Supporting Information

Inclusion of Picolines by a Substituted Binaphthyl Diol Host: Selectivity and Structure

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^{1}H-NMR Spectra

Table 1S. X-Ray data and refinement parameters for **V-IX**

Compound	**H.2PIC:3PIC(0.21:0.79)**	**H.3PIC**	**H.4PIC**	**H.3PIC**	**H.4PIC**
Structure	**V**	**VI**	**VII**	**VIII**	**IX**
Comment	Similar to **IV**	Same as **II**	Same as **III**	Same as **II**	Same as **III**
Empirical formula	$C_{52}H_{37}NO_2$	$C_{58}H_{44}N_2O_2$	$C_{52}H_{37}NO_2$	$C_{58}H_{44}N_2O_2$	$C_{52}H_{37}NO_2$
Formula weight	707.83	800.95	707.83	800.95	707.83
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/n$	$P2_1/c$	$P2_1/n$
a [Å]	9.873(2)	16.709(4)	9.9384(6)	16.6896(3)	9.9367(6)
b [Å]	20.894(6)	11.588(2)	20.7758(12)	11.5679(2)	20.7808(13)
c [Å]	18.825(6)	22.298(9)	18.8529(11)	22.3133(5)	18.8561(12)
α [°]	90	90	90	90	90
β [°]	99.15(3)	95.08(1)	100.60(1)	95.14(3)	100.66(1)
γ [°]	90	90	90	90	90
V[Å^3]	3833.85(18)	4300.7(2)	3826.2(4)	4290.56(18)	3826.4(4)
Z	4	4	4	4	4
Temperature(K)	173	173	173	173	173
D_{calc}(g/cm^{-3})	1.226	1.237	1.229	1.240	1.229
μ(Mo-Kα)(mm^{-1})	0.074	0.074	0.074	0.074	0.074
F(000)	1488	1688	1488	1688	1488.0
Crystal size/mm	0.09x0.18x0.29	0.09x0.16x0.24	0.09x0.12x0.24	0.08x0.16x0.21	0.1x0.12x0.28
Reflections collected	8782	18447	44983	8756	27993
Independent reflections	8782	9465	9631	8756	8755
Observed reflections [I>2s(I)]	6668	7131	6536	5673	5861
Parameters	498	569	505	569	505
Goodness-of-fit F^2	1.032	1.035	1.018	1.016	1.019
R_1[I>2s(I)][a]	0.0467	0.0475	0.0476	0.0496	0.0458
wR_2(all data)[b]	0.1213	0.1370	0.1224	0.1380	0.1212

Table 2S. ^{1}H-NMR values for **H.2PIC/3PIC**, **H.2PIC/4PIC**, **H.3PIC/4PIC**

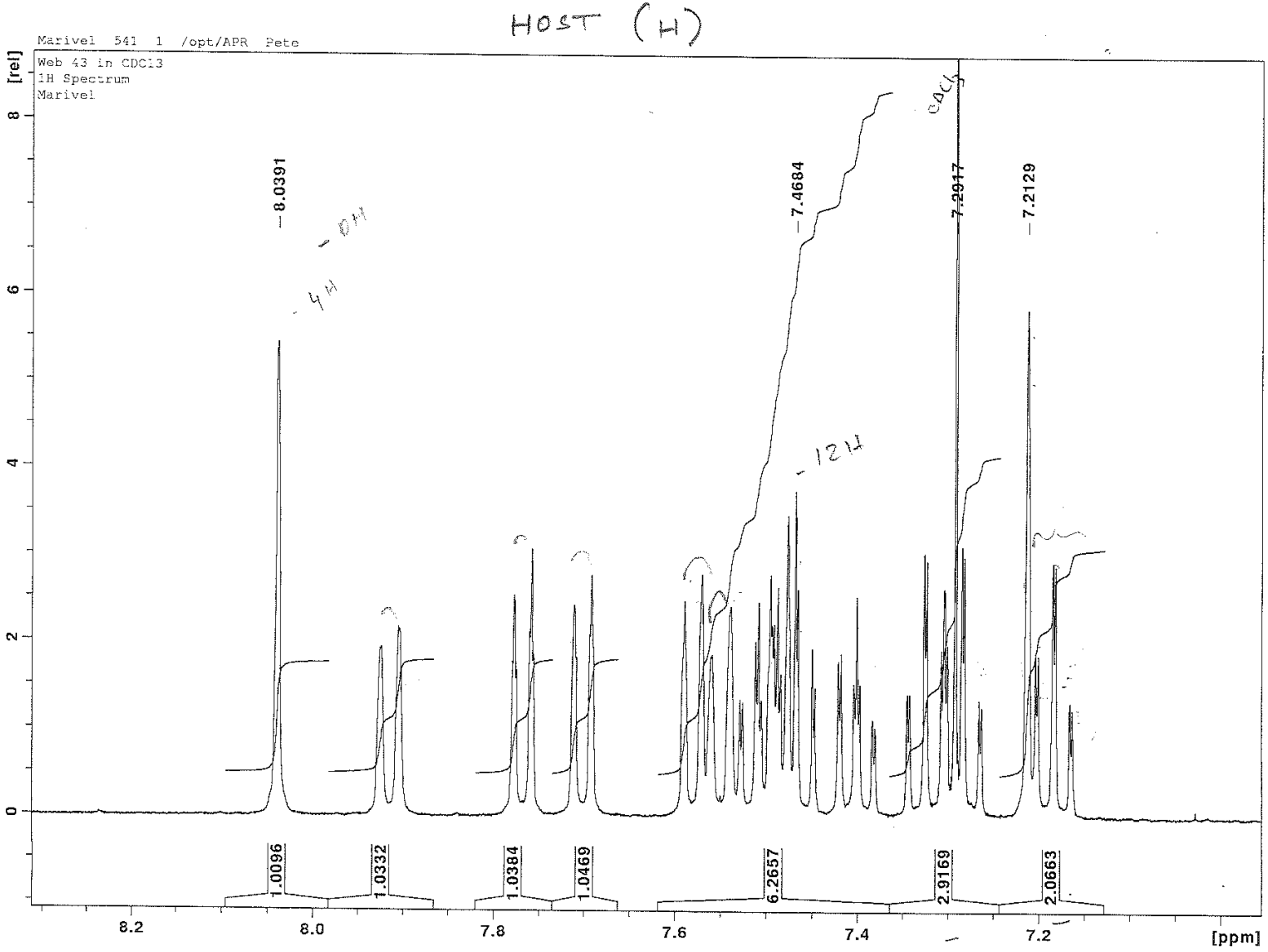
H.2PIC/3PIC	X_{3PIC}	0.10	-	0.20	0.30	0.40	-	0.50	0.60	0.70	0.80	0.90	1.0
	Z_{3PIC}	0.15	-	0.47	0.58	0.67	-	0.76	0.85	0.87	0.93	0.99	1.0
H.2PIC/4PIC	X_{4PIC}	0.10	0.15	0.20	0.30	0.40	-	0.50	0.60	0.70	0.80	0.90	1.0
	Z_{4PIC}	0.02	0.74	0.91	0.92	0.97	-	0.98	0.98	-	-	-	1.0
H.3PIC/4PIC	X_{4PIC}	0.10	-	0.20	0.30	0.40	0.45	0.50	0.60	0.70	0.80	0.90	1.0
	Z_{4PIC}	0.04	-	0.09	0.18	0.27	0.90	0.93	-	-	-	-	1.0

Table 3S. ^{1}H-NMR values of three-guest competition experiment, **H.2PIC/3PIC/4PIC**

Name of the experiment	***Mole fraction**	**2PIC**	**3PIC**	**4PIC**	**Structure**	**Comment**
A	Z_{Sol}	0.60	0.20	0.20	**IX**	Same as **III** (**H.4PIC**)
	X_{NMR}	0.12	0.09	0.78		
B	Z_{Sol}	0.40	0.40	0.20		
	X_{NMR}	0.03	0.20	0.77		
C	Z_{Sol}	0.40	0.20	0.40		
	X_{NMR}	0.03	0.08	0.89		
D	Z_{Sol}	0.20	0.60	0.20	**VIII**	Same as **II** (**H.3PIC**)
	X_{NMR}	0.01	0.82	0.17		
E	Z_{Sol}	0.20	0.40	0.40		
	X_{NMR}	0.01	0.11	0.88		
F	Z_{Sol}	0.20	0.20	0.60		
	X_{NMR}	0.01	0.07	0.92		
G	Z_{Sol}	0.33	0.33	0.33		
	X_{NMR}	0.02	0.11	0.86		

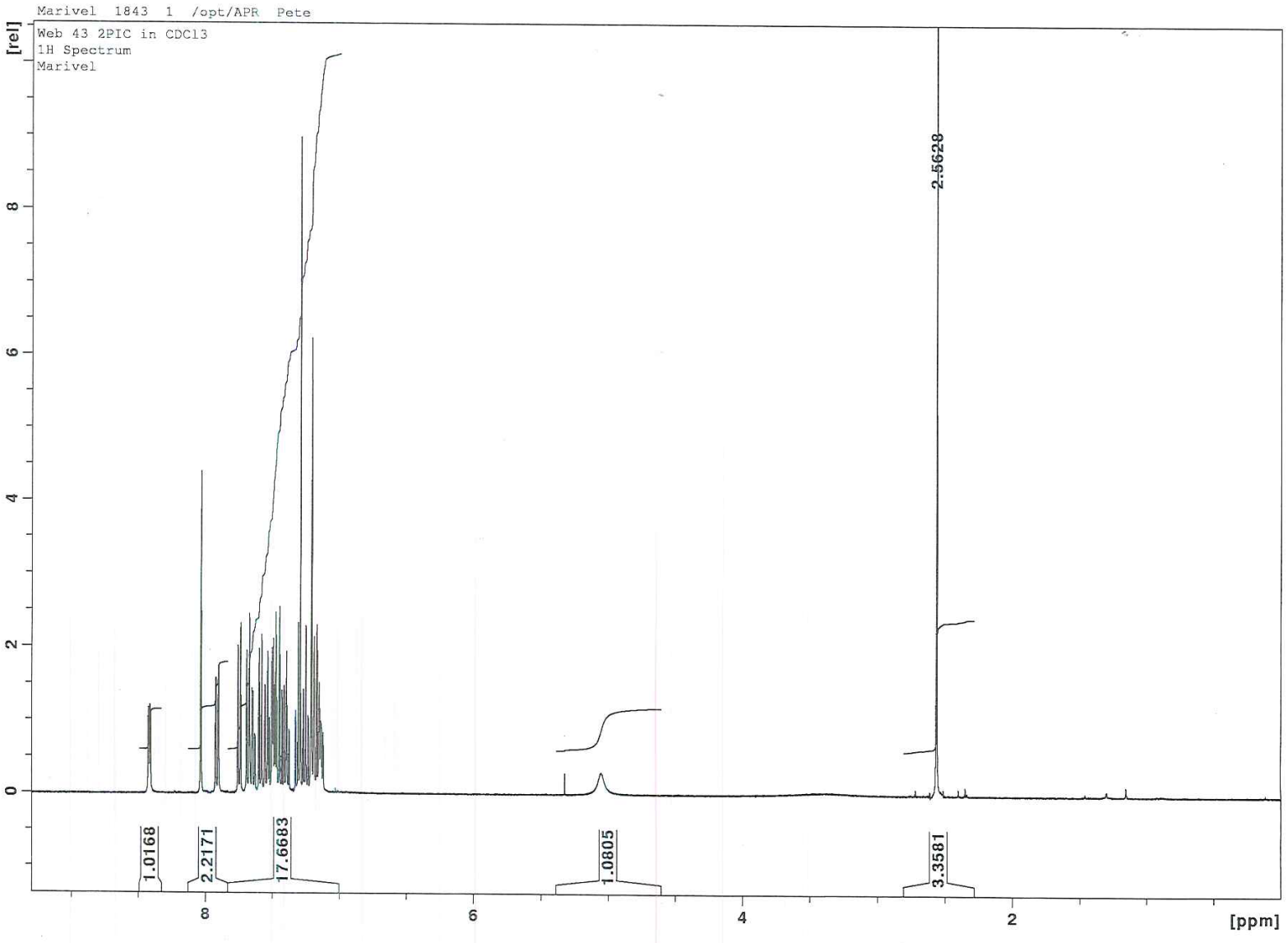
*Z_{Sol} = Mole fraction in solution mixture, X_{NMR} = Mole fraction in crystals, obtained by ^{1}H-NMR

1. HOST (H)



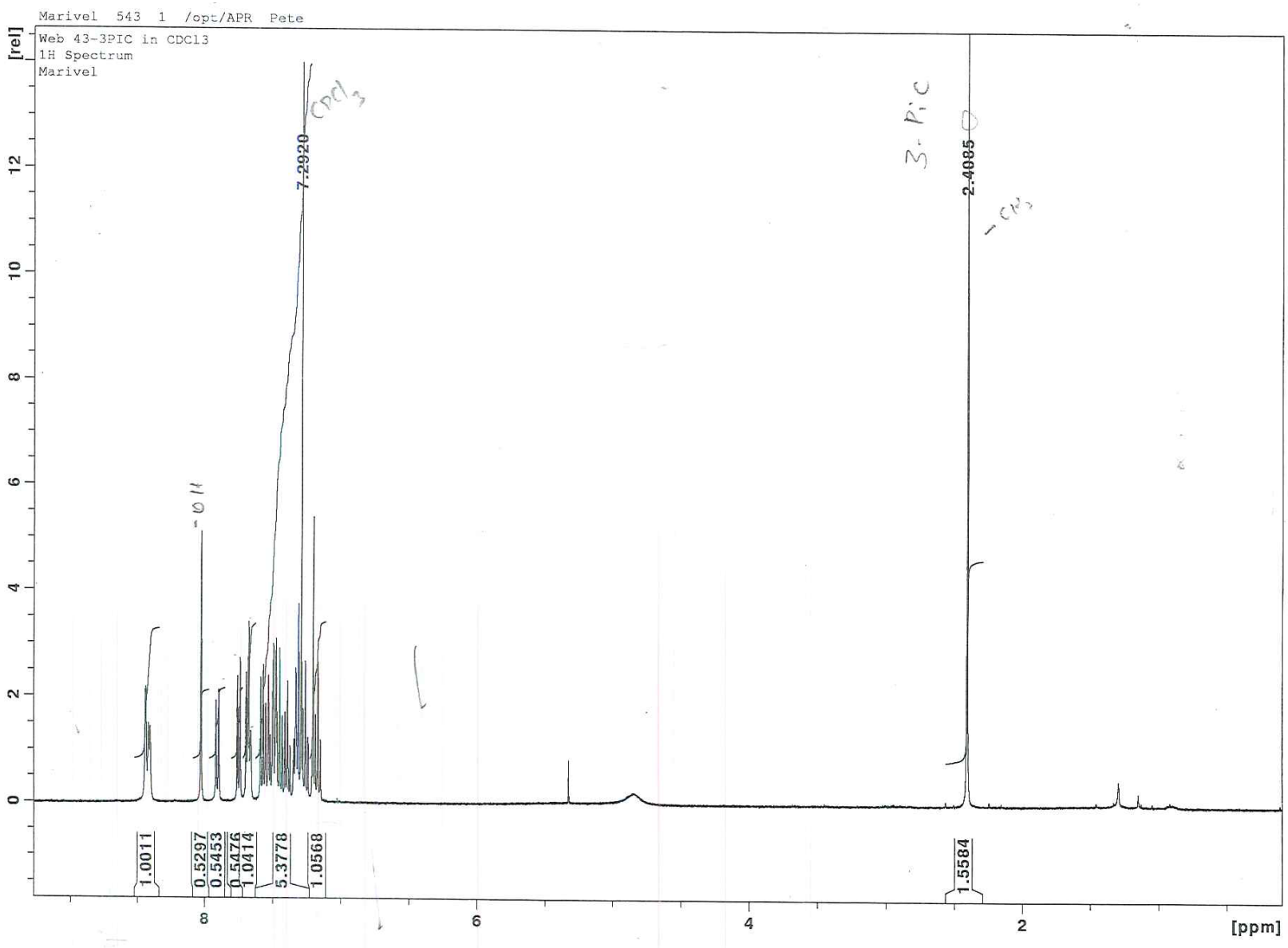
^{1}H-NMR (400 MHz) spectrum of **Host** (**H**) in $CDCl_3$ at 25°C

2. H.2PIC (I)



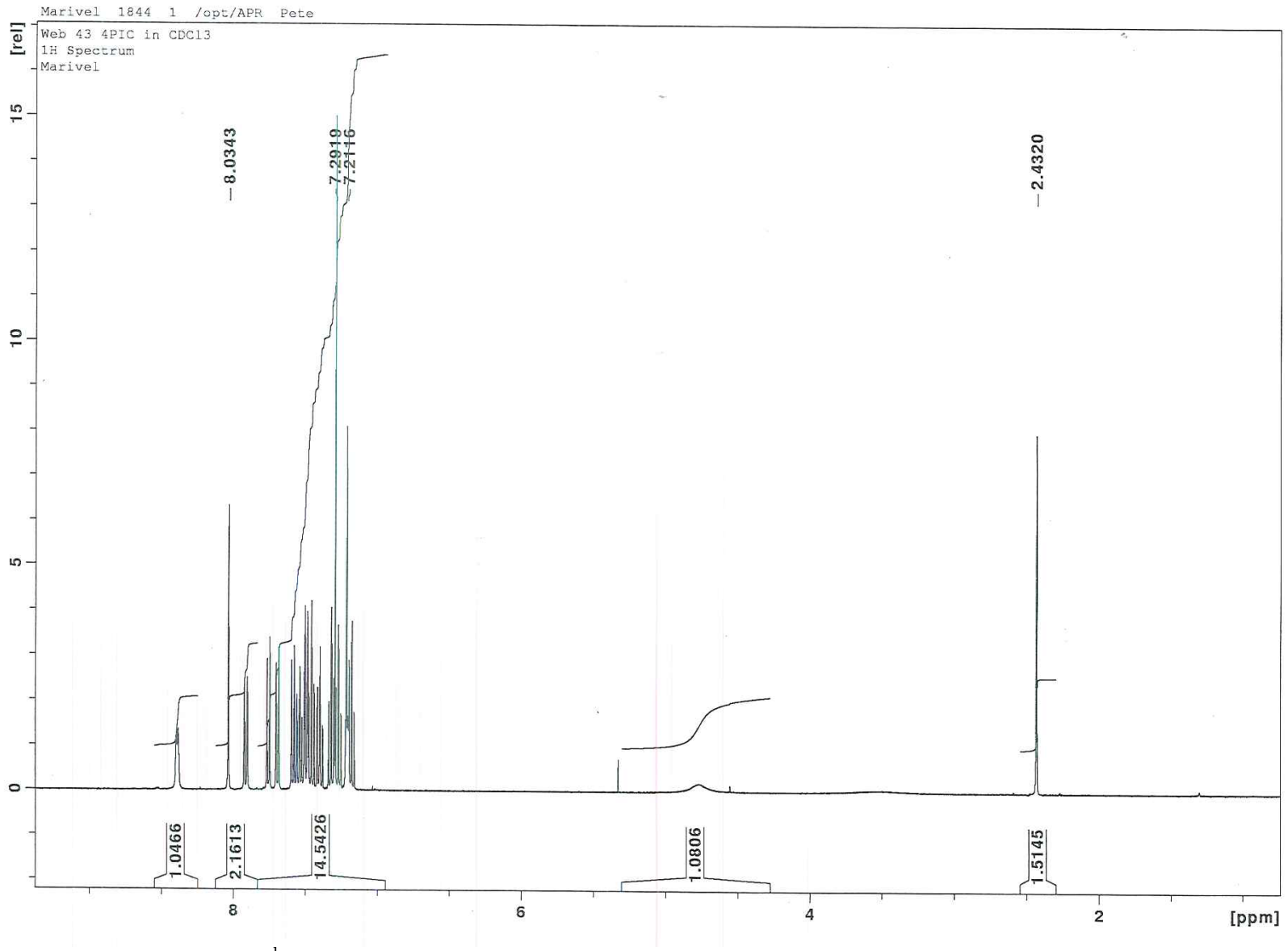
^{1}H-NMR (400 MHz) spectrum of **H.2PIC** (**I**) in $CDCl_3$ at 25°C

3. H.3PIC



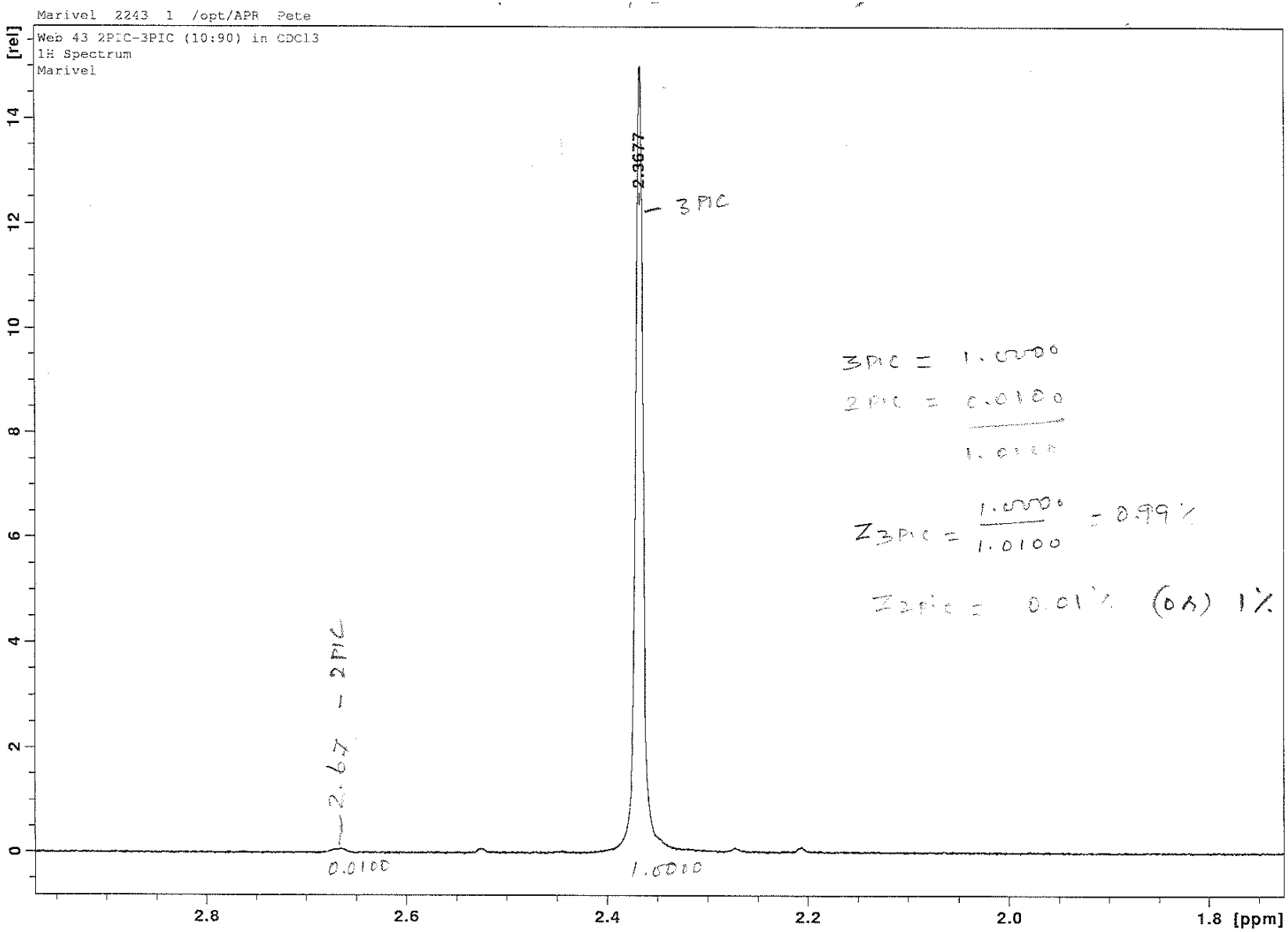
^{1}H-NMR (400 MHz) spectrum of **H.3PIC (II)** in $CDCl_3$ at 25°C

4. H.4PIC



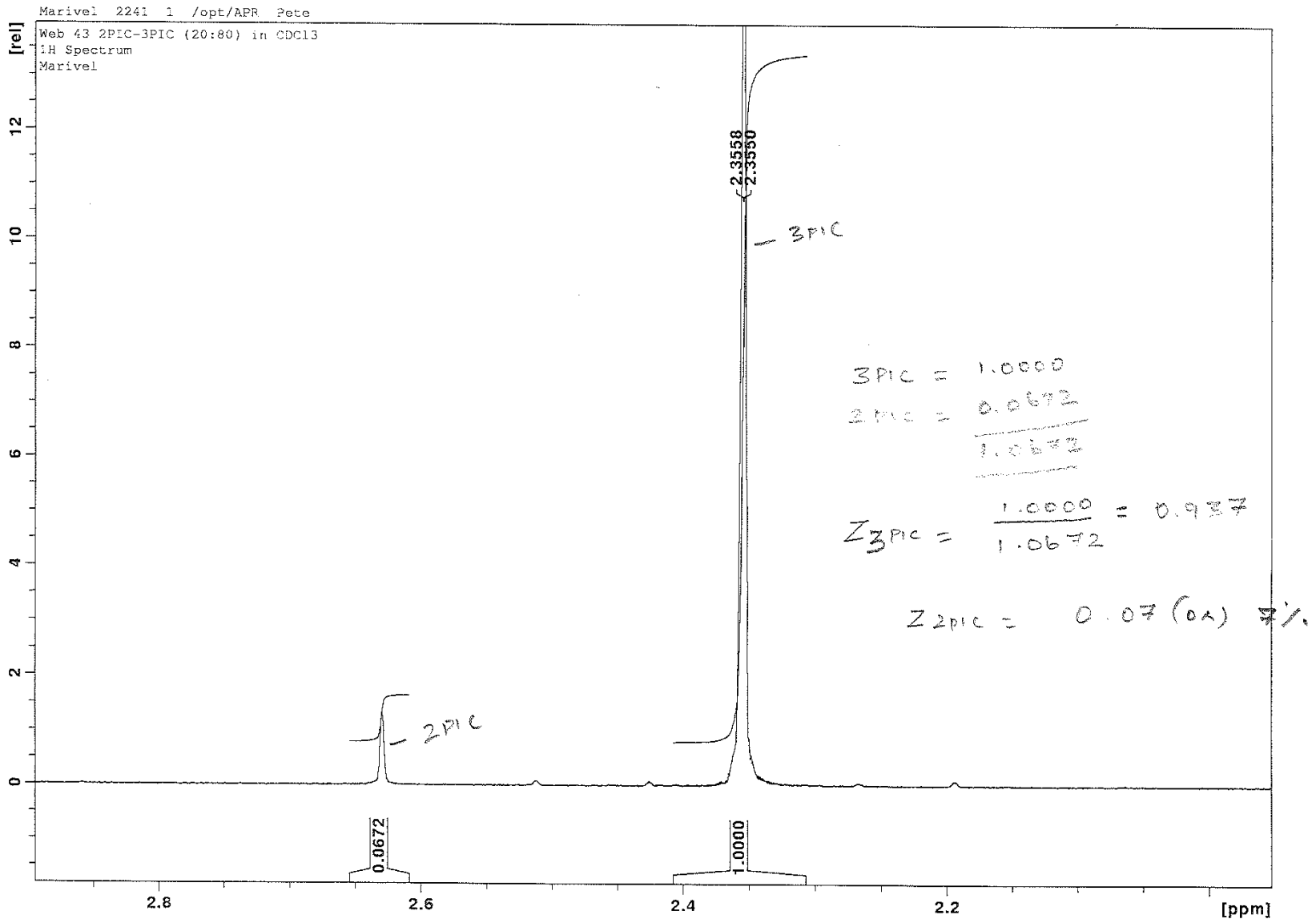
^{1}H-NMR (400 MHz) spectrum of **H.4PIC** (**III**) in $CDCl_3$ at 25°C

1a. H.2PIC/3PIC (0.1:0.9)



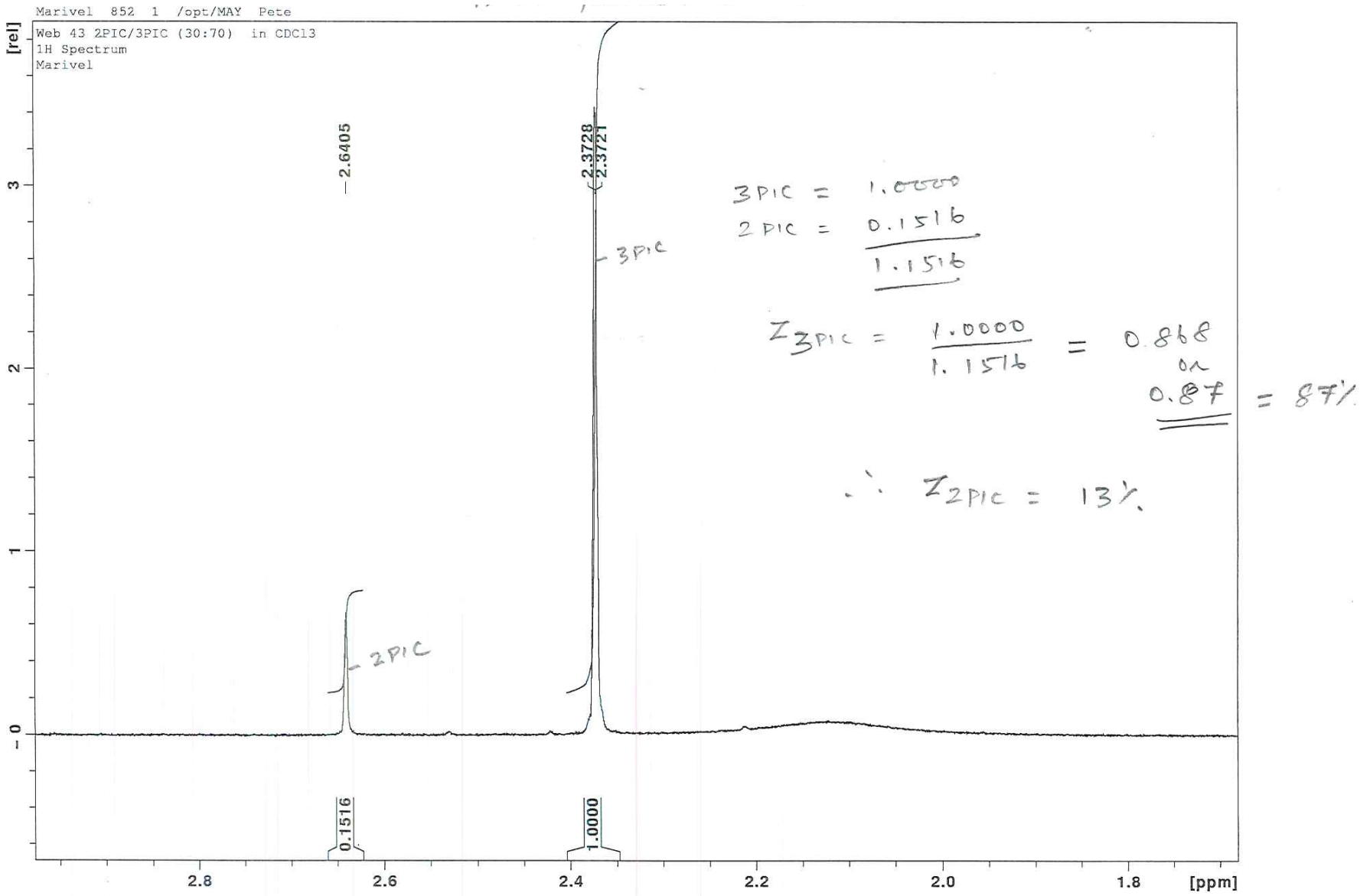
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.1:0.9)** in $CDCl_3$ at 25°C

1b. H.2PIC/3PIC (0.2:0.8)



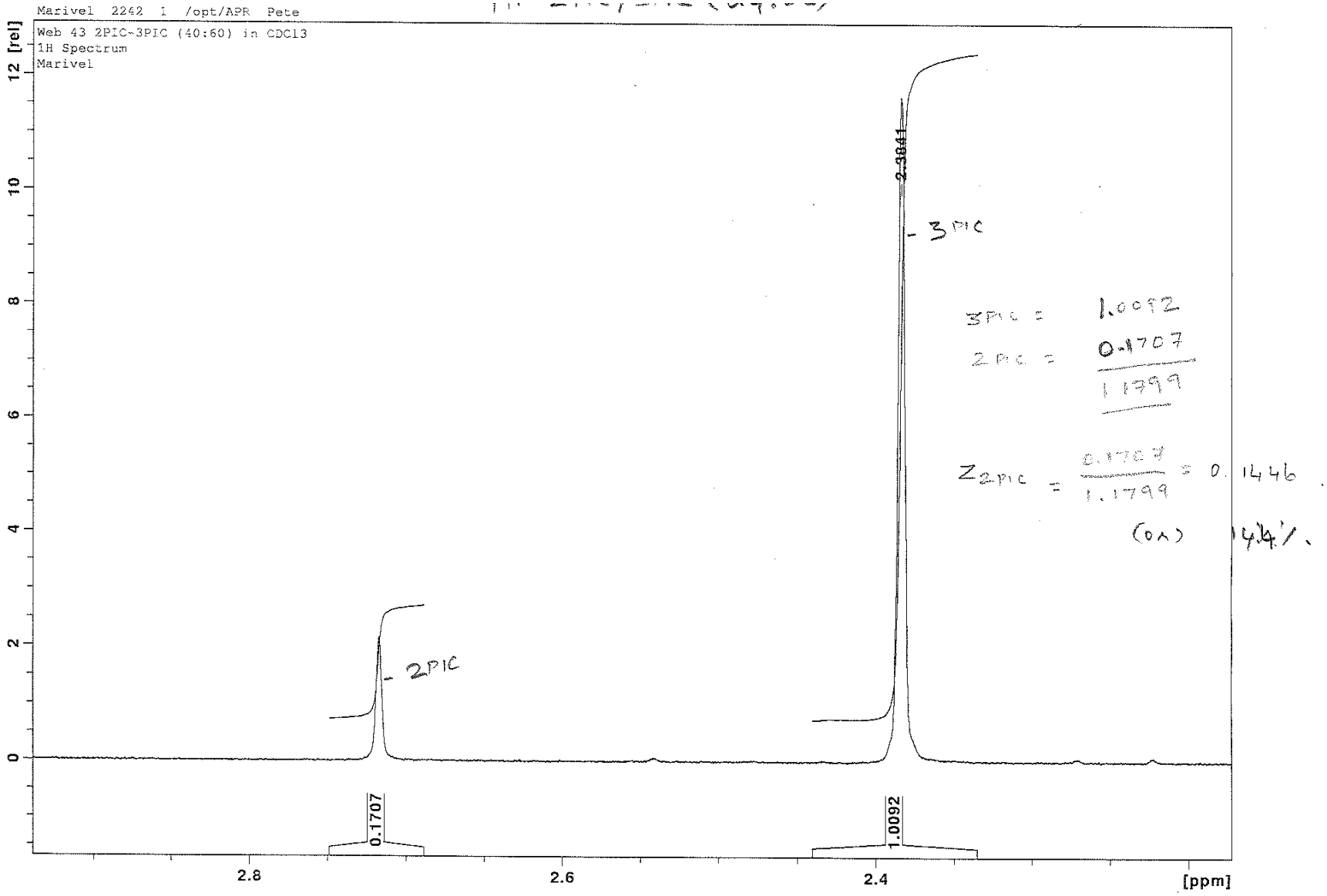
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.2:0.8)** in $CDCl_3$ at 25°C

1c. H.2PIC/3PIC (0.3:0.7)



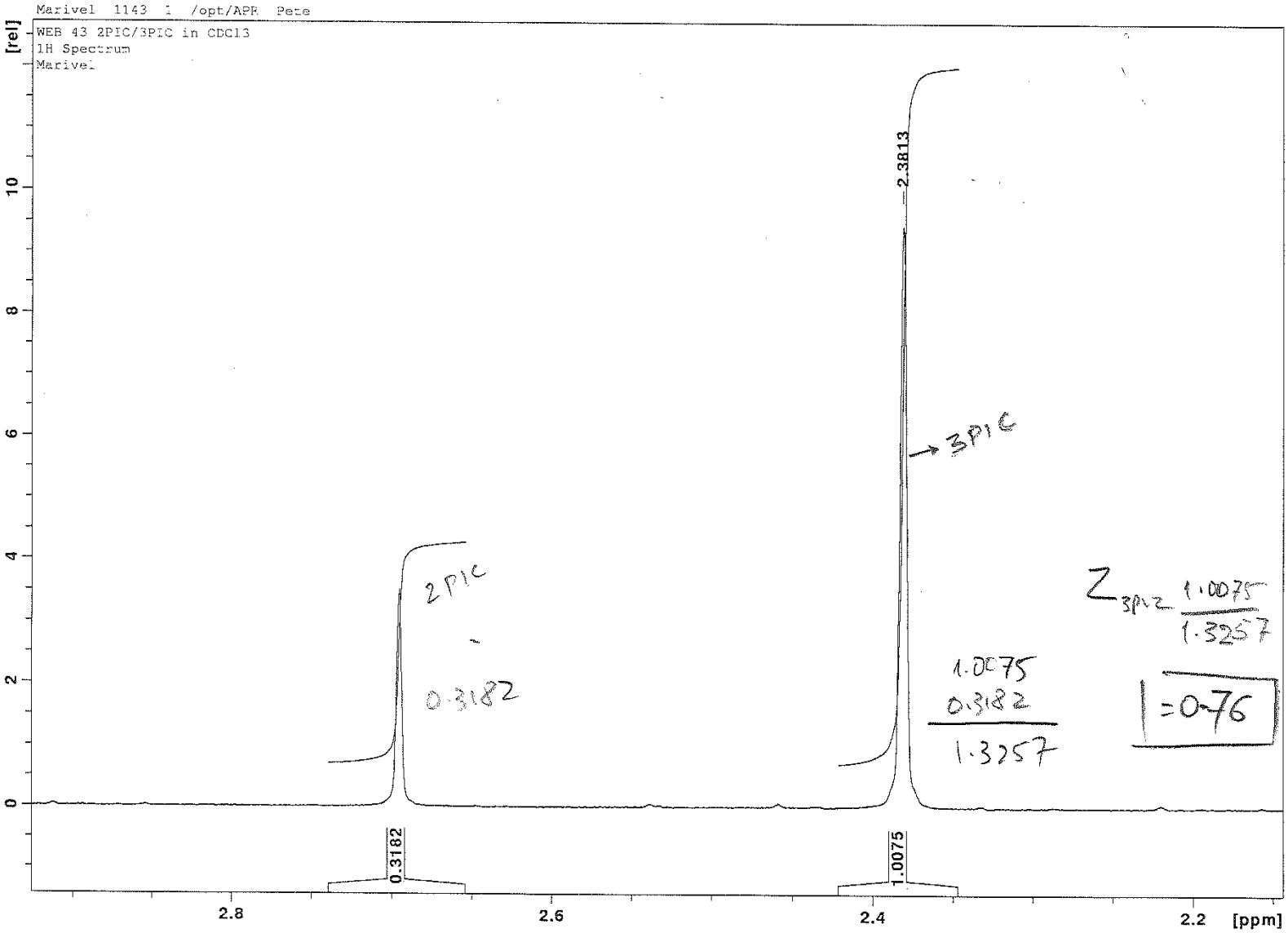
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.3:0.7)** in $CDCl_3$ at 25°C

1d. H.2PIC/3PIC (0.4:0.6)



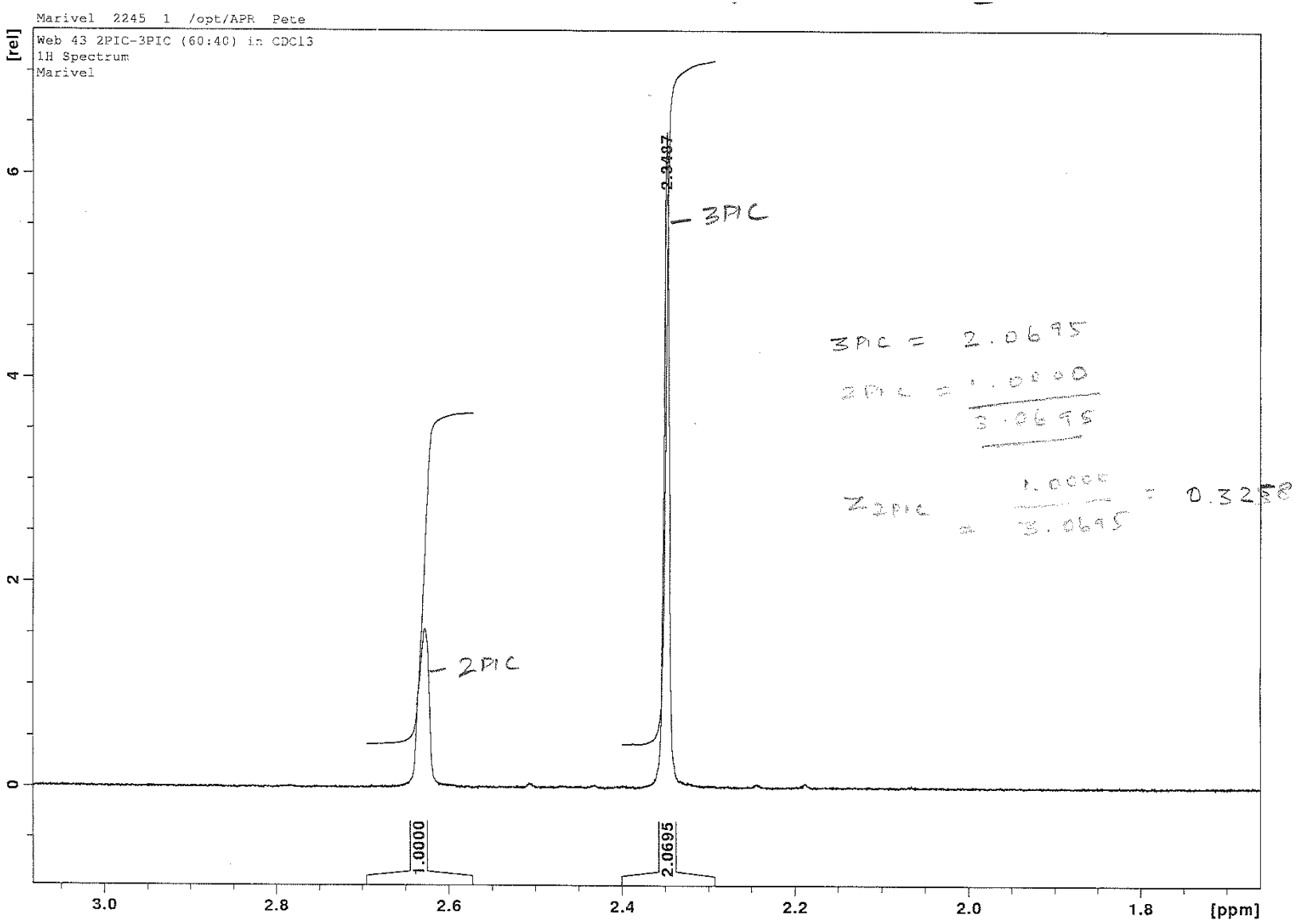
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.4:0.6)** in $CDCl_3$ at 25°C

1e. H.2PIC/3PIC (0.5:0.5)



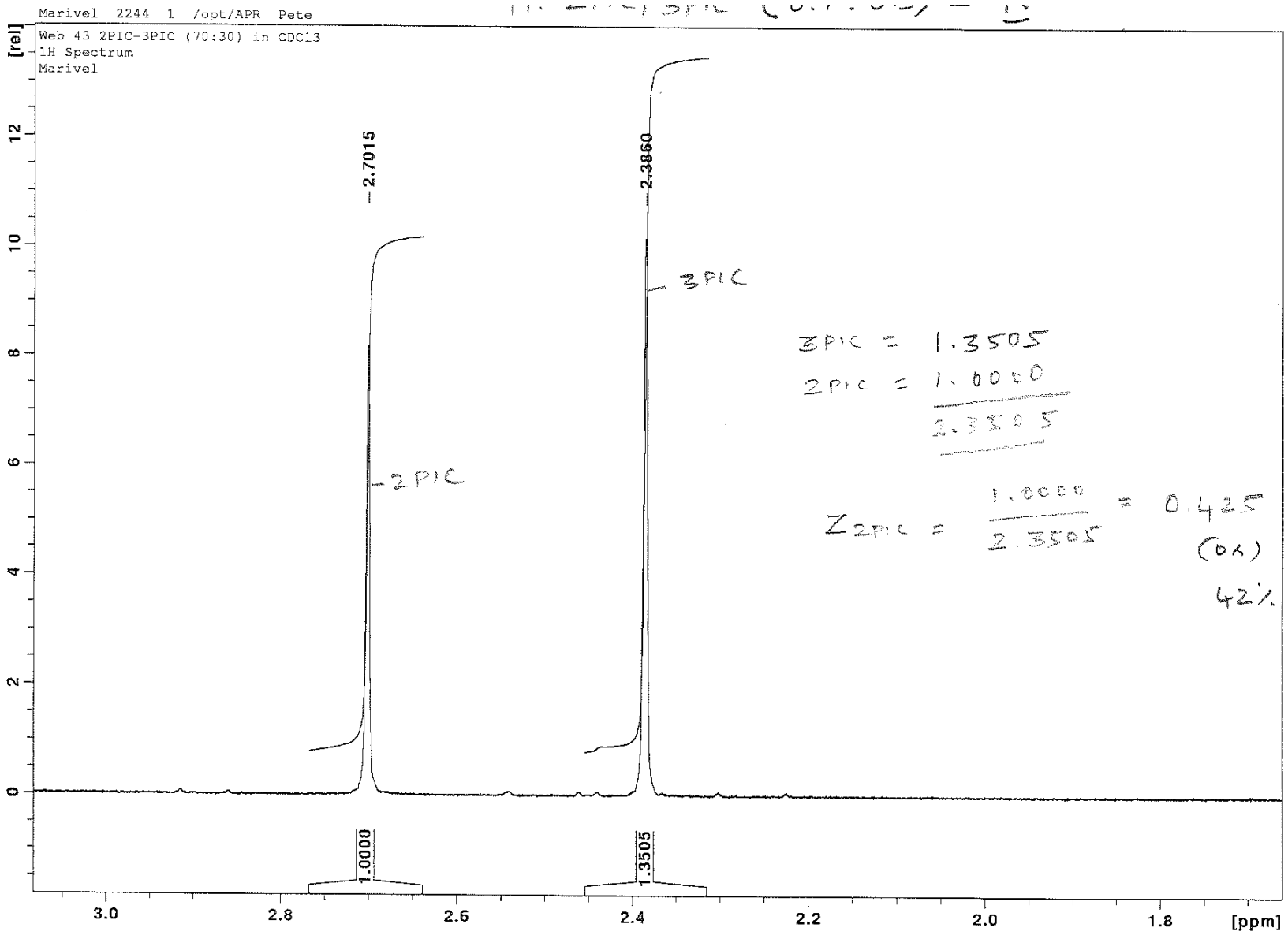
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.5:0.5)** in $CDCl_3$ at 25°C

1f. H.2PIC/3PIC (0.6:0.4) - V



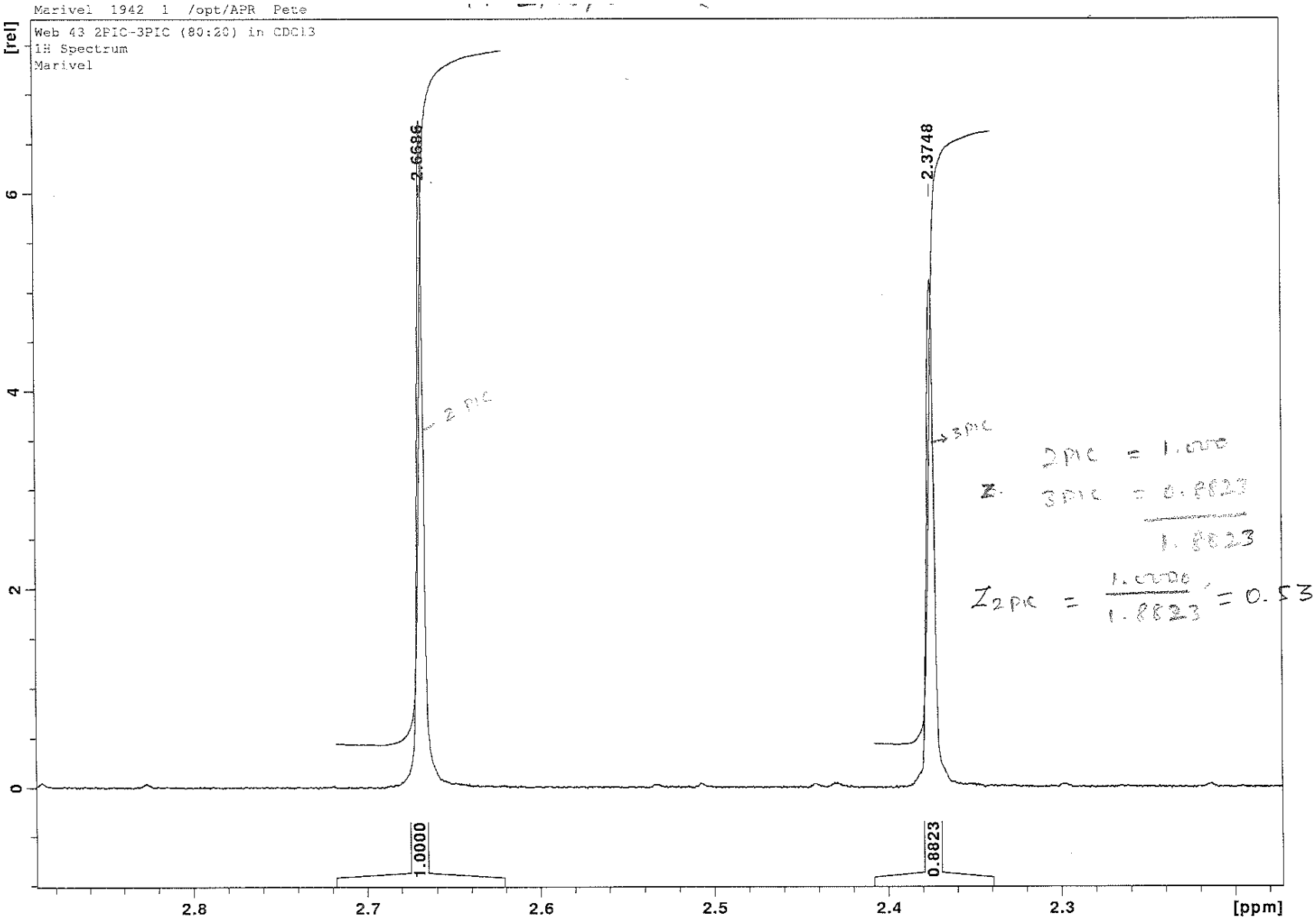
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.6:0.4)** in $CDCl_3$ at 25°C

1g. H.2PIC/3PIC (0.7:0.3) - IV



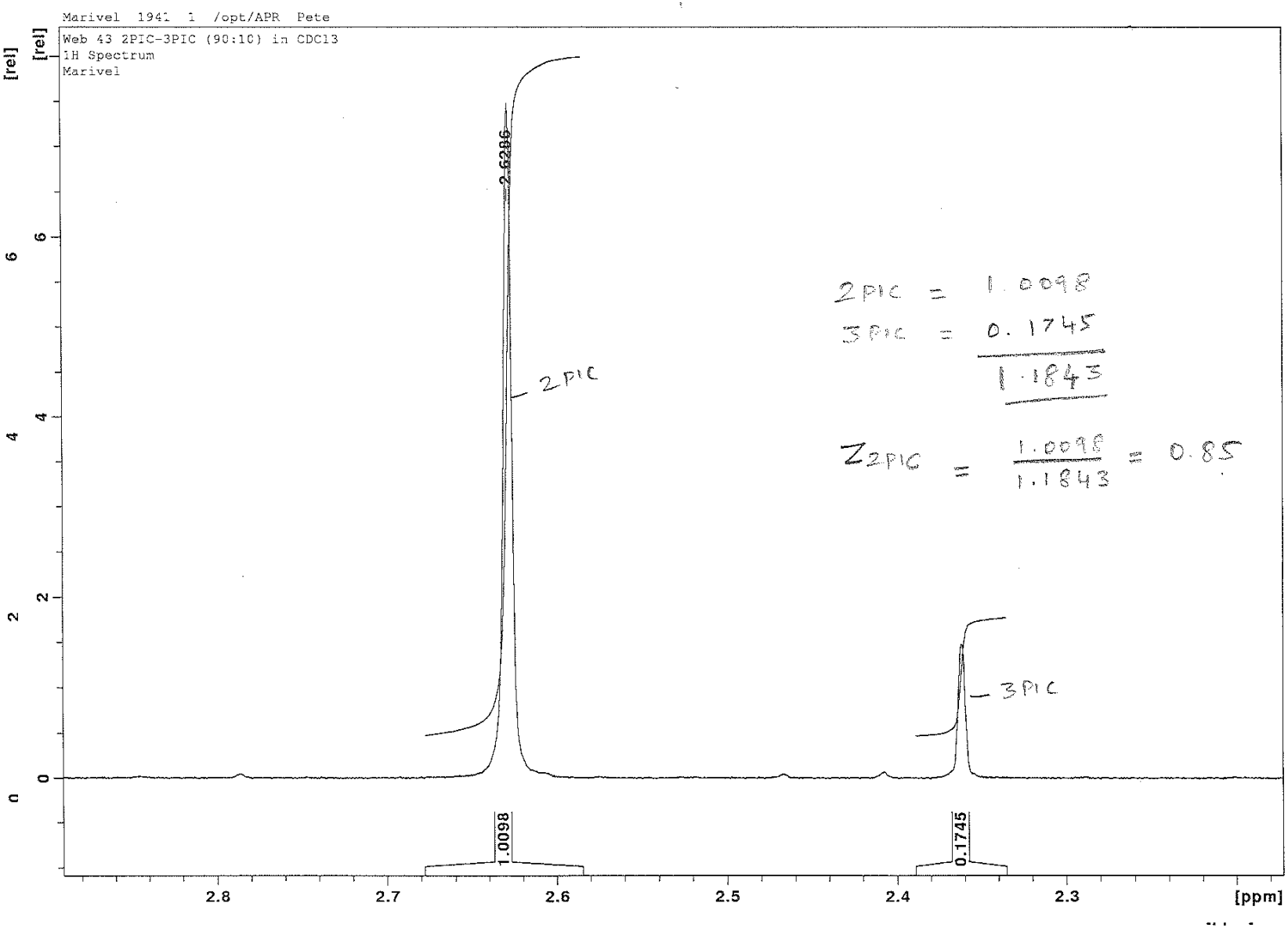
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.7:0.3)** in $CDCl_3$ at 25°C

1h. H.2PIC/3PIC (0.8:0.2)



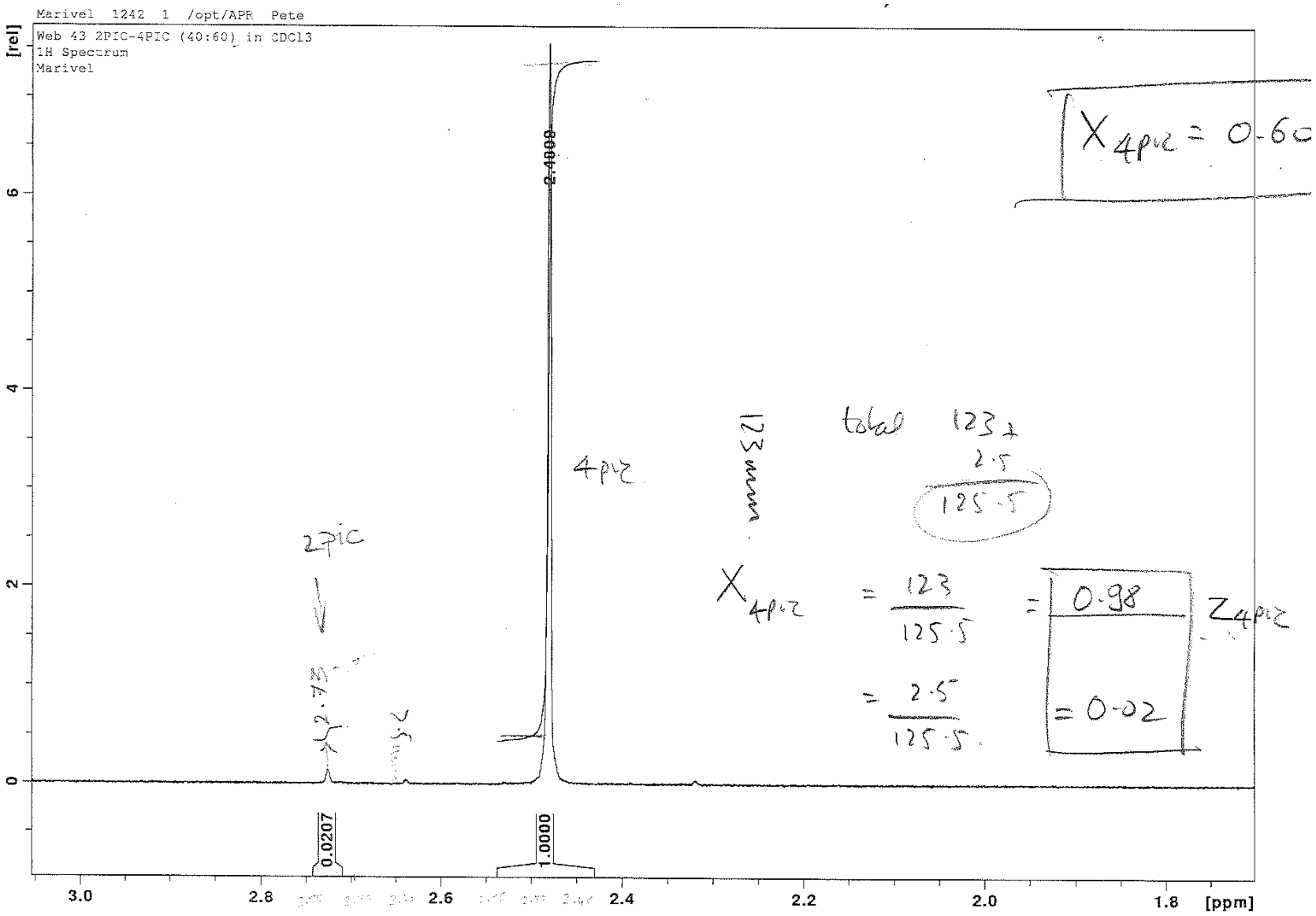
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.8:0.2)** in $CDCl_3$ at 25°C

1i. H.2PIC/3PIC (0.9:0.1)



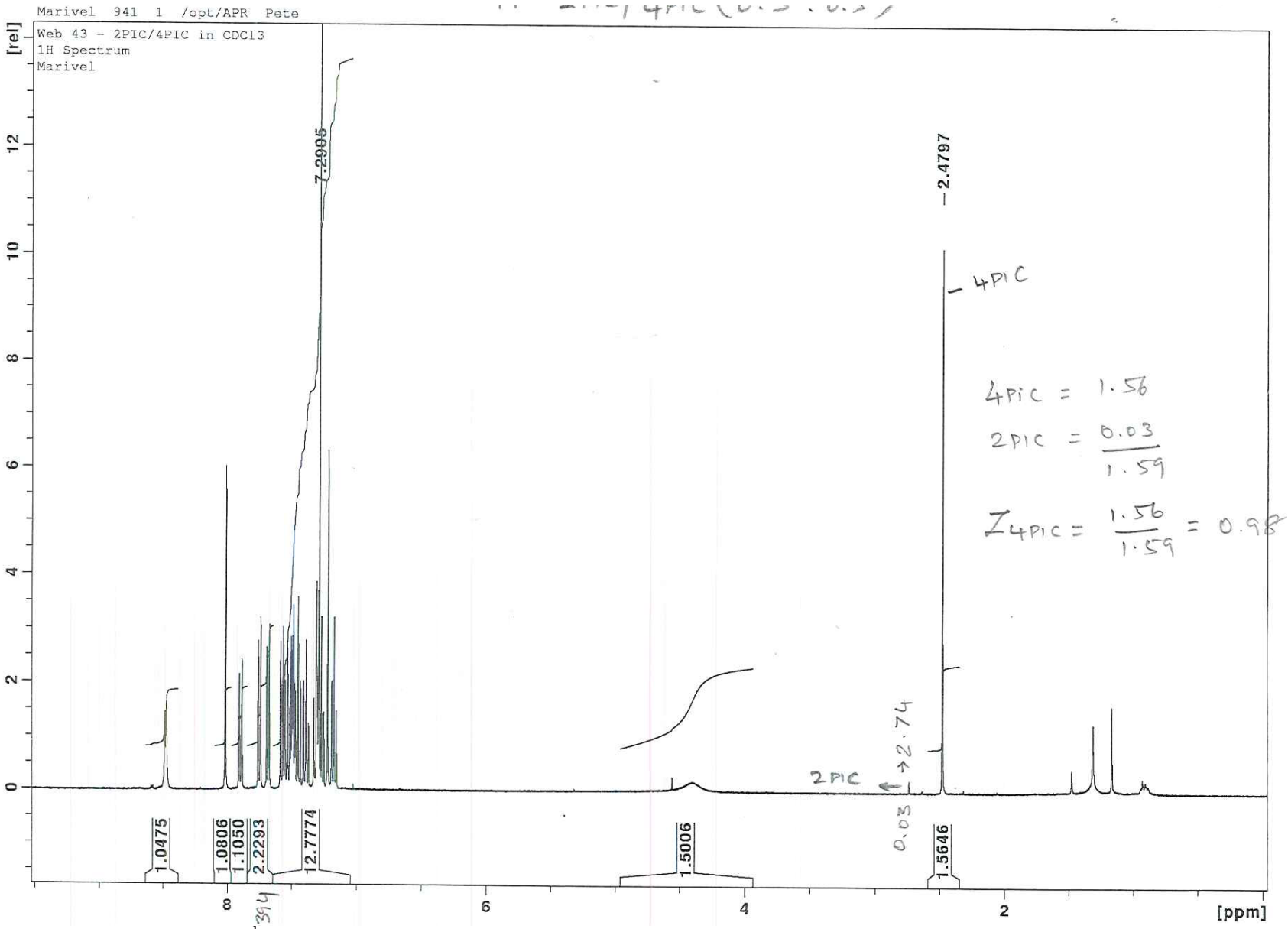
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC (0.9:0.1)** in $CDCl_3$ at 25°C

2a. H.2PIC/4PIC (0.4:0.6)



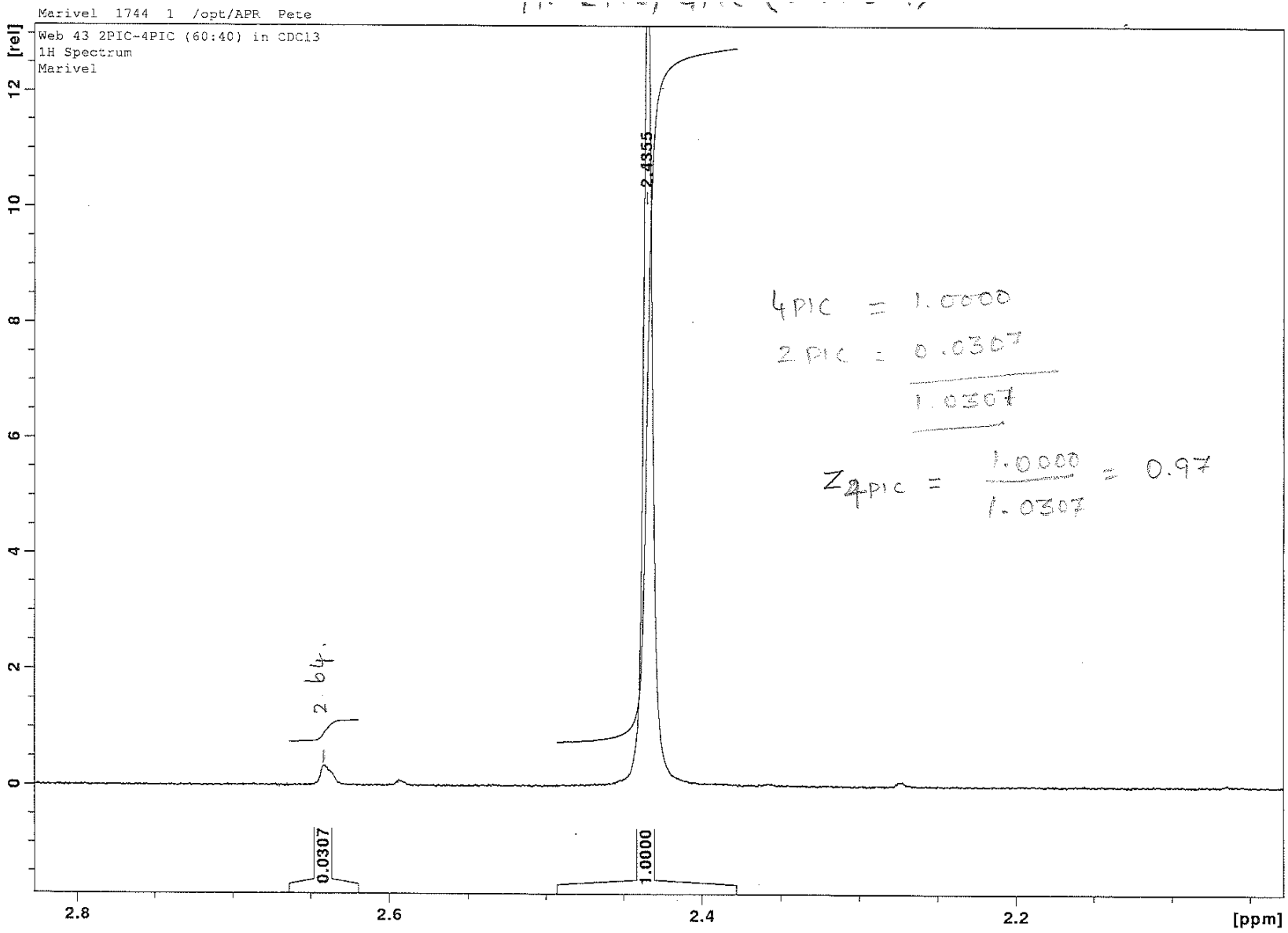
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.4:0.6)** in $CDCl_3$ at 25°C

2b. H.2PIC/4PIC (0.5:0.5)



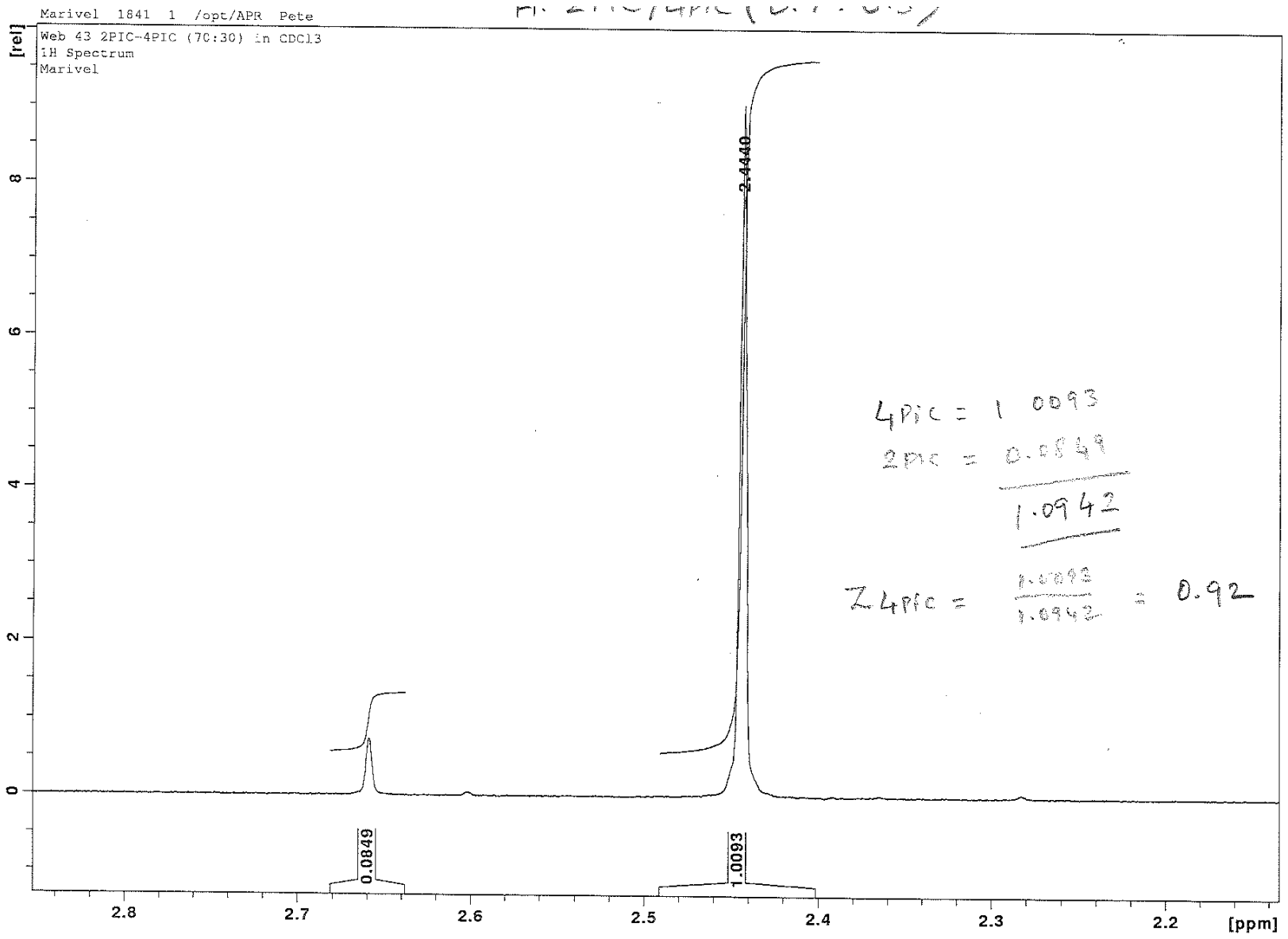
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.5:0.5)** in $CDCl_3$ at 25°C

2c. H.2PIC/4PIC (0.6:0.4)



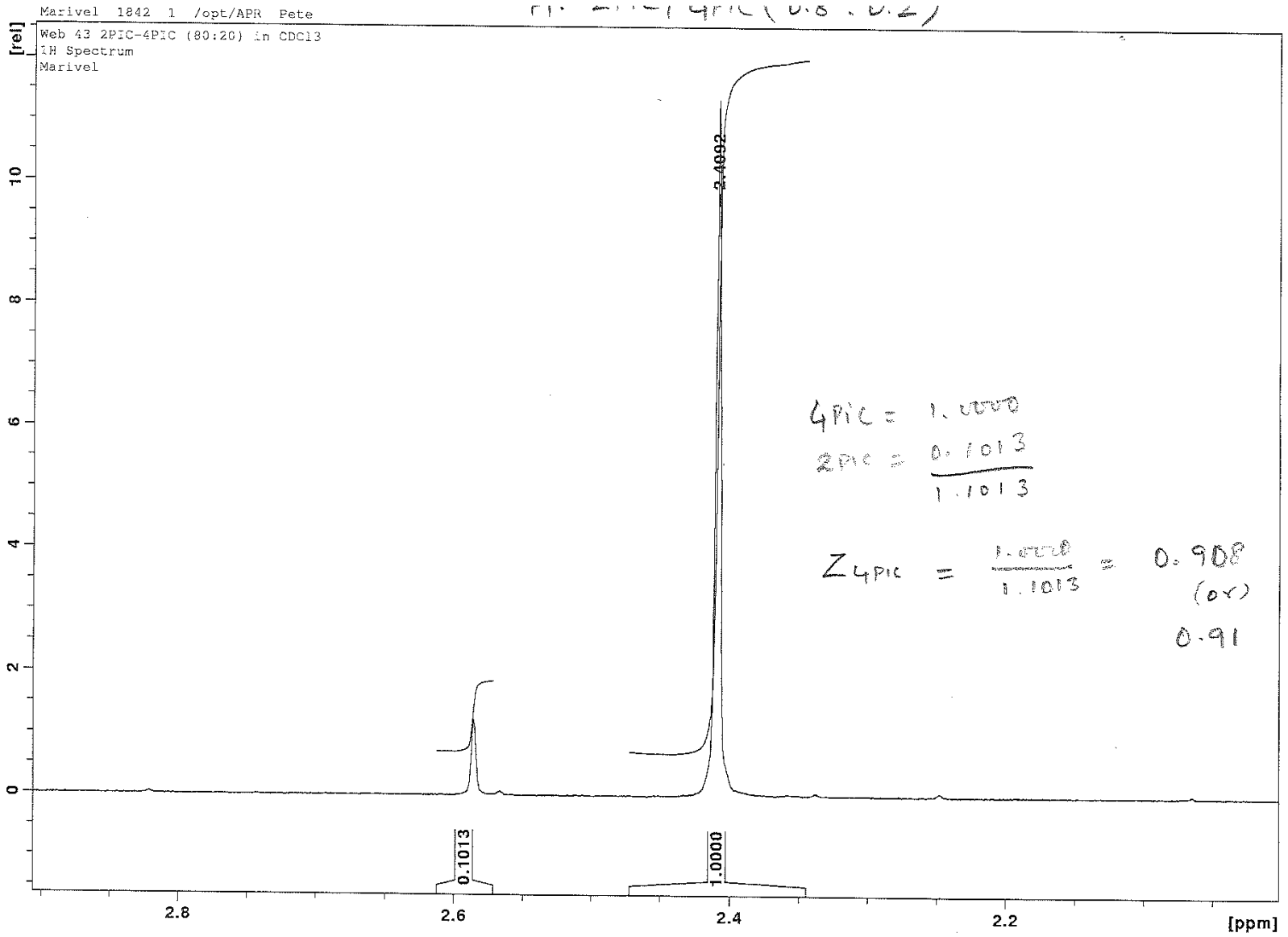
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.6:0.4)** in $CDCl_3$ at 25°C

2d. H.2PIC/4PIC (0.7:0.3)



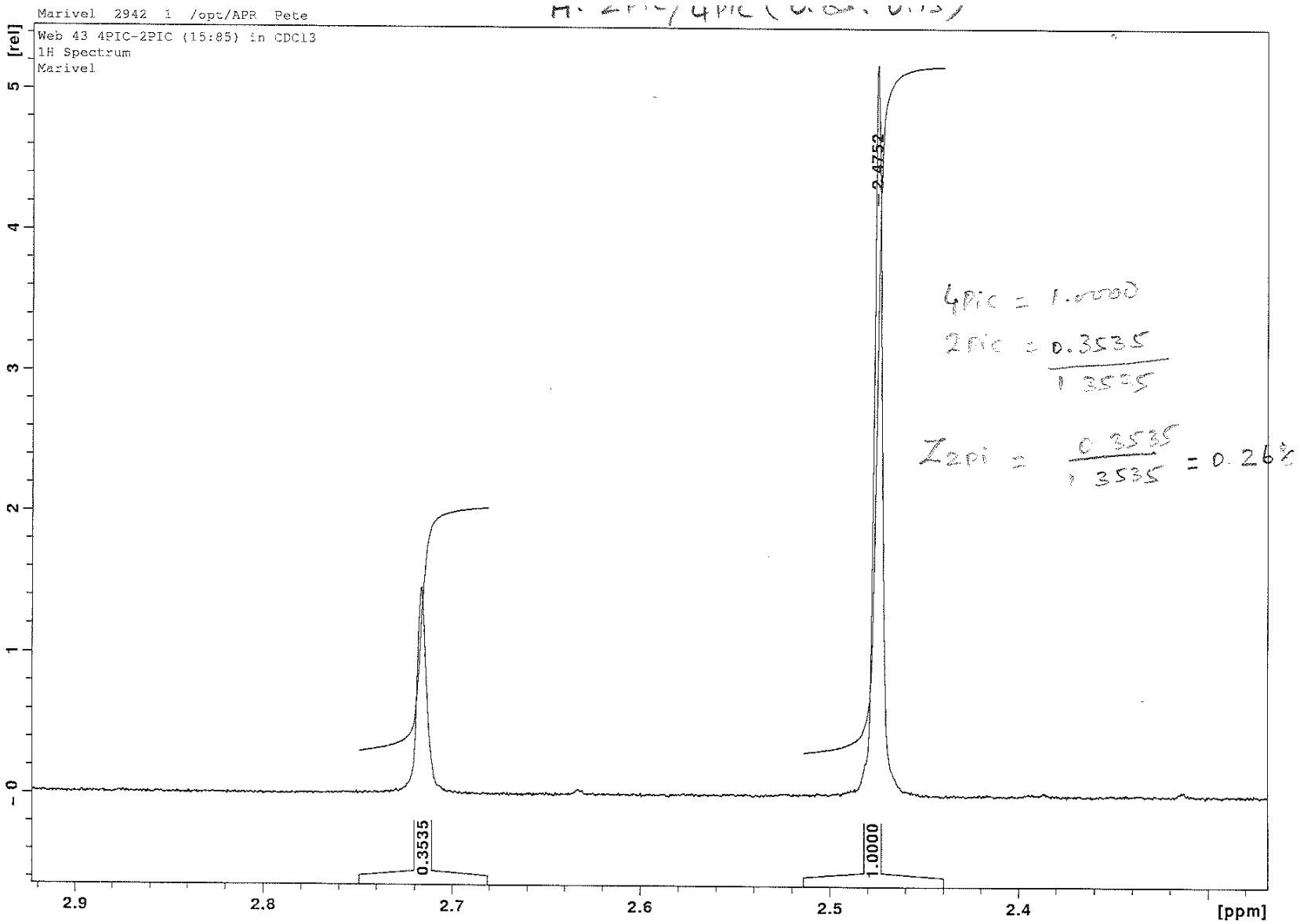
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.7:0.3)** in $CDCl_3$ at 25°C

2e. H.2PIC/4PIC (0.8:0.2)



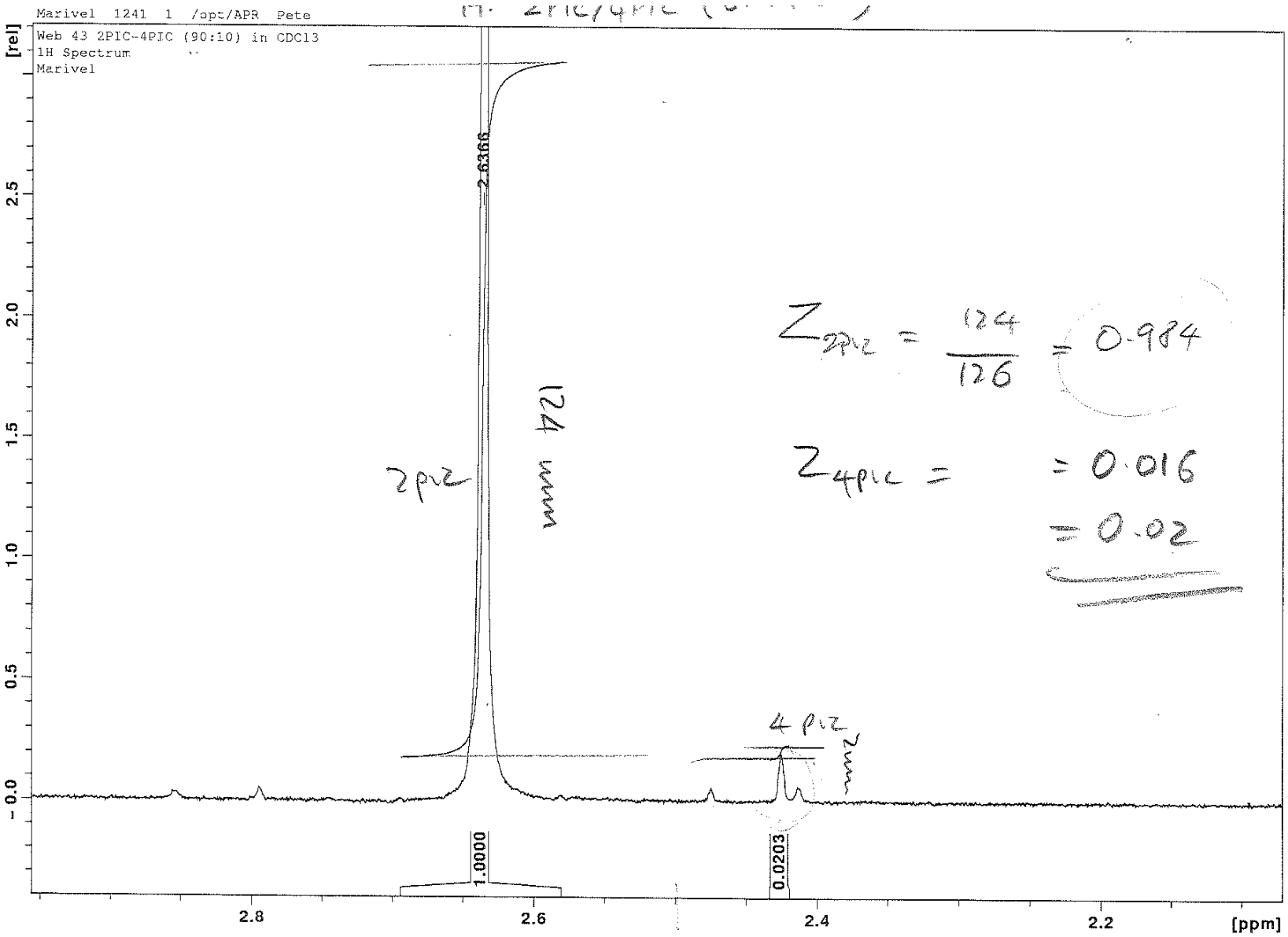
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.8:0.2)** in $CDCl_3$ at 25°C

2f. H.2PIC/4PIC (0.85:0.15)



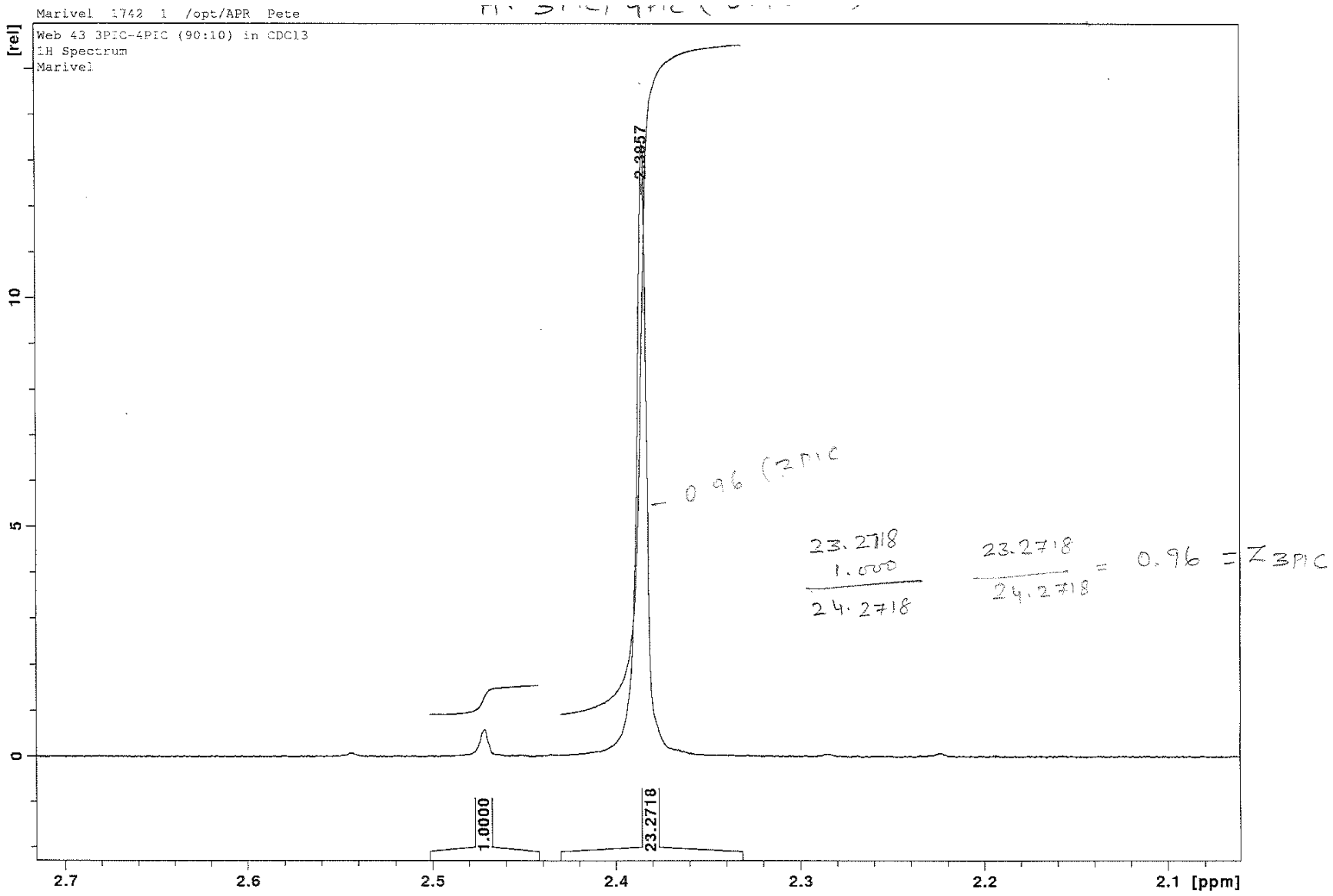
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.85:0.15)** in $CDCl_3$ at 25°C

2g. H.2PIC/4PIC (0.9:0.1)



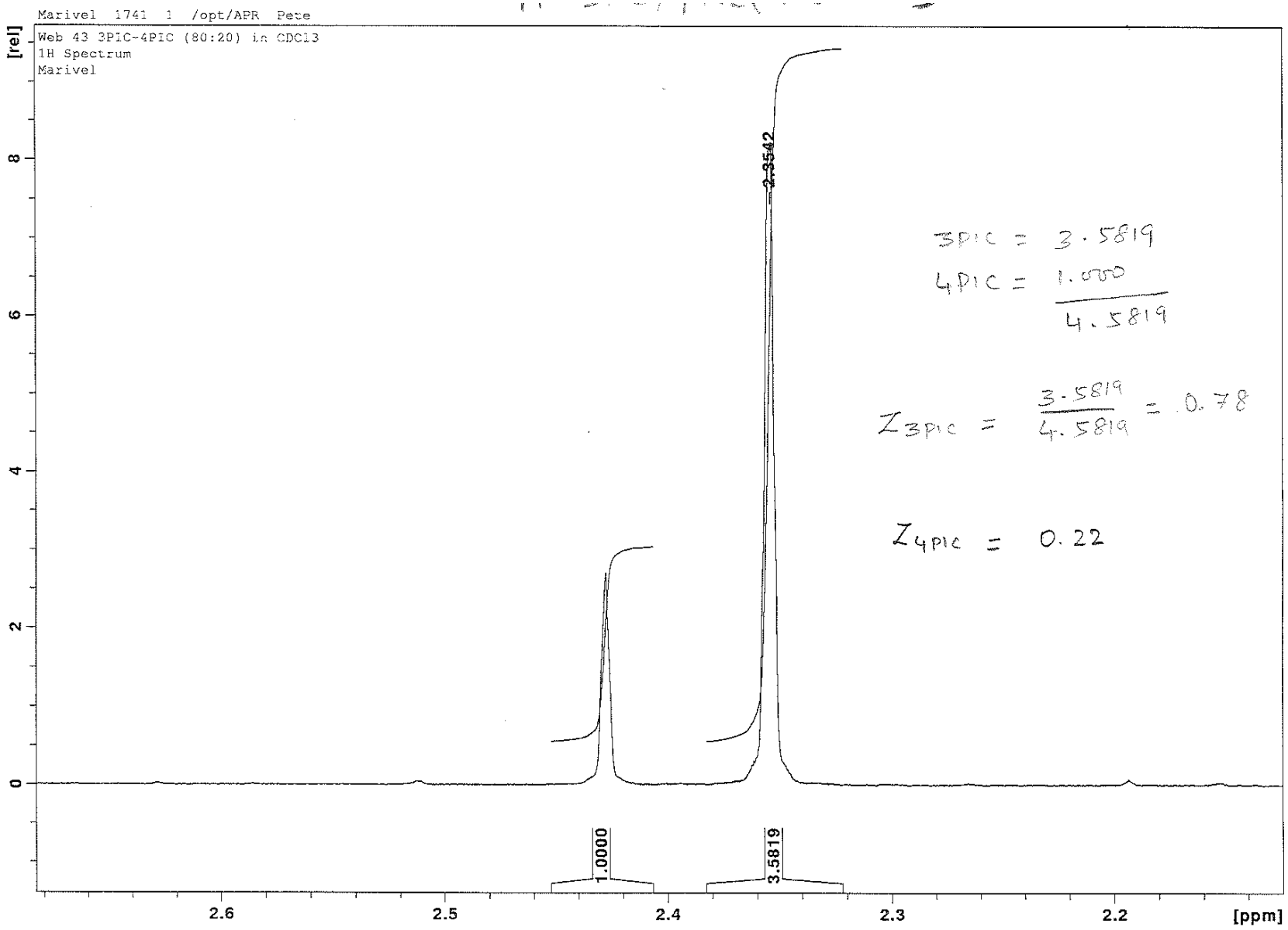
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/4PIC (0.9:0.1)** in $CDCl_3$ at 25°C

3a. H.3PIC/4PIC (0.9:0.1)



^{1}H-NMR (400 MHz) spectrum of **H.3PIC/4PIC (0.9:0.1)** in $CDCl_3$ at 25°C

3b. H.3PIC/4PIC (0.8:0.2)

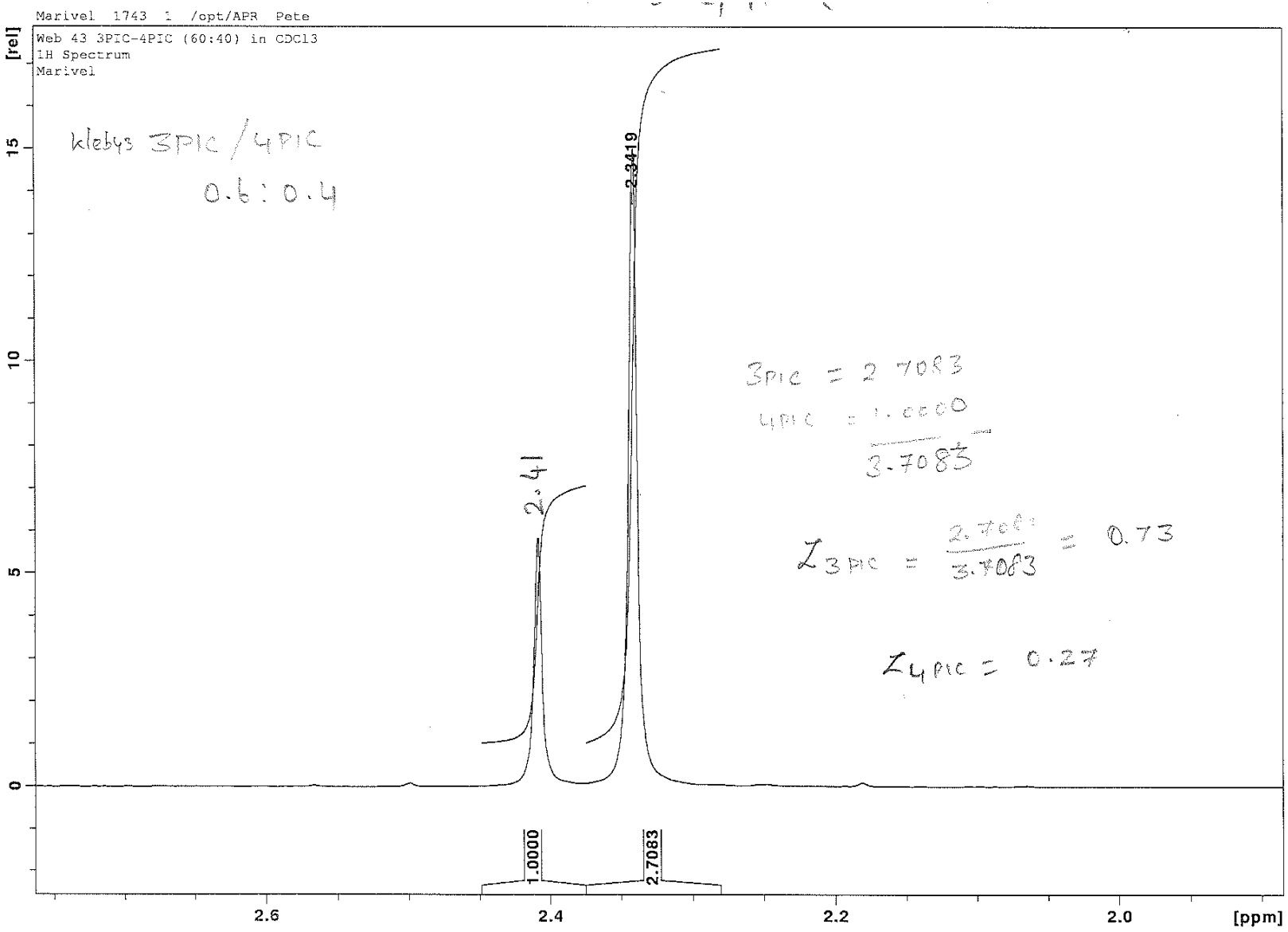


^{1}H-NMR (400 MHz) spectrum of **H.3PIC/4PIC (0.8:0.2)** in $CDCl_3$ at 25°C

3c. H.3PIC/4PIC (0.7:0.3)

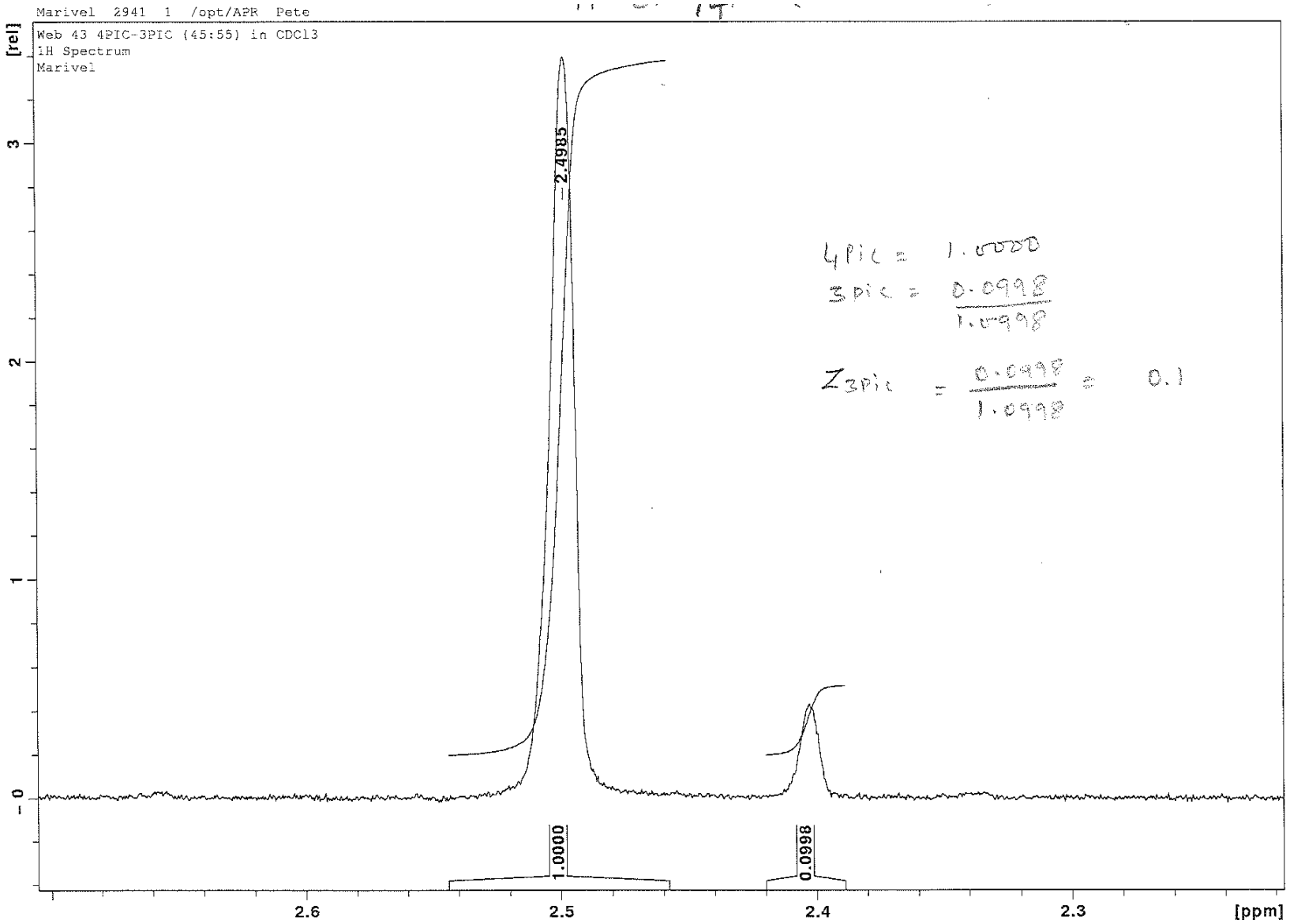
^{1}H-NMR (400 MHz) spectrum of **H.3PIC/4PIC (0.7:0.3)** in $CDCl_3$ at 25°C

3d. H.3PIC/4PIC (0.6:0.4) contains mixture of **H.3PIC (VI)** and **H.4PIC (VII)**



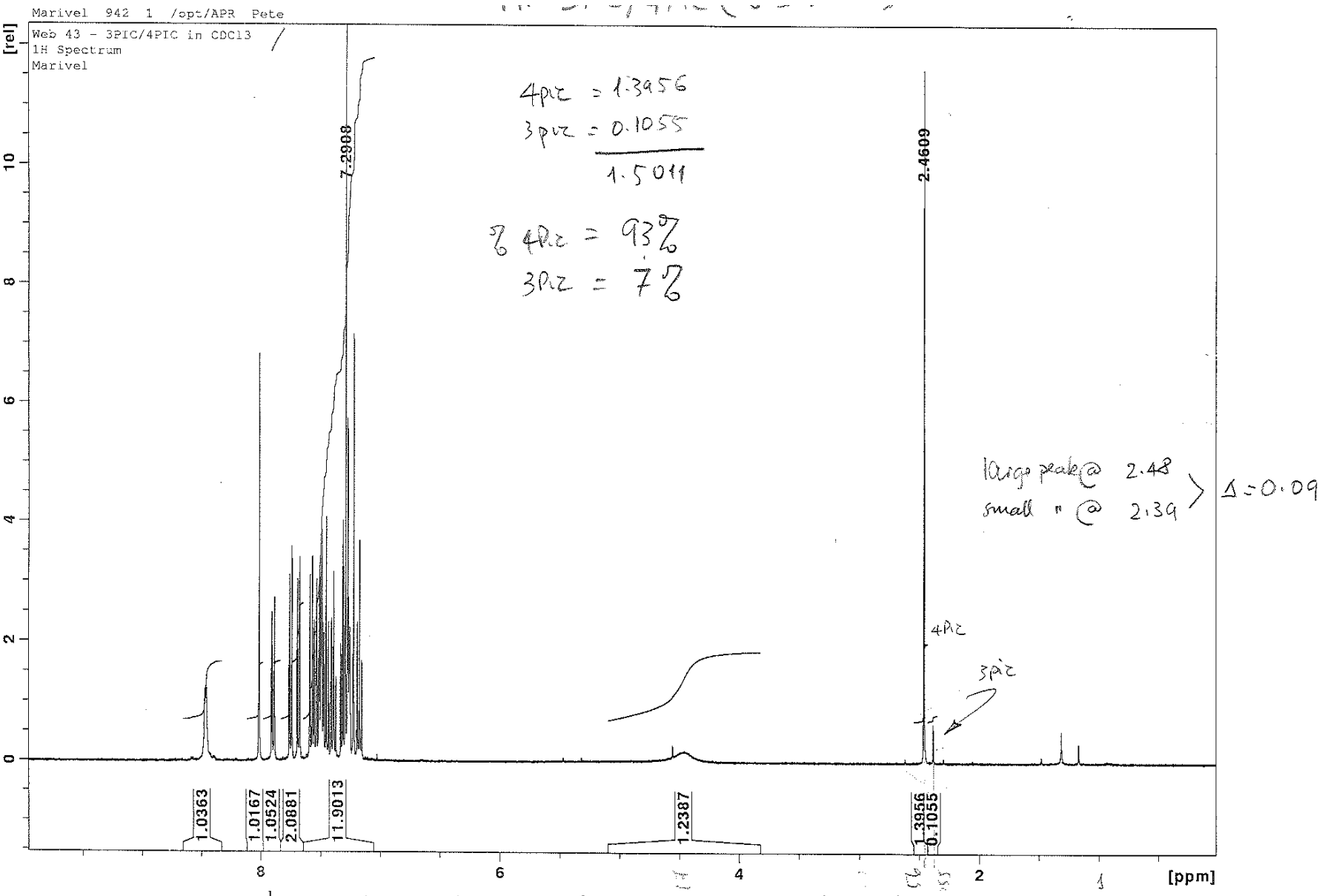
^{1}H-NMR (400 MHz) spectrum of **H.3PIC/4PIC (0.6:0.4)** in $CDCl_3$ at 25°C

3e. H.3PIC/4PIC (0.55:0.45)



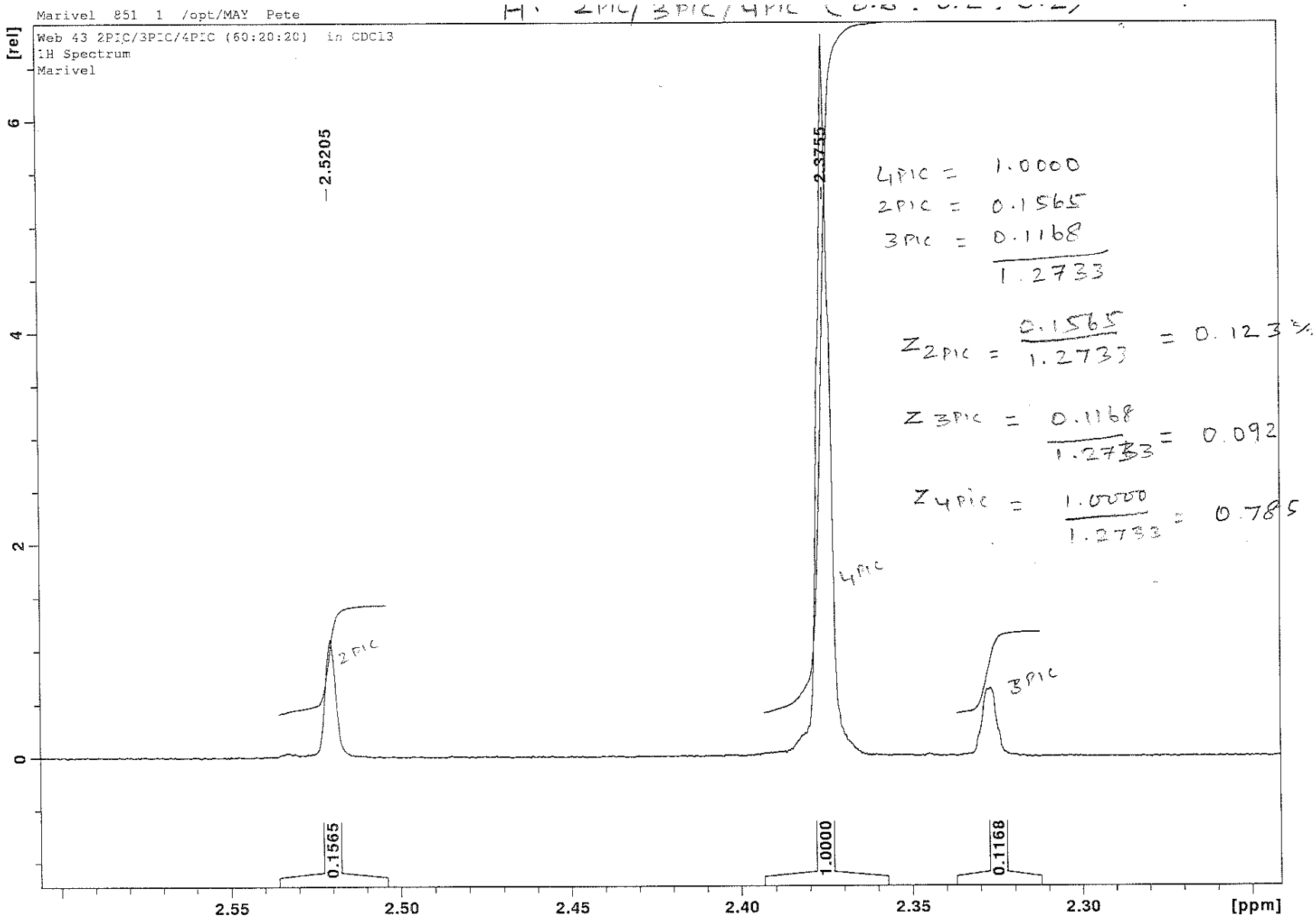
^{1}H-NMR (400 MHz) spectrum of **H.3PIC/4PIC (0.55:0.45)** in $CDCl_3$ at 25°C

3f. H.3PIC/4PIC (0.5:0.4)



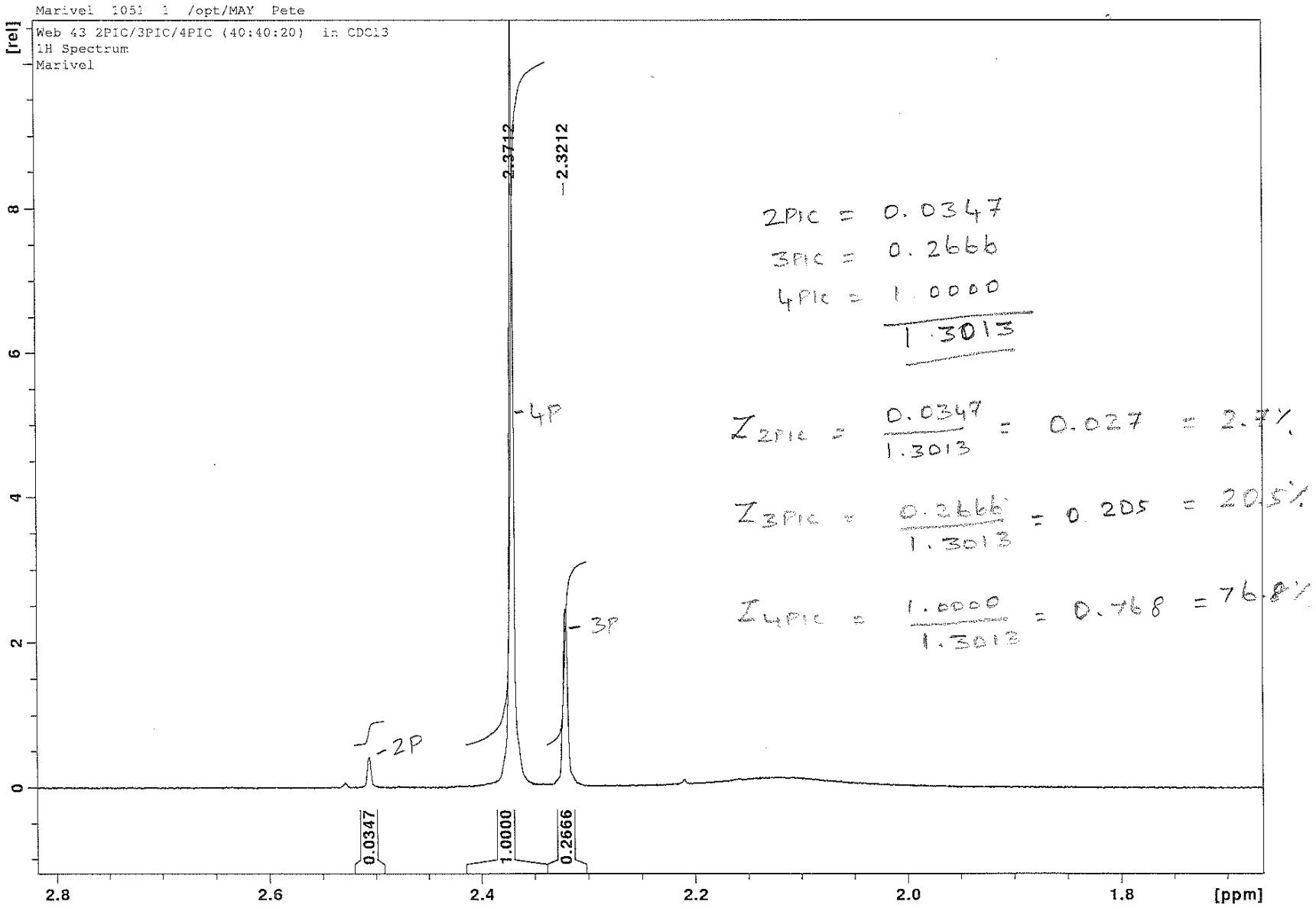
^{1}H-NMR (400 MHz) spectrum of **H.3PIC/4PIC (0.5:0.4)** in $CDCl_3$ at 25°C

4a. H.2PIC/3PIC/4PIC (0.6:0.2:0.2) –'A'



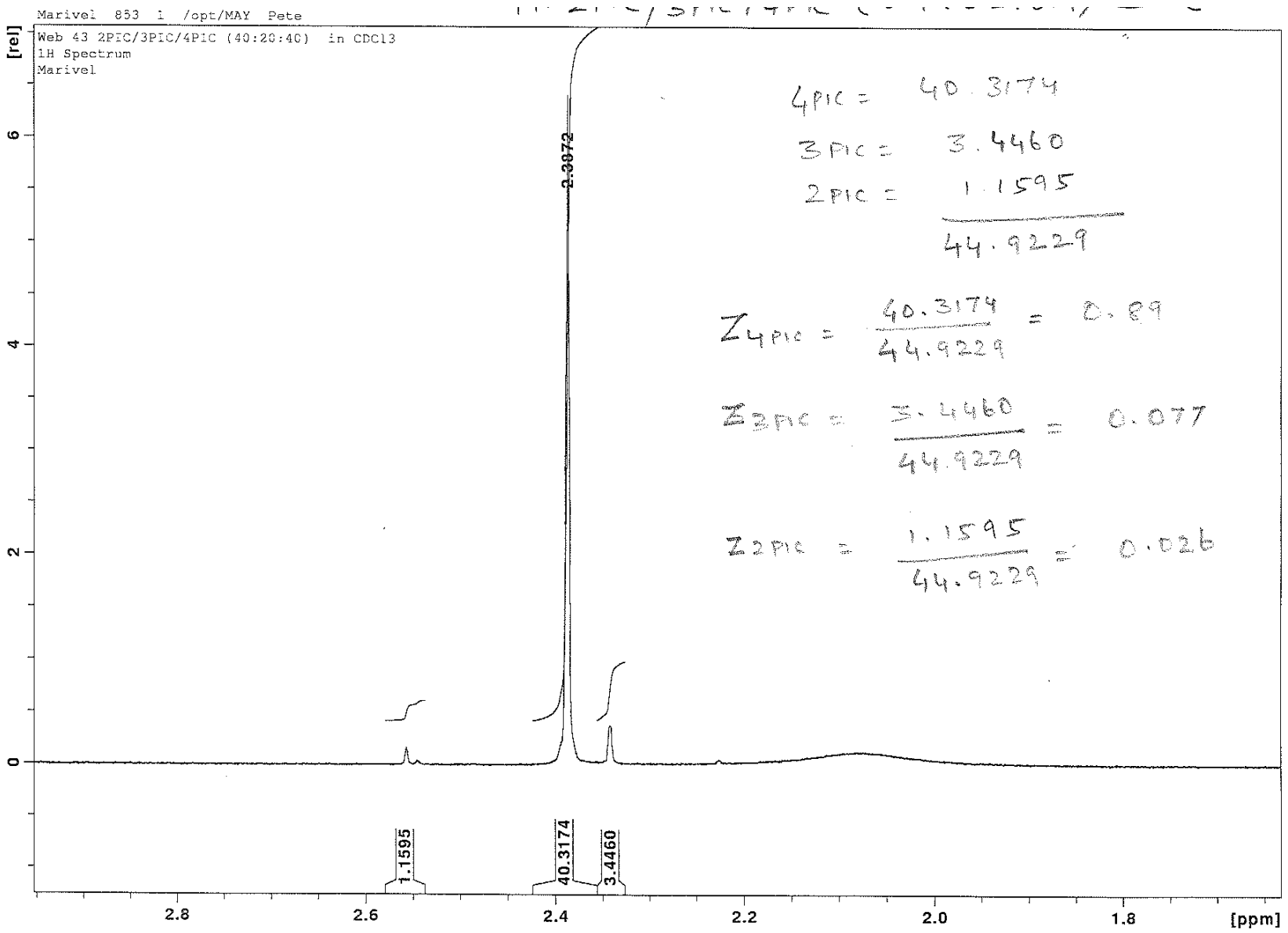
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.6:0.2:0.2)** in $CDCl_3$ at 25°C

4b. H.2PIC/3PIC/4PIC (0.4:0.4:0.2) – 'B' - IX



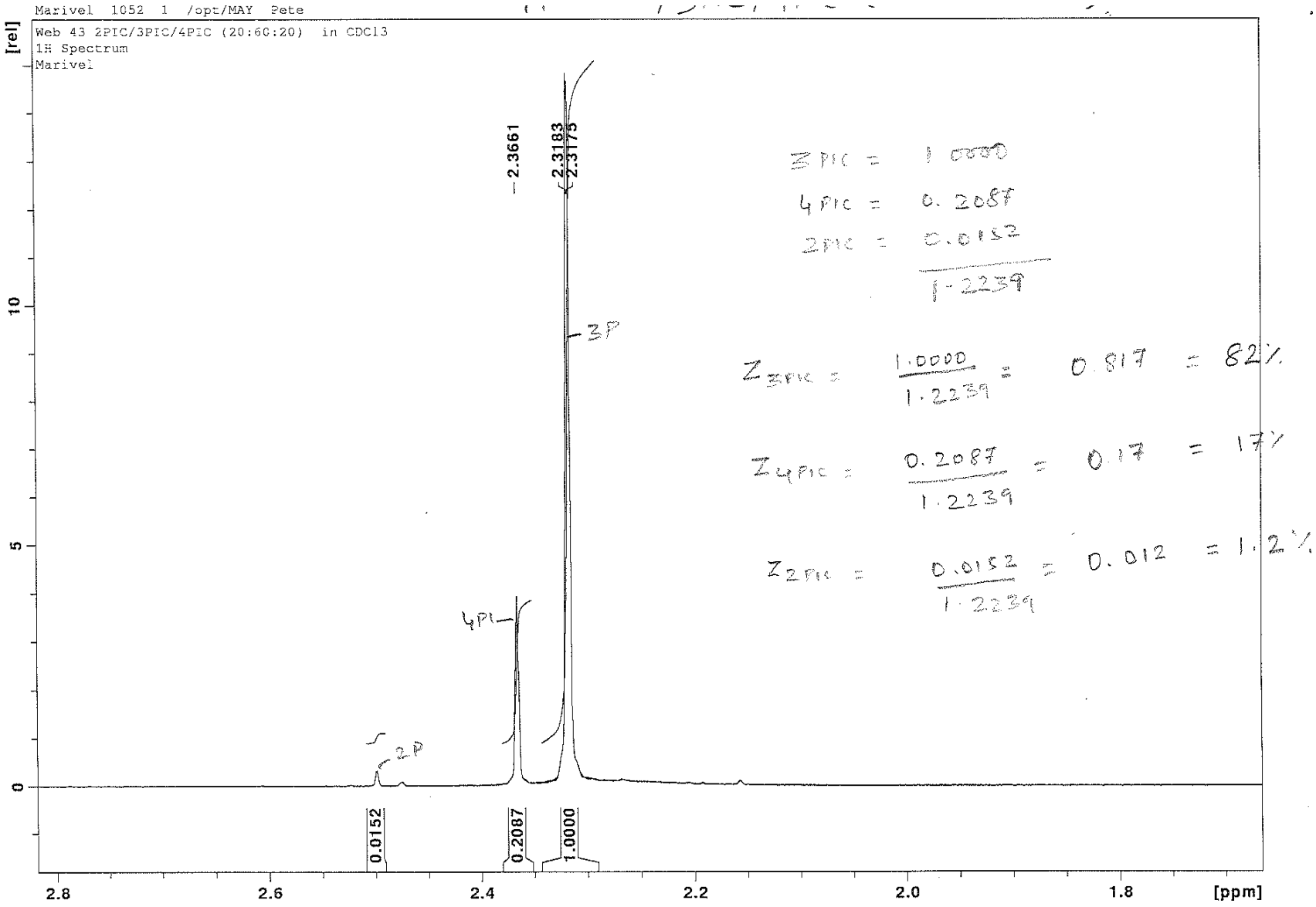
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.4:0.4:0.2)** in $CDCl_3$ at 25°C

4c. H.2PIC/3PIC/4PIC (0.4:0.2:0.4) – 'C'



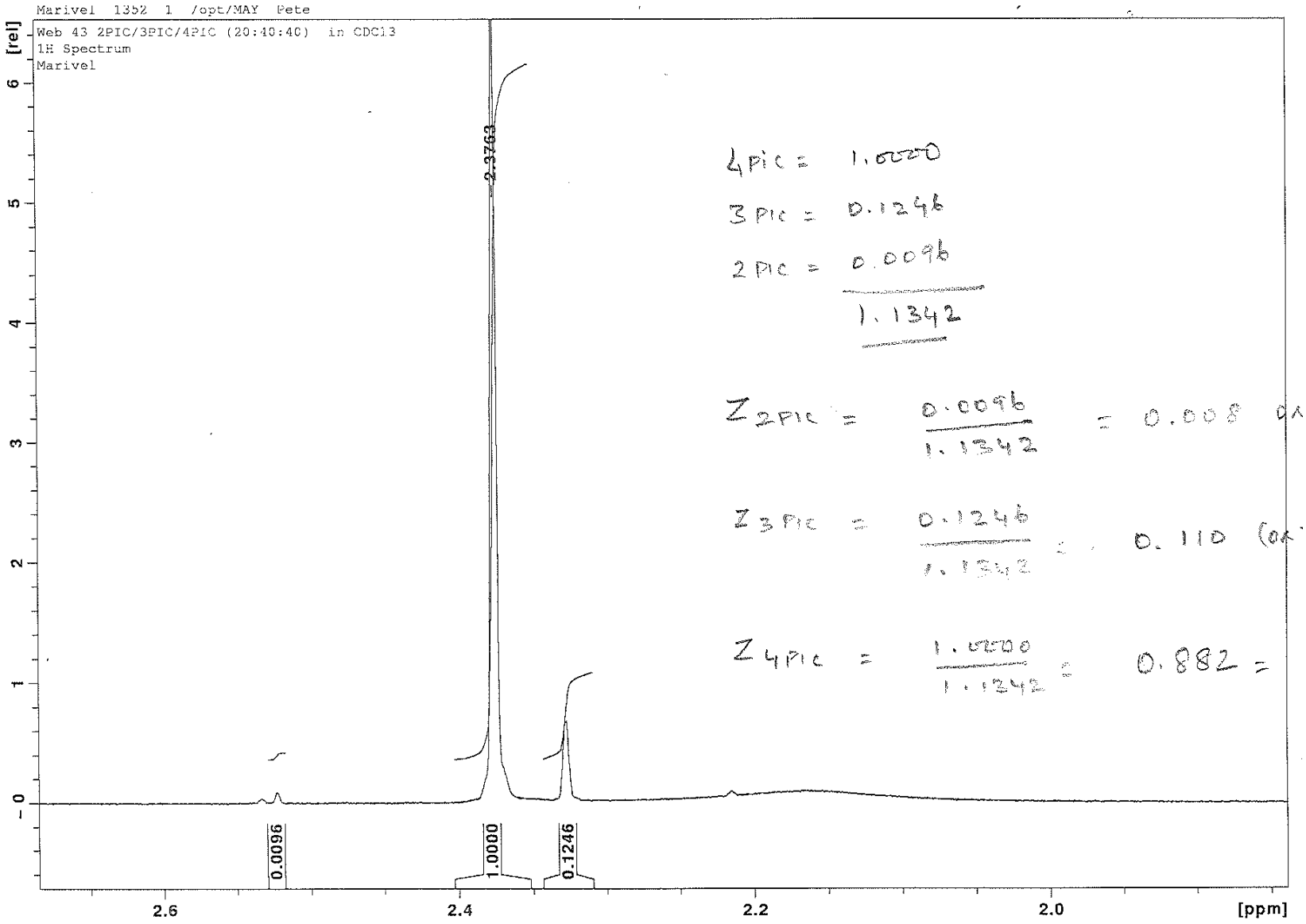
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.4:0.2:0.4)** in $CDCl_3$ at 25°C

4d. H.2PIC/3PIC/4PIC (0.2:0.6:0.2) – 'D' - VIII



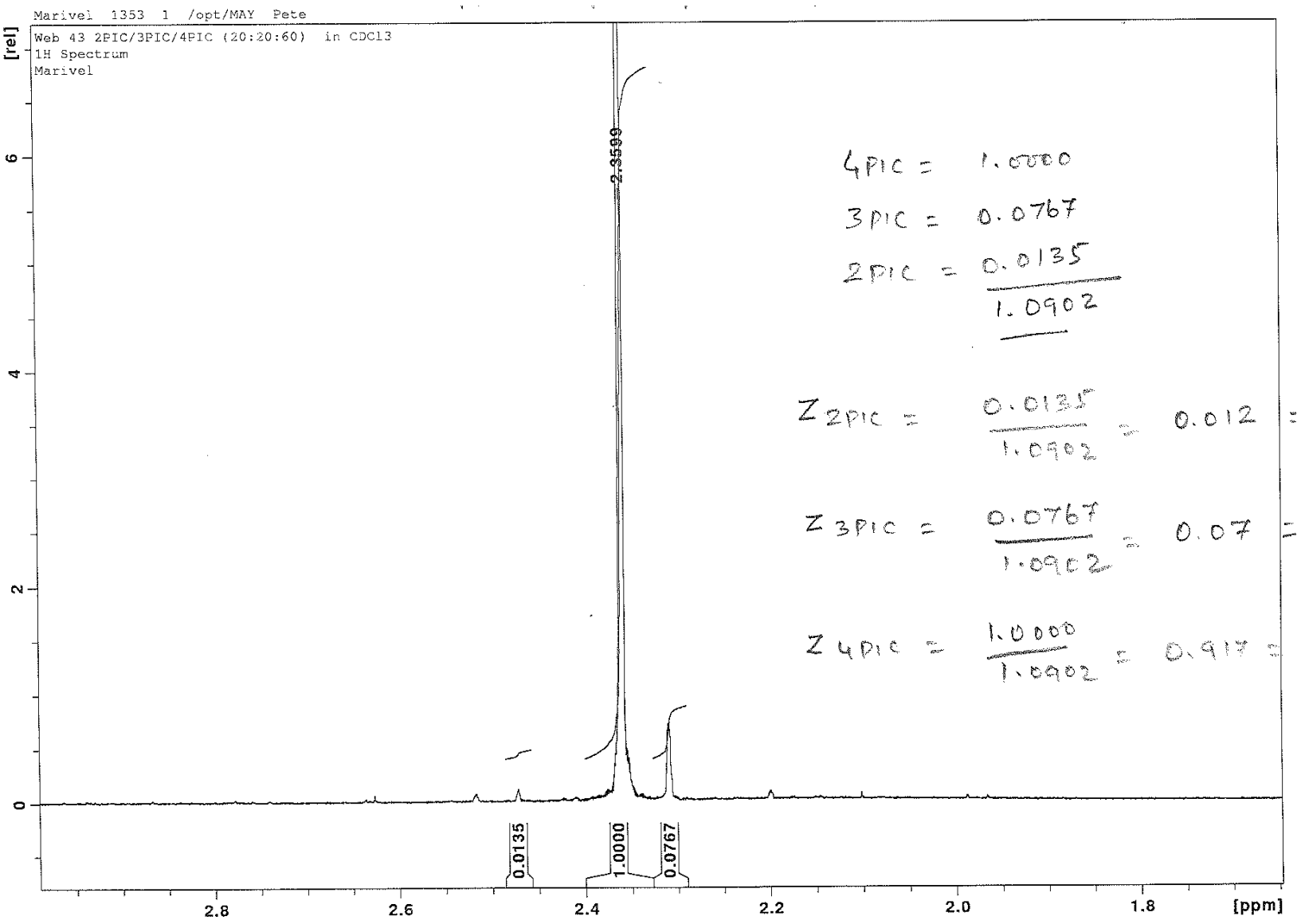
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.2:0.6:0.2)** in $CDCl_3$ at 25°C

4e. H.2PIC/3PIC/4PIC (0.2:0.4:0.4) – 'E'



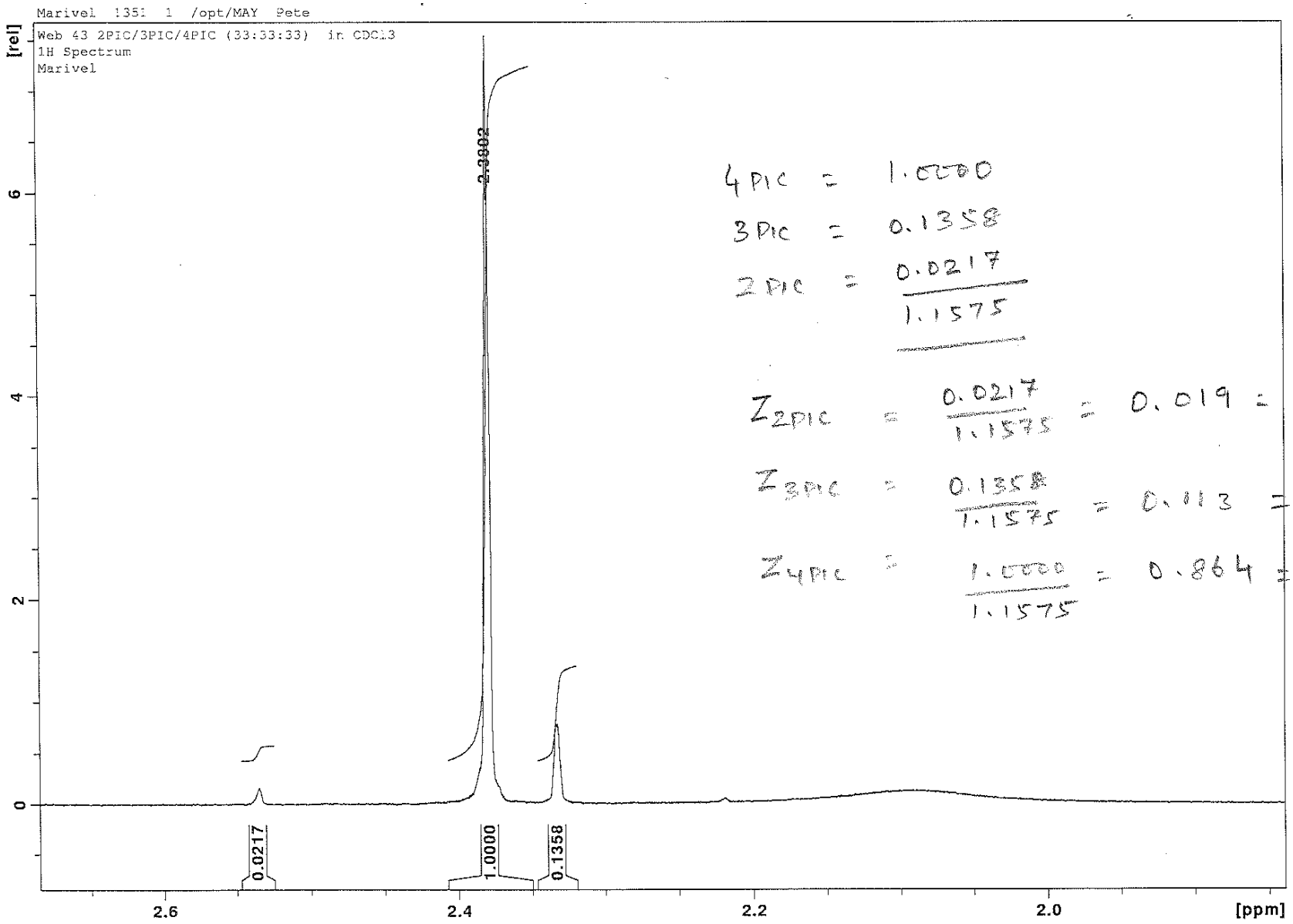
^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.2:0.4:0.4)** in $CDCl_3$ at 25°C

4f. H.2PIC/3PIC/4PIC (0.2:0.2:0.6) – 'F'



^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.2:0.2:0.6)** in $CDCl_3$ at 25°C

4g. H.2PIC/3PIC/4PIC (0.33:0.33:0.33) – 'G'



^{1}H-NMR (400 MHz) spectrum of **H.2PIC/3PIC/4PIC (0.33:0.33:0.33)** in $CDCl_3$ at 25°C