

¹H NMR and ¹³C NMR spectral data with peak Assignments

3-hydroxy-3-methylbutyronitrile: These NMR spectra compared favorably with that reported in *J. Org. Chem.* **1996**, *62*, 4087.

3-ethyl-3-hydroxypentanenitrile: These spectra compared favorably with that reported in *J. Org. Chem.* **1968**, *33*, 3402.

3-hydroxy-3-methylpentanenitrile: The boiling point compared favorably to that reported in *Bull. Chim. Belg.* **1932**, *41*, 251. The ¹H and ¹³C NMR spectra do not appear to have been reported. ¹H NMR (CDCl₃): δ 0.97 (t, 3H), 1.35 (s, 3H), 1.66 (m, 2H), 2.18 (bs, 1H), 2.51 (d, 2H). ¹³C NMR (CDCl₃): δ 8.1 (CH₃CH₂), 26.1 (CH₃C(OH)), 30.8 (CH₂CN), 34.2 (CH₂CH₃), 71.3 (COH), 117.8 (CN).

3-phenyl-3-hydroxypropionitrile: ¹H NMR compared favorably to that reported in *Synth. Comm.* **1994**, *24*, 1433. ¹³C NMR compared favorably to that reported in *Tetrahedron* **1994**, *35*, 3447.

3-(4-chlorophenyl)-3-hydroxypropionitrile: ¹H NMR compared favorably with that reported in *J. Org. Chem.* **1991**, *56*, 1381.

3-hydroxy-4-methylhexanenitrile: These NMR spectra compared favorably with that reported in *J. Org. Chem.* **1995**, *60*, 5973.

3-cyclohexyl-3-hydroxypropionitrile: ¹H NMR compared favorably to that reported in *J. Chem. Soc. Perkins Trans 1.* **1991**, 1931.

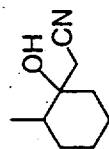
3-(4-methoxyphenyl)-3-hydroxypropionitrile: ¹H NMR compared favorably with that reported in *Bull. Chem. Soc. Japan* **1994**, *67*, 1126.

3-hydroxy-4,4-dimethylpentanenitrile: These NMR spectra compared favorably with that reported in *J. Org. Chem.* **1995**, *60*, 5973.

3-(2,5-dimethoxyphenyl)-3-hydroxypropionitrile: ¹H NMR compared favorably with that reported in *J. Org. Chem.* **1995**, *60*, 2261.

2,3-diphenyl-3-hydroxypropionitrile: These NMR spectra compared favorably with that reported in *J. Org. Chem.* **1995**, *60*, 2261.

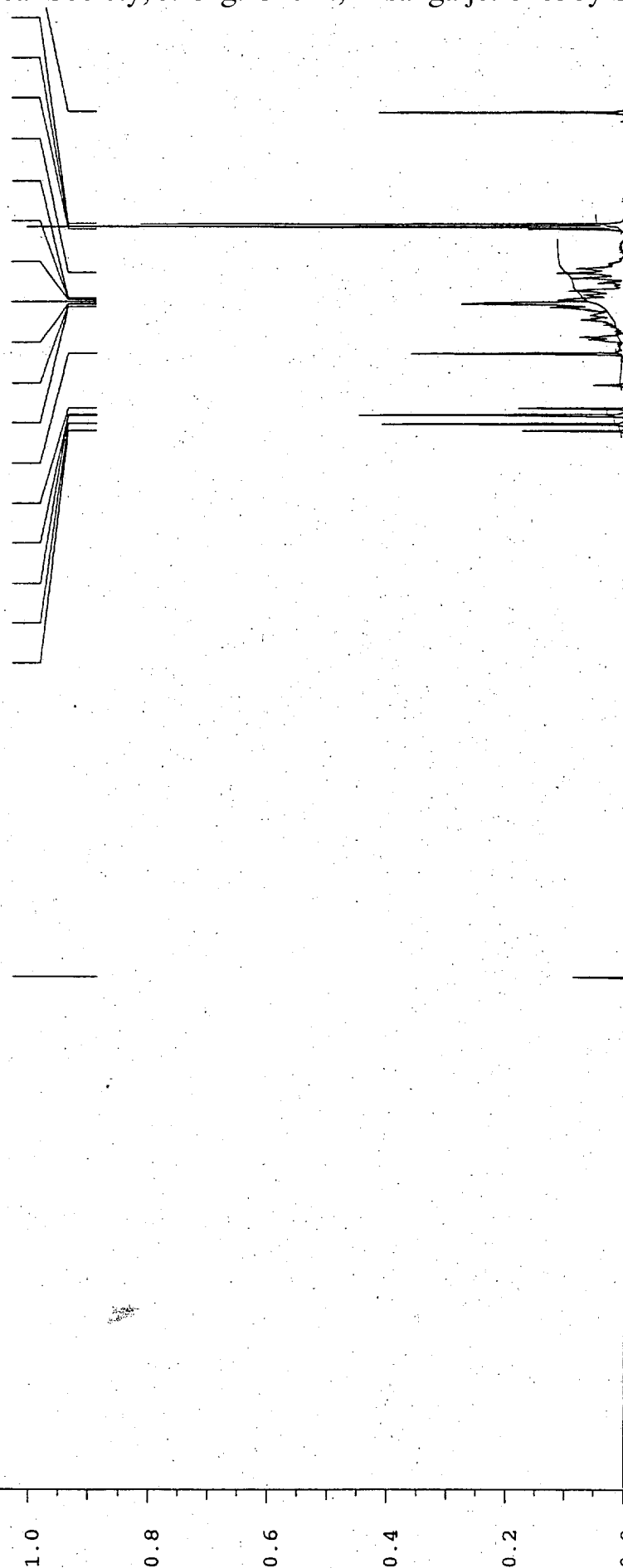
2-methylcy=0 + MeCN; fraction # 4: CDC13



r.i.

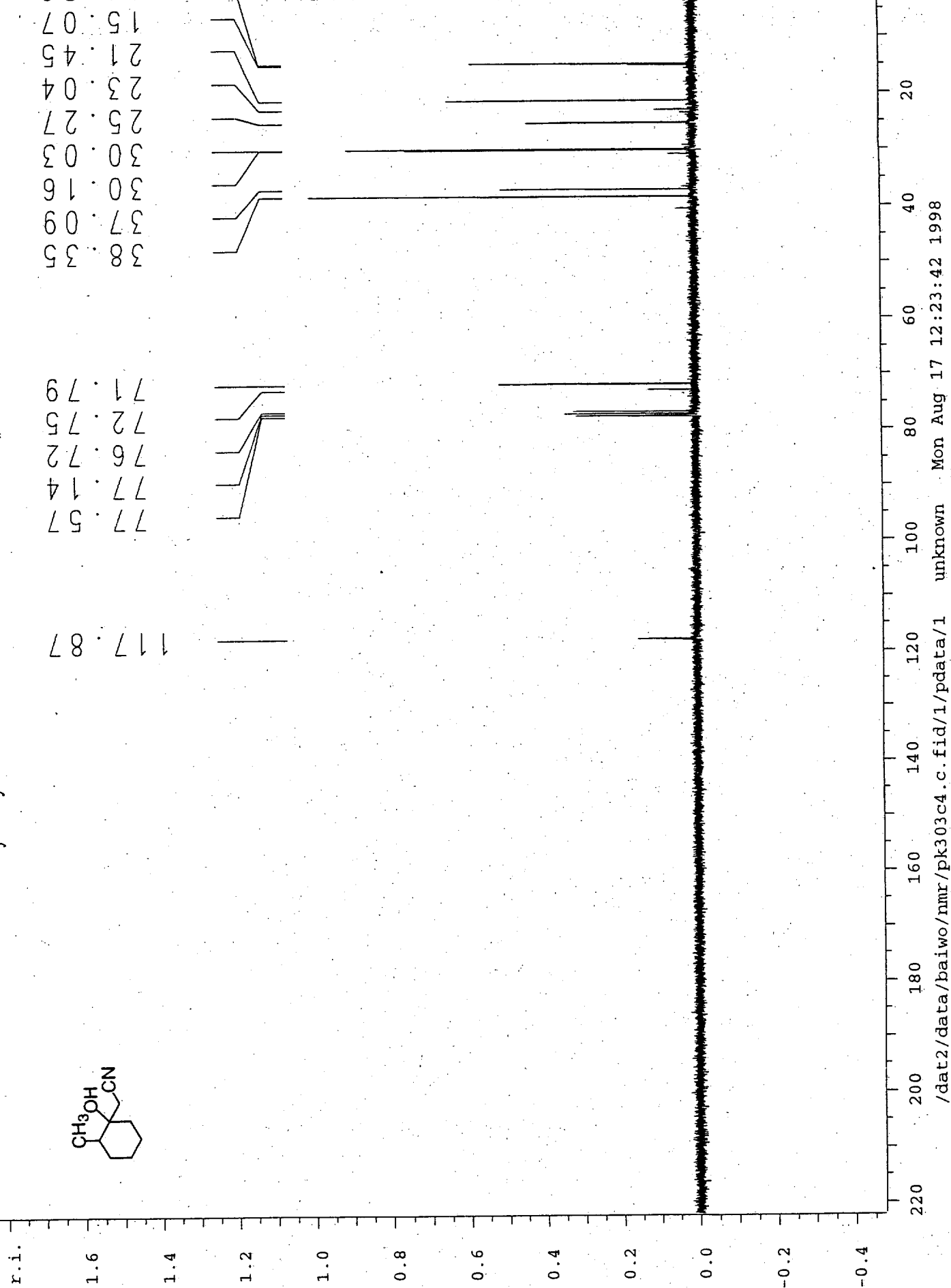
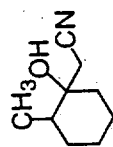
7.30

2.65
2.60
2.52
2.52
2.46
2.01
1.61
1.60
1.59
1.58
1.56
1.55
1.54
1.33
0.97
0.96
0.90



2.00
0.64
7.69
2.99

2-methylcy=0 + MeCN; fraction # 4: CDCl3



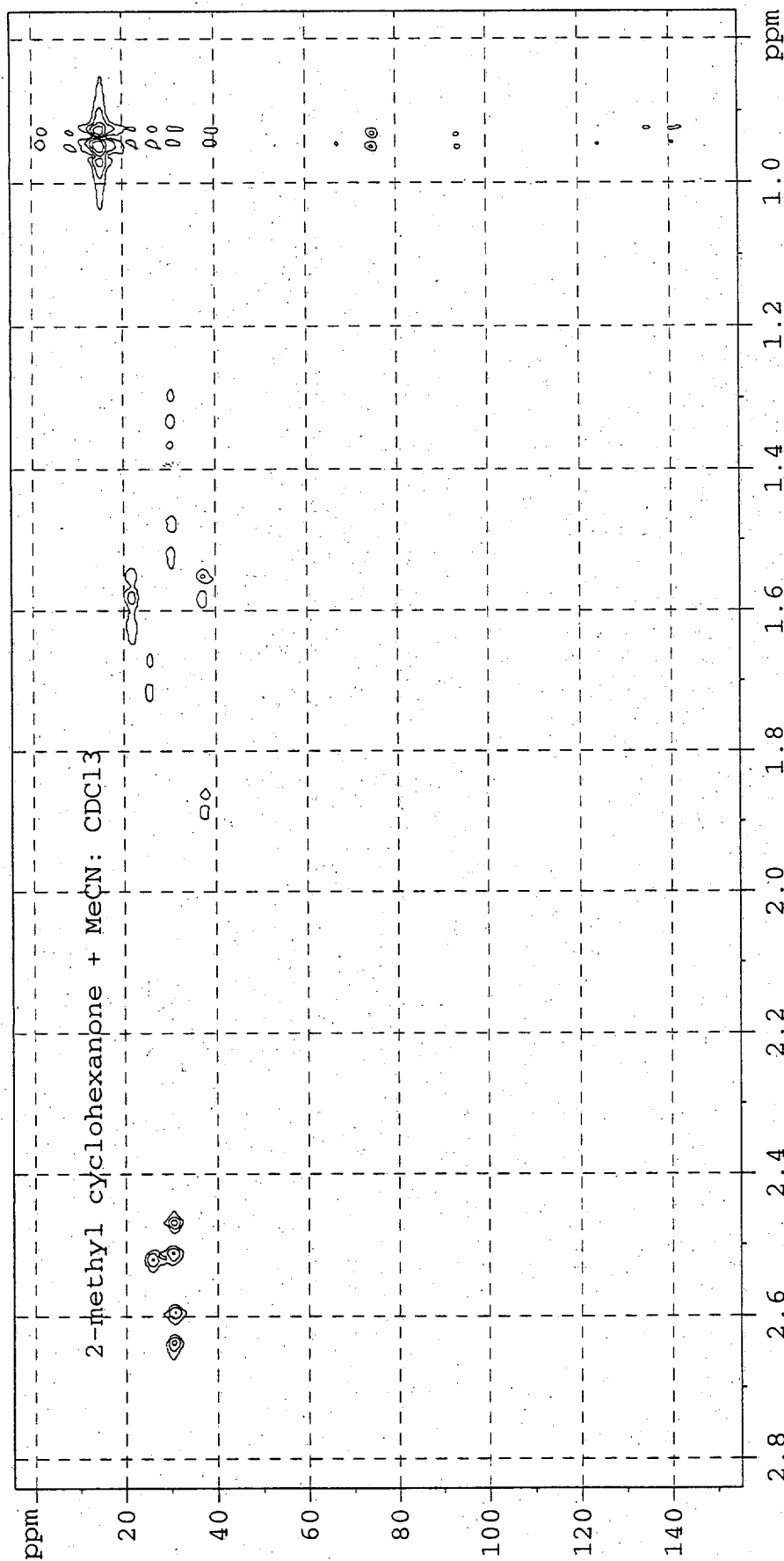
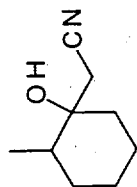
Mass spectrum of 2,4-dichlorobenzonitrile. The x-axis represents the mass-to-charge ratio (m/z) from 40 to 200, and the y-axis represents relative intensity from 0 to 100. The base peak is at m/z 113.1. Other significant peaks are labeled at m/z 55.3, 68.1, 84.0, 95.1, 124.1, 138.1, 153.1, 169.0, and 181.0.

m/z	Relative Intensity (%)
55.3	~35
68.1	~30
84.0	~25
95.1	~85
113.1	100
124.1	~20
138.1	~10
153.1	~5
169.0	~2
181.0	~2

Mass	Int%	Dev ppm	12 C	1 H	13 13c	14 N	16 O
153.11551	2.78	0.97	9	15	0	1	1
152.10811	2.59	3.77	9	14	0	1	1
138.09325	6.10	9.88	8	12	0	1	1
136.11354	4.67	6.70	9	14	0	1	0
135.10547	3.20	4.96	9	13	0	1	0
134.09729	2.21	2.36	9	12	0	1	0
125.08238	2.38	No matches found					
124.07621	12.36	-0.22	7	10	0	1	1
120.08133	8.88	0.02	8	10	0	1	0
114.10040	7.87	3.58	6	13	1	0	1
113.18467	3.29	No matches found					
113.17806	13.43	No matches found					
113.17127	4.64	No matches found					
113.16002	2.68	No matches found					
113.15853	17.97	No matches found					
113.09720	100.00	4.94	7	13	0	0	1
112.16670	2.06	No matches found					
112.08929	8.45	4.21	7	12	0	0	1
111.06822	2.84	-1.75	6	9	0	1	1
110.06131	10.09	6.55	6	8	0	1	1
109.08959	8.57	4.06	7	11	0	1	0
108.16710	2.50	No matches found					
108.08213	13.27	7.41	7	10	0	1	0
97.06612	3.60	8.01	6	9	0	0	1
97.05254	8.23	-2.28	5	7	0	1	1
96.09028	6.31	8.80	6	11	1	0	0
96.04560	34.40	6.86	5	6	0	1	1
96.02857	6.59	No matches found					
95.08724	70.09	No matches found					
95.08474	19.59	No matches found					
95.07307	5.77	-4.52	6	9	0	1	0
95.06831	10.49	-7.54	5	8	1	1	0
95.06322	3.43	No matches found					
94.07829	5.05	0.43	7	10	0	0	0
94.06926	3.31	No matches found					
94.06530	7.20	-3.95	6	8	0	1	0
93.07131	2.63	9.46	7	9	0	0	0
85.10335	2.61	No matches found					
84.05950	3.65	No matches found					
84.04706	11.75	No matches found					
83.05178	3.53	No matches found					
83.03924	6.41	No matches found					
82.06784	3.32	No matches found					
81.07314	2.30	No matches found					
81.06035	4.44	No matches found					
79.05754	5.20	No matches found					
77.04197	2.80	No matches found					
71.08581	3.69	-3.67	5	11	0	0	0
71.05064	5.28	No matches found					
70.07871	21.15	6.50	5	10	0	0	0
70.07362	2.67	-2.31	4	9	1	0	0
70.04245	11.70	8.35	4	6	0	0	1
70.03660	2.44	No matches found					
70.03069	2.37	No matches found					
69.07445	2.65	No matches found					
69.07014	22.26	-4.15	5	9	0	0	0
69.05922	5.05	No matches found					

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PROCNO 1

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MeCOEt + MeCN : CDC13

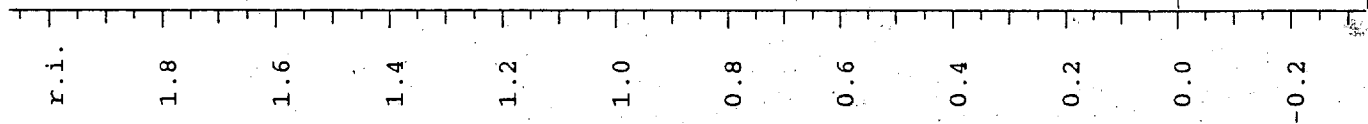
7.28



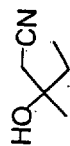
2.56
2.52
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1.67
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0.97
0.95



1.97
0.90
1.97
2.97
3.00

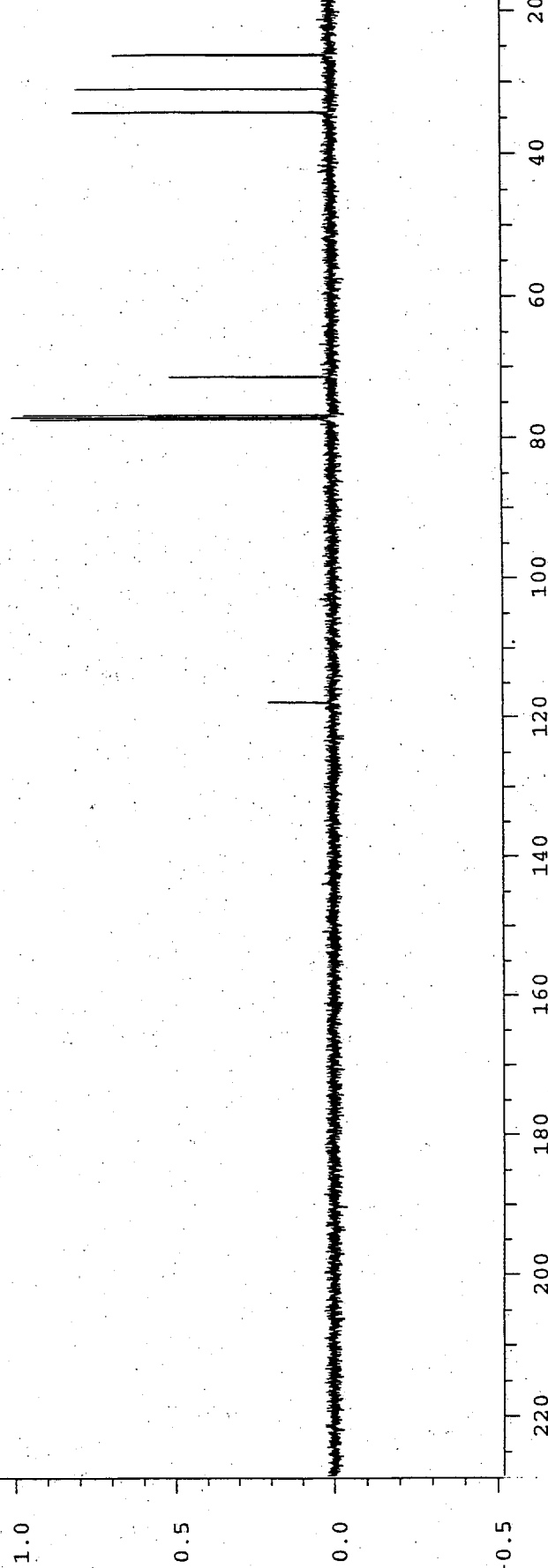


MeCOEt + MeCN : CDC13



r.i.

117.81
77.40
77.08
76.76
71.34
34.16
30.83
26.10
8.10



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameter

Date_ 990204

Time 9.37

INSTRUM spect

PROBHD 5 mm QNP 31P

