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Supporting Information

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Supporting Information:

Selective Chemical Rescue of a Thyroid Hormone Receptor Mutant, TRβ(H435Y), Identified in Pituitary Carcinoma and Resistance to Thyroid Hormone.

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EXPERIMENTAL:

All compounds were purchased from Acros Organics (Morris Plains, NJ) and Aldrich Chemical Co. (Milwaukee, WI) unless otherwise mentioned. NMR spectra were recorded on Bruker DRX-400 MHz spectrometer at the University of Delaware NMR facility. Mass spectrometry was carried out at University of Delaware mass spectrometry laboratory. All the designed oligonucleotides for mutagenesis were purchased from Ranson Hill Biosciences Inc. Human Embryonic Kidney cells (HEK293) were obtained from ATCC (American Type Culture Collection). Transactivation response assays were performed using the Dual-Luciferase Assay System (Promega # E1960) following the manufacturer's protocol. Solvents THF, ether and methylene chloride were distilled from Na or K. Silica gel (60 Å) and TLC plates (60 Å, 250 μm) were purchased from Sillicycle (Quebec, Canada) and Bodman Industries (Aston, Pa) respectively.

Construction of mutants

pSG5hTRβ (wt) encodes for the "wild-type" receptor isoforms which are constuitively expressed when transfected into mammalian cells. pSG5hTRβ (H435A), pSG5hTRβ (H435L), pSG5hTRβ (H435Y), pSG5hTRβ (H435Q) were created from pSG5hTRβ (wt) using Quickchange mutagenesis kit (Stratagene) following manufacturers protocol. The mutagenic oligonucleotides primers were:

TRwt GG ATG ATA GGA GCC TGC **CAT** GCC AGC CGC TTC C

H435Y f GG ATG ATA GGA GCC TGC **TAT** GCC AGC CGC TTC C

H435Y r G GAA GCG GCT GGC **ATA** GCA GGC TCC TAT CAT CC.

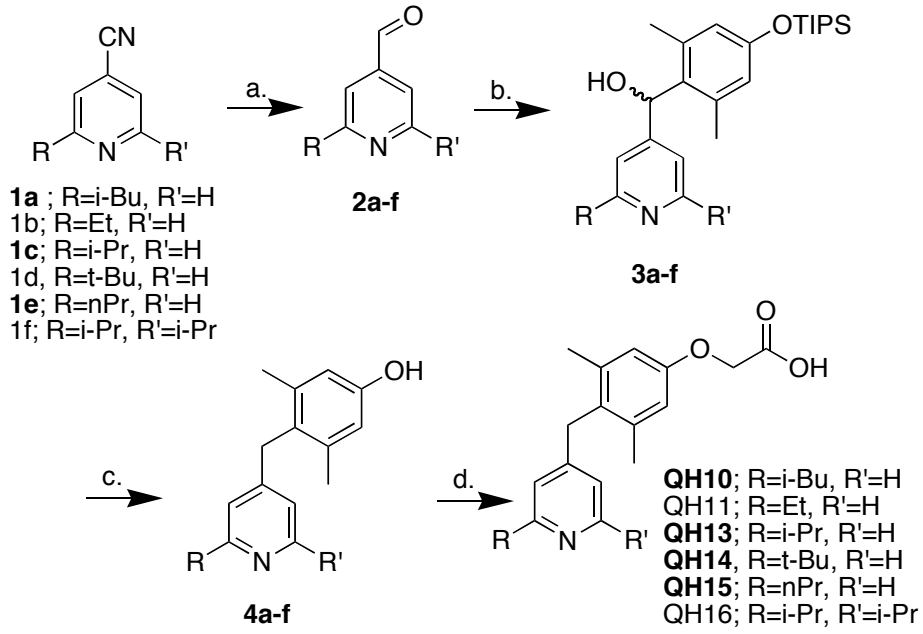
The constructs were sequenced over the entire coding region of the TR to confirm the presence of only the desired mutation.

Evaluation of biological activities

Twenty-four hours prior to transfection, HEK 293 cells were seeded at a density of 45,000 cells per well in 24-well culture plates and grown in Dulbecco's Modified Eagle Medium (DMEM) supplemented with 10% fetal bovine serum (FBS) and gentamycin. Four hours prior to transfection, the medium was changed to DMEM containing 10% charcoal-resin stripped FBS. Transfections were performed using $CaPO_4$ method with 0.08 μg of TR, 0.17 μg of TRE-Luc, 0.03 μg of Renilla-Luc as internal standard per well. Six hours after transfection, the medium was removed and replaced with DMEM with 10% charcoal-resin stripped FBS containing appropriate concentrations of ligand. The cells were allowed to incubate for 36h before harvesting by passive lysis buffer. Cell extracts were immediately assayed by the Dual Luciferase Assay (Promega) with a Wallac Microbeta luminometer. All experiments were run in triplicate and normalized to the highest activation of wild type TRβ at 50nM T_3. Activity is reported in relative light unit (RLU), determined as the ratio of the inducible firefly luciferase luminescence divided by the luminescence of the renilla luciferase control and normalized by RLU of wild type TRβ at 50 nM T_3. Dose-response data were analyzed by nonlinear regression analysis using GraphPad Prism.

Synthesis of QH10-QH16.

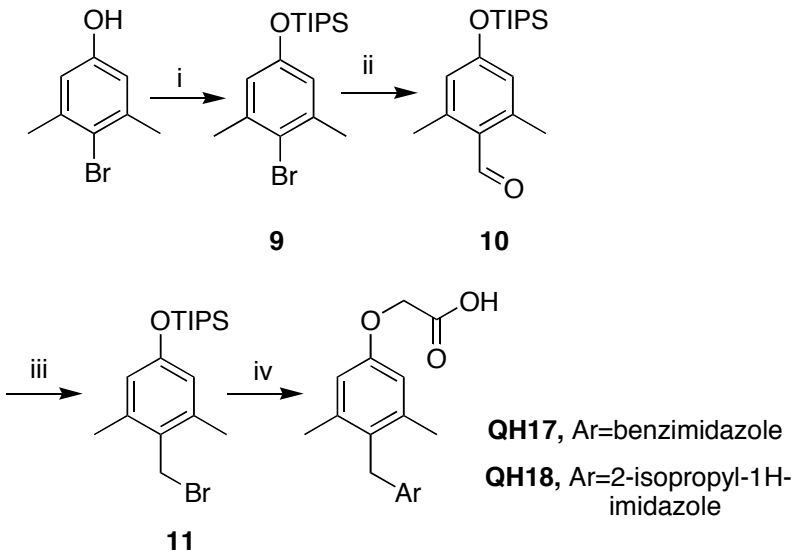
Pyridyl analogs were derived from the corresponding 2-substituted-4-cyanopyridines by nucleophilic radical addition to 4-cyanopyridine by alkyl radicals generated by silver-promoted radical decarboxylation of corresponding carboxylic acids providing an efficient entry into the 2-alkylpyridine series (Scheme 1).[23] The resulting intermediates, **1a-f**, were reduced to aldehydes by DIBAL, which was then coupled with aryl lithium derived from (4-bromo-3,5-dimethyl-phenoxy)-triisopropyl-silane to give alcohols, **3a-f**. The oxoacetic acid side chain was introduced by alkylating the phenol with ethyl-2-bromoacetate followed by hydrogenation to afford the target molecules. The phenyl analog **QH9** was synthesized starting from 1-bromo-3-isopropyl-benzene following the analogous synthetic scheme used to synthesize GC-1 from 4-bromo-2-isopropylanisole.



Scheme S1. Synthesis of Pyridyl ligands. a. Dibal-H, -78C, H+ b. n-BuLi, (4-Bromo-3,5-dimethyl-phenoxy)-triisopropyl-silane c. Zn/HCOOH d. i. Cs_2CO_3, $BrCH_2CO_2Bn$ ii. H2, 10%Pd/C, 9%AcOH/EtOH.

Synthesis of QH17-QH18.

2-Isobutyl-pyridine-4-carbaldehyde, (2a). To a solution of 2-isobutyl-isonicotinonitrile (1.6 g, 9.8 mmol) in toluene (11 mL) at -78° C, and was added drop-wise via syringe 1M DIBAL in hexanes (11.3 mL, 11.3 mmol). The reaction mixture was warmed to 5°C, stirred for 5 min, and cooled to -78°C before adding CH_3OH (11 mL). The mixture was warmed to 5°C and stirred for 5 min before 25% aqueous rochelle's salt (potassium sodium tartrate) was added. After 3 min the reaction mixture was acidified to pH <1.0 with 10% aqueous H_2SO_4. The aqueous solution was made basic by slow addition of solid K_2CO_3 and extracted with EtOAc. The extracts were dried over $MgSO_4$, concentrated, filtered and evaporated under reduced pressure, and the residue was purified by flash column chromatography (silica gel, 2% MeOH/CH_2Cl_2) to give pure product, **2a** (1.0g, 7.84 mmol, 77%). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 0.90 (d, *J*=7.2 Hz, 6H), 2.13 (m, *J*=6.7 Hz, 1H), 2.76 (d, *J*=7.1 Hz, 2H), 7.50 (d, *J*=3.9 Hz, 2H), 8.77 (dd, *J*=1.8 Hz, *J*=3.9 Hz, 1H), 10.0 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz), δ 22.6, 25.7, 36.3, 119.4, 119.9, 142.3, 150.5, 169.4, 192.1; HRMS (CI) calculated for $C_{10}H_{13}NO$ (M^+) 163.0997 found 163.0992.



2-Isopropyl-pyridine-4-carbaldehyde, (2c). This compound was synthesized in 78% yield from 2-isopropyl-isonicotinonitrile following the protocol used to prepare 2a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.34 (d, *J*=6.9 Hz, 6H), 3.20 (heptet, *J*=6.9 Hz, 1H), 7.52 (dd, *J*=1.4 Hz, *J*=4.9 Hz, 1H), 7.60 (d, *J*=0.8 Hz, 1H), 8.80 (d, *J*=4.9 Hz, 1H), 10.07 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 13.9, 31.5, 119.9, 120.9, 142.3, 150.7, 165.6, 192.1, HRMS (CI) calculated for $C_9H_{12}NO$ (MH^+) 149.0841, found 149.0849.

2-*tert*-Butyl-pyridine-4-carbaldehyde, (2d). This compound was synthesized in 81% yield from 2-tert-butyl-isonicotinonitrile following the protocol used to prepare 2a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.38 (s, 9H), 7.48 (dd, *J*=1.4 Hz, *J*=4.9 Hz, 1H), 7.72 (d, *J*=1.2 Hz, 1H), 8.80 (dd, *J*=0.6 Hz, *J*=4.8 Hz 1H), 10.0 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 30.3, 38.0, 118.0, 119.6, 142.1, 150.2, 171.5, 192.4; HRMS (CI) calculated for $C_{10}H_{13}NO$ (M^+) 163.0997, found 163.0989.

2-Propyl-pyridine-4-carbaldehyde, (2e). This compound was synthesized in 75% yield from 2-Propyl-isonicotinonitrile following the protocol used to prepare 2a. 1H-NMR (CDCl3, 400 MHz) δ 0.98 (t, J=7.4Hz, 3H), 1.8 (hextet, J=7.5 Hz, 2H), 2.89 (t, J=7.4 Hz, 2H), 7.51 (d, J=1.6 Hz, 1H), 7.54 (d, J=0.9 Hz, 1H), 8.7 (dd, J=4.9 Hz, J=0.4 Hz, 1H), 10.0 (s, 1H), 13C-NMR (CDCl3, 100 MHz) δ 12.8, 21.9, 39.1, 118.4, 120.1, 141.0, 149.6, 163.1, 190.9; HRMS (CI) calculated for C9H11NO, 149.0841, found 150.0920(MH+).

2,6-Diisopropyl-pyridine-4-carbaldehyde, (2f). This compound was synthesized from 2,6-diisopropyl-isonicotinonitrile in 75% yield following the protocol used to prepare 2a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.30 (d, *J*=6.8 Hz, 12H), 3.10 (heptet, *J*=6.8 Hz, 2H), 7.36 (s, 2H), 10.0 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 22.6, 36.5, 116.5, 140.1, 168.5, 192.7; HRMS (CI) calculated for $C_{12}H_{17}NO$ (M^+) 191.1310, found 192.1388.

[2,6-Dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-(2-isobutyl-pyridin-4-yl)-methanol, (3a). To a solution of (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane (2.4 g, 6.8 mmol) in 17 mL of dry tetrahydrofuran at -78°C was added 13.9 mL of n-butyllithium (2.5 M in hexane). The reaction mixture was stirred for 30 min at -78°C and then **2a** (1.1 g, 6.6 mmol) was added. The reaction mixture was stirred for 1 h at -78°C and for 6 h at room temperature. The mixture was diluted with 30 mL of ether, washed with 35 mL of water and 5×10 mL of brine. The organic portion was dried ($MgSO_4$), filtered, and evaporated under reduced pressure, and the residue was purified by flash chromatography (silica gel, 90:10 hexane/ethyl acetate) to yield **3a** (1.88 g, 4.4 mmol, 67%) as an oil. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 0.85 (d, *J*=6.8 Hz, 6H), 1.06-1.10 (m, 18H), 1.22 (heptet, *J*=5.2 Hz, 3H), 2.04 (m, *J*=6.7 Hz, 1H), 2.15 (s,

6H), 2.56 (d, *J*-5.6 Hz, 2H), 6.17 (s, 1H), 6.53 (s, 2H), 6.94-6.96 (m, 1H), 7.01 (s, 1H), 8.35 (d, *J*=5.6 Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) 12.9, 20.9, 22.5, 29.5, 47.7, 70.0, 118.2, 120.4, 120.7, 131.5, 138.8, 149.1, 153.3, 155.6, 161.5; HRMS (CI) calculated for $C_{27}H_{43}NO_2Si$ 442.3141, found 442.3120 (MH^+).

[2,6-Dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-(2-ethyl-pyridin-4-yl)-methanol, (3b). This compound was synthesized in 63% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-isobutyl-isonicotinonitrile following the protocol used to prepare **3a**. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.11 (d, *J*=8.0 Hz, 18H), 1.19-1.28 (m, 6H), 2.17 (s, 6H), 2.78 (q, *J*=8.0 Hz, 2H), 6.19 (s, 1H), 6.55 (s, 2H), 6.98-7.01 (m, 1H), 7.14 (s, 1H), 8.3 (d, *J*=4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.0, 18.2, 20.9, 70.2, 118.5, 119.3, 120.8, 131.4, 131.5, 138.8, 148.6, 155.8, 163.4; HRMS (CI) calculated for $C_{25}H_{39}NO_2Si$ (MH) 413.2985, found 413.2740.

[2,6-Dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-(2-isopropyl-pyridin-4-yl)-methanol, (3c). This compound was synthesized in 68% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-isopropyl-isonicotinonitrile following the protocol used to prepare 3a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.04 (d, *J*=6.9 Hz, 18H), 1.18 (heptet, *J*=7.1 Hz, 3H), 1.35-1.42 (m, 6H), 2.13 (s, 6H), 3.60 (heptet, *J*=7.6 Hz, 1H), 6.33 (s, 1H), 6.53 (s, 2H), 7.44 (d, *J*=6.3 Hz, 1H), 7.70 (s, 1H), 8.35 (d, *J*=6.1 Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 12.6, 21.0, 22.2, 32.9, 69.7, 120.9, 121.0, 121.5, 130.2, 138.7, 139.7, 156.3, 162.2, 166.6; HRMS (CI) calculated for $C_{26}H_{41}NO_2Si$ 427.2907, found 428.2978 (MH^+).

(2-*tert*-Butyl-pyridin-4-yl)-[2,6-Dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-methanol, (3d). This compound was synthesized in 66% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-*tert*-butyl-isonicotinonitrile following the protocol used to prepare 3a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.09 (d, *J*=7.2 Hz, 18H), 1.23 (heptet, *J*=6.8 Hz, 3H), 1.31 (s, 9H), 2.16 (s, 6H), 6.17 (s, 1H), 6.55 (s, 2H), 6.90-6.91 (m, 1H) 7.33 (s, 1H), 8.35 (d, *J*=5.1 Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 12.9, 20.9, 30.4, 37.5, 70.1, 116.3, 118.1, 120.7, 131.7, 138.7, 148.4, 153.2, 155.5, 169.3; HRMS (CI) calculated for $C_{27}H_{43}NO_2Si$ 442.3141, found 442.3130(MH^+).

[2,6-Dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-(2-propyl-pyridin-4-yl)-methanol, (3e). This compound was synthesized from in 66% yield (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-propyl-isonicotinonitrile following the protocol used to prepare 3a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 0.88 (t, *J*=7.4 Hz, 3H), 1.10 (d, *J*=7.2 Hz, 18H), 1.23 (heptet, *J*=7.5 Hz, 3H), 1.67 (sextet, *J*=7.5 Hz, 2H), 2.15 (s, 6H), 2.66 (t, *J*=7.5 Hz, 2H), 6.17 (s, 1H), 6.54 (s, 2H), 6.94 (d, *J*=5.1 Hz, 1H), 7.01 (s, 1H), 8.24 (d, *J*=5.2Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 12.9, 18.1, 20.8, 23.3, 69.6, 118.4, 119.9, 120.6, 131.8, 138.7, 148.7, 153.9, 155.5, 162.1; HRMS (CI) calculated for $C_{26}H_{41}NO_2Si$ 427.2907, found 428.2969 (MH^+).

(2,6-Diisopropyl-pyridin-4-yl)-[2,6-dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-methanol, (3f). This compound was synthesized in 65% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-diisopropyl-isonicotinonitrile following the protocol used to prepare 3a. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.11 (d, *J*=7.1 Hz, 18H), 1.18-1.27 (m, 15H), 2.16 (s, 6H), 3.0 (heptet, *J*=6.9 Hz, 2H), 6.17 (s, 1H), 6.56 (s, 2H), 6.89 (s, 2H), ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 12.9, 21.0, 22.8, 36.4, 70.1, 114.5, 120.6, 132.1, 138.8, 153.7, 155.4, 166.6; HRMS (CI) calculated for $C_{29}H_{47}NO_2Si$ 469.3376, found 467.3353(M^+).

4-(2-Isobutyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenol, (4a). Zinc (780 mg, 12 mmol) was added to a solution of **3a** (530 mg, 1.2 mmol) in formic acid (3.6 mL). The mixture was vigorously stirred under reflux over night and then filtered. The filter cake was washed with formic acid and the filtrate was concentrated under reduced pressure. The residue was taken up in H_2O (2 mL) and the pH was adjusted to 9 with saturated Na_2CO_3. The solution was extracted with EtOAc (3×2mL), dried over $MgSO_4$, filtered, and concentrated under reduced pressure to give **4a** (216 mg, 0.9 mmol, 75%). ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 0.88 (d, *J*=6.6 Hz, 6H), 2.03 (m, *J*=6.5 Hz, 1H), 2.13 (s, 6H), 2.60 (d, *J*=7.2 Hz, 2H), 3.94 (s, 1H), 6.60 (s, 2H), 6.78-6.8 (m, 2H), 8.3 (d, *J*=5.1 Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 20.5, 22.6, 29.5, 34.0 47.2, 115.5, 121.0, 123.5, 126.7, 138.6, 148.7, 150.7, 155.2, 161.4; HRMS (CI) calculated for $C_{18}H_{23}NO$ (M) 269.1780, found 269.1773.

4-(2-Ethyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenol, (4b). This compound was synthesized in 64% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-isobutyl-isonicotinonitrile following the protocol used to prepare **4a**. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.25 (t, *J*=8.4 Hz, 3H), 2.14 (s, 6H), 2.77 (q, *J*=8.0 Hz, 2H), 3.94 (s, 1H), 6.60 (s, 2H), 6.76 (d, *J*=5.6 Hz, 1H), 6.87 (s, 1H), 8.3 (d, *J*=5.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.3, 20.5, 30.9, 34.3, 115.5, 119.6, 120.8, 126.2, 138.6, 148.8, 151.5, 157.6, 163.8; HRMS (CI) calculated for $C_{16}H_{19}NO$ 241.1467, found 241.1477(M^+).

4-(2-Isopropyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenol, (4c). This compound was synthesized in 69% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-isopropyl-isonicotinonitrile following the protocol used to prepare **4a**. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.26 (d, *J*=6.9 Hz, 6H), 2.15 (s, 6H), 3.01 (heptet, *J*=6.9 Hz, 1H), 3.94 (s, 2H), 6.59 (s, 2H), 6.72 (d, *J*=4.4, 1H), 6.9 (s, 1H), 8.3 (d, *J*=5.1 Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 20.5, 22.8, 34.1, 36.1, 115.3, 120.6, 120.9, 126.9, 138.8, 148.7, 150.9, 154.8, 167.2; HRMS (CI) calculated for $C_{17}H_{21}NO$ (M) 255.1623, found 255.1632.

4-(2-*tert*-Butyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenol, (4d). This compound was synthesized in 60% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-*tert*-butyl-isonicotinonitrile following the protocol used to prepare **4a**. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.34 (s, 9H), 2.14 (s, 6H), 3.95 (s, 2H), 6.60 (s, 2H), 6.68 (s, 1H), 7.12 (s, 1H), 8.37 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 20.5, 30.4, 34.3, 37.4, 115.3, 119.3, 120.4, 127.0, 138.8, 148.6, 150.6, 154.9, 169.1; HRMS (CI) calculated for $C_{18}H_{23}NO$ (M) 269.1780, found 269.1783.

3,5-Dimethyl-4-(2-propyl-pyridin-4-ylmethyl)-phenol, (4e). This compound was synthesized in 66% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-propyl-isonicotinonitrile following the protocol used to prepare **4a**. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.8 (m, 3H), 1.6 (hextet, *J*=7.4 Hz, 2H), 2.1 (s, 6H), 2.6 (triplet, *J*=7.2 Hz, 2H), 3.9 (s, 2H), 6.6 (s, 2H), 6.7 (dd, *J*=1.2 Hz, *J*=5.1 Hz, 1H), 6.8 (s, 1H), 8.3 (d, *J*=5.2Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 12.2, 20.4, 22.9, 35.2, 49.4, 115.4, 121.0, 122.6, 127.1, 138.6, 148.8, 151.2, 155.3, 165.2; HRMS (CI) calculated for $C_{17}H_{21}NO$ (M) 255.1623, found 255.1596 (M^+).

4-(2,6-Diisopropyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenol, (4f). This compound was synthesized in 61% yield from (4-bromo-3, 5-dimethyl-phenoxy)-triisopropyl-silane and 2-diisopropyl-isonicotinonitrile following the protocol used to prepare **4a**. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.21-1.29 (m, 12H), 2.2 (s, 6H), 2.92 (heptet, *J*=6.6 Hz, 2H), 3.9 (s, 2H), 6.46-6.61 (m, 4H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 20.5, 22.6, 29.5, 34.1, 113.5, 114.2, 115.5, 116.4, 117.5, 139.6, 154.6, 166.1; HRMS (CI) calculated for $C_{20}H_{27}NO$ (M) 297.2093, found 297.2090.

[4-(2-Isobutyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenoxy]-acetic acid, (QH10). To cesium carbonate (5.72 g, 17.6 mmol) and **4a** (941 mg, 3.5 mmol) in 27 mL of DMF was added bromo-acetic acid benzyl ester (1.0 g, 4.4 mmol). The reaction mixture was stirred for 30 min at room temperature, poured into 35 mL of cold 1N HCl, and extracted with ethyl acetate. The combined organic portions were dried ($MgSO_4$) and evaporated under reduced pressure to yield crude product. To the above ester (842.3 mg, 2.02 mmol) in 16 mL of methanol was added 11 mL of 1N NaOH. The reaction mixture was stirred for 3 h, then acidified with 12 mL of 2N HCl, and extracted with ethyl acetate (3×30mL). The combined organic layer was dried ($MgSO_4$) and evaporated under reduced pressure to give **QH10** (612 mg, 1.79 mmol, 89%) as oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.86 (d, *J*=6.6 Hz, 6H), 1.9 (heptet, *J*=7.1 Hz, 1H), 2.13 (s, 6H), 2.66 (d, *J*=7.2 Hz, 2H), 3.99 (s, 2H), 4.64 (s, 2H), 6.68 (s, 2H), 6.88 (s, 1H), 6.92 (s, 1H), 8.45 (d, *J*=4.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) 14.4, 20.7, 22.5, 34.6, 44.9, 69.3, 114.7, 121.5, 122.0, 126.7, 138.5, 146.3, 155.5, 157.2, 164.9, 179.1; HRMS (CI) calculated for $C_{20}H_{25}NO_3$ (MH^+) 299.1521 found 299.1514.

[4-(2-Ethyl -pyridin-4-ylmethyl)-3,5-dimethyl-phenoxy]-acetic acid, (QH11). This compound was synthesized from 3,5-dimethyl-4- (2-isobutyl-pyridin-4-ylmethyl)-phenol following the protocol used to prepare **QH10**. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ^{1}H 1.2-1.3 (m, 3H), 2.12 (s, 6H), 2.71-2.91 (m, 2H), 3.97 (s, 2H), 4.57 (s, 2H), 6.67 (s, 2H), 6.87 (s, 1H), 6.96 (broad s, 1H), 8.41 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) 20.7, 28.3, 29.7, 34.7, 67.1, 114.7, 118.1, 121.6, 123.4, 127.0, 138.5, 156.9, 161.1, 162.8, 188.0; HRMS (CI) calculated for $C_{20}H_{25}NO$ (M) 299.1521, found 298.1443 ($M-H^+$).

[4-(2-Isopropyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenoxy]-acetic acid, (QH13). This compound was synthesized in 93% yield from 3,5-dimethyl-4- (2-isopropyl-pyridin-4-ylmethyl)-phenol following the protocol used to prepare **QH10**. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.20 (d, *J*=6.9 Hz, 6H), 2.10 (s, 6H), 3.21 (heptet, *J*=6.9 Hz, 1H), 4.01 (s, 2H), 4.62 (s, 2H), 6.68 (s, 2H), 6.85 (d, *J*=5.2 Hz, 1H), 7.06 (s, 1H), 8.45 (d, *J*=4.9 Hz, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz), δ 20.7, 22.6, 34.5, 34.8, 60.1, 114.7, 121.2, 121.7, 126.9, 138.5, 146.3, 154.2, 157.1, 165.5, 171.1; HRMS (CI) calculated for $C_{19}H_{23}NO_3$ (M) 313.1638 found 313.1680.

[4-(2-*tert*-butyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenoxy]-acetic acid QH14. This compound was synthesized in 93% yield from 3,5-dimethyl-4- (2-*tert*-butyl-pyridin-4-ylmethyl)-phenol following the protocol used to prepare QH10. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.53 (s, 9H), 2.16 (s, 6H), 4.16 (s, 2H), 4.67 (s, 2H), 6.69 (s, 2H), 7.09 (s, 1H), 7.45 (s, 1H), 8.78 (s, 1H), ^{13}C-NMR ($CDCl_3$, 100 MHz), δ 20.7, 29.9, 34.5, 37.2, 65.7, 114.6, 120.2, 121.1, 127.2, 138.5, 146.7, 153.9, 156.8, 167.1, 173.2; HRMS (CI) calculated for $C_{20}H_{25}NO_3$ (M) 327.1831 found 327.1825.

[3,5-Dimethyl-4-(2-propyl-pyridin-4-ylmethyl)-phenoxy]-acetic acid, (QH15). This compound was synthesized in 94% yield from 3,5-dimethyl-4- (2-propyl-pyridin-4-ylmethyl)-phenol following the protocol used to prepare **QH10**. ^{1}H-NMR ($CDCl_3$, 250 MHz) δ 0.98 (t, *J*=7.3 Hz, 3H), 1.6-1.7 (m, 2H), 2.40 (s, 6H), 2.83 (t, *J*=7.5 Hz, 2H), 3.75 (s, 2H), 4.7 (s, 2H), 6.6 (s, 2H), 7.27 (s, 2H), 8.7 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 12.8, 18.0, 26.1, 26.7, 32.9, 46.6, 118.7, 119.2, 119.3, 132.5, 136.0, 145.5, 149.8, 156.2, 167.5, 177.7; HRMS (CI) calculated for $C_{20}H_{25}NO$ (M) 313.1678, found 313.1681(M^+).

[4-(2,6-Diisopropyl-pyridin-4-ylmethyl)-3,5-dimethyl-phenoxy]-acetic acid, (QH16). This compound was synthesized in 94% yield from 3,5-dimethyl-4- (2-diisopropyl-pyridin-4-ylmethyl)-phenol following the protocol used to prepare QH10. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.2-1.3(m, 12H), 2.38 (s, 6H), 3.07 (heptet, *J*=6.7 Hz, 2H), 3.78 (s, 2H), 4.68 (s, 2H), 6.58 (s, 2H), 7.18 (s, 2H); ^{13}C-NMR ($CDCl_3$, 100 MHz) 20.5, 22.8, 34.2, 36.2, 66.8, 115.3, 120.6, 121.0, 126.9, 138.8, 148.8, 151.0, 154.9, 167.2, 179.1; HRMS (CI) calculated for $C_{22}H_{29}NO_3$ (M) 355.2147 found 354.2055($M-H^+$).

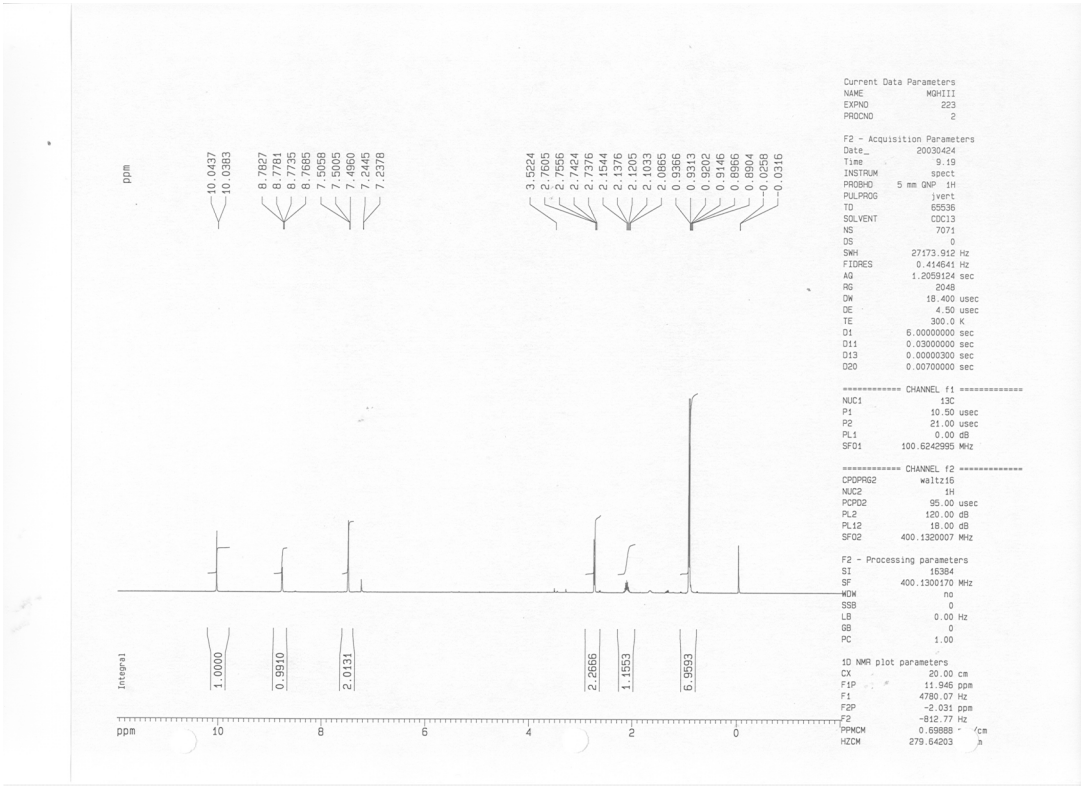
(4-Benzoimidazol-1-ylmethyl-3,5-dimethyl-phenoxy)-acetic acid, QH17. QH17 was made from 4-Bromomethyl-3,5-dimethyl-phenoxy)-triisopropyl-silane: To a solution of 2,6-dimethyl-4-(triisopropyl-silanyloxy)-benzaldehyde (250mg, 0.8 mmol) in 2.5 mL ethanol was added $NaBH_4$ (80mg, 2.1 mmol). After stirring for 2 hr at room temperature, the reaction mixture was quenched with 3 mL of water, and then diluted with 7 mL of ether. The organic portion was dried ($MgSO_4$), filtered and evaporated under reduced pressure to give crude [2,6-dimethyl-4-(triisopropyl-silanyloxy)-phenyl]-methanol. To the crude alcohol in 2.5 mL of dry ether was added pyridine (15 μL) and PBr_3 (95 μL). The reaction mixture was stirred at room temperature for 3 hrs and then diluted with 3 mL of ether and washed with 2 mL of water and 3×2 mL of brine. The organic portion was dried ($MgSO_4$), filtered and evaporated under reduced pressure to give 4-Bromomethyl-3,5-dimethyl-phenoxy)-triisopropyl-silane. The compound was not stable to storage and therefore was directly used in next reaction without any purification.

To a solution of (4-bromomethyl-3,5-dimethyl-phenoxy)-triisopropyl-silane (50 mg, 0.2 mmol), NaH (8 mg, 0.3 mmol) in 0.8 mL of THF was a 1*H*-Benzoimidazole (23 mg, 0.2 mmol). After stirring for 2 hr at room temperature, the reaction mixture was diluted with 5 mL of ether and washed with 2 mL of water and 3×2 mL of brine. The organic portion was dried ($MgSO_4$), filtered and evaporated under reduced pressure to give 4-Benzoimidazol-1-ylmethyl-3,5-dimethyl-phenol, which was carried to the next step. To a solution of cesium carbonate (150 mg, 0.5 mmol) and 4-Benzoimidazol-1-ylmethyl-3,5-dimethyl-phenol (10.0 mg, 0.04 mmol) in 1.0 mL of DMF was added ethyl bromoacetate (85mg, 0.06 mmol). The reaction mixture was stirred for 30 min at room temperature, poured into 0.5 mL of cold 1N HCl, and extracted with ethyl acetate. The combined organic portions were dried ($MgSO_4$) and evaporated to yield crude (4-benzoimidazol-1-ylmethyl-3,5-dimethyl-phenoxy)-acetic acid ethyl ester. To this ester in 0.2 mL of methanol was added 0.2 mL of 1N NaOH. The reaction mixture was stirred for 3 h, then acidified with 0.3 mL of 2N HCl, and extracted with ethyl acetate (1×1 mL). The combined organic layer was dried ($MgSO_4$) and evaporated under reduced pressure and the residue was purfied by flash chromatography (reverse phase silica gel, 10%MeOH/H_2O) to give **QH17** (4.5 mg, 0.02 mmol, 71%).

^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.2 (s, 6H), 4.6 (s, 2H), 5.2 (s, 2H), 6.6 (s, 2H), 7.35-7.36 (m, 4H), 8.4 (s, 1H), ^{13}C NMR ($CDCl_3$, 100 MHz), δ 20.7, 34.3, 67.5, 114.5, 119.0, 128.6, 128.8, 135.5, 138.8, 148.8, 156.3, 169.2; HRMS (CI) calculated for $C_{18}H_{18}N_2O_3$ 310.1317, found 309.1245 ($M-H^+$).

[4-(2-Isopropyl-imidazol-1-ylmethyl)-3,5-dimethyl-phenoxy]-acetic acid, QH18. This compound was prepared in 74% yield from **11** following the protocol for **QH17**. ^{1}H-NMR δ 1.3 (d, *J*=8.6 Hz, 6H), 2.4 (s, 6H), 3.0 (heptet, *J*=8.1 Hz, 1H), 4.7 (s, 2H), 6.6 (s, 2H), 7.2 (s, 2H); ^{13}C NMR ($CDCl_3$) δ 20.7, 22.7, 34.1, 36.2, 67.1, 114.4, 120.7, 128.7, 138.7, 135.4, 149.9, 156.3, 169.2; MS (CI) found 302.1 (M^+).

2a.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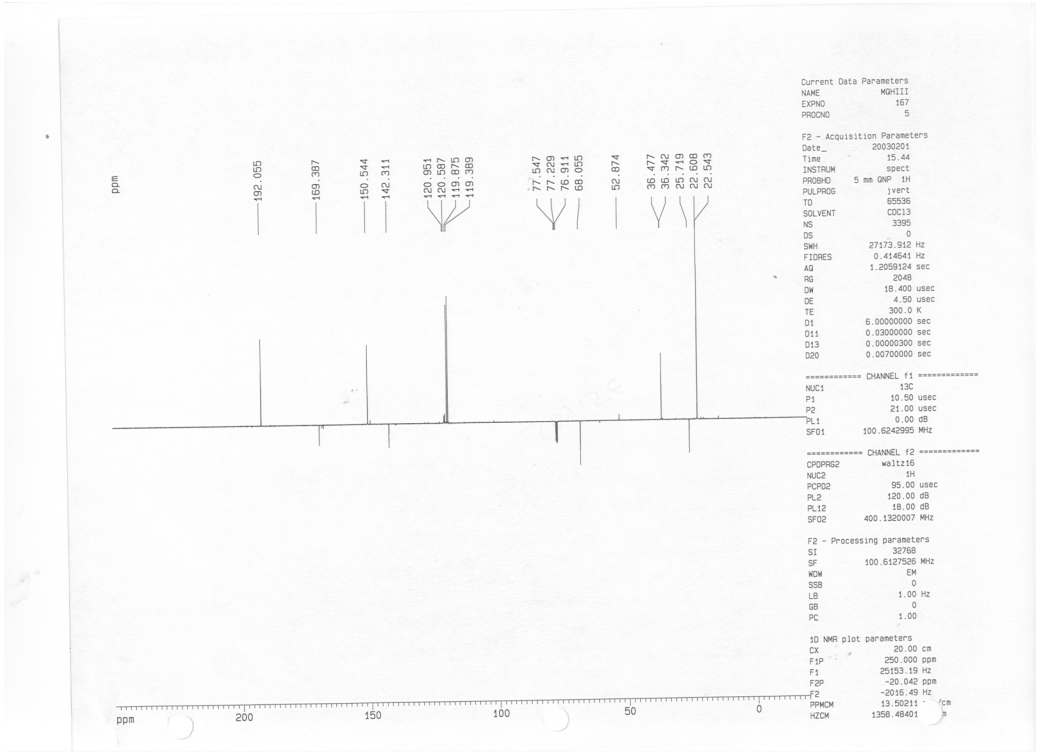
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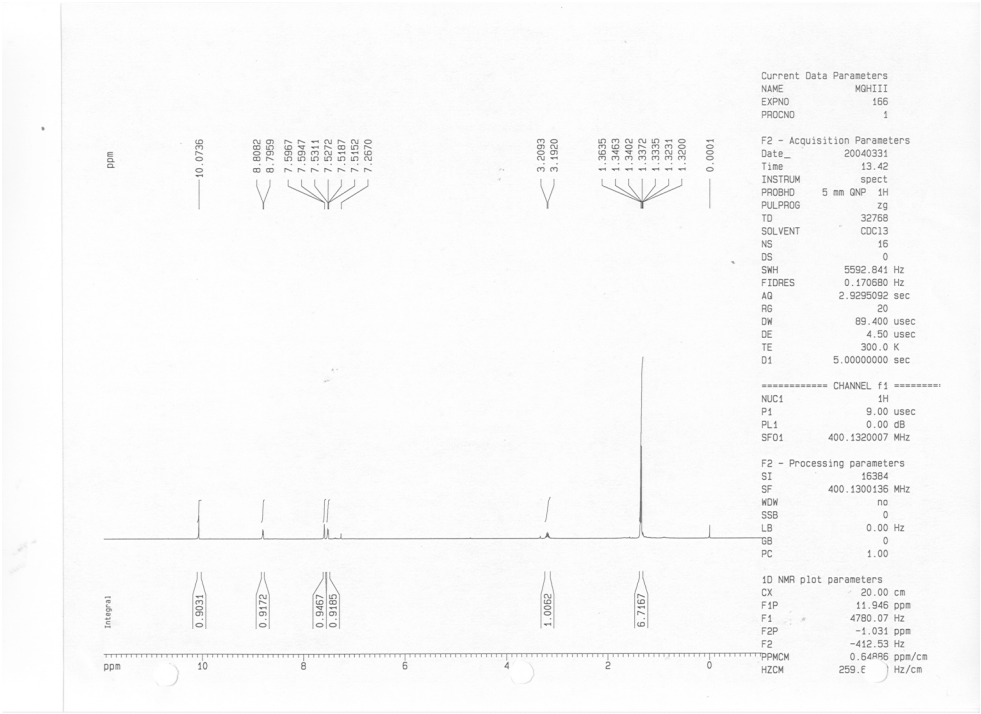
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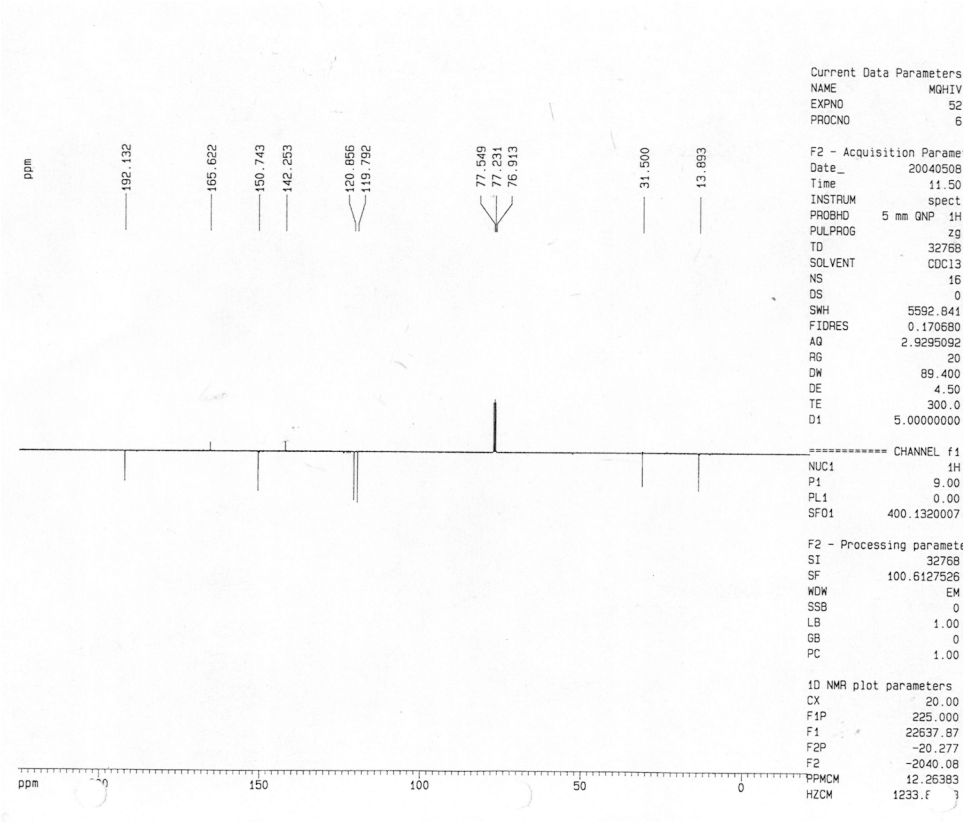
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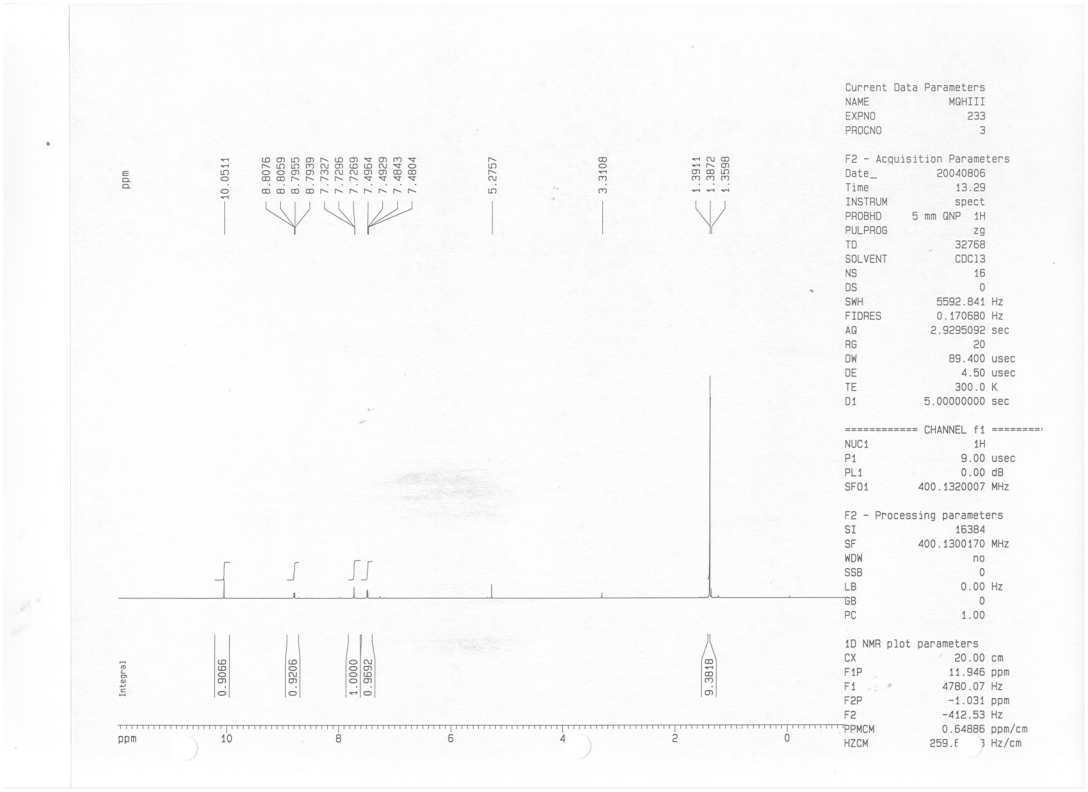
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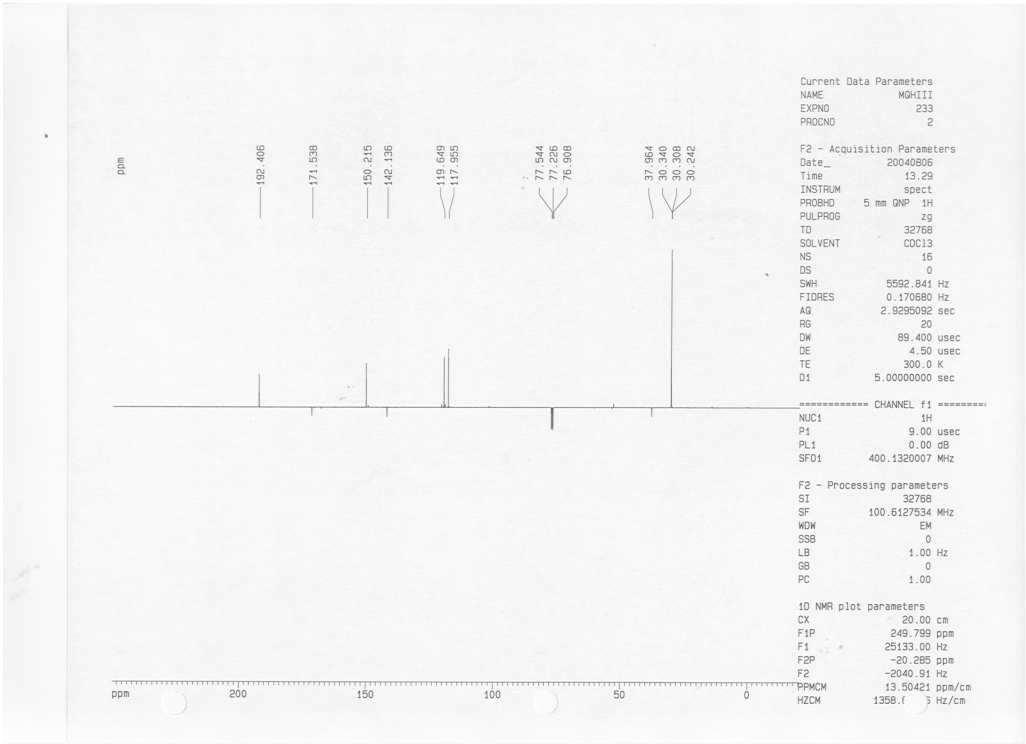
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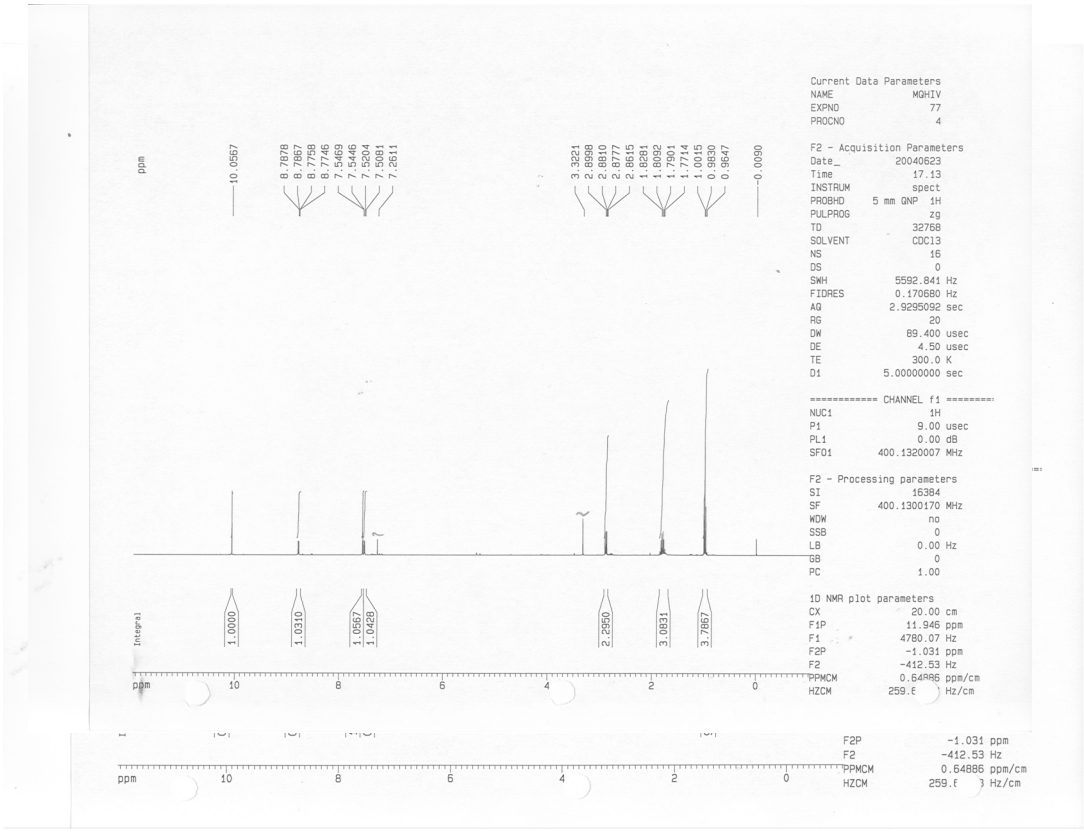
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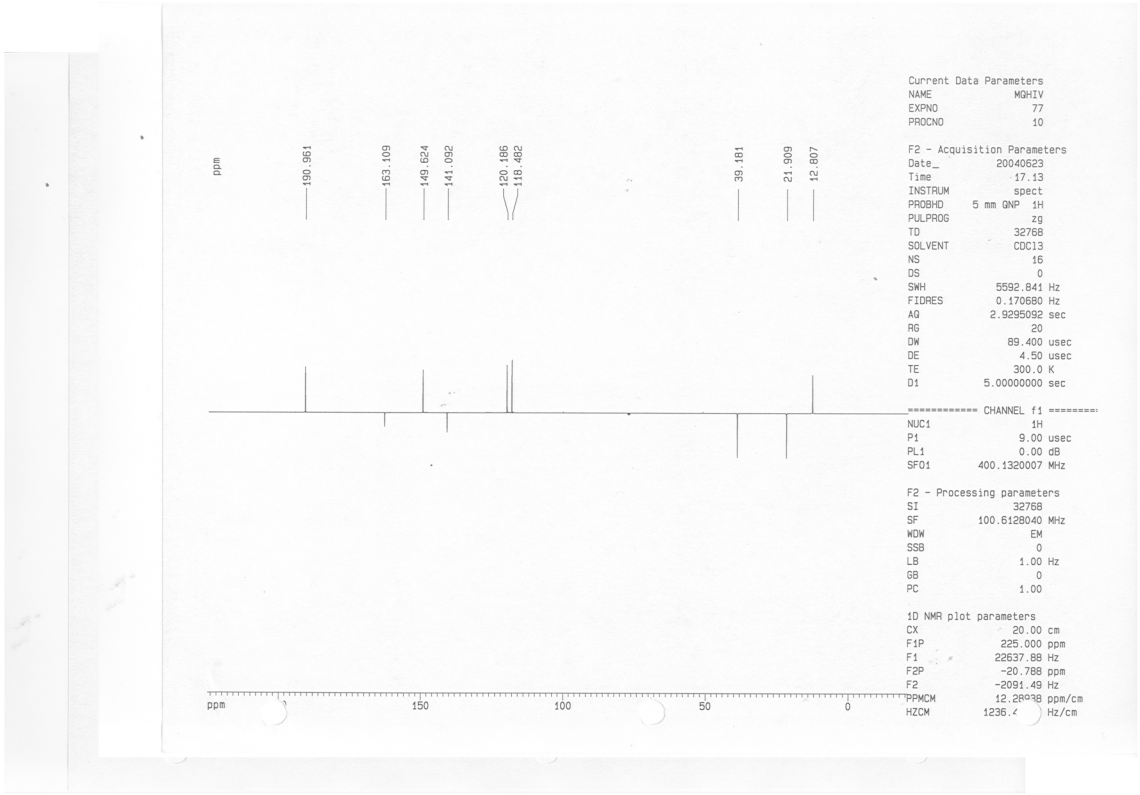
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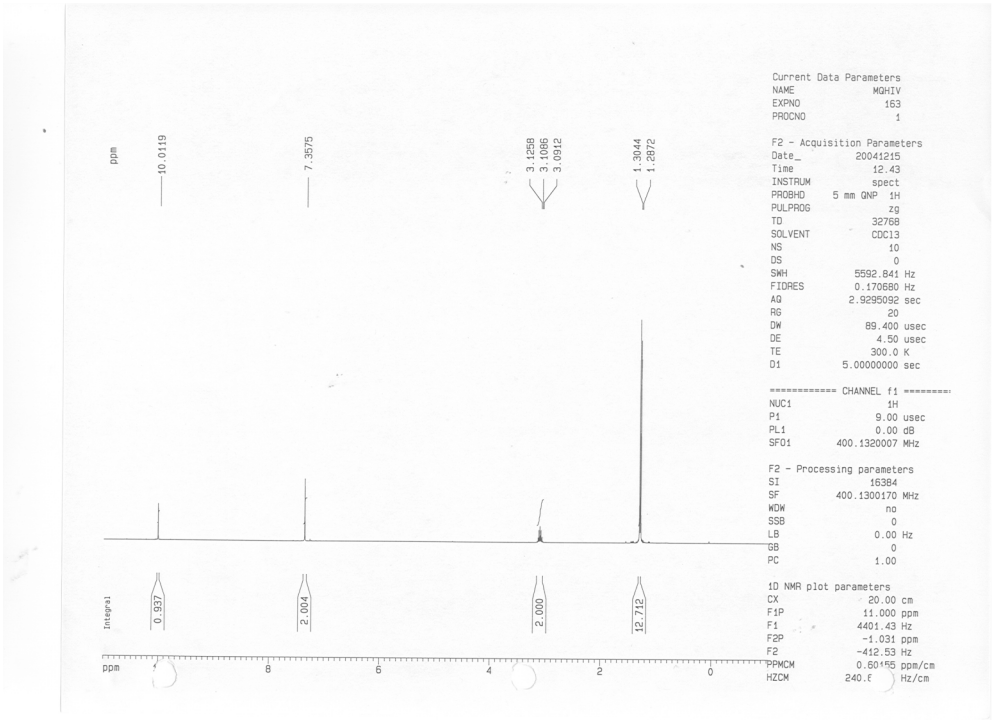
2f.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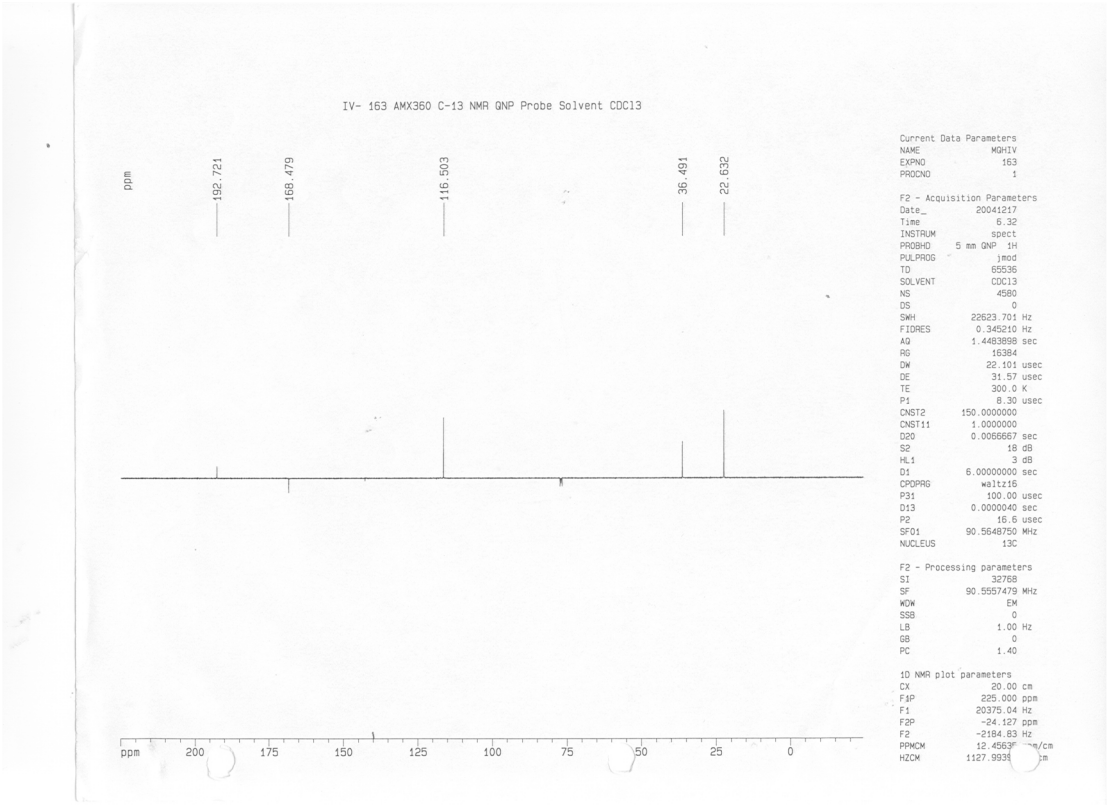
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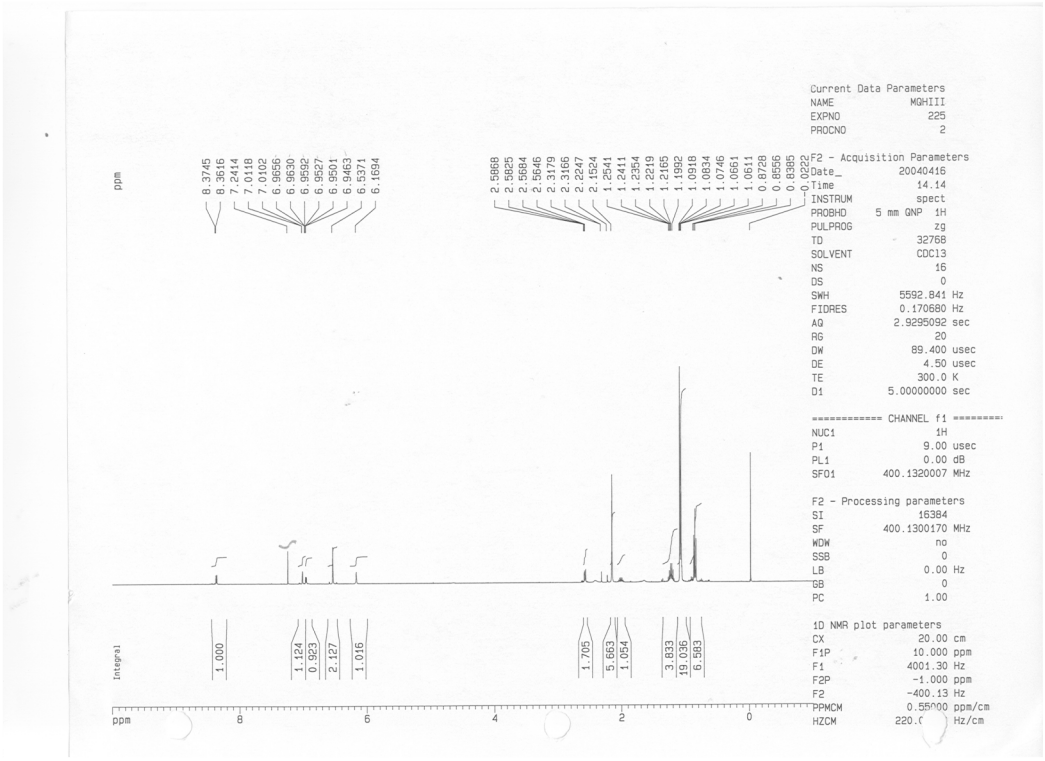
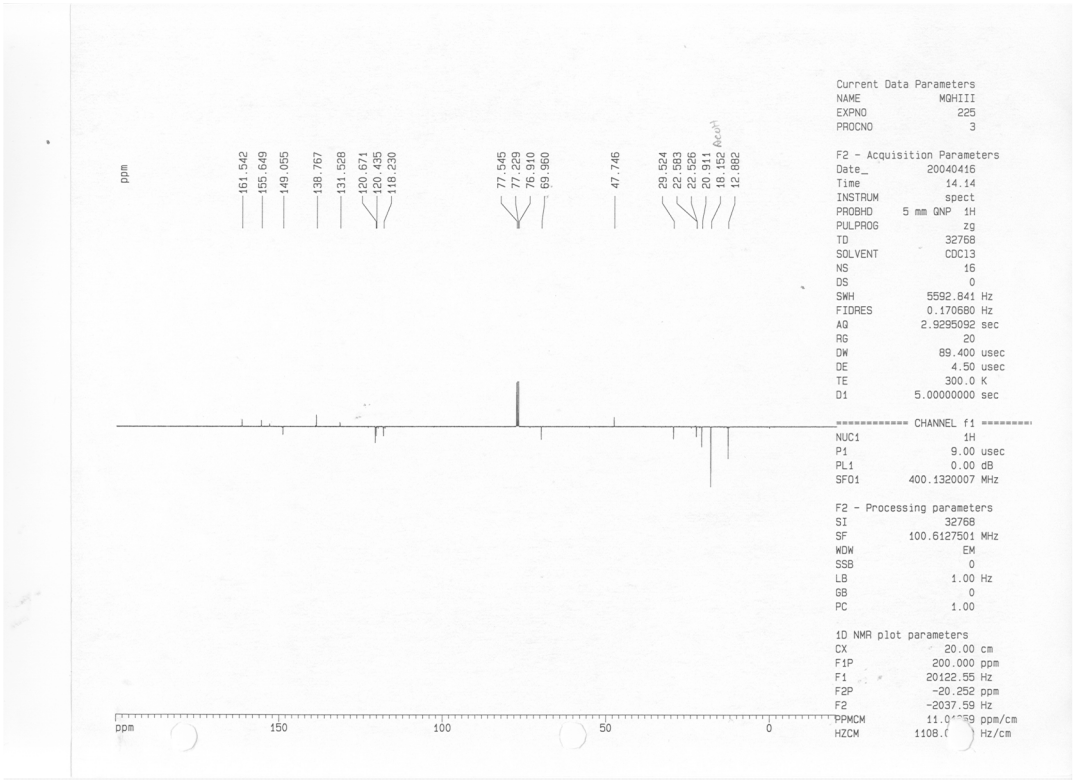
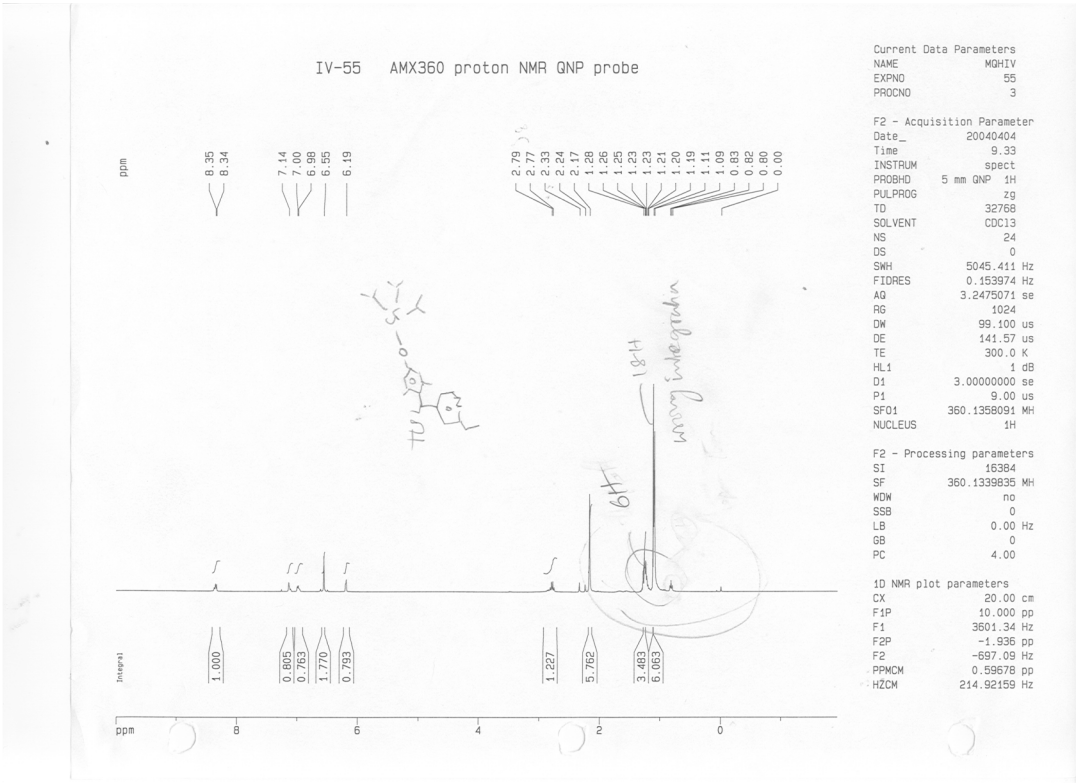
ppm
200
175
150
125
100
75
50
25
0
Current Data Parameters
NAME MQHIV
EXPNO 163
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041217
Time 6.32
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 4580
DS 0
SWH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4483898 sec
RG 16384
DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.30 usec
CNST2 150.0000000
CNST11 1.0000000
D20 0.0066667 sec
S2 18 dB
HL1 3 dB
D1 6.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.6 usec
SFO1 90.5648750 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.5557479 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 225.000 ppm
F1 20375.04 Hz
F2P -24.127 ppm
F2 -2184.83 Hz
PPMCM 12.4563 ppm/cm
HZCM 1127.9939 Hz/cm

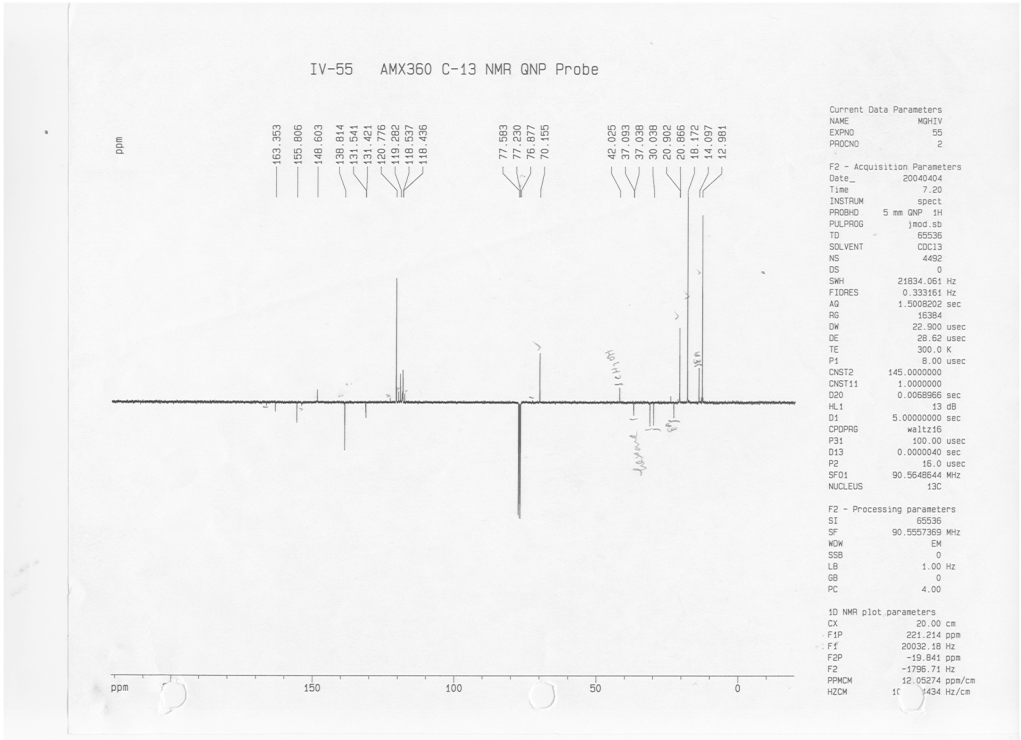
3a.


ppm
8.3745
8.3616
7.2414
7.0118
7.0102
6.9656
6.9630
6.9592
6.9527
6.9501
6.9463
6.5371
6.1694
2.5868
2.5825
2.5684
2.5646
2.3179
2.3166
2.2247
2.1524
2.1541
2.1411
2.1354
2.1219
2.1165
1.1992
1.0918
1.0834
1.0746
1.0661
1.0611
0.8728
0.8556
0.8385
0.0222
Integral
1.000
1.124
0.923
2.127
1.016
1.705
5.663
1.054
3.833
19.036
6.583
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIII
EXPNO 225
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040416
Time 14.14
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.0 Hz/cm

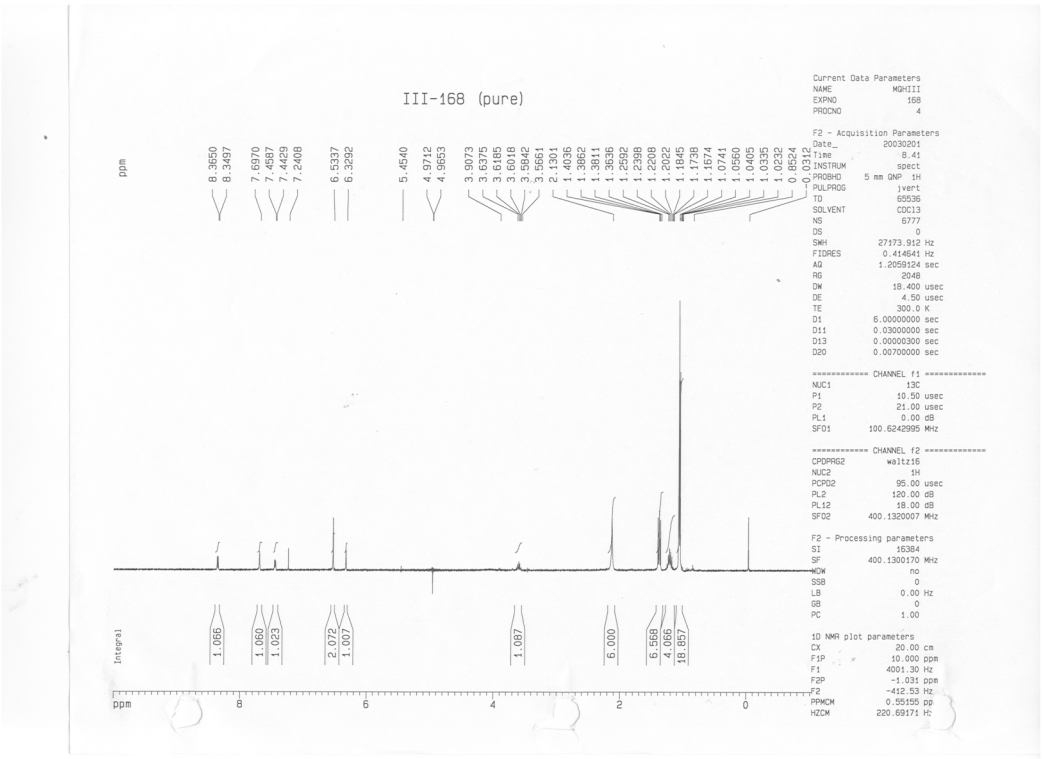

ppm
161.542
155.649
149.055
138.767
131.528
120.671
120.435
118.230
77.545
77.229
76.910
69.960
47.746
29.524
22.583
22.526
20.911
18.152
12.882
Acetone
ppm
150
100
50
0
Current Data Parameters
NAME MQHIII
EXPNO 225
PROCNO 3
F2 - Acquisition Parameters
Date_ 20040416
Time 14.14
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127501 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.252 ppm
F2 -2037.59 Hz
PPMCM 11.0[illegible]9 ppm/cm
HZCM 1108.[illegible] Hz/cm

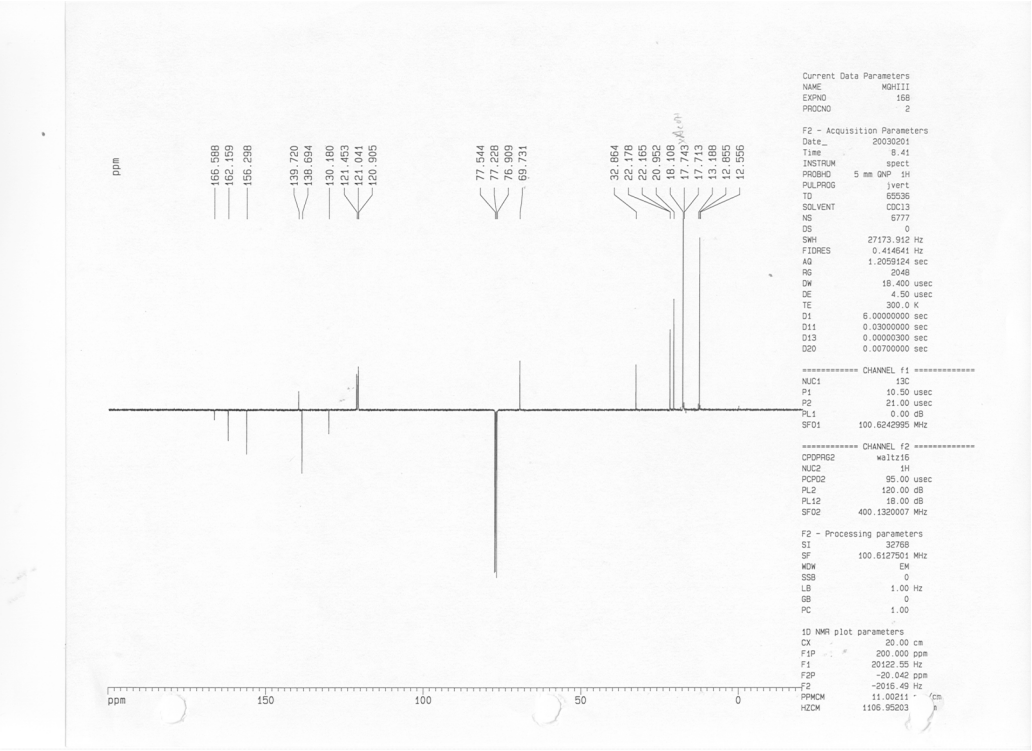
3b.


IV-55 AMX360 proton NMR QNP probe
ppm
8.35
8.34
7.14
7.00
6.98
6.55
6.19
2.79
2.77
2.33
2.24
2.17
1.28
1.26
1.25
1.23
1.23
1.21
1.20
1.19
1.11
1.09
0.83
0.82
0.80
0.00
Integral
1.000
0.805
0.763
1.770
0.793
1.227
5.762
3.483
6.063
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 55
PROCNO 3
F2 - Acquisition Parameter
Date_ 20040404
Time 9.33
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 5045.411 Hz
FIDRES 0.153974 Hz
AQ 3.2475071 se
RG 1024
DW 99.100 us
DE 141.57 us
TE 300.0 K
HL1 1 dB
D1 3.00000000 se
P1 9.00 us
SFO1 360.1358091 MH
NUCLEUS 1H
F2 - Processing parameters
SI 16384
SF 360.1339835 MH
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 pp
F1 3601.34 Hz
F2P -1.936 pp
F2 -697.09 Hz
PPMCM 0.59678 pp
HZCM 214.92159 Hz

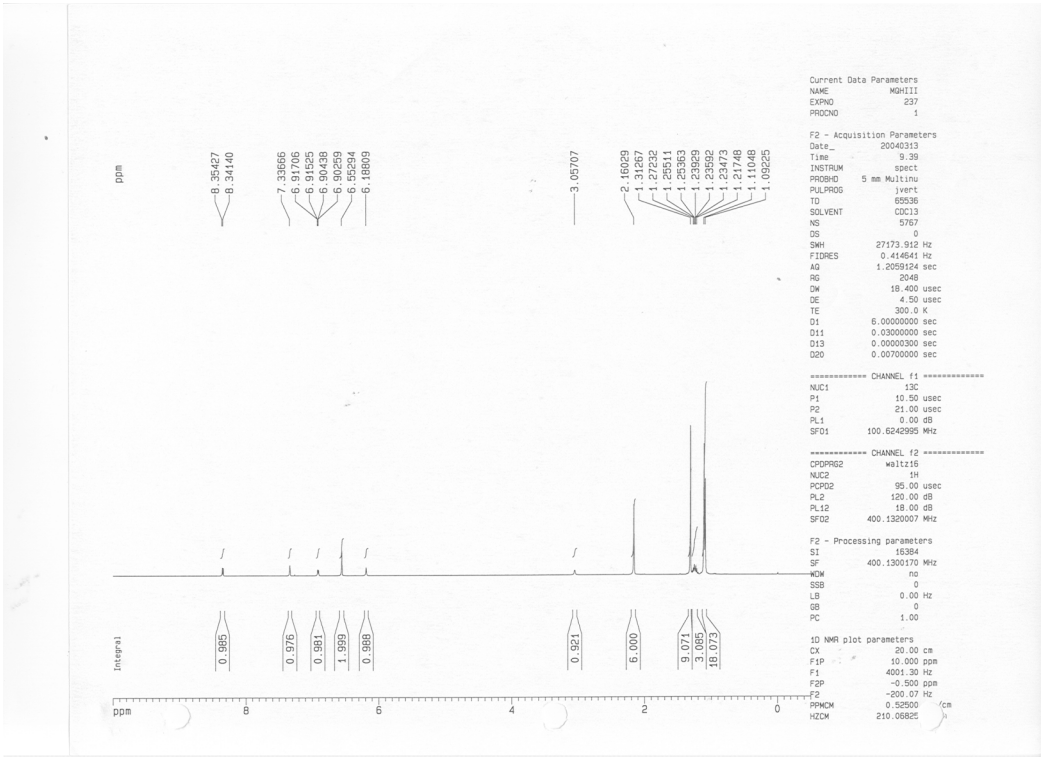

IV-55 AMX360 C-13 NMR QNP Probe
ppm
163.353
155.806
148.603
138.814
131.541
131.421
120.776
119.282
118.537
118.436
77.583
77.230
76.877
70.155
42.025
37.093
37.038
30.038
20.902
20.866
18.172
14.097
12.981
ppm
150
100
50
0
Current Data Parameters
NAME MQHIV
EXPNO 55
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040404
Time 7.20
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod.sb
TD 65536
SOLVENT CDCl3
NS 4492
DS 0
SWH 21834.061 Hz
FIDRES 0.333161 Hz
AQ 1.5008202 sec
RG 16384
DW 22.900 usec
DE 28.62 usec
TE 300.0 K
P1 8.00 usec
CNST2 145.0000000
CNST11 1.0000000
D20 0.0068966 sec
HL1 13 dB
D1 5.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648644 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 65536
SF 90.5557369 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 20.00 cm
F1P 221.214 ppm
F1 20032.18 Hz
F2P -19.841 ppm
F2 -1796.71 Hz
PPMCM 12.05274 ppm/cm
HZCM 1 1434 Hz/cm

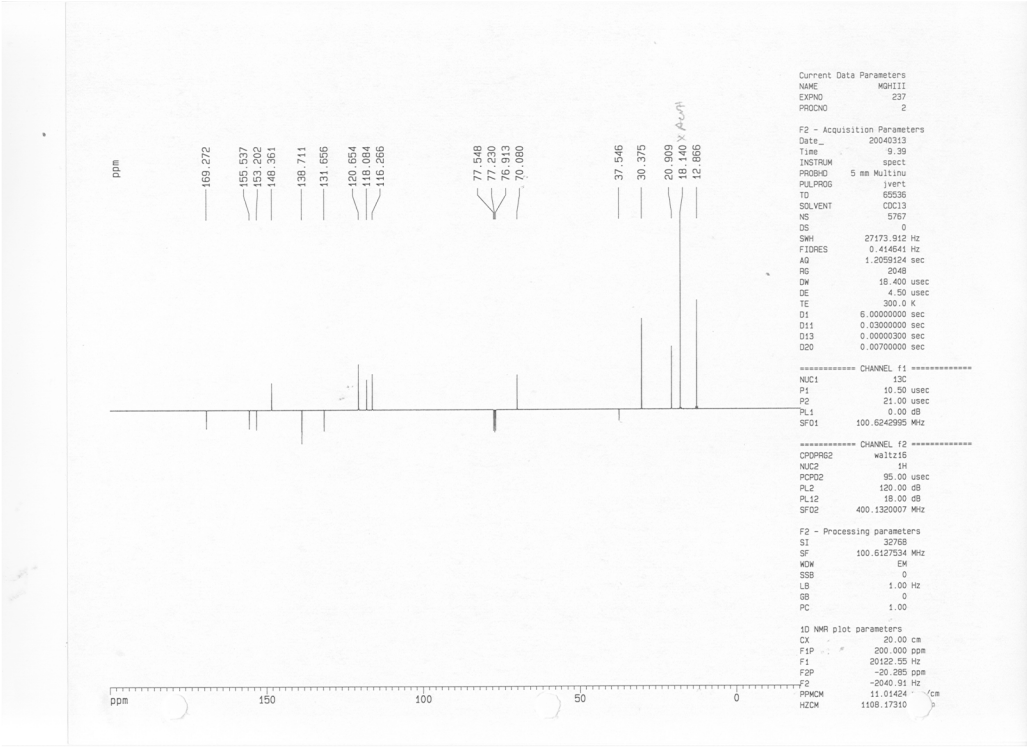
3c.


III-168 (pure)
ppm
8.3650
8.3497
7.6970
7.4587
7.4429
7.2408
6.5337
6.3292
5.4540
4.9712
4.9653
3.9073
3.6375
3.6185
3.6018
3.5842
3.5661
2.1301
1.4036
1.3862
1.3811
1.3636
1.2592
1.2398
1.2208
1.2022
1.1845
1.1738
1.1674
1.0741
1.0560
1.0405
1.0335
1.0232
0.8824
0.0312
Integral
1.066
1.060
1.023
2.072
1.007
1.087
6.000
6.568
4.066
18.857
Current Data Parameters
NAME MQHIII
EXPNO 168
PROCNO 4
F2 - Acquisition Parameters
Date_ 20030201
Time 8.41
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 6777
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 pp
HZCM 220.69171 Hz

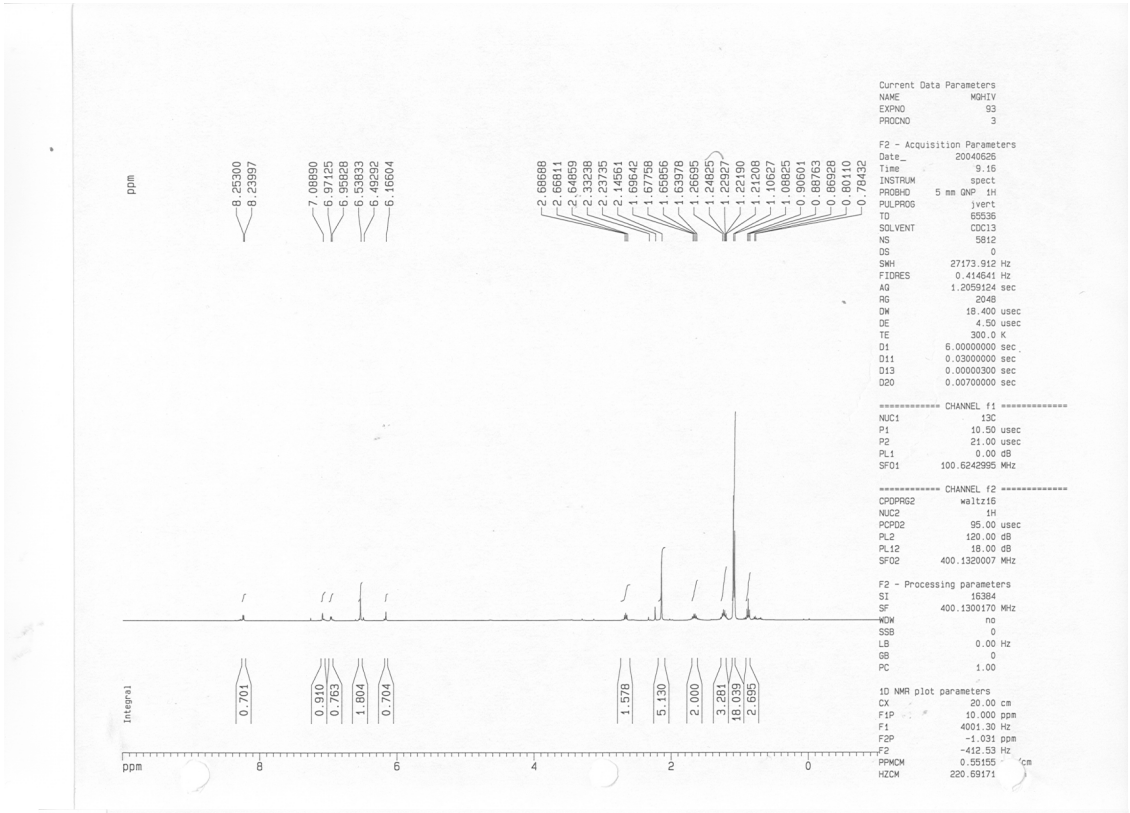

ppm
166.588
162.159
156.298
139.720
138.694
130.180
121.453
121.041
120.905
77.544
77.228
76.909
69.731
32.864
22.178
22.165
20.952
18.109
17.743
17.713
13.188
12.855
12.556
Current Data Parameters
NAME MQHIII
EXPNO 168
PROCNO 2
F2 - Acquisition Parameters
Date_ 20030201
Time 8.41
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 6777
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127501 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.042 ppm
F2 -2016.49 Hz
PPMCM 11.00211
HZCM 1106.95203

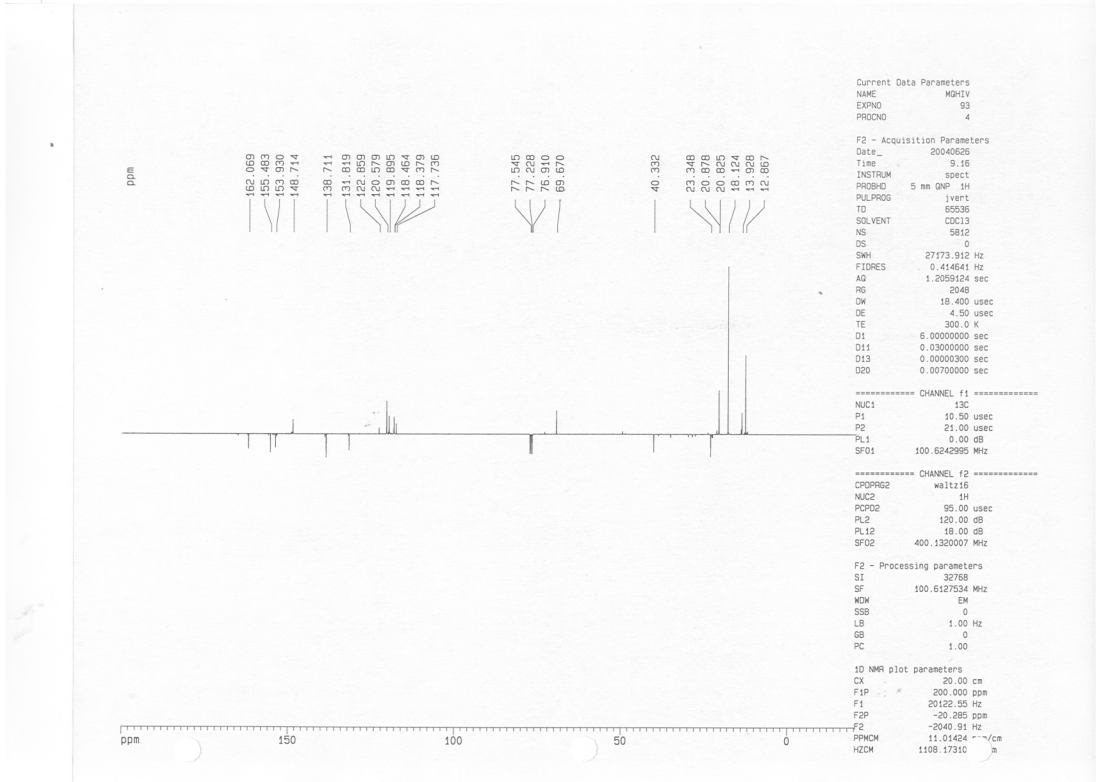
3d.


ppm
8.35427
8.34140
7.33666
6.91706
6.91525
6.90438
6.90259
6.55294
6.18809
3.05707
2.16029
1.31267
1.27232
1.25511
1.25363
1.23929
1.23592
1.23473
1.21748
1.11048
1.09225
Integral
0.985
0.976
0.981
1.999
0.988
0.921
6.000
9.071
3.085
18.073
ppm
8
6
4
2
0
Current Data Parameters
NAME MGHIII
EXPNO 237
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040313
Time 9.39
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5767
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 /cm
HZCM 210.06825

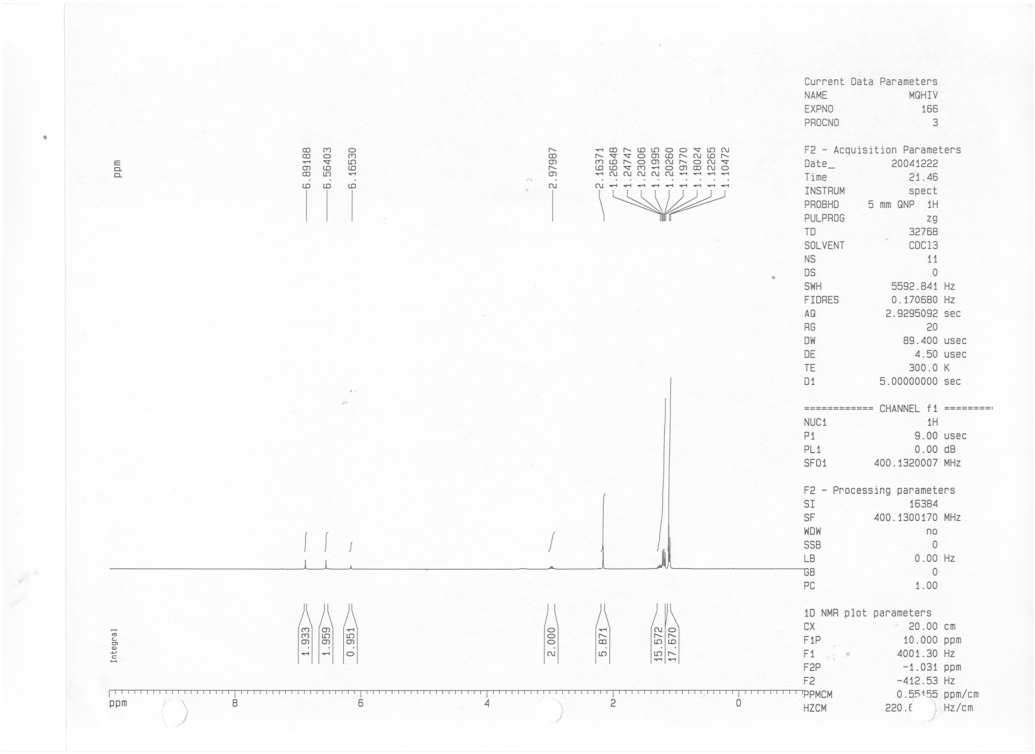

ppm
169.272
155.537
153.202
148.361
138.711
131.656
120.654
118.084
116.266
77.548
77.230
76.913
76.080
37.546
30.375
20.909
18.140
12.866
ppm
150
100
50
0
Current Data Parameters
NAME MGHIII
EXPNO 237
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040313
Time 9.39
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5767
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.285 ppm
F2 -2040.91 Hz
PPMCM 11.01424 /cm
HZCM 1108.17310

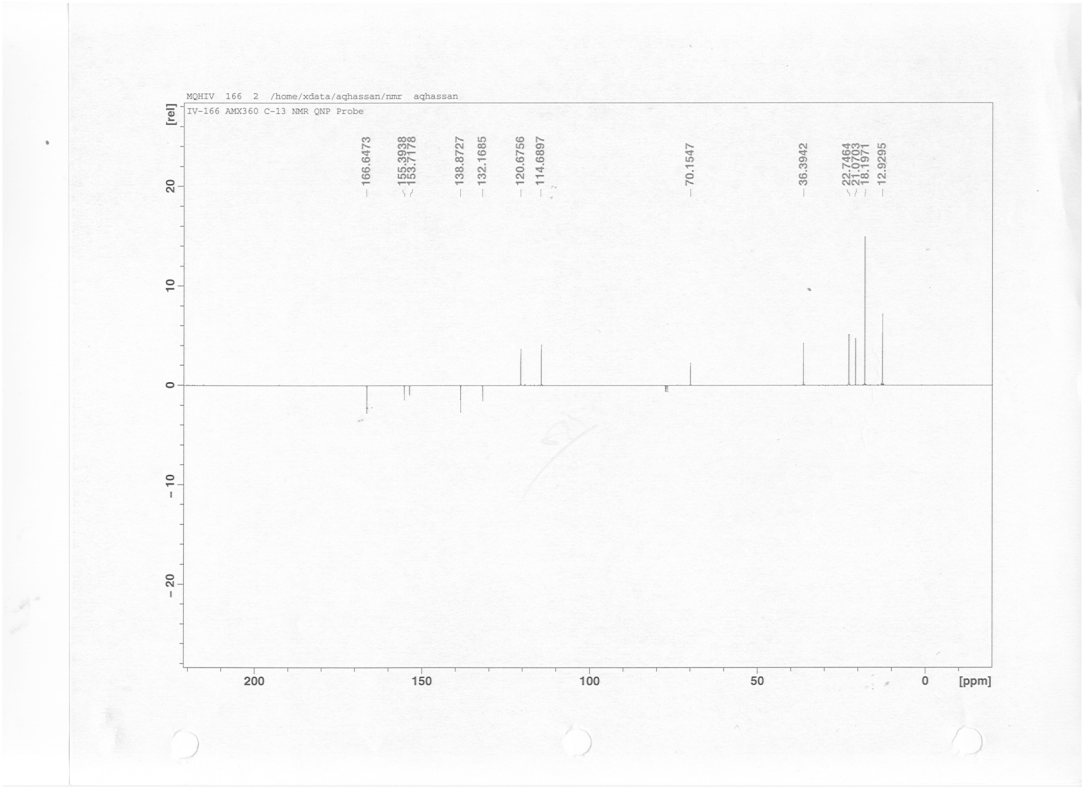
3e.


ppm
8.25300
8.23997
7.08890
6.97125
6.95828
6.53833
6.49292
6.16604
2.68688
2.66811
2.64859
2.33238
2.23735
2.14561
1.69642
1.67758
1.65856
1.63978
1.26695
1.24825
1.22927
1.22190
1.21208
1.10627
1.08825
0.90601
0.88763
0.86928
0.80110
0.78432
Integral
0.701
0.910
0.763
1.804
0.704
1.578
5.130
2.000
3.281
18.039
2.695
ppm
8
6
4
2
0
Current Data Parameters
NAME MGHIV
EXPNO 93
PROCNO 3
F2 - Acquisition Parameters
Date_ 20040626
Time 9.16
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5812
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.69171 Hz

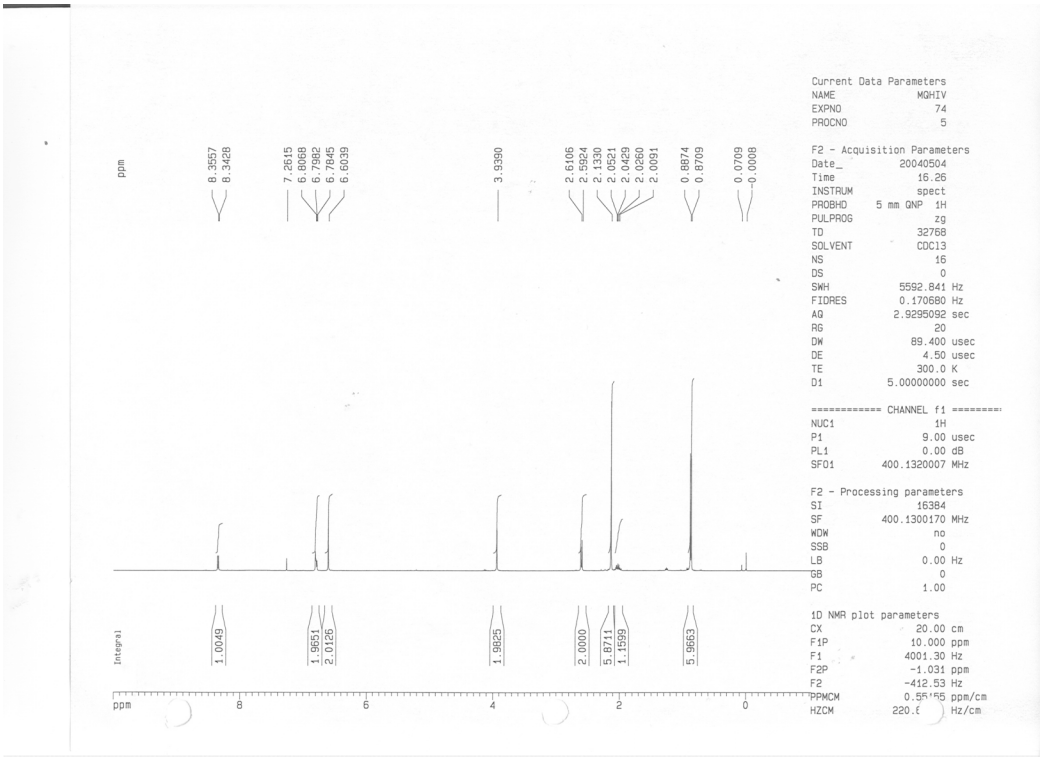

ppm
162.069
155.483
153.930
148.714
138.711
131.819
122.859
120.579
119.695
118.464
118.379
117.736
77.545
77.228
76.910
69.670
40.332
23.348
20.678
20.625
18.124
13.928
12.867
ppm
150
100
50
0
Current Data Parameters
NAME MGHIV
EXPNO 93
PROCNO 4
F2 - Acquisition Parameters
Date_ 20040626
Time 9.16
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5812
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.285 ppm
F2 -2040.91 Hz
PPMCM 11.01424 ppm/cm
HZCM 1108.17310 Hz

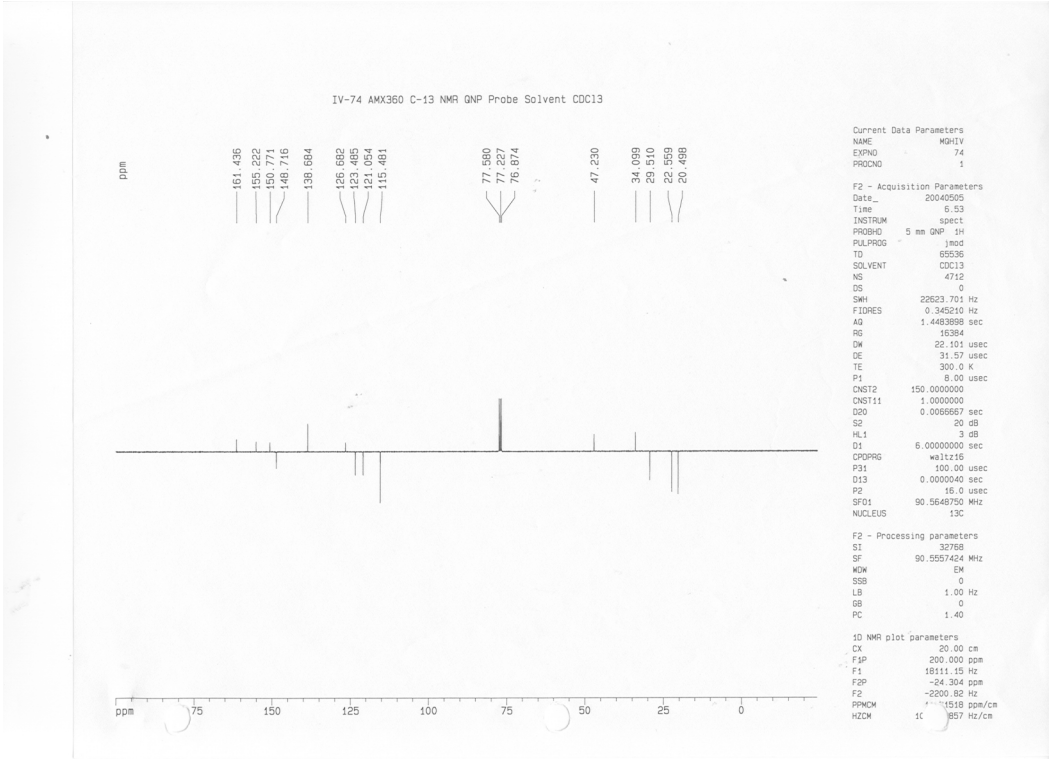
3f.


ppm
6.89188
6.56403
6.16530
2.97987
2.16371
1.26648
1.24747
1.23006
1.21995
1.20260
1.19770
1.18024
1.12265
1.10472
Integral
1.933
1.959
0.951
2.000
5.871
15.572
17.670
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 166
PROCNO 3
F2 - Acquisition Parameters
Date_ 20041222
Time 21.46
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.6 Hz/cm

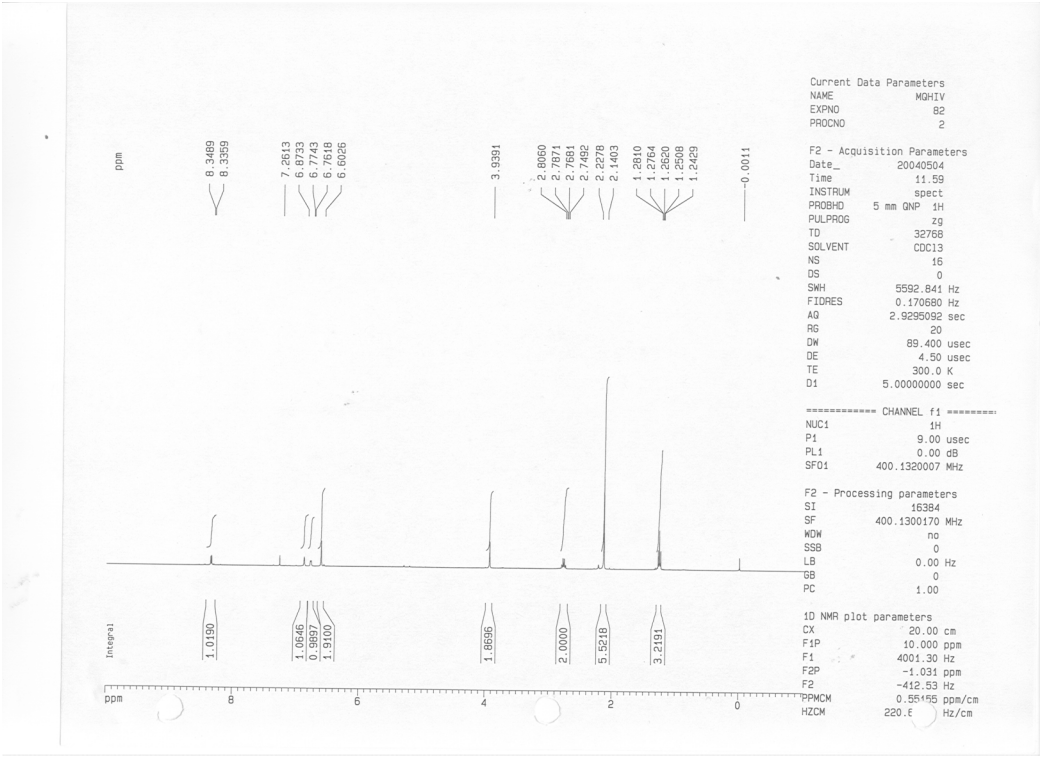

MQHIV 166 2 /home/xdata/aqhassan/nmr aqhassan
IV-166 AMX360 C-13 NMR QNP Probe
[rel]
20
10
0
-10
-20
166.6473
155.3938
153.7178
138.8727
132.1685
120.6756
114.6897
70.1547
36.3942
22.7464
21.0703
18.1971
12.9295
200
150
100
50
0
[ppm]

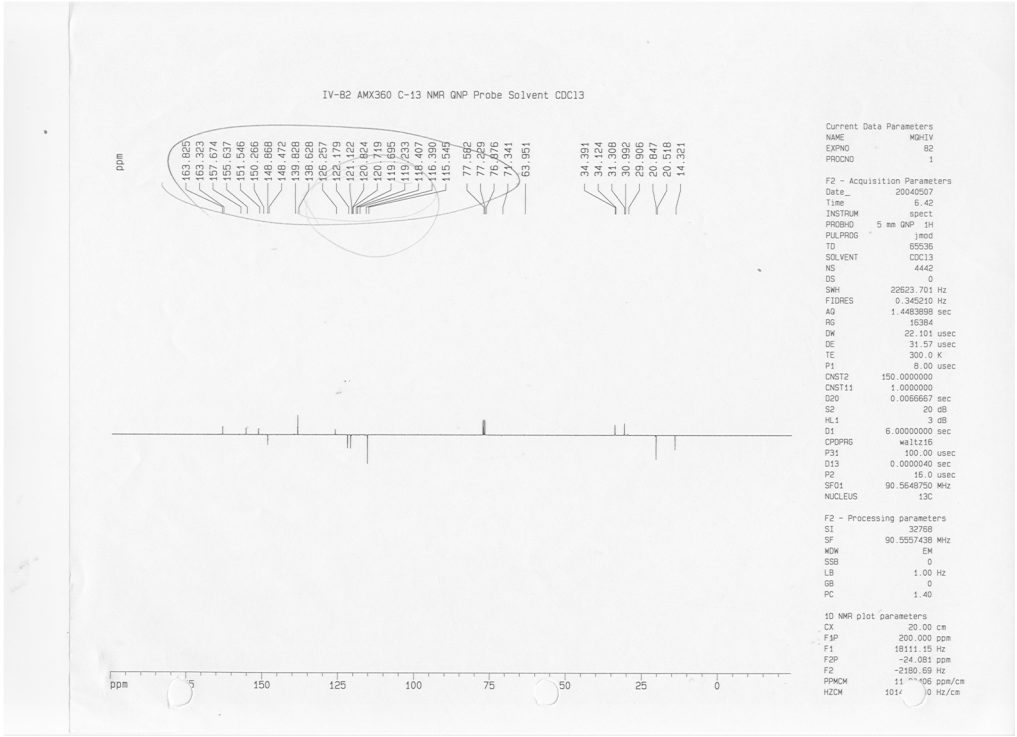
4a.


ppm
8.3557
8.3428
7.2615
6.8068
6.7982
6.7845
6.6039
3.9990
2.6106
2.5924
2.1330
2.0521
2.0429
2.0260
2.0091
0.8874
0.8709
0.0709
-0.0008
Integral
1.0049
1.9651
2.0126
1.9825
2.0000
5.8711
1.1599
5.9663
Current Data Parameters
NAME MQHIV
EXPNO 74
PROCNO 5
F2 - Acquisition Parameters
Date_ 20040504
Time 16.26
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.6 Hz/cm

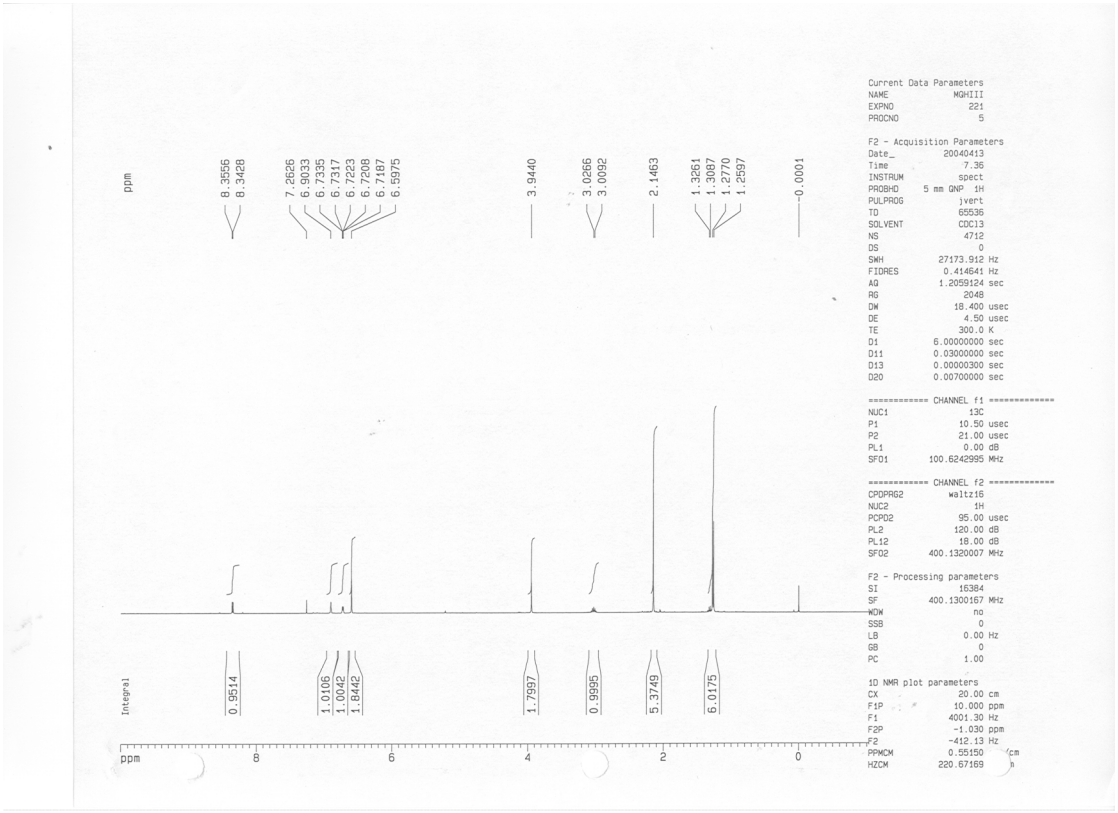

IV-74 AMX360 C-13 NMR QNP Probe Solvent CDCl3
ppm
161.436
155.222
150.771
148.716
138.684
126.682
123.485
121.054
115.481
77.580
77.227
76.874
47.230
34.099
29.510
22.559
20.498
Current Data Parameters
NAME MQHIV
EXPNO 74
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040505
Time 6.53
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 4712
DS 0
SWH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4483898 sec
RG 16384
DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.00 usec
CNST2 150.0000000
CNST11 1.0000000
D20 0.0066667 sec
SI 20 dB
HL1 3 dB
D1 6.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648750 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.5557424 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 18111.15 Hz
F2P -24.304 ppm
F2 -2200.82 Hz
PPMCM 1518 ppm/cm
HZCM 1857 Hz/cm

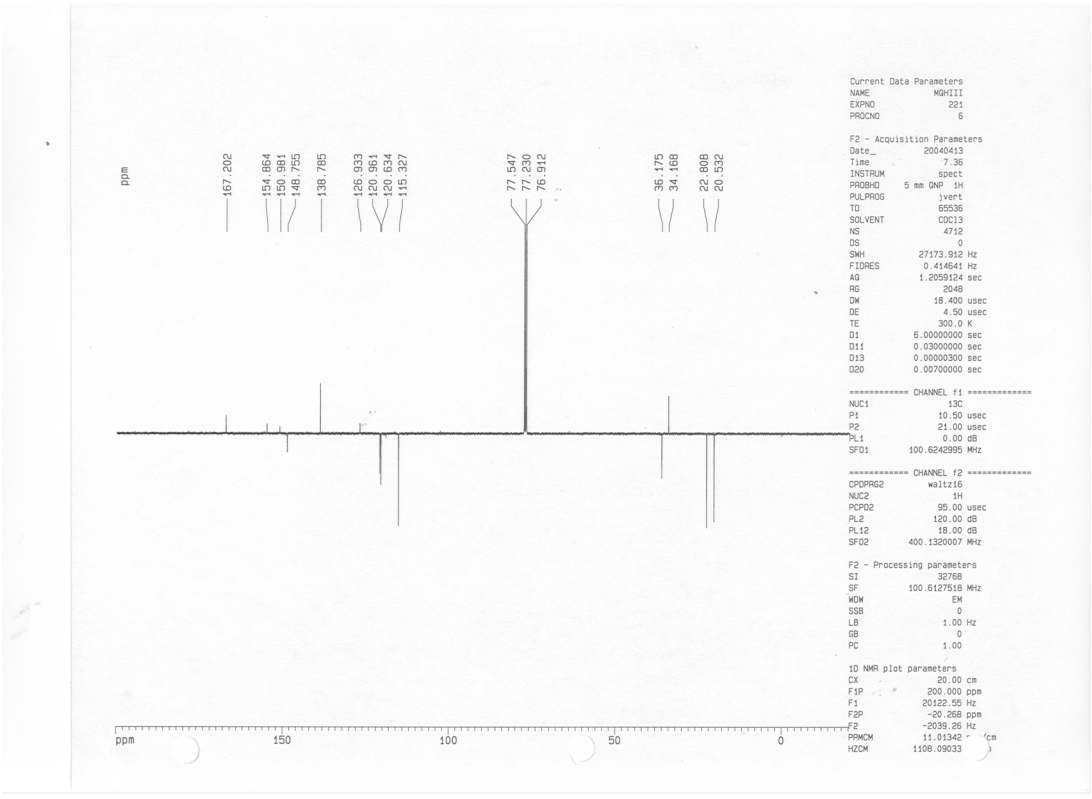
4b.


ppm
8.3489
8.3359
7.2613
6.8733
6.7743
6.7618
6.6026
3.9391
2.8060
2.7971
2.7681
2.7492
2.2278
2.1403
1.2810
1.2764
1.2620
1.2508
1.2429
-0.0011
Integral
1.0190
1.0646
0.9897
1.9100
1.8696
2.0000
5.5218
3.2191
Current Data Parameters
NAME MQHIV
EXPNO 82
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040504
Time 11.59
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.6 Hz/cm

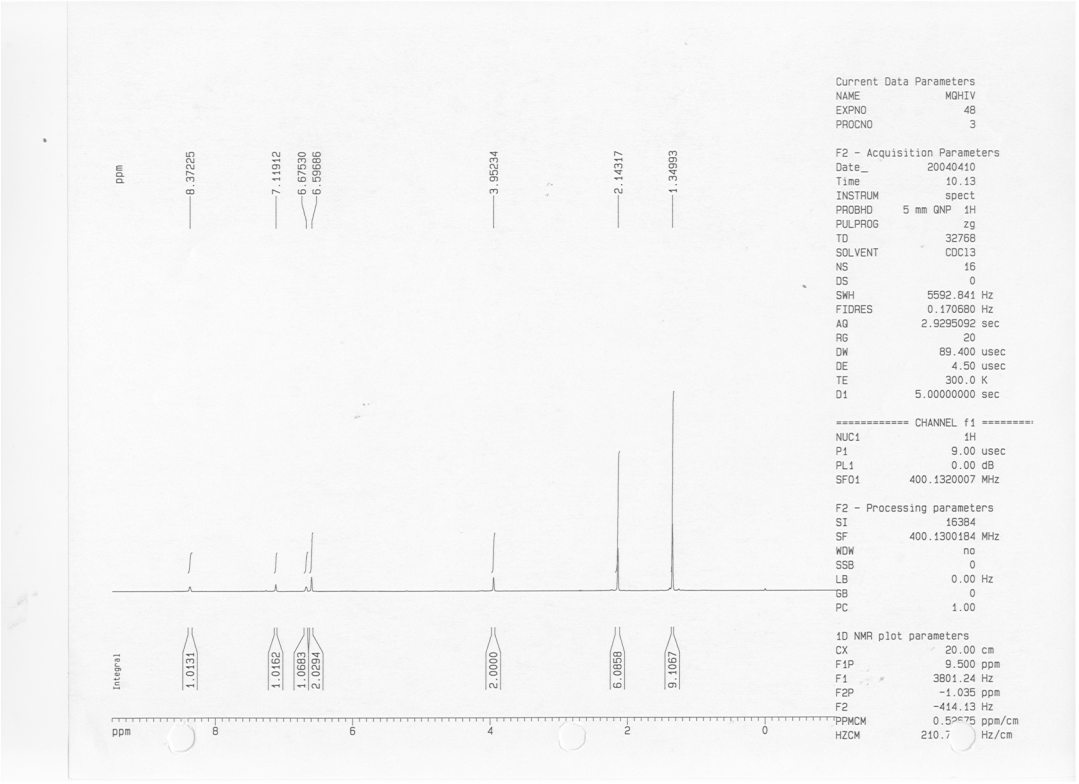

IV-82 AMX360 C-13 NMR QNP Probe Solvent CDCl3
ppm
163.825
163.323
157.674
155.637
151.546
150.266
148.868
148.472
139.828
138.628
126.257
122.179
121.122
120.824
120.719
119.695
119.233
118.407
116.390
115.545
77.582
77.269
76.476
74.341
63.951
34.391
34.124
31.308
30.992
29.906
20.647
20.518
14.321
Current Data Parameters
NAME MQHIV
EXPNO 82
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040507
Time 6.42
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 4442
DS 0
SWH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4483898 sec
RG 16384
DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.00 usec
CNST2 150.0000000
CNST11 1.0000000
D20 0.0066667 sec
S2 20 dB
HL1 3 dB
D1 6.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648750 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.5557438 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 18111.15 Hz
F2P -24.081 ppm
F2 -2180.69 Hz
PPMCM 11.[illegible]06 ppm/cm
HZCM 1014.[illegible]0 Hz/cm

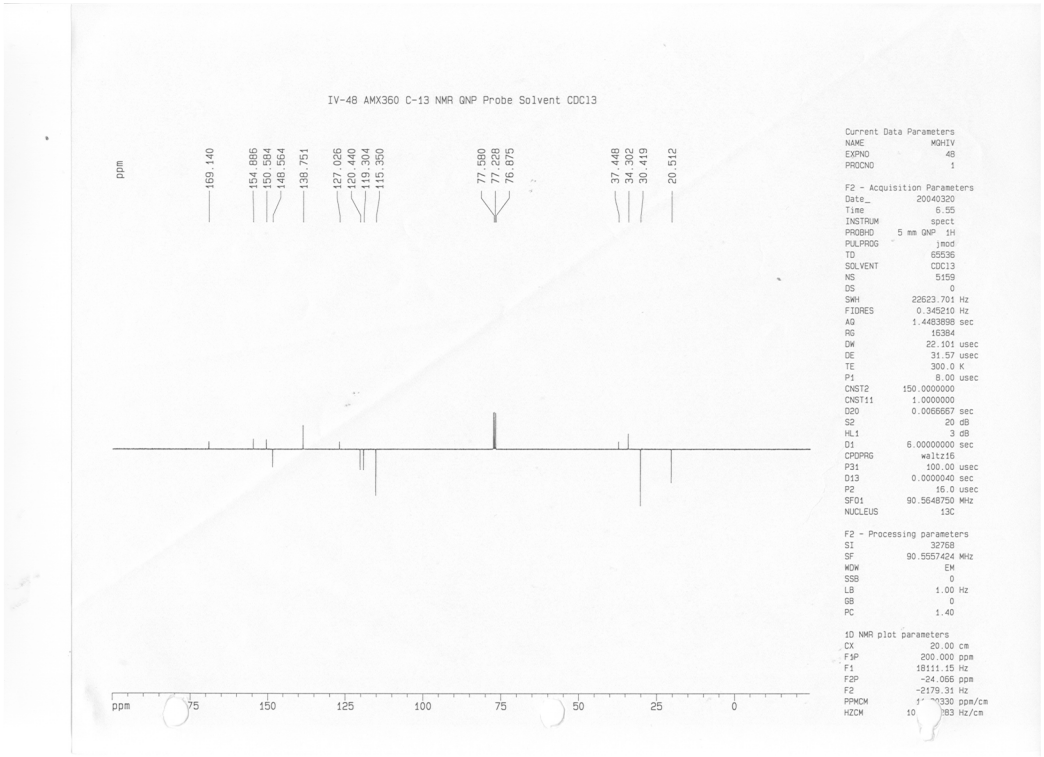
4c.


ppm
8.3556
8.3428
7.2626
6.9033
6.7335
6.7317
6.7223
6.7208
6.7187
6.5975
3.9440
3.0266
3.0092
2.1463
1.3261
1.3087
1.2770
1.2597
0.0001
Integral
0.9514
1.0106
1.0042
1.8442
1.7997
0.9995
5.3749
6.0175
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIII
EXPNO 221
PROCNO 5
F2 - Acquisition Parameters
Date_ 20040413
Time 7.36
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 4712
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300167 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.030 ppm
F2 -412.13 Hz
PPMCM 0.55150 ppm/cm
HZCM 220.67169 Hz/cm

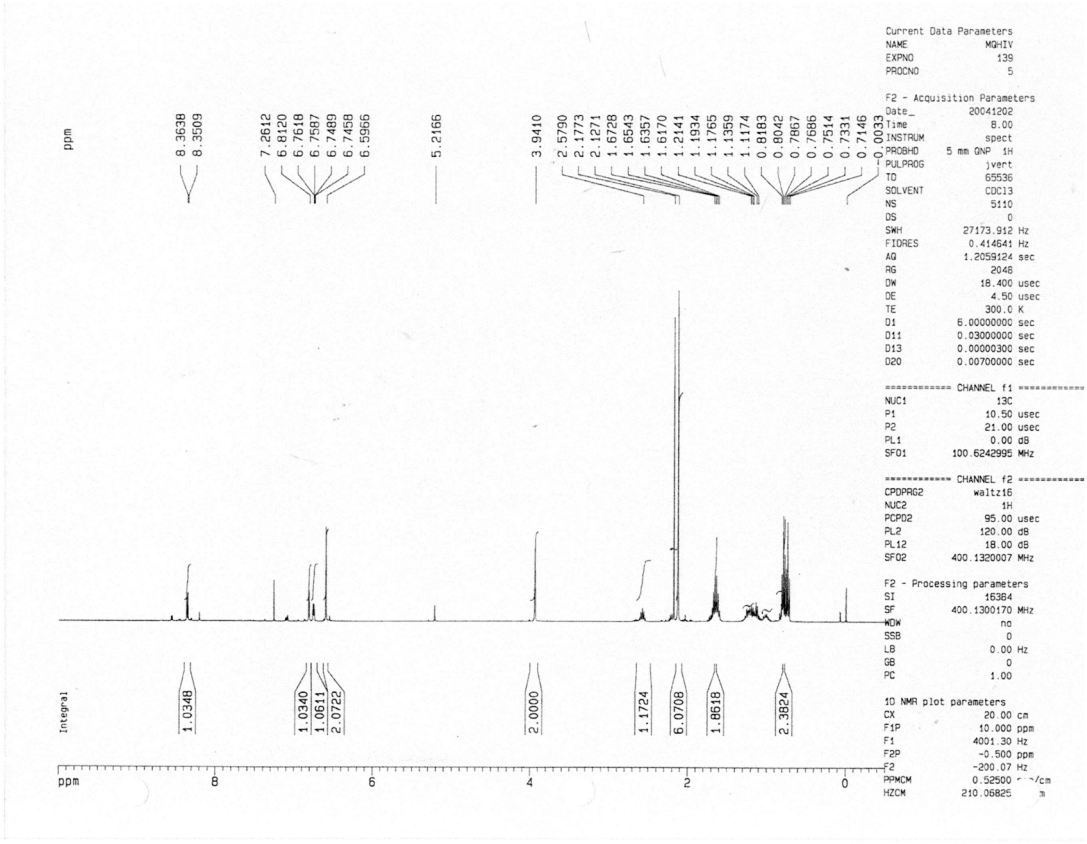

ppm
167.202
154.864
150.981
148.755
138.785
126.933
120.961
120.634
115.327
77.547
77.230
76.912
36.175
34.168
22.808
20.532
ppm
150
100
50
0
Current Data Parameters
NAME MQHIII
EXPNO 221
PROCNO 6
F2 - Acquisition Parameters
Date_ 20040413
Time 7.36
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 4712
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127518 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.268 ppm
F2 -2039.26 Hz
PPMCM 11.01342 ppm/cm
HZCM 1108.09033 Hz/cm

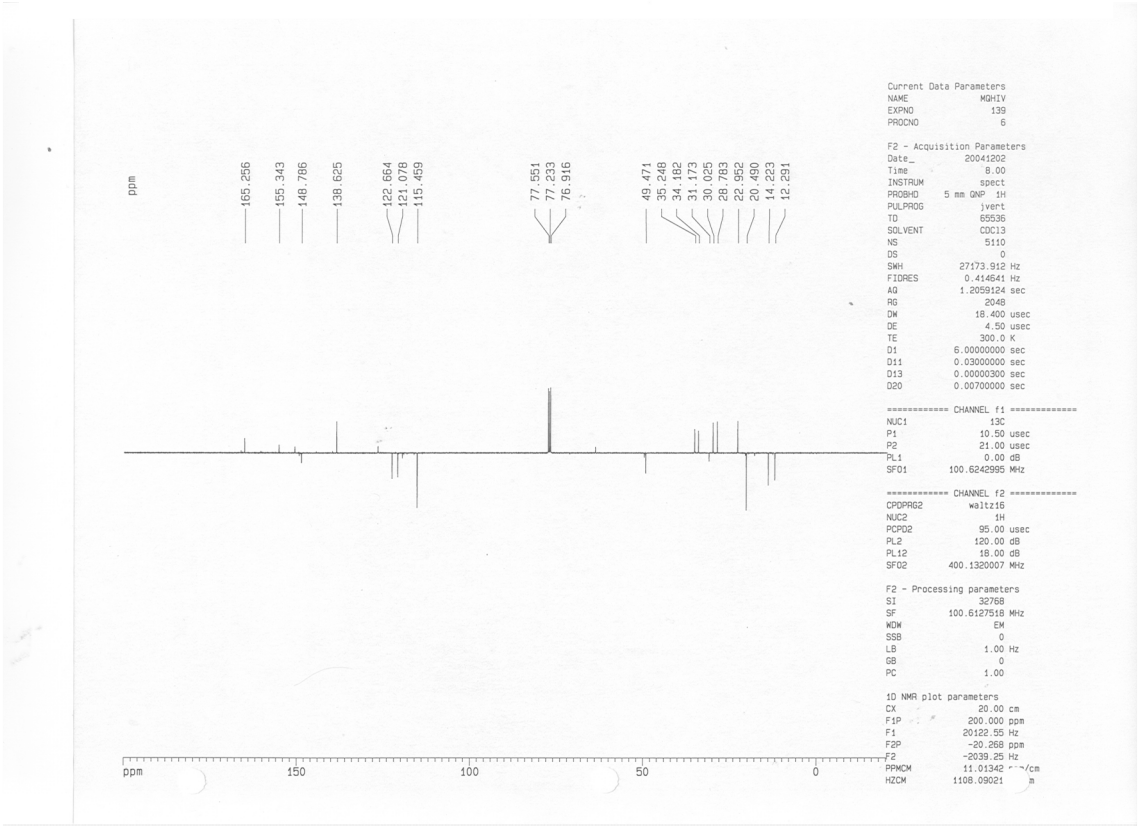
4d.


ppm
8.37225
7.11912
6.67530
6.59686
3.95234
2.14317
1.34993
Integral
1.0131
1.0162
1.0683
2.0294
2.0000
6.0658
9.1067
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 48
PROCNO 3
F2 - Acquisition Parameters
Date_ 20040410
Time 10.13
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300184 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 9.500 ppm
F1 3801.24 Hz
F2P -1.035 ppm
F2 -414.13 Hz
PPMCM 0.52675 ppm/cm
HZCM 210.7 Hz/cm

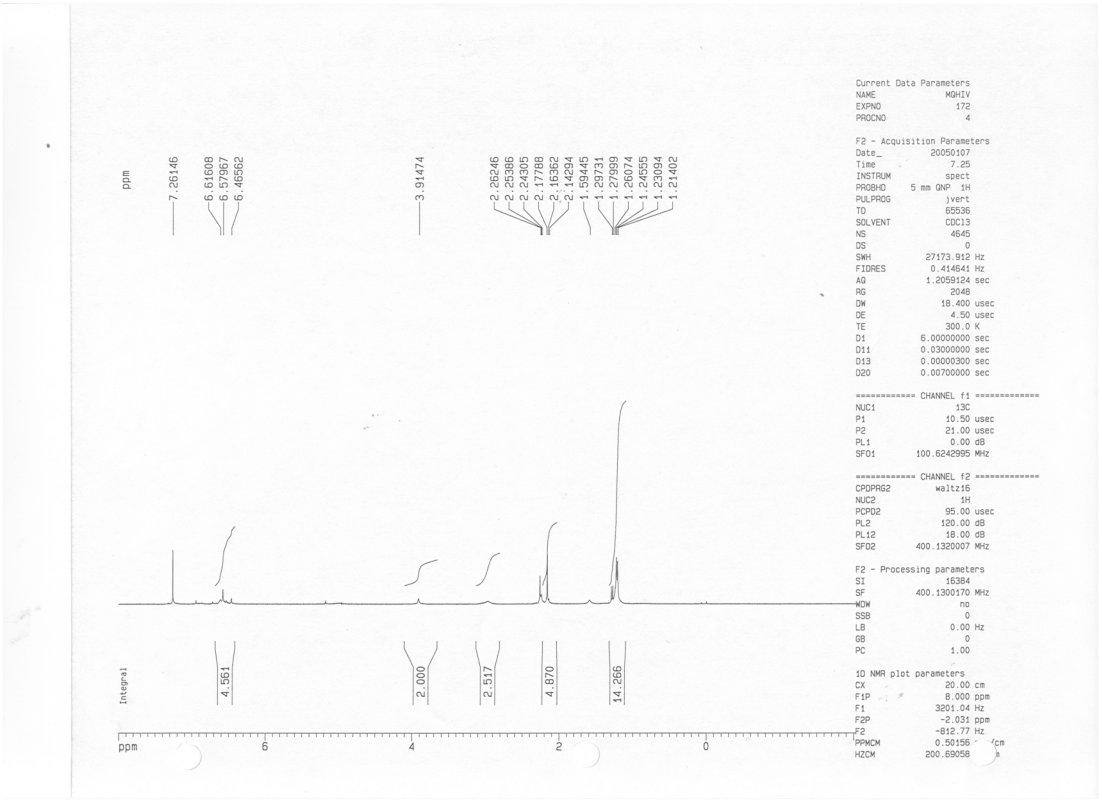

IV-48 AMX360 C-13 NMR QNP Probe Solvent CDCl3
ppm
169.140
154.886
150.584
148.564
138.751
127.026
120.440
119.304
115.350
77.580
77.228
76.875
37.448
34.302
30.419
20.512
ppm
175
150
125
100
75
50
25
0
Current Data Parameters
NAME MQHIV
EXPNO 48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040320
Time 6.55
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 5159
DS 0
SWH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4483898 sec
RG 16384
DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.00 usec
CNST2 150.0000000
CNST11 1.0000000
D20 0.0066667 sec
S2 20 dB
HL1 3 dB
D1 6.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648750 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.5557424 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 18111.15 Hz
F2P -24.066 ppm
F2 -2179.31 Hz
PPMCM 1.00330 ppm/cm
HZCM 10.083 Hz/cm

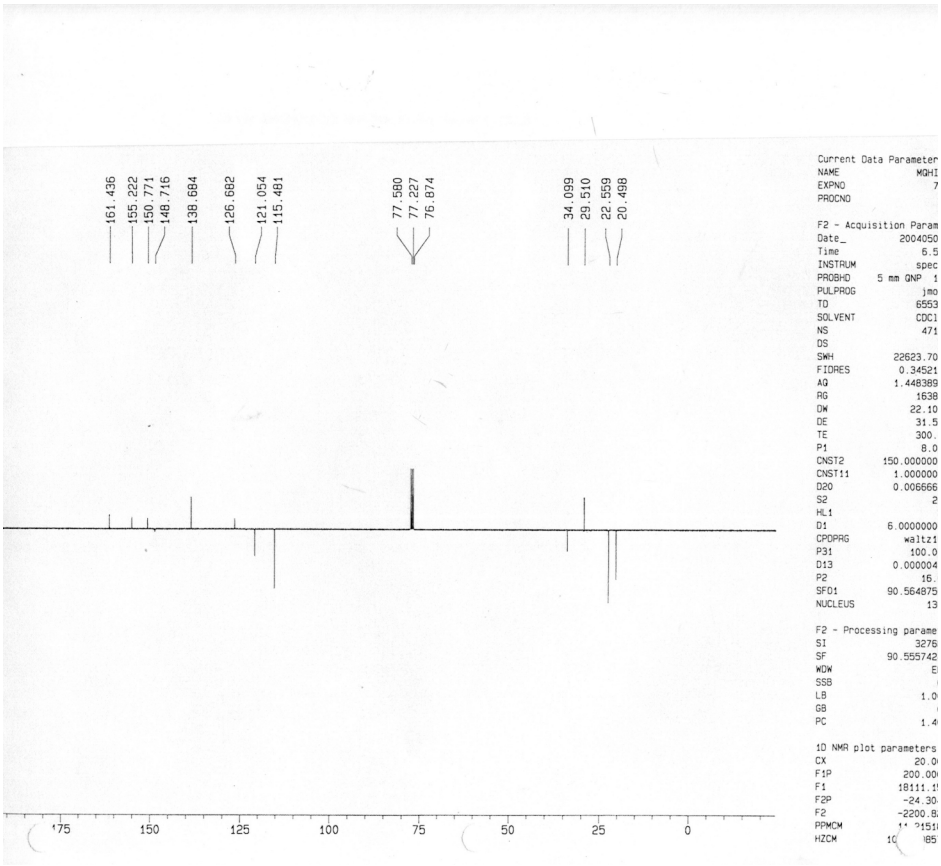
4e.


ppm
8.3638
8.3509
7.2612
6.8120
6.7618
6.7587
6.7489
6.7458
6.5966
5.2166
3.9410
2.5790
2.1773
2.1271
1.6728
1.6543
1.6357
1.6170
1.2141
1.1934
1.1765
1.1359
1.1174
0.8183
0.8042
0.7867
0.7686
0.7514
0.7331
0.7146
0.0033
Integral
1.0348
1.0340
1.0611
2.0722
2.0000
1.1724
6.0708
1.8618
2.3824
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 139
PROCNO 5
F2 - Acquisition Parameters
Date_ 20041202
Time 8.00
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5110
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500
HZCM 210.06825

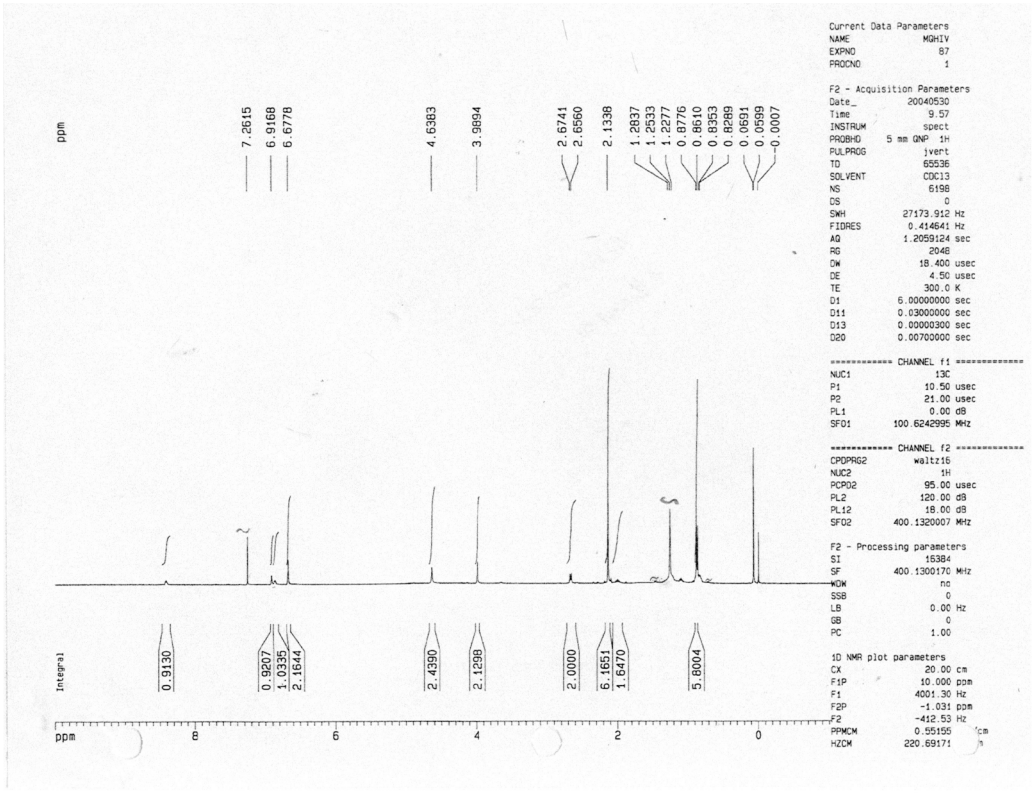

ppm
165.256
155.343
148.786
138.625
122.664
121.078
115.459
77.551
77.233
76.916
49.471
35.248
34.182
31.173
30.025
28.783
22.952
20.490
14.223
12.291
ppm
150
100
50
0
Current Data Parameters
NAME MQHIV
EXPNO 139
PROCNO 6
F2 - Acquisition Parameters
Date_ 20041202
Time 8.00
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5110
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127518 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.268 ppm
F2 -2039.25 Hz
PPMCM 11.01342
HZCM 1108.09021

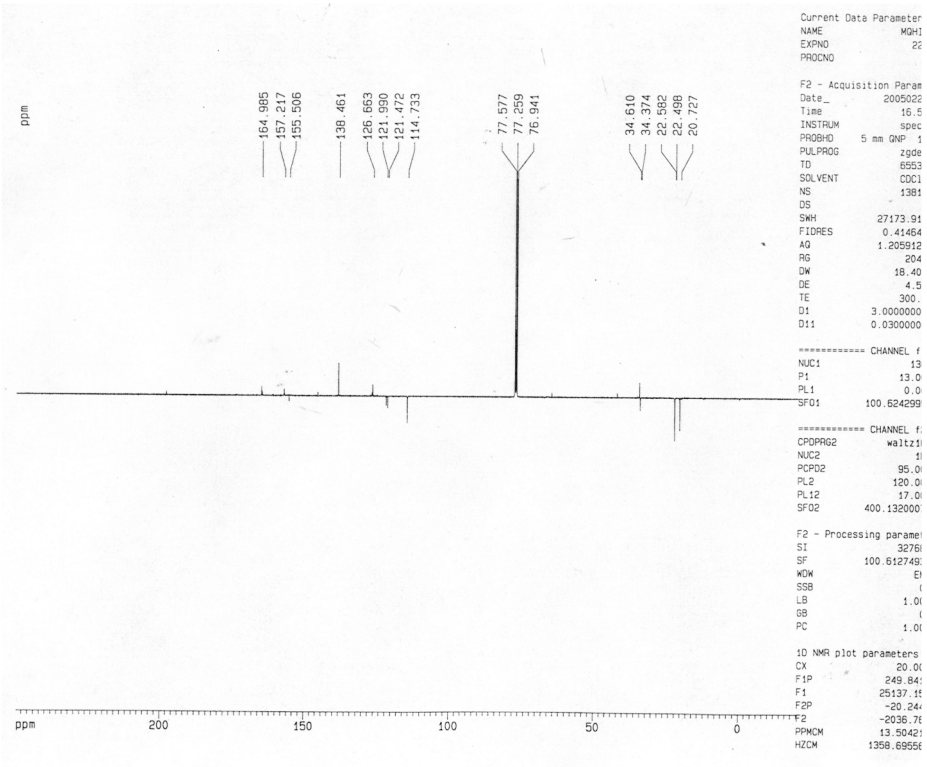
4f.


ppm
7.26146
6.61608
6.57967
6.46562
3.91474
2.26246
2.25386
2.24305
2.17788
2.16362
2.14294
1.59445
1.29731
1.27999
1.26074
1.24555
1.23094
1.21402
Integral
4.561
2.000
2.517
4.870
14.266
ppm
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 172
PROCNO 4
F2 - Acquisition Parameters
Date_ 20050107
Time 7.26
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 4545
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -2.031 ppm
F2 -812.77 Hz
PPMCM 0.50156 /cm
HZCM 200.69058

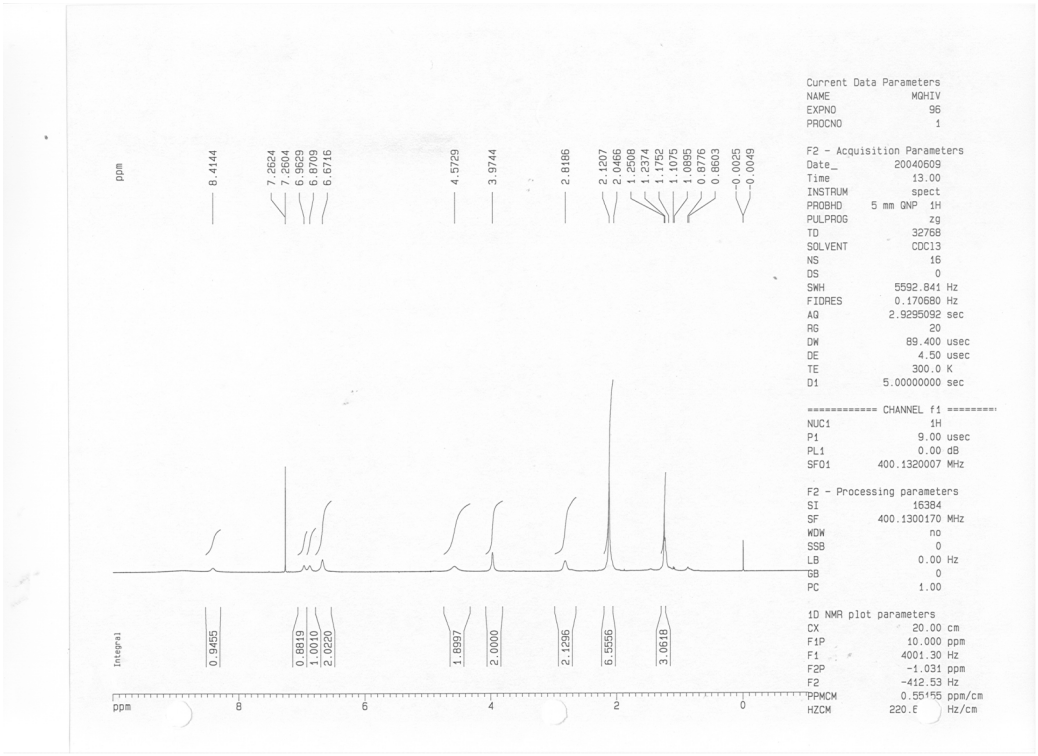

161.436
155.222
150.771
148.716
138.684
126.682
121.054
115.481
77.580
77.227
76.874
34.099
29.510
22.559
20.498
175
150
125
100
75
50
25
0
Current Data Parameter
NAME MQHI
EXPNO 7
PROCNO
F2 - Acquisition Param
Date_ 2004050
Time 6.5
INSTRUM spec
PROBHD 5 mm QNP 1
PULPROG jmo
TD 6553
SOLVENT CDCl
NS 471
DS
SWH 22623.70
FIDRES 0.34521
AQ 1.448389
RG 1638
DW 22.10
DE 31.5
TE 300.
P1 8.0
CNST2 150.000000
CNST11 1.000000
D20 0.006666
S2 2
HL1
D1 6.0000000
CPDPRG waltz1
P31 100.0
D13 0.000004
P2 16.
SFO1 90.564875
NUCLEUS 13
F2 - Processing parame
SI 3276
SF 90.555742
WDW E
SSB
LB 1.0
GB
PC 1.4
1D NMR plot parameters
CX 20.0
F1P 200.00
F1 18111.1
F2P -24.30
F2 -2200.8
PPMCM 11.2151
HZCM 10 165

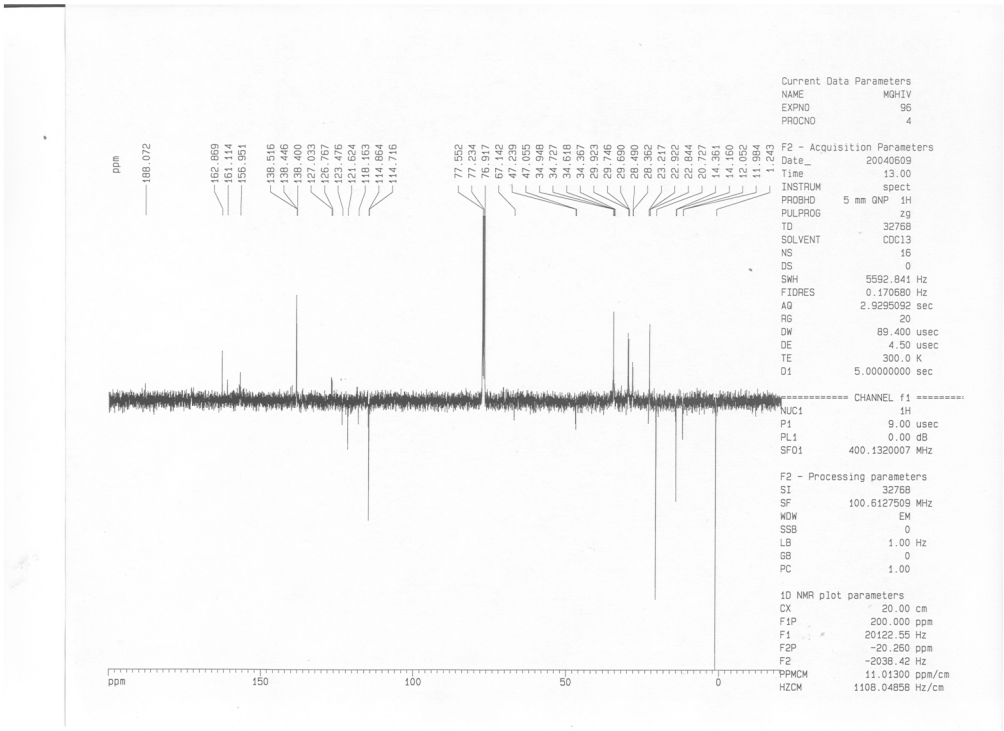
QH10.


ppm
7.2615
6.9168
6.6778
4.6383
3.9894
2.6741
2.6560
2.1338
1.2837
1.2533
1.2277
0.8776
0.8610
0.8353
0.8289
0.0691
0.0599
-0.0007
Integral
0.9130
0.9207
1.0335
2.1644
2.4390
2.1298
2.0000
6.1651
1.6470
5.8004
Current Data Parameters
NAME MQH1V
EXPNO 87
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040530
Time 9.57
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 6198
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW nd
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.69171 Hz/cm

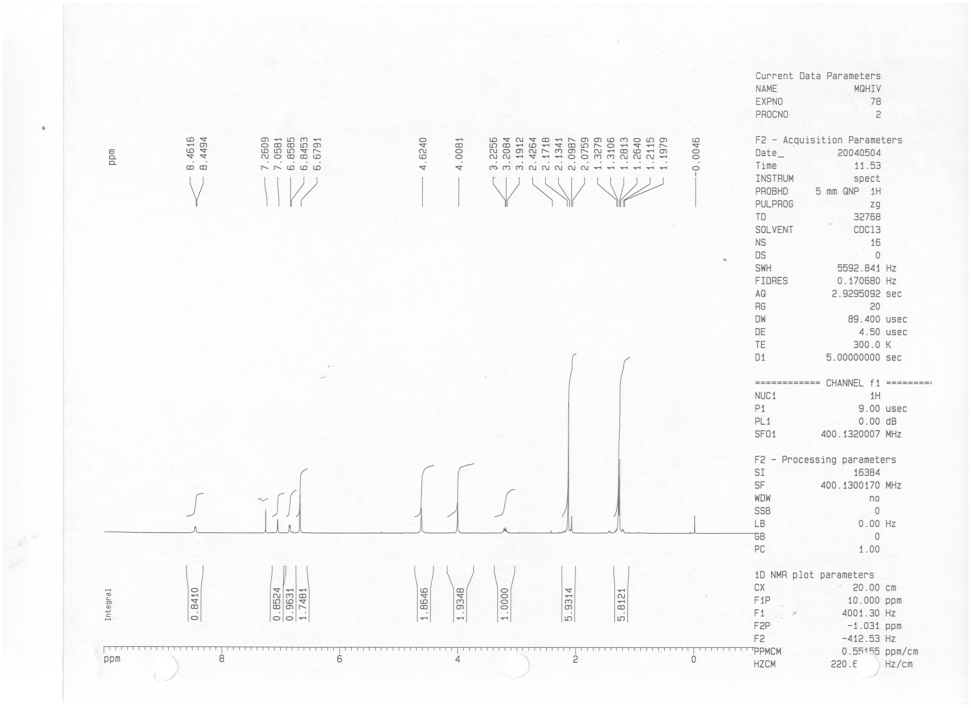

ppm
164.985
157.217
155.506
138.461
126.663
121.990
121.472
114.733
77.577
77.259
76.941
34.610
34.374
22.582
22.498
20.727
Current Data Parameter
NAME MQH1
EXPNO 22
PROCNO
F2 - Acquisition Param
Date_ 2005022
Time 16.5
INSTRUM spec
PROBHD 5 mm QNP 1
PULPROG zgde
TD 6553
SOLVENT CDCl
NS 1381
DS
SWH 27173.91
FIDRES 0.41464
AQ 1.205912
RG 204
DW 18.40
DE 4.5
TE 300.
D1 3.0000000
D11 0.0300000
CHANNEL f
NUC1 13
P1 13.0
PL1 0.0
SFO1 100.624299
CHANNEL f
CPDPRG2 waltz1
NUC2 1
PCPD2 95.0
PL2 120.0
PL12 17.0
SFO2 400.132000
F2 - Processing parame
SI 3276
SF 100.612749
WDW E
SSB
LB 1.0
GB
PC 1.0
1D NMR plot parameters
CX 20.0
F1P 249.84
F1 25137.1
F2P -20.24
F2 -2036.7
PPMCM 13.5042
HZCM 1358.6955

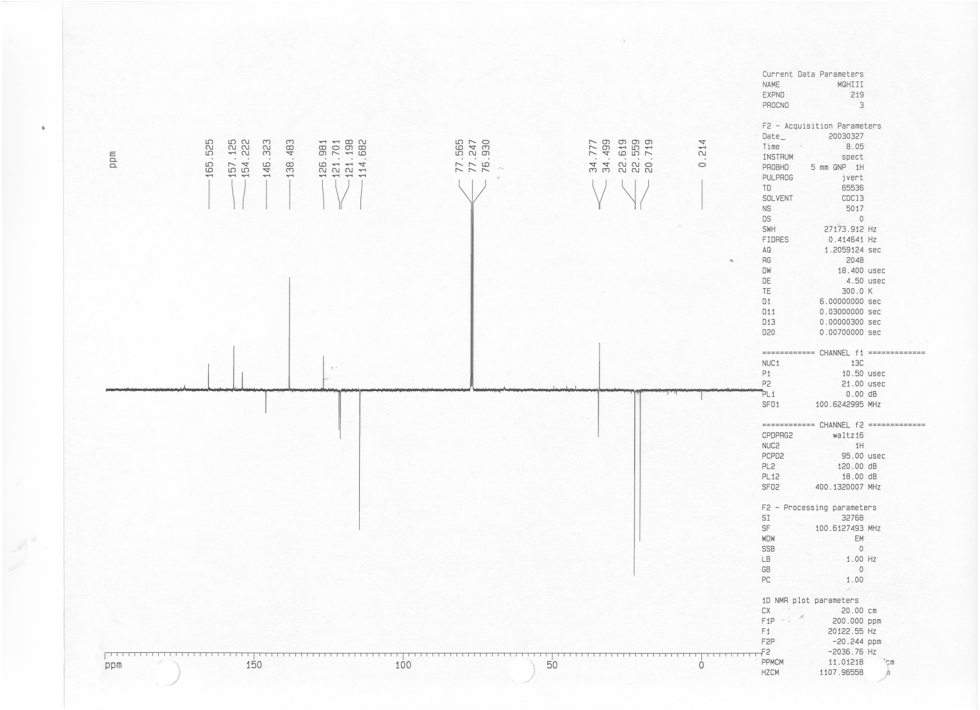
QH11.


ppm
8.4144
7.2624
7.2604
6.9629
6.8709
6.6716
4.5729
3.9744
2.8186
2.1207
2.0466
1.2508
1.2374
1.1752
1.1075
1.0895
0.8776
0.8603
-0.0025
-0.0049
Integral
0.9455
0.8819
1.0010
2.0220
1.8997
2.0000
2.1296
6.5556
3.0618
ppm
8
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 96
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040609
Time 13.00
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.6 Hz/cm

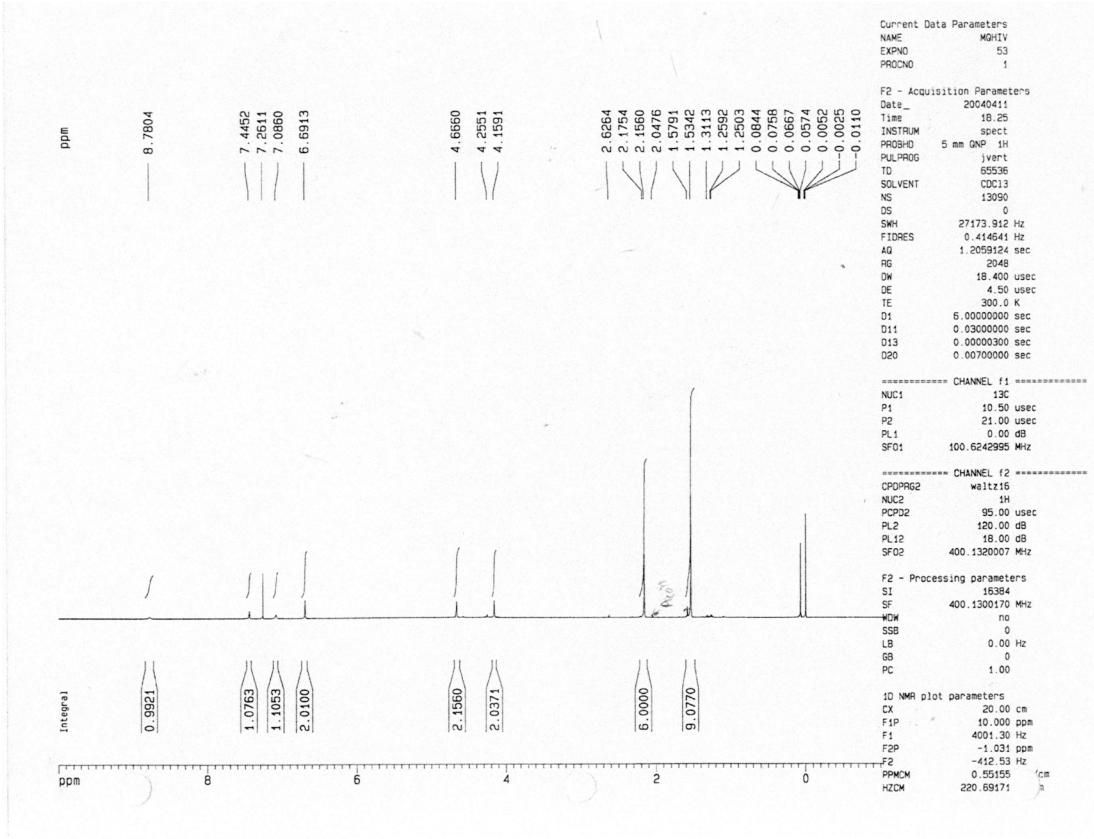

ppm
188.072
162.869
161.114
156.951
138.516
138.446
138.400
127.033
126.767
123.476
121.624
118.163
114.864
114.716
77.552
77.234
76.917
67.142
47.239
47.055
34.948
34.727
34.618
34.367
29.923
29.746
29.690
28.480
28.352
23.227
22.922
22.844
20.727
14.361
14.160
12.052
11.984
1.243
ppm
150
100
50
0
Current Data Parameters
NAME MQHIV
EXPNO 96
PROCNO 4
F2 - Acquisition Parameters
Date_ 20040609
Time 13.00
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.260 ppm
F2 -2038.42 Hz
PPMCM 11.01300 ppm/cm
HZCM 1108.04858 Hz/cm

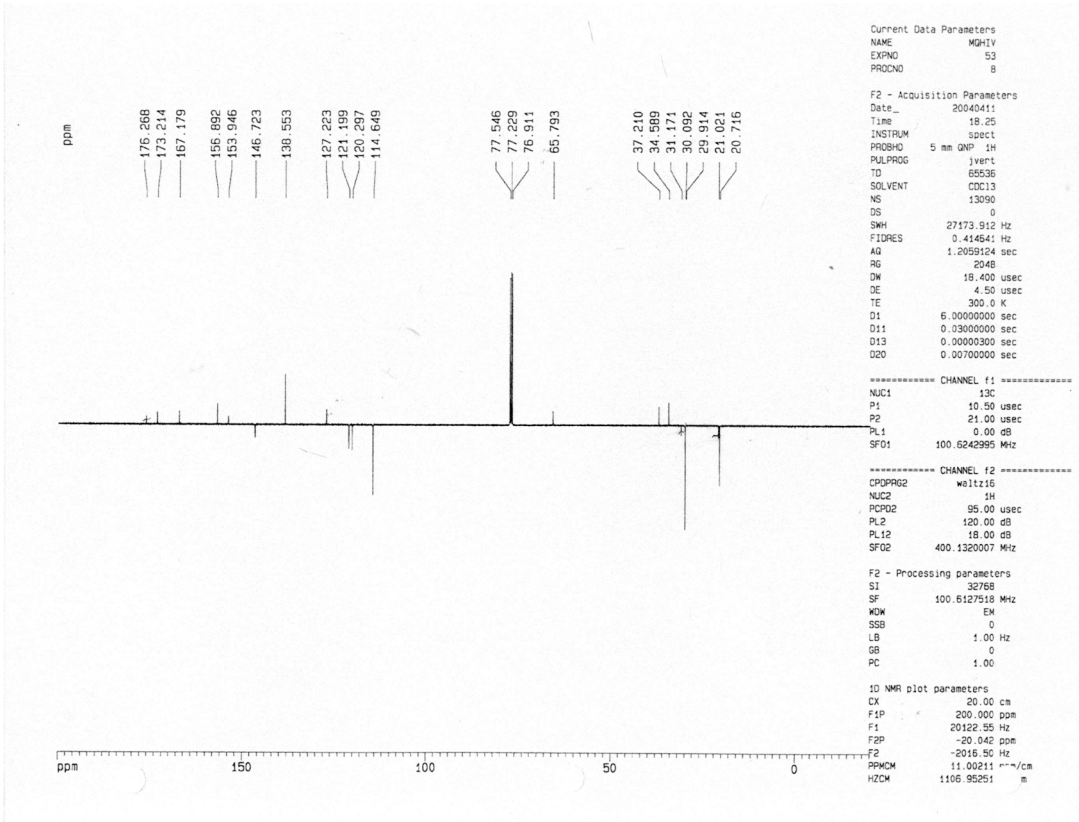
QH13.


ppm
8.4616
8.4494
7.2609
7.0581
6.8585
6.6453
6.6791
4.6240
4.0081
3.2256
3.2084
3.1912
2.4264
2.1718
2.1341
2.0987
2.0759
1.3379
1.3106
1.2813
1.2640
1.2115
1.1979
0.0046
Integral
0.8410
0.8524
0.9581
1.7481
1.8646
1.9348
1.0000
5.9314
5.8121
Current Data Parameters
NAME MQHIV
EXPNO 78
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040504
Time 11.53
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55455 ppm/cm
HZCM 220.6 Hz/cm

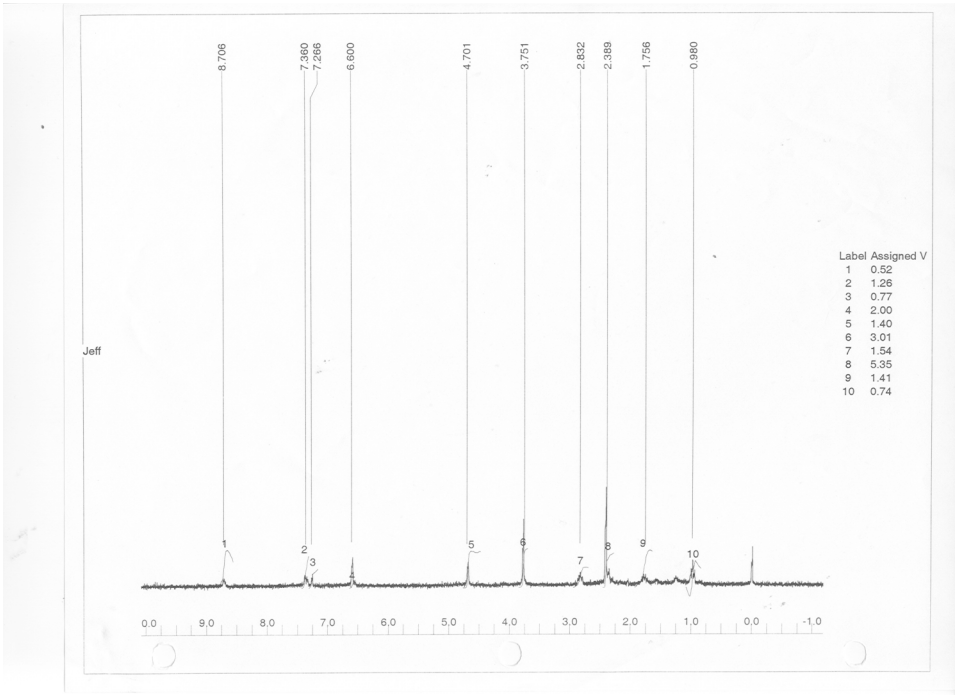

ppm
165.525
157.125
154.222
146.323
138.483
126.981
121.701
121.198
114.682
77.565
77.247
76.930
34.777
34.499
22.619
22.559
20.719
0.214
Current Data Parameters
NAME MQHIII
EXPNO 219
PROCNO 3
F2 - Acquisition Parameters
Date_ 20030327
Time 8.05
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5017
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127493 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.244 ppm
F2 -2036.76 Hz
PPMCM 11.01218 ppm/cm
HZCM 1107.98558 Hz/cm

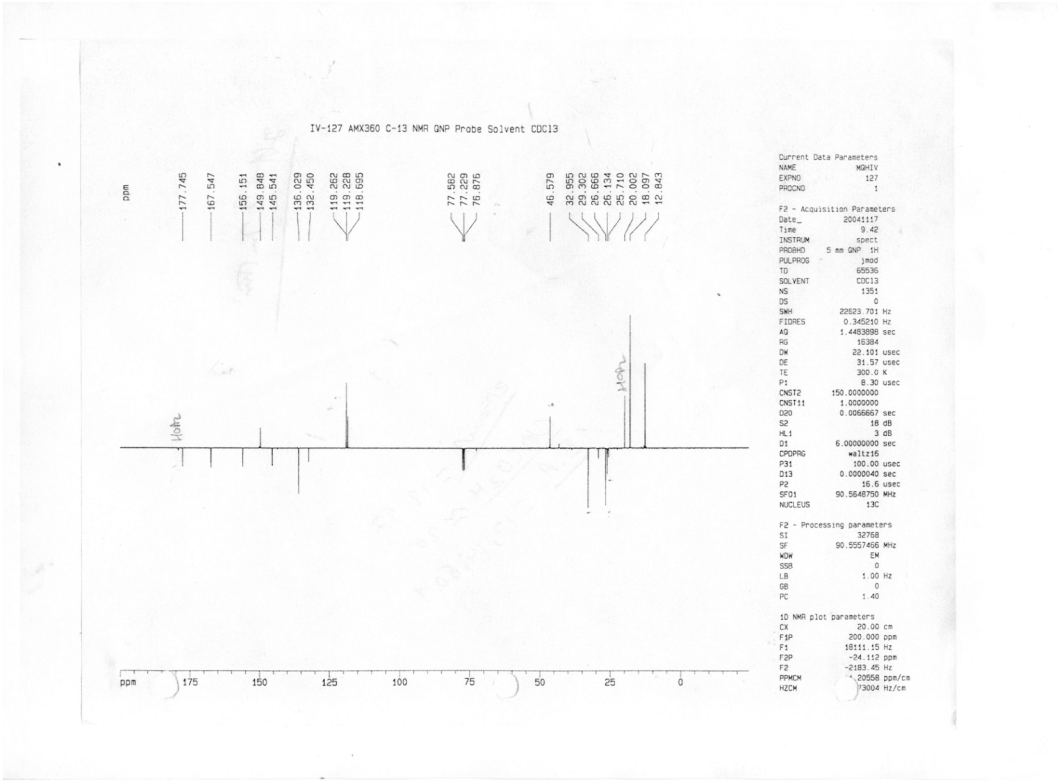
QH14.


ppm
8.7804
7.4452
7.2611
7.0860
6.6913
4.6660
4.2551
4.1591
2.6264
2.1754
2.1560
2.0476
1.5791
1.5342
1.3113
1.2592
1.2503
0.0844
0.0758
0.0667
0.0574
0.0052
-0.0025
-0.0110
Integral
0.9921
1.0763
1.1053
2.0100
2.1560
2.0371
6.0000
9.0770
Current Data Parameters
NAME MQHIV
EXPNO 53
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040411
Time 18.25
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 13090
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SF01 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220.69171 Hz

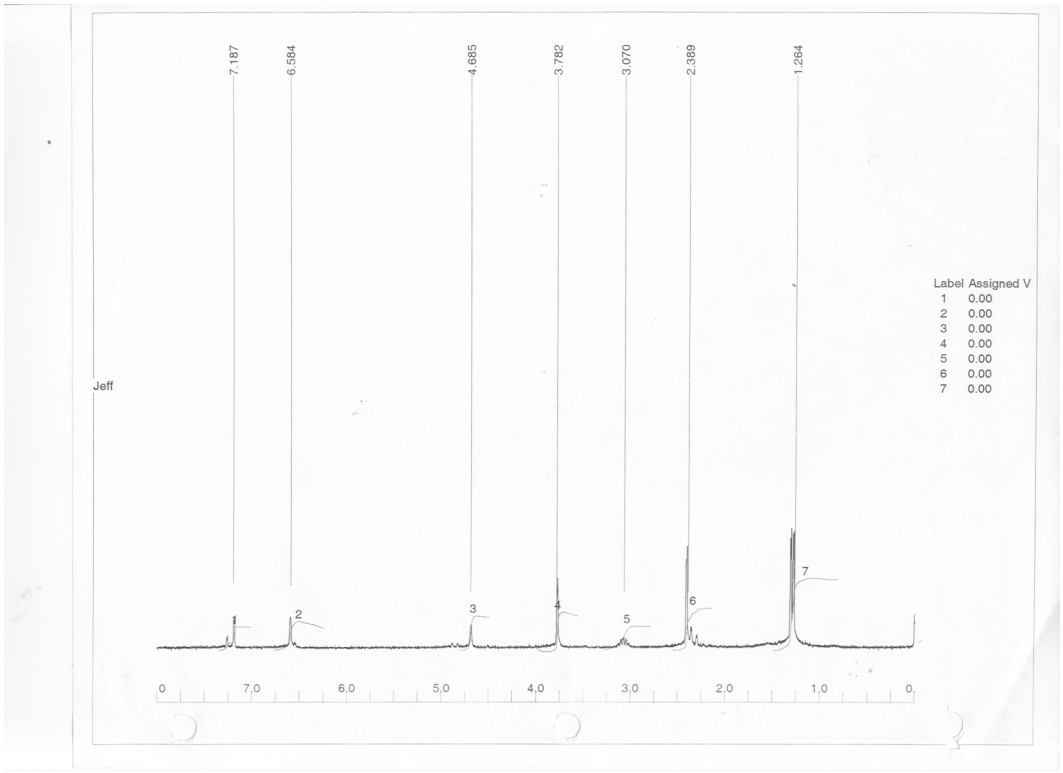

ppm
176.268
173.214
167.179
156.892
153.946
146.723
138.553
127.223
121.199
120.297
114.649
77.546
77.229
76.911
65.793
37.210
34.589
31.171
30.092
29.914
21.021
20.716
Current Data Parameters
NAME MQHIV
EXPNO 53
PROCNO 8
F2 - Acquisition Parameters
Date_ 20040411
Time 18.25
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 13090
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SF01 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127518 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.042 ppm
F2 -2016.50 Hz
PPMCM 11.00211 ppm/cm
HZCM 1106.95251 Hz

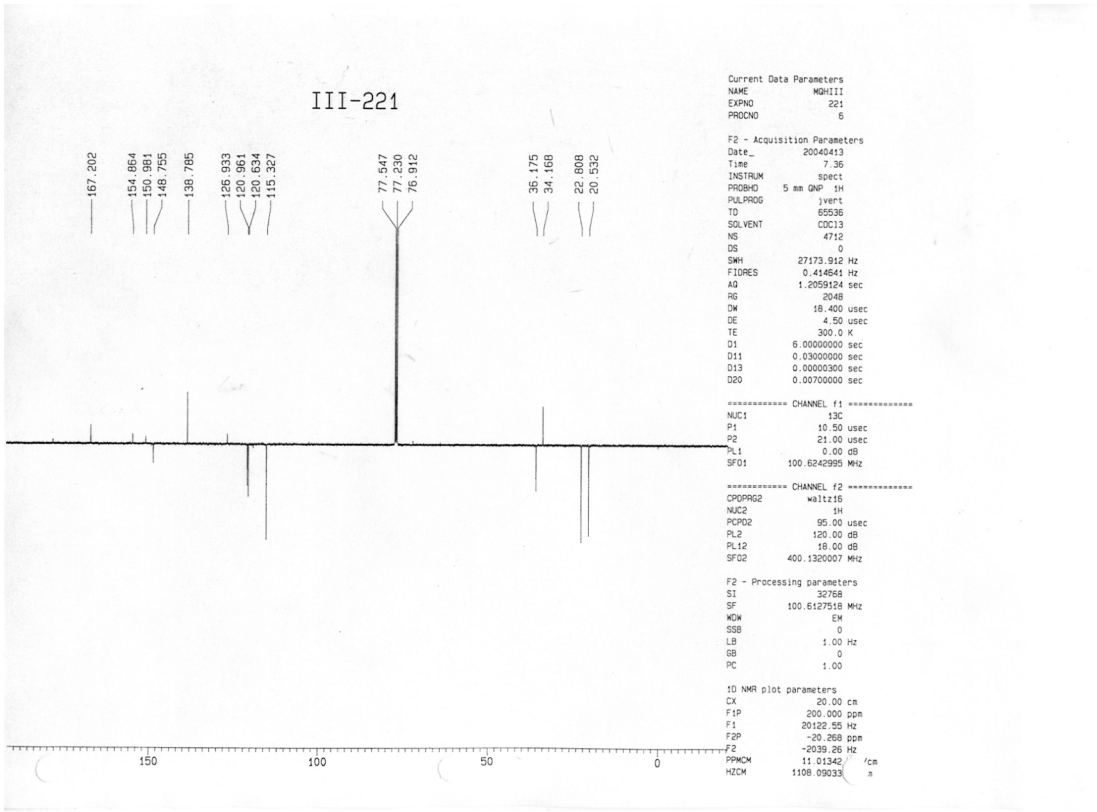
QH15.


8.706
7.360
7.266
6.600
4.701
3.751
2.832
2.389
1.756
0.980
Jeff
Label Assigned V
1 0.52
2 1.26
3 0.77
4 2.00
5 1.40
6 3.01
7 1.54
8 5.35
9 1.41
10 0.74
0.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0

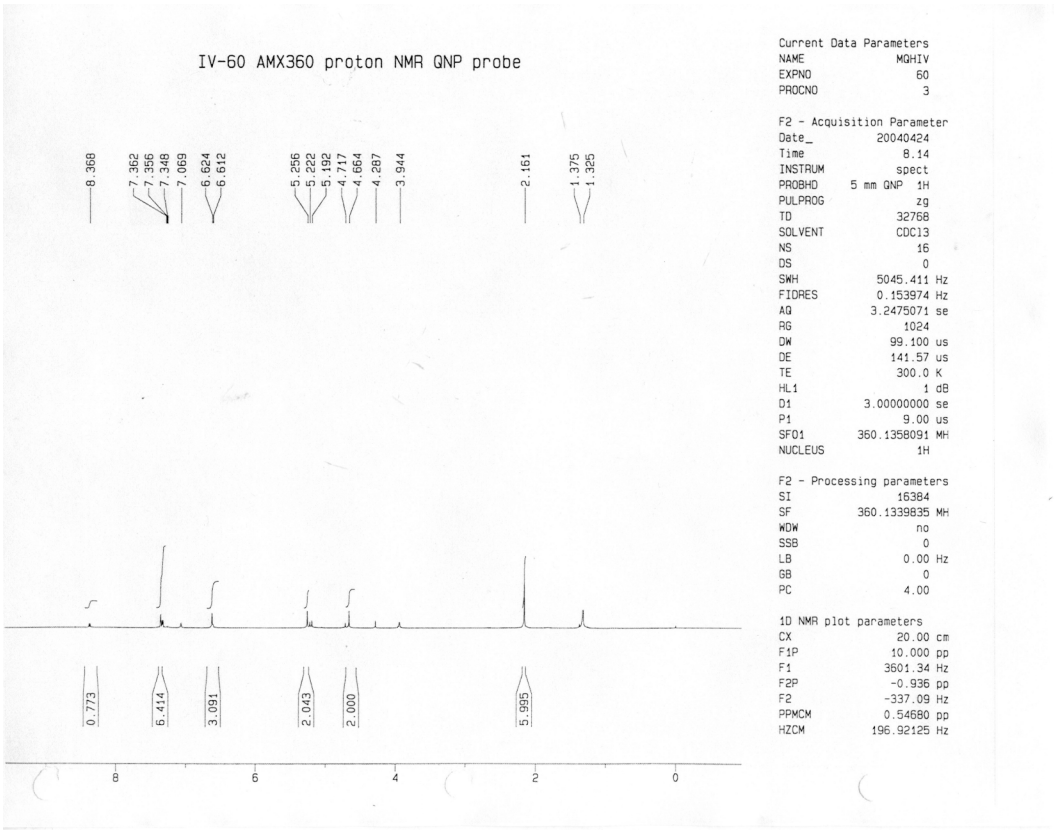

IV-127 AMX360 C-13 NMR QNP Probe Solvent CDCl3
ppm
177.745
167.547
156.151
149.848
145.541
136.029
132.450
119.262
119.228
118.695
77.582
77.269
76.876
46.579
32.965
29.302
26.666
26.134
25.710
20.002
18.097
12.843
Current Data Parameters
NAME MQHIV
EXPNO 127
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041117
Time 9.42
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1351
DS 0
SWH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4483898 sec
RG 16384
DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.30 usec
CNST2 150.0000000
CNST11 1.0000000
D20 0.0066667 sec
S2 18 dB
HL1 3 dB
D1 6.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.6 usec
SFO1 90.5648750 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.5557456 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 18111.15 Hz
F2P -24.112 ppm
F2 -2183.45 Hz
PPMCM 10.20558 ppm/cm
HZCM 7730.04 Hz/cm
ppm 175 150 125 100 75 50 25 0

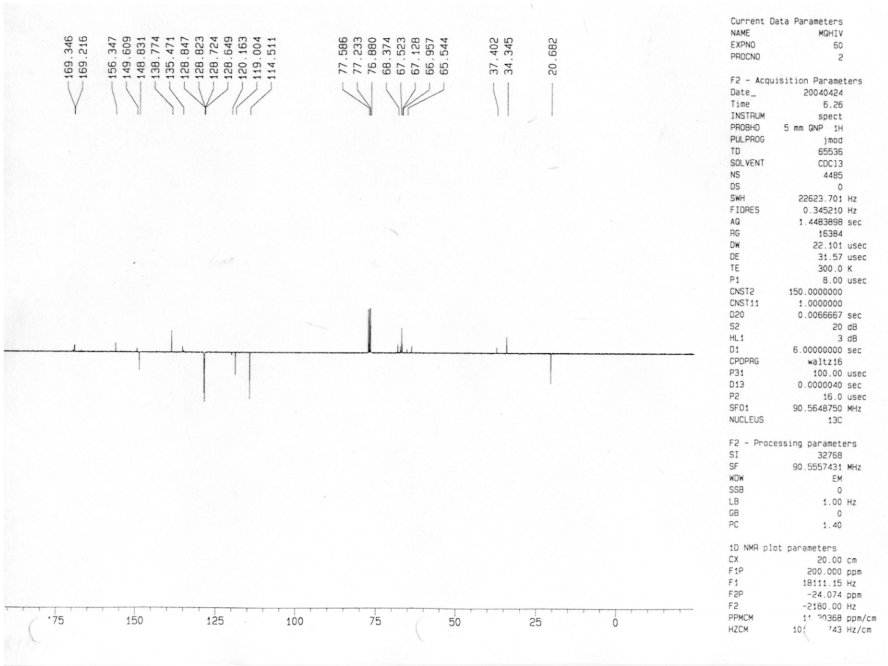
QH16.


7.187
6.584
4.685
3.782
3.070
2.389
1.264
Jeff
Label Assigned V
1 0.00
2 0.00
3 0.00
4 0.00
5 0.00
6 0.00
7 0.00
2
3
4
5
6
7
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

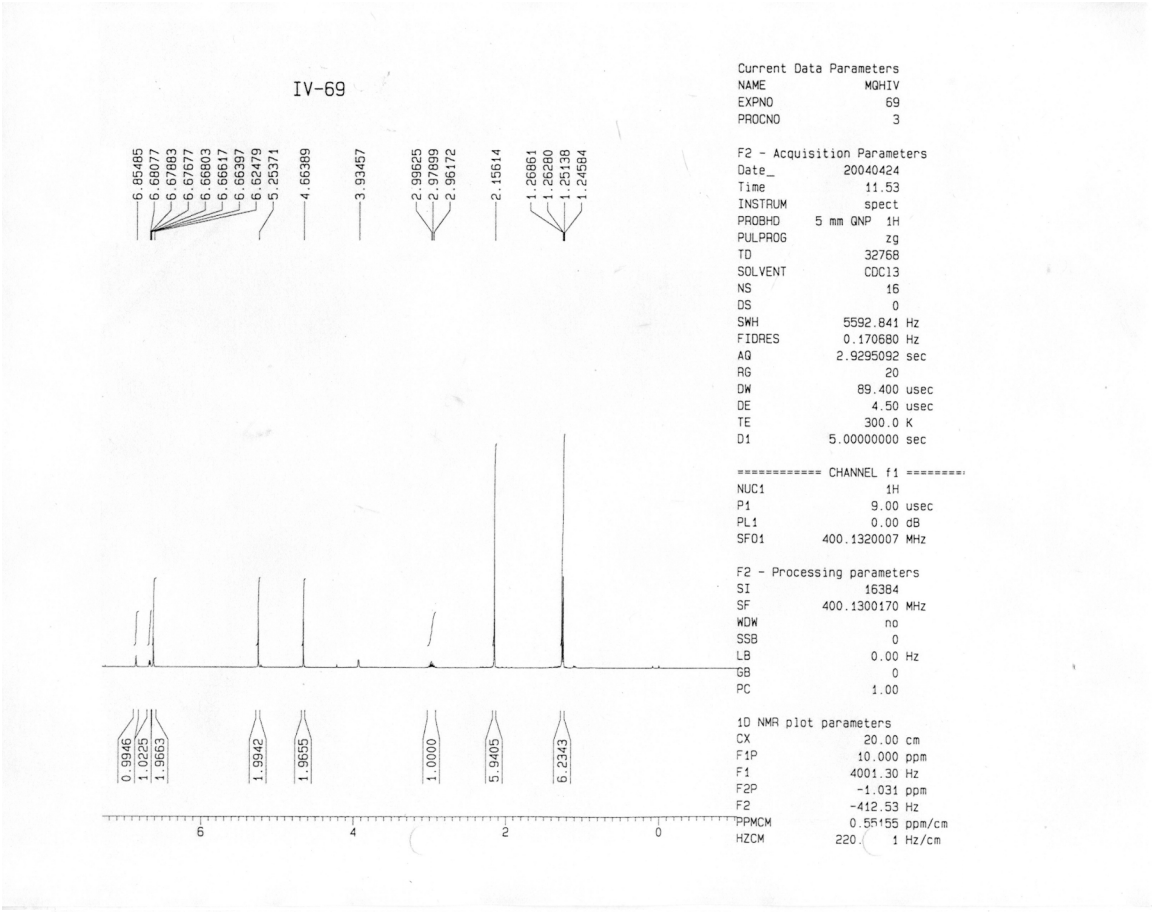

III-221
167.202
154.864
150.981
148.755
138.785
126.933
120.961
120.634
115.327
77.547
77.230
76.912
36.175
34.168
22.808
20.532
150
100
50
0
Current Data Parameters
NAME MQHIII
EXPNO 221
PROCNO 6
F2 - Acquisition Parameters
Date_ 20040413
Time 7.36
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 4712
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
CHANNEL f1
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127518 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.268 ppm
F2 -2039.26 Hz
PPMCM 11.01342 /cm
HZCM 1108.09033 /

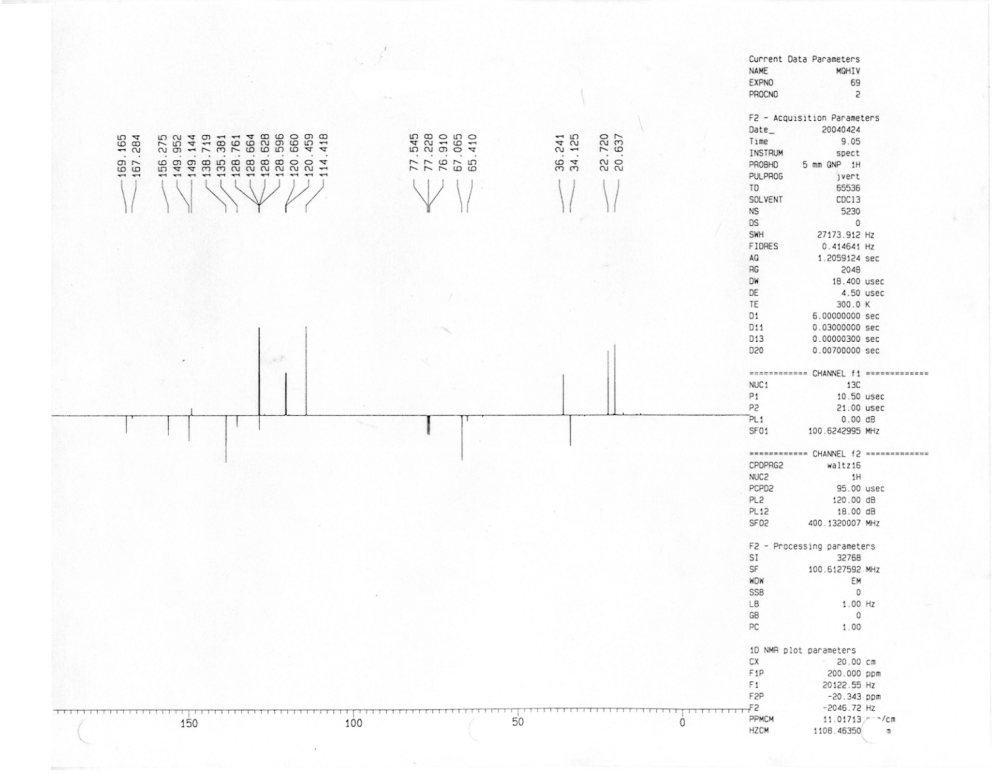
QH17.


IV-60 AMX360 proton NMR QNP probe
8.368
7.362
7.356
7.348
7.069
6.624
6.612
5.256
5.222
5.192
4.717
4.664
4.287
3.944
2.161
1.375
1.325
0.773
6.414
3.091
2.043
2.000
5.995
8
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 60
PROCNO 3
F2 - Acquisition Parameter
Date_ 20040424
Time 8.14
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5045.411 Hz
FIDRES 0.153974 Hz
AQ 3.2475071 se
RG 1024
DW 99.100 us
DE 141.57 us
TE 300.0 K
HL1 1 dB
D1 3.00000000 se
P1 9.00 us
SFO1 360.1358091 MH
NUCLEUS 1H
F2 - Processing parameters
SI 16384
SF 360.1339835 MH
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 pp
F1 3601.34 Hz
F2P -0.936 pp
F2 -337.09 Hz
PPMCM 0.54680 pp
HZCM 196.92125 Hz


169.346
169.216
156.347
149.609
148.831
138.774
135.471
128.847
128.823
128.724
128.649
120.163
119.004
114.511
77.586
77.233
76.880
68.374
67.523
67.128
66.957
65.544
37.402
34.345
20.682
175
150
125
100
75
50
25
0
Current Data Parameters
NAME MQHIV
EXPNO 60
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040424
Time 6.26
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 4485
DS 0
SWH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4483898 sec
RG 16384
DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.00 usec
CNST2 150.0000000
CNST11 1.0000000
D20 0.0066667 sec
S2 20 dB
HL1 3 dB
D1 6.00000000 sec
CPDPRG waltz16
P31 100.00 usec
D13 0.0000040 sec
P2 16.0 usec
SFO1 90.5648750 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.5557431 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 18111.15 Hz
F2P -24.074 ppm
F2 -2180.00 Hz
PPMCM 11.20368 ppm/cm
HZCM 101.[illegible]743 Hz/cm

QH18.


IV-69
6.85485
6.68077
6.67883
6.67677
6.66803
6.66617
6.66397
6.62479
5.25371
4.66389
3.93457
2.99625
2.97899
2.96172
2.15614
1.26861
1.26280
1.25138
1.24584
0.9946
1.0225
1.9663
1.9942
1.9655
1.0000
5.9405
6.2343
6
4
2
0
Current Data Parameters
NAME MQHIV
EXPNO 69
PROCNO 3
F2 - Acquisition Parameters
Date_ 20040424
Time 11.53
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 20
DW 89.400 usec
DE 4.50 usec
TE 300.0 K
D1 5.00000000 sec
========== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 16384
SF 400.1300170 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.031 ppm
F2 -412.53 Hz
PPMCM 0.55155 ppm/cm
HZCM 220. 1 Hz/cm


169.165
167.284
156.275
149.952
149.144
138.719
135.381
128.761
128.664
128.628
128.596
120.660
120.459
114.418
77.545
77.228
76.910
67.065
65.410
36.241
34.125
22.720
20.637
150
100
50
0
Current Data Parameters
NAME MQHIV
EXPNO 69
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040424
Time 9.05
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 5230
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SFO1 100.6242995 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -20.343 ppm
F2 -2046.72 Hz
PPMCM 11.01713 ppm/cm
HZCM 1108.46350 Hz