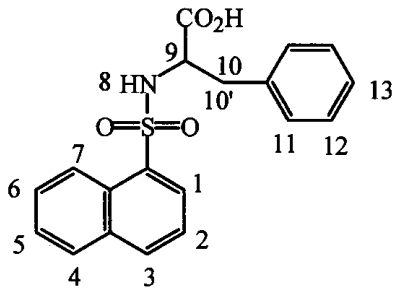
Supporting Information Contents

Complexation-induced ^{1}H NMR shifts of naph-D/L-phe:β-CD complexes.



- **NMR of the Naph-D-phe:β-CD Complex**

The proton shifts observed upon complexation with β-CD

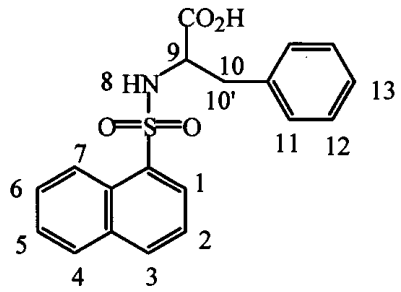
Proton	Naph-D-phe	N-D-P+β–CD	Δδ
1	7.89	7.94	+0.05
2	7.38	7.45	+0.07
3	7.97	8.01	+0.04
4	7.82	7.83	+0.01
5	7.46	7.52	+0.06
6	7.46	7.52	+0.06
7	8.10	8.13	+0.03
9	3.63	obscured	
10	2.80	2.99	+0.19
10'	2.45	2.46	+0.01
11	6.60	6.58	-0.02
12	6.60	6.58	-0.02
13	6.60	6.58	-0.02

- **NMR of the Naph-L-phe:β-CD Complex**

The proton shifts observed upon complexation with β-CD

Proton	Naph-L-phe	N-L-P+β–CD	Δδ
1	7.90	7.92	+0.02
2	7.39	7.44	+0.05
3	7.98	8.00	+0.02
4	7.83	7.85	+0.02
5	7.47	7.51	+0.04
6	7.47	7.51	+0.04
7	8.11	8.08	-0.03
9	3.64	obscured	
10	2.80	3.03	+0.23
10'	2.46	2.47	+0.01
11	6.61	6.54	-0.07
12	6.61	6.54	-0.07
13	6.61	6.54	-0.07

Complexation-induced ^{1}H NMR shifts of naph-D/L-phe:γ-CD complexes.



- **NMR of the Naph-D-phe:γ-CD Complex**

The proton shifts observed upon complexation with γ-CD

Proton	Naph-D-phe	N-D-P+γ-CD	Δδ
1	7.89	7.94	+0.05
2	7.38	7.39	+0.01
3	7.97	7.94	-0.03
4	7.82	7.73	-0.09
5	7.46	7.50	+0.04
6	7.46	7.50	+0.04
7	8.10	8.00	-0.10
9	3.63	obscured	
10	2.80	2.82	+0.02
10'	2.45	2.30	-0.15
11	6.60	6.38	-0.22
12	6.60	6.25	-0.35
13	6.60	6.25	-0.35

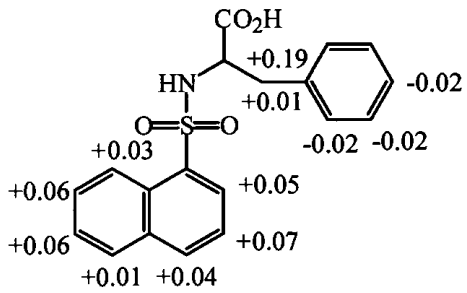
- **NMR of the Naph-L-phe:γ-CD Complex**

The proton shifts observed upon complexation with γ-CD

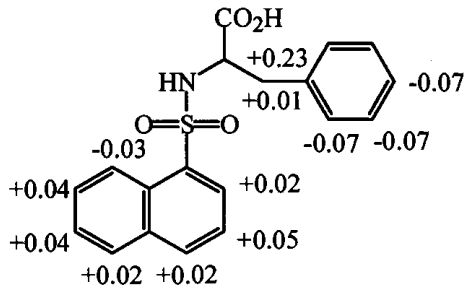
Proton	Naph-L-phe	N-L-P+γ-CD	Δδ
1	7.90	7.90	0.00
2	7.39	7.43	+0.04
3	7.98	7.92	-0.06
4	7.83	7.72	-0.11
5	7.47	7.50	+0.03
6	7.47	7.50	+0.03
7	8.11	8.07	-0.04
9	3.64	obscured	
10	2.80	2.81	+0.01
10'	2.46	2.32	-0.14
11	6.61	6.39	-0.22
12	6.61	6.23	-0.38
13	6.61	6.23	-0.38

Complexation-induced ^{1}H NMR shifts of naph-D/L-phe:β- and γ-CD complexes (figures).

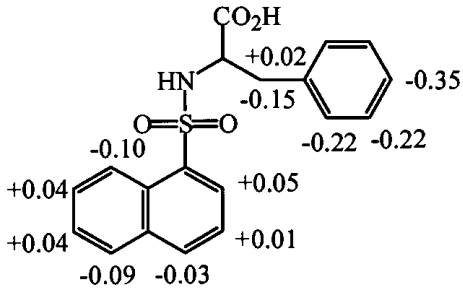
Naph-D-phe+βCD



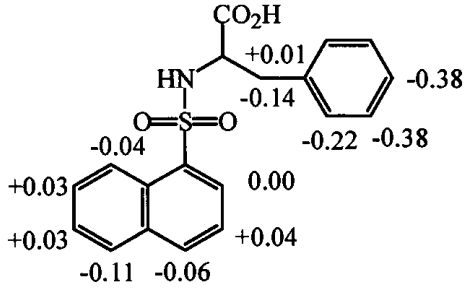
Naph-L-phe+βCD



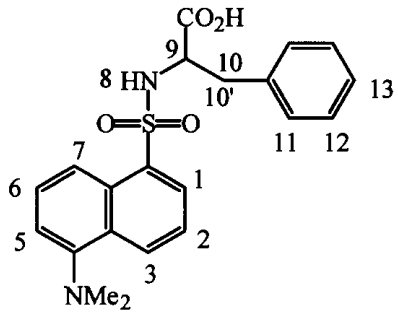
Naph-D-phe+γCD



Naph-L-phe+γCD



Complexation-induced ^{1}H NMR shifts of dans-D/L-phe:β-CD complexes.



- **NMR of the Dans-D-phe:β-CD Complex**

The proton shifts observed upon complexation with β-CD

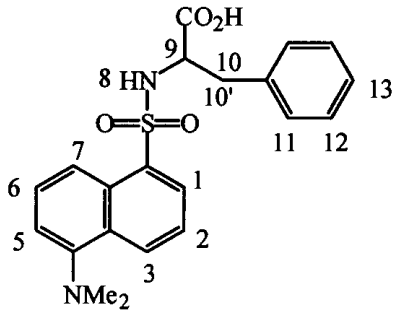
Proton	Dans-D-phe	D-D-P+β–CD	Δδ
1	8.06	8.07	+0.01
2	7.56	7.59	+0.03
3	8.34	8.44	+0.10
5	7.32	7.27	-0.05
6	7.48	7.59	+0.11
7	7.94	8.02	+0.08
9	3.71	obscured	
10	2.91	3.03	+0.12
10'	2.53	2.61	+0.08
11	6.71	6.82	+0.11
12	6.64	6.69	+0.05
13	6.64	6.69	+0.05

- **NMR of the Dans-L-phe:β-CD Complex**

The proton shifts observed upon complexation with β-CD

Proton	Dans-L-phe	D-L-P+β–CD	Δδ
1	8.06	8.10	+0.04
2	7.56	7.64	+0.08
3	8.34	8.45	+0.11
5	7.32	7.28	-0.04
6	7.48	7.56	+0.08
7	7.94	8.00	+0.06
9	3.71	obscured	?
10	2.91	2.94	+0.03
10'	2.53	2.42	-0.11
11	6.71	6.81	+0.10
12	6.64	6.65	+0.01
13	6.64	6.65	+0.01

Complexation-induced ^{1}H NMR shifts of dans-D/L-phe:γ-CD complexes.



- **NMR of the Dans-D-phe:γ-CD Complex**

The proton shifts observed upon complexation with γ-CD

Proton	Dans-D-phe	D-D-P+γCD	Δδ
1	8.06	8.07	+0.01
2	7.56	7.57	+0.01
3	8.34	8.37	+0.03
5	7.32	7.29	-0.03
6	7.48	7.61	+0.13
7	7.94	7.82	-0.12
9	3.71	obscured	
10	2.91	2.93	+0.02
10'	2.53	2.37	-0.15
11	6.71	6.57	-0.14
12	6.64	6.37	-0.27
13	6.64	6.37	-0.27

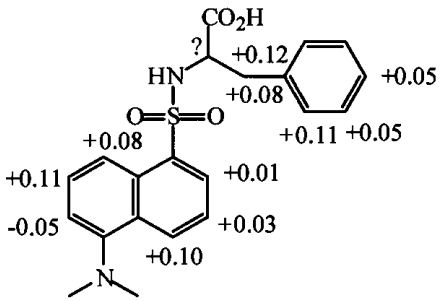
- **NMR of the Dans-L-phe:γ-CD Complex**

The proton shifts observed upon complexation with γ-CD

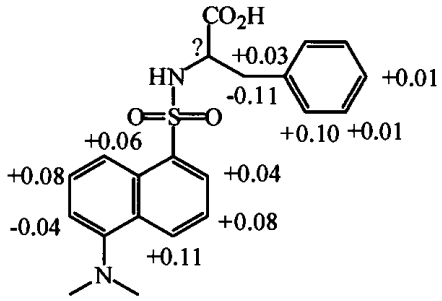
Proton	Dans-L-phe	D-L-P+γCD	Δδ
1	8.06	8.03	-0.03
2	7.56	7.57	+0.01
3	8.34	8.33	-0.01
5	7.32	7.30	-0.02
6	7.48	7.60	+0.12
7	7.94	7.94	0.00
9	3.71	obscured	
10	2.91	3.00	+0.09
10'	2.53	2.58	+0.05
11	6.71	6.59	-0.12
12	6.64	6.38	-0.26
13	6.64	6.38	-0.26

Complexation-induced ^{1}H NMR shifts of dans-D/L-phe:β- and γ-CD complexes (figures).

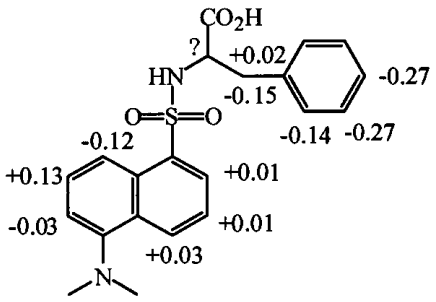
Dans-D-phe+β–CD



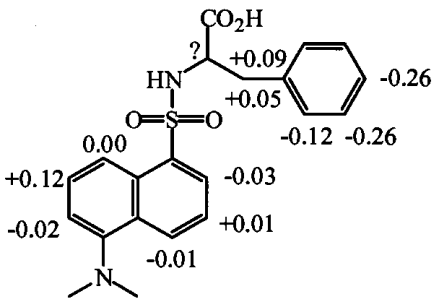
Dans-L-phe+β–CD



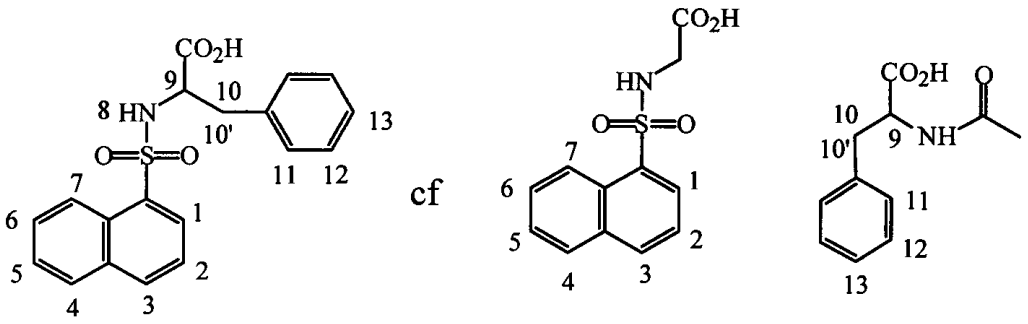
Dans-D-phe+γ–CD



Dans-L-phe+γ–CD



^{1}H NMR shifts of naph-D/L-phe compared to model compounds.



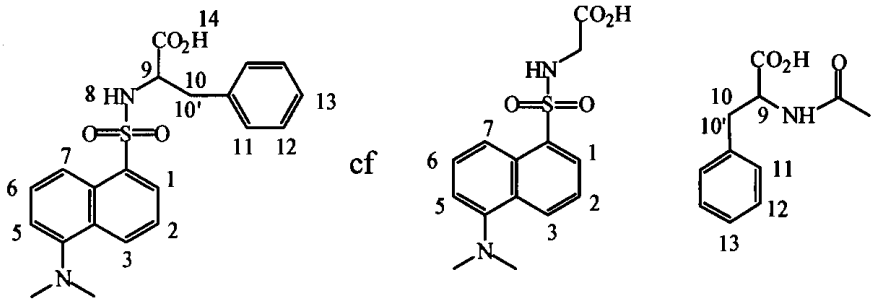
- **Naph-D-phe c.f. (naph-gly and phe-ac)**

Proton	N-D-P	Models	Δδ
1	7.89	8.08 or 8.07	-0.19 or –0.18
2	7.38	7.48	-0.10
3	7.97	8.08 or 8.07	-0.11 or –0.10
4	7.82	7.93	-0.11
5	7.46	7.54	-0.08
6	7.46	7.62	-0.16
7	8.10	8.43	-0.33
9	3.63	4.27	-0.64
10	2.80	3.02	-0.22
10'	2.45	2.74	-0.29
11	6.60	7.24 to 7.10	-0.64 to -0.50
12	6.60	7.24 to 7.10	-0.64 to -0.50
13	6.60	7.24 to 7.10	-0.64 to -0.50

- **Naph-L-phe c.f. (naph-gly and phe-ac)**

Proton	N-L-P	Models	Δδ
1	7.90	8.08 or 8.07	-0.18 or -0.17
2	7.39	7.48	-0.09
3	7.98	8.08 or 8.07	-0.10 or -0.09
4	7.83	7.93	-0.10
5	7.47	7.54	-0.07
6	7.47	7.62	-0.15
7	8.11	8.43	-0.32
9	3.64	4.27	-0.63
10	2.80	3.02	-0.22
10'	2.46	2.74	-0.28
11	6.61	7.24 to 7.10	-0.63 to -0.49
12	6.61	7.24 to 7.10	-0.63 to -0.49
13	6.61	7.24 to 7.10	-0.63 to -0.49

^{1}H NMR shifts of dans-D/L-phe compared to model compounds



- **Dans-D-phe c.f. (dans-gly and phe-ac)**

Proton	D-D-P	Models	Δδ
1	8.06	8.24	-0.18
2	7.56	7.68	-0.12
3	8.34	8.49	-0.15
5	7.32	7.41	-0.09
6	7.48	7.70	-0.22
7	7.94	8.31	-0.37
9	3.71	4.27	-0.56
10	2.91	3.02	-0.11
10'	2.53	2.74	-0.21
11	6.71	7.24 to 7.10	-0.53 to -0.39
12	6.64	7.24 to 7.10	-0.60 to -0.46
13	6.64	7.24 to 7.10	-0.60 to -0.46

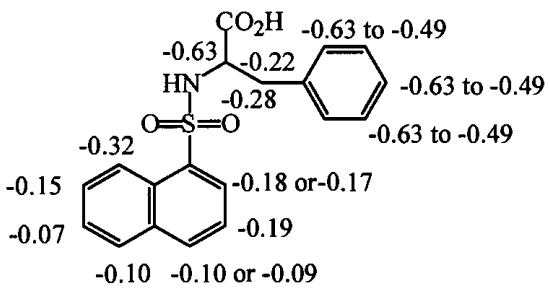
- **Dans-L-phe c.f. (dans-gly and phe-ac)**

Proton	D-L-P	Models	Δδ
1	8.06	8.24	-0.18
2	7.56	7.68	-0.12
3	8.34	8.49	-0.15
5	7.32	7.41	-0.09
6	7.48	7.70	-0.22
7	7.94	8.31	-0.37
9	3.71	4.27	-0.56
10	2.91	3.02	-0.11
10'	2.53	2.74	-0.21
11	6.71	7.24 to 7.10	-0.53 to -0.39
12	6.64	7.24 to 7.10	-0.60 to -0.46
13	6.64	7.24 to 7.10	-0.60 to -0.46

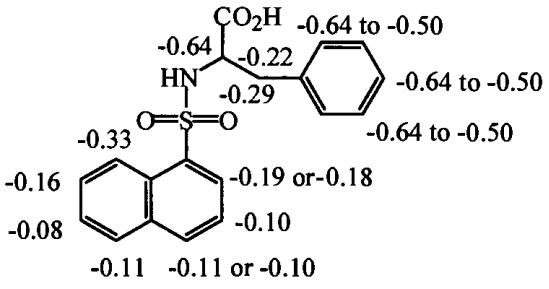
^{1}H NMR shifts of naph- and dans- D/L-phe compared to model compounds (figures).

Naph-D/L-phe c.f. Models

naph-L-phe cf models

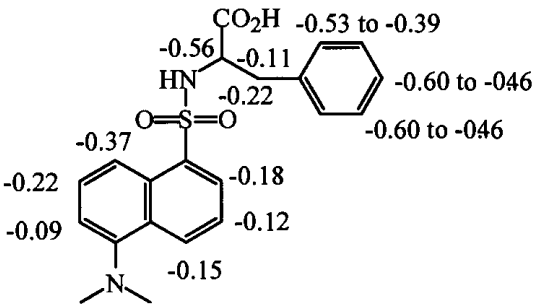


naph-D-phe cf models

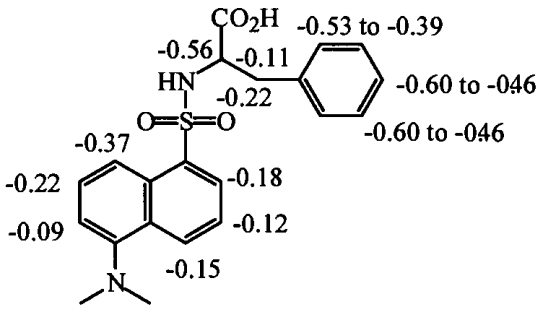


Dans-D/L-phe c.f. Models

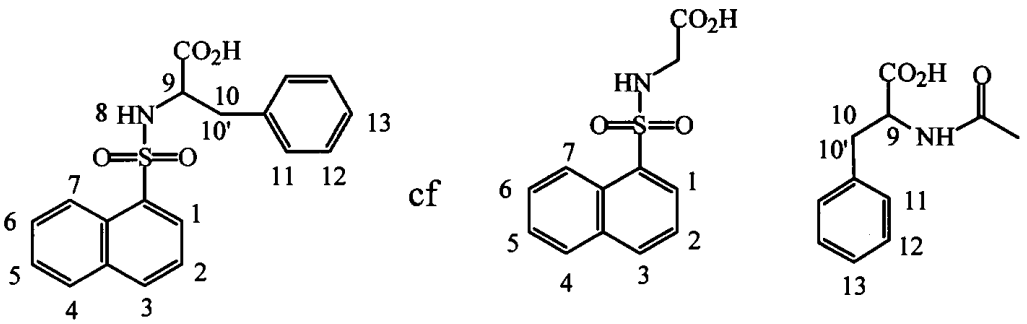
dans-L-phe cf models



dans-D-phe cf models



^{1}H NMR shifts of naph-D/L-phe:β-CD complexes compared to model compounds



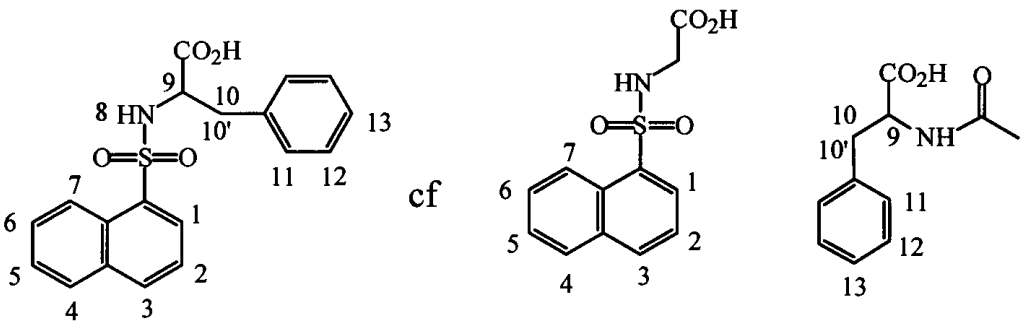
- **Naph-D-phe + β–CD c.f. (naph-gly and phe-ac)**

Proton	N-D-P+β–CD	Models	Δδ
1	7.94	8.08 or 8.07	-0.14 or –0.13
2	7.45	7.48	-0.03
3	8.00	8.08 or 8.07	-0.08 or –0.07
4	7.85	7.93	-0.08
5	7.51	7.54	-0.03
6	7.51	7.62	-0.11
7	8.08	8.43	-0.35
9	obscured	4.27	
10	3.03	3.02	+0.01
10'	2.47	2.74	-0.27
11	6.54	7.24 to 7.10	-0.70 to -0.56
12	6.54	7.24 to 7.10	-0.70 to -0.56
13	6.54	7.24 to 7.10	-0.70 to -0.56

- **Naph-L-phe + β–CD c.f. (naph-gly and phe-ac)**

Proton	N-L-P+β–CD	Models	Δδ
1	7.92	8.08 or 8.07	-0.16 or -0.15
2	7.44	7.48	-0.04
3	8.00	8.08 or 8.07	-0.08 or -0.07
4	7.85	7.93	-0.08
5	7.51	7.54	-0.03
6	7.51	7.62	-0.11
7	8.08	8.43	-0.35
9	obscured	4.27	
10	3.03	3.02	+0.01
10'	2.47	2.74	-0.27
11	6.54	7.24 to 7.10	-0.70 to -0.56
12	6.54	7.24 to 7.10	-0.70 to -0.56
13	6.54	7.24 to 7.10	-0.70 to -0.56

^{1}H NMR shifts of naph-D/L-phe:γ-CD complexes compared to model compounds



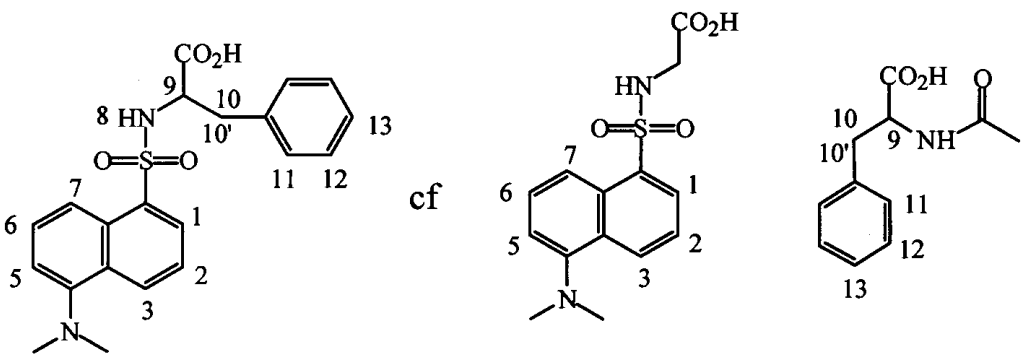
- **Naph-D-phe + γ–CD c.f. (naph-gly and phe-ac)**

Proton	N-D-P+γ–CD	Models	Δδ
1	7.94	8.08 or 8.07	-0.14 or –0.13
2	7.39	7.48	-0.09
3	7.94	8.08 or 8.07	-0.14 or –0.13
4	7.73	7.93	-0.20
5	7.50	7.54	-0.04
6	7.50	7.62	-0.12
7	8.00	8.43	-0.43
9	obscured	4.27	
10	2.82	3.02	-0.20
10'	2.30	2.74	-0.44
11	6.38	7.24 to 7.10	-0.86 to -0.72
12	6.25	7.24 to 7.10	-0.99 to -0.85
13	6.25	7.24 to 7.10	-0.99 to -0.85

- **Naph-L-phe + γ–CD c.f. (naph-gly and phe-ac)**

Proton	N-L-P+γ–CD	Models	Δδ
1	7.90	8.08 or 8.07	-0.18 or -0.17
2	7.43	7.48	-0.05
3	7.92	8.08 or 8.07	-0.16 or -0.15
4	7.72	7.93	-0.21
5	7.50	7.54	-0.04
6	7.50	7.62	-0.12
7	8.07	8.43	-0.36
9	obscured	4.27	
10	2.81	3.02	-0.21
10'	2.32	2.74	-0.42
11	6.39	7.24 to 7.10	-0.85 to -0.71
12	6.23	7.24 to 7.10	-1.01 to -0.87
13	6.23	7.24 to 7.10	-1.01 to -0.87

^{1}H NMR shifts of dans-D/L-phe:β-CD complexes compared to model compounds



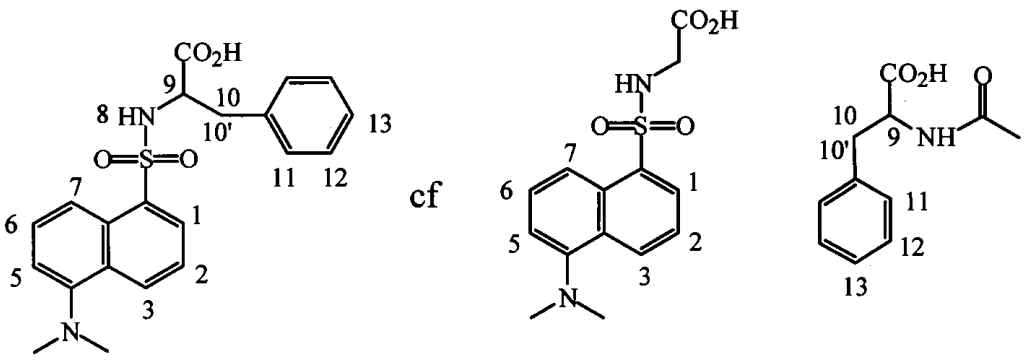
- **Dans-D-phe + β–CD c.f. (dans-gly and phe-ac)**

Proton	N-D-P+β–CD	Models	Δδ
1	8.07	8.24	-0.17
2	7.59	7.68	-0.09
3	8.44	8.49	-0.05
5	7.27	7.41	-0.14
6	7.59	7.70	-0.11
7	8.02	8.31	-0.29
9	obscured	4.27	
10	3.03	3.02	+0.01
10'	2.61	2.74	-0.13
11	6.82	7.24 to 7.10	-0.42 to -0.28
12	6.69	7.24 to 7.10	-0.55 to -0.41
13	6.69	7.24 to 7.10	-0.55 to -0.41

- **Dans-L-phe + β–CD c.f. (dans-gly and phe-ac)**

Proton	D-L-P+β–CD	Models	Δδ
1	8.10	8.24	-0.14
2	7.64	7.68	-0.04
3	8.45	8.49	-0.04
5	7.28	7.41	-0.13
6	7.56	7.70	-0.16
7	8.00	8.31	-0.31
9	obscured	4.27	
10	2.94	3.02	-0.08
10'	2.42	2.74	-0.32
11	6.81	7.24 to 7.10	-0.43 to -0.29
12	6.65	7.24 to 7.10	-0.59 to -0.45
13	6.65	7.24 to 7.10	-0.59 to -0.45

^{1}H NMR shifts of dans-D/L-phe:γ-CD complexes compared to model compounds



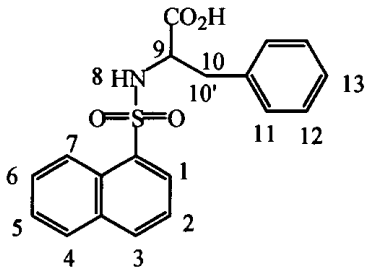
- **Dans-D-phe + γ–CD c.f. (dans-gly and phe-ac)**

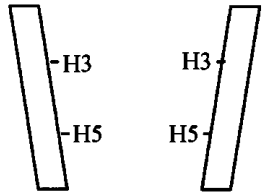
Proton	D-D-P+γ–CD	Models	Δδ
1	8.07	8.24	-0.17
2	7.57	7.68	-0.11
3	8.37	8.49	-0.12
5	7.29	7.41	-0.12
6	7.61	7.70	-0.09
7	7.82	8.31	-0.49
9	obscured	4.27	
10	2.93	3.02	-0.09
10'	2.37	2.74	-0.37
11	6.57	7.24 to 7.10	-0.67 to -0.53
12	6.37	7.24 to 7.10	-0.87 to -0.73
13	6.37	7.24 to 7.10	-0.87 to -0.73

- **Dans-L-phe + γ–CD c.f. (dans-gly and phe-ac)**

Proton	D-L-P+γ–CD	Models	Δδ
1	8.03	8.24	-0.21
2	7.57	7.68	-0.11
3	8.33	8.49	-0.16
5	7.30	7.41	-0.11
6	7.60	7.70	-0.10
7	7.94	8.31	-0.35
9	obscured	4.27	
10	3.00	3.02	-0.02
10'	2.58	2.74	-0.16
11	6.59	7.24 to 7.10	-0.65 to -0.51
12	6.38	7.24 to 7.10	-0.86 to -0.72
13	6.38	7.24 to 7.10	-0.86 to -0.72

NOE's Observed in Naph-D/L-phe+β and γ-CD Complexes





Naph-L-phe+βCD	Peak Intensity
$H_3 \leftrightarrow 3$	(m)
$H_3 \leftrightarrow 4$	(w)
$H_3 \leftrightarrow 2$	(m)
$H_3 \leftrightarrow 5,6$	(m)
$H_3 \leftrightarrow 11,12,13$	(s)
$H_5 \leftrightarrow 11,12,13$	(s)
$H_5 \leftrightarrow 10$	(w)

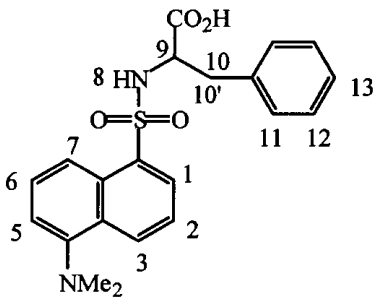
Naph-L-phe+γCD	Peak Intensity
$H_{3/5} \leftrightarrow 7$	(m)
$H_{3/5} \leftrightarrow 3,1$	(s)
$H_{3/5} \leftrightarrow 4$	(w)
$H_{3/5} \leftrightarrow 5,6$	(m)
$H_{3/5} \leftrightarrow 2$	(m)
$H_{3/5} \leftrightarrow 11$	(s)
$H_{3/5} \leftrightarrow 12,13$	(s)
$H_{3/5} \leftrightarrow 10$	(m)
$H_{3/5} \leftrightarrow 10'$	(m)

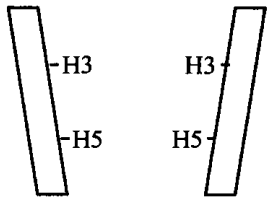
Naph-D-phe+βCD	Peak Intensity
$H_3 \leftrightarrow 7$	(w)
$H_3 \leftrightarrow 3$	(m)
$H_3 \leftrightarrow 1$	(w)
$H_3 \leftrightarrow 4$	(m)
$H_3 \leftrightarrow 5,6$	(w)
$H_3 \leftrightarrow 2$	(m)
$H_3 \leftrightarrow 11,12,13$	(s)
$H_5 \leftrightarrow 1$	(w)
$H_5 \leftrightarrow 11,12,13$	(s)
$H_5 \leftrightarrow 10$	(m)
$11,12,13 \leftrightarrow 10'$	(m)

Naph-D-phe+γCD	Peak Intensity
$H_3 \leftrightarrow 7$	(m)
$H_3 \leftrightarrow 3,1$	(m)
$H_3 \leftrightarrow 4$	(w)
$H_3 \leftrightarrow 5,6$	(m)
$H_3 \leftrightarrow 2$	(m/w)
$H_3 \leftrightarrow 11$	(s)
$H_3 \leftrightarrow 12,13$	(s)
$H_5 \leftrightarrow 1,3$	(m)
$H_5 \leftrightarrow 5,6$	(m)
$H_5 \leftrightarrow 2$	(m/w)
$H_5 \leftrightarrow 11$	(s)
$H_5 \leftrightarrow 12,13$	(s)
$H_5 \leftrightarrow 10$	(m)
$11 \leftrightarrow 10'$	(m)

(w) = weak; (m) = medium; (s) = strong

NOE's Observed in Dans-D/L-phe+β and γ-CD Complexes





Dans-L-phe+βCD	Peak Intensity
$H_3 \leftrightarrow 3$	(m)
$H_3 \leftrightarrow 7$	(w)
$H_3 \leftrightarrow 2$	(w)
$H_3 \leftrightarrow 6$	(m)
$H_3 \leftrightarrow 5$	(s/m)
$H_3 \leftrightarrow 11,12,13$	(s)
$H_5 \leftrightarrow 11$	(s)
$NMe_2 \leftrightarrow 3$	(m)
$NMe_2 \leftrightarrow 5$	(m)
$NMe_2 \leftrightarrow 12,13$	(m)
$H_{3/5} \leftrightarrow NMe_2$	(m)
$11 \leftrightarrow 10'$	(m)

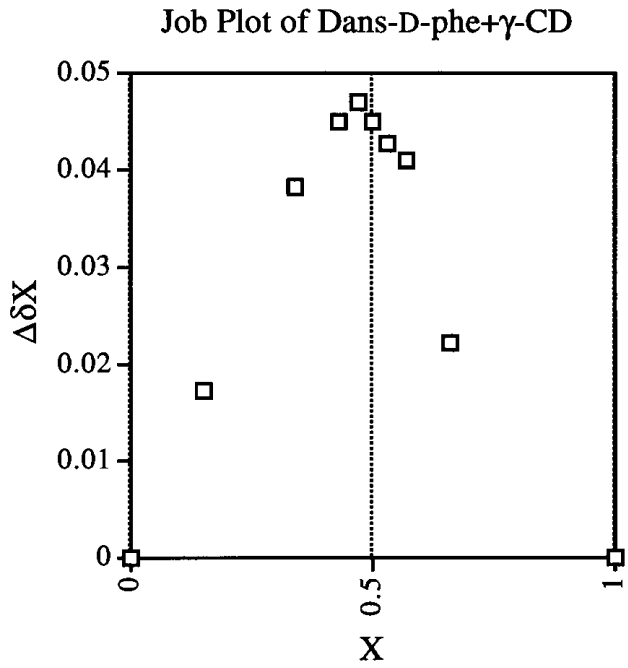
Dans-L-phe+γCD	Peak Intensity
$H_{3/5} \leftrightarrow 1$	(m)
$H_3 \leftrightarrow 7$	(m)
$H_{3/5} \leftrightarrow 2,6$	(s)
$H_{3/5} \leftrightarrow 11,12,13$	(s)
$NMe_2 \leftrightarrow 12,13$	(m)
$NMe_2 \leftrightarrow 3$	(m)
$NMe_2 \leftrightarrow 5$	(m)
$11 \leftrightarrow 10$	(w)
$11 \leftrightarrow 10'$	(m)

Dans-D-phe+βCD	Peak Intensity
$H_3 \leftrightarrow 3$	(w)
$H_3 \leftrightarrow 7$	(w)
$H_3 \leftrightarrow 2,6$	(m)
$H_3 \leftrightarrow 5$	(m)
$H_3 \leftrightarrow 11,12,13$	(m)
$H_5 \leftrightarrow 5$	(w)
$H_5 \leftrightarrow 11$ or 12	(w)
$NMe_2 \leftrightarrow 3$	(m)
$NMe_2 \leftrightarrow 5$	(m)

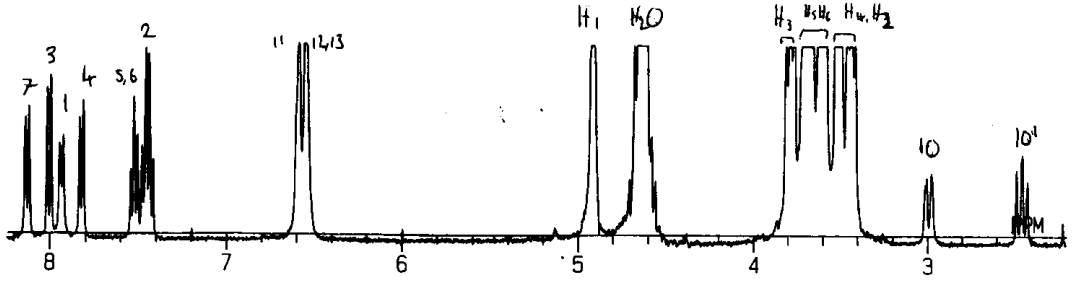
Dans-D-phe+γCD	Peak Intensity
$H_3 \leftrightarrow 1$	(w)
$H_3 \leftrightarrow 2,6$	(m)
$H_3 \leftrightarrow 5$	(w)
$H_3 \leftrightarrow 11,12,13$	(s)
$H_5 \leftrightarrow 1$	(m/w)
$H_5 \leftrightarrow 7$	(w)
$H_5 \leftrightarrow 2,6$	(w)
$H_5 \leftrightarrow 11,12,13$	(s)
$NMe_2 \leftrightarrow 12,13$	(m)
$NMe_2 \leftrightarrow 3$	(m)
$NMe_2 \leftrightarrow 5$	(m)
$11 \leftrightarrow 10'$	(m)

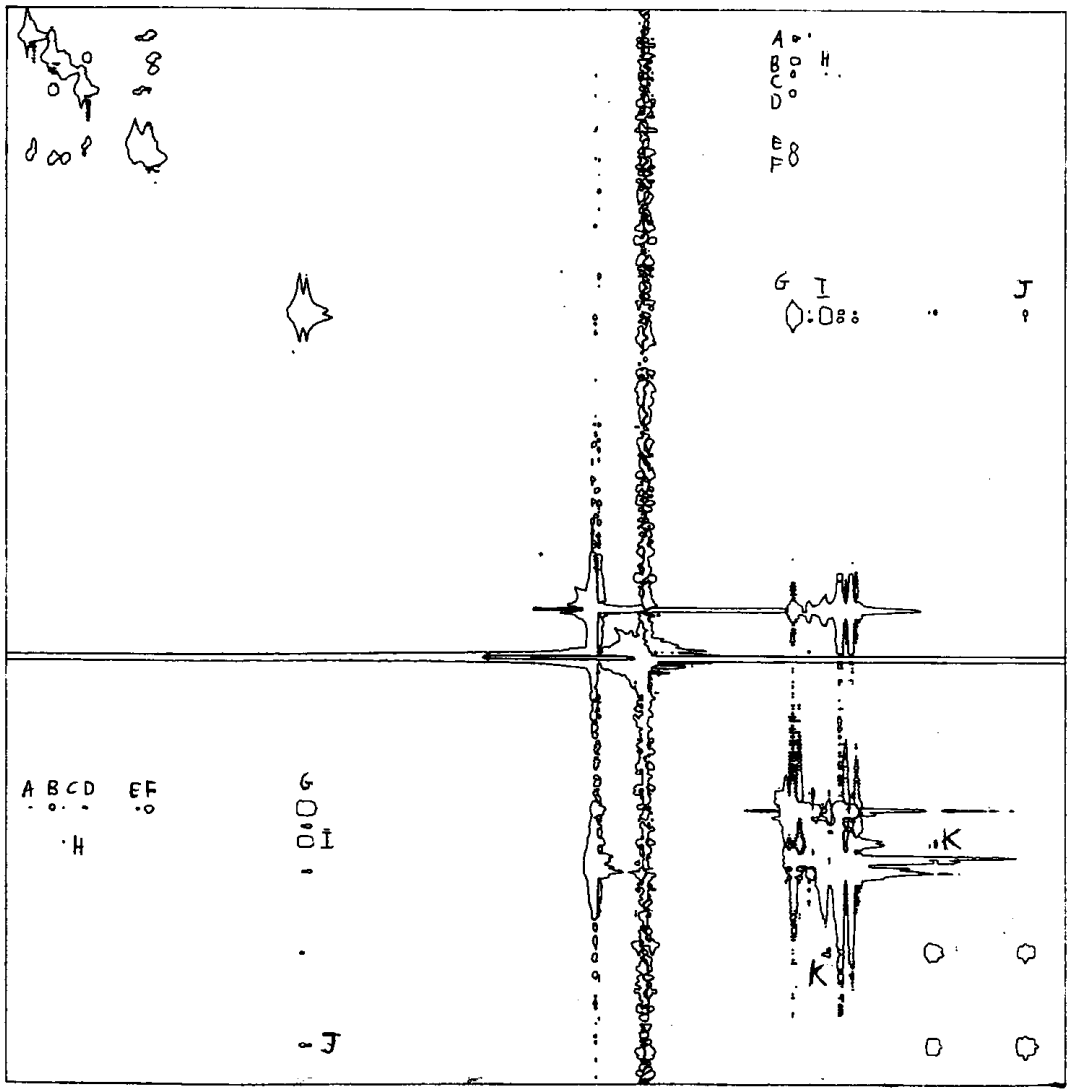
(w) = weak; (m) = medium; (s) = strong

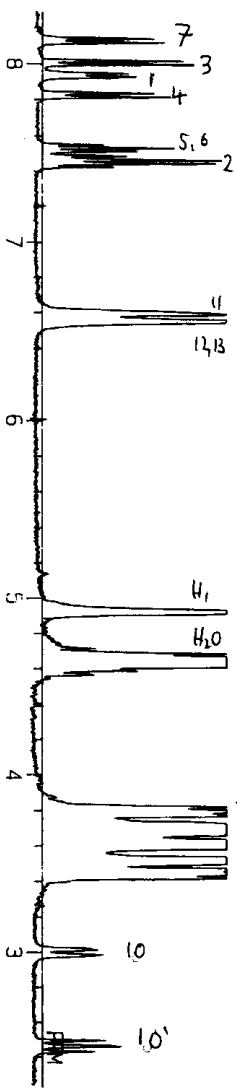
^{1}H NMR Job Plot of the Dans-D-phe+γ-CD Complex



Job plot of the dans-D-phe+γ-CD complex; total concentration = 20mM

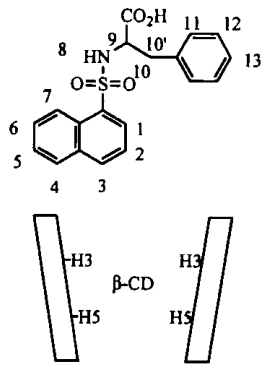


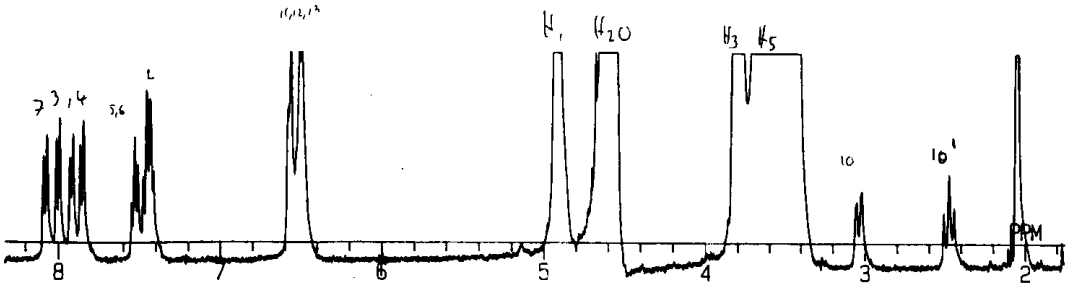


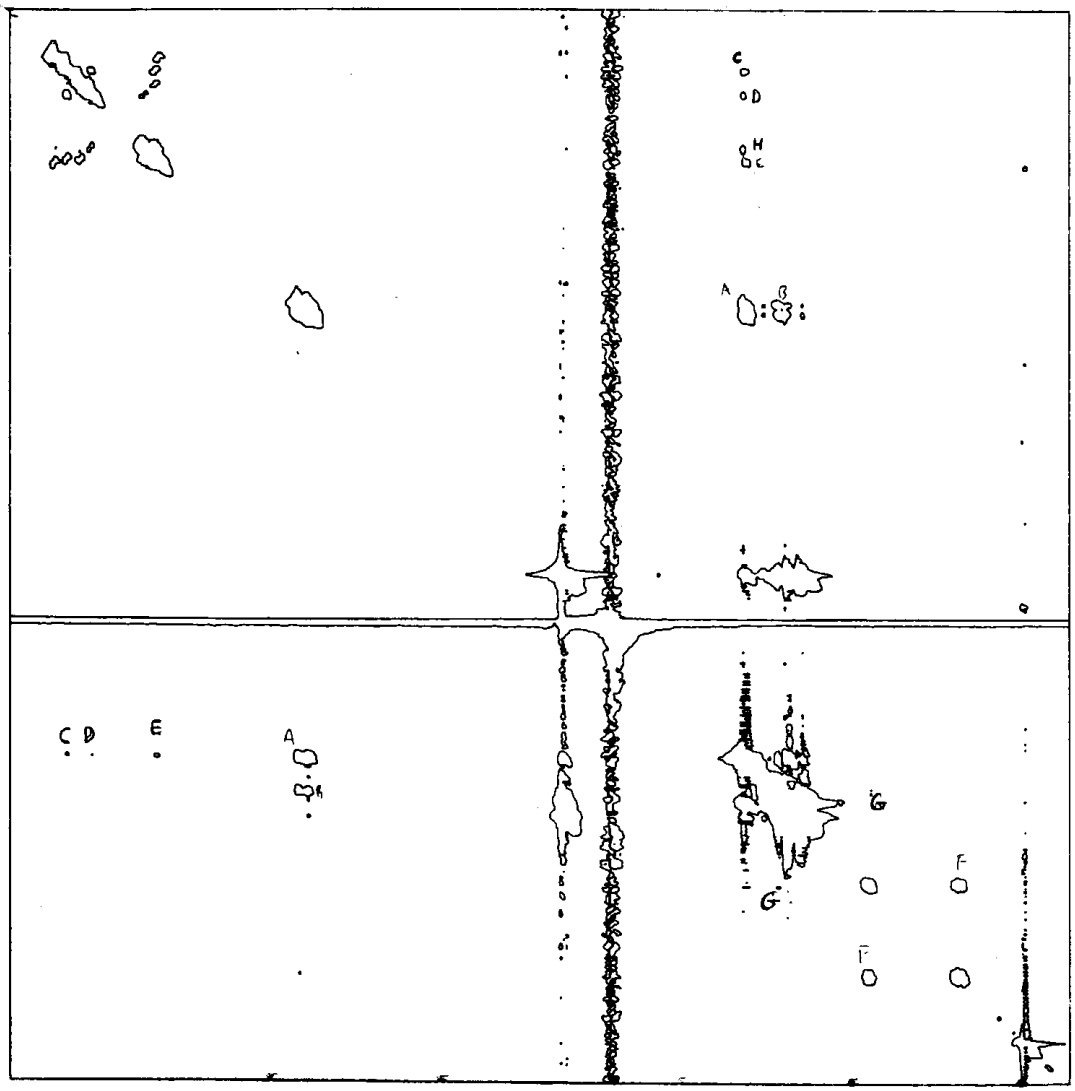


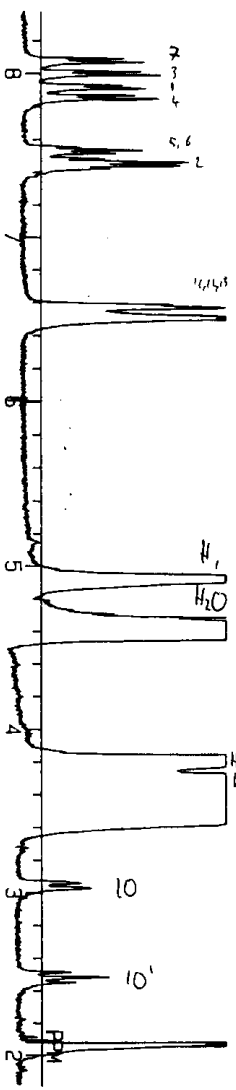

```
02-OCT-99 07:50:17
DFILE 209910021
COMNT RX052_N-D-P+BCD_KBUFF_991002
EXMOD VPHROEH
OBNUC 1H
OBFIN      10453.1 Hz
POINT         1024
FREQU       3909.3 Hz
CLPNT         1024
TODAT          512
CLFRQ       3909.3 Hz
SCANS            16
ACQTM         0.131 sec
PD            2.369 sec
PW1           44.0 us
PW2           22.0 us
PW3           40.5 us
PI1           0.010 ms
PI2           0.256 ms
PI3         450.000 ms
IRATN           511
OBATN           100
CTEMP         23.2 c
CSPED            9 Hz
SLVNT D2O
LOOP1           1200
XS        -145.0719 Hz
CXS       -160.3424 Hz
XE        2412.7740 Hz
CXE       2420.4060 Hz
TH          1.40000
DET           10.0 us
DELAY        135.0 us
OPERATOR :
```

naph-D-phe



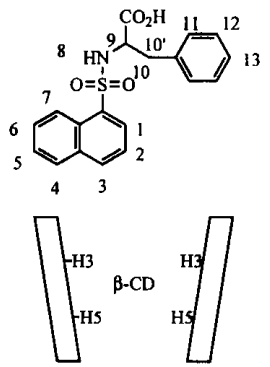




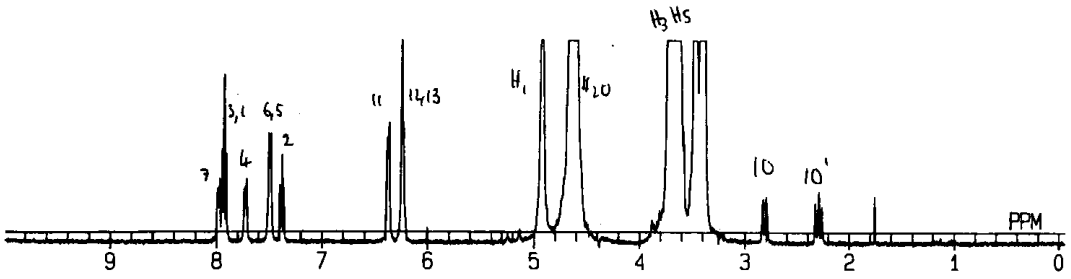


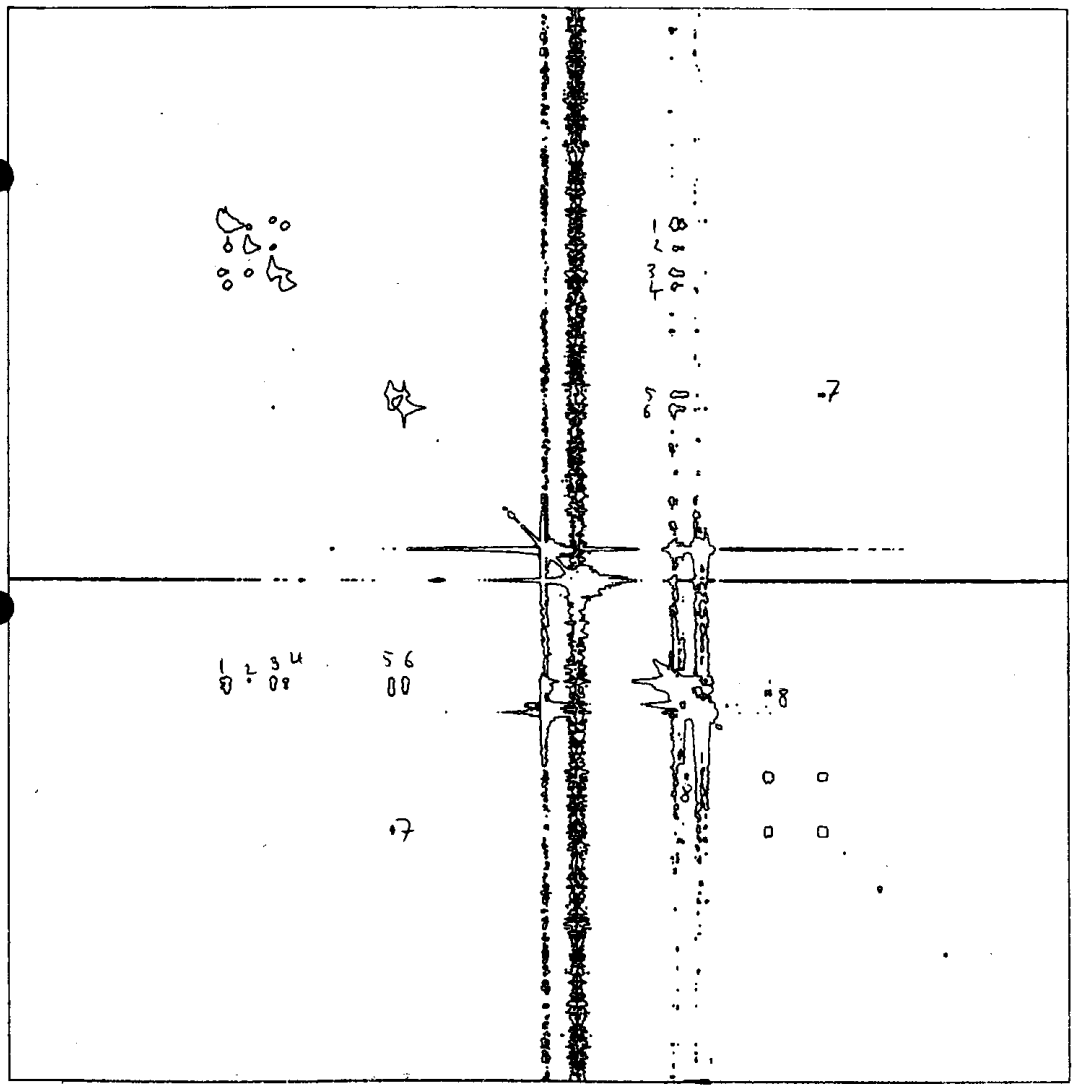
01-OCT-99 06: 31: 27
DFILE 209910011
COMNT RX052_N-L-P+BCD_KBUFF_9
EXMOD VPHROEH
OBNUC 1H
OBFIN 10398.4 Hz
POINT 1024
FREQU 3799.4 Hz
CLPNT 1024
TODAT 512
CLFRQ 3799.4 Hz
SCANS 16
ACQTM 0.135 sec
PD 2.365 sec
PW1 44.0 us
PW2 22.0 us
PW3 40.5 us
PI1 0.010 ms
PI2 0.263 ms
PI3 450.000 ms
IRATN 511
OBATN 100
CTEMP 23.9 c
CSPED 8 Hz
SLVNT D2O
LOOP1 1200
XS -126.1517 Hz
CXS -146.5588 Hz
XE 2626.9230 Hz
CXE 2623.2190 Hz
TH 1.40000
DET 10.0 us
DELAY 135.0 us
OPERATOR :

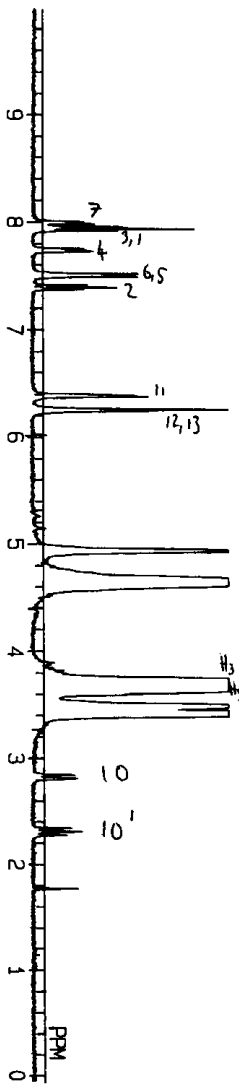
naph-L-phe



S18





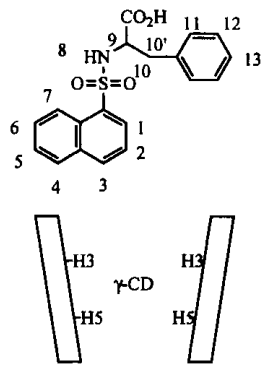


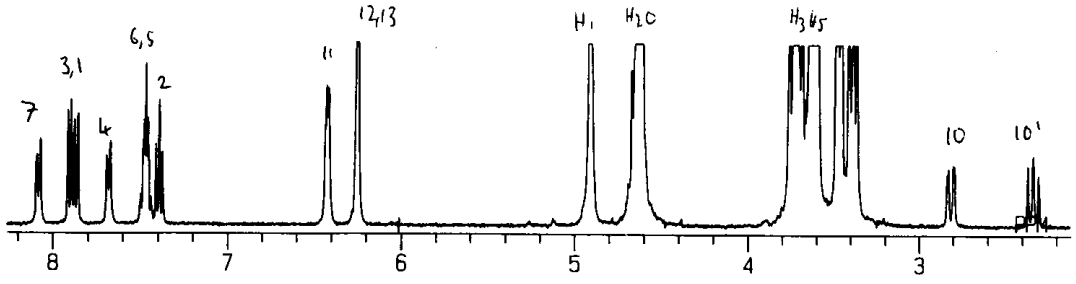
08-SEP-99 06: 22: 08
DFILE 209909081
COMNT ROESY_NAPTH-D-PHE/GCD_KBUFF_990907
EXMOD VPHROEH
OBNUC 1H

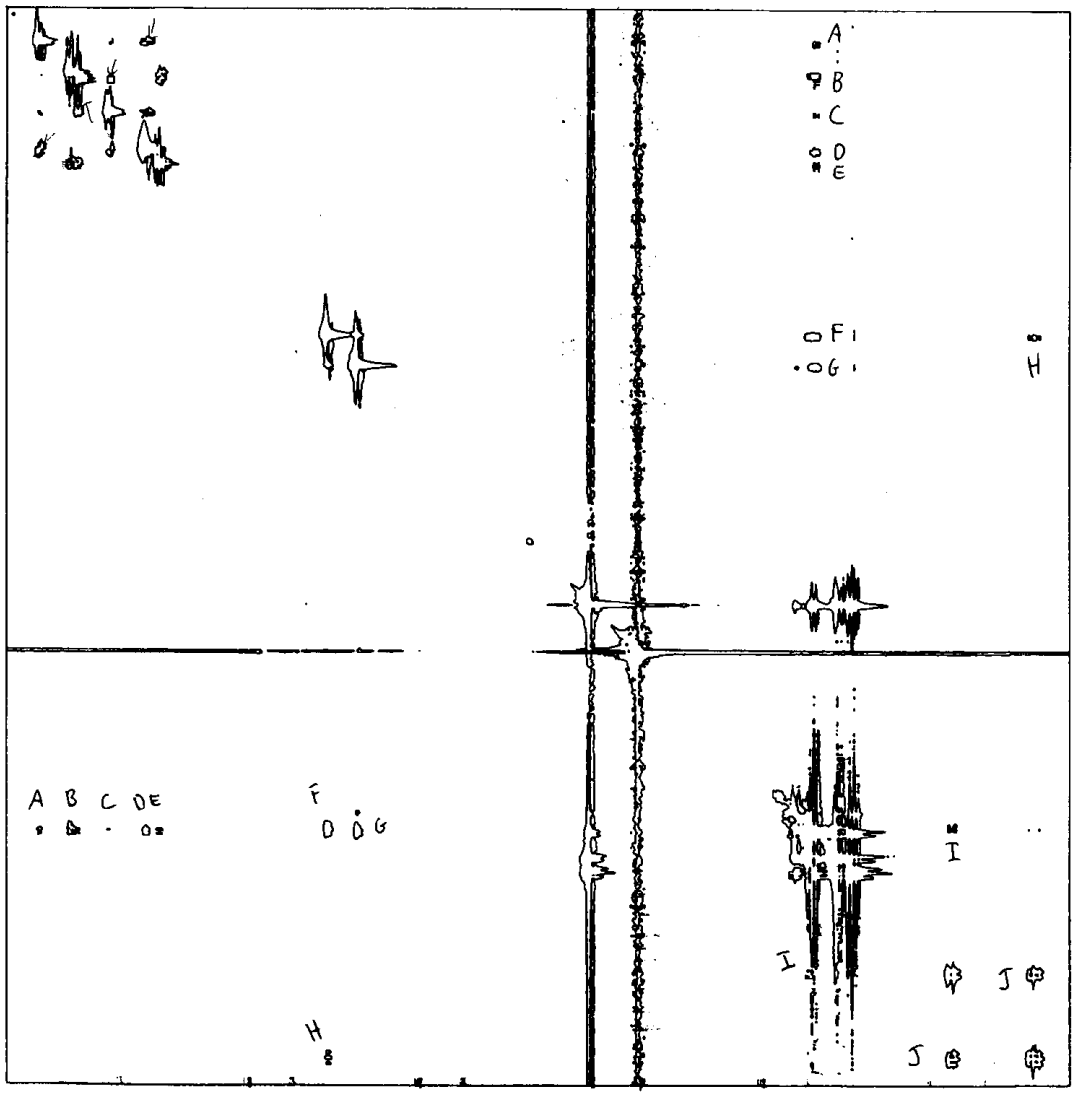
OBFIN	10492.2 Hz
POINT	1024
FREQU	4019.3 Hz
CLPNT	1024
TODAT	512
CLFRQ	4019.3 Hz
SCANS	16
ACQTM	0.127 sec
PD	2.373 sec
PW1	43.0 us
PW2	21.5 us
PW3	41.0 us
PI1	0.010 ms
PI2	0.249 ms
PI3	450.000 ms
IRATN	511
OBATN	100
CTEMP	23.2 c
CSPED	10 Hz
SLVNT	D2O
LOOP1	1200
XS	-3.9250 Hz
CXS	-1.9625 Hz
XE	4011.4430 Hz
CXE	4015.3750 Hz
TH	0.70000
DET	10.0 us
DELAY	110.0 us

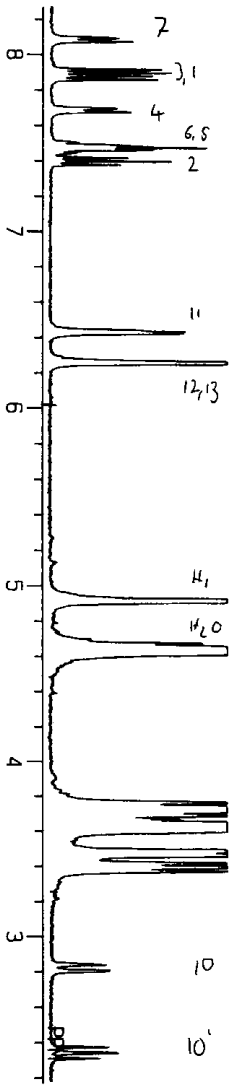
OPERATOR : _____

naph-D-phe







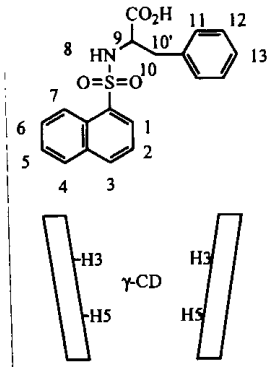


17-DEC-99 06: 35: 34
DFILE 209912171
COMNT ROESYOF_N-L-P: GCD_KBUFF_991217
EXMOD VPHROEH
OBNUC 1H

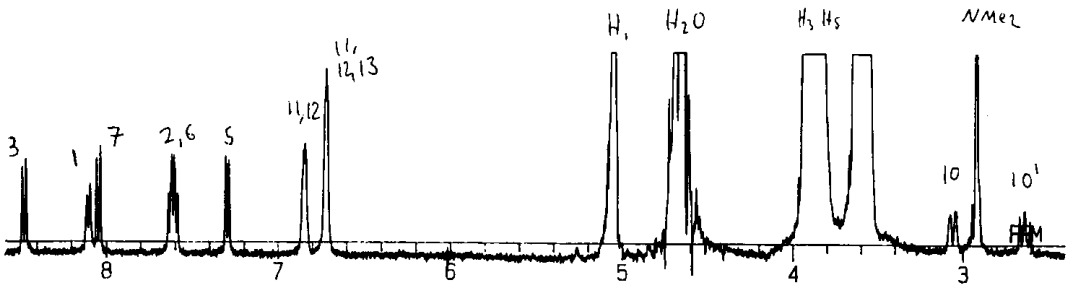
OBFIN	10578.1 Hz
POINT	1024
FREQU	2517.6 Hz
CLPNT	1024
TODAT	512
CLFRQ	2517.6 Hz
SCANS	16
ACQTM	0.203 sec
PD	2.297 sec
PW1	47.0 us
PW2	23.5 us
PW3	39.0 us
PI1	0.010 ms
PI2	0.397 ms
PI3	450.000 ms
IRATN	511
OBATN	100
CTEMP	23.7 c
CSPED	11 Hz
SLVNT	D2O
LOOP1	1200
XS	-7.3759 Hz
CXS	-18.4395 Hz
XE	2453.6990 Hz
CXE	2436.4670 Hz
TH	1.20000
DET	10.0 us
DELAY	185.0 us

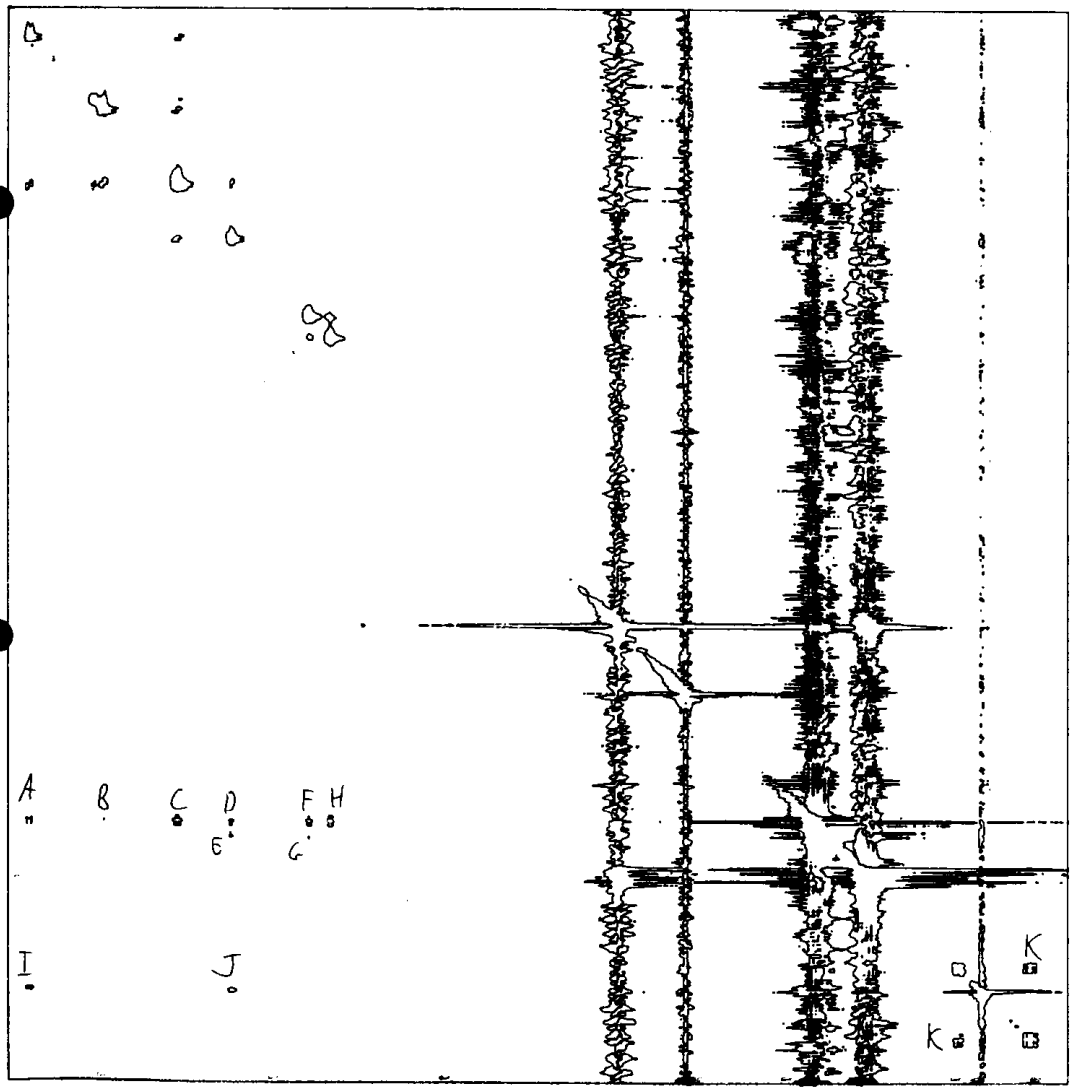
OPERATOR : _____

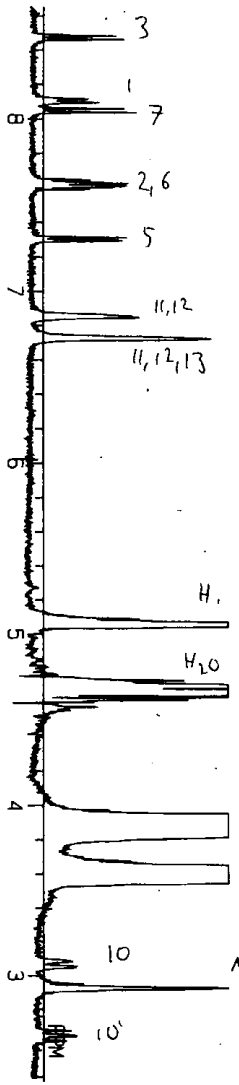
naph-L-phe



S20





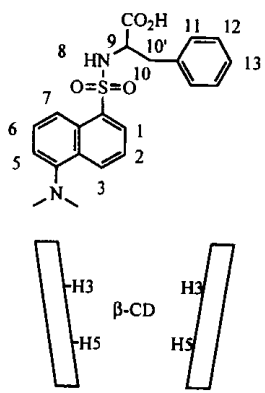


11-NOV-99 07: 07: 42
DFILE OR0133R1
COMNT 991110, OR0133R1-2, DNS-D-PHE+BETA-CD, 35C
EXMOD VPHROEH
OBNUC 1H

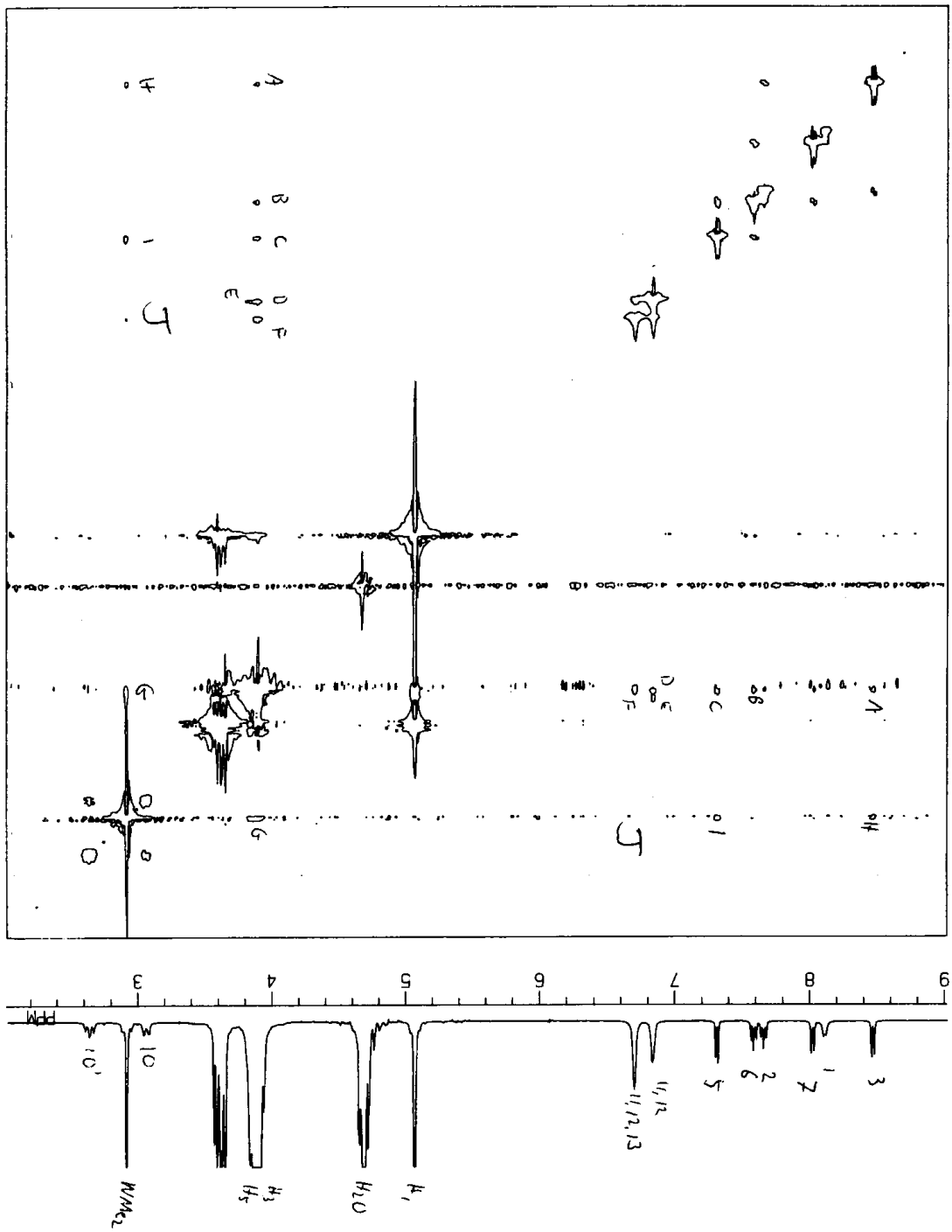
OBFIN	10671.9 Hz
POINT	1024
FREQU	2768.5 Hz
CLPNT	1024
TODAT	512
CLFRQ	2768.5 Hz
SCANS	16
ACQTM	0.185 sec
PD	2.315 sec
PW1	61.0 us
PW2	30.5 us
PW3	32.0 us
PI1	0.010 ms
PI2	0.361 ms
PI3	450.000 ms
IRATN	230
OBATN	100
CTEMP	34.9 c
CSPED	9 Hz
SLVNT	D2O
LOOP1	1200
XS	-24.3330 Hz
CXS	-33.7952 Hz
XE	2471.1460 Hz
CXE	2506.2500 Hz
TH	4.00000
DET	10.0 us
DELAY	169.0 us

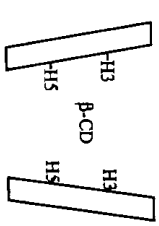
OPERATOR : _____

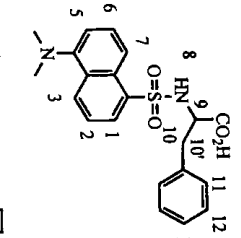
dans-D-phe



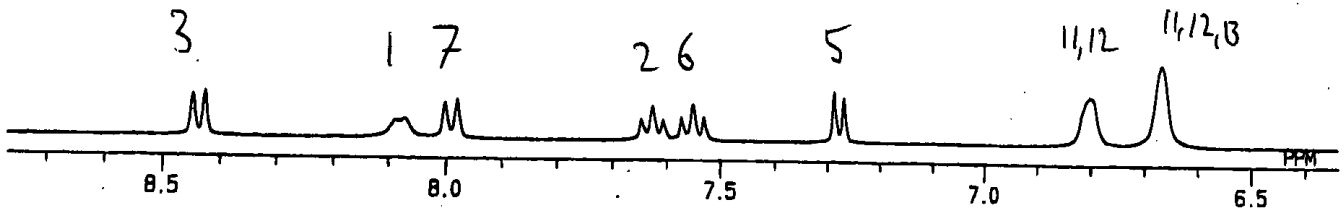
S21

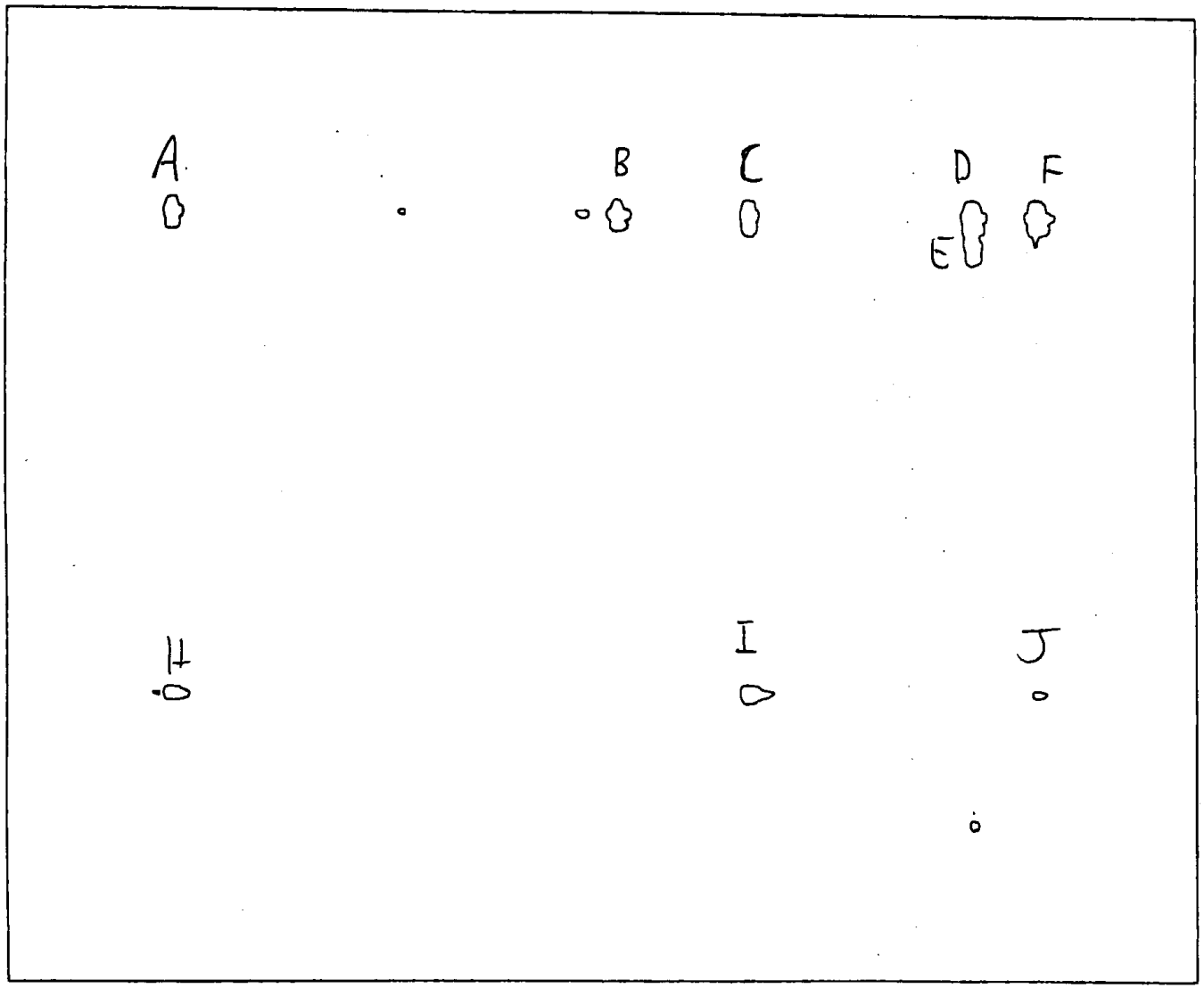


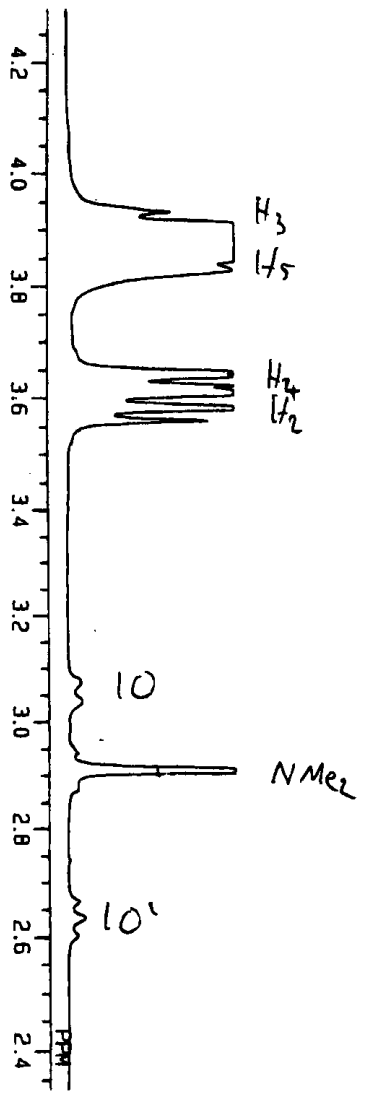


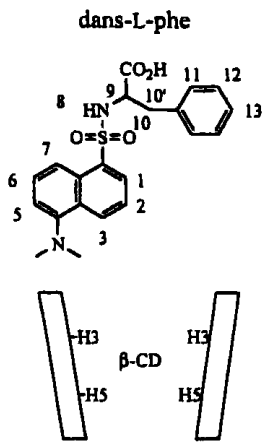


dans-L-phe

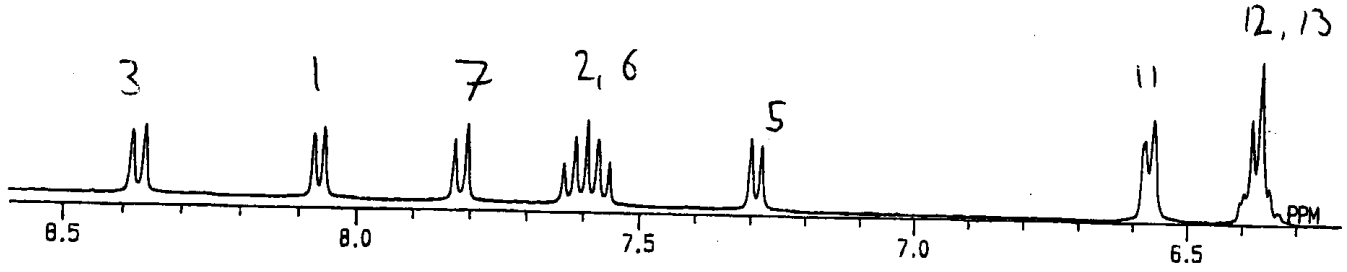

3
1 7
2 6
5
11,12
11,12,13
8.5
8.0
7.5
7.0
6.5
PPM

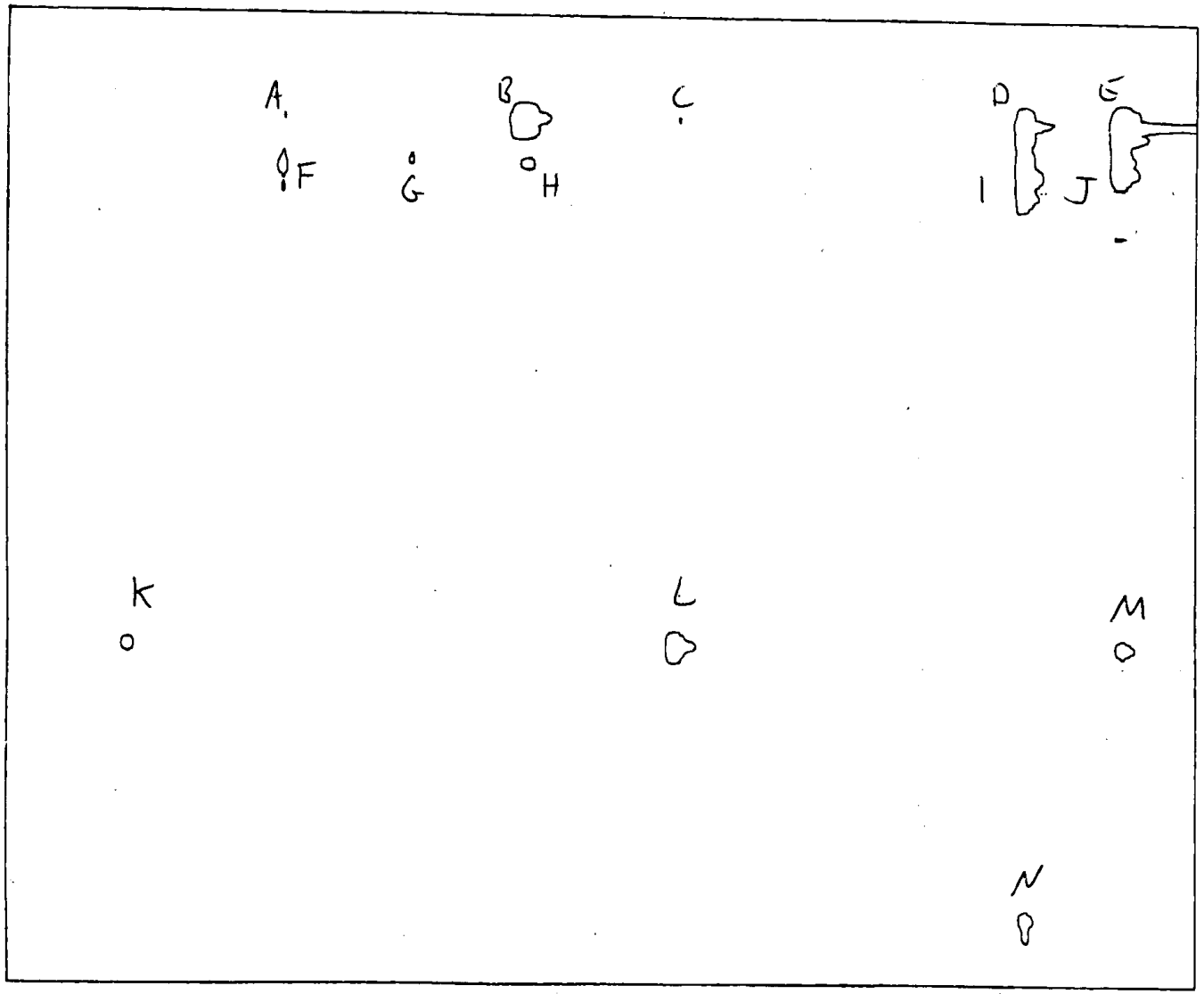

A
B
C
D
F
E
H
I
J

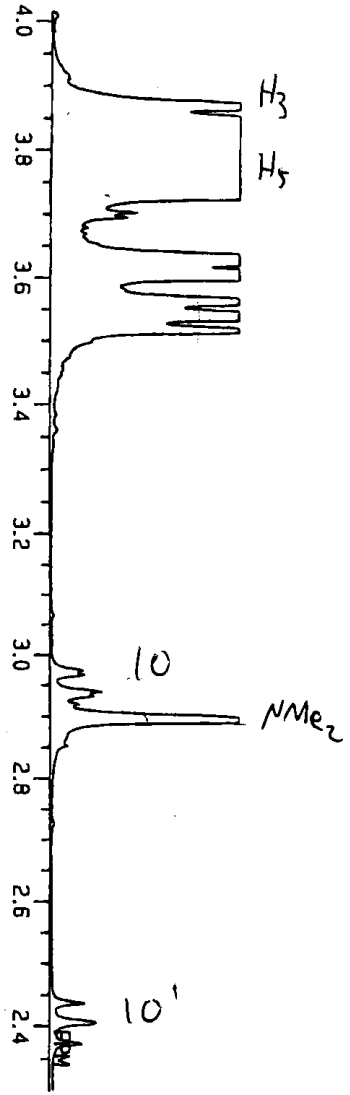

4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
PPM
H3
H5
H2
H4
10
NMe2
10'


dans-L-phe
CO2H
HN
O=S=O
β-CD
H3
H5

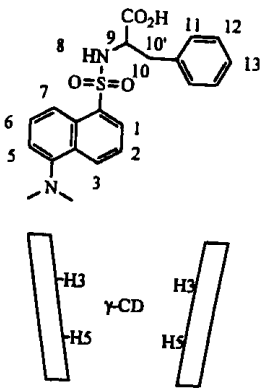
S23

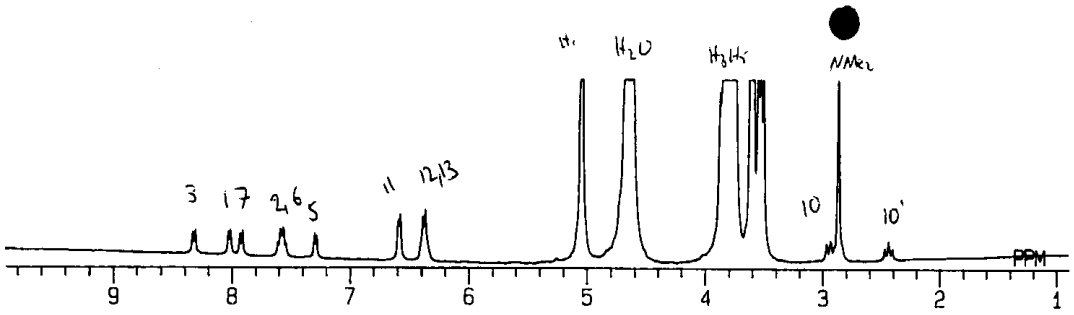

3
1
7
2, 6
5
11
12, 13
8.5
8.0
7.5
7.0
6.5
PPM

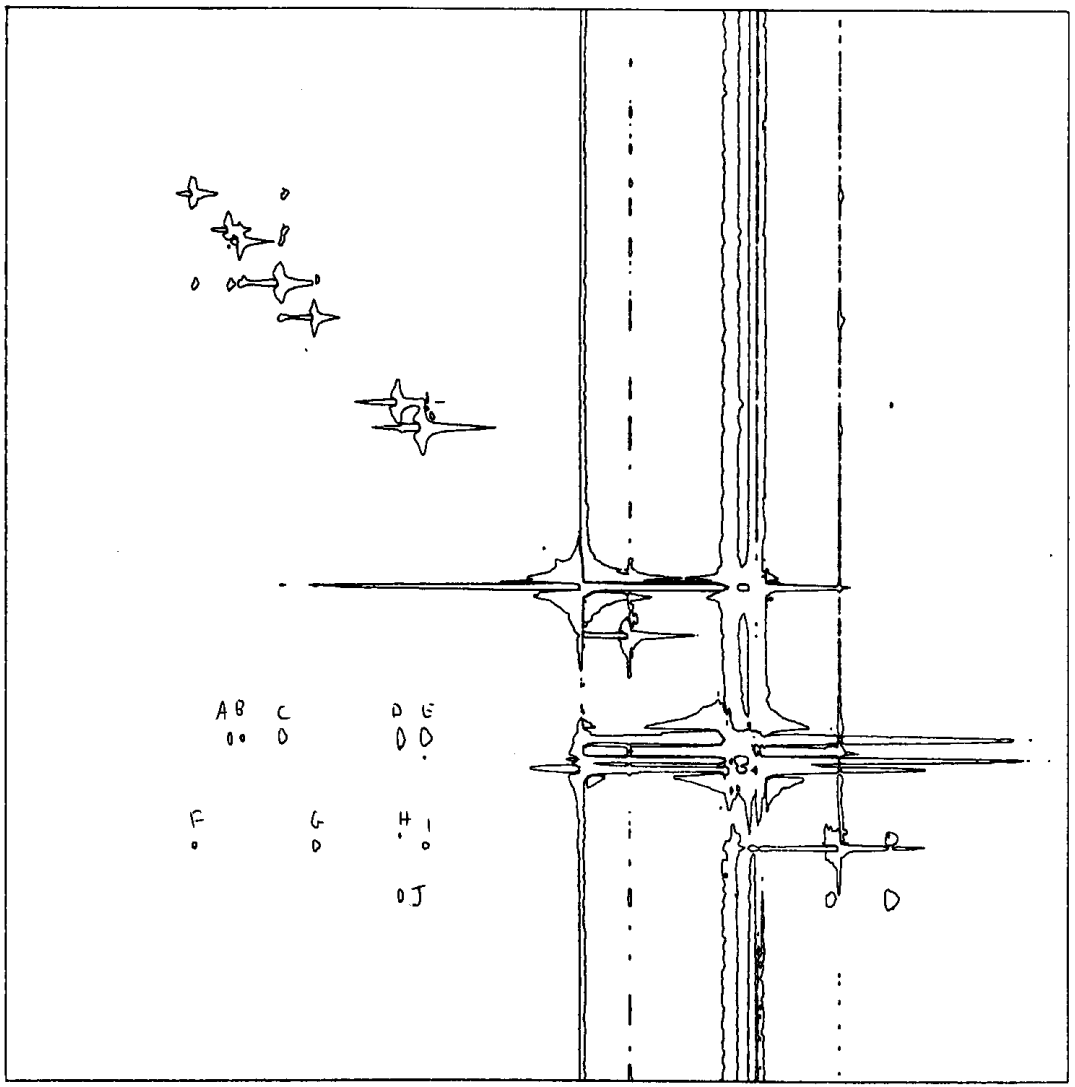

A.
B
C.
D
I
J
F
G
H
K
L
M
N
O

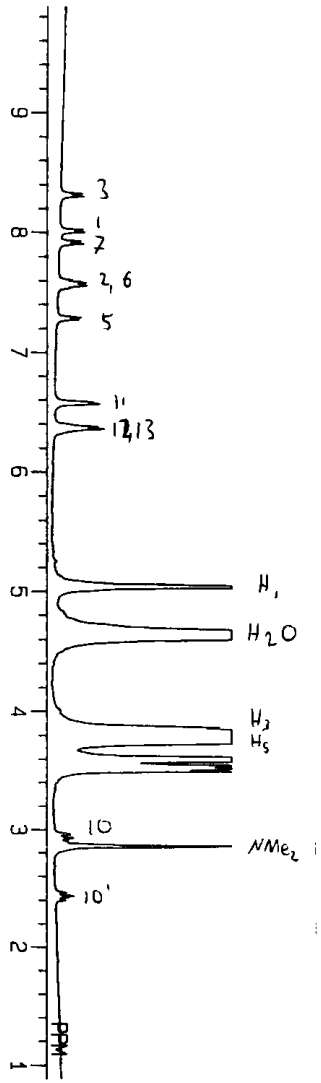

4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
H3
H5
10
NMe2
10'

dans-D-phe

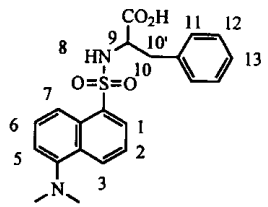

CO2H
11
12
8
9
10'
HN
10
13
O=S=O
7
6
1
5
2
N
3
H3
H5
γ-CD
H3
H5

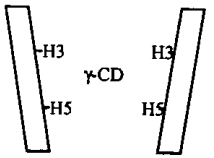

3
17
2,6
5
11
12,13
H_1
H_2O
H_3H_5
NMe_2
10
10'
PPM
9
8
7
6
5
4
3
2
1


A B C D E
F G H I
J


3
17
2, 6
5
11
12,13
H_1
H_2O
H_2
H_5
10
NMe_2
10'
PPM

dans-L-phe


CO_2H
HN
O=S=O
11
12
13
10'
9
8
10
7
6
5
1
2
3
N


H3
H5
γ-CD
H3
H5