Supporting Information

Assessment of amination reactions via nucleophilic aromatic substitution using conventional and eco-friendly energies

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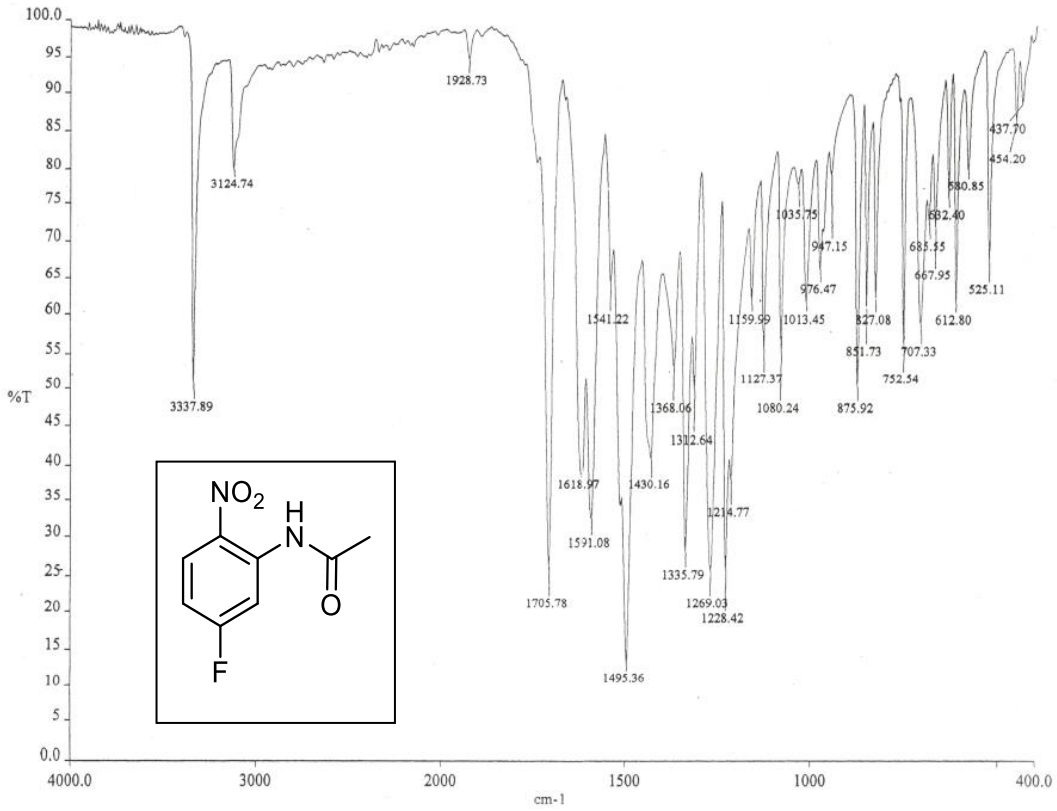
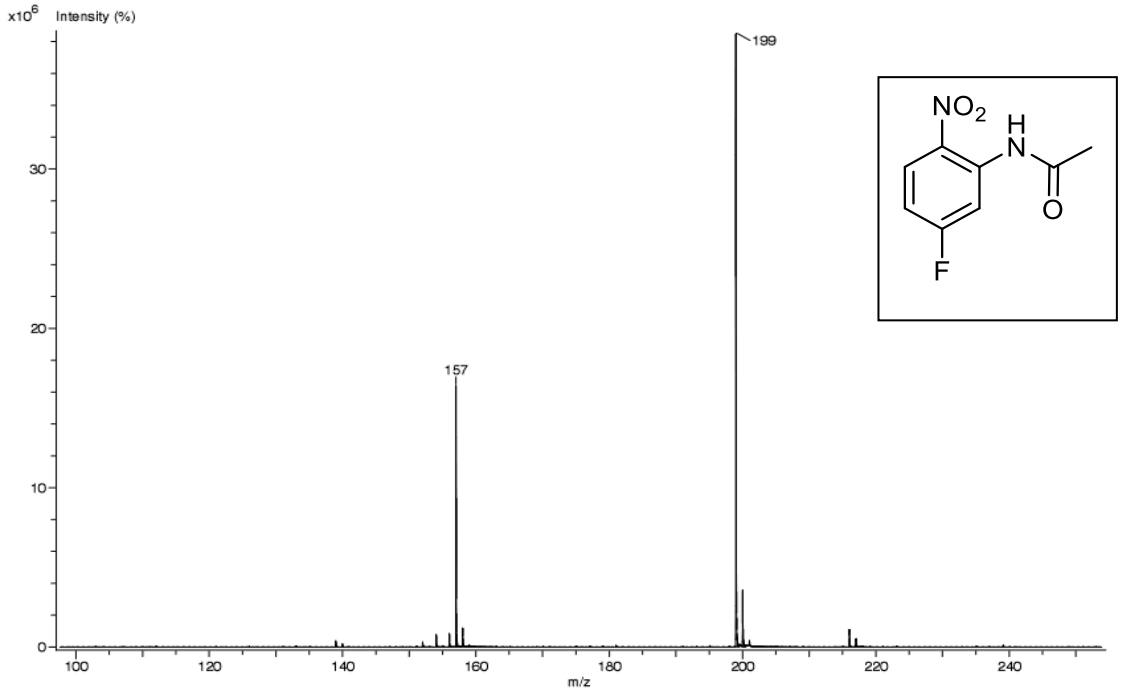
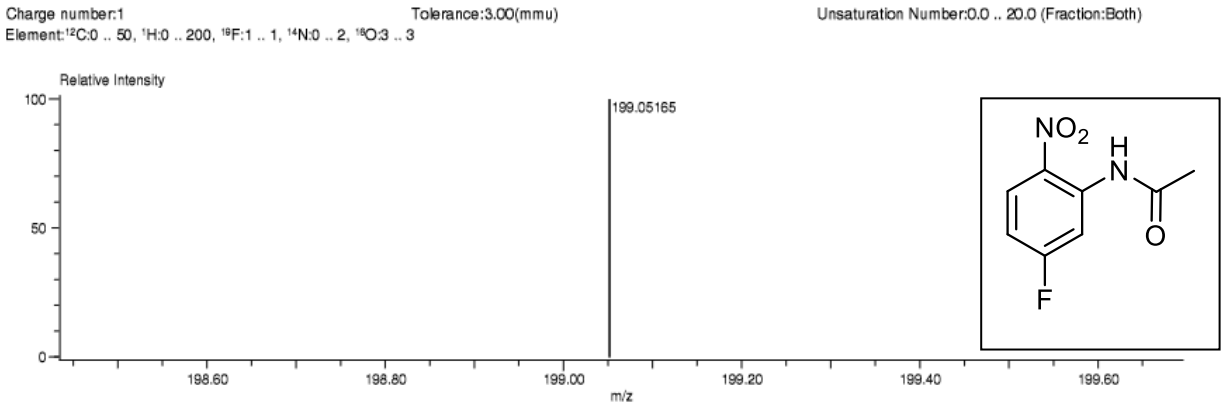


N-(5-Fluoro-2-nitrophenyl)acetamide **1a**

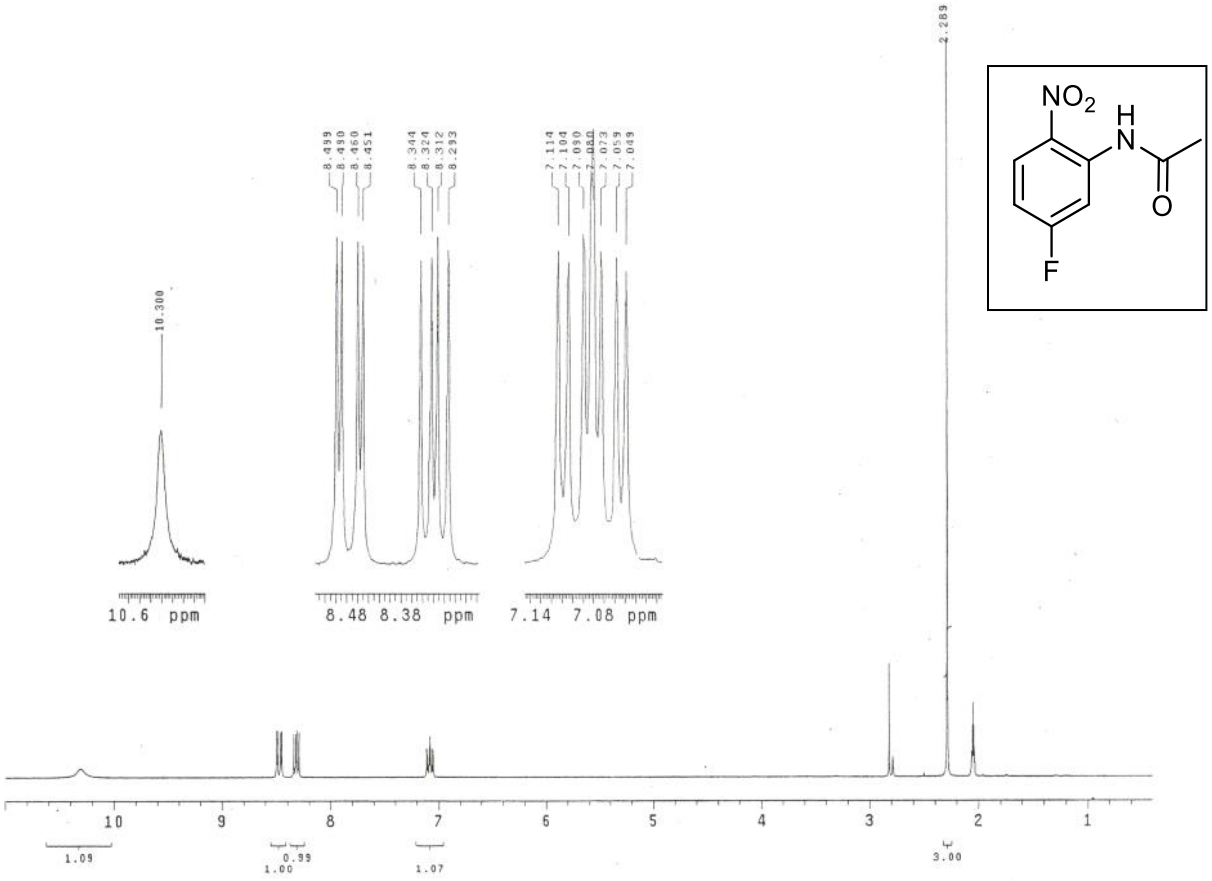


N-(5-Fluoro-2-nitrophenyl)acetamide **1a**

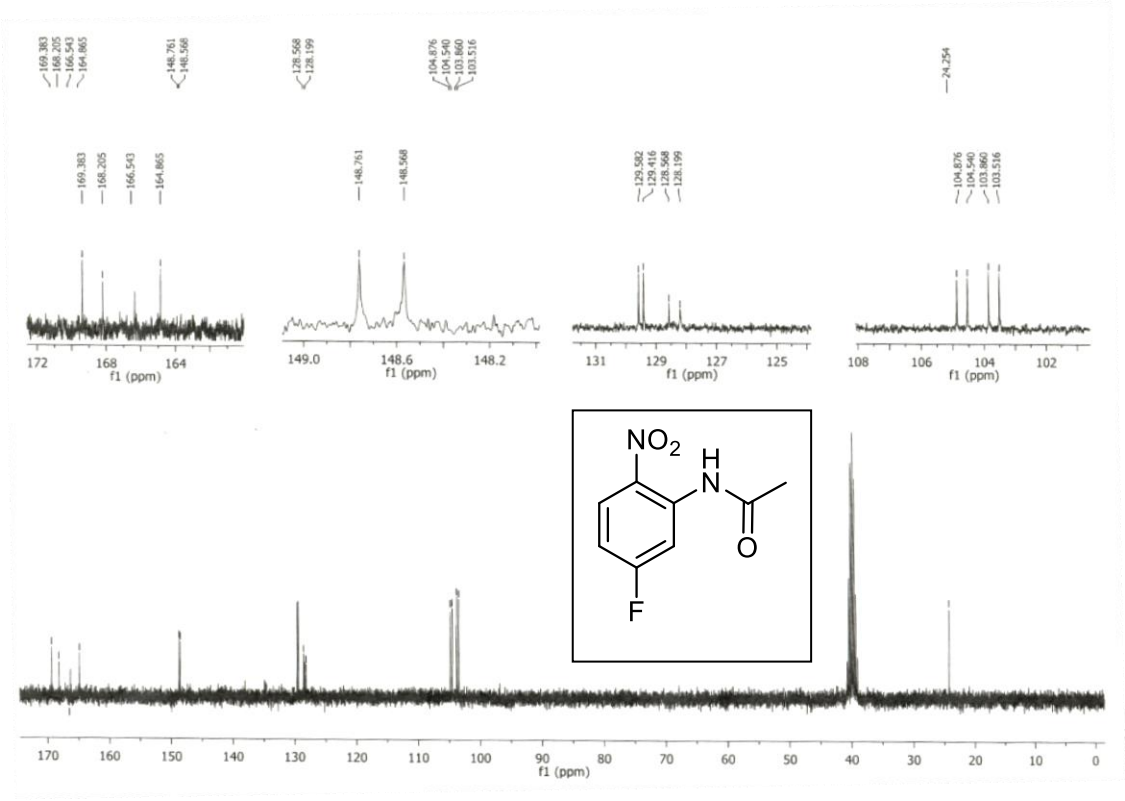


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
199.05165	182405.88	199.05190	-0.24	-1.22	$^{12}C_6{}^1H_8{}^{19}F_1{}^{14}N_2{}^{16}O_3$	5.5

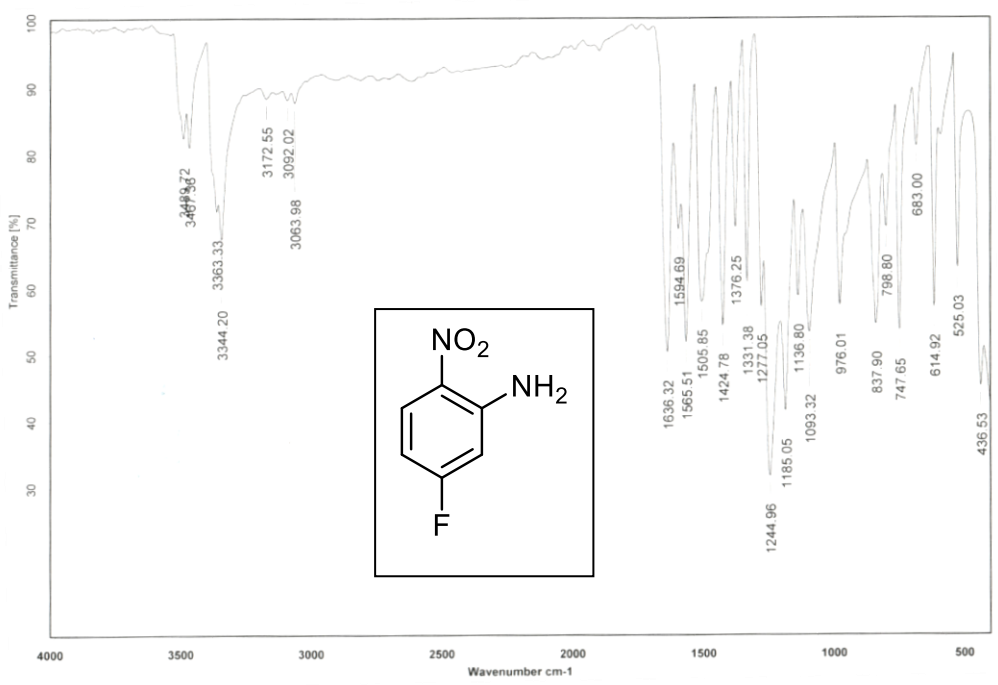
N-(5-Fluoro-2-nitrophenyl)acetamide **1a**



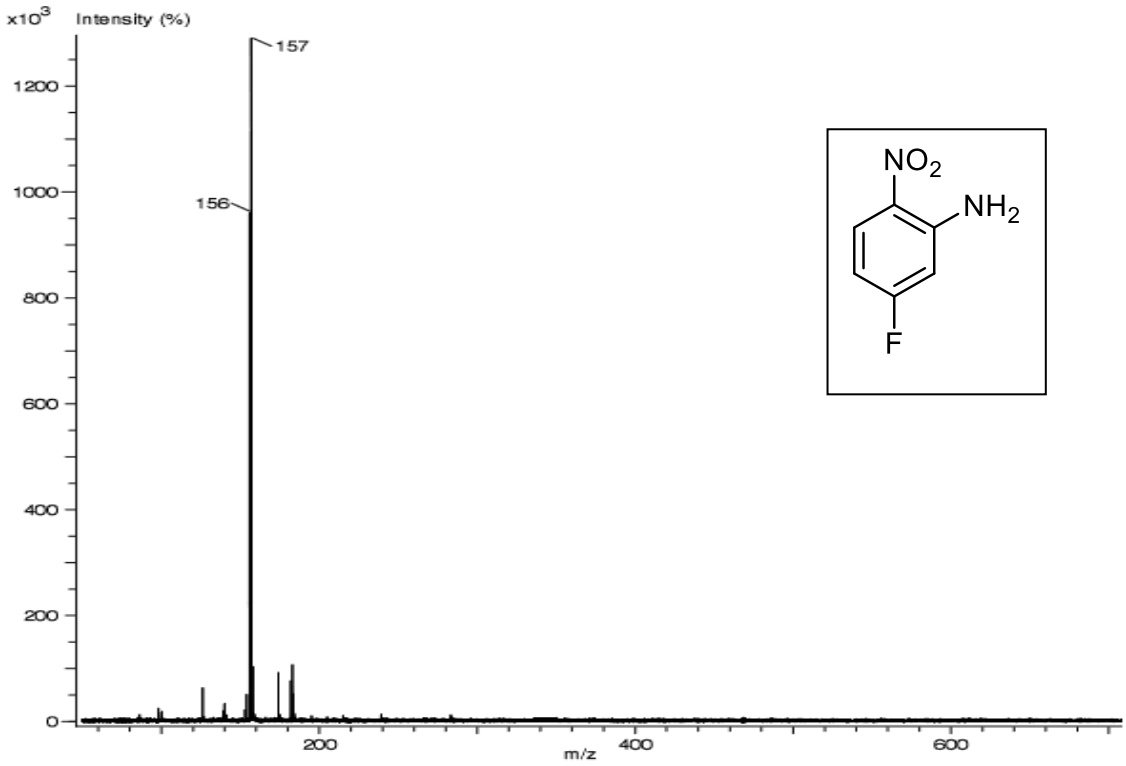
N-(5-Fluoro-2-nitrophenyl)acetamide **1a**



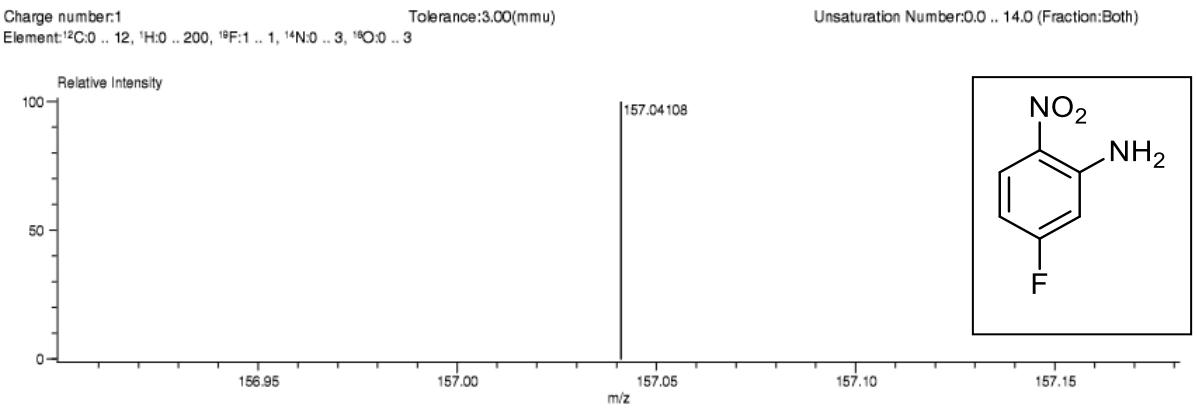
N-(5-Fluoro-2-nitrophenyl)acetamide **1a**



5-Fluoro-2-nitroaniline **4a**

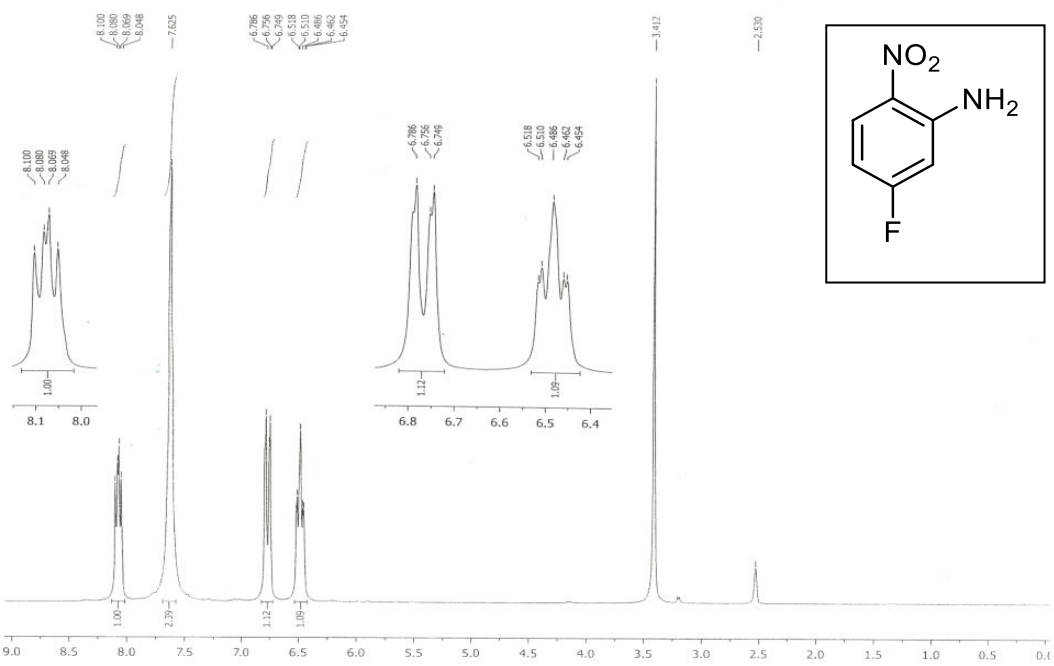


5-Fluoro-2-nitroaniline **4a**

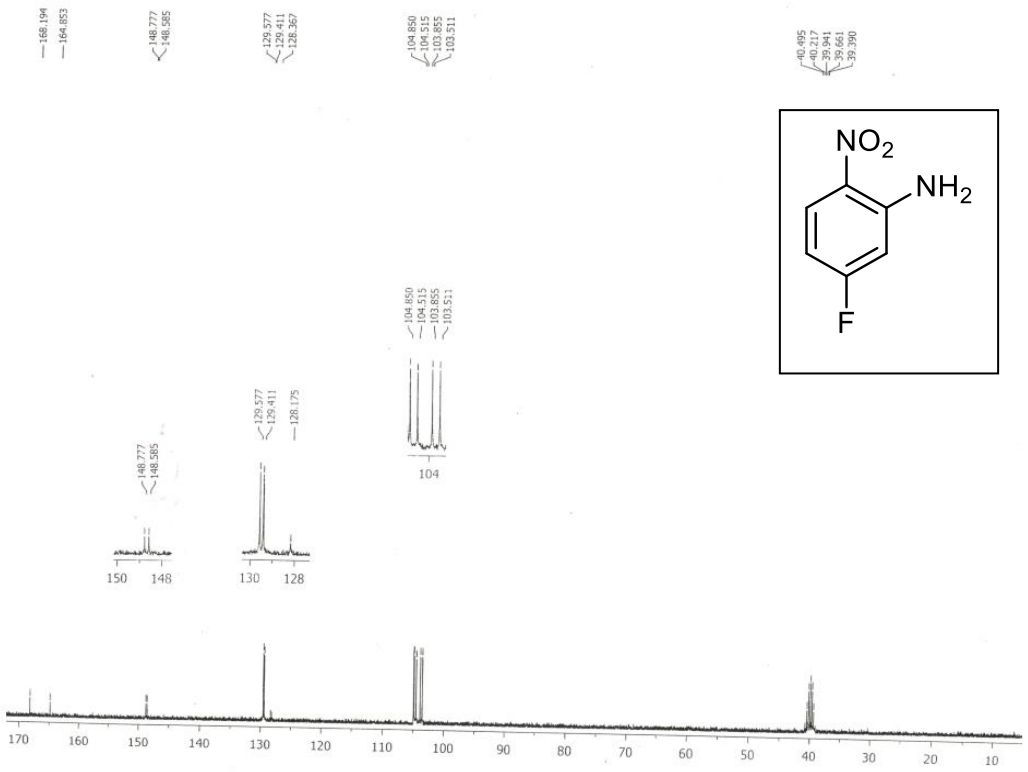


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
157.04108	5744.00	157.04133	-0.25	-1.59	$^{12}C_6{}^1H_8{}^{19}F_1{}^{14}N_2{}^{16}O_2$	4.5

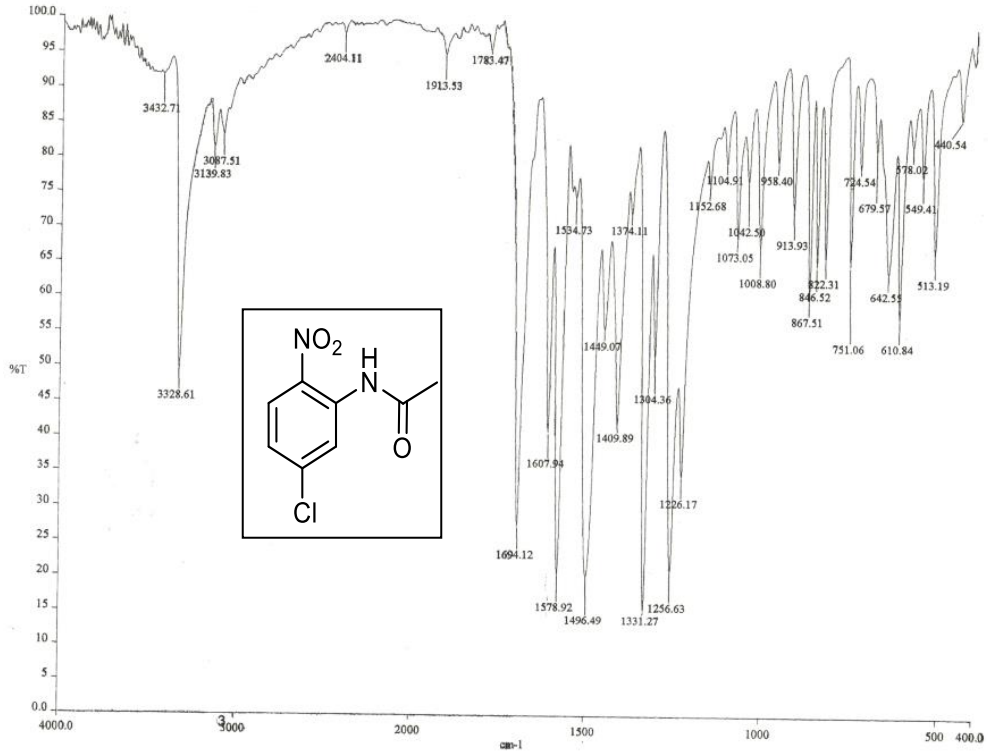
5-Fluoro-2-nitroaniline **4a**



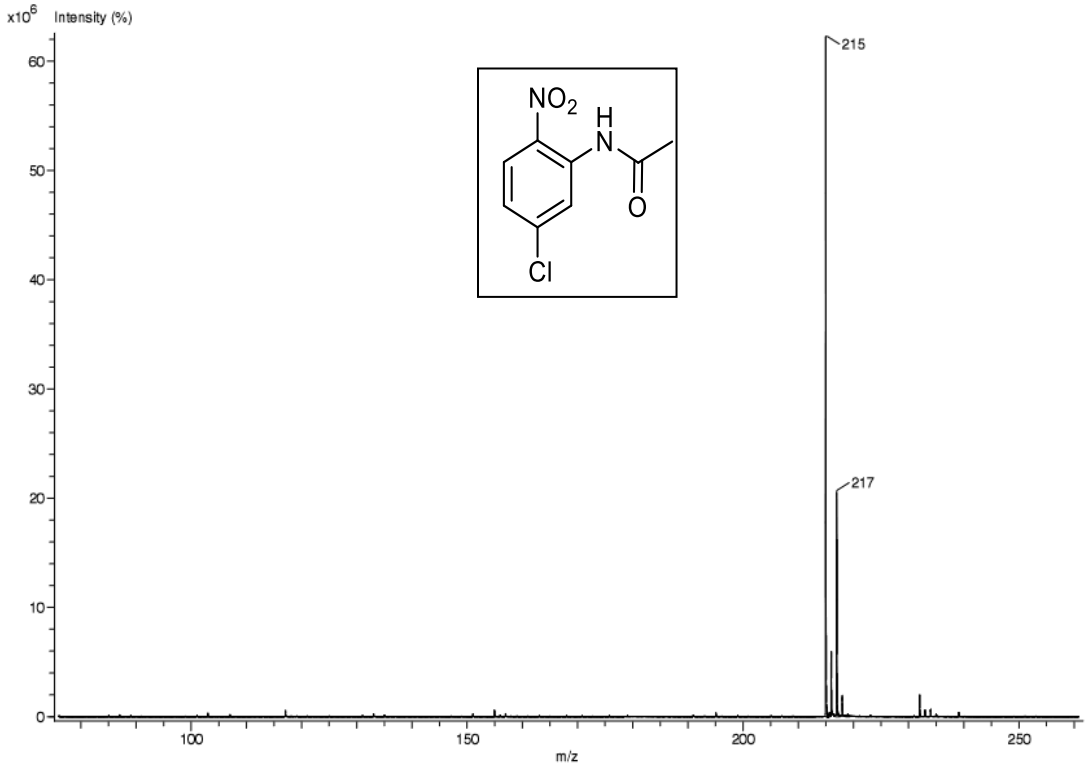
5-Fluoro-2-nitroaniline **4a**



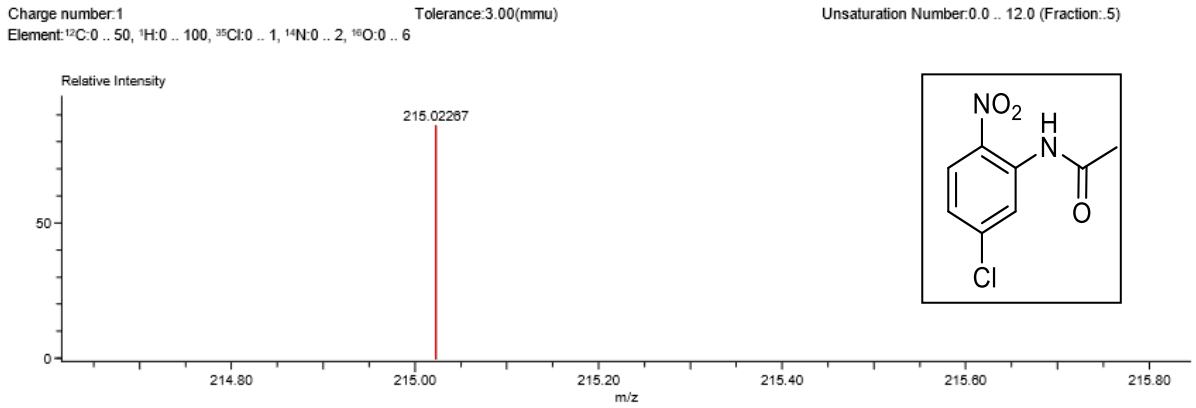
5-Fluoro-2-nitroaniline **4a**



N-(5-Chloro-2-nitrophenyl)acetamide **1b**

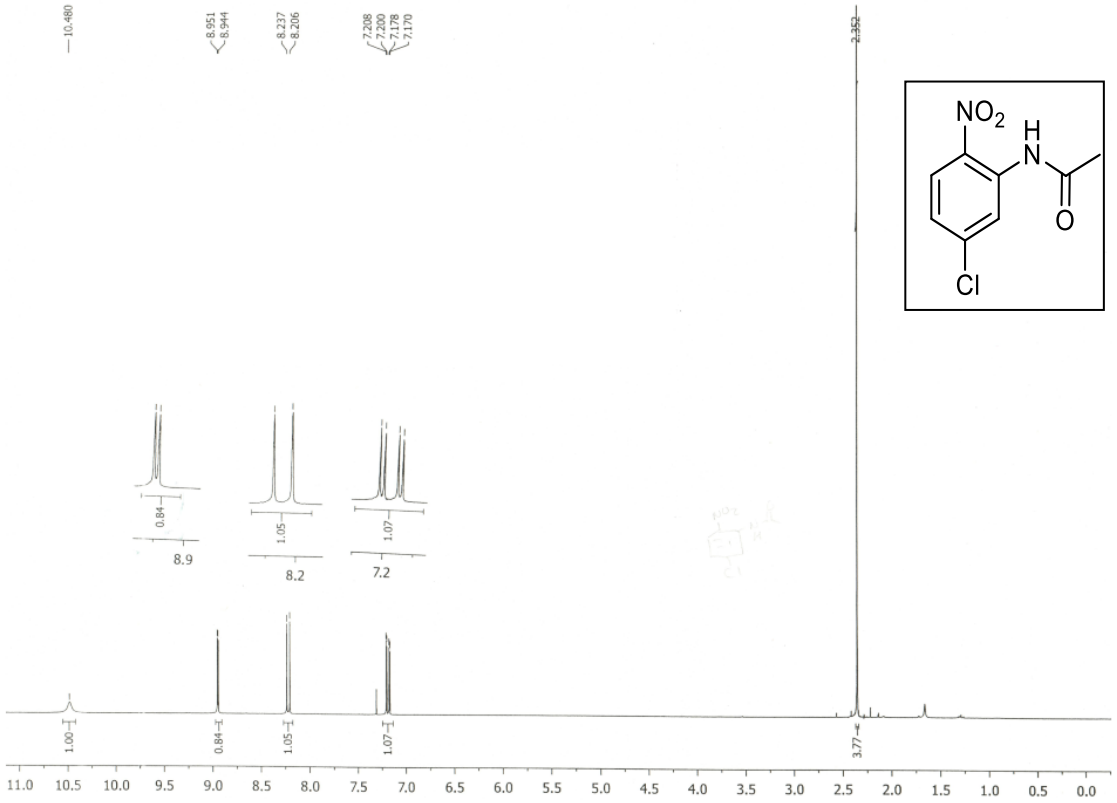


N-(5-Chloro-2-nitrophenyl)acetamide(**1b**

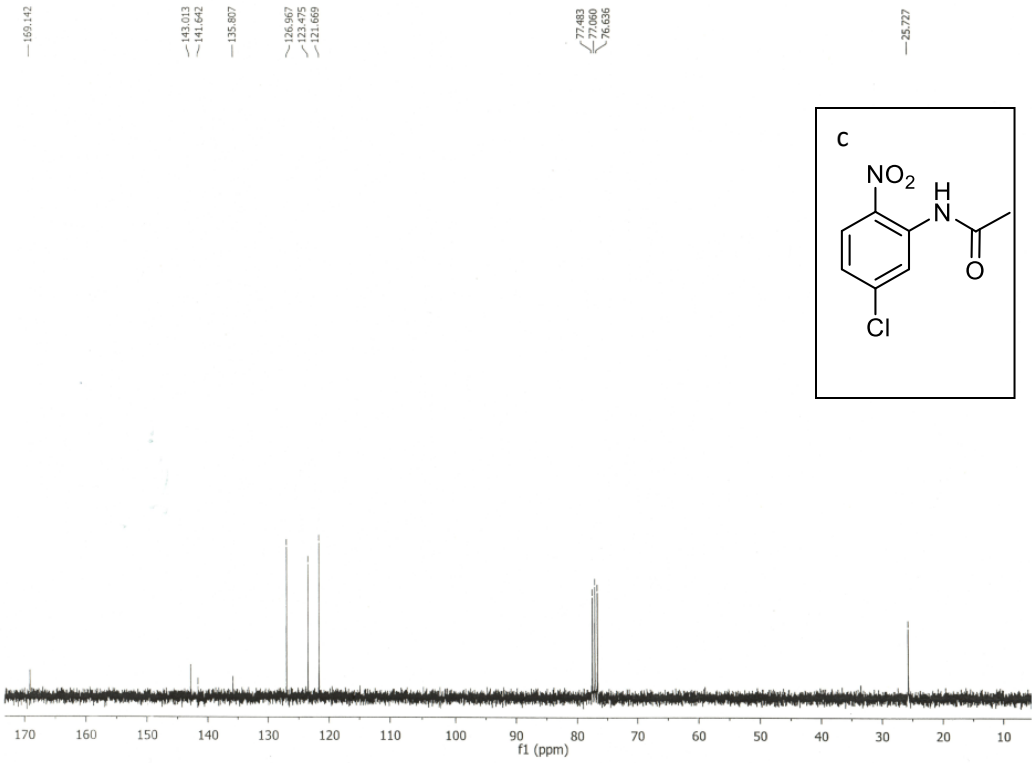


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
215.02267	102033.13	215.02234	0.33	1.51	$^{12}C_8{}^{1}H_8{}^{35}Cl_1{}^{14}N_2{}^{16}O_3$	5.5

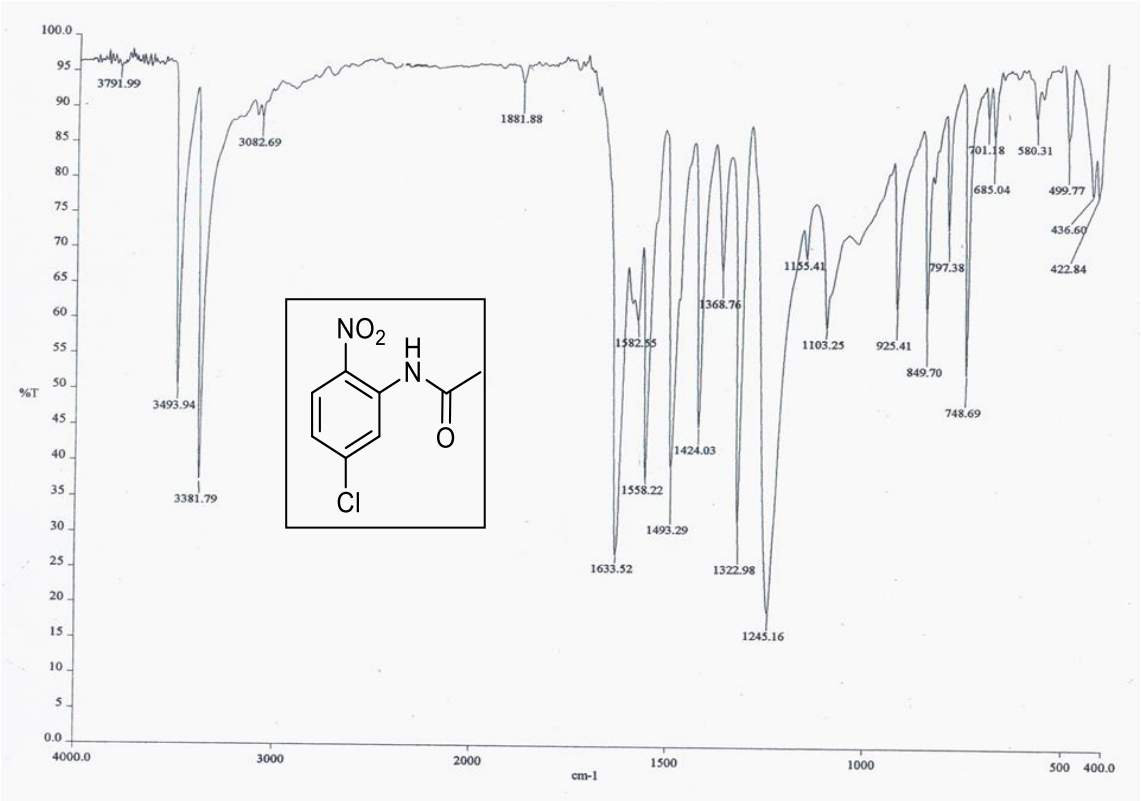
N-(5-Chloro-2-nitrophenyl)acetamide **1b**



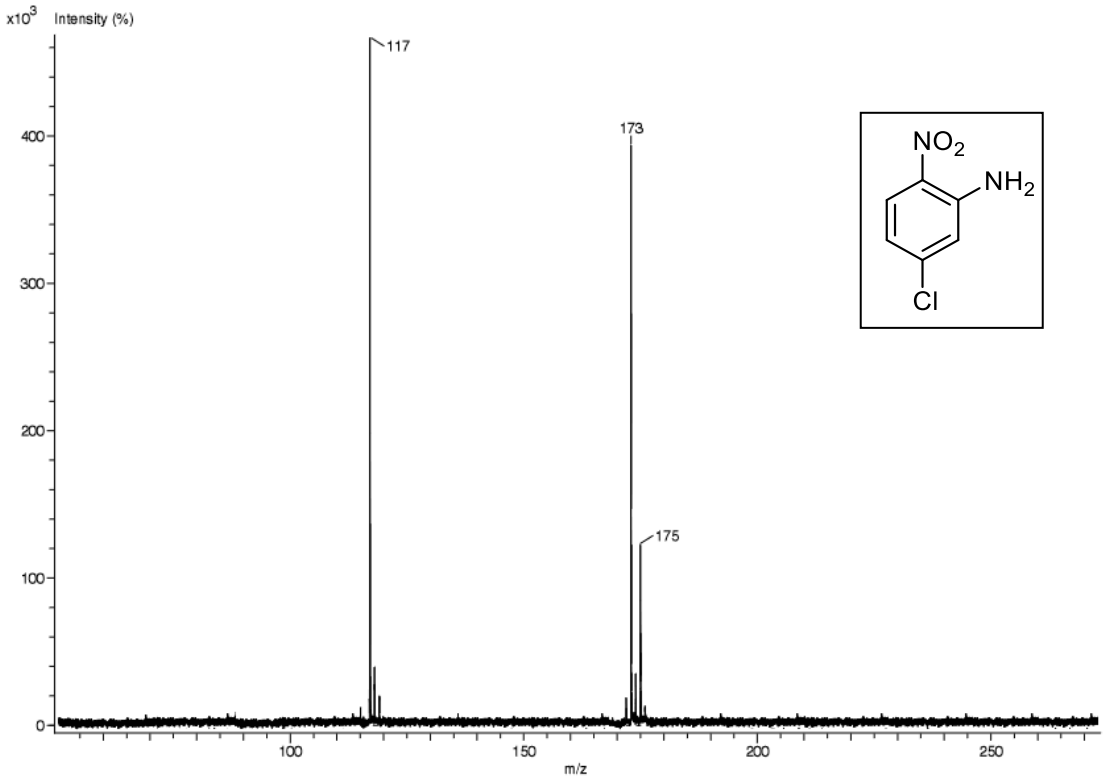
N-(5-Chloro-2-nitrophenyl)acetamide **1b**



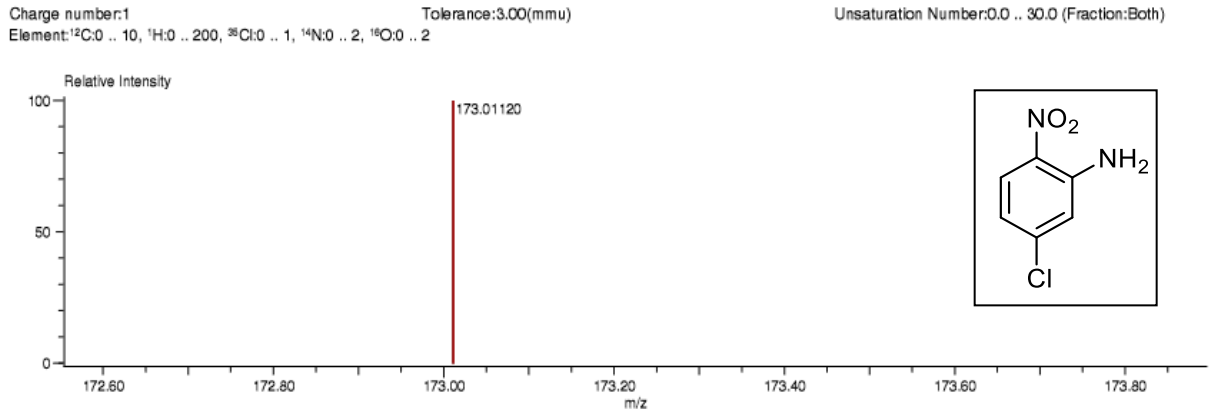
N-(5-Chloro-2-nitrophenyl)acetamide **1b**



5-Chloro-2-nitroaniline **4b**

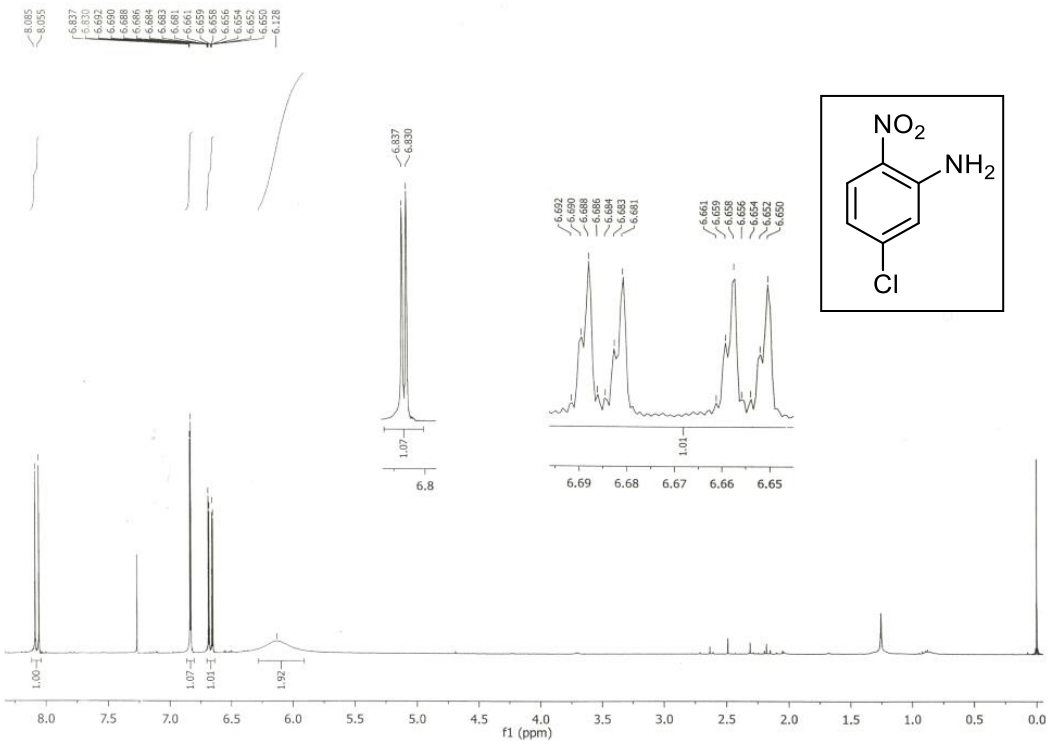


5-Chloro-2-nitroaniline **4b**

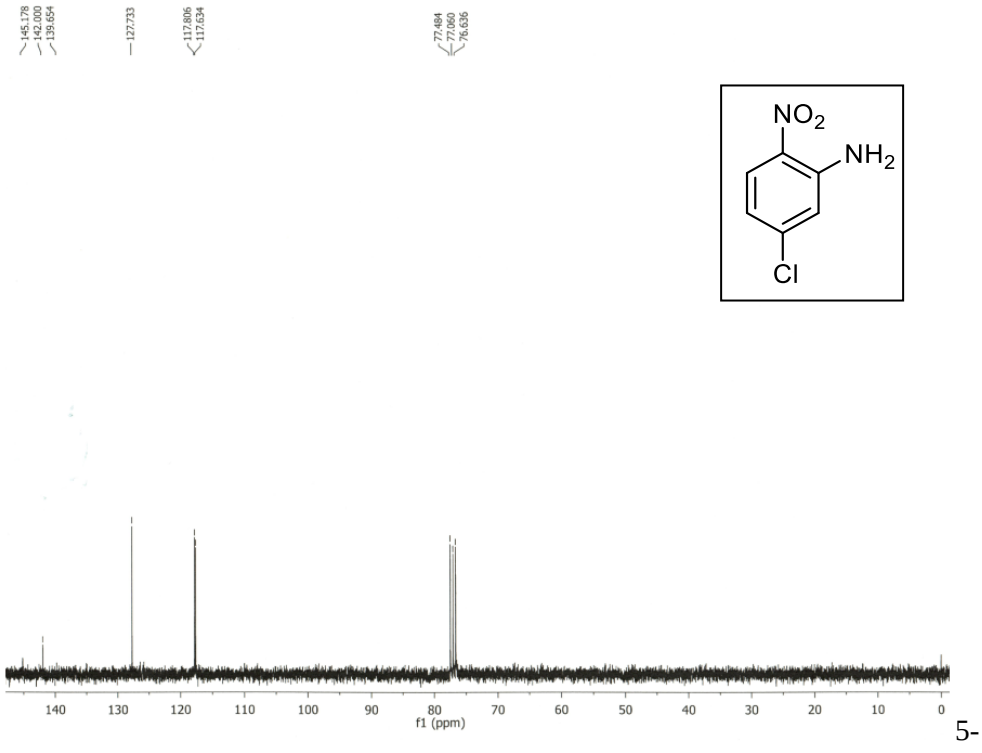


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
173.01120	1433254.00	173.01178	-0.58	-3.33	$^{12}C_6{}^{1}H_5{}^{35}Cl_1{}^{14}N_2{}^{16}O_2$	4.5

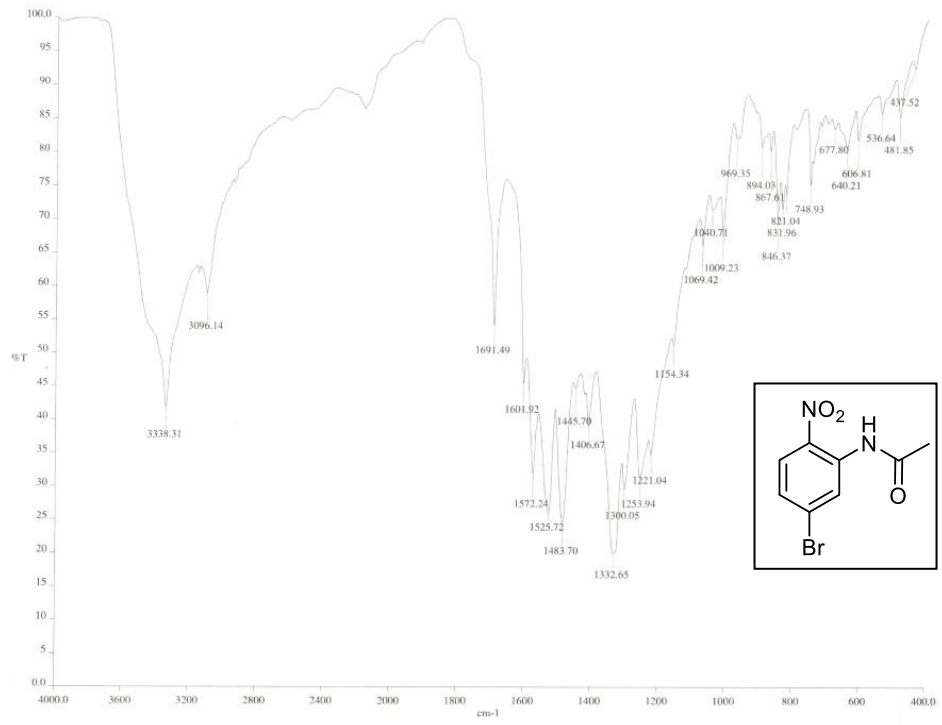
5-Chloro-2-nitroaniline **4b**



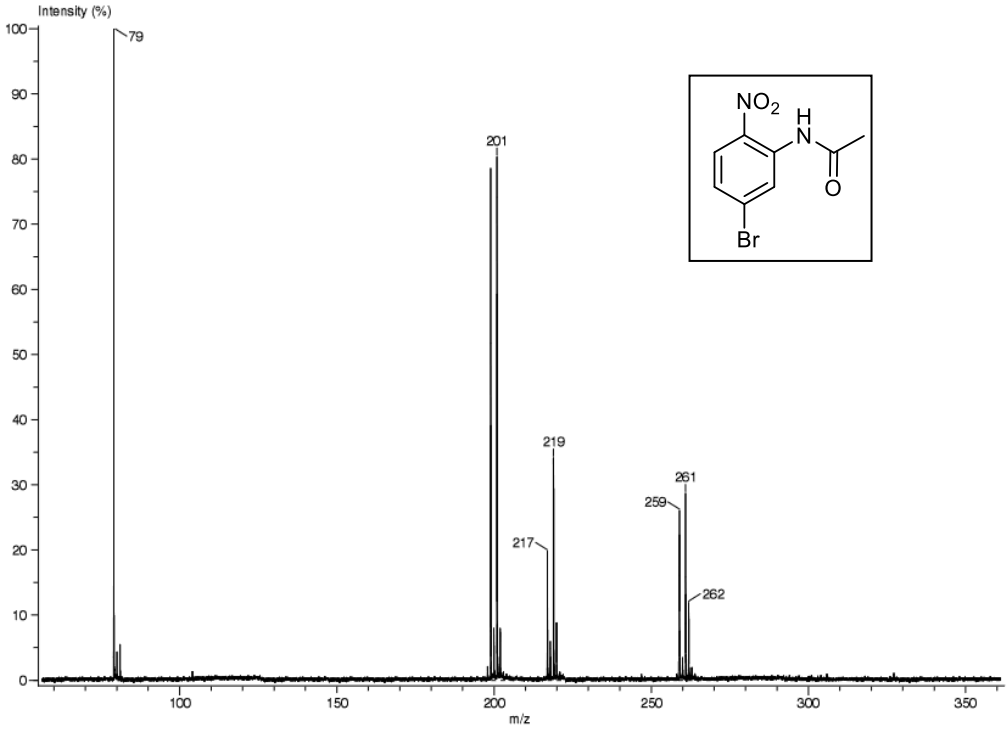
5-Chloro-2-nitroaniline **4b**



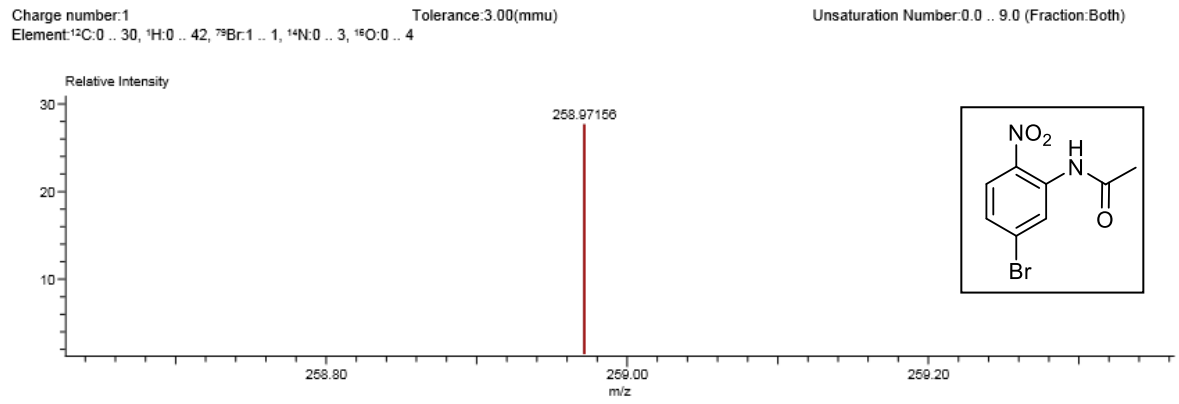
5-Chloro-2-nitroaniline **4b**



N-(5-Bromo-2-nitrophenyl)acetamide **1c**

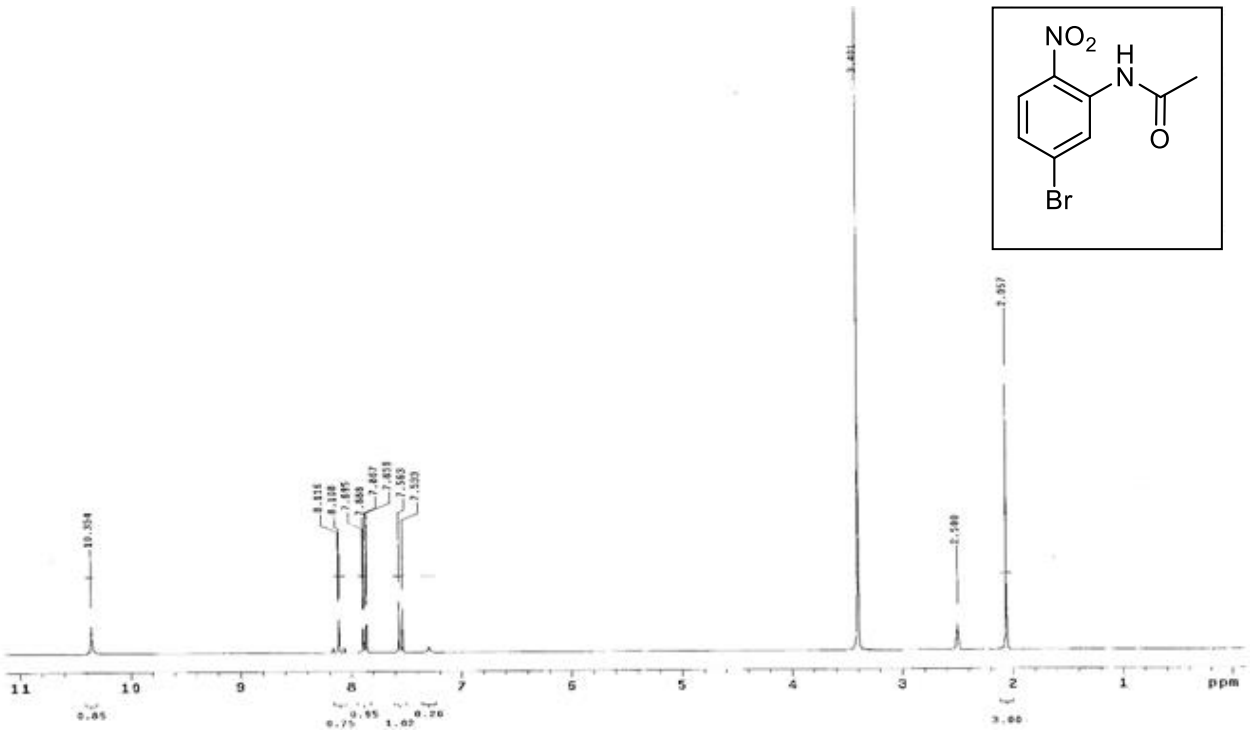


N-(5-Bromo-2-nitrophenyl)acetamide **1c**

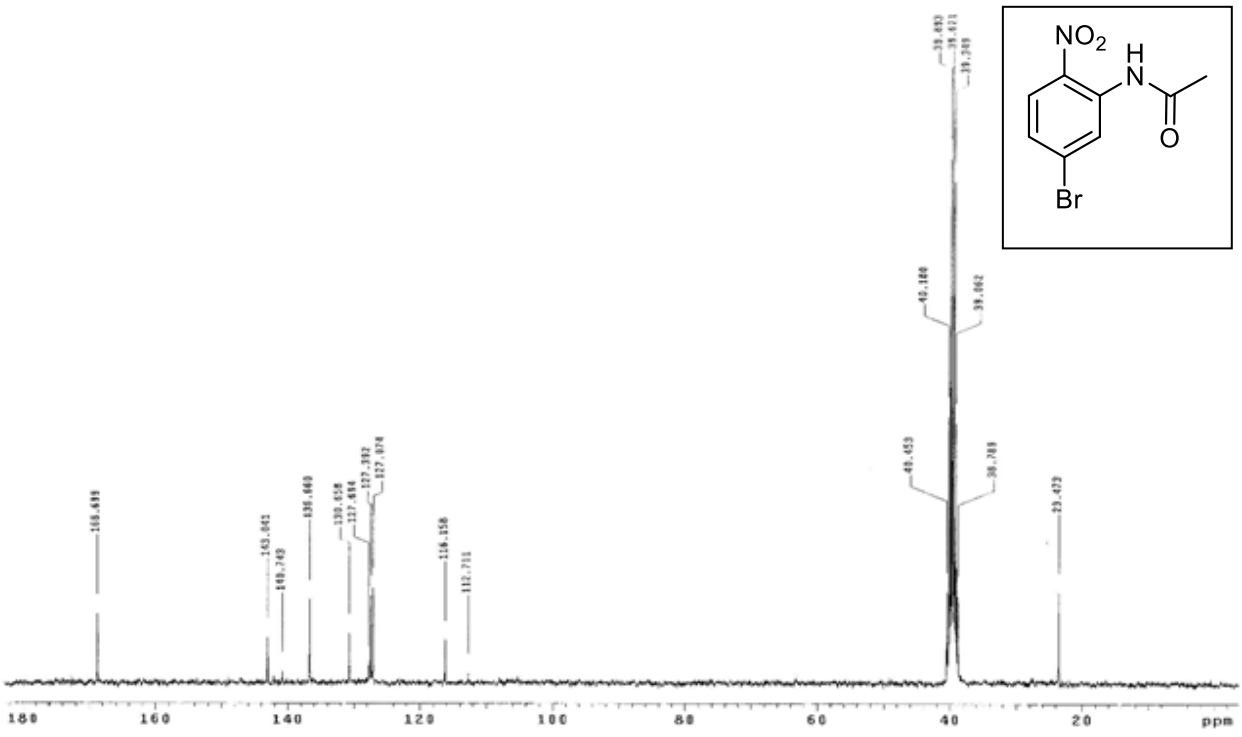


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
258.97156	105486.35	258.97183	-0.27	-1.03	$^{12}C_8{}^1H_8{}^{79}Br_1{}^{14}N_2{}^{16}O_3$	5.5

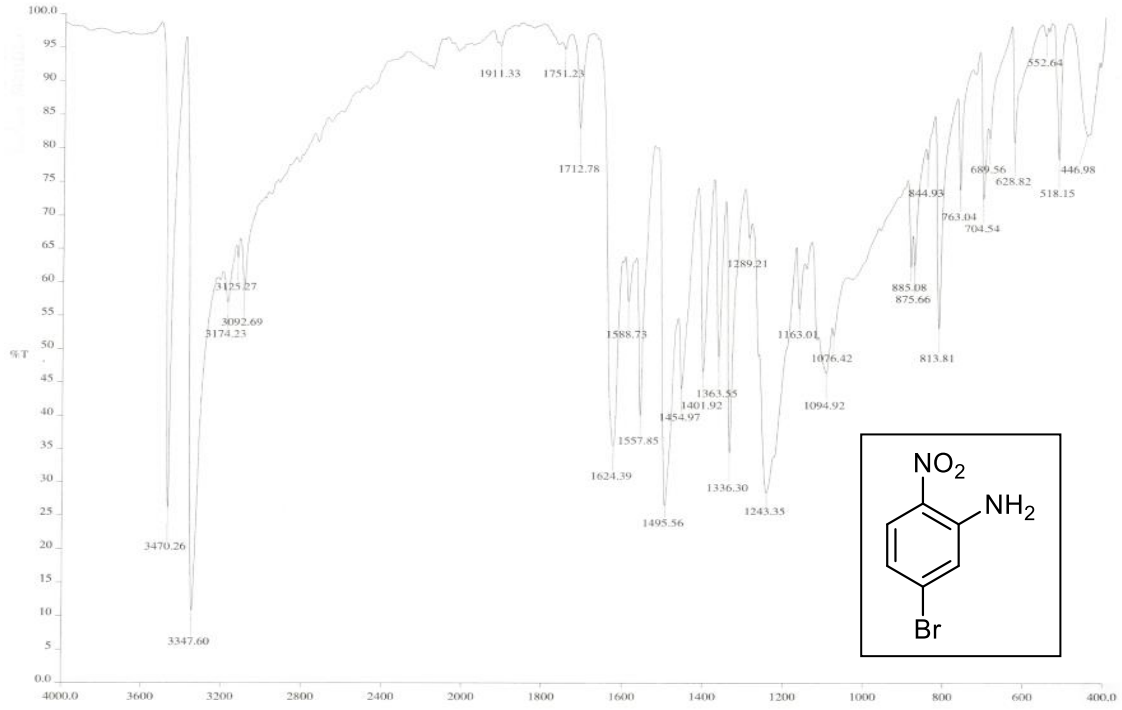
N-(5-Bromo-2-nitrophenyl)acetamide **1c**



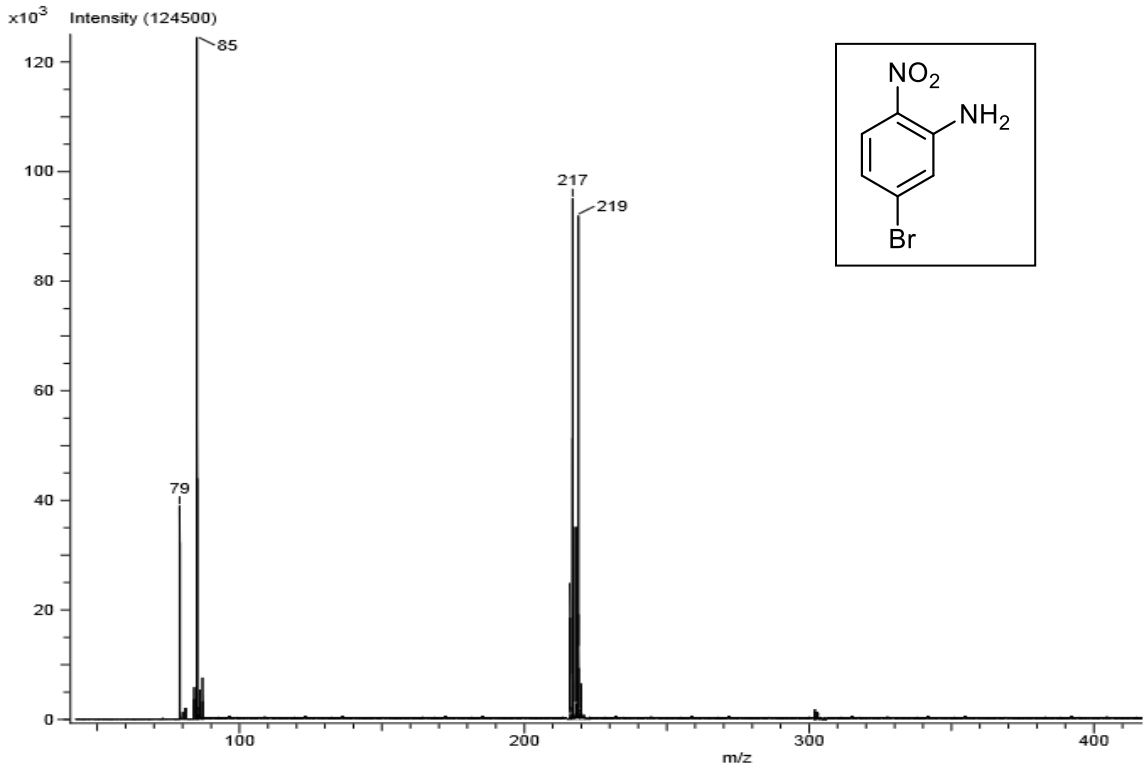
N-(5-Bromo-2-nitrophenyl)acetamide **1c**



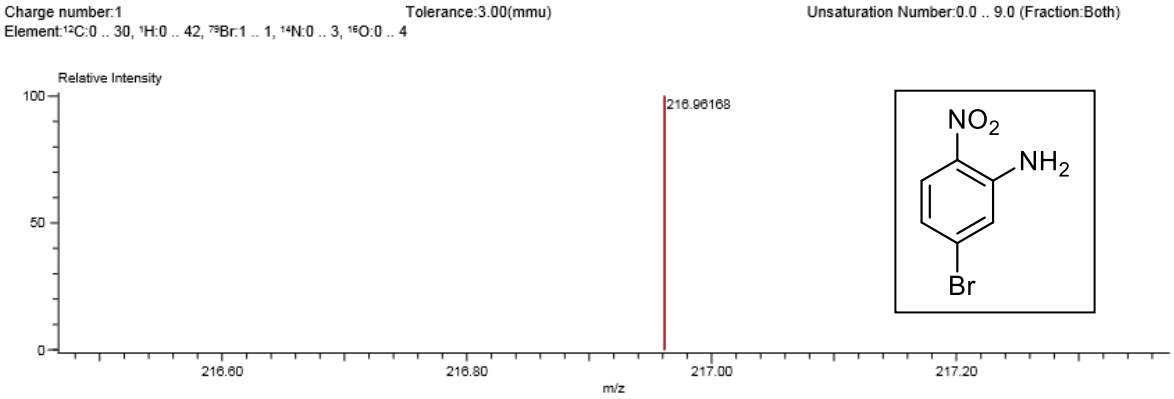
N-(5-Bromo-2-nitrophenyl)acetamide **1c**



5-Bromo-2-nitroaniline **4c**

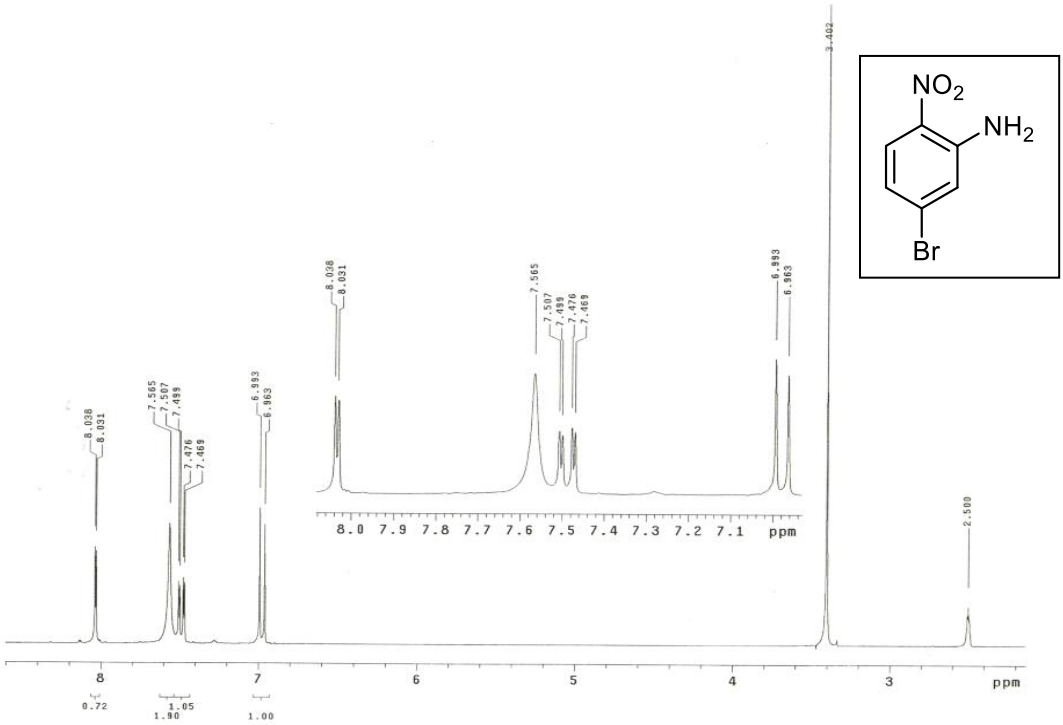


5-Bromo-2-nitroaniline **4c**

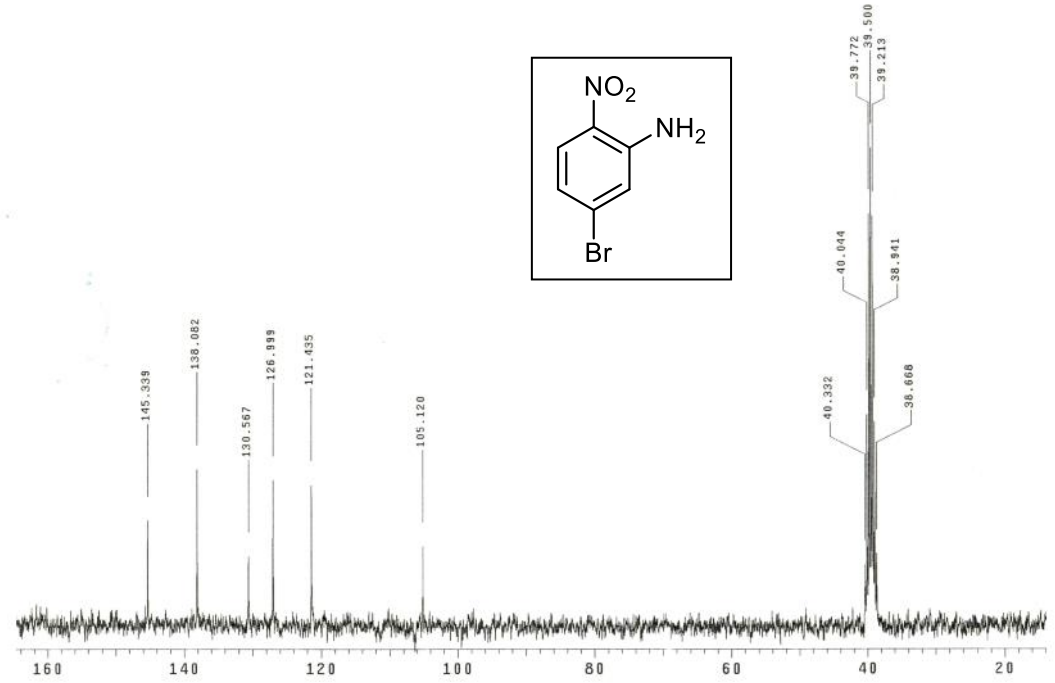


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
216.96168	381471.03	216.96127	0.41	1.91	$^{12}C_6{}^{1}H_5{}^{79}Br_1{}^{14}N_2{}^{16}O_2$	4.5

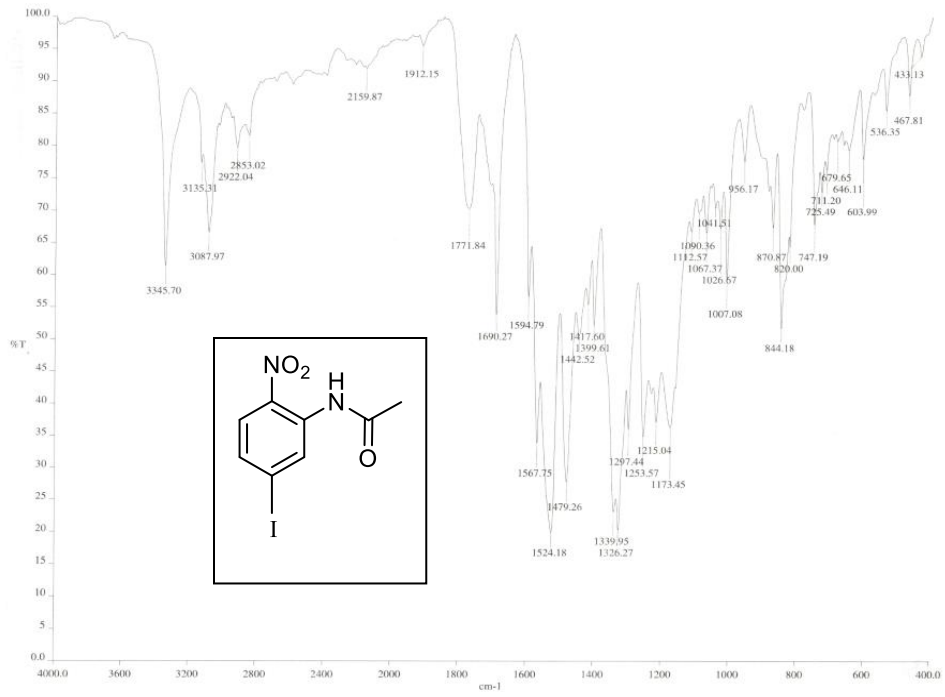
5-Bromo-2-nitroaniline **4c**



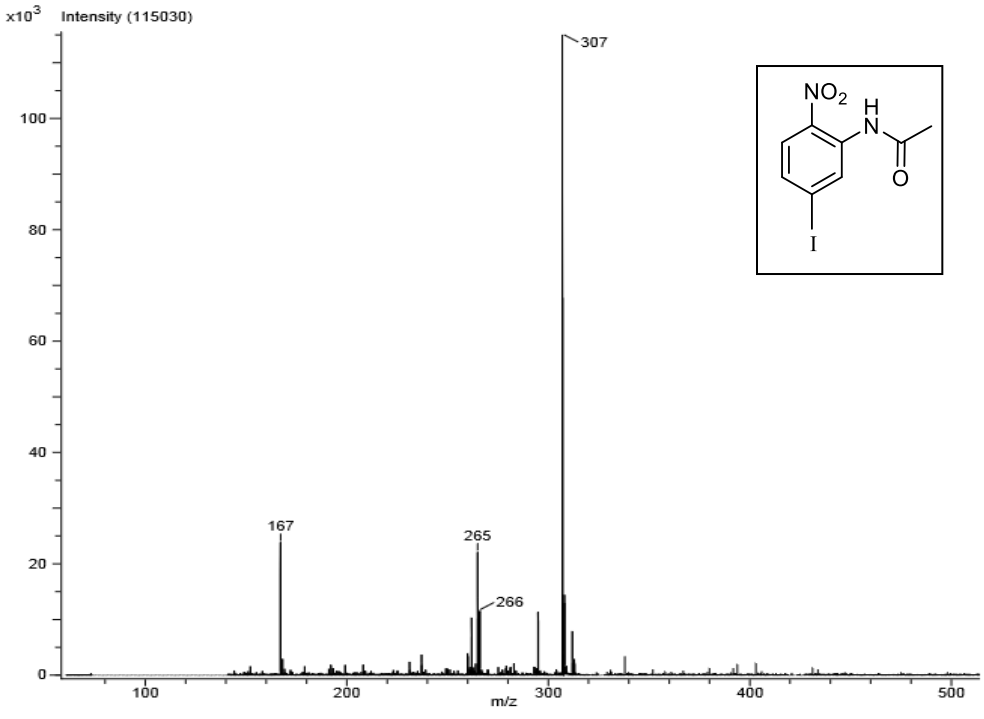
5-Bromo-2-nitroaniline **4c**



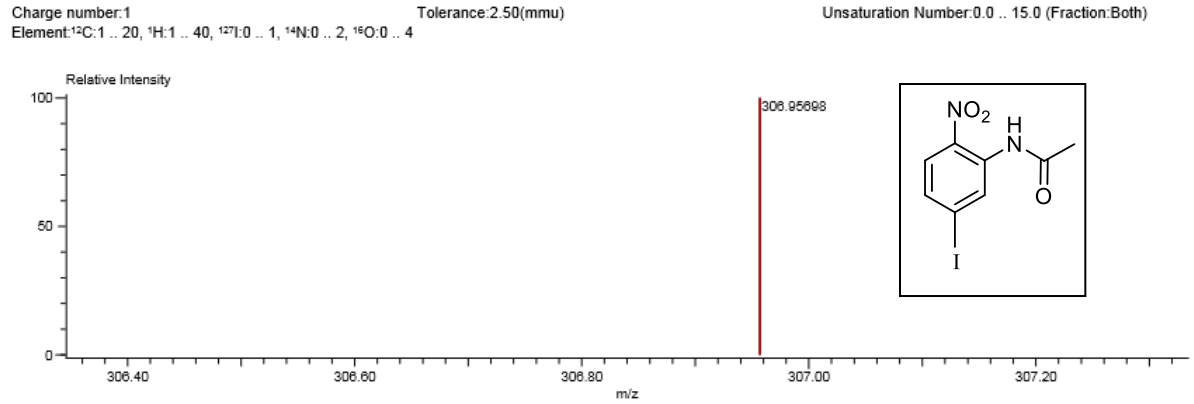
5-Bromo-2-nitroaniline **4c**



N-(5-Iodo-2-nitrophenyl)acetamide **1d**

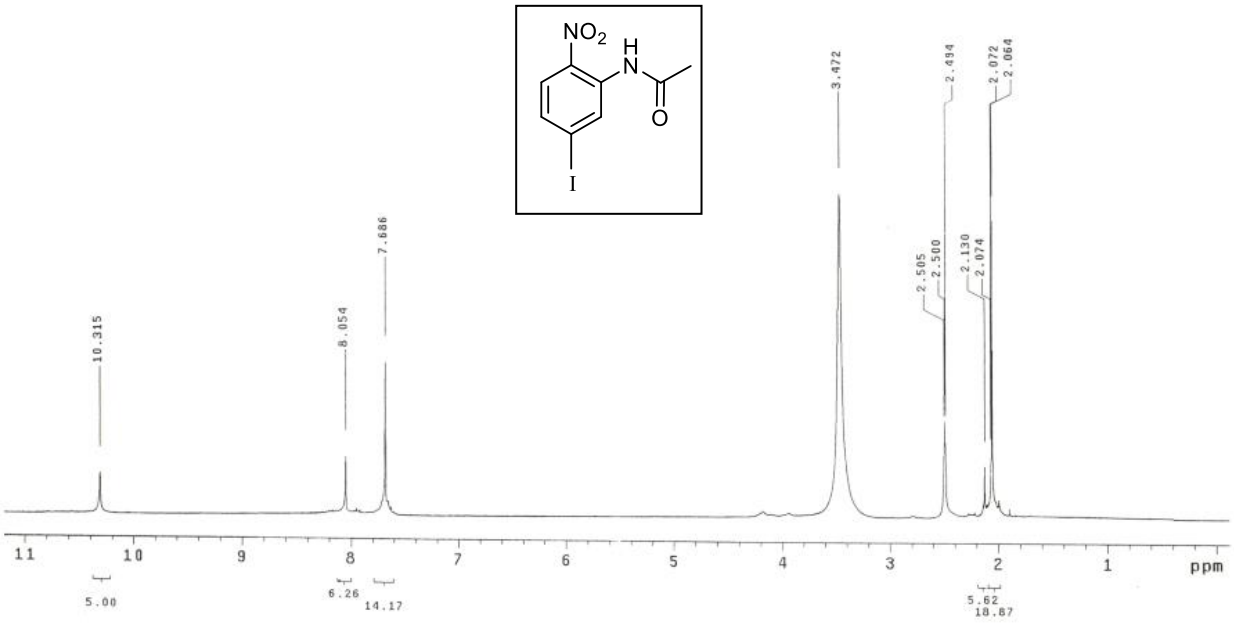


N-(5-Iodo-2-nitrophenyl)acetamide **1d**

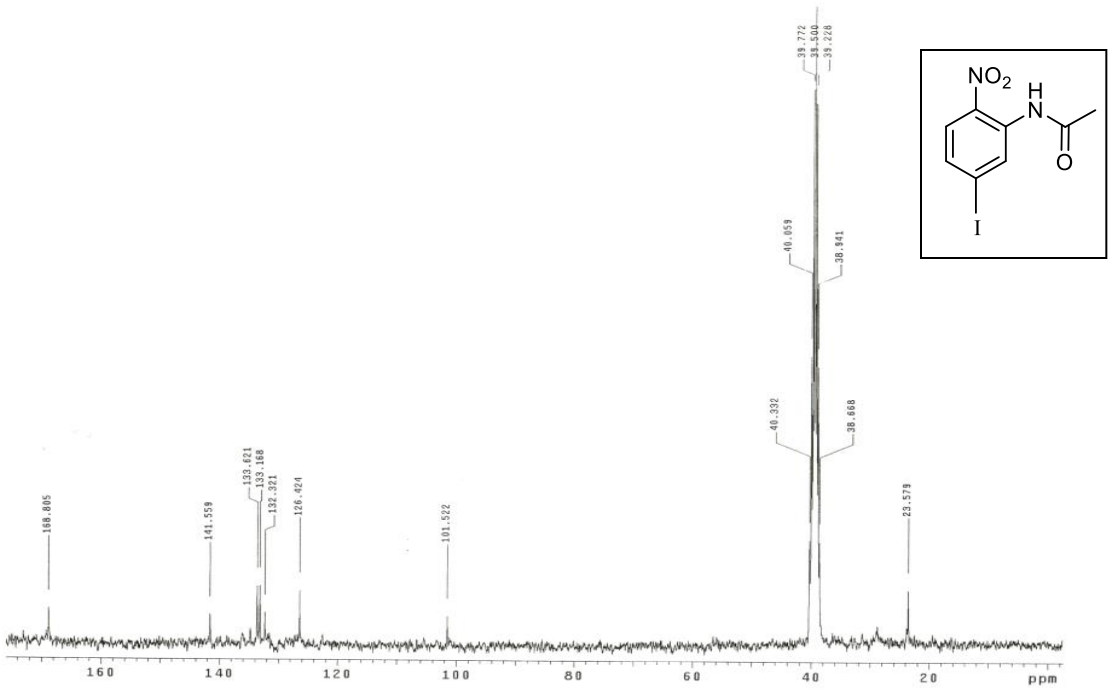


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
306.95698	396880.56	306.95796	-0.98	-3.20	$^{12}C_8{}^{1}H_8{}^{127}I_1{}^{14}N_2{}^{16}O_3$	5.5

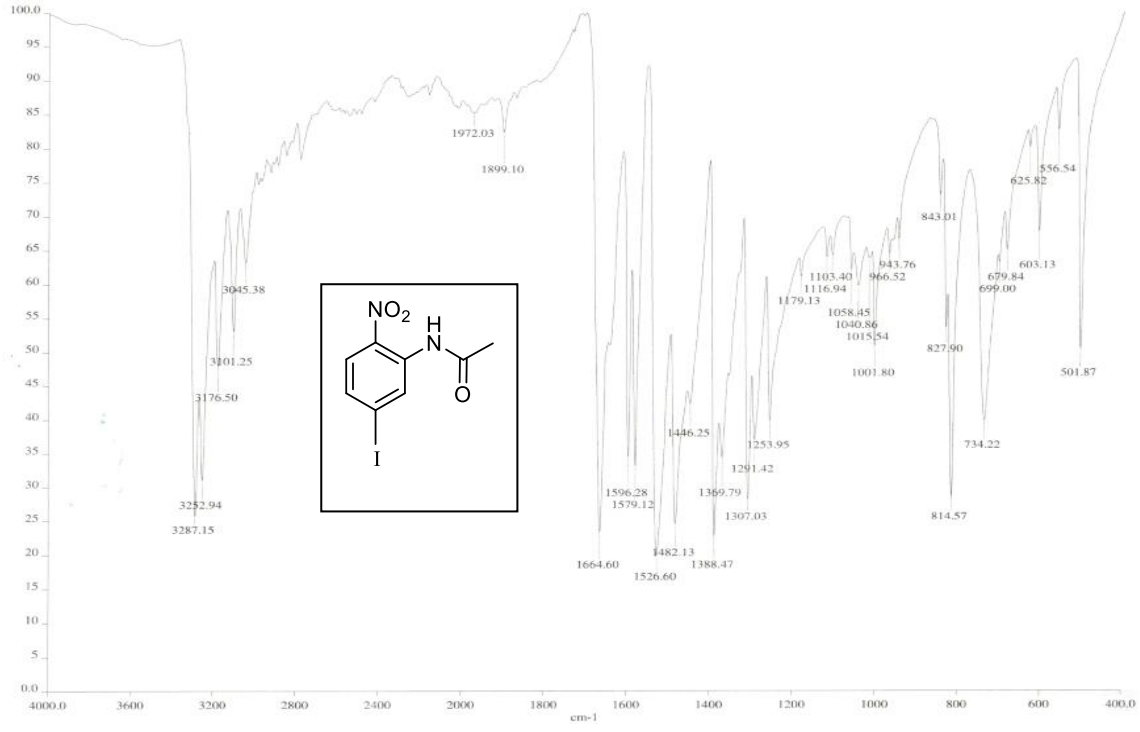
N-(5-Iodo-2-nitrophenyl)acetamide **1d**



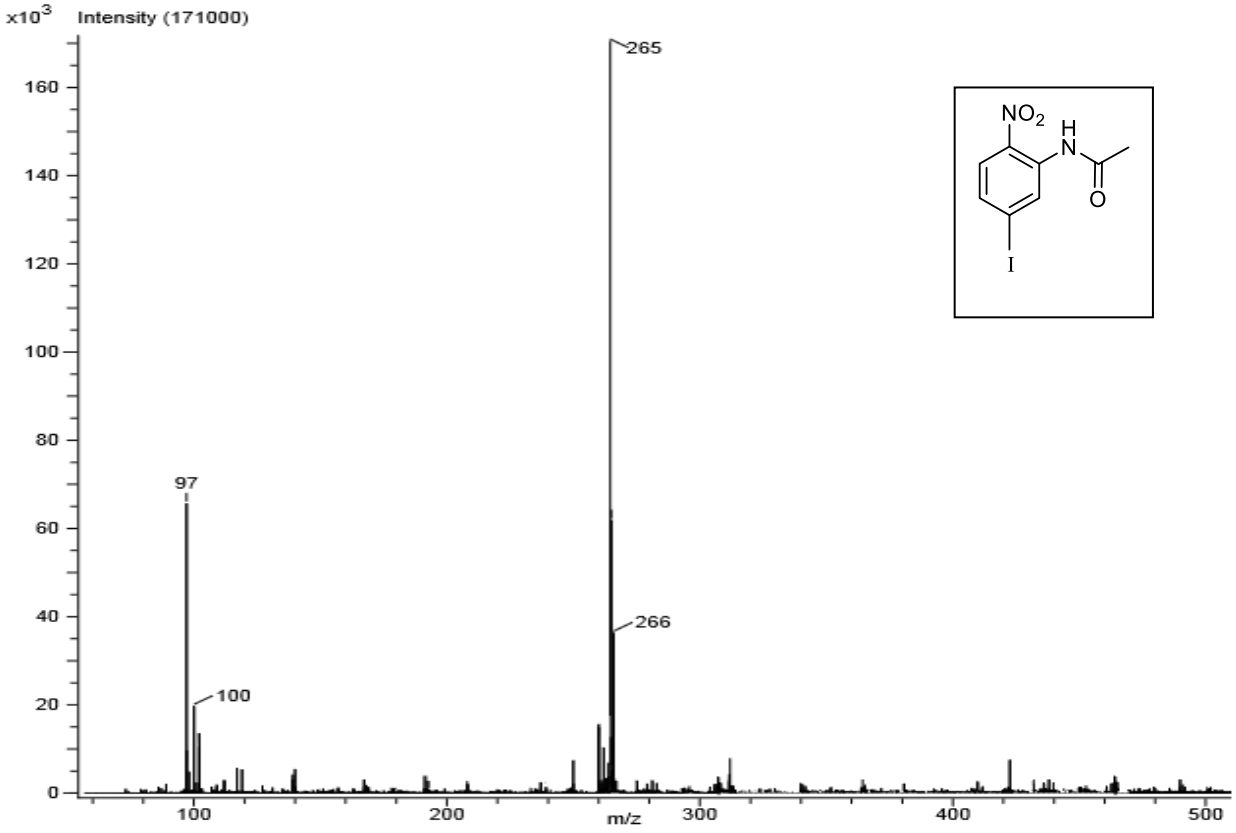
N-(5-Iodo-2-nitrophenyl)acetamide **1d**



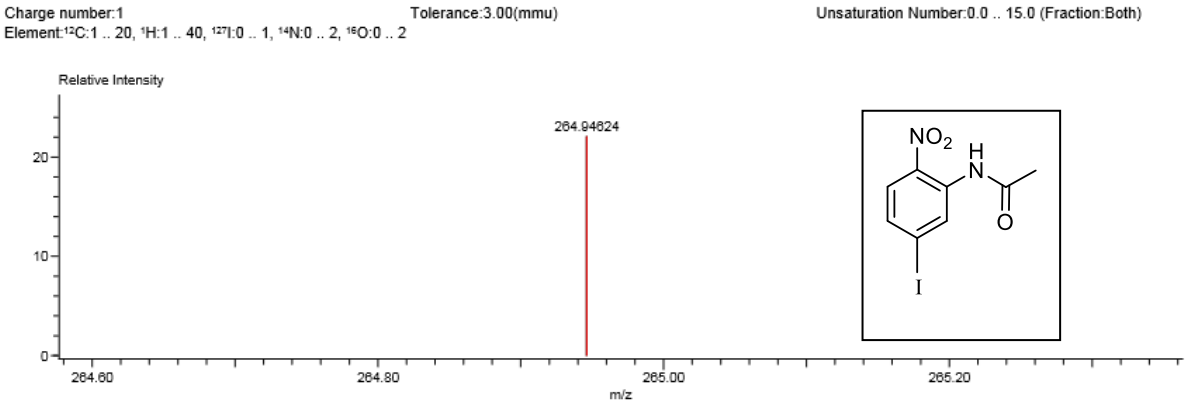
N-(5-Iodo-2-nitrophenyl)acetamide **1d**



5-Iodo-2-nitroaniline **4d**

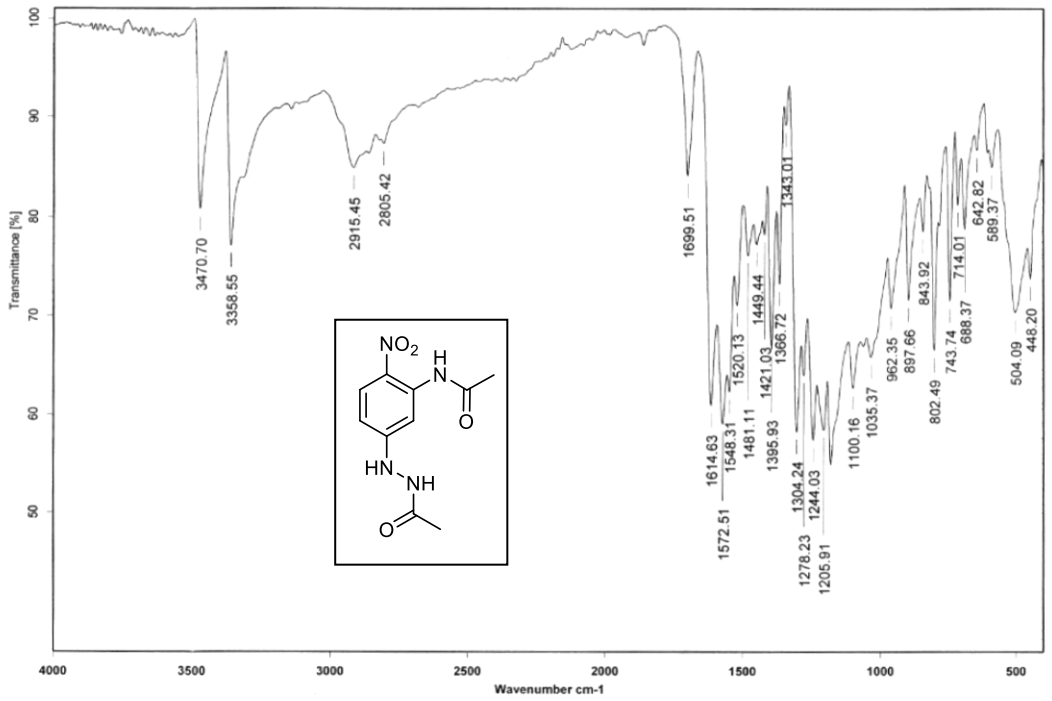


5-Iodo-2-nitroaniline **4d**

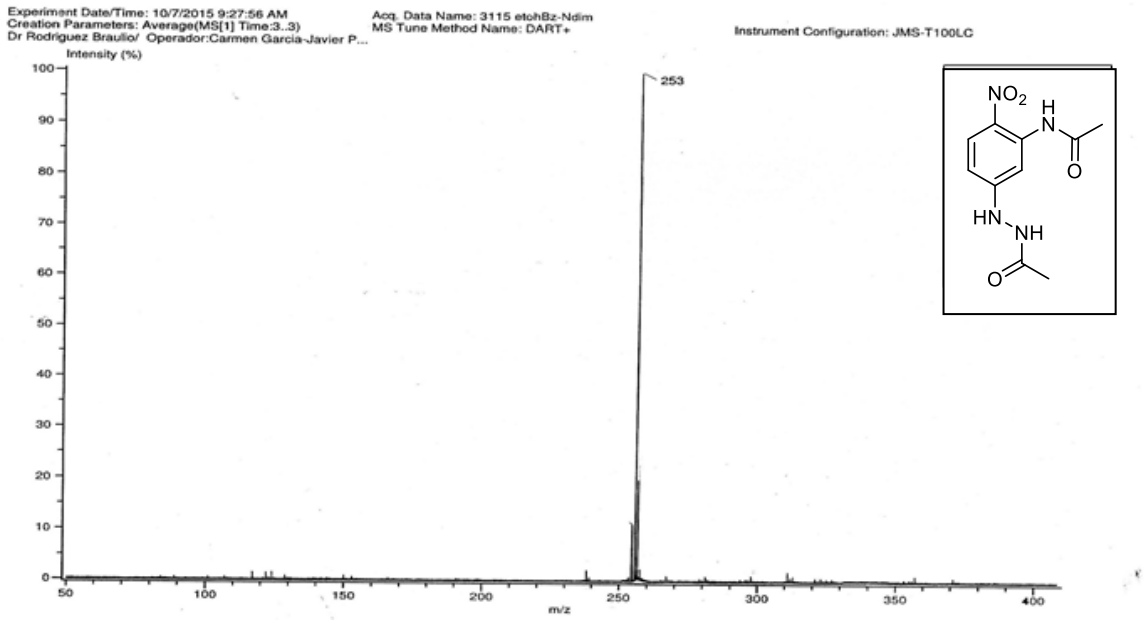


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
264.94624	264648.50	264.94739	-1.15	-4.35	$^{12}C_6{}^{1}H_6{}^{127}I_1{}^{14}N_2{}^{16}O_2$	4.5

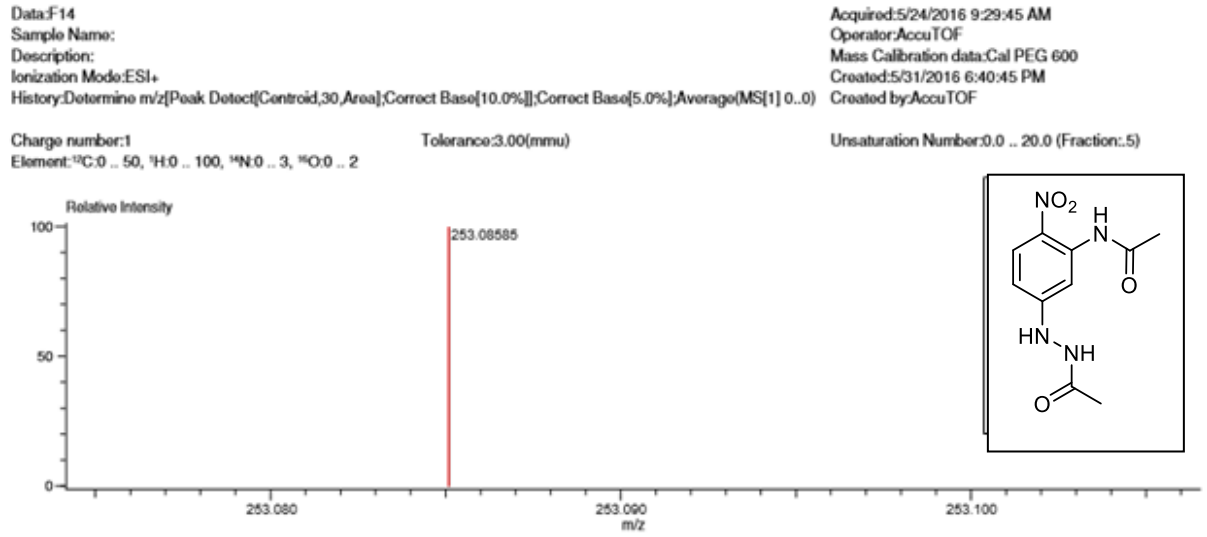
5-Iodo-2-nitroaniline **4d**



N-(5-(2-Acetylhydrazino)-2-nitrophenyl)acetamide **3a**

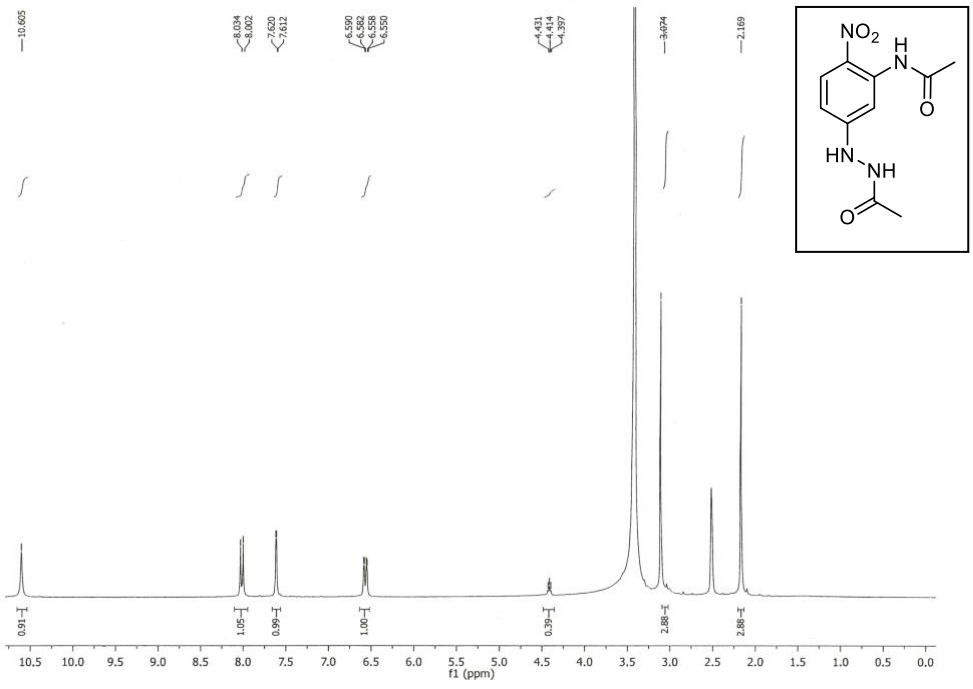


N-(5-(2-Acetylhydrazino)-2-nitrophenyl)acetamide **3a**

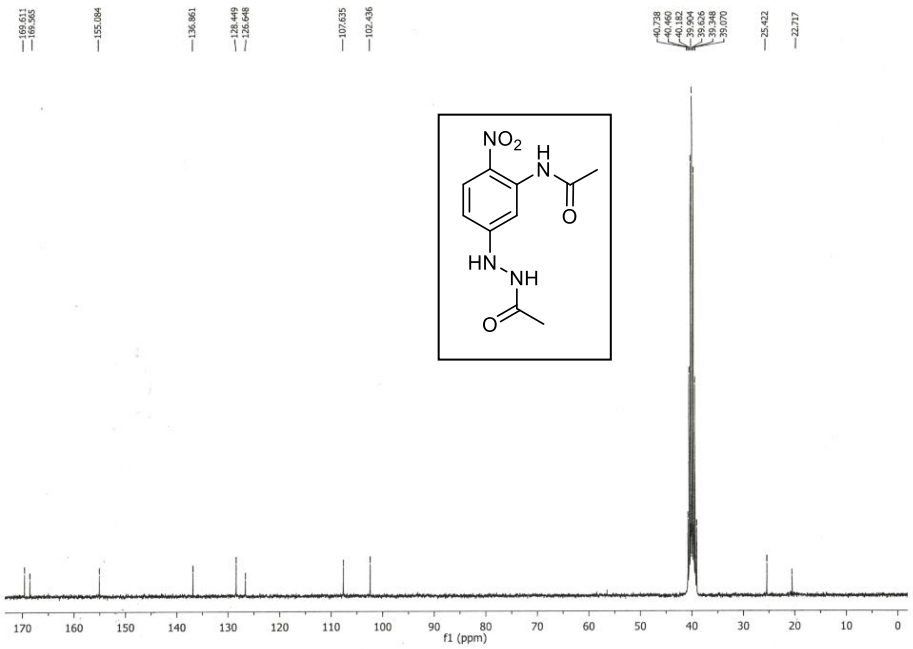


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
253.08550	2369.51	253.08585	0.30	1.34	$^{12}C_{10}{}^{1}H_{12}{}^{14}N_4{}^{16}O_4$	5.5

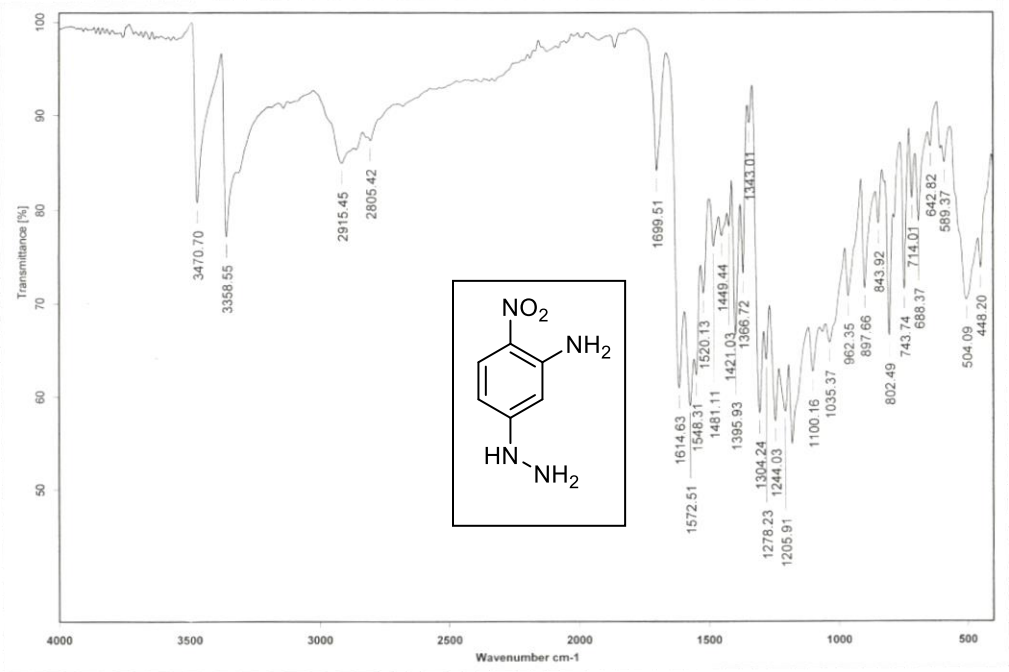
N-(5-(2-Acetylhydrazino)-2-nitrophenyl)acetamide **3a**



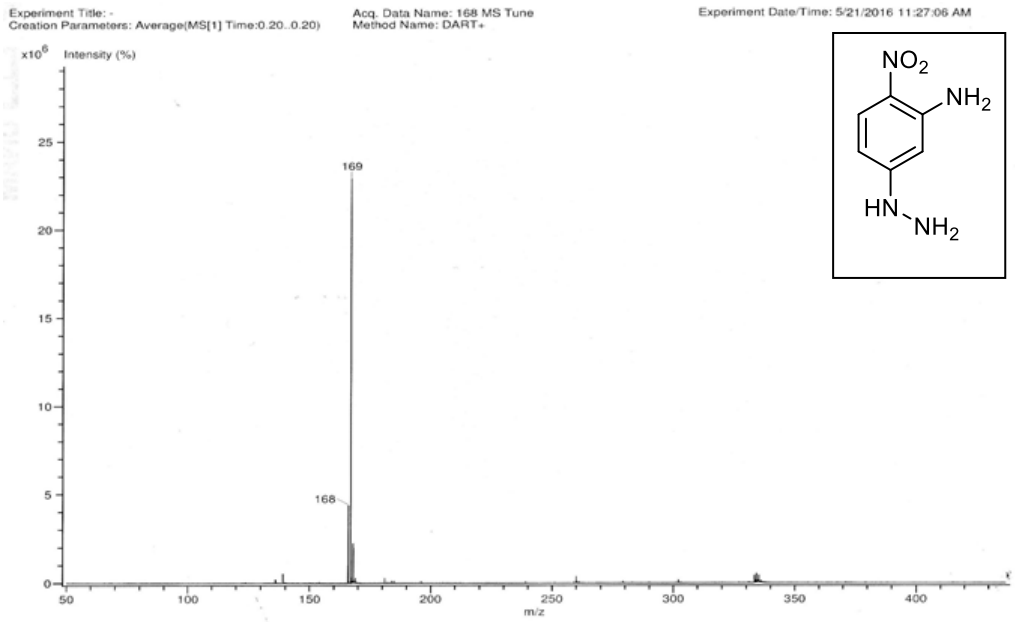
N-(5-(2-Acetylhydrazino)-2-nitrophenyl)acetamide **3a**



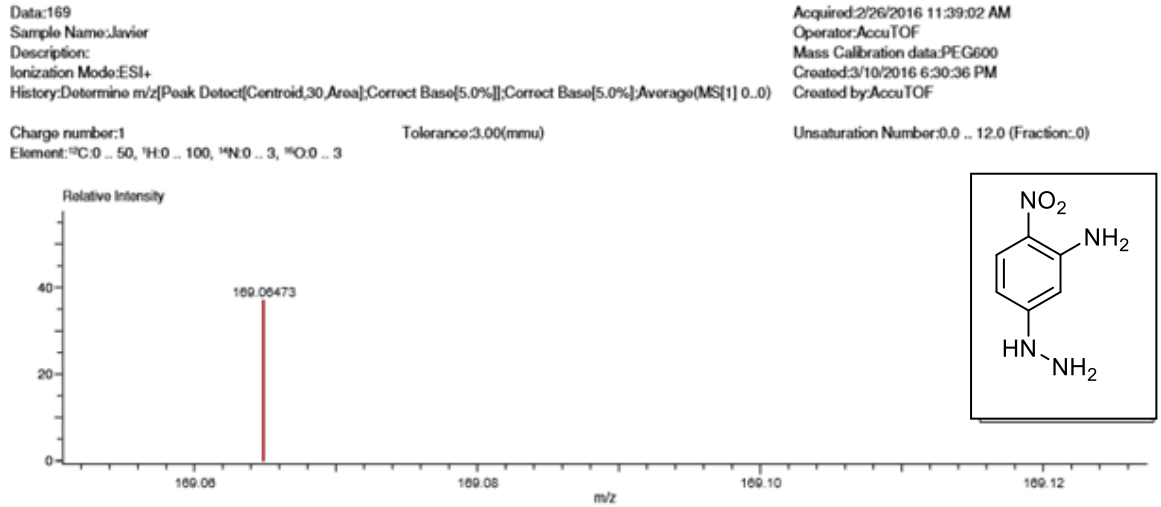
N-(5-(2-Acetylhydrazino)-2-nitrophenyl)acetamide **3a**



3-Amino-4-nitrophenylhydrazine **5a**

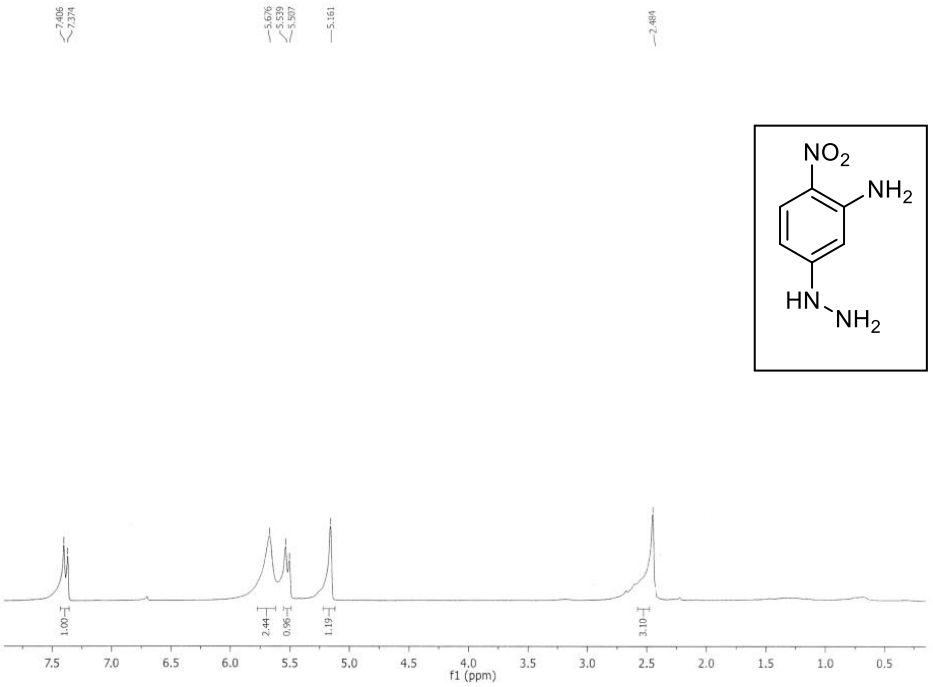


3-Amino-4-nitrophenylhydrazine **5a**

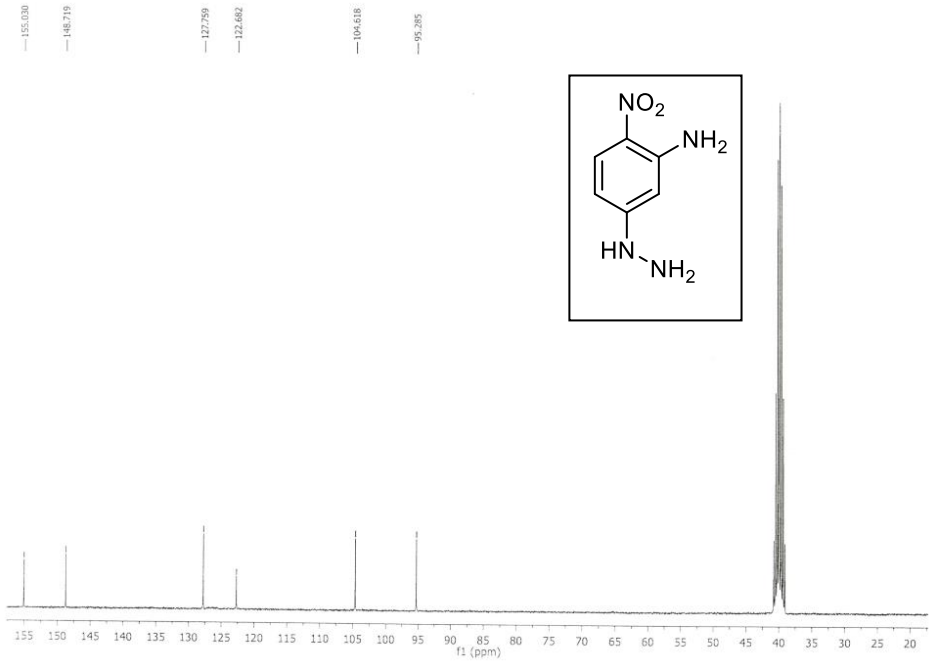


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
169.06473	751800.75	169.06451	0.22	1.31	$^{13}C_6{}^{1}H_8{}^{14}N_4{}^{16}O_2$	5.0

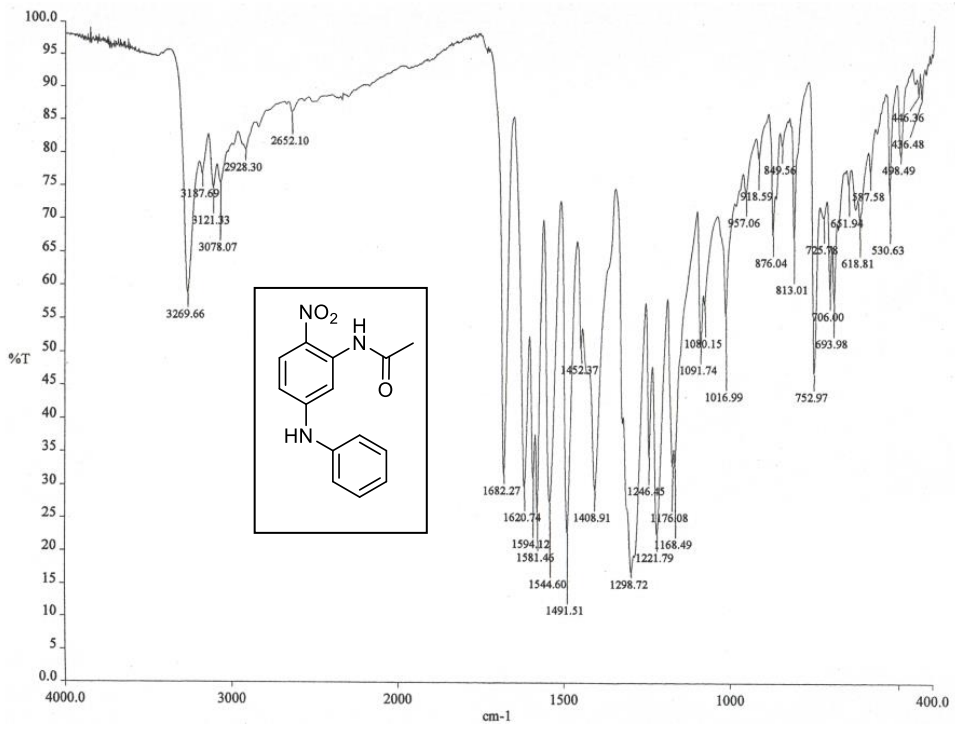
3-Amino-4-nitrophenylhydrazine **5a**



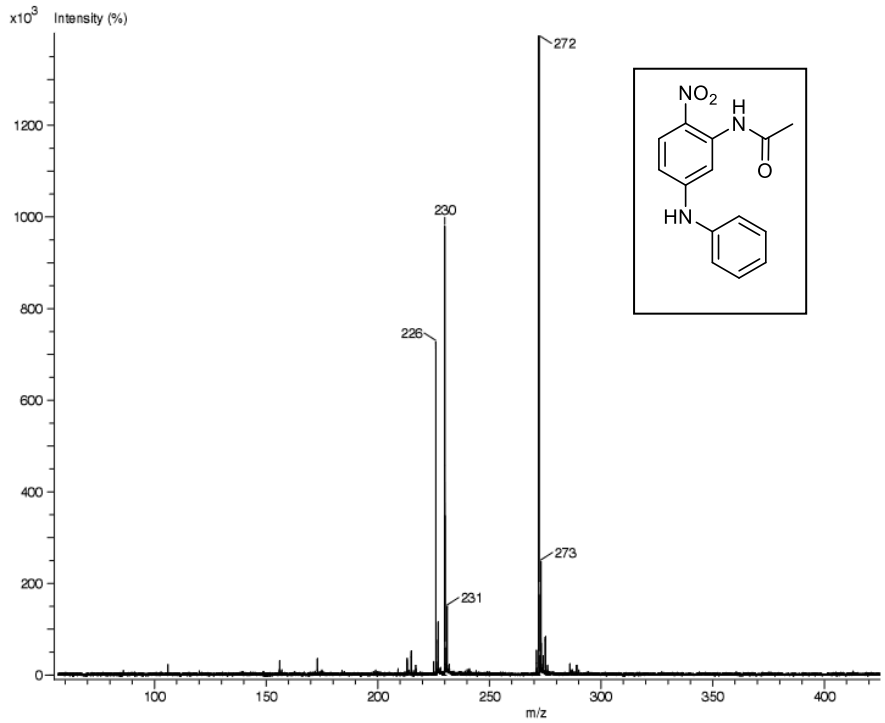
3-Amino-4-nitrophenylhydrazine **5a**



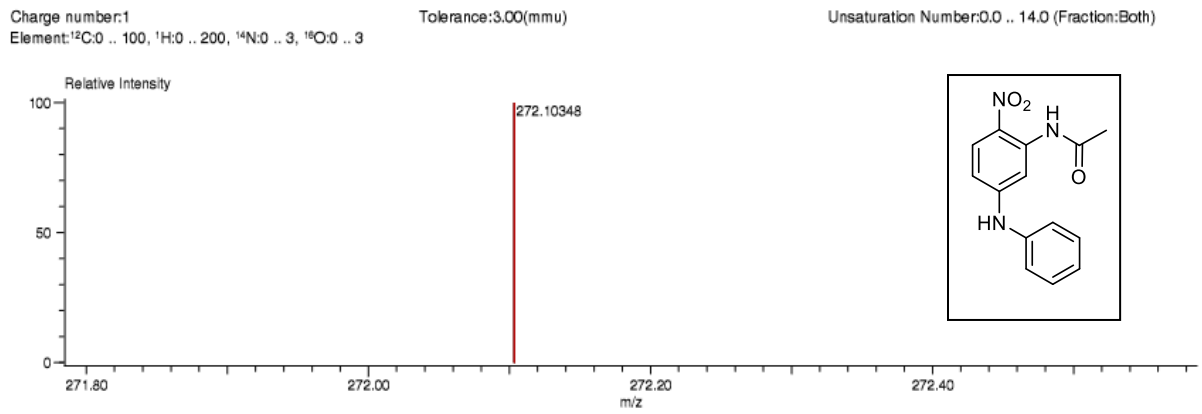
3-Amino-4-nitrophenylhydrazine **5a**



N-(2-Nitro-5-(phenylamino)phenyl)acetamide **3b**

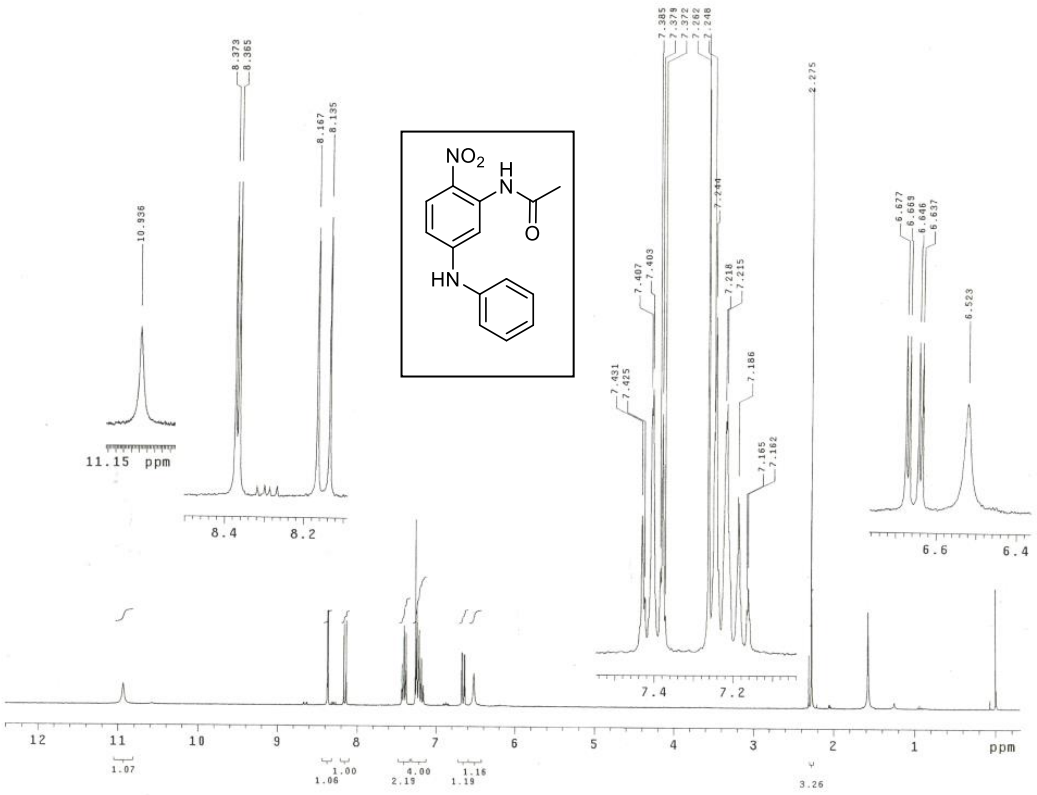


N-(2-Nitro-5-(phenylamino)phenyl)acetamide **3b**

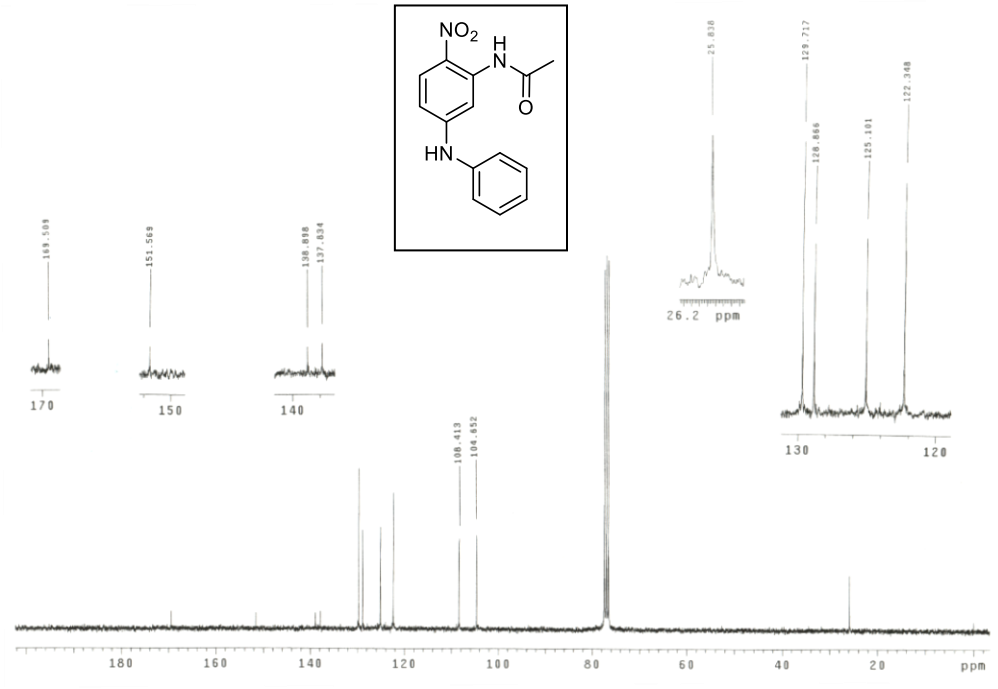


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
272.10348	54445.25	272.10352	-0.04	-0.13	$^{12}C_{14}{}^{1}H_{14}{}^{14}N_3{}^{16}O_3$	9.5

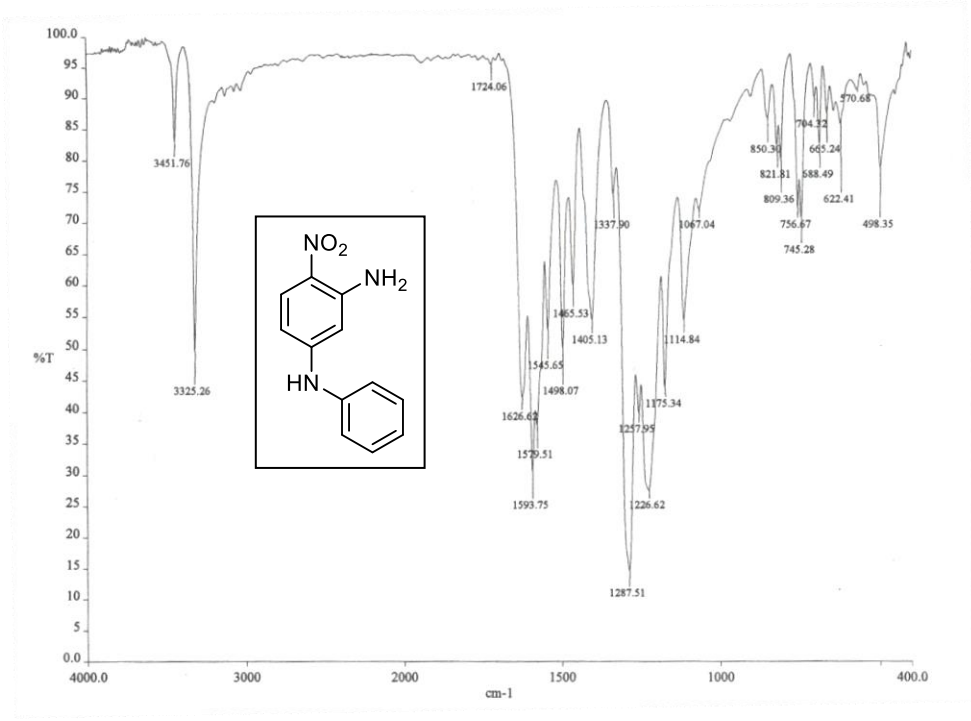
N-(2-Nitro-5-(phenylamino)phenyl)acetamide **3b**



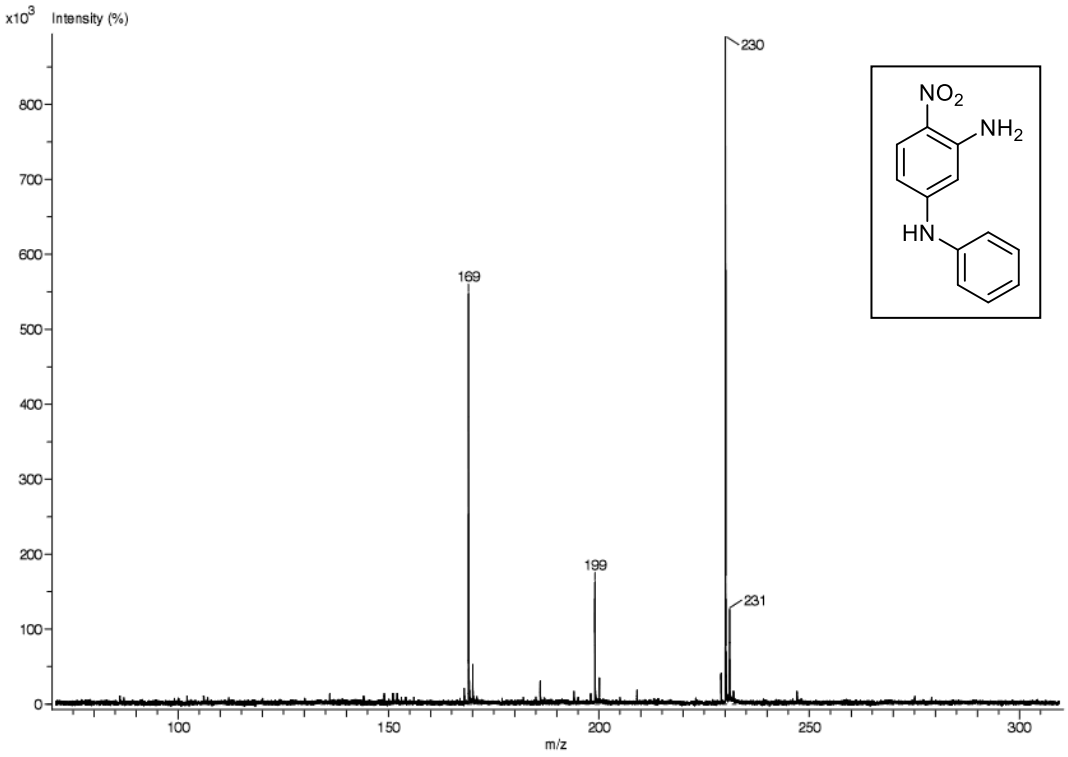
N-(2-Nitro-5-(phenylamino)phenyl)acetamide **3b**



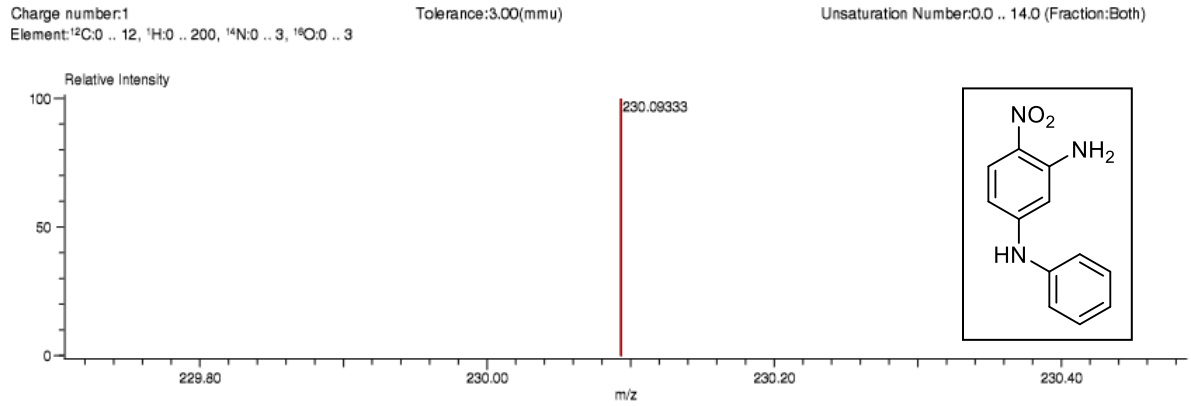
N-(2-Nitro-5-(phenylamino)phenyl)acetamide **3b**



2-Nitro-5-anilinoaniline **5b**

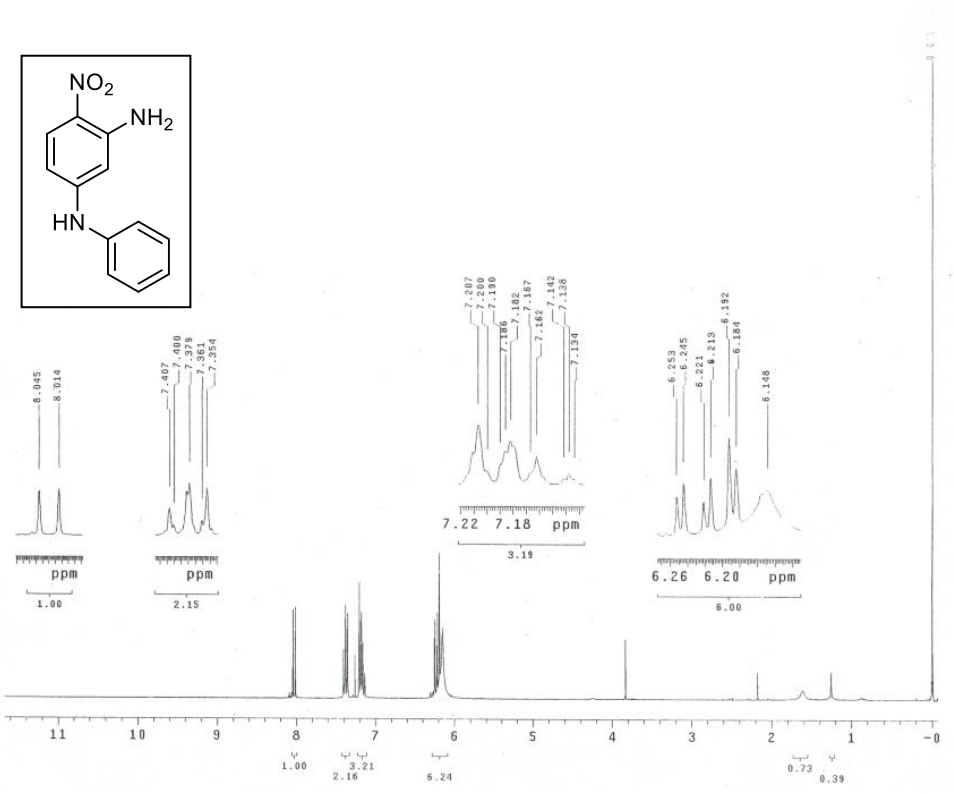


2-Nitro-5-anilinoaniline **5b**

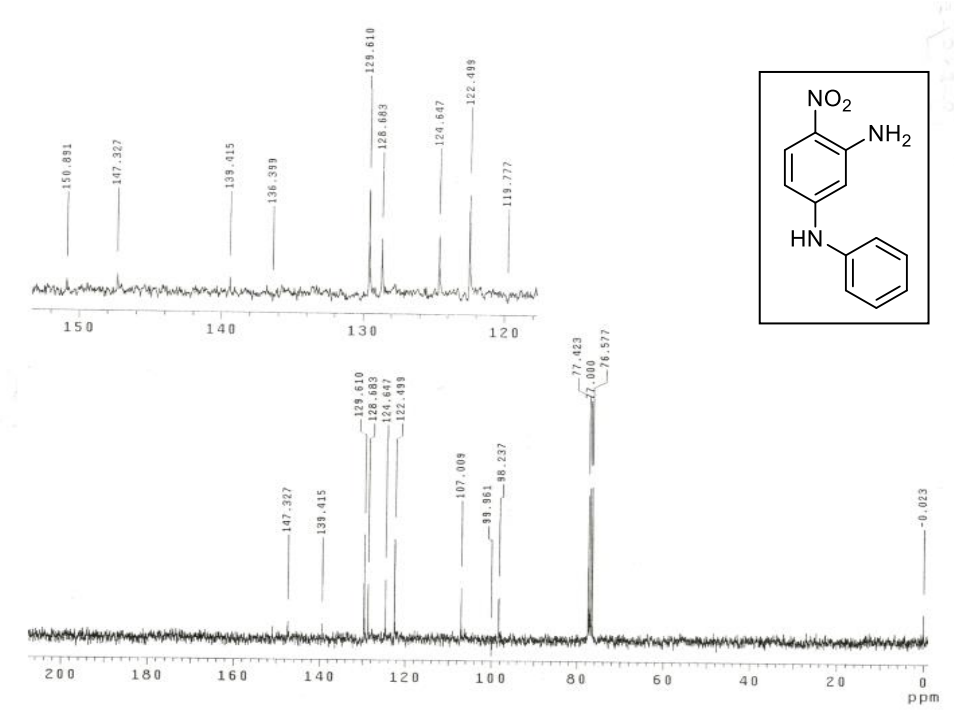


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
230.09333	48614.38	230.09295	0.38	1.67	$^{12}C_{12}{}^{1}H_{12}{}^{14}N_{3}{}^{16}O_{2}$	8.5

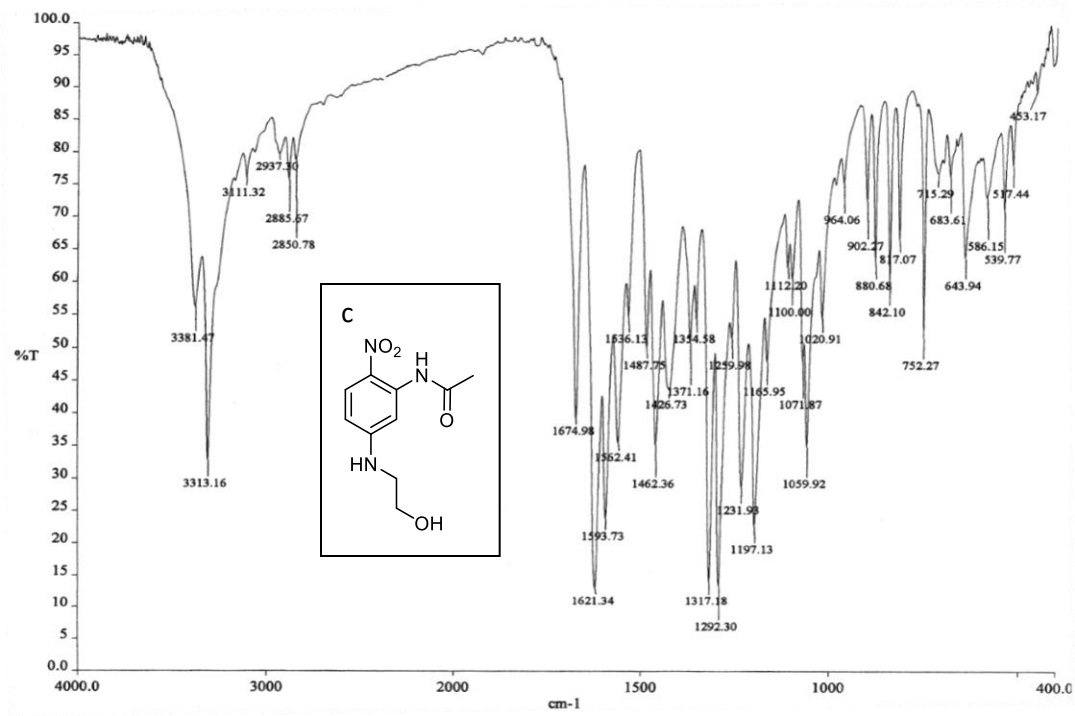
2-Nitro-5-anilinoaniline **5b**



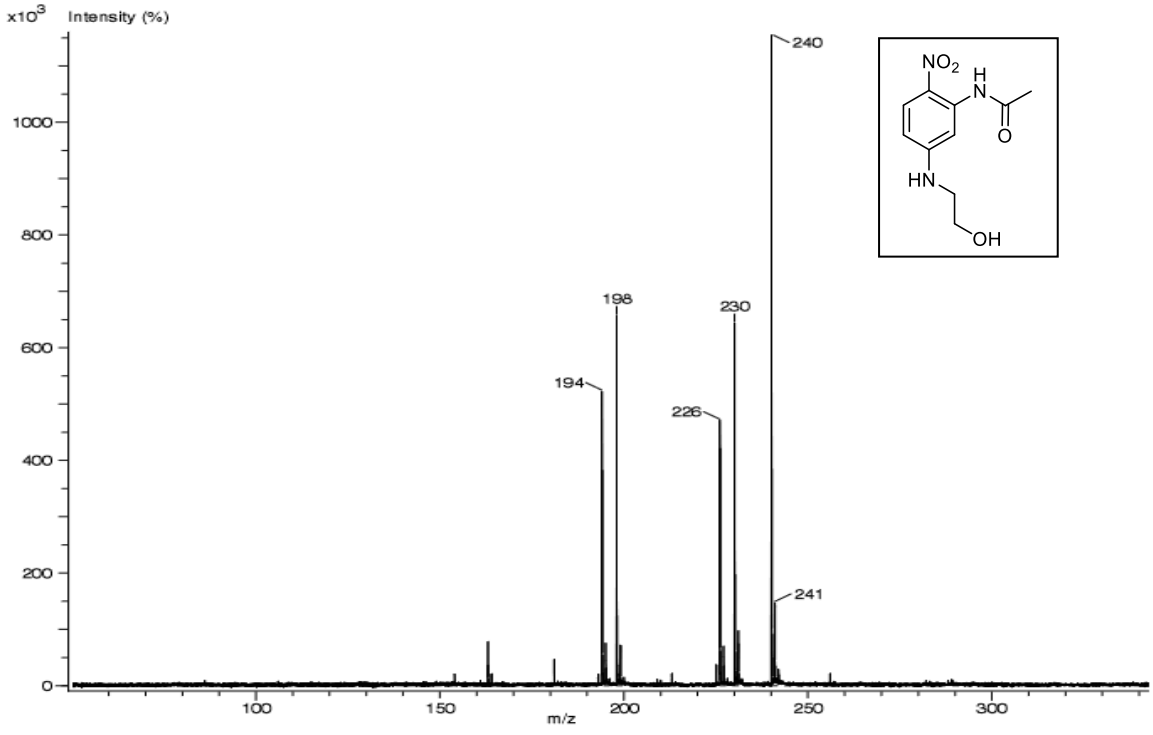
2-Nitro-5-anilinoaniline **5b**



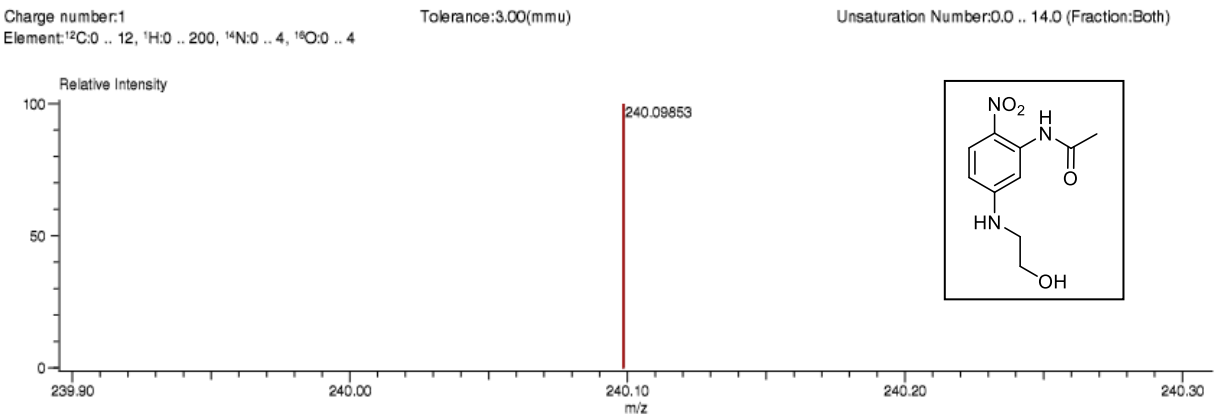
2-Nitro-5-anilinoaniline **5b**



N-(5-(2-Hydroxyethylamino)-2-nitrophenyl)acetamide **3c**

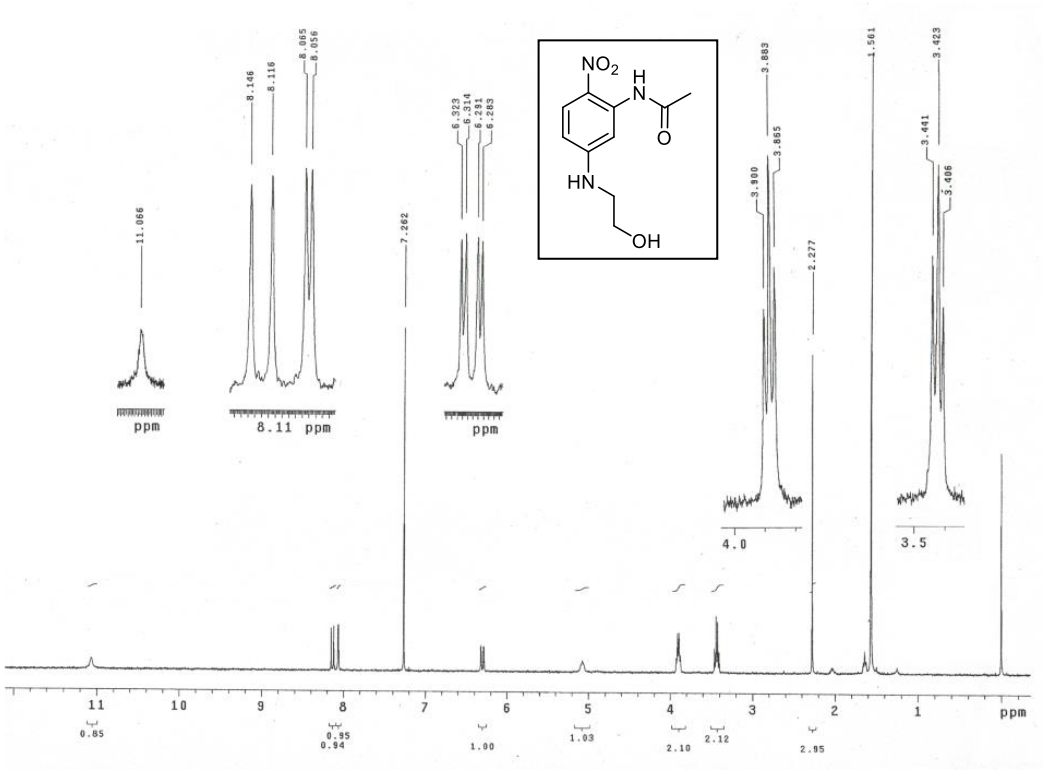


N-(5-(2-Hydroxyethylamino)-2-nitrophenyl)acetamide **3c**

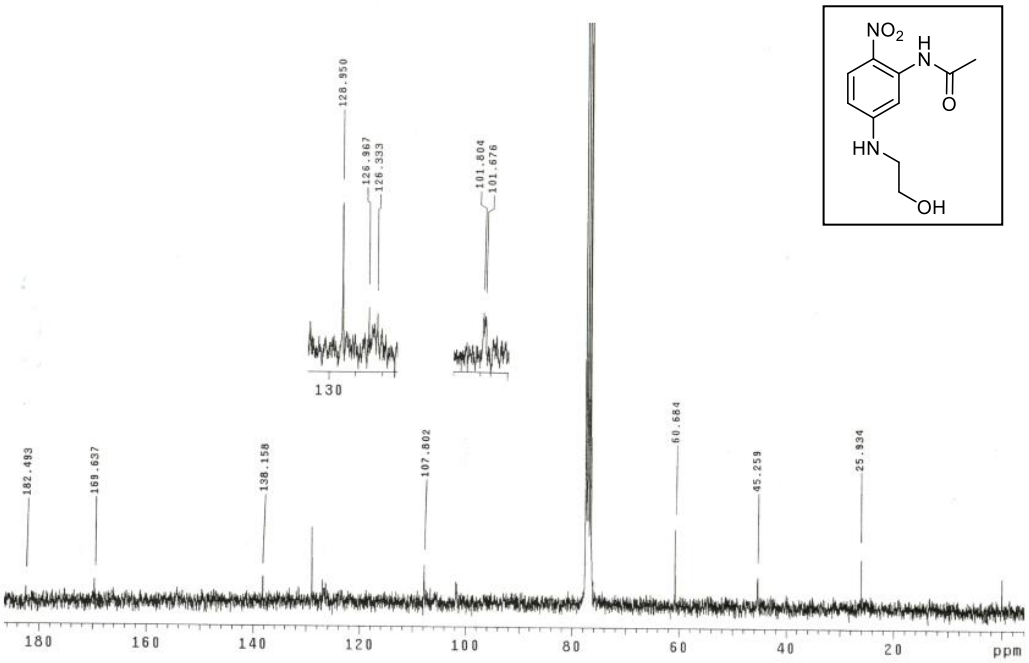


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
240.09853	23085.75	240.09843	0.10	0.42	$^{12}C_{10}{}^{1}H_{14}{}^{14}N_{3}{}^{16}O_{4}$	5.5

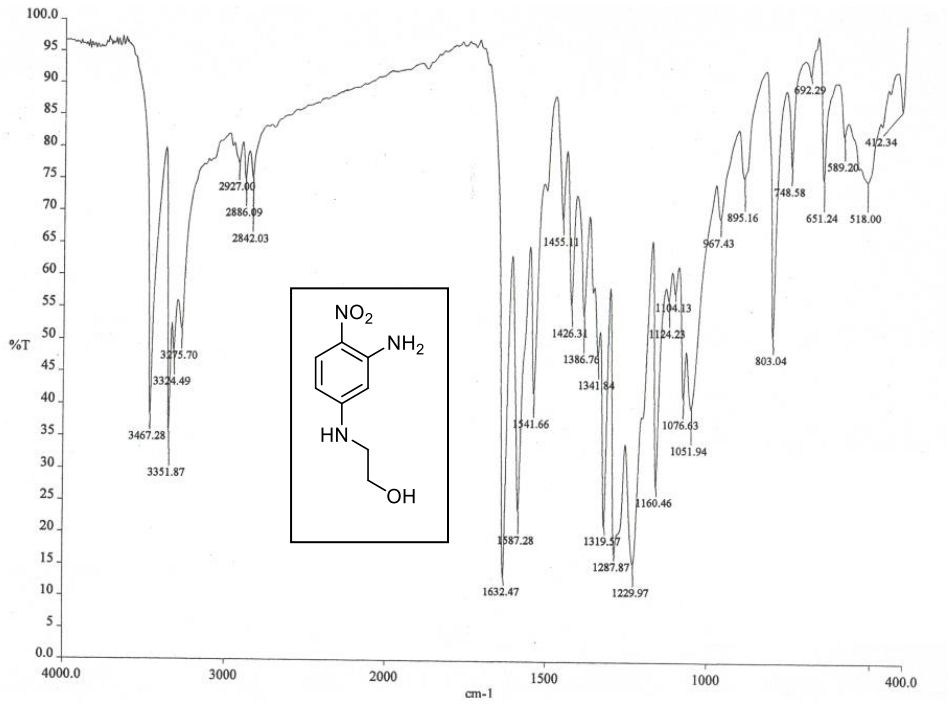
N-(5-(2-Hydroxyethylamino)-2-nitrophenyl)acetamide **3c**



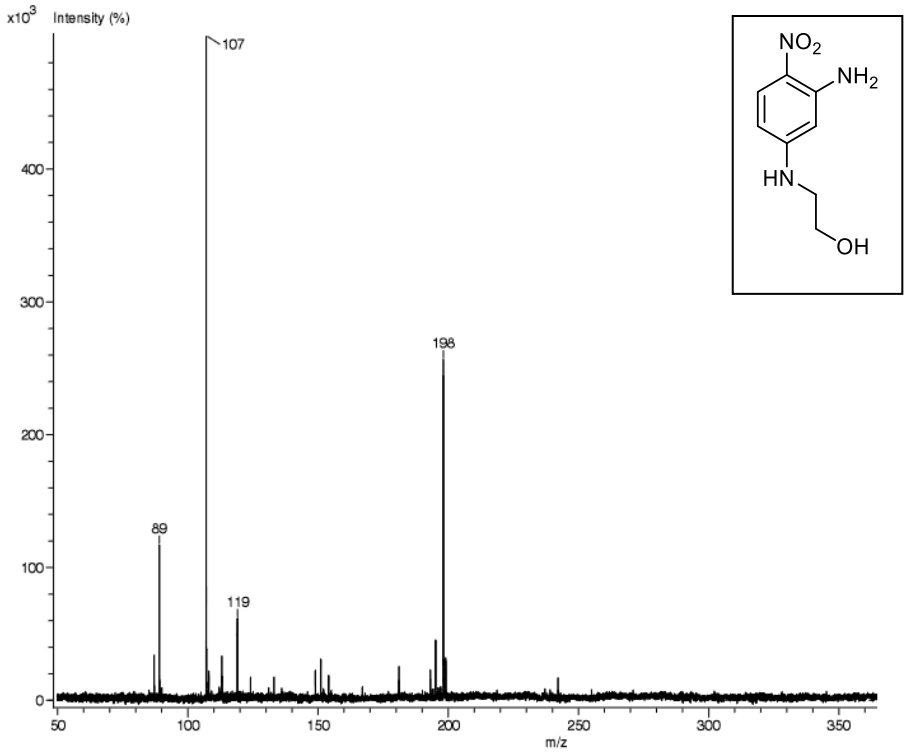
N-(5-(2-Hydroxyethylamino)-2-nitrophenyl)acetamide **3c**



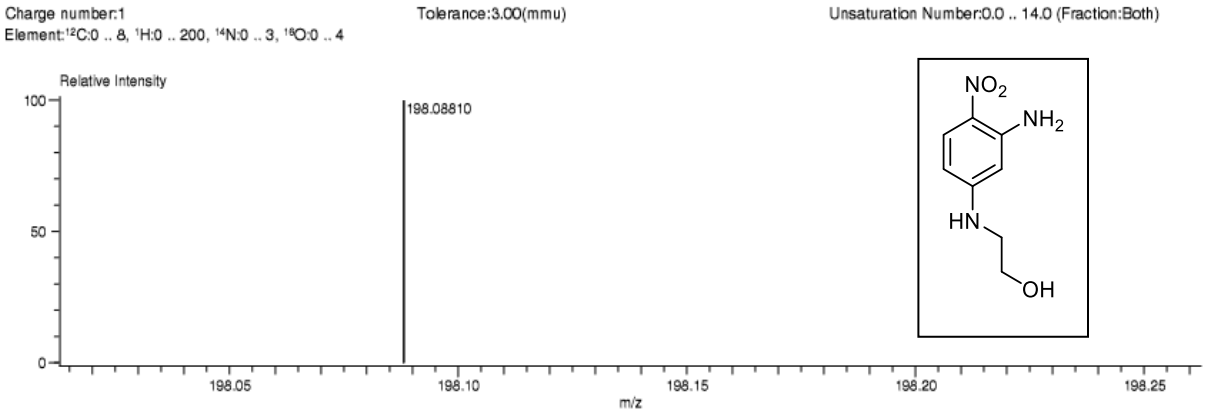
N-(5-(2-Hydroxyethylamino)-2-nitrophenyl)acetamide **3c**



5-(2-Hydroxyethylamino)-2-nitroaniline **5c**

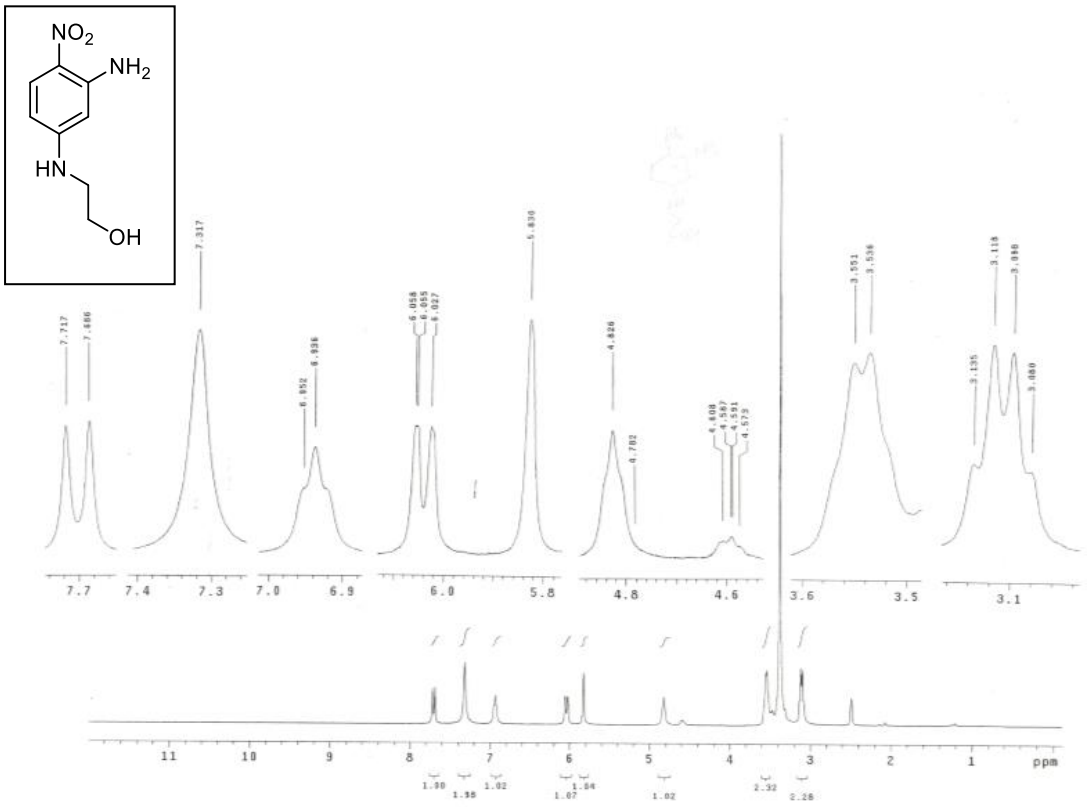


5-(2-Hydroxyethylamino)-2-nitroaniline **5c**

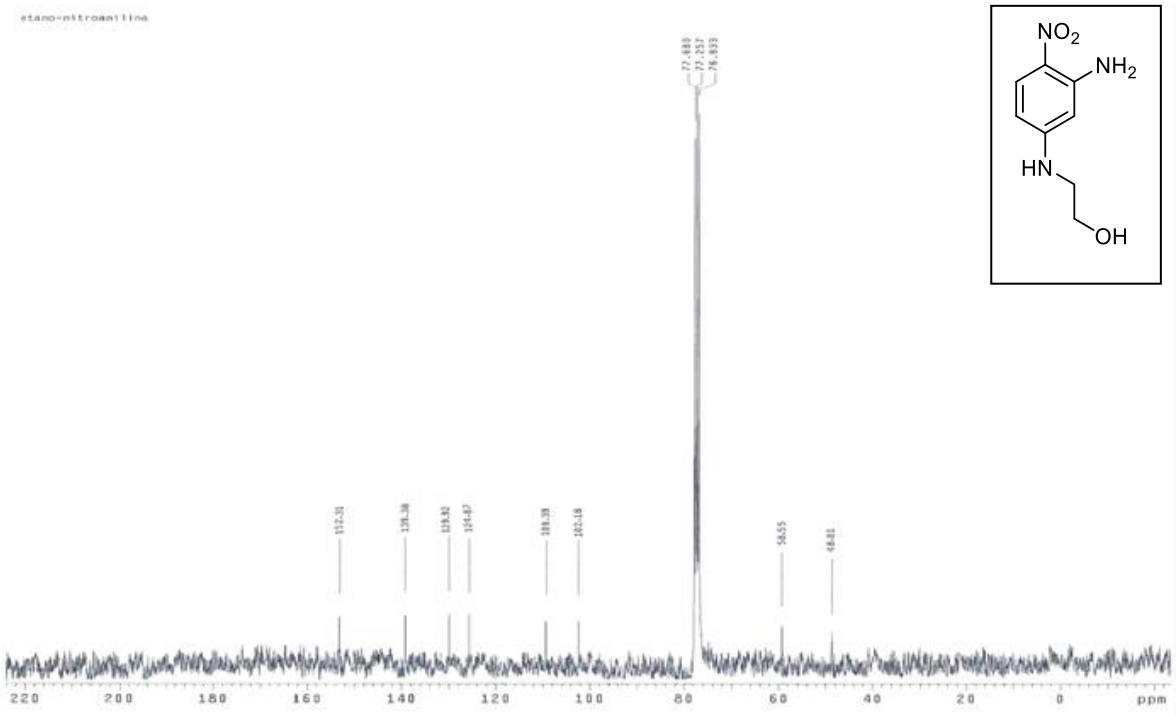


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
198.08810	16035.25	198.08787	0.24	1.20	$^{12}C_6{}^{1}H_{12}{}^{14}N_3{}^{16}O_3$	4.5

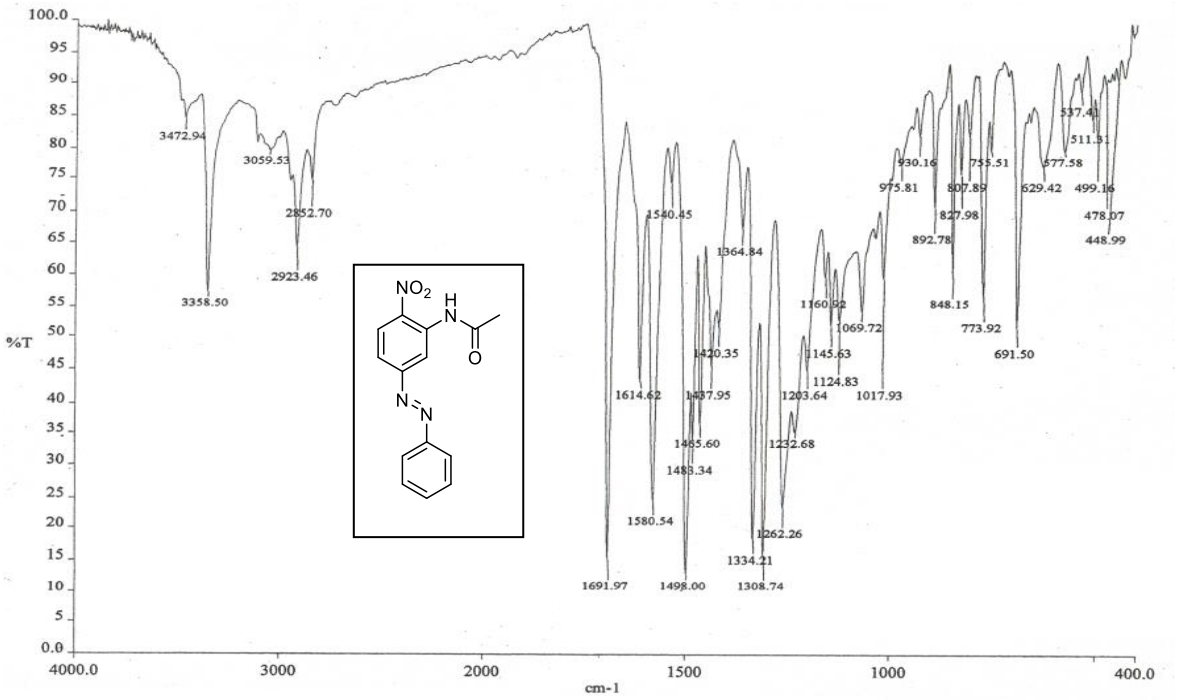
5-(2-Hydroxyethylamino)-2-nitroaniline **5c**



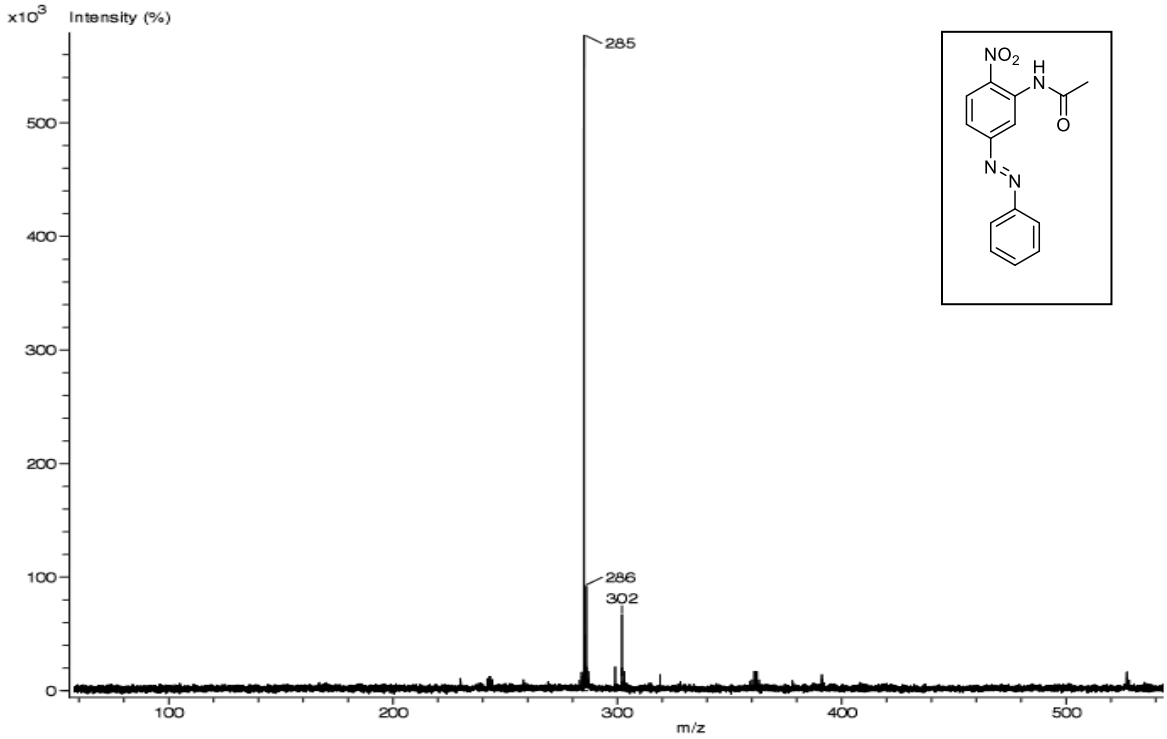
5-(2-Hydroxyethylamino)-2-nitroaniline **5c**



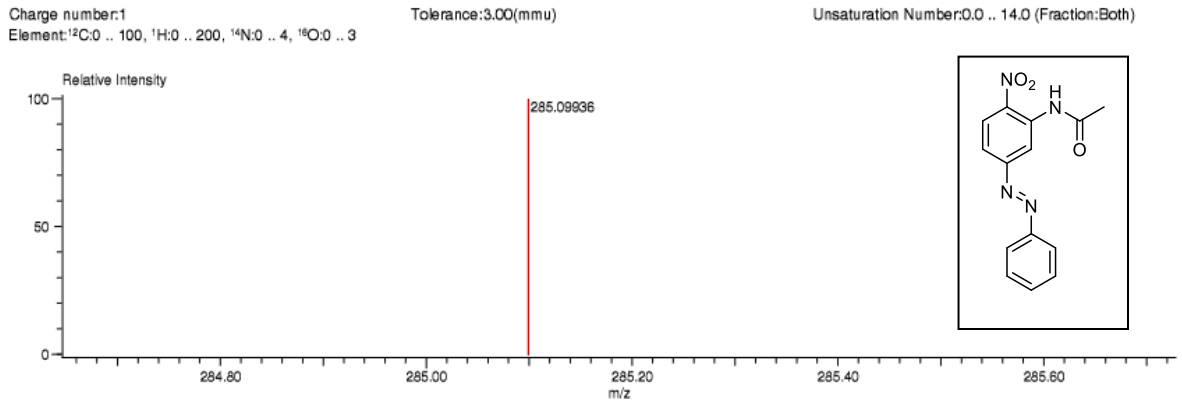
5-(2-Hydroxyethylamino)-2-nitroaniline **5c**



N-(2-Nitro-5-(phenyldiazenyl)phenyl)acetamide **3d**

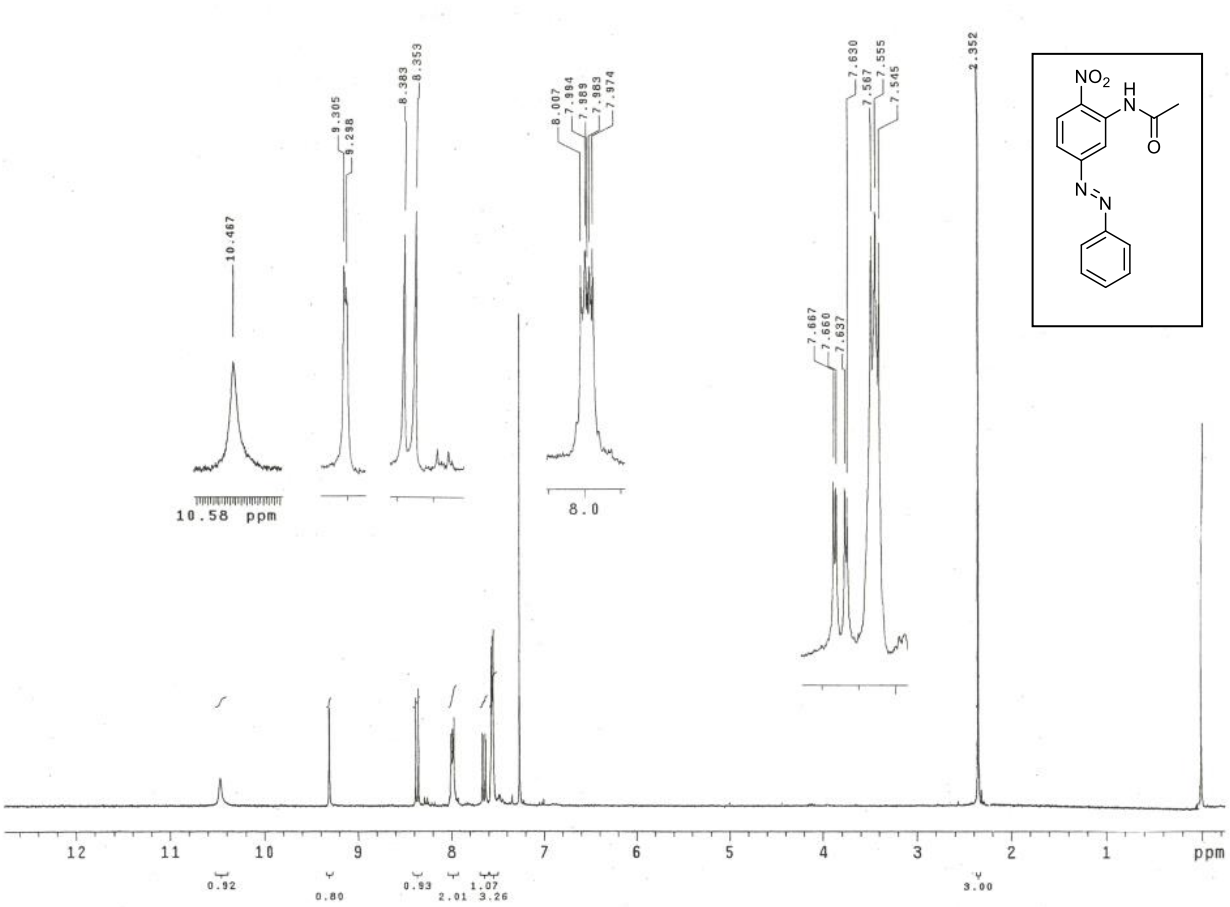


N-(2-Nitro-5-(phenyldiazenyl)phenyl)acetamide **3d**

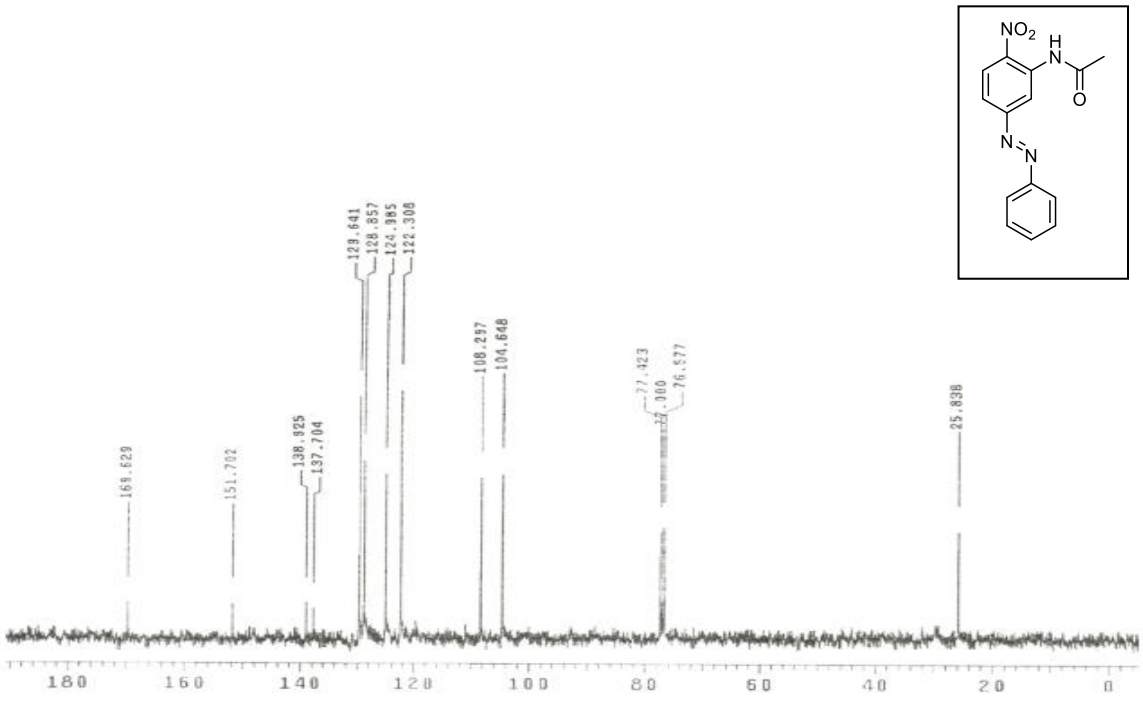


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
285.09936	33896.50	285.09876	0.59	2.07	$^{12}C_{14}{}^{1}H_{13}{}^{14}N_{4}{}^{16}O_{3}$	10.5

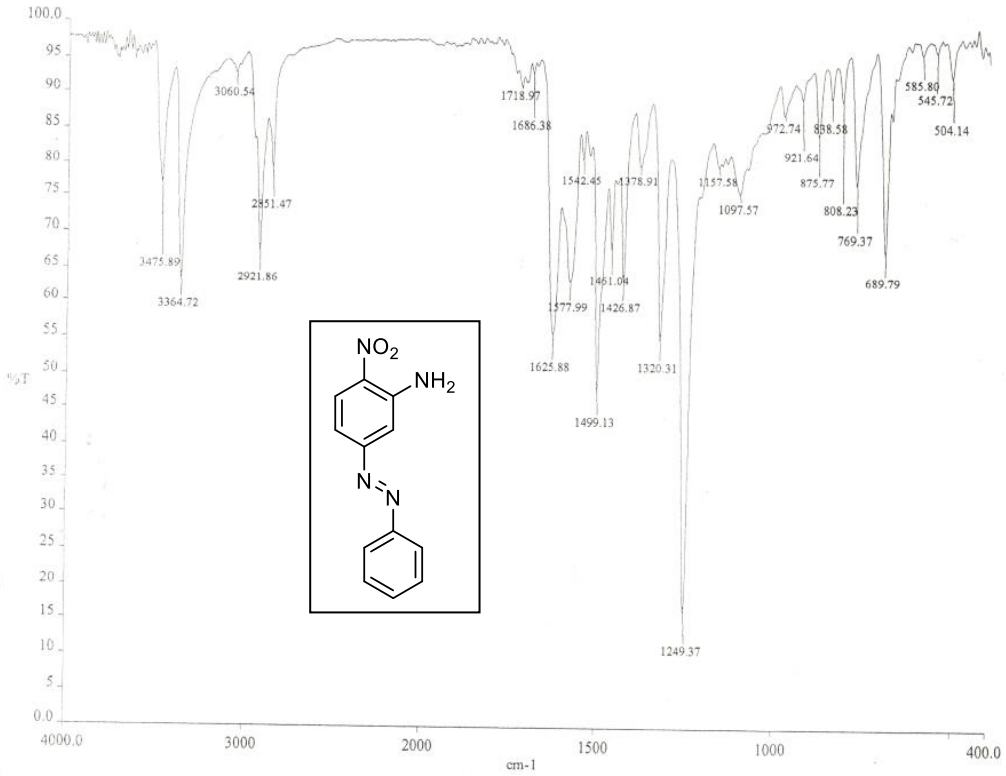
N-(2-Nitro-5-(phenyldiazenyl)phenyl)acetamide **3d**



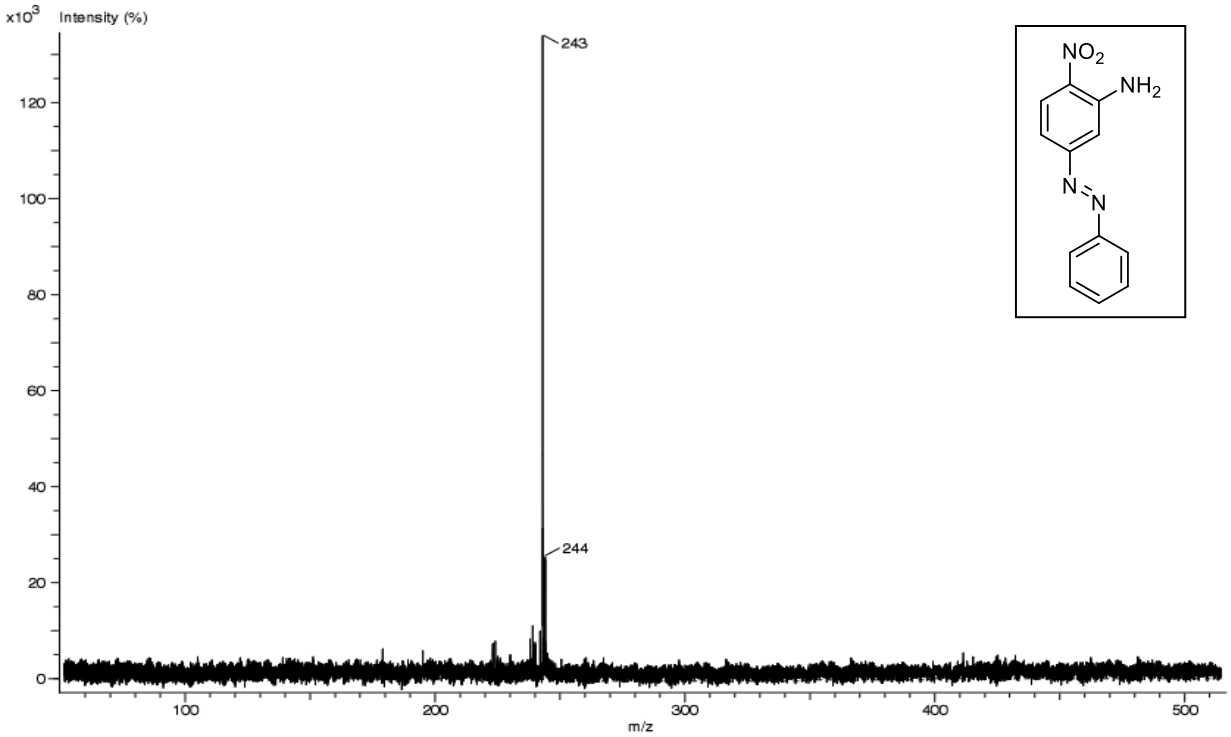
N-(2-Nitro-5-(phenyldiazenyl)phenyl)acetamide **3d**



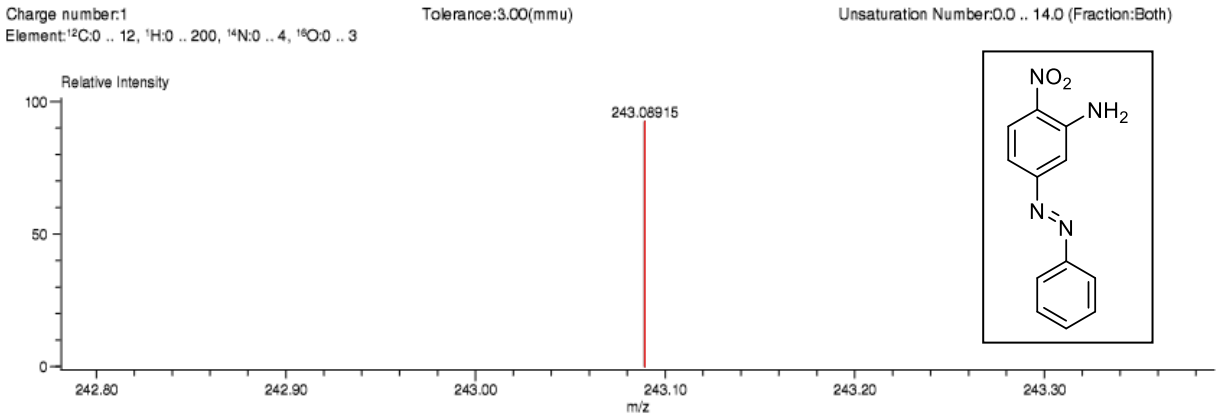
N-(2-Nitro-5-(phenyldiazenyl)phenyl)acetamide **3d**



2-Nitro-5-(phenyldiazenyl)aniline **5d**

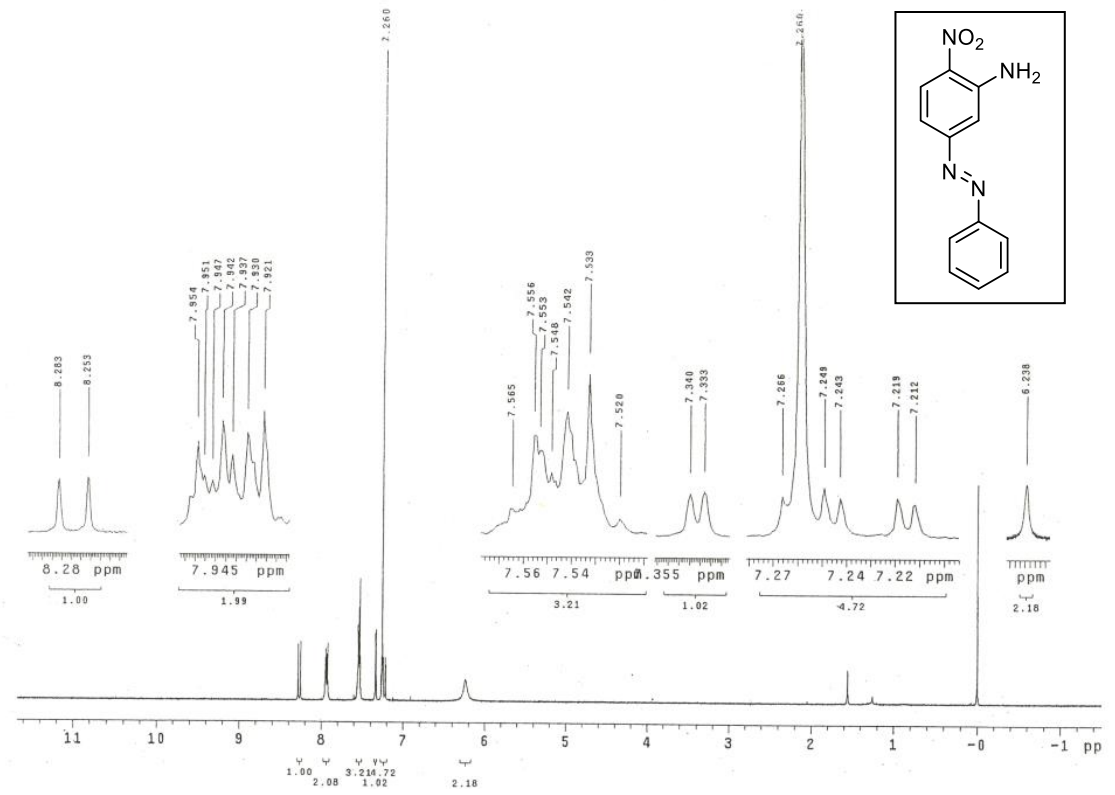


2-Nitro-5-(phenyldiazenyl)aniline **5d**

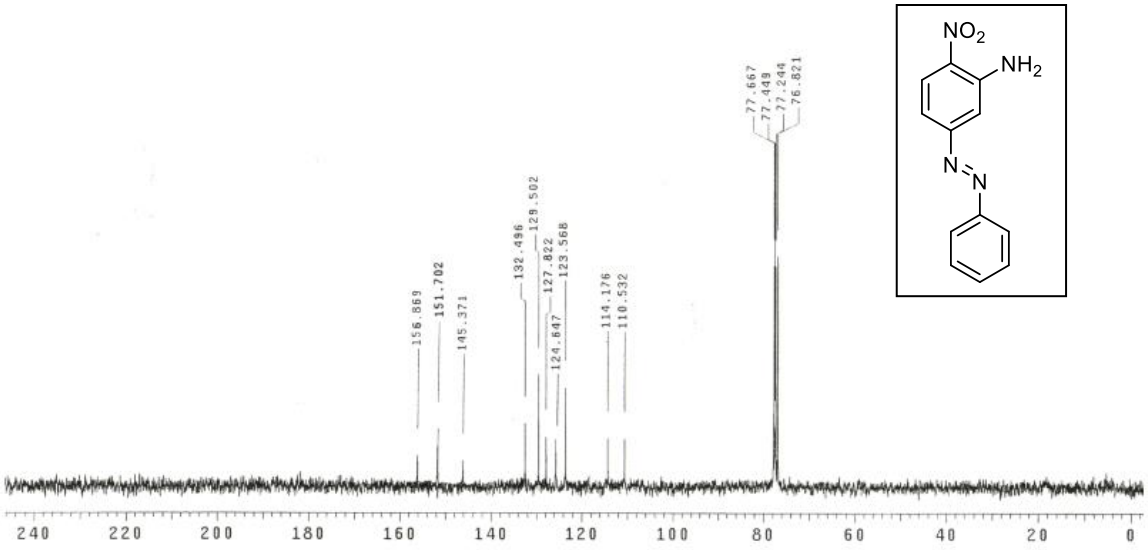


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
243.08915	1080.13	243.08820	0.95	3.90	$^{12}C_{12}{}^{1}H_{11}{}^{14}N_{4}{}^{16}O_{2}$	9.5

2-Nitro-5-(phenyldiazenyl)aniline **5d**



2-Nitro-5-(phenyldiazenyl)aniline **5d**



2- Nitro-5-(phenyldiazenyl)aniline **5d**