

Supporting information

Title: 2-Deoxyglycoside conjugates of lupane triterpenoids with high cytotoxic activity – synthesis, activity, and pharmacokinetic profile.

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1) Tables of ^{13}C NMR spectra of new compounds.

carbon	Compound			
	11a	11b	15a	15b
1	38.51	38.29	38.52	38.71
2	21.96	21.57	23.58	26.66
3	82.63	81.42	80.66	78.38
4	38.40	38.25	37.72	38.59
5	55.74	55.41	55.37	55.14
6	18.14	17.99	18.08	17.97
7	34.89	37.71	34.74	34.63
8	41.27	41.14	41.32	41.13
9	51.11	50.89	50.90	50.82
10	37.12	36.98	37.09	36.95
11	21.19	21.01	21.28	21.01
12	27.64	27.47	27.77 ^a	27.22
13	45.15	45.16	42.74	42.52
14	45.16	45.12	45.52 [*]	45.97 [*]
15	29.08	28.90	27.36 ^a	27.59
16	33.66	33.49	32.03	32.17
17	53.05	53.01	46.06 [*]	45.39 [*]
18	171.83	172.66	170.98	174.56
19	145.66	145.54	146.35	145.84
20	25.08	24.87	25.14	24.86
21	207.29	207.96	208.24	210.03
22	47.60	47.41	48.14	48.27
23	28.50	28.22	27.88	27.59
24	16.31	16.13	16.50	15.79
25	16.64 [*]	16.47 [*]	16.83 ^b	16.49
26	16.76 [*]	16.61 [*]	16.73 ^b	16.49
27	15.89	15.76	15.88	15.15
28	174.86	174.88	70.81	70.27
29	19.98	19.74	20.00	19.58
30	20.10	19.86	20.52	20.29
COOCH ₃	52.48	52.41	-	-
AcO: CH ₃ 1	20.90	-	21.29	-
AcO: CH ₃ 2	20.77	-	20.83	-
AcO: CH ₃ 3	20.73	-	20.76	-
AcO: CH ₃ 4	-	-	20.71	-
AcO: C=O 1	170.43	-	172.48	-
AcO: C=O 2	170.33	-	170.42	-
AcO: C=O 3	170.10	-	170.23	-
AcO: C=O 4	-	-	169.96	-
1'	93.64	93.30	97.77	97.70
2'	30.73	32.94	29.96	32.17
3'	66.39	65.34	65.35	64.86
4'	66.75	68.82	65.98	68.04
5'	67.02	69.85	66.82	70.21
6'	62.47	62.45	62.14	61.70

carbon	Compound			
	12a	13a	13b	14a
1	38.56	38.52	38.53	38.55
2	22.00	21.99	22.00	21.98
3	82.66	82.66	82.67	82.59
4	38.42	38.40	38.41	38.42
5	55.77	55.73	55.76	55.72
6	18.16	18.12	18.17	18.15
7	34.91	34.87	34.91	34.68
8	41.32	41.21	41.33	41.57
9	51.15	51.10	51.12	50.99
10	37.15	37.08	37.15	37.16
11	21.25	21.03	21.17	21.03
12	27.68	27.57	27.66	27.45
13	45.13	45.15	45.26	46.14
14	45.12	45.05	45.18	45.52
15	29.09	28.85	29.11	27.98
16	33.54	33.44	33.44	28.37
17	52.98	52.74	52.83	58.46
18	171.83	171.89	171.90	168.12
19	145.62	145.55	145.87	150.61
20	25.11	25.09	25.09	25.90
21	207.26	207.22	207.41	194.25
22	47.64	47.41	47.67	189.24
23	28.53	28.50	28.52	28.52
24	16.64	16.44	16.71	16.70
25	16.78	16.74	16.78	16.78
26	16.32	16.30	16.31	16.34
27	15.87	15.80	15.84	16.08
28	174.31	173.86	178.32	170.97
29	19.95	19.89	19.96	19.74
30	20.16	20.23	20.07	19.80
COOCH ₂ CH ₃	61.01	-	-	-
COOCH ₂ CH ₃	14.16	-	-	-
COOCH ₃	-	-	-	53.37
COOCH ₂ Ph	-	66.52	-	-
Ph: C 1	-	135.79	-	-
Ph: C 2, 4, 6	-	128.36	-	-
Ph: C 3, 5	-	128.57	-	-
AcO: CH ₃ 1	20.90	20.89	20.89	20.91
AcO: CH ₃ 2	20.77	20.75	20.75	20.77
AcO: CH ₃ 3	20.72	20.72	20.72	20.74
AcO: C=O 1	170.46	170.46	170.81	170.46
AcO: C=O 2	170.33	170.32	170.67	170.30
AcO: C=O 3	170.09	170.09	170.45	170.09
1'	93.67	93.67	93.67	93.69
2'	30.76	30.76	30.75	30.77
3'	66.41	66.41	66.44	66.40
4'	66.78	66.77	66.79	66.76
5'	67.07	67.05	67.04	67.09
6'	62.48	62.47	62.49	62.45

carbon	Compound		carbon	Compound			
	16a	16b		17a	18	19a	20
1	38.50	38.76	1	39.15	39.11	39.17	39.12
2	21.91	22.21	2	25.75	25.68	25.76	25.68
3	82.53	82.86	3	89.18	89.15	89.20	89.15
4	38.43	38.67	4	39.34	39.30	39.33	39.29
5	55.82	56.08	5	55.80	55.78	55.80	55.77
6	18.15	18.41	6	18.50	18.49	18.49	18.48
7	33.99	34.24	7	35.12	35.11	35.12	35.11
8	40.99	41.29	8	41.43	41.53	41.56	41.56
9	50.76	50.95	9	51.34	51.34	51.36	51.34
10	37.16	37.41	10	37.20	37.20	37.20	37.19
11	19.75	19.98	11	21.46	21.47	21.51	21.52
12	21.75	22.11	12	27.92	27.91	27.94	27.93
13	50.73	50.73	13	45.44	45.43	45.44	45.42
14	46.06	46.29	14	45.43	45.43	45.38	45.38
15	26.73	27.31	15	29.36	29.91	29.34	29.38
16	26.73	28.35	16	33.95	33.95	33.80	33.80
17	77.21	52.73	17	53.31	53.31	53.23	53.23
18	209.16	212.52	18	171.99	171.91	172.18	172.10
22	170.97	-	19	145.93	145.94	145.87	145.88
23	28.47	28.72	20	25.35	25.36	25.36	25.36
24	16.46	16.79	21	207.42	207.39	207.56	207.53
25	16.60	16.83	22	47.88	47.88	47.90	47.90
26	16.28	16.52	23	28.35	28.37	28.35	28.67
27	15.92	16.10	24	16.90	16.90	16.88	16.89
28	67.97	69.77	25	17.04	17.04	17.05	17.04
COOCH ₂ Ph	66.92	-	26	16.53	16.52	16.54	16.52
Ph: C 1	135.80	-	27	16.19	16.19	16.19	16.19
Ph: C 2, 4, 6	128.34	-	28	175.15	175.15	174.57	174.57
Ph: C 3, 5	128.50	-	29	20.25	20.26	20.20	20.20
AcO: CH ₃ 1	20.89	21.10	30	20.38	20.39	20.42	20.42
AcO: CH ₃ 2	20.81	21.03	COOCH ₂ CH ₃	-	-	61.27	61.27
AcO: CH ₃ 3	20.73	20.96	COOCH ₂ CH ₃	-	-	14.42	14.42
AcO: CH ₃ 4	20.73	20.93	COOCH ₃	52.71	52.71	-	-
AcO: CH ₃ 5	20.68	20.93	AcO: CH ₃ 1	21.30	21.11	21.31	21.11
AcO: CH ₃ 6	20.68	20.93	AcO: CH ₃ 2	21.11	-	21.11	-
AcO: C=O 1	170.47	170.86	AcO: C=O 1	170.61	170.12	170.61	170.12
AcO: C=O 2	170.41	170.86	AcO: C=O 2	170.51	-	170.51	-
AcO: C=O 3	170.34	170.75	1'	99.77	99.98	99.77	99.98
AcO: C=O 4	170.23	170.65	2'	36.13	42.01	36.13	42.01
AcO: C=O 5	170.10	170.51	3'	65.91	47.14	65.91	47.15
AcO: C=O 6	169.86	170.35	4'	75.36	77.28	75.36	77.28
1'	93.62	93.92	5'	69.47	67.72	69.47	67.72
2'	29.76	30.13	6'	17.63	18.03	17.64	18.03
3'	66.40	66.75					
4'	66.94	66.84					
5'	67.98	67.29					
6'	62.46	62.52					
1''	98.13	98.04					
2''	30.73	31.00					
3''	65.98	66.38					
4''	66.76	66.75					
5''	67.02	67.06					
6''	62.37	62.10					

carbon	Compound				
	21a	22	23	21b	24a
1	39.15	39.09	39.31	38.89	38.95
2	25.76	25.67	26.46	25.49	25.56
3	89.17	89.14	88.12	88.93	88.18
4	39.33	39.28	39.44	39.07	39.10
5	55.78	55.75	55.35	55.23	55.57
6	18.46	18.44	18.40	18.23	18.26
7	35.11	35.08	35.11	34.87	34.89
8	41.46	41.45	41.47	41.30	41.32
9	51.33	51.31	51.35	51.09	51.10
10	37.15	37.14	37.20	36.93	36.98
11	21.30	21.30	21.30	21.12	21.19
12	27.86	27.83	27.86	27.67	27.70
13	45.46	45.44	45.48	45.31	45.36
14	45.32	45.32	45.32	45.19	45.19
15	29.14	29.12	29.11	29.15	29.15
16	33.73	33.71	33.72	33.49	33.42
17	53.18	53.17	53.18	52.67	52.86
18	172.22	172.14	172.23	172.07	171.36
19	145.81	145.83	145.82	145.80	146.01
20	25.37	25.36	25.36	25.09	25.12
21	207.52	207.49	207.52	207.45	206.90
22	47.70	47.68	47.69	47.77	47.64
23	28.35	28.35	28.23	28.08	28.09
24	16.69	16.69	16.70	16.68	16.73
25	17.04	17.01	17.05	16.81	16.83
26	16.54	16.50	16.57	16.27	16.29
27	16.13	16.12	16.12	15.92	15.93
28	174.15	174.15	174.16	178.60	178.95
29	20.17	20.15	20.16	19.98	19.98
30	20.51	20.50	20.50	20.09	20.11
COOCH ₂ Ph	66.80	66.79	66.79	-	-
Ph: C 1	136.06	136.06	136.07	-	-
Ph: C 2, 4, 6	128.63	128.60	128.61	-	-
Ph: C 3, 5	128.85	128.84	128.85	-	-
AcO: CH ₃ 1	21.32	21.11	21.34	21.05	21.21
AcO: CH ₃ 2	21.13	-	-	20.85	-
AcO: C=O 1	170.61	170.12	170.81	170.42	170.36
AcO: C=O 2	170.51	-	-	170.32	-
1'	99.77	99.98	97.01	99.50	99.12
2'	36.14	42.00	129.42	35.85	29.75
3'	65.92	47.14	128.26	65.65	24.25
4'	75.37	77.28	71.32	75.09	73.83
5'	69.48	67.71	64.70	69.24	66.62
6'	17.65	18.03	18.18	17.36	17.73

carbon	Compound			
	27a	28a	29a	30a
1	38.53	38.63	38.54	38.72
2	27.42	22.71	22.19	22.79
3	82.83	83.30	82.83	83.31
4	38.41	38.35	38.42	38.36
5	55.81	55.88	55.81	55.96
6	18.47	18.24	18.18	18.32
7	34.85	34.93	34.90	35.01
8	41.29	41.29	41.32	41.34
9	51.12	51.10	51.12	51.20
10	37.12	37.15	37.13	37.16
11	21.47	21.21	21.24	21.33
12	27.65	27.65	27.67	27.75
13	45.15	45.16	45.14	45.22
14	45.15	45.14	45.11	45.11
15	29.37	29.10	29.08	26.16
16	33.69	33.69	33.54	33.62
17	53.04	53.04	52.97	52.98
18	171.7	171.69	171.90	171.87
19	145.65	145.65	145.60	145.61
20	25.36	25.09	25.09	25.17
21	207.15	207.15	207.30	207.27
22	47.61	47.61	47.63	47.72
23	28.51	28.19	28.52	28.29
24	16.32	16.24	16.31	16.24
25	16.75	16.74	16.74	16.73
26	16.64	16.45	16.62	16.72
27	15.89	15.86	15.87	15.83
28	174.88	174.89	174.31	174.31
29	19.99	20.00	19.94	19.94
30	20.39	20.13	20.15	20.17
COOCH ₂ CH ₃	-	-	61.01	61.08
COOCH ₂ CH ₃	-	-	14.15	14.23
COOCH ₃	52.45	52.44	-	-
AcO: CH ₃ 1	21.18	20.87	21.24	20.99
AcO: CH ₃ 2	21.45	20.62	21.20	20.70
AcO: CH ₃ 3	20.92	20.62	20.93	20.60
AcO: CH ₃ 4	20.87	20.62	20.63	20.60
AcO: CH ₃ 5	20.87	20.51	20.60	20.42
AcO: CH ₃ 6	20.52	-	20.54	-
AcO: C=O 1	170.54	170.74	170.54	170.73
AcO: C=O 2	170.35	170.34	170.35	170.33
AcO: C=O 3	170.18	170.21	170.18	170.20
AcO: C=O 4	170.12	170.08	170.12	170.07
AcO: C=O 5	169.66	169.50	169.66	169.49
AcO: C=O 6	169.24	-	169.24	-
1'	93.12	91.20	93.11	91.20
2'	34.85	130.82	34.84	130.83
3'	69.88	127.84	69.88	127.86
4'	77.89	73.64	77.87	73.73
5'	68.67	67.55	68.66	67.63
6'	62.90	63.13	62.90	63.21
1''	101.32	102.50	101.31	102.51
2''	69.21	68.82	69.21	68.90
3''	71.09	70.86	71.09	70.94
4''	66.72	66.83	66.71	66.80
5''	70.54	70.70	70.54	70.78
6''	60.86	61.21	60.86	61.29

carbon	Compound		
	31a	32	31b
1	38.51	38.44	38.54
2	22.20	22.07	22.15
3	82.84	82.49	82.77
4	38.39	38.42	38.41
5	55.78	55.71	55.81
6	18.13	18.12	18.22
7	34.85	34.84	34.83
8	41.21	41.20	41.32
9	51.08	51.07	51.15
10	37.07	37.06	37.13
11	21.02	21.02	21.34
12	27.56	27.54	27.68
13	45.16	45.13	45.25
14	45.05	45.04	45.20
15	28.85	28.85	29.68
16	33.45	33.44	33.58
17	52.90	52.89	54.00
18	171.96	171.84	171.51
19	145.52	145.55	145.24
20	25.08	25.09	25.08
21	207.26	207.22	208.47
22	47.41	47.40	47.85
23	28.50	28.50	28.52
24	16.42	16.34	16.32
25	16.71	16.72	16.78
26	16.30	16.42	16.78
27	15.80	15.81	15.89
28	173.86	173.86	173.45
29	19.88	19.88	20.04
30	20.22	20.23	20.11
COOCH ₂ Ph	66.52	66.51	-
Ph: C 1	135.52	135.78	-
Ph: C 2, 4, 6	128.36	128.35	-
Ph: C 3, 5	128.57	128.57	-
AcO: CH ₃ 1	21.20	20.92	21.07
AcO: CH ₃ 2	21.60	20.77	21.00
AcO: CH ₃ 3	20.80	20.71	20.80
AcO: CH ₃ 4	20.70	20.66	20.70
AcO: CH ₃ 5	20.62	20.52	20.62
AcO: CH ₃ 6	20.51	-	20.30
AcO: C=O 1	170.53	170.58	170.58
AcO: C=O 2	170.35	170.31	170.38
AcO: C=O 3	170.18	170.25	170.21
AcO: C=O 4	170.12	170.07	170.03
AcO: C=O 5	169.65	169.41	169.18
AcO: C=O 6	169.22	-	169.25
1'	93.12	93.06	93.05
2'	34.85	40.82	34.83
3'	69.81	46.13	69.81
4'	77.86	80.07	77.89
5'	68.66	69.85	68.61
6'	62.90	63.09	62.91
1"	101.31	99.78	101.32
2"	69.21	69.03	69.18
3"	71.09	71.05	71.03
4"	66.72	66.80	66.72
5"	70.54	70.74	70.38
6"	60.85	60.95	60.87

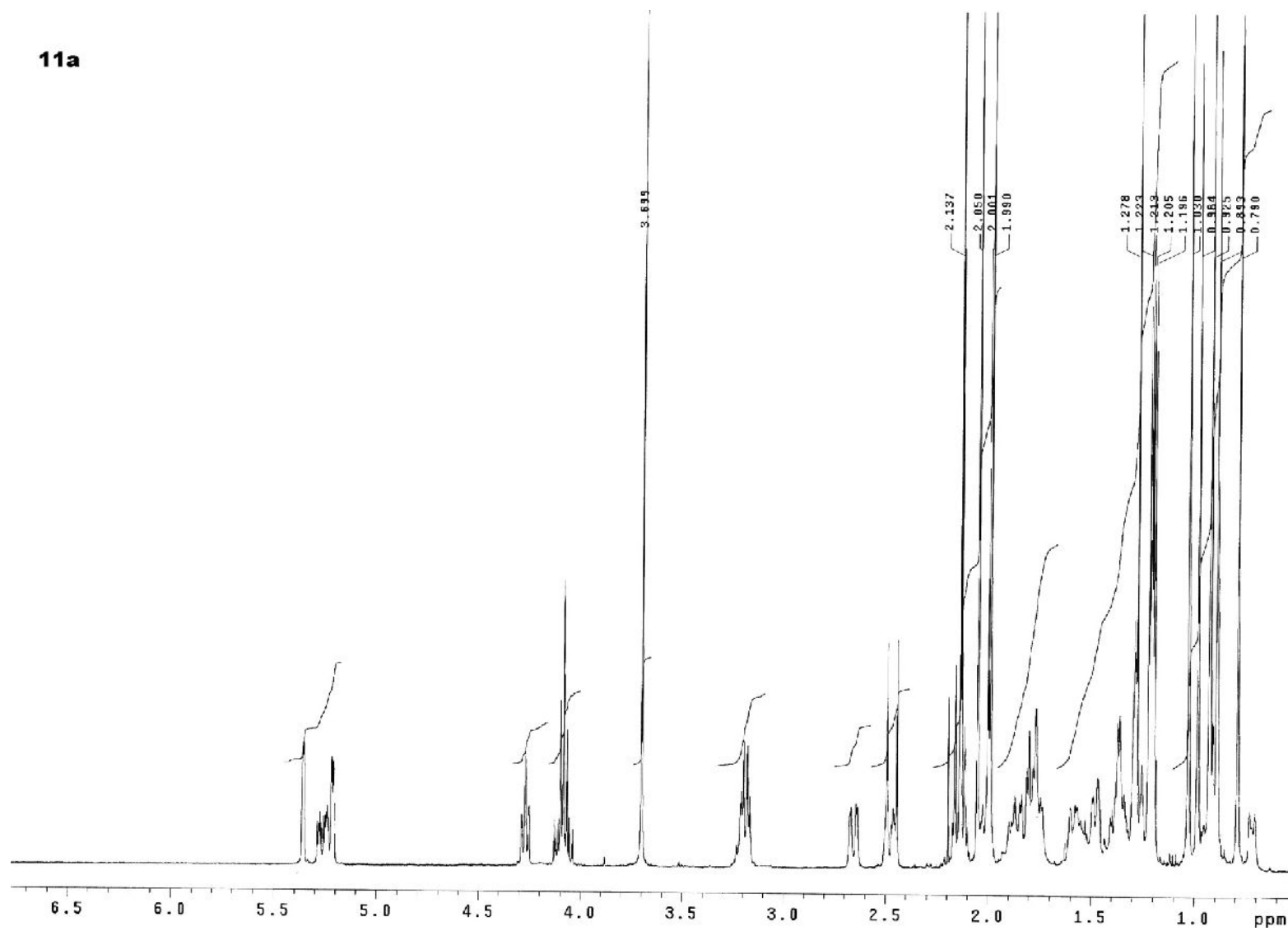
carbon	Compound			
	12b	13c	14b	16c
1	38.28	38.34	38.33	38.30
2	21.57	21.63	21.59	21.54
3	81.45	81.53	81.38	81.36
4	34.67	38.28	38.27	38.22
5	55.39	55.46	55.41	55.48
6	17.95	18.02	17.99	17.97
7	34.67	34.76	34.50	34.02
8	41.15	41.20	41.44	40.77
9	50.88	50.97	50.78	50.59
10	36.95	37.02	37.02	36.98
11	21.02	21.04	20.85	19.49
12	27.45	27.52	27.81*	21.54
13	45.14	45.14	46.15	49.72
14	45.05	45.15	45.49	47.00
15	28.85	28.97	28.22*	26.85
16	33.30	33.42	27.32*	30.42
17	52.93	52.87	58.41	52.37
18	172.92	173.33	168.09	214.35
19	145.46	145.34	150.54	-
20	24.84	24.88	25.72	-
21	208.14	208.38	194.26	-
22	47.41	47.75	189.27	-
23	28.16	28.25	28.24	28.14
24	16.52	16.61	16.53	15.69
25	16.40	16.45	16.61	16.40
26	16.06	16.14	16.15	16.03
27	15.68	15.75	15.96	15.58
28	174.30	176.50	171.59	65.91
29	19.82	19.83	19.50	-
30	19.60	19.78	19.58	-
COOCH ₂ CH ₃	61.03	-	-	-
COOCH ₂ CH ₃	13.84	-	-	-
COOCH ₃	-	-	53.29	-
1'	93.30	93.35	93.35	93.85
2'	32.88	33.00	32.97	32.34
3'	65.30	65.37	65.35	65.30
4'	68.64	68.95	68.89	68.68
5'	69.95	69.84	69.91	69.71
6'	62.21	62.57	62.54	62.31
1''	-	-	-	97.85
2''	-	-	-	32.90
3''	-	-	-	65.10
4''	-	-	-	68.48
5''	-	-	-	69.94
6''	-	-	-	62.31

carbon	Compound					
	17b	25	19b	26	21c	24b
1	38.85	38.92	38.85	38.95	38.76	38.83
2	27.19	25.54	25.47	25.56	25.38	25.50
3	78.87	88.70	88.52	88.71	88.43	88.01
4	38.80	38.99	38.99	39.02	38.89	39.04
5	55.32	55.51	55.47	55.53	55.37	55.29
6	18.20	18.14	18.17	18.15	18.09	18.18
7	34.87	34.81	34.81	34.84	34.75	34.85
8	41.25	41.21	41.25	41.26	41.15	41.25
9	51.09	51.02	51.04	51.06	50.98	51.08
10	37.18	36.87	36.89	36.90	36.79	36.91
11	21.16	21.10	21.18	21.16	21.09	21.12
12	27.64	27.58	27.61	27.62	27.54	27.62
13	45.22	45.20	45.20	45.20	45.18	45.19
14	45.19	45.14	45.11	45.11	45.16	45.18
15	29.09	29.00	29.01	29.00	29.07	29.07
16	33.66	33.60	33.47	33.47	33.66	33.51
17	53.07	53.04	52.99	52.97	53.41	52.87
18	171.96	172.30	172.38	172.39	171.59	172.86
19	145.66	145.59	145.58	145.56	145.01	145.47
20	25.06	24.98	25.02	25.01	24.86	24.99
21	207.38	207.63	207.71	207.67	209.09	208.01
22	47.59	47.52	47.57	47.57	48.05	47.81
23	27.92	27.94	28.01	27.98	27.86	27.84
24	16.23	16.19	16.16	16.23	16.00	16.19
25	16.72	16.67	16.72	16.70	16.63	16.74
26	16.63	16.54	16.56	16.55	16.44	16.59
27	15.92	15.84	15.87	15.85	15.76	15.86
28	174.90	174.88	174.33	174.32	176.51	176.59
29	19.96	19.86	19.85	19.84	19.82	19.91
30	20.02	19.98	20.07	20.05	19.82	19.98
1'	98.32	96.42	100.12	96.46	100.03	99.06
2'	37.55	29.53	38.10	29.56	37.93	30.10
3'	69.02	48.68	69.05	48.66	68.72	25.50
4'	77.90	53.39	78.01	53.41	77.73	71.96
5'	67.35	65.13	67.55	65.12	67.58	69.49
6'	17.65	17.98	17.44	18.04	17.26	17.63

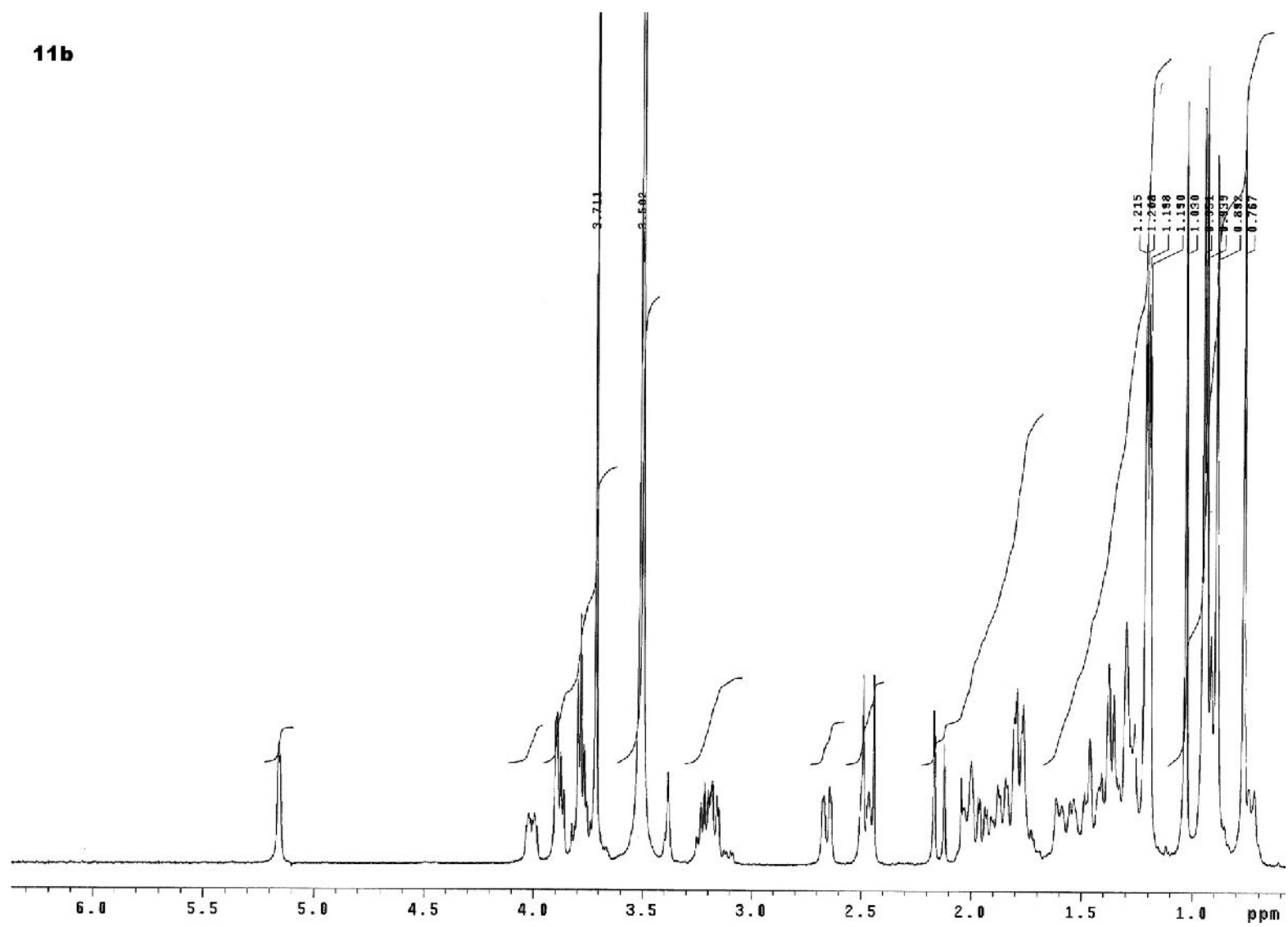
carbon	Compound				
	27b	28b	29b	30b	31c
1	38.71	39.09	38.53	39.01	38.28
2	22.03	27.15	22.01	27.26	22.54
3	82.43	78.87	82.66	78.91	81.71
4	38.58	38.99	38.42	38.82	38.28
5	55.86	55.55	55.77	55.58	55.52
6	18.39	18.40	18.15	18.17	18.06
7	35.12	35.08	34.91	35.02	34.79
8	41.46	41.47	41.32	41.35	41.22
9	51.31	51.29	51.17	51.14	51.01
10	37.56	37.37	37.25	37.40	37.04
11	21.41	21.35	21.25	21.34	21.08
12	27.86	27.82	27.68	27.73	27.58
13	45.53	45.52	45.13	45.26	45.16
14	45.46	45.46	45.13	45.15	45.16
15	29.31	29.27	29.11	29.23	29.55
16	33.90	33.85	33.54	33.66	34.79
17	52.73	53.36	52.98	53.06	52.87
18	172.81	172.87	171.95	172.12	172.13
19	145.89	145.88	145.62	145.82	145.37
20	25.28	25.23	25.11	25.14	24.93
21	208.16	208.18	207.31	207.35	208.63
22	47.81	47.77	47.64	47.59	48.27
23	28.62	28.05	28.53	28.28	28.28
24	16.49	16.11	16.32	16.42	16.14
25	16.96	16.88	16.73	16.81	16.52
26	16.86	16.80	16.64	16.53	16.23
27	16.14	15.56	15.86	15.47	15.78
28	175.20	175.20	174.35	174.67	176.50
29	20.14	20.09	19.95	19.98	19.82
30	20.27	20.21	20.16	20.21	19.82
COOCH ₂ CH ₃	-	-	61.01	61.03	-
COOCH ₂ CH ₃	-	-	14.13	14.17	-
COOCH ₃	53.77	52.72	-	-	-
1'	93.38	95.60	93.49	95.74	94.00
2'	37.56	132.96	37.50	132.63	37.04
3'	67.63	126.33	67.67	126.12	67.30
4'	82.43	72.99	82.66	73.06	82.10
5'	71.23	70.34	71.22	70.39	71.23
6'	61.96	62.10	62.03	62.05	61.59
1''	103.82	104.13	103.84	104.09	103.43
2''	71.44	71.49	71.41	71.67	71.09
3''	73.77	73.66	73.70	73.59	73.44
4''	69.41	69.12	69.43	69.15	69.10
5''	75.56	74.89	75.56	74.91	75.58
6''	61.88	61.74	61.92	61.69	61.63

2) Copies of ^1H NMR spectra of new compounds.

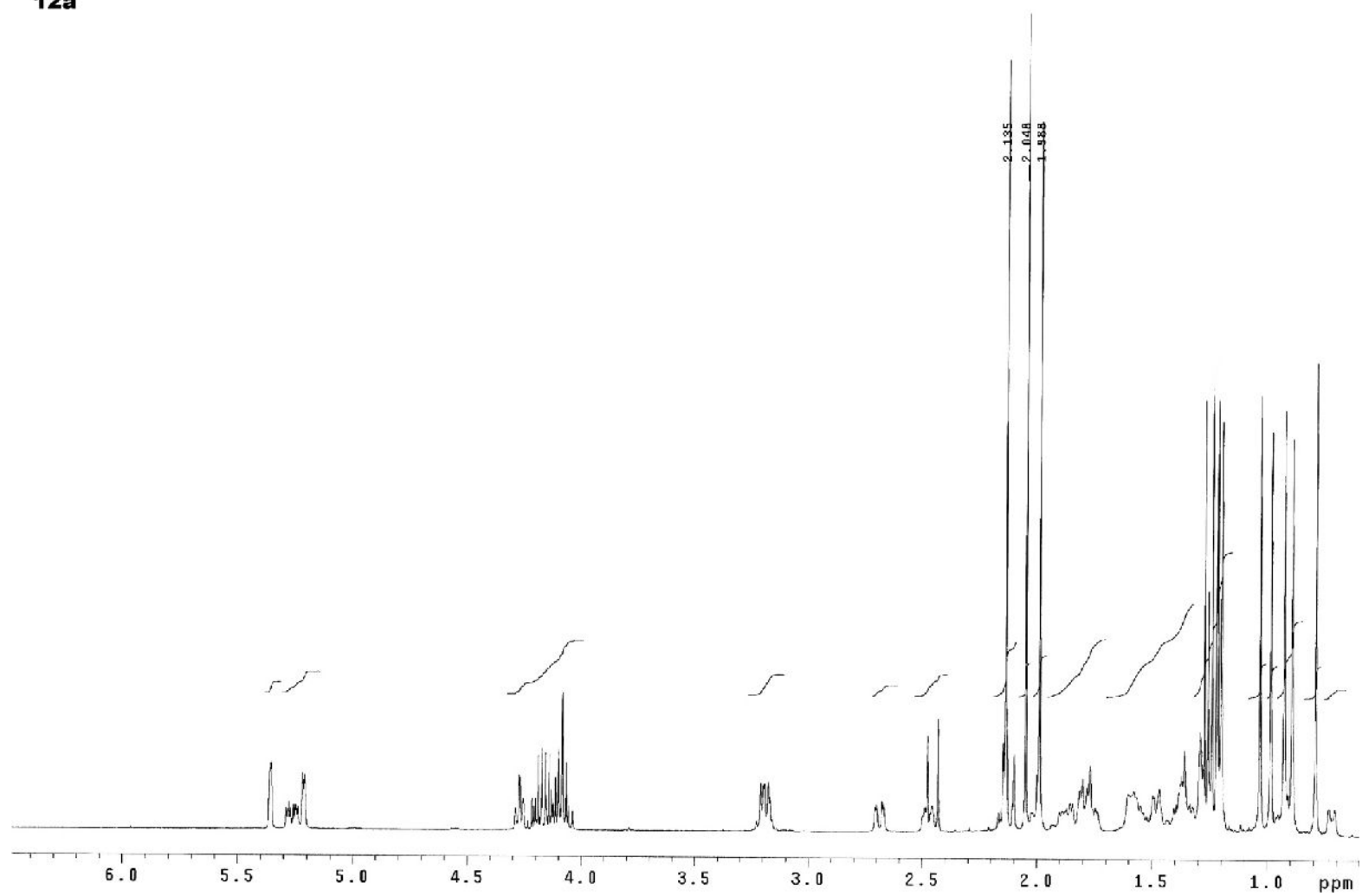
11a



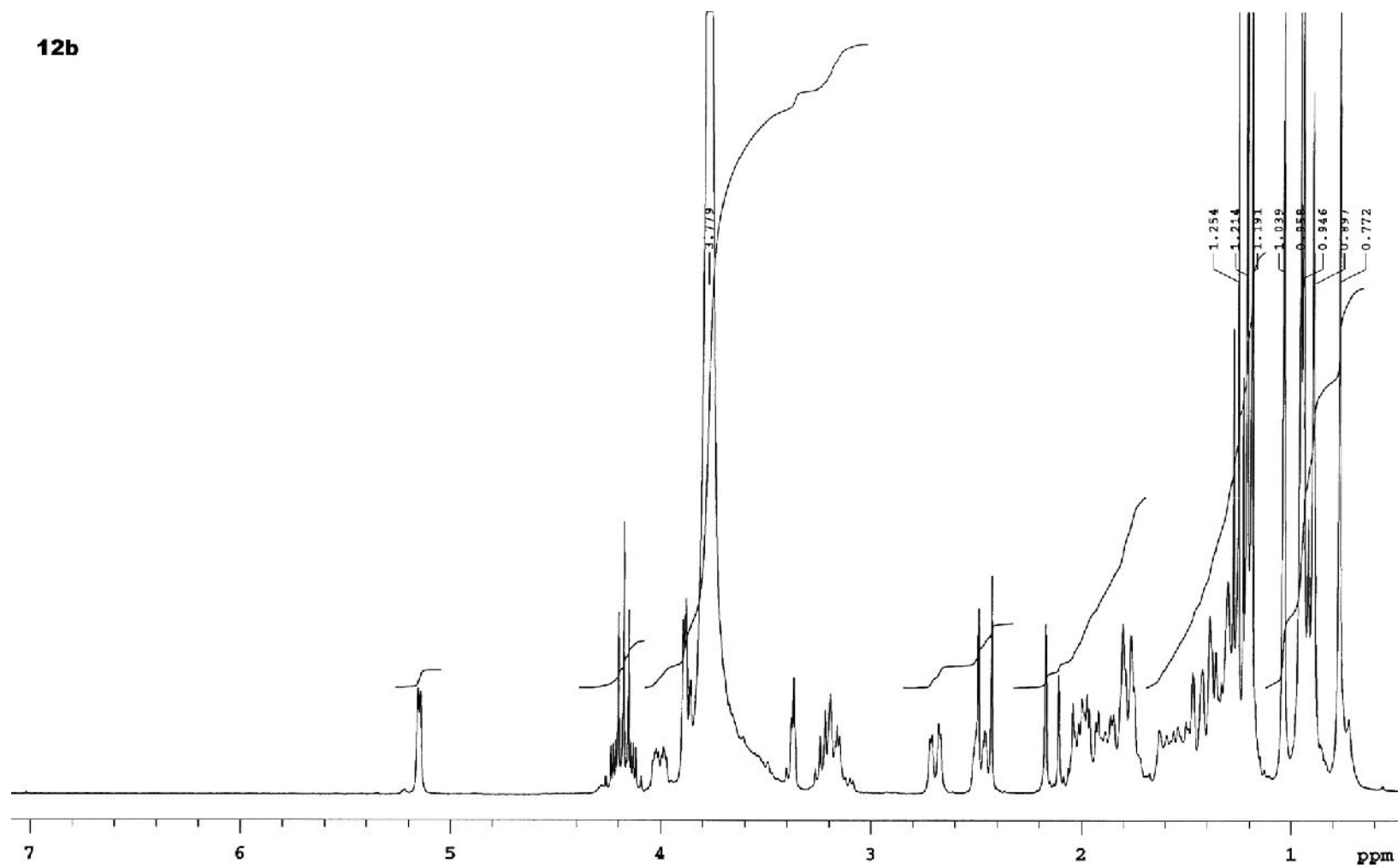
11b



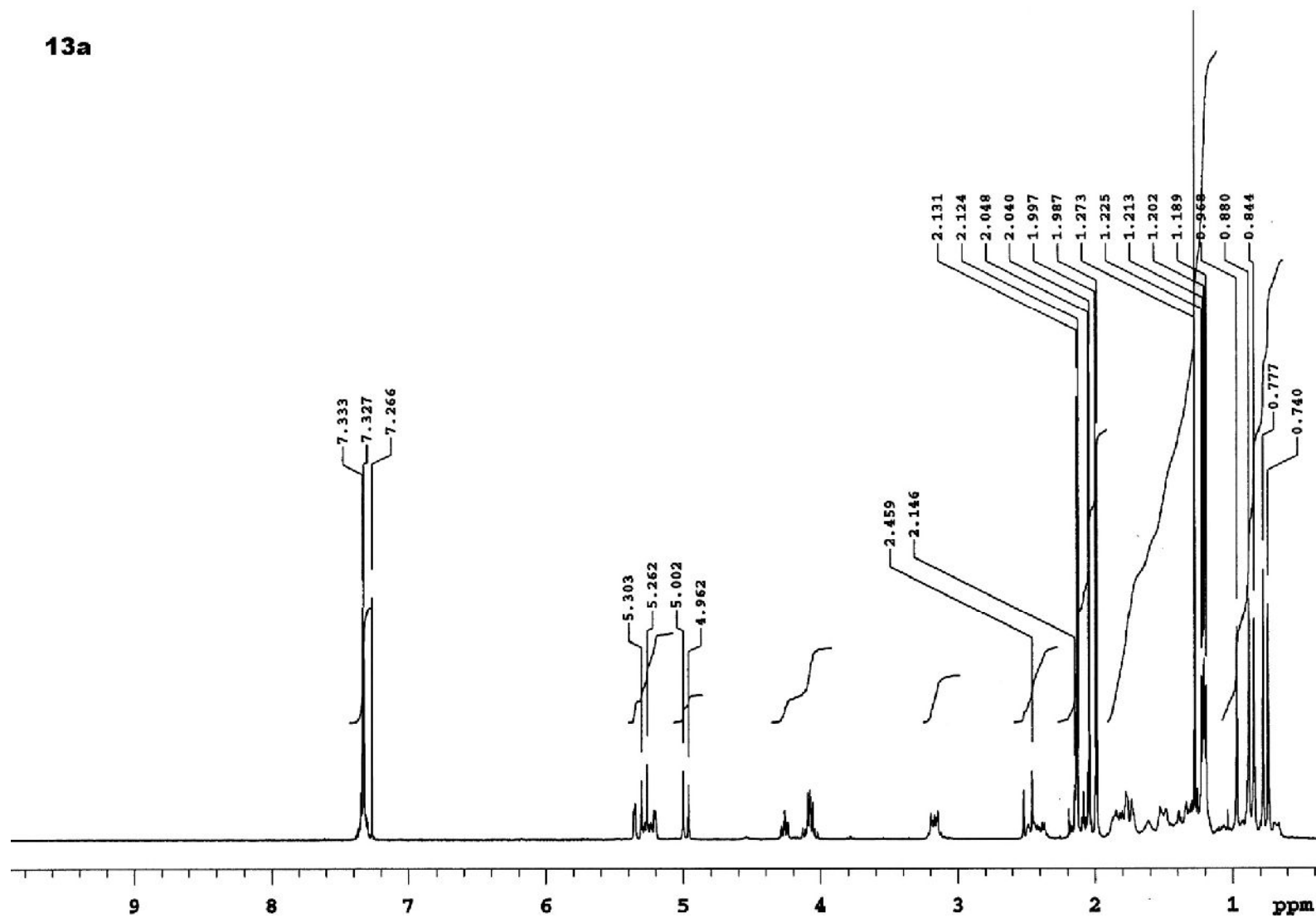
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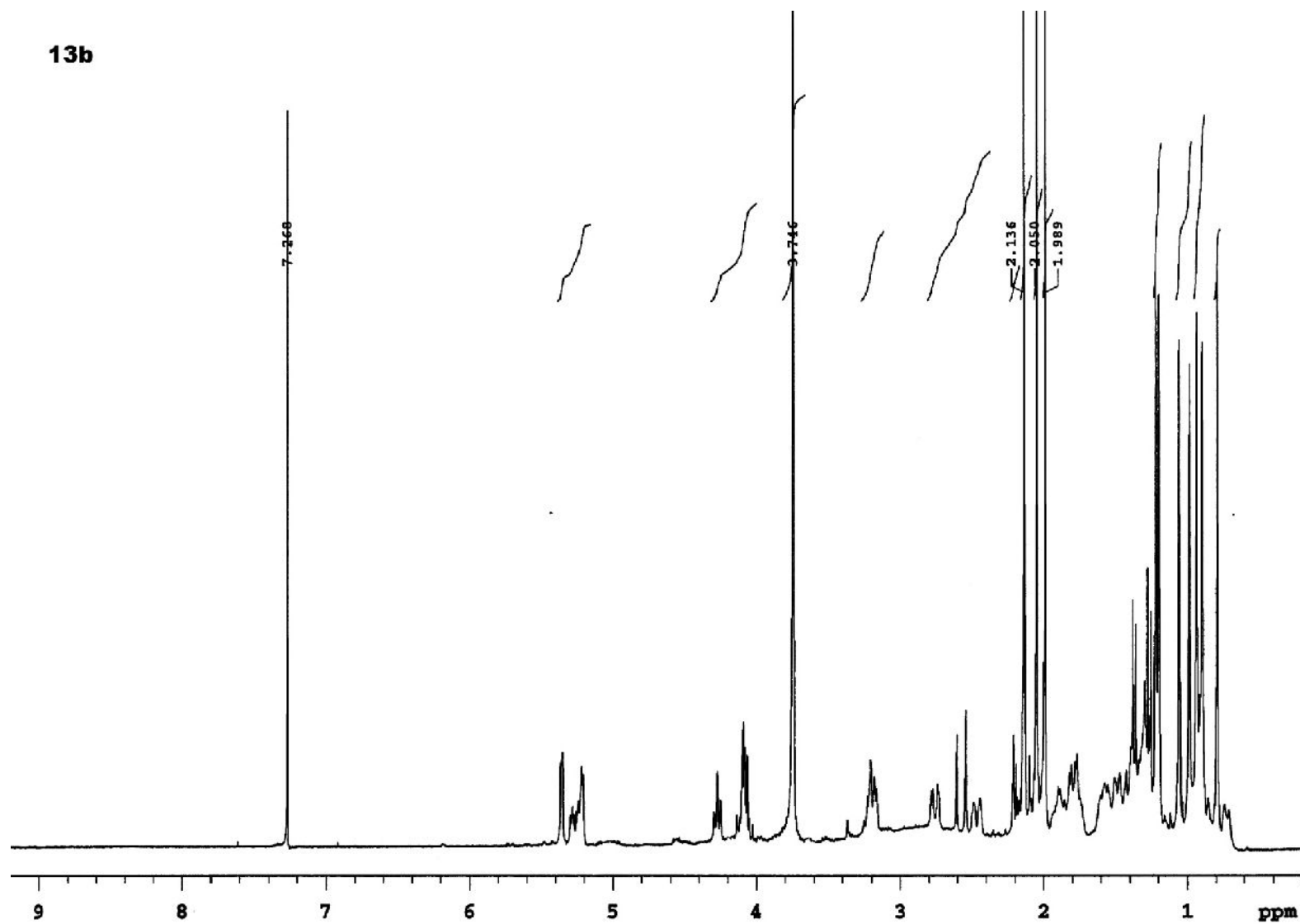
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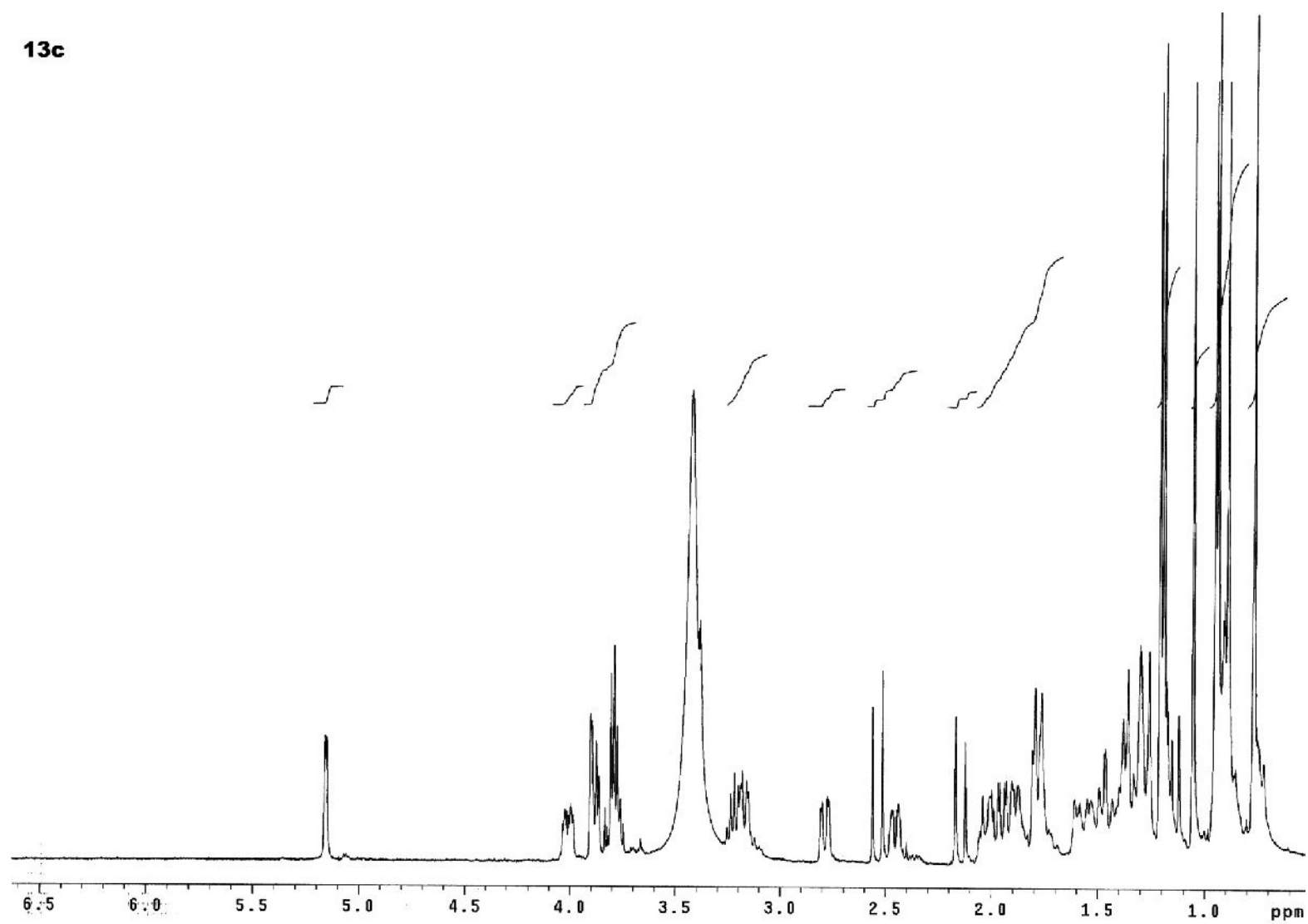
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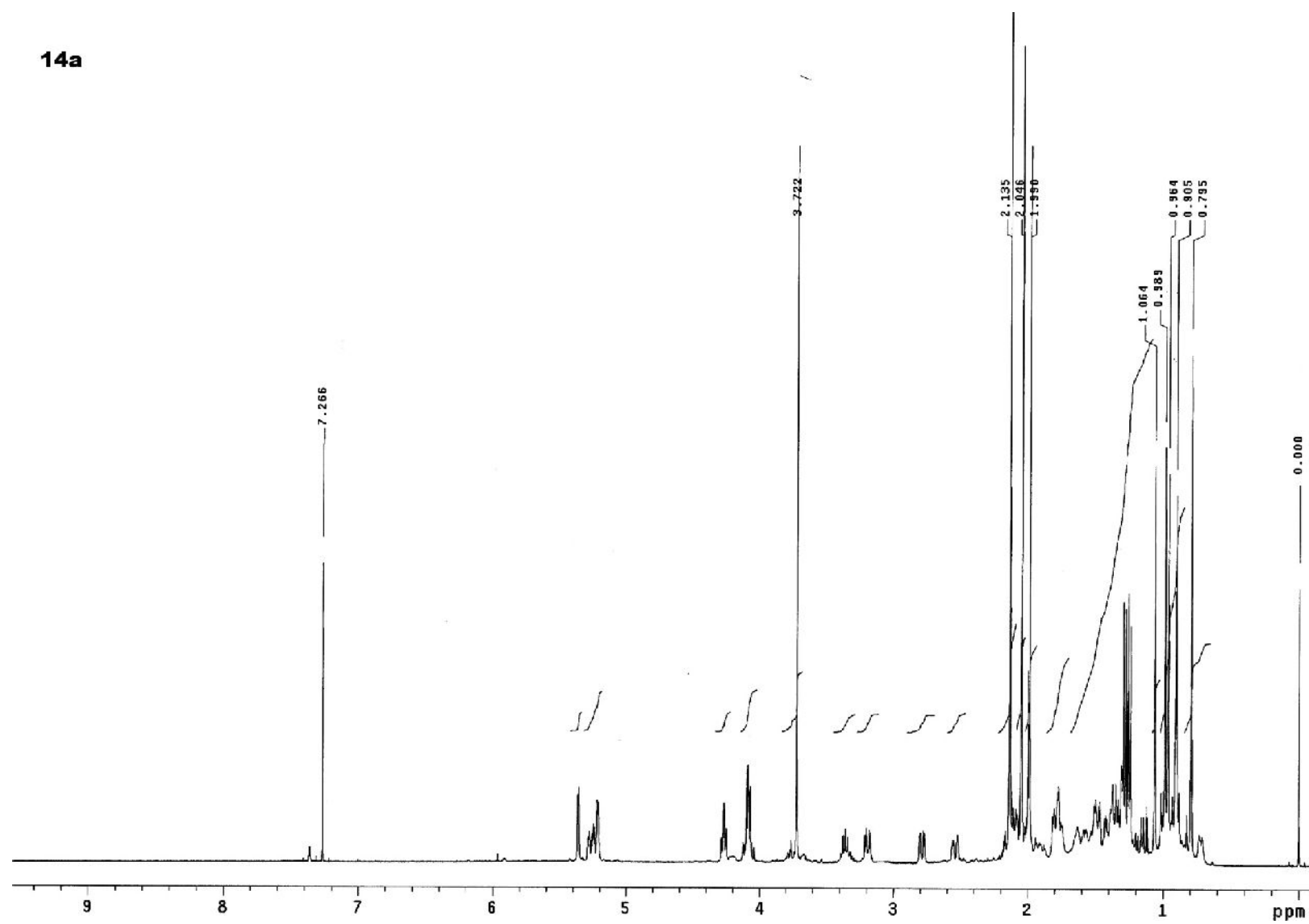
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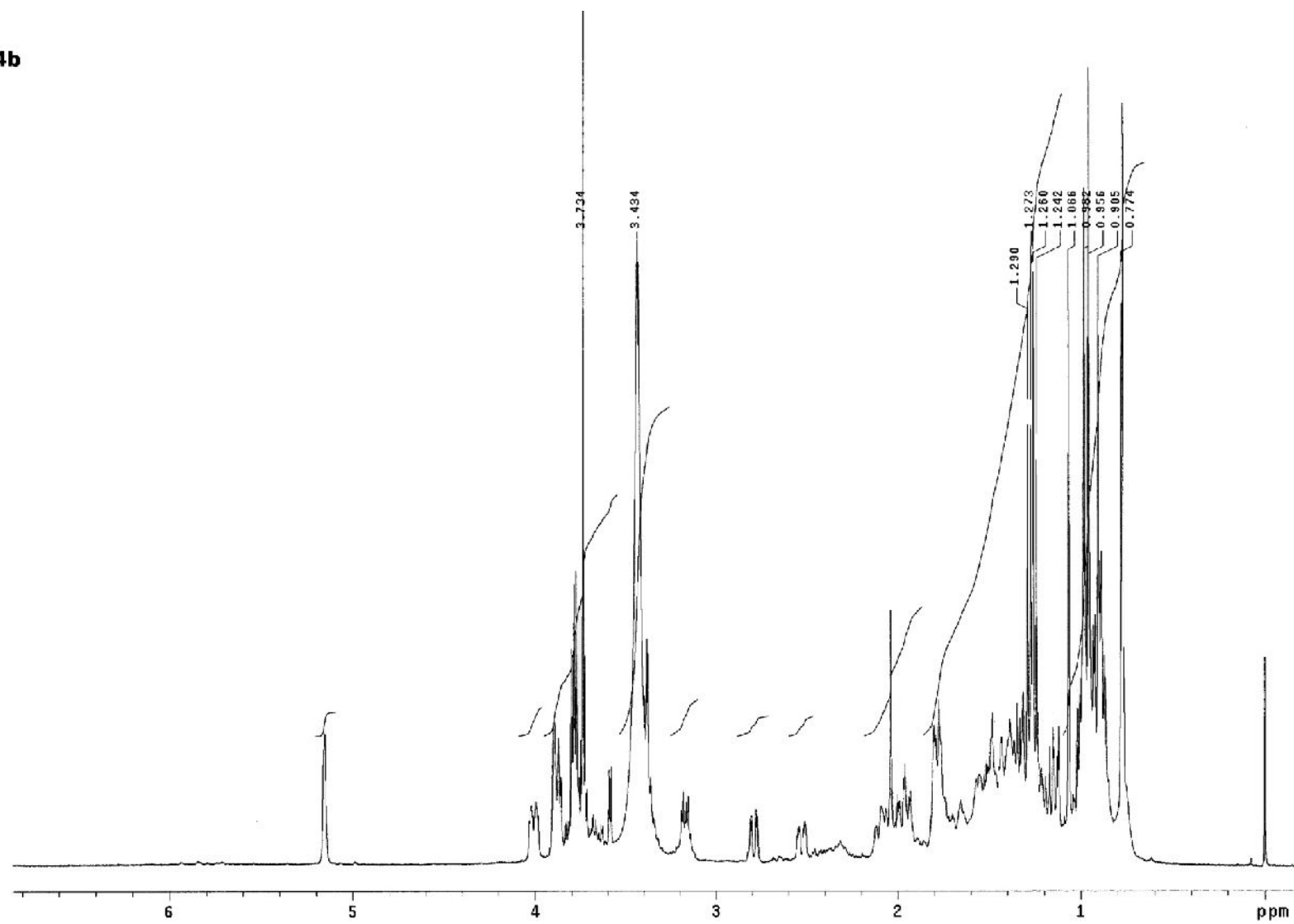
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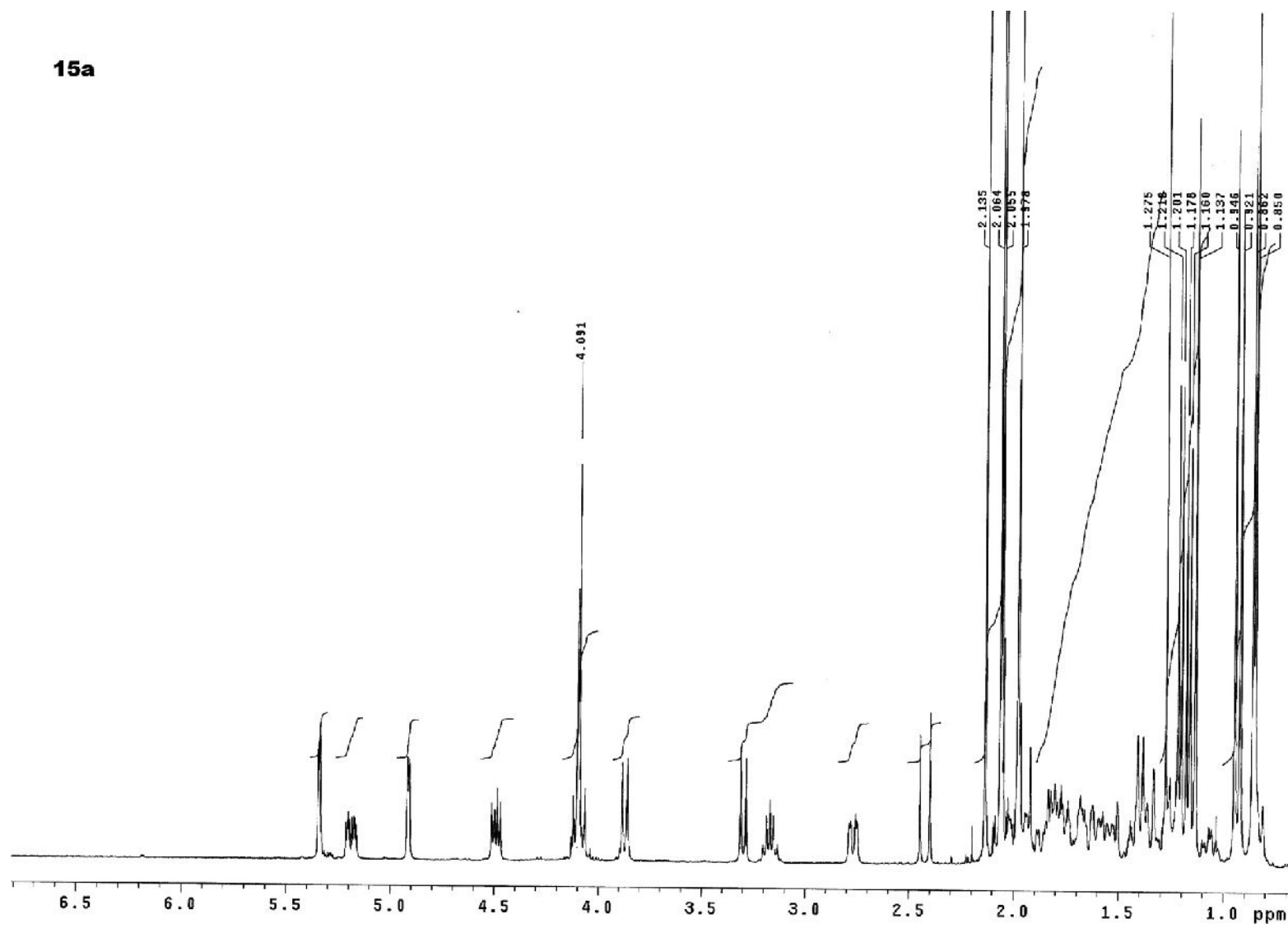
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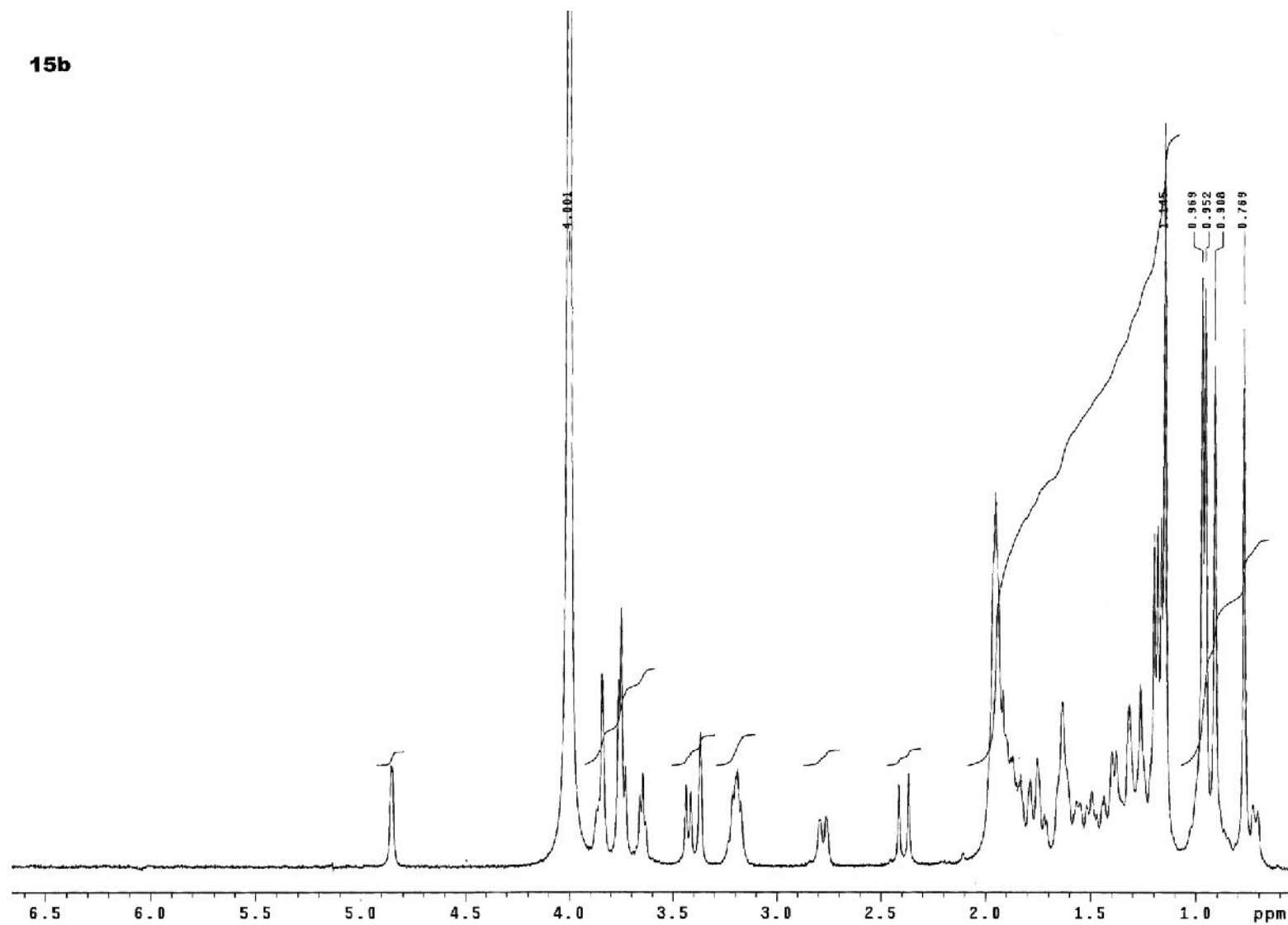
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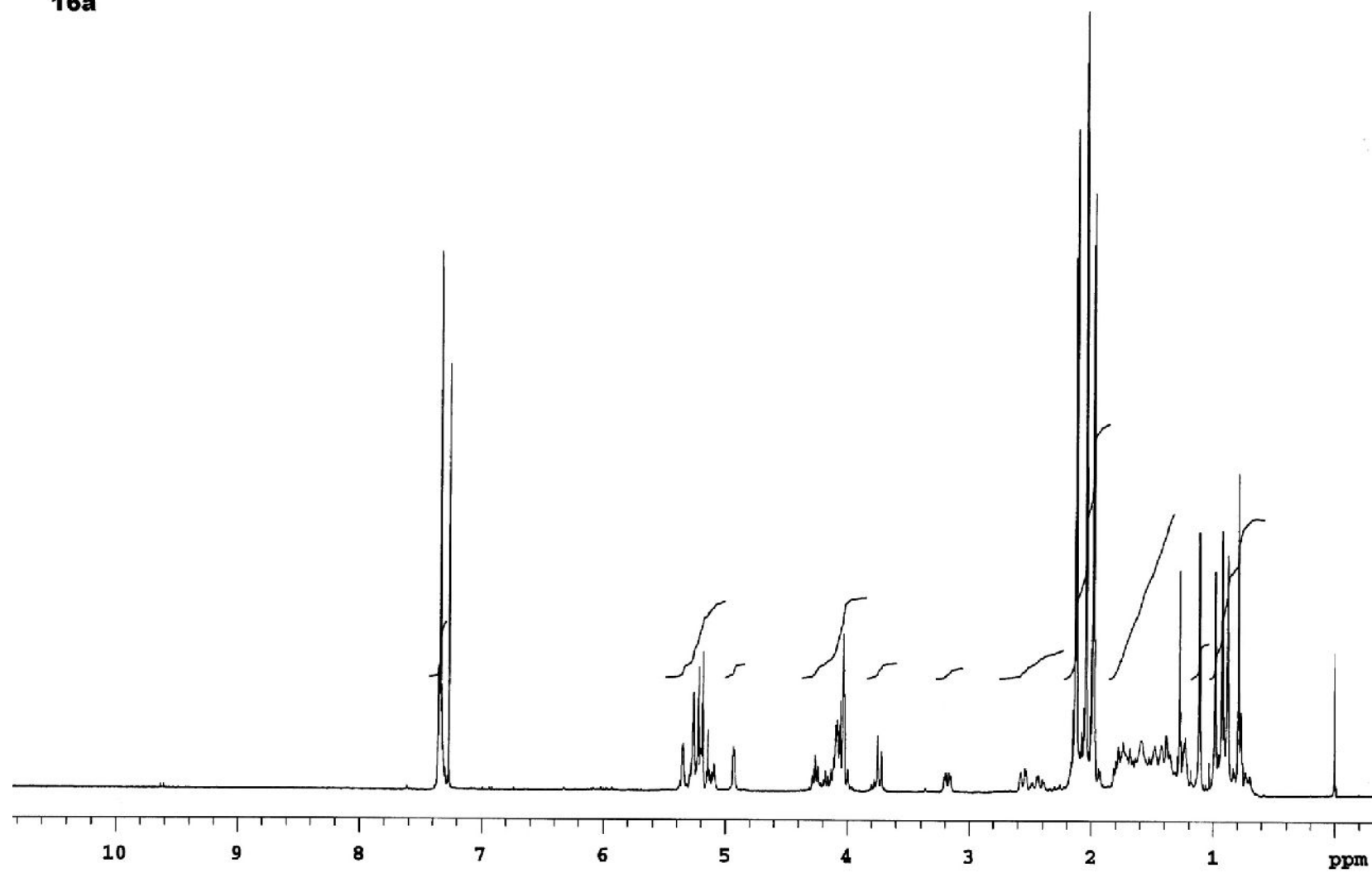
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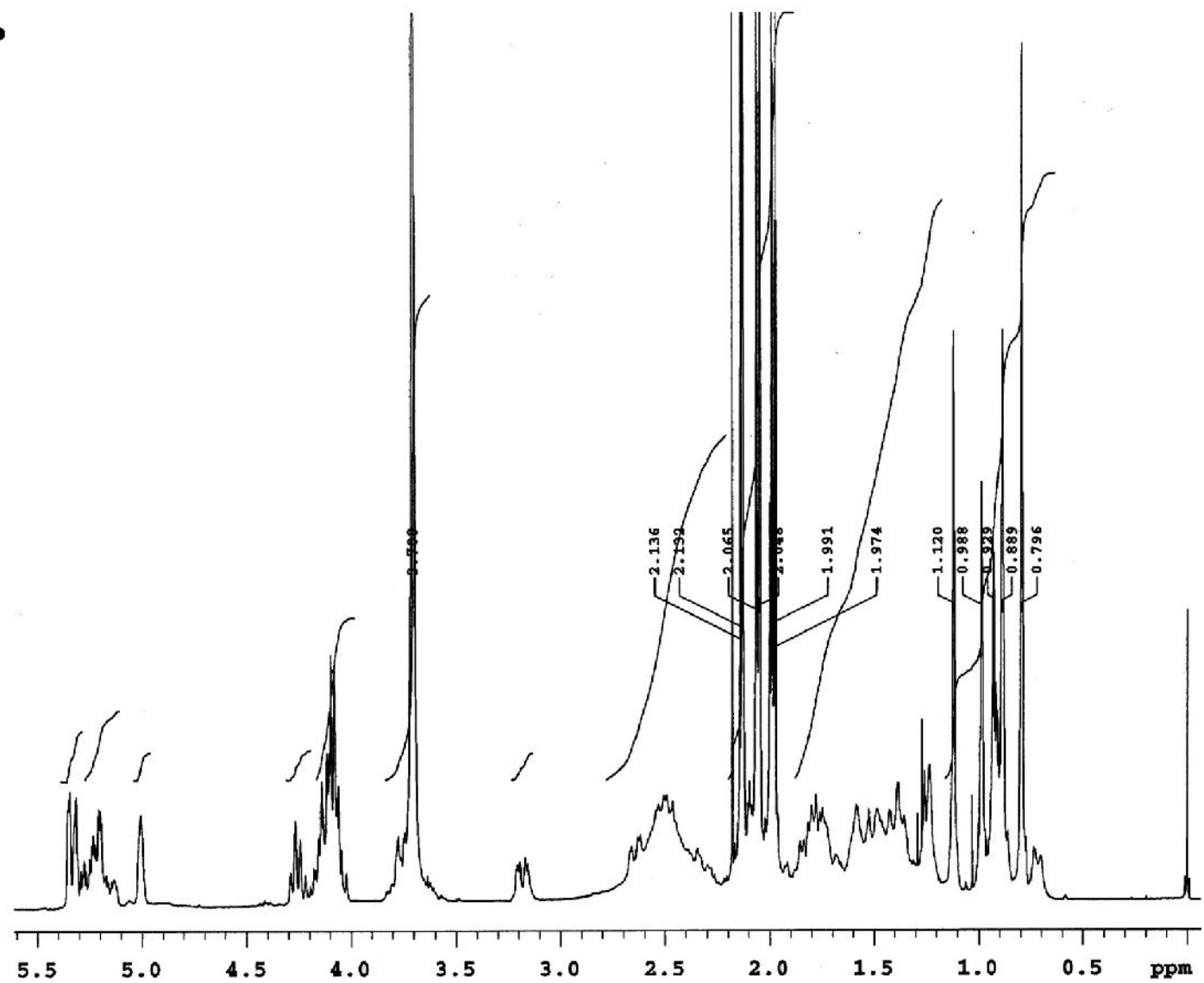
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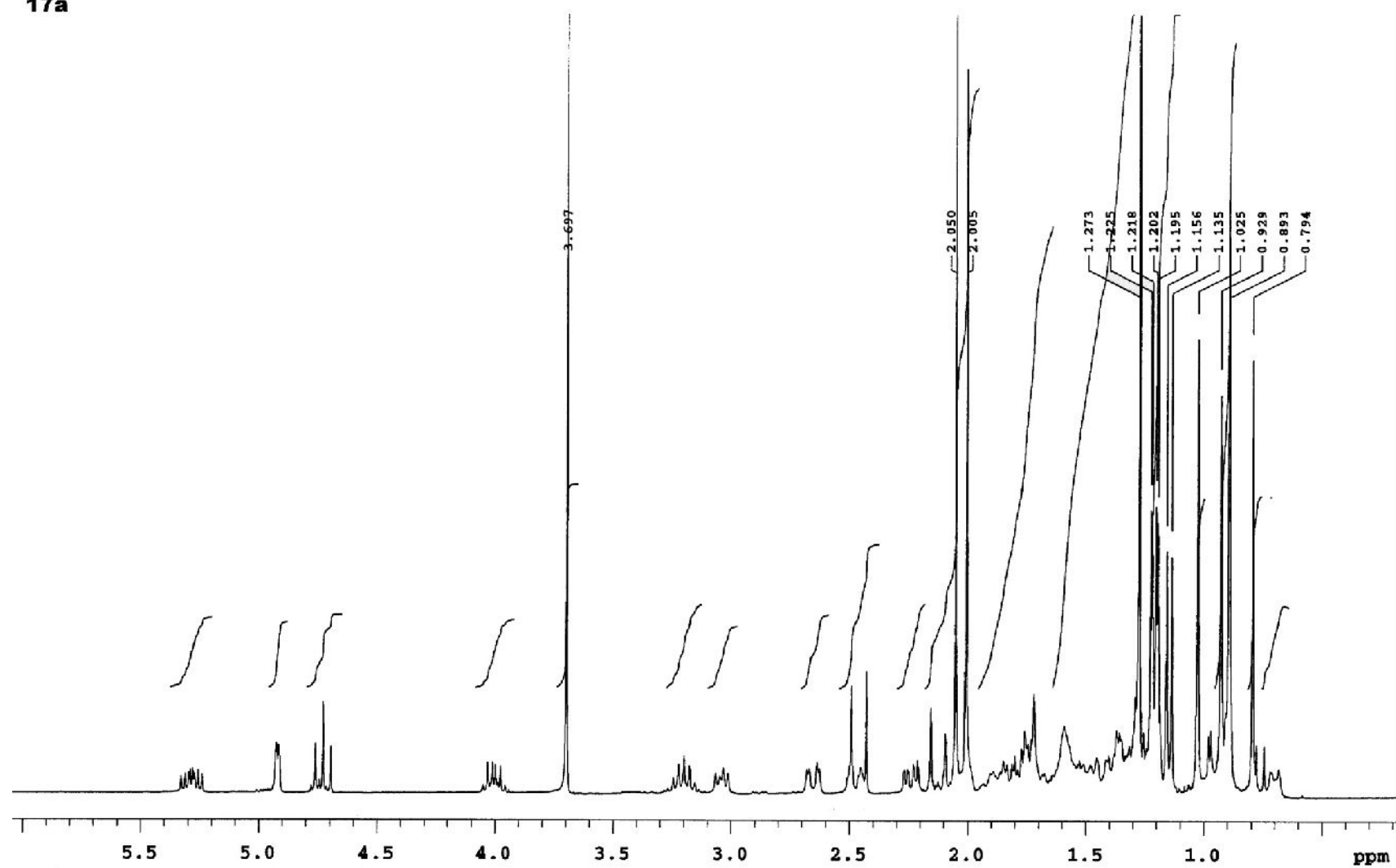
16a



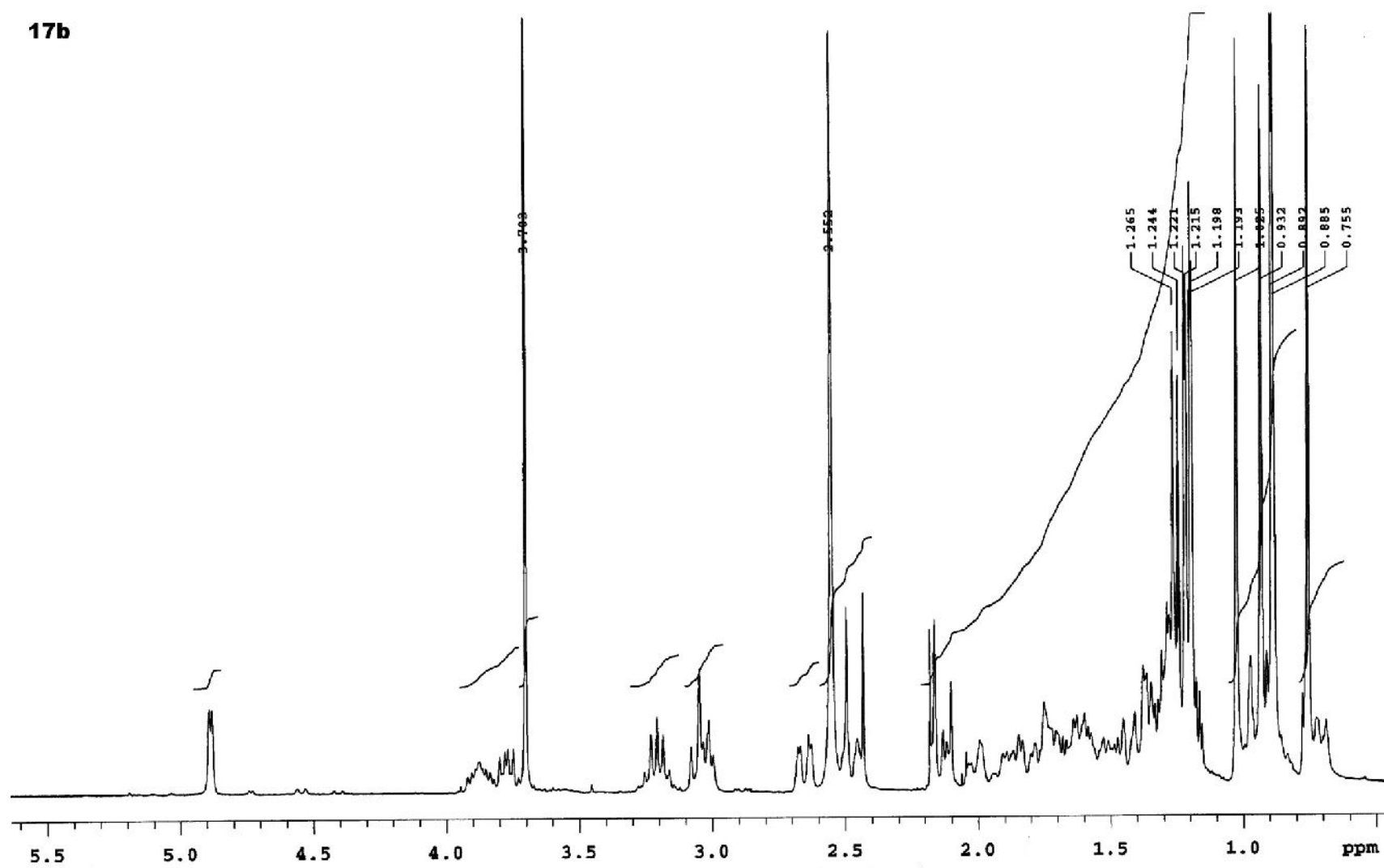
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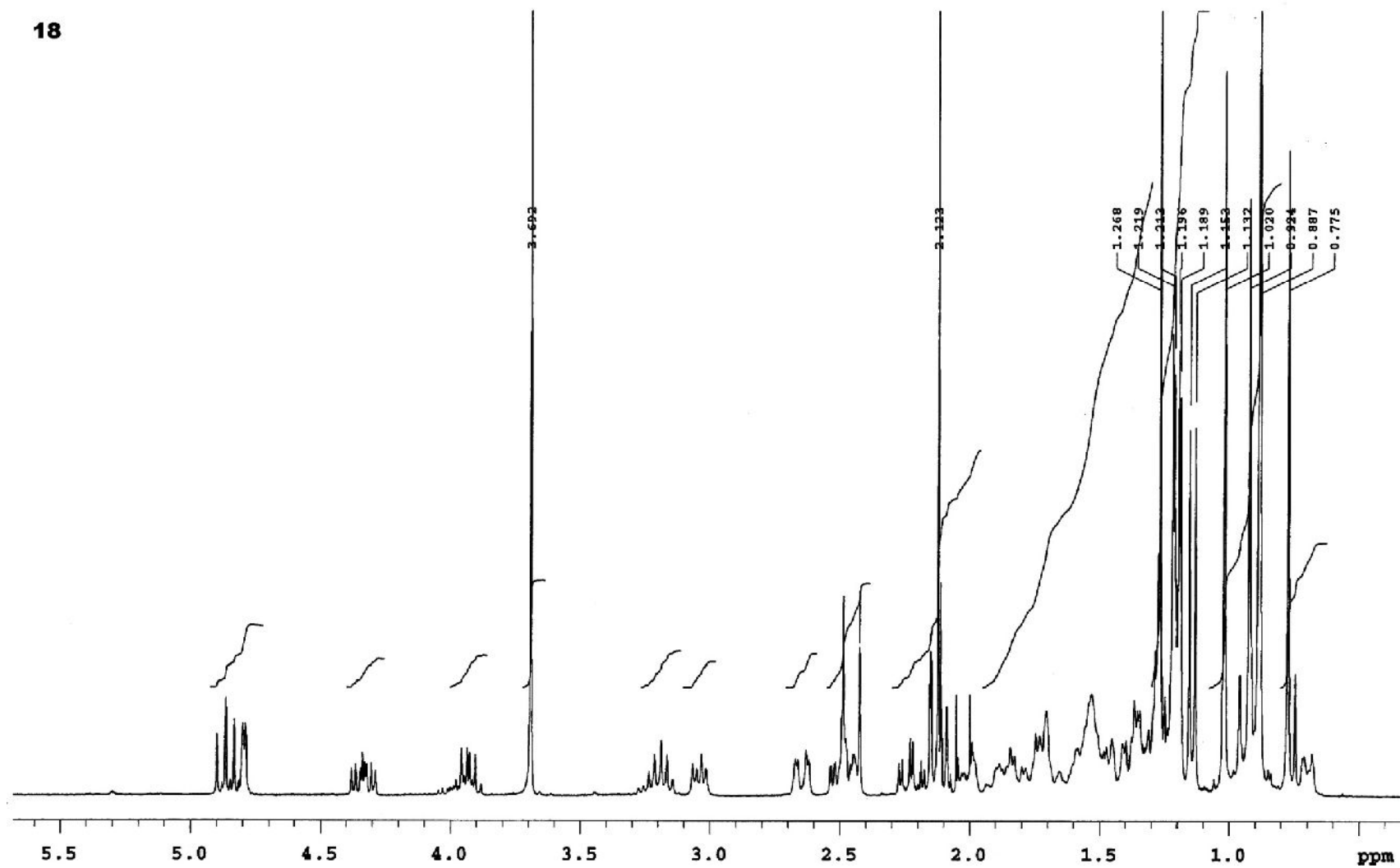
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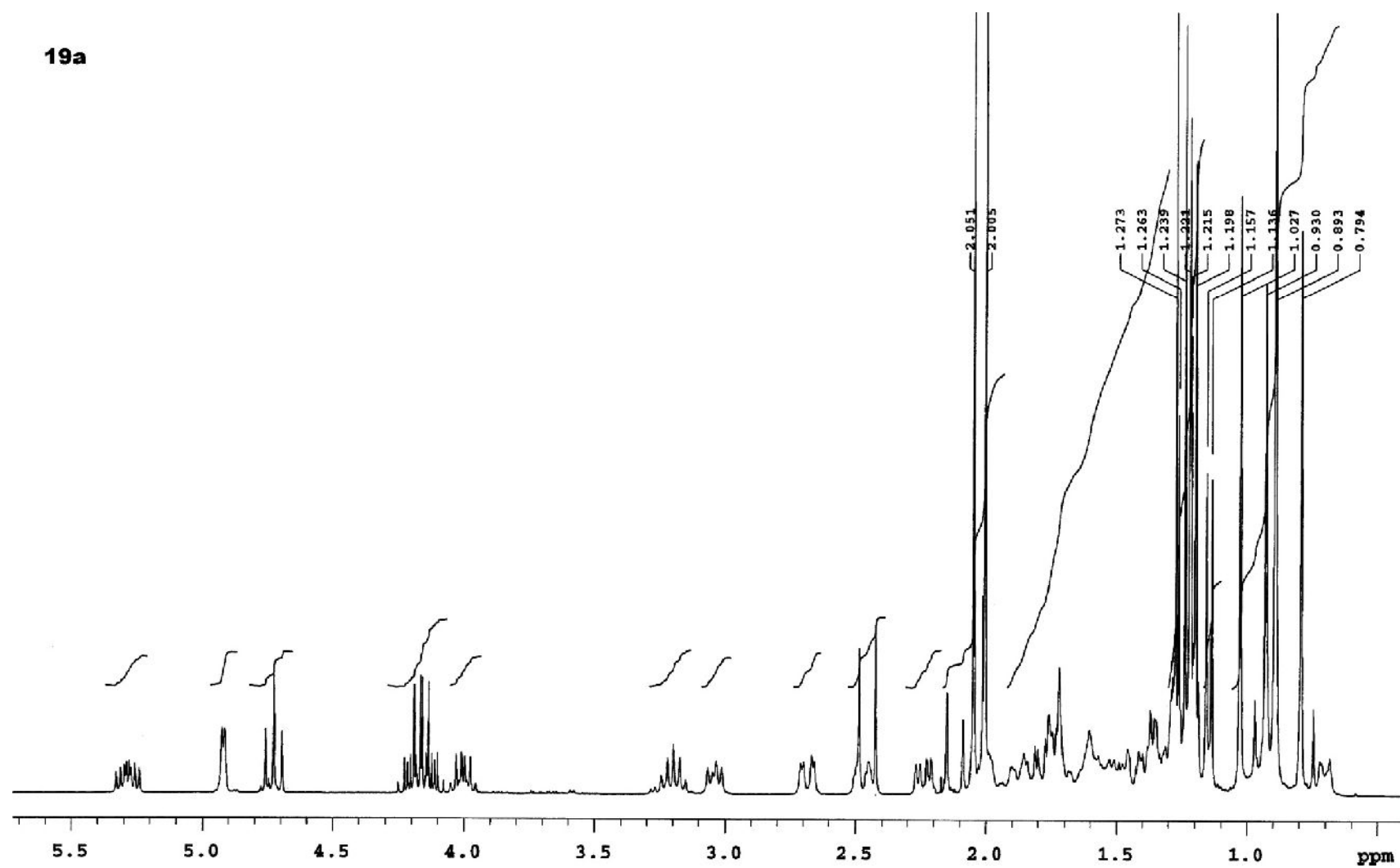
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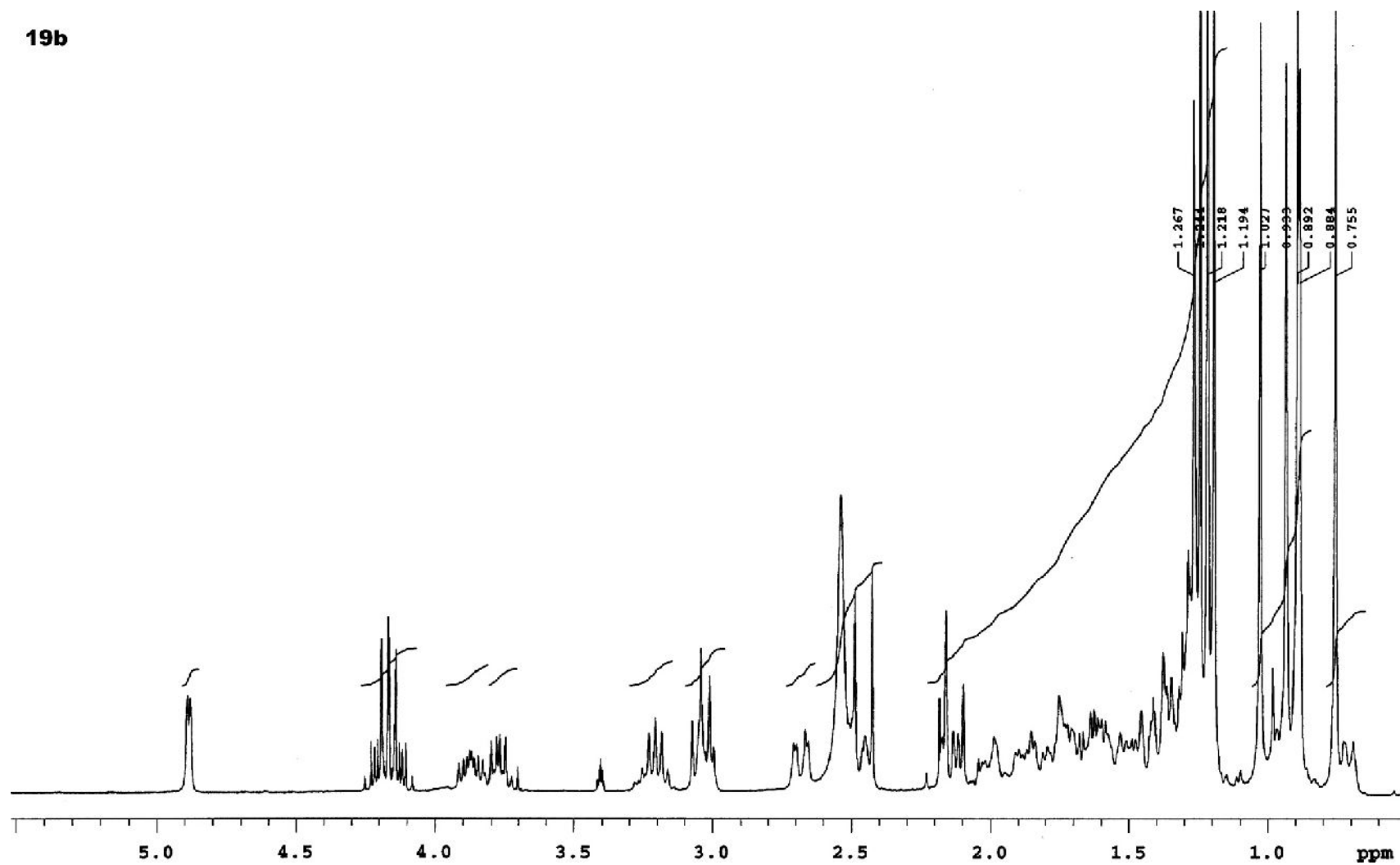
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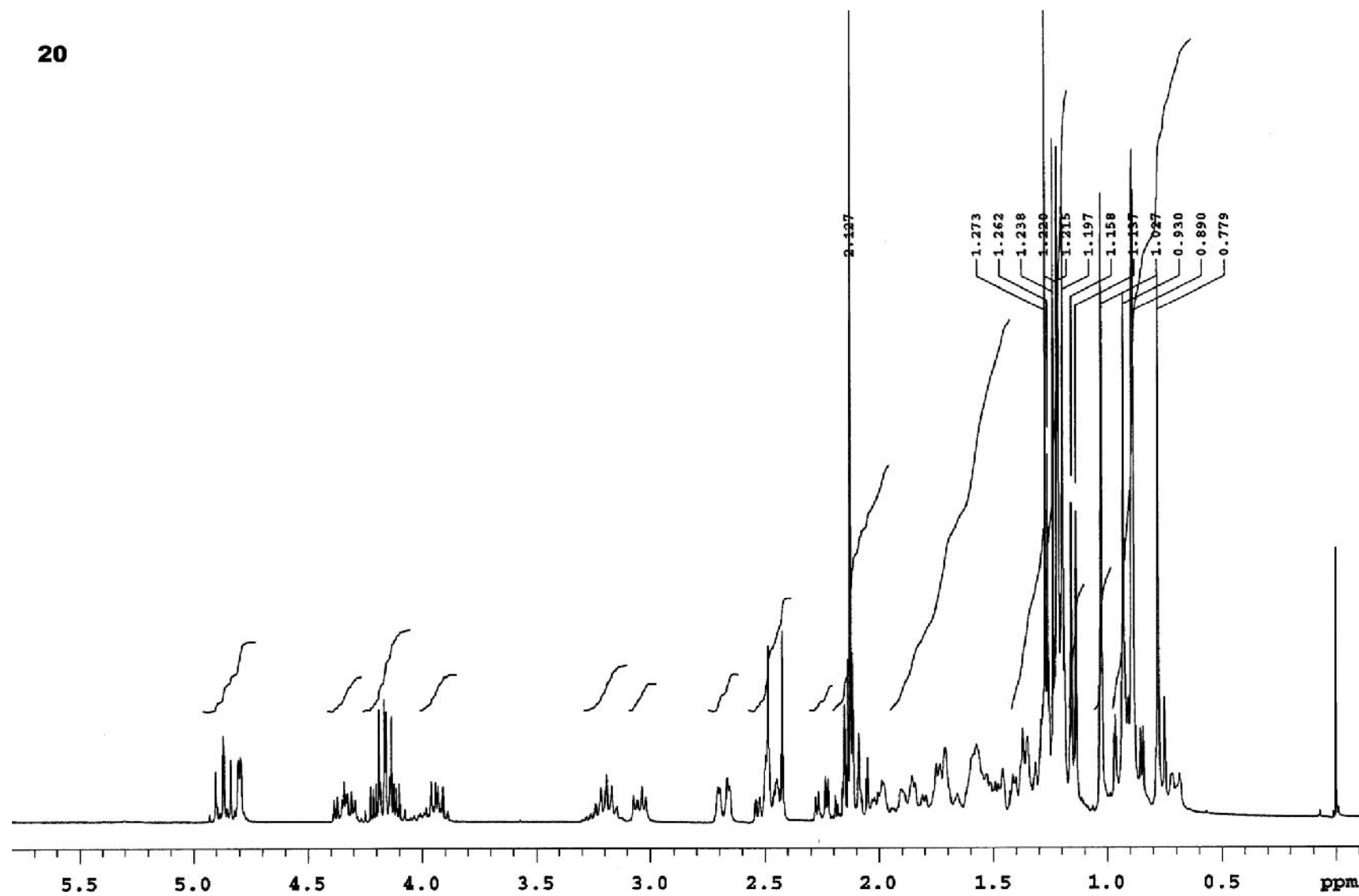


19a

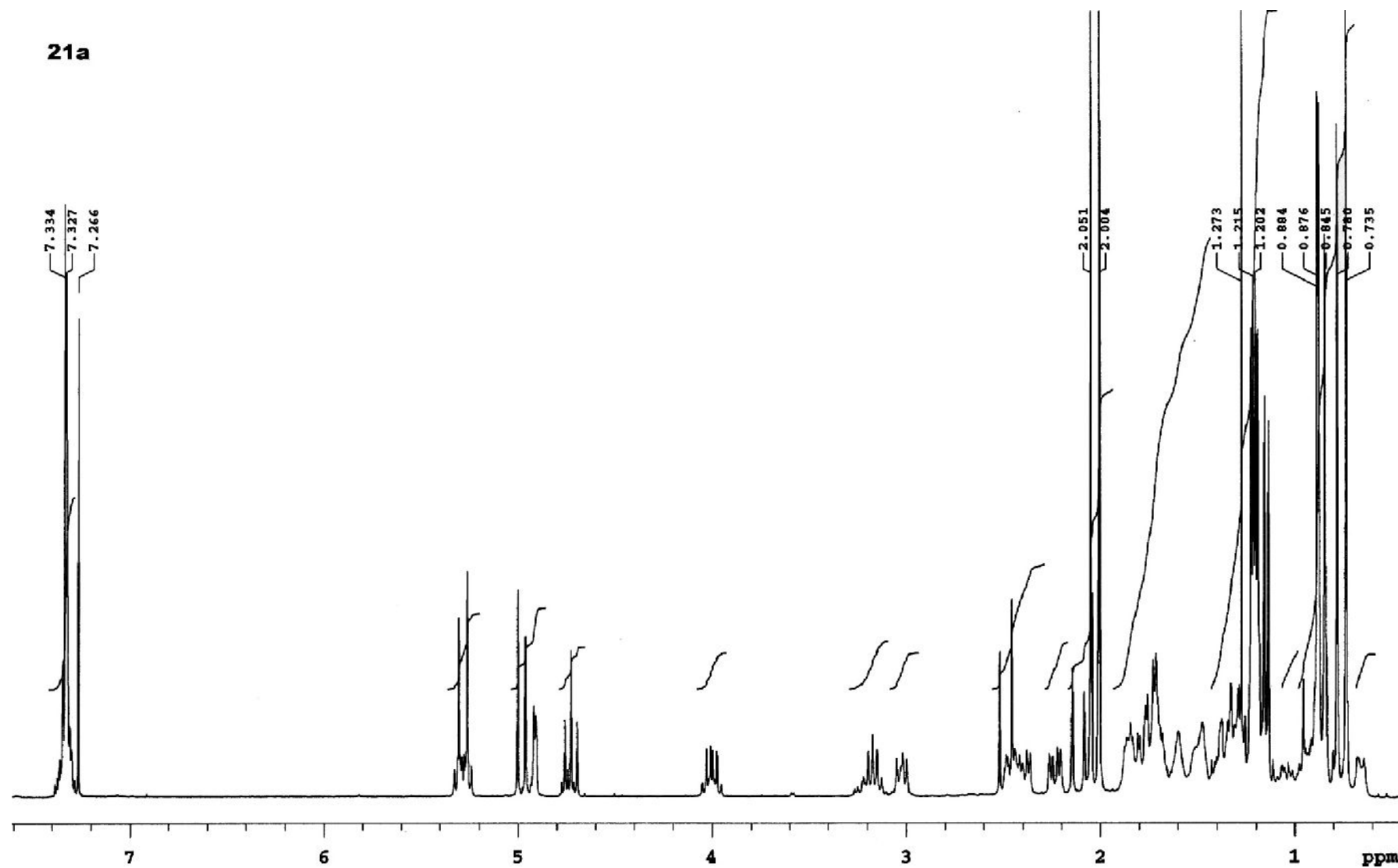


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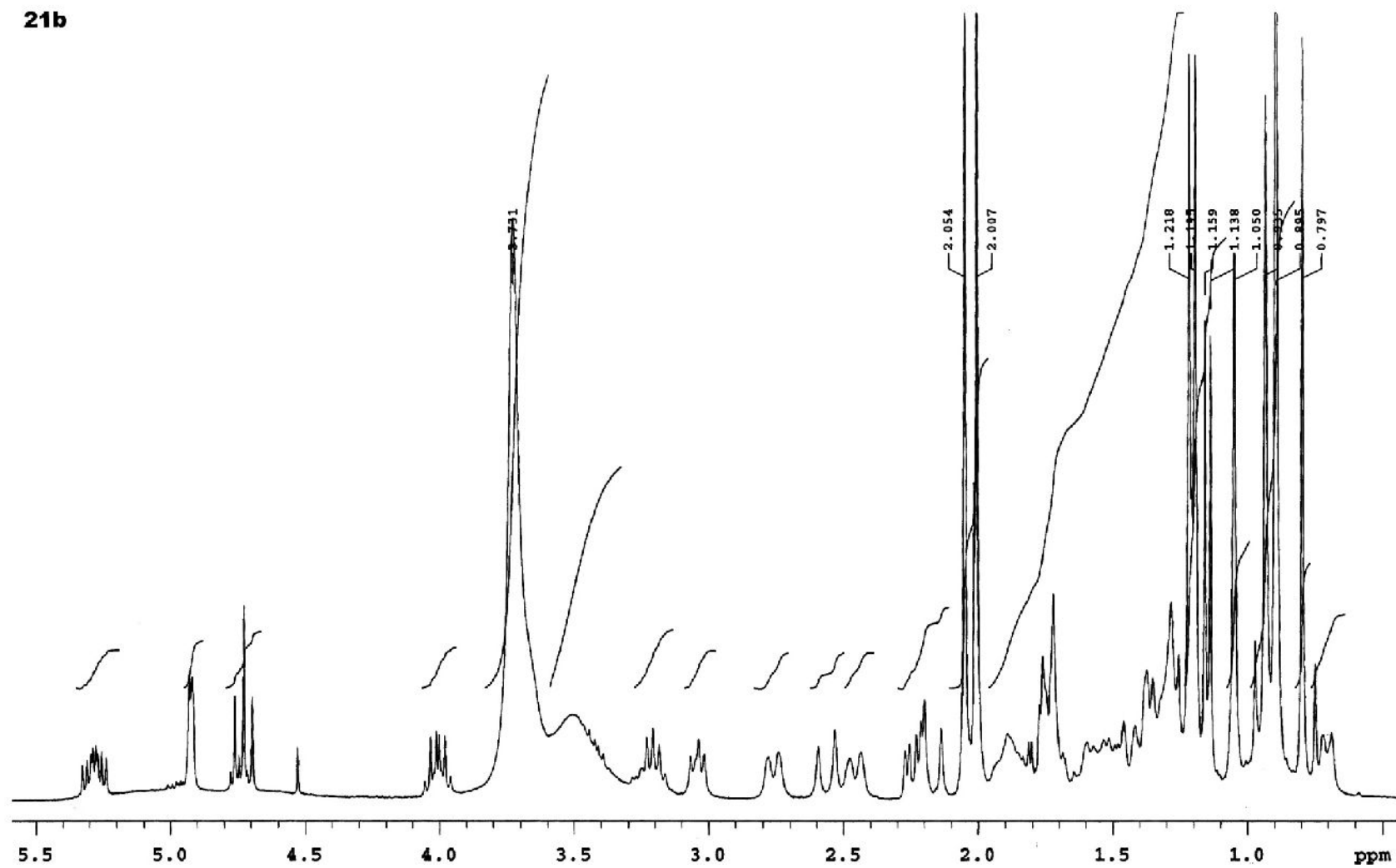


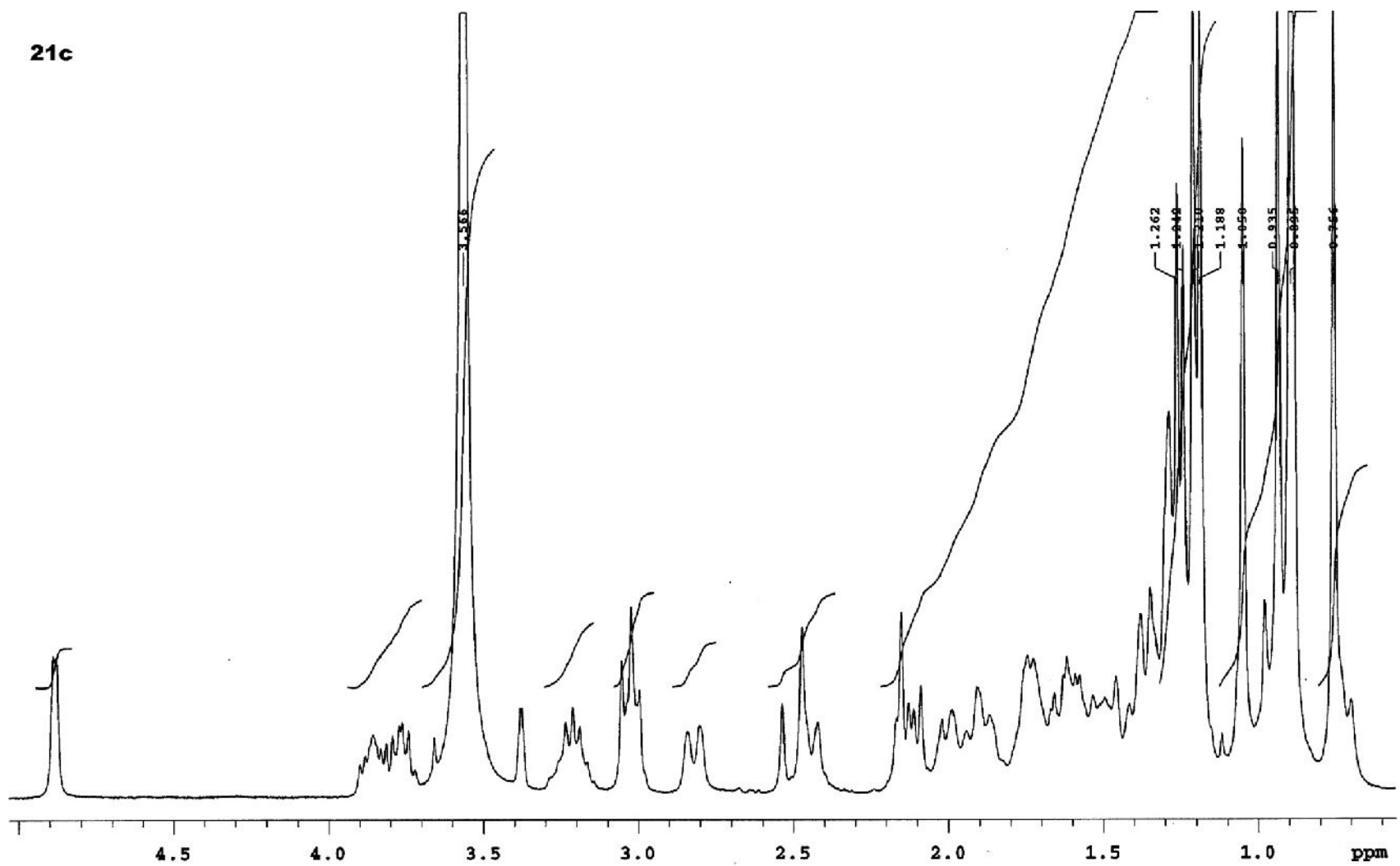


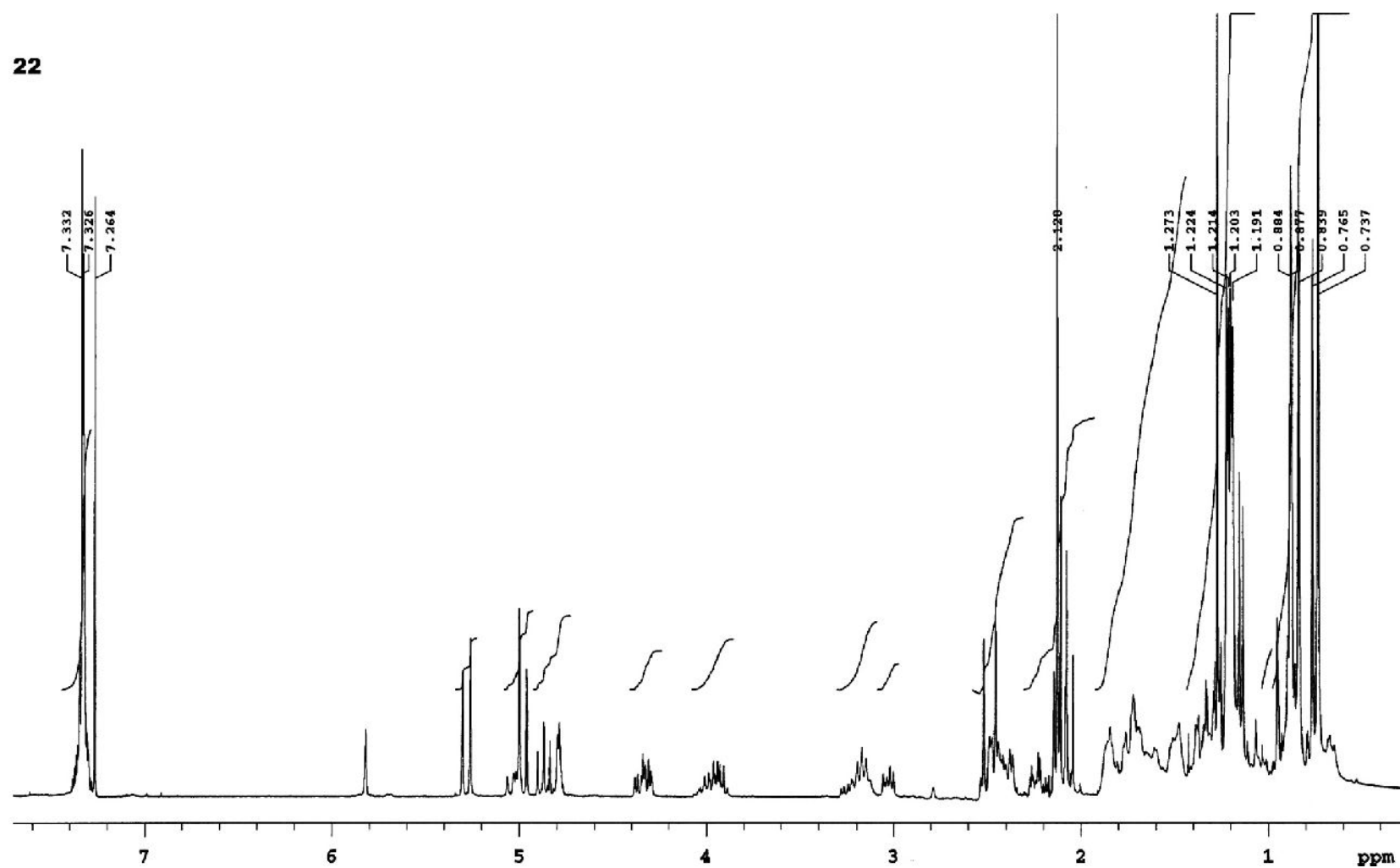
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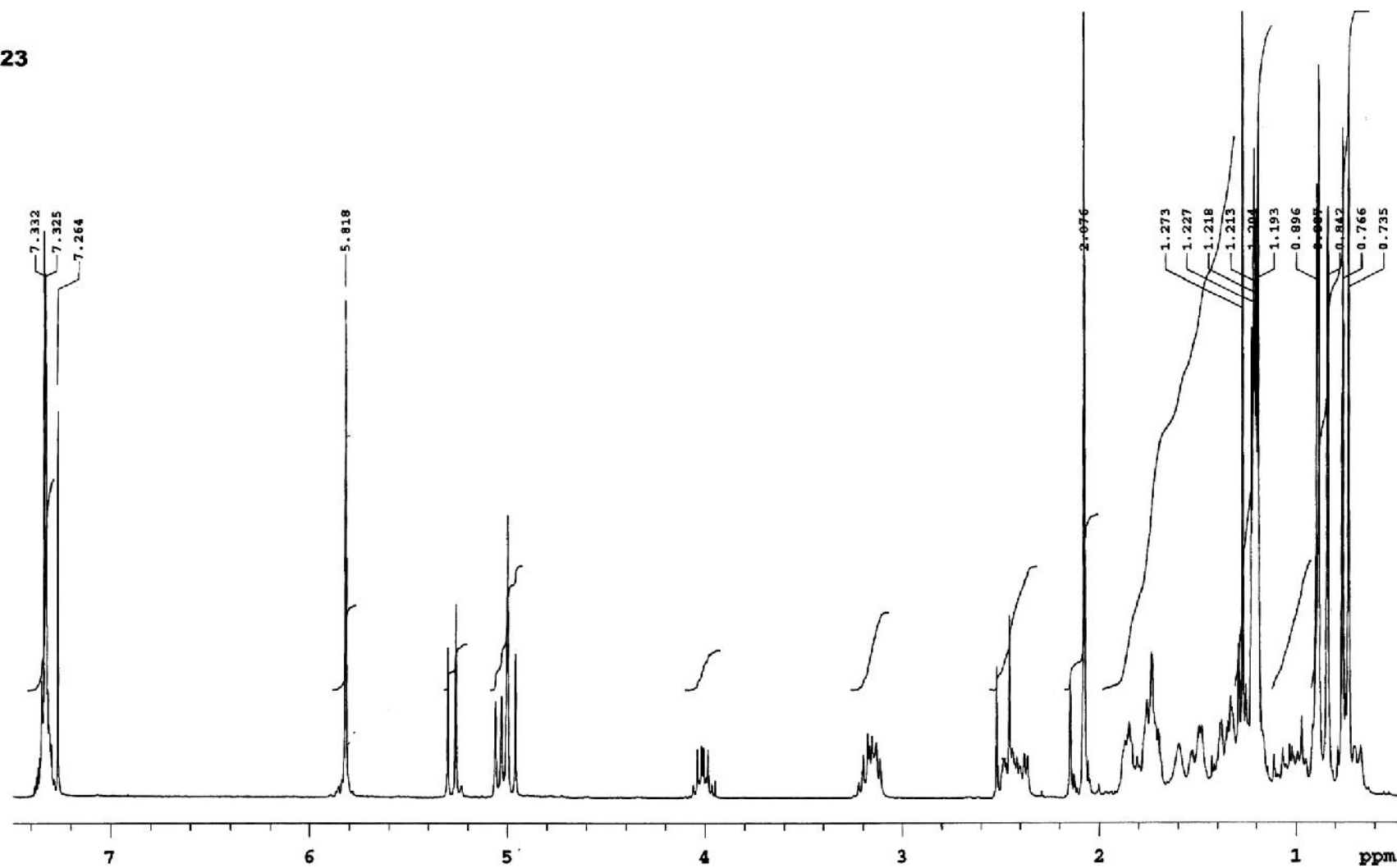


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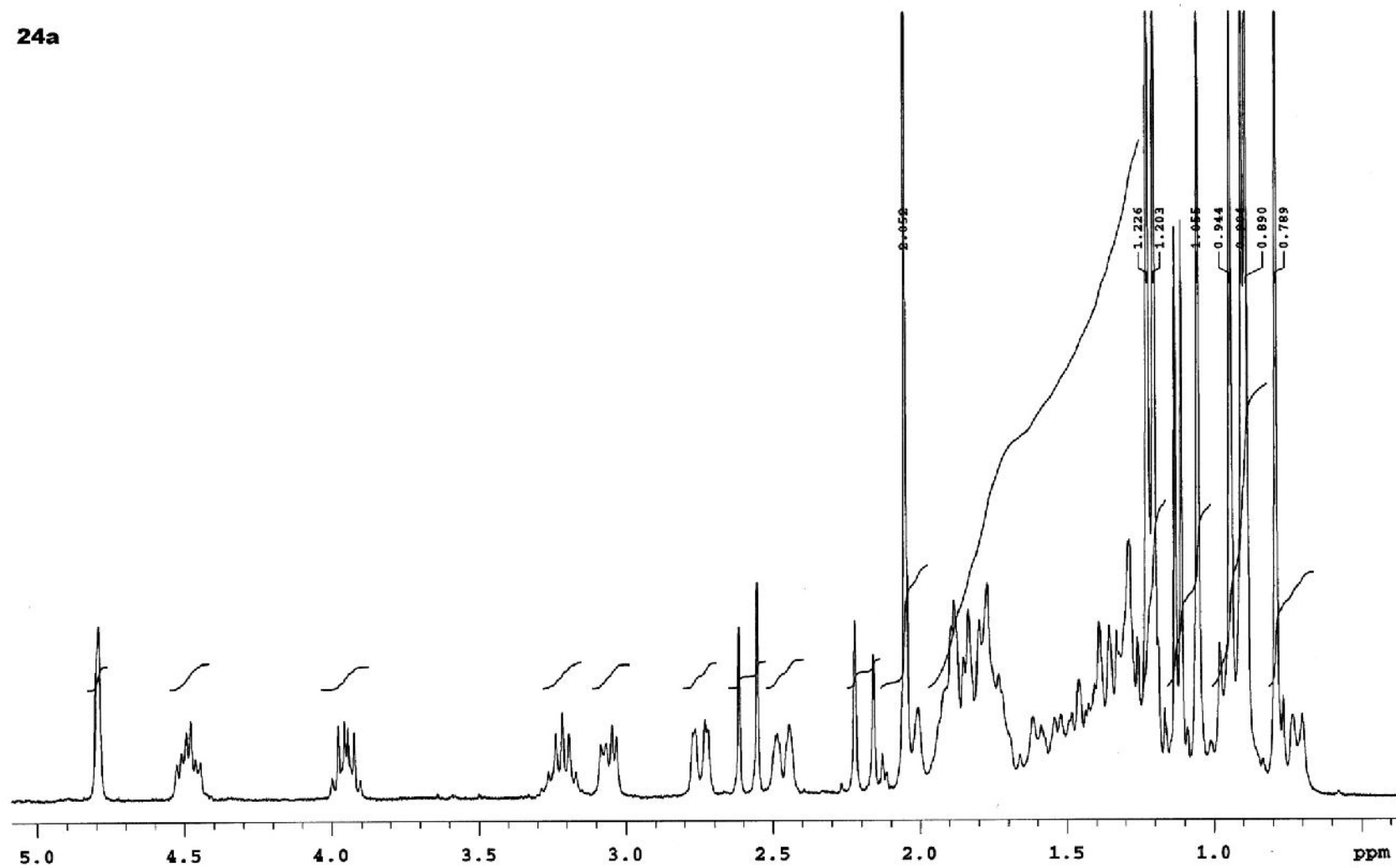




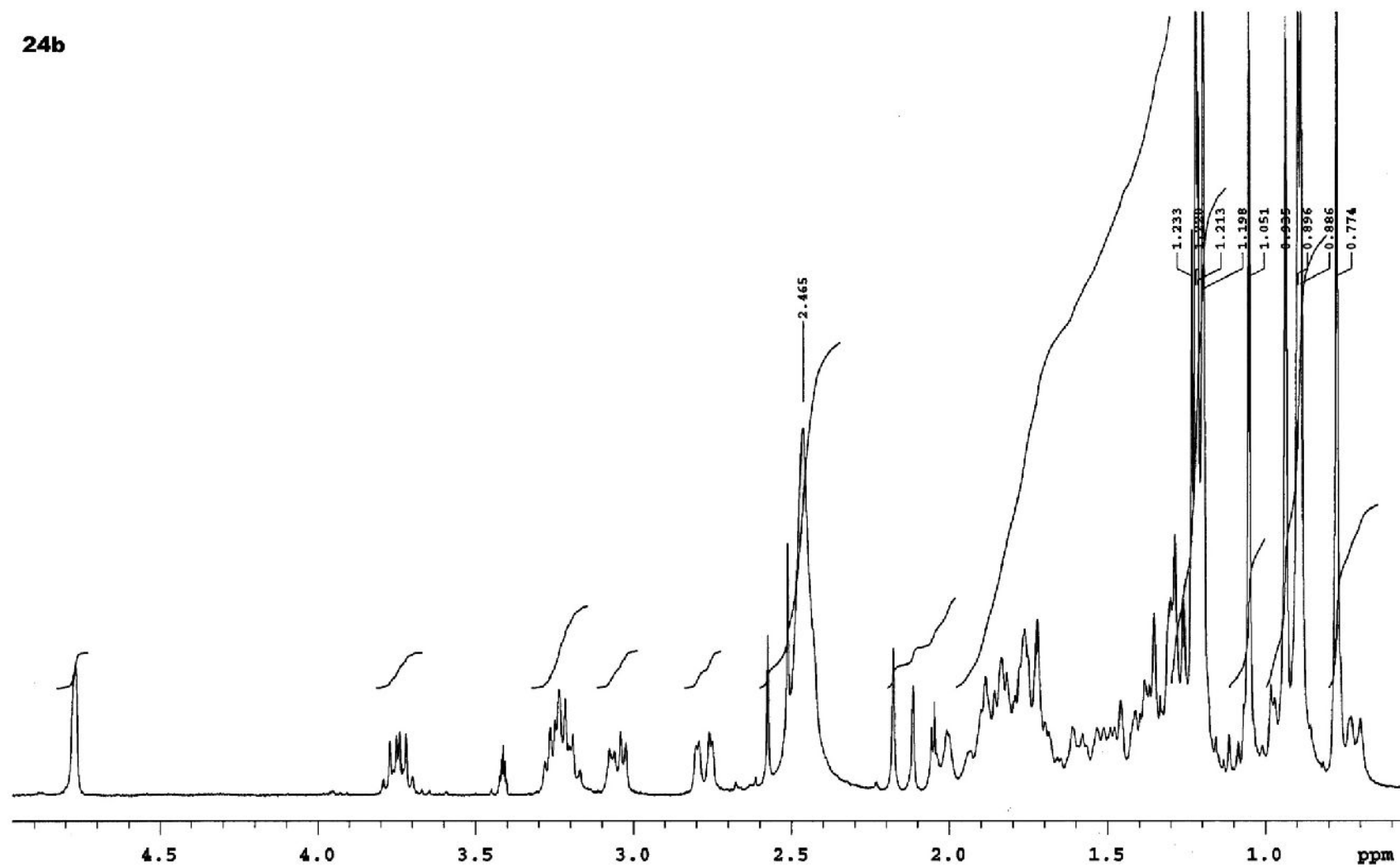




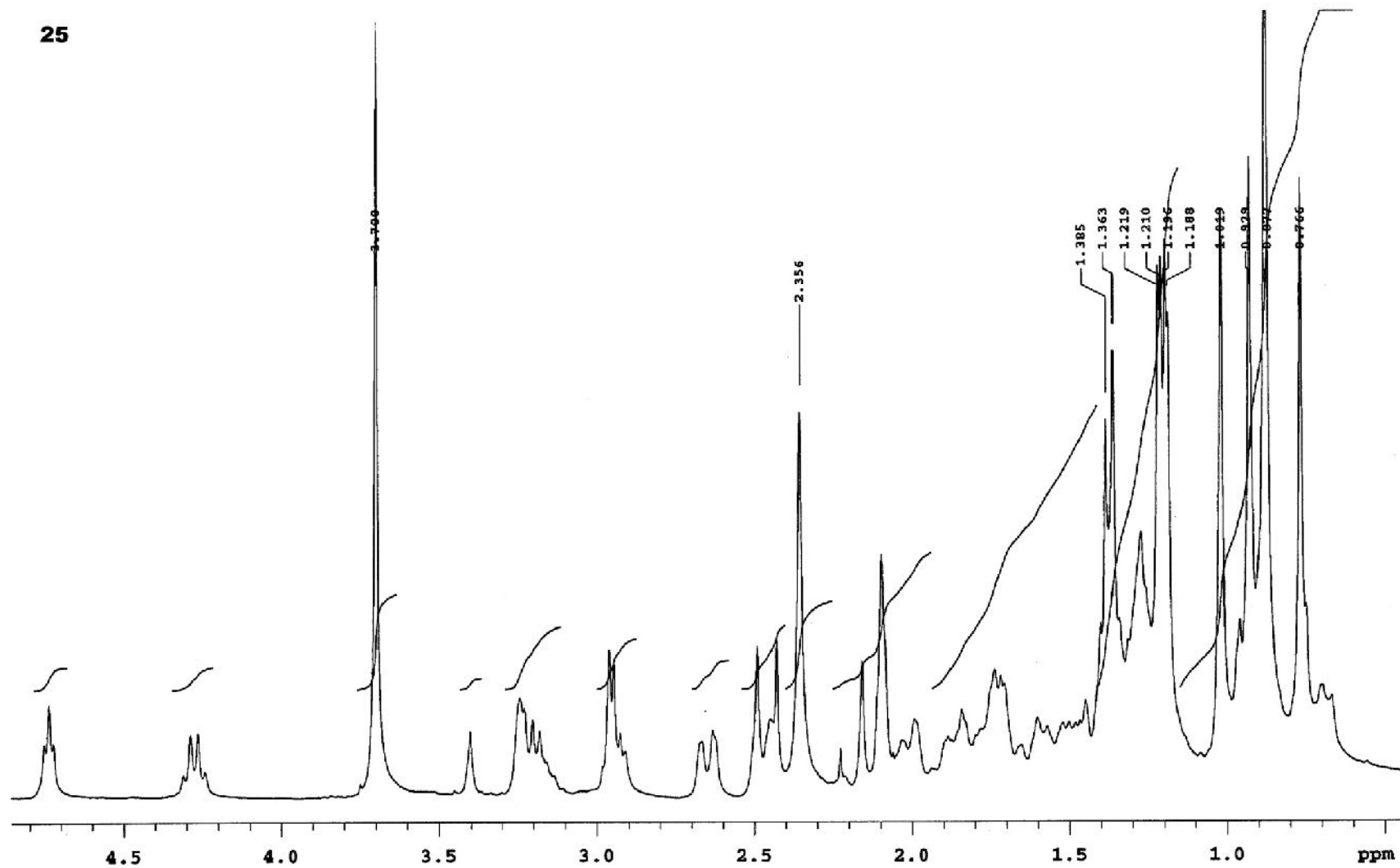
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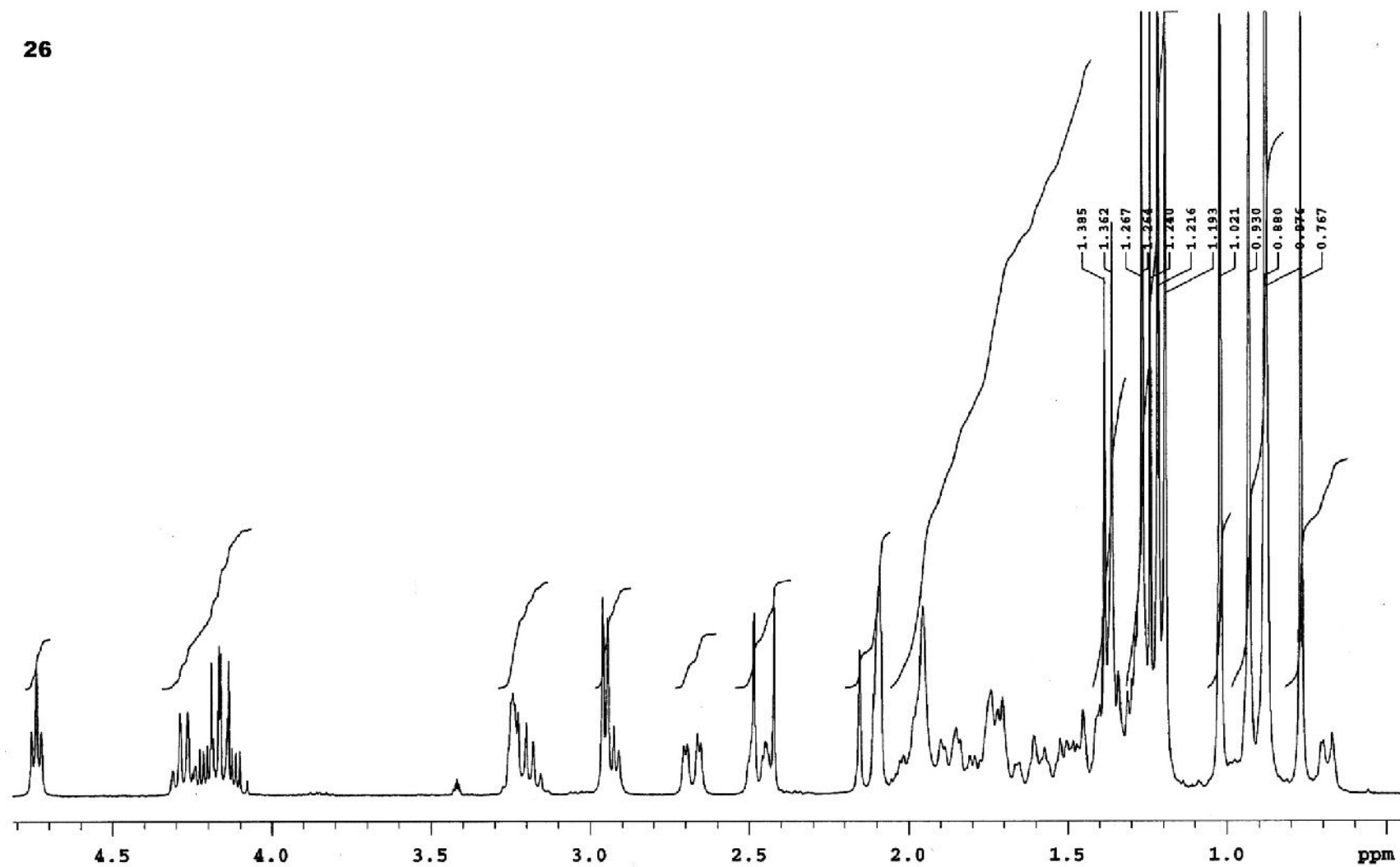


24b

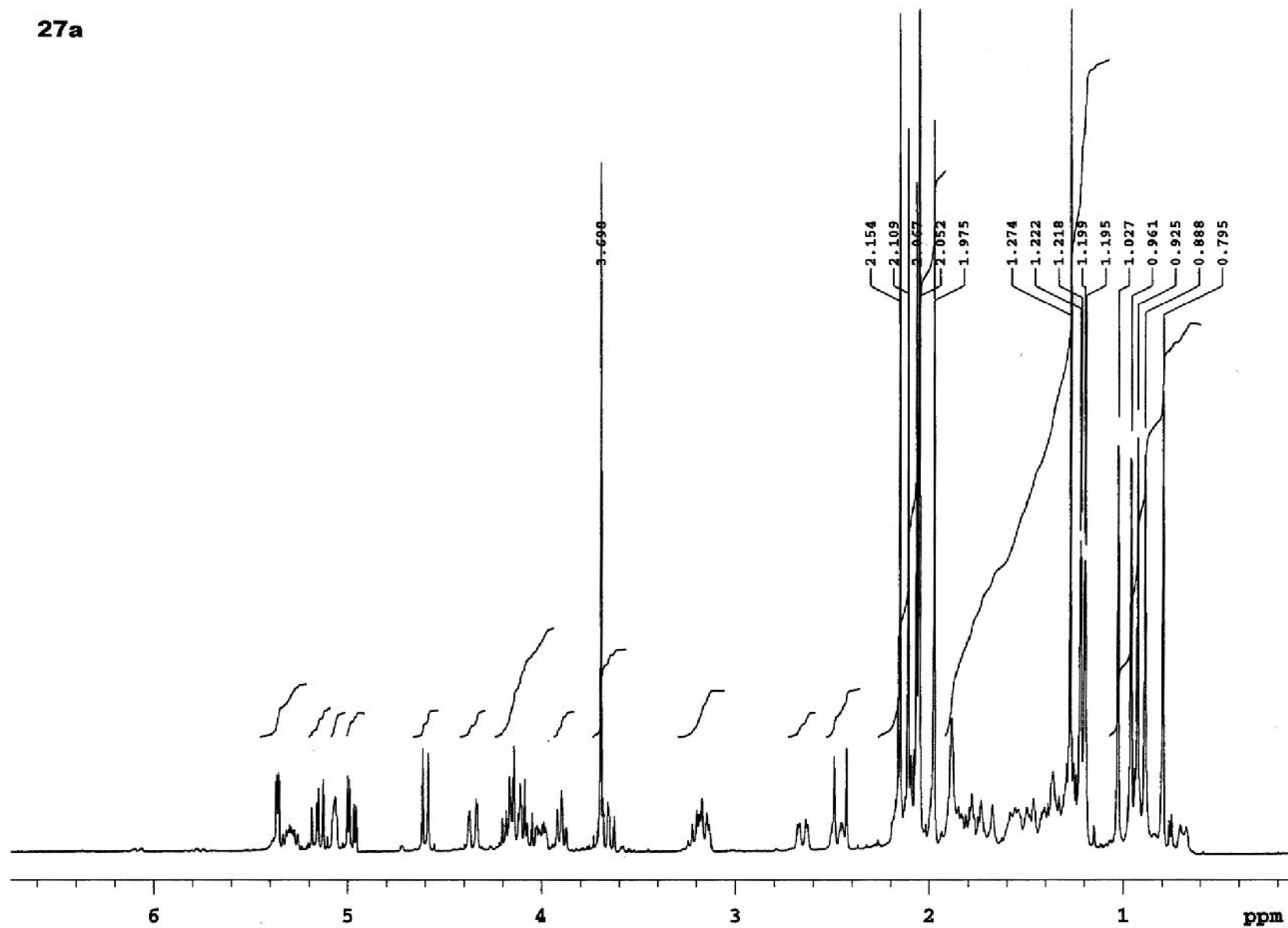


25

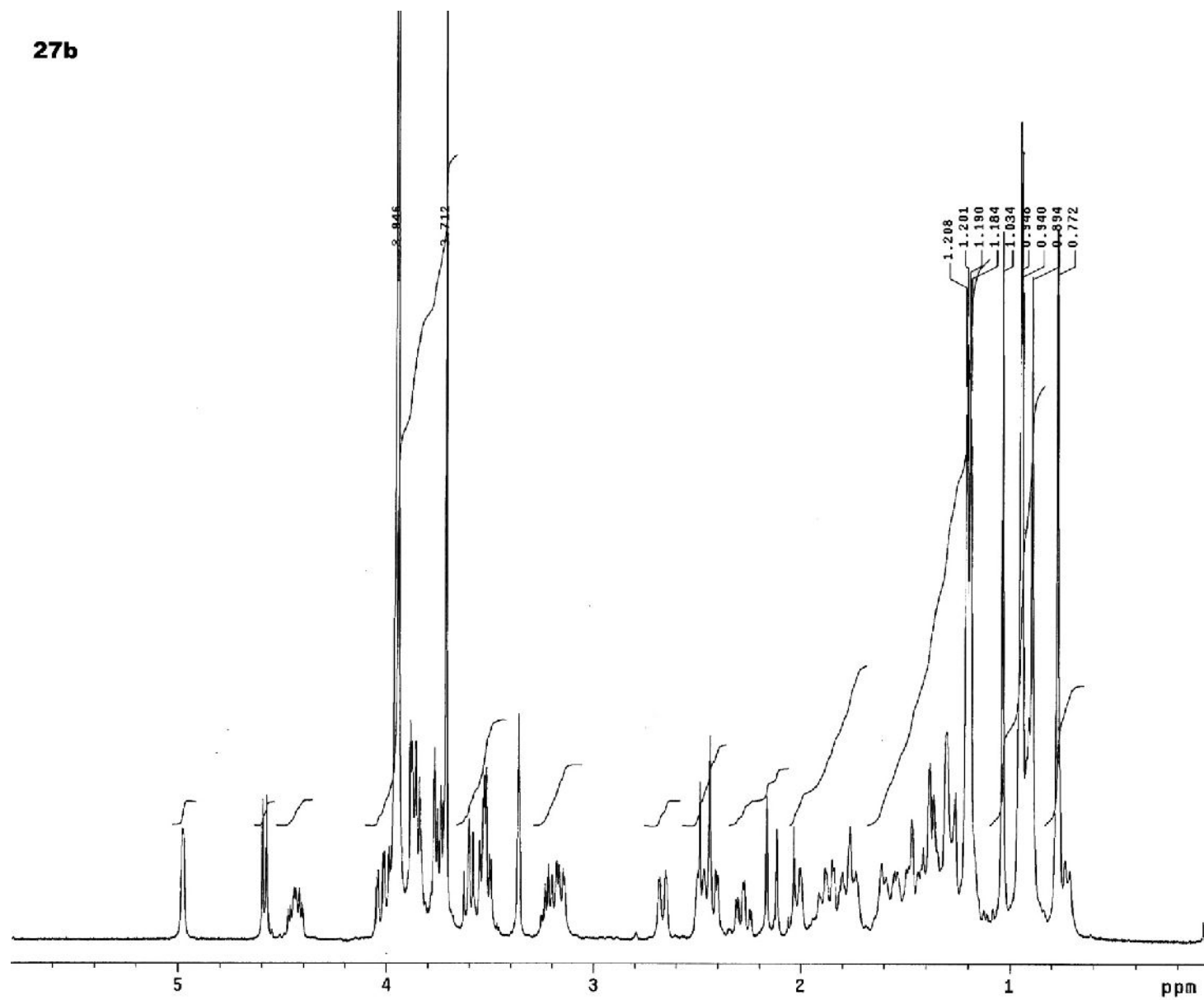




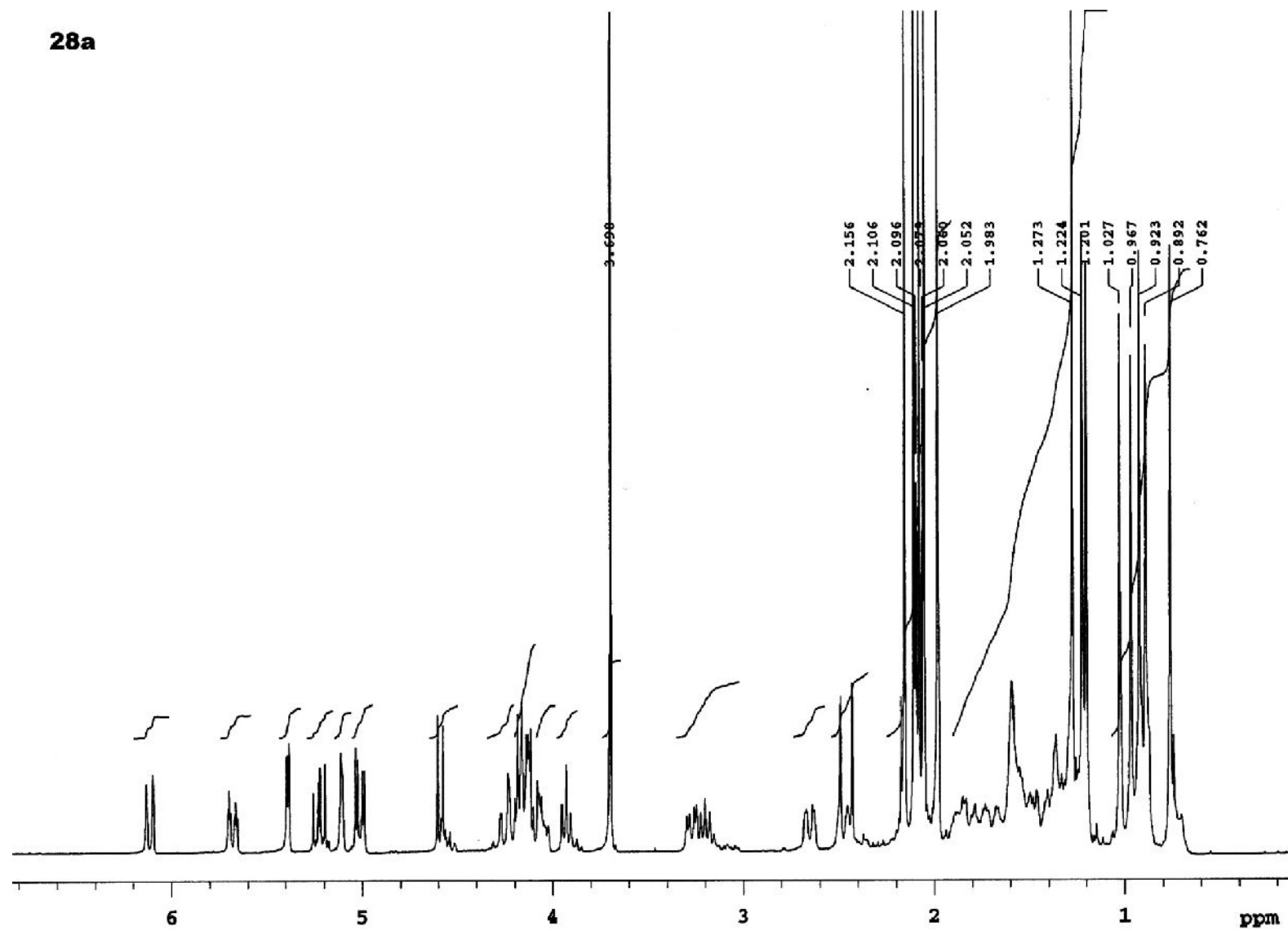
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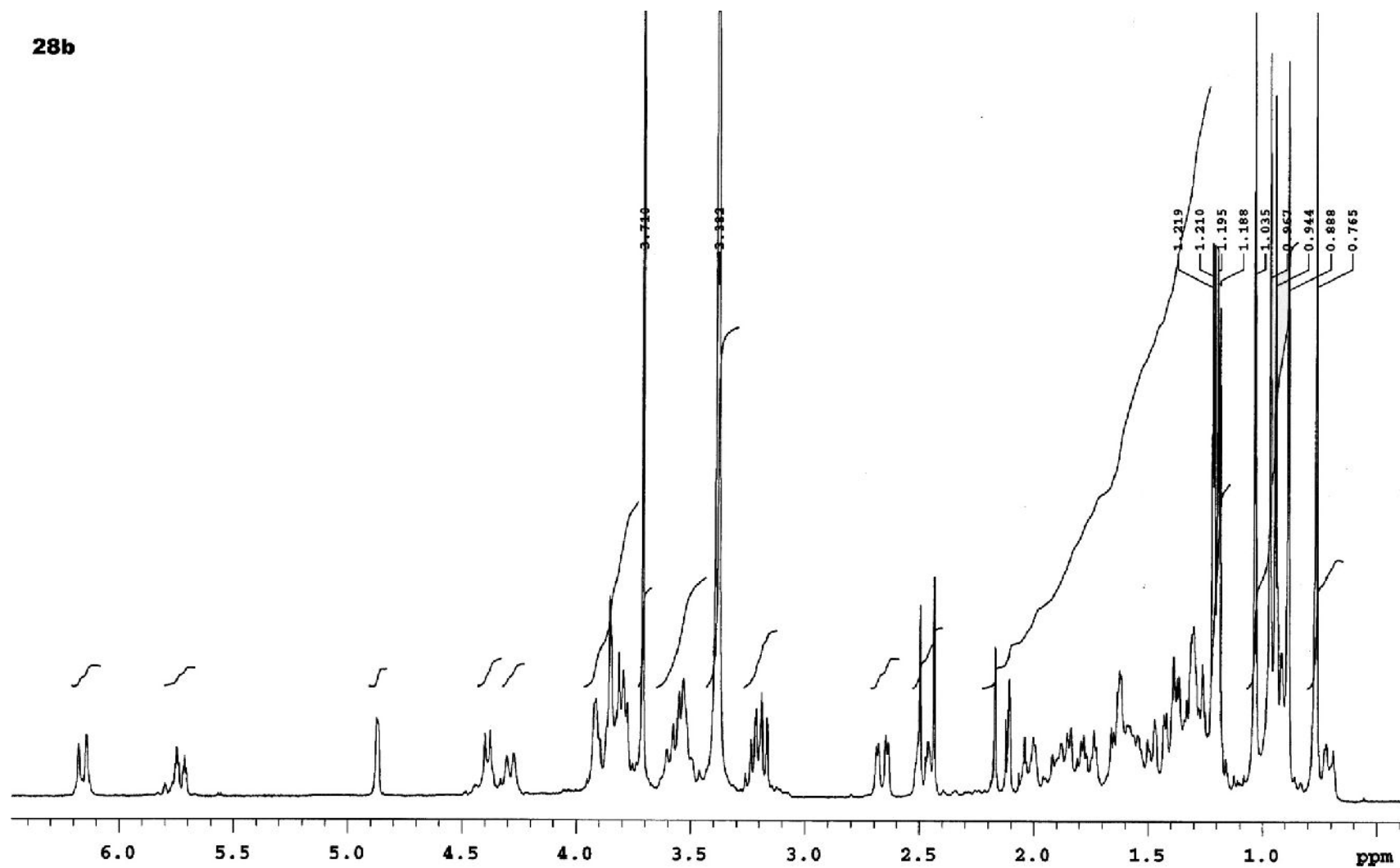
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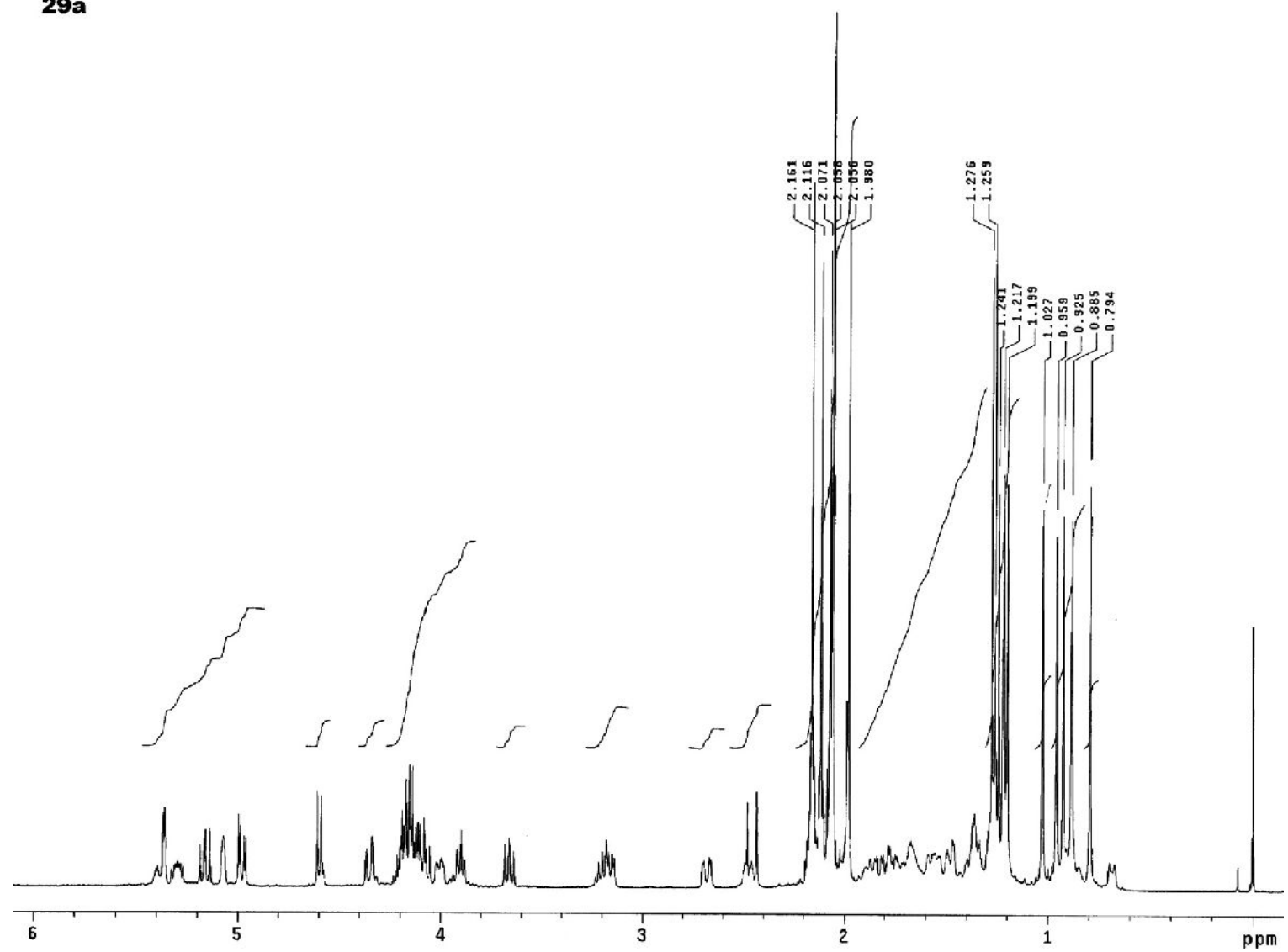
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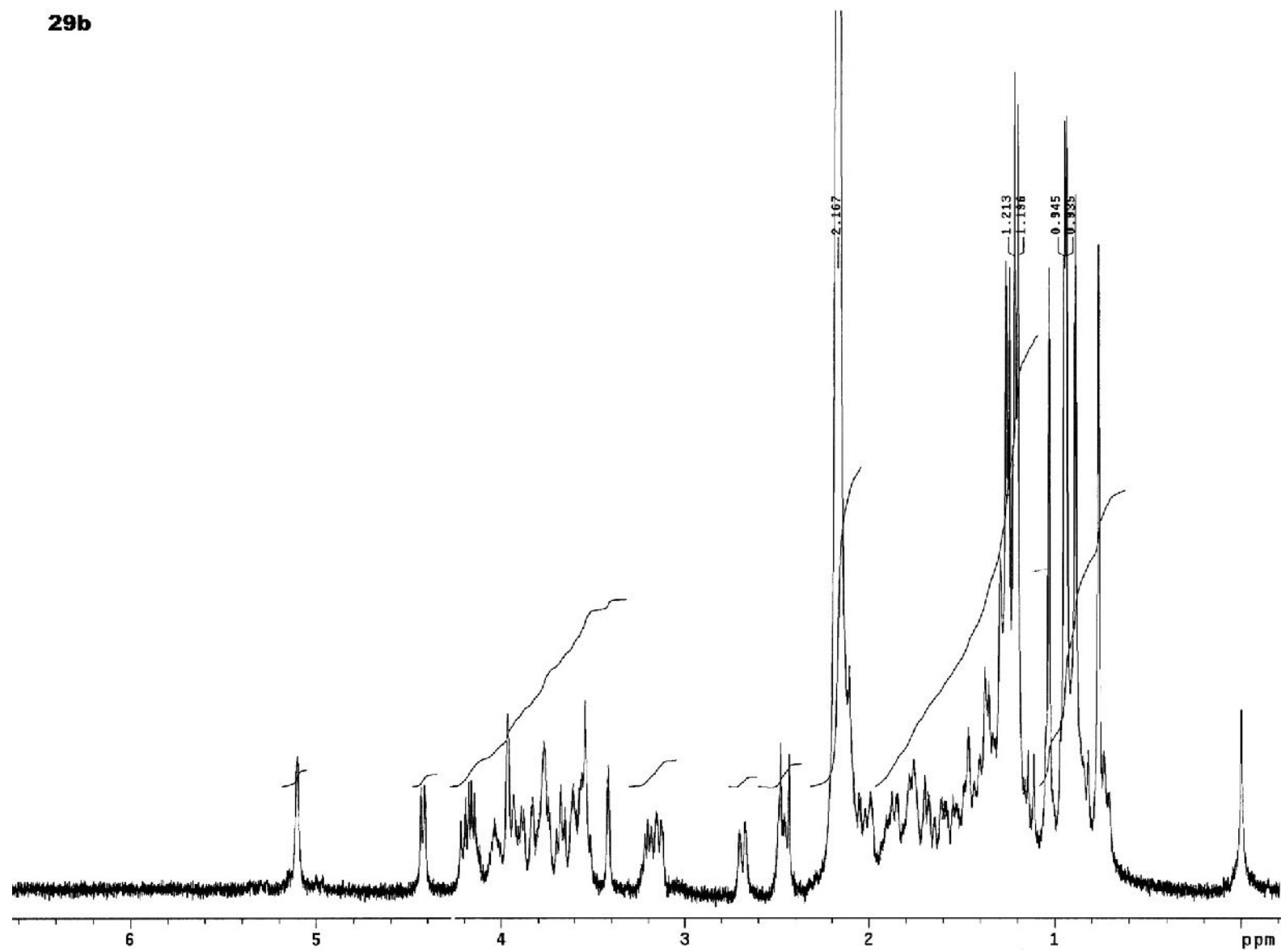
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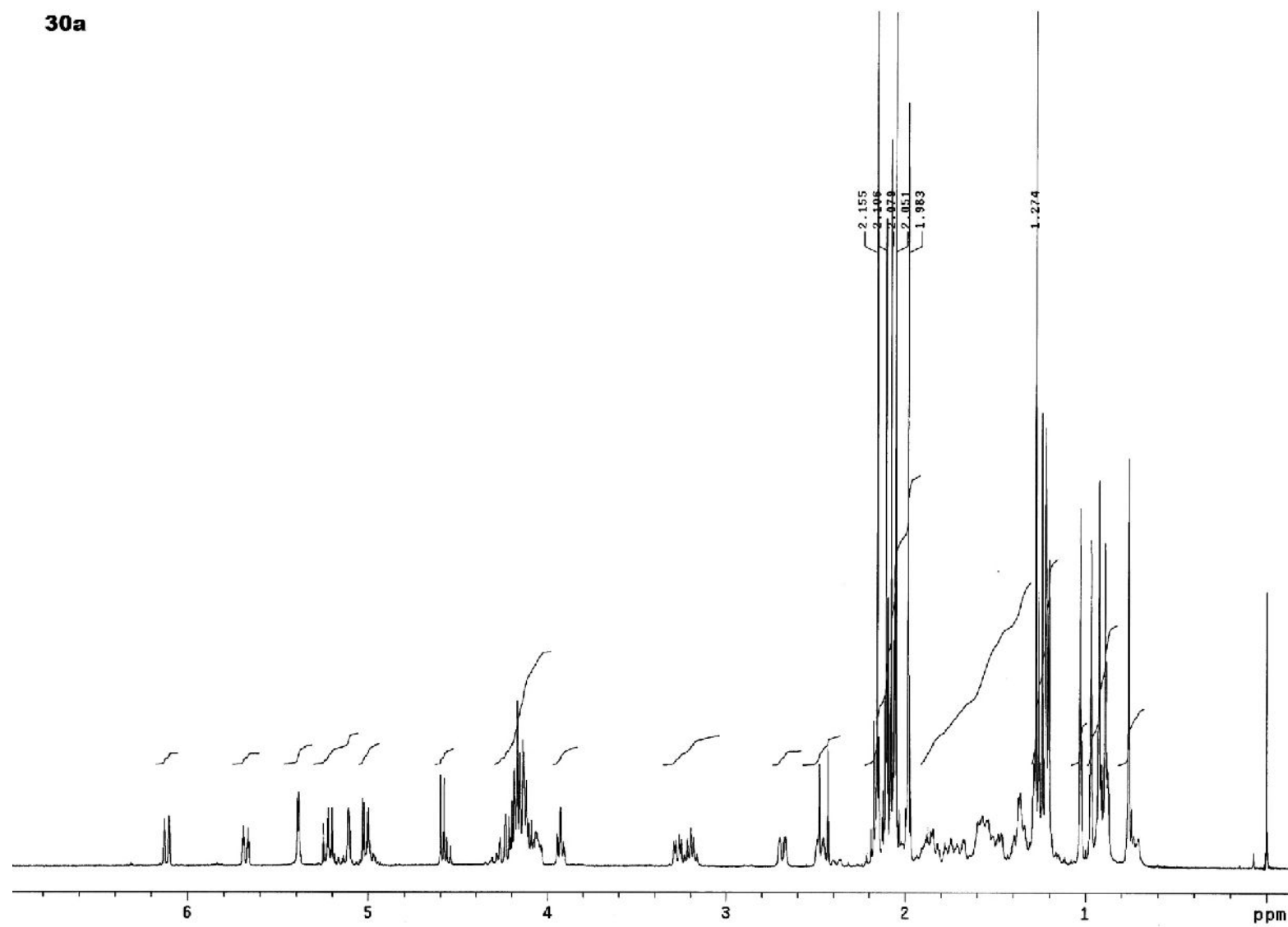
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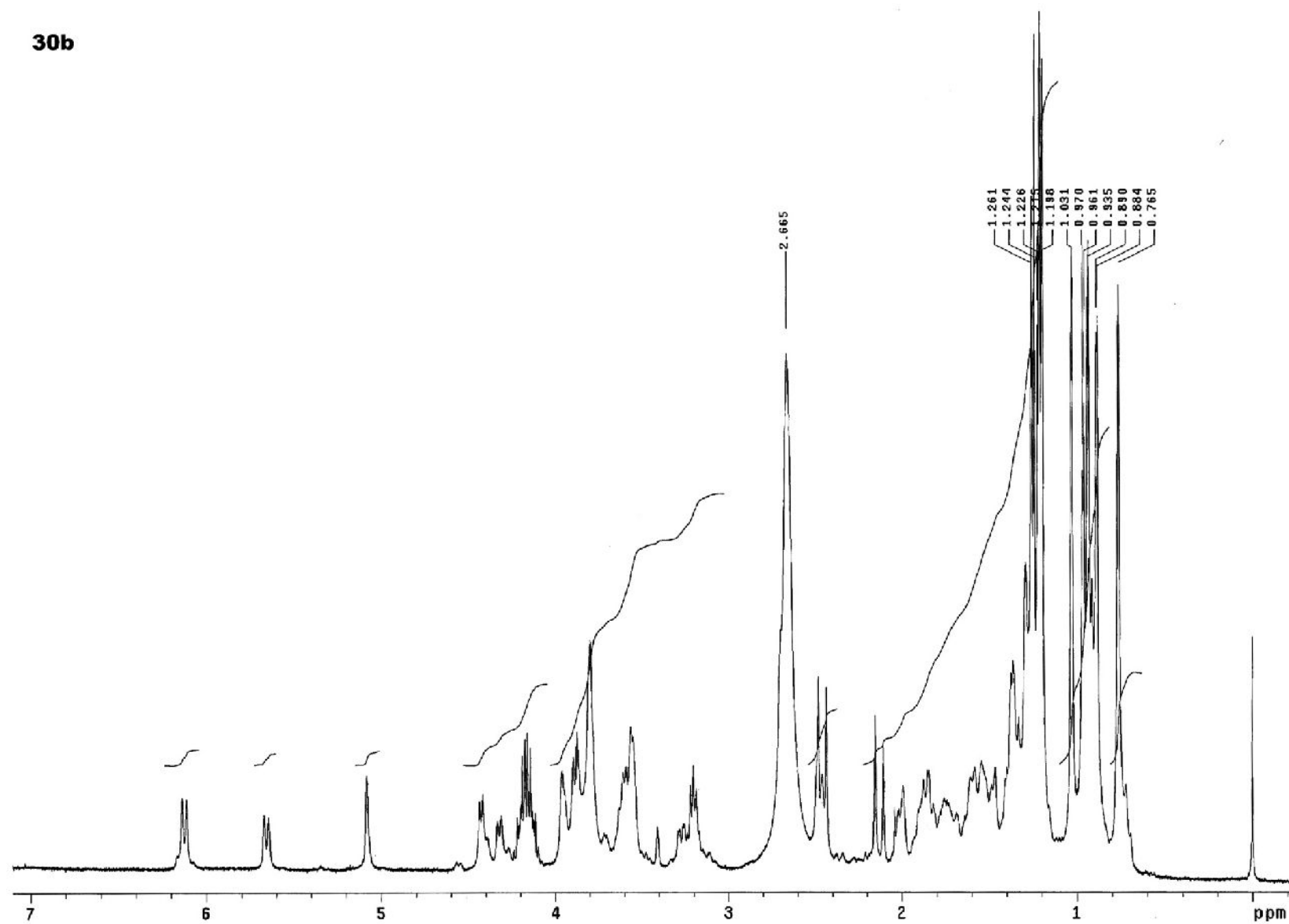
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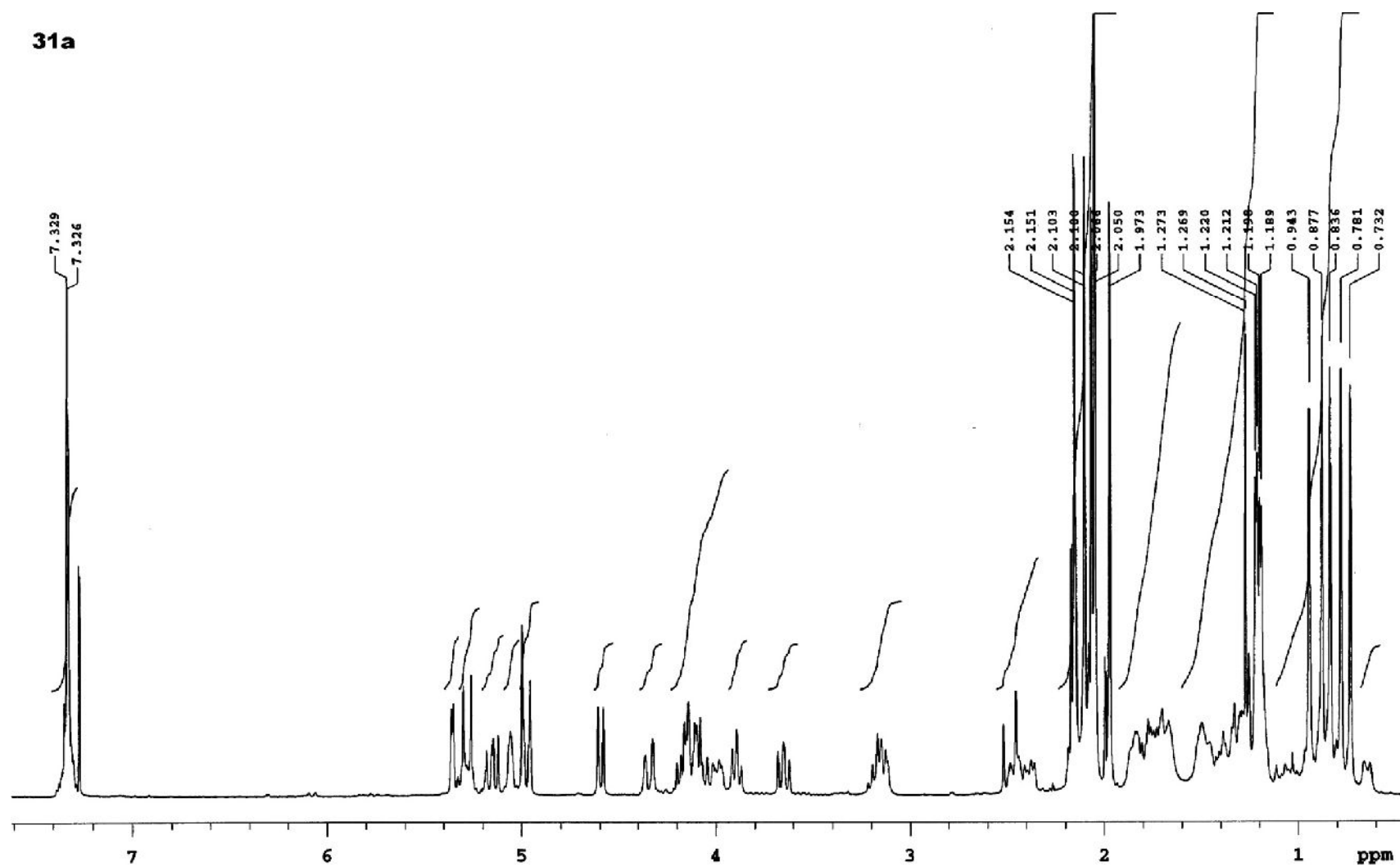
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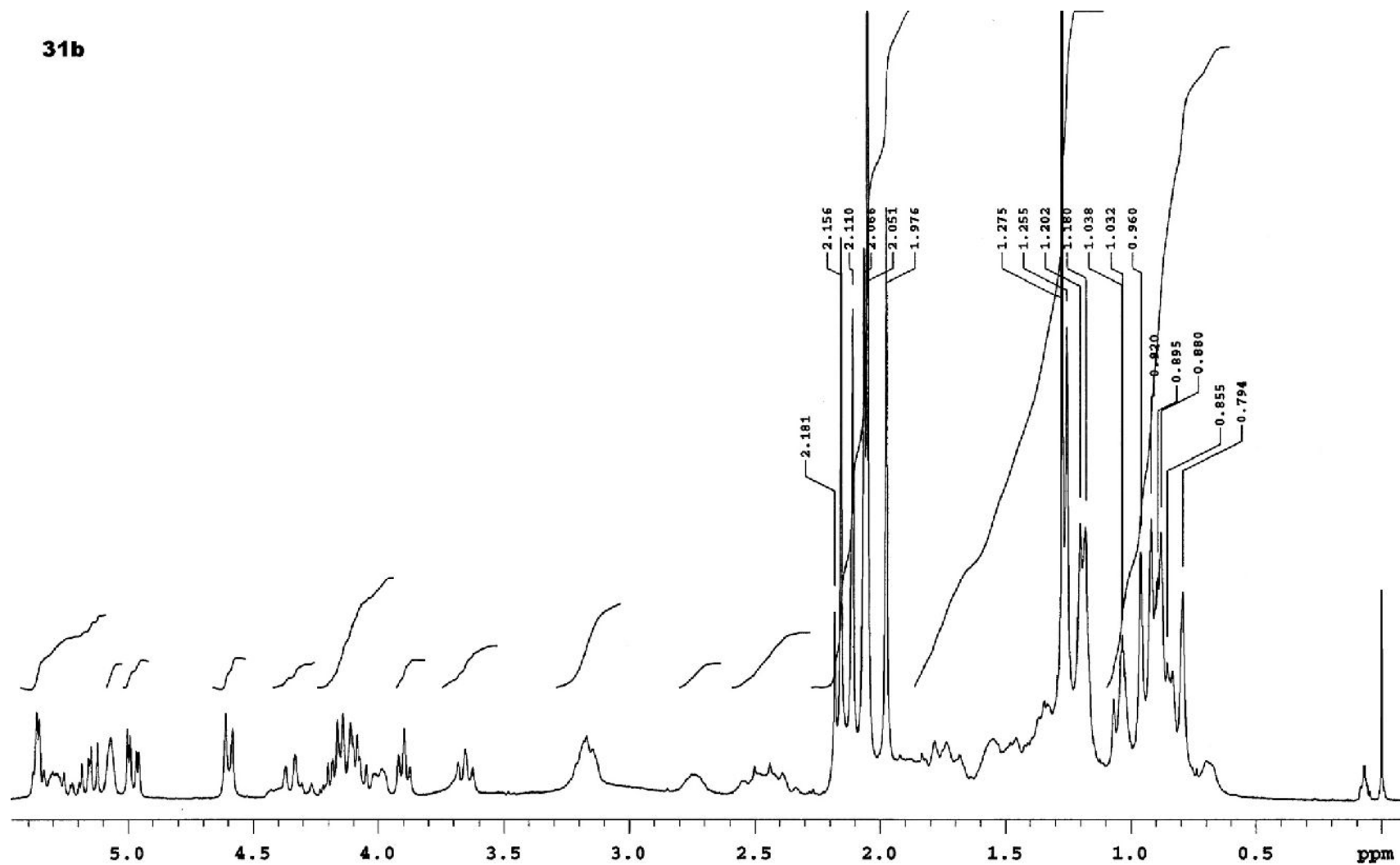
30b



31a



31b



31c

