

Supporting Information for:

Synthesis of Novel Symmetrical and Unsymmetrical Pyrazines

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Table of Contents:

General Experimental Section:.....	S2	Amino Diol 3e : ¹³ C Spectrum.....	S18
Experimental Procedures:.....	S3	Pyrazine 4a : ¹ H Spectrum.....	S19
Amino Diol 3a : ¹ H Spectrum.....	S9	Pyrazine 4a : ¹³ C Spectrum.....	S20
Amino Diol 3a : ¹³ C Spectrum.....	S10	Pyrazine 4b : ¹ H Spectrum.....	S21
Amino Diol 3b : ¹ H Spectrum.....	S11	Pyrazine 4b : ¹³ C Spectrum	S22
Amino Diol 3b : ¹³ C Spectrum.....	S12	Pyrazine 4c : ¹ H Spectrum.....	S23
Amino Diol 3c : ¹ H Spectrum.....	S13	Pyrazine 4c : ¹³ C Spectrum	S24
Amino Diol 3c : ¹³ C Spectrum.....	S14	Pyrazine 4d : ¹ H Spectrum.....	S25
Amino Diol 3d : ¹ H Spectrum.....	S15	Pyrazine 4d : ¹³ C Spectrum	S26
Amino Diol 3d : ¹³ C Spectrum.....	S16	Pyrazine 4e : ¹ H Spectrum.....	S27
Amino Diol 3e : ¹ H Spectrum.....	S17	Pyrazine 4e : ¹³ C Spectrum	S28

General Experimental Section:

^1H NMR and ^{13}C NMR spectra were obtained as solutions in the deuterated solvents specified at 400 MHz and 100 MHz respectively. ^{13}C multiplicities were determined with the aid of a JVERT pulse sequence, differentiating the signals for methyl and methane carbons as 'd', from methylene and quaternary carbons as 'u'. The infrared (IR) spectra were determined as films or nujol mulls. R_f values indicated refer to thin layer chromatography (TLC) on 2.5 x 10 cm, 250 μm silica gel plates. Column chromatography was carried out as indicated on either silica gel or basic alumina. The solvent mixtures reported are volume/volume mixtures. All glassware was oven dried. All reactions were stirred magnetically, under dry N_2 , unless otherwise noted.

Experimental Procedures:

Amino diols **3a**: In a 25 mL round bottom flask, *S*-(-)-2-amino-3-phenyl-1-propanol (**2a**) (1.1 g, 13 mmol) was combined with cyclohexene oxide (**1a**) (1.47 g, 15 mmol). The flask was sealed and the reaction was allowed to proceed for 2 weeks, at which point the mixture was subjected to bulb-to-bulb distillation (pot = 100 °C, 2 mmHg) to remove unreacted amino alcohol and epoxide, followed by column chromatography of the residue (acetone/ CH₂Cl₂/NH₄OH) over basic alumina to give the diastereomeric amino diols **3a** (1.1 g, 34% yield) as a viscous, pale yellow oil. TLC: $R_f = 0.59$ (5:44:1 MeOH/CH₂Cl₂/NH₄OH). IR (film) 3352, 2930, 2861, and 1454 cm⁻¹; ¹H NMR (CD₃OD) δ 0.78-1.01 (m, 1H), 1.15 (m, 3H), 1.55 (m, 2H), 1.80 (m, 2H), 2.24-2.36 (m, 1H), 2.57-2.74 (m, 1H), 2.832 (m, 1H), 3.11 (m, 1H), 3.22-3.43 (m, 1H), and 7.13 (m, 5H); ¹³C NMR (CD₃OD) δ d 40.40, 58.82, 59.48, 74.67, 75.17, 127.20, 127.32, 129.43, 129.45, 129.59, 130.38, 130.46; u 25.59, 25.76, 31.61, 31.82, 35.07, 35.11, 37.81, 39.69; HRMS calcd for C₁₅H₂₃NNaO₂: 272.163, obsd: 272.163 [M+Na].

Amino diols **3c**: Trans-anethole oxide (**1b**) (2.7 g, 16.4 mmol) was combined neat with *R*-2-amino-1-butanol (**2b**) (1.5 g, 16.4 mmol). After a week of stirring under nitrogen at room temperature, the reaction mixture was diluted with 20 mL of methanol and evaporated onto 6 g of basic alumina. An alumina column was then run with a 0-40% acetone/ CH₂Cl₂/NH₄OH gradient. The eluted fractions still had traces of amino alcohol, therefore the residue after evaporation was then subjected to bulb-to-bulb distillation (2 mm Hg, Pot = 115 °C, pot residue) to give the amino diols **3c** (1.5 g, 36% yield). TLC: $R_f = 0.41$, (5:44:1 MeOH/CH₂Cl₂/NH₄OH); IR (film): 3386, 2965, 1512, and 1248 cm⁻¹; ¹H NMR (CD₃OD) δ 0.82 (t, $J = 7.4$ Hz, 1H), 0.88 (t, $J = 7.6$ Hz, 1H), 1.01

(t, $J = 6$ Hz, 3H), 1.25-1.45 (m, 1H), 1.45-1.65 (m, 1H), 1.89 (m, 1H), 2.39 (m, 1H), 3.30-3.60 (m, 2H), 3.65-3.75 (m, 2H), 4.00 (m, 1H), 6.90 (m, 2H), 7.25 (m, 2H); ^{13}C NMR (CD_3OD) δ d 8.88, 9.59, 18.12, 18.62, 54.24, 56.61, 57.27, 63.70, 64.61, 69.84, 113.03, 129.41, 129.61; u 22.13, 24.66, 25.11, 67.47, 130.99, 131.96, 158.94; HRMS calcd for $\text{C}_{14}\text{H}_{23}\text{NNaO}_3$: 276.158, obsd: 276.158 [M+Na].

Amino diols **3d**: Trans-anethole oxide (**1b**) (2.7 g, 16.4 mmol) and *S*-(-)-2-amino-3-phenyl-1-propanol (**2a**) (2.5g, 16.4 mmol) were combined with 5 mL MeOH and the solution was stirred for two weeks at room temperature under nitrogen. The reaction mixture was then taken directly to bulb-to-bulb distillation (2 mm Hg, pot = 100 °C, bottom fraction) and the residue was passed through a short alumina column (acetone/ $\text{CH}_2\text{Cl}_2/\text{NH}_4\text{OH}$) to give the amino diols **3d** (1.37 g, 30% yield).

TLC: $R_f = 0.54$, (5:44:1 MeOH/ $\text{CH}_2\text{Cl}_2/\text{NH}_4\text{OH}$); IR (film): 3385, 2931, 1512, and 1248 cm^{-1} ; ^1H NMR (CDCl_3) δ 0.9-1.0 (m, 4H), 1.2 (s, 1H), 2.4-3.0 (m, 3H), 3.0-4.0 (m, 4H), 6.7-7.4 (m, 11H). ^{13}C NMR (CDCl_3) δ d 19.12, 29.19, 30.88, 55.21, 56.77, 57.54, 64.21, 64.74, 70.12, 70.21, 113.64, 113.84, 126.27, 126.42, 126.57, 128.42, 128.50, 128.57, 128.60, 128.81, 128.94, 129.19, 129.24, 129.33, 129.41; u 30.51, 37.69, 38.86, 39.55, 53.43, 53.81, 62.04, 63.89, 64.21, 131.19, 131.48, 158.78, 159.01; HRMS calcd for $\text{C}_{19}\text{H}_{26}\text{N}_1\text{O}_3$: 316.191, obsd: 316.192 [M+H].

Amino diol **3e**: Following the procedure of Taguchi,⁸ cyclohexene oxide (**1a**) (10 g, 0.10 mol) and 6.0 ml conc. NH_4OH (29% aq.) were combined. The flask was sealed and the reaction was allowed to stir for 5 days. The white slurry was then vacuum filtered with 3 x 25 mL rinses of Et_2O and evaporated to give amino diols **3e** (3.1 g, 29% purified yield). TLC: $R_f = 0.28$ (5:44:1 MeOH/ $\text{CH}_2\text{Cl}_2/\text{NH}_4\text{OH}$). MP: 150-151 °C (Lit = 153 °C); IR

(film) 3336, 2929, 2855, 1449 cm^{-1} ; ^1H NMR (CDCl_3) δ 0.90-1.05 (m, 1H), 1.15-1.35 (m, 3H), 1.65-1.80 (m, 2H), 1.95-2.10 (m, 2H), 2.30-2.40 (m, 1H), 3.15-3.25 (m, 1H). ^{13}C NMR (CDCl_3) δ d 59.28, 74.11; u 24.49, 24.92, 31.20, 33.88; HRMS calcd for $\text{C}_{12}\text{H}_{23}\text{NNaO}_2$: 236.163, obsd: 236.163 [M+Na].

Pyrazine 4a: Oxalyl chloride (2.13 g, 14.0 mmol) diluted to 10 mL with CH_2Cl_2 was added to a 100 mL round bottom flask in a -40°C bath. DMSO (1.31 g, 16.9 mmol diluted to 10 mL with CH_2Cl_2) over the course of one minute with gas evolution. Amino diols **3a** (250 mg, 0.92 mmol in 10 mL CH_2Cl_2) were then added. The reaction was allowed to proceed with the temperature being kept between -20°C and -40°C . After 2h, triethylamine (5 mL, 35.8 mmol) was then added with accompanying exotherm to give a turbid yellow solution. The mixture was allowed to warm to 0°C over the course of 30 min, and the mixture was then partitioned between water and CH_2Cl_2 . The combined organic extract was dried over Na_2SO_4 . TLC indicated the absence of amino diols **3a**. The CH_2Cl_2 solution was decanted into a 250 mL round bottom flask, to which was added 20 mL of absolute EtOH and $\text{NH}_2\text{OH} \cdot \text{HCl}$ (88 mg, 1.27 mmol). The round bottom flask was fitted with a distillation apparatus and the mixture was heated until the bulk of the CH_2Cl_2 had distilled out. The mixture was then kept at reflux for two hours with an air condenser. The brown solution was then concentrated onto flash silica gel and chromatographed on flash silica gel with a MTBE/PE gradient to give 88 mg of crude pyrazine **4a**. This was then further purified via TLC mesh chromatography (1:1 MTBE/PE) to give 48 mg of pyrazine **4a** as a pale yellow oil, 23% yield overall from **3a**.

Pyrazine 4c: Oxalyl chloride (2.13 g, 14.0 mmol) diluted to 10 mL with CH_2Cl_2 was added to a 100 mL round bottom flask in a -40°C bath. DMSO (1.31 g, 16.9 mmol

diluted to 10 mL with CH₂Cl₂) over the course of one minute with gas evolution. Amino diols **3c** (250 mg, 0.99 mmol) in 10 mL CH₂Cl₂ were then added. The reaction was allowed to proceed with the temperature being kept between -20 °C and -40 °C. After 2h, triethylamine (5mL, 35.8 mmol) was then added with accompanying exotherm to give a turbid yellow solution. The mixture was allowed to warm to 0 °C over the course of 30 min, and the mixture was then partitioned between water and CH₂Cl₂. The combined organic extract was dried over Na₂SO₄. TLC indicated the absence of amino diols **3c**. The CH₂Cl₂ solution was decanted into a 250 mL round bottom flask, to which was added 20 mL of absolute EtOH and NH₂OH · HCl (88 mg, 1.27 mmol). The round bottom flask was fitted with a distillation apparatus and the mixture was heated until the bulk of the CH₂Cl₂ had distilled out. The mixture was then kept at reflux for two hours with an air condenser. The brown solution was then concentrated onto flash silica gel and chromatographed on flash silica gel with a MTBE/PE gradient to give crude pyrazine **4c**. This was then further purified via TLC mesh chromatography (1:1 MTBE/PE) to give 25 mg of pyrazine **4c** as a, 20% yield overall from **3c**. TLC: *R_f* = 0.50, (MTBE); IR (film): 2970, 1610, 1514, 1382, and 1250 cm⁻¹; ¹H NMR (CDCl₃) δ 1.33 (t, *J* = 13.2 Hz, 3H), 2.59 (s, 3H), 2.82 (q, *J* = 7.6, 13.2 Hz, 2H), 3.85 (s, 3H), 6.98 (d, *J* = 9.6 Hz, 2H), 7.51 (d, *J* = 9.6 Hz, 2H), 8.26 (s, 1H); ¹³C NMR (CDCl₃) δ d 13.77, 22.84, 55.38, 113.82, 130.41, 140.51; u 28.36, 131.44, 148.23, 152.39, 155.18, 159.91; HRMS calcd for C₁₄H₁₇N₂O: 229.134, obsd: 229.133 [M+H].

Pyrazine **4d**: Oxalyl chloride (2.13 g, 14.0 mmol diluted to 10 mL with CH₂Cl₂) was added to a 100 mL round bottom flask in a -40 °C bath. DMSO (1.31 g, 16.9 mmol diluted to 10 mL with CH₂Cl₂) over the course of one minute with gas evolution. Amino

diols **3d** (315 mg, 1.0 mmol in 10 mL CH₂Cl₂) were then added. The reaction was allowed to proceed with the temperature being kept between -20 °C and -40 °C. After 2h, triethylamine (5 mL, 35.8 mmol) was then added with accompanying exotherm to give a turbid yellow solution. The mixture was allowed to warm to 0 °C over the course of 30 min, and the mixture was then partitioned between water and CH₂Cl₂. The combined organic extract was dried over Na₂SO₄. TLC indicated the absence of amino diols **3d**. The CH₂Cl₂ solution was decanted into a 250 mL round bottom flask, to which was added 20 mL of absolute EtOH and NH₂OH · HCl (88 mg, 1.27 mmol). The round bottom flask was fitted with a distillation apparatus and the mixture was heated until the bulk of the CH₂Cl₂ had distilled out. The mixture was then kept at reflux for two hours with an air condenser. The brown solution was then concentrated onto flash silica gel and chromatographed on flash silica gel with a MTBE/PE gradient to give crude pyrazine **4d**. This was then further purified via TLC mesh chromatography (1:1 MTBE/PE) to give 25 mg of pyrazine **4d** as a pale yellow oil, 15% yield overall from **3d**.

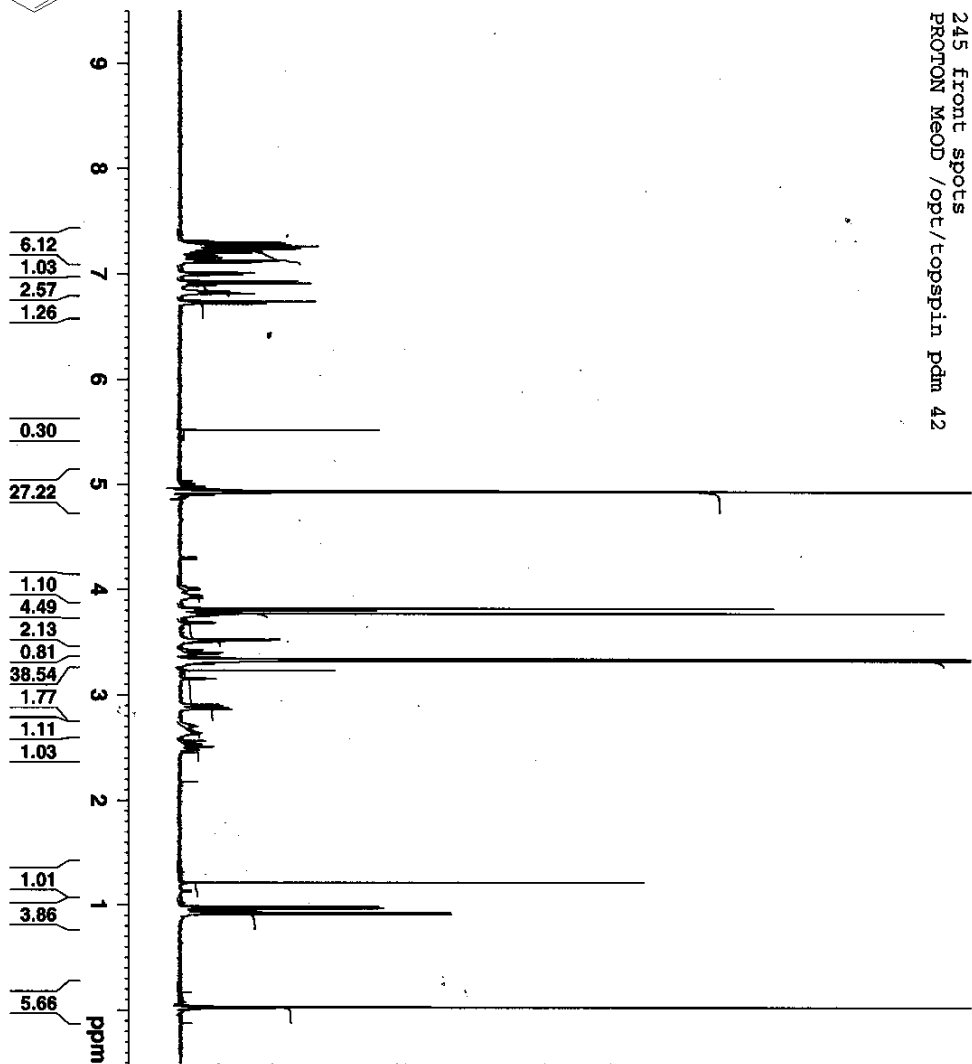
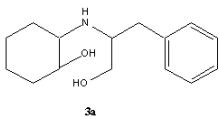
TLC: R_f = 0.52, (MTBE); IR (film): 2920, 2360, 1514, and 1251 cm⁻¹; ¹H NMR (CDCl₃) δ 1.02 (s, 3H), 1.49 (s, 2H), 2.42 (s, 3H), 3.04 (s, 1H), 3.69 (s, 3H), 4.01 (s, 2H), 6.83 (d, J = 6.4 Hz, 2H), 7.00-7.20 (m, 5H), 7.37 (d, J = 6.8 Hz, 2H), 8.07 (s, 1H); ¹³C NMR (CDCl₃) δ d 22.70, 26.80, 55.20, 113.64, 126.40, 128.48, 128.84, 130.30, 141.07; u 41.51, 131.02, 138.53, 148.44, 152.54, 159.81; HRMS calcd for C₁₉H₁₈N₂NaO: 313.132, obsd: 313.133[M+Na].

Pyrazine **4e**:

Amino diol **3e** (213 mg, 1.0 mmol) was suspended in 20 mL CH₂Cl₂, then DMSO was added dropwise until complete dissolution was observed (~5 drops). Meanwhile, 6.3 mL

of a 1.63 M oxalyl chloride/ CH₂Cl₂ solution was cooled to -78 °C. DMSO (1.2 mL diluted to 10 mL with CH₂Cl₂) was added dropwise over 5 min with stirring. The solution of amino diol **3e** was then added over 5 min, and the reaction was kept at -78 °C for an additional 2 h. Triethylamine (5 mL) was then added, and after 15 min the reaction was allowed to come to room temperature (~2 h). The mixture was then partitioned between water and CH₂Cl₂. The organic extract was dried over Na₂SO₄ then decanted into another flask, to which was added 20 mL abs EtOH and NH₂OH · HCl (78 mg, 1.12 mmol). The mixture then had 95 mL solvent distilled out of it by fractional distillation and was refluxed at 90 °C (bath temp) for an additional 2 h. The mixture was then concentrated and the residue was chromatographed to give pyrazine **4e** as a white solid (80 mg, 43% yield from amino diol **7**). MP: 103-104 °C. Lit = 105-106 °C.¹² TLC: *R_f* = 0.62, (MTBE); ¹H NMR (CDCl₃) δ 1.90 (m, 2H), 2.85 (m, 2H); ¹³C NMR (CDCl₃) δ u 22.98, 32.02, 149.33; HRMS calcd for C₁₂H₁₆N₂: 188.131, obsd: 188.131 [M+].

Amino Diols 3a: ¹H Spectrum



245 front spots
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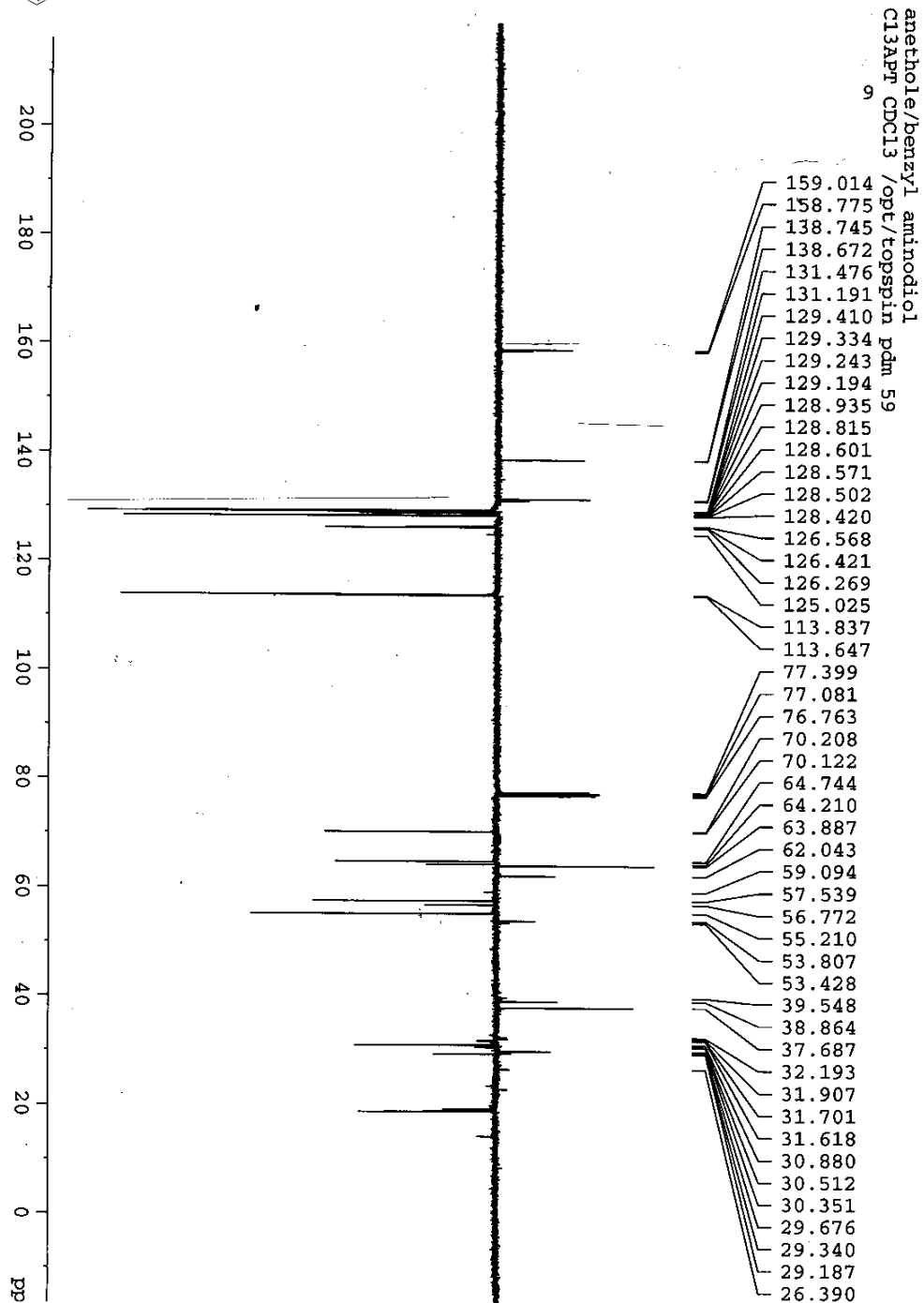
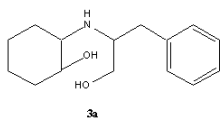
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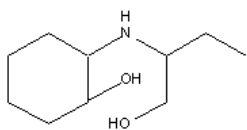
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Amino Diols 3a: ¹³C Spectrum



Amino Diols **3b**: ¹³C Spectrum



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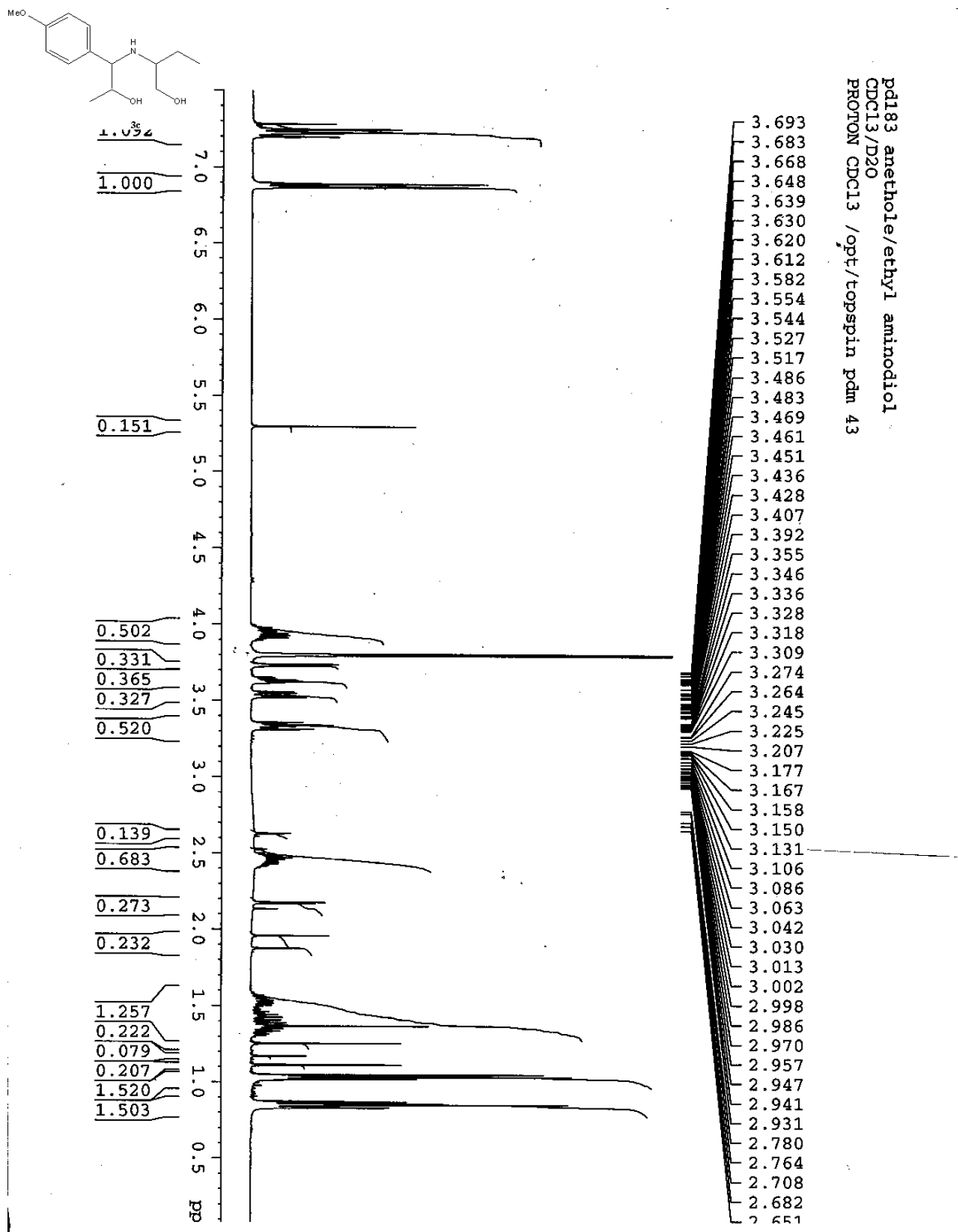
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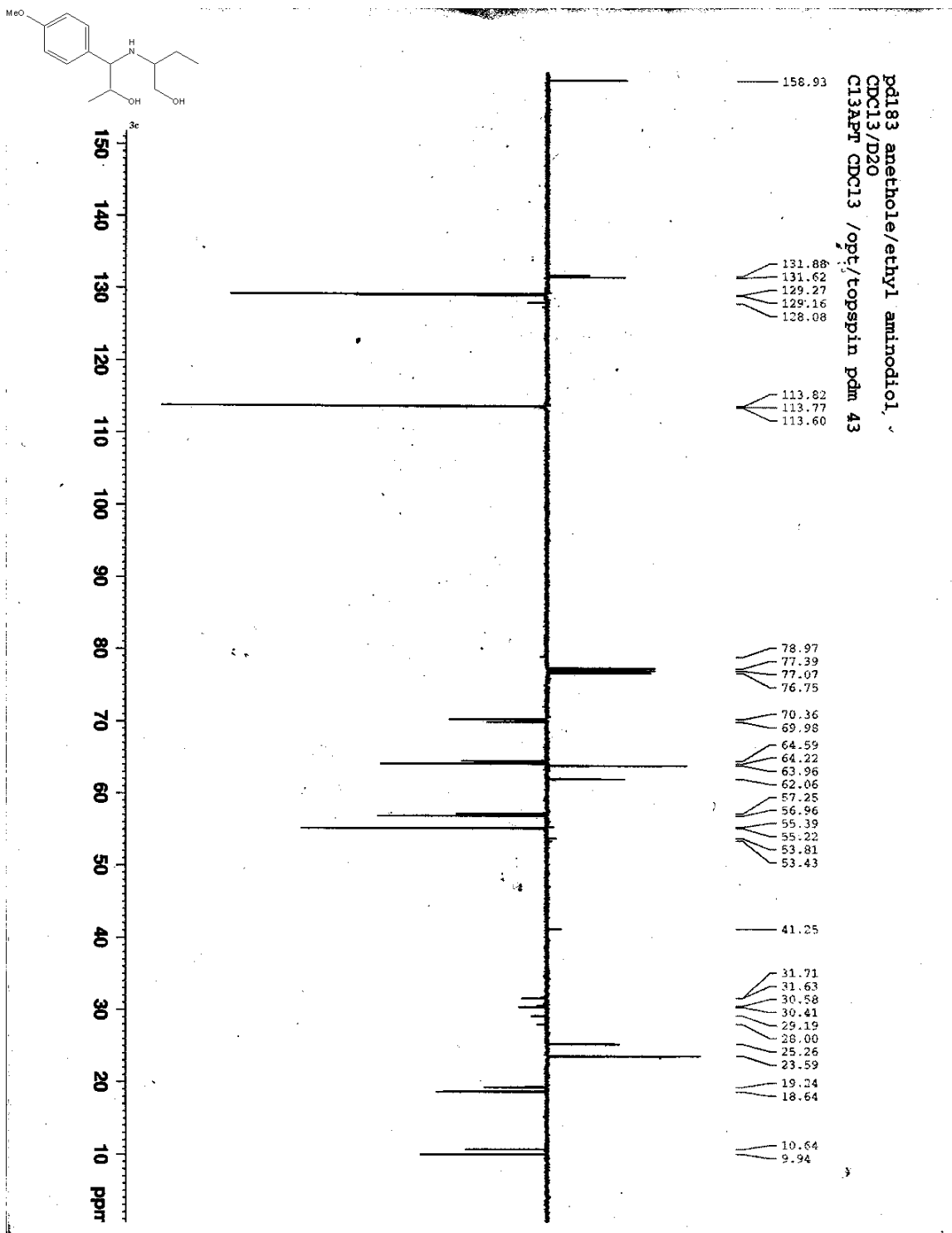
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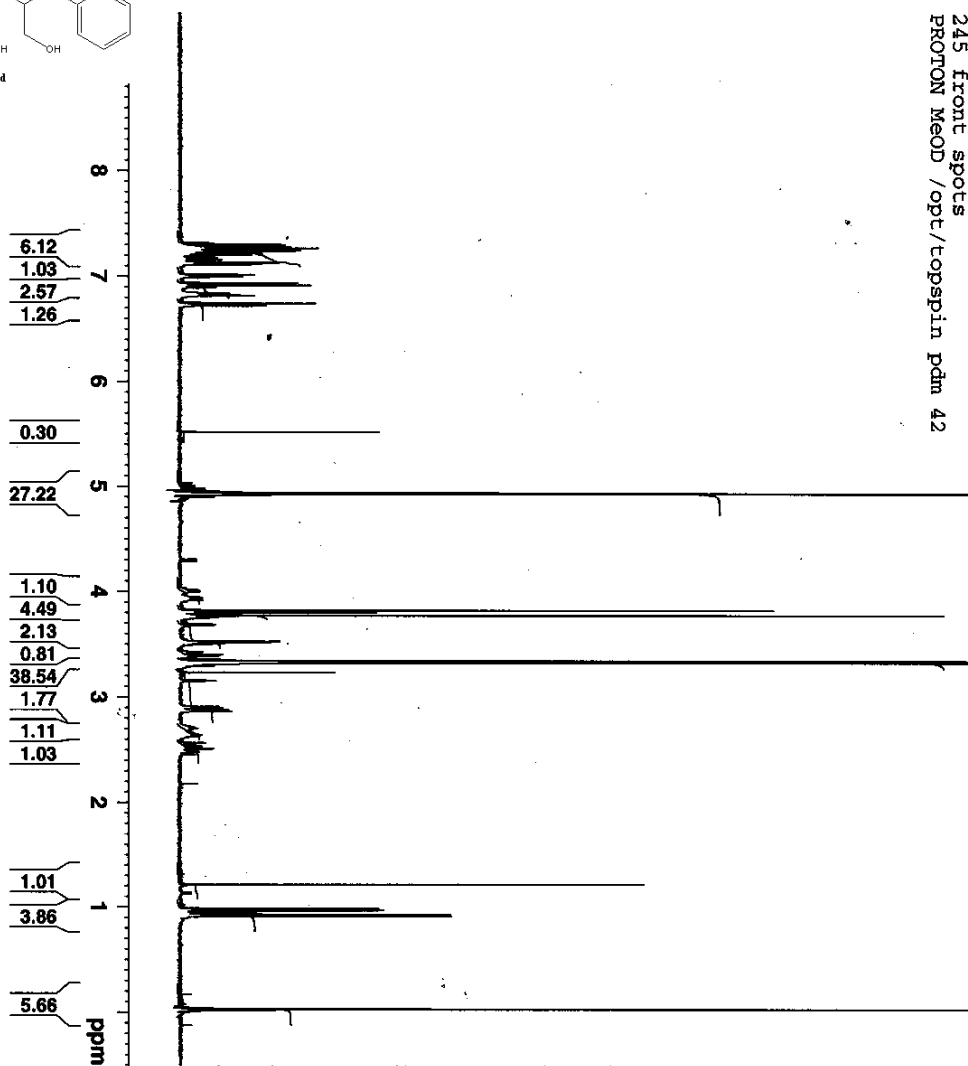
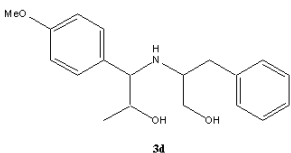
Amino Diols 3c: ¹H Spectrum



Amino Diols 3c: ¹³C Spectrum



Amino Diols **3d**: ¹H Spectrum



245 front spots
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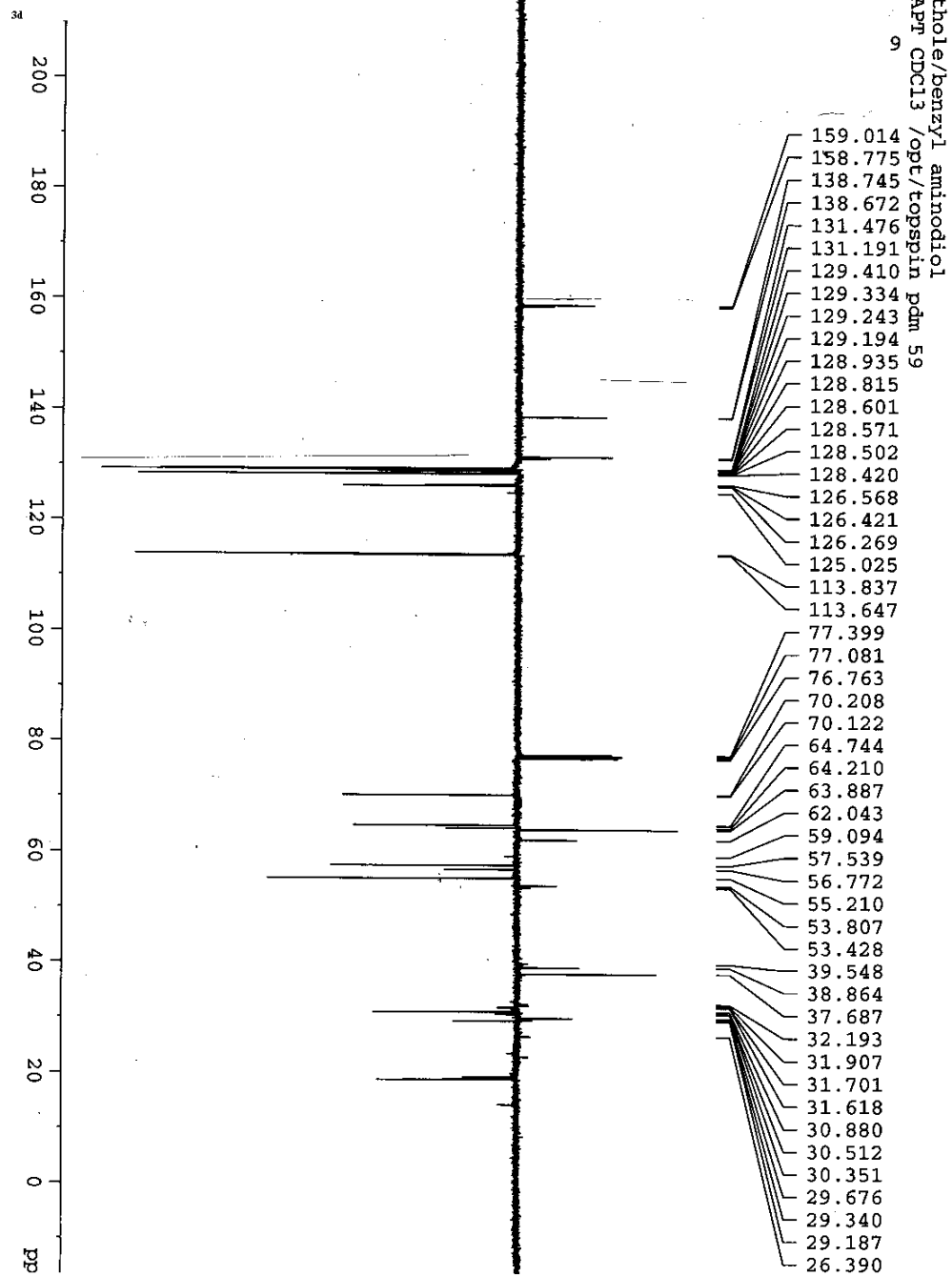
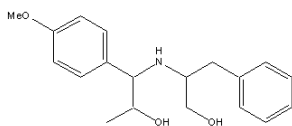
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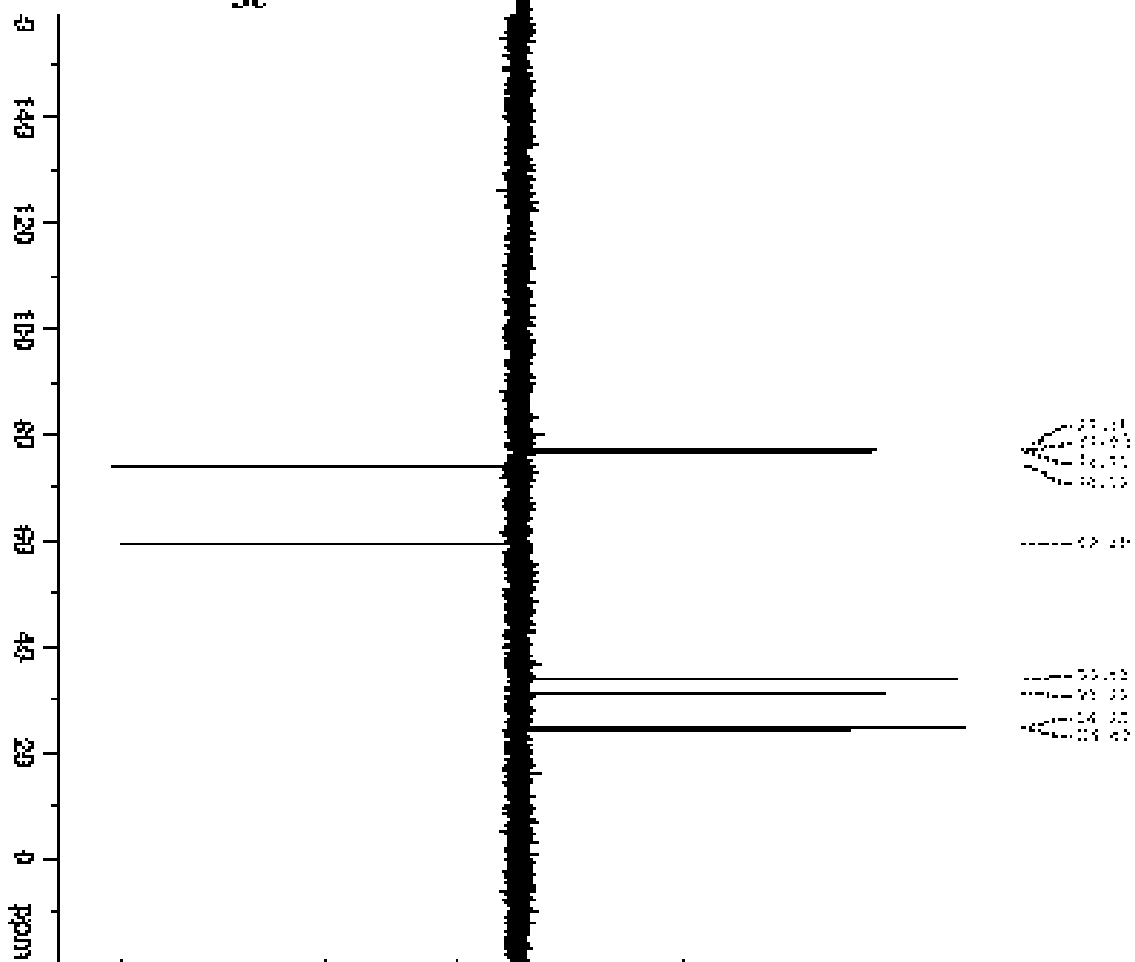
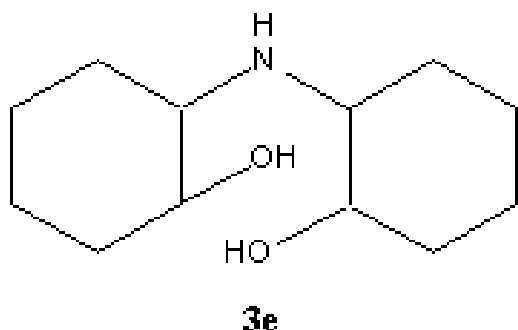
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Amino Diols **3d**: ^{13}C Spectrum



Amino Diol **3e**: ^{13}C Spectrum



BRUMER

National Super Magnetron
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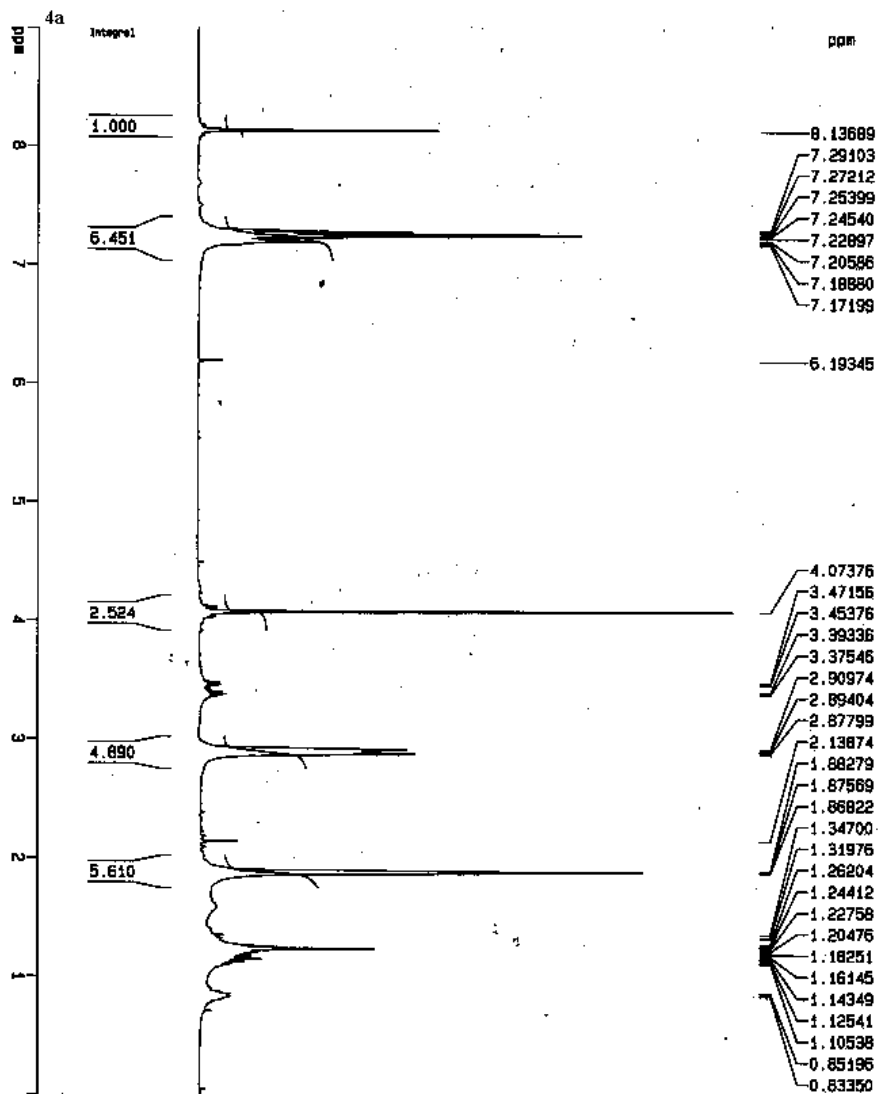
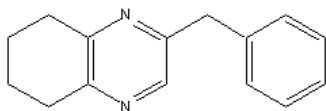
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cyclohexane-1-amino diol

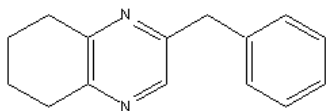
Pyrazine 4a ¹H Spectrum:



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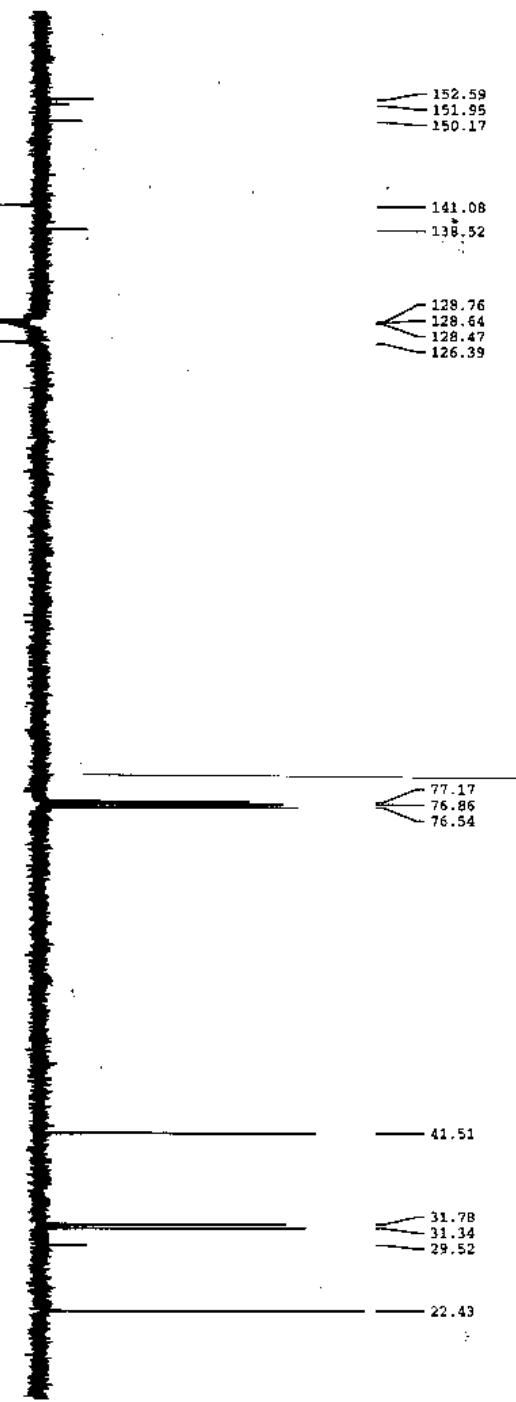
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Pyrazine 4a ¹³C Spectrum:



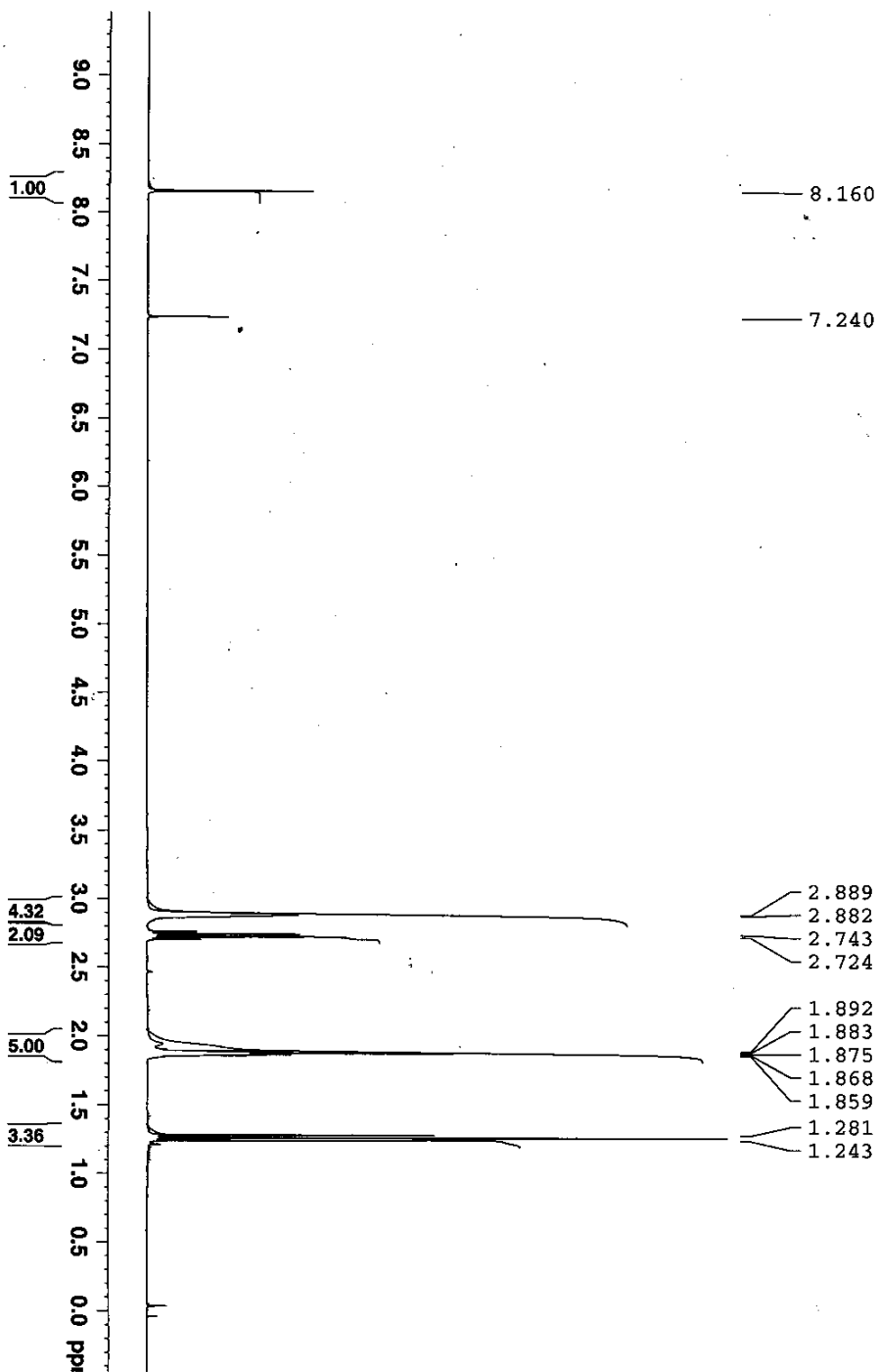
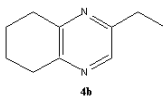
4a

150
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80
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60
50
40
30
20
ppm



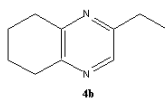
pd225jv after column
C13APT CDC13 /opt/topspin pdm 50

Pyrazine 4b ¹H Spectrum:

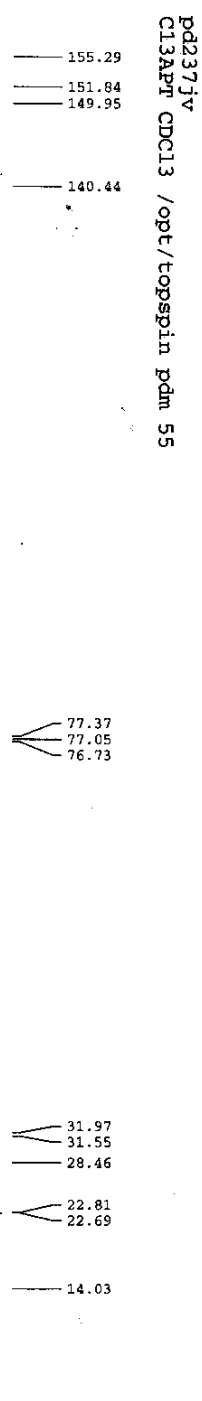


pd237
PROTON CDCl3 /opt/topspin pdm 55

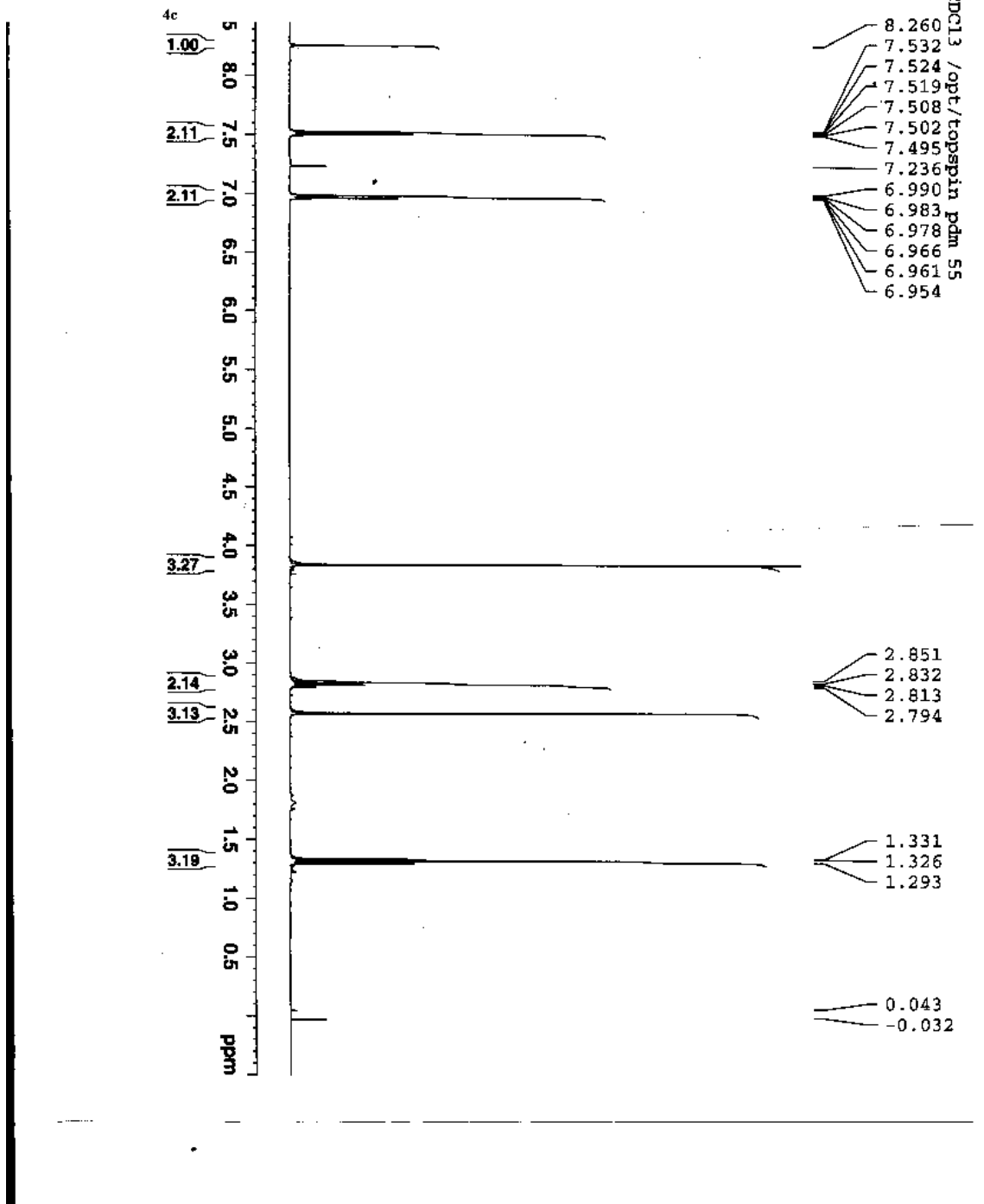
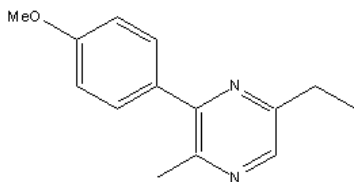
Pyrazine 4b ¹³C Spectrum:



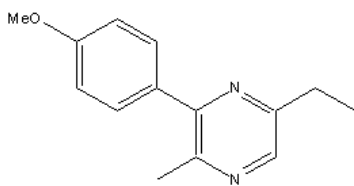
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



Pyrazine 4c ¹H Spectrum:



Pyrazine 4c ¹³C Spectrum:

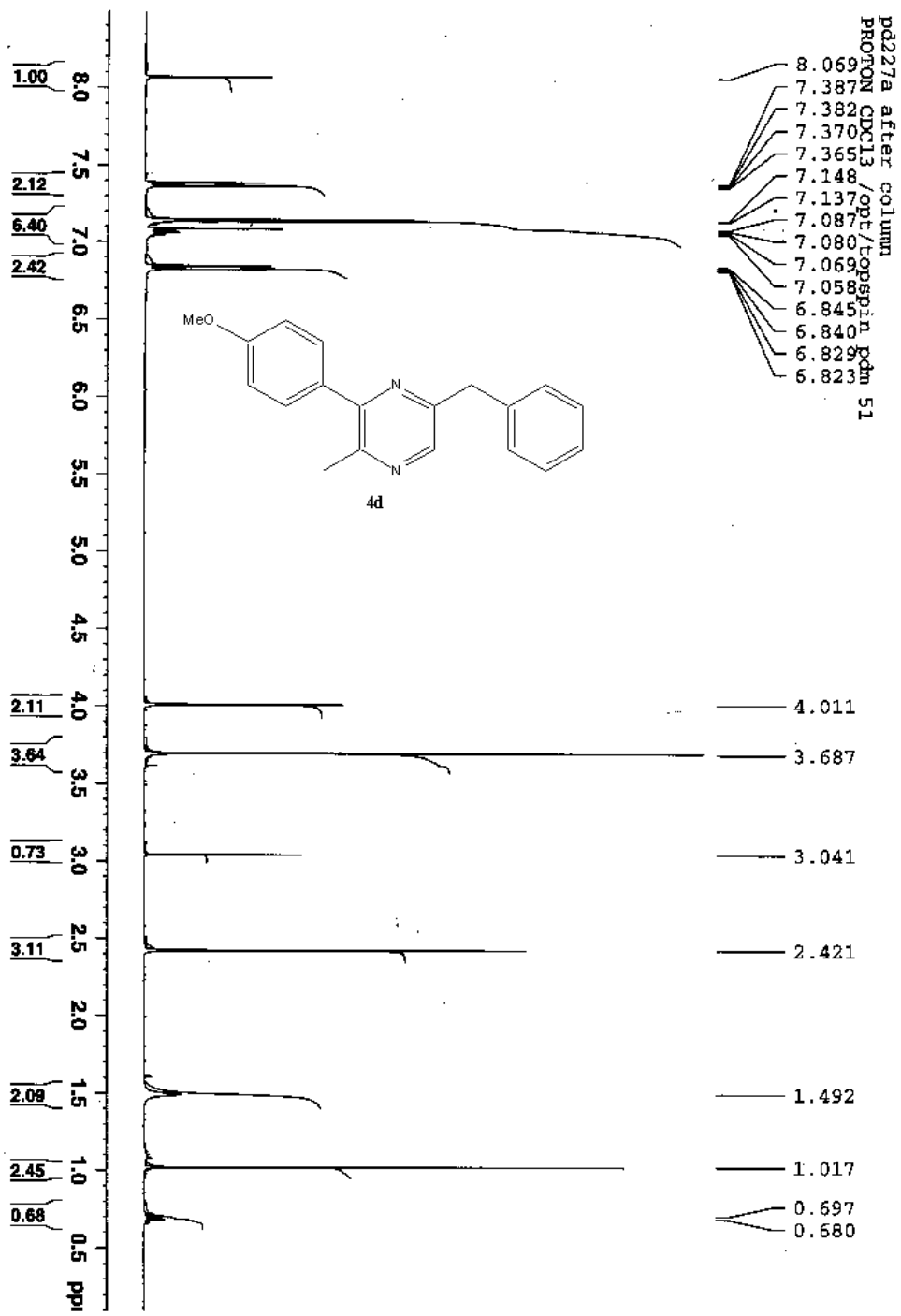


¹³C NMR spectrum showing chemical shifts in ppm (150 to 10) on the x-axis.

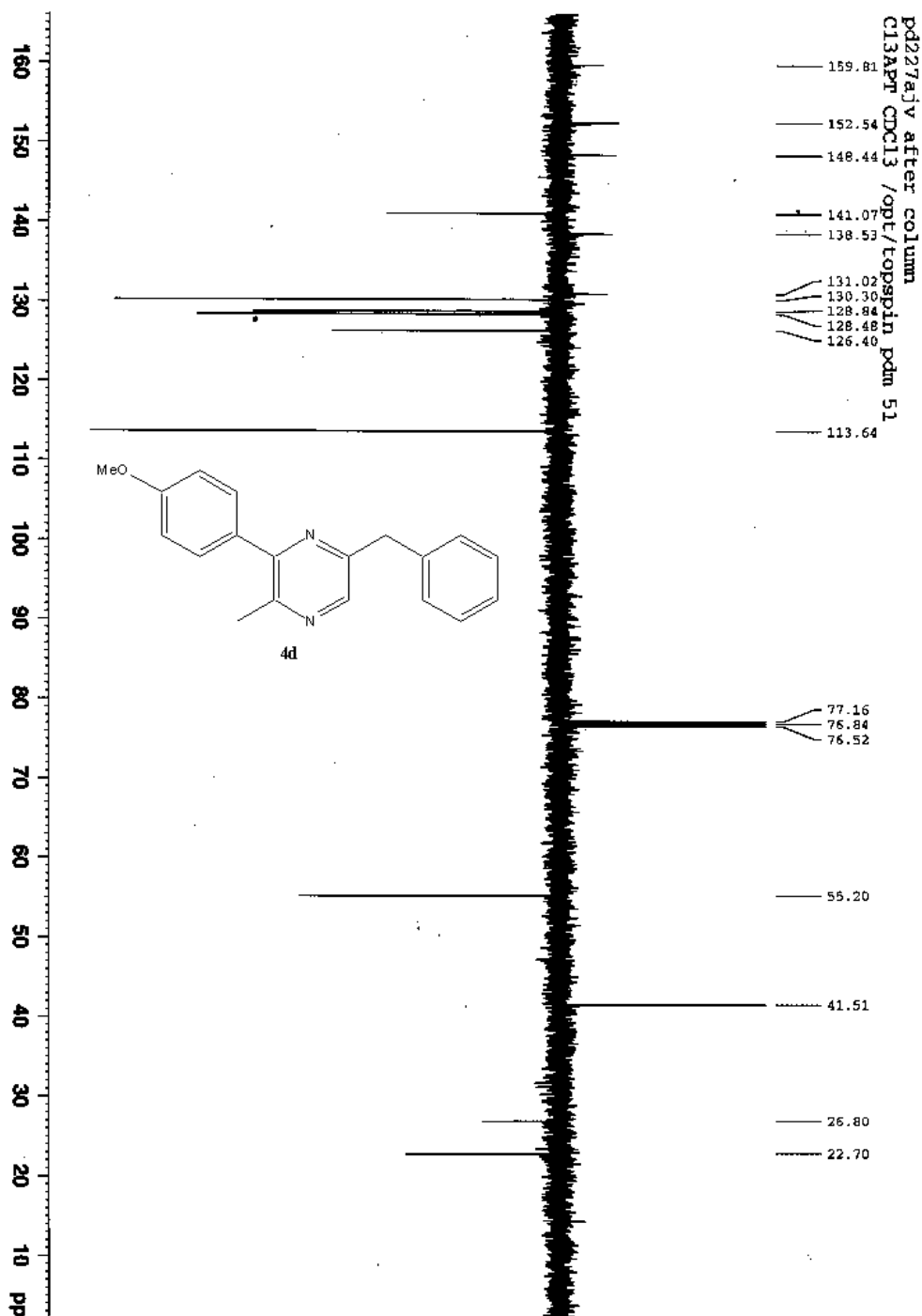


pd249jv
C13APT CDCl3 /opt/cogspin pdm 55

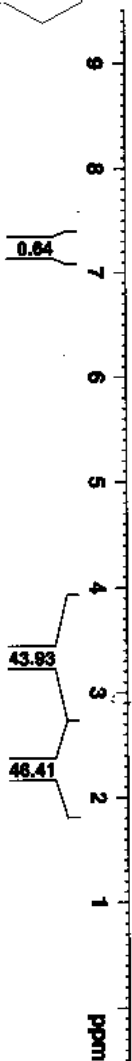
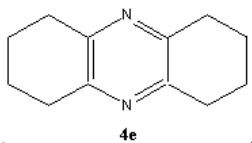
Pyrazine 4d ¹H Spectrum:



Pyrazine 4d ¹³C Spectrum:



Pyrazine 4e ¹H Spectrum:



Current Data Parameters
 NAME: pd231a
 EXPR: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20051111
 Time: 1.58
 INSTRUM: spect
 PROBRD: 5 mm PABBO BB-
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWE: 4006.410 Hz
 FIDRES: 0.061133 Hz
 AQ: 8.1789427 sec
 RG: 50.8
 DW: 124.800 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec
 TDO: 1

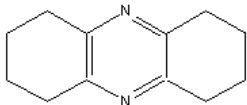
===== CHANNEL f1 =====
 NUC1: ¹H
 P1: 10.25 usec
 PL: -2.00 dB
 SFO1: 400.1318006 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



pd231a
 PROTON CDCl3 /opt/topspin pdm 25

Pyrazine 4e ¹³C Spectrum:



4e

200 180 160 140 120 100 80 60 40 20 0 ppm

PC 1.40

CSB 0

LB 1.00 Hz

SSB 0

WDW EM

SI 32768

SP 100.6126261 MHz

F2 - Processing parameters

SFO2 400.1315005 MHz

FIL2 16.20 dB

PCPD2 -2.00 dB

MPC2 80.00 usec

CHPRG2 waltr216

==== CHANNEL F2 =====

SFO1 100.6228298 MHz

PL1 -3.00 dB

P2 15.20 usec

F1 7.60 usec

MPC1 13C

==== CHANNEL F1 =====

TDI 1

DELTA 0.00000968 sec

d20 5.00000000 sec

d1 5.00000000 sec

CMSTR1 1.00000000

TE 300.0 K

DE 5.00 usec

TM 20.850 usec

RG 16384

AQ 1.3664756 sec

FTURES 0.365918 Hz

SRH 23980.814 Hz

NS 128

SOLVENT MeOD

TD 65836

FIDUCIOS 5

PROBHD 5 mm BBO BB-

INSTRUM spect

Flow 15.1

Date_ 20050817

F2 - Acquisition Parameters

PROCNO 1

EXPNO 1

NAMES pkl149jvert

Current Data Parameters

1



48.15
47.93
47.72
47.51
47.30
47.08
46.87
30.63
22.09

pkl149jvert
C13APT MeOD /opt/topspin pdm 47