text{CF}}=3\text{Hz}$, C), 162.5(d, $J_{\text{CF}}=245\text{Hz}$, C).

$^{19}\text{F-NMR}$ (CDCl_3 , 376.5 MHz) δ : -115.0.

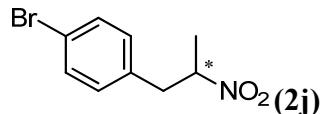


1-chloro-4-(2-nitropropyl)benzene

$[\alpha]_D^{25} = +57.4^\circ$ (C 0.5, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.55(d, $J= 6.8\text{Hz}$, 3H, CH₃), 2.99(dd, $J_1=14.0\text{Hz}, J_2=6.4\text{Hz}$, 1H, PhCH), 3.28(dd, $J_1=14.0\text{Hz}, J_2=7.6\text{Hz}$, 1H, PhCH), 4.74(m, 1H, CHNO₂), 7.09(d, $J_1=8.4\text{Hz}$, 2H, aromatic H), 7.27~7.30(m, 2H, aromatic H).

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.8(CH₃), 40.4(CH₂), 84.2(CH), 129.0(2×CH), 130.3(2×CH), 133.5(C), 133.9(C).

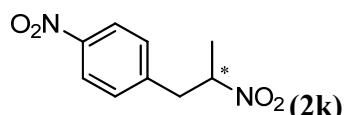


1-bromo-4-(2-nitropropyl)benzene

$[\alpha]_D^{25} = +87.2^\circ$ (C 0.6, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.55(d, $J= 7.2\text{Hz}$, 3H, CH₃), 2.98(dd, $J_1=14.0\text{Hz}, J_2=6.4\text{Hz}$, 1H, PhCH), 3.26(dd, $J_1=14.0\text{Hz}, J_2=8.0\text{Hz}$, 1H, PhCH), 4.75 (m, 1H, CHNO₂), 7.03(d, $J=8.0\text{Hz}$, 2H, aromatic H), 7.43(d, $J=8.0\text{Hz}$, 2H, aromatic H).

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.8(CH₃), 40.5(CH₂), 84.1(CH), 121.5(C), 130.6 (2×CH), 131.9 (2×CH), 134.5(C).

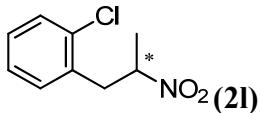


1-nitro-4-(2-nitropropyl)benzene

$[\alpha]_D^{25} = +30.5^\circ$ (C 0.27, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.61(d, $J= 6.4\text{Hz}$, 3H, CH₃), 3.15(dd, $J_1=14.0\text{Hz}, J_2=6.0\text{Hz}$, 1H, PhCH), 3.42(dd, $J_1=14.0\text{Hz}, J_2=8.4\text{Hz}$, 1H, PhCH), 4.84 (m, 1H, CHNO₂), 7.35(d, $J=8.8\text{Hz}$, 2H, aromatic H), 8.17(d, $J=8.8\text{Hz}$, 2H, aromatic H).

¹³C-NMR (CDCl₃, 100 MHz) δ: 19.1(CH₃), 40.6(CH₂), 83.7(CH), 124.1 (2×CH), 129.9 (2×CH), 142.9(C), 147.4(C).

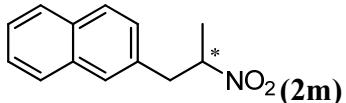


1-chloro-2-(2-nitropropyl)benzene

$[\alpha]_D^{25} = -8.1^\circ$ (C 0.1, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.59(d, *J*= 6.8Hz, 3H, CH₃), 3.19(dd, *J*₁=14.0Hz, *J*₂=6.0Hz, 1H, PhCH), 3.40(dd, *J*₁=14.0Hz, *J*₂=7.6Hz, 1H, PhCH), 4.92 (m, 1H, CHNO₂), 7.16~7.25(m, 3H, aromatic *H*), 7.37~7.39(m, 1H, aromatic *H*).

¹³C-NMR (CDCl₃, 100 MHz) δ: 19.1(CH₃), 38.9(CH₂), 82.7(CH), 127.2(CH), 129.1(CH), 129.8(CH), 131.4(CH), 133.5(C), 134.1(C).

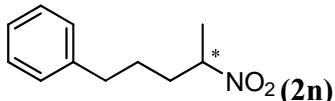


2-(2-nitropropyl)naphthalene

$[\alpha]_D^{25} = +51.6^\circ$ (C 0.5, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.56 (d, *J*= 6.8Hz, 3H, CH₃), 3.15(dd, *J*₁=14.0Hz, *J*₂=6.8Hz, 1H, PhCH), 3.48(dd, *J*₁=14.0Hz, *J*₂=7.6Hz, 1H, PhCH), 4.86(m, 1H, CHNO₂), 7.27(dd, *J*₁=8.4Hz, *J*₂=1.6Hz, 1H, aromatic *H*), 7.44~7.49(m, 2H, aromatic *H*), 7.61(s, 1H, aromatic *H*), 7.77~7.82(m, 3H, aromatic *H*);

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.9(CH₃), 41.3(CH₂), 84.4(CH), 126.1(CH), 126.4(CH), 126.8(CH), 127.6(CH), 127.7(CH), 127.9(CH), 128.6(CH), 132.6(C), 132.9(C), 133.5(C).

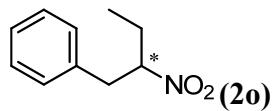


(4-nitropentyl)benzene

$[\alpha]_D^{25} = +20.8^\circ$ (C 0.22, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.50(d, *J*= 6.8Hz, 3H, CH₃), 1.62~1.69(m, 2H, PhCH₂CH₂), 1.75(m, 1H, PhCH₂CH₂CH), 2.02(m, 1H, PhCH₂CH₂CH), 2.64(t, *J*=7.6Hz, PhCH₂), 4.56(m, 1H, CHNO₂), 7.13~7.21(m, 3H, aromatic *H*), 7.26~7.29(m, 2H, aromatic *H*);

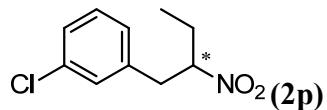
¹³C-NMR (CDCl₃, 100 MHz) δ: 19.2(CH₃), 27.3(CH₂), 34.6(CH₂), 35.1(CH₂), 83.4(CH), 126.1(CH), 128.3(2×CH), 128.5(2×CH), 141.1(C).



[α]_D²⁵ = +24.5° (C 0.22, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 0.91(t, *J*= 7.2Hz, 3H, CH₃), 1.76(m, 1H, CH₃CH), 1.95(m, 1H, CH₃CH), 2.95(dd, *J*₁=14.0Hz, *J*₂=6.0Hz, 1H, Ph-CH), 3.18(dd, *J*₁=14.0Hz, *J*₂=8.4Hz, 1H, Ph-CH), 4.55(m, 1H, CHNO₂), 7.07~7.09(m, 2H, aromatic H), 7.15~7.25(m, 3H, aromatic H);

¹³C-NMR (CDCl₃, 100 MHz) δ: 10.2(CH₃), 26.8(CH₂), 39.7(CH₂), 91.4(CH), 127.4(CH), 128.8(2×CH), 128.9(2×CH), 134.7(C).

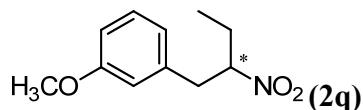


1-chloro-3-(2-nitrobutyl)benzene

[α]_D²⁵ = +84.1° (C 0.6, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 0.99(t, *J*= 6.8Hz, 3H, CH₃), 1.84(m, 1H, CH₃CH), 2.02(m, 1H, CH₃CH), 2.99(dd, *J*₁=14.0Hz, *J*₂=5.6Hz, 1H, Ph-CH), 3.23(dd, *J*₁=14.0Hz, *J*₂=8.8Hz, 1H, Ph-CH), 4.62(m, 1H, CHNO₂), 7.02~7.05(m, 1H, aromatic H), 7.16(s, 1H, aromatic H), 7.22~7.25(m, 2H, aromatic H);

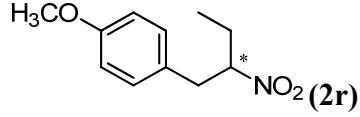
¹³C-NMR (CDCl₃, 100 MHz) δ: 10.2(CH₃), 26.9(CH₂), 39.2(CH₂), 90.9(CH), 127.1(CH), 127.7(CH), 129.0(CH), 130.1(CH), 134.6(C), 137.7(C).



1-methoxy-3-(2-nitrobutyl)benzene

[α]_D²⁵ = +47.6° (C 0.5, CHCl₃).

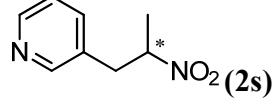
¹H-NMR (CDCl₃, 400 MHz) δ: 0.92(t, *J*= 7.2Hz, 3H, CH₃), 1.74(m, 1H, CH₃CH), 1.94(m, 1H, CH₃CH), 2.92(dd, *J*₁=14.0Hz, *J*₂=6.0Hz, 1H, Ph-CH), 3.17(dd, *J*₁=14.0Hz, *J*₂=8.4Hz, 1H, Ph-CH), 3.71(s, 3H, OCH₃), 4.56(m, 1H, CHNO₂), 6.62(dd, *J*₁=*J*₂=2.0Hz, 1H, aromatic H), 6.66(dd, *J*=7.6Hz, *J*₂=2.0Hz, 1H, aromatic H), 6.72(dd, *J*₁=8.0Hz, *J*₂=2.0Hz, 1H, aromatic H), 7.14(dd, *J*₁=8.0Hz, *J*₂=7.6Hz, 1H, aromatic H);
¹³C-NMR (CDCl₃, 100 MHz) δ: 10.2(CH₃), 26.8(CH₂), 39.7(CH₂), 55.2(OCH₃), 91.2(CH), 112.6(CH), 114.7(CH), 121.1(CH), 129.8(CH), 137.2(C), 159.9(C).



1-methoxy-4-(2-nitrobutyl)benzene

[α]_D²⁵ = +31.7° (C 0.5, CHCl₃).

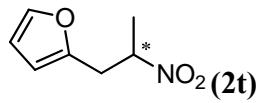
¹H-NMR (CDCl₃, 400 MHz) δ: 0.99(t, *J*= 7.2Hz, 3H, CH₃), 1.81(m, 1H, CH₃CH), 2.02(m, 1H, CH₃CH), 2.97(dd, *J*₁=14.4Hz, *J*₂=5.6Hz, 1H, Ph-CH), 3.19(dd, *J*₁=14.4Hz, *J*₂=8.4Hz, 1H, Ph-CH), 3.78(s, 3H, OCH₃), 4.59(m, 1H, CHNO₂), 6.84(d, *J*=8.4Hz, 2H, aromatic H), 7.07(d, *J*=8.4Hz, 2H, aromatic H);
¹³C-NMR (CDCl₃, 100 MHz) δ: 10.2(CH₃), 26.7(CH₂), 38.9(CH₂), 55.2(OCH₃), 91.6(CH), 114.2(2×CH), 129.9(2×CH), 127.7(C), 158.9(C).



3-(2-nitropropyl)pyridine

[α]_D²⁵ = -5.4° (C 0.1, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.64(d, *J*= 6.8Hz, 3H, CH₃), 3.14(dd, *J*₁=14.4Hz, *J*₂=5.2Hz, 1H, Pyridyl-CH), 3.48(dd, *J*₁=14.4Hz, *J*₂=8.8Hz, 1H, Pyridyl-CH), 4.82(m, 1H, CHNO₂), 7.49(dd, *J*₁=8.0Hz, *J*₂=5.6Hz, 1H, aromatic H), 7.75(d, *J*=8.0Hz, 1H, aromatic H), 8.50(s, 1H, aromatic H), 8.53(d, *J*=5.6Hz, 1H, aromatic H);
¹³C-NMR (CDCl₃, 100 MHz) δ: 19.2(CH₃), 37.5(CH₂), 83.2(CH), 125.5(CH), 133.9(C), 139.6(CH), 146.6(CH), 147.8(CH).

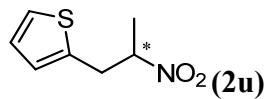


2-(2-nitropropyl)furan

$[\alpha]_D^{25} = +61.8^\circ$ (C 0.4, CHCl₃).

¹H-NMR (CDCl₃, 400 MHz) δ: 1.57(d, *J*= 6.4Hz, 3H, CH₃), 3.08(dd, *J*₁=15.2Hz, *J*₂=6.8Hz, 1H, Furyl-CH), 3.48(dd, *J*₁=15.2Hz, *J*₂=7.2Hz, 1H, Furyl-CH), 4.85(m, 1H, CHNO₂), 6.12(d, *J*=3.2Hz, 1H, aromatic H), 6.29(dd, *J*₁=3.2Hz, *J*₂=1.6Hz, 1H, aromatic H), 7.34(d, *J*=1.6Hz, 1H, aromatic H);

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.8(CH₃), 33.4(CH₂), 81.8(CH), 108.0(CH), 110.5(CH), 142.3(CH), 149.4(C).



2-(2-nitropropyl)thiophene

$[\alpha]_D^{25} = +79.6^\circ$ (C 0.42, CHCl₃).

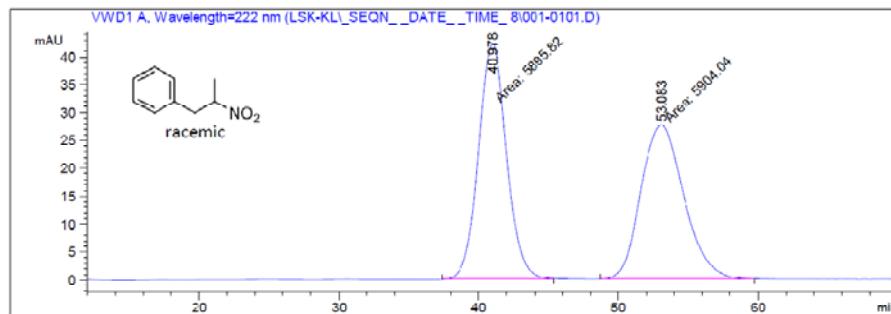
¹H-NMR (CDCl₃, 400 MHz) δ: 1.59(d, *J*= 6.4Hz, 3H, CH₃), 3.25(dd, *J*₁=15.2Hz, *J*₂=6.4Hz, 1H, Thienyl-CH), 3.54(dd, *J*₁=15.2Hz, *J*₂=7.6Hz, 1H, Thienyl-CH), 4.85(m, 1H, CHNO₂), 6.85(dd, *J*₁=3.2Hz, *J*₂=0.8Hz, 1H, aromatic H), 6.94(dd, *J*₁=5.6Hz, *J*₂=3.2Hz, 1H, aromatic H), 7.20(dd, *J*₁=5.6Hz, *J*₂=0.8Hz, 1H, aromatic H);

¹³C-NMR (CDCl₃, 100 MHz) δ: 18.7(CH₃), 35.0(CH₂), 84.2(CH), 125.0(CH), 126.8(CH), 127.2(CH), 137.1(C).

5 References

- [1] (a) A. Fryszkowska, K. Fisher, J. M. Gardiner and G. M. Stephens, *J. Org. Chem.* , 2008, 73, 4295–4298; (b) Y. Kawai, Y. Inab and N. Tokitoh, *Tetrahedron: Asymmetry* , 2001, 12, 309-318.
- [2] A. Bhattacharjya, R. Mukhopadhyay and S. C. Pakrashi, *Synthesis*, 1985, 886-887.
- [3] (a) S. Li, K. Huang, B. Cao, J. Zhang, W. Wu and X. Zhang, *Angew. Chem. Int. Ed.* , 2012, 51, 8573-8576; (b) S. Li, K. Huang, J. Zhang, W. Wu and X. Zhang, *Chem. Eur. J.* , 2013, 19, 10840 -10844.
- [4] (a) J. Xiang, E.-X. Sun, C.-X. Lian, W.-C. Yuan, J. Zhu, Q. Wang and J. Deng, *Tetrahedron*, 2012, 68, 4609-4620; (b) E. Burda, T. Reß, T. Winkler, C. Giese, X. Kostrov, T. Huber, W. Hummel and H. Gręger, *Angew. Chem. Int. Ed.* , 2013, 52, 9323 -9326; (c) R. R. Bak, A. F. McAnda, A. J. Smallridge and M. A. Trewhella, *Australian Journal of Chemistry*, 1996, 49, 1257-1260; (d) Y. Yanto, C. K. Winkler, S. Lohr, M. Hall, K. Faber and A. S. Bommarius, *Org. Lett.*, 2011, 13, 2540-2543.

6 Representative HPLC traces

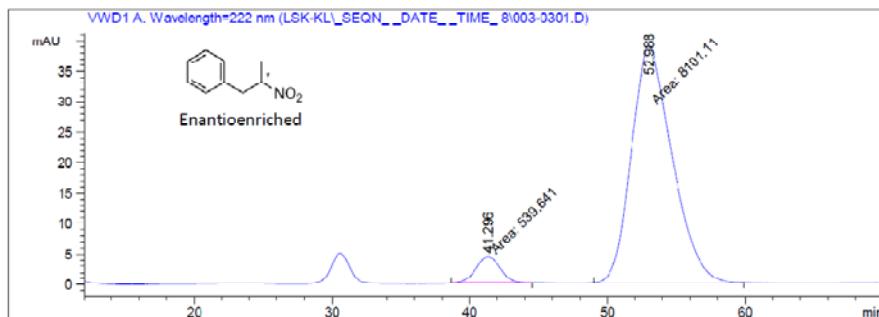


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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	40.978	MM	2.3364	5895.81641		42.05685	49.9651
2	53.083	MM	3.5690	5904.04248		27.57126	50.0349

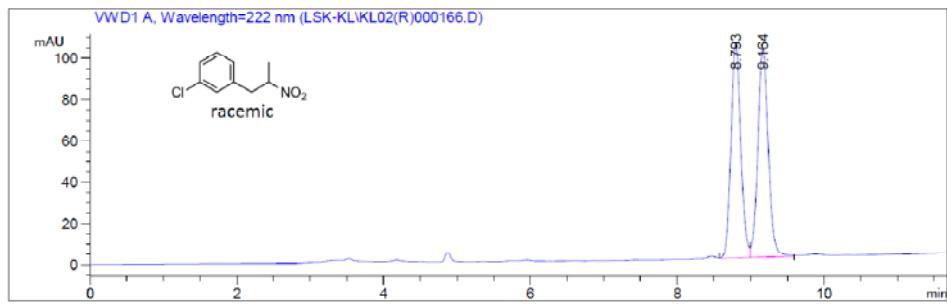


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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	41.296	MM	2.0825	539.64117		4.31888	6.2453
2	52.988	MM	3.4493	8101.11377		39.14381	93.7547

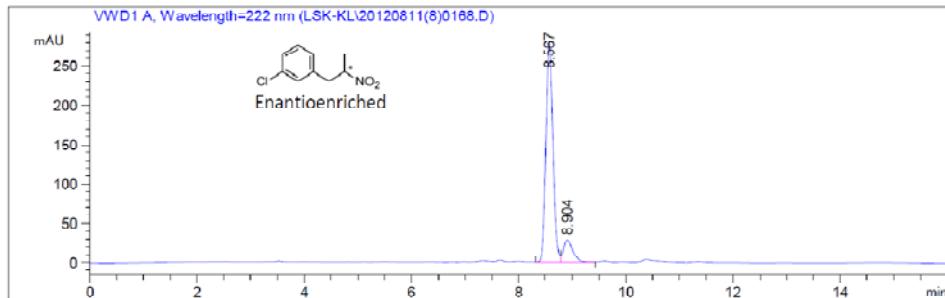


Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	8.793	VV	0.1437	965.58356	103.55462	49.0421	
2	9.164	VB	0.1524	1003.30518	100.87052	50.9579	

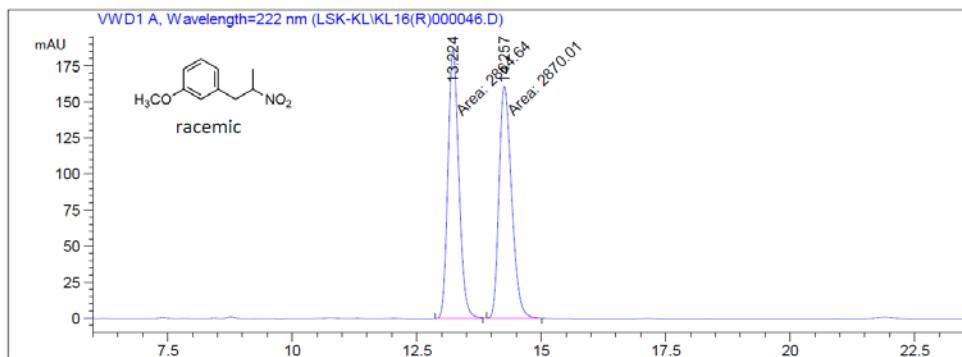


Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	8.567	VV	0.1437	2566.23975	279.01001	87.4688	
2	8.904	VV	0.1793	367.65329	29.40752	12.5312	

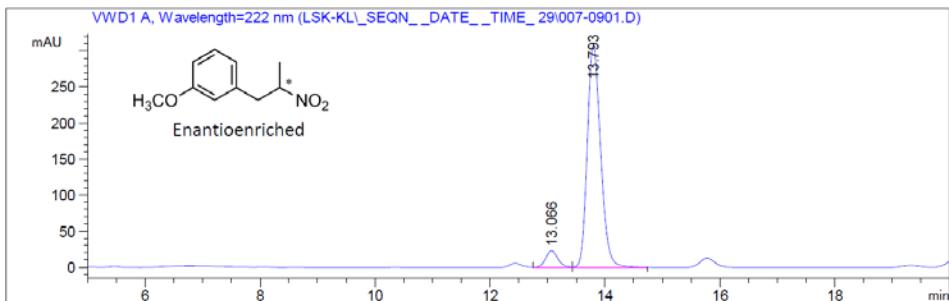


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	13.224	MM	0.2556	2864.64	380	186.77107	49.9532
2	14.257	MM	0.2960	2870.01	074	161.58247	50.0468

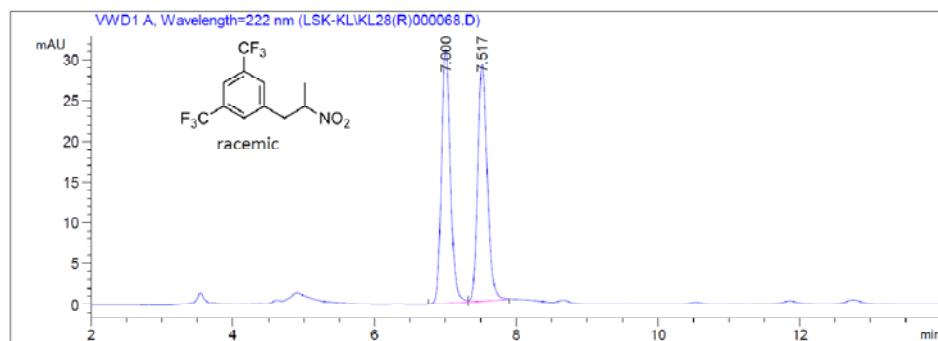


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	13.066	VV	0.2231	333.04150	22.96572	6.3028	
2	13.793	VB	0.2501	4950.98584	308.06375	93.6972	

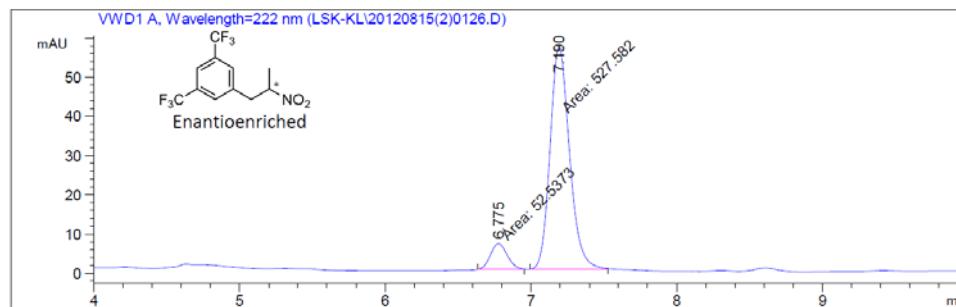


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	%
1	7.000	BV	0.1337	271.79367	31.20340	50.0781	
2	7.517	VB	0.1434	270.94540	29.15437	49.9219	

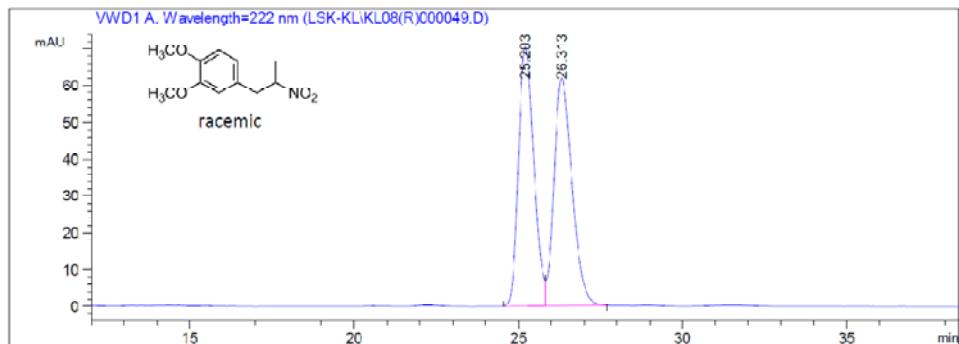


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	%
1	6.775	MM	0.1329	52.53727	6.58839	9.0563	
2	7.190	MM	0.1549	527.58179	56.75214	90.9437	

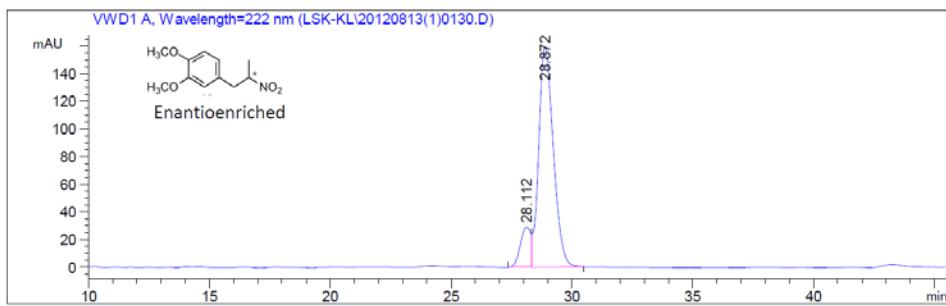


Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	25.203	BV	0.5101	2308.92651	70.51905	49.2855	
2	26.313	VB	0.5918	2375.86816	61.91747	50.7145	

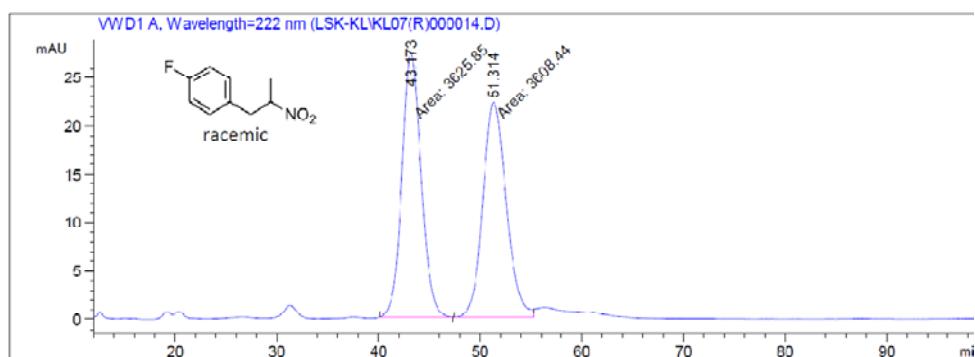


Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	28.112	BV	0.4649	875.57520	29.07660	11.5820	
2	28.872	VB	0.6447	6684.24219	159.51347	88.4180	

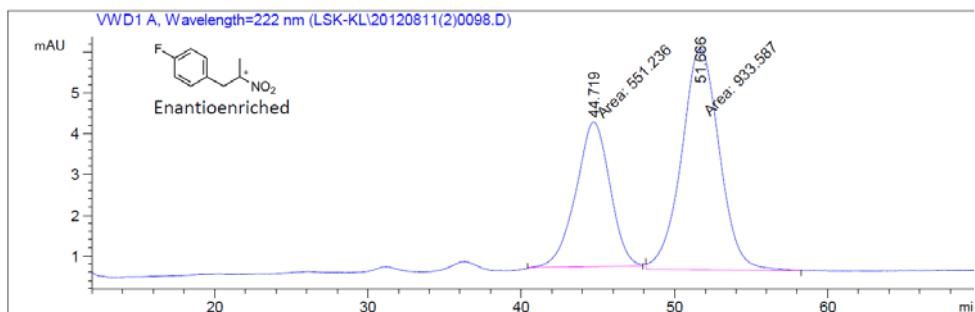


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	%
1	43.173	MM	2.2105	3625.85449	27.33820	50.1204	
2	51.314	MM	2.7046	3608.44141	22.23676	49.8796	

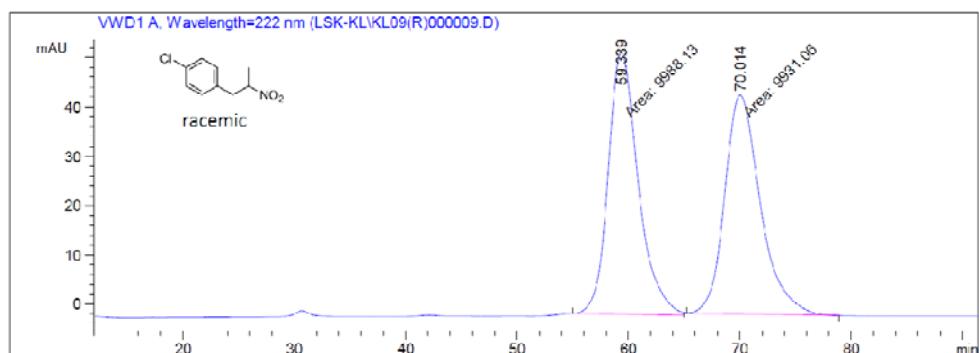


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	%
1	44.719	MM	2.5830	551.23560	3.55684	37.1247	
2	51.666	MM	2.8643	933.58698	5.43223	62.8753	

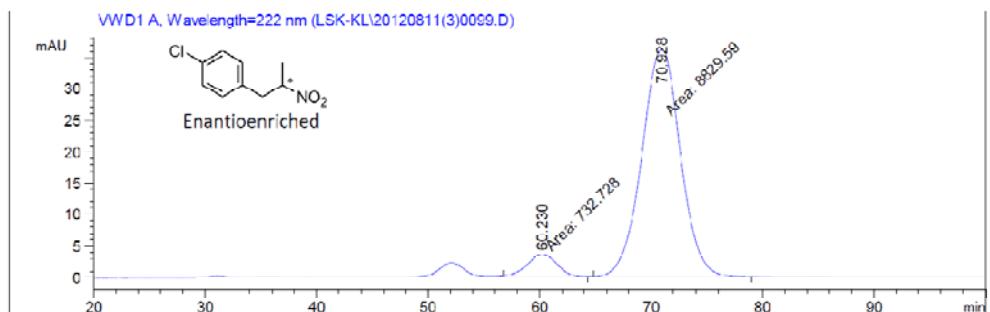


Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	59.339	MM	3.1346	9900.13104	53.10644	50.1403	
2	70.014	MM	3.7303	9931.05957	44.37114	49.8567	

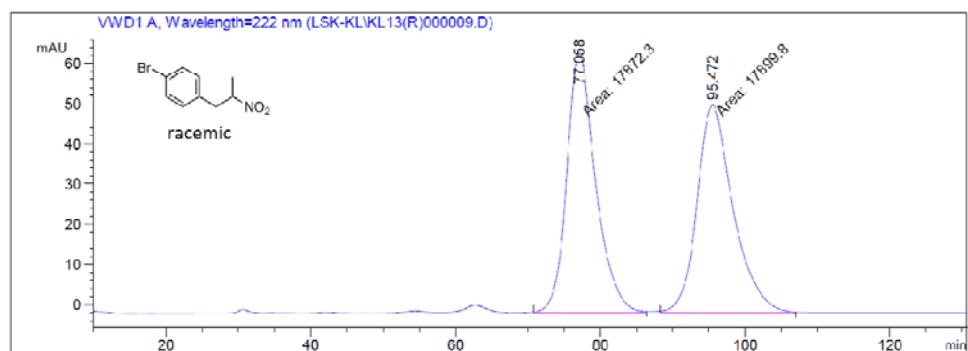


Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	60.230	MM	3.3304	732.72821	3.66685	7.6627	
2	70.928	MM	4.0432	8829.58887	36.39711	92.3373	

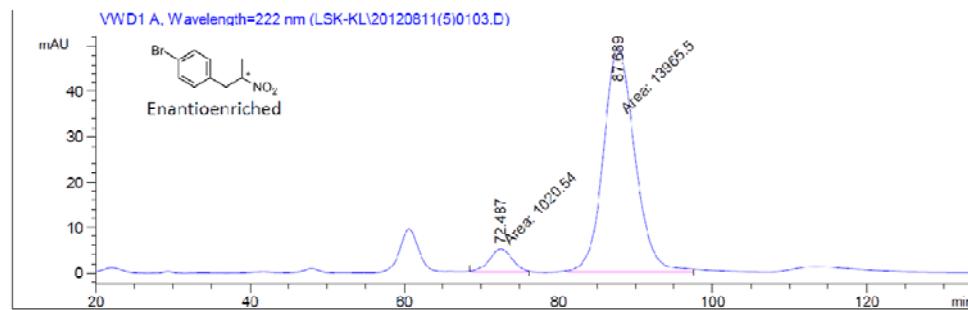


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with TSTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	77.058	MM	4.5957	1.7872e4		64.81572	49.9615
2	95.472	MM	5.7768	1.7699e4		51.64314	50.0385

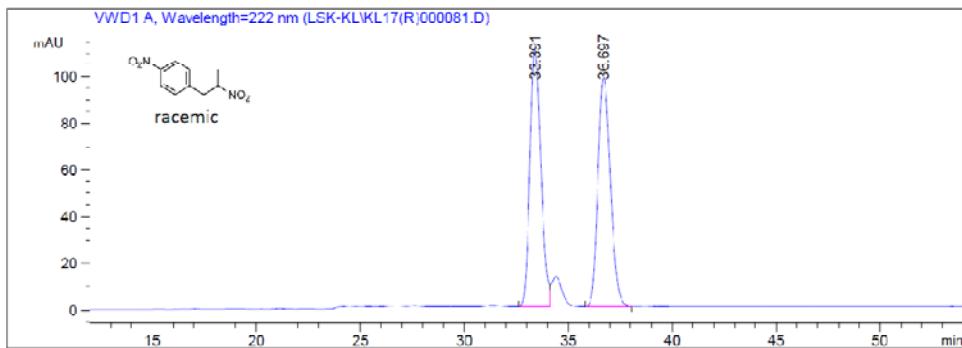


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	72.487	MM	3.3687	1.02053760		5.04909	6.8099
2	87.689	MM	4.7021	1.39655e4		49.50137	93.1901

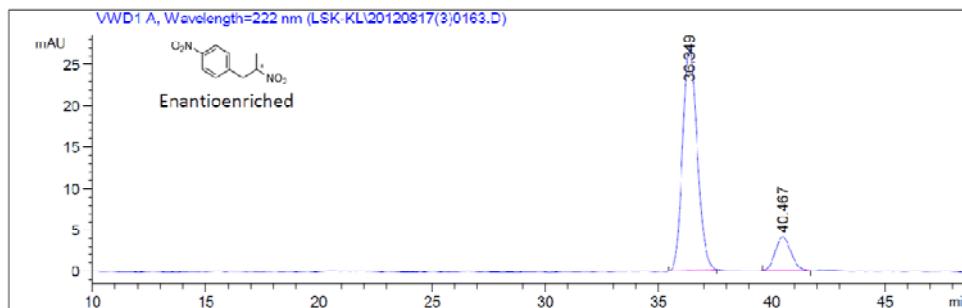


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

#	RetTime	Type	Width	Area	Height	Area %
	[min]		[min]	[mAU]	[mAU]	%
1	33.391	BV	0.5761	4102.07129	111.15654	49.9969
2	36.697	BB	0.6533	4102.57061	98.21953	50.0031

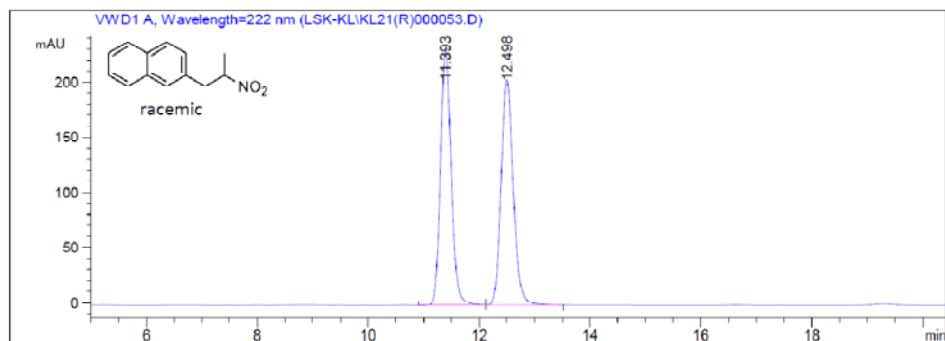


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

#	RetTime	Type	Width	Area	Height	Area %
	[min]		[min]	[mAU]	[mAU]	%
1	36.349	BB	0.7021	1219.45569	27.12606	85.7866
2	40.467	BB	0.7230	202.04327	4.15597	14.2134

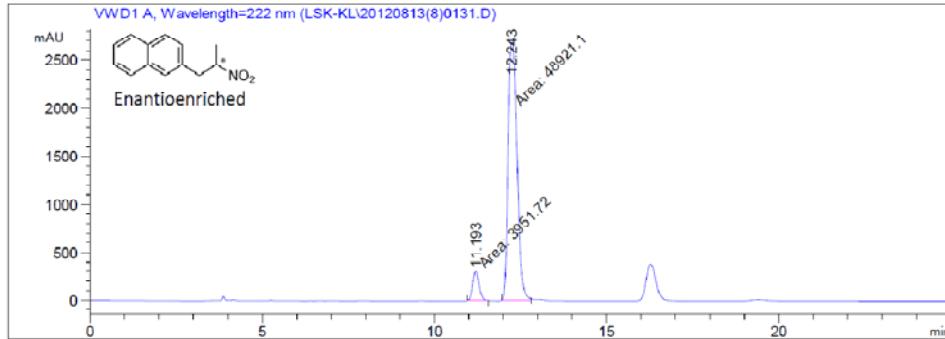


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	11.393	VV	0.2065	3135.80076	233.04440	49.9651	
2	12.490	VB	0.2359	3140.17627	204.50464	50.0349	

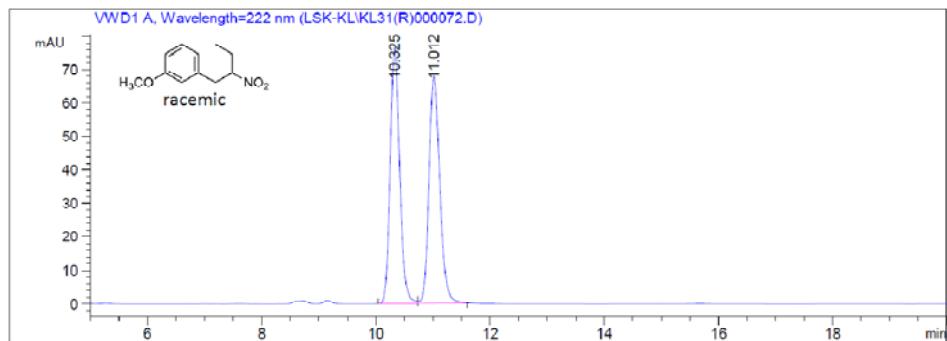


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Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	11.193	MM	0.2159	3951.72144	305.11908	7.4740	
2	12.243	MM	0.3031	4.89211e4	2689.92993	92.5260	

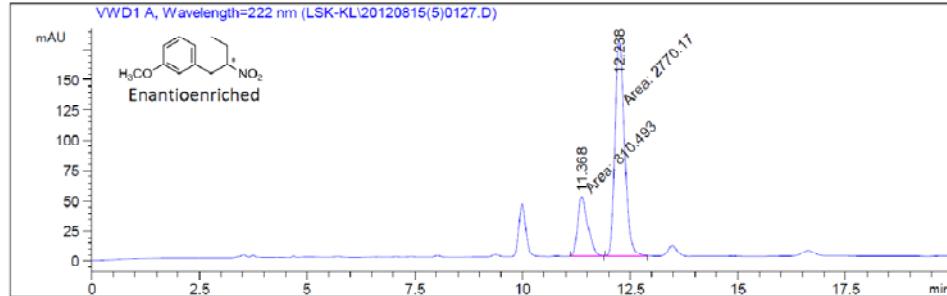


Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	10.325	BV	0.1791	888.96930	76.60941	49.9515	
2	11.012	VB	0.2013	890.69470	67.81270	50.0485	

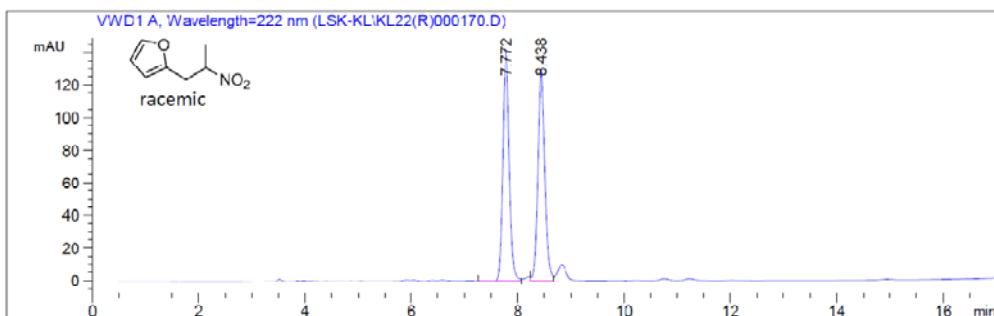


Area Percent Report

Sorted By : Signal
 Multipliqr : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	11.368	MM	0.2728	810.49298	49.52109	22.6352	
2	12.238	MM	0.2586	2770.17456	178.54398	77.3648	

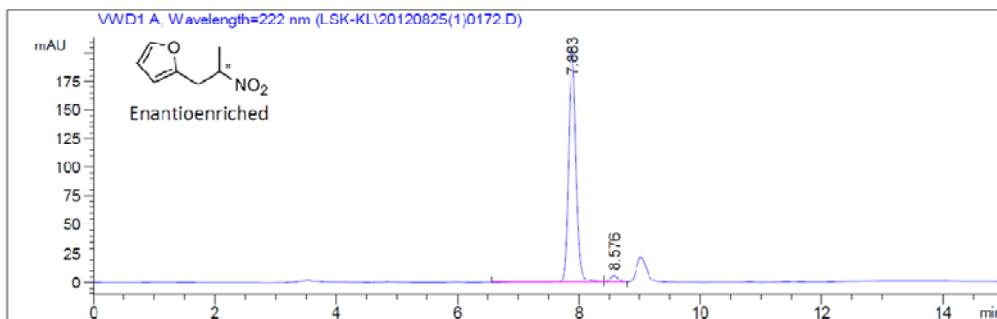


Area Percent Report
=====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with TSTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.772	VV	0.1296	1187.38208		142.02644	50.0095
2	8.438	VV	0.1412	1186.93323		130.36206	49.9905

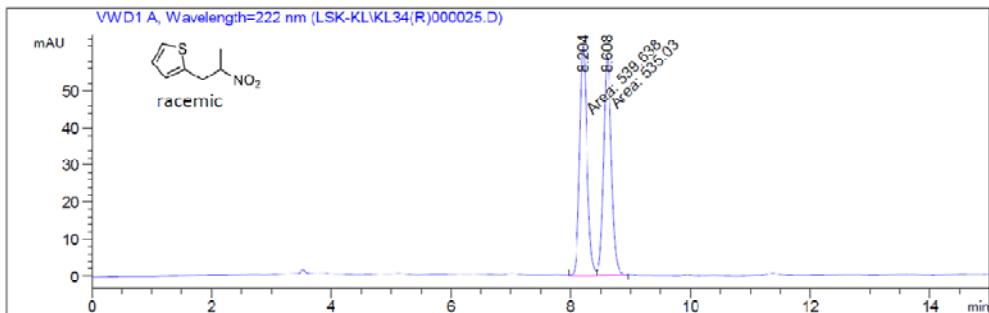


Area Percent Report
=====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	7.883	VV	0.1308	1750.20386		203.78961	96.7969
2	8.576	VV	0.1487	57.91647		5.886507	3.2031

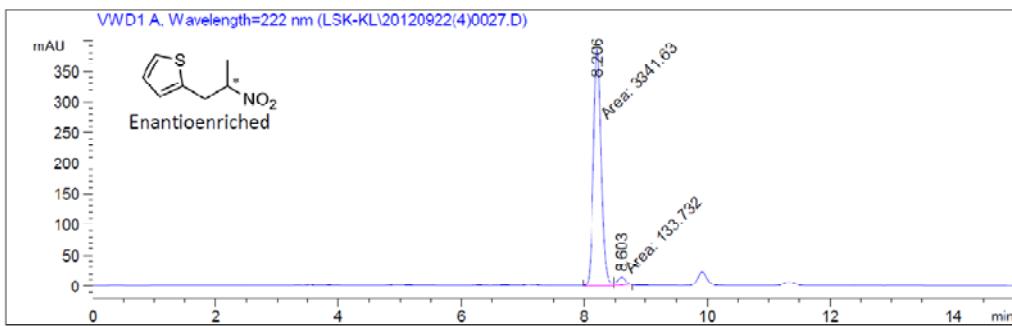


Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	8.204	MM	0.1448	539.63837	62.10995	50.2144	
2	8.608	MM	0.1514	535.02985	58.90245	49.7856	

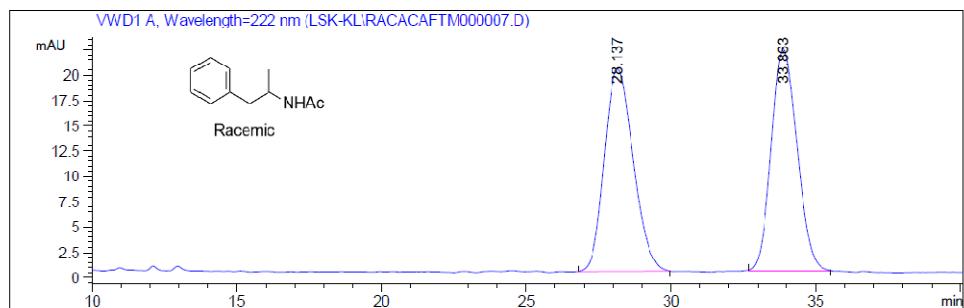


Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	8.206	MM	0.1446	3341.62720	385.06290	96.1520	
2	8.603	MM	0.1563	133.73155	14.26393	3.8480	

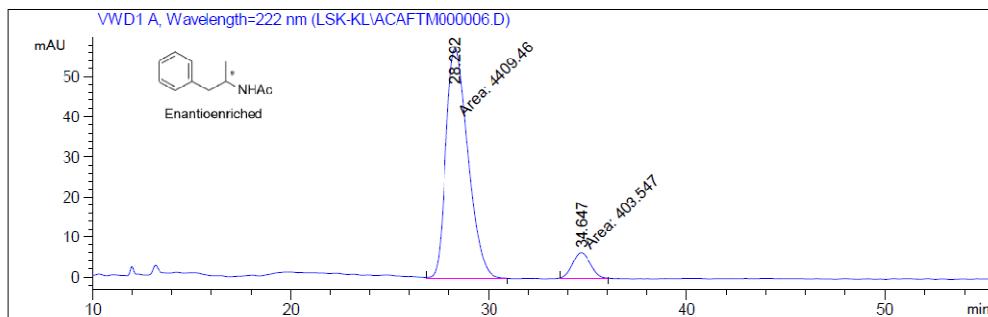


=====
Area Percent Report
=====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with TSTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	28.137	BB	1.0806	1393.45105		20.07576	50.5255
2	33.863	BB	0.9618	1364.46399		21.97265	49.4745

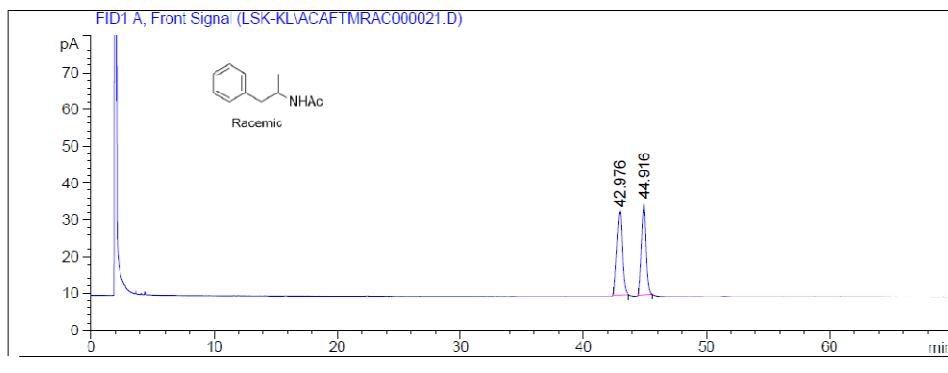


=====
Area Percent Report
=====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=222 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	28.292	MM	1.2821	4409.45898		57.32087	91.6155
2	34.647	MM	1.0602	403.54724		6.34377	8.3845

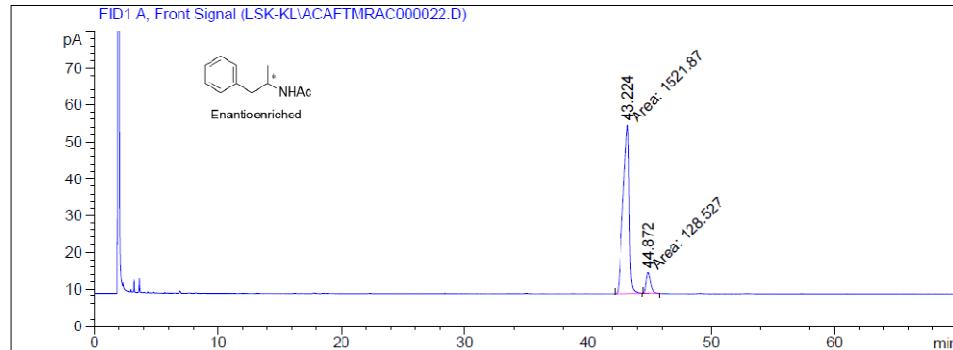


```
=====
Area Percent Report
=====
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ μ l] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	42.976	BB	0.3391	656.50165	22.85561	50.09132
2	44.916	BB	0.3090	654.10791	24.89106	49.90868



```
=====
Area Percent Report
=====
```

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ μ l] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A, Front Signal

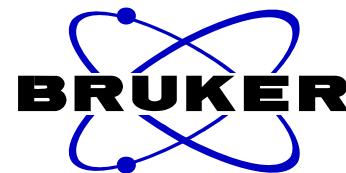
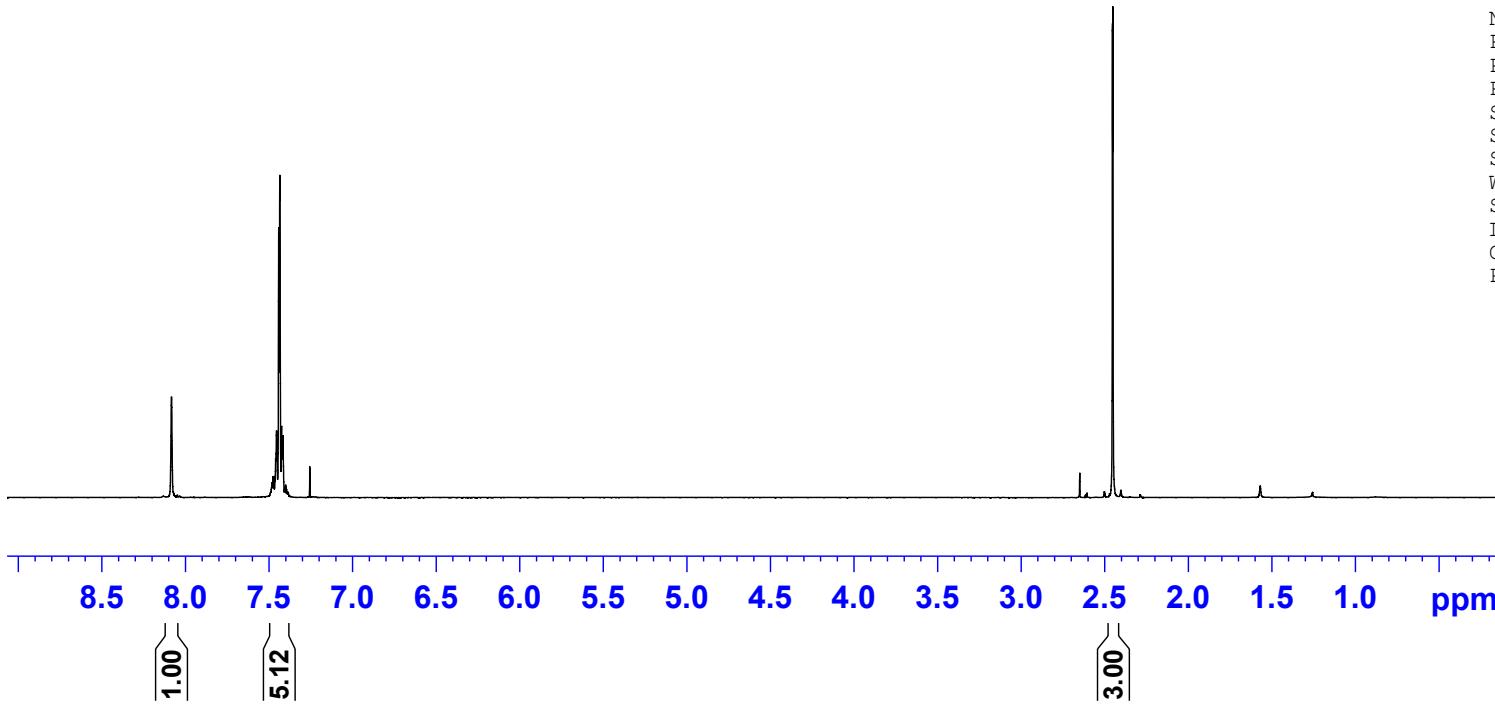
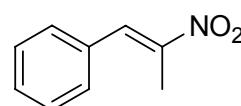
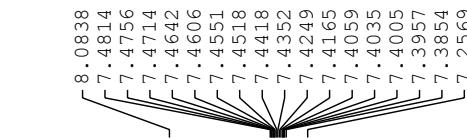
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	43.224	MM	0.5570	1521.86682	45.53423	92.21236
2	44.872	MM	0.3945	128.52672	5.42969	7.78764

7 NMR spectra

7.1 NMR spectra of α,β -Disubstituted Nitroalkenes

7.2 NMR spectra of α -chiral nitroalkanes

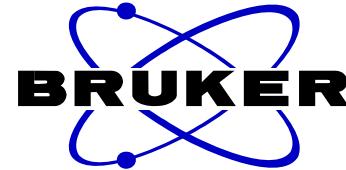
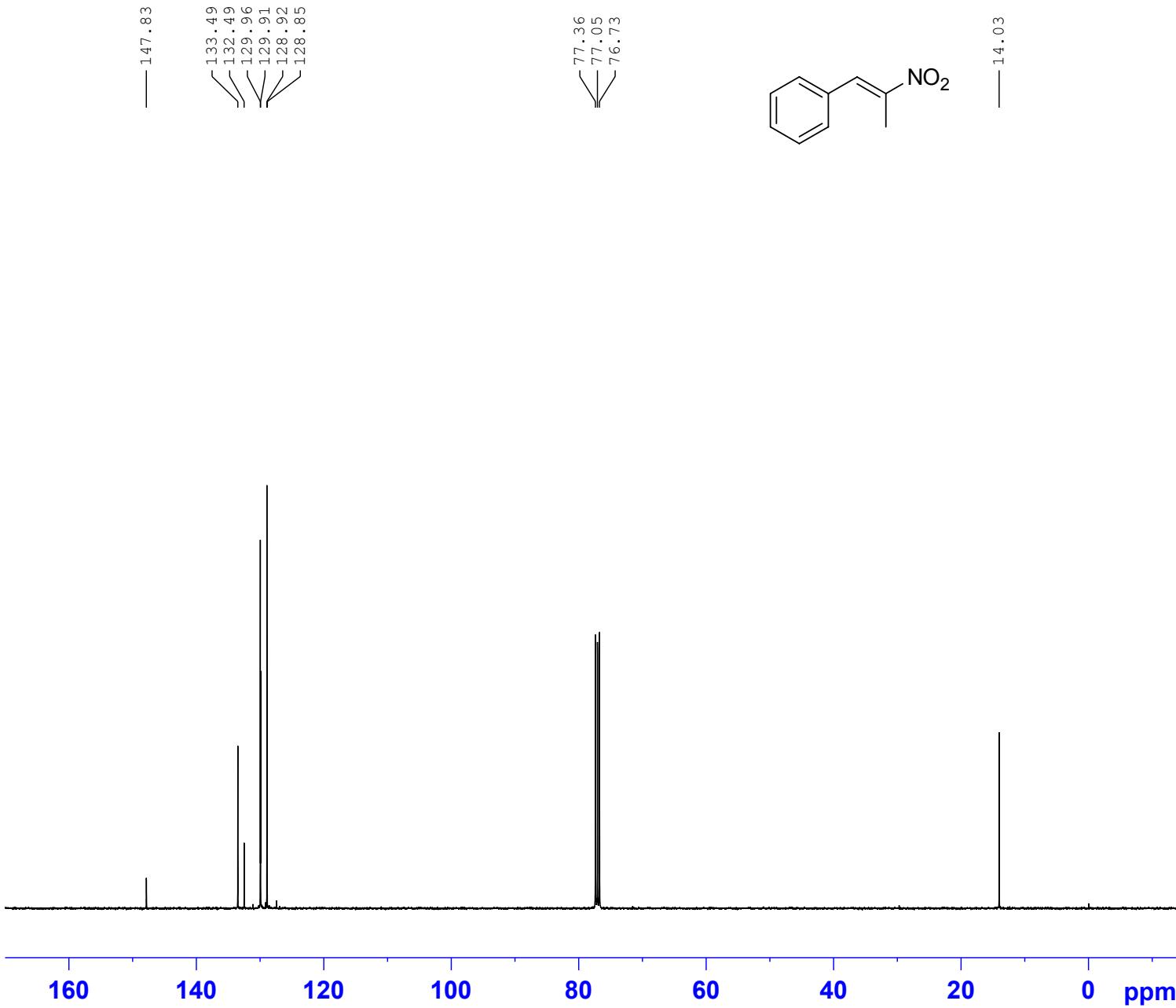
KL01
PROTON CDC13 {E:\NMR Data} skl 28



NAME Jun23-2011
EXPNO 6
PROCNO 1
Date_ 20110623
Time 17.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 302.3 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL01
C13CPD CDC13 {E:\NMR Data} skl 28



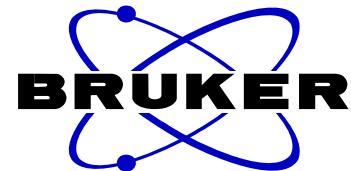
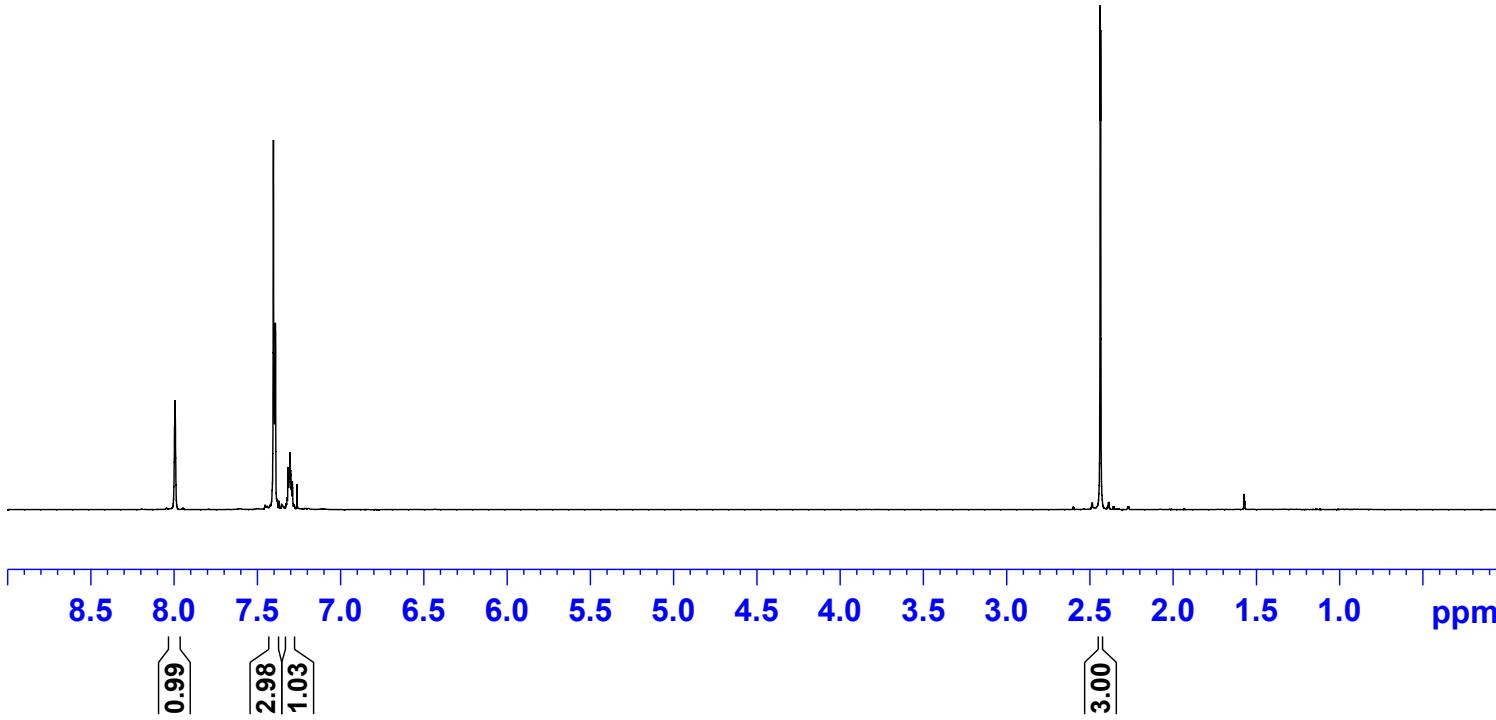
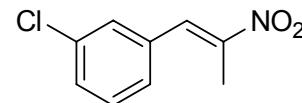
NAME Jun23-2011
EXPNO 7
PROCNO 1
Date_ 20110623
Time 20.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 304.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127664 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL02
PROTON CDCl₃ {E:\NMR Data} skl 28

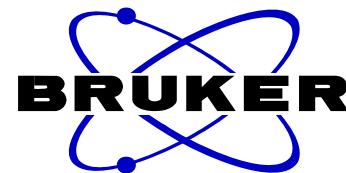
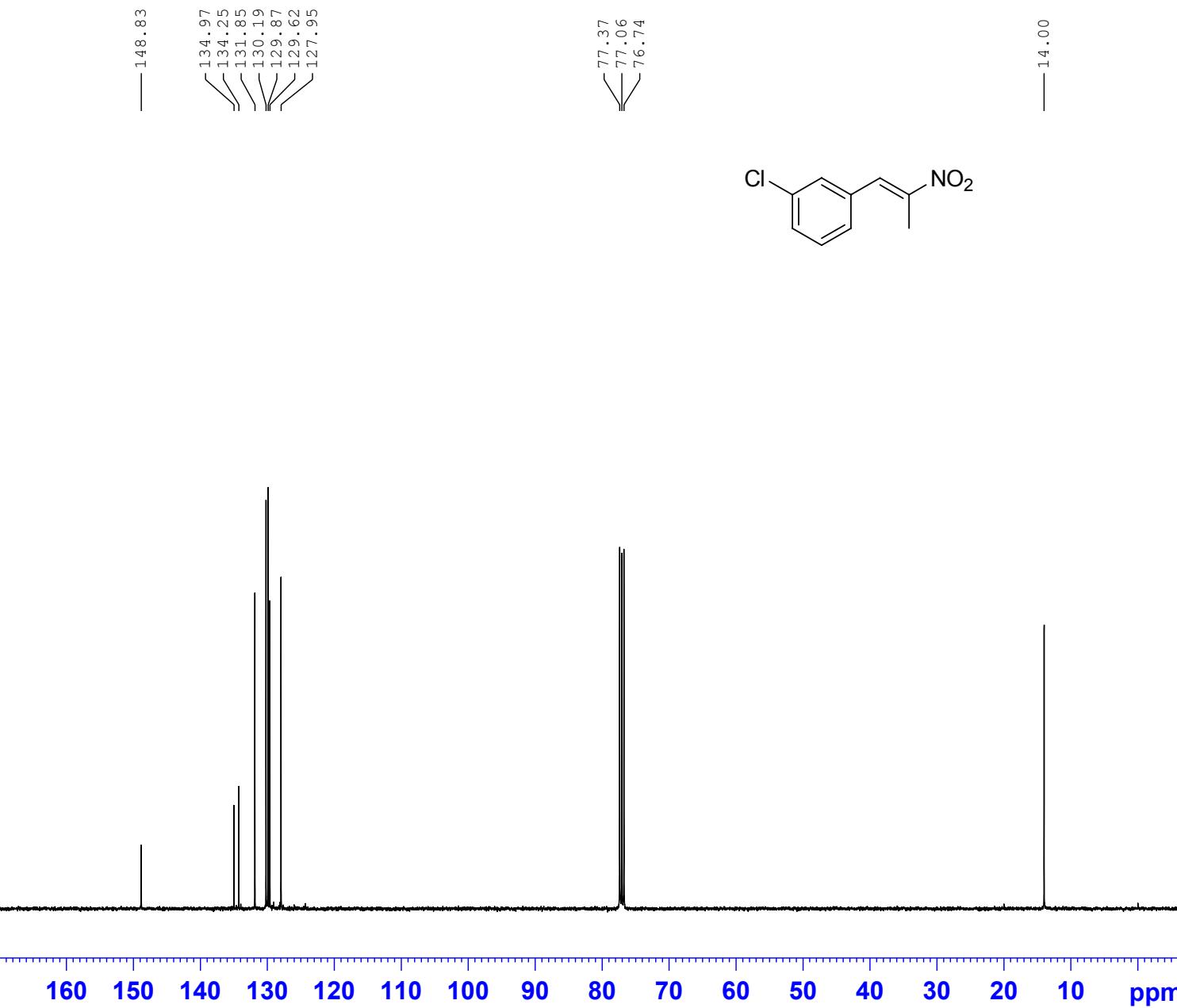
7.9955
7.4042
7.3996
7.3949
7.3918
7.3155
7.3119
7.3048
7.3009
7.2991
7.2952
7.2900
7.2622



NAME Jun29-2011
EXPNO 5
PROCNO 1
Date_ 20110629
Time 18.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 302.4 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL02
C13CPD CDC13 {E:\NMR Data} skl 28



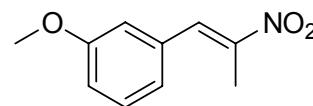
NAME Jun29-2011
EXPNO 6
PROCNO 1
Date_ 20110701
Time_ 5.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

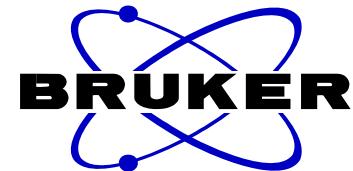
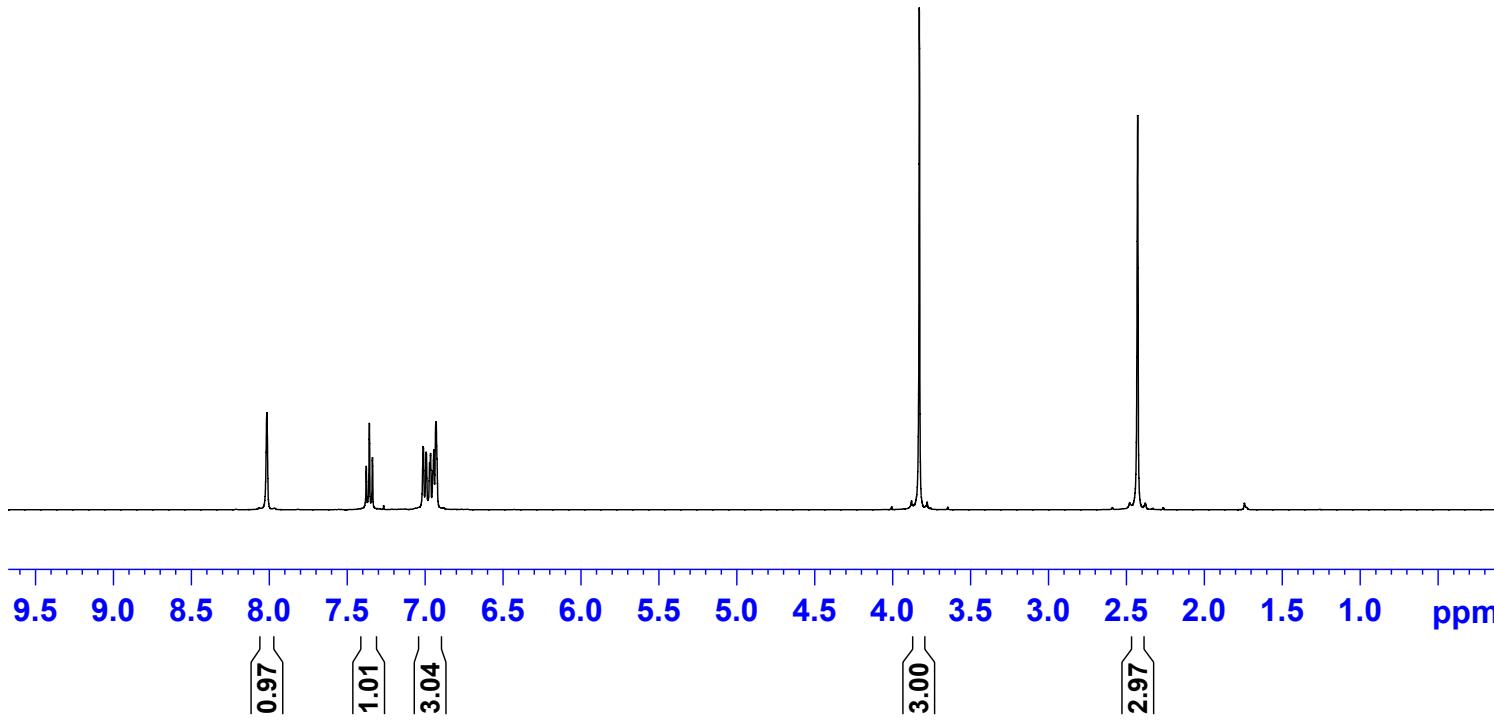
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127661 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL16
PROTON CDCl₃ {E:\NMR Data} skl 28

8.0151
7.3771
7.3574
7.3375
7.3375
7.2660
7.0120
6.9929
6.9707
6.9647
6.9498
6.9441
6.9292



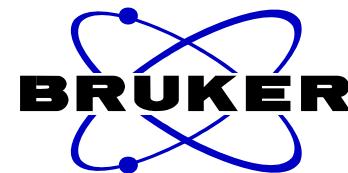
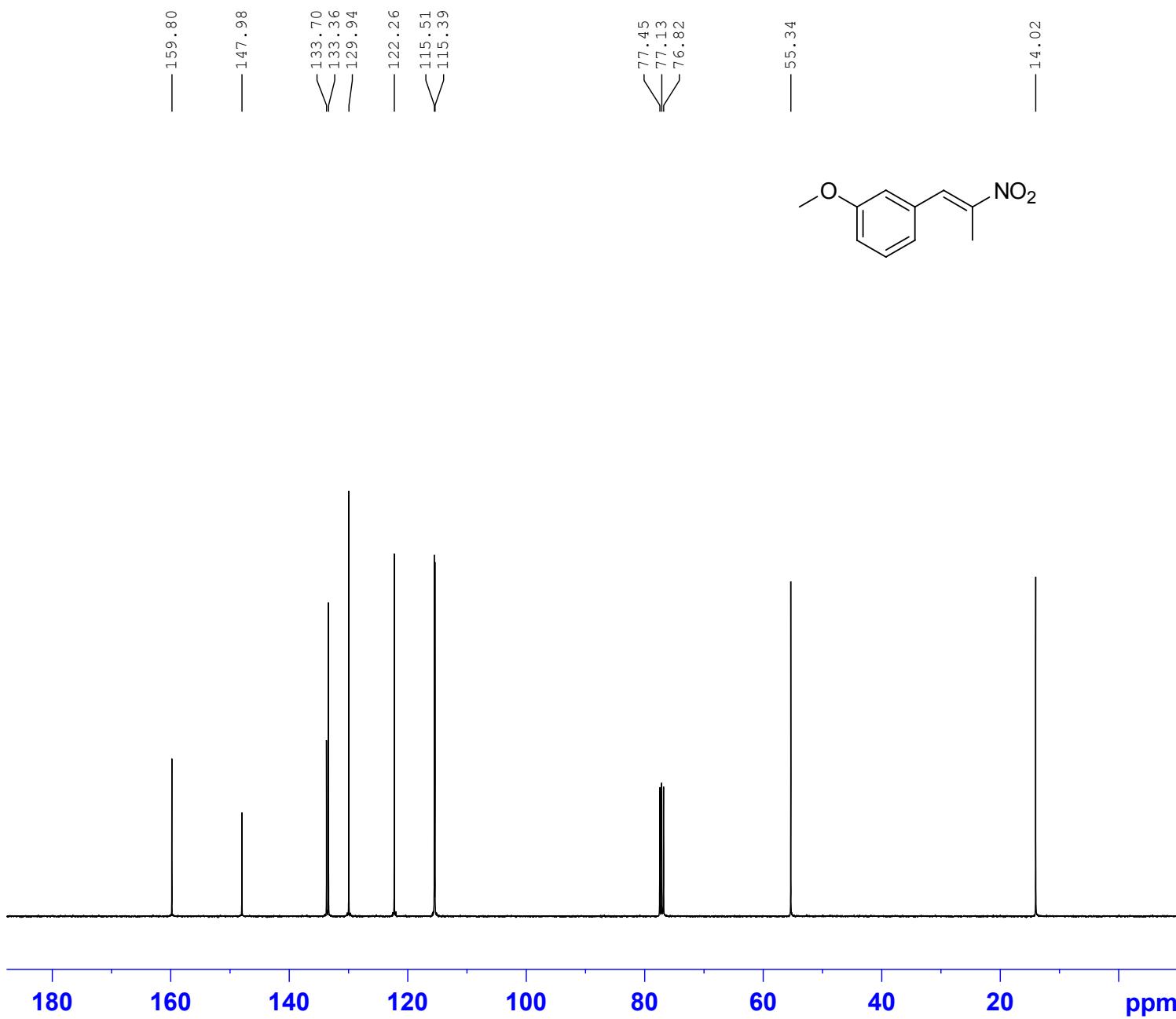
3.8286
2.4275



NAME Jul22-2012
EXPNO 3
PROCNO 1
Date_ 20120722
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 300.4 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL16
C13CPD CDC13 {E:\NMR Data} skl 28

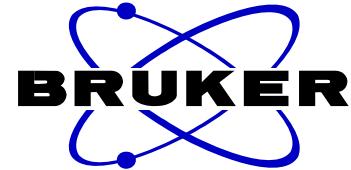


NAME Jul22-2012
EXPNO 5
PROCNO 1
Date_ 20120722
Time 19.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

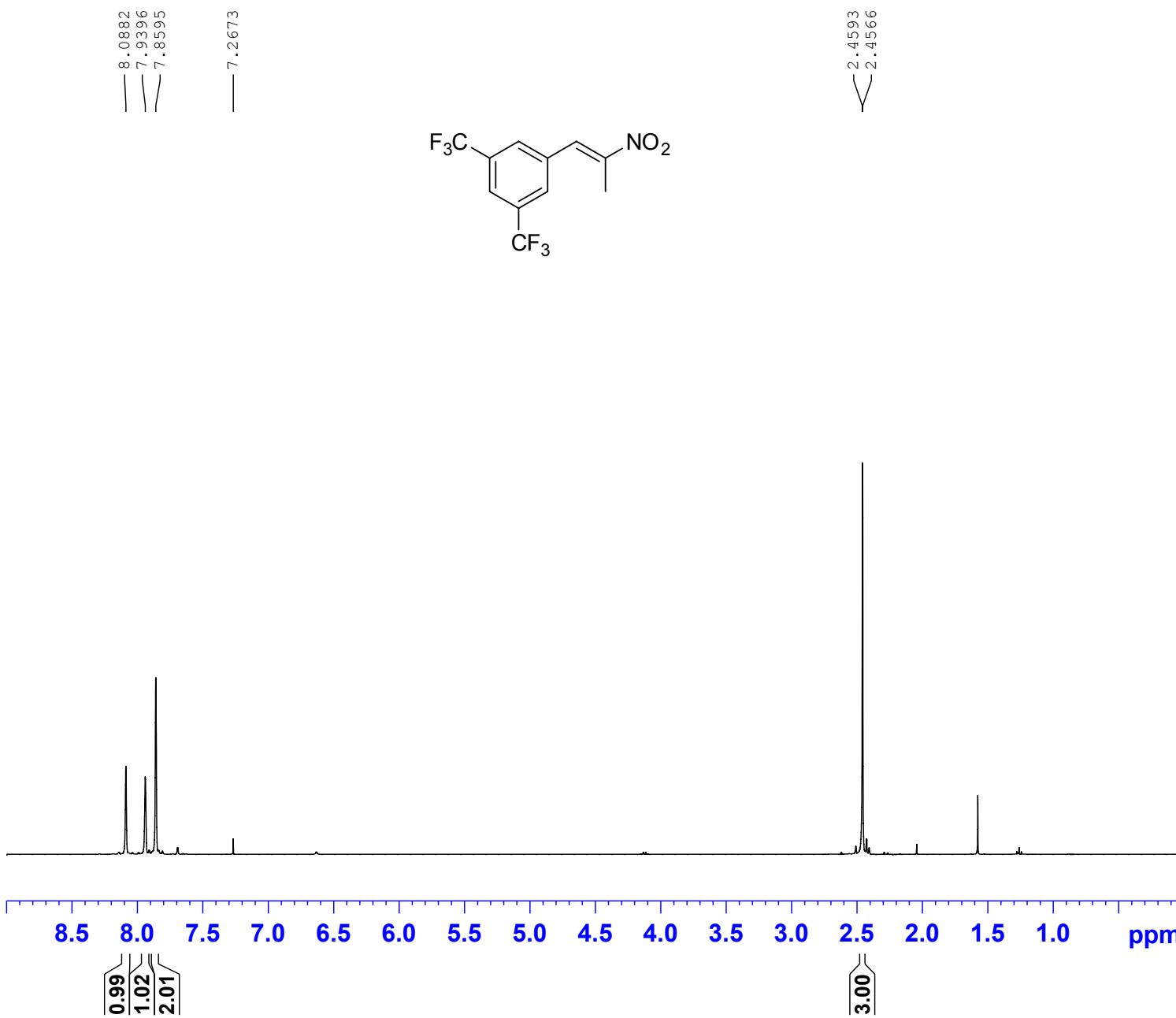
KL28
PROTON CDC13 {E:\NMR Data} skl 28



NAME Jul28-2012
EXPNO 11
PROCNO 1
Date_ 20120729
Time 10.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.0000000 sec
TDO 1

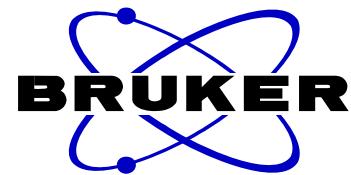
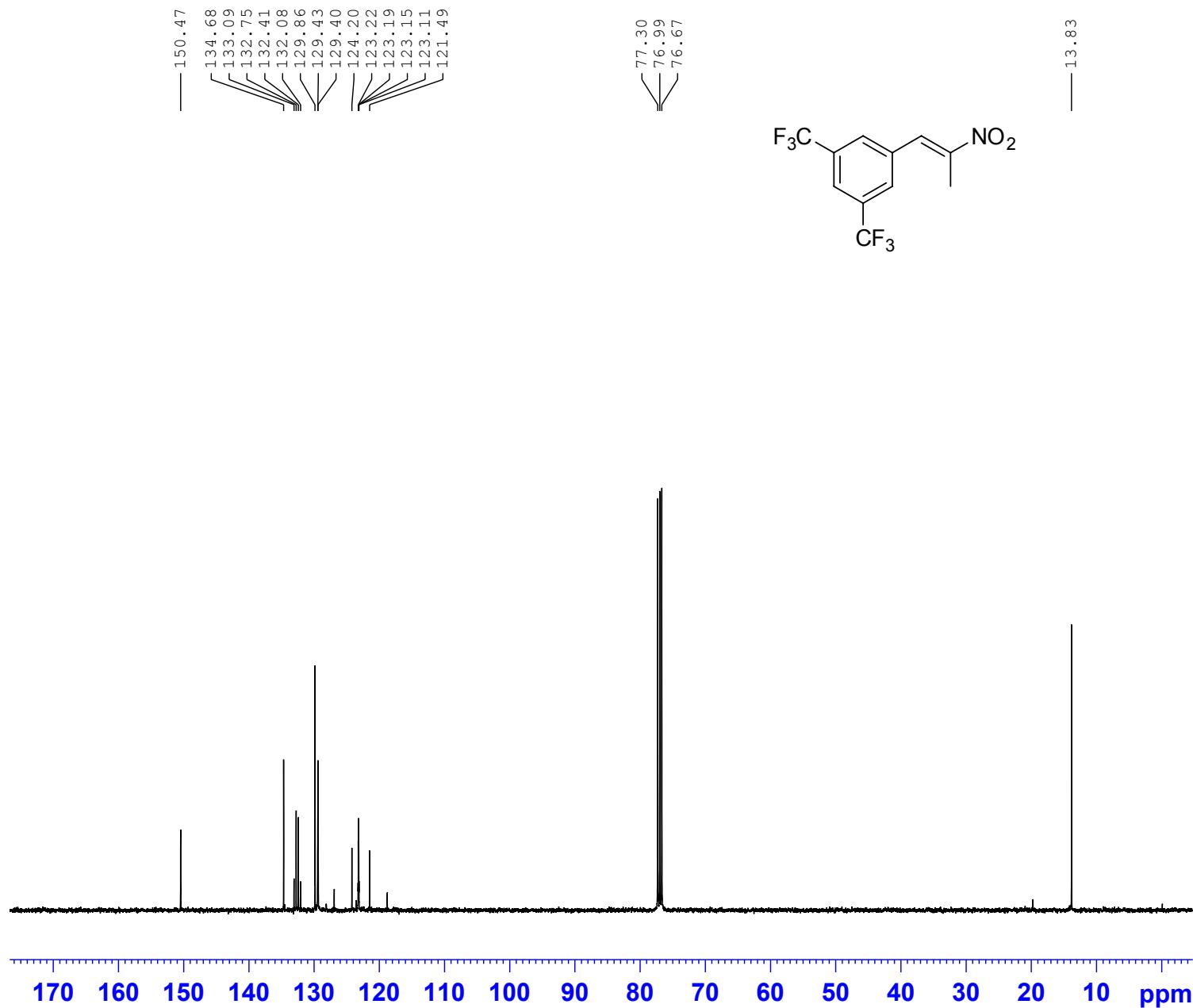
===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300069 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



KL28

C13CPD32 CDC13 {E:\NMR Data} skl 28

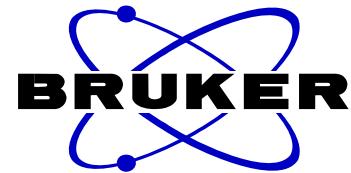


NAME Jul28-2012
EXPNO 14
PROCNO 1
Date_ 20120729
Time 12.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

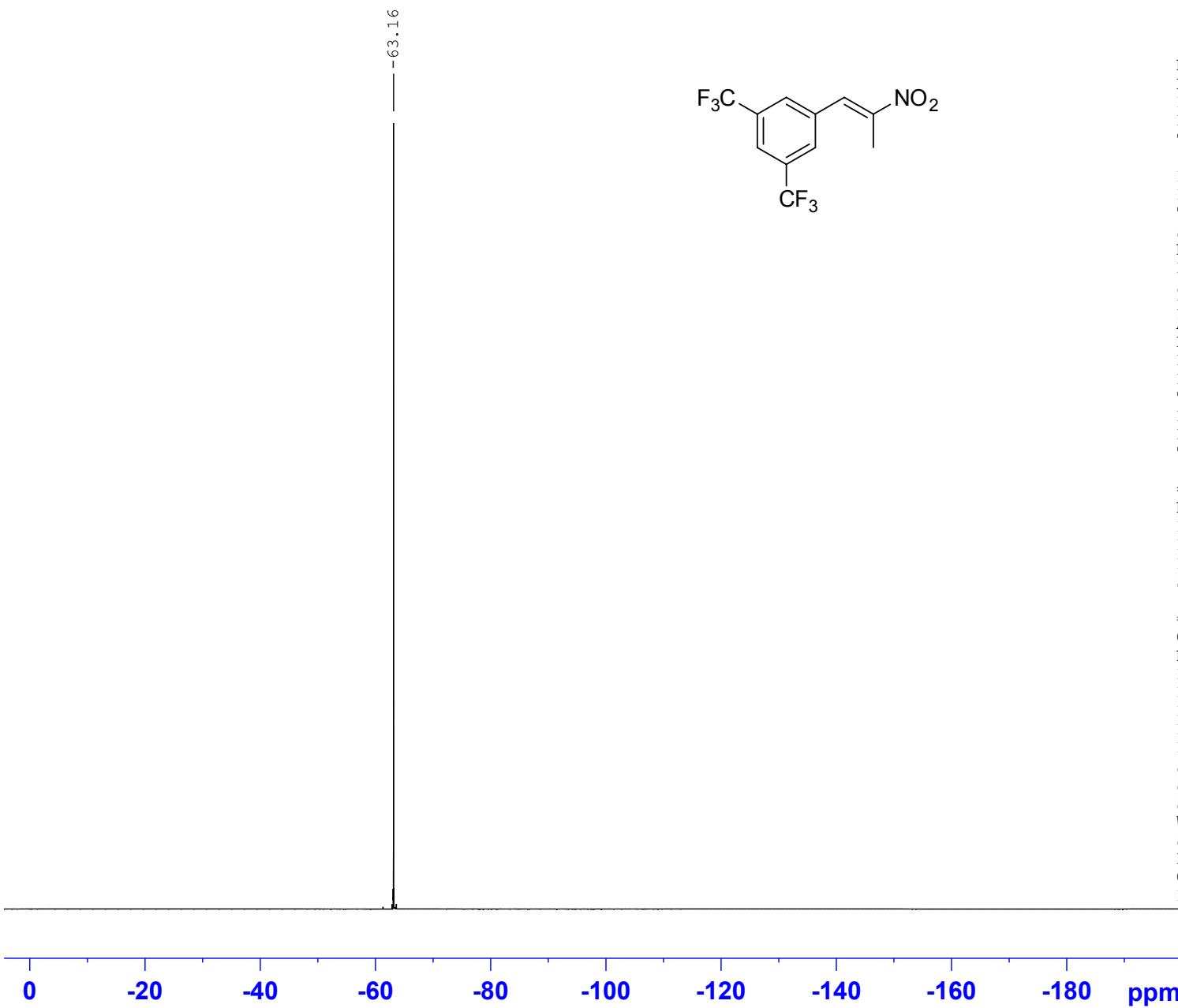
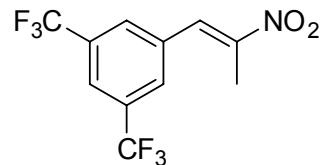
KL28
f19cpd.medchem CDC13 {E:\NMR Data} skl 28



NAME Jul28-2012
EXPNO 13
PROCNO 1
Date_ 20120729
Time 11.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc60
TD 131072
SOLVENT CDC13
NS 128
DS 4
SWH 93750.000 Hz
FIDRES 0.715256 Hz
AQ 0.6991007 sec
RG 512
DW 5.333 usec
DE 6.50 usec
TE 302.3 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

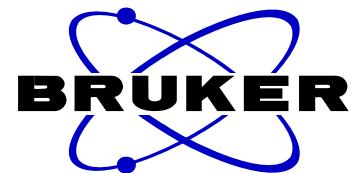
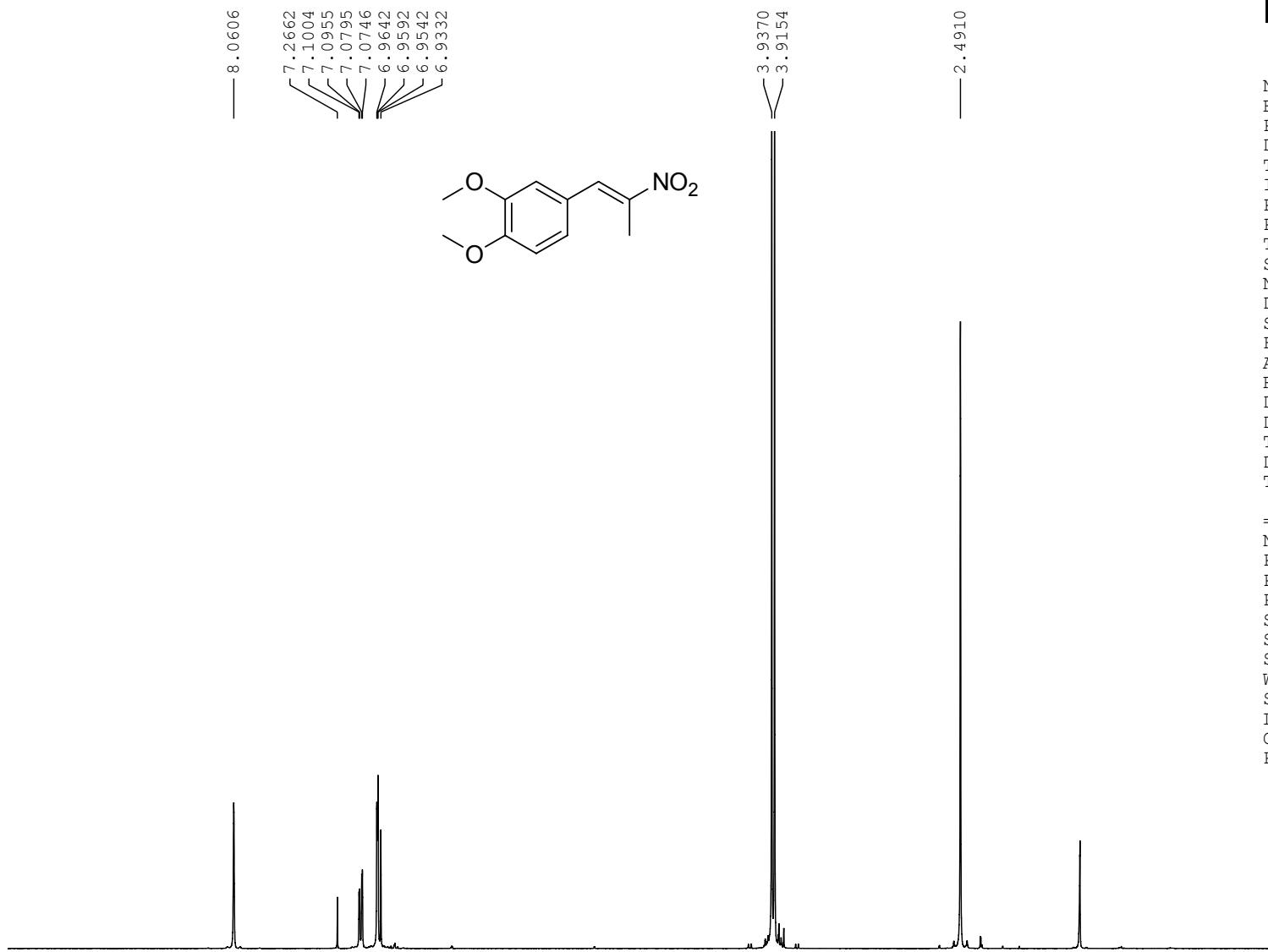
===== CHANNEL f1 ======
NUC1 19F
P1 14.00 usec
PL1 1.50 dB
PL1W 35.56558990 W
SFO1 376.4569512 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
SFO2 400.1316005 MHz
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.87 Hz
GB 0
PC 1.00



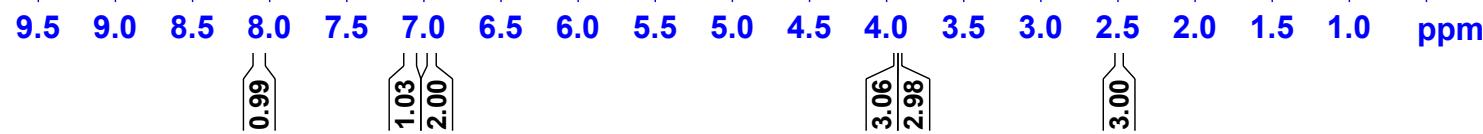
KL08

PROTON CDCl₃ {E:\NMR Data} skl 44

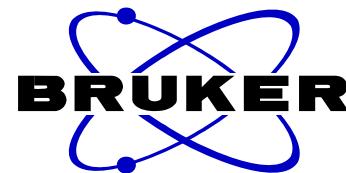
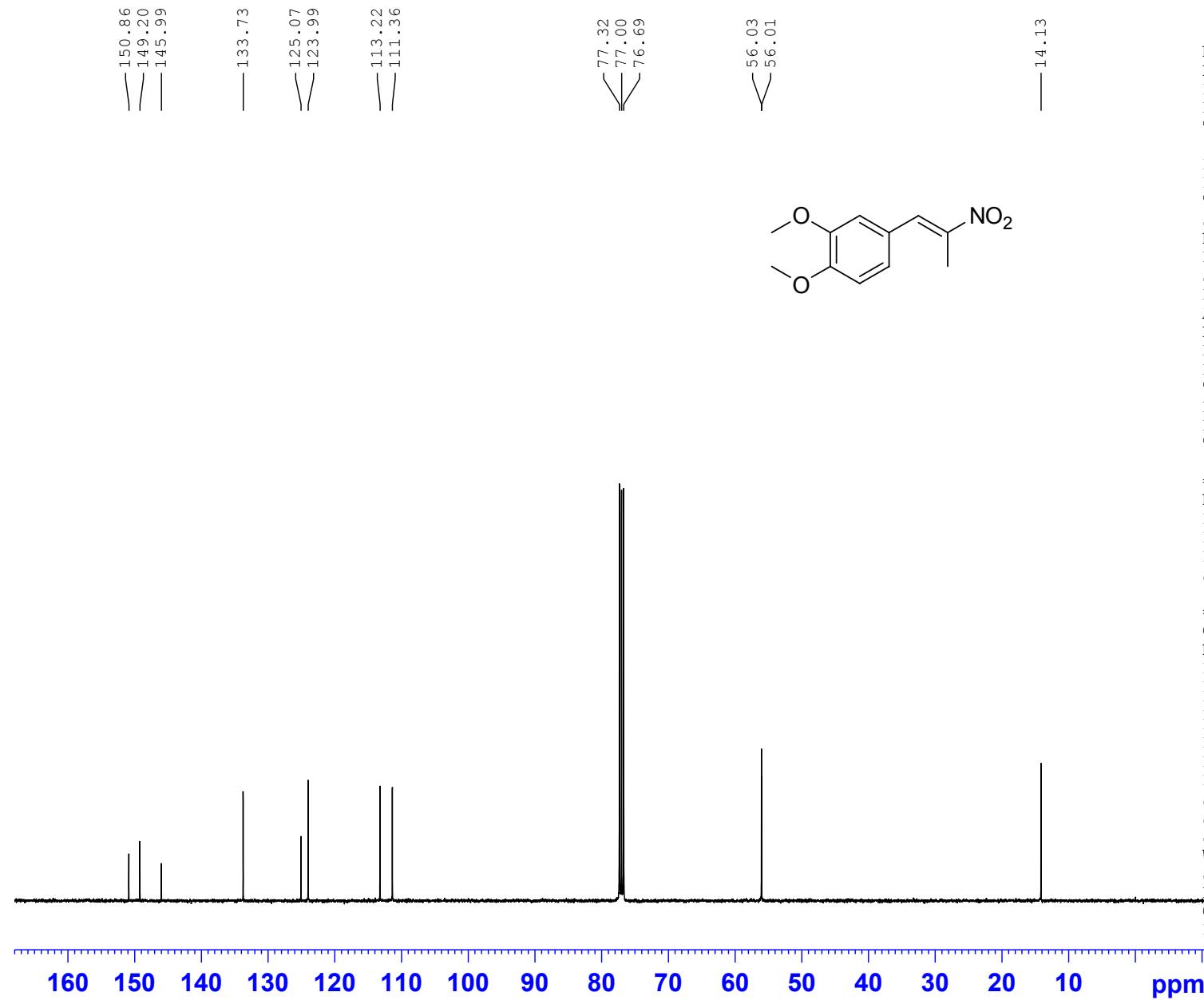


NAME Jul17-2012
EXPNO 13
PROCNO 1
Date_ 20120718
Time 9.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.50 usec
TE 303.6 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



KL08
C13CPD CDC13 {E:\NMR Data} skl 44

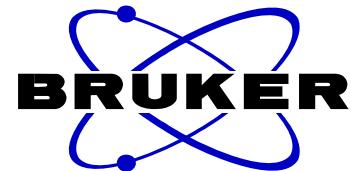
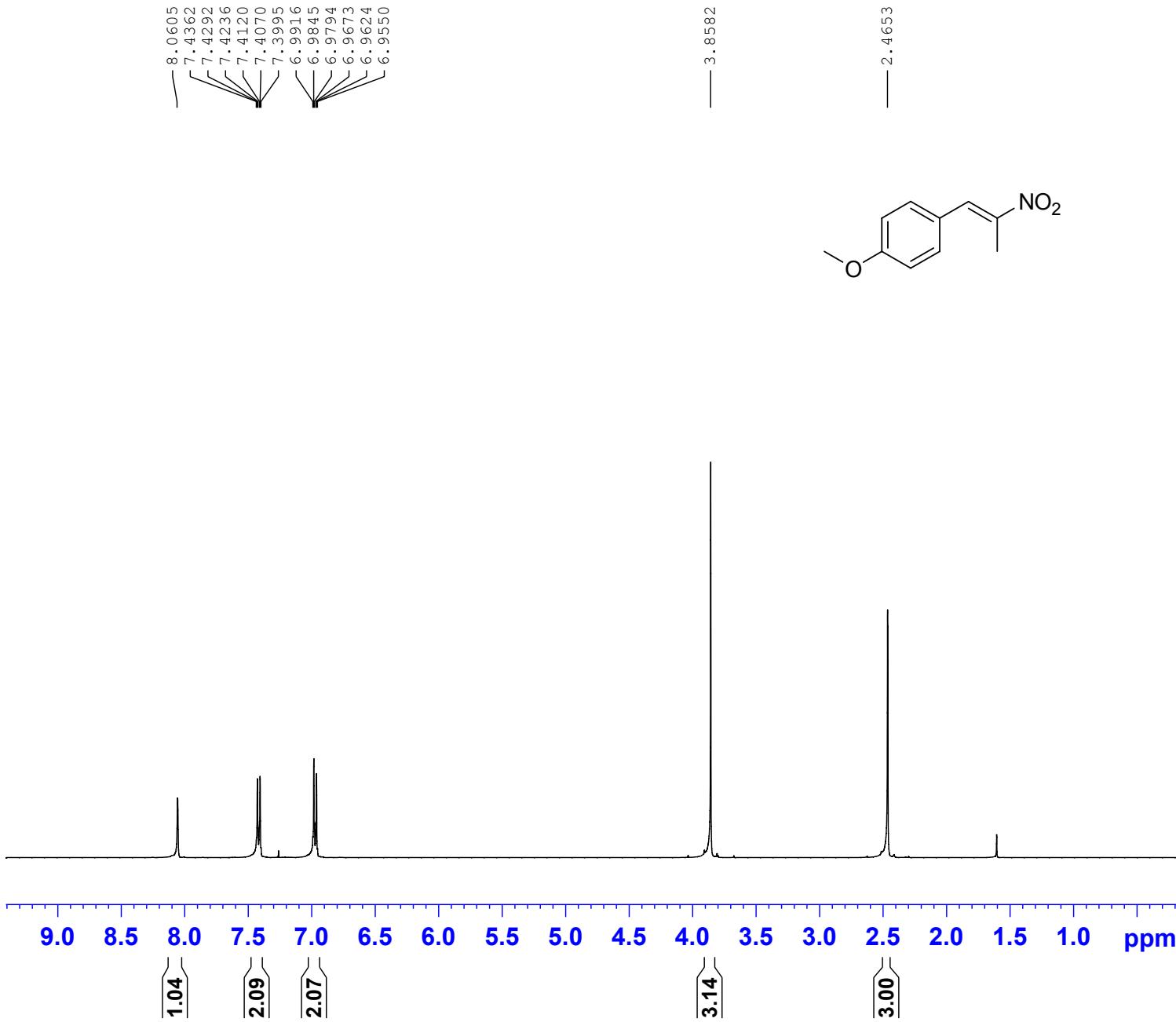
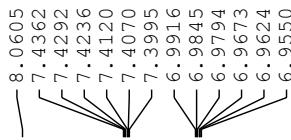


NAME Jul17-2012
EXPNO 9
PROCNO 1
Date_ 20120718
Time 0.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 306.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

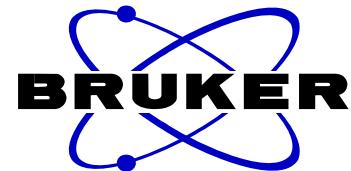
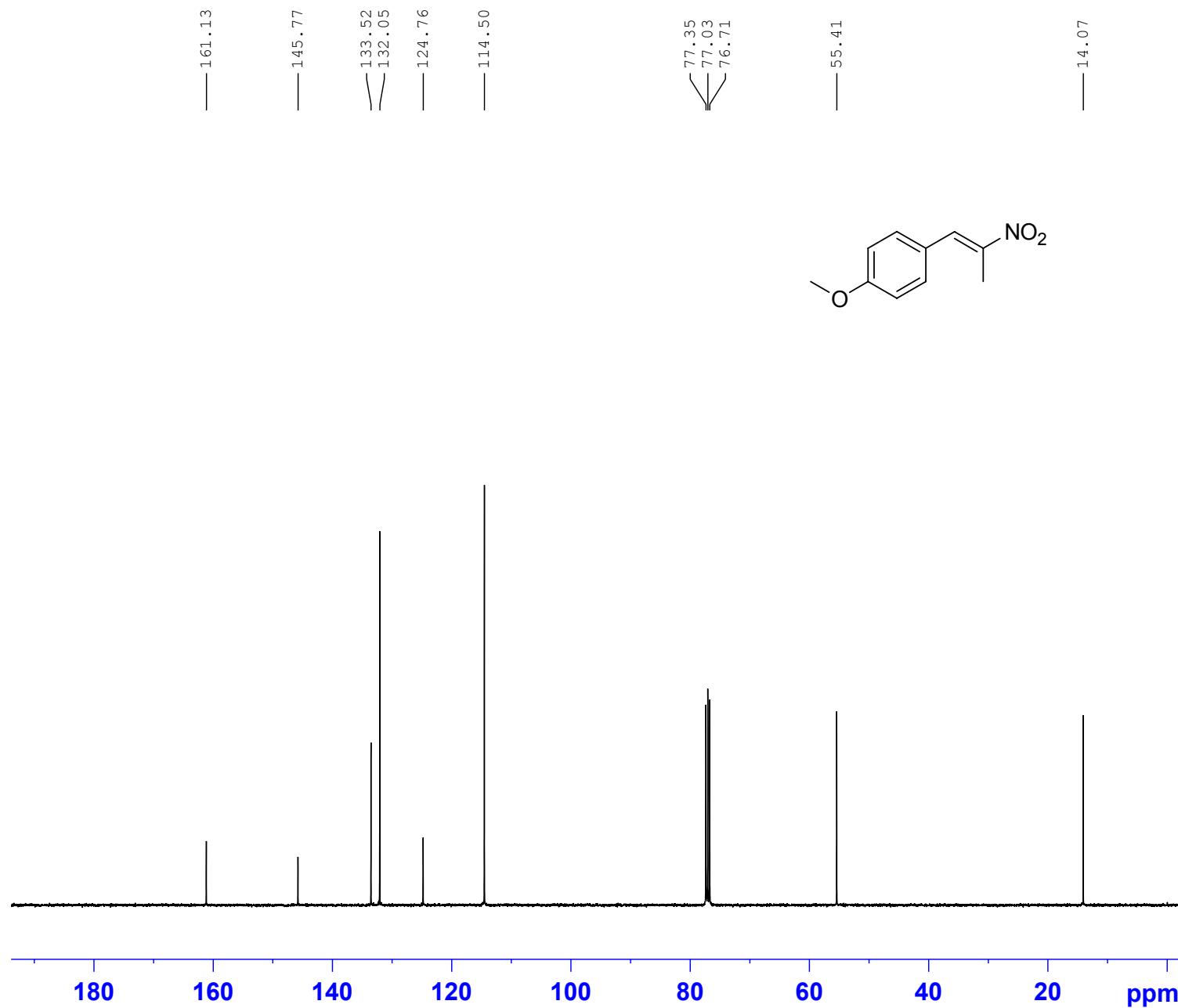
KL06
PROTON CDCl₃ {E:\NMR Data} skl 14



NAME Jul16-2012
EXPNO 11
PROCNO 1
Date_ 20120716
Time 21.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 304.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL06
C13CPD CDC13 {E:\NMR Data} skl 14



NAME Jul16-2012
EXPNO 13
PROCNO 1
Date_ 20120716
Time 22.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 306.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

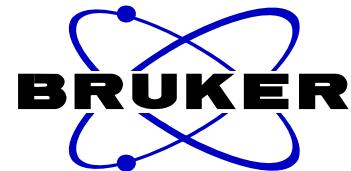
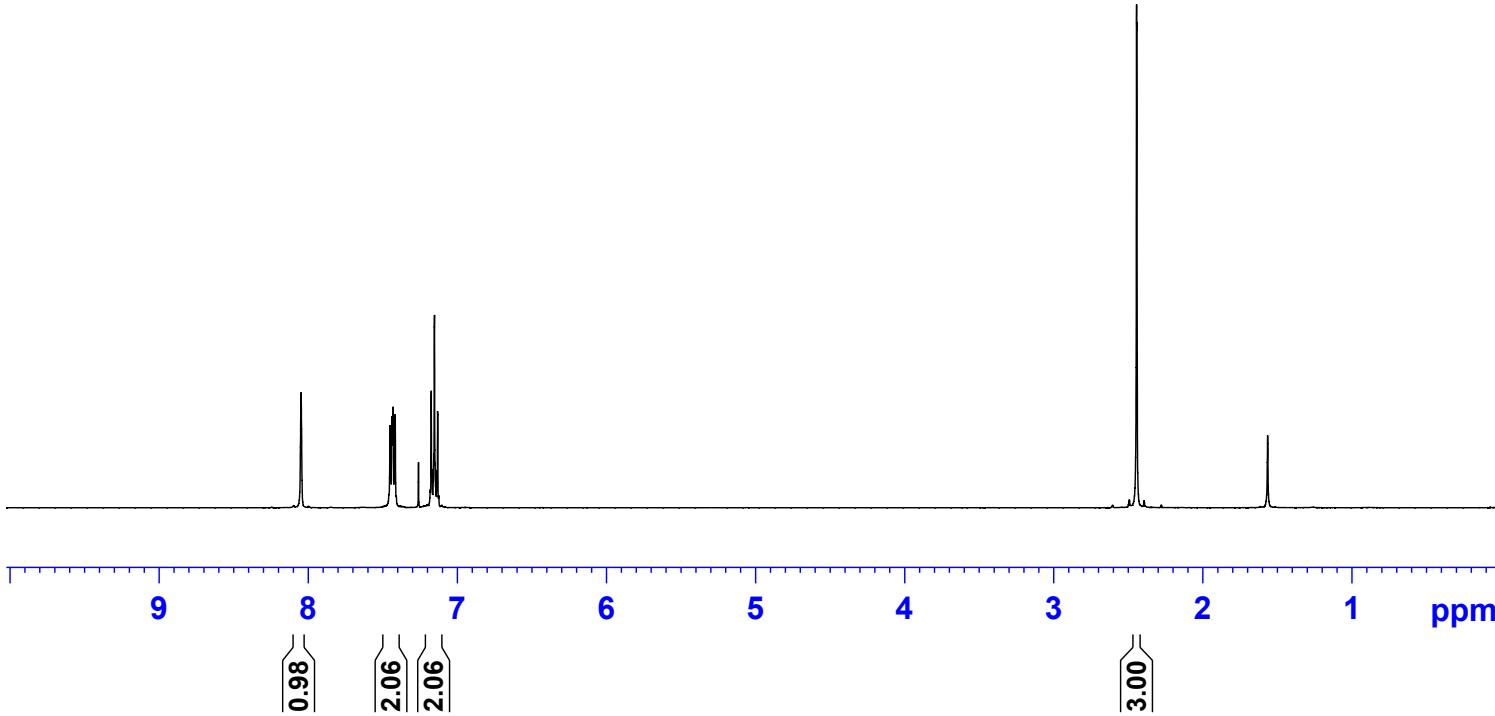
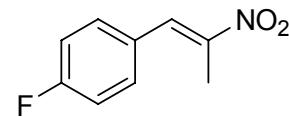
===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL07

PROTON CDC13 {E:\NMR Data} skl 15

8.0479
7.4516
7.4467
7.4383
7.4342
7.4300
7.4215
7.4168
7.2605
7.1822
7.1749
7.1696
7.1576
7.1535
7.1489
7.1370
7.1319

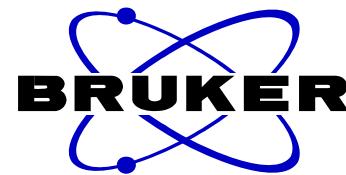
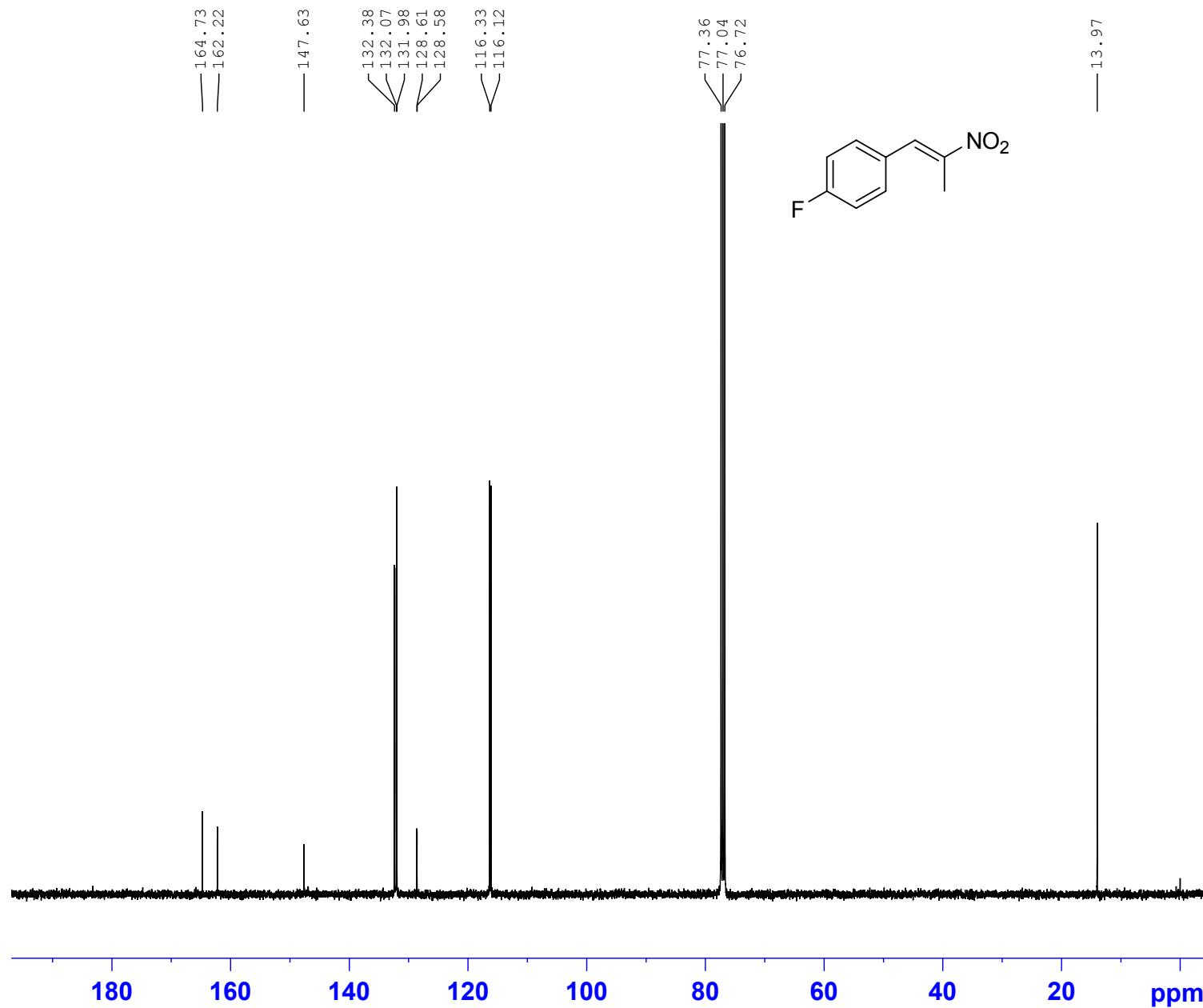


NAME Jul16-2012
EXPNO 14
PROCNO 1
Date_ 20120716
Time 22.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.50 usec
TE 304.9 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL07
C13CPD CDC13 {E:\NMR Data} skl 15

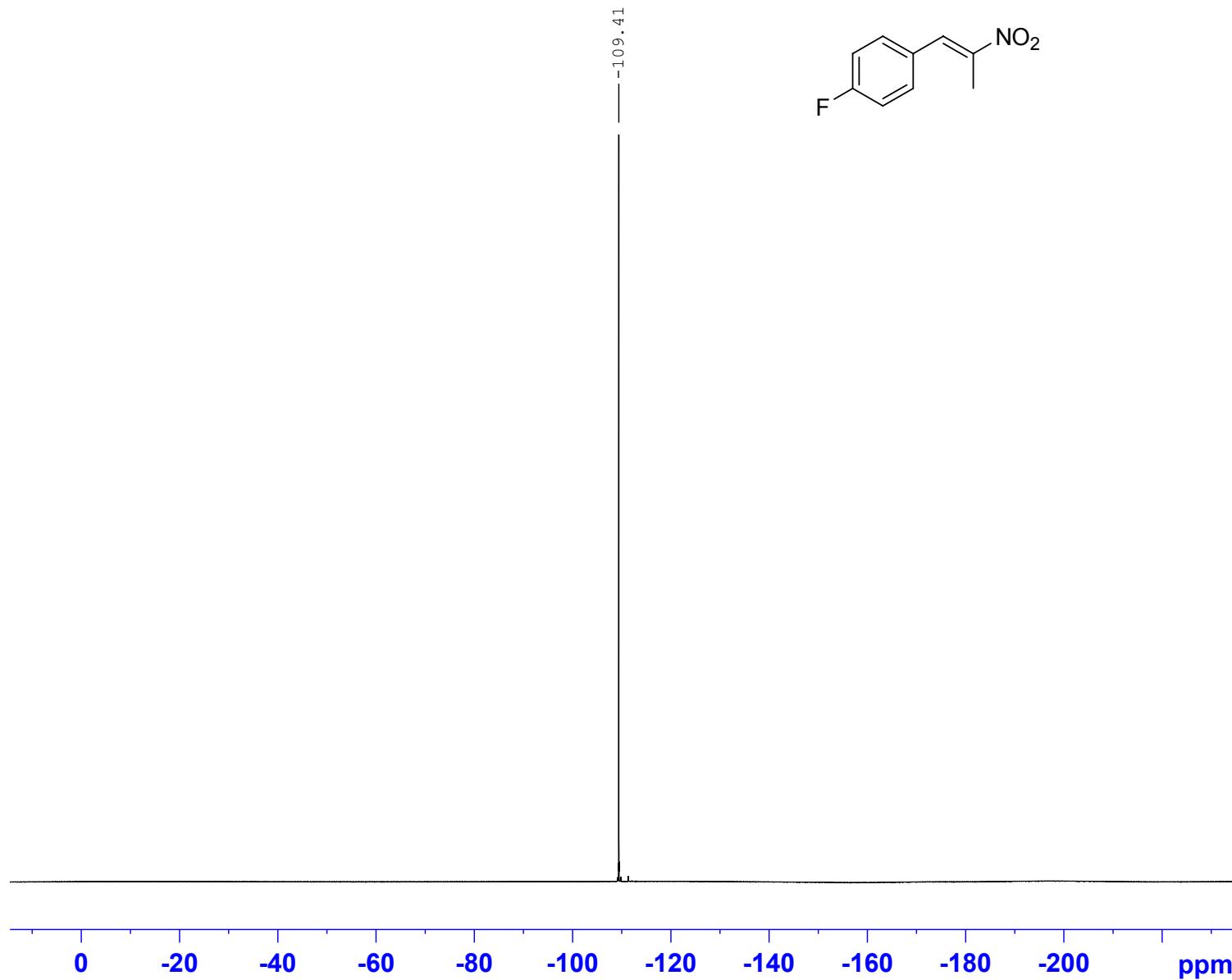
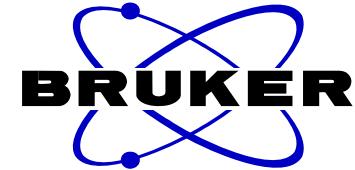


NAME Jul16-2012
EXPNO 16
PROCNO 1
Date_ 20120717
Time 1.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 306.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

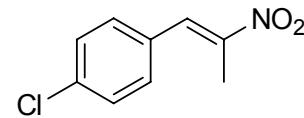
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127643 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL07
f19cpd.medchem CDC13 {E:\NMR Data} skl 15

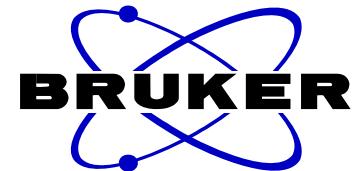
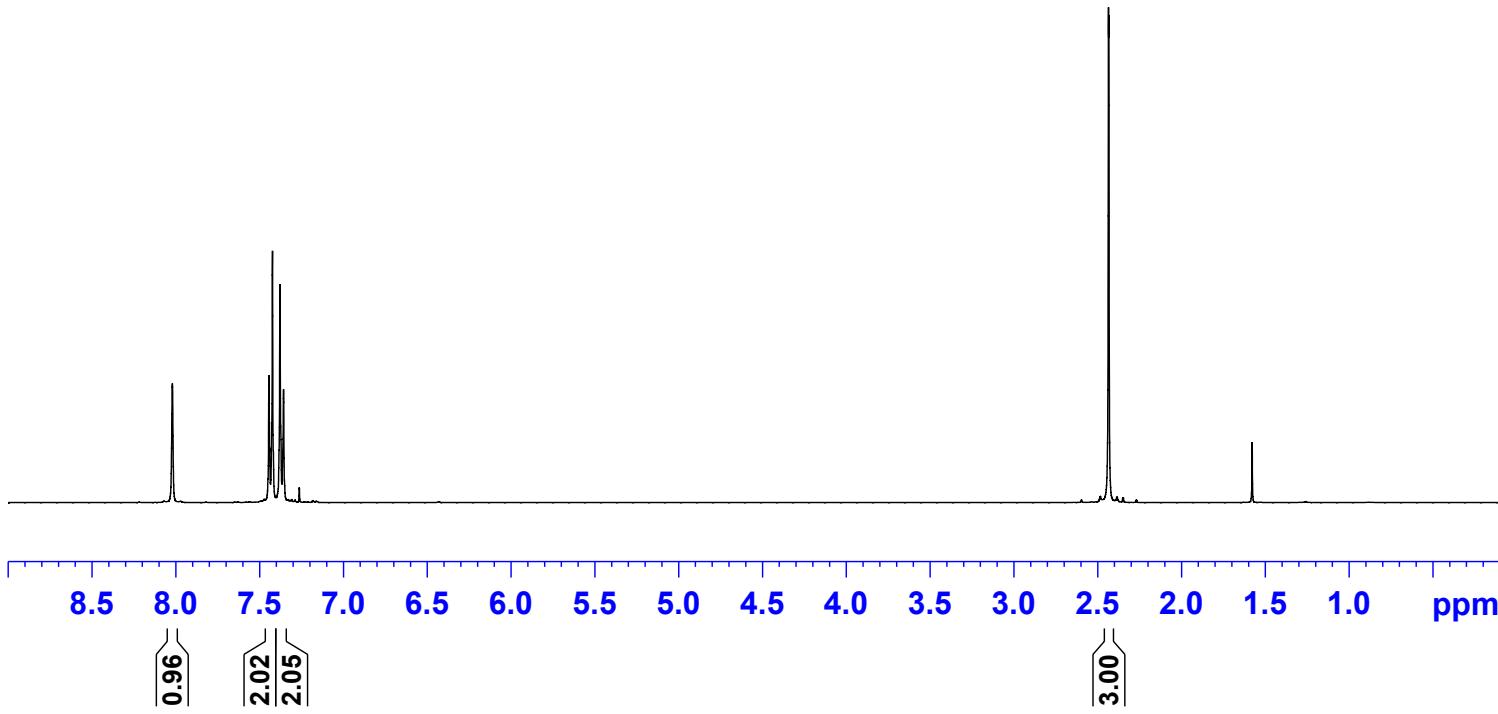


KL09
PROTON CDCl₃ {E:\NMR Data} skl 45

8.0204
7.4444
7.4397
7.4279
7.4230
7.3783
7.3570



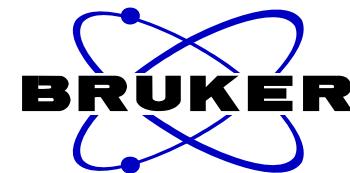
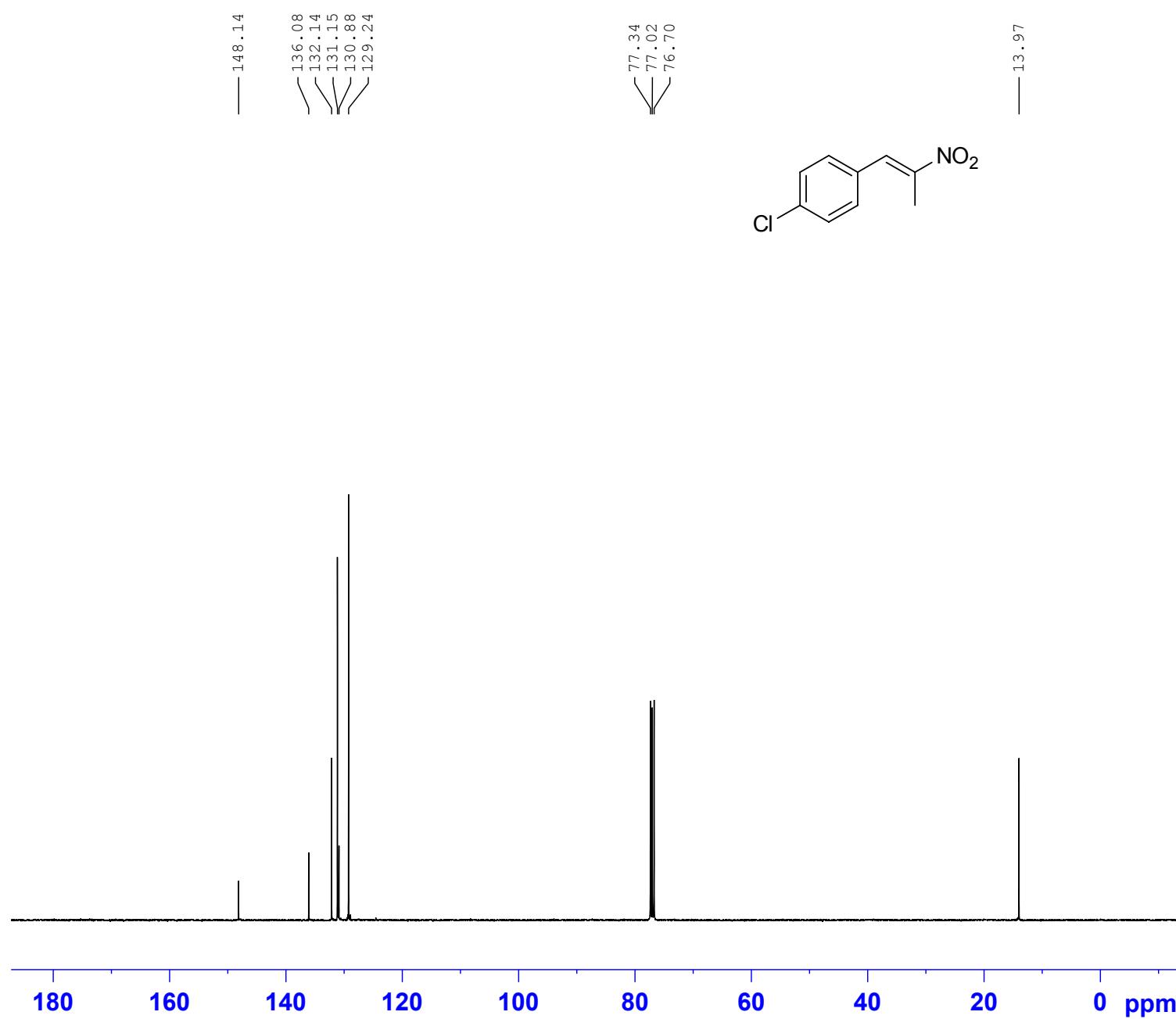
2.4355
2.4334



NAME Jul17-2012
EXPNO 10
PROCNO 1
Date_ 20120718
Time 0.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 304.8 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL09
C13CPD CDC13 {E:\NMR Data} skl 45

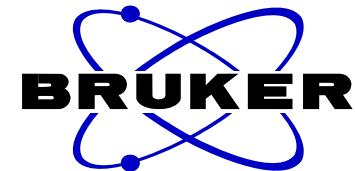
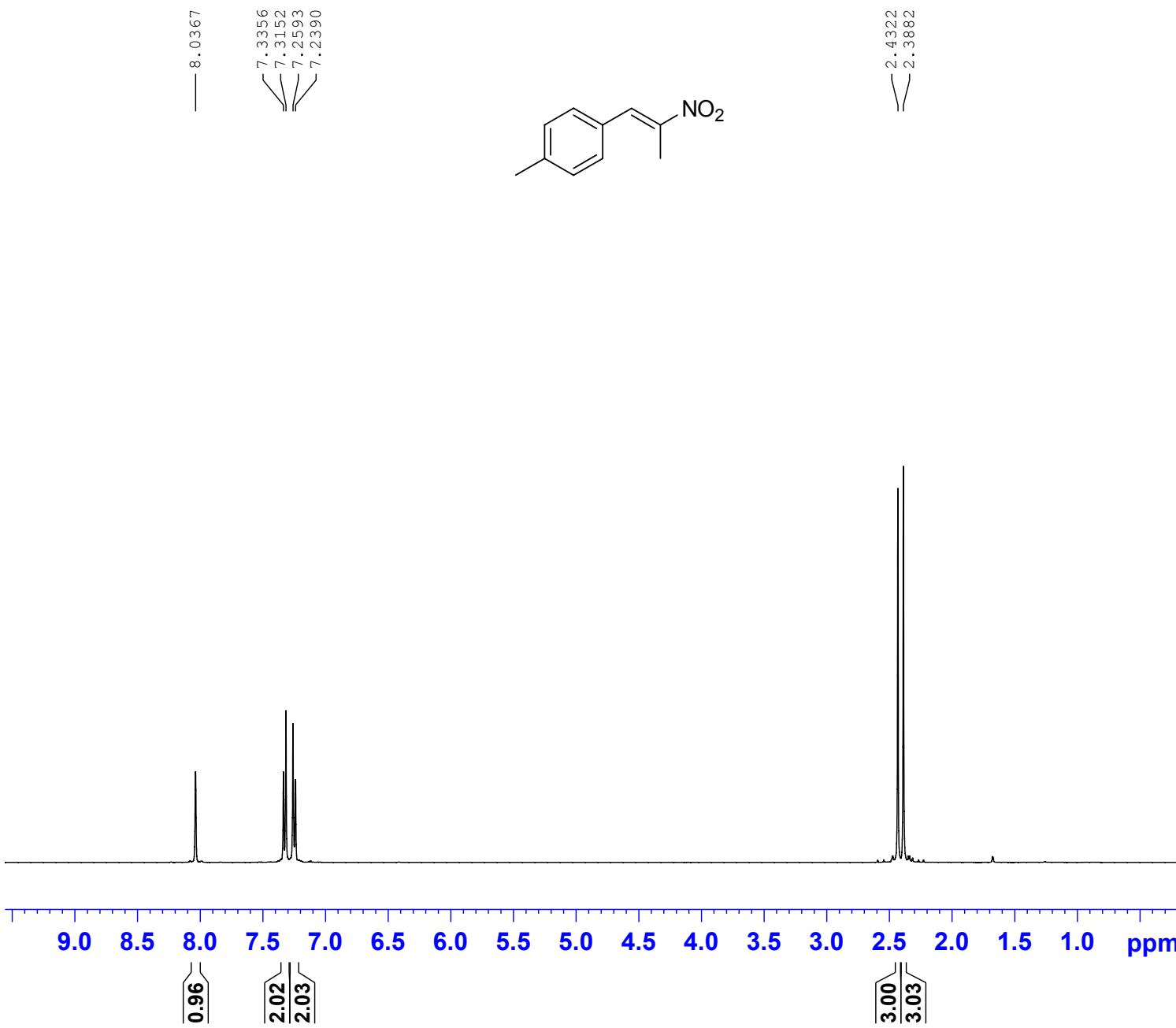


NAME Jul17-2012
EXPNO 12
PROCNO 1
Date_ 20120718
Time 3.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 306.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

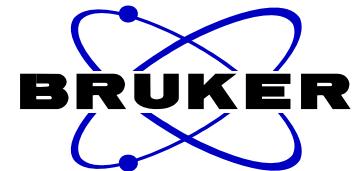
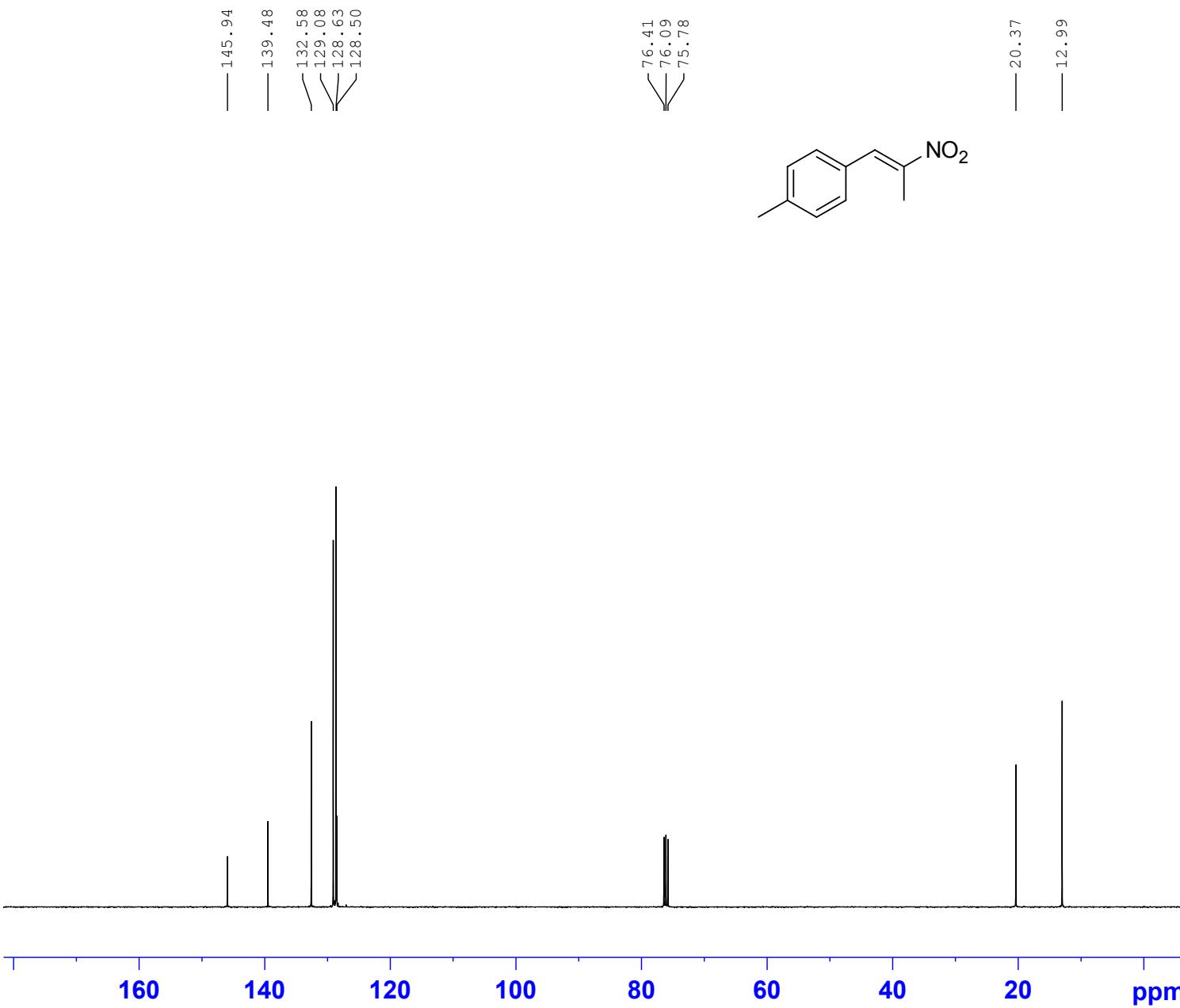
KL12
PROTON CDC13 {E:\NMR Data} skl 44



NAME Jul19-2012
EXPNO 14
PROCNO 1
Date_ 20120720
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 301.7 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL12
C13CPD CDC13 {E:\NMR Data} skl 44



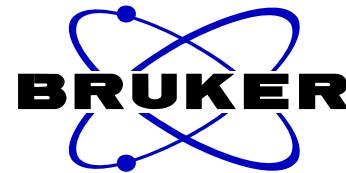
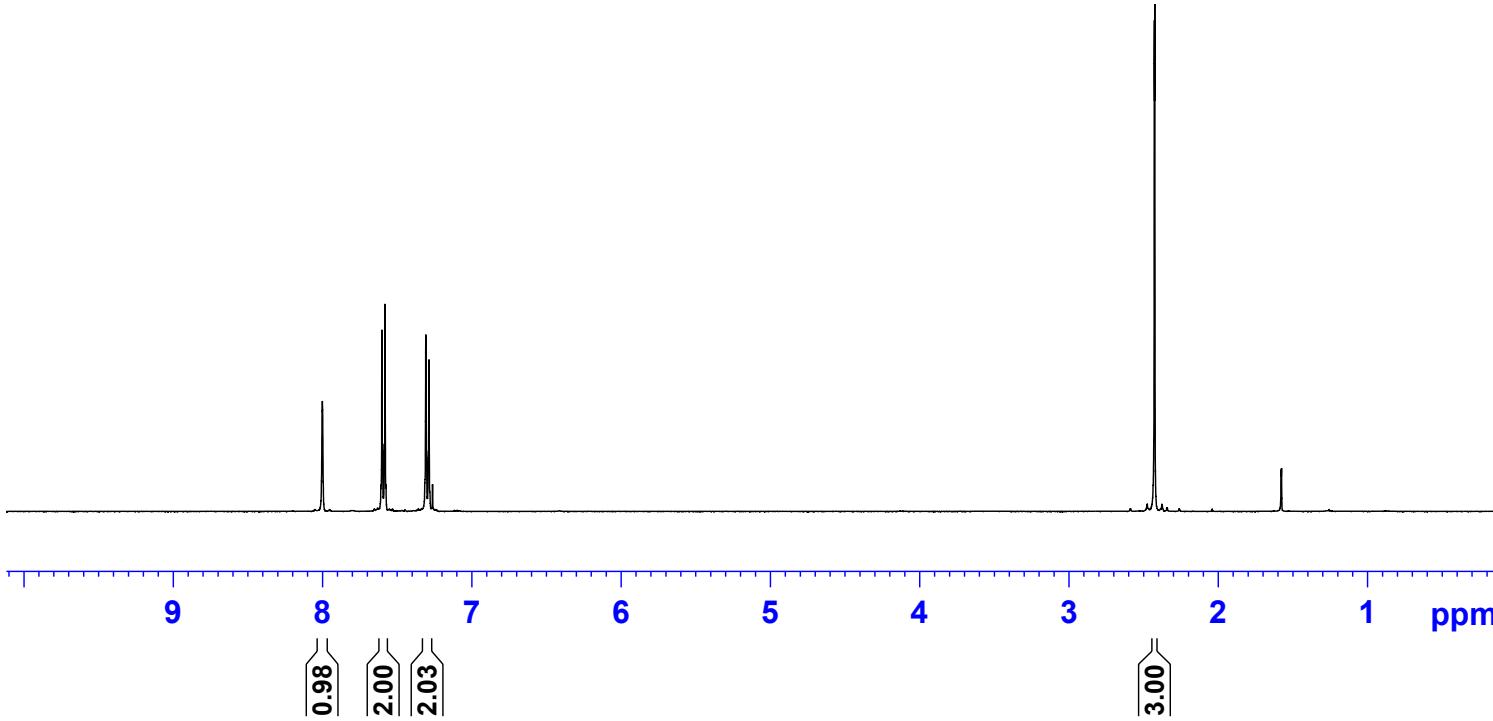
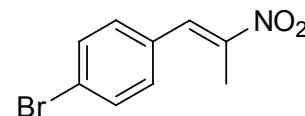
NAME Jul19-2012
EXPNO 10
PROCNO 1
Date_ 20120720
Time 5.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.5 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL13
PROTON CDC13 {E:\NMR Data} skl 45

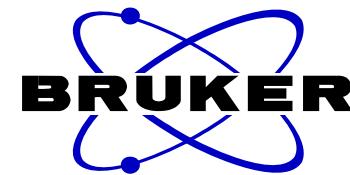
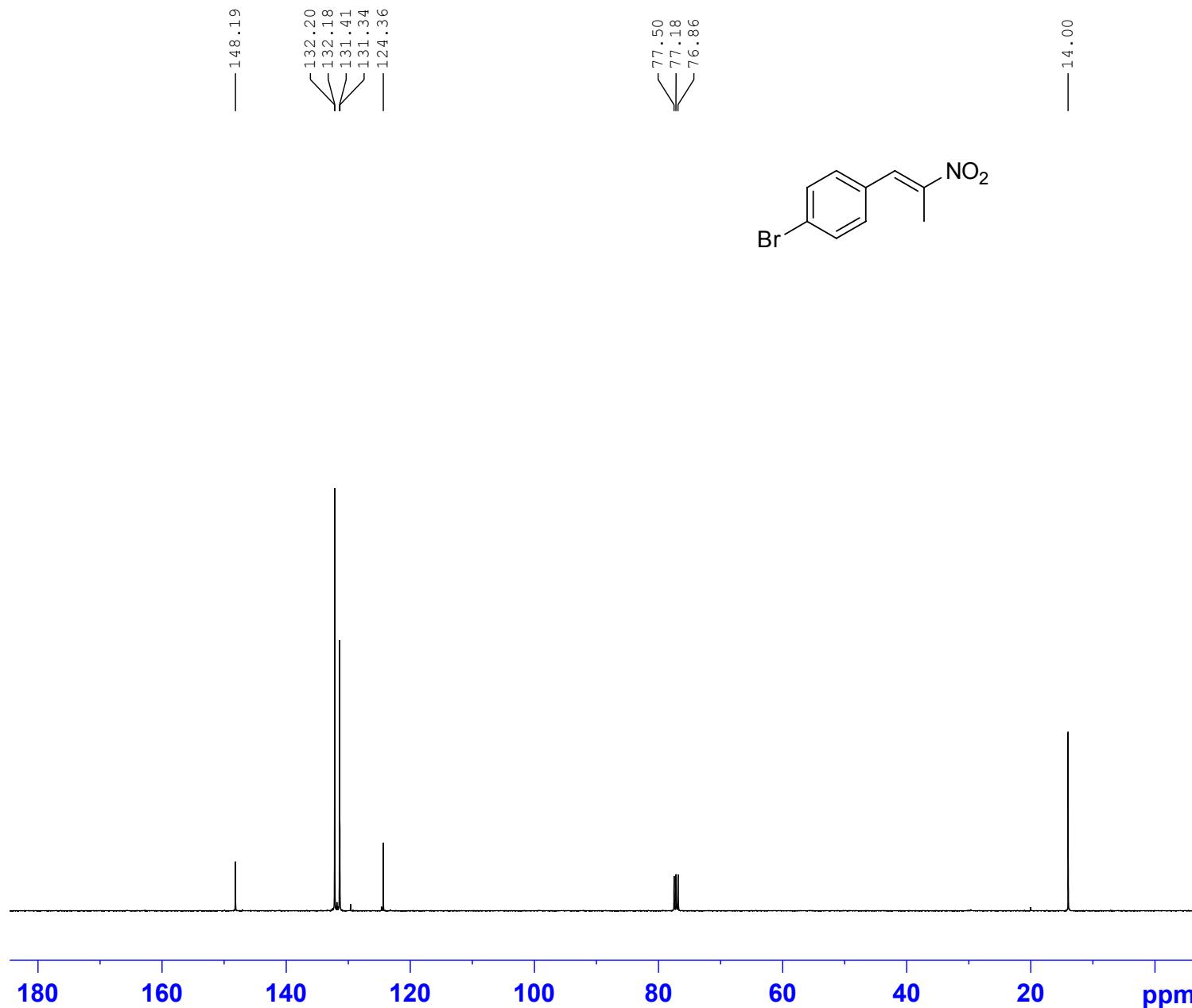
8.0011
7.6085
7.6025
7.5980
7.5860
7.5813
7.5753
7.3133
7.3081
7.2871
7.2632



NAME Jul19-2012
EXPNO 11
PROCNO 1
Date_ 20120720
Time 6.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 302.1 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL13 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 1



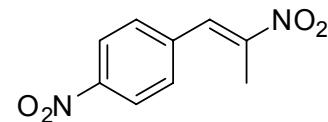
NAME Aug02-2012
EXPNO 3
PROCNO 1
Date_ 20120803
Time 2.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

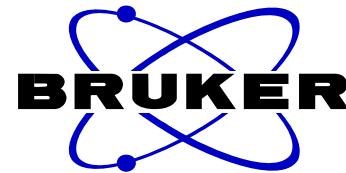
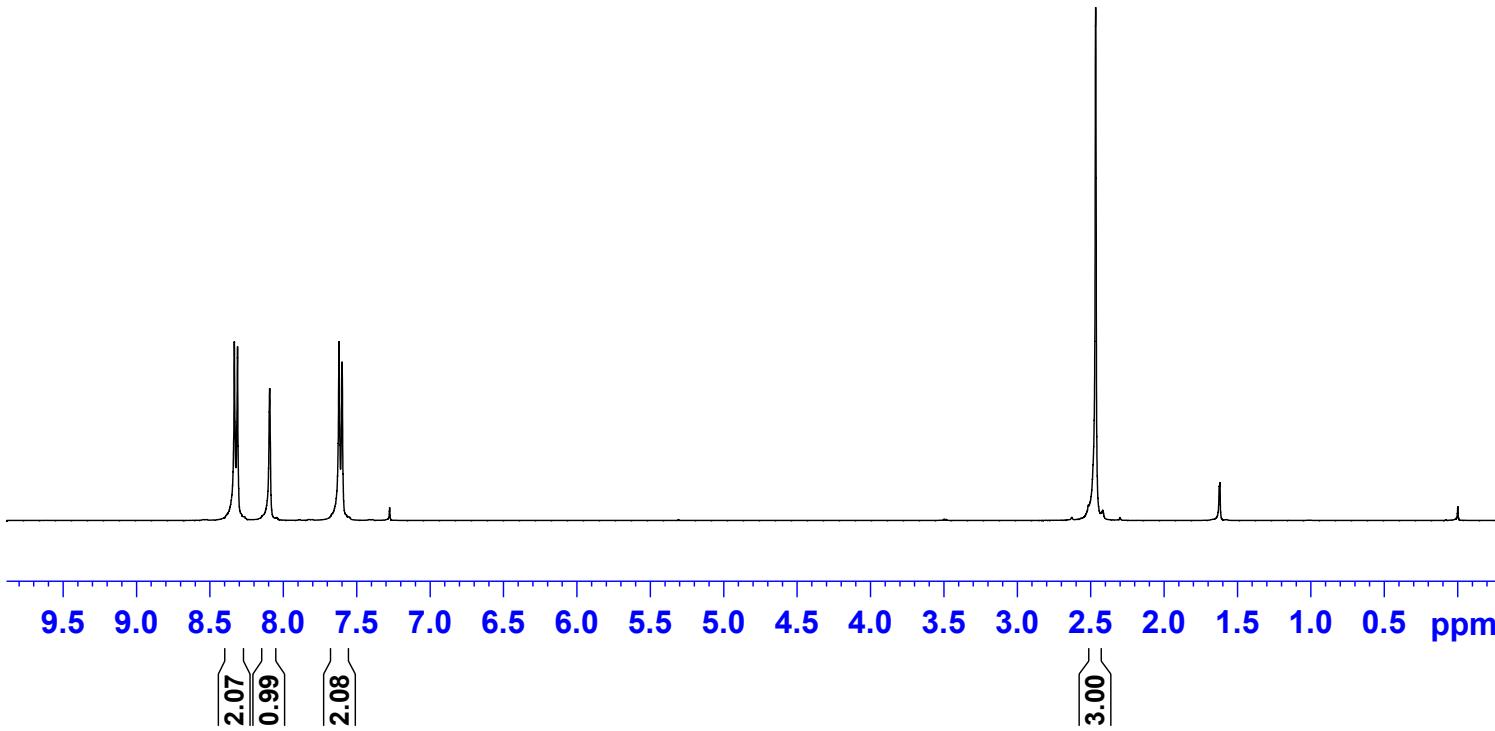
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL17
PROTON CDC13 {E:\NMR Data} skl 3

8.3342
8.3124
8.0935
7.6213
7.5997
7.2762



— 2.4667 —

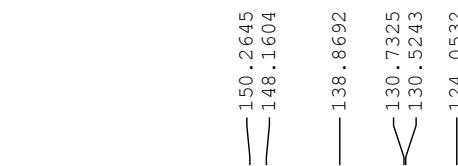


NAME Jul21-2012
EXPNO 3
PROCNO 1
Date_ 20120721
Time 21.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 299.9 K
D1 1.0000000 sec
TDO 1

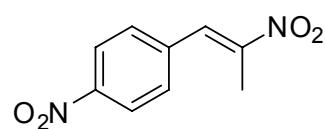
===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL17

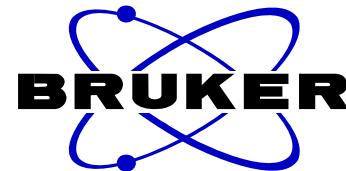
C13CPD CDC13 {E:\NMR Data} skl 3



77.3604
77.0429
76.7250



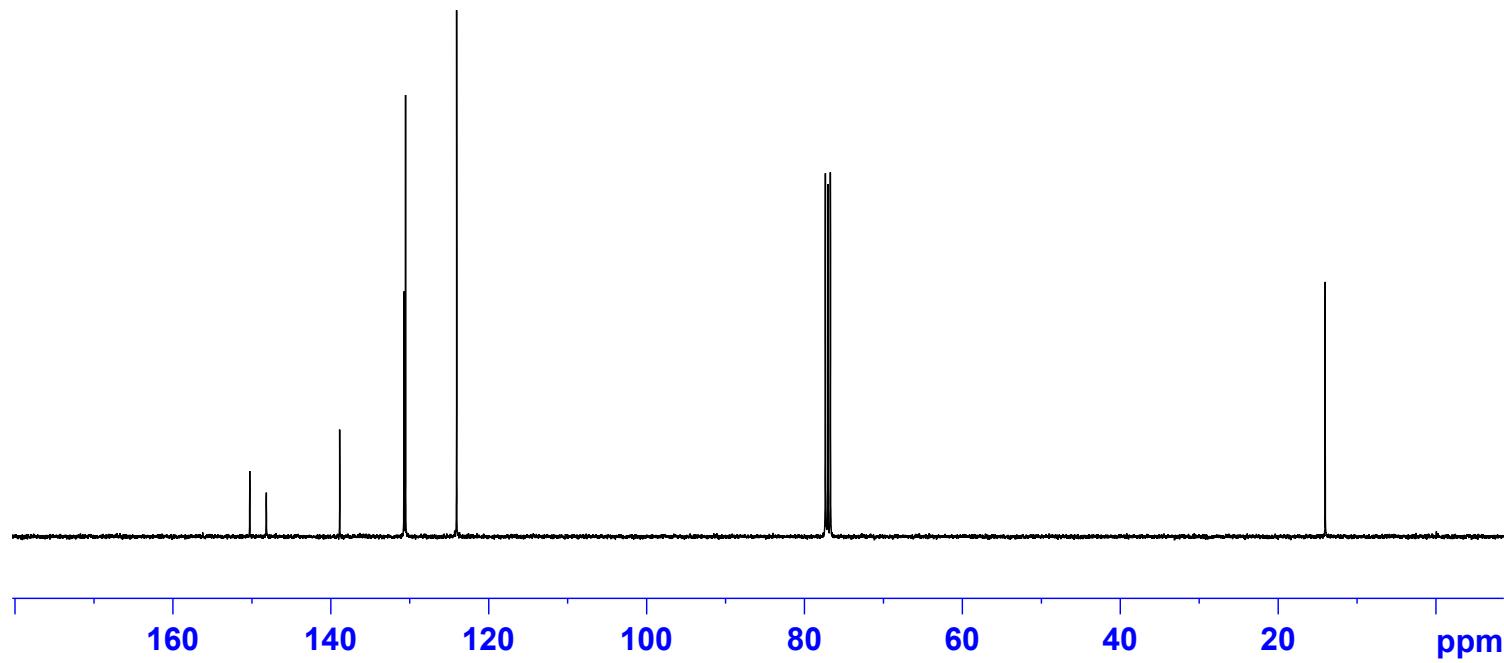
14.0432



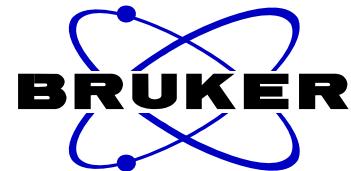
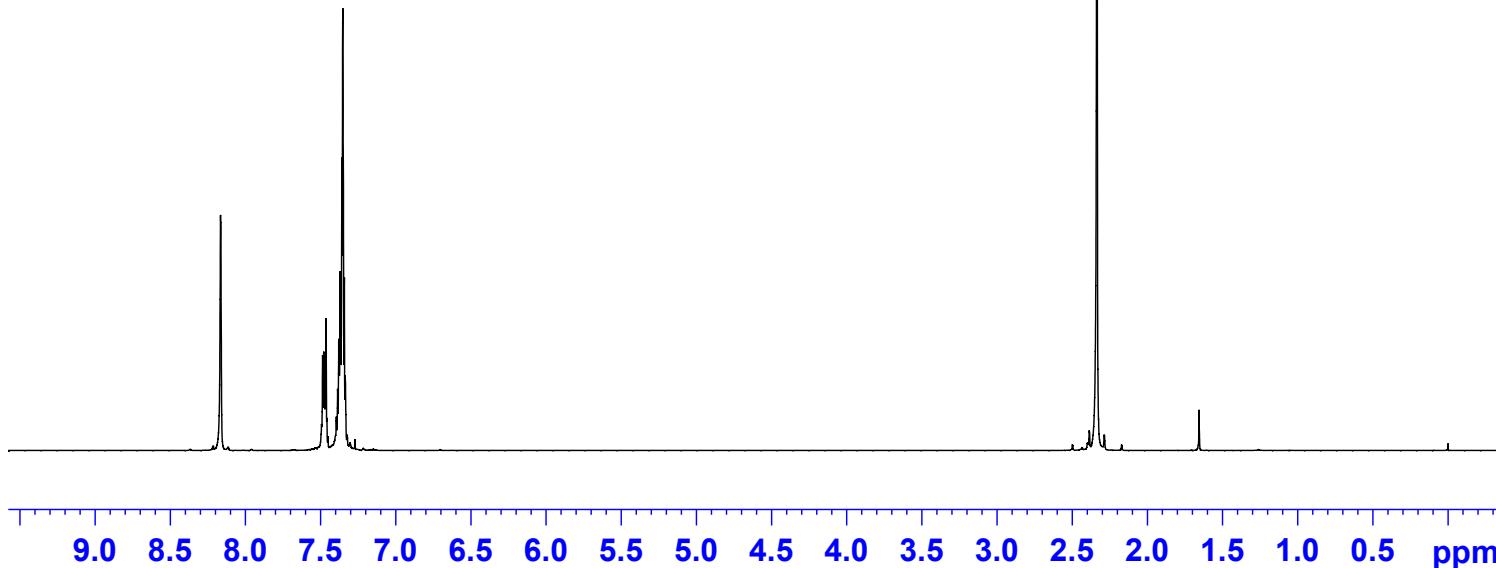
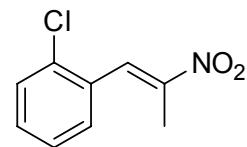
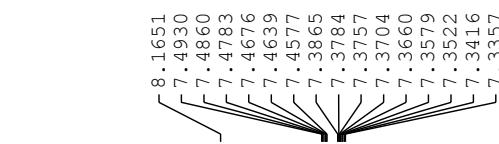
NAME Jul21-2012
EXPNO 9
PROCNO 1
Date_ 20120722
Time 2.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 301.6 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



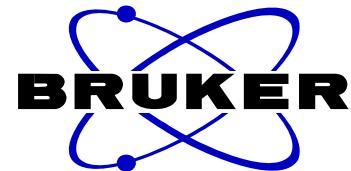
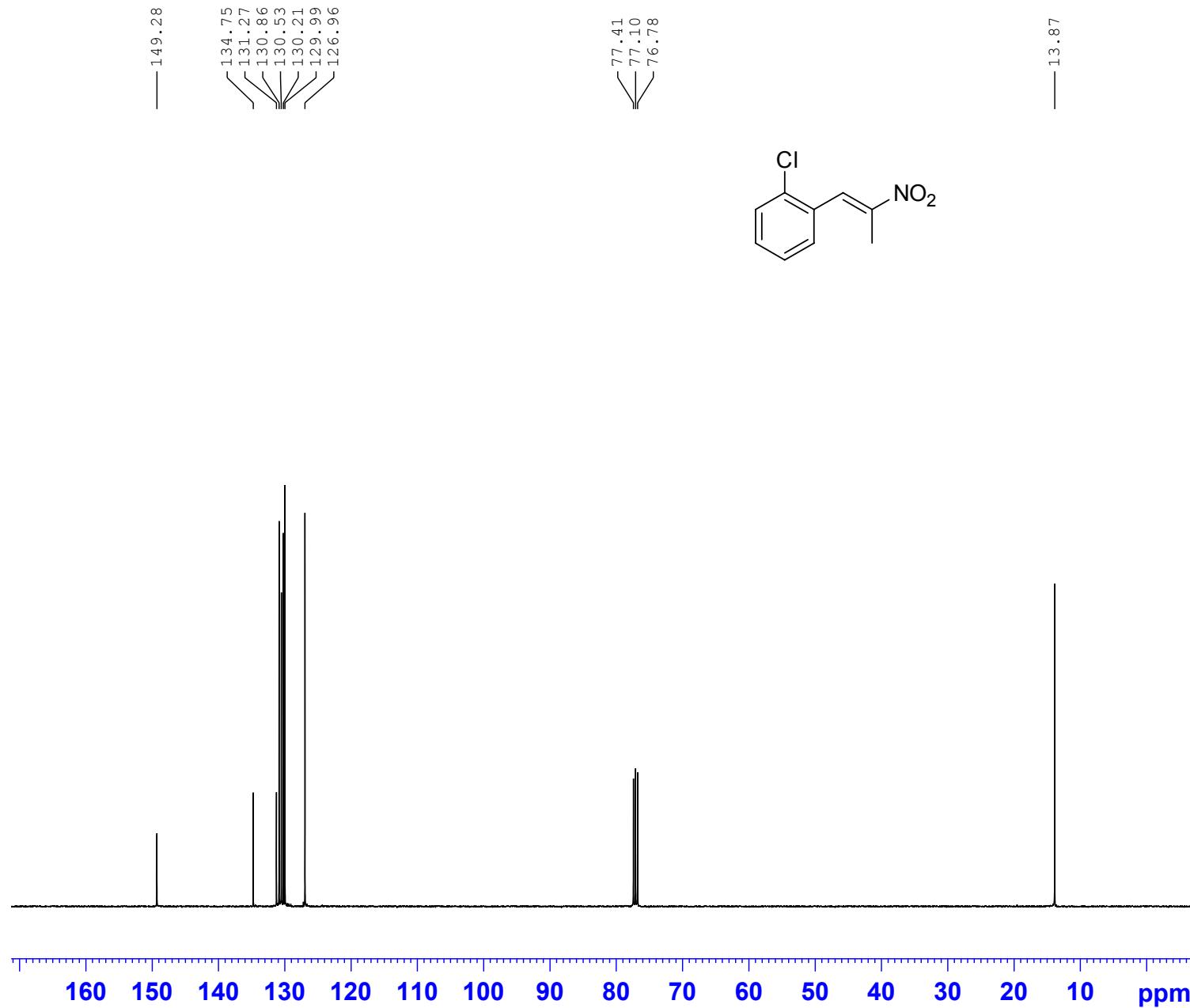
KL10
PROTON CDC13 {E:\NMR Data} skl 27



NAME Jul18-2012
EXPNO 1
PROCNO 1
Date_ 20120718
Time 17.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 304.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL10
C13CPD CDC13 {E:\NMR Data} skl 27



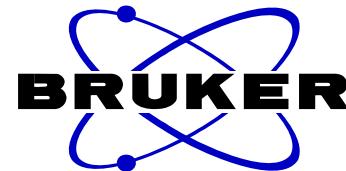
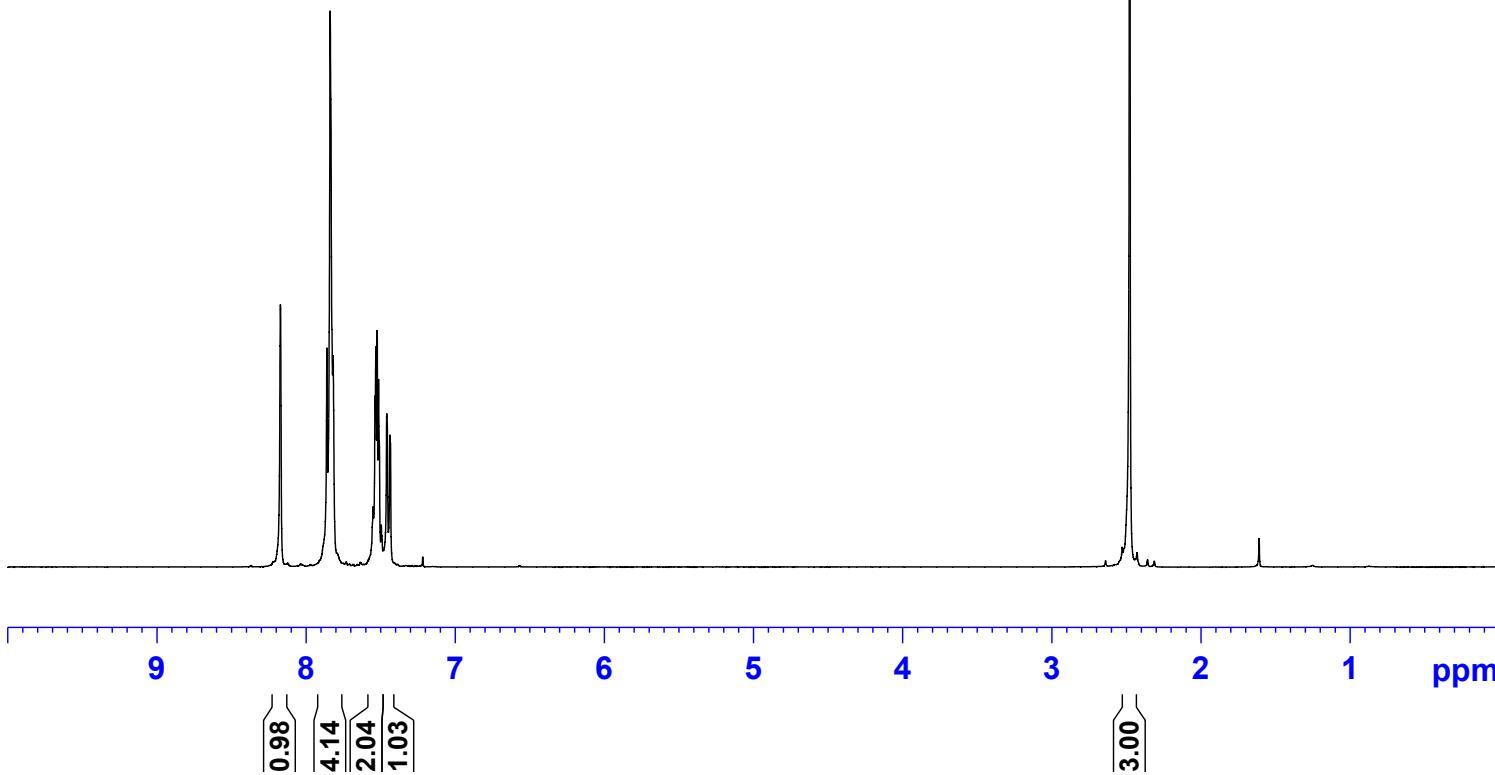
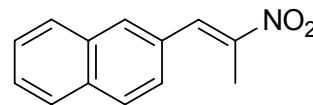
NAME Jul18-2012
EXPNO 4
PROCNO 1
Date_ 20120718
Time 20.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 306.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL21
PROTON CDC13 {E:\NMR Data} skl 44

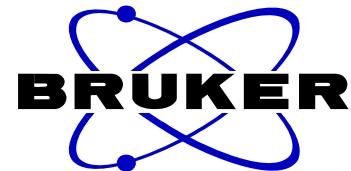
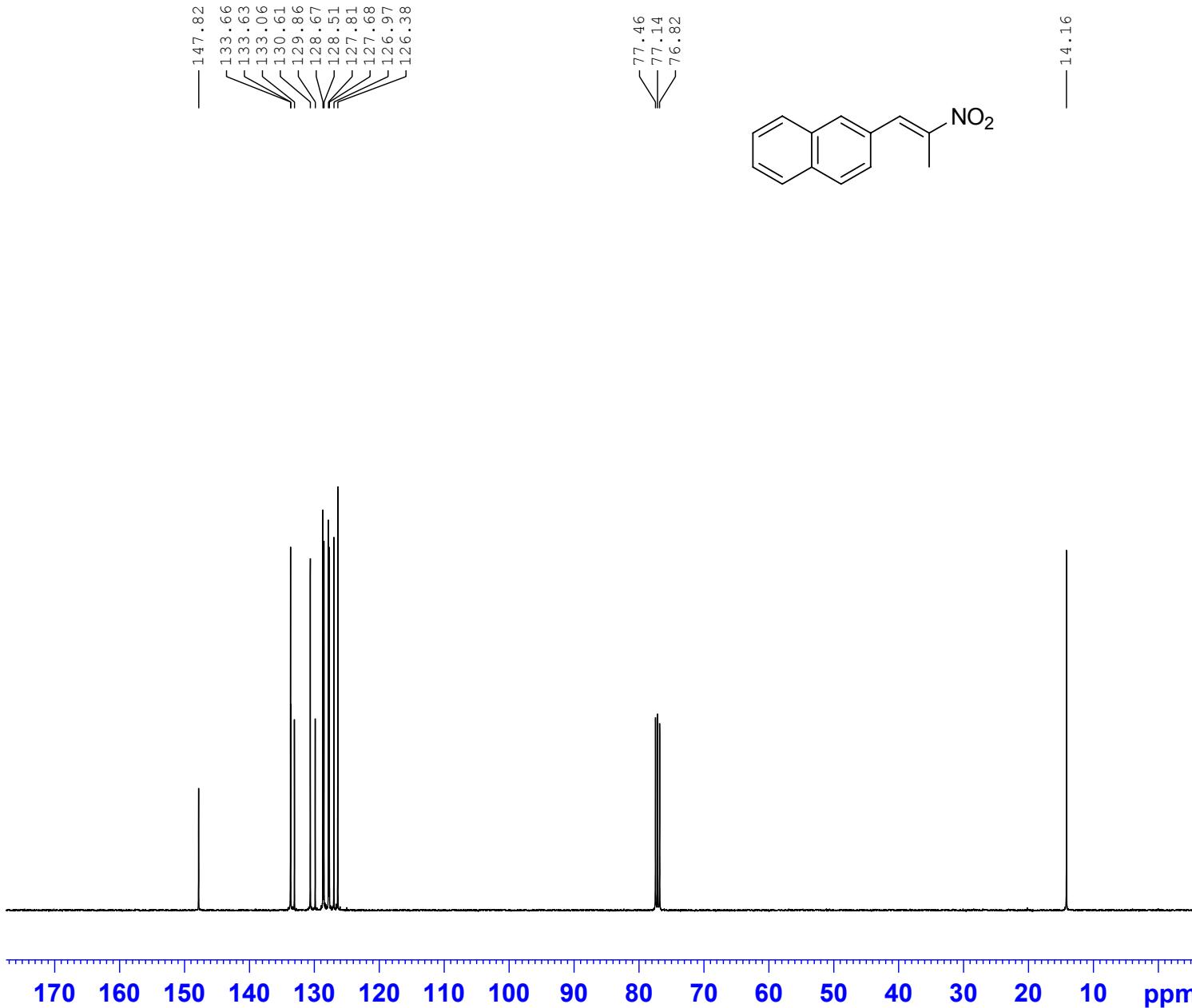
8.1726
7.8611
7.8390
7.8199
7.5514
7.5388
7.5333
7.5241
7.5149
7.5098
7.4965
7.4925
7.4600
7.4565
7.4386
7.4355



NAME Jul24-2012
EXPNO 4
PROCNO 1
Date_ 20120725
Time 1.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 302.7 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300262 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL21
C13CPD CDC13 {E:\NMR Data} skl 44



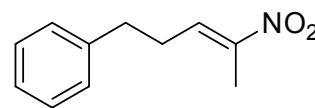
NAME Jul24-2012
EXPNO 6
PROCNO 1
Date_ 20120725
Time 4.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

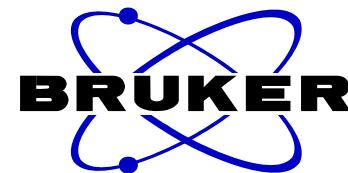
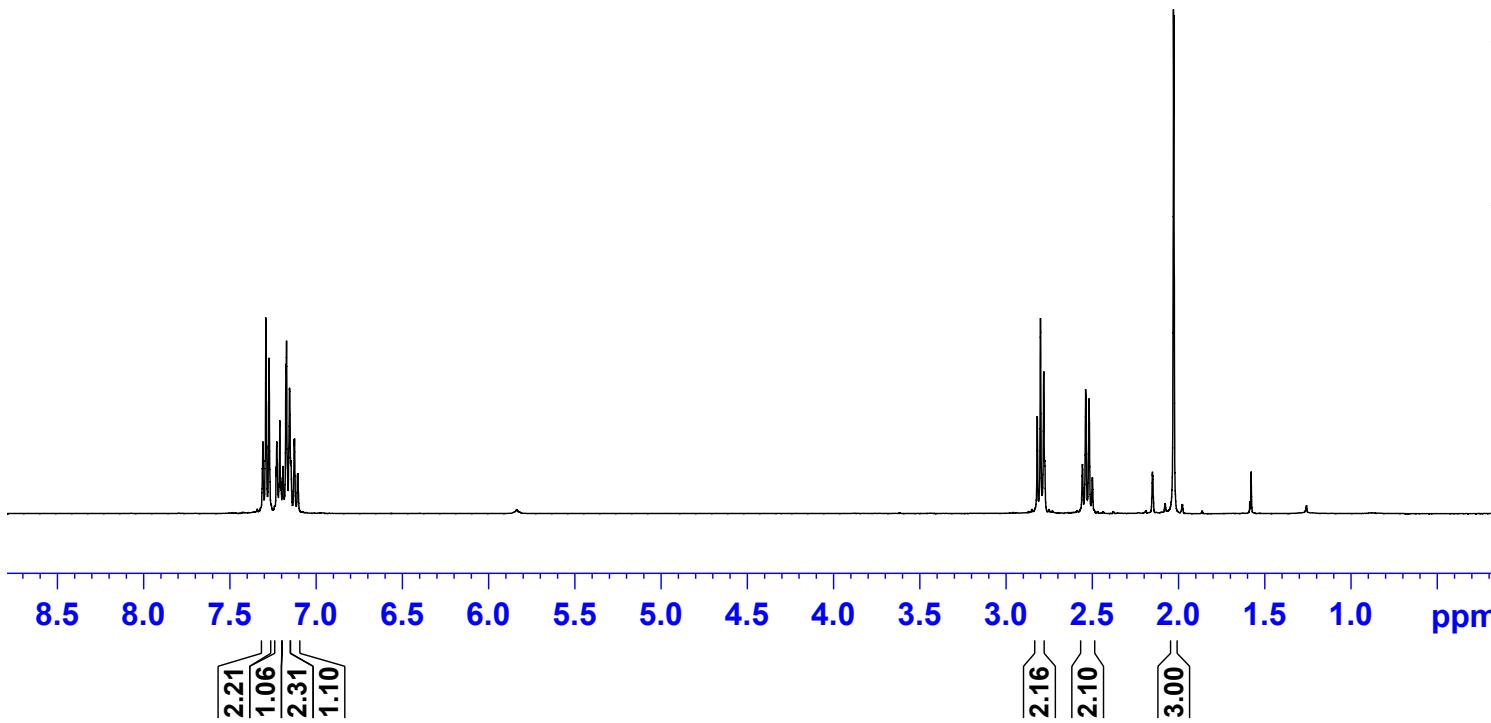
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL26
PROTON CDCl₃ {E:\NMR Data} skl 44

7.3115
7.3091
7.3053
7.2957
7.2916
7.2761
7.2727
7.2321
7.2284
7.2252
7.2156
7.2101
7.2041
7.1953
7.1918
7.1752
7.1717
7.1544
7.1475
7.1452
7.1276
7.1252
7.1079
7.1055

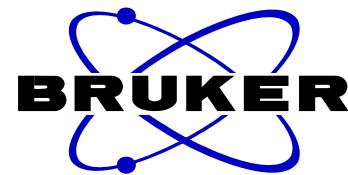
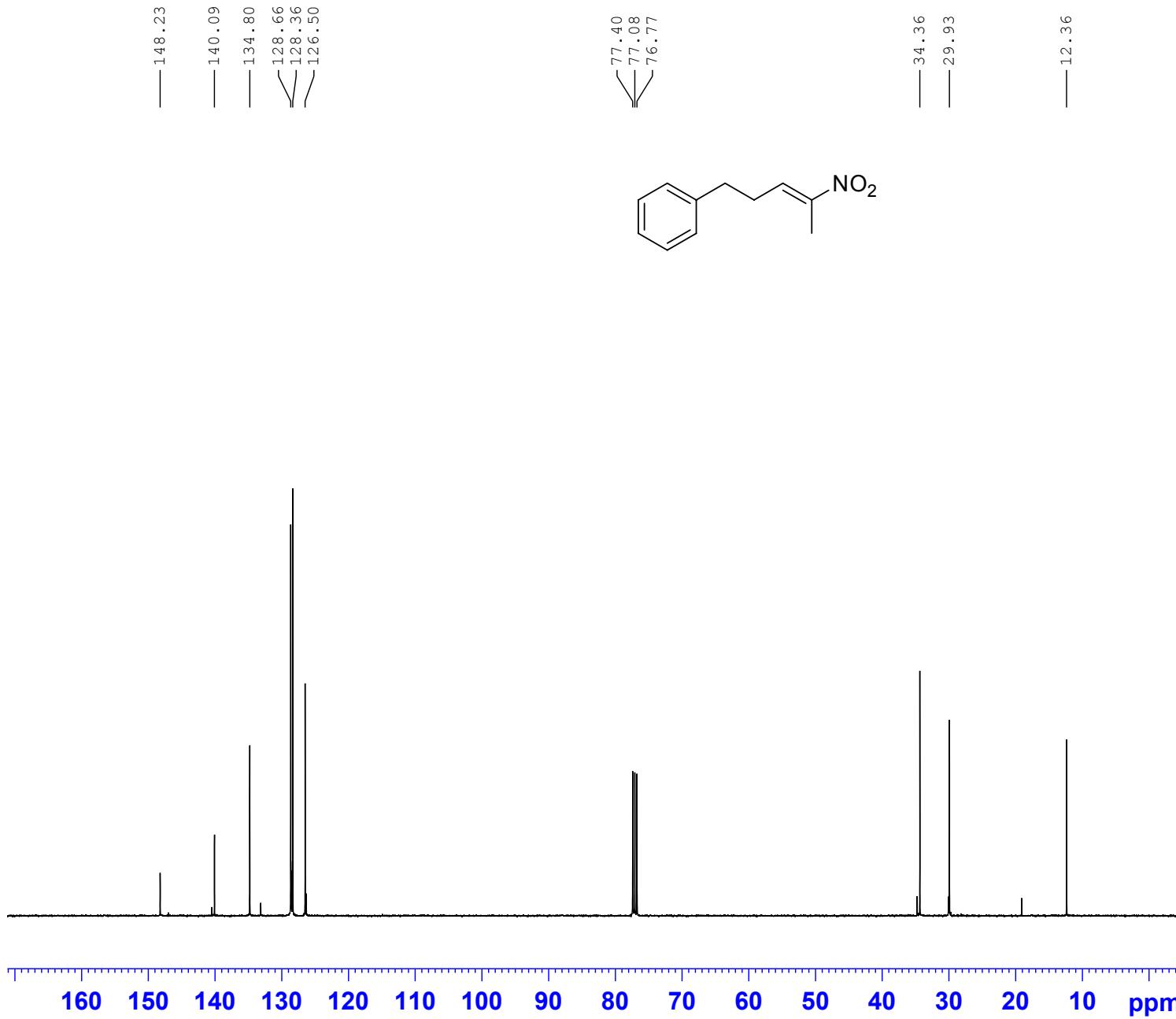


2.8190
2.8004
2.7816
2.5571
2.5386
2.5370
2.5191
2.4998
2.0292
2.0269



NAME Aug07-2012
EXPNO 4
PROCNO 1
Date_ 20120807
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 301.5 K
D1 1.0000000 sec
TDO 1

KL26
C13CPD32 CDC13 {E:\NMR Data} skl 44



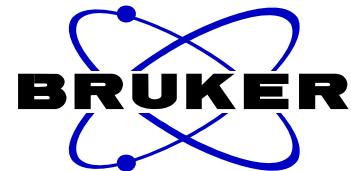
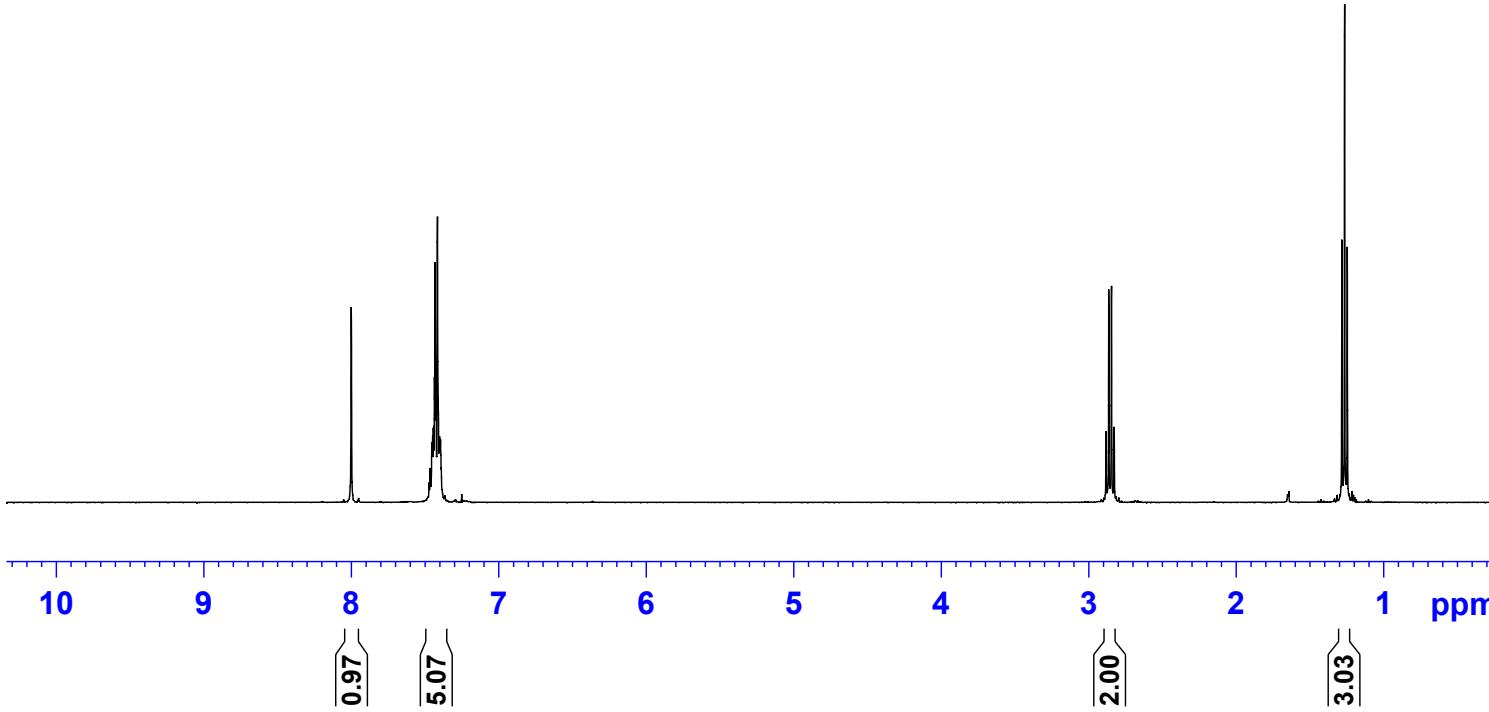
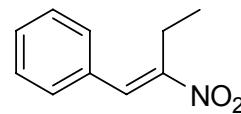
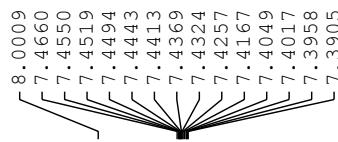
NAME Aug07-2012
EXPNO 7
PROCNO 1
Date_ 20120808
Time 7.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL29

PROTON CDC13 {E:\NMR Data} skl 14

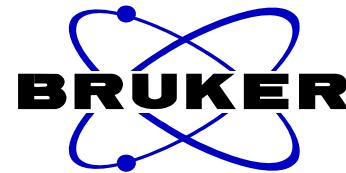
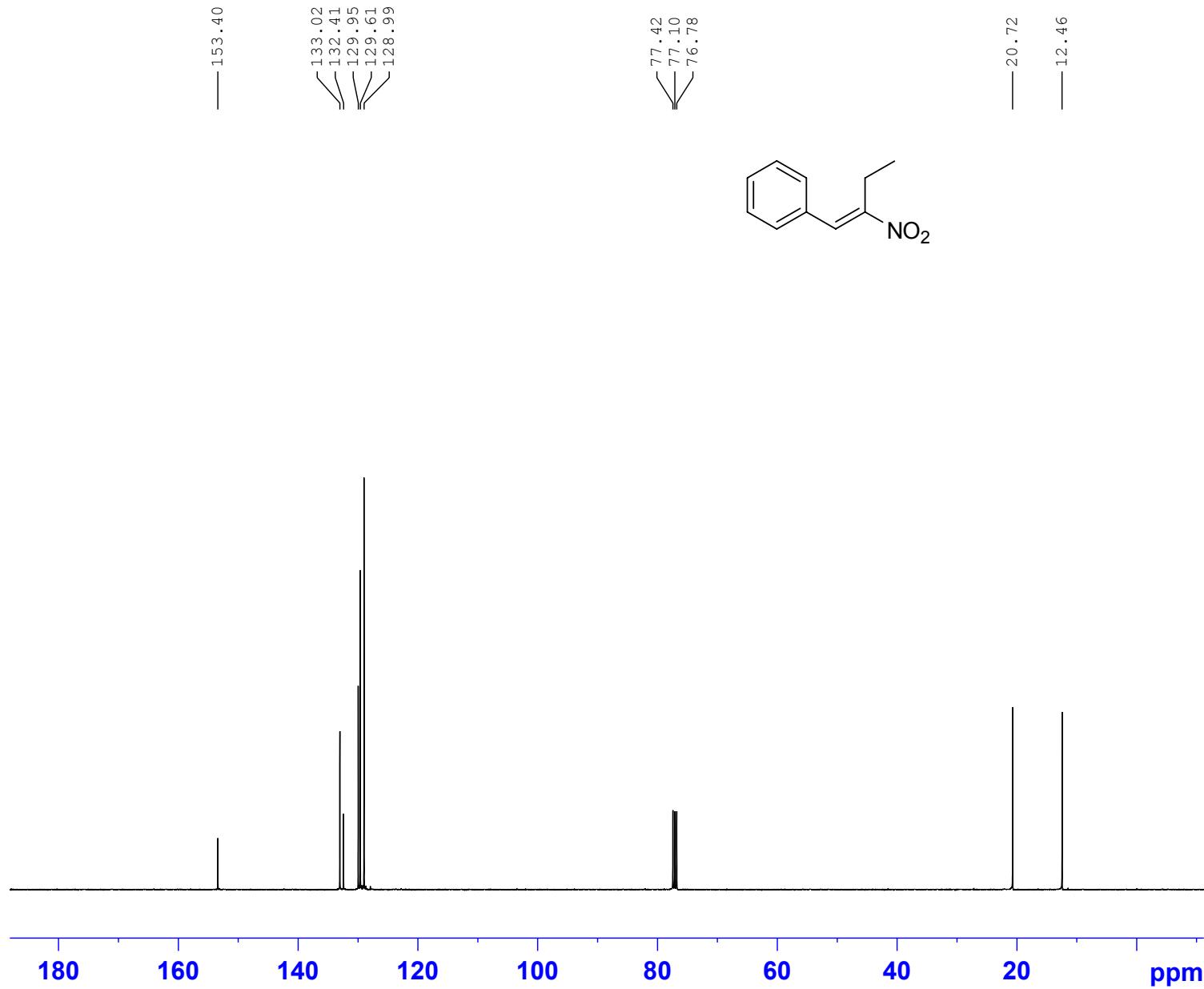


NAME Aug10-2012
EXPNO 8
PROCNO 1
Date_ 20120811
Time 15.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 50.8
DW 60.800 usec
DE 6.50 usec
TE 303.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300127 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL29
C13CPD32 CDC13 {E:\NMR Data} skl 14



NAME Aug10-2012
EXPNO 3
PROCNO 1
Date_ 20120811
Time 3.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

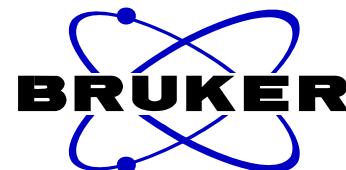
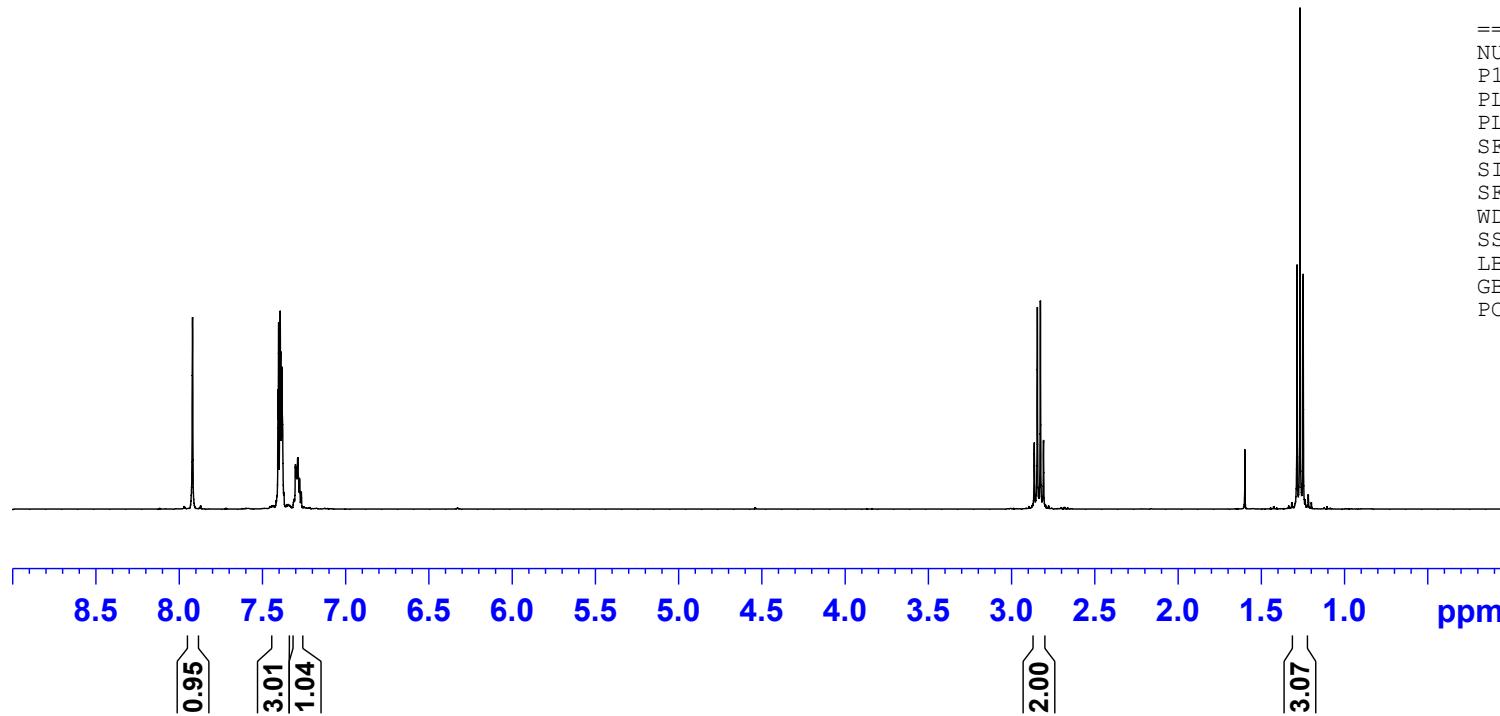
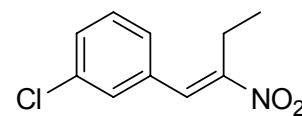
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL30
PROTON CDCl₃ {E:\NMR Data} skl 45

7.9189
7.4051
7.4018
7.3957
7.3919
7.3895
7.3862
7.3850
7.3818
7.3720
7.3693
7.3664
7.3004
7.2970
7.2961
7.2934
7.2907
7.2874
7.2853
7.2822
7.2758
7.2743
7.2649

2.8633
2.8448
2.8263
2.8079

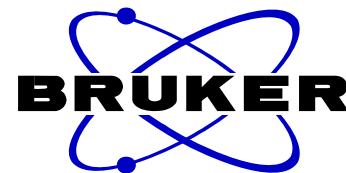
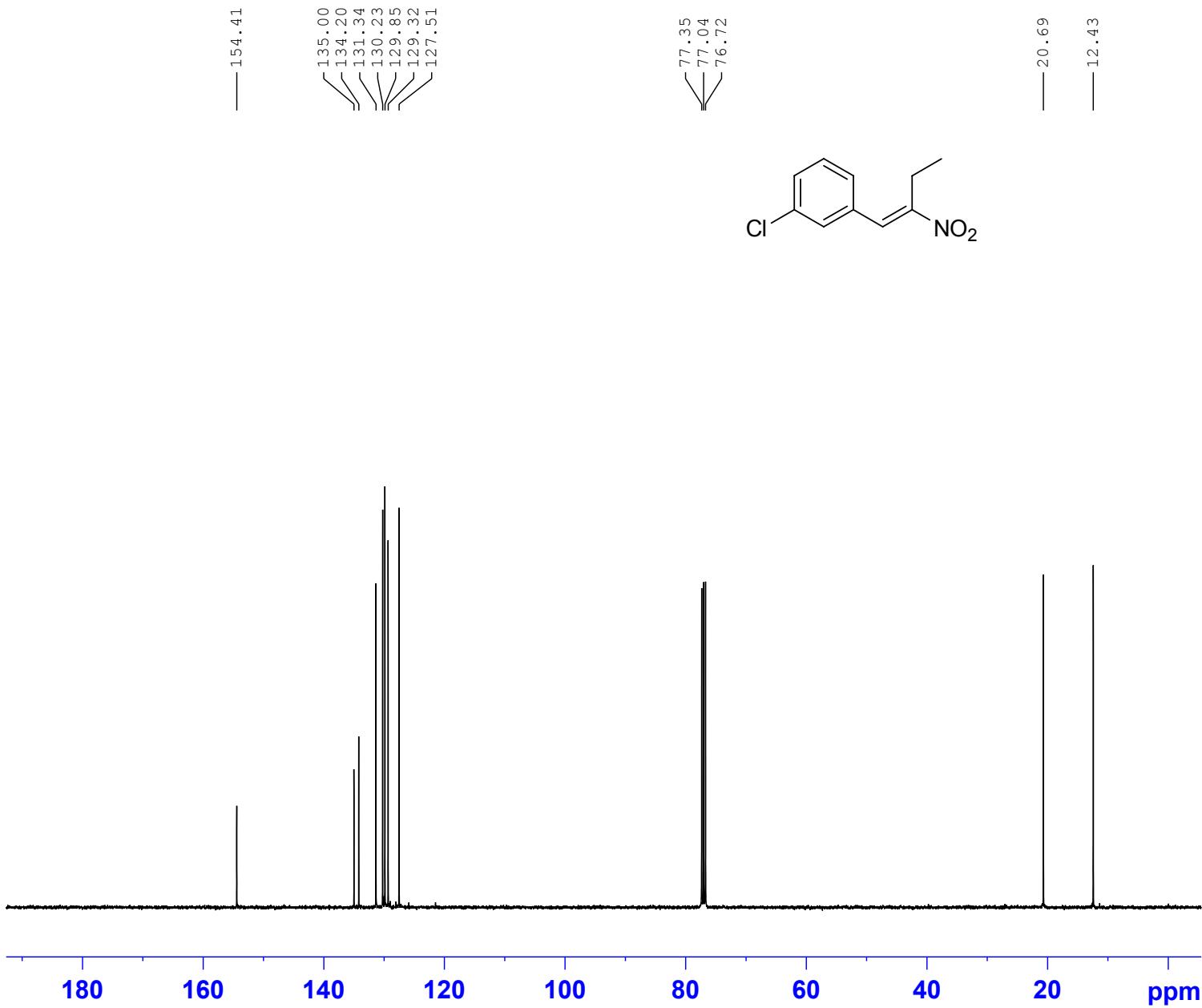
1.2850
1.2665
1.2480



NAME Aug11-2012
EXPNO 6
PROCNO 1
Date_ 20120812
Time 3.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 304.1 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL30
C13CPD32 CDC13 {E:\NMR Data} skl 45



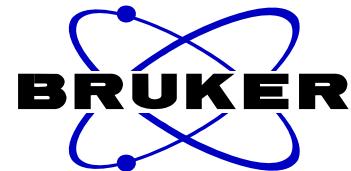
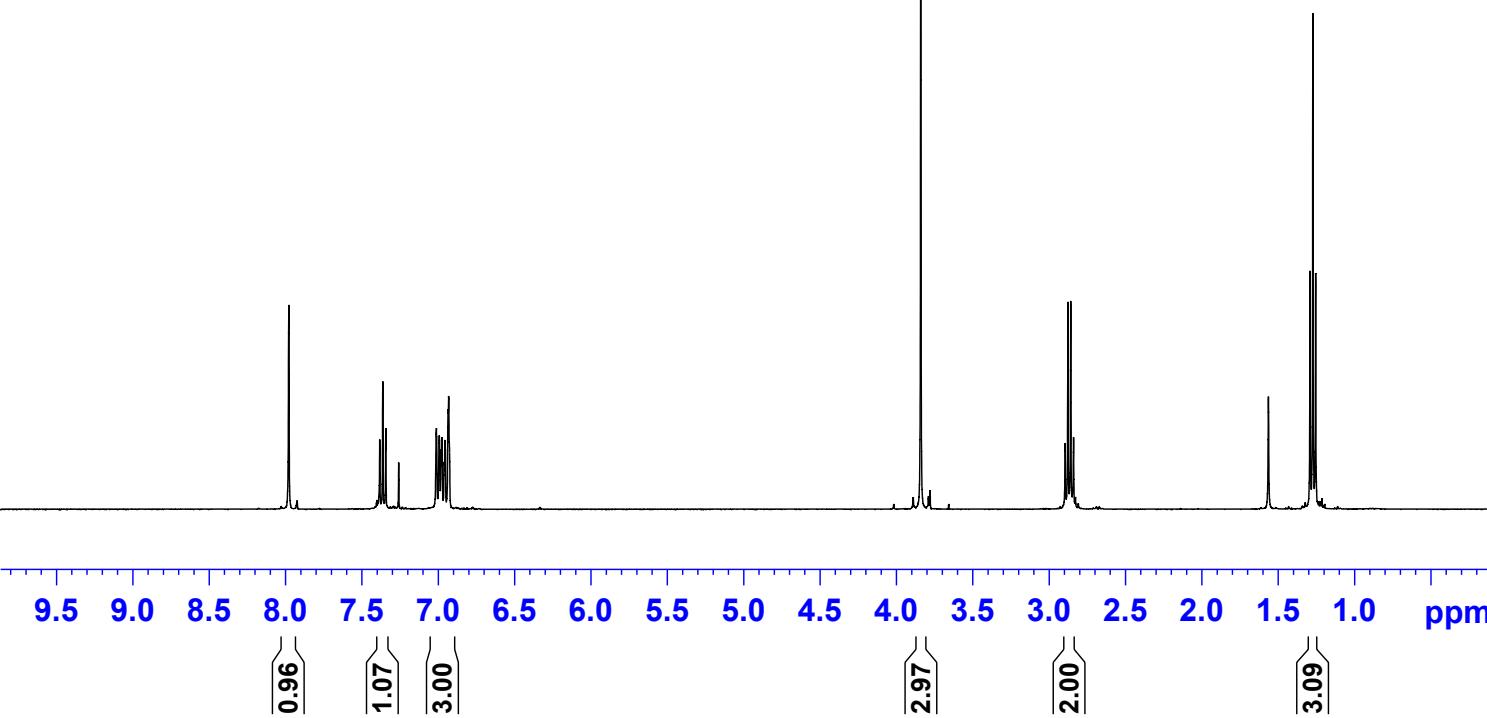
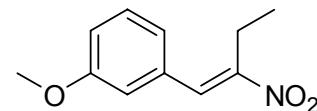
NAME Aug11-2012
EXPNO 8
PROCNO 1
Date_ 20120812
Time 5.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL31
PROTON CDC13 {E:\NMR Data} skl 46

7.9787
7.3831
7.3632
7.3433
7.2588
7.0122
6.9929
6.9815
6.9753
6.9753
6.9607
6.9547
6.9359
6.9317

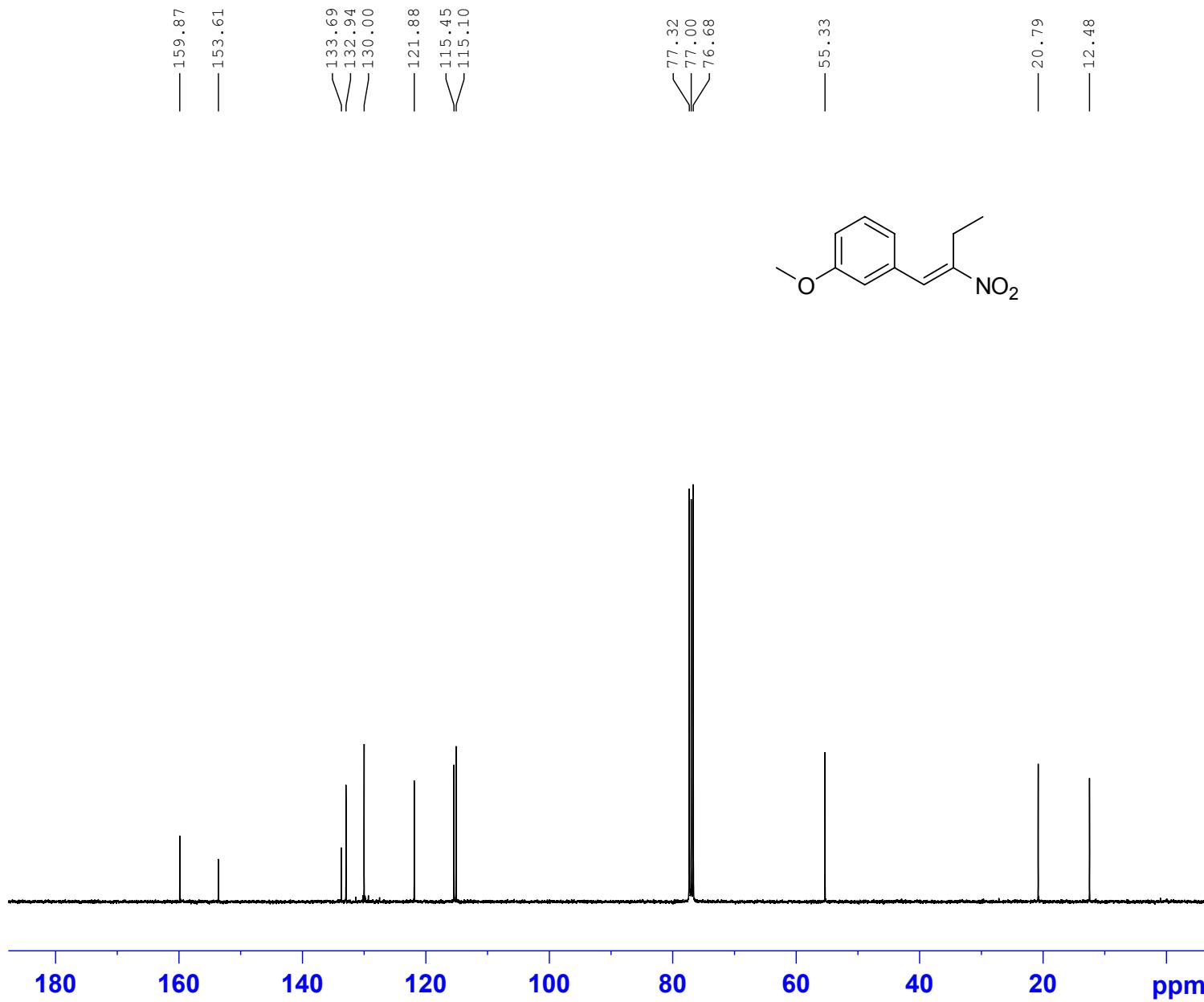


NAME Aug11-2012
EXPNO 9
PROCNO 1
Date_ 20120812
Time 5.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.50 usec
TE 303.9 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300102 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL31
C13CPD32 CDC13 {E:\NMR Data} skl 46

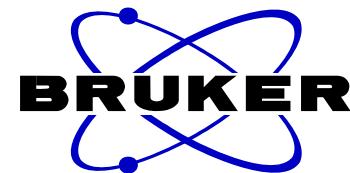
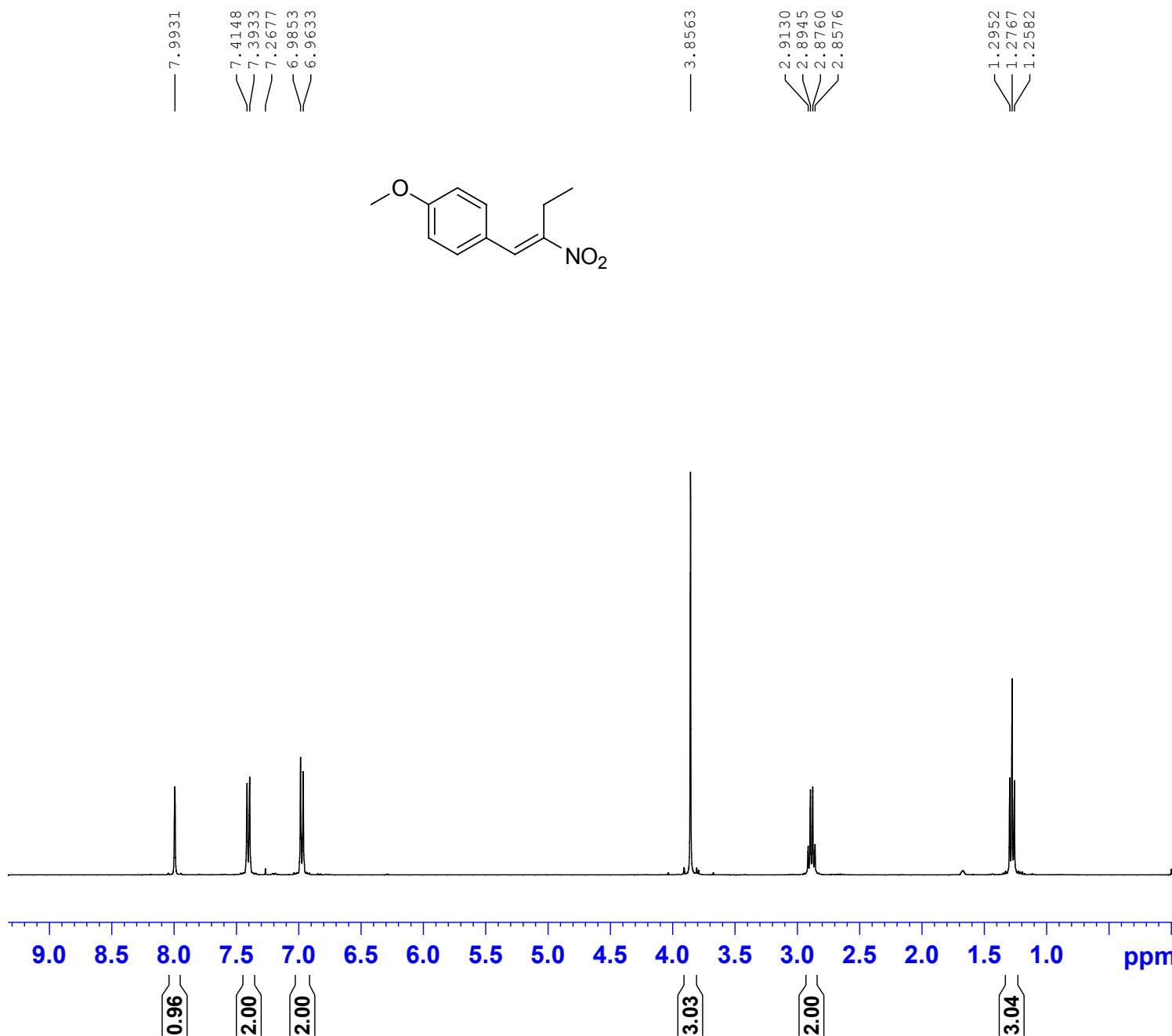


NAME Aug11-2012
EXPNO 11
PROCNO 1
Date_ 20120812
Time 7.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

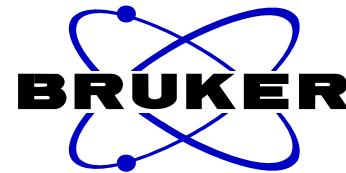
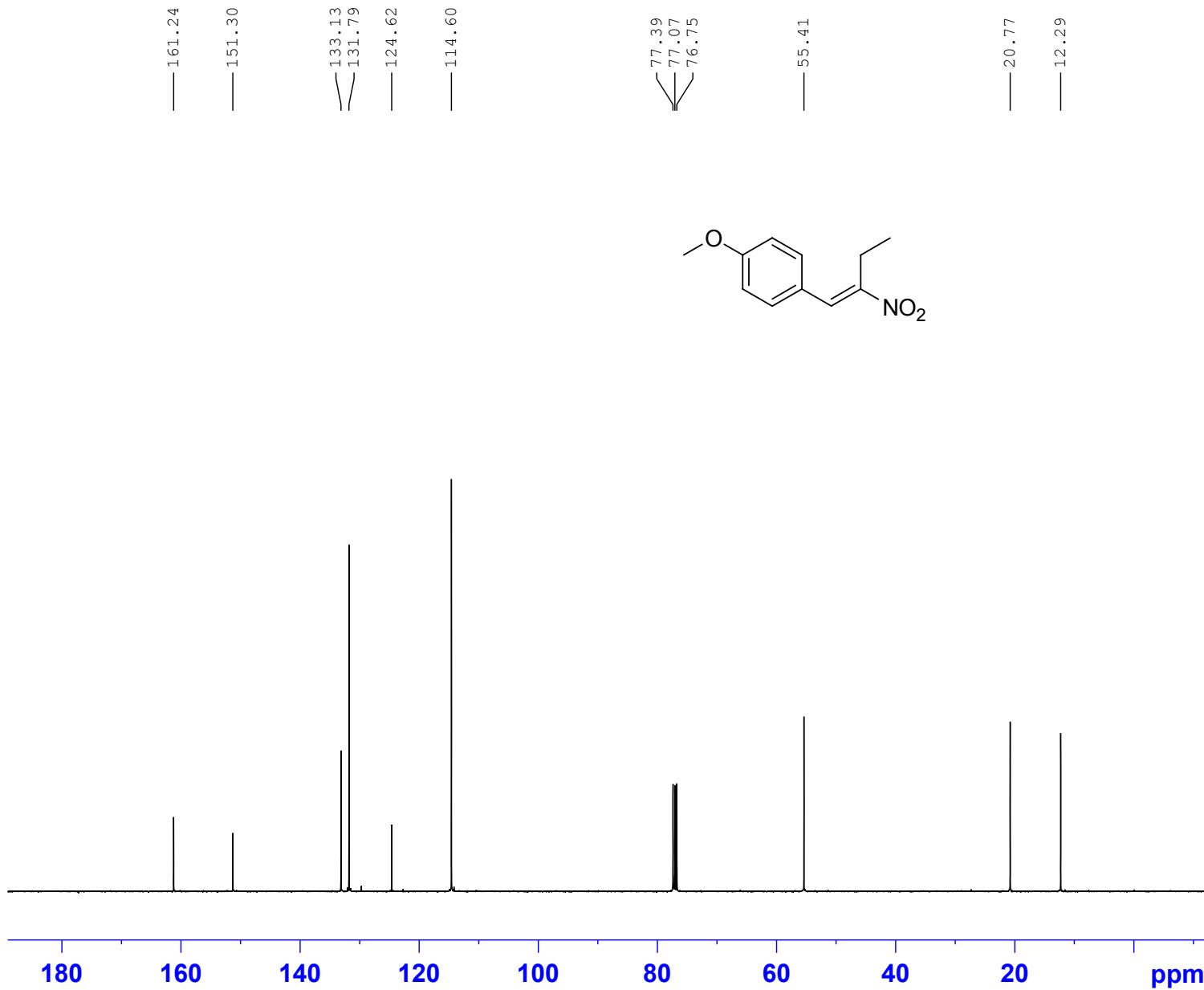
KL32
PROTON CDCl₃ {E:\NMR Data} skl 27



NAME Aug13-2012
EXPNO 5
PROCNO 1
Date_ 20120813
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 301.5 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL32
C13CPD CDC13 {E:\NMR Data} skl 27



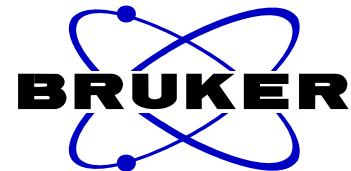
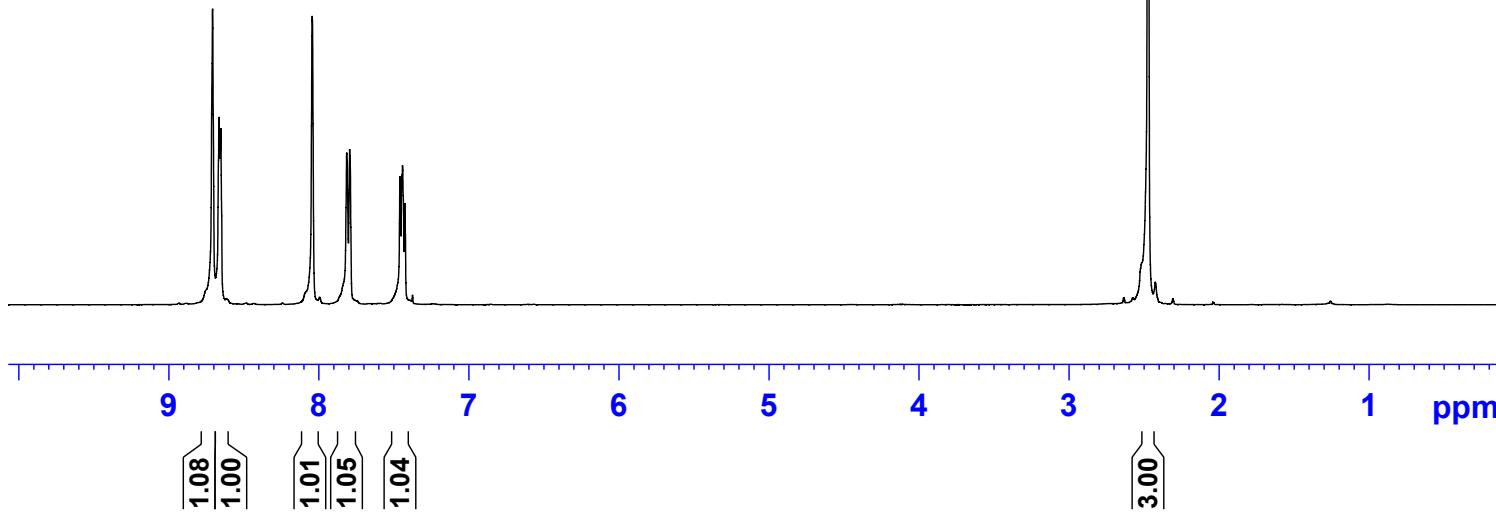
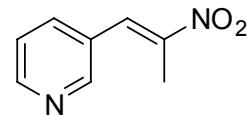
NAME Aug13-2012
EXPNO 7
PROCNO 1
Date_ 20120813
Time 21.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 304.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL23
PROTON CDC13 {E:\NMR Data} skl 28

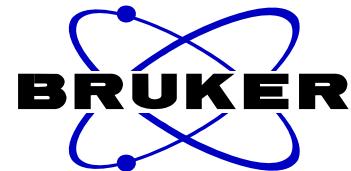
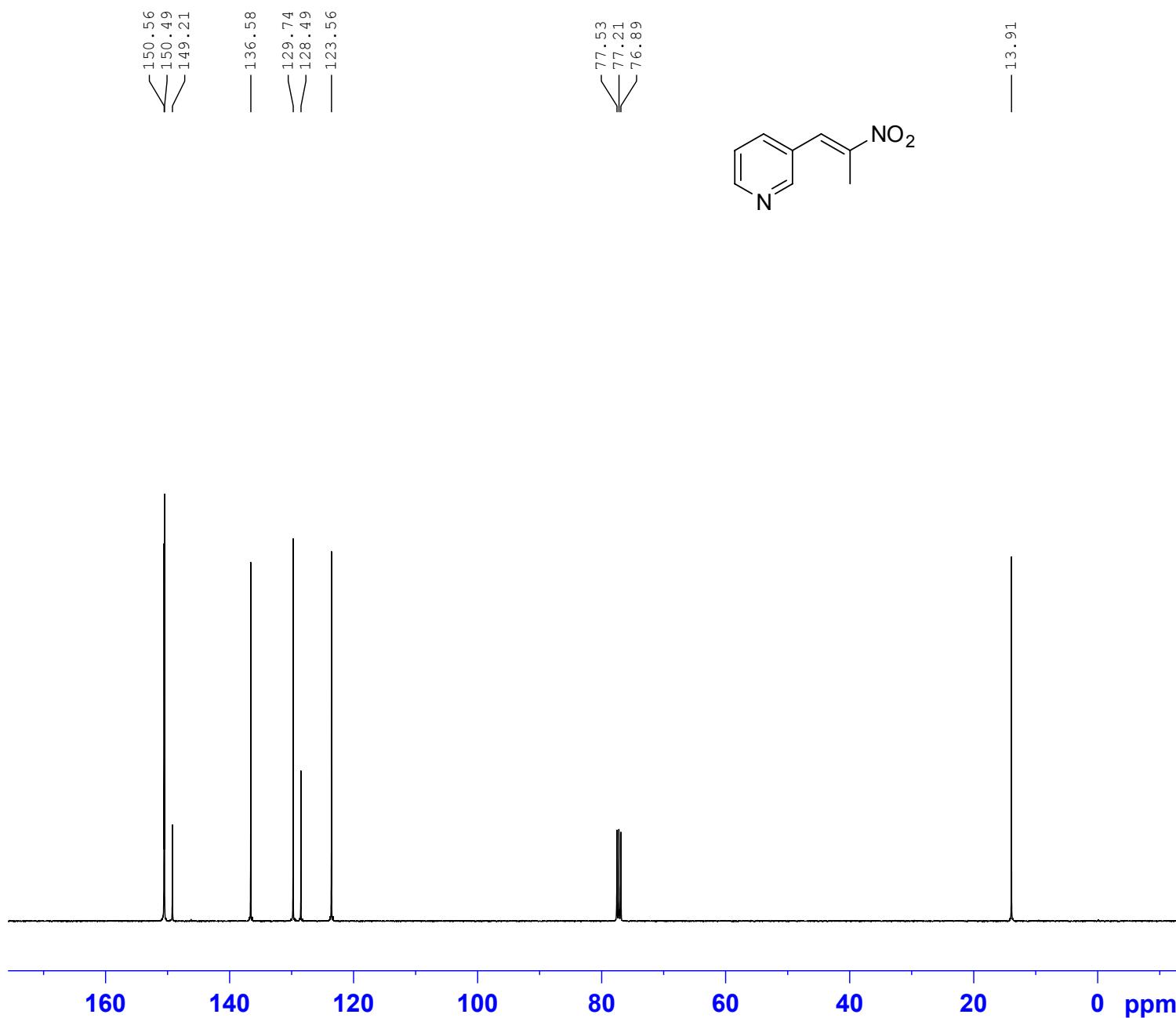
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8.6645
8.6582
8.6529
8.0431
7.8136
7.8102
7.4412
7.4435
7.4464
7.4564
7.4586
7.7937



NAME Jul25-2012
EXPNO 8
PROCNO 1
Date_ 20120726
Time 9.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1299640 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL23
C13CPD CDC13 {E:\NMR Data} skl 28

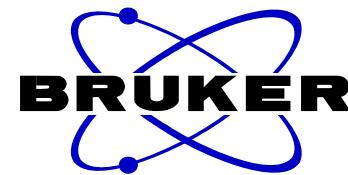
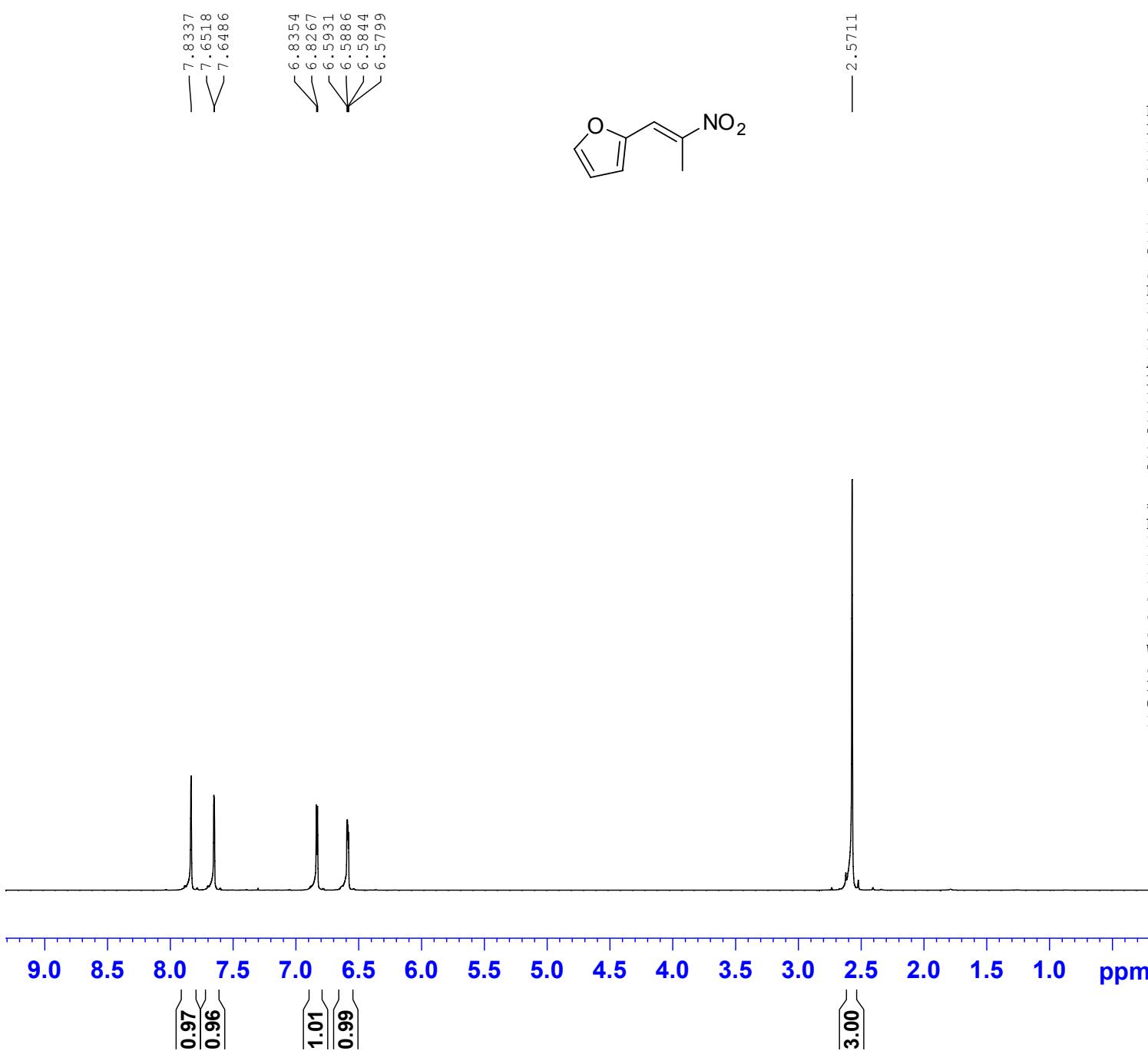


NAME Jul25-2012
EXPNO 7
PROCNO 1
Date_ 20120726
Time 4.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.6 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL22

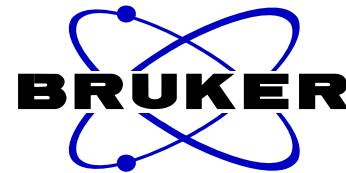
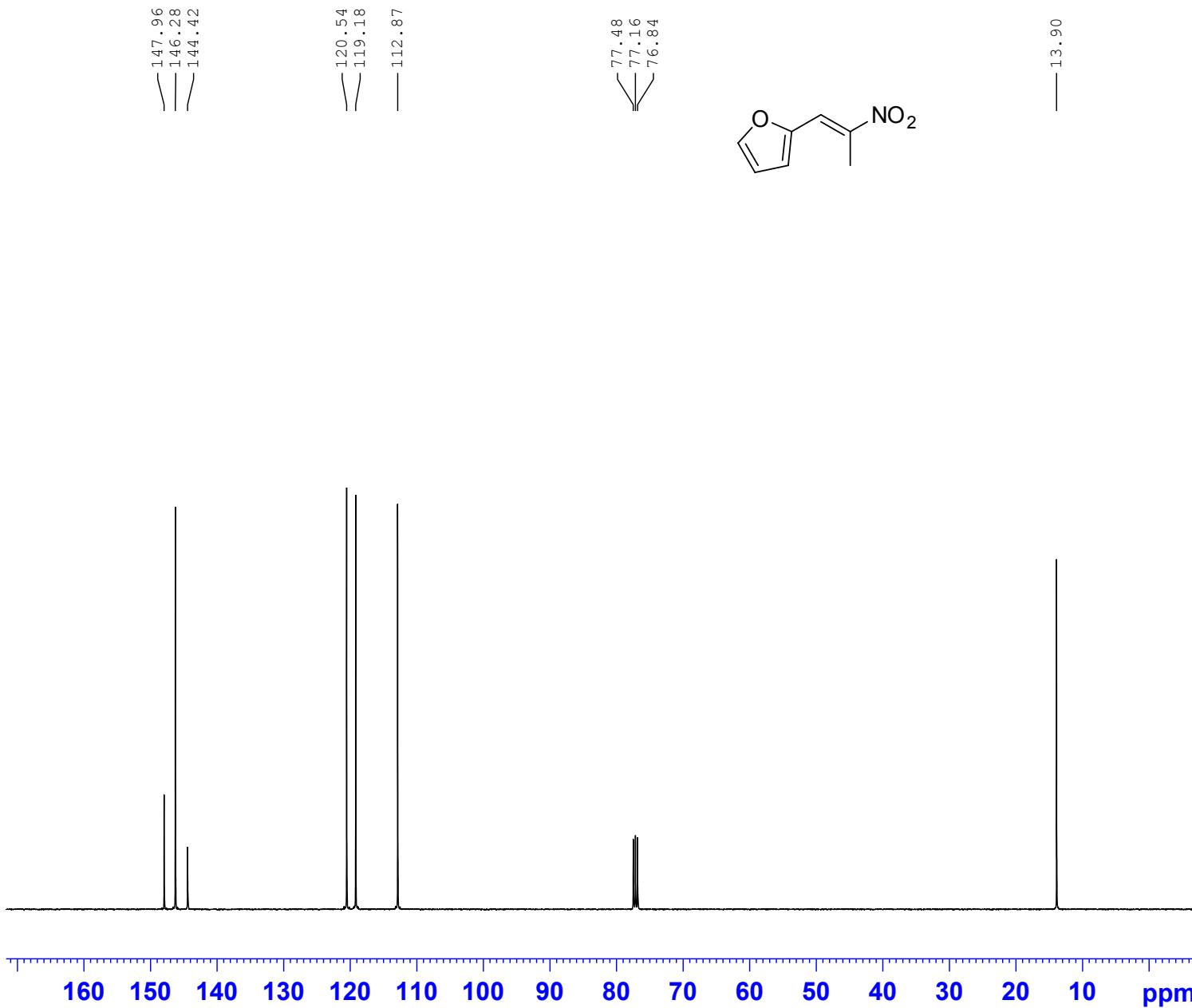
PROTON CDCl₃ {E:\NMR Data} skl 44

NAME Jul25-2012
 EXPNO 9
 PROCNO 1
 Date_ 20120726
 Time 9.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 32
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 40.3
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1299933 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL22
C13CPD CDC13 {E:\NMR Data} skl 44

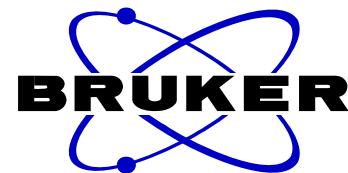
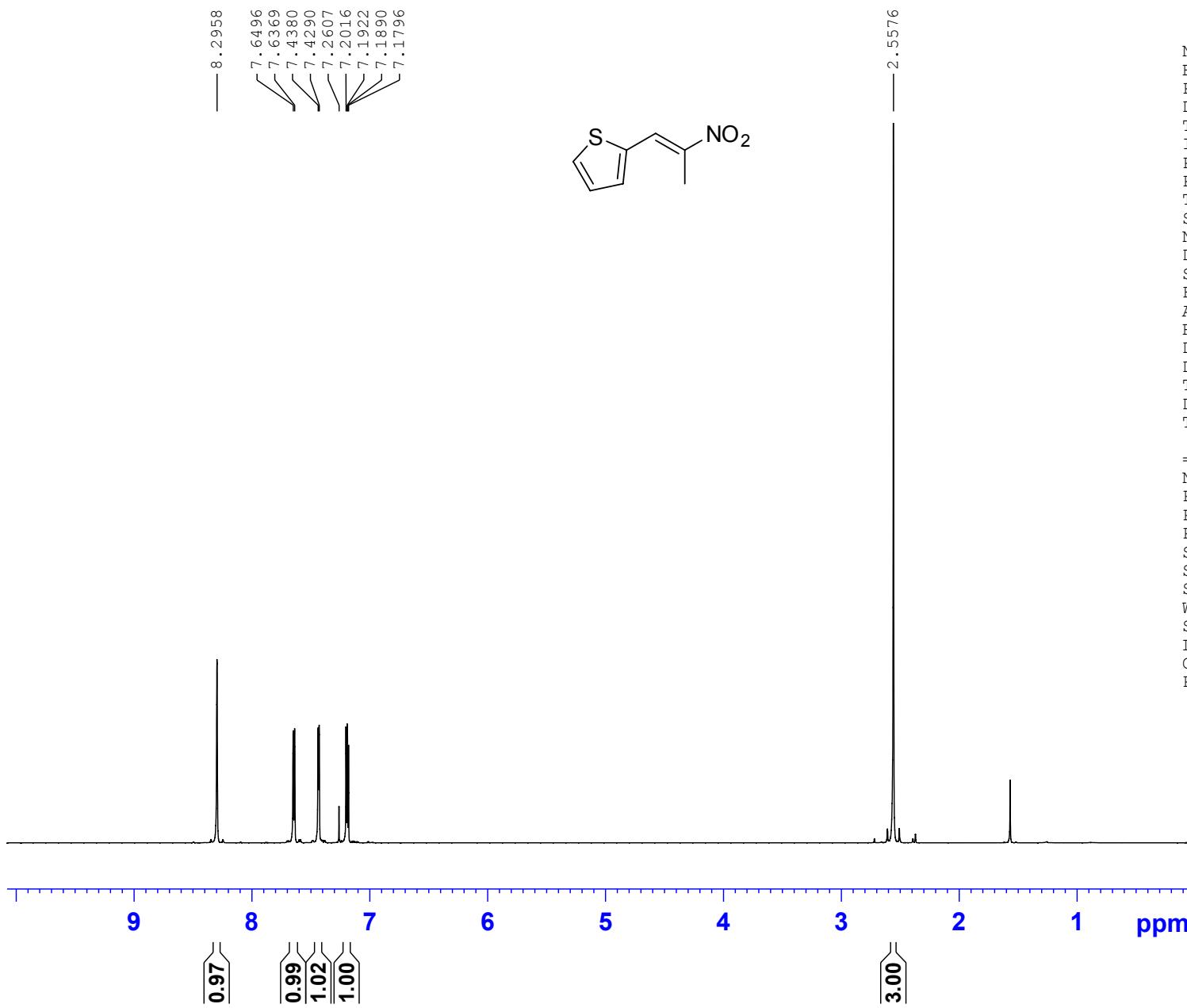


NAME Jul25-2012
EXPNO 5
PROCNO 1
Date_ 20120726
Time 0.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.9 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

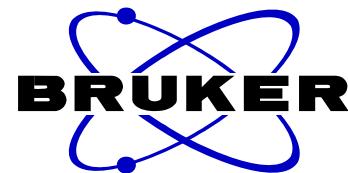
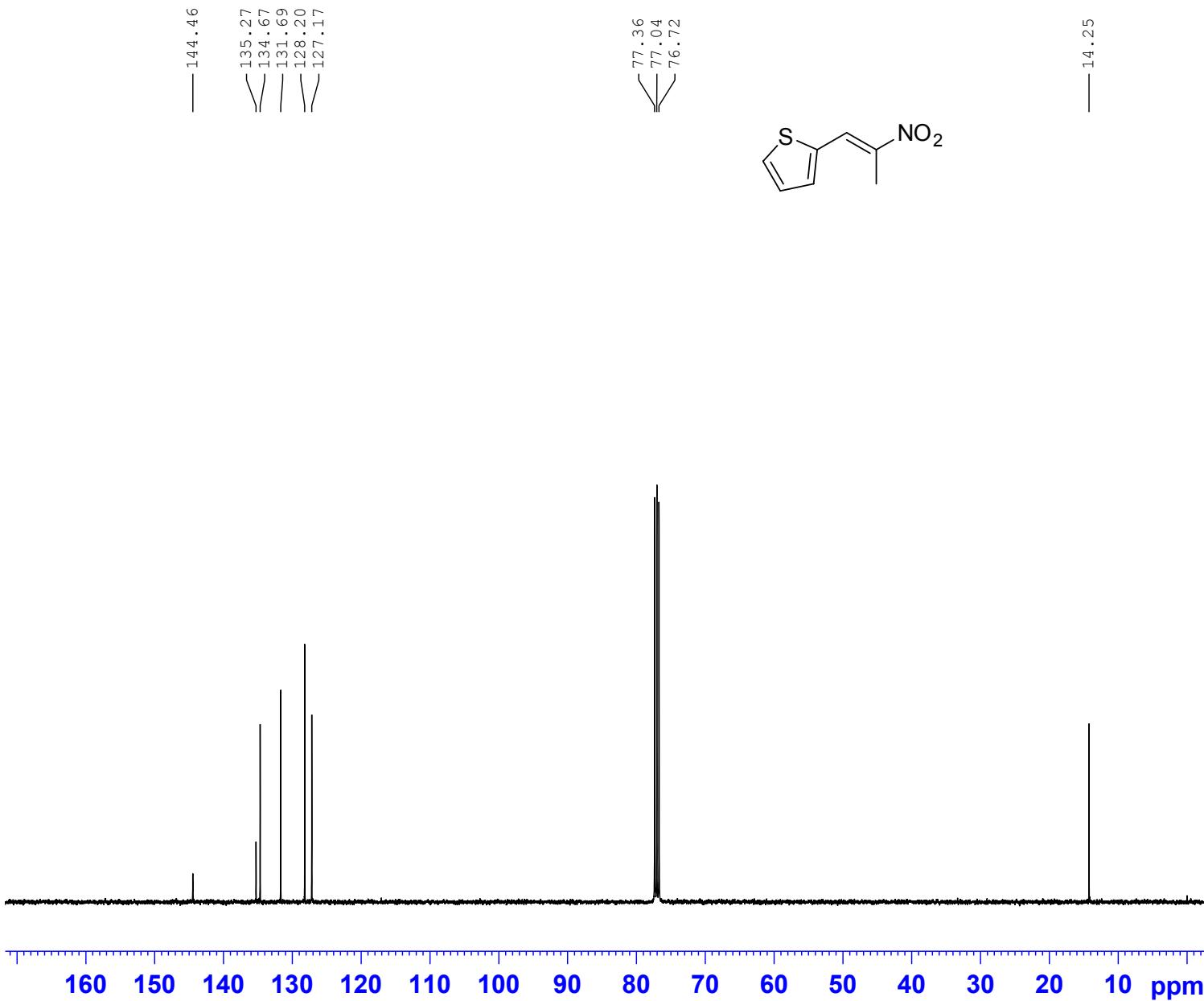
KL34
PROTON CDC13 {E:\NMR Data} skl 27



NAME Sep21-2012
EXPNO 10
PROCNO 1
Date_ 20120922
Time 6.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 6.50 usec
TE 302.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL34
C13CPD CDC13 {E:\NMR Data} skl 27



NAME Sep21-2012
EXPNO 12
PROCNO 1
Date_ 20120922
Time 7.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.6 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127668 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

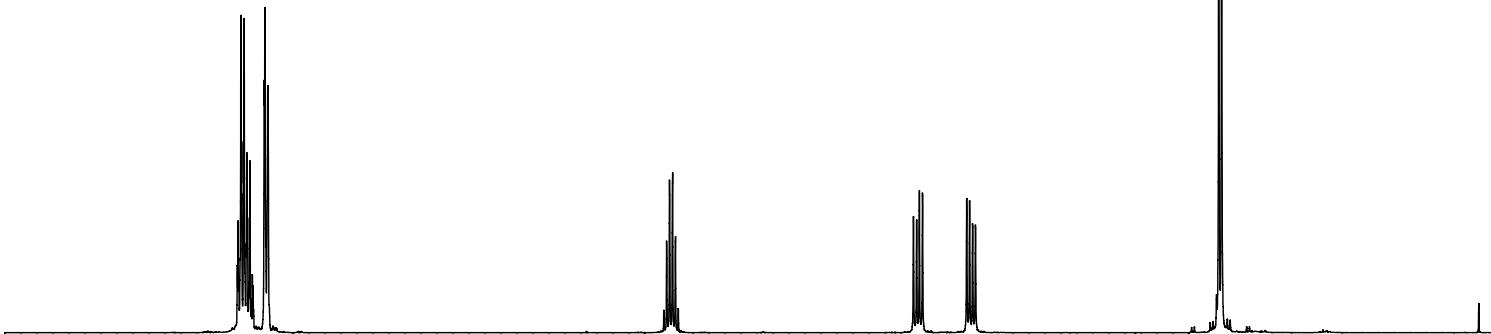
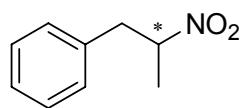
KL01 REDUCTION

PROTON CDCl₃ {E:\NMR Data} skl 28

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7.3054
7.3001
7.2959
7.2852
7.2816
7.2761
7.2687
7.2650
7.2610
7.2536
7.2473
7.2391
7.2323
7.2287
7.2256
7.1624
7.1584
7.1534
7.1418
7.1321

4.8057
4.7892
4.7720
4.7540
4.7368
4.7203
3.3334
3.3146
3.2980
3.2797
3.0190
3.0023
2.9841
2.9669

1.5331
1.5164



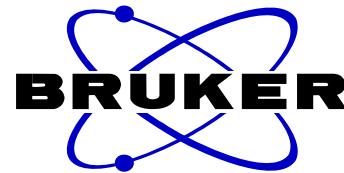
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

3.00 / 1.96

0.99

1.00 / 1.01

3.00



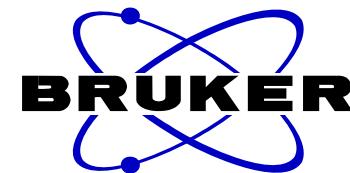
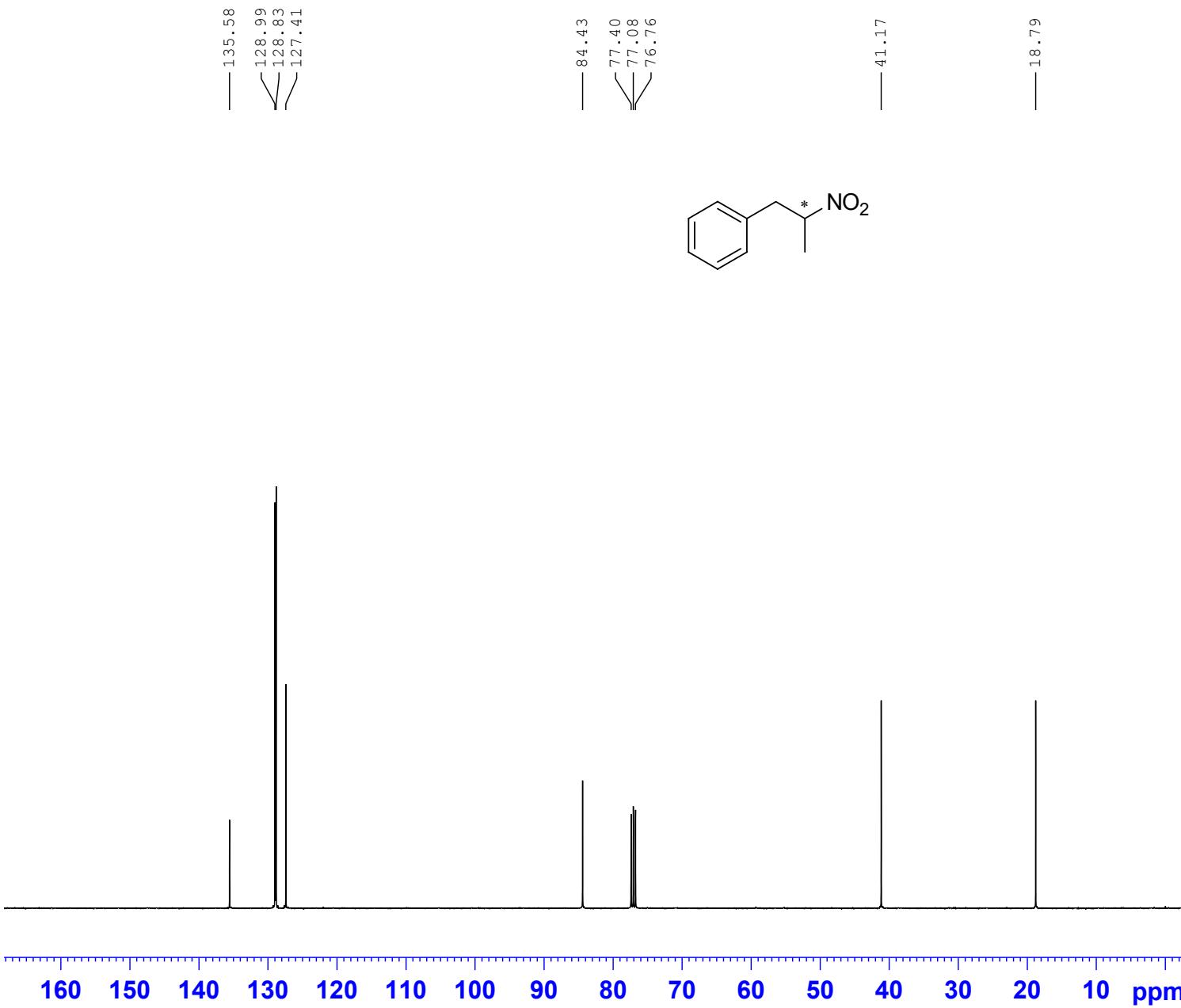
Jun29-2011

NAME 3
EXPNO 1
PROCNO 1
Date_ 20110629
Time 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 301.9 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====

NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300206 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL01 REDUCTION
C13CPD CDC13 {E:\NMR Data} skl 44

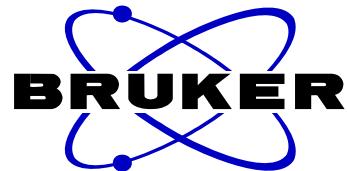
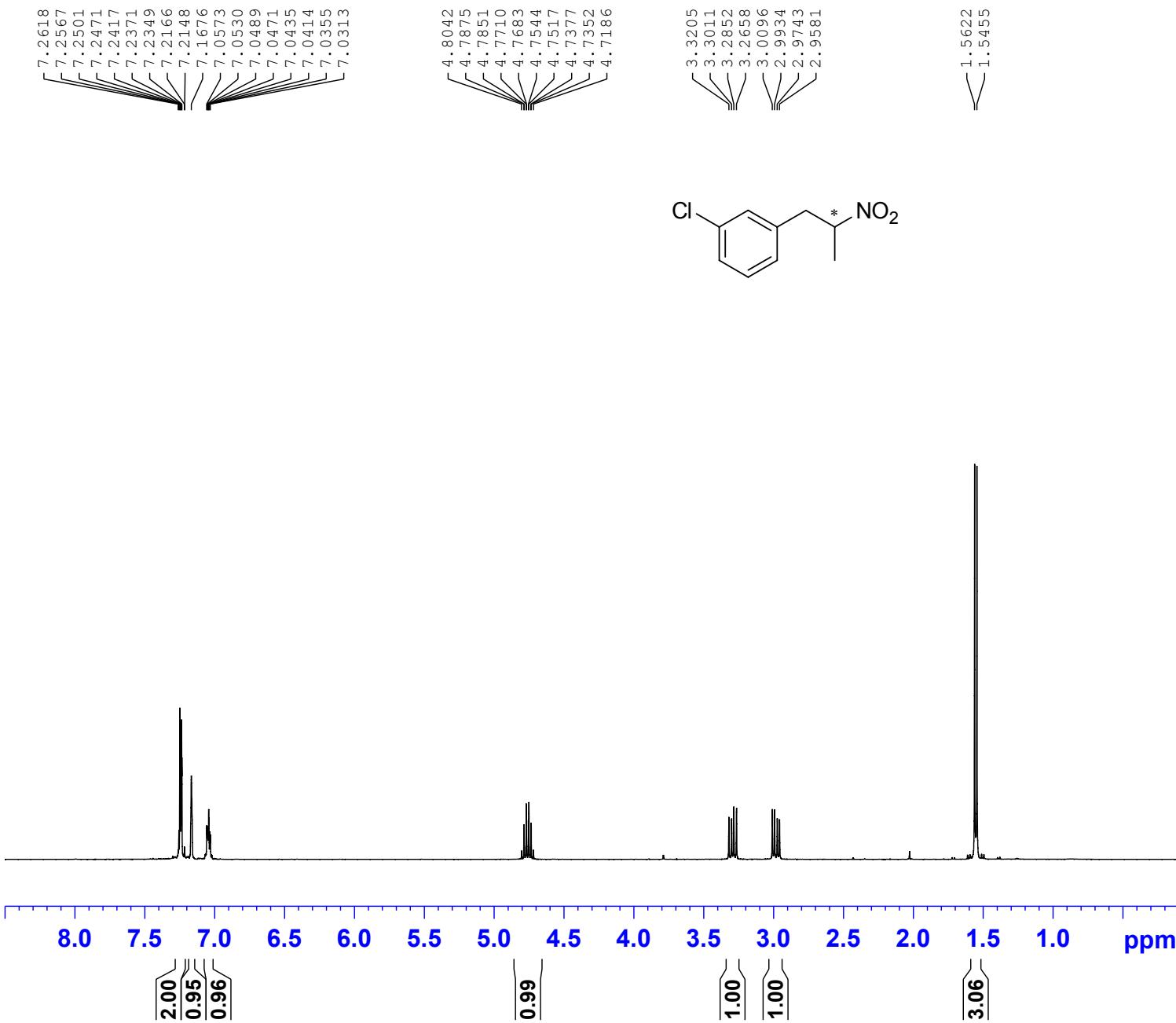


NAME Jun30-2011
EXPNO 3
PROCNO 1
Date_ 20110701
Time 19.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 304.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

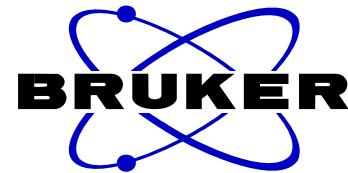
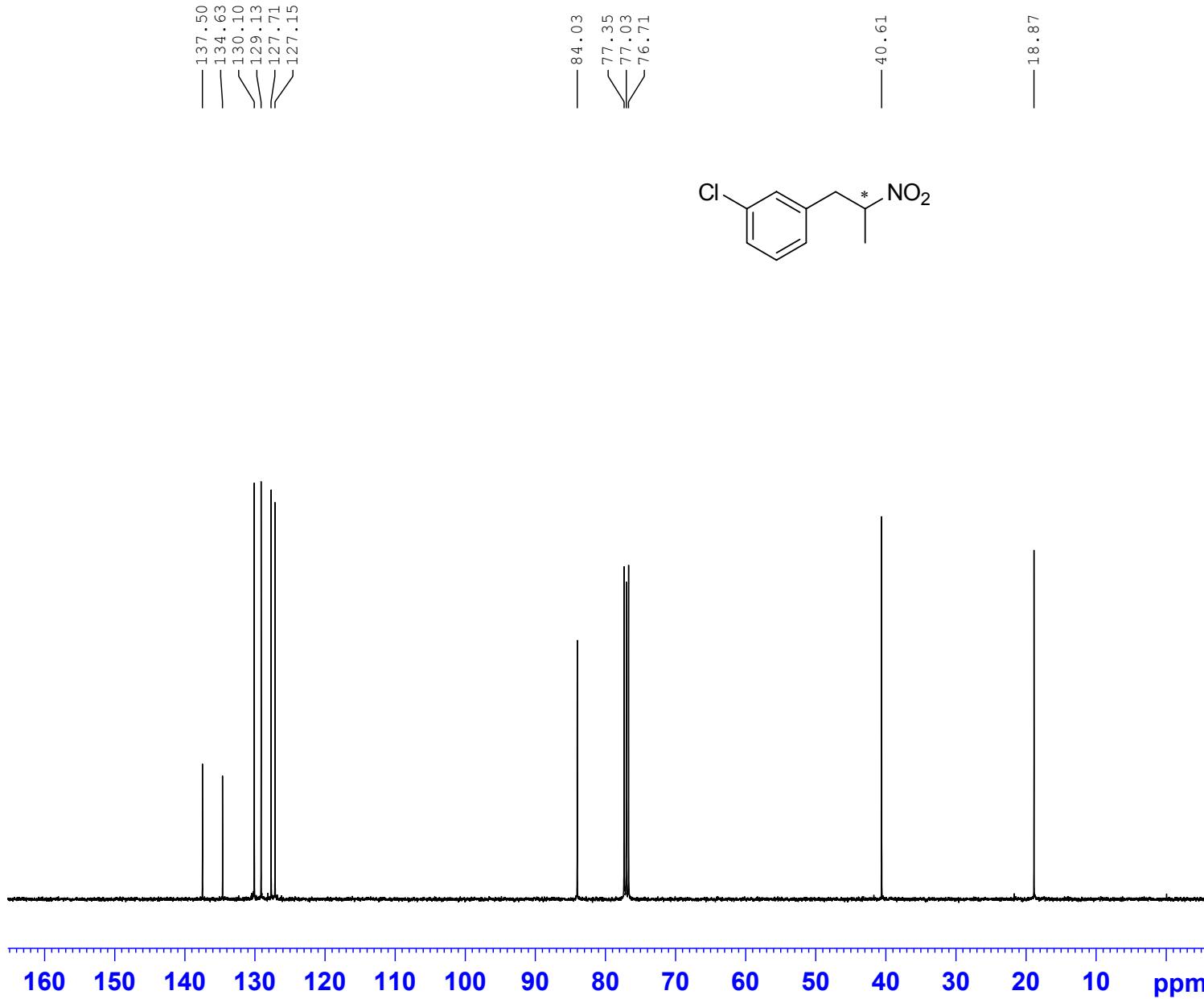
KL02 REDUCTION
PROTON CDC₁₃ {E:\NMR Data} skl 14



NAME Jul01-2011
EXPNO 9
PROCNO 1
Date_ 20110702
Time 9.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 302.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL02 REDUCTION
C13CPD CDC13 {E:\NMR Data} skl 14

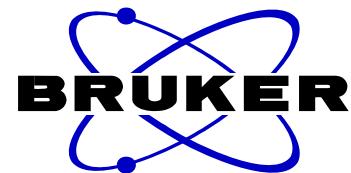
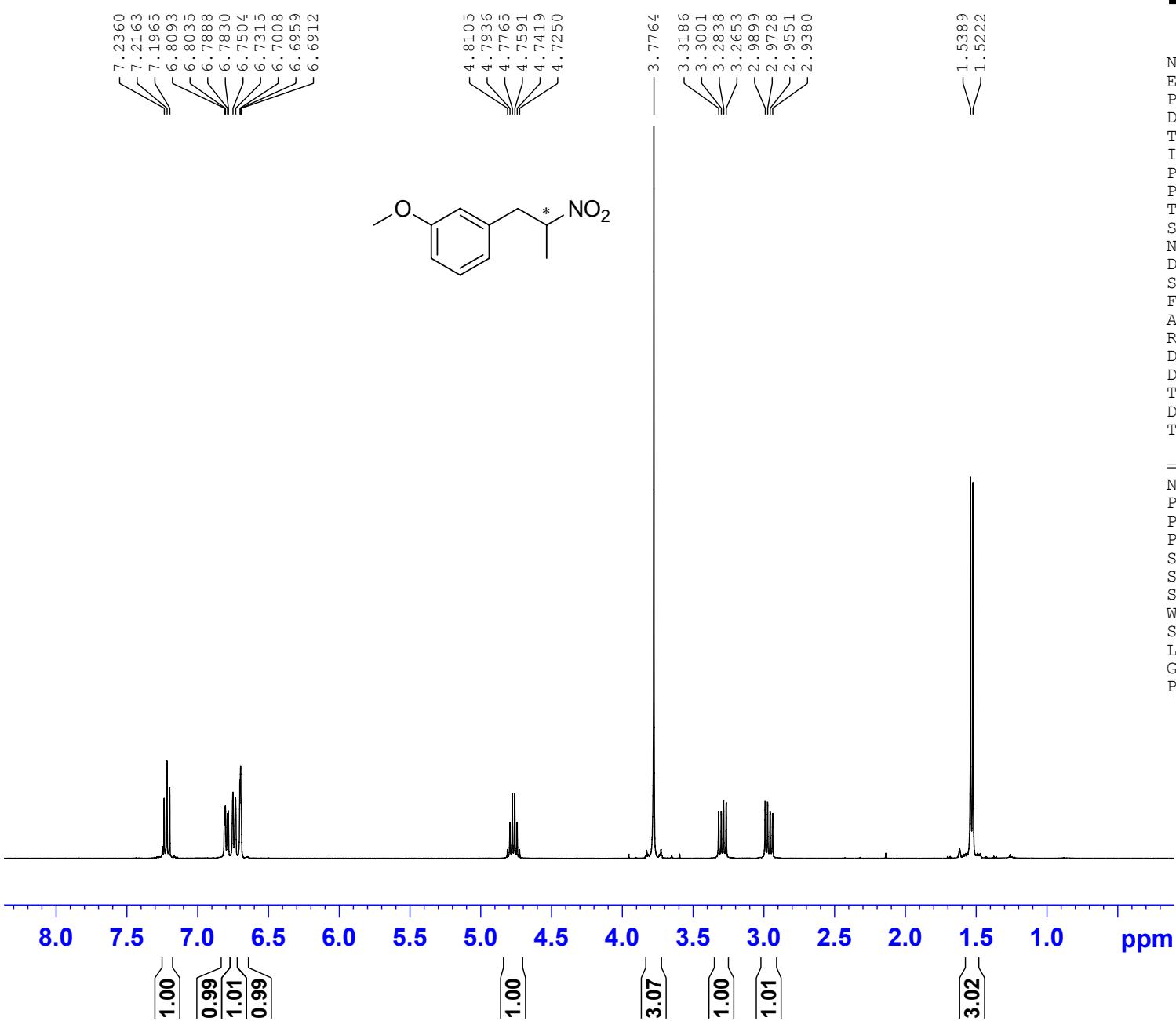


NAME Jul01-2011
EXPNO 10
PROCNO 1
Date_ 20110702
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 304.1 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL16 (R)
PROTON CDC13 {E:\NMR Data} skl 44

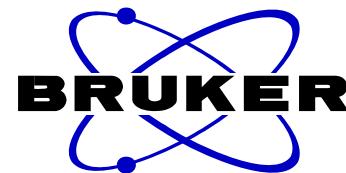
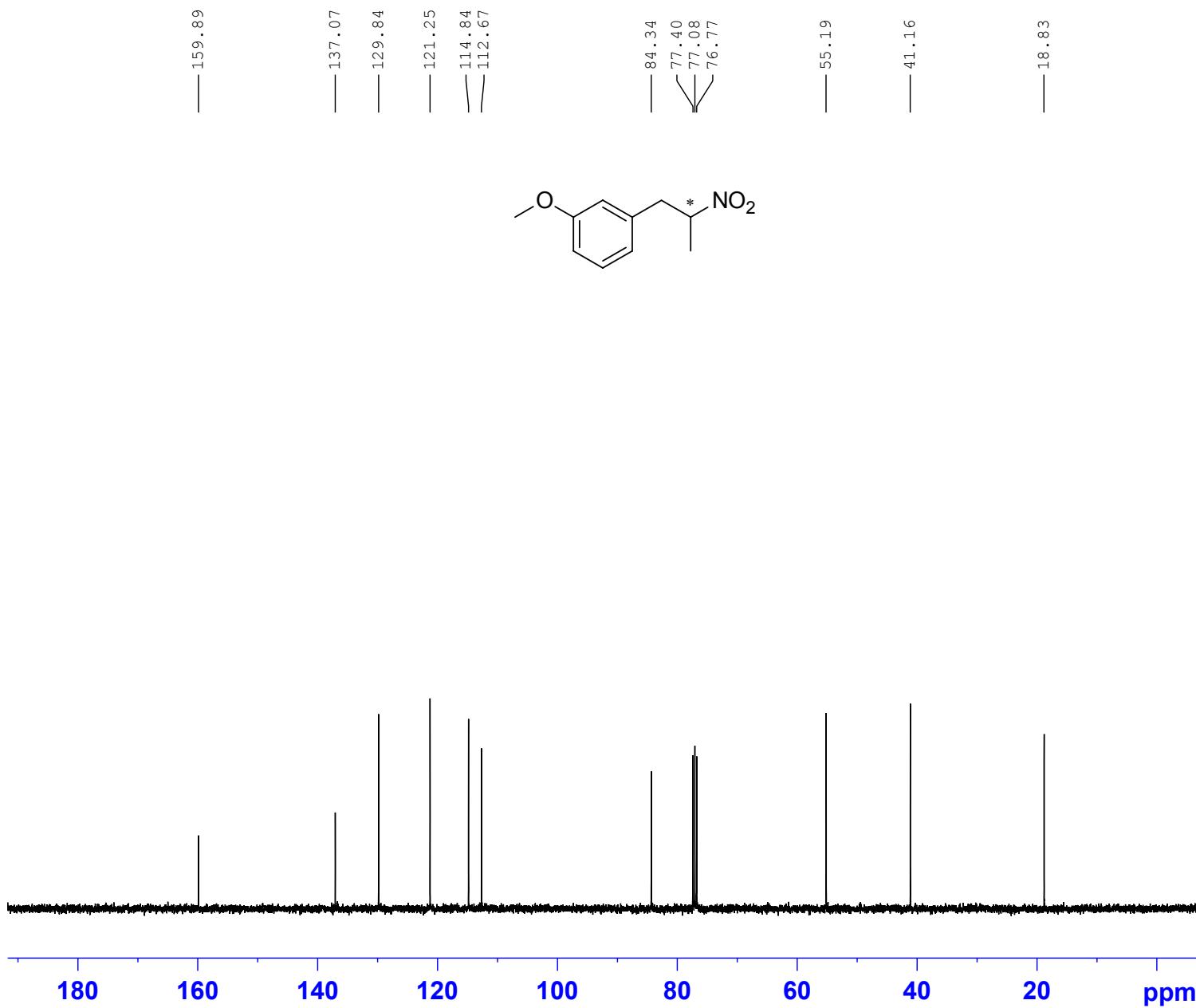


NAME Jul29-2012
EXPNO 10
PROCNO 1
Date_ 20120730
Time 3.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 300.8 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

Parameter	Value
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300142 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL16 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 44



NAME Jul29-2012
EXPNO 12
PROCNO 1
Date_ 20120730
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

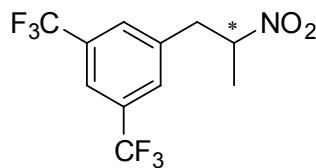
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL28 (R)

PROTON CDC13 {E:\NMR Data} skl 4

— 7.8093
— 7.6412

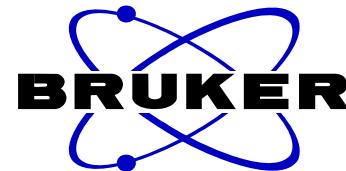
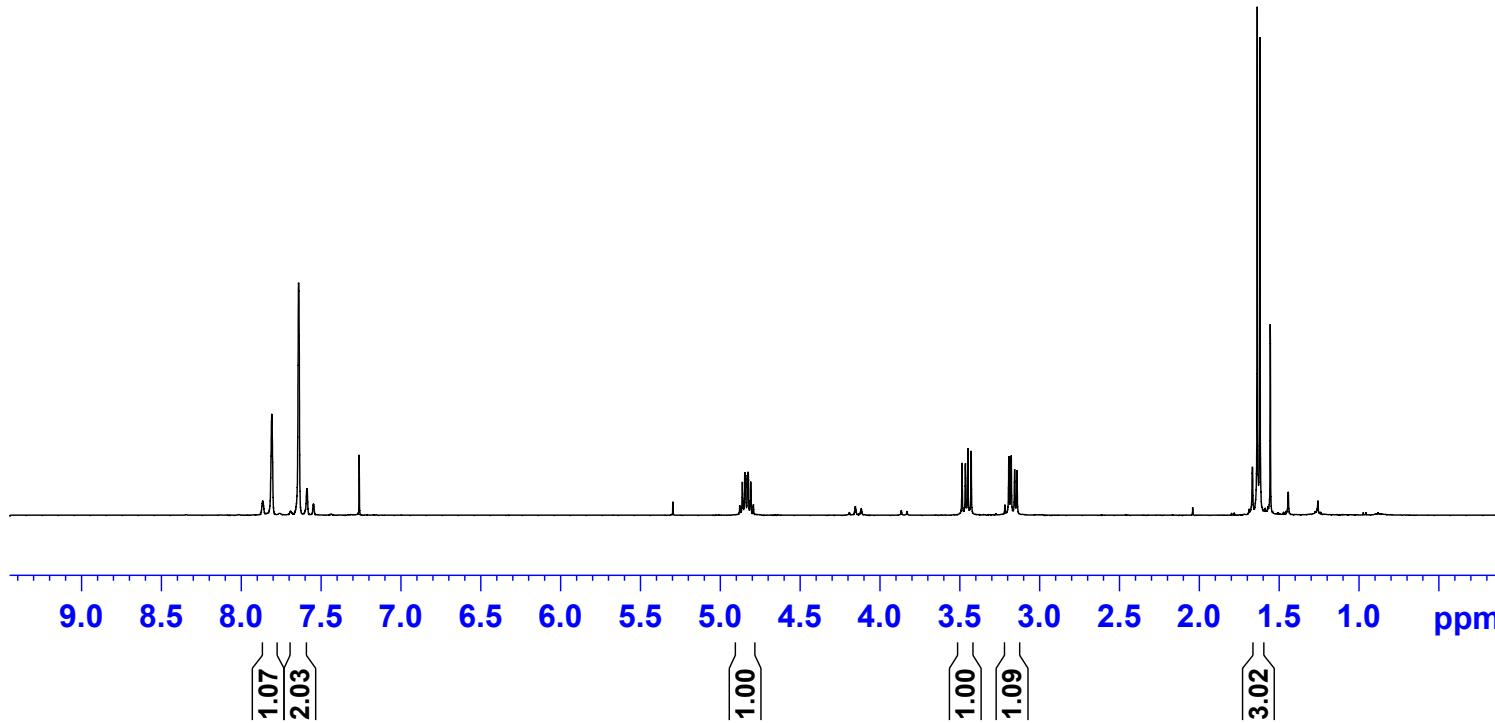
— 7.2616



4.8623
4.8475
4.8456
4.8414
4.8309
4.8268
4.8249
4.8101

3.4866
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3.4505
3.4297
3.1934
3.1790
3.1573
3.1429

1.6380
1.6213

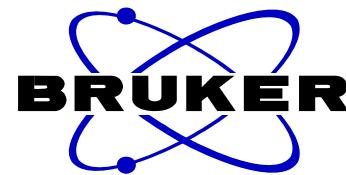
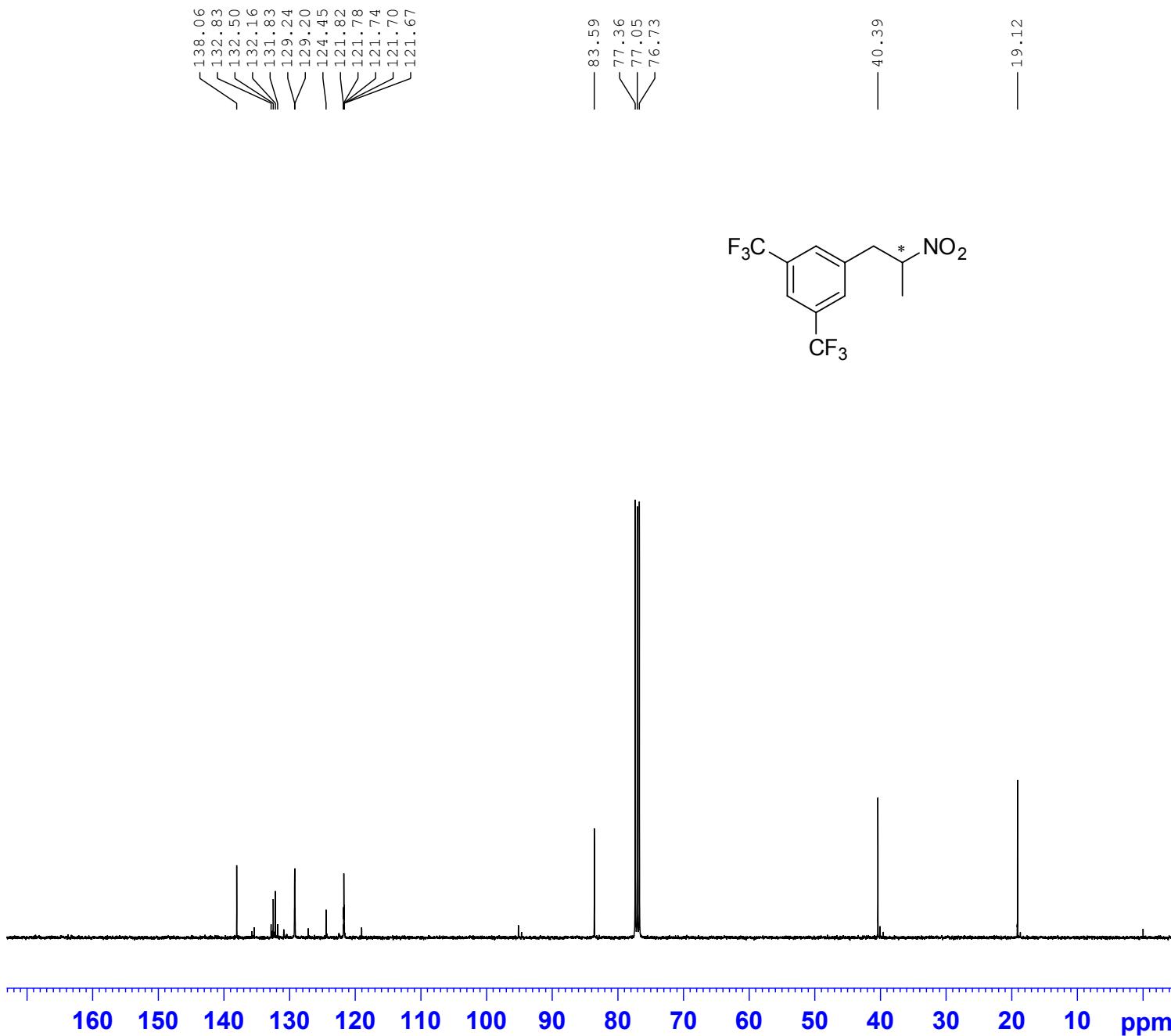


NAME Aug01-2012
EXPNO 15
PROCNO 1
Date_ 20120802
Time 5.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 6.50 usec
TE 300.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL28 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 4

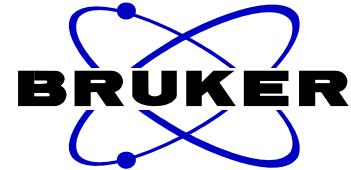


NAME Aug01-2012
EXPNO 17
PROCNO 1
Date_ 20120802
Time 8.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127634 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

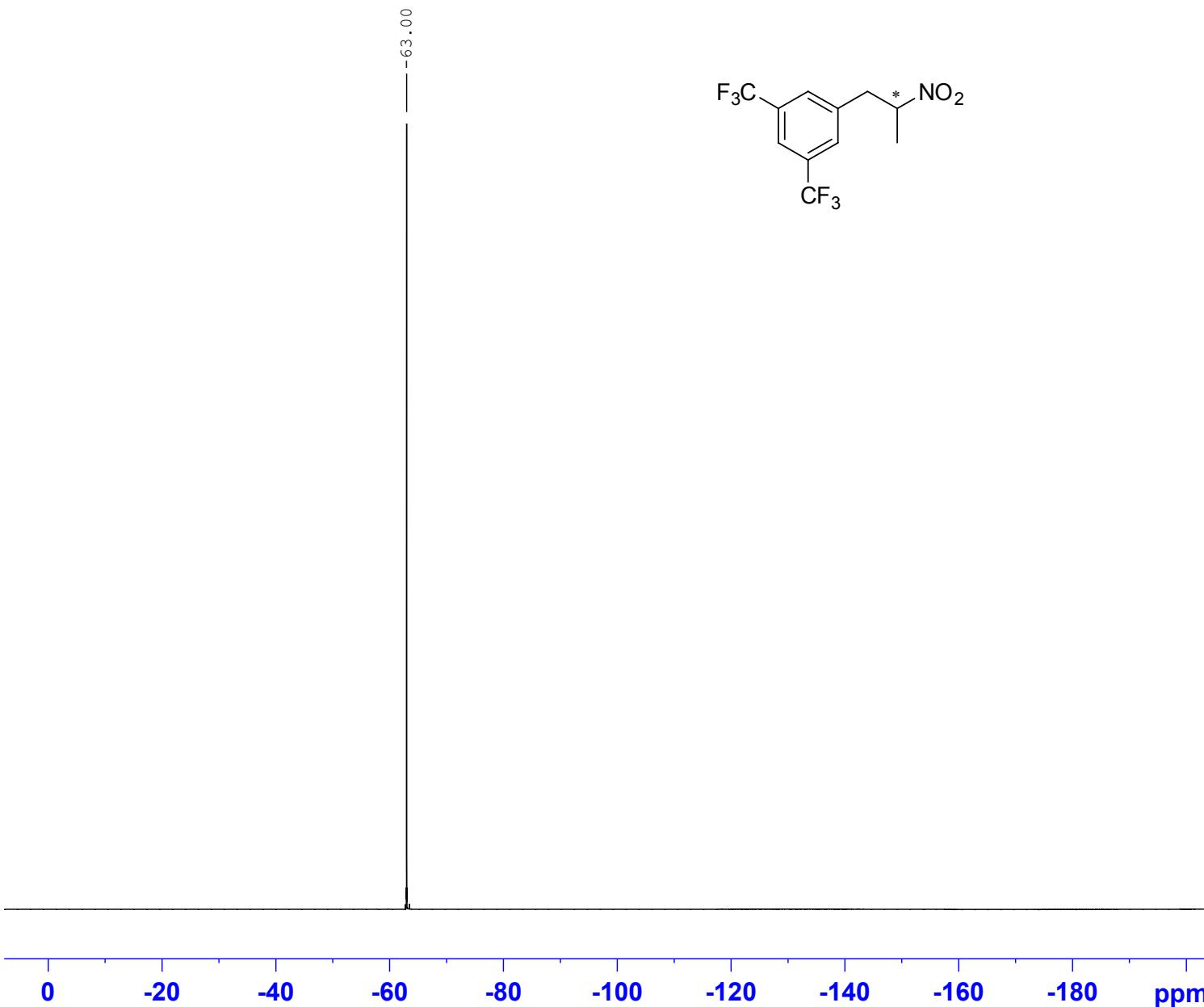
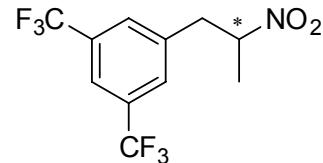
KL28 (R)
f19cpd.medchem CDC13 {E:\NMR Data} skl 4



NAME Aug01-2012
EXPNO 18
PROCNO 1
Date_ 20120802
Time 8.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc60
TD 131072
SOLVENT CDC13
NS 128
DS 4
SWH 93750.000 Hz
FIDRES 0.715256 Hz
AQ 0.6991007 sec
RG 912
DW 5.333 usec
DE 6.50 usec
TE 302.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 19F
P1 14.00 usec
PL1 1.50 dB
PL1W 35.56558990 W
SFO1 376.4569512 MHz

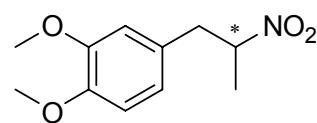
===== CHANNEL f2 ======
CPDPKG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
SFO2 400.1316005 MHz
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.87 Hz
GB 0
PC 1.00



KL08 (R)
PROTON CDC13 {E:\NMR Data} skl 10

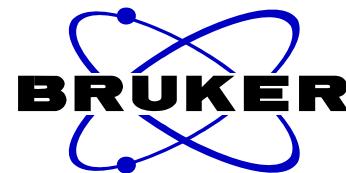
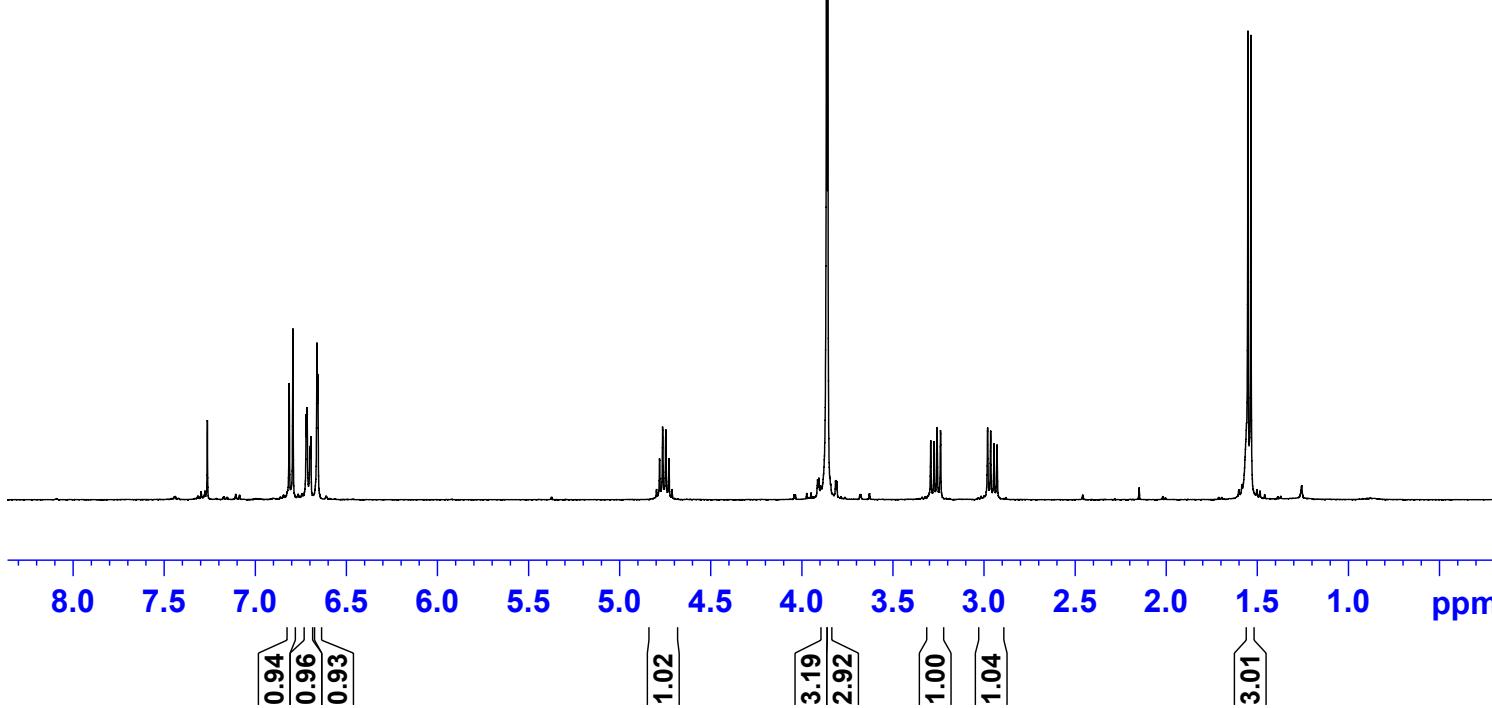
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6.7930
6.7200
6.7150
6.6996
6.6947
6.6609
6.6561

4.7804
4.7635
4.7457
4.7286



3.8639
3.8573
3.2921
3.2734
3.2569
3.2382
2.9799
2.9632
2.9448
2.9280

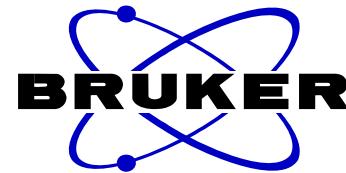
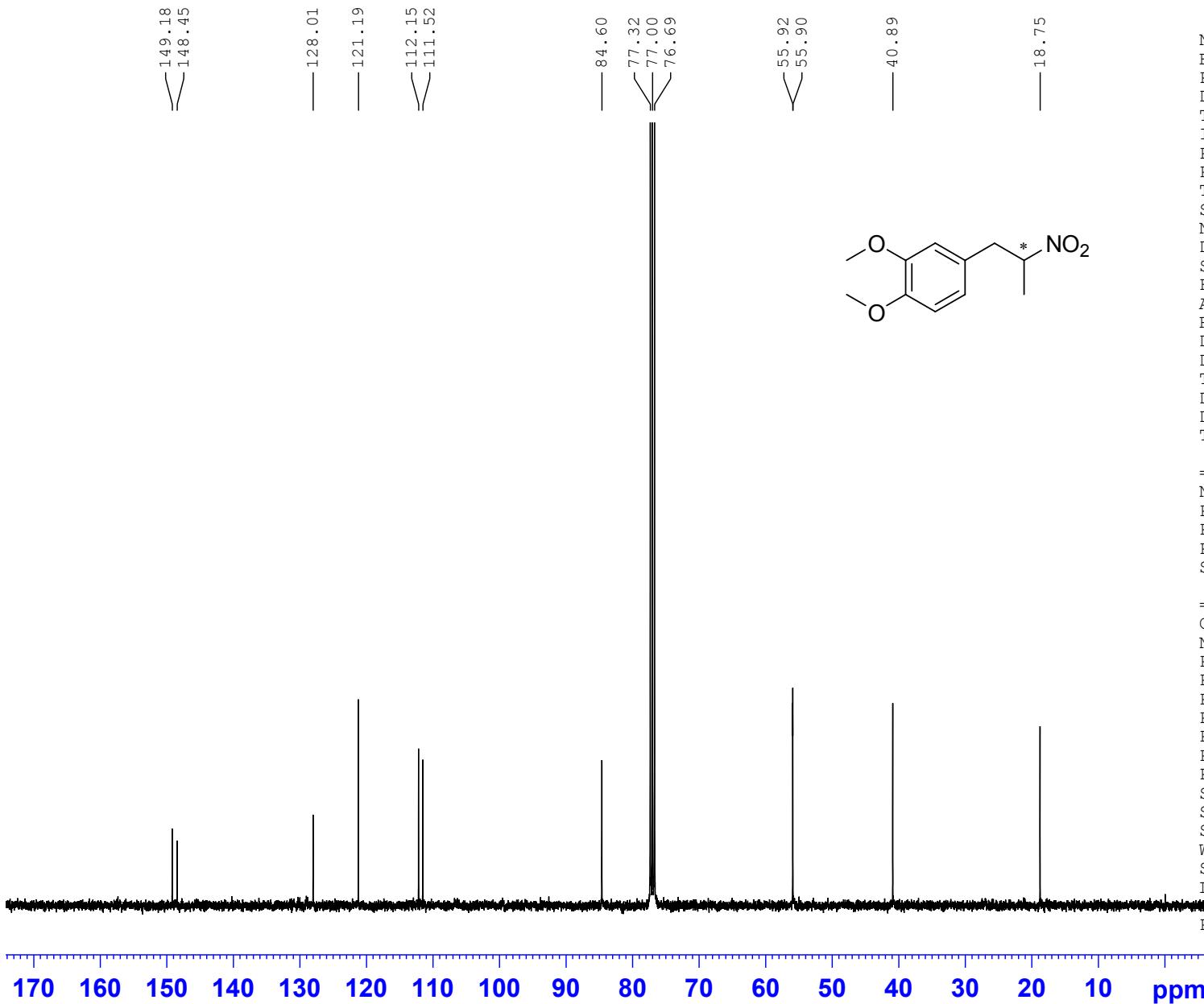
1.5514
1.5348



NAME Jul27-2012
EXPNO 4
PROCNO 1
Date_ 20120727
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 6.50 usec
TE 301.4 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL08 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 8



NAME Jul27-2012
EXPNO 12
PROCNO 1
Date_ 20120728
Time 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
EB 0
PC 1.40

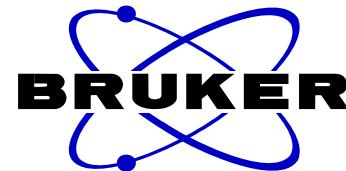
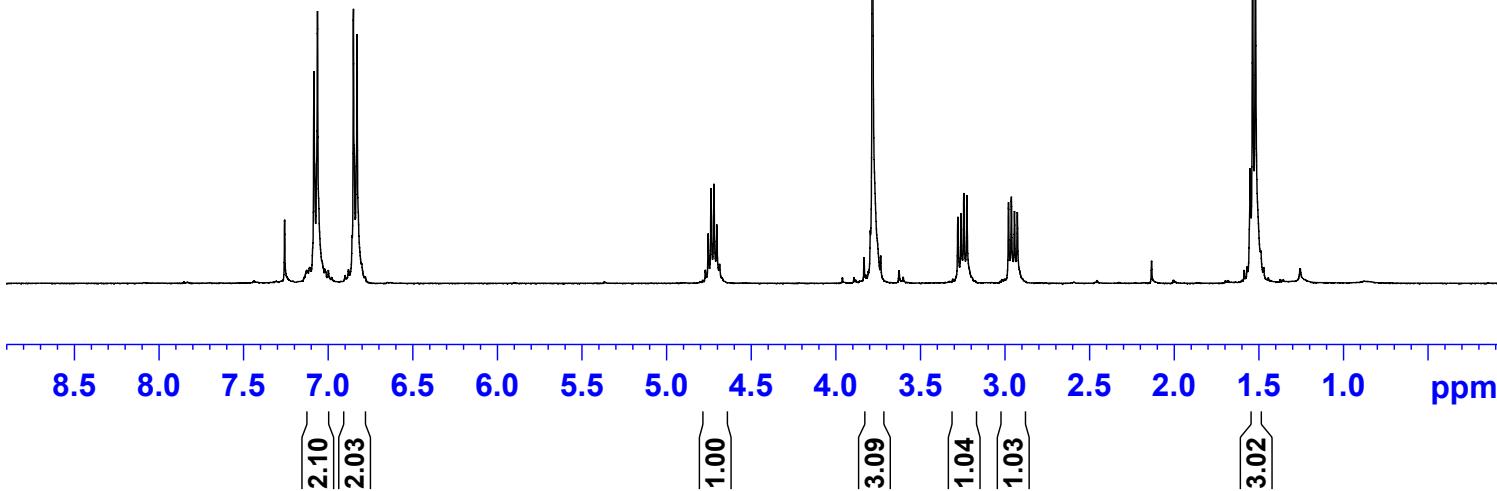
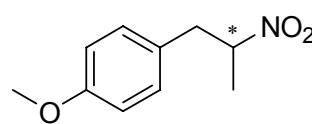
KL06 (R)
PROTON CDC13 {E:\NMR Data} skl 9

7.2572
7.0845
7.0635
6.8583
6.8512
6.8298
6.8028

4.7546
4.7376
4.7206
4.7036

3.7842
3.2793
3.2607
3.2442
3.2255
2.9797
2.9629
2.9445
2.9277

1.5372
1.5207

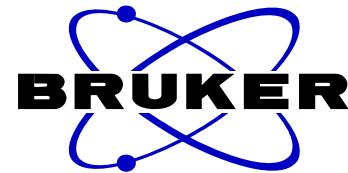
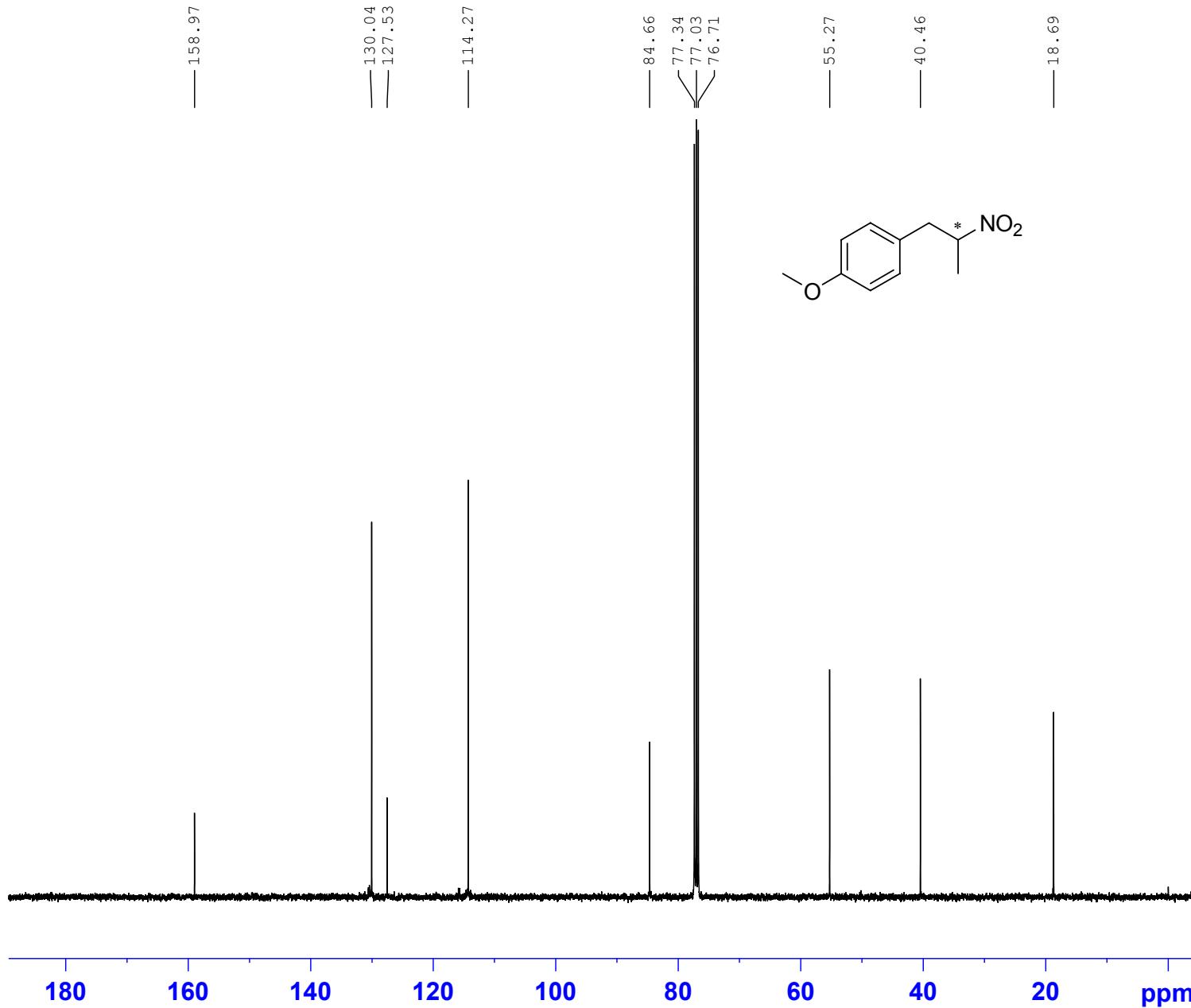


NAME Jul27-2012
EXPNO 3
PROCNO 1
Date_ 20120727
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 6.50 usec
TE 301.5 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300108 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL06 (R)
C13CPD CDC13 {E:\NMR Data} skl 6



NAME Jul27-2012
EXPNO 7
PROCNO 1
Date_ 20120728
Time 8.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127663 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL07 (R)

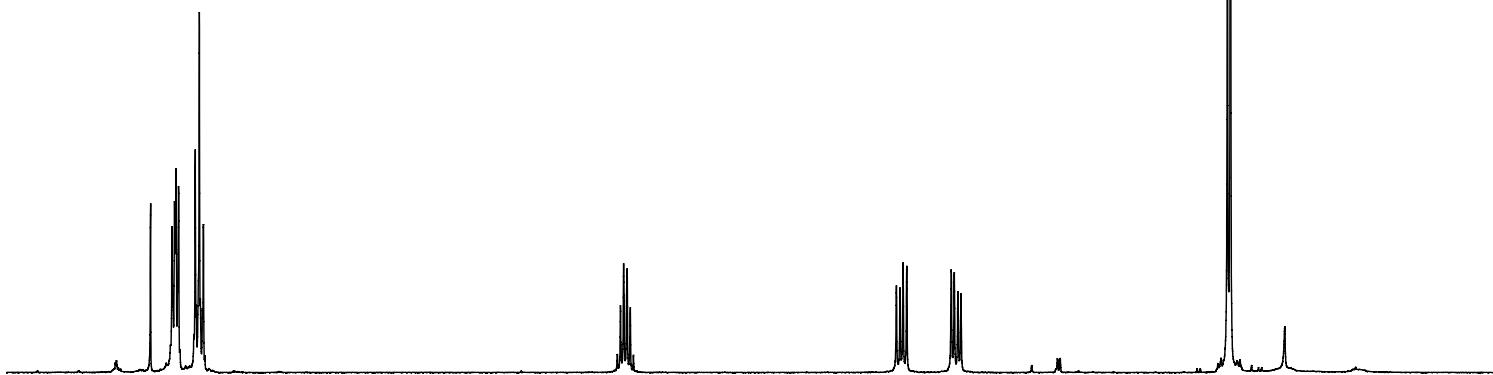
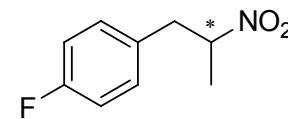
PROTON CDC13 {E:\NMR Data} skl 7

7.2590
7.1454
7.1402
7.1320
7.1241
7.1158
7.1108
7.0295
7.0224
7.0170
7.0009
6.9956
6.9842
6.9793

4.7719
4.7554
4.7386
4.7363
4.7196

3.3116
3.2921
3.2761
3.2567
3.0212
3.0052
2.9858
2.9698

1.5593
1.5431

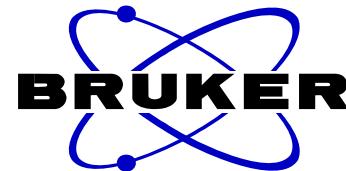


2.03
1.94

1.00

1.01
1.01

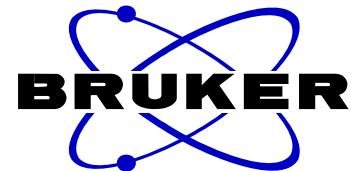
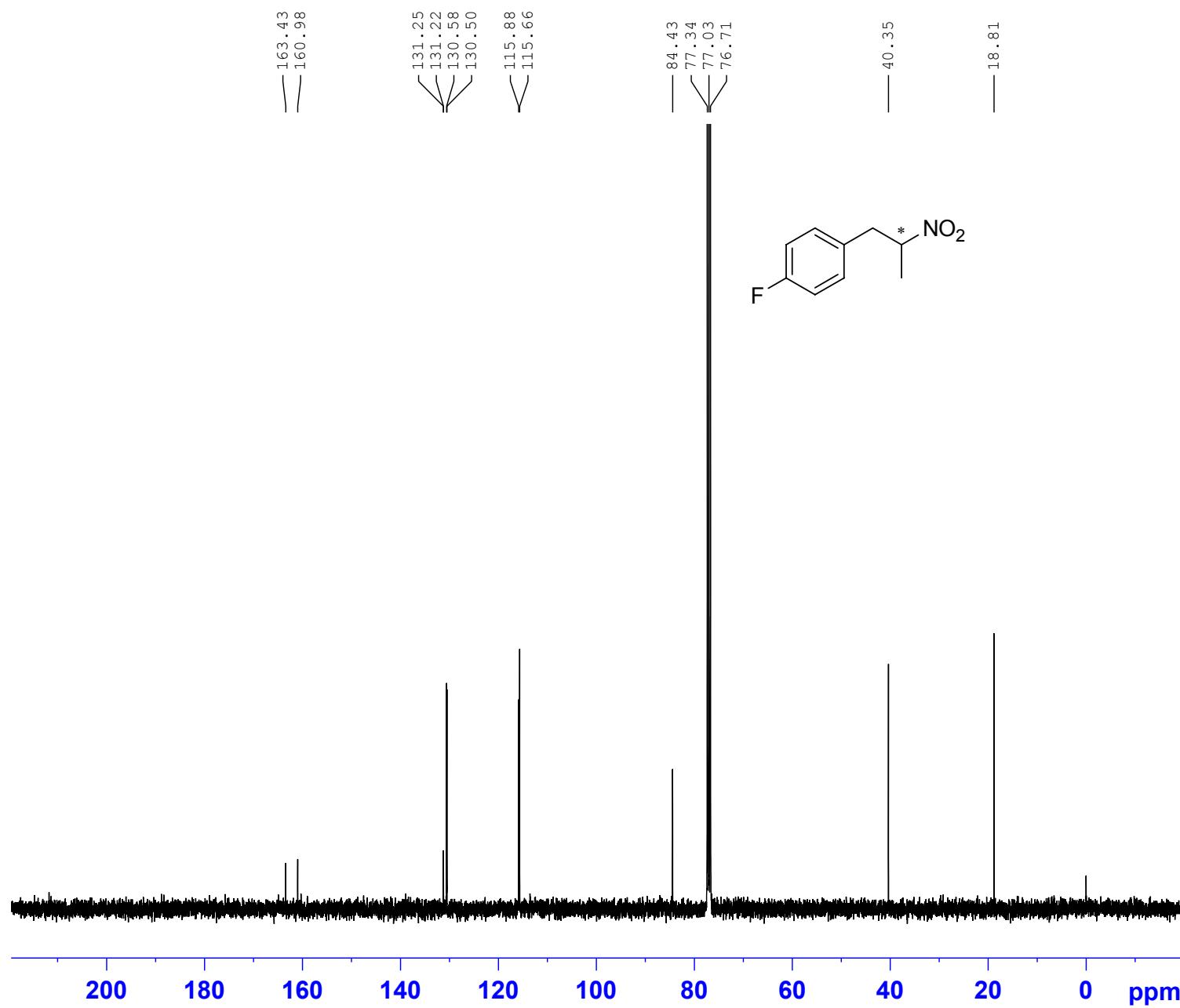
3.74



NAME Jul27-2012
EXPNO 1
PROCNO 1
Date_ 20120727
Time 11.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL07 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 7

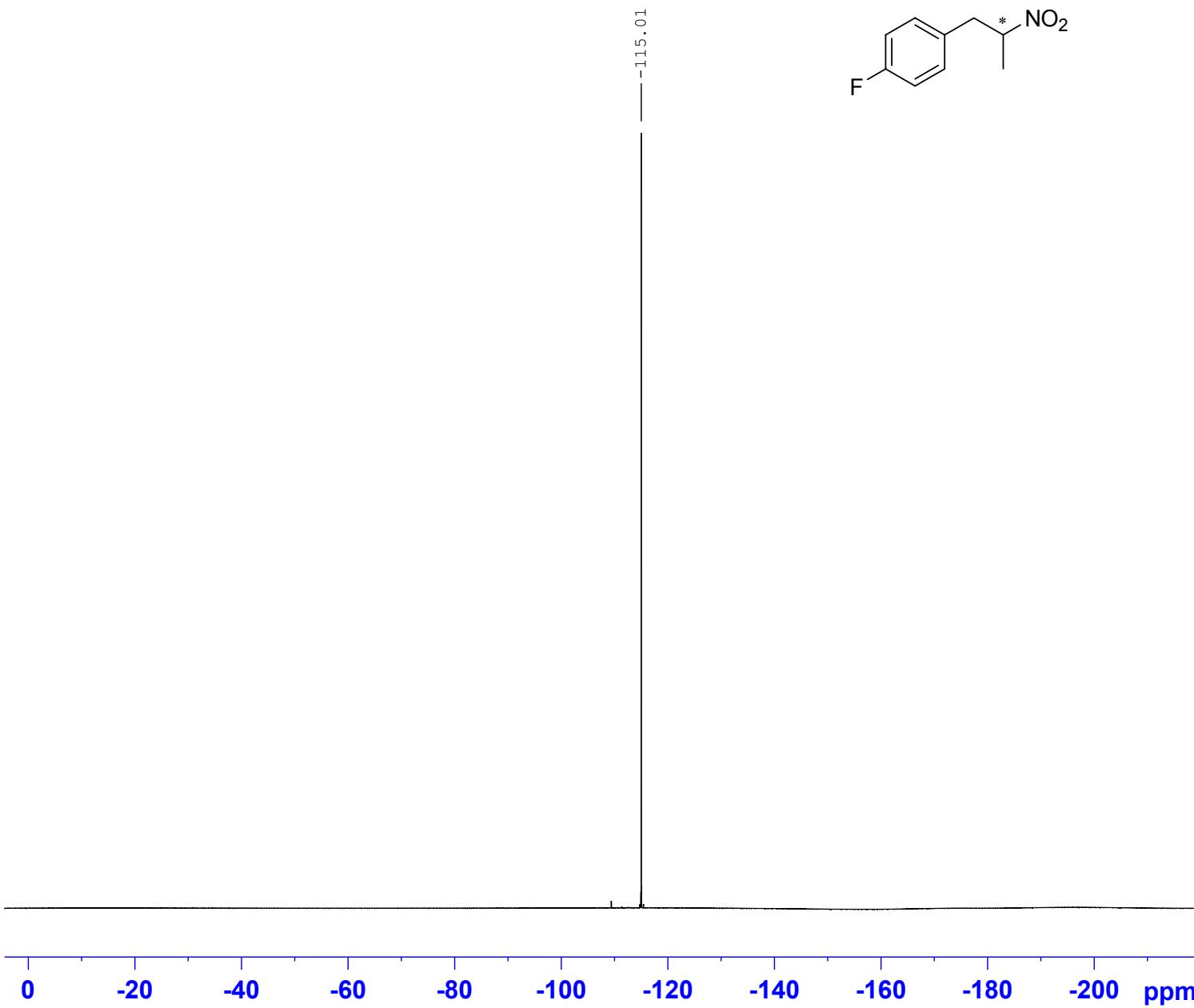


NAME Jul27-2012
EXPNO 9
PROCNO 1
Date_ 20120728
Time 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127658 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL07 (R)
f19cpd.medchem CDC13 {E:\NMR Data} skl 7



NAME Jul27-2012
EXPNO 10
PROCNO 1
Date_ 20120728
Time 9.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc60
TD 131072
SOLVENT CDC13
NS 128
DS 4
SWH 93750.000 Hz
FIDRES 0.715256 Hz
AQ 0.6991007 sec
RG 1030
DW 5.333 usec
DE 6.50 usec
TE 303.9 K
D1 3.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 19F
P1 14.00 usec
PL1 1.50 dB
PL1W 35.56558990 W
SFO1 376.4569512 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
SFO2 400.1316005 MHz
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.87 Hz
GB 0
PC 1.00

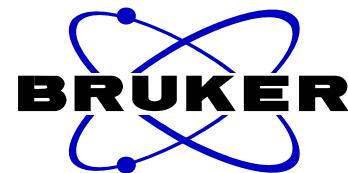
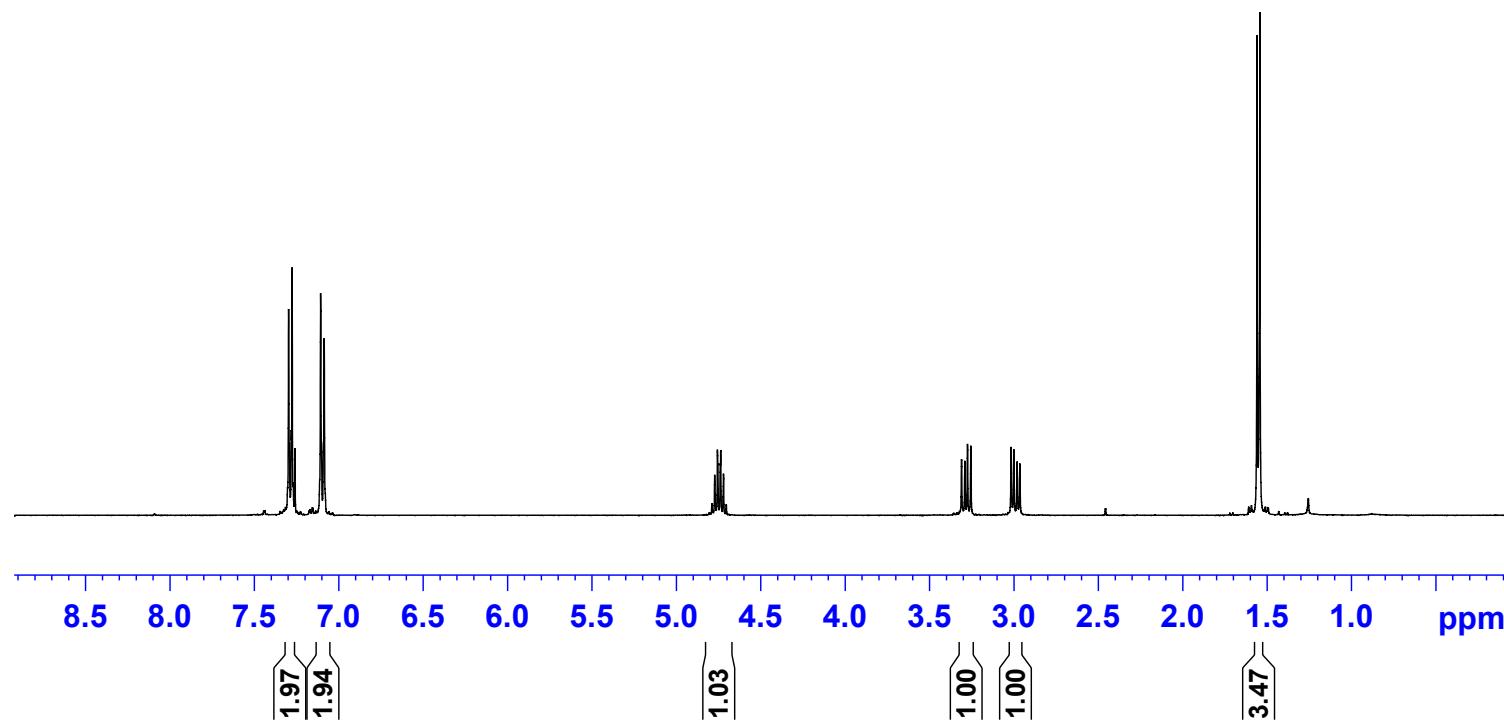
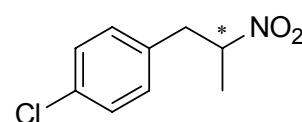
KL09 (R)
PROTON CDC13 {E:\NMR Data} skl 8

7.3028
7.2967
7.2920
7.2804
7.2757
7.2695
7.2587
7.1068
7.0859

4.7725
4.7559
4.7535
4.7392
4.7367
4.7202

3.3099
3.2904
3.2745
3.2551
3.0161
3.0000
2.9808
2.9647

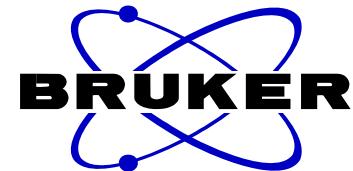
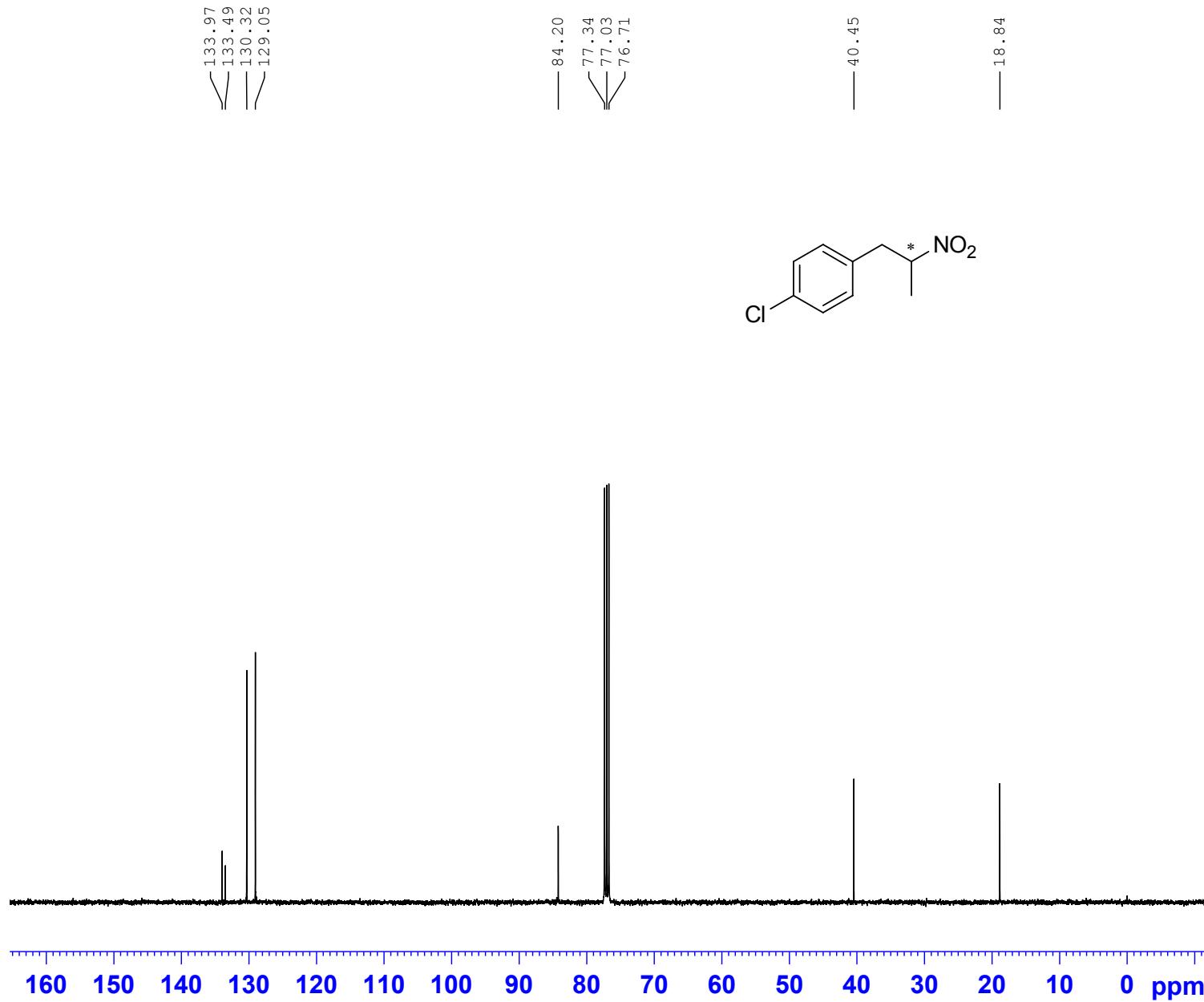
1.5595
1.5429



NAME Jul27-2012
EXPNO 2
PROCNO 1
Date_ 20120727
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL09 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 9

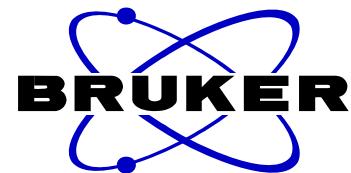
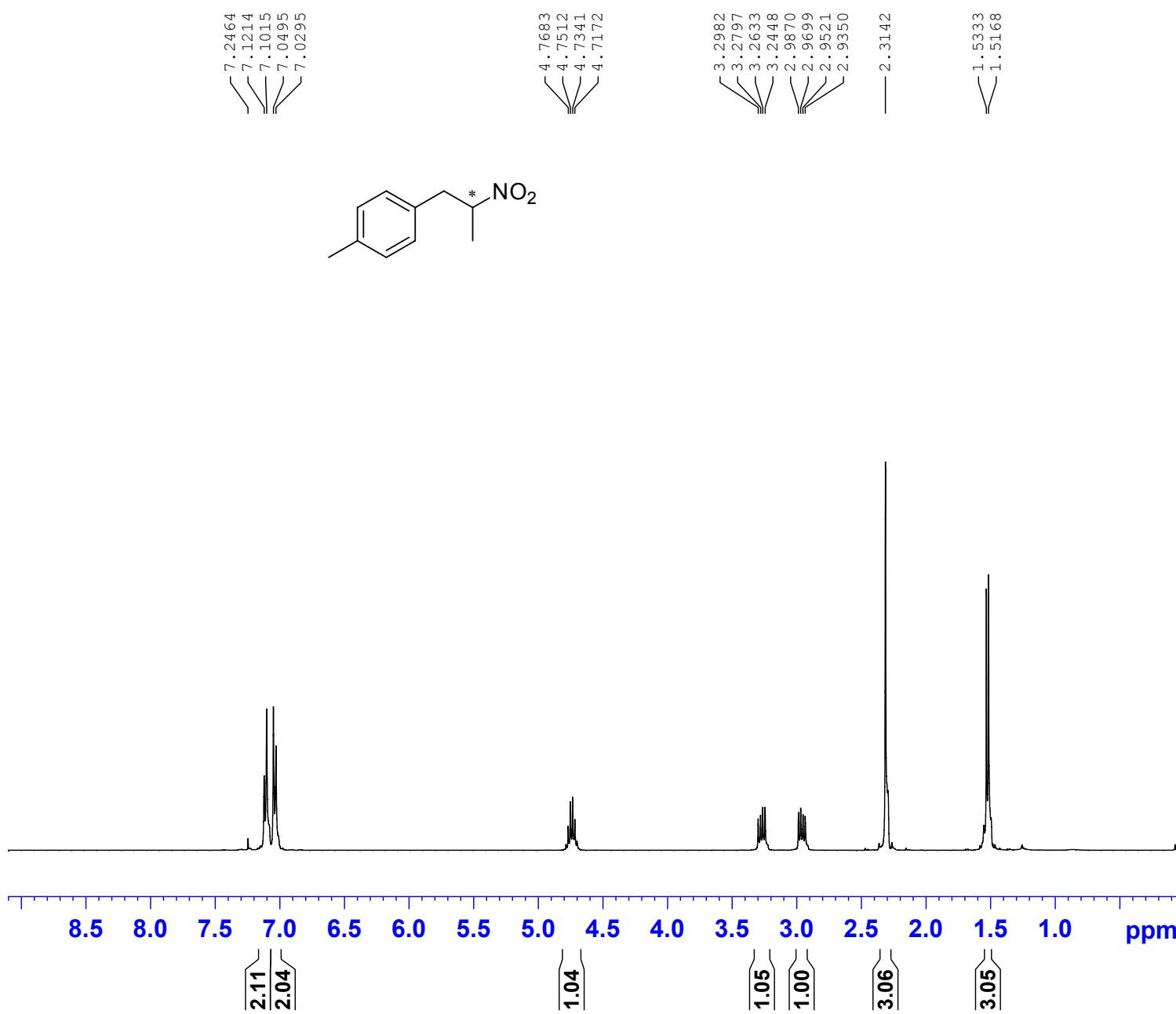


NAME Jul27-2012
EXPNO 14
PROCNO 1
Date_ 20120728
Time 12.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127662 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL12 (R)
PROTON CDC13 {E:\NMR Data} skl 12

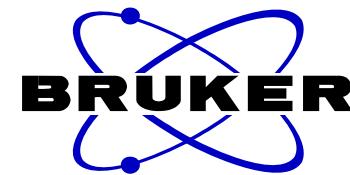
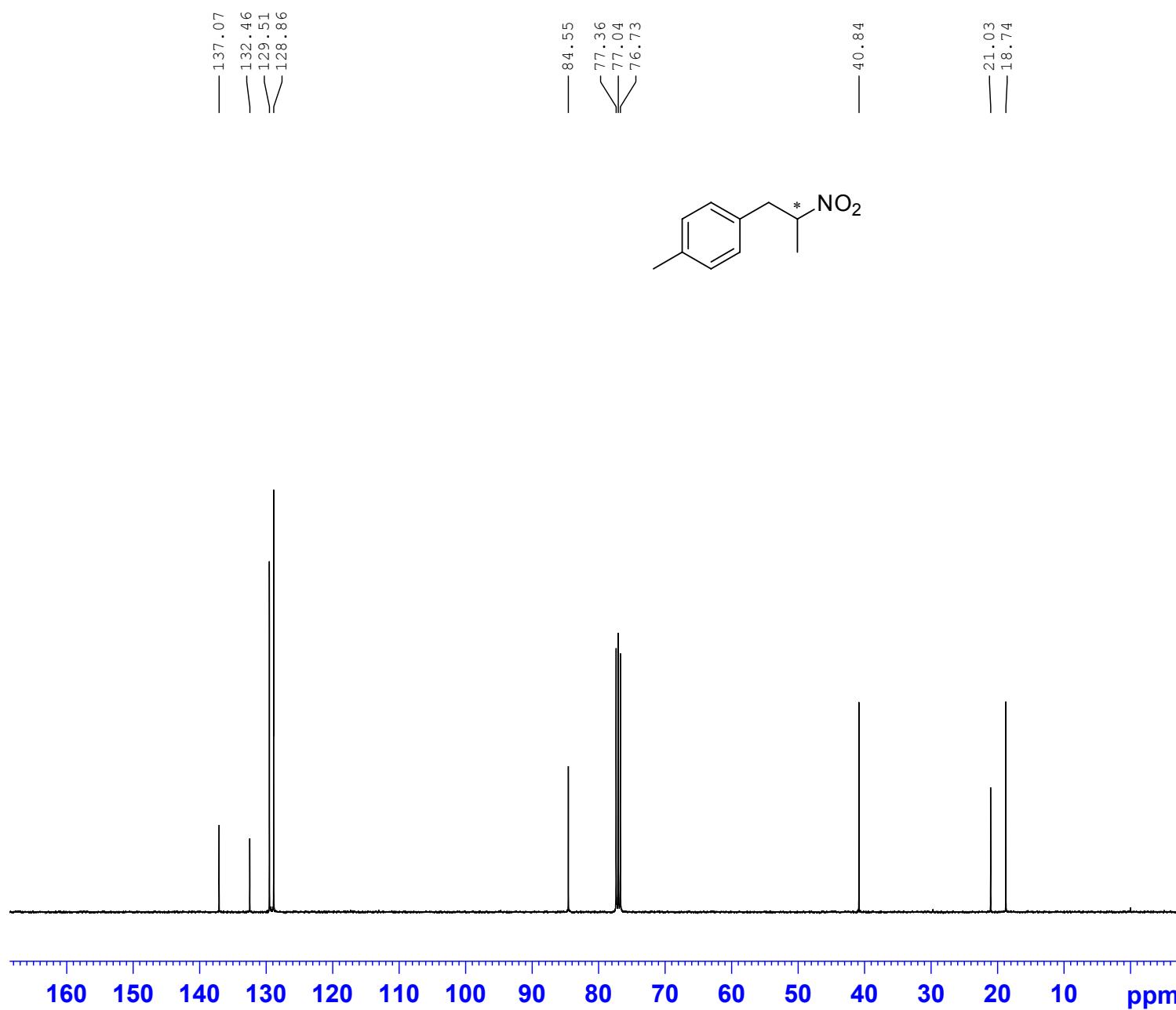


NAME Jul28-2012
EXPNO 1
PROCNO 1
Date_ 20120729
Time 3.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 301.3 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300157 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL12 (R)
C13CPD CDC13 {E:\NMR Data} skl 12

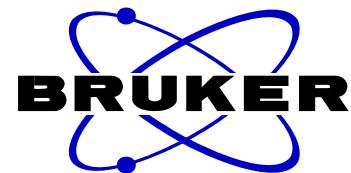
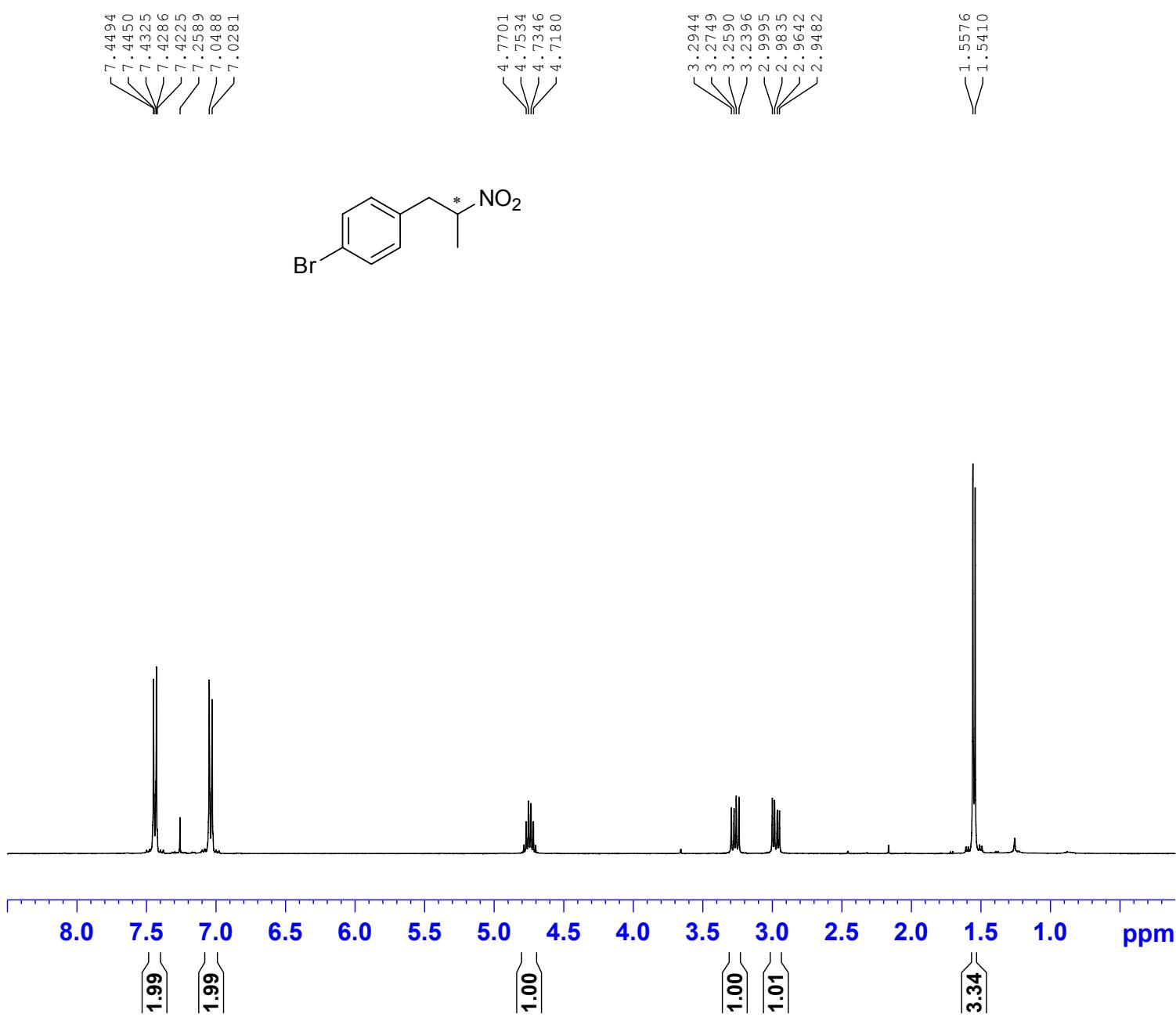


NAME Jul28-2012
EXPNO 3
PROCNO 1
Date_ 20120729
Time 6.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

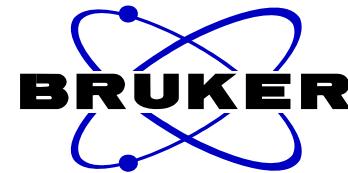
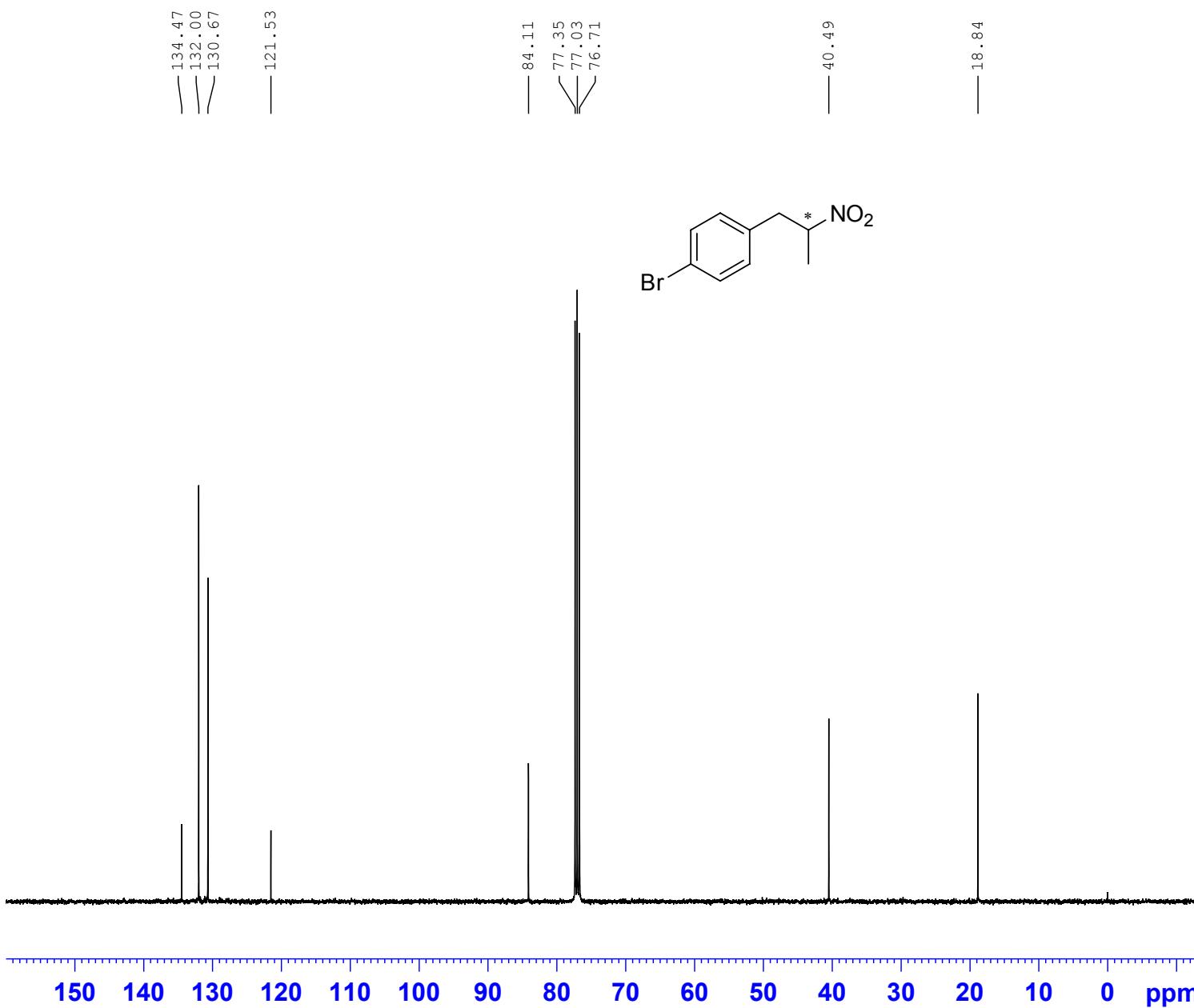
===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127678 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL13 (R)
PROTON CDC13 {E:\NMR Data} skl 13



KL13 (R)
C13CPD CDC13 {E:\NMR Data} skl 13

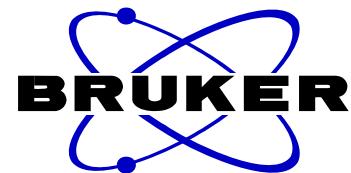
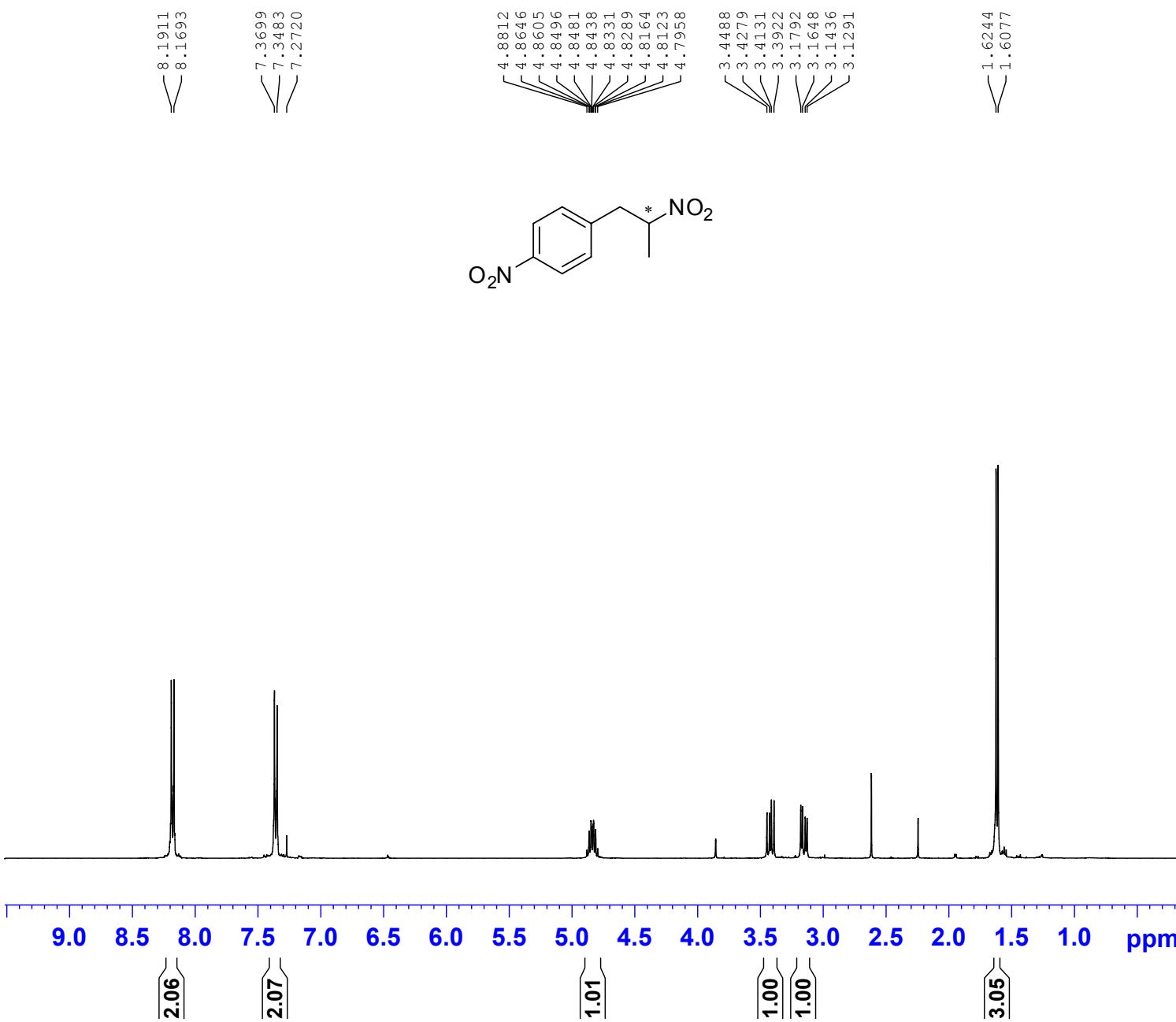


NAME Jul28-2012
EXPNO 6
PROCNO 1
Date_ 20120729
Time 8.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127671 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

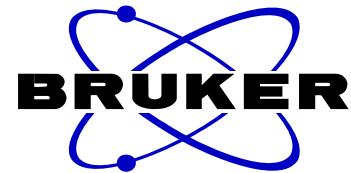
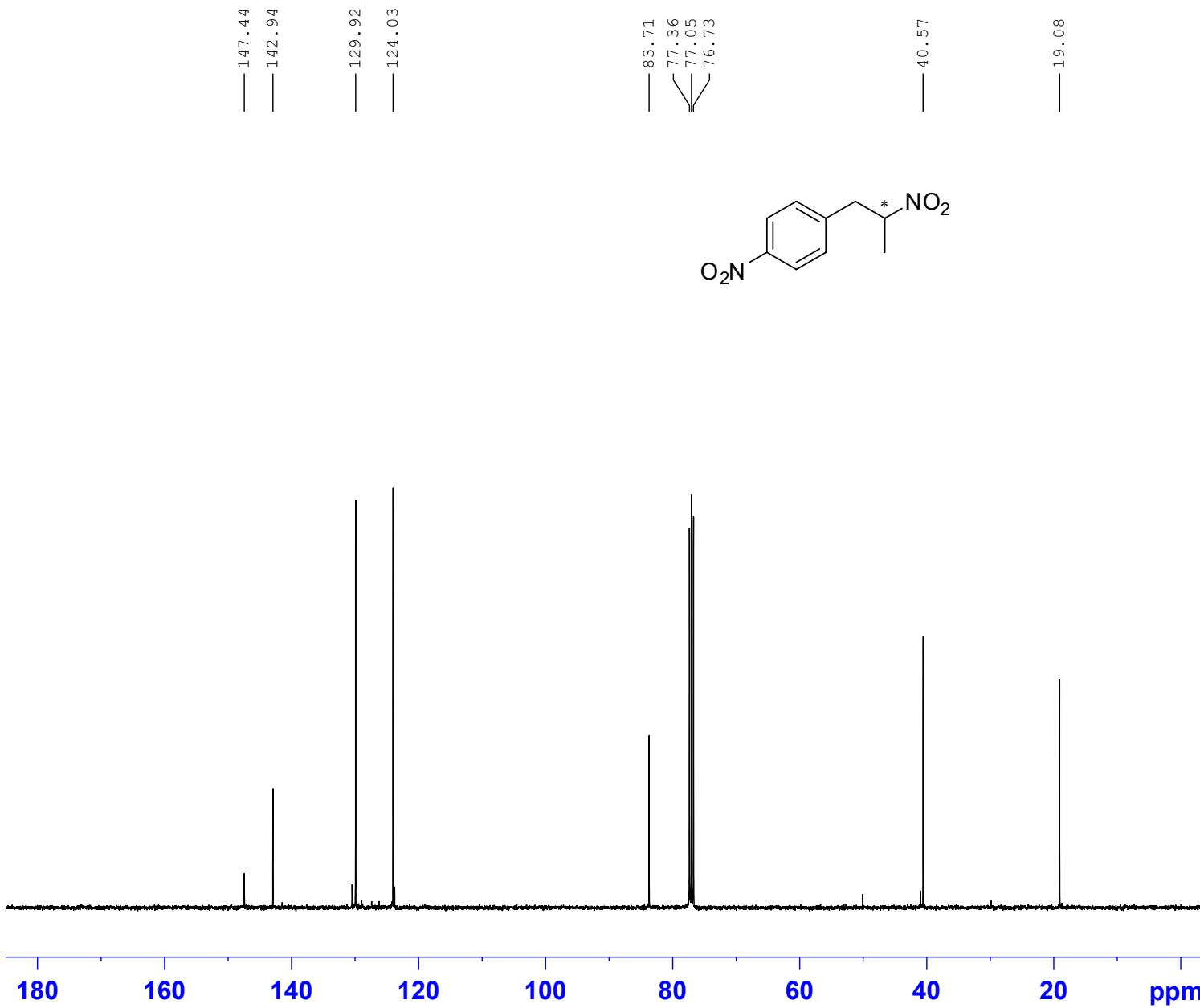
KL17 (R)
PROTON CDC13 {E:\NMR Data} skl 45



NAME Jul29-2012
EXPNO 13
PROCNO 1
Date_ 20120730
Time 4.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 300.5 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL17 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 45

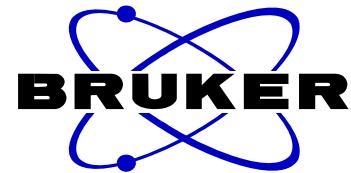
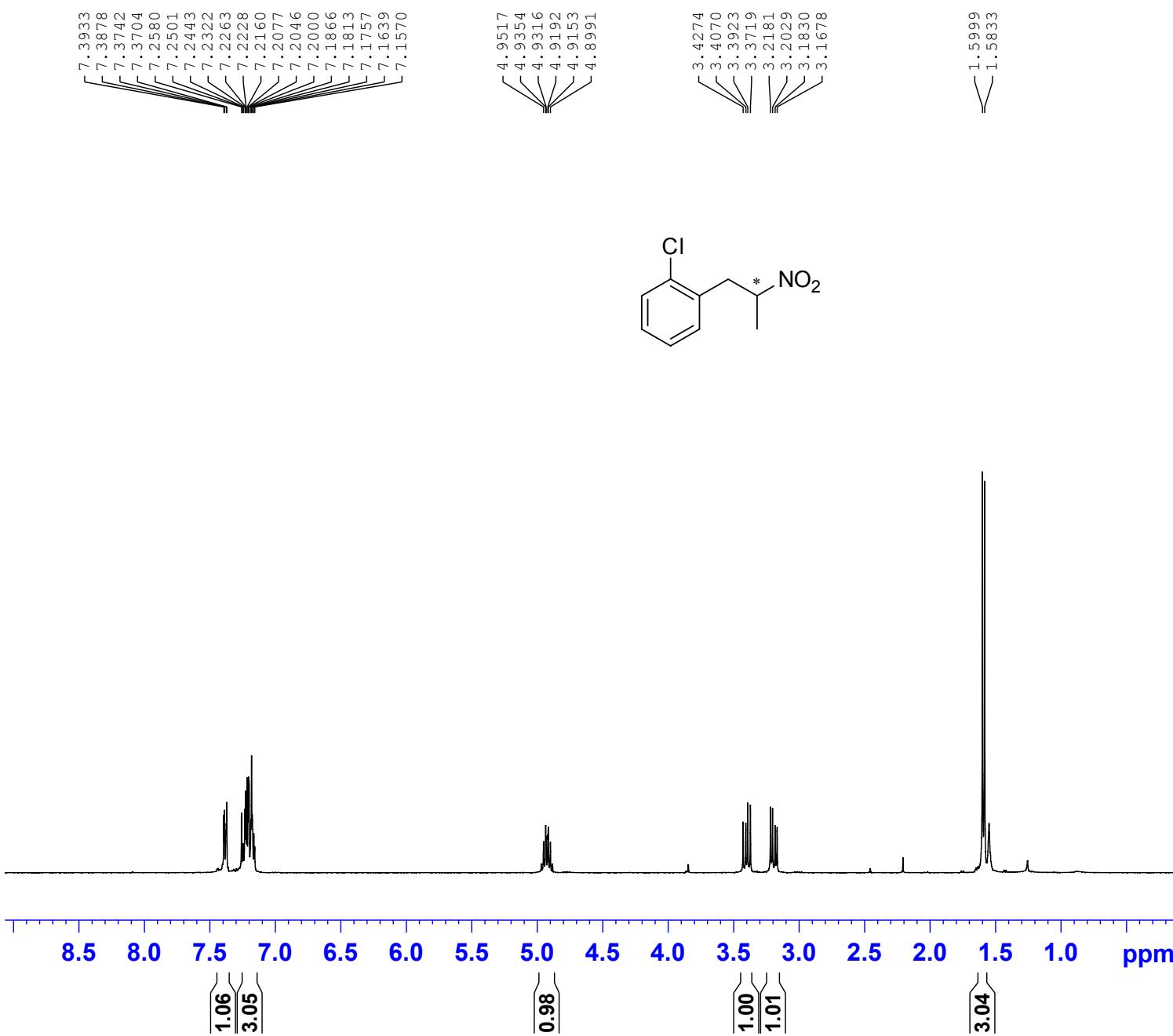


NAME Jul29-2012
EXPNO 16
PROCNO 1
Date_ 20120730
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL10 (R)
PROTON CDC13 {E:\NMR Data} skl 11



NAME Jul27-2012
EXPNO 5
PROCNO 1
Date_ 20120727
Time 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.50 usec
TE 301.5 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

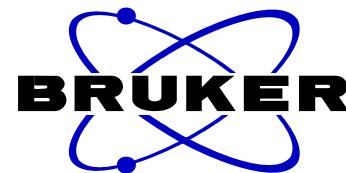
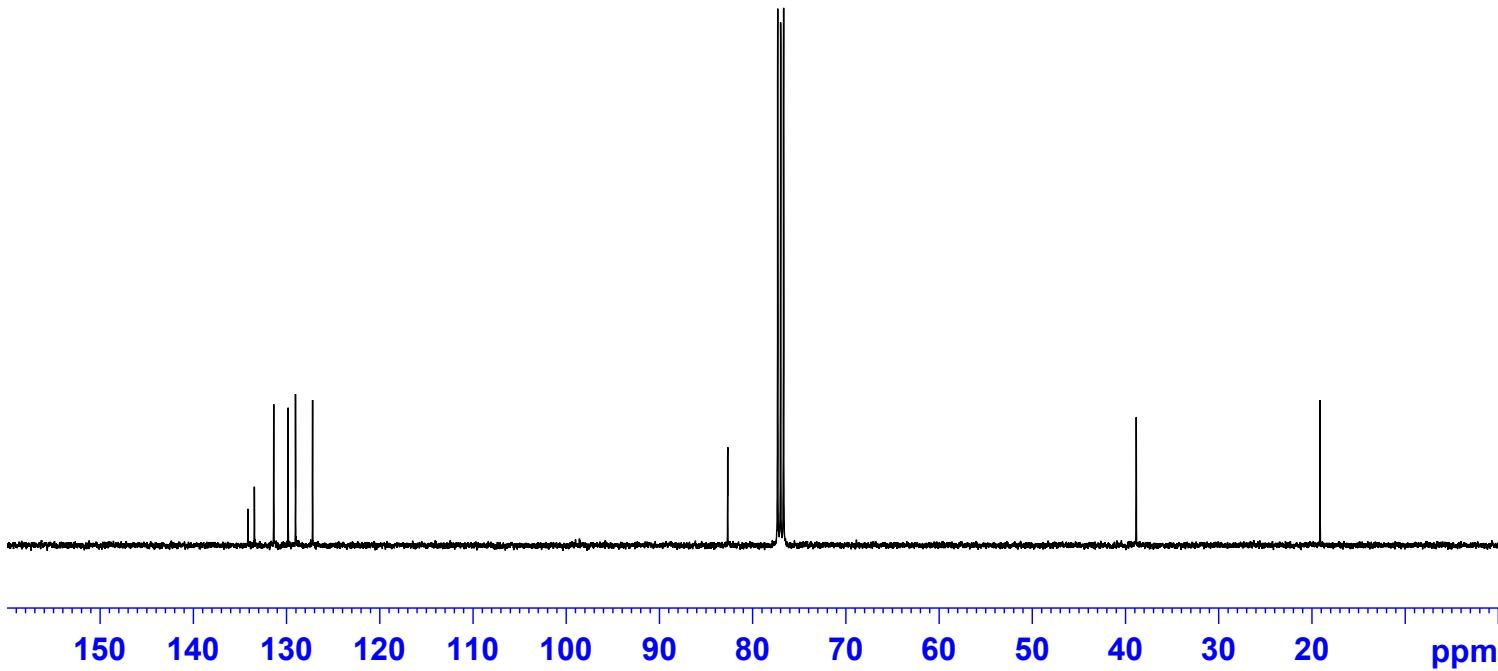
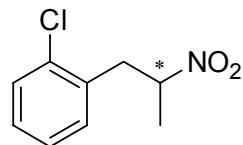
KL10 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 10

134.1445
133.4517
131.3816
129.8337
129.0410
127.2103

82.6772
77.3167
76.9996
76.6819

38.8440

19.1182

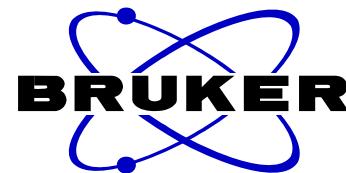
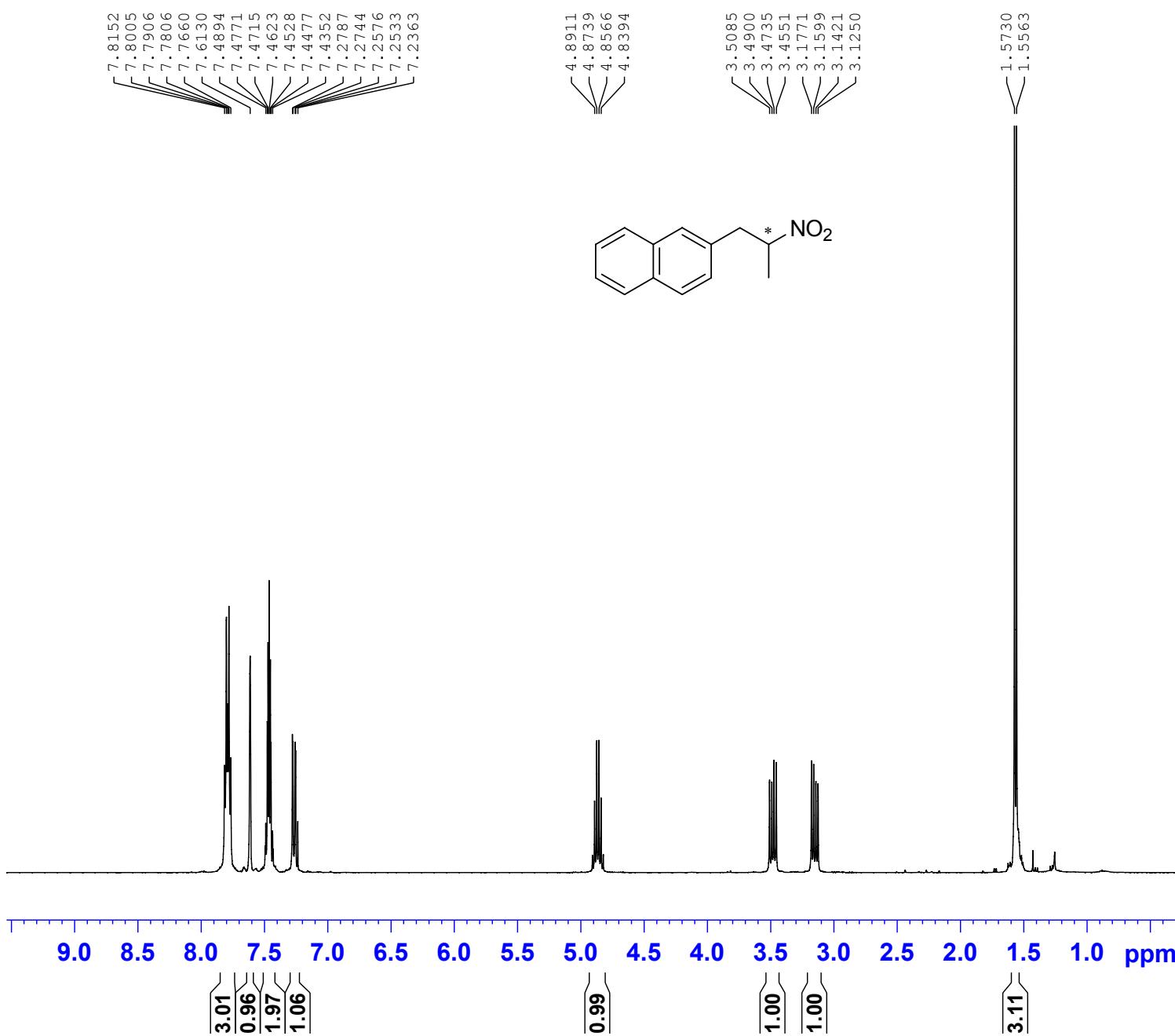


NAME Jul27-2012
EXPNO 16
PROCNO 1
Date_ 20120728
Time 14.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL21 (R)
PROTON CDC13 {E:\NMR Data} skl 21

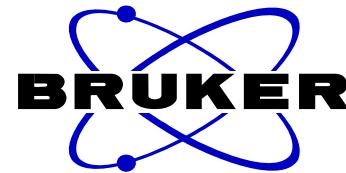
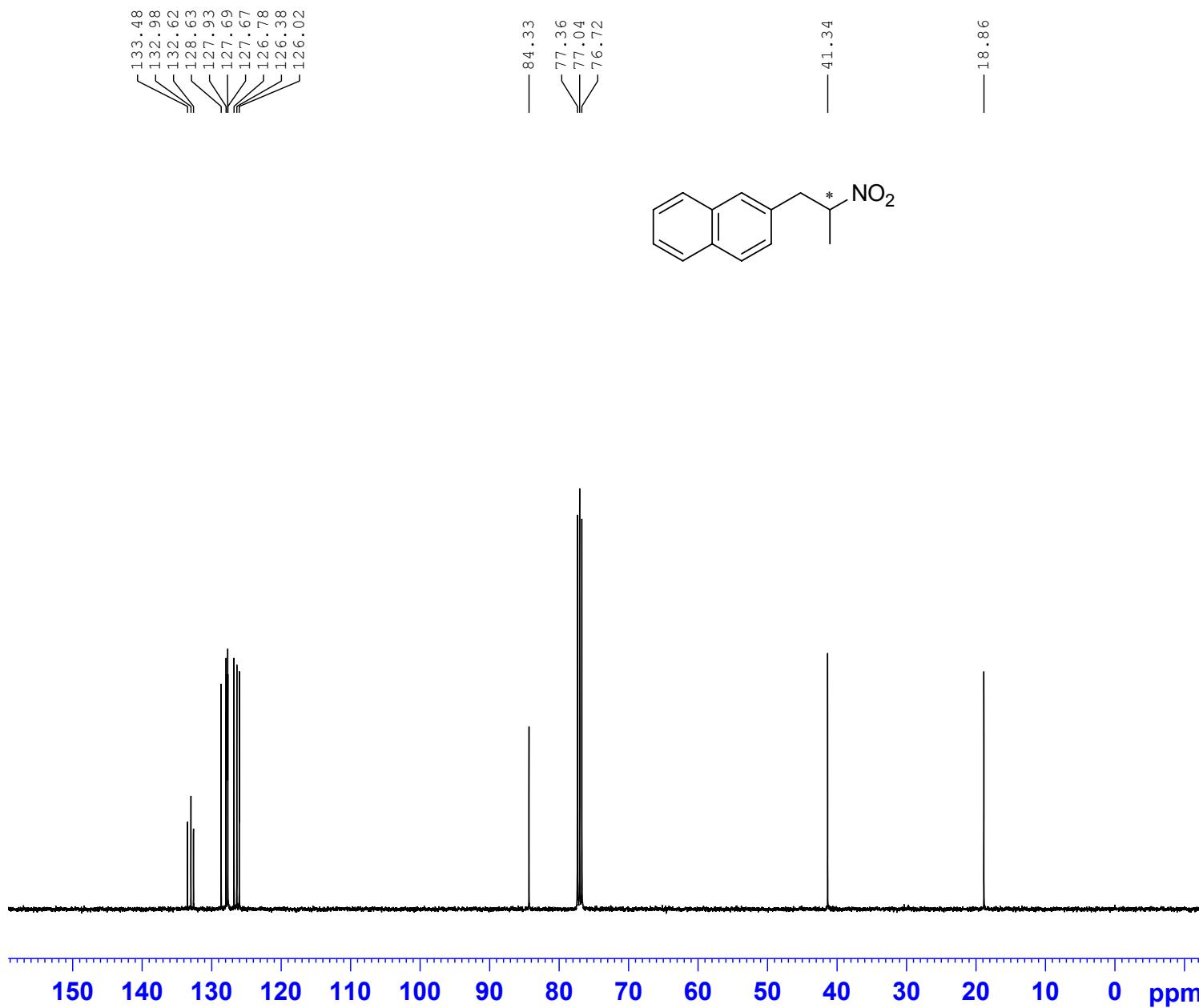


NAME Jul30-2012
EXPNO 4
PROCNO 1
Date_ 20120730
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 301.1 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300193 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL21 (R)
C13CPD CDC13 {E:\NMR Data} skl 21

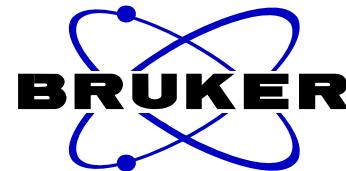
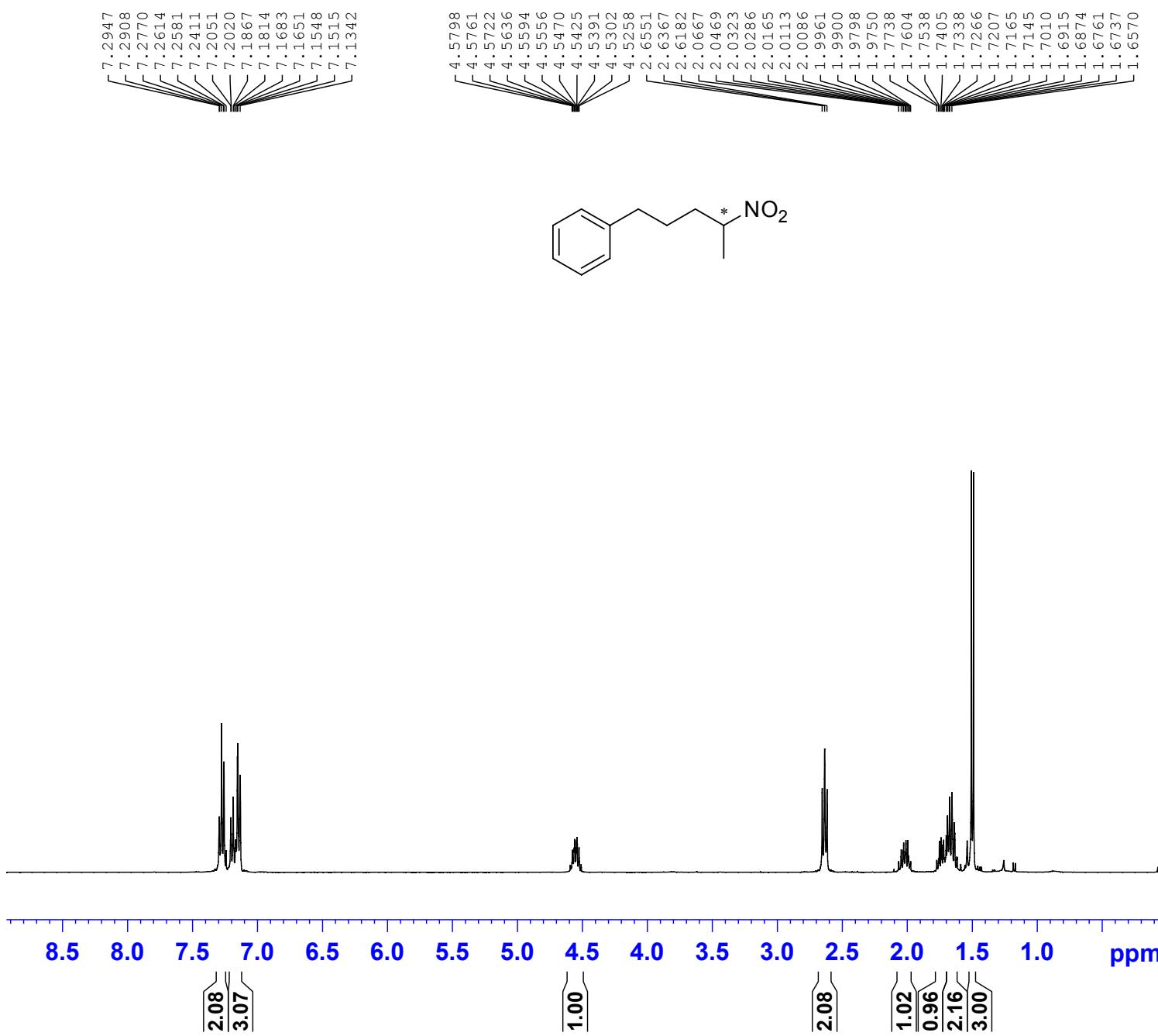


NAME Jul30-2012
EXPNO 12
PROCNO 1
Date_ 20120731
Time 0.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL26 (R)
PROTON CDC13 {E:\NMR Data} skl 28

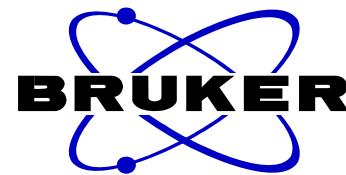


NAME Aug08-2012
EXPNO 5
PROCNO 1
Date_ 20120808
Time 19.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 304.8 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300173 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

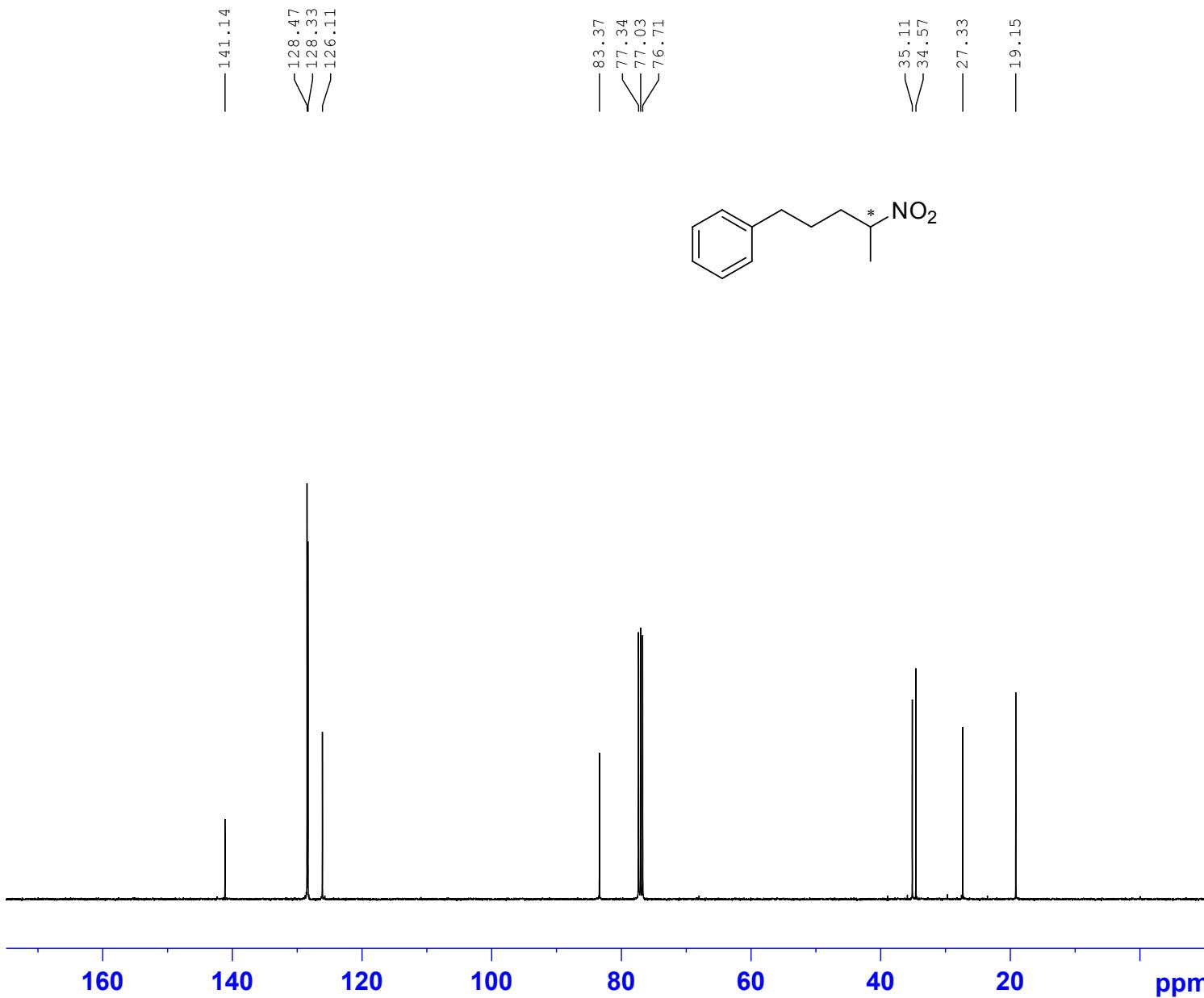
KL26 (R)
C13CPD CDCl₃ {E:\NMR Data} skl 28



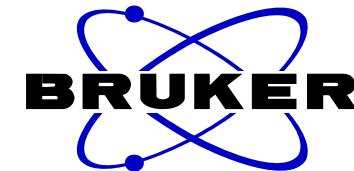
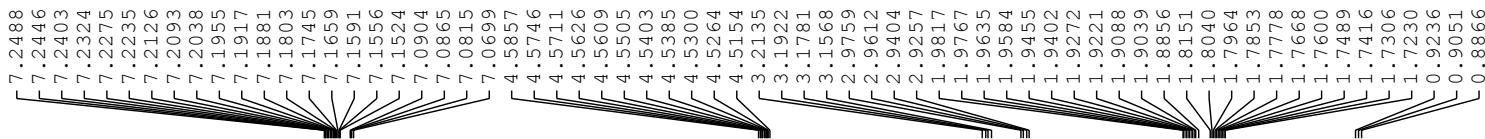
NAME Aug08-2012
EXPNO 7
PROCNO 1
Date_ 20120808
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 306.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

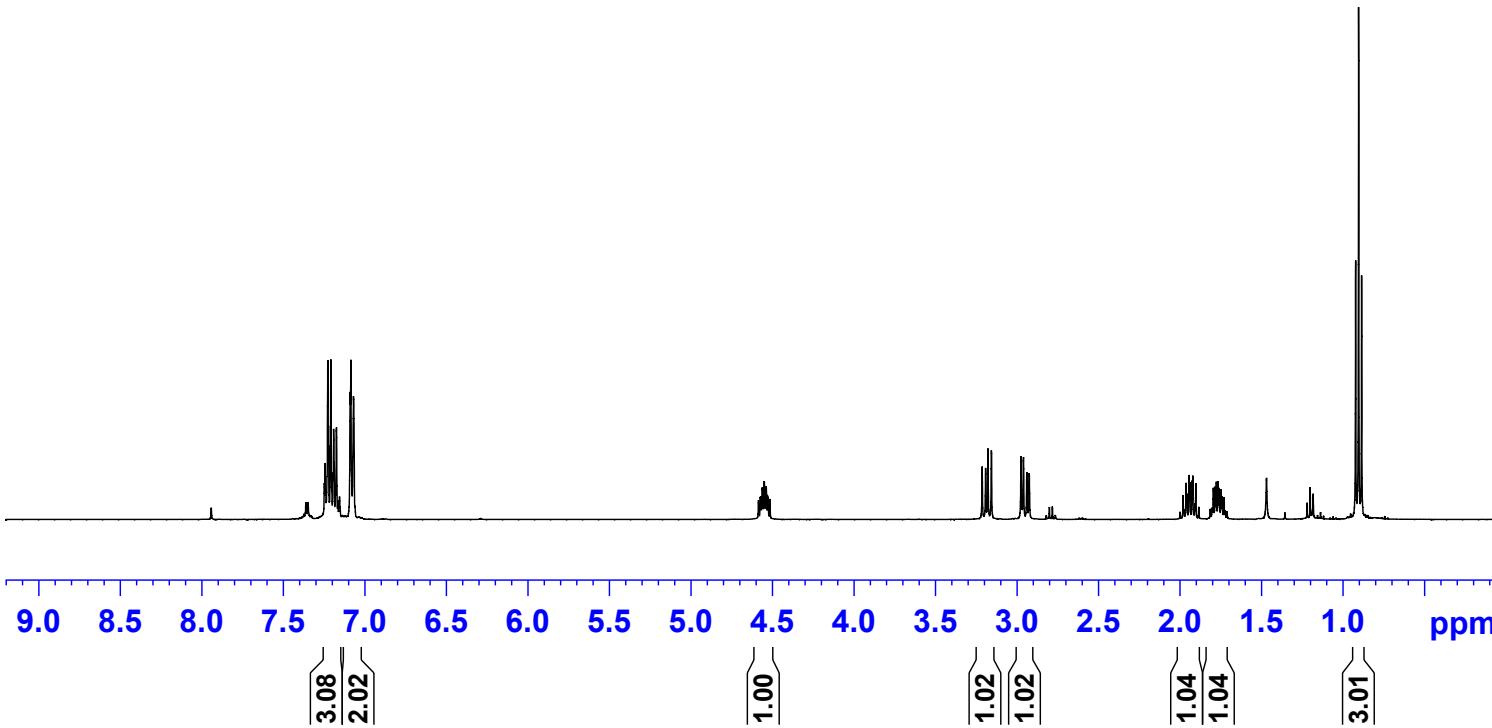


KL29 (R)
PROTON CDC13 {E:\NMR Data} skl 44

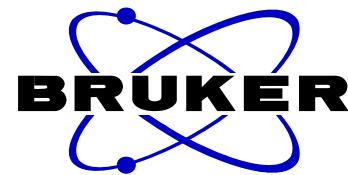
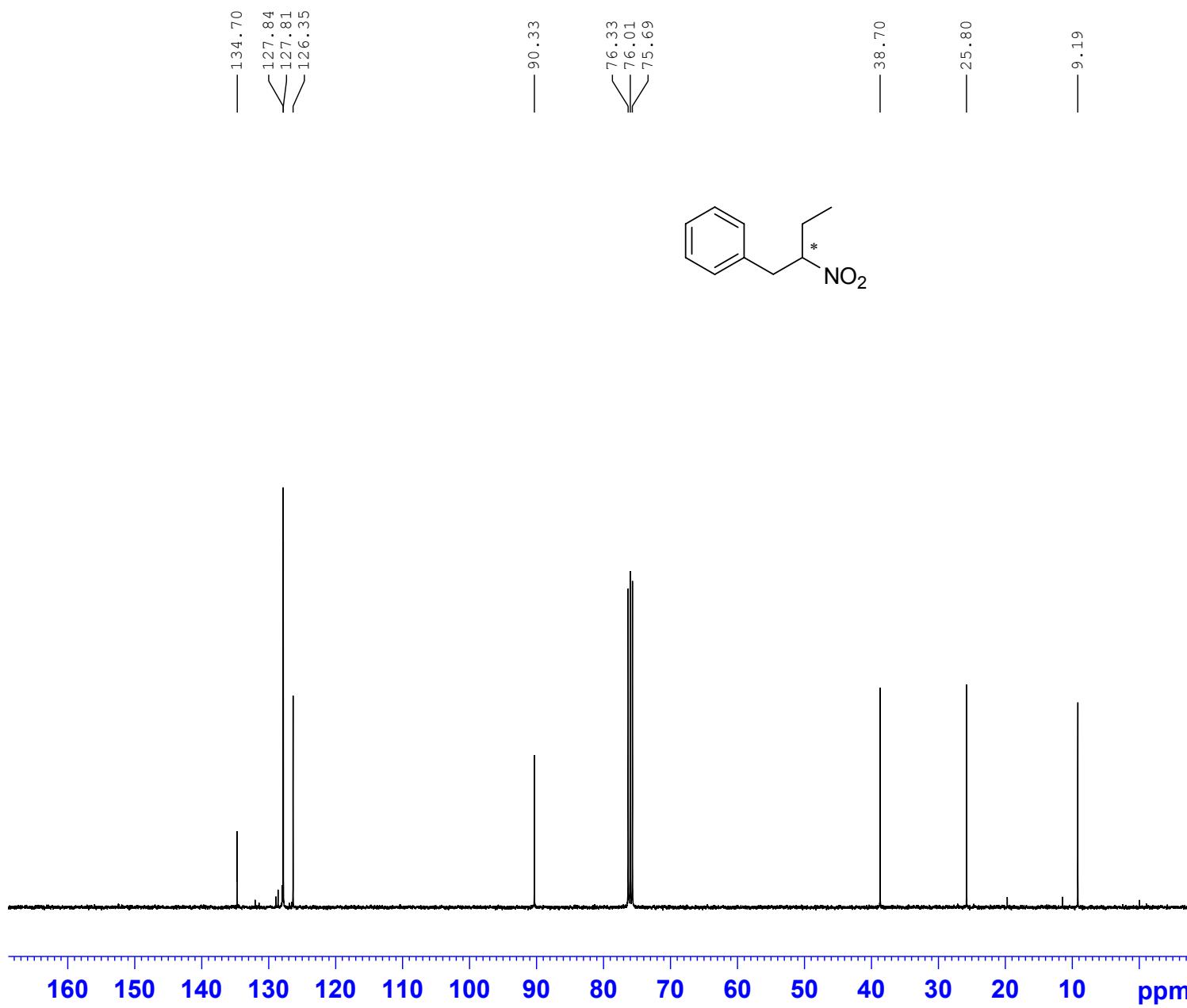


NAME Aug11-2012
EXPNO 3
PROCNO 1
Date_ 20120812
Time 1.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 304.3 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300434 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



KL29 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 44

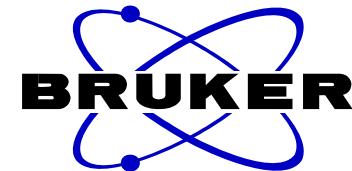
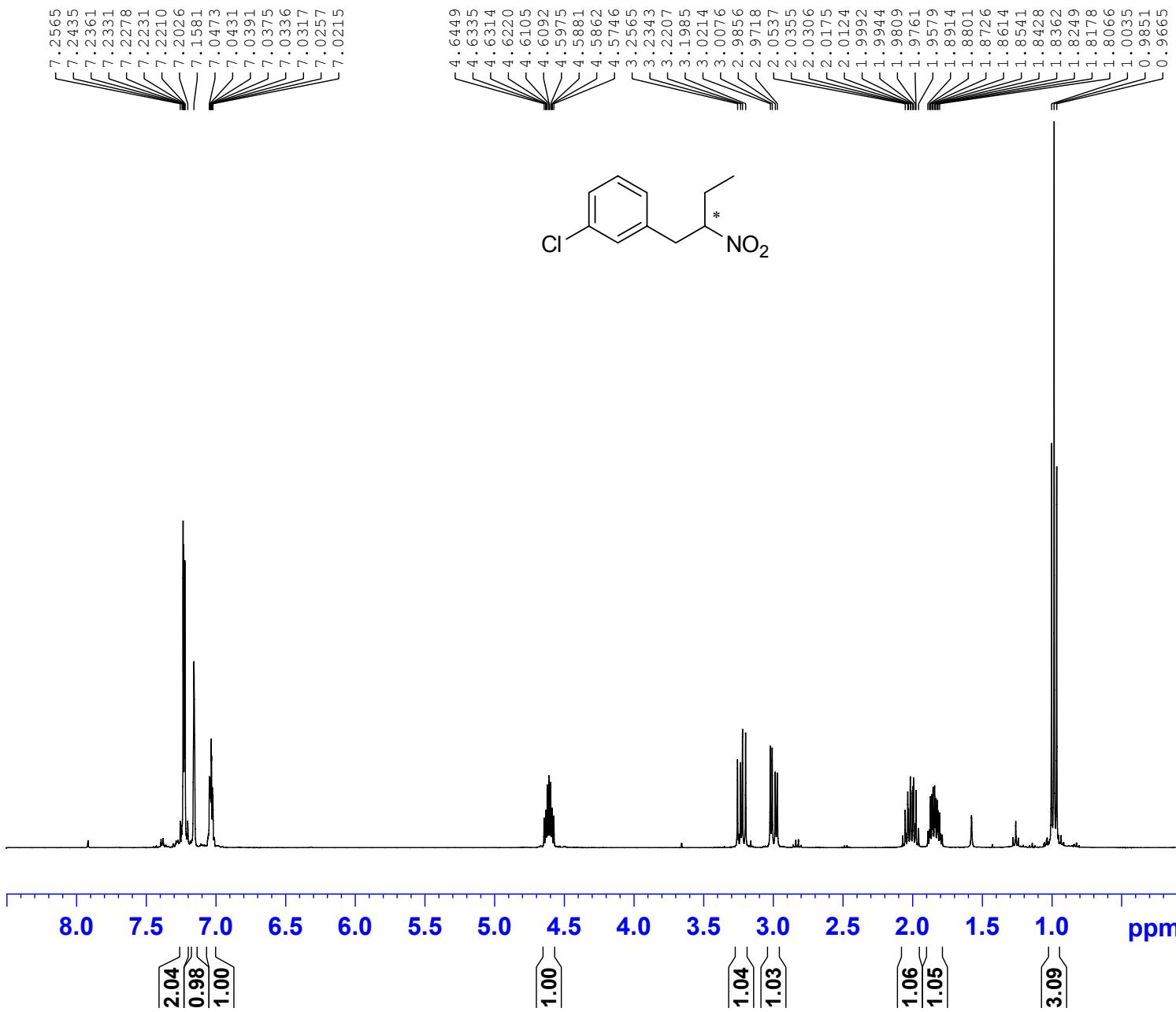


NAME Aug11-2012
EXPNO 5
PROCNO 1
Date_ 20120812
Time 3.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128699 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

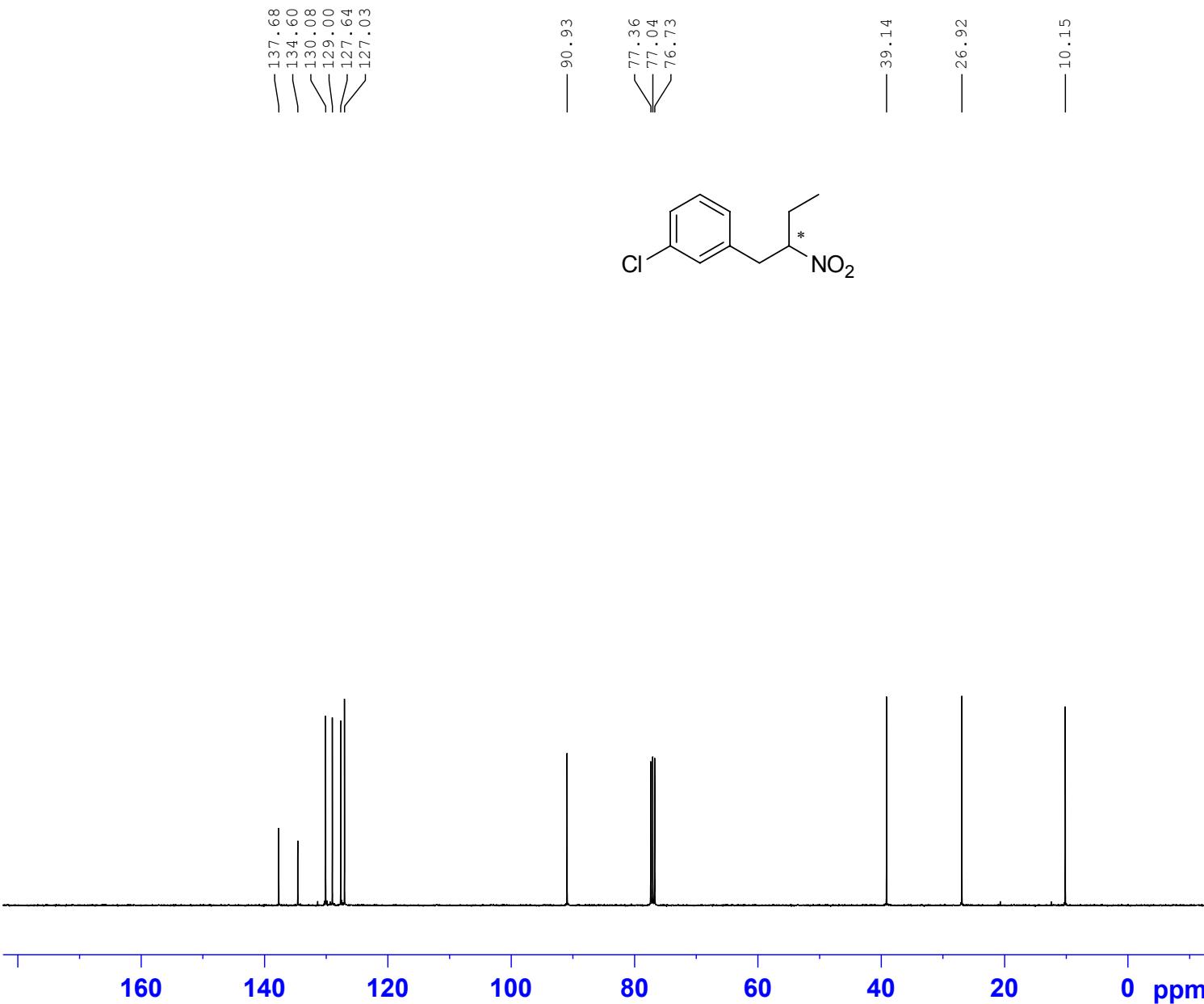
KL30 (R)
PROTON CDC13 {E:\NMR Data} skl 27



NAME Aug12-2012
EXPNO 1
PROCNO 1
Date_ 20120812
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL30 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 27



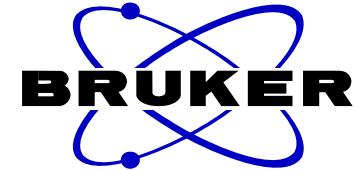
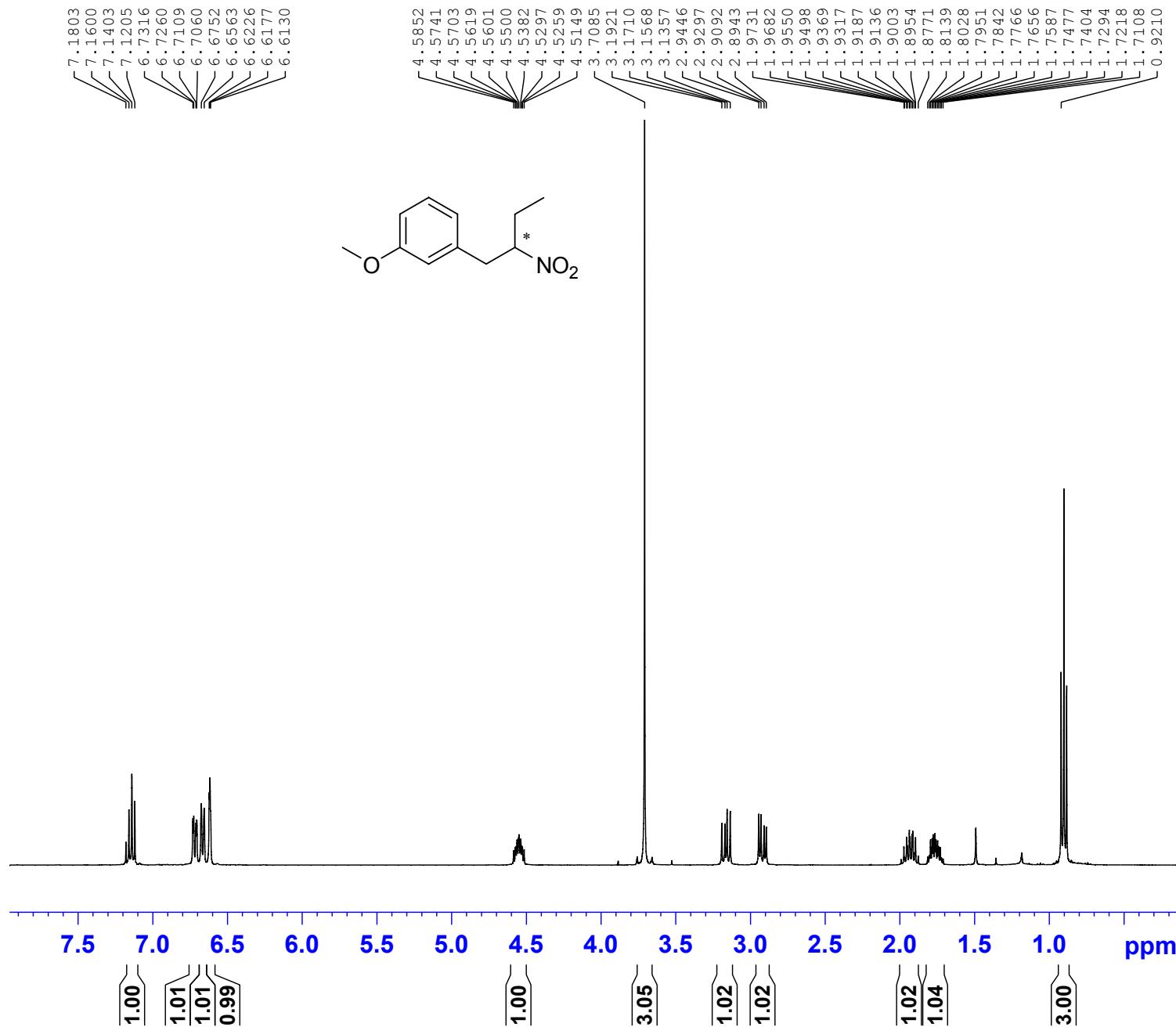
NAME Aug12-2012
EXPNO 5
PROCNO 1
Date_ 20120812
Time 13.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL31 (R)

PROTON CDC13 {E:\NMR Data} skl 28

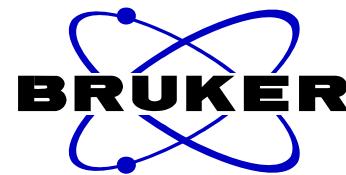
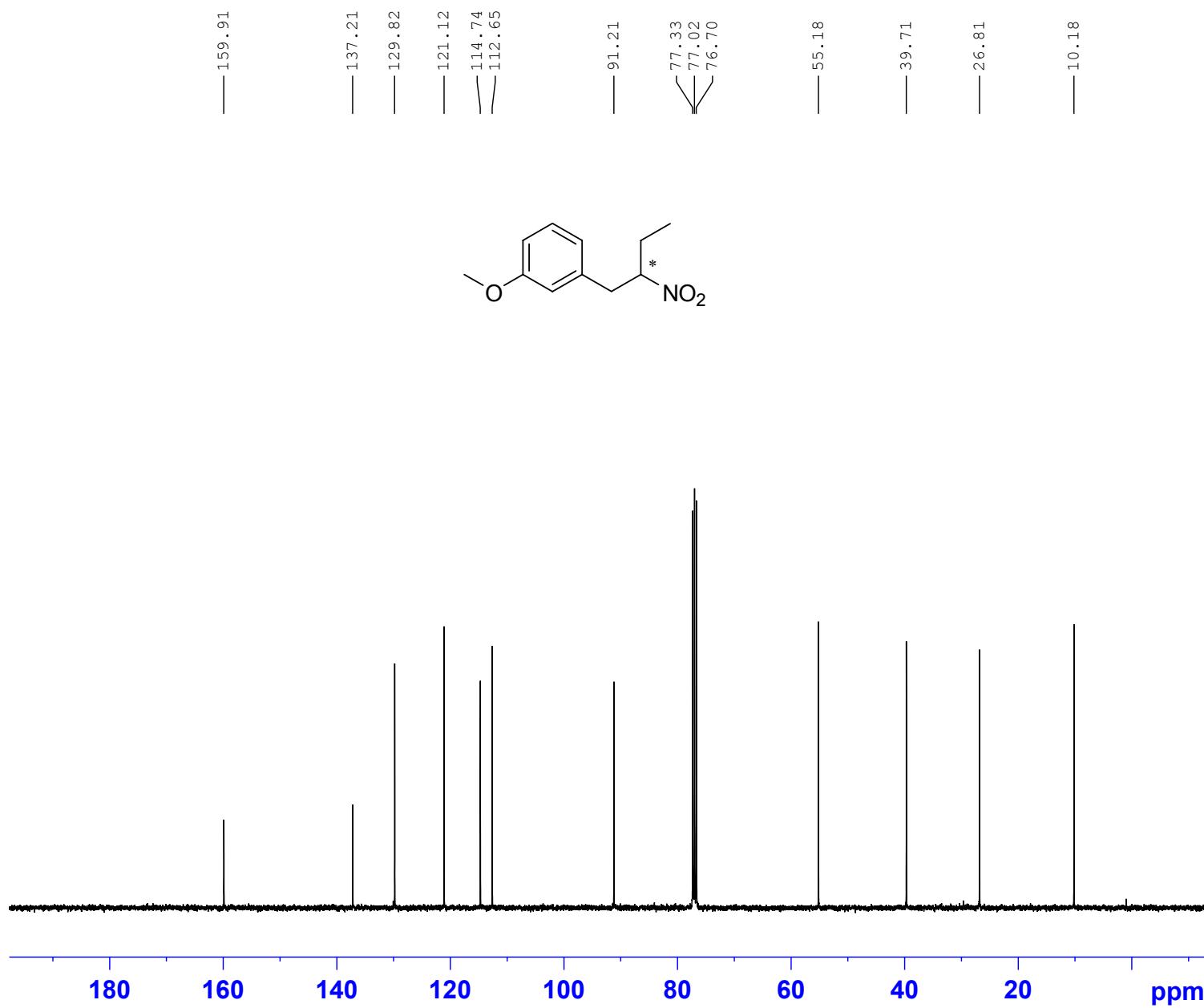


NAME Aug12-2012
 EXPNO 2
 PROCNO 1
 Date_ 20120812
 Time 10.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 44
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 161
 DW 60.800 usec
 DE 6.50 usec
 TE 303.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300417 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL31 (R)
C13CPD32 CDC13 {E:\NMR Data} skl 28



NAME Aug12-2012
EXPNO 9
PROCNO 1
Date_ 20120812
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.5 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

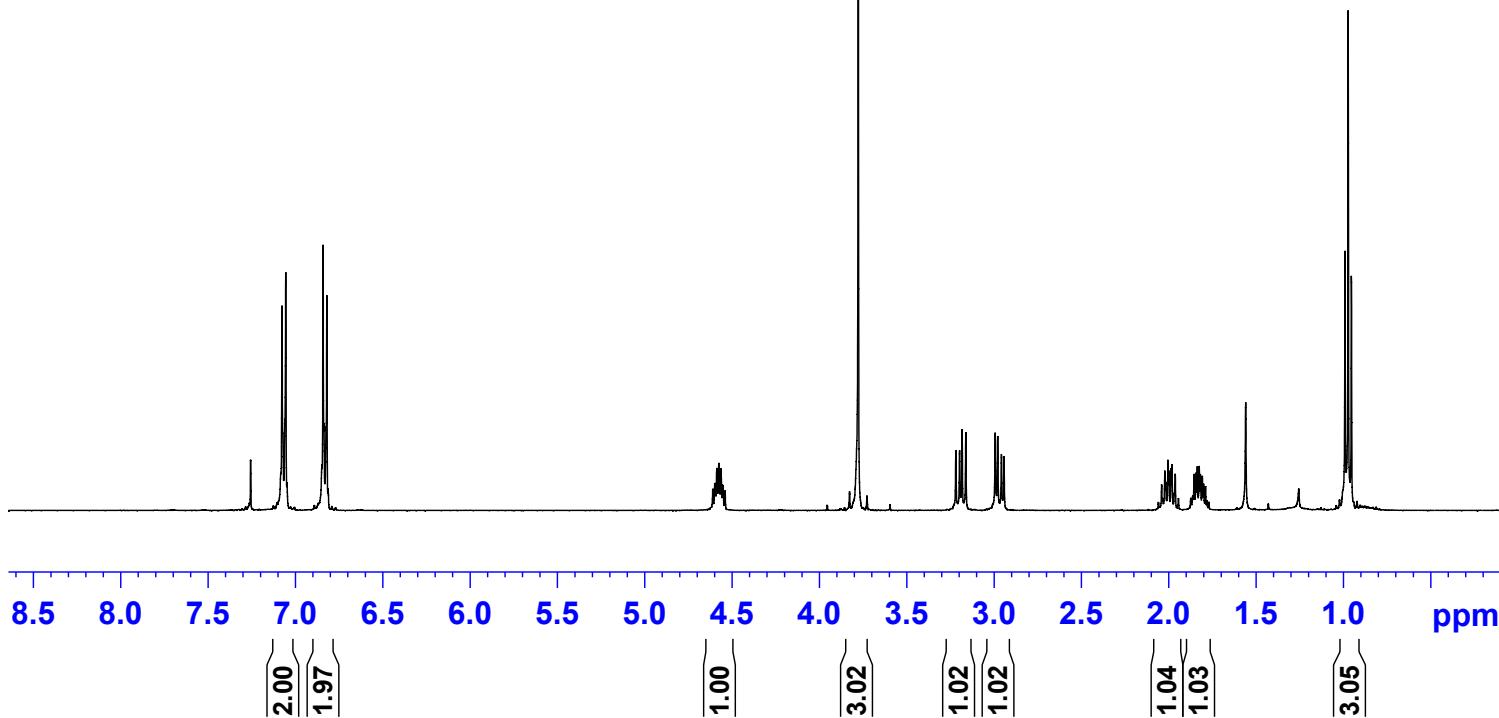
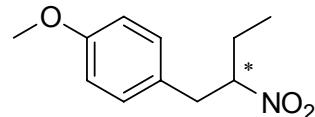
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL32 (R)

PROTON CDC13 {E:\NMR Data} skl 14

7.2569
7.0839
7.0772
7.0558
6.8494
6.8420
6.8370
6.8253
6.8205

4.6109
4.5996
4.5965
4.5868
4.5757
4.5645
4.5548
4.5517
4.5405
3.7783

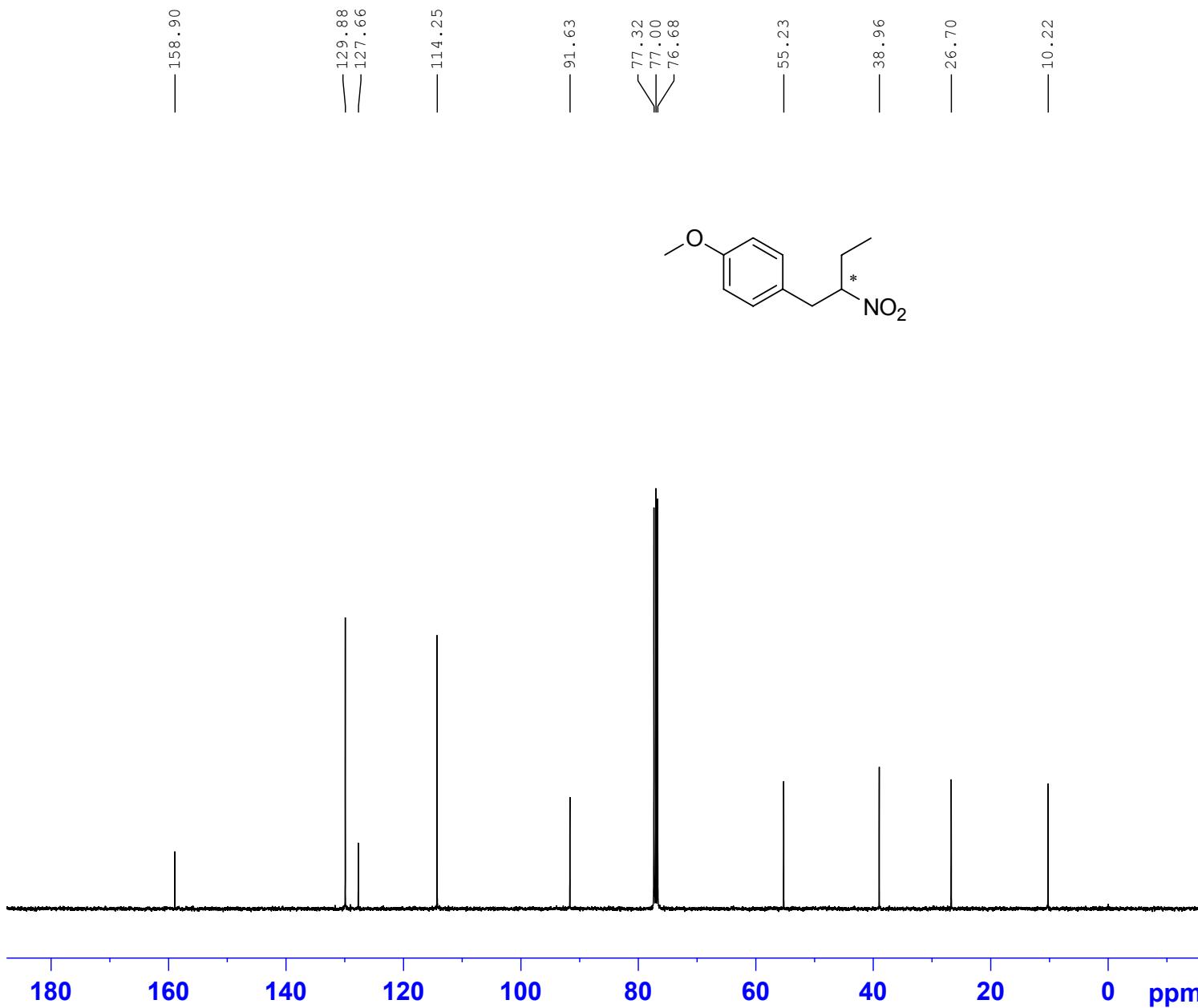


NAME Aug13-2012
EXPNO 3
PROCNO 1
Date_ 20120813
Time 19.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 301.5 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300112 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

KL32 (R)
C13CPD CDC13 {E:\NMR Data} skl 14



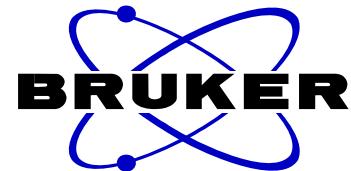
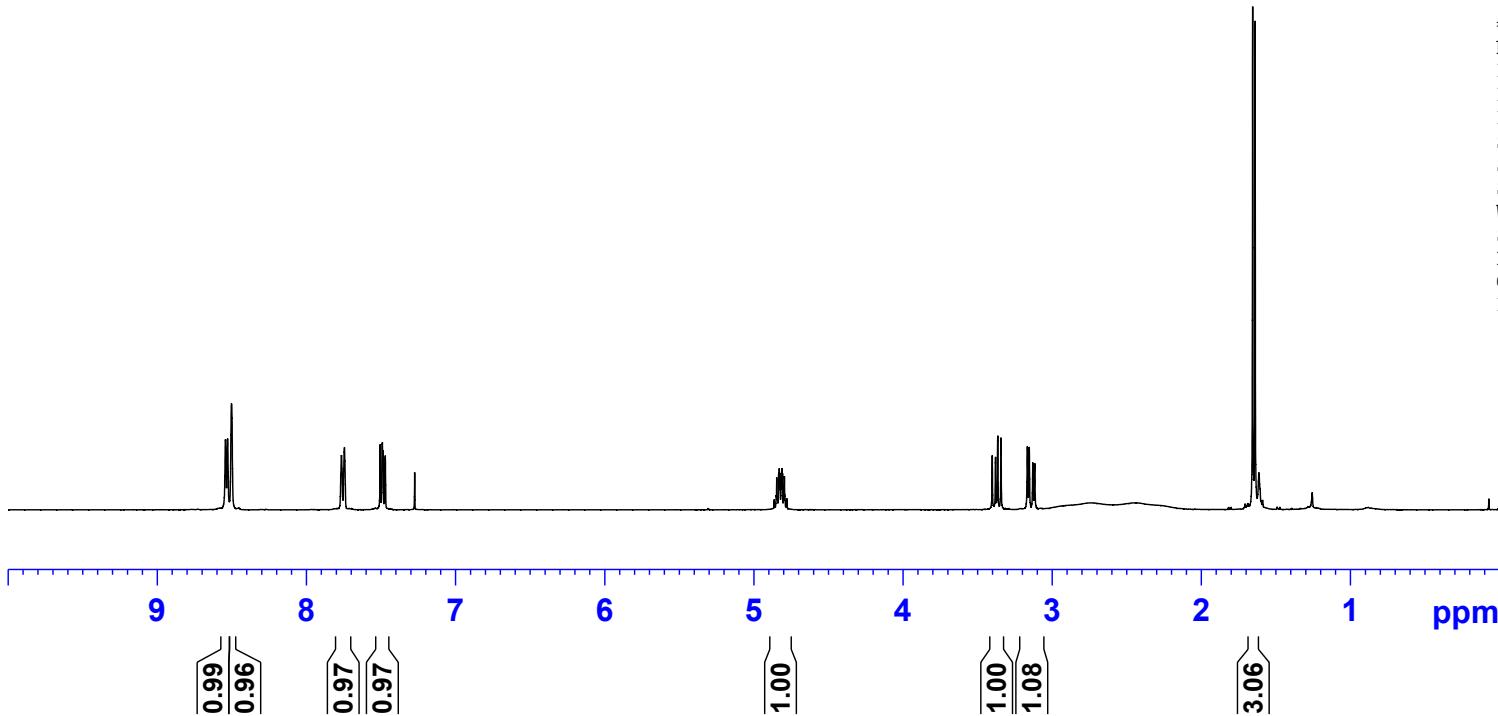
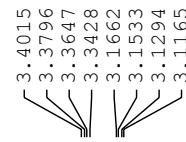
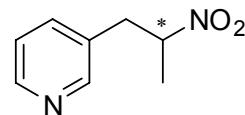
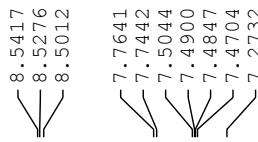
NAME Aug13-2012
EXPNO 11
PROCNO 1
Date_ 20120814
Time 2.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 305.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

KL23 (R)

PROTON CDC13 {E:\NMR Data} skl 2

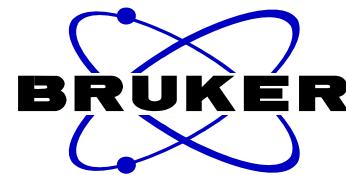


NAME Aug01-2012
EXPNO 5
PROCNO 1
Date_ 20120801
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 300.7 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300047 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

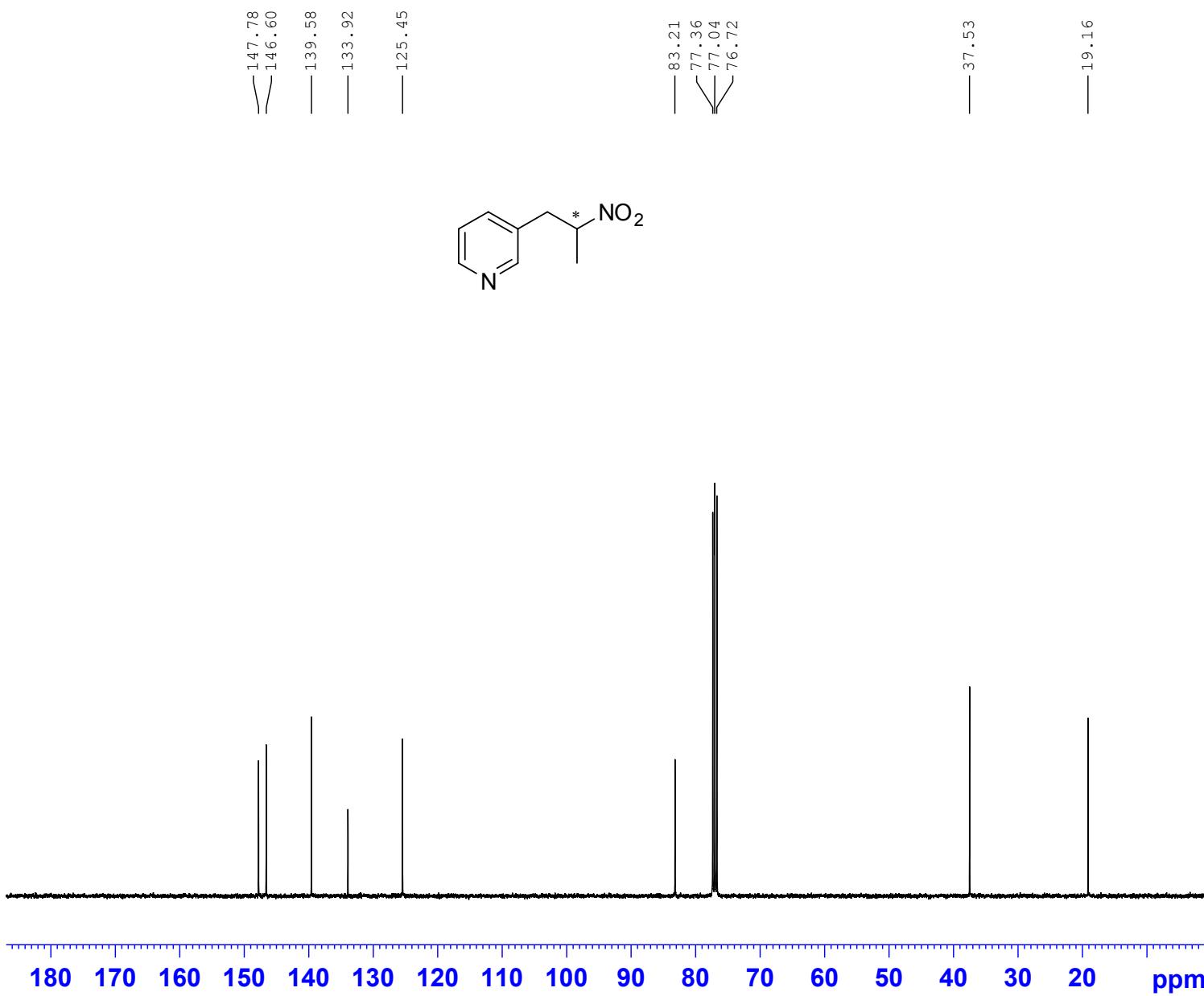
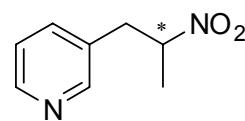
KL23 (R)
C13CPD CDC13 {E:\NMR Data} skl 2



NAME Aug01-2012
EXPNO 10
PROCNO 1
Date_ 20120802
Time 2.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

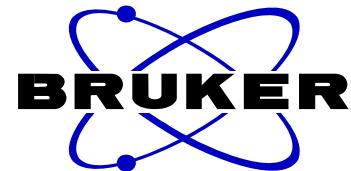
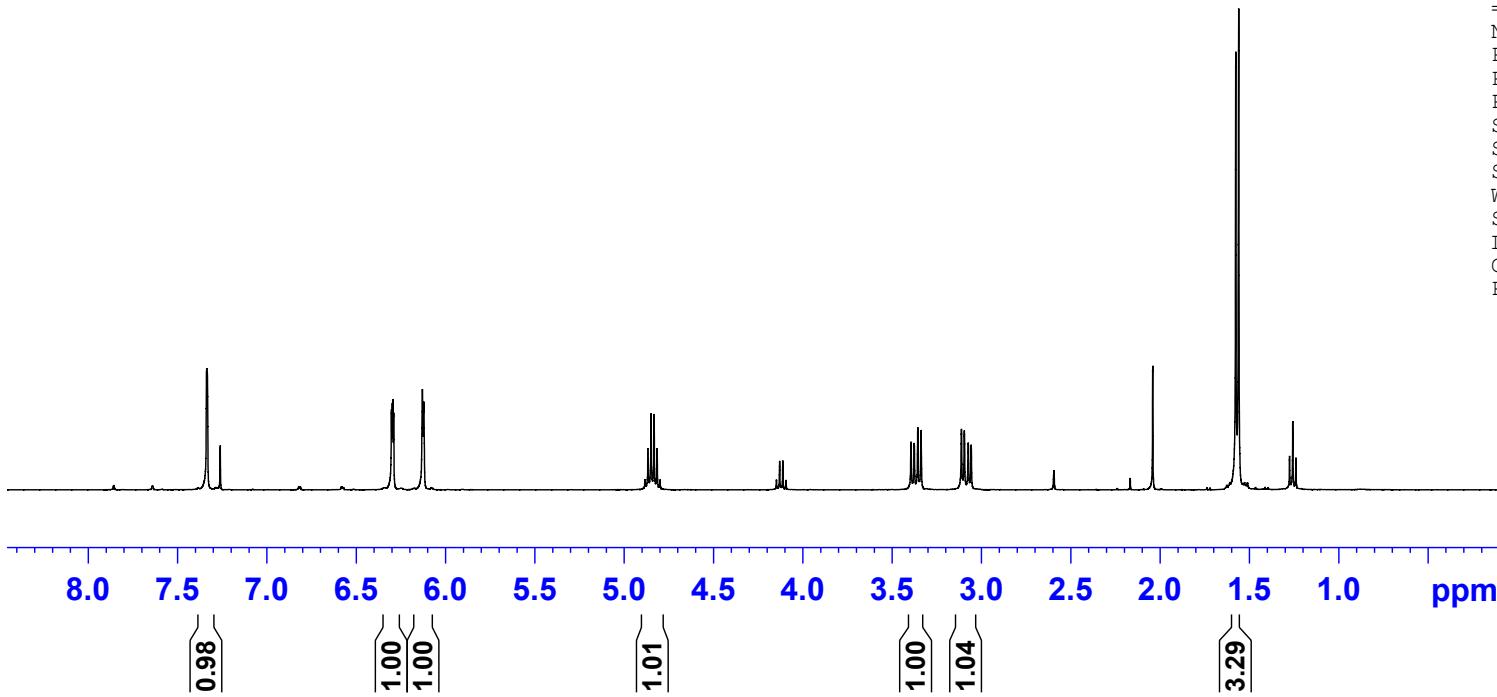
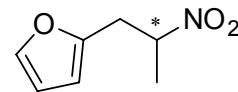
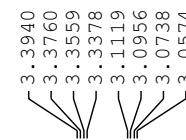
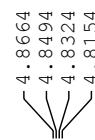
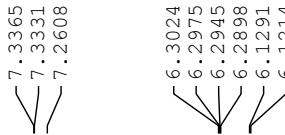
===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



KL22 (R)

PROTON CDC13 {E:\NMR Data} skl 1

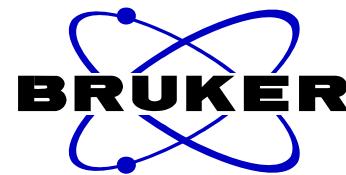
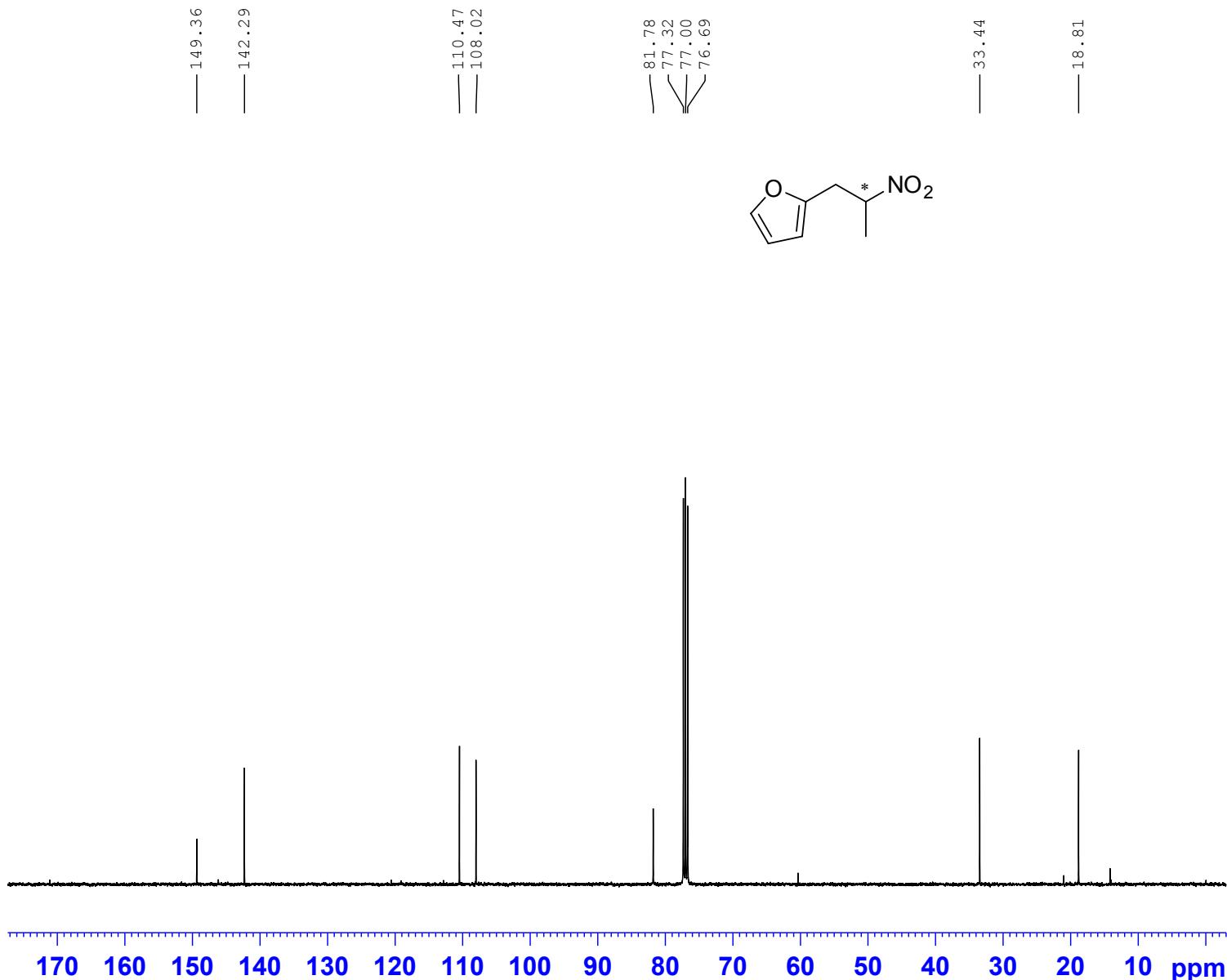


NAME Aug01-2012
EXPNO 6
PROCNO 1
Date_ 20120801
Time 22.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 44
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.50 usec
TE 301.3 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====

NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL22 (R)
C13CPD CDC13 {E:\NMR Data} skl 1



NAME Aug01-2012
EXPNO 8
PROCNO 1
Date_ 20120802
Time 1.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 302.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

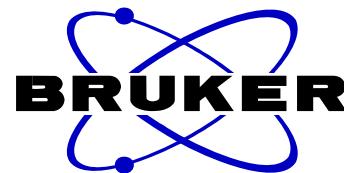
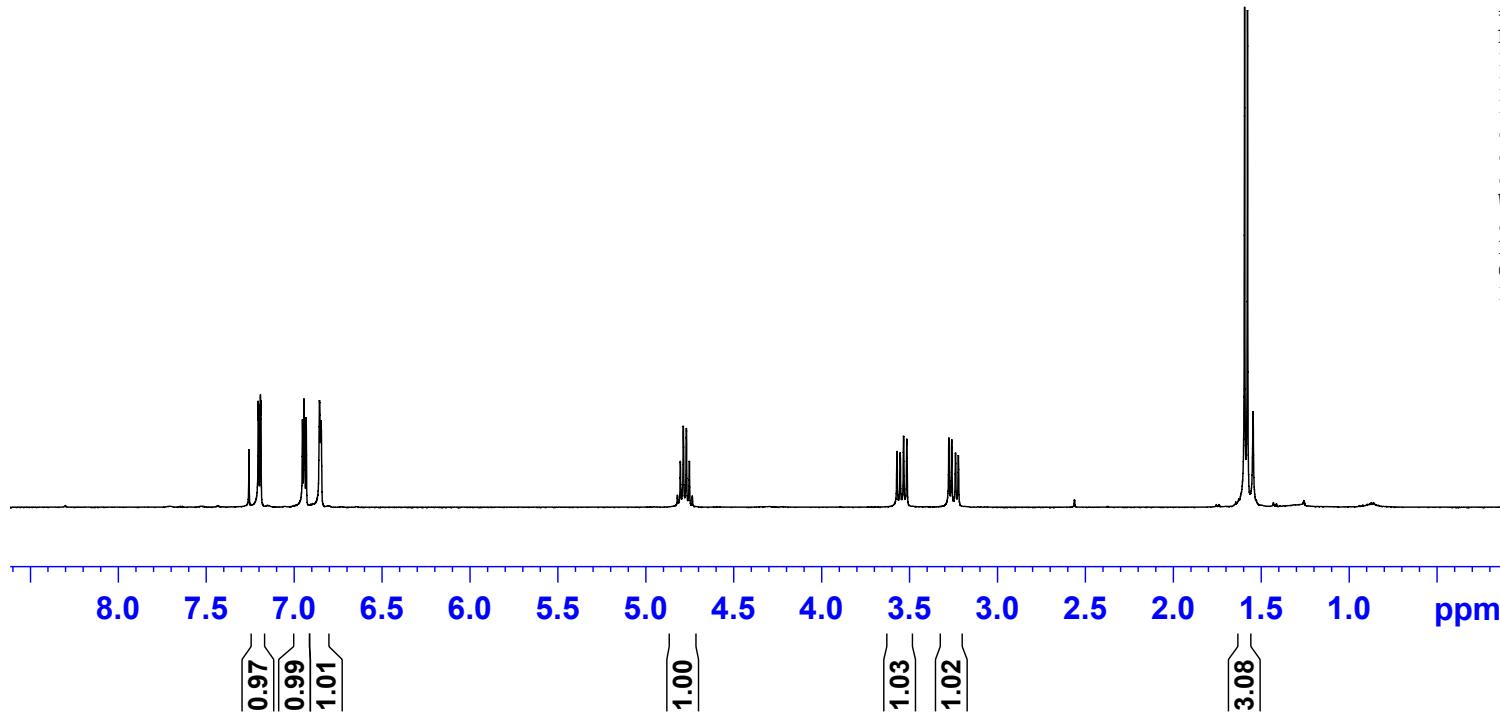
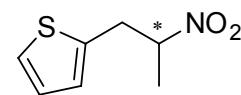
KL34 (R)
PROTON CDC13 {E:\NMR Data} skl 28

7.2570
7.2045
7.2018
7.1916
7.1889
6.9526
6.9439
6.9398
6.9311
6.8557
6.8547
6.8474

4.8033
4.7864
4.7690
4.7520

3.5714
3.5529
3.5337
3.5152
3.2760
3.2599
3.2383
3.2222

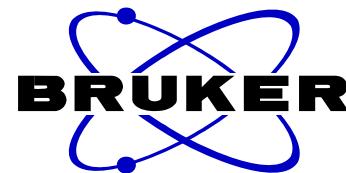
1.5943
1.5776



NAME Sep21-2012
EXPNO 1
PROCNO 1
Date_ 20120921
Time 17.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.50 usec
TE 302.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KL34 (R)
C13CPD CDC13 {E:\NMR Data} skl 28



NAME Sep21-2012
EXPNO 9
PROCNO 1
Date_ 20120922
Time 6.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 303.7 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 ======
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
PL1W 75.02186584 W
SFO1 100.6228298 MHz

===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 18.23 dB
PL13 19.00 dB
PL2W 31.17179108 W
PL12W 0.29563907 W
PL13W 0.24760634 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127663 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

