

Liver-Targeted Prodrugs of 2'-C-Methyladenosine for Therapy of Hepatitis C Virus Infection

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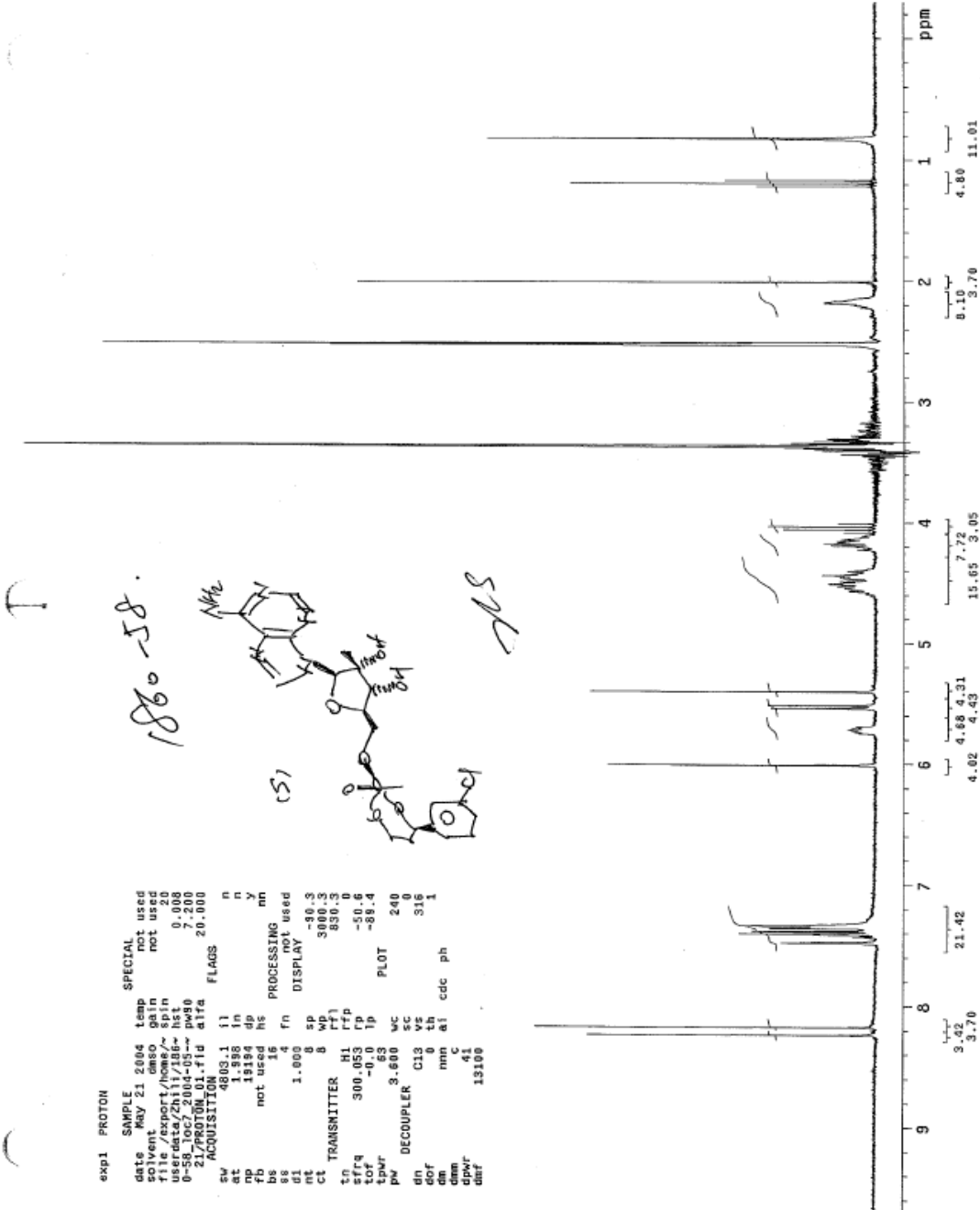
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SUPPORTING INFORMATION

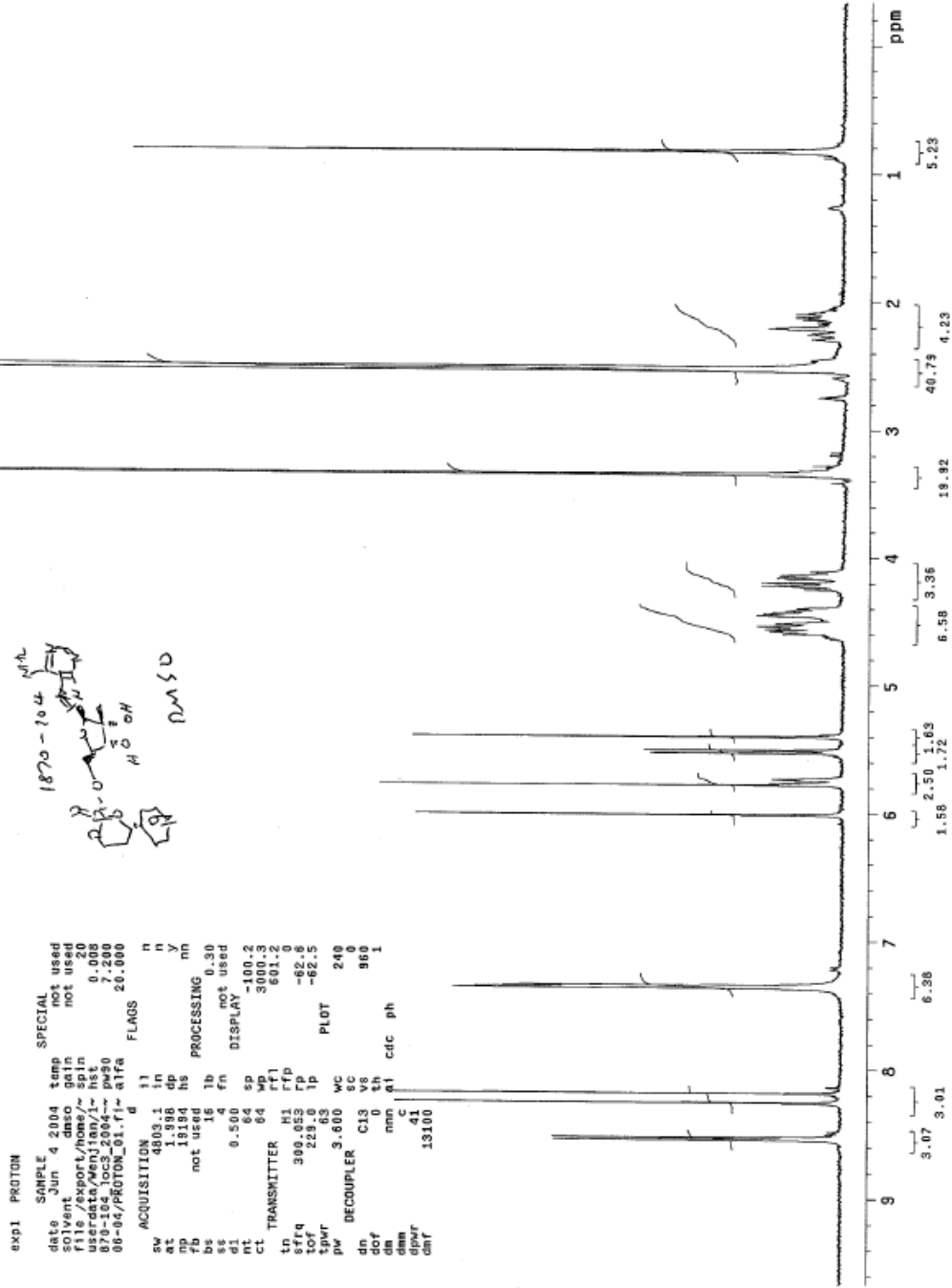
A. Elemental analysis data for compounds **6a-6s**, **7**, **8**, **9a-c**, **9f-g**, **9i** and **9p**.

Cpd	Calcd for	Calcd			Found		
		C	H	N	C	H	N
6a	C ₂₀ H ₂₃ ClN ₅ O ₇ P	45.34	4.76	13.22	45.67	4.53	13.21
6b	C ₂₀ H ₂₂ N ₅ O ₇ Cl ₂ P·1.7 CF ₃ CO ₂ H·2.7 H ₂ O	35.63	3.72	8.88	35.17	3.55	8.80
6c	C ₂₀ H ₂₂ N ₅ O ₇ Cl ₂ P·1.0 H ₂ O·1.0 CF ₃ CO ₂ H	38.95	3.71	10.32	38.56	3.52	10.57
6d	C ₂₀ H ₂₃ BrN ₅ O ₇ P·1.5 H ₂ O·0.1 CH ₂ Cl ₂	40.79	4.46	11.83	40.49	4.46	11.49
6e	C ₂₀ H ₂₃ N ₅ O ₇ BrP·1.5 H ₂ O·0.4 CF ₃ CO ₂ H	39.72	4.23	11.14	39.44	4.55	11.18
6f	C ₂₀ H ₂₃ N ₅ O ₇ FP·0.4 CF ₃ CO ₂ H	46.18	4.36	12.94	46.09	4.39	13.01
6g	C ₂₀ H ₂₂ N ₅ O ₇ F ₂ P·0.75 H ₂ O	45.59	4.50	13.29	45.49	4.08	13.30
6h	C ₂₀ H ₂₂ F ₂ N ₅ O ₇ P·0.3 CH ₂ Cl ₂	45.25	4.23	13.00	45.07	3.94	12.69
6i	C ₂₀ H ₂₂ F ₂ N ₅ O ₇ P·1.5 H ₂ O·0.1 C ₆ H ₁₄	45.07	4.85	12.76	45.04	5.25	12.59
6j	C ₂₀ H ₂₂ N ₅ O ₇ PCl·0.8 CF ₃ CO ₂ ·0.9 H ₂ O	40.71	3.89	10.99	40.46	3.93	10.98
6k	C ₂₀ H ₂₂ N ₅ O ₇ BrFP·3.4 H ₂ O·2.2 CF ₃ CO ₂ H·0.1 EtOAc	33.27	3.58	7.82	32.94	3.24	7.52
6l	C ₂₁ H ₂₃ N ₆ O ₇ P·1.1 H ₂ O	48.30	4.86	16.09	48.53	5.11	15.75
6m	C ₂₁ H ₂₃ N ₆ O ₇ P·1.0 H ₂ O·0.1 EtOAc	48.47	4.84	16.15	48.89	4.42	15.68
6n	C ₁₉ H ₂₃ N ₆ O ₇ P·2.0 H ₂ O·1.0 CF ₃ CO ₂ H	40.14	4.49	13.37	40.36	4.92	13.63
6o	C ₁₉ H ₂₃ N ₆ O ₇ P·1.5 H ₂ O·0.4 EtOAc	45.76	15.54	5.44	45.88	15.19	5.09
6p	C ₁₉ H ₂₃ N ₆ O ₇ P·2.5H ₂ O	43.60	5.39	16.06	43.35	5.54	16.05
6q	C ₁₉ H ₂₂ N ₆ O ₇ BrP·1.0 H ₂ O·0.4 EtOAc	40.52	4.49	13.76	40.39	4.22	13.42
6r	C ₂₀ H ₂₅ N ₆ O ₈ P·1.0 CF ₃ CO ₂ H·1.2 H ₂ O	41.03	4.44	13.05	40.96	4.97	13.70
6s	C ₂₀ H ₂₅ N ₆ O ₇ P·1.2 H ₂ O	46.73	5.37	16.35	46.64	5.21	16.15
7	C ₂₄ H ₃₂ H ₇ O ₈ P·1.7H ₂ O·3CF ₃ CO ₂ H·0.1 (C ₂ H ₅) ₂ O	37.92	4.07	10.32	37.65	3.72	9.87
8	C ₂₆ H ₃₃ N ₅ O ₉ CIP·0.8 CF ₃ CO ₂ H	46.22	4.75	9.76	46.00	4.84	9.97
9a	C ₂₁ H ₂₁ N ₅ O ₈ CIP·1.0 H ₂ O	45.38	4.17	12.60	45.21	3.97	12.41
9b	C ₂₁ H ₂₀ C ₁₂ N ₅ O ₈ P	44.07	3.52	12.39	43.68	3.90	12.43
9c	C ₂₁ H ₂₀ ClN ₅ O ₈ P·1.0 H ₂ O·0.5 imidazole	43.28	3.87	13.46	43.28	3.92	13.79
9f	C ₂₁ H ₂₁ N ₅ O ₈ FP·0.7 CH ₂ Cl ₂	44.87	3.89	12.06	44.67	3.86	12.01
9g	C ₂₁ H ₂₀ N ₅ O ₈ F ₂ P·1.0 H ₂ O	45.25	3.98	12.56	44.88	3.74	12.47
9i	C ₂₁ H ₂₀ F ₂ N ₅ O ₈ P·1.5 H ₂ O	44.53	4.09	12.36	44.31	3.75	12.18
9p	C ₂₀ H ₂₁ N ₆ O ₈ P·1.0 H ₂ O	45.98	4.44	16.09	45.82	4.43	15.97

B. ¹H NMR Spectrum of Compound 6a.



C. ¹H NMR Spectrum of Compound 6p.

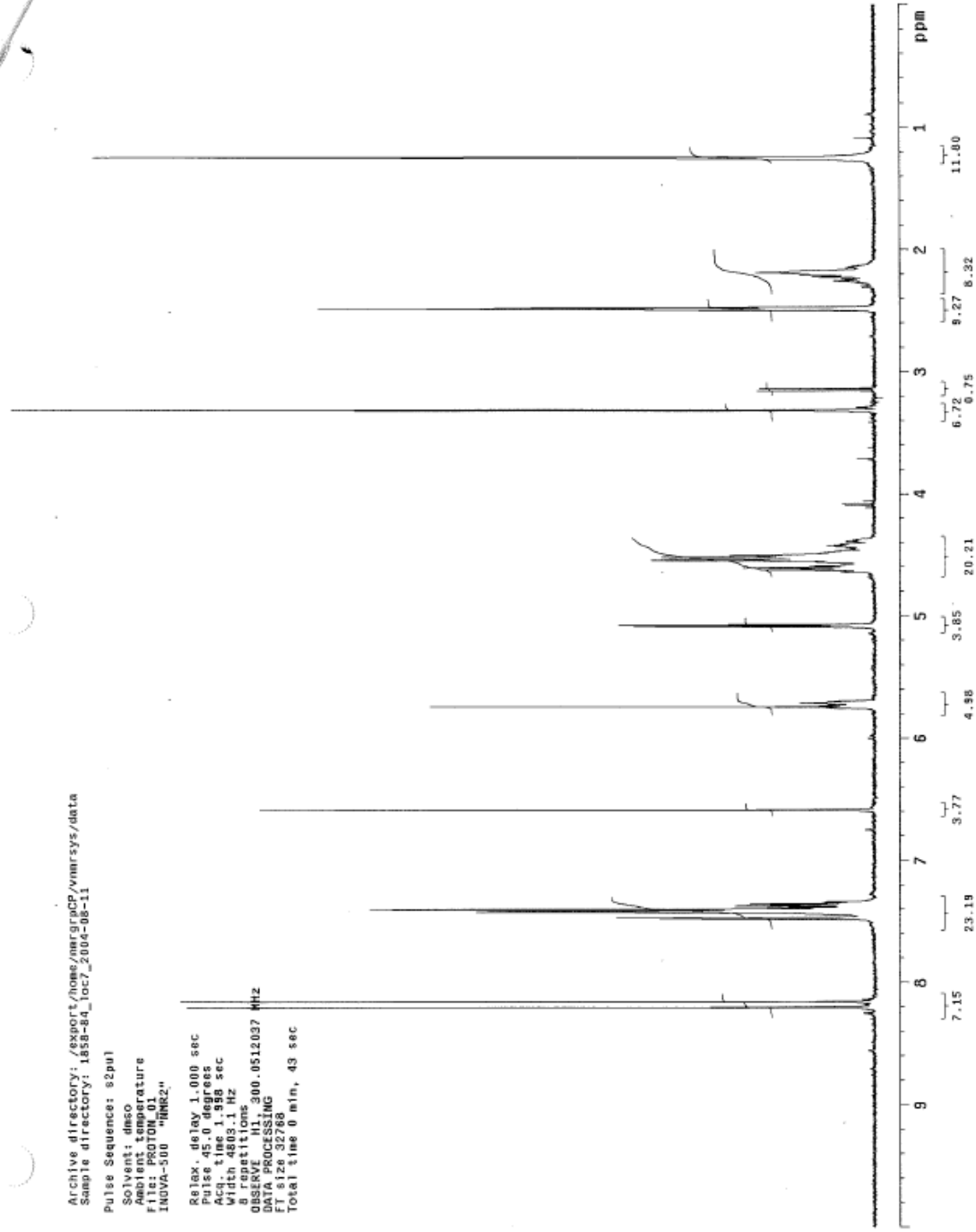


D. ¹H NMR Spectrum of Compound 9a.

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E. ¹H NMR Spectrum of Compound **9p**.

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