Copper-Catalyzed Decarboxylative C-N Cross-Coupling for N-Arylation

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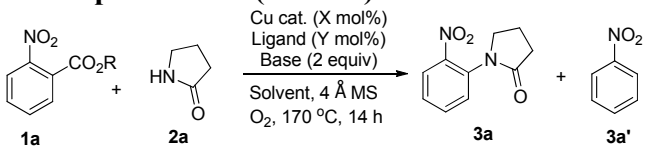
Supporting information

Contents:

I. General Information: All reagents and solvents were used as supplied. ^{1}H NMR spectra were recorded using an internal deuterium lock at ambient temperature on a Varian 400 MHz spectrometer. An internal reference of δ_H 7.26 was used for $CDCl_3$. Data are presented as follows: chemical shift (in ppm on the δ scale relatively to δ_{TMS} = 0), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintuplet, m = mutiplet, br = broad, dd = doublet of doublet, dt = doublet of triplet, dq = doublet of quartet), coupling constant (*J*/Hz) and integration. ^{13}C NMR spectra were recorded on a Varian 400 MHz spectrometer. An internal reference of δ_C 77.0 was used for $CDCl_3$. High resolution mass spectra were recorded using a Agilent 6220 mass spectrometer with electrospray ionization source and Agilent 1200 liquid chromatograph. The resolution of the MS system was approximately 11000 (FWHM definition).

II. Reaction optimization (Table 1).

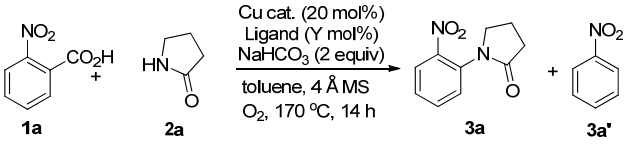


1a **2a** **3a** **3a'**

Entry[a]	R	Cu cat. (X)	Ligand (Y)	Base	Solvent	Conversion [%][b]	**3a** [%][b]	**3a'** [%][b]
1	K,Na	$CuCl_2$ (20)	bpy (50)	$NaHCO_3$	NMP	100	0	>98
2	H	$CuCl_2$ (20)	bpy (50)	$NaHCO_3$	NMP	100	0	>98
3	H	$CuCl_2$ (20)	bpy (50)	$NaHCO_3$	DMA	100	0	>98
4	H	$CuCl_2$ (20)	bpy (50)	$NaHCO_3$	DMSO	100	0	95
5	K	$CuCl_2$ (20)	bpy (50)	$NaHCO_3$	toluene	69	31	38
6	Na	$CuCl_2$ (20)	bpy (50)	$NaHCO_3$	toluene	53	20	32
7	H	$CuCl_2$ (20)	bpy (50)	$KHCO_3$	toluene	18	17	trace
8	H	$CuCl_2$ (20)	bpy (50)	Li_2CO_3	toluene	100	52	48
9	H	$CuCl_2$ (20)	bpy (50)	Na_2CO_3	toluene	84	53	21
10	H	$CuCl_2$ (20)	bpy (50)	K_2CO_3	toluene	100	trace	>98
11	H	$CuCl_2$ (20)	bpy (50)	Cs_2CO_3	toluene	100	0	>98
12	H	$CuCl_2$ (20)	bpy (50)	K_3PO_4	toluene	8	16	52
13	H	$CuCl_2$ (20)	bpy (50)	NaOtBu	toluene	30	17	13
14	H	$CuCl_2$ (20)	bpy (50)	KOtBu	toluene	65	34	31
15	H	$CuCl_2$ (100)	none	$NaHCO_3$	toluene	100	45	55
16	H	none	bpy (50)	$NaHCO_3$	toluene	trace	0	trace
17	H	$CuCl_2$ (20)	bpy (50)	none	toluene	100	0	>98

[a] Unless otherwise noted, all reactions were carried out in sealed pressure vessels under oxygen atmosphere; 1.0 equiv of **1a,** 5.0 equiv of **2a**. [b] Conversion and yields were determined by ^{1}H NMR analysis using mesitylene as internal standard. bpy = 2,2′-Bipyridine, NMP = *N*-Methylpyrrolidinone, DMA = *N*, *N*-Dimethylacetamide, DMSO = Dimethyl sulfoxide.

III. Reaction optimization (Table 2).



1a **2a** **3a** **3a'**

Entry[a]	Cu cat.	Ligand (Y)	Conversion [%]	**3a** [%][b]	**3a'** [%][b]
1	Cu_2O	bpy (50)	trace	0	trace
2	CuI	bpy (50)	29	7	21
3	$CuBr_2$	bpy (50)	44	34	9
4	$Cu(TFA)_2{\cdot}H_2O$	bpy (50)	82	30	50
5	$Cu(BF_4)_2$	bpy (50)	84	47	35
6	CuF_2	bpy (50)	95	55	43
7	$CuCl_2$	pyr (50)	64	11	53
8	$CuCl_2$	Ph_3N (50)	16	7	8
9	$CuCl_2$	SIPr (50)	22	8	13
10	$CuCl_2$	TMEDA (50)	20	trace	19
11	$CuCl_2$	Ac-ILe-OH (50)	42	34	7
12	$CuCl_2$	bqu(50)	trace	0	trace
13	$CuCl_2$	bpy (20)	73	56	17

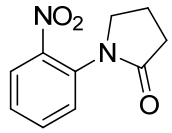
[a] Unless otherwise noted, all reactions were carried out in sealed pressure vessels under oxygen atmosphere; 1.0 equiv of **1a,** 5.0 equiv of **2a**. [b] Conversion and yields were determined by ^{1}H NMR analysis using mesitylene as internal standard. bpy = 2,2'-Bipyridine, SIPr = 1,3-Bis(2,6-di-i-propylphenyl)imidazolidin-2-ylidene, TMEDA = *N*,*N*,*N*',*N*'-Tetramethylethylenediamine, Ac-Ile-OH = *N*-Acetyl-*L*-isoleucine, bqu = 2,2'-Biquinoline.

IV. General procedure:

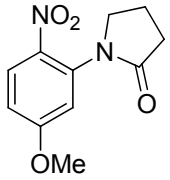
A solution of **1a** (84 mg, 0.5 mmol), **2a** (213 mg, 2.50 mmol), $CuCl_2$ (13 mg, 0.1 mmol), 1,10-phenanthroline (18 mg, 0.1 mmol), $NaHCO_3$ (84 mg, 1.0 mmol), 4 Å molecular sieves (50 mg) in anhydrous anisole (2 mL) was added into an oven-dried pressure vessel. The vessel was purged with oxygen and was sealed. The mixture was heated at 170 ℃ for 14 h before being cooled to ambient temperature.[1] The reaction mixture was diluted with EtOAc (2 mL) and was acidified with 1 N HCl solution (2 mL). The mixture was then filtered through a short plug of celite and the filtrate was extracted with EtOAc (3 x 5 mL). The combined organic phases were washed with brine (5 mL), dried over anhydrous $MgSO_4$, concentrated under the reduced pressure. The residue was

[1] The authors did not experience hazard for small scale reactions; however, for large reaction scales using a closed system, the production of CO_2 can be dangerous.

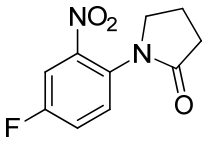
purified by flash chromatography on 8 g silica gel with 0-100 % EtOAc/heptane afforded compound **3a** as a white solid (76 mg, 73%).



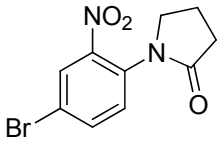
1-(2-nitrophenyl) pyrrolidin-2-one (3a).[2] ^{1}H NMR (400 MHz, $CDCl_3$) 8.00 - 7.58 (m, 1 H), 7.68 - 7.60 (m, 1 H), 7.46 - 7.38 (m, 1 H), 7.36 (d, 1 H), 3.89 (t, J = 6.95 Hz, 2 H), 2.55 (t, J = 7.96 Hz, 2 H), 2.36 - 2.20 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 145.7, 133.7, 132.3, 127.5, 127.4, 125.5, 50.1, 31.2, 19.0; HRMS (Cl/NH_3) *m/z* calcd for C10H11N2O3 $[M+H]^+$ 207.0691 found 207.0690.



1-(5-methoxy-2-nitrophenyl) pyrrolidin-2-one (3b). (118 mg, 76%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 9.09 Hz, 4 H) 6.88 (dd, J = 9.22, 2.65 Hz, 4 H) 6.80 (d, J = 2.53 Hz, 1 H) 3.89 (s, 3 H) 3.84 (t, J = 6.95 Hz, 2 H) 2.55 (t, J = 7.96 Hz, 2 H) 2.22 - 2.32 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 163.7, 138.9, 134.8, 127.9, 113.6, 112.5, 56.1, 50.3, 31.2, 19.1; HRMS (Cl/NH_3) *m/z* calcd for C11H12N2O4 $[M+H]^+$ 237.0870 found 237.0879.



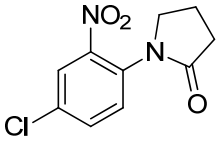
1-(4-fluoro-2-nitrophenyl)pyrrolidin-2-one (3c). (92 mg, 82%), pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (ddd, J = 7.86, 2.31, 0.95 Hz, 1 H), 7.40 - 7.32 (m, 2 H), 3.90 - 3.78 (m, 2 H), 2.58 - 2.48 (m, 2 H), 2.34 - 2.20 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 160.2 (d, J = 251 Hz), 146.2 (d, J = 8 Hz), 129.5 (d, J = 8 Hz), 128.7, 121.0 (d, J = 22 Hz), 113.2 (d, J = 27 Hz), 50.2, 31.0, 19.0; HRMS (Cl/NH_3) *m/z* calcd for C10H10FN2O3 [M+H]+ 225.0676 found 225.0675.



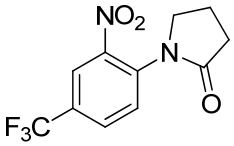
1-(4-bromo-2-nitrophenyl)pyrrolidin-2-one (3d). (77 mg, 54%), white solid. ^{1}H NMR (400 MHz ,$CDCl_3$) δ 8.10 (d, J = 2.3 Hz, 1 H), 7.75 (dd, J = 2.3, 8.5 Hz, 1 H), 7.23 (d, J = 8.5 Hz, 1 H), 3.92 - 3.82 (m, 2 H), 2.60 - 2.51 (m, 2 H), 2.34 - 2.19 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 145.9, 136.6, 131.2, 128.5, 128.4,

[2] a) W. Deng, Y-F. Wang, Y. Zou, L. Liu, Q-X. Guo *Tetrahedron Lett.* 2004, **45**, 2311; b) B. Renger *Synthesis* 1985, 856.

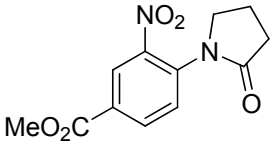
120.2, 50.0, 31.1, 19.0. HRMS (Cl/NH_3) *m/z* calcd for C10H10BrN2O3 $[M+H]^+$ 284.9875 found 284.9870.



1-(4-chloro-2-nitrophenyl)pyrrolidin-2-one (3e). (80 mg, 67%), pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 2.40 Hz, 1 H), 7.60 (dd, *J* = 8.59, 2.40 Hz, 1 H), 7.30 (d, *J* = 8.59 Hz, 1 H), 3.92 - 3.83 (m, 2 H), 2.61 - 2.50 (m, 2 H), 2.34 - 2.21 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ175.1, 145.8, 133.7, 133.1, 130.7, 128.4, 125.7, 50.1, 31.1, 19.0; HRMS (Cl/NH_3) *m/z* calcd for C10 H11N2O3Cl $[M+H]^+$ 241.0380 found 241.0372.

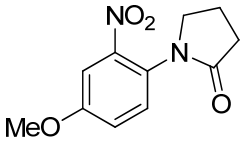


1-(2-nitro-4-(trifluoromethyl)phenyl)pyrrolidin-2-one (3f). [3] (89 mg, 65%), pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 1.52 Hz, 1 H), 7.87 (dd, *J* = 8.34, 1.77 Hz, 1 H), 7.48 (d, *J* = 8.34 Hz, 1 H), 3.90 - 4.02 (m, 2 H), 2.57 (t, *J* = 7.96 Hz, 2 H), 2.25 - 2.38 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 145.1, 135.2, 130.0, 129.1, 126.7, 123.0, 122.6 (q, *J* = 270 Hz), 50.0, 31.1, 19.0; HRMS (Cl/NH_3) *m/z* calcd for C11H10F3N2O3 $[M+H]^+$ 275.0644 found 275.0643.

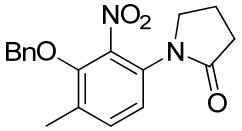


methyl 3-nitro-4-(2-oxopyrrolidin-1-yl)benzoate (3g).[4] (91 mg, 69%), pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 1.89 Hz, 1 H), 8.24 (dd, *J* = 8.34, 1.89 Hz, 1 H), 7.40 (d, *J* = 8.34 Hz, 1 H), 3.94 (s, 3 H), 3.94 - 3.58 (m, 2H), 2.54 (t, *J* = 7.96 Hz, 2 H), 2.28 (t, *J* = 7.52 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ174.5, 164.5, 144.9, 135.7, 134.1, 128.6, 126.7, 125.7, 52.8, 49.6, 31.2, 19.0; HRMS (Cl/NH_3) *m/z* calcd for C12H13N2O5 $[M+H]^+$ 265.0746 found 265.0817.

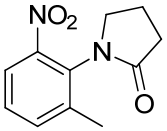
[3] C. Cheng, G. Sun, J. Wan, C. Sun *Synlett* 2009, 2663.
[4] V. R. Atigadda, W. Brouillette, F. Duarte, S. M. Ali, Y. S. Babu, S. Bantia, P. Chand, N. Chu, J. A. Montgomery, D. A. Walsh *J. Med. Chem.* 1999, **42**, 2332.



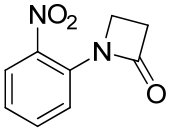
1-(4-methoxy-2-nitrophenyl)pyrrolidin-2-one (3h). (73 mg, 62%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 2.8 Hz, 1 H), 7.31 - 7.27 (m, 1 H), 7.21 - 7.15 (m, 1 H), 3.88 (s, 3 H), 3.84 (t, *J* = 6.9 Hz, 2 H), 2.59 - 2.49 (m, 2 H), 2.26 (t, *J* = 7.6 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.1, 158.6, 146.4, 129.4, 125.0, 120.1, 110.2, 56.0, 50.4, 31.0, 19.0; HRMS (Cl/NH3) *m/z* calcd for C11H13N2O4 $[M+H]^+$ 237.0875 found 237.0876.



1-(3-(benzyloxy)-4-methyl-2-nitrophenyl)pyrrolidin-2-one (3i). (85 mg, 52%), white solid. ^{1}H NMR (400 MHz ,$CDCl_3$) δ 7.52 - 7.29 (m, 5 H), 7.03 (d, *J* = 8.2 Hz, 1 H), 5.04 (s, 2 H), 3.77 (t, *J* = 6.9 Hz, 2 H), 2.53 (t, *J* = 8.1 Hz, 2 H), 2.36 (s, 3 H), 2.29 - 2.11 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 150.0, 143.7, 136.0, 133.4, 133.4, 130.0, 128.6, 128.5, 128.2, 123.1, 76.8, 50.9, 30.8, 19.1, 16.3; HRMS (Cl/NH3) *m/z* calcd for C18H19N2O4 $[M+H]^+$ 326.1267 found 327.1344.



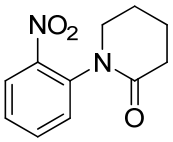
1-(2-methyl-6-nitrophenyl)pyrrolidin-2-one (3j). (37mg, 34%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.83 Hz, 1 H), 7.55 - 7.49 (m, 1 H), 7.36 (t, *J* = 7.96 Hz, 1 H), 3.81 - 3.71 (m, 1 H), 3.68 (dd, *J* = 8.21, 4.80 Hz, 1 H), 2.51 (t, *J* = 8.02 Hz, 2 H), 2.31 (s, 3H), 2.36 - 2.12 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 147.4, 139.4, 135.6, 130.8, 128.3, 123.1, 49.2, 30.7, 19.4, 17.6; HRMS (Cl/NH3) *m/z* calcd for C11H13N2O3 $[M+H]^+$ 221.0925 found 221.0926.



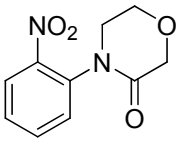
1-(2-nitrophenyl) azetidin-2-one (4a).[5] (64 mg, 67%), pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 8.34, 1.01 Hz, 1 H), 7.71 (dd, *J* = 8.21, 1.39 Hz, 1 H), 7.53 - 7.46 (m, 1 H), 7.13 - 7.19 (m, 1 H), 3.66 (t, *J* = 4.80 Hz, 2 H), 3.12 (t, *J* = 4.80 Hz, 2 H); ^{13}C NMR (100 MHz, CDCl3) δ 165.7, 140.7, 133.4, 131.1, 125.1,

[5] J. Lange, A. C. Bissember, M. G. Banwell, I. A. Cade *Aust. J. Chem.* 2011, **64**, 454.

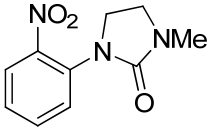
124.7, 122.4, 40.8, 37.3; HRMS (Cl/NH3) *m/z* calcd for C9H9N2O3 $[M+H]^+$ 193.0535 found 193.0608.



1-(2-nitrophenyl)piperidin-2-one (4b).[6] (68 mg, 62%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 8.08, 1.52 Hz, 1 H), 7.65 (td, *J* = 7.77, 1.39 Hz, 1 H), 7.49 - 7.41 (m, 1 H), 7.33 (dd, 1 H) 3.70 (t, *J* = 5.81 Hz, 2 H), 2.51 (t, 2 H), 2.10-1.83 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 146.5, 136.7, 134.1, 129.3, 128.2, 125.2, 51.6, 32.5, 23.2, 21.0; HRMS (Cl/NH3) *m/z* calcd for C11H13N2O3 $[M+H]^+$ 221.0921 found 221.0932.

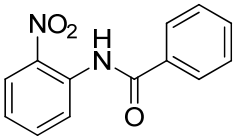


4-(2-nitrophenyl)morpholin-3-one (4c).[7] (53 mg, 48%), pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.21, 1.39 Hz, 1 H), 7.70 (td, *J* = 7.77, 1.39 Hz, 1 H), 7.48 - 7.57 (m, 1 H), 7.39 (dd, *J* = 7.96, 1.14 Hz, 1 H), 4.32 (s, 2 H), 4.09 (t, *J* = 5.05 Hz, 2 H), 3.82 (br. s., 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 146.4, 134.6, 134.5, 129.0, 128.9, 125.5, 68.5, 63.9, 50.0; HRMS (Cl/NH3) *m/z* calcd for C10H11N2O4 $[M+H]^+$ 223.0714 found 223.0721.

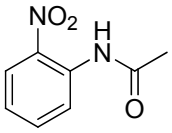


1-methyl-3-(2-nitrophenyl) imidazolidin-2-one (4d). (62 mg, 56%), yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.34 Hz, 1 H), 7.57 (t, *J* = 8.0 Hz, 1 H), 7.31 (d, *J* = 7.83 Hz, 2 H), 3.89 (t, *J* = 7.83 Hz, 2 H), 3.63 - 3.51 (m, 2 H), 2.89 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 145.1, 133.4, 133.2, 125.6, 125.5, 125.4, 45.0, 44.3, 31.3; HRMS (Cl/NH3) *m/z* calcd for C10H12N3O3 $[M+H]^+$ 222.0873 found 222.0878.

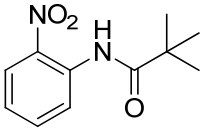
[6] H. Moehrle, J. Mehrens, *Zeitschrift fuer Naturforschung, B: Chemical Sciences* 1998, **53**, 37.
[7] D. Dorsch, Dieter, B. Cezanne, W. Mederski, C. Tsaklakidis, H. Wurziger, PCT Int. Appl. 2005, WO 2005016899 A1 20050224.



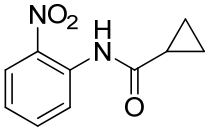
N-(2-nitrophenyl)benzamide (4e).[8] (88 mg, 73%), light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.35 (br.s., NH), 9.02 (d, *J* = 8.59 Hz, 1 H) 8.29 (dd, *J* = 8.46, 1.52 Hz, 1 H), 8.10 - 7.93 (m, 2 H), 7.73 (s, 1 H), 7.61 (d, *J* = 7.45 Hz, 1 H) 7.58 - 7.51 (m, 2 H), 7.23 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 136.4, 136.2, 135.3, 134.0, 132.6, 129.0, 127.4, 125.9, 123.3, 122.1; HRMS (Cl/NH3) *m/z* calcd for C13H11N2O3 $[M+H]^+$ 243.0764 found 243.0768.



N-(2-nitrophenyl)acetamide (4f).[9] (39 mg, 44%), light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 10.30 (br.s., NH), 8.77 (dd, *J* = 8.46, 1.26 Hz, 1 H), 8.21 (dd, *J* = 8.46, 1.52 Hz, 1 H), 7.65 (s, 1 H), 7.21 - 7.15 (m, 1 H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 136.3, 136.0, 134.9, 125.7, 123.2, 122.1, 25.6; HRMS (Cl/NH3) *m/z* calcd for C8H9N2O3 $[M+H]^+$ 181.0613 found 181.0605.



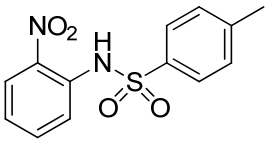
N-(2-nitrophenyl)pivalamide (4g).[10] (72 mg, 65%), yellow solid. ^{1}H NMR (400 MHz ,$CDCl_3$) δ 10.73 (br.s., 1 H), 8.83 (dd, *J* = 0.9, 8.5 Hz, 1 H), 8.23 (dd, *J* = 1.4, 8.5 Hz, 1 H), 7.71 - 7.59 (m, 1 H), 7.16 (dt, *J* = 1.3, 7.9 Hz, 1 H), 1.36 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.9, 136.3, 136.0, 135.4, 125.8, 122.9, 122.1, 40.6, 27.4; HRMS (Cl/NH3) *m/z* calcd for C11H15N2O3 $[M+H]^+$ 223.1083 found 223.1080.



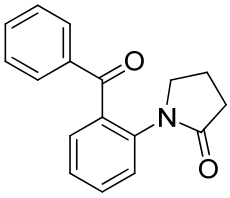
N-(2-nitrophenyl)cyclopropanecarboxamide (4h). [11] (54 mg, 52%), yellow solid. ^{1}H NMR (400 MHz ,$CDCl_3$) δ 10.59 (br.s., NH), 8.78 (dd, *J* = 1.3, 8.6 Hz, 1 H), 8.21 (dd, *J* = 1.6, 8.5 Hz, 1 H), 7.62 (ddd, *J* = 1.3, 7.3, 8.5 Hz, 1 H), 7.15 (ddd, *J* = 1.3, 7.2, 8.5 Hz, 1 H), 1.67 (tt, *J* = 4.5, 7.8 Hz, 1 H), 1.17 - 1.10 (m, 2 H), 0.98 -

[8] S. Darvesh, R. S. McDonald, K. V. Darvesh, D. Mataija, S. Mothana, H. Cook, K. M. Carneiro, N. Richard, R. Walsh, E. Martin, *Bioorgan. Med. Chem.* 2006, **14**, 4586.
[9] J. Jiao, X-R. Zhang, N-H. Chang, J. Wang, J-F. Wei, X-Y. Shi, Z-G. Chen, *J. Org. Chem.***76**, 1180.
[10] J. R. Gage, J. M. Wagner, *J. Org. Chem.* 1995, **60**, 2613.
[11] P. Zhang, E. A. Terefenko, C. C. McComas, P. E. Mahaney, A. Vu, E. Trybulski, E. Koury, G. Johnston, J. Bray, D. Deecher *Bioorg. Med. Chem Lett.* 2008, **18**, 6067.

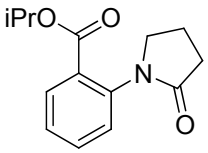
0.91 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 136.0, 135.9, 135.1, 125.7, 122.9, 122.2, 16.9, 8.9; HRMS (Cl/NH3) *m/z* calcd for C10H11N2O3 $[M+H]^+$ 207.0770 found 207.0771.



4-methyl-N-(2-nitrophenyl)benzenesulfonamide (4j).[12] (98 mg, 67%), yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 9.84 (br.s., NH), 8.10 (dd, *J* = 8.46, 1.52 Hz, 1 H), 7.84 (dd, *J* = 8.46, 1.01 Hz, 1 H), 7.73 (d, *J* = 8.34 Hz, 1 H), 7.61 - 7.54 (m, 1 H), 7.29 - 7.22 (m, 2 H), 7.18 - 7.10 (m, 1 H), 2.38 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 137.0, 135.8, 135.7, 133.9, 130.0, 127.2, 126.1, 123.7, 121.0, 21.5; HRMS (Cl/NH3) *m/z* calcd for C13H13N2O4S $[M+H]^+$ 293.0591 found 293.0591.



1-(2-benzoylphenyl)pyrrolidin-2-one (5b).[13] (78 mg, 59%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.1 Hz, 2 H), 7.59 - 7.48 (m, 3 H), 7.46 - 7.39 (m, 2 H), 7.34 (dt, *J* = 0.9, 7.5 Hz, 1 H), 7.29 (d, *J* = 8.0 Hz, 1 H), 3.81 - 3.73 (m, 2 H), 2.20 (t, *J* = 8.0 Hz, 2 H), 1.88 (dq, *J* = 7.3, 7.5 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.7, 174.4, 137.3, 137.2, 135.5, 132.7, 131.6, 130.1, 129.8, 128.1, 126.4, 125.2, 50.6, 31.2, 18.5; HRMS (Cl/NH3) *m/z* calcd for C17H16NO2 $[M+H]^+$ 266.1181 found 266.1186.



isopropyl 2-(2-oxopyrrolidin-1-yl)benzoate (5c).[14] (60 mg, 48%), colorless viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 1.3, 7.8 Hz, 1 H), 7.55 - 7.49 (m, 1 H), 7.37 - 7.30 (m, 1 H), 7.27 - 7.20 (m, 1 H), 5.26 - 5.13 (m, 1 H), 3.84 (t, *J* = 7.0 Hz, 2 H), 2.54 (t, *J* = 8.1 Hz, 2 H), 2.29 - 2.15 (m, 2 H), 1.35 (d, *J* = 6.3 Hz, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 165.5, 138.2, 132.5, 131.1, 129.0, 127.1, 127.0, 68.6, 50.9, 31.6, 21.9, 18.9; HRMS (Cl/NH3) *m/z* calcd for C14H18NO3 $[M+H]^+$ 248.1287 found 248.1279.

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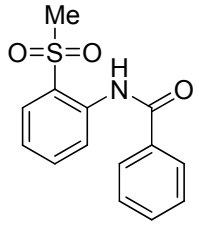
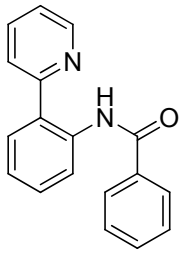
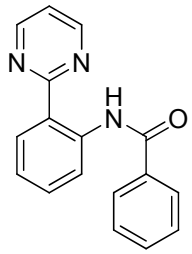
[12] R. A. Bunce, C. L. Smith, C. L. Knight, *Org. Prep. Proced. Int.* 2004, **36**, 482.
[13] S. Barroso, G. Blay, L. Cardona, I. Fernandez, B. Garcia, J. R. Pedro, *J. Org. Chem.* 2004, **69**, 6821.
[14] H, Suzuki, Hitomi; T. Murashima, *J. Chem. Soc., Perkin Trans. 1* 1994, 903.



N-(2-(methylsulfonyl)phenyl)benzamide (5d).[15] (70 mg, 51%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.56 - 10.37 (br.s., NH), 8.67 (dd, *J* = 1.0, 8.5 Hz, 1 H), 8.03 - 7.95 (m, 3 H), 7.71 (s, 1 H), 7.60 (d, *J* = 7.3 Hz, 1 H), 7.57 - 7.50 (m, 2 H), 7.35 - 7.28 (m, 1 H), 3.09 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 137.2, 135.5, 133.5, 132.6, 129.4, 129.0, 127.4, 127.3, 124.4, 123.0, 44.3; HRMS (Cl/NH3) *m/z* calcd for C14H13NO3S $[M+H]^+$ 276.0694 found 276.0690.



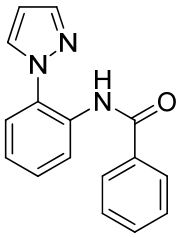
***N*-(2-(pyridin-2-yl)phenyl)benzamide (5e)**.[16] (106 mg, 77%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.27 (br.s., NH), 8.79 (d, *J* = 8.3 Hz, 1 H), 8.74 - 8.62 (m, 1 H), 8.09 - 7.95 (m, 2 H), 7.90 - 7.78 (m, 2 H), 7.73 (d, *J* = 8.0 Hz, 1 H), 7.55 - 7.44 (m, 4 H), 7.33 - 7.27 (m, 1 H), 7.24 - 7.17 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 158.2, 147.2, 138.1, 137.8, 135.7, 131.5, 130.2, 128.7, 128.6, 127.3, 125.5, 123.5, 123.0, 121.9, 121.9; HRMS (Cl/NH3) *m/z* calcd for C18H15N2O $[M+H]^+$ 275.1184 found 275.1184.



***N*-(2-(pyrimidin-2-yl)phenyl)benzamide (5f).** (44 mg, 63%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.50 (br.s., 1 H), 8.93 (dd, *J* = 0.5, 8.3 Hz, 1 H),

[15] F. Babudri, S. Florio, A. Vitrani, L. Di Nunno, *J. Chem. Soc., Perkin Trans. 1* 1984, 1899.
[16] A. John, K. M. Nicholas, *J. Org. Chem.* 2011, **76**, 4158.

8.84 (d, *J* = 4.9 Hz, 3 H), 8.66 (dd, *J* = 1.4, 8.1 Hz, 1 H), 8.08 (dd, *J* = 1.5, 7.9 Hz, 2 H), 7.61 - 7.47 (m, 3 H), 7.29 - 7.18 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 165.1, 156.4, 140.1, 136.0, 132.3, 131.6, 130.7, 128.6, 127.4, 123.2, 122.8, 121.0, 118.5; HRMS (Cl/NH3) *m/z* calcd for C17H14N3O $[M+H]^+$ 276.1137 found 276.1143.



***N*-(2-(1H-pyrazol-1-yl)phenyl)benzamide (5g).** (47 mg, 65%), white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.31 (br. s., 1 H), 8.72 (dd, *J* = 1.1, 8.3 Hz, 1 H), 8.03 - 7.91 (m, 2 H), 7.87 (dd, *J* = 2.1, 4.6 Hz, 2 H), 7.54 - 7.45 (m, 3 H), 7.45 - 7.39 (m, 1 H), 7.38 (dd, *J* = 1.3, 8.0 Hz, 1 H), 7.24 - 7.16 (m, 1 H), 6.52 (t, *J* = 2.2 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 141.1, 134.8, 131.8, 131.8, 130.2, 129.1, 128.6, 128.0, 127.3, 124.0, 122.9, 122.1, 107.3; HRMS (Cl/NH3) *m/z* calcd for C16H14N3O $[M+H]^+$ 264.1137 found 264.1134.

V. Selected ^{1}H and ^{13}C NMR spectra:

ZHANGYUT-001-EXP012-proton

10/31/2011 11:31:14 AM

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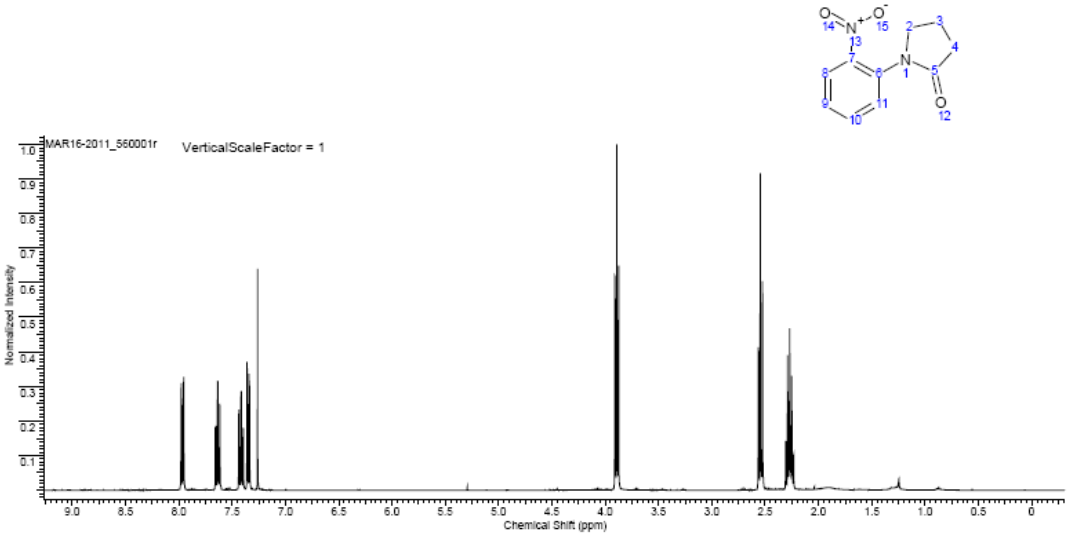

ZHANGYUT-001-EXP012-carbon

10/31/2011 11:27:50 AM

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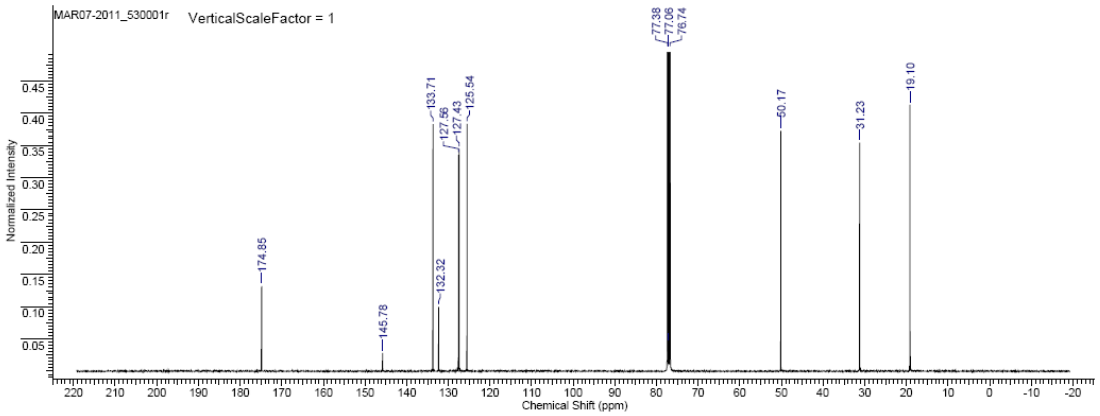

ZHANGYUT-001-EXP049-1-pdt

4/27/2011 8:40:06 AM

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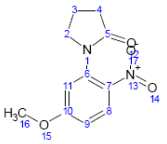

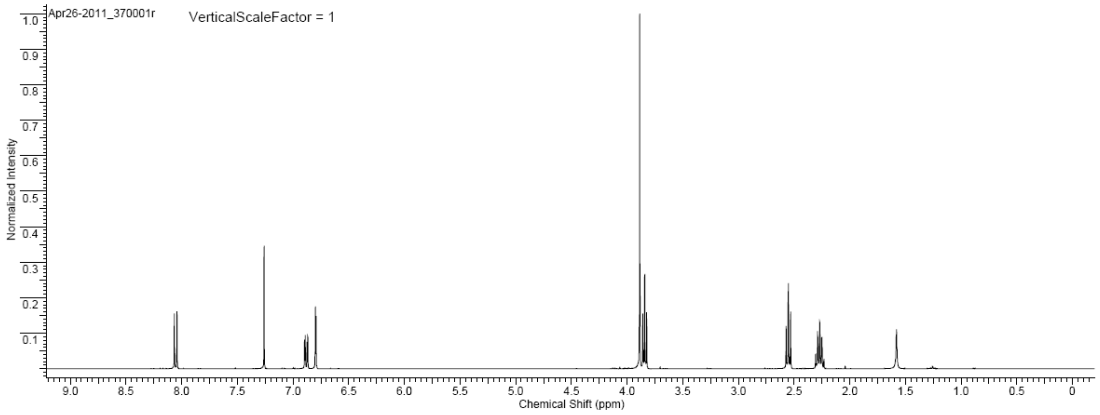

ZHANGYUT-001-EXP049-carbon

10/31/2011 11:05:14 AM

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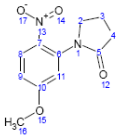

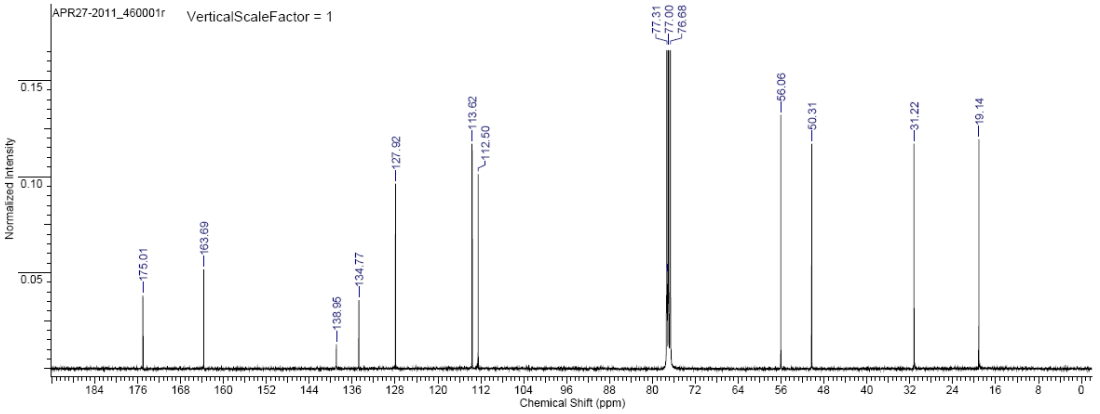

ZHANGYUT-002-EXP081-pdt

11/11/2011 2:27:12 PM

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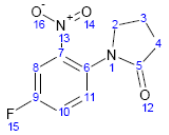

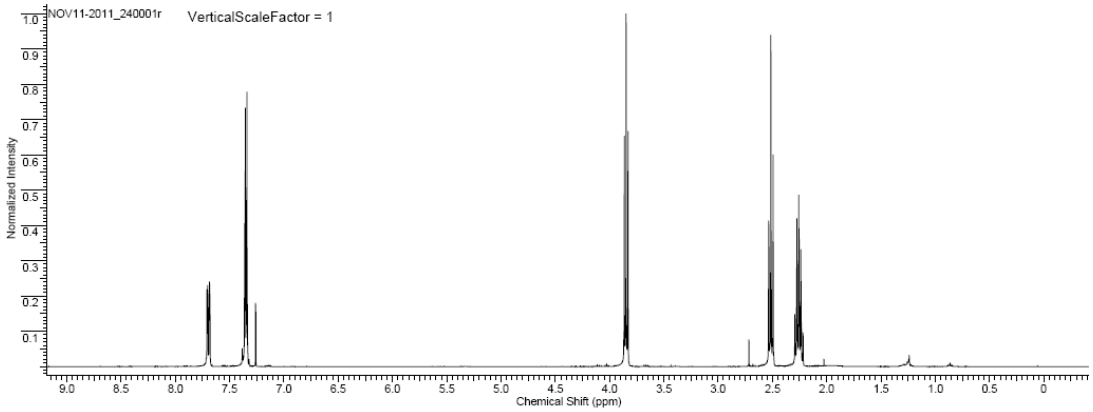

ZHANGYUT-002-EXP081-pdt

11/17/2011 2:55:05 PM

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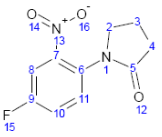
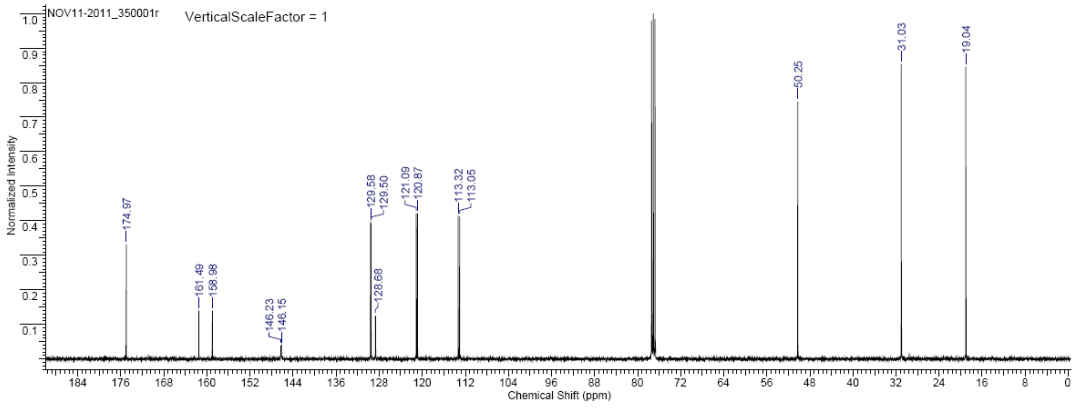
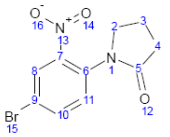


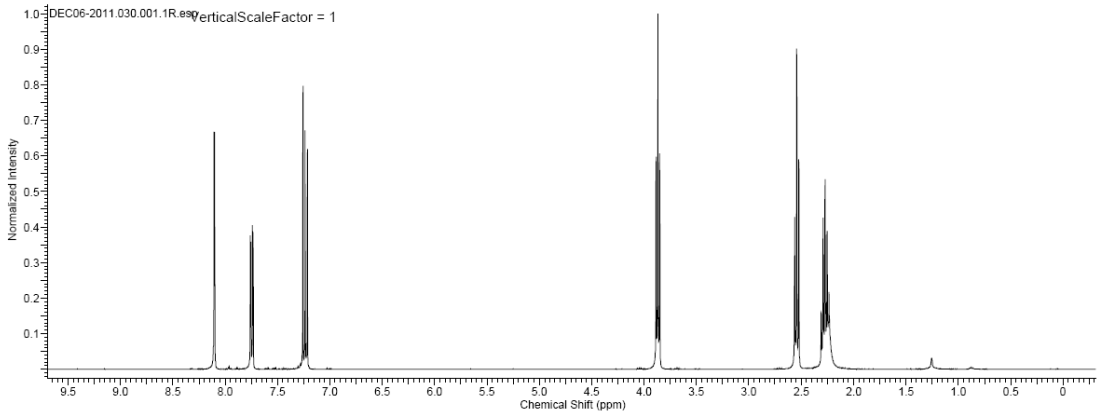


ZHANGYUT-002-EXP068-pdt

12/6/2011 11:14:39 AM

Formula $C_{10}H_9BrN_2O_3$	*FW*	285.0941					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP068-ISO1 Project ZHANGYUT Name FLOW				
Date	06 Dec 2011 10:19:28	*Date Stamp*	06 Dec 2011 10:19:28				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC06-2011.30_201112061025.02\DEC06-2011\30\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	574.70	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2461.5276
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

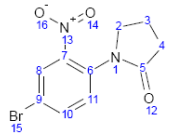


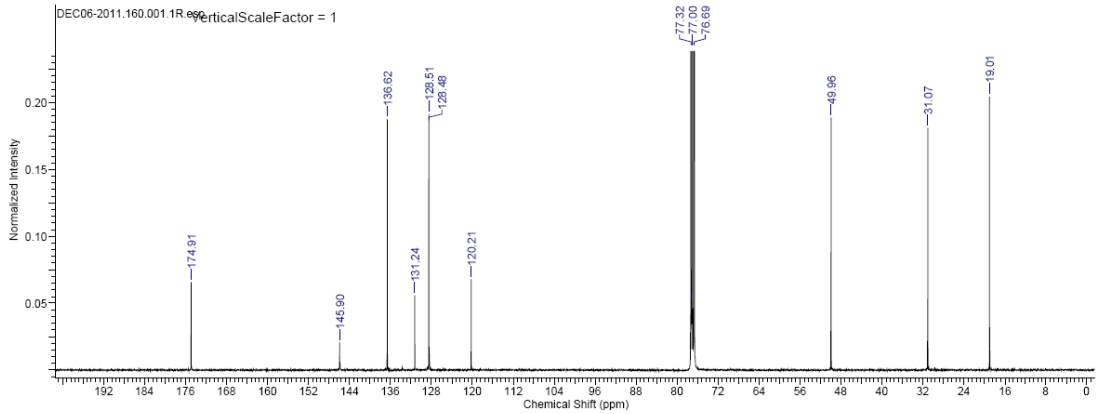


ZHANGYUT-002-EXP068-pdt

12/7/2011 9:12:30 AM

Formula $C_{10}H_9BrN_2O_3$	*FW*	285.0941					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP068-CARBON Name ZHANGYUT Project FLOW				
Date	06 Dec 2011 23:56:32	*Date Stamp*	06 Dec 2011 23:56:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.DEC06-2011.160_201112070000.02\DEC06-2011\160\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	5000	*Origin*	av400a
Original Points Count	32768	*Owner*	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	9195.20	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10057.2246
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		

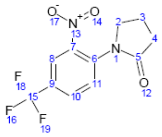


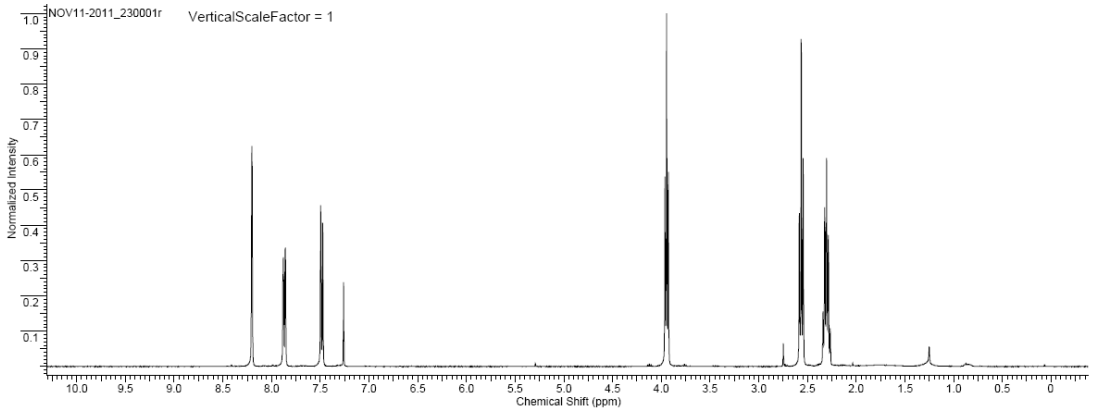


ZHANGYUT-002-EXP080-pdt

11/11/2011 2:18:12 PM

Formula $C_{11}H_9F_3NO_2$	*FW*	274.1960					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP080-ISO Project ZHANGYUT Name FLOW				
Date	11 Nov 2011 18:52:48	*Date Stamp*	11 Nov 2011 18:52:48				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV11-2011.230_201111111405.02\NOV11-2011_230001r						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	181.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.6541
Sweep Width (Hz)	8278.02	*Temperature (degree C)*	27.000				

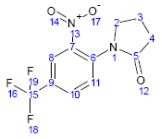


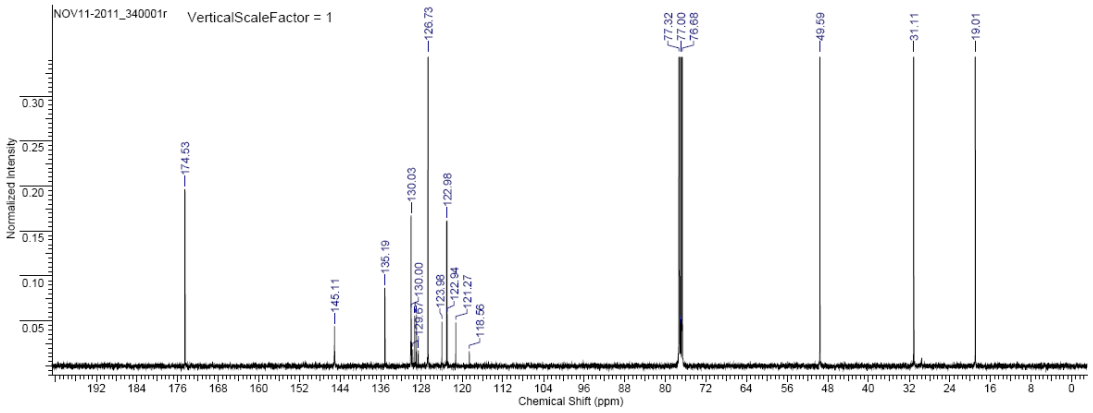


ZHANGYUT-002-EXP080-pdt

11/22/2011 4:32:25 PM

Formula $C_{11}H_9F_3NO_2$	*FW*	274.1960					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP080-CARBON Project ZHANGYUT Name FLOW				
Date	12 Nov 2011 03:09:52	*Date Stamp*	12 Nov 2011 03:09:52				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV11-2011.340_201111112220.01\NOV11-2011_340001r						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	3200	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10057.4990
Sweep Width (Hz)	23980.63	*Temperature (degree C)*	27.000				

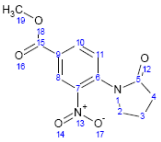


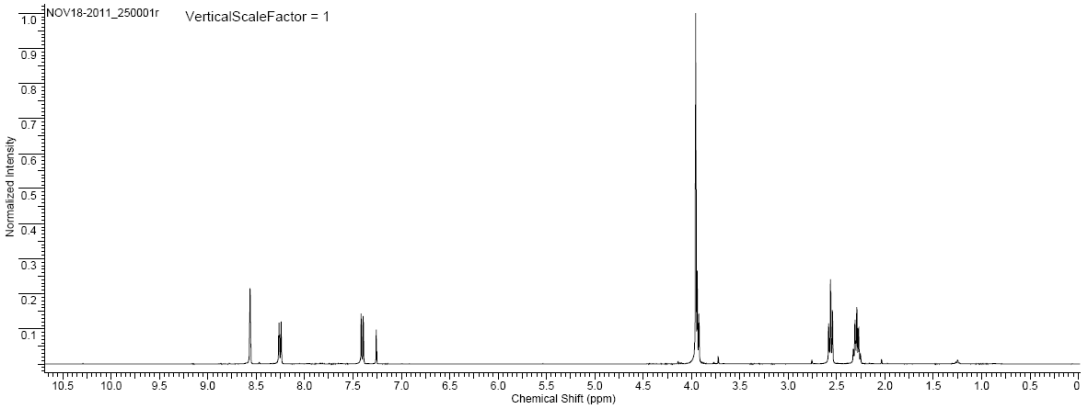


ZHANGYUT-002-EXP079-pdt

11/18/2011 4:01:33 PM

Formula $C_{12}H_{16}N_2O_5$	*FW* 264.2341						
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP079-ISO Project ZHANGYUT Name FLOW				
Date	18 Nov 2011 20:11:44	*Date Stamp*	18 Nov 2011 20:11:44				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV18-2011.250_201111181515.01\NOV18-2011_250001r						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	181.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.1484
Sweep Width (Hz)	8278.02	*Temperature (degree C)*	27.000				

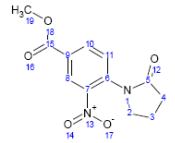


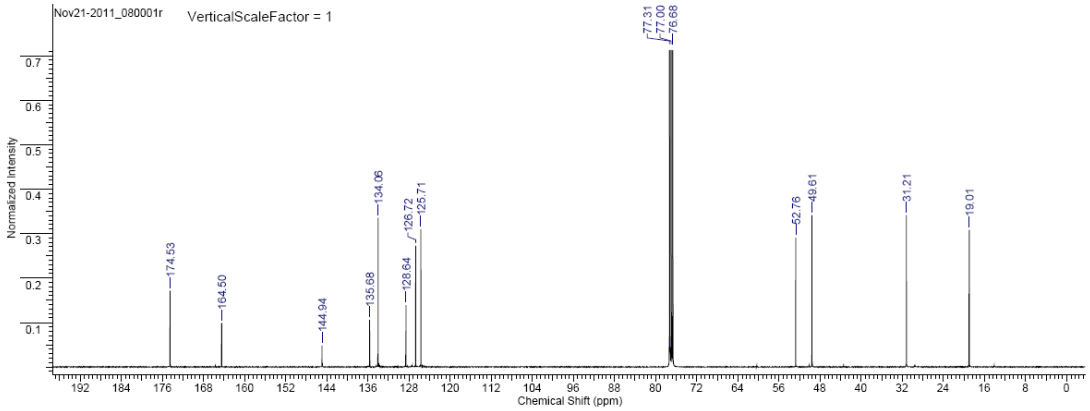


ZHANGYUT-002-EXP079-pdt

11/22/2011 2:00:26 PM

Formula $C_{12}H_{16}N_2O_5$	*FW* 264.2341						
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP079-CARBON Name ZHANGYUT Project FLOW				
Date	22 Nov 2011 04:50:08			*Date Stamp*	22 Nov 2011 04:50:08		
File Name	\\phusca-s6001\usca-lab-prod\Inbox\USCA-ANALYTICS\nmr\av400a\current\Nov21-2011_080001r					*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	6000	*Origin*	av400a	*Original Points Count*	32768
Owner	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	9195.20
SW(cyclical) (Hz)	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10055.0293	*Sweep Width (Hz)*	23980.08
Temperature (degree C)	27.000						

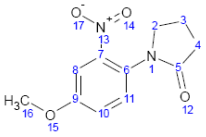


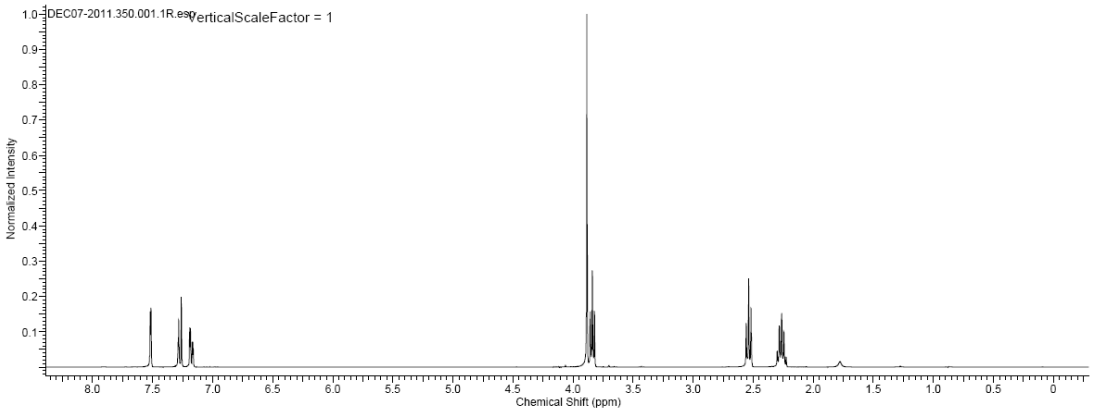


ZHANGYUT-002-EXP094-pdt

12/8/2011 9:59:07 AM

Formula $C_{11}H_{12}N_2O_4$	*FW*	236.2240					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP094-ISO Project ZHANGYUT Name FLOW				
Date	07 Dec 2011 18:10:56	*Date Stamp*	07 Dec 2011 18:10:56				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC07-2011.350_201112071815.01\DEC07-2011\350\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	128.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2473.8958
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

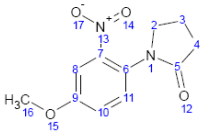


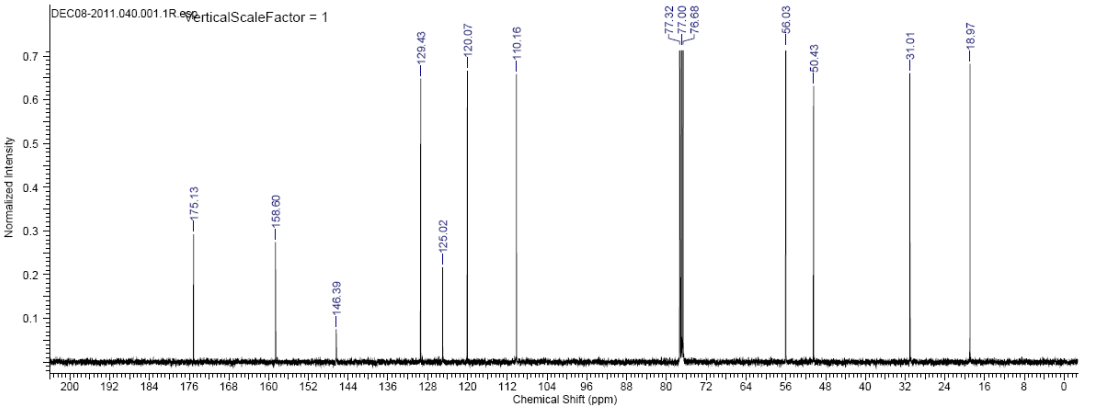


ZHANGYUT-002-EXP094-pdt

12/8/2011 9:58:00 AM

Formula $C_{11}H_{12}N_2O_4$	*FW*	236.2240					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP094-CARBON Project ZHANGYUT Name FLOW				
Date	08 Dec 2011 09:28:16	*Date Stamp*	08 Dec 2011 09:28:16				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC08-2011.40_201112080930.02\DEC08-2011\40\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	512	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10054.7549
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.63	*Temperature (degree C)*	27.000		

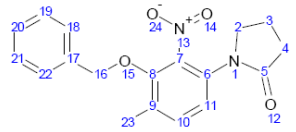


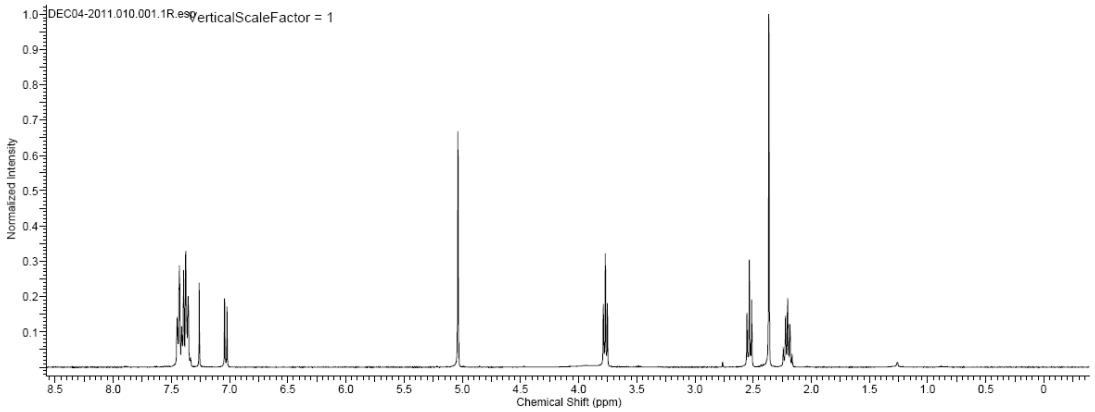


ZHANGYUT-002-EXP098-pdt

12/6/2011 8:47:02 AM

Formula $C_{10}H_{10}N_2O_4$	*FW* 326.3465						
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP098-2-ISO2 Project ZHANGYUT Name FLOW				
Date	04 Dec 2011 09:09:04	*Date Stamp*	04 Dec 2011 09:09:04				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC04-2011.10_201112040910.02\DEC04-2011\10\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	362.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.2747
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

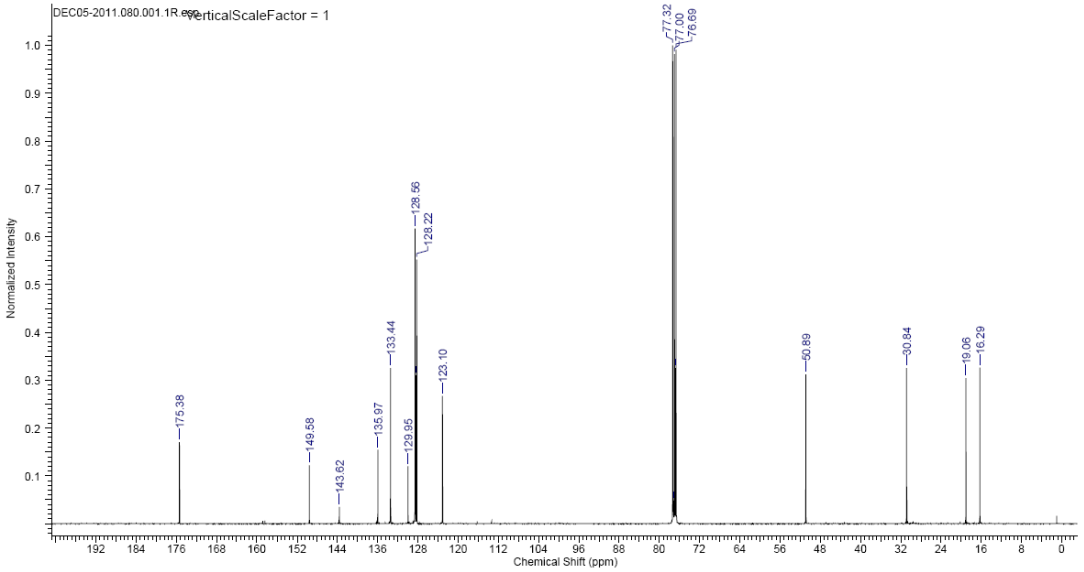




ZHANGYUT-002-EXP098-pdt

12/6/2011 8:38:59 AM

Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP098-CARBON-2 Name ZHANGYUT Project FLOW				
Date	05 Dec 2011 22:52:32	*Date Stamp*	05 Dec 2011 22:52:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.DEC05-2011.80_201112052255.02\DEC05-2011\80\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	5000	*Origin*	av400a
Original Points Count	32768	*Owner*	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	7298.20	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10055.0381
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.08	*Temperature (degree C)*	27.000		

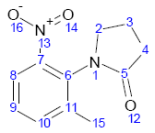


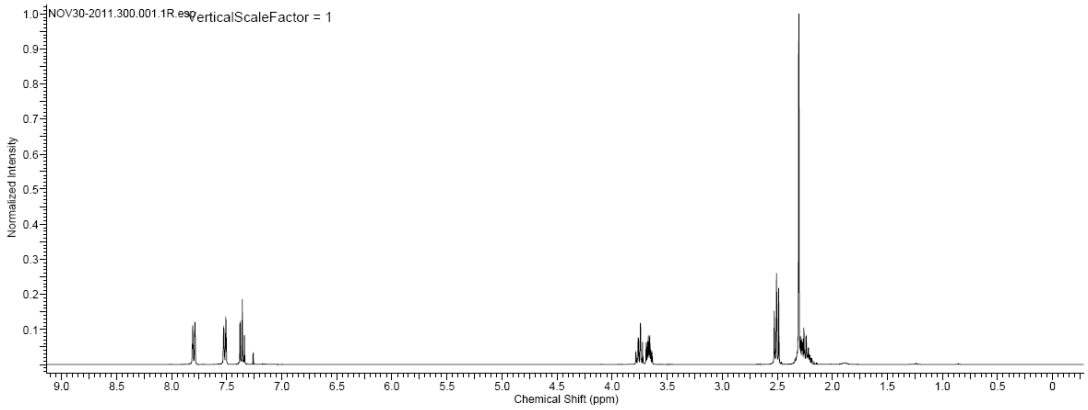
ZHANGYUT-003-EXP082-pdt

12/23/2011 3:05:05 PM

Formula $C_{11}H_{12}NO_3$	FW	220.2246

Acquisition Time (sec)	3.9584	Comment	Notebook ZHANGYUT-002-EXP082-ISO Project ZHANGYUT Name FLOW				
Date	30 Nov 2011 15:24:32	Date Stamp	30 Nov 2011 15:24:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV30-2011.300_201111301525.01\NOV30-2011\300\PDATA\1\1R						
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	32	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	65536	Pulse Sequence	zg30
Receiver Gain	71.80	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2462.6538
Spectrum Type	STANDARD	Sweep Width (Hz)	8278.02	Temperature (degree C)	27.000		



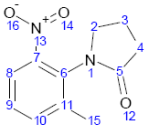


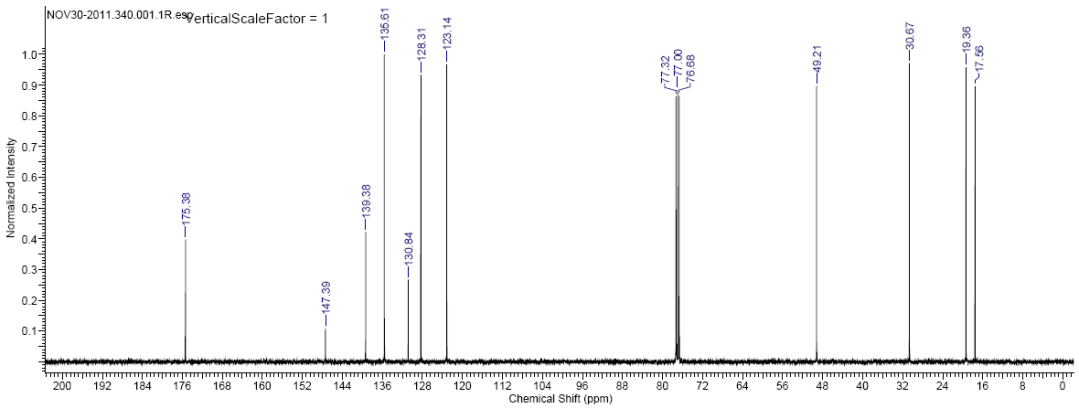
ZHANGYUT-003-EXP082-pdt

12/23/2011 3:07:20 PM

Formula $C_{11}H_{12}NO_3$	FW	220.2246

Acquisition Time (sec)	1.3664	Comment	Notebook ZHANGYUT-002-EXP082-CARBON Project ZHANGYUT Name FLOW				
Date	30 Nov 2011 17:26:08	Date Stamp	30 Nov 2011 17:26:08				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV30-2011.340_201111301730.02\NOV30-2011\340\PDATA\1\1R						
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	512	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	131072	Pulse Sequence	zgpg30
Receiver Gain	4096.00	SW(cyclical) (Hz)	23980.81	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10049.2656
Spectrum Type	STANDARD	Sweep Width (Hz)	23980.63	Temperature (degree C)	27.000		

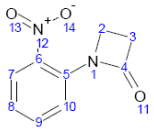


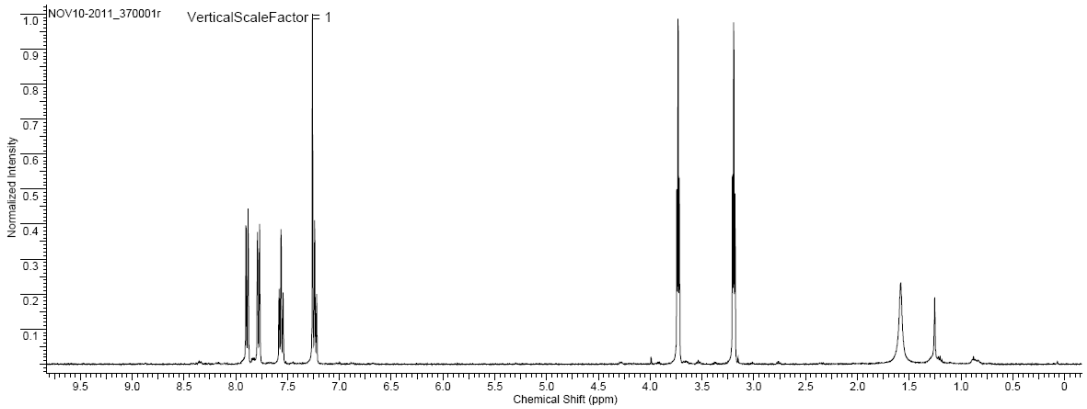


ZHANGYUT-002-EXP095-pdt

11/11/2011 2:30:36 PM

Formula $C_9H_8N_2O_3$	*FW*	192.1714					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP095-ISO2 Project ZHANGYUT Name FLOW				
Date	10 Nov 2011 22:56:00	*Date Stamp*	10 Nov 2011 22:56:00				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\1564499_AV400D.NOV10-2011.370_201111101800.01\NOV10-2011_370001r						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	574.70	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.7803
Sweep Width (Hz)	8278.02	*Temperature (degree C)*	27.000				

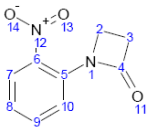


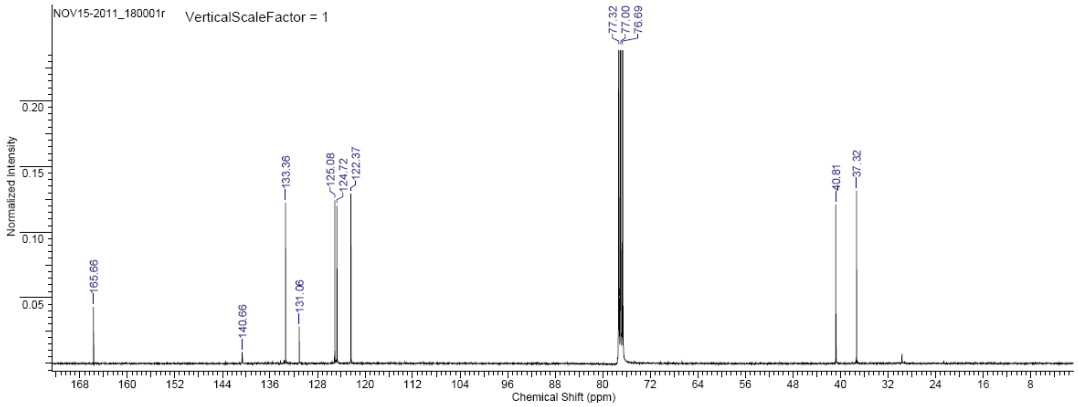


ZHANGYUT-002-EXP095-pdt

11/16/2011 10:57:33 AM

Formula $C_9H_8N_2O_3$	*FW*	192.1714					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP095-CARBON Name ZHANGYUT Project FLOW				
Date	16 Nov 2011 03:52:32	*Date Stamp*	16 Nov 2011 03:52:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.NOV15-2011.180_201111152255.01\NOV15-2011_180001r						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	5000	*Origin*	av400a
Original Points Count	32768	*Owner*	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	7298.20	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10057.9561
Sweep Width (Hz)	23980.08	*Temperature (degree C)*	27.000				

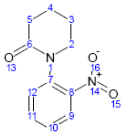


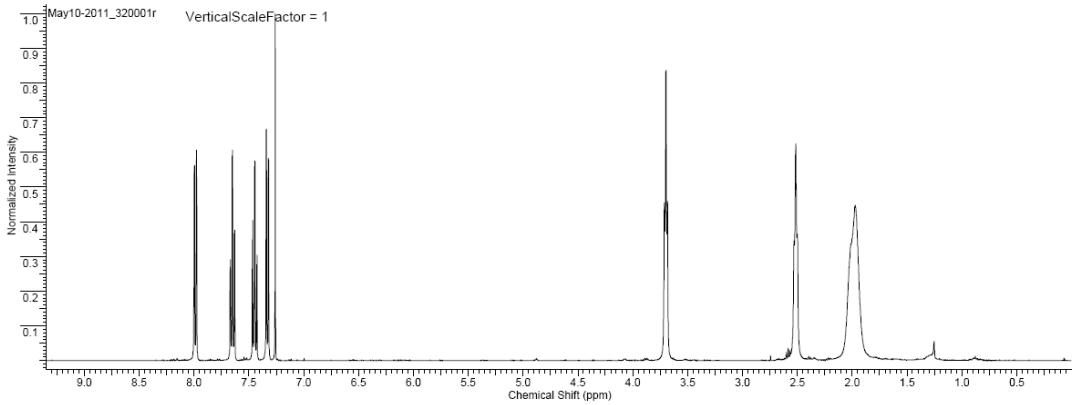


ZHANGYUT-001-EXP066-pdt

5/10/2011 4:19:40 PM

Formula $C_{11}H_{12}N_2O_3$	*FW*	220.2246					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-001-EXP066-ISO Name ZHANGYUT Project FLOW				
Date	10 May 2011 19:26:56			*Date Stamp*	10 May 2011 19:26:56		
File Name	\\phusca-s6001\usca-lab-prod\Inbox\USCA-ANALYTICS\nmr\av400b\current\May10-2011_320001r					*Frequency (MHz)*	400.34
Nucleus	1H	*Number of Transients*	32	*Origin*	av400b	*Original Points Count*	32768
Owner	av400b	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	181.00
SW(cyclical) (Hz)	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2458.4312	*Sweep Width (Hz)*	8277.89
Temperature (degree C)	27.000						

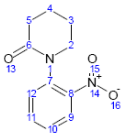


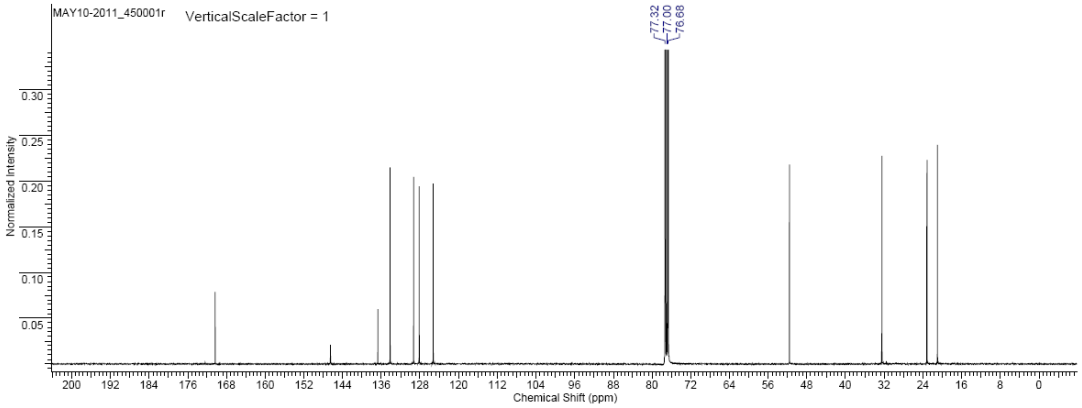


ZHANGYUT-001-EXP066-carbon

5/11/2011 7:59:33 AM

Formula $C_{11}H_{12}N_2O_3$	*FW*	220.2246					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-001-EXP066-ISO-C Name ZHANGYUT Project FLOW				
Date	11 May 2011 00:02:08	*Date Stamp*	11 May 2011 00:02:08				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.MAY10-2011.450_201105102005.01\MAY10-2011_450001r						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	2048	*Origin*	av400a
Original Points Count	32768	*Owner*	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	6502.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10055.7607
Sweep Width (Hz)	23980.08	*Temperature (degree C)*	27.000				

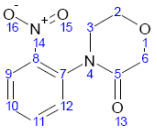


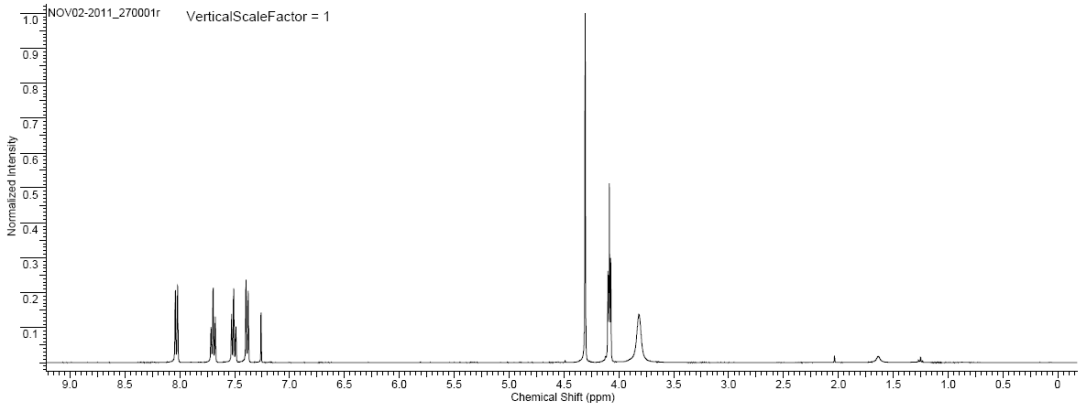


ZHANGYUT-002-EXP0784-proton

11/4/2011 6:37:34 PM

Formula $C_{16}H_{10}N_2O_4$	*FW* 222.1974						
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP084-ISO Project ZHANGYUT Name FLOW				
Date	02 Nov 2011 19:52:32	*Date Stamp*	02 Nov 2011 19:52:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV02-2011.270_201111021605.02\NOV02-2011_270001r						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	181.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.4014
Sweep Width (Hz)	8278.02	*Temperature (degree C)*	27.000				

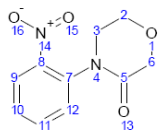


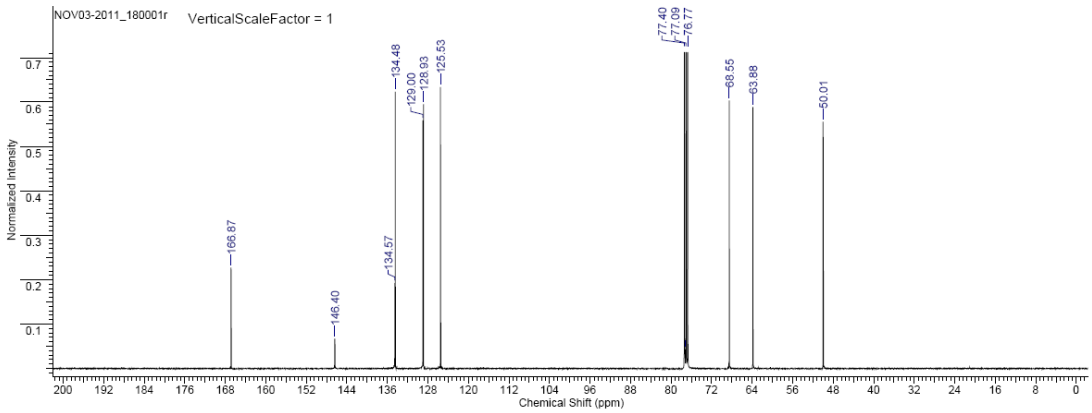


ZHANGYUT-002-EXP084-carbon

11/4/2011 9:00:28 AM

Formula $C_{16}H_{10}N_2O_4$	*FW* 222.1974						
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP084-CARBON Name ZHANGYUT Project FLOW				
Date	03 Nov 2011 23:04:32	*Date Stamp*	03 Nov 2011 23:04:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.NOV03-2011.180_201111031905.02\NOV03-2011_180001r						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	av400a
Original Points Count	32768	*Owner*	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	9195.20	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10060.8027
Sweep Width (Hz)	23980.08	*Temperature (degree C)*	27.000				

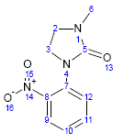


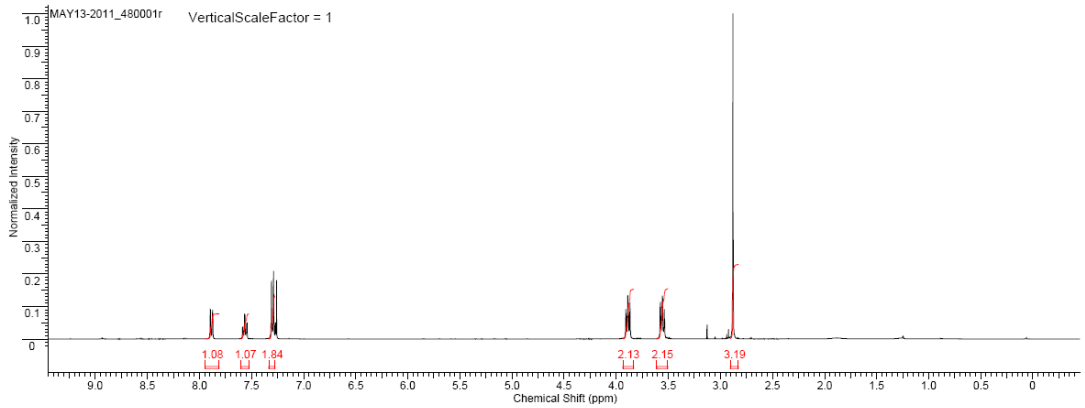


ZHANGYUT-001-EXP072-iso

5/16/2011 8:23:46 AM

Formula $C_{10}H_{11}N_3O_3$	FW	221.2126					
Acquisition Time (sec)	3.9584	Comment	Notebook ZHANGYUT-001-EXP072-ISO Name ZHANGYUT Project FLOW				
Date	13 May 2011 20:58:40	Date Stamp	13 May 2011 20:58:40				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.MAY13-2011.480_201105131700.02\MAY13-2011_480001r						
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4	Origin	av400a
Original Points Count	32768	Owner	av400a	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	114.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2461.9592
Sweep Width (Hz)	8277.89	Temperature (degree C)	27.000				

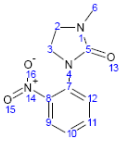


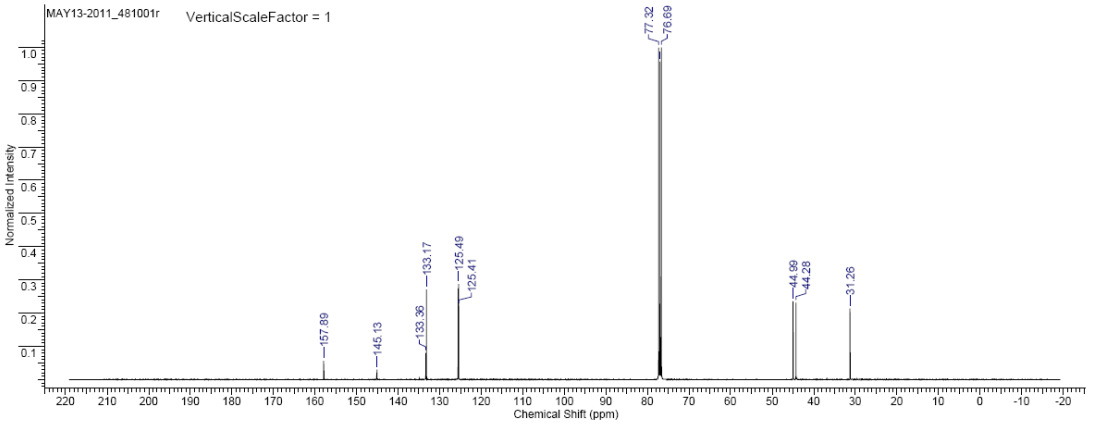


ZHANGYUT-001-EXP072-carbon

5/16/2011 8:26:14 AM

Formula $C_{10}H_{11}N_3O_3$	FW	221.2126					
Acquisition Time (sec)	1.3664	Comment	Notebook ZHANGYUT-001-EXP072-C Name ZHANGYUT Project FLOW			Date	14 May 2011 00:57:36
Date Stamp	14 May 2011 00:57:36	File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.MAY13-2011.481_201105132100.01\MAY13-2011_481001r				
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	3000	Origin	av400a
Original Points Count	32768	Owner	av400a	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	13004.00	SW(cyclical) (Hz)	23980.81	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10054.2969
Sweep Width (Hz)	23980.08	Temperature (degree C)	27.000				

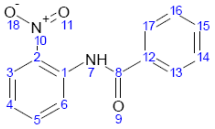


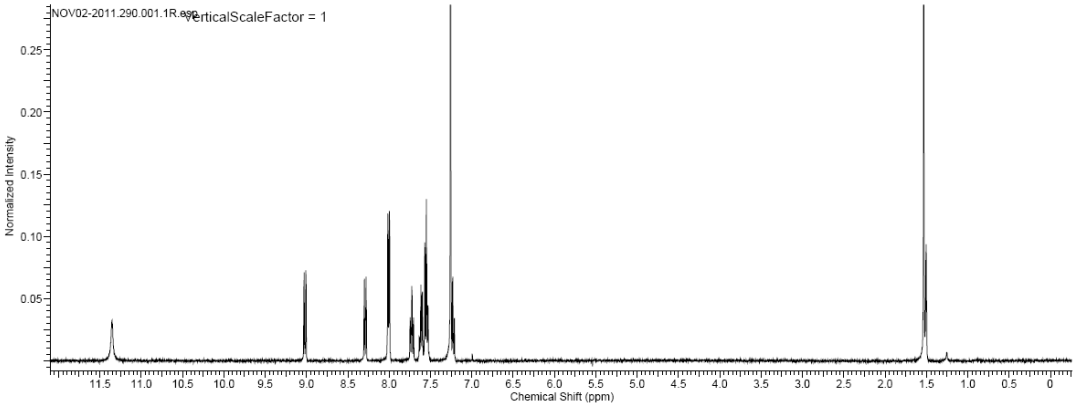


ZHANGYUT-002-EXP085-pdt

12/23/2011 3:21:41 PM

Formula $C_{13}H_{16}N_2O_3$	*FW* 242.2301						
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP085-ISO Project ZHANGYUT Name FLOW				
Date	02 Nov 2011 16:11:44	*Date Stamp*	02 Nov 2011 16:11:44				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV02-2011.290_201111021625.02\NOV02-2011\290\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	1149.40	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.5273
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

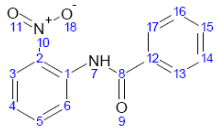


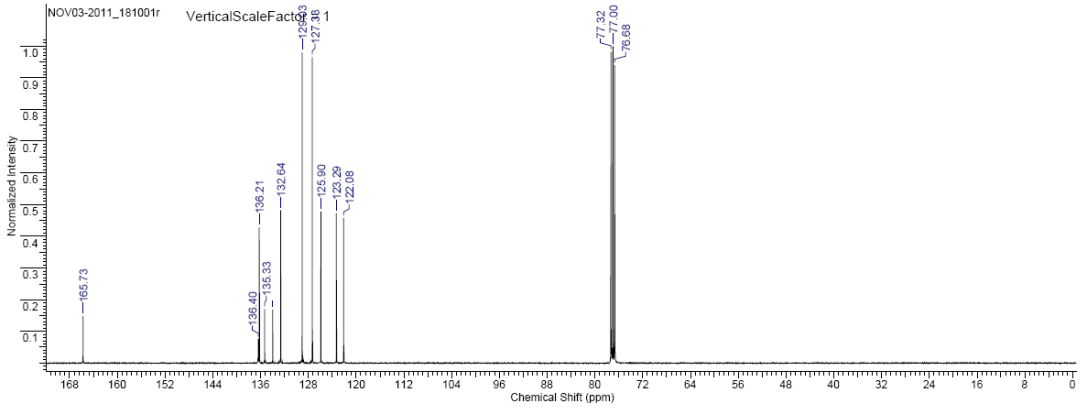


ZHANGYUT-002-EXP085-carbon

11/4/2011 9:03:19 AM

Formula $C_{13}H_{16}N_2O_3$	*FW* 242.2301						
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP085-CARBON Name ZHANGYUT Project FLOW				
Date	04 Nov 2011 00:08:32	*Date Stamp*	04 Nov 2011 00:08:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400A.NOV03-2011.181_201111032010.02\NOV03-2011_181001r						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	av400a
Original Points Count	32768	*Owner*	av400a	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	9195.20	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10055.7607
Sweep Width (Hz)	23980.08	*Temperature (degree C)*	27.000				

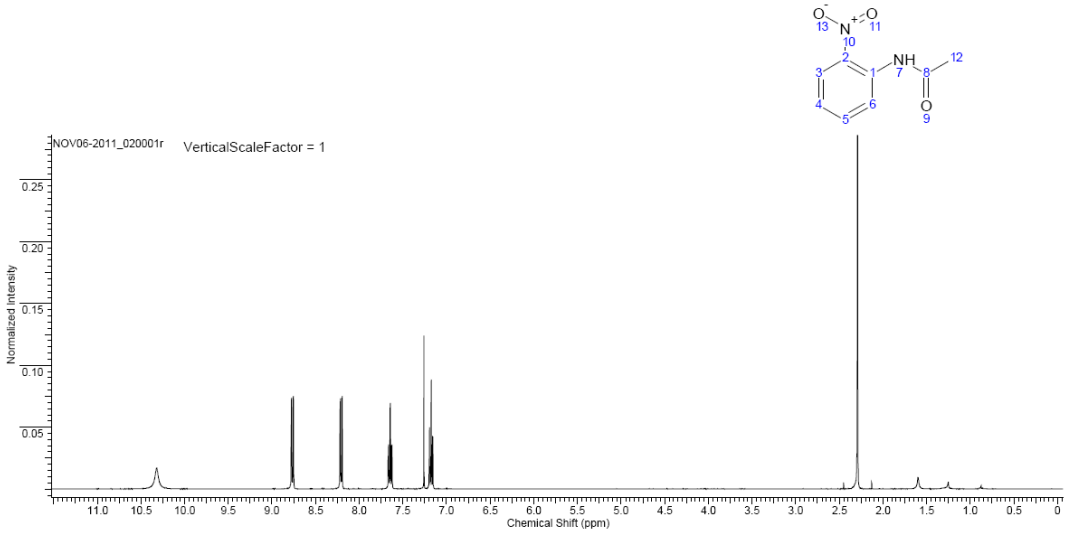




ZHANGYUT-002-EXP086-pdt

11/6/2011 12:54:59 PM

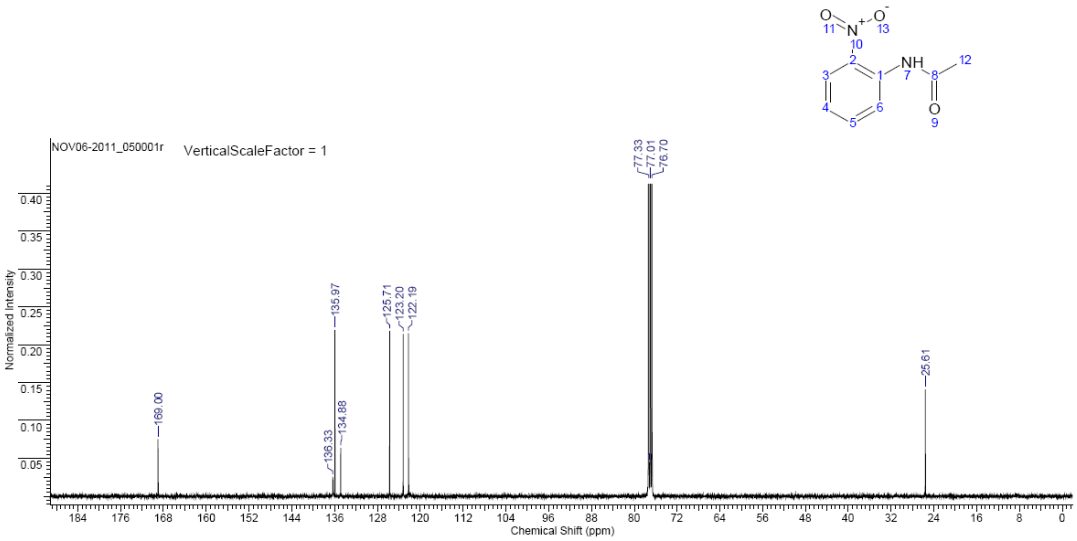
Formula $C_9H_8N_2O_3$	*FW*	180.1607					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP086-ISO Project ZHANGYUT Name FLOW				
Date	06 Nov 2011 17:18:56	*Date Stamp*	06 Nov 2011 17:18:56				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV06-2011.20_201111061230.02\NOV06-2011_020001r						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	362.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.4014
Sweep Width (Hz)	8278.02	*Temperature (degree C)*	27.000				



ZHANGYUT-002-EXP086-carbon

11/7/2011 8:42:44 AM

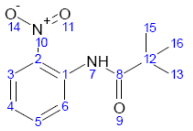
Formula $C_9H_8N_2O_3$	*FW*	180.1607					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP086-CARBON Project ZHANGYUT Name FLOW				
Date	07 Nov 2011 00:46:56	*Date Stamp*	07 Nov 2011 00:46:56				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV06-2011.50_201111062000.02\NOV06-2011_050001r						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	6250	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10060.8027
Sweep Width (Hz)	23980.63	*Temperature (degree C)*	27.000				

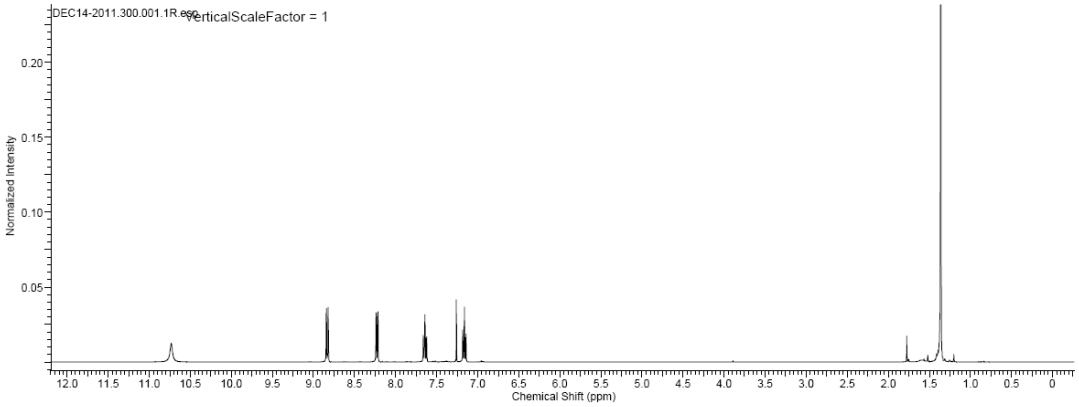


ZHANGYUT-003-EXP001-pdt

12/23/2011 3:24:59 PM

Formula $C_{11}H_{14}N_2O_3$	*FW*	222.2405					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-003-EXP001-ISO2 Project ZHANGYUT Name FLOW				
Date	14 Dec 2011 16:02:56	*Date Stamp*	14 Dec 2011 16:02:56				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC14-2011.300_201112141605.01\DEC14-2011\300\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	228.10	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2461.6433
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

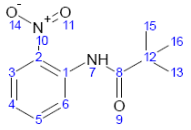


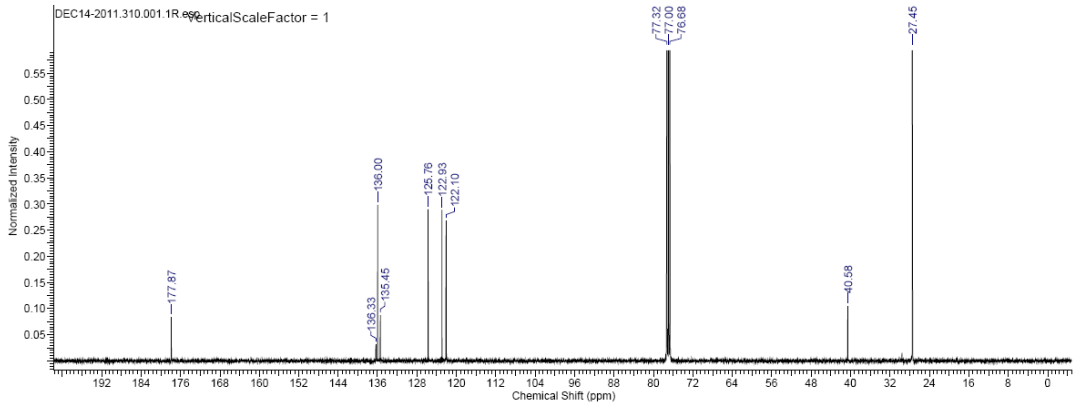


ZHANGYUT-003-EXP001-pdt

12/15/2011 8:46:23 AM

Formula $C_{11}H_{14}N_2O_3$	*FW*	222.2405					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-003-EXP001-ISO2-CARBON Project ZHANGYUT Name FLOW				
Date	14 Dec 2011 22:31:12	*Date Stamp*	14 Dec 2011 22:31:12				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC14-2011.310_201112142235.02\DEC14-2011\310\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	3500	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30
Receiver Gain	1625.50	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10058.7803
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.63	*Temperature (degree C)*	27.000		

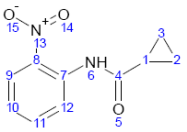


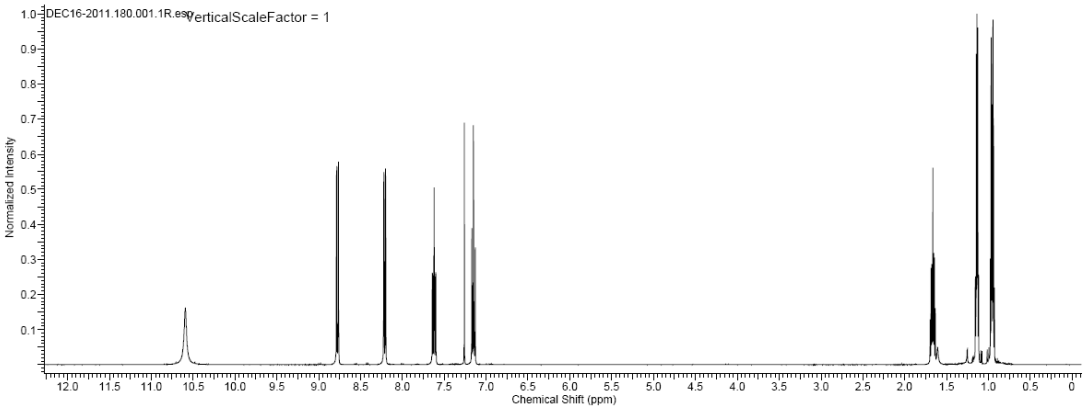


ZHANGYUT-003-EXP004-pdt

12/19/2011 9:21:34 AM

Formula $C_{10}H_{10}N_2O_3$	*FW*	206.1980					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-003-EXP004-ISO1 Project ZHANGYUT Name FLOW				
Date	16 Dec 2011 16:15:44	*Date Stamp*	16 Dec 2011 16:15:44				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\1655342_AV400D.DEC16-2011.180_201112161620.01\DEC16-2011\180\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	228.10	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2461.7695
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

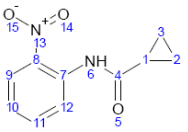


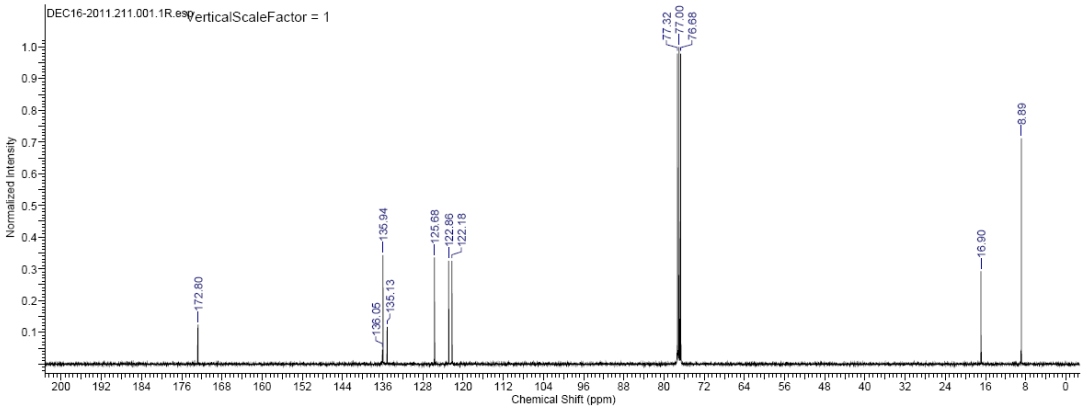


ZHANGYUT-003-EXP004-pdt

12/19/2011 1:10:34 PM

Formula $C_{10}H_{10}N_2O_3$	*FW*	206.1980					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-003-EXP004-ISO1-CARBON Project ZHANGYUT Name FLOW				
Date	17 Dec 2011 08:02:56	*Date Stamp*	17 Dec 2011 08:02:56				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC16-2011.211_201112170805.02\DEC16-2011\211\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	3500	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10058.0479
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.63	*Temperature (degree C)*	27.000		

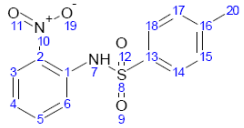


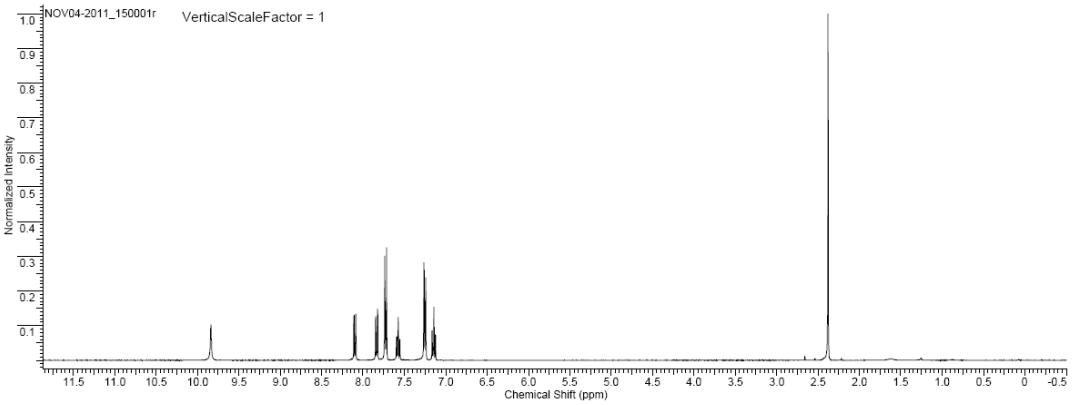


ZHANGYUT-002-EXP088-pdt

11/10/2011 4:21:39 PM

Formula $C_{13}H_{12}NO_2S_4$	*FW*	292.3104					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-002-EXP088-ISO Project ZHANGYUT Name FLOW				
Date	04 Nov 2011 14:09:04	*Date Stamp*	04 Nov 2011 14:09:04				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.NOV\04-2011.150_201111041020.01\NOV04-2011_150001r						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	128.00	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2462.7148
Sweep Width (Hz)	8278.02	*Temperature (degree C)*	27.000				

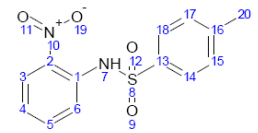


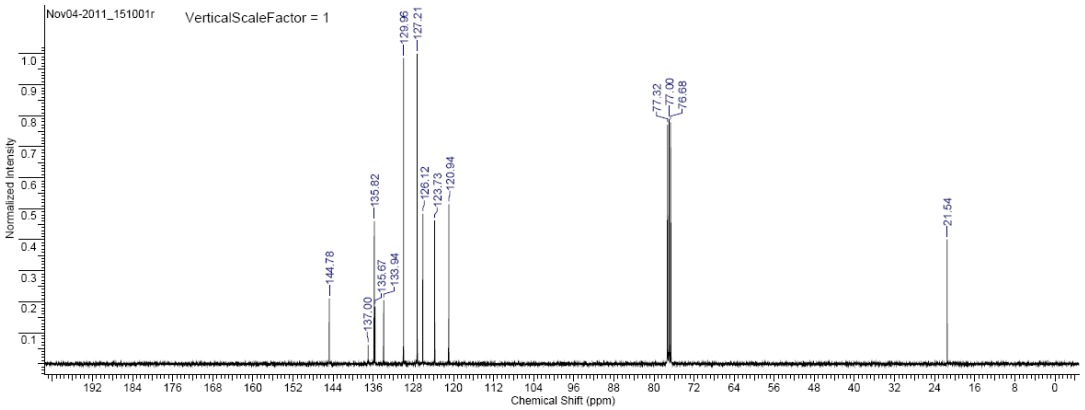


ZHANGYUT-002-EXP088-pdt

11/10/2011 4:27:41 PM

Formula $C_{13}H_{12}NO_2S_4$	*FW*	292.3104					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-002-EXP088-CARBON Project ZHANGYUT Name FLOW				
Date	05 Nov 2011 09:42:24			*Date Stamp*	05 Nov 2011 09:42:24		
File Name	\\phusca-s6001\usca-lab-prod\Inbox\USCA-ANALYTICS\nmr\av400d\current\Nov04-2011_151001r					*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	1024	*Origin*	av400d	*Original Points Count*	32768
Owner	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30	*Receiver Gain*	4096.00
SW(cyclical) (Hz)	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10056.4014	*Sweep Width (Hz)*	23980.63
Temperature (degree C)	27.000						

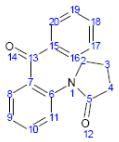


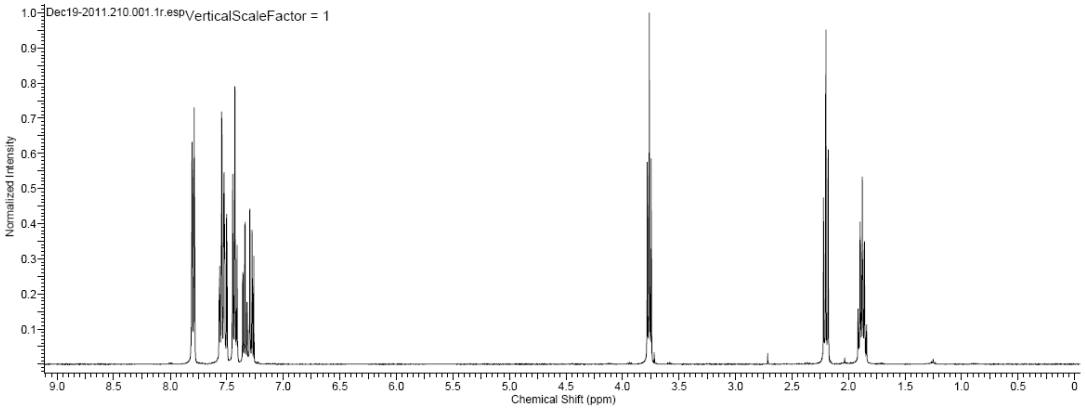


ZHANGYUT-002-EXP090-pdt

12/19/2011 3:51:50 PM

Formula $C_{17}H_{15}NO_2$	***FW***	265.3065					
Acquisition Time (sec)	3.9584	***Comment***	Notebook ZHANGYUT-002-EXP90-ISO2 Project ZHANGYUT Name FLOW				
Date	19 Dec 2011 15:33:04			***Date Stamp***	19 Dec 2011 15:33:04		
File Name	\\phusca-s6001\usca-lab-prod\Inbox\USCA-ANALYTICS\nmr\av400d\current\Dec19-2011\210\pdata\1\1r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	32	***Origin***	av400d	***Original Points Count***	32768
Owner	av400d	***Points Count***	65536	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2461.8958	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8278.02	***Temperature (degree C)***	27.000				

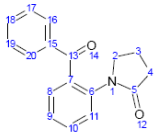


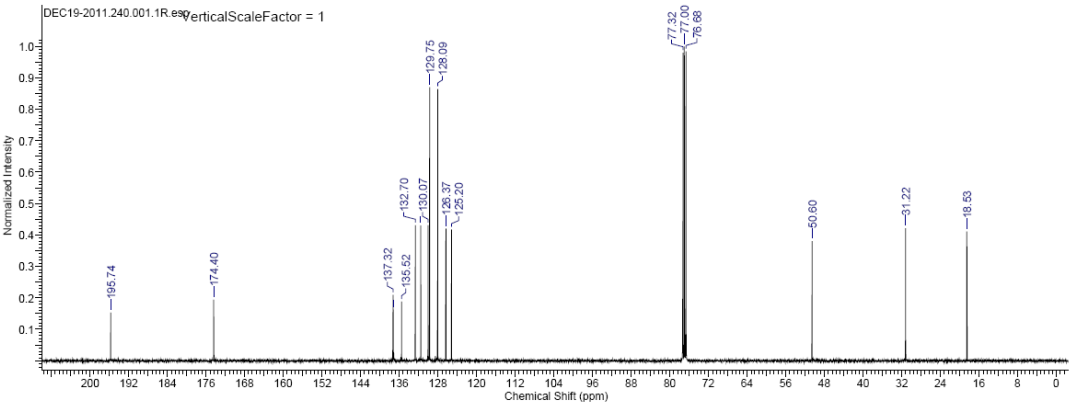


ZHANGYUT-002-EXP090-pdt

1/27/2012 12:09:04 PM

Formula $C_{17}H_{15}NO_2$	***FW***	265.3065					
Acquisition Time (sec)	1.3664	***Comment***	Notebook ZHANGYUT-002-EXP090-ISO2-CARBON Project FLOW Name ZHANGYUT				
Date	20 Dec 2011 00:28:32	***Date Stamp***	20 Dec 2011 00:28:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.DEC19-2011.240_201112200030.01\DEC19-2011\240\PDATA\1\1R						
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	3500	***Origin***	av400d
Original Points Count	32768	***Owner***	av400d	***Points Count***	131072	***Pulse Sequence***	zgpg30
Receiver Gain	2048.00	***SW(cyclical) (Hz)***	23980.81	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	10054.7549
Spectrum Type	STANDARD	***Sweep Width (Hz)***	23980.63	***Temperature (degree C)***	27.000		

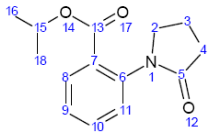


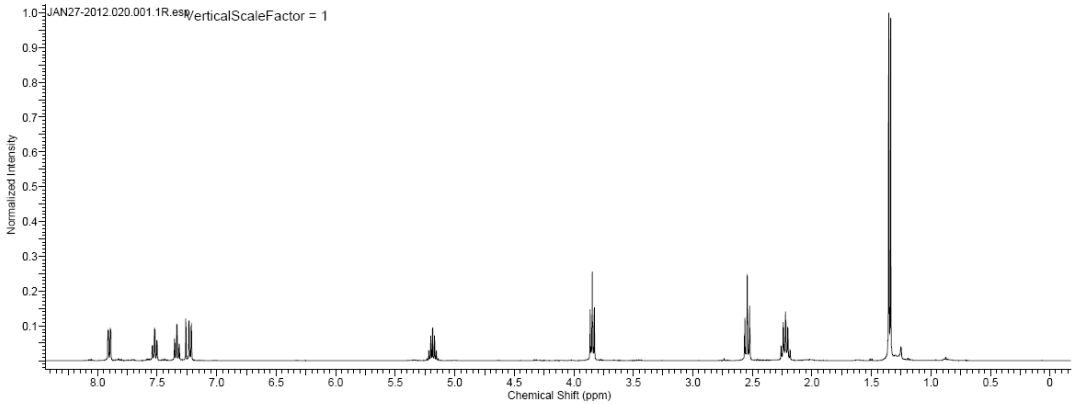


ZHANGYUT-003-EXP036-pdt

1/27/2012 8:55:35 AM

Formula $C_{14}H_{15}NO_3$	FW 247.2897						
Acquisition Time (sec)	3.9584	Comment	Notebook ZHANGYUT-003-EXP036-ISO Project FLOW Name ZHANGYUT				
Date	27 Jan 2012 08:13:36	Date Stamp	27 Jan 2012 08:13:36				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN27-2012.20_201201270815.01\JAN27-2012\20\PDATA\1\1R						
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	32	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	65536	Pulse Sequence	zg30
Receiver Gain	161.30	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2461.7695
Spectrum Type	STANDARD	Sweep Width (Hz)	8278.02	Temperature (degree C)	27.000		

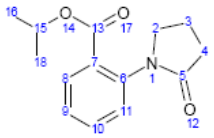


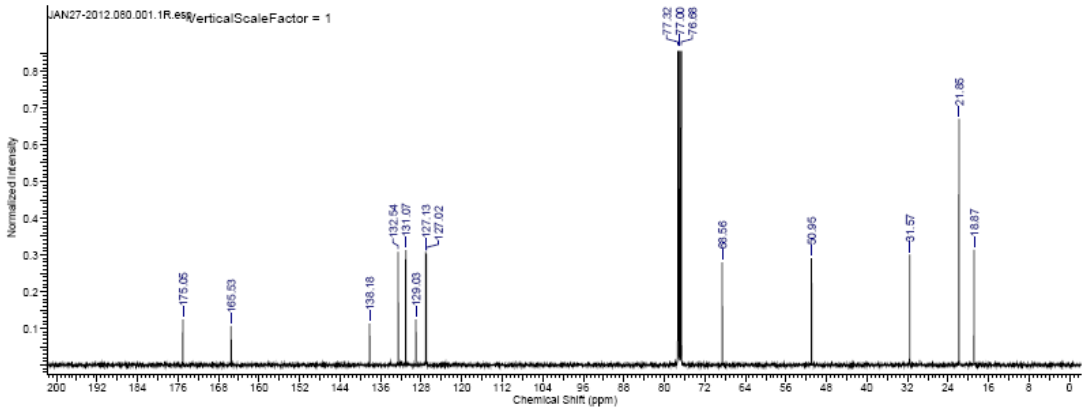


ZHANGYUT-003-EXP036.pdt

1/30/2012 8:42:22 AM

Formula $C_{14}H_{15}NO_3$	FW 247.2897						
Acquisition Time (sec)	1.3664	Comment	Notebook ZHANGYUT-003-EXP036-ISO-CARBON Project FLOW Name ZHANGYUT				
Date	27 Jan 2012 23:52:16	Date Stamp	27 Jan 2012 23:52:16				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN27-2012.80_201201272355.02\JAN27-2012\80\PDATA\1\1R						
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	5000	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	131072	Pulse Sequence	zgpg30
Receiver Gain	1625.50	SW(cyclical) (Hz)	23980.81	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10056.9502
Spectrum Type	STANDARD	Sweep Width (Hz)	23960.63	Temperature (degree C)	27.000		

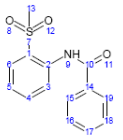


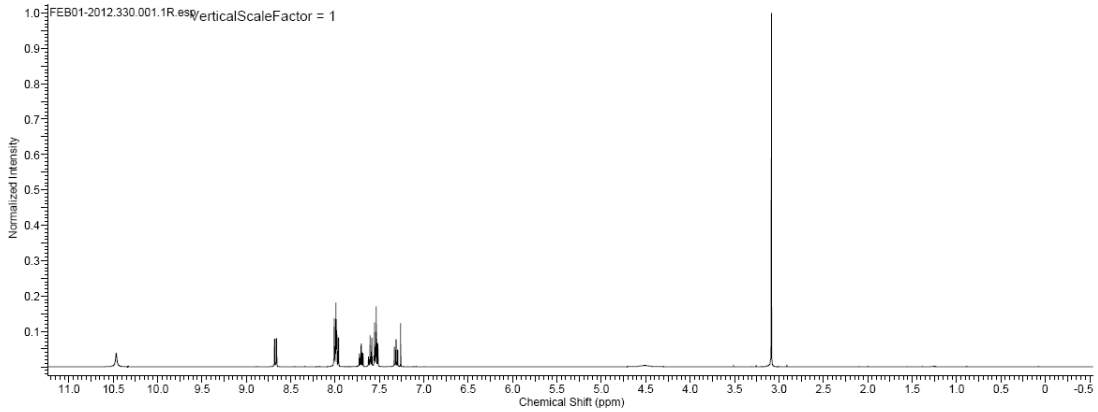


ZHANGYUT-003-EXP035.pdt

2/2/2012 8:27:54 AM

Formula $C_{14}H_{13}NO_3S$	*FW*	275.3229					
Acquisition Time (sec)	3.9584	*Comment*	Notebook ZHANGYUT-003-EXP035-2-ISO2 Project FLOW Name ZHANGYUT				
Date	01 Feb 2012 16:30:40	*Date Stamp*	01 Feb 2012 16:30:40				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.FEB01-2012.330_201202011635.02\FEB01-2012\330\PDATA\1\1R						
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	228.10	*SW(cyclical) (Hz)*	8278.15	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2461.8960
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8278.02	*Temperature (degree C)*	27.000		

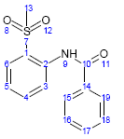


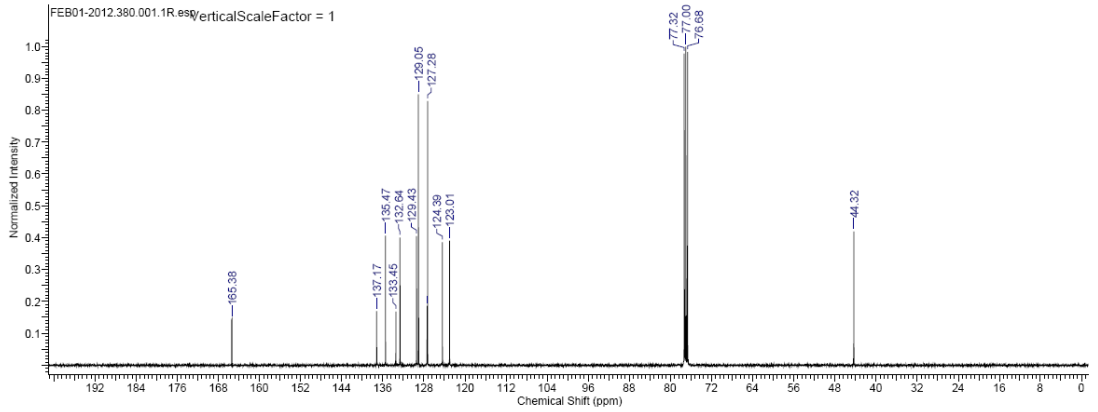


ZHANGYUT-003-EXP035.pdt

2/2/2012 8:31:37 AM

Formula $C_{14}H_{13}NO_3S$	*FW*	275.3229					
Acquisition Time (sec)	1.3664	*Comment*	Notebook ZHANGYUT-003-EXP035-2-ISO2-CARBON Project FLOW Name ZHANGYUT				
Date	01 Feb 2012 23:22:24	*Date Stamp*	01 Feb 2012 23:22:24				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.FEB01-2012.380_201202012325.02\FEB01-2012\380\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	4500	*Origin*	av400d
Original Points Count	32768	*Owner*	av400d	*Points Count*	131072	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SW(cyclical) (Hz)*	23980.81	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10056.7676
Spectrum Type	STANDARD	*Sweep Width (Hz)*	23980.63	*Temperature (degree C)*	27.000		



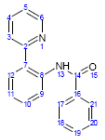


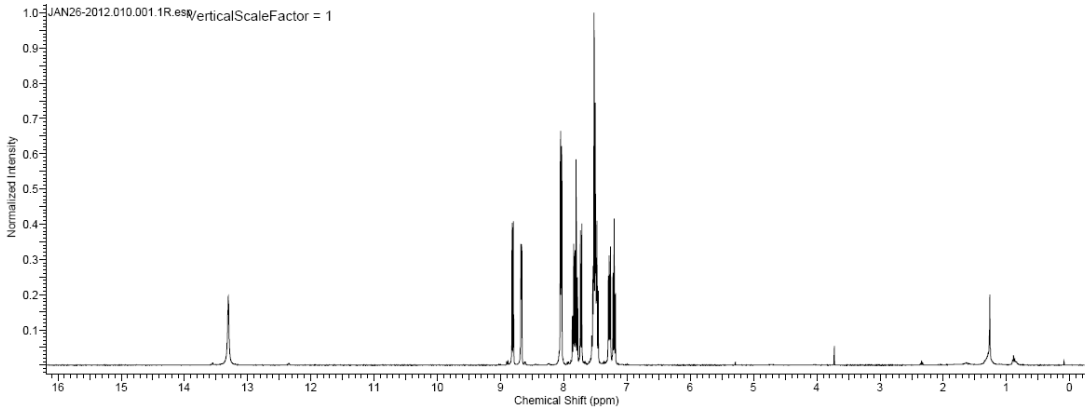
ZHANGYUT-003-EXP029-pdt

1/27/2012 9:01:15 AM

Formula $C_{10}H_{14}NO_2$	FW	274.3166

Acquisition Time (sec)	3.9584	Comment	Notebook ZHANGYUT-003-EXP029-ISO1C Project FLOW Name ZHANGYUT				
Date	26 Jan 2012 08:17:52	Date Stamp	26 Jan 2012 08:17:52				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN26-2012.10_201201260820.01\JAN26-2012\10\PDATA\1\1R						
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	32	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	65536	Pulse Sequence	zg30
Receiver Gain	128.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2461.7698
Spectrum Type	STANDARD	Sweep Width (Hz)	8278.02	Temperature (degree C)	27.000		



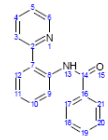


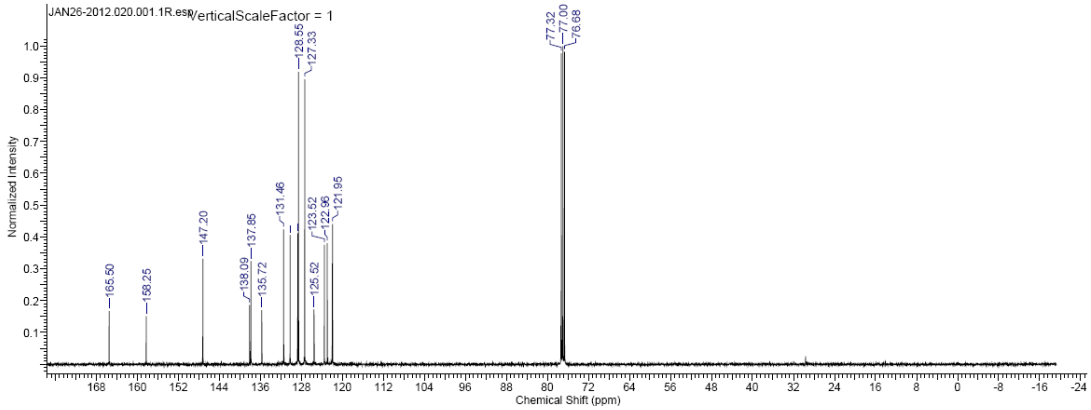
ZHANGYUT-003-EXP029-pdt

1/27/2012 8:41:43 AM

Formula $C_{10}H_{14}NO_2$	FW	274.3166

Acquisition Time (sec)	1.3664	Comment	Notebook ZHANGYUT-003-EXP029-ISO1C-CARBON Project FLOW Name ZHANGYUT				
Date	26 Jan 2012 23:05:20	Date Stamp	26 Jan 2012 23:05:20				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN26-2012.20_201201262310.02\JAN26-2012\20\PDATA\1\1R						
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	4200	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	131072	Pulse Sequence	zgpg30
Receiver Gain	1625.50	SW(cyclical) (Hz)	23980.81	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10054.5723
Spectrum Type	STANDARD	Sweep Width (Hz)	23980.63	Temperature (degree C)	27.000		

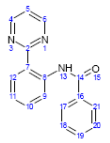


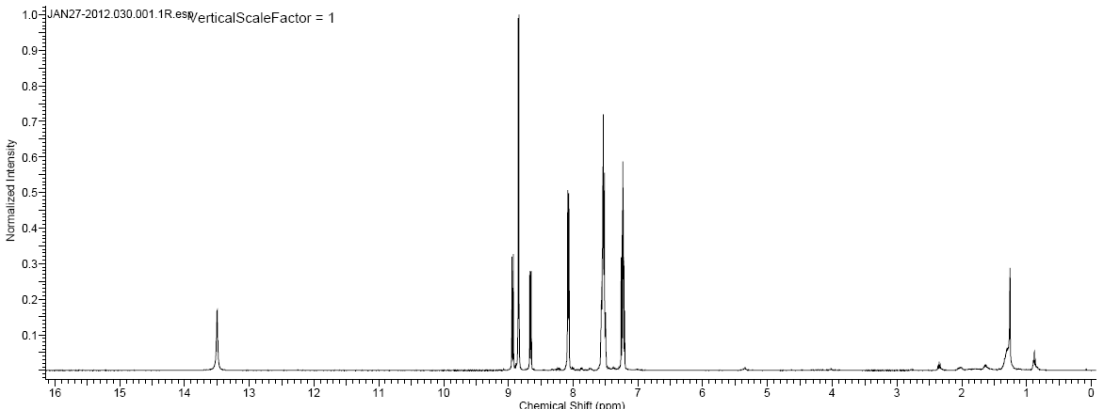


ZHANGYUT-003-EXP039-pdt

1/27/2012 9:14:09 AM

Formula $C_{17}H_{13}N_3O$	FW	275.3046					
Acquisition Time (sec)	3.9584	Comment	Notebook ZHANGYUT-003-EXP039-ISO2A Project FLOW Name ZHANGYUT				
Date	27 Jan 2012 08:24:16	Date Stamp	27 Jan 2012 08:24:16				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN27-2012.30_201201270825.02\JAN27-2012\30\PDATA\1\1R						
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	32	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	65536	Pulse Sequence	zg30
Receiver Gain	181.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2461.8960
Spectrum Type	STANDARD	Sweep Width (Hz)	8278.02	Temperature (degree C)	27.000		

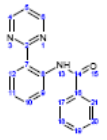


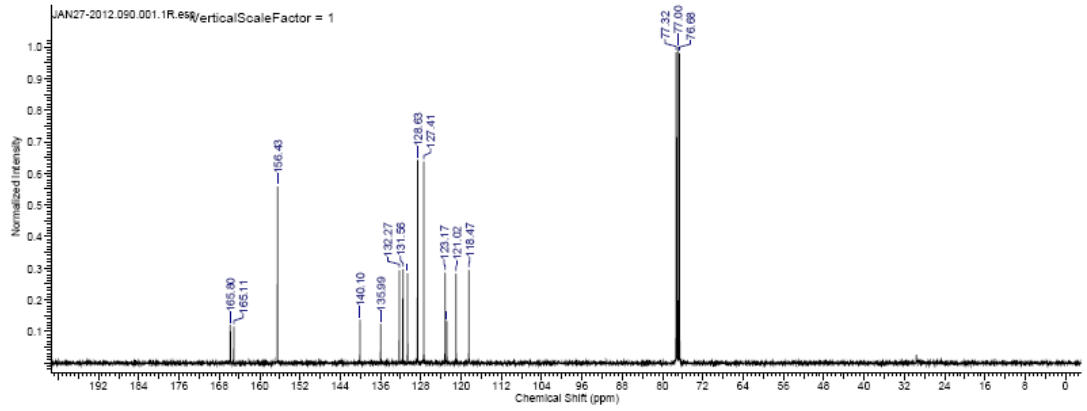


ZHANGYUT-003-EXP039.pdt

1/30/2012 9:09:49 AM

Formula $C_{17}H_{13}N_3O$	FW	275.3046					
Acquisition Time (sec)	1.3664	Comment	Notebook ZHANGYUT-003-EXP039-ISO-CARBON Project FLOW Name ZHANGYUT				
Date	28 Jan 2012 04:04:00	Date Stamp	28 Jan 2012 04:04:00				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN27-2012.90_201201280405.02\JAN27-2012\90\PDATA\1\1R						
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	4300	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	131072	Pulse Sequence	zgpg30
Receiver Gain	4096.00	SW(cyclical) (Hz)	23980.81	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10056.4014
Spectrum Type	STANDARD	Sweep Width (Hz)	23980.63	Temperature (degree C)	27.000		

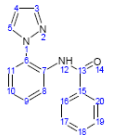


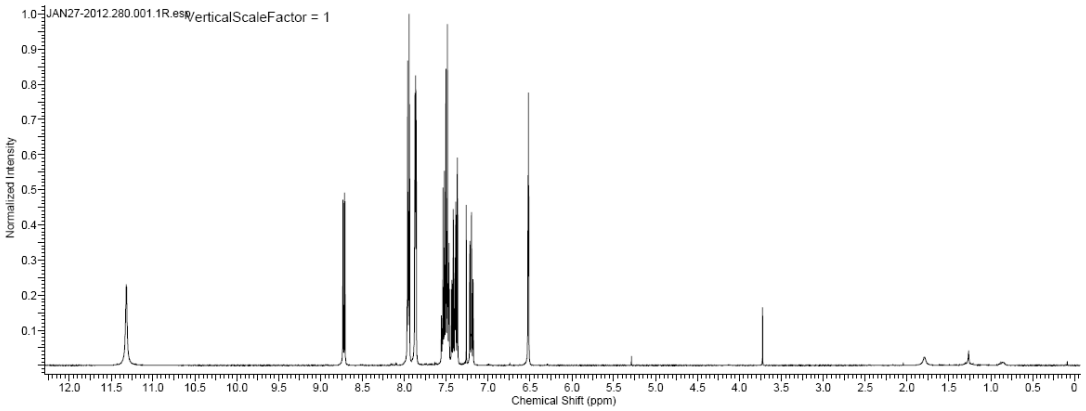


ZHANGYUT-003-EXP030.pdt

1/27/2012 3:43:49 PM

Formula $C_{16}H_{13}NO$	FW	263.2939					
Acquisition Time (sec)	3.9584	Comment	Notebook ZHANGYUT-003-EXP030-ISOA Project FLOW Name ZHANGYUT				
Date	27 Jan 2012 13:46:24	Date Stamp	27 Jan 2012 13:46:24				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN27-2012.280_201201271350.02\JAN27-2012\280\PDATA\1\1R						
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	32	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	65536	Pulse Sequence	zg30
Receiver Gain	128.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2461.8960
Spectrum Type	STANDARD	Sweep Width (Hz)	8278.02	Temperature (degree C)	27.000		





ZHANGYUT-003-EXP030.pdt

1/30/2012 8:37:20 AM

Formula $C_{16}H_{13}NO$	FW	263.2939					
Acquisition Time (sec)	1.3664	Comment	Notebook ZHANGYUT-003-EXP030-ISO-CARBON Project FLOW Name ZHANGYUT				
Date	28 Jan 2012 08:28:32	Date Stamp	28 Jan 2012 08:28:32				
File Name	C:\DOCUME~1\ZHANGYUT\LOCALS~1\TEMP\AWM_TEMP\AV400D.JAN27-2012.380_201201280830.02\JAN27-2012\380\PDATA\1\1R						
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	4500	Origin	av400d
Original Points Count	32768	Owner	av400d	Points Count	131072	Pulse Sequence	zgpg30
Receiver Gain	1625.50	SW(cyclical) (Hz)	23980.81	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10055.3037
Spectrum Type	STANDARD	Sweep Width (Hz)	23980.63	Temperature (degree C)	27.000