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SUPPORTING INFORMATION

Platinum- and Acid-Catalyzed Enyne Metathesis Reactions: Mechanistic Studies and Applications to the Syntheses of Streptorubin B and Metacycloprodigiosin

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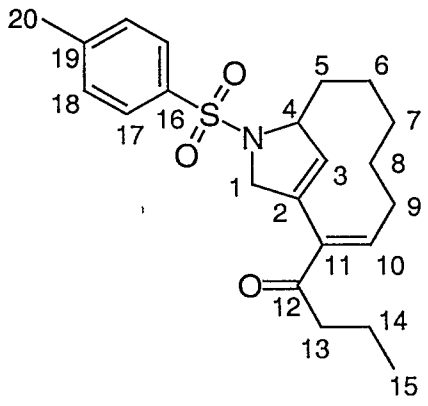
Instrumentation and Spectra Formats. NMR: Spectra were recorded on a Bruker AC 200, AMX 300, DPX 300, AMX 400 or DMX 600 spectrometer in $CDCl_3$ unless stated otherwise. Chemical shifts (δ) are given in ppm relative to TMS, coupling constants (*J*) in Hz. The multiplicity in the ^{13}C NMR spectra refers to the geminal protons (DEPT). IR: Nicolet FT-7199, wavenumbers in cm^{-1}. MS: Finnigan MAT 8200 (70 eV); HR-MS: Finnigan MAT SSQ 7000 (70 eV). Elemental analyses: Dornis & Kolbe, Mülheim.



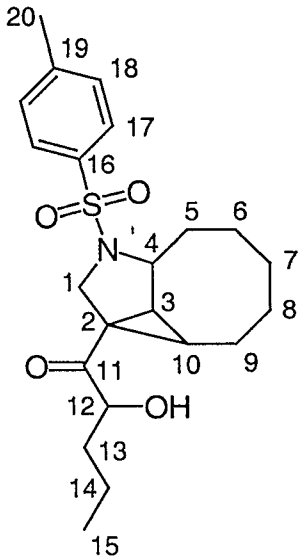
The ^{1}H and ^{13}C NMR data of compound **16**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for $^{1}J(C,H)$ and for $^{n}J(C,H)$.

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H	
1a/1b	58.5 (dd)	143/148	4.35 (dt, J = 14.4, 2.2)	4.24 (ddd, J = 14.4, 4.8, 1.6)
2	132.6 (s)	-	-	
3	131.6 (d)	168	5.31 (dt, J = 2.2, 1.7)	
4	67.3 (d)	144	4.73 (m)	
5a/5b	35.3 (t)	128	2.23 (m)	1.43
6a/6b	19.1 (t)	125	1.48	1.43
7a/7b	28.5 (t)	126	1.60	1.14 (m)
8a/8b	27.5 (t)	128	1.54	1.49
9a/9b	25.5 (t)	126	2.30	2.07 (dtd, J = 14.7, 7.0, 4.1)
10	145.6 (d)	155	6.88 (dd, J = 8.4, 6.9)	
11	138.6 (s)	-		
12	199.5 (s)	-		
13a/13b	40.4 (t)	125	2.42 (dt, J = 16.5, 7.4)	2.32 (dt, J = 16.5, 7.4)
14	17.7 (t)	128	1.51 (sext, J = 7.4)	
15	13.7 (q)	126	0.83 (t, J = 7.4)	
16	135.2 (s)	-		
17	127.2 (d)	164		
18	129.8 (d)	160		
19	143.4 (s)	-		
20	21.5 (q)	127		



The ^{1}H and ^{13}C NMR data of compound **22**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H).

MS (EI) *m/z* (rel intensity) 405 ([M^{+}]), 334 (16), 332 (15), 277 (13), 250 (100), 232 (15), 178 (10), 155 (34), 148 (13), 106 (10), 91 (67), 55 (12), 43 (11).

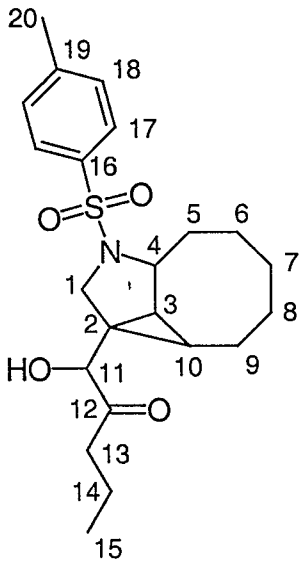
HR-MS ($C_{22}H_{31}NSO_4$): *calcd.* 405.19738; *found* 405.1955.

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H	
1a/1b	48.9 (dd)	151/136	3.85 (d, J = 10.0)	3.52 (d, J = 10.0)
2	34.1 (s)	-		
3	39.0 (d)	171	2.22 (dd, J = 8.7, 4.5)	
4	59.7 (d)	137	3.45 (td, J = 4.5, 1.5)	
5a/5b	32.5 (t)	127	2.54 (dt, J = 13.6, 5.2)	1.47
6a/6b	19.1 (t)	127	1.63	1.44
7a/7b	25.5 (t)	128	1.91	1.36
8	26.4 (t)	128	1.58	
9a/9b	19.4 (t)	127	2.11 (dddd, J= 14, 13, 10, 8)	1.81 (dq, J = 14.0, 3.8)
10	34.3 (d)	157	1.50 (ddd, J = 12.9, 8.5, 4.3)	
11	209.5 (s)	-		
12a/12b	74.3 (d)	145	4.26 (ddd, J = 7.1, 6.4, 3.3)	3.30 (d, J = 6.4)
13a/13b	36.1 (t)	127	1.67	1.36
14a/14b	18.1 (t)	127	1.42	1.32
15	13.8 (q)	125	0.93 (t, J = 7.2)	
16	131.2 (s)	-		
17	127.9 (d)	164	7.63	
18	129.9 (d)	160	7.34	
19	144.3 (s)	-		
20	21.6 (q)	127	2.43 (s)	



The ^{1}H and ^{13}C NMR data of compound **21**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H).

MS (ESI/pos. in CH_3OH) *m/z* (rel intensity) 406 ([M+H$^+$] 25), 428 ([M+Na$^+$] 100).

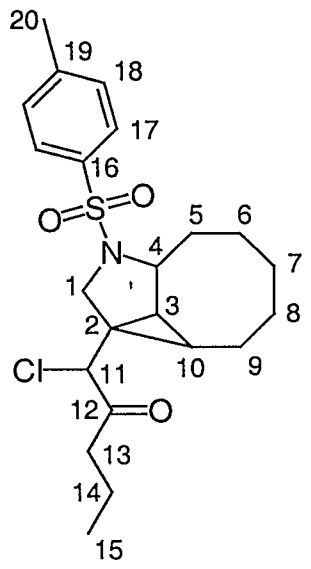
MS (EI) *m/z* (rel intensity) 405 ([M$^+$], 5), 334 (100), 304 (85), 250 (92), 232 (32), 163 (30), 155 (67), 91 (84), 71 (17), 55 (11), 43 (21).

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H	
1a/1b	47.9 (dd)	148/138	3.24 (d, J = 9.7)	3.14 (dd, J = 9.7, 0.4)
2	28.7 (s)	-		
3	30.2 (d)	166	1.48 (dd, J = 8.5, 4.3)	
4	60.9 (d)	136	3.51 (td, J = 4.5, 1.0)	
5a/5b	32.7 (t)	126	2.50	1.45
6a/6b	19.2 (t)	125	1.62	1.45
7a/7b	25.52 (t)	125	1.91 (m)	1.42
8	26.8 (t)	125	1.60	
9a/9b	18.9 (t)	127	2.06 (m)	1.84 (dq, J = 14.1, 3.7)
10	25.49 (d)	152	0.98 (ddd, J = 12.4, 8.5, 4.1)	
11	80.1 (d)	145	3.52 (s)	
12	210.1 (s)	-		
13a/13b	40.1 (t)	125	2.51 (dt, J = 17.3, 7.3)	2.39 (dtd, J = 17.3, 7.2, 0.4)
14	16.9 (t)	129	1.64 (sext, J = 7.3)	
15	13.8 (q)	126	0.91 (t, J = 7.4)	
16	131.5 (s)	-		
17	127.9 (d)	165	7.60	
18	129.7 (d)	160	7.31	
19	143.8 (s)	-		
20	21.5 (q)	127	2.41 (s)	



The ^{1}H and ^{13}C NMR data of compound **26**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H).

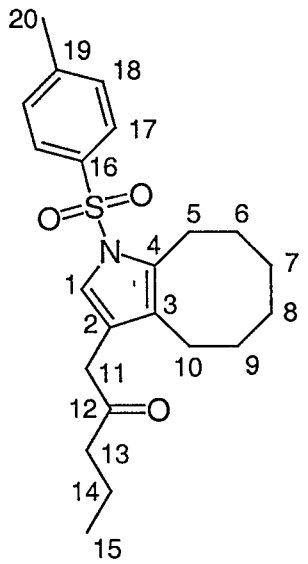
MS (EI) *m/z* (rel intensity) 423 ([M^+] 2), 388 (99), 352 (10), 304 (100), 268 (13), 232 (41), 217 (89), 205 (10), 184 (6), 155 (20), 91 (17), 43 (10).

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H	
1a/1b	49.4 (dd)	151/139	3.58 (d, J = 10.4)	3.48 (dd, J = 10.4, 0.6)
2	28.5 (s)	-		
3	32.4 (d)	166	1.41	
4	60.4 (d)	137	3.51 (td, J = 4.4, 1.1)	
5a/5b	32.7 (t)	127	2.50	1.41
6a/6b	19.1 (t)	127	1.59	1.42
7a/7b	25.6 (t)	124	1.88 (m)	1.34 (m)
8	26.6 (t)	125	1.54	
9a/9b	19.2 (t)	128	2.00 (m)	1.81 (dq, J = 13.9, 3.7)
10	28.8 (d)	152	0.97 (ddd, J = 12.5, 8.6, 4.0)	
11	69.6 (d)	150	3.90 (s)	
12	202.4 (s)	-		
13	41.6 (t)	126	2.47 (td, J = 7.2, 1.6)	
14	17.0 (t)	129	1.58	
15	13.6 (q)	126	0.89 (t, J = 7.4)	
16	131.7 (s)	-		
17	128.0 (d)	165	7.65	
18	129.6 (d)	161	7.32	
19	143.7 (s)	-		
20	21.6 (q)	127	2.41 (s)	



The ^{1}H and ^{13}C NMR data of compound **24**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H).

MS (EI) *m/z* (rel intensity) 387 ([M^+] 23), 359 (7), 316 (100), 232 (15), 160 (18), 91 (11)

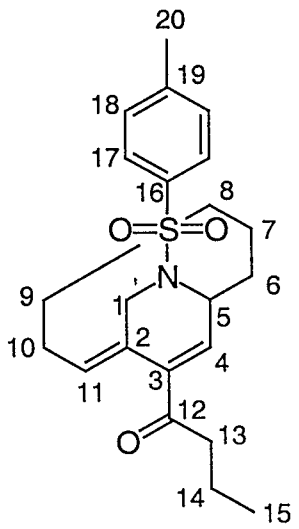
HR-MS ($C_{22}H_{29}NSO_3$): *calcd.* 387.186826; *found* 387.1855

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H
1	119.8 (d)	192	7.13 (s)
2	118.8 (s)	-	
3	126.3 (s)	-	
4	131.3 (s)	-	
5	23.5 (t)	128	2.75 (m)
6	29.4 (t)	126	1.49 (m)
7	25.5 (t)	125	1.23 (m)
8	26.1 (t)	125	1.29 (m)
9	30.0 (t)	126	1.44 (m)
10	23.2 (t)	126	2.31 (m)
11	39.7 (t)	127	3.38 (m)
12	208.3 (s)	-	
13	43.4 (t)	125	2.37 (t, J = 7.3)
14	17.2 (t)	129	1.54 (sext., J = 7.3)
15	13.6 (q)	126	0.85 (t, J = 7.4)
16	136.9 (s)	-	
17	126.5 (d)	166	7.60
18	129.8 (d)	161	7.23
19	144.5 (s)	-	
20	21.5 (q)	128	2.37 (s)



The ^{1}H and ^{13}C NMR data of compound **25**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H).

MS (EI) *m/z* (rel intensity) 387 ([M^{+}]), 304 (10), 248 (17), 232 (100), 155 (29), 150 (21), 91 (48), 83 (16), 71 (11), 55 (11), 43 (15).

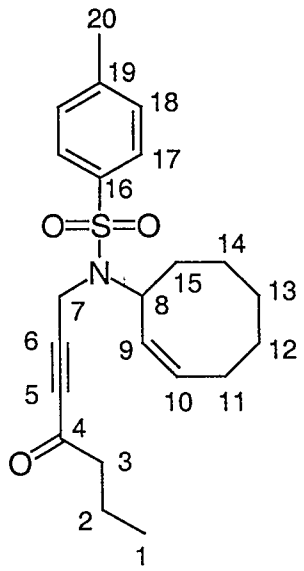
HR-MS ($C_{22}H_{29}NSO_3$): *calcd.* 387.18682; *found* 387.1856

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H	
1a/1b	45.3 (dd)	147/139	4.51 (d, J = 10.9)	3.31 (dd, J = 10.9, 1.5)
2	127.3 (s)	-		
3	143.9 (s)	-		
4	136.0 (d)	162	6.51 (d, J = 7.1)	
5	54.2 (d)	138	4.58 (dt, J = 7.0, 4.0)	
6a/6b	35.3 (t)	127	2.04 (dddd, J = 14.7, 13.5, 4.4, 1.4)	1.59 (m)
7a/7b	25.2 (t)	125	1.48	0.94 (td, J = 13.5, 9.5)
8a/8b	25.6 (t)	125	1.74	1.40
9a/9b	27.8 (t)	127	1.76	1.02 (qd, J = 12.5, 3.8)
10a/10b	29.0 (t)	129	2.39	2.29 (m)
11	135.9 (d)	155	5.58 (ddd, J = 11.6, 5.7, 1.4)	
12	198.2 (s)	-		
13	40.3 (t)	126	2.49 (t, J = 7.3)	
14	17.9 (t)	129	1.50 (sext., J = 7.5)	
15	13.6 (q)	126	0.83 (t, J = 7.4)	
16	135.1 (s)	-		
17	127.3 (d)	165	7.65	
18	126.7 (d)	160	7.26	
19	143.4 (s)	-	2.38 (s)	
20	21.5 (q)	127		

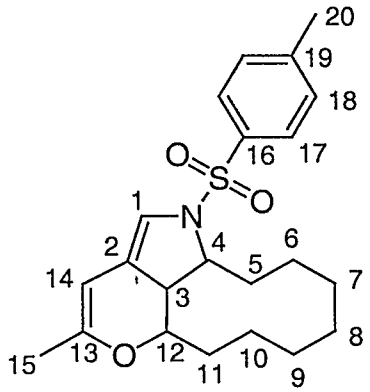


The ^{1}H and ^{13}C NMR data of compound **12**. All assignments are unambiguous, except where indicated by *, and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H). Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker AMX 300

position	δ_C	^{1}J (C,H)	δ_H	
1	13.4 (q)	126	0.86 (t, J = 7.4)	
2	17.2 (t)	128	1.55 (sext., J = 7.4)	
3	47.0 (t)	128	2.33 (t, J = 7.3)	
4	187.0 (s)	-		
5	83.0 (s)	-		
6	87.6 (s)	-		
7a/7b	33.0 (t)	144	4.30 (d, J = 19.2)	4.21 (d, J = 19.2)
8	55.7 (d)	137	4.83 (qd, J = 8.1, 1.0)	
9	127.5 (d)	n.d.	5.46 (ddd, J = 10.8, 8.2, 0.9)	
10	130.8 (d)	157	5.61 (dddd, J = 10.7, 9.5, 7.7, 1.2)	
11	26.2 (t)*	124		
12	28.7 (t)	128		
13	25.9 (t)*	124		
14	24.4 (t)	124		
15	34.3 (t)	128		
16	137.4 (s)	-		
17	127.5 (d)	164	7.71	
18	129.4 (d)	160	7.23	
19	143.4 (s)	-		
20	21.4 (q)	127	2.37 (s)	



The ^{1}H and ^{13}C NMR data of compound **35**. All assignments are unambiguous and were made using COSY, NOESY and $^{13}C,^{1}H$-chemical shift correlated NMR spectra (the latter optimized for ^{1}J(C,H) and for ^{n}J(C,H).

Arbitrary numbering as shown.

Solvent: $CDCl_3$

Spectrometer: Bruker DMX 600

position	δ_C	^{1}J (C,H)	δ_H	
1	120.8 (d)	187	6.18 (d, J = 1.9)	
2	116.8 (s)	-		
3	50.5 (d)	132	2.99 (ddd, J = 11.4, 6.0, 1.9)	
4	65.4 (d)	134	3.35 (td, J = 11.6, 3.3)	
5a/5b	34.6 (t)	129	2.51 (m)	1.84 (m)
6a/6b	20.1 (t)	127	1.58 (m)	1.33
7a/7b	27.3 (t)	126	1.51	1.34
8a/8b	23.3 (t)	125	1.39	0.92
9a/9b	20.0(t)	126	1.43	1.33
10a/10b	23.1 (t)	127	1.51	1.05 (m)
11a/11b	26.5 (t)	128	1.10 (m)	0.98 (m)
12	73.7 (d)	147	4.61 (dt, J = 5.8, 4.3)	
13	151.2 (s)	-		
14	93.5 (d)	165	5.19 (s)	
15	20.7 (q)	128	1.73 (s)	
16	131.2 (s)	-		
17	128.3 (d)	165	7.63	
18	129.5 (d)	161	7.31	
19	143.9 (s)	-		
20	21.5 (q)	127	2.40 (s)	

Table 1. Infrared Absorptions of New Compounds (cm^{-1})

Product	IR
5	3365, 3083, 2926, 2854, 1699, 1575, 1506, 1461, 1376, 1338, 1112, 1067, 961, 801, 750, 694
7	3360, 3346, 3088, 2952, 2925, 2913, 2854, 1568, 1495, 1465, 1454, 1432, 1202, 822, 744, 712
9	3439, 3252, 2927, 2856, 1646, 1599, 1494, 1442, 1321, 1162, 1153, 812, 670, 573
10	3277, 3065, 3026, 2928, 2856, 2121, 1648, 1598, 1495, 1451, 1336, 1162, 1094, 812, 664, 577
11	3025, 2929, 2857, 2242, 1718, 1650, 1598, 1495, 1435, 1240, 1258, 1162, 1092, 816, 752, 664, 586
12	3026, 2963, 2931, 2859, 2215, 1677, 1598, 1495, 1456, 1350, 1162, 1092, 1052, 813, 664, 583
13	3023, 2999, 2948, 2926, 2873, 1715, 1616, 1597, 1493, 1459, 1471, 1435, 1341, 1261, 1242, 1157, 1090, 1058, 813, 670, 544
16	3064, 2961, 2932, 2871, 1689, 1669, 1597, 1494, 1460, 1442, 1401, 1342, 1162, 1096, 1061, 1041, 1017, 815, 671, 594
17	3064, 3028, 2932, 2870, 1712, 1657, 1598, 1494, 1461, 1404, 1339, 1305, 1161, 1096, 1063, 1046, 815, 670, 548
18	3539, 3062, 3029, 2928, 2868, 1657, 1598, 1494, 1400, 1335, 1306, 1289, 1160, 1096, 1061, 1017, 814, 671, 548
19	3064, 2931, 2868, 1597, 1491, 1468, 1458, 1340, 1285, 1199, 1161, 1119, 1095, 1068, 1016, 1004, 815, 768, 691, 671, 583, 548
20	2953, 2926, 2868, 1657, 1598, 1494, 1464, 1343, 1163, 1094, 1042, 1017, 814, 709, 671, 580, 548
21	3064, 3028, 2963, 2930, 2864, 2255, 2116, 2091, 1711, 1597, 1494, 1461, 1402, 1344, 1166, 1092, 913, 815, 734, 673, 583, 550
22	3057, 3030, 2960, 2922, 2865, 1679, 1597, 1493, 1461, 1403, 1345, 1171, 1094, 1063, 955, 816, 671, 585, 551

Table 1. Infrared Absorptions of New Compounds (cm^{-1}), *continued*

24	3144, 3066, 3031, 2929, 2858, 1767, 1718, 1597, 1495, 1454, 1363, 1172, 1120, 1091, 1072, 1010, 814, 670, 580
25	3064, 3030, 2959, 2932, 2873, 2255, 1684, 1661, 1598, 1494, 1495, 1341, 1305, 1162, 1095, 913, 815, 733, 676, 549
26	3024, 2962, 2928, 2865, 1724, 1596, 1493, 1462, 1384, 1334, 1305, 1159, 1104, 1063, 1023, 820, 673
27	3025, 2929, 2859, 2226, 2649, 1598, 1495, 1451, 1338, 1305, 1162, 1093, 1052, 912, 810, 662, 578
28	3277, 2946, 2923, 2852, 1653, 1598, 1495, 1455, 1439, 1326, 1157, 1069, 1042, 812, 741, 670, 569, 548
29	3265, 3068, 3010, 2937, 2912, 2845, 2125, 1646, 1598, 1494, 1471, 1456, 1339, 1290, 1165, 1091, 902, 819, 735, 721, 659, 548
30	3417, 3325, 3016, 2962, 2933, 2867, 2246, 2206, 1675, 1597, 1492, 1475, 1460, 1445, 1337, 1287, 1222, 1162, 1090, 1053, 813, 661
31	3058, 2929, 2865, 1755, 1716, 1691, 1668, 1613, 1598, 1494, 1465, 1442, 1343, 1257, 1161, 1095, 1053, 815, 736, 670
32	2935, 2866, 1708, 1598, 1471, 1445, 1361, 1334, 1205, 1164, 1095, 1059, 813, 669, 548
33	3065, 2933, 2858, 1712, 1653, 1597, 1491, 1466, 1342, 1288, 1254, 1201, 1163, 1094, 1050, 815, 771, 691, 670, 586
34	2928, 2860, 1714, 1599, 1549, 1494, 1463, 1342, 1304, 1164, 1095, 1049, 815, 672, 590, 547
36	3219, 3065, 3030, 2964, 2931, 2867, 1598, 1493, 1460, 1380, 1340, 1305, 1162, 1095, 1055, 1018, 877, 812, 671, 588

Table 2. Mass Spectral Data of New Compounds

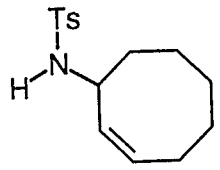
Product	MS (EI) *m/z* (rel. intensity)
5	219 ([M$^+$] 62), 190 (18), 176 (100), 162 (68), 148 (27), 134 (18), 120 (24), 106 (52), 93 (13), 80 (18), 41 (9)
7	219 ([M$^+$] 62), 190 (18), 176 (100), 162 (68), 148 (27), 134 (18), 120 (24), 106 (52), 93 (13), 80 (18), 41 (9)
9	279 ([M$^+$], 24), 236 (17), 155 (33), 124 (100), 108 (14), 91 (73), 80 (18), 65 (19), 55 (15), 41 (19), 30 (19)
10	317 ([M$^+$] 2), 235 (88), 170 (11), 162 (28), 155 (49), 118 (10), 106 (14), 91 (93), 80 (100), 67 (22), 55 (16), 39 (36)
11	375 ([M$^+$] 1), 193 (54), 261 (17), 234 (15), 220 (33), 188 (10), 155 (33), 138 (100), 106 (16), 91 (77), 79 (10), 67 (16), 41 (16)
12	387 ([M$^+$] 2), 305 (95), 262 (27), 232 (48), 162 (12), 155 (32), 150 (100), 122 (13), 91 (87), 80 (28), 71 (23), 65 (15), 55 (15), 43 (28)
13	375 ([M$^+$] 91), 343 (51), 316 (10), 300 (15), 220 (100), 188 (61), 160 (89), 118 (17), 91 (99), 80 (18), 65 (20), 41 (13)
16	387 ([M$^+$] 54), 316 (10), 232 (100), 162 (41), 155 (12), 91 (38), 80 (12), 71 (34), 43 (23)
17	389 ([M$^+$] 6), 318 (100), 234 (28), 155 (13), 91 (32), 80 (8), 71 (9), 43 (29)
18	391 ([M$^+$] 5), 319 (98), 318 (100), 264 (12), 248 (14), 234 (46), 218 (11), 164 (57), 155 (40), 91 (89), 80 (35), 67 (10), 65 (11), 55 (20), 43 (17)
19	527 ([M$^+$] 2), 373 (100), 344 (12), 330 (48), 316 (20), 288 (100), 276 (12), 261 (27), 234 (15(, 218 (76), 191 (10), 155 (36), 134 (19), 107 (11), 91 (66), 80 (19), 67 (18), 65 (13), 60 (20), 55 (15), 41 (15)
20	375 ([M$^+$] 68), 332 (15), 318 (60), 304 (16), 291 (100), 277 (27), 263 (16), 248 (41), 234 (79), 220 (18), 155 (58), 136 (11), 109 (16), 91 (94), 80 (49), 67 (16), 55 (23), 41 (23)
27	373 ([M$^+$] 3), 316 (11), 291 (81), 248 (100), 235 (59), 218 (37), 155 (45), 136 (20), 109 (26), 91 (75), 80 (28), 67 (44), 55 (33), 41 (29)
28	307 ([M$^+$] 45), 236 (32), 223 (30), 210 (9), 155(57), 152 (91), 136 (23), 91 (100), 80 (25), 68 (31), 65 (21), 55 (17), 41 (29), 30 (20)

Table 2. Mass Spectral Data of New Compounds, *continued*

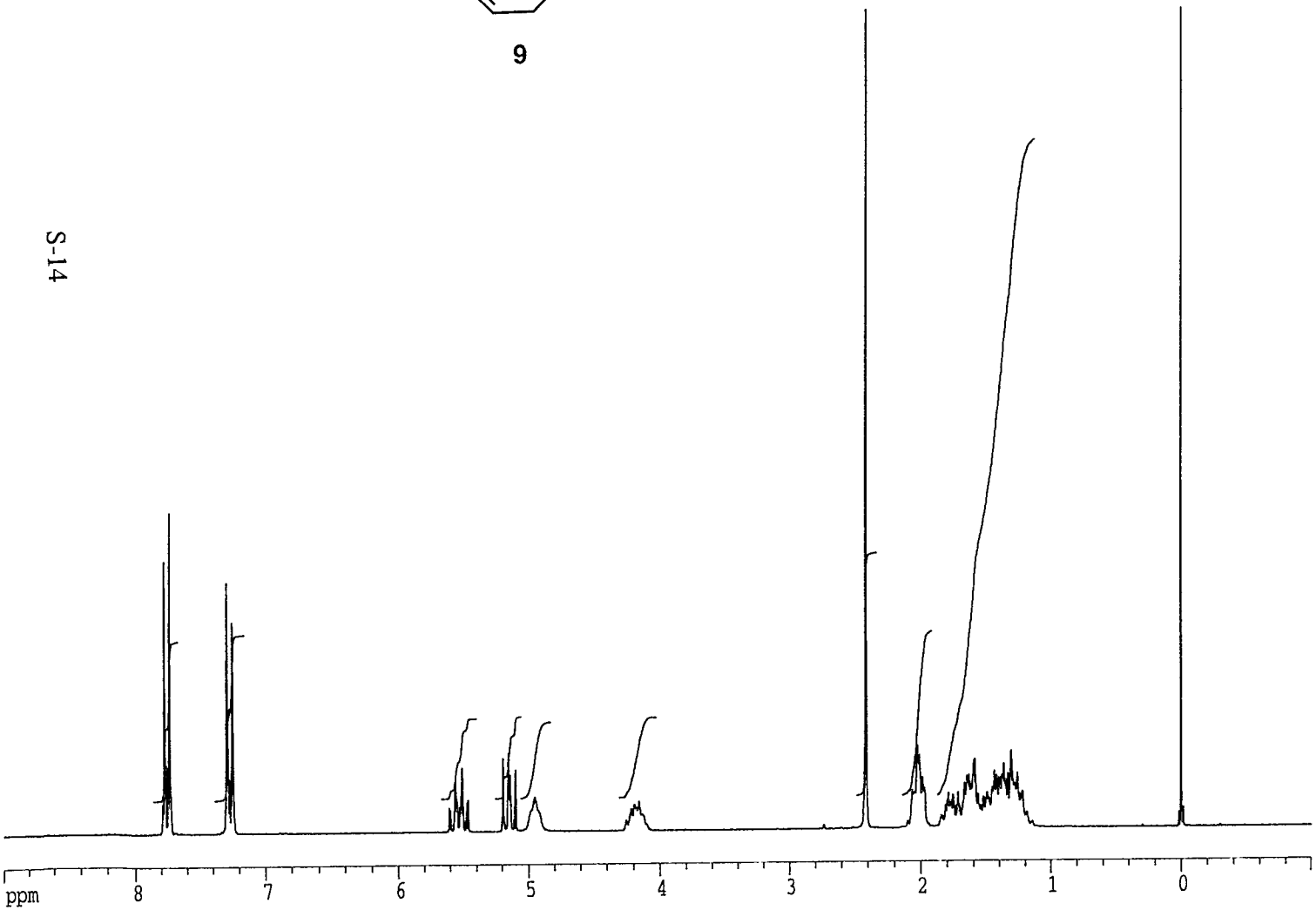
29	345 ([M^+] 18), 261 (11), 235 (100), 190 (44), 155 (32), 118 (12), 106 (39), 91 (74), 80 (48), 67 (18), 55 (15), 41 (23)
30	387 ([M^+] 12), 277 (100), 232 (89), 148 (27), 122 (58), 81 (11), 67 (11), 43 (30)
31	387 ([M^+] 46), 232 (100), 148 (17), 91 (31), 43 (26)
32	389 ([M^+] 6), 346 (100), 234 (34), 155 (17), 91 (34), 80 (9), 43 (13)
33	527 ([M^+]), 373 (96), 305 (19), 275 (67), 260 (80), 248 (11), 235 (15), 221 (13), 218 (67), 155 (46), 120 (12), 106 (20), 94 (100), 91 (83), 65 (30), 60 (46), 55 (22), 41 (22)
34	375 ([M^+] 51), 346 (29), 319 (12), 305 (23), 291 (12), 263 (100), 248 (20), 234 (33), 155 (42), 108 (19), 91 (78), 80 (27), 69 (11), 55 (23), 41 (22)
36 [a]	556 [$M+H^+$], 573 [$M+NH_4^+$], 578 [$M+Na^+$], 594 [$M+K^+$]

[a] MS (ESI/pos. in CH_3CN).

SZI-SA-030-01



9



Current Data Parameters

NAME	AP150F
EXPNO	118
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970415
Time	22.30
INSTRUM	ac200
PROBHD	
PULPROG	X51.AU
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4032.258 Hz
FIDRES	0.123055 Hz
AQ	4.0632820 sec
RG	10
DW	124.000 usec
DE	155.00 usec
TE	300.0 K
P1	10.10 usec
HL1	83 dB
D1	1.00000000 sec
DE	155.00 usec
SFO1	200.1332390 MHz
NUCLEUS	1H

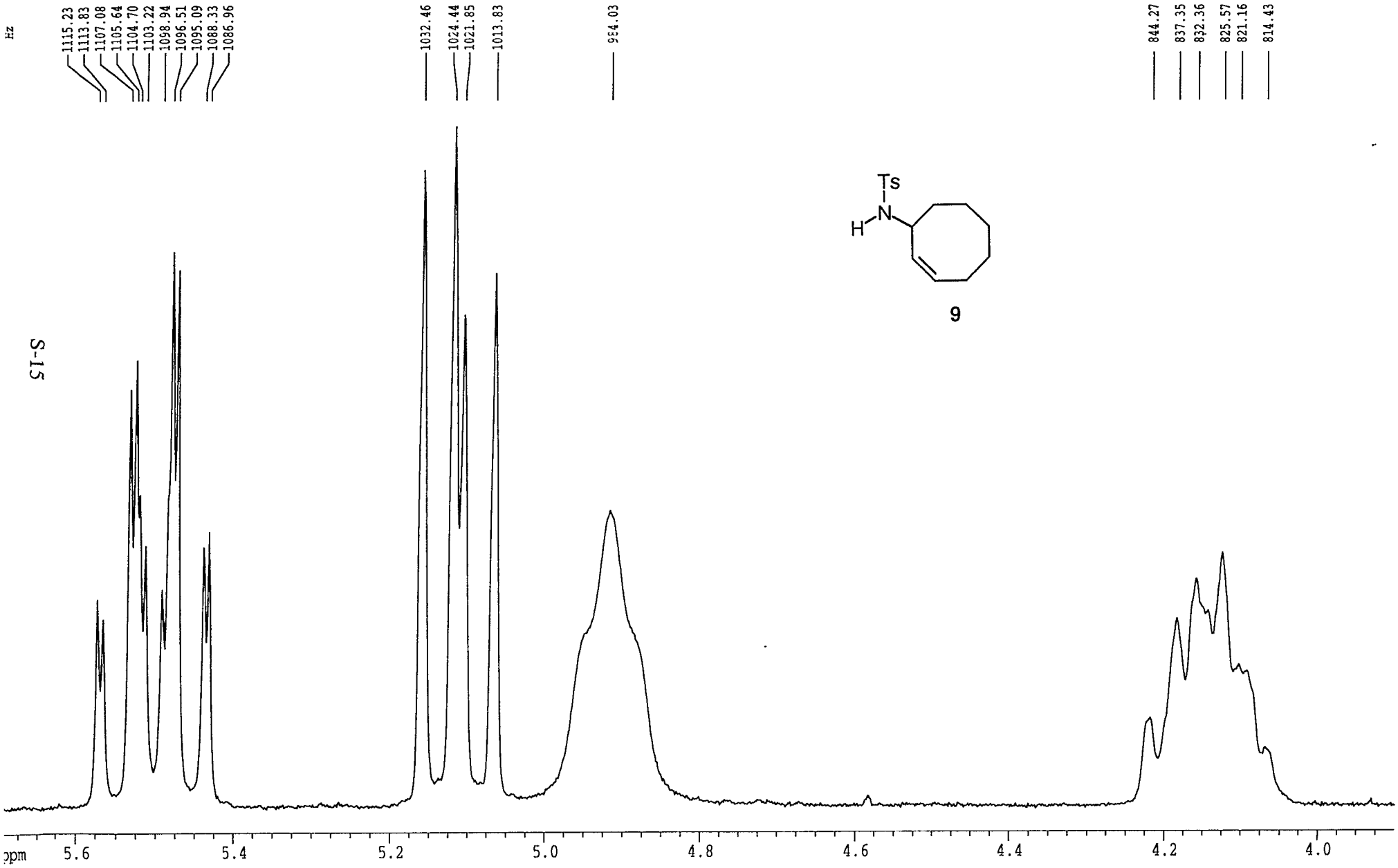
F2 - Processing parameters

SI	16384
SF	200.1323382 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	0.00

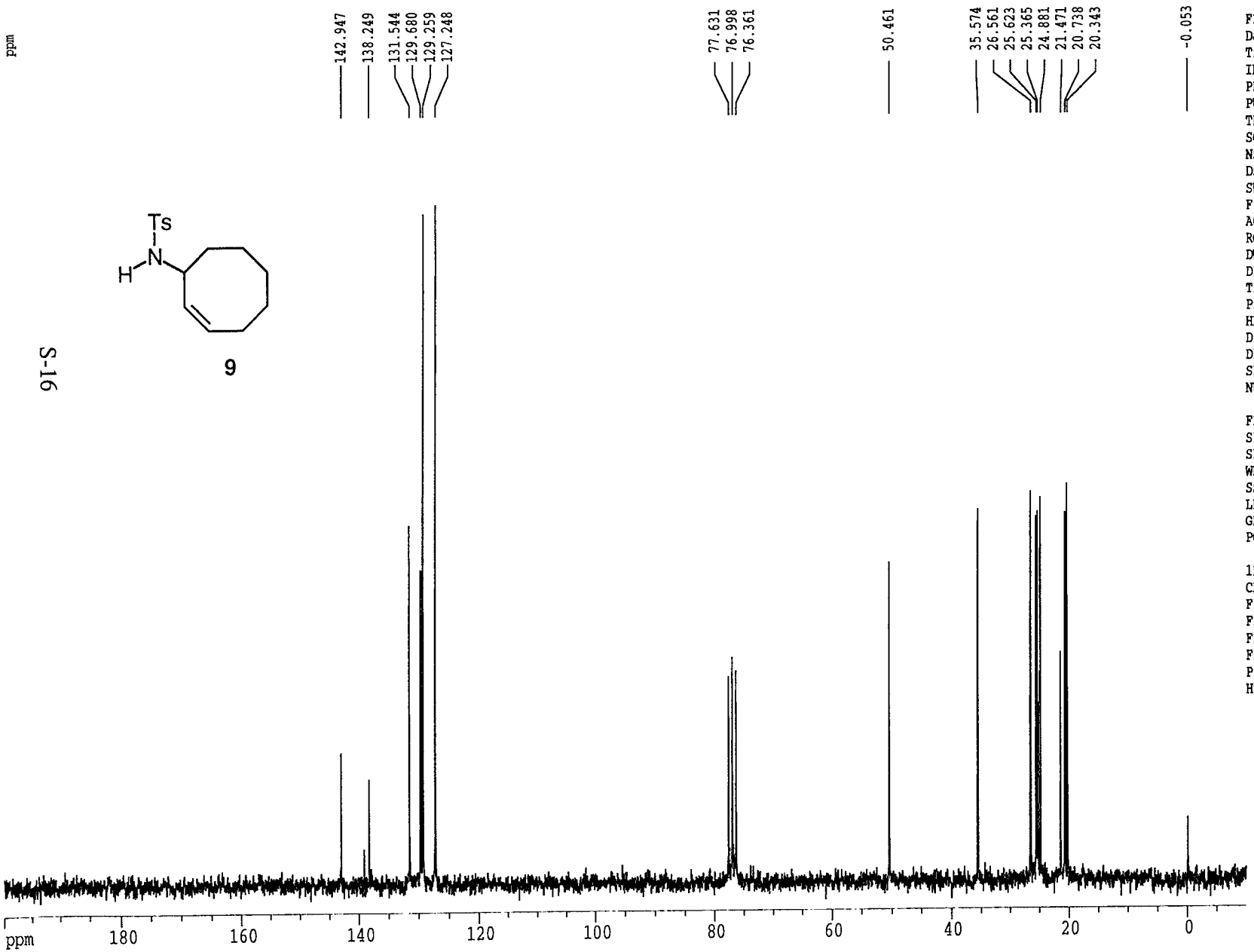
1D NMR plot parameters

CX	20.00 cm
F1P	9.000 ppm
F1	1801.19 Hz
F2P	-1.000 ppm
F2	-200.13 Hz
PPMCM	0.50000 ppm/cm
HZCM	100.06617 Hz/cm

SZI-SA-030-01


Hz
1115.23
1113.83
1107.08
1105.64
1104.70
1103.22
1098.94
1096.51
1095.09
1088.33
1086.96
1032.46
1024.44
1021.85
1013.83
984.03
844.27
837.35
832.36
825.57
821.16
814.43
Ts
N
H
9
ppm
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0

SZI-SA-031-03



Current Data Parameters

NAME	AP151F
EXPNO	119
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970416
Time	0.17
INSTRUM	ac200
PROBHD	
PULPROG	X60.AU
TD	32768
SOLVENT	CDCl3
NS	1568
DS	0
SWH	14285.714 Hz
FIDRES	0.435965 Hz
AQ	1.1469300 sec
RG	640
DW	35.000 usec
DE	46.30 usec
TE	300.0 K
P1	15.50 usec
HL1	20 dB
D1	0.00100000 sec
DE	46.30 usec
SFO1	50.3287650 MHz
NUCLEUS	13C

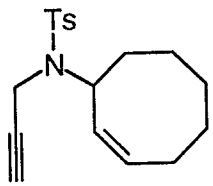
F2 - Processing parameters

SI	16384
SF	50.3233180 MHz
WDW	EM
SSB	0
LB	1.60 Hz
GB	0
PC	2.00

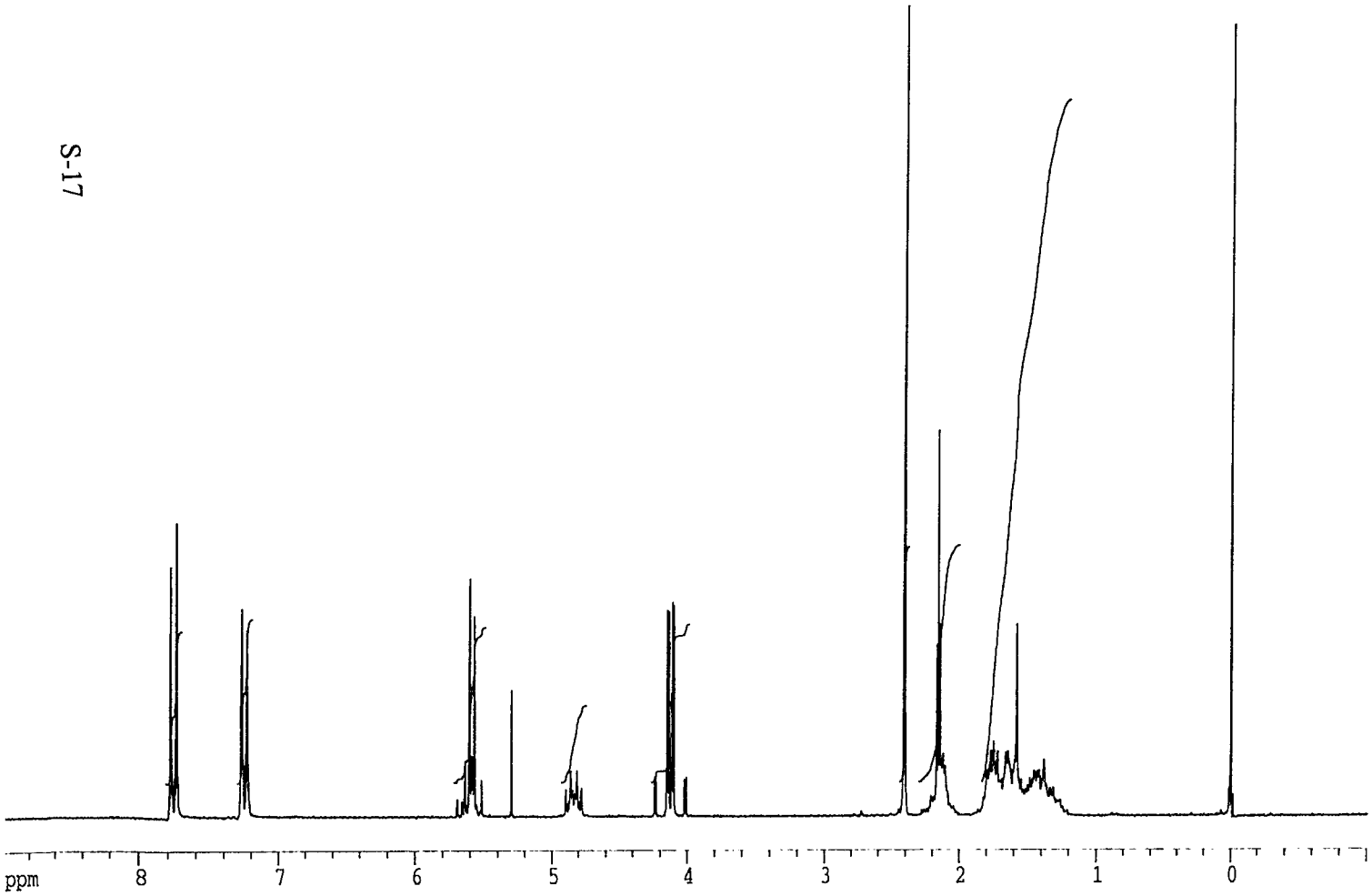
1D NMR plot parameters

CX	22.00 cm
F1P	200.000 ppm
F1	10064.66 Hz
F2P	-10.000 ppm
F2	-503.23 Hz
PPMCM	9.54545 ppm/cm
HZCM	480.35892 Hz/cm

SZI-SA-032-01



10



Current Data Parameters

NAME	AG130F
EXPNO	102
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970813
Time	10.39
INSTRUM	ac200
PROBHD	
PULPROG	X59.AU
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4032.258 Hz
FIDRES	0.123055 Hz
AQ	4.0632820 sec
RG	40
DW	124.000 usec
DE	155.00 usec
TE	300.0 K
P1	10.10 usec
HL1	83 dB
D1	1.00000000 sec
DE	155.00 usec
SFO1	200.1332390 MHz
NUCLEUS	1H

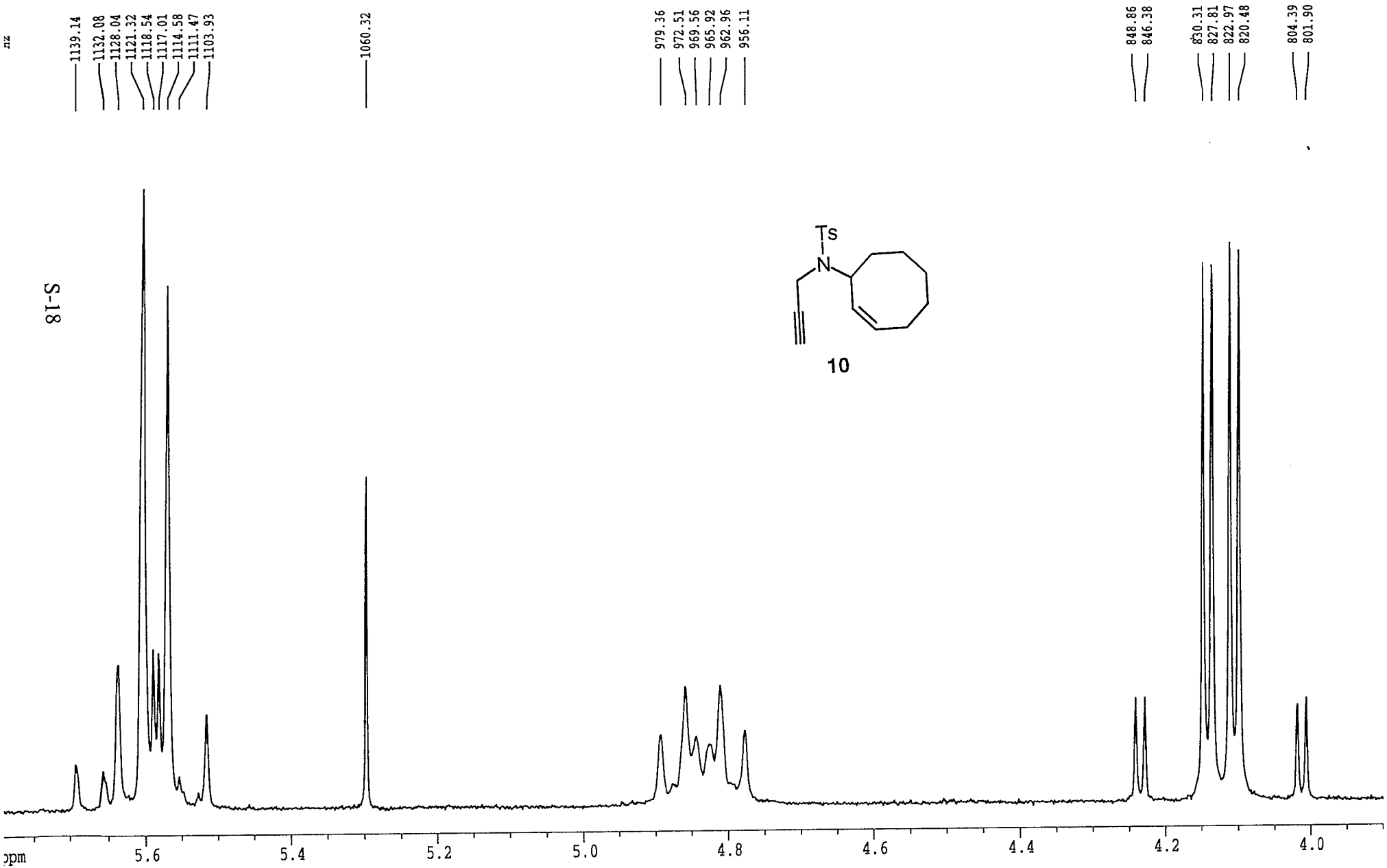
F2 - Processing parameters

SI	16384
SF	200.1323402 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

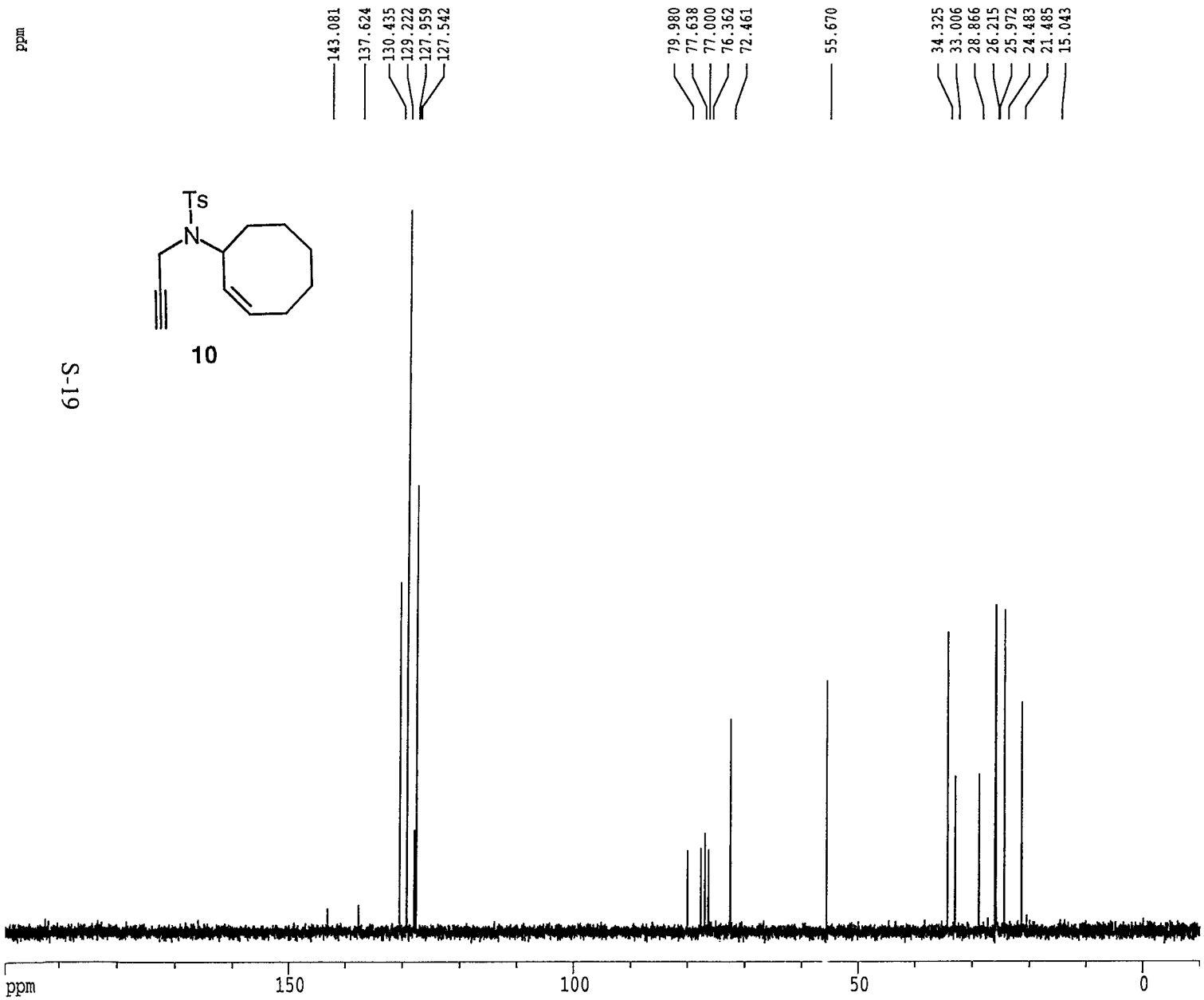
1D NMR plot parameters

CX	20.00 cm
F1P	9.000 ppm
F1	1801.19 Hz
F2P	-1.000 ppm
F2	-200.13 Hz
PPMCM	0.50000 ppm/cm
HZCM	100.06617 Hz/cm

SZI-SA-032-01


1139.14
1132.08
1128.04
1121.32
1118.54
1117.01
1114.58
1111.47
1103.93
1060.32
979.36
972.51
969.56
965.92
962.96
956.11
848.86
846.38
830.31
827.81
822.97
820.48
804.39
801.90
Ts
N
10
ppm
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0

SZI-SA-032-01



Current Data Parameters

NAME	AG110F
EXPNO	144
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970812
Time	19.55
INSTRUM	ac200
PROBHD	
PULPROG	X60.AU
TD	32768
SOLVENT	CDCl3
NS	1568
DS	0
SWH	14285.714 Hz
FIDRES	0.435965 Hz
AQ	1.1469300 sec
RG	640
DW	35.000 usec
DE	46.30 usec
TE	300.0 K
P1	15.50 usec
HL1	20 dB
D1	0.00100000 sec
DE	46.30 usec
SFO1	50.3287650 MHz
NUCLEUS	13C

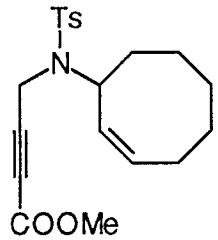
F2 - Processing parameters

SI	16384
SF	50.3233180 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

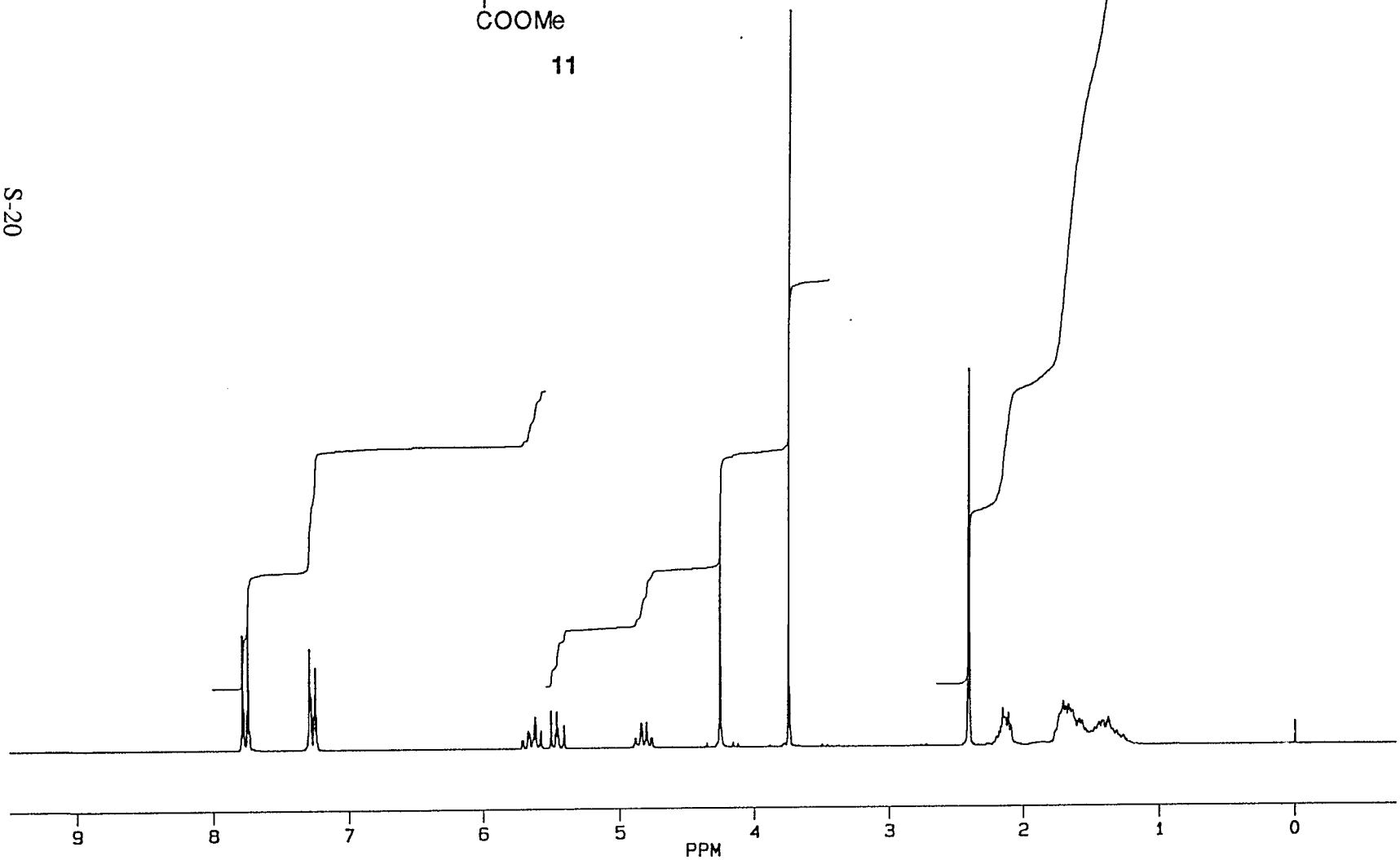
1D NMR plot parameters

CX	20.00 cm
F1P	200.000 ppm
F1	10064.66 Hz
F2P	-10.000 ppm
F2	-503.23 Hz
PPMCM	10.50000 ppm/cm
HZCM	528.39484 Hz/cm

SZI-SA-010-02



11



JL100F.103
AU PROG:
X59.AU
DATE 10-7-96
TIME 10:07

SA.NA SZISA010
SA.NO JL10 103
SOLVENT CDCl3
SF 200.132
SY 80.0
O1 3239.000
SI 32768
TD 32768
SW 4032.258
HZ/PT .246

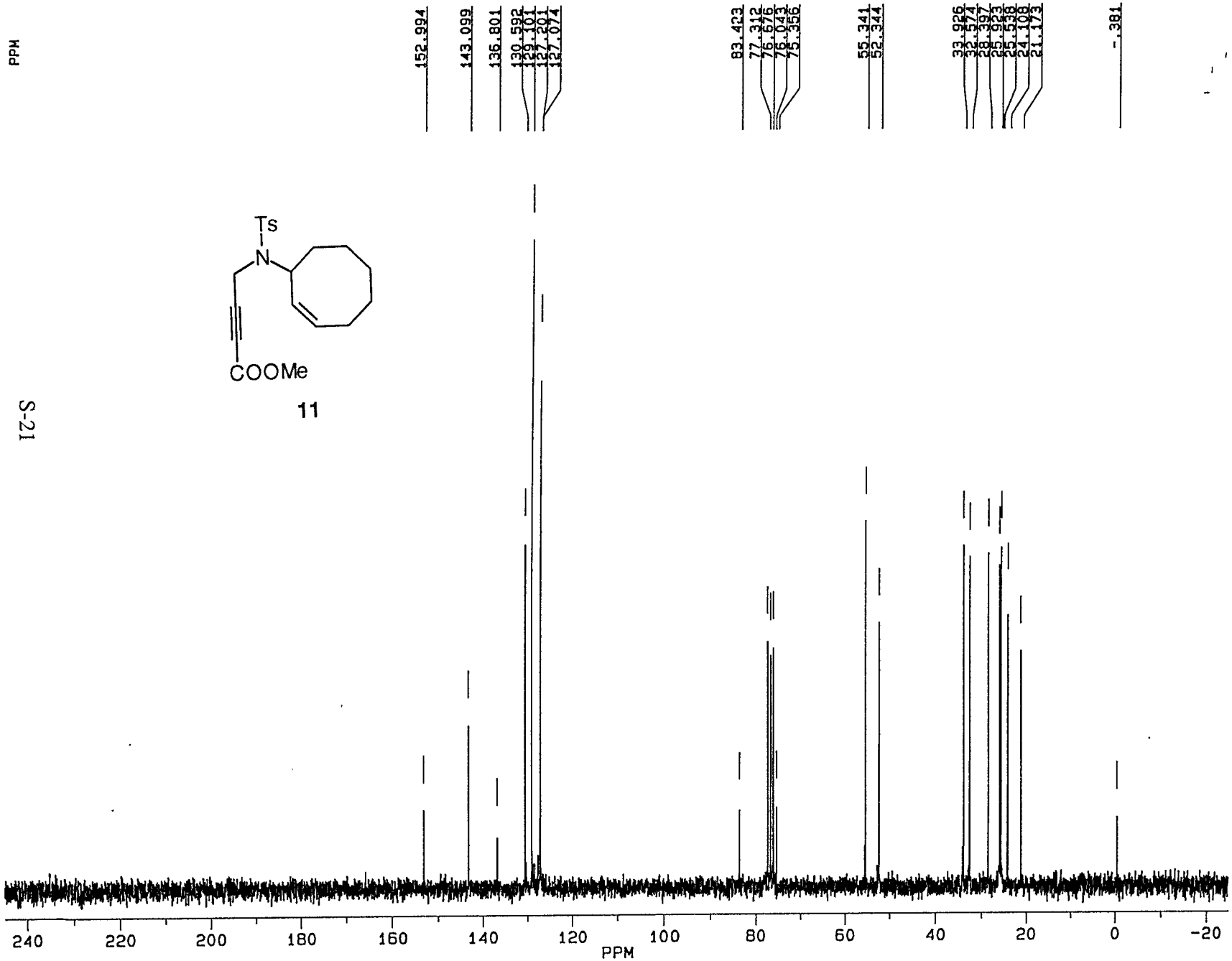
PW 0.0
RD 0.0
AQ 4.063
RG 10
NS 32
TE 300

FW 5100
O2 2228.997
DP 63L PO

LB 0.0
GB .180
CX 22.65
CY 12.00
F1 1900.21H
F2 -149.39H
HZ/CM 90.490
PPM/CM .452
SR 2337.01

D7 .0002000
D1 1.0000000
PO 3.40
RGA
RD 0.0
PW 0.0
DE 155.00
NS 32
DS 0

SZI-SA-010-01



MY071F.139
AU PROG:
X53.AU
DATE 7-5-96
TIME 23:52

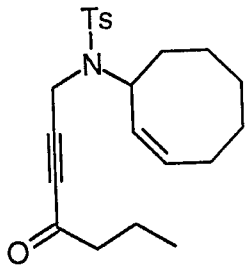
SA.NA SZISA010
SA.NO MY07 139
SOLVENT CDCl3
SF 50.323
SY 50.0
O1 1765.000
SI 32768
TD 32768
SW 14285.714
HZ/PT .872

PW 0.0
RD 0.0
AQ 1.147
RG 640
NS 1568
TE 300

FW 17900
O2 3239.000
DP 20H CPD

LB .800
GB 0.0
CX 22.65
CY 12.00
F1 245.015P
F2 -24.985P
HZ/CM 599.881
PPM/CM 11.921
SR -3665.39

SZI-SA-090-06



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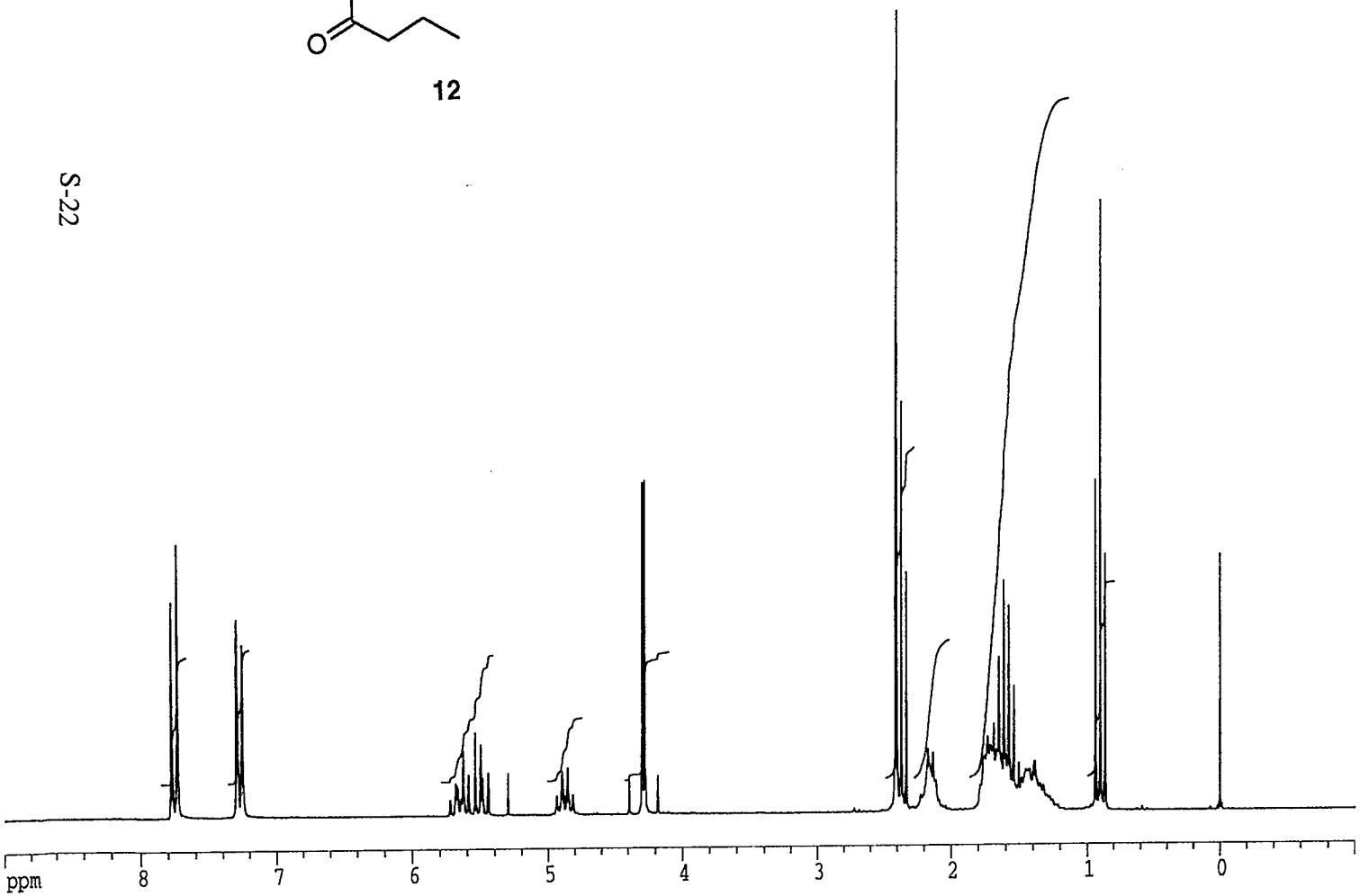


Current Data Parameters

NAME	AP160F
EXPNO	150
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970417
Time	9.01
INSTRUM	ac200
PROBHD	
PULPROG	X59.AU
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4032.258 Hz
FIDRES	0.123055 Hz
AQ	4.0632820 sec
RG	8
DW	124.000 usec
DE	155.00 usec
TE	300.0 K
P1	10.10 usec
HL1	83 dB
D1	1.00000000 sec
DE	155.00 usec
SFO1	200.1332390 MHz
NUCLEUS	1H

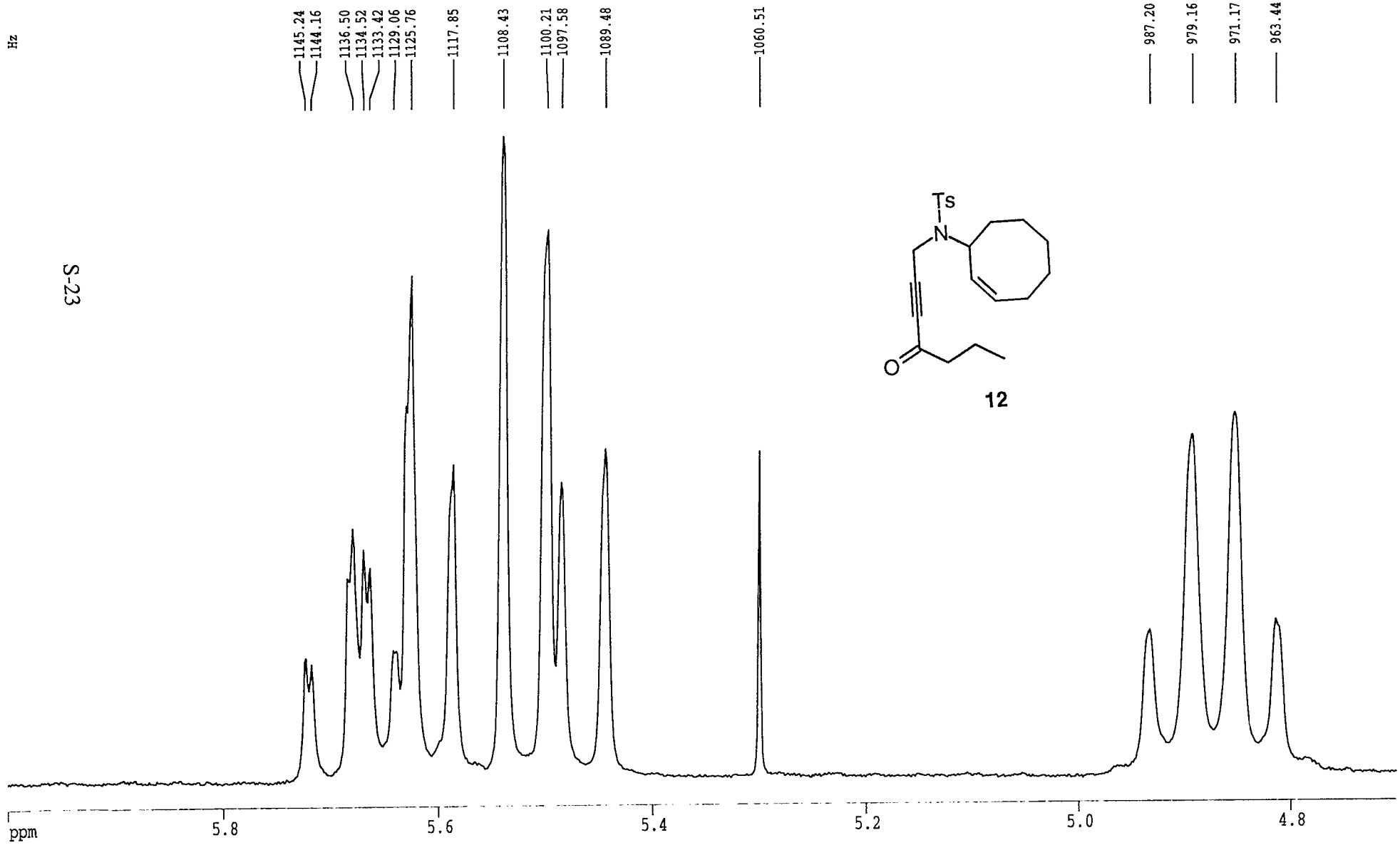
F2 - Processing parameters

SI	16384
SF	200.1323358 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	9.000 ppm
F1	1801.19 Hz
F2P	-1.000 ppm
F2	-200.13 Hz
PPMCM	0.50000 ppm/cm
HZCM	100.06617 Hz/cm

SZI-SA-090-06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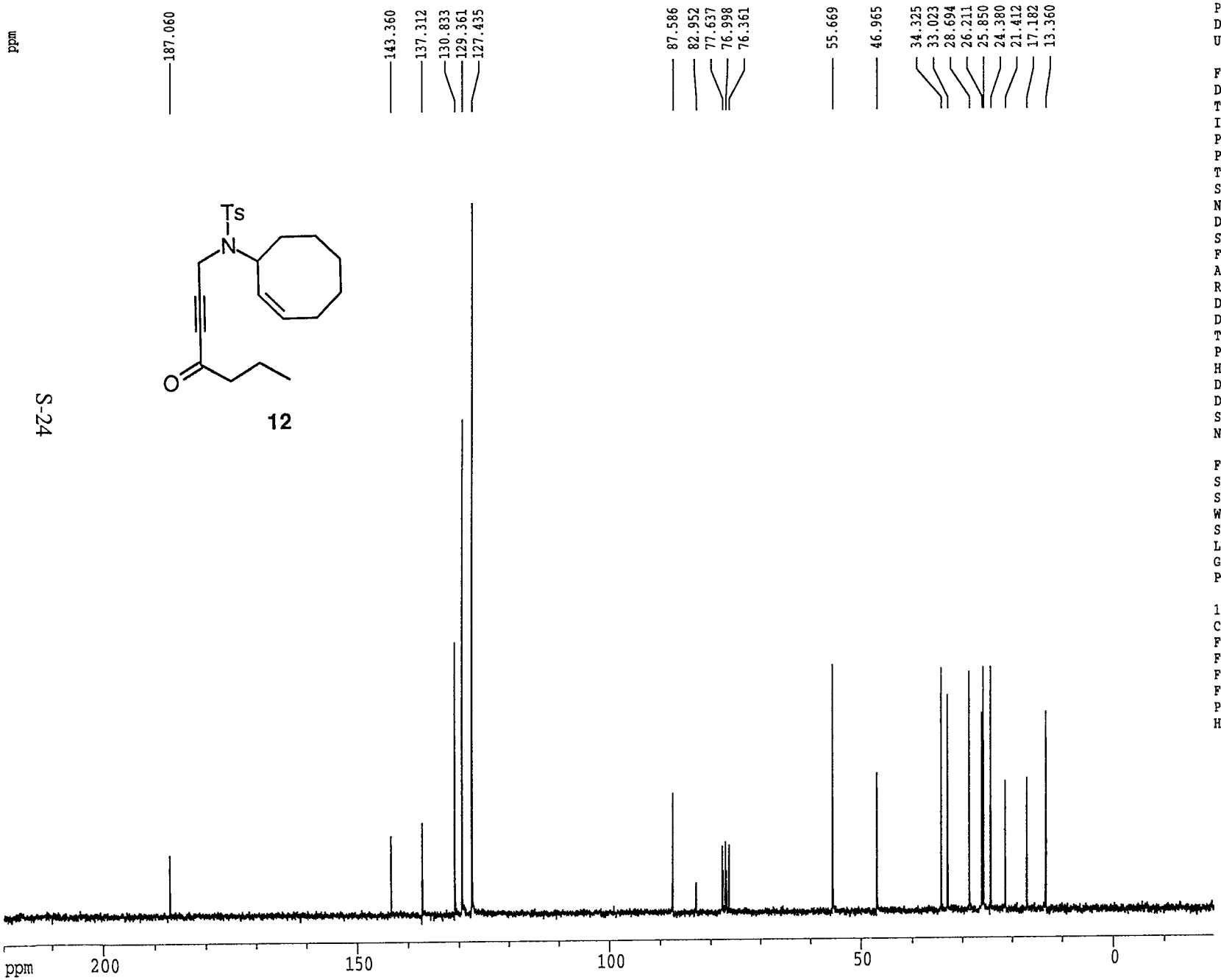
1144.16
1136.50
1134.52
1133.42
1129.06
1125.76
1117.85
1108.43
1100.21
1097.58
1089.48
1060.51
987.20
979.16
971.17
963.44
Ts
N
O
12
ppm
5.8
5.6
5.4
5.2
5.0
4.8

SZI-SA-090-06



Current Data Parameters

NAME	AP161F
EXPNO	150
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

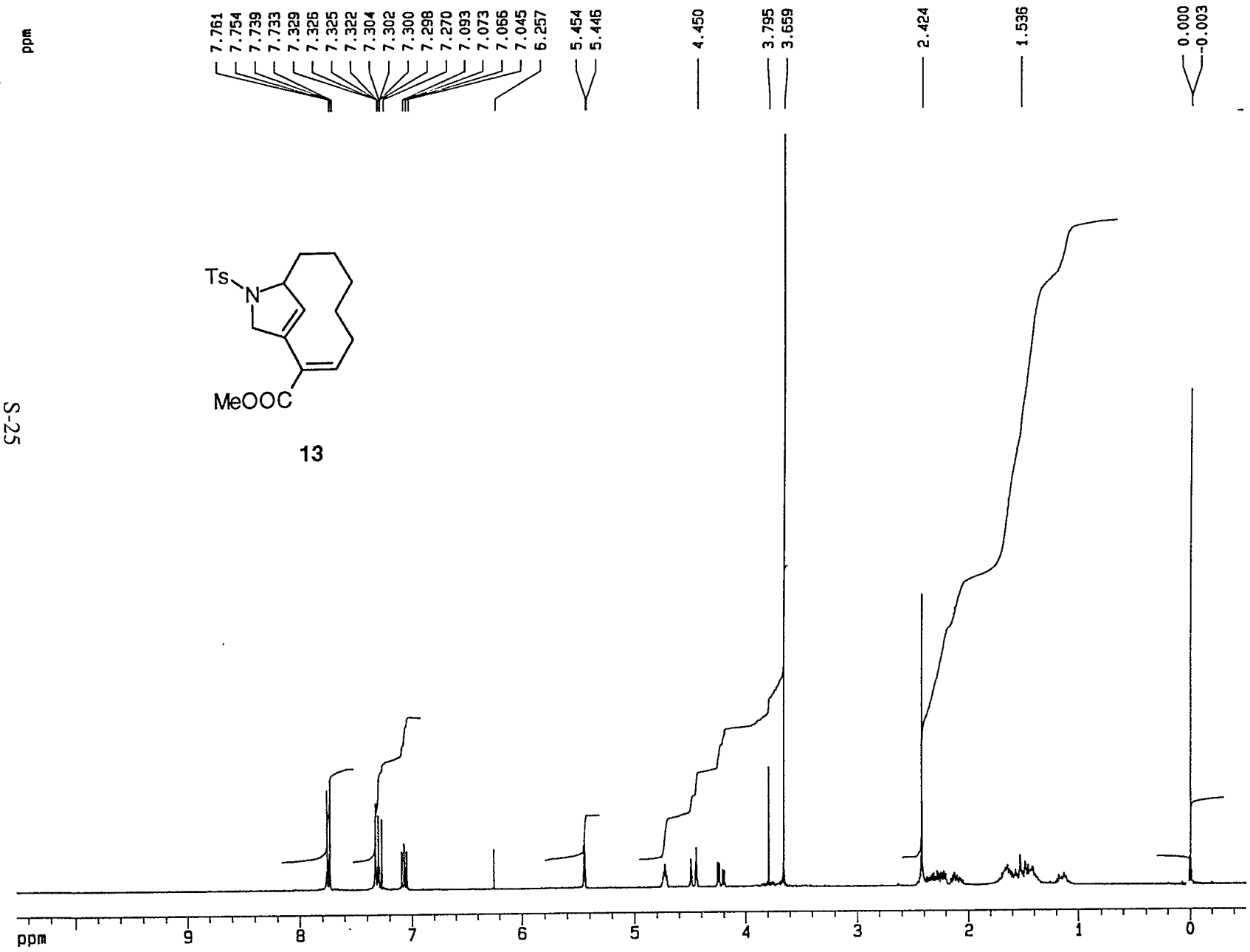
Date_	970417
Time	10.17
INSTRUM	ac200
PROBHD	
PULPROG	X60.AU
TD	32768
SOLVENT	CDCl3
NS	1568
DS	0
SWH	14285.714 Hz
FIDRES	0.435965 Hz
AQ	1.1469300 sec
RG	640
DW	35.000 usec
DE	46.30 usec
TE	300.0 K
P1	15.50 usec
HL1	20 dB
D1	0.00100000 sec
DE	46.30 usec
SFO1	50.3287650 MHz
NUCLEUS	13C

F2 - Processing parameters

SI	16384
SF	50.3233206 MHz
WDW	EM
SSB	0
LB	0.80 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.00 cm
F1P	220.000 ppm
F1	11071.13 Hz
F2P	-20.000 ppm
F2	-1006.47 Hz
PPMCM	10.90909 ppm/cm
HZCM	548.98169 Hz/cm



Current Data Parameters

NAME	aug23104
EXPNO	10
PROCNO	1
DU	u
USER	et

F2 - Acquisition Parameters

Date	960824
Time	0.37
PULPROG	zg30
SOLVENT	CDCl3
AQ	2.6214736 sec
DW	80.0 usec
RG	512
NUCLEUS	1H
SFO1	300.1349393 MHz
SFO2	360.1319532 MHz
TE	302.0 K
HL1	0 dB
D1	1.0000000 sec
P1	6.8 usec
DE	100.0 usec
SFO1	300.1349393 MHz
SWH	6249.97 Hz
TD	32768
NS	32
DS	2

F2 - Processing parameters

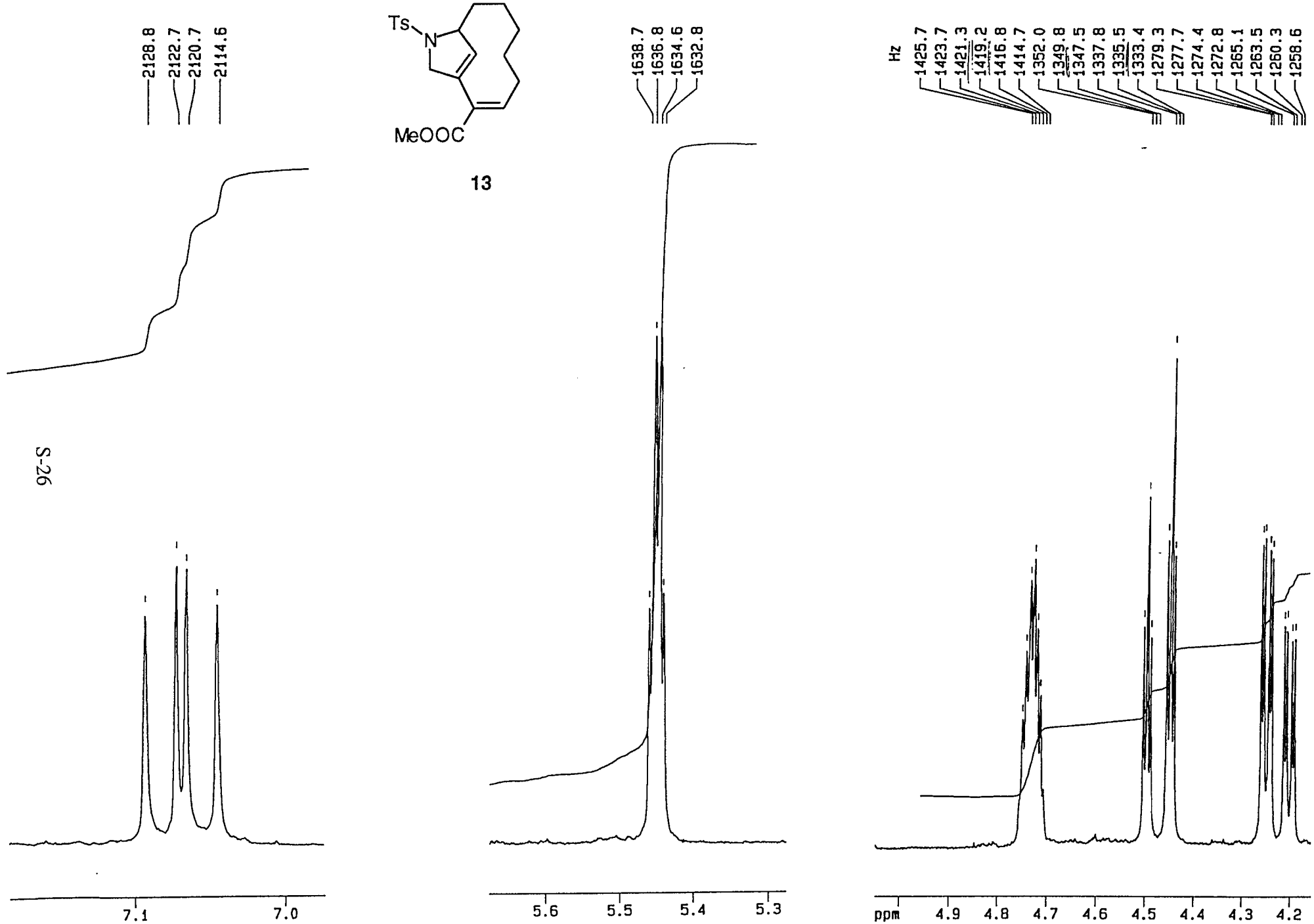
SI	32768
SF	300.1333645 MHz
SR	3364.45 Hz
HZpPT	0.1907 Hz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	8.00

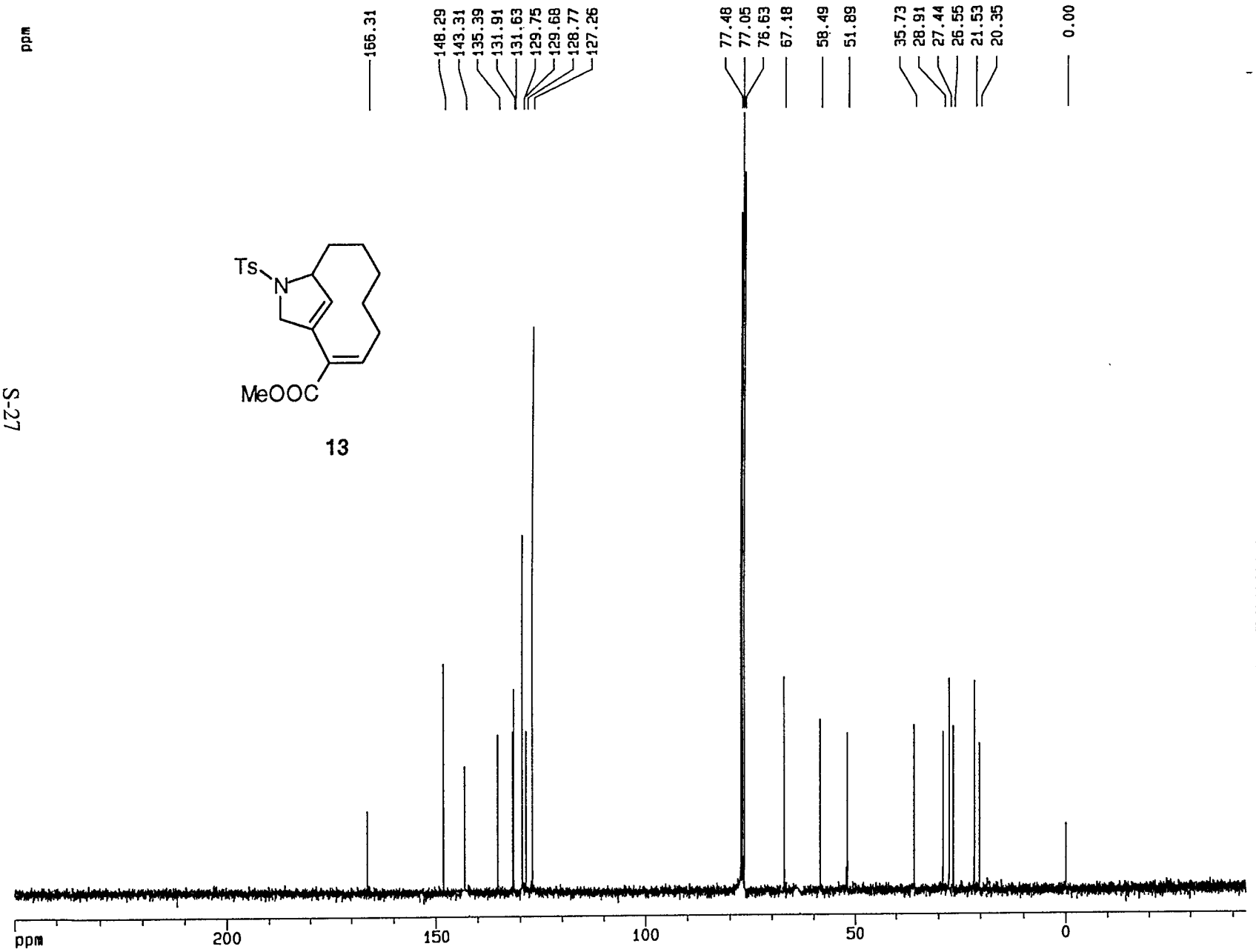
1D NMR plot parameters

CX	22.10 cm
CY	14.00 cm
F1P	10.500 ppm
F1	3151.40 Hz
F2P	-0.500 ppm
F2	-150.07 Hz
PPMCM	0.49774 ppm/cm
HZCM	149.38765 Hz/cm

SZI-SA-027-20

SZI-SA-027-20


Ts
N
MeOOC
13
2128.8
2122.7
2120.7
2114.6
1638.7
1636.8
1634.6
1632.8
Hz
1425.7
1423.7
1421.3
1419.2
1416.8
1414.7
1352.0
1349.8
1347.5
1337.8
1335.5
1333.4
1279.3
1277.7
1274.4
1272.8
1265.1
1263.5
1260.3
1258.6
7.1
7.0
5.6
5.5
5.4
5.3
ppm
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2



Current Data Parameters

NAME	aug23104
EXPNO	11
PROCNO	1
DU	u
USER	et

F2 - Acquisition Parameters

Date	960824
Time	0.46
PULPROG	zgdc15
SOLVENT	CDCl3
AQ	0.9830652 sec
DW	15.0 usec
RG	16384
NUCLEUS	13C
SFO1	75.4815977 MHz
SFO2	300.1344003 MHz
TE	302.0 K
D11	0.0300000 sec
P31	100.0 usec
S2	27 dB
HL1	0 dB
D1	0.0300000 sec
P1	5.7 usec
DE	21.4 usec
SFO1	75.4815977 MHz
SWH	33333.16 Hz
TD	65536
NS	8000
DS	16

F2 - Processing parameters

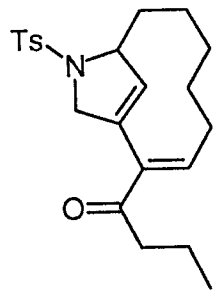
SI	32768
SF	75.4685900 MHz
SR	-1409.97 Hz
HZpPT	1.0172 Hz
WDW	EM
SSB	0
LB	0.80 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.10 cm
CY	14.00 cm
F1P	250.000 ppm
F1	18867.15 Hz
F2P	-42.900 ppm
F2	-3237.60 Hz
PPMCM	13.25339 ppm/cm
HZCM	1000.21490 Hz/cm

SZI-SA-027-20

SZI-SA-092-02



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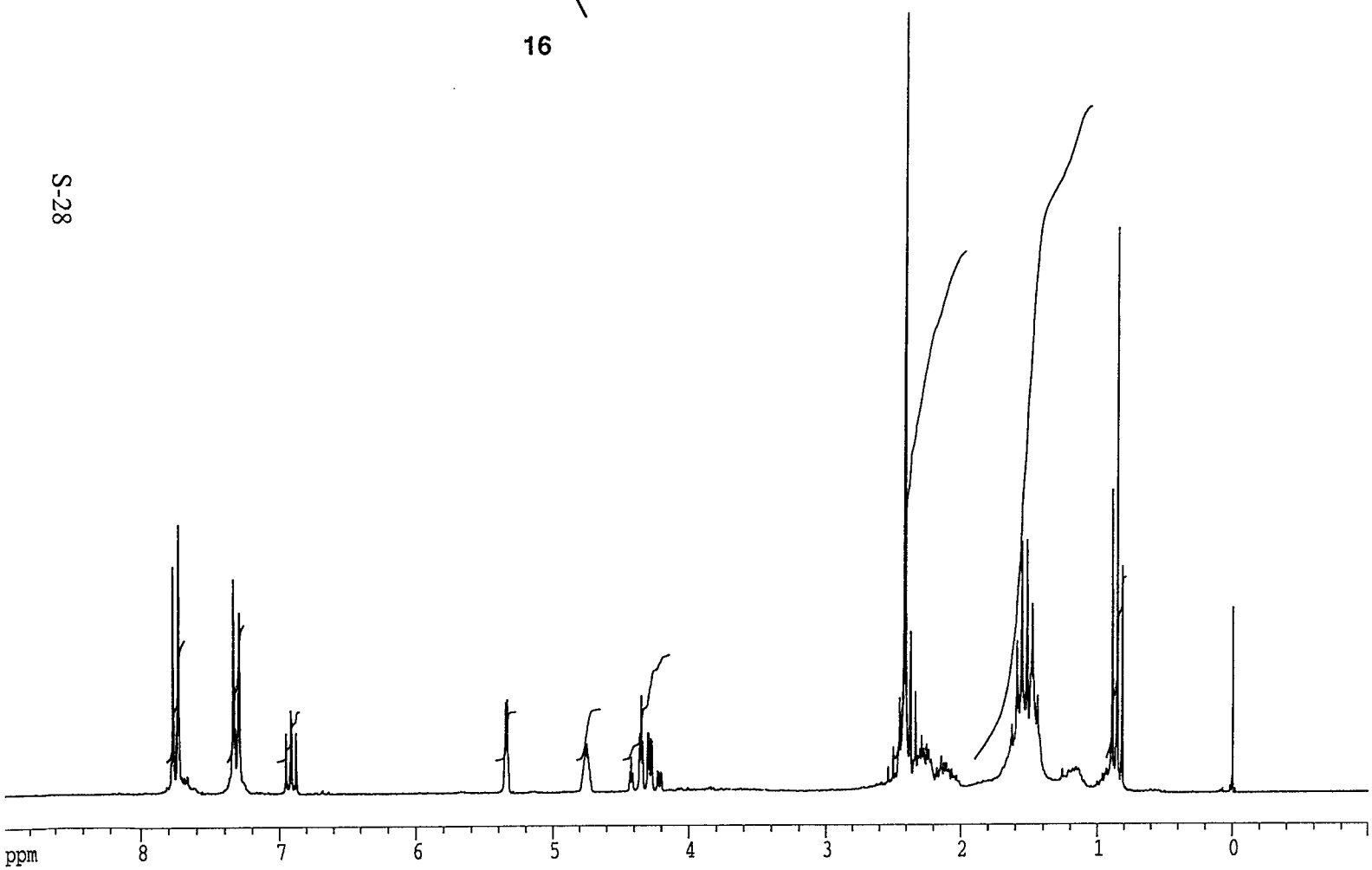


Current Data Parameters

NAME	AP160F
EXPNO	151
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970417
Time	10.58
INSTRUM	ac200
PROBHD	
PULPROG	X59.AU
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4032.258 Hz
FIDRES	0.123055 Hz
AQ	4.0632820 sec
RG	4
DW	124.000 usec
DE	155.00 usec
TE	300.0 K
P1	10.10 usec
HL1	83 dB
D1	1.00000000 sec
DE	155.00 usec
SFO1	200.1332390 MHz
NUCLEUS	1H

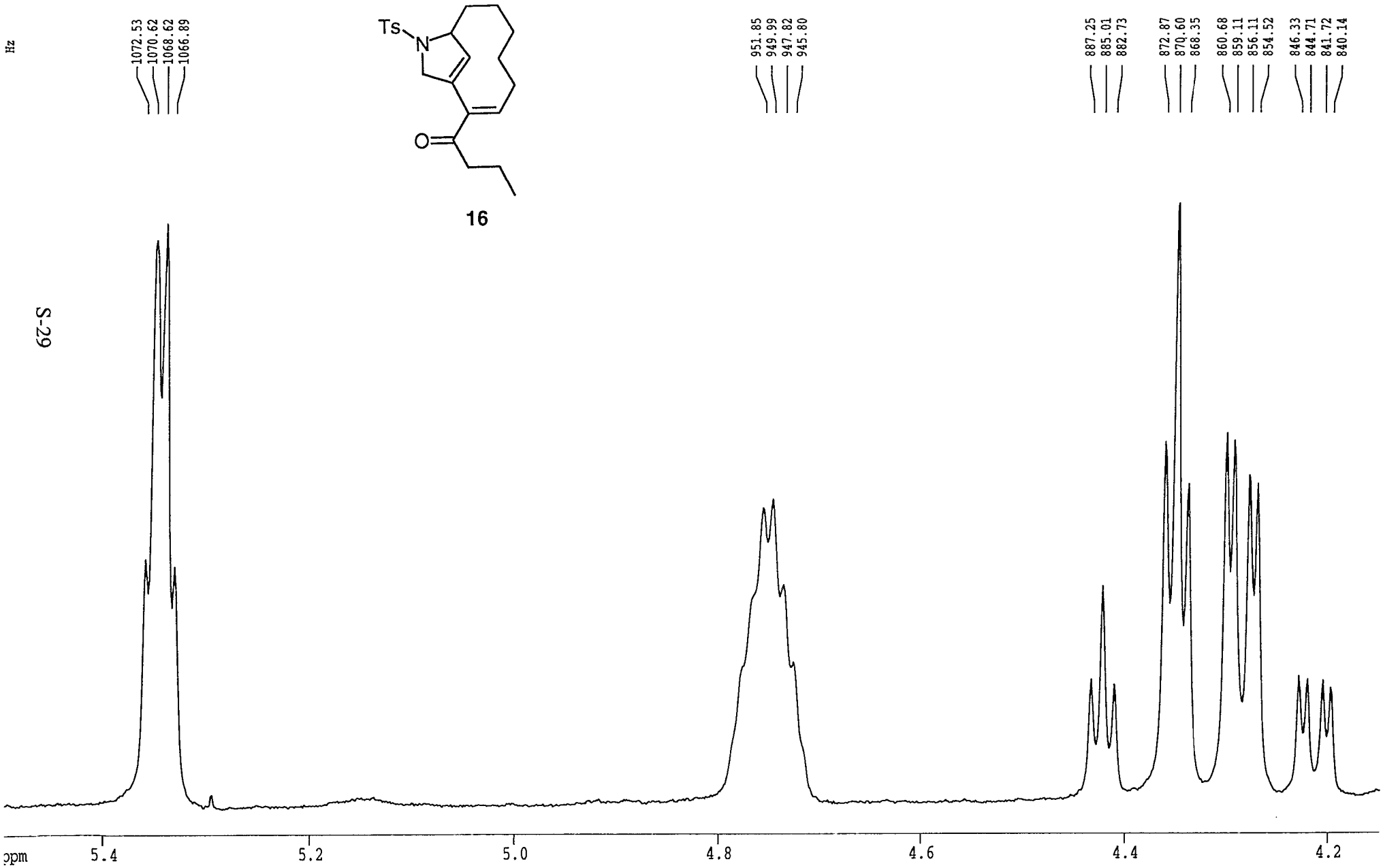
F2 - Processing parameters

SI	16384
SF	200.1323333 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

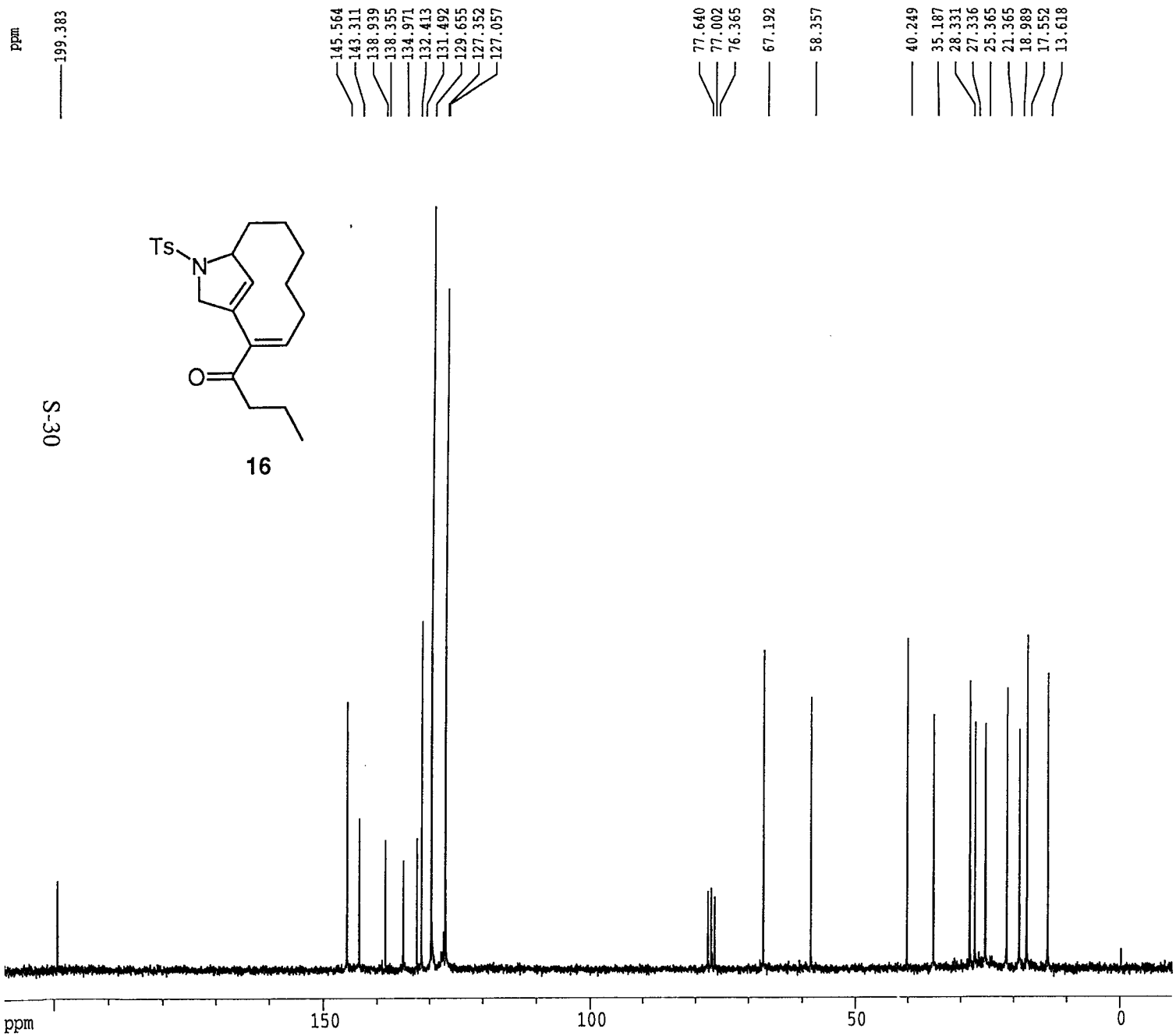
1D NMR plot parameters

CX	21.00 cm
F1P	9.000 ppm
F1	1801.19 Hz
F2P	-1.000 ppm
F2	-200.13 Hz
PPMCM	0.47619 ppm/cm
HZCM	95.30112 Hz/cm

SZI-SA-092-02


Hz
1072.53
1070.62
1068.62
1066.89
Ts
N
O
16
951.85
949.99
947.82
945.80
887.25
885.01
882.73
872.87
870.60
868.35
860.68
859.11
856.11
854.52
846.33
844.71
841.72
840.14
ppm
5.4
5.2
5.0
4.8
4.6
4.4
4.2

SZI-SA-092-02



Current Data Parameters

NAME	AP161F
EXPNO	151
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	970417
Time	11.32
INSTRUM	ac200
PROBHD	
PULPROG	X60.AU
TD	32768
SOLVENT	CDCl3
NS	1568
DS	0
SWH	14285.714 Hz
FIDRES	0.435965 Hz
AQ	1.1469300 sec
RG	400
DW	35.000 usec
DE	46.30 usec
TE	300.0 K
P1	15.50 usec
HL1	20 dB
D1	0.00100000 sec
DE	46.30 usec
SFO1	50.3287650 MHz
NUCLEUS	13C

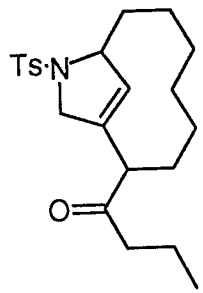
F2 - Processing parameters

SI	16384
SF	50.3233224 MHz
WDW	EM
SSB	0
LB	0.80 Hz
GB	0
PC	2.00

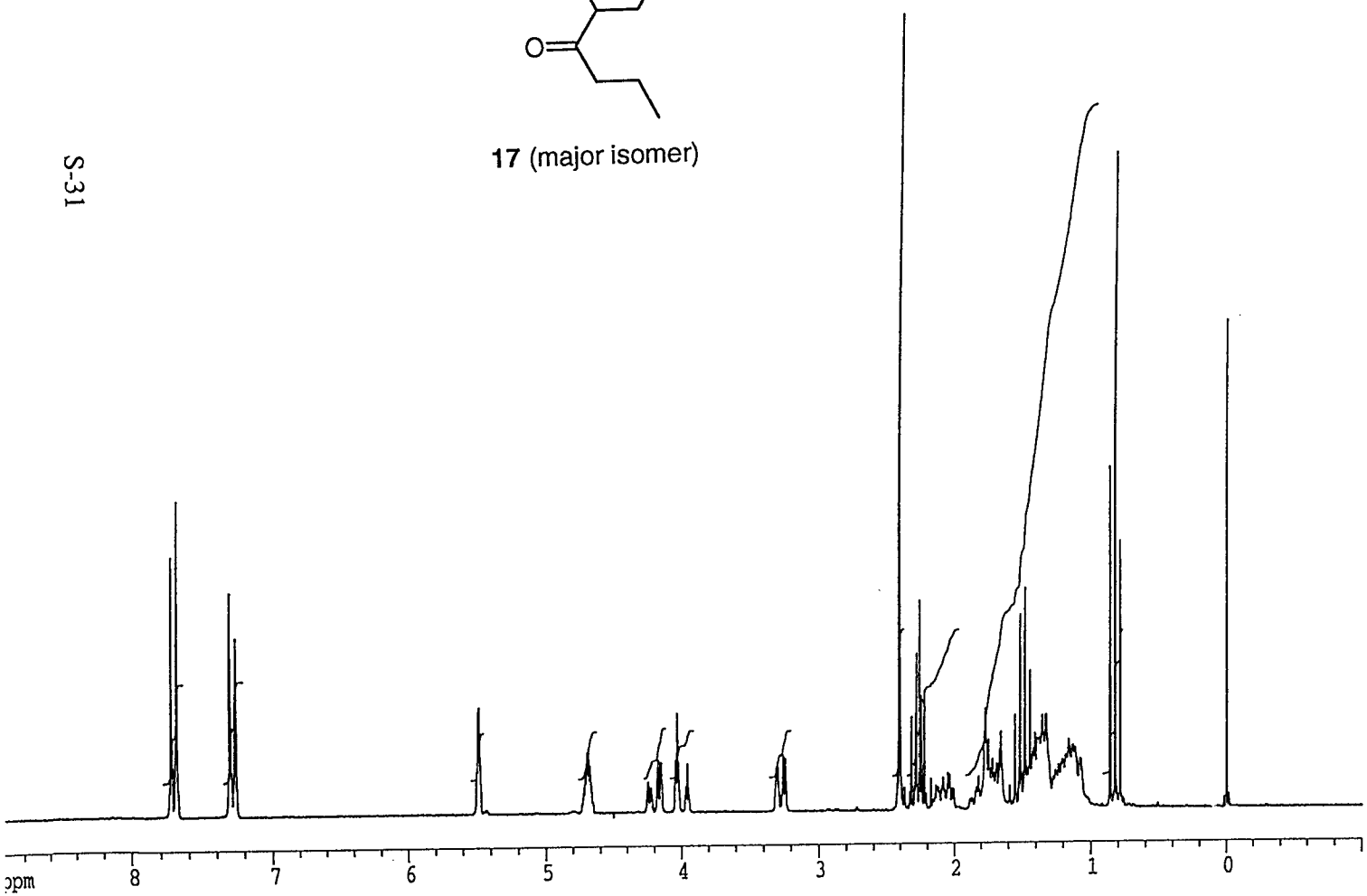
1D NMR plot parameters

CX	20.00 cm
F1P	210.000 ppm
F1	10567.90 Hz
F2P	-10.000 ppm
F2	-503.23 Hz
PPMCM	11.00000 ppm/cm
HZCM	553.55652 Hz/cm

SZI-SB-011-01



17 (major isomer)



Current Data Parameters

NAME	N0120F
EXPNO	107
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	971112
Time	14.16
INSTRUM	ac200
PROBHD	
PULPROG	X51.AU
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4032.258 Hz
FIDRES	0.123055 Hz
AQ	4.0632820 sec
RG	16
DW	124.000 usec
DE	155.00 usec
TE	300.0 K
P1	10.10 usec
HL1	83 dB
D1	1.00000000 sec
DE	155.00 usec
SFO1	200.1332390 MHz
NUCLEUS	1H

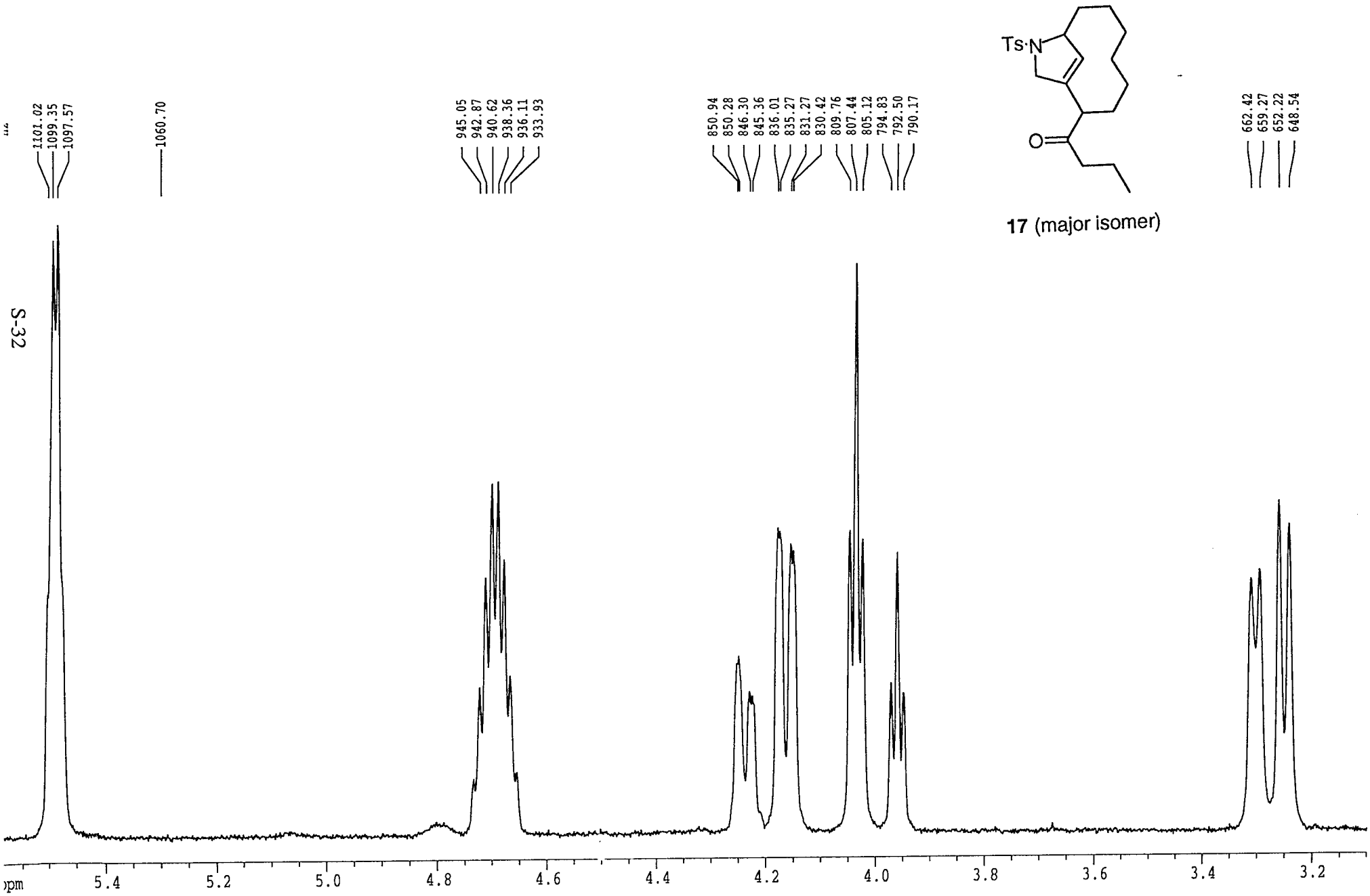
F2 - Processing parameters

SI	16384
SF	200.1323377 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

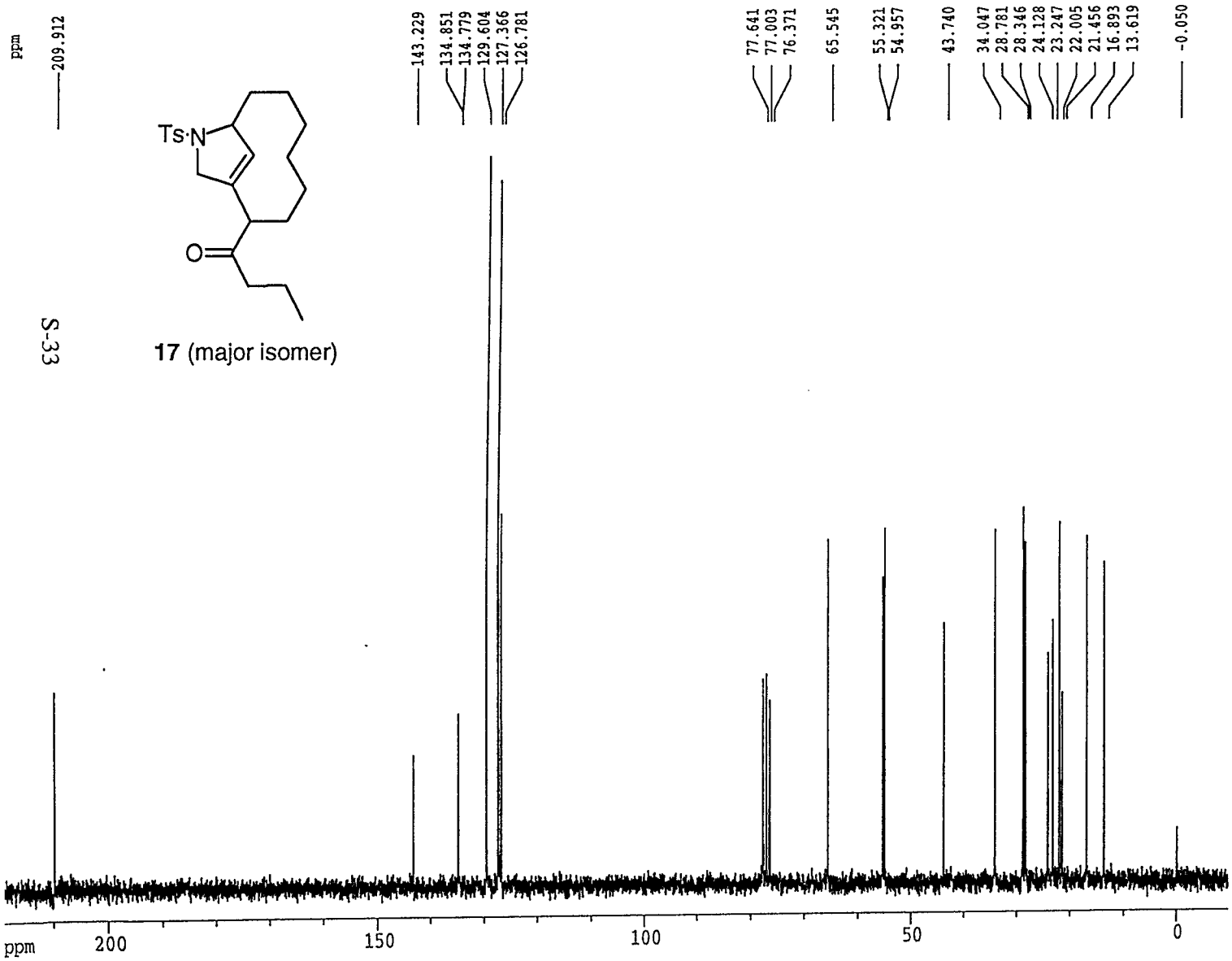
1D NMR plot parameters

CX	20.00 cm
F1P	9.000 ppm
F1	1801.19 Hz
F2P	-1.000 ppm
F2	-200.13 Hz
PPMCM	0.50000 ppm/cm
HZCM	100.06617 Hz/cm

SZI-SB-011-01


1101.02
1099.35
1097.57
1060.70
945.05
942.87
940.62
938.36
936.11
933.93
850.94
850.28
846.30
845.36
836.01
835.27
831.27
830.42
809.76
807.44
805.12
794.83
792.50
790.17
662.42
659.27
652.22
648.54
Ts·N
O
17 (major isomer)
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2

SZI-SB-011-01



Current Data Parameters

NAME	N0121F
EXPNO	107
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	971112
Time	14.49
INSTRUM	ac200
PROBHD	
PULPROG	X60.AU
TD	32768
SOLVENT	CDCl3
NS	1568
DS	0
SWH	14285.714 Hz
FIDRES	0.435965 Hz
AQ	1.1469300 sec
RG	640
DW	35.000 usec
DE	46.30 usec
TE	300.0 K
P1	15.50 usec
HL1	20 dB
D1	0.00100000 sec
DE	46.30 usec
SFO1	50.3287650 MHz
NUCLEUS	13C

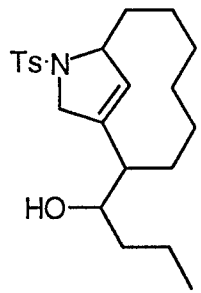
F2 - Processing parameters

SI	16384
SF	50.3233180 MHz
WDW	EM
SSB	0
LB	0.80 Hz
GB	0
PC	2.00

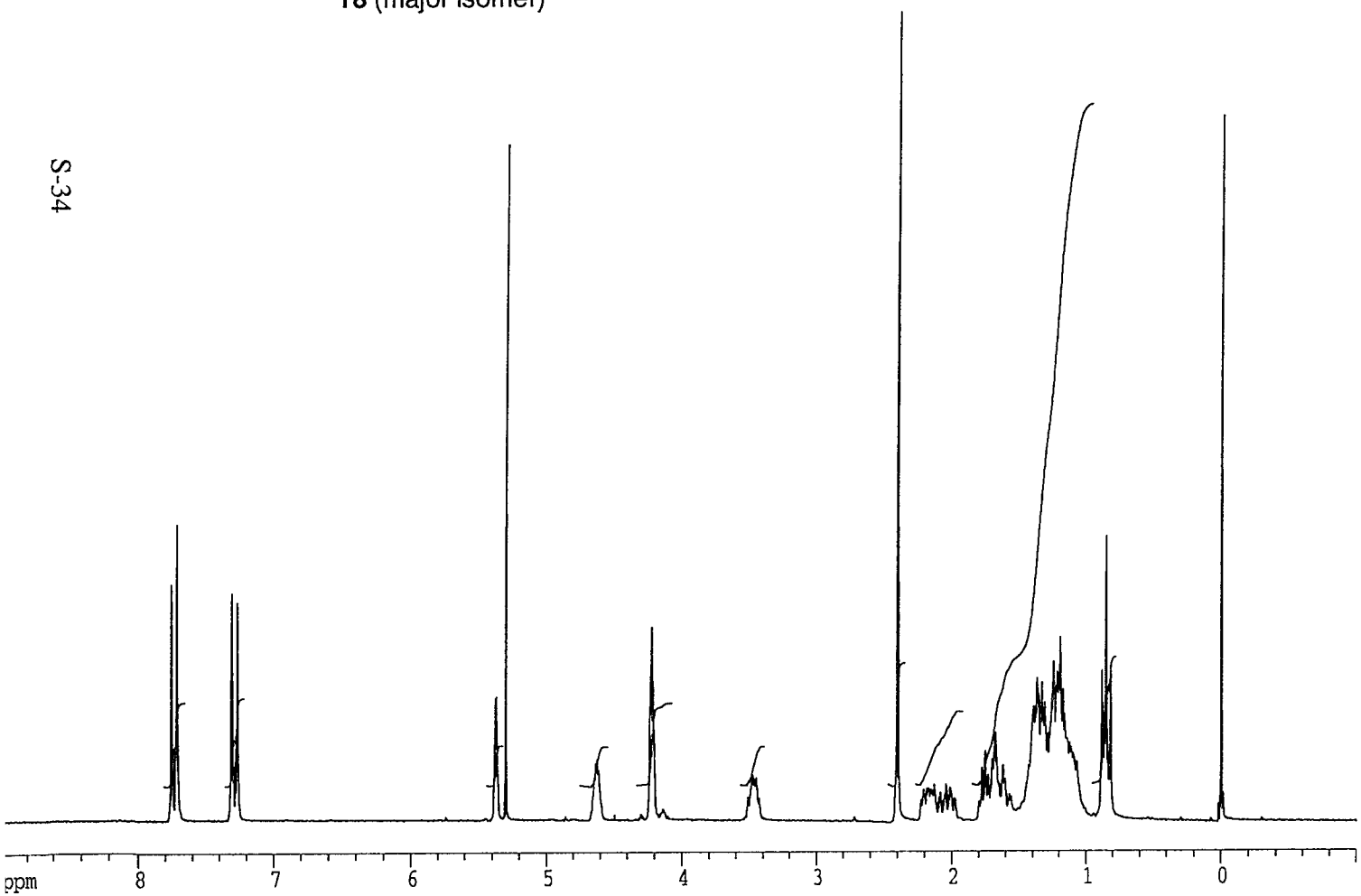
1D NMR plot parameters

CX	20.00 cm
F1P	220.000 ppm
F1	11071.13 Hz
F2P	-10.000 ppm
F2	-503.23 Hz
PPMCM	11.50000 ppm/cm
HZCM	578.71814 Hz/cm

SZI-SA-188-01



18 (major isomer)



Current Data Parameters

NAME	OK230F
EXPNO	135
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_ -	971024
Time	4.10
INSTRUM	ac200
PROBHD	
PULPROG	X51.AU
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4032.258 Hz
FIDRES	0.123055 Hz
AQ	4.0632820 sec
RG	16
DW	124.000 usec
DE	155.00 usec
TE	300.0 K
P1	10.10 usec
HL1	83 dB
D1	1.00000000 sec
DE	155.00 usec
SFO1	200.1332390 MHz
NUCLEUS	1H

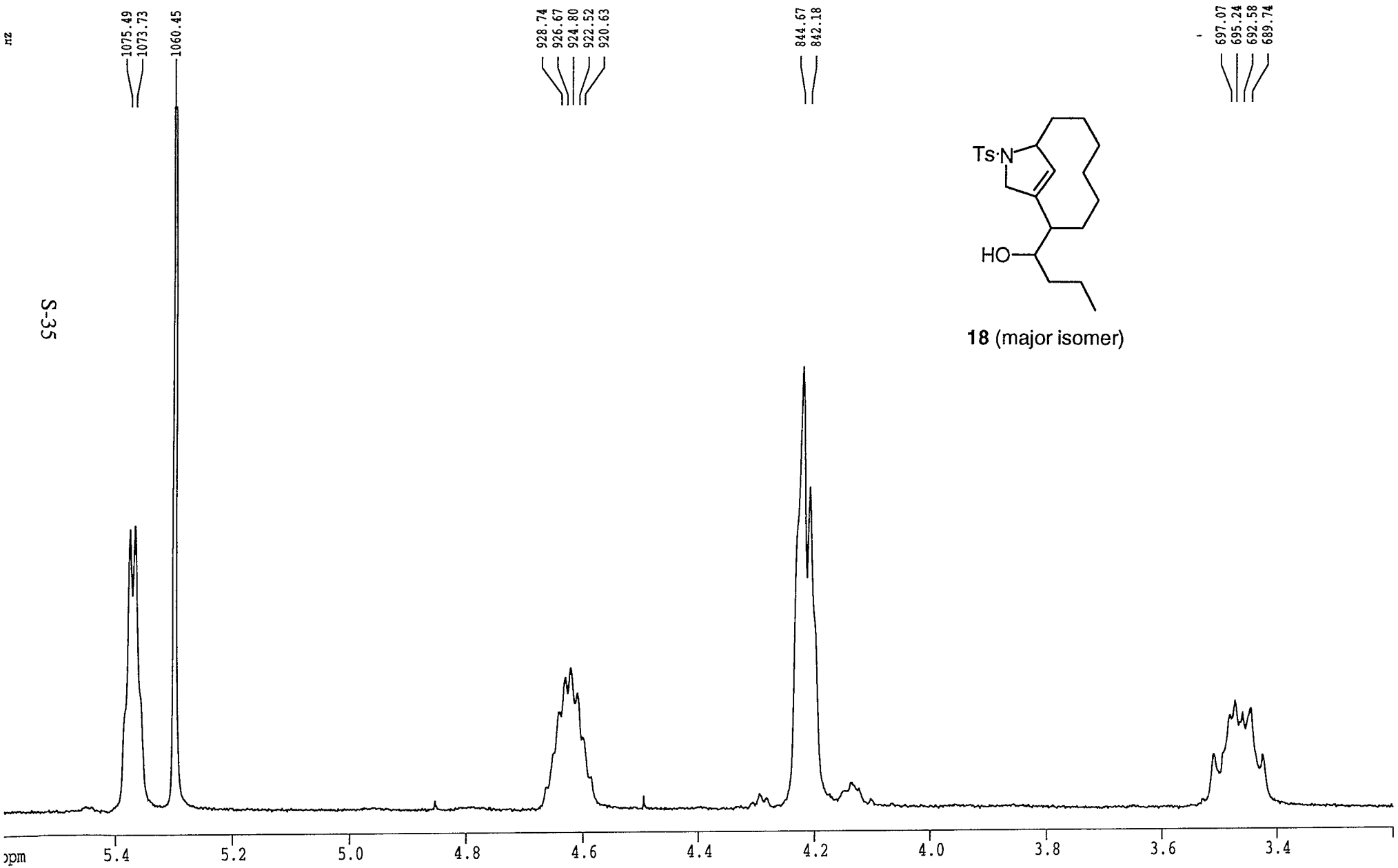
F2 - Processing parameters

SI	16384
SF	200.1323395 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	0.60

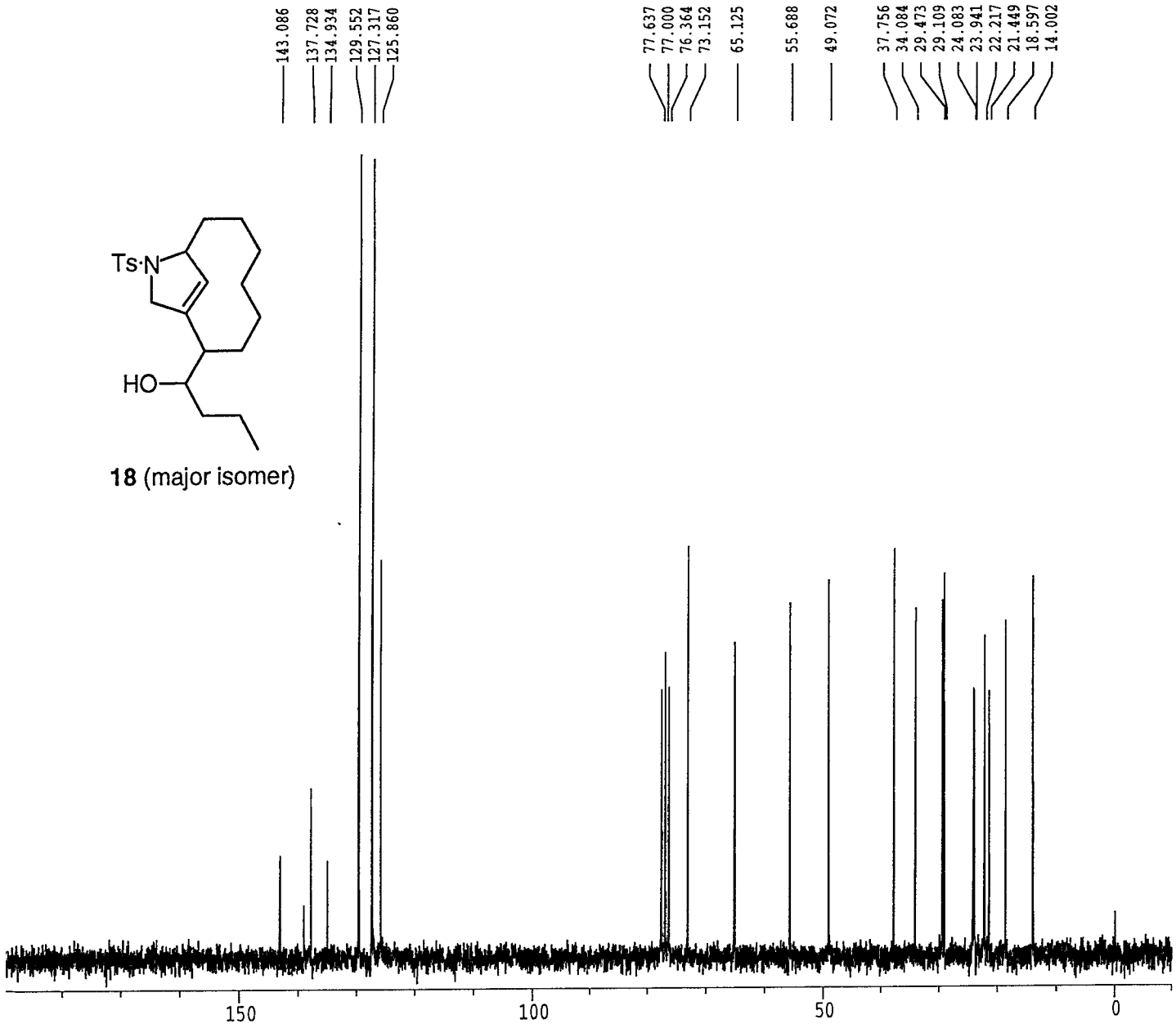
1D NMR plot parameters

CX	20.00 cm
F1P	9.000 ppm
F1	1801.19 Hz
F2P	-1.000 ppm
F2	-200.13 Hz
PPMCM	0.50000 ppm/cm
HZCM	100.06617 Hz/cm

SZI-SA-188-01


1075.49
1073.73
1060.45
928.74
926.67
924.80
922.52
920.63
844.67
842.18
697.07
695.24
692.58
689.74
Ts·N
HO
18 (major isomer)
ppm
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4

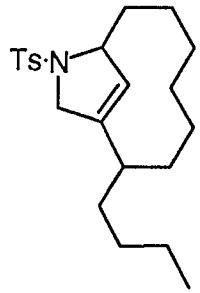
SZI-SA-188-01



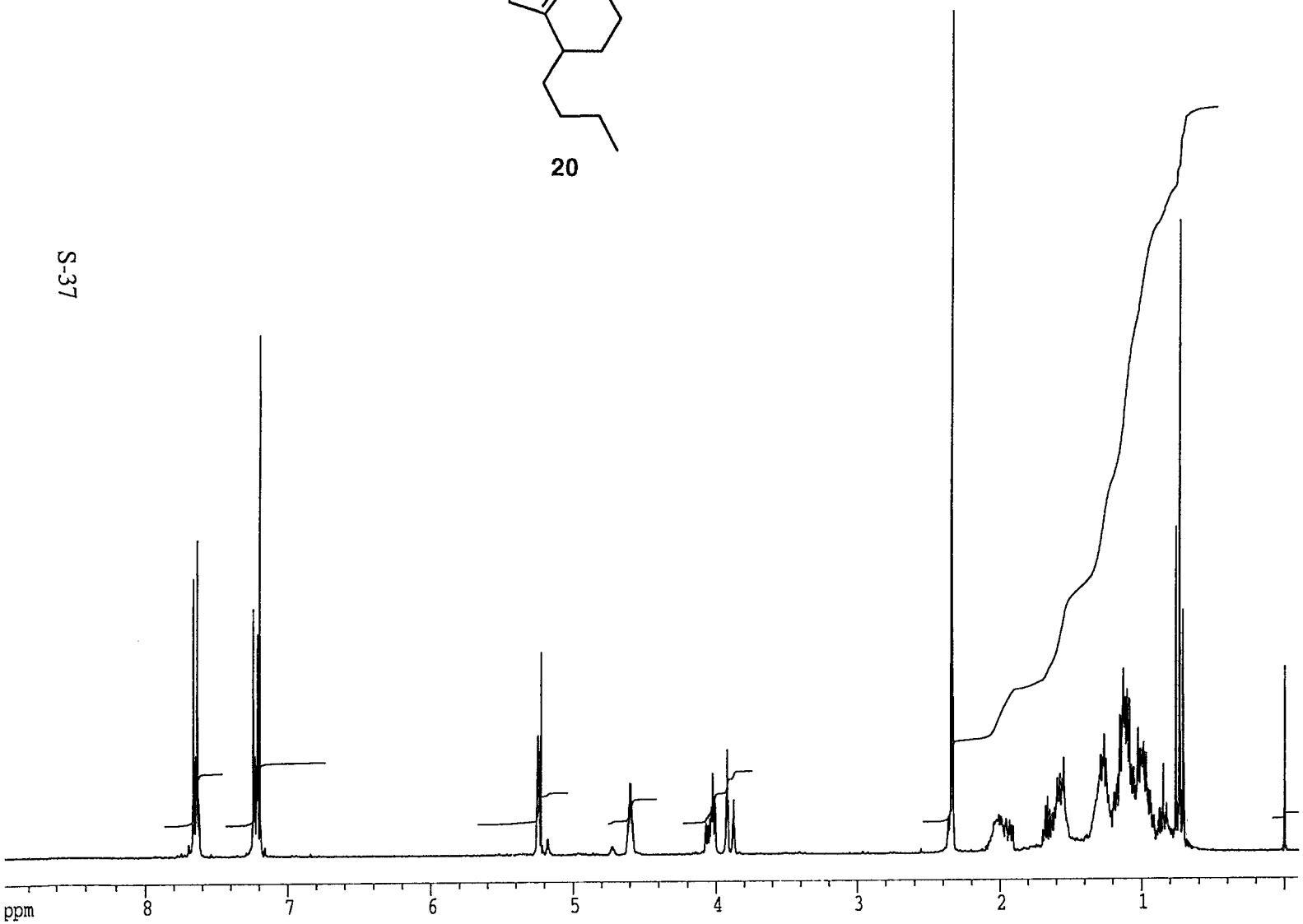
18 (major isomer)

```
Current Data Parameters
NAME            OK231F
EXPNO              135
PROCNO               1
DU                 mpi
USER               szi

F2 - Acquisition Parameters
Date_    -       971024
Time               4.43
INSTRUM          ac200
PROBHD
PULPROG          X60.AU
TD                32768
SOLVENT           CDCl3
NS                 1568
DS                    0
SWH           14285.714 Hz
FIDRES         0.435965 Hz
AQ           1.1469300 sec
RG                  640
DW               35.000 usec
DE               46.30 usec
TE               300.0 K
P1               15.50 usec
HL1                 20 dB
D1          0.00100000 sec
DE               46.30 usec
SFO1         50.3287650 MHz
NUCLEUS             13C

F2 - Processing parameters
SI                16384
SF           50.3233180 MHz
WDW                 EM
SSB                  0
LB                0.80 Hz
GB                   0
PC                2.00

1D NMR plot parameters
CX                21.00 cm
F1P             210.000 ppm
F1            10567.90 Hz
F2P            -10.000 ppm
F2             -503.23 Hz
PPMCM          10.47619 ppm/cm
HZCM         527.19666 Hz/cm
```

SZI-SB-074-01



20



Current Data Parameters

NAME	mar10103
EXPNO	10
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

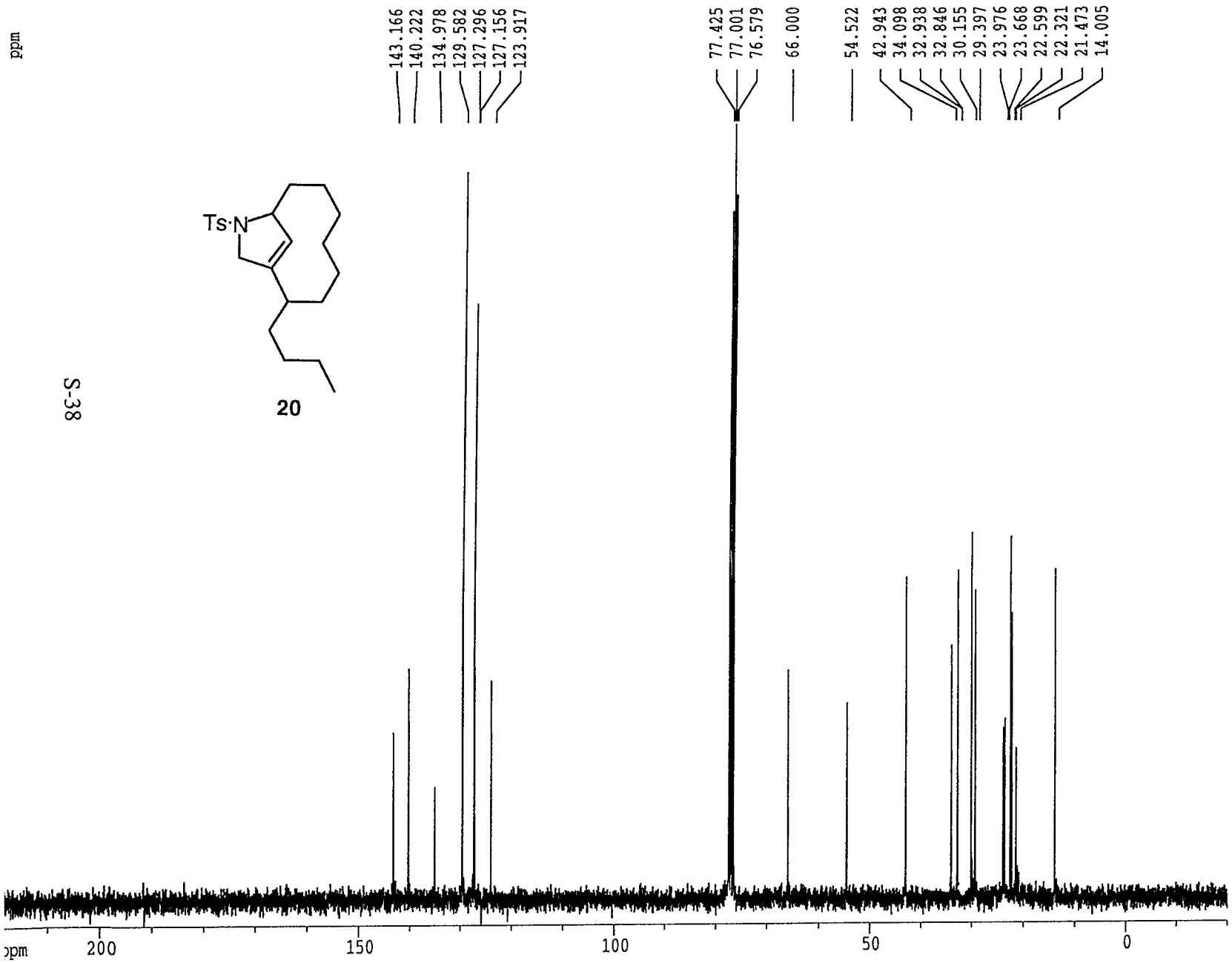
Date_	980310
Time	11.59
INSTRUM	amx300
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	2
SWH	6249.967 Hz
FIDRES	0.190734 Hz
AQ	2.6214900 sec
RG	512
DW	80.000 usec
DE	100.00 usec
TE	302.0 K
HL1	0 dB
D1	1.00000000 sec
P1	6.75 usec
DE	100.00 usec
SFO1	300.1349393 MHz
NUCLEUS	1H

F2 - Processing parameters

SI	32768
SF	300.1333881 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	5.00

1D NMR plot parameters

CX	21.00 cm
F1P	9.000 ppm
F1	2701.20 Hz
F2P	-0.100 ppm
F2	-30.01 Hz
PPMCM	0.43333 ppm/cm
HZCM	130.05782 Hz/cm



NAME	mar10103
EXPNO	11
PROCNO	1
DU	mpi
USER	szi

F2 - Acquisition Parameters

Date_	980310
Time _	12.28
INSTRUM	amx300
PROBHD	5 mm QNP 1H
PULPROG	zgdc30
TD	65536
SOLVENT	CDCl3
NS	6000
DS	16
SWH	31249.998 Hz
FIDRES	0.476837 Hz
AQ	1.0486259 sec
RG	16384
DW	16.000 usec
DE	22.86 usec
TE	302.0 K
D11	0.03000000 sec
CPDPRG	waltz16
P31	100.00 usec
S2	27 dB
HL1	0 dB
D1	0.03000000 sec
P1	5.68 usec
DE	22.86 usec
SFO1	75.4734422 MHz
NUCLEUS	13C

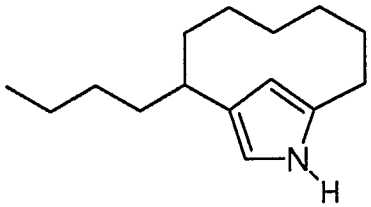
F2 - Processing parameters

SI	32768
SF	75.4685943 MHz
WDW	EM
SSB	0
LB	0.80 Hz
GB	0
PC	2.00

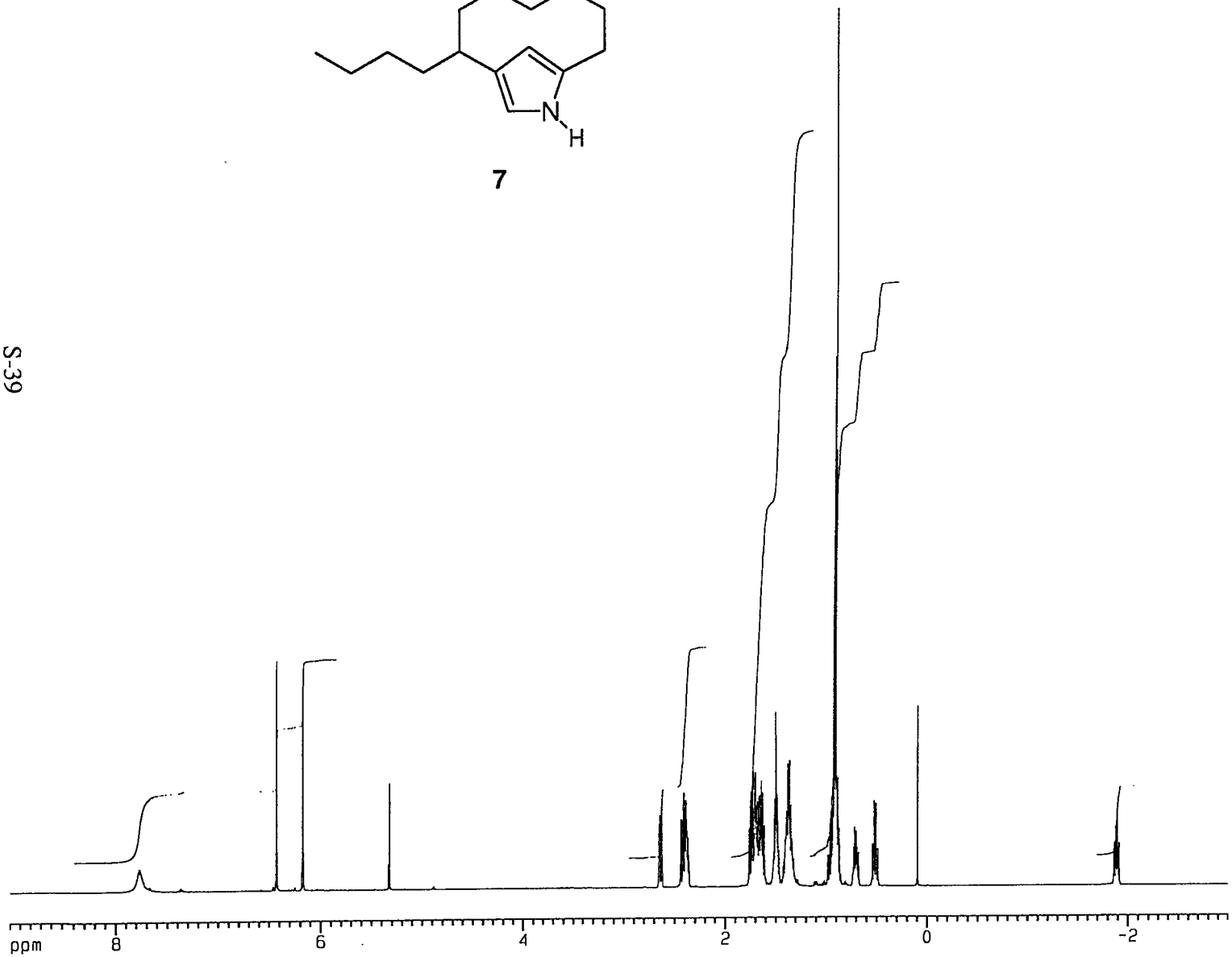
1D NMR plot parameters

CX	22.10 cm
F1P	220.000 ppm
F1	16603.09 Hz
F2P	-20.000 ppm
F2	-1509.37 Hz
PPMCM	10.85973 ppm/cm
HZCM	819.56848 Hz/cm

SZI-SB-074-01



7



Current Data Parameters

NAME	szi08201
EXPNO	10
PROCNO	1
DU	v
USER	wir

F2 - Acquisition Parameters

Date_	980318
Time	12.18
INSTRUM	dmx600
PROBHD	5 mm TXI 13C
PULPROG	zg30
TD	65536
SOLVENT	Tol
NS	32
DS	2
SWH	12019.230 Hz
AQ	2.7263477 sec
RG	64
DW	41.600 usec
DE	4.50 usec
TE	303.0 K
D1	1.00000000 sec
P1	9.00 usec
DE	4.50 usec
SFO1	600.2230011 MHz
NUC1	1H
PL1	0.00 dB

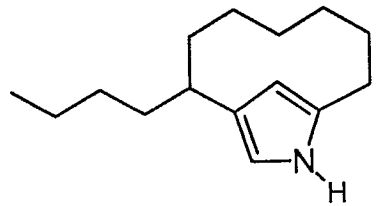
F2 - Processing parameters

SI	65536
SF	600.2200221 MHz
SR	22.14 Hz
WDW	GM
SSB	0
LB	-0.30 Hz
GB	0.18
PC	4.00

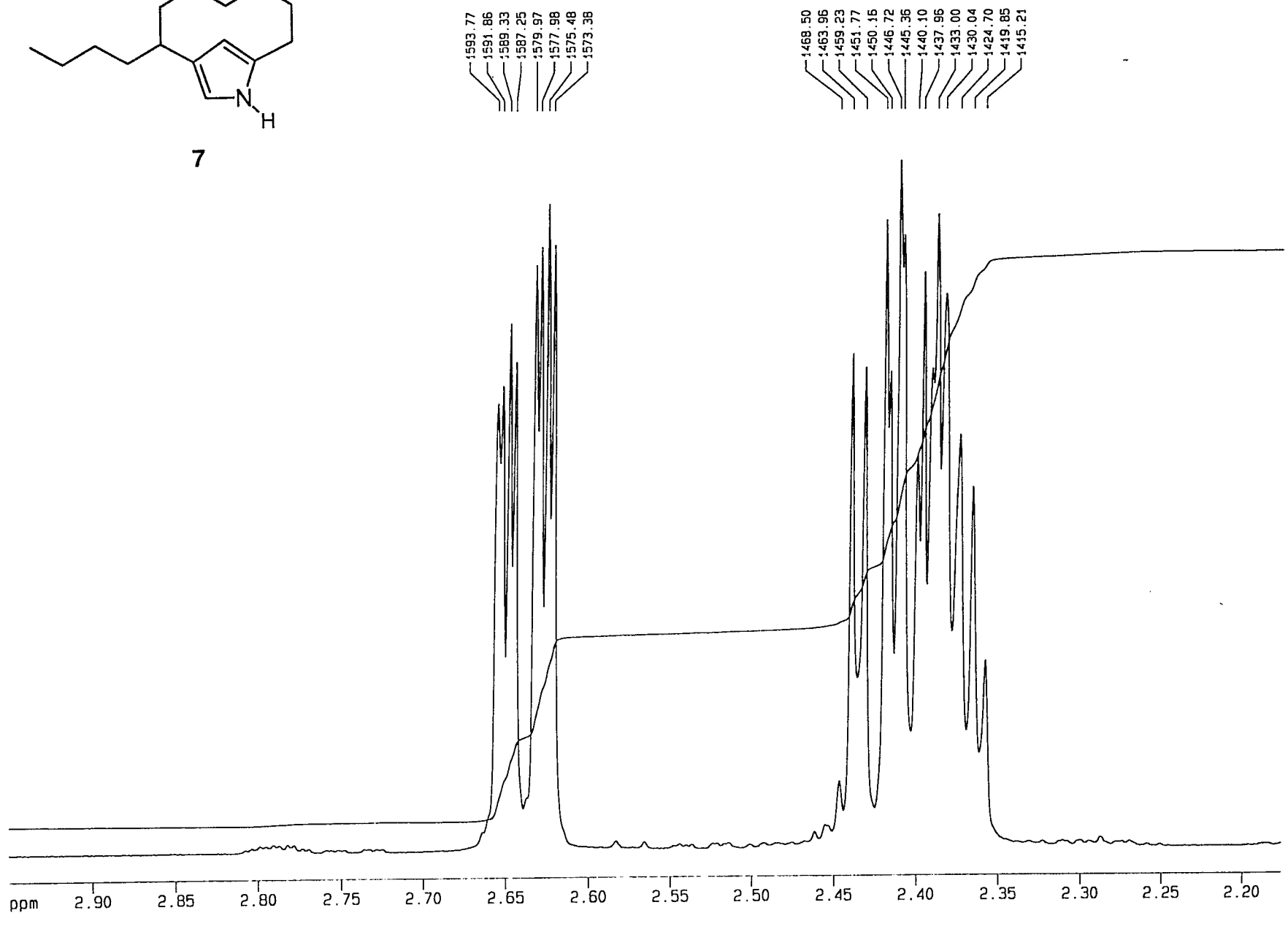
1D NMR plot parameters

CX	20.00 cm
CY	15.00 cm
F1P	9.000 ppm
F1	5401.98 Hz
F2P	-3.000 ppm
F2	-1800.66 Hz
PPMCM	0.60000 ppm/cm
HZCM	360.13202 Hz/cm

SZI-SB-082-01


N
H

7


1593.77
1591.86
1589.33
1587.25
1579.97
1577.98
1575.48
1573.38
1468.50
1463.96
1459.23
1451.77
1450.16
1446.72
1445.36
1440.10
1437.96
1433.00
1430.04
1424.70
1419.85
1415.21
wir/szi08201/10/1
Y exp. factor: 8
Int. plot exp. factor: 3
1770.56 Hz to 1306.20 Hz
20.000 Hz/cm changed!
ppm
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
2.20