SUPPORTING INFORMATION

Isolation of Ugi Four-Component Condensation Primary Adducts: A Straightforward Route to Isocoumarins

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EXPERIMENTAL

General

Melting points were determined in open capillary tubes with a Büchi 512 apparatus and are uncorrected. IR spectra were measured on a Perkin-Elmer Spectrum BX spectrophotometer for potassium bromide discs. NMR spectra were recorded on a Varian Gemini 200 operating at 200 MHz and 50.33 MHz for ^{1}H and ^{13}C acquisitions, respectively. Chemical shifts (δ) are reported in ppm relative to chloroform (δ = 7.26, 77.23).

3-(N-Cyclohexyl)amino-4-[N-(2,2-dimethoxy-2-phenyl)ethyl]amino-1*H*-isochromen-1-one (**13a**)

A solution of phenacylamine dimethyl acetal (**11**) (362 mg, 2.0 mmol) and cyclohexyl isocyanide (**12a**) (218 mg, 2.0 mmol) in MeOH (1.0 mL) was added to a solution of 2-formylbenzoic acid (**10**) (278 mg, 1.85 mmol) in MeOH (2.8 mL). The resulting mixture was stirred for 18 h at rt and then cooled and filtered. The collected product was washed with a little cold pentane and dried in a oven at 50 °C to give 641 mg (82%) of **13a**. Yellow crystals, mp 148.5-150 °C (EtOH).
^{1}H NMR: δ 8.04 (d, 1H), 7.63-7.38 (m, 6H), 7.06-6.95 (m, 2H), 4.69 (d, *J* = 8.8 Hz, 1H), 3.44 (m, 1H), 3.28 (s, 6H), 3.18 (s, 2H), 1.92-0.86 (m, 11H).
^{13}C NMR: δ 160.8, 154.0, 141.0, 140.0, 134.7, 130.4, 128.2, 127.2, 121.8, 117.9, 114.0, 102.7, 97.5, 55.3, 50.0, 49.2, 34.1, 25.7, 25.1.
IR: 3362, 2928, 2845, 1731, 1264, 1604, 1554, 1482, 1473, 1042, 762, 705 cm^{-1}.
Anal. Calcd. for $C_{25}H_{30}N_2O_4$: C, 71.07; H, 7.16; N, 6.63. Found: C, 70.91; H, 7.15; N, 6.77.

3-(N-*tert*-Butyl)amino-4-[N-(2,2-dimethoxy-2-phenyl)ethyl]amino-1*H*-isochromen-1-one (**13b**)

This compound (**13b**) was prepared analogously to **13a** by employing *tert*-butyl isocyanide (**12b**) in the place of cyclohexyl isocyanide (**12a**). Yield 72%, yellow crystals, mp 138-139 °C (*i*-Pr_2O).
^{1}H NMR: δ 8.05 (d, 1H), 7.63-7.36 (m, 8H), 7.08-6.89 (m, 2H), 5.09 (s, 1H), 3.27 (s, 6H), 3.19 (s, 2H), 1.91 (brs, 1H), 1.29 (s, 9H).
^{13}C NMR: δ 160.6, 155.1, 140.6, 139.8, 134.6, 130.3, 128.2, 128.1, 127.1, 122.1, 118.1, 114.4, 102.6, 98.8, 53.2, 52.2, 49.1, 30.4.
IR: 3334, 2965, 1732, 1627, 1604, 1553, 1484, 1456, 1137, 1042, 762, 667 cm^{-1}.
Anal. Calcd. for $C_{23}H_{28}N_2O_4$: C, 69.67; H, 7.12; N, 7.07. Found: C, 69.89; H, 6.99; N, 7.15.

N-Cyclohexyl-2-(2,2-dimethoxy-2-phenyl)ethyl-1,3-dihydro-1-oxoisoindol-3-carboxamide (**14a**)

A drop of aq. HCl (37% HCl : water = 1:2) was added to a solution of **13a** (211 mg, 0.5 mmol) in THF (3.3 mL). The yellow color quickly disappeared. After 2 min the reaction mixture was

cautiously diluted with cold water under stirring to give **14a** in almost quantitative yield. White crystals, mp 223-225 °C from EtOH/water (2:1). Variations of the mp value were observed depending upon the heating rate.
^{1}H NMR: δ 7.46-7.23 (m, 9H), 5.94 (d, *J* = 8.4 Hz, 1H), 4.78 (s, 1H), 4.59 (d, *J* = 14.6 Hz, 1H), 3.68 (m, 1H), 3.51 (d, *J* = 14.6 Hz, 1H), 3.28 (s, 3H), 3.26 (s, 3H), 1.98-0.82 (m, 10H).
^{13}C NMR: δ 168.4, 166.3, 141.0, 138.1, 131.5, 129.6, 128.1, 127.9, 126.7, 123.0, 121.9, 102.1, 64.7, 49.3, 48.7, 44.6, 33.1, 32.4, 25.3, 25.2, 25.0.
IR: 3317, 2931, 2850,1700, 1684, 1670, 1532, 1411, 1318, 1127, 1072, 1047, 731 cm^{-1}.
Anal. Calcd. for $C_{25}H_{30}N_2O_4$: C, 71.07; H, 7.16; N, 6.63. Found: C, 71.05; H, 7.32; N, 6.47.

N-*tert*-Butyl-2-(2,2-dimethoxy-2-phenyl)ethyl-1,3-dihydro-1-oxoisoindol-3-carboxamide (**14b**)

This compound (**14b**) was prepared analogously to **14a** by employing compound **13b** as the starting material in the place of **13a**. Yield: almost quantitative. An analytical sample was obtained from EtOH/water (1:1). The product melted at about 188 °C then resolidified and melted again at 197-198 °C.
^{1}H NMR: δ 7.49-7.20 (m, 9H), 5.54 (s, 1H), 4.63 (d, *J* = 14.7 Hz, 1H), 4.59 (s, 1H), 3.49 (d, *J* = 14.7 Hz, 1H), 3.30 (s, 3H), 3.23 (s, 3H), 1.25 (s, 9H).
^{13}C NMR: δ 168.7, 166.2, 141.3, 138.7, 131.8, 130.0, 128.5, 128.3, 128.2, 127.0, 123.5, 121.9, 102.0, 65.2, 51.8, 49.5, 48.9, 45.1, 28.7.
IR: 3301, 2963, 1695, 1664, 1542, 1404, 1128, 1050, 735, 699 cm^{-1}.
Anal. Calcd. for $C_{23}H_{28}N_2O_4$: C, 69.67; H, 7.12; N, 7.07. Found: C, 69.72; H, 7.25; N, 7.00.

N-Cyclohexyl-1,3-dihydro-1-oxo-2-phenacylisoindol-3-carboxamide (**15a**)

A solution of **13a** (211 mg, 0.5 mmol) in THF (5.3 mL) was treated with six drops of aq. HCl (HCl 37% : water = 1:2). The resulting solution was allowed to stand at rt for 5d and then cautiously diluted with cold water under stirring to give **15a** in almost quantitative yield as white crystals. An analytical sample was obtained from EtOH/water (1:1). The product softened at about 177 °C and melted at 183-185 °C.
The same product **15a** was obtained starting from **14a** in the same conditions.
^{1}H NMR: δ 8.00 (d, 1H), 7.83-7.44 (m, 8H), 7.31 (d, *J* = 8.1 Hz, 1H), 5.15 (s, 1H), 5.11 (d, *J* = 17.9 Hz, 1H), 4.87 (d, *J* = 17.9 Hz, 1H), 3.64 (m, 1H), 1.93-0.90 (m, 10H).
^{13}C NMR: δ 194.1, 170.0, 166.4, 141.9, 134.5, 134.1, 132.5, 129.8, 129.0, 128.9, 128.1, 123.8, 122.9, 66.3, 49.6, 48.8, 32.8, 32.6, 25.5, 25.1, 24.9.
IR: 3278, 2938, 2856, 1701, 1690, 1651, 1545, 1408, 1228, 1004, 751, 690 cm^{-1}.
Anal. Calcd. for $C_{23}H_{24}N_2O_3$: C, 73.38; H, 6.43; N, 7.44. Found: C, 73.52; H, 6.27; N, 7.57.

N-*tert*-Butyl-1,3-dihydro-1-oxo-2-phenacylisoindol-3-carboxamide (**15b**)

This compound (**15b**) was prepared analogously to **15a** starting from **13b** or **14b**. Yield: nearly quantitative. White crystals, mp 155-156 °C from EtOH/water (1:1).
^{1}H NMR: δ 8.02 (d, 1H), 7.86-7.44 (m, 8H), 7.06 (s, 1H), 5.10 (d, *J* = 17.9 Hz, 1H), 5.05 (s, 1H), 4.87 (d, *J* = 17.9 Hz, 1H), 1.24 (s, 9H).
^{13}C NMR: δ 193.9, 170.0, 166.6, 142.1, 134.5, 134.1, 132.5, 129.8, 128.9, 128.1, 123.8, 122.*7*, 67.0, 51.7, 49.6, 28.6.
IR: 3315, 2967, 1700, 1695, 1669, 1533, 1419, 1226, 1006, 735, 690 cm^{-1}.
Anal. Calcd. for $C_{21}H_{22}N_2O_3$: C, 71.98; H, 6.33; N, 7.99. Found: C, 72.09; H, 6.15; N, 7.85.

3-(N-Substituted)amino-4-arylamino-1*H*-isochromen-1-ones (**17**)

A small flask containing a solution of 2-formylbenzoic acid (**10**)(540 mg, 3.6 mmol) in MeOH (4 mL) was poured into an oil bath (bath temperature 80 °C). When the solution began to boil a solution of the isocyanide **12** (3.8 mmol) and the aniline **16** (3.8 mmol) in MeOH (1 mL) was added and the flask lifted and maintained at such a distance from the oil surface that the temperature dropped to 40 °C within 15 min. The flask was then transferred to another bath and maintained at 40 °C (reaction mixture temperature) for 45 min. The flask was removed from the bath and allowed to cool at rt. A small magnetic bar was poured into the flask and stirring was started. After 15 min stirring at rt the reaction mixture was cooled with an ice bath and filtered to give almost pure **17**. Unless otherwise stated analytical samples were obtained from EtOH.

3-(N-Cyclohexyl)amino-4-(N-phenyl)amino-1*H*-isochromen-1-one (**17a**)

Yield 57%. Yellow crystals, mp 140-141 °C.
^{1}H NMR: δ 8.10 (d, 1H), 7.44 (m, 1H), 7.27-7.05 (m, 4H), 6.84-6.57 (m, 3H), 4.81 (d, *J* = 9.2 Hz, 1H), 4.69 (s, 1H), 3.73 (m, 1H), 2.10-1.01 (m, 10H).
^{13}C NMR: δ 160.7, 155.2, 146.3, 141.0, 135.0, 130.2, 129.5, 122.7, 119.2, 118.9, 114.4, 113.2, 91.7, 50.6, 34.3, 25.6, 25.1.
IR: 3371, 3347, 2932, 2853, 1713, 1700, 1623, 1604, 1552, 1494, 1241, 1087, 767, 748 cm^{-1}.
Anal. Calcd. for $C_{21}H_{22}N_2O_2$: C, 75.42; H, 6.63; N, 8.38. Found: C, 75.35; H, 6.51; N, 8.51.

3-(N-Cyclohexyl)amino-4-[N-(4-fluoro)phenyl]amino-1*H*-isochromen-1-one (**17b**)

Yield 58%. Yellow crystals, mp 151-152 °C from MeOH.
^{1}H NMR: δ 8.10 (d, 1H), 7.45 (m, 1H), 7.15-6.82 (m, 4H), 6.67-6.53 (m, 2H), 4.83 (d, *J* = 9.1 Hz, 1H), 4.65 (s, 1H), 3.72 (m, 1H), 2.07-1.01 (m, 10H).
^{13}C NMR: δ 160.5, 156.1 (d, $^{1}J_{CF}$ = 236 Hz), 155.0, 142.2, 140.6, 134.8, 130.0, 122.4, 118.8, 115.8 (d, $^{2}J_{CF}$ = 23 Hz), 114.1, 113.6 (d, $^{3}J_{CF}$ = 7 Hz), 91.6, 50.2, 33.9, 25.1, 24.6.
IR: 3376, 3340, 2937, 2853, 1709, 1696, 1624, 1606, 1555, 1508, 1483, 1336, 1215, 818, 759 cm^{-1}.
Anal. Calcd. for $C_{21}H_{21}FN_2O_2$: C, 71.57; H, 6.01; N, 7.95. Found: C, 71.79; H, 6.11; N, 7.79.

4-[N-(3-Chloro)phenyl]amino-3-(N-cyclohexyl)amino-1*H*-isochromen-1-one (**17c**)

Yield 62%. Yellow crystals, mp 156-158 °C.
^{1}H NMR: δ 8.08 (d, 1H), 7.47 (m, 1H), 7.15-7.03 (m, 3H), 6.78-6.48 (m, 3H), 4.80 (s, 1H), 4.73 (d, *J* = 8.8 Hz, 1H), 3.73 (m, 1H), 2.06-1.02 (m, 10H).
^{13}C NMR: δ 160.6, 155.0, 147.6, 140.6, 135.3, 135.1, 130.6, 130.3, 122.8, 119.0, 114.4, 113.1, 111.4, 90.8, 50.6, 34.3, 25.6, 25.0.
IR: 3409, 3342, 2930, 2844, 1712, 1696, 1605, 1594, 1551, 1473, 1334, 1160, 1086, 848, 763, 678 cm^{-1}.
Anal. Calcd. for $C_{21}H_{21}ClN_2O_2$: C, 68.38; H, 5.74; N, 7.59. Found: C, 68.12; H, 5.56; N, 7.72.

4-[N-(4-Chloro)phenyl]amino-3-(N-cyclohexyl)amino-1*H*-isochromen-1-one (**17d**)

Yield 68%. Yellow crystals, mp 173-175 °C.
^{1}H NMR: δ 8.10 (d, 1H), 7.45 (m, 1H), 7.20-6.98 (m, 4H), 6.66-6.53 (m, 2H), 4.76 (d, *J* = 8.8 Hz, 1H), 4.74 (s, 1H), 3.72 (m, 1H), 2.07-1.00 (m, 10H).
^{13}C NMR: δ 160.6, 155.1, 145.0, 140.7, 135.0, 130.2, 129.4, 123.4, 122.8, 119.1, 114.4, 114.3, 91.4, 50.6, 34.3, 25.6, 25.0.
IR: 3367, 3302, 2925, 2853, 1723, 1624, 1603, 1550, 1492, 1482, 1305, 1094, 818, 767 cm^{-1}.
Anal. Calcd. for $C_{21}H_{21}ClN_2O_2$: C, 68.38; H, 5.74; N, 7.59. Found: C, 68.22; H, 5.90; N, 7.43.

4-[N-(4-Fluoro)phenyl]amino-3-[N-(4-methyl)phenyl]amino-1*H*-isochromen-1-one (**17e**)

Yield 64%. Yellow crystals, mp 163-165 °C.
^{1}H NMR: δ 8.13 (d, 1H), 7.50 (m, 1H), 7.24-7.03 (m, 6H), 7.01-6.81 (m, 3H), 6.72-6.57 (m, 2H), 4.82 (s, 1H), 2.31 (s, 3H).
^{13}C NMR: δ 159.7, 156.4 (d, $^{1}J_{CF}$ = 236 Hz), 152.0, 141.9, 139.7, 135.1, 134.9, 132.8, 130.0, 129.5, 123.6, 119.7, 119.6, 115.8 (d, $^{2}J_{CF}$ =23 Hz), 115.4, 114.0 (d, d, $^{3}J_{CF}$ = 7 Hz), 94.0, 20.5.
IR: 3379, 3336, 3032, 1724, 1634, 1605, 1556, 1508, 1482, 1385, 1329, 1206, 824, 759 cm^{-1}.
Anal. Calcd. for $C_{22}H_{17}FN_2O_2$: C, 73.32; H, 4.75; N, 7.77. Found: C, 73.54; H, 4.62; N, 7.89.

3-(N-Cyclohexyl)amino-4-[N-(4-methyl)phenyl]amino-1*H*-isochromen-1-one (**17f**)

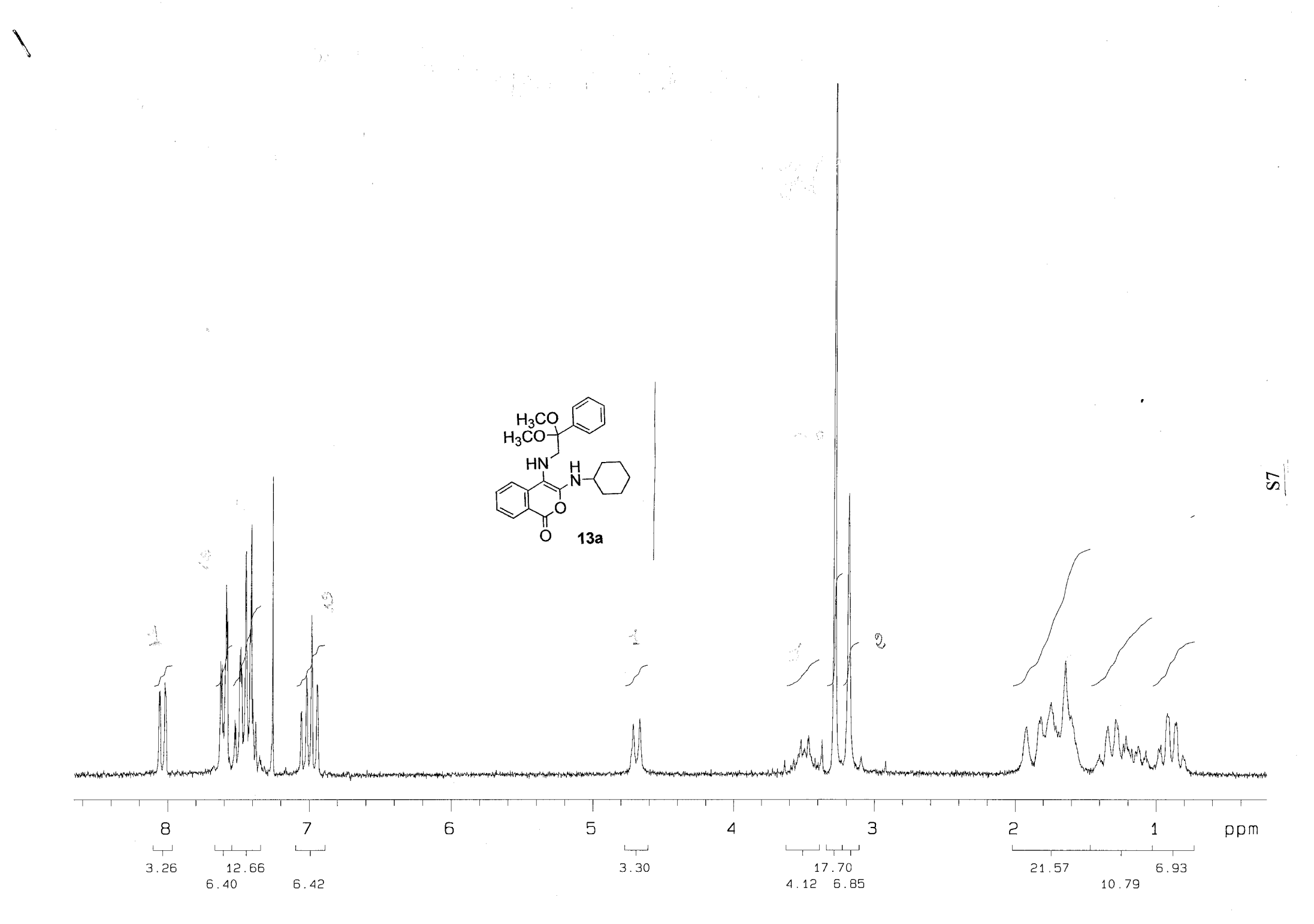
Yield 82%. Yellow crystals, mp 148-149 °C from MeOH.
^{1}H NMR: δ 8.10 (d, 1H), 7.43 (m, 1H), 7.15-6.92 (m, 4H), 6.63-6.50 (m, 2H), 4.83 (d, *J* = 9.1 Hz, 1H), 4.57 (s, 1H), 3.72 (m, 1H), 2.25 (s, 3H), 2.05-1.03 (m, 10H).
^{13}C NMR: δ 160.6, 155.0, 143.7, 140.8, 134.7, 129.9, 129.8, 122.3, 119.0, 114.1, 113.0, 91.7, 50.2, 33.9, 25.2, 24.6, 20.2.
IR: 3370, 3304, 2923, 2854, 1724, 1615, 1603, 1556, 1514, 1482, 1307, 1243, 1094, 810, 755 cm^{-1}.
Anal. Calcd. for $C_{22}H_{24}N_2O_2$: C, 75.83; H, 6.94; N, 8.04. Found: C, 75.99; H, 7.05; N, 7.87.

N-Cyclohexyl-2-(3-chloro)phenyl-1,3-dihydro-1-oxoisoindol-3-carboxamide (**18c**)

This compound (**18c**) was prepared analogously to **14a** by employing compound **17c** as the starting material in the place of **13a**. Yield: almost quantitative. An analytical sample was obtained from EtOH. White crystals, mp 223-224 °C.
^{1}H NMR: δ 7.98 (m, 1H), 7.82-7.13 (m, 7H), 5.98 (d, *J* = 8.4 Hz, 1H), 5.56 (s, 1H), 3.69 (m, 1H), 1.73-0.77 (m, 10H).
^{13}C NMR: δ 168.1, 166.2, 140.2, 139.2, 137.4, 135.2, 133.3, 130.2, 129.4, 125.1, 124.2, 122.7, 119.9, 117.4, 65.5, 48.7, 32.4, 32.3, 25.2, 24.6.
IR: 3265, 3078, 2935, 2854, 1712, 1660, 1595, 1485, 1369, 1359, 1245, 1106, 768, 730, 677 cm^{-1}.
Anal. Calcd. for $C_{21}H_{21}ClN_2O_2$: C, 68.38; H, 5.74; N, 7.59. Found: C, 68.12; H, 5.54; N, 7.66.

N-Cyclohexyl-1,3-dihydro-2-(4-methyl)phenyl-1-oxoisoindol-3-carboxamide (**18f**)

This compound (**18f**) was prepared analogously to **14a** by employing compound **17f** as the starting material in the place of **13a**. Yield: almost quantitative. An analytical sample was obtained from EtOH. White crystals, mp 227-228 °C.
^{1}H NMR: δ 7.84-7.42 (m, 6H), 7.25-7.12 (m, 2H), 5.75 (d, *J* = 8.4 Hz, 1H), 5.58 (s, 1H), 3.63 (m, 1H), 2.35 (s, 3H), 1.65-0.72 (m, 10H).
^{13}C NMR: δ 167.9, 166.5, 140.3, 135.3, 134.9, 132.7, 130.9, 129.8, 129.1, 124.0, 122.6, 120.2, 65.6, 48.6, 32.5, 25.4, 24.7, 24.6, 21.1.
IR: 3267, 3078, 2923, 2853, 1702, 1653, 1554, 1517, 1374, 1245, 1106, 806, 723 cm^{-1}.
Anal. Calcd. for $C_{22}H_{24}N_2O_2$: C, 75.83; H, 6.94; N, 8.04. Found: C, 75.88; H, 6.71; N, 7.91.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HN
H
N
O
O
13a
8
7
6
5
4
3
2
1
ppm
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6.40
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4.12
6.85
21.57
6.93
10.79

STANDARD 1H OBSERVE

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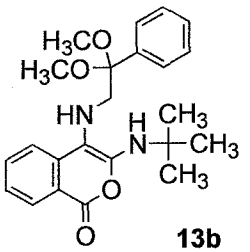


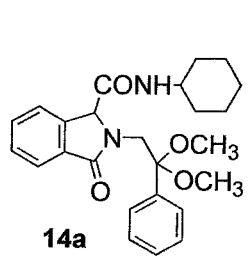
13b

8 7 6 5 4 3 2 ppm

3.81 21.33 7.56 3.56 20.72 7.19 4.72 31.12

prodotto giallo trattato con HCl

Pulse Sequence: s2pul



14a

S9

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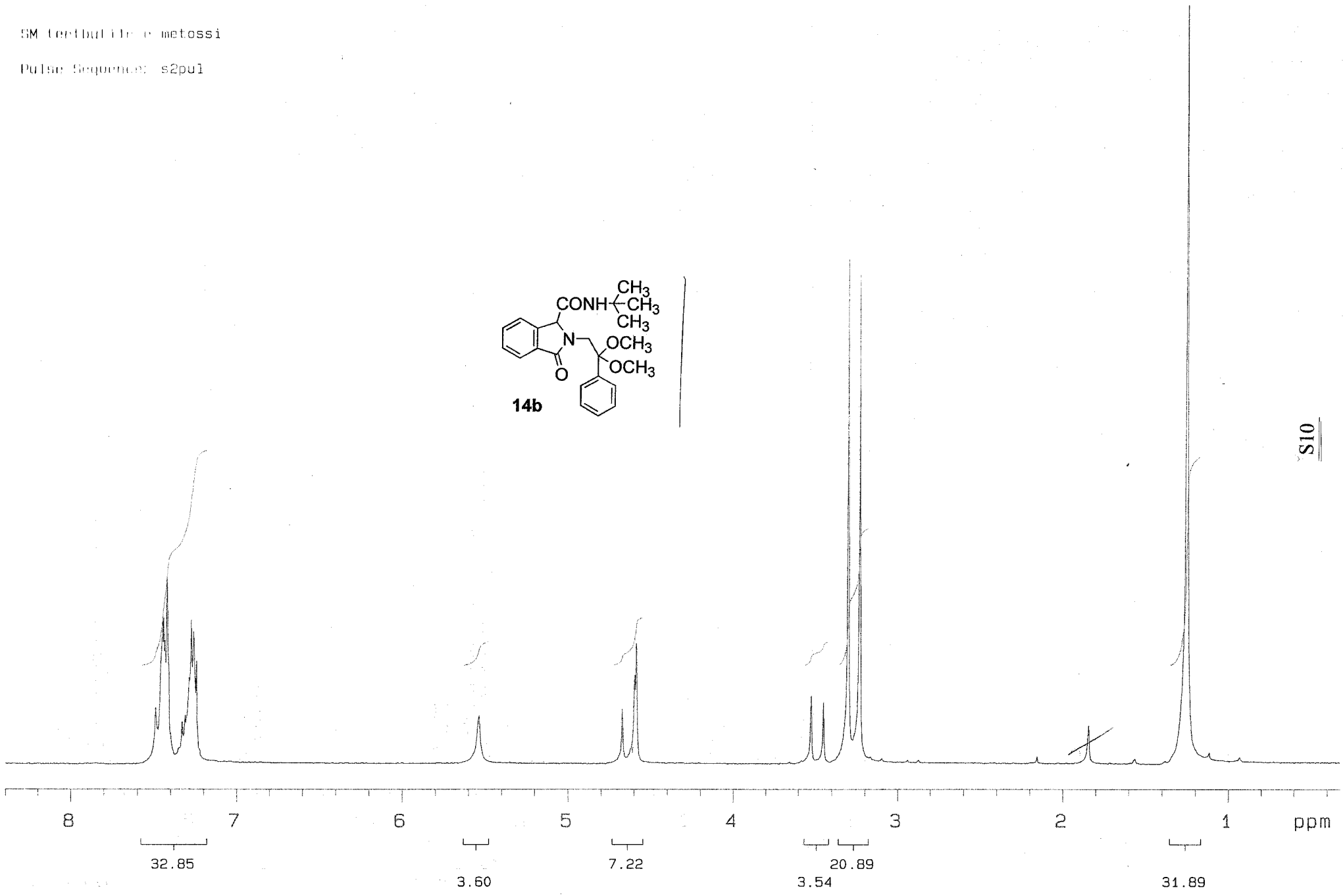
SM terbutilic e metossi
Pulse Sequence: s2pul
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CH3
CH3
N
OCH3
OCH3
O
14b
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5
4
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ppm
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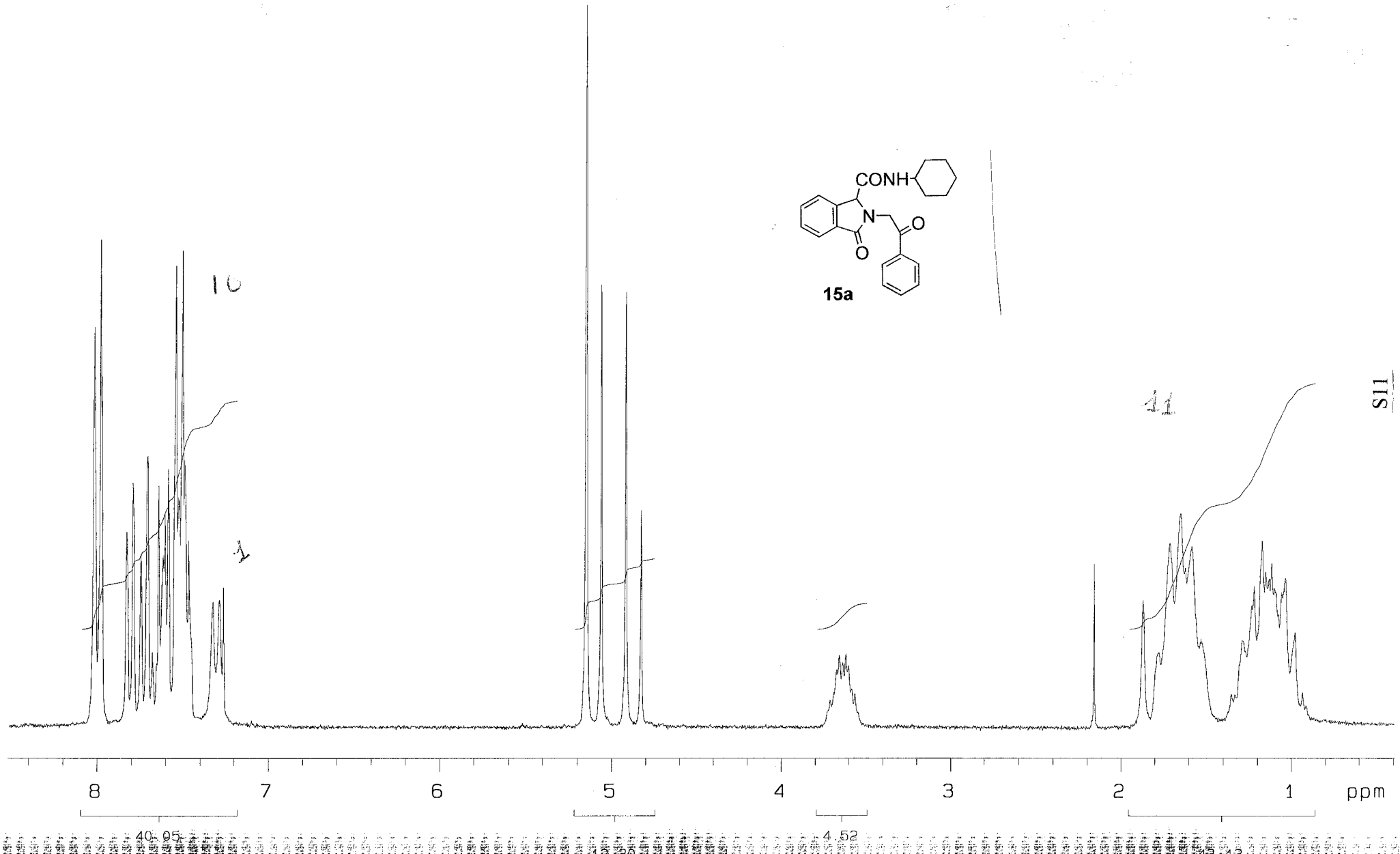
20.89
31.89


CONH
N
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O
15a
10
1
11
8
7
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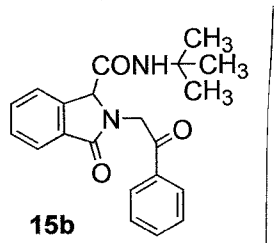
25.13

SM tert butile deprotetto

Pulse Sequence: s2pul



15b

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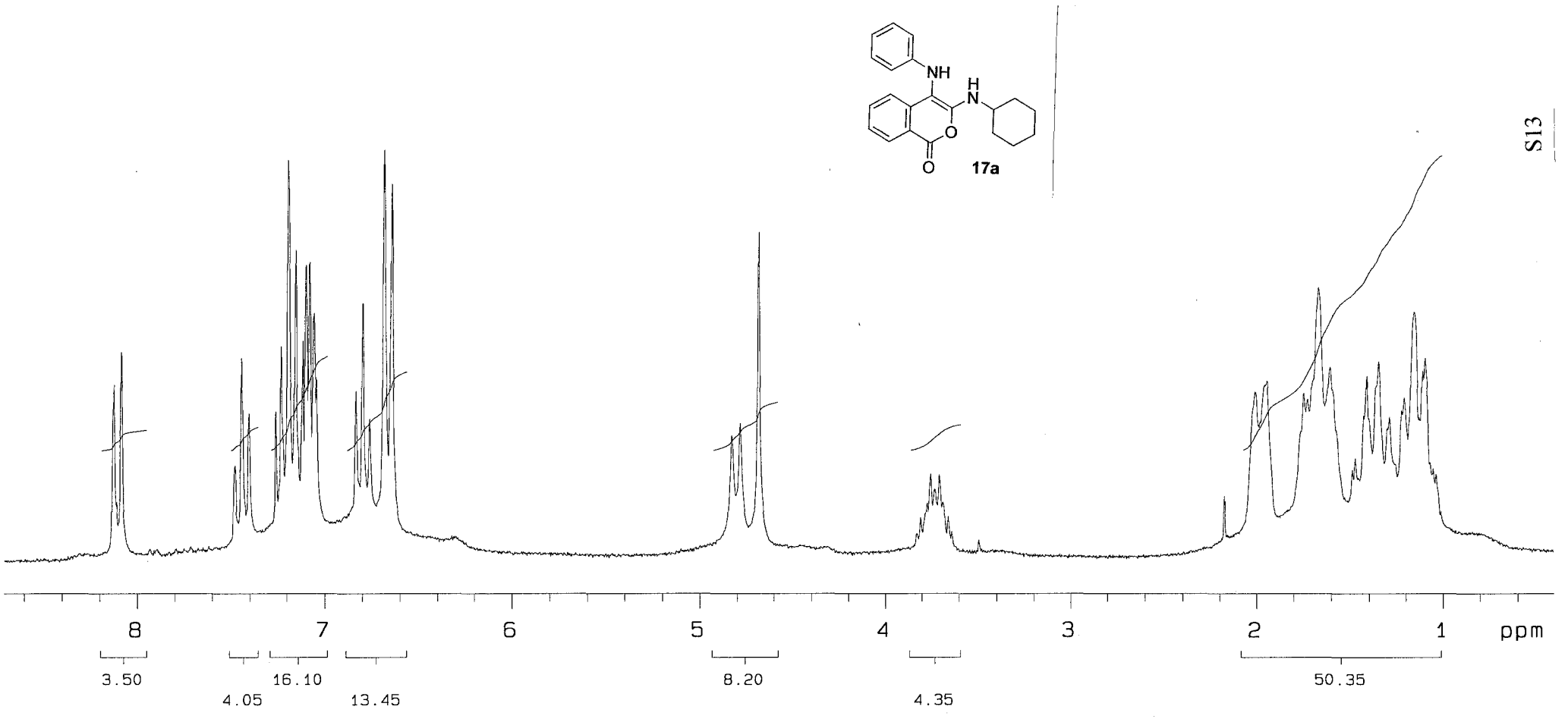

giallo parafluoro e cicloesile novembre 2009

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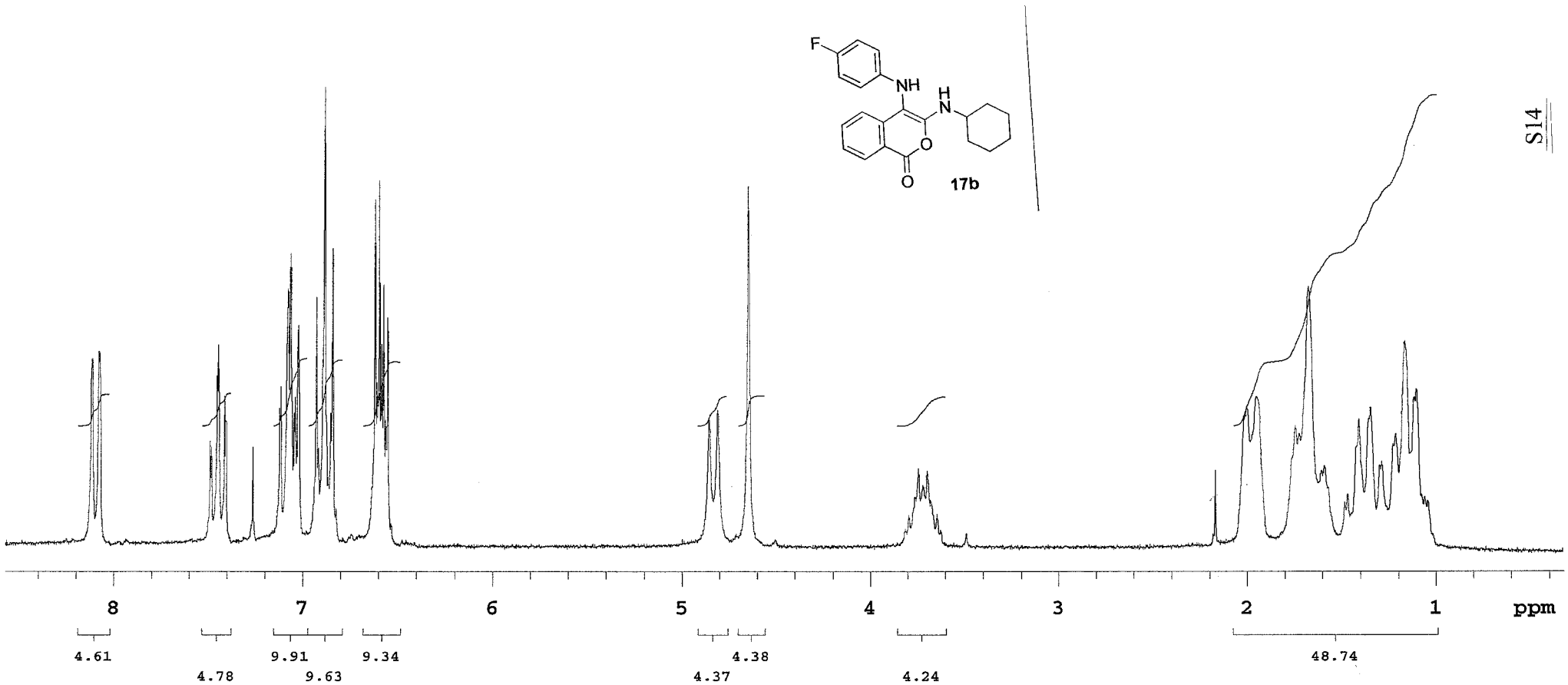

CC01

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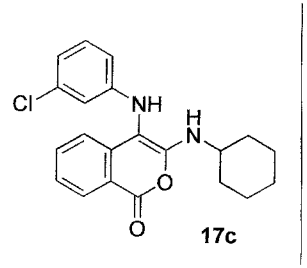

17c

9 8 7 6 5 4 3 2 1 ppm

2.94 4.06 12.38 3.35 2.92 4.09 8.99 4.34 56.93

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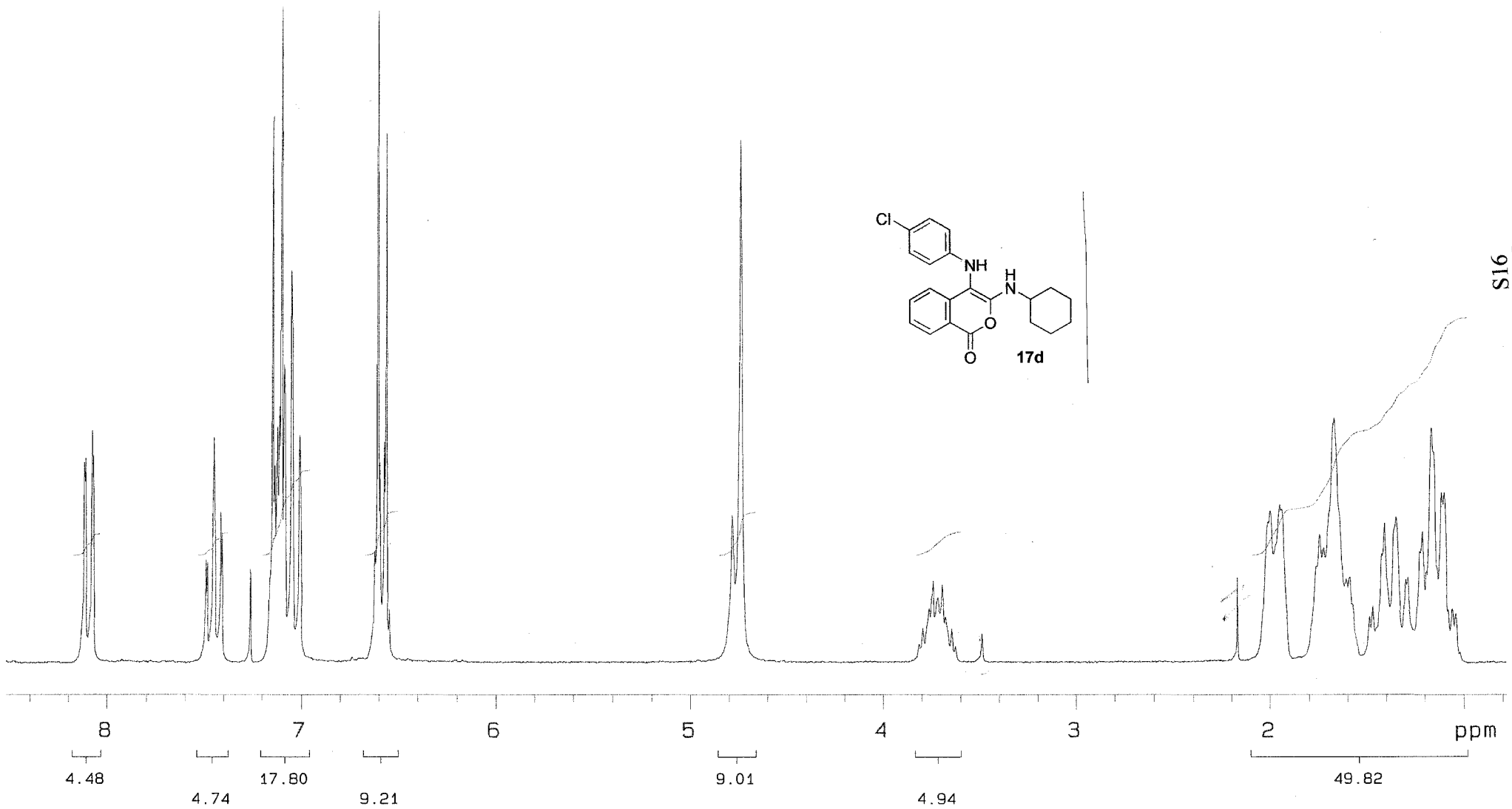
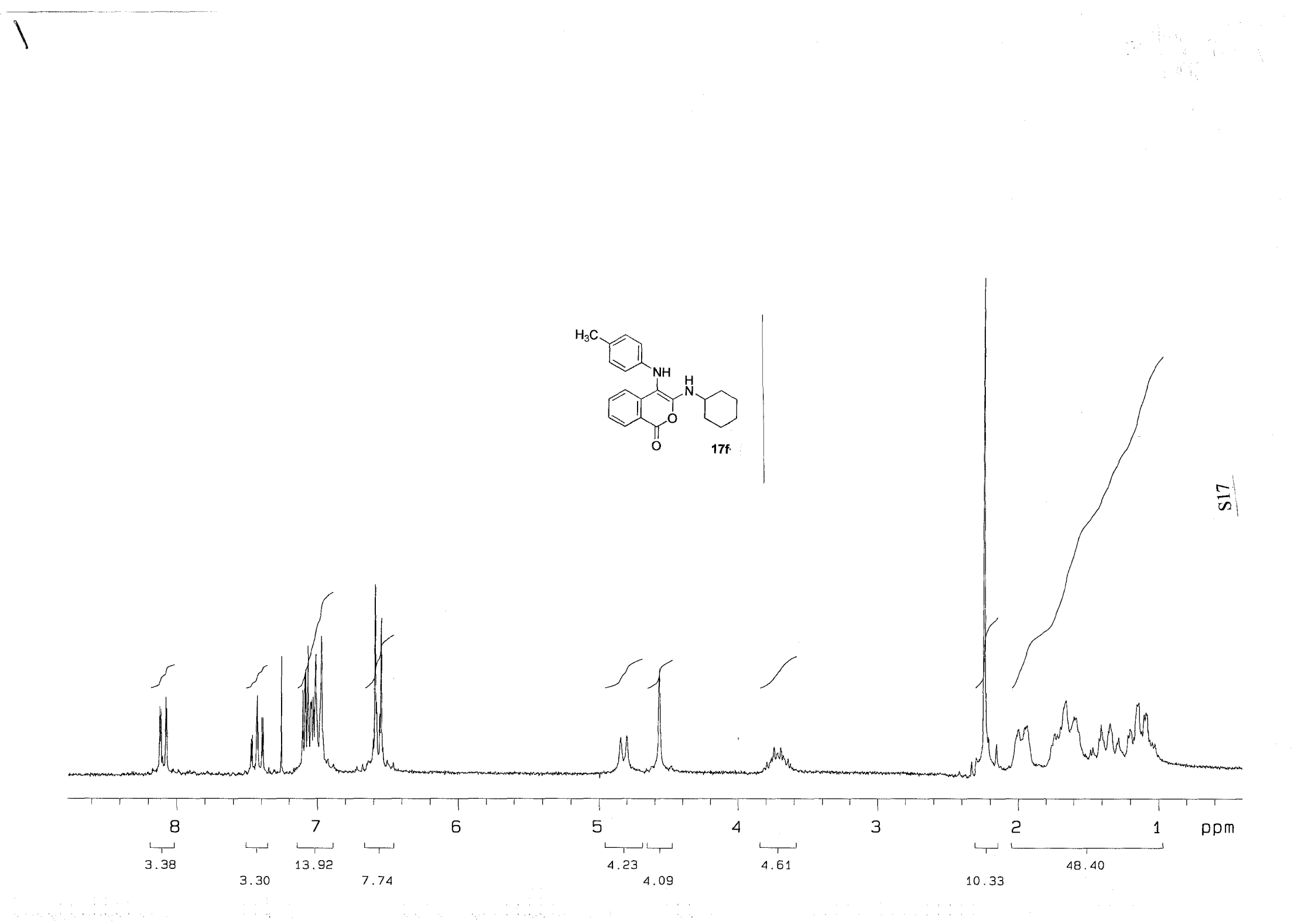
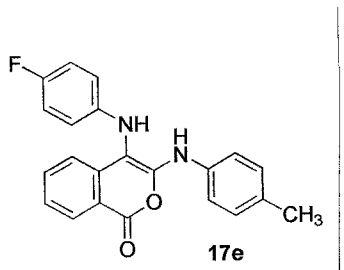



H3C
NH
H
N
O
O
17f
8
7
6
5
4
3
2
1
ppm
3.38
3.30
13.92
7.74
4.23
4.09
4.61
10.33
48.40

SM_Giallo parafluoro tolile novembre2009

Pulse Sequence: s2pul



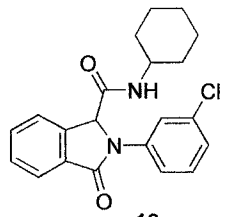
17e

8 7 6 5 4 3 2 ppm

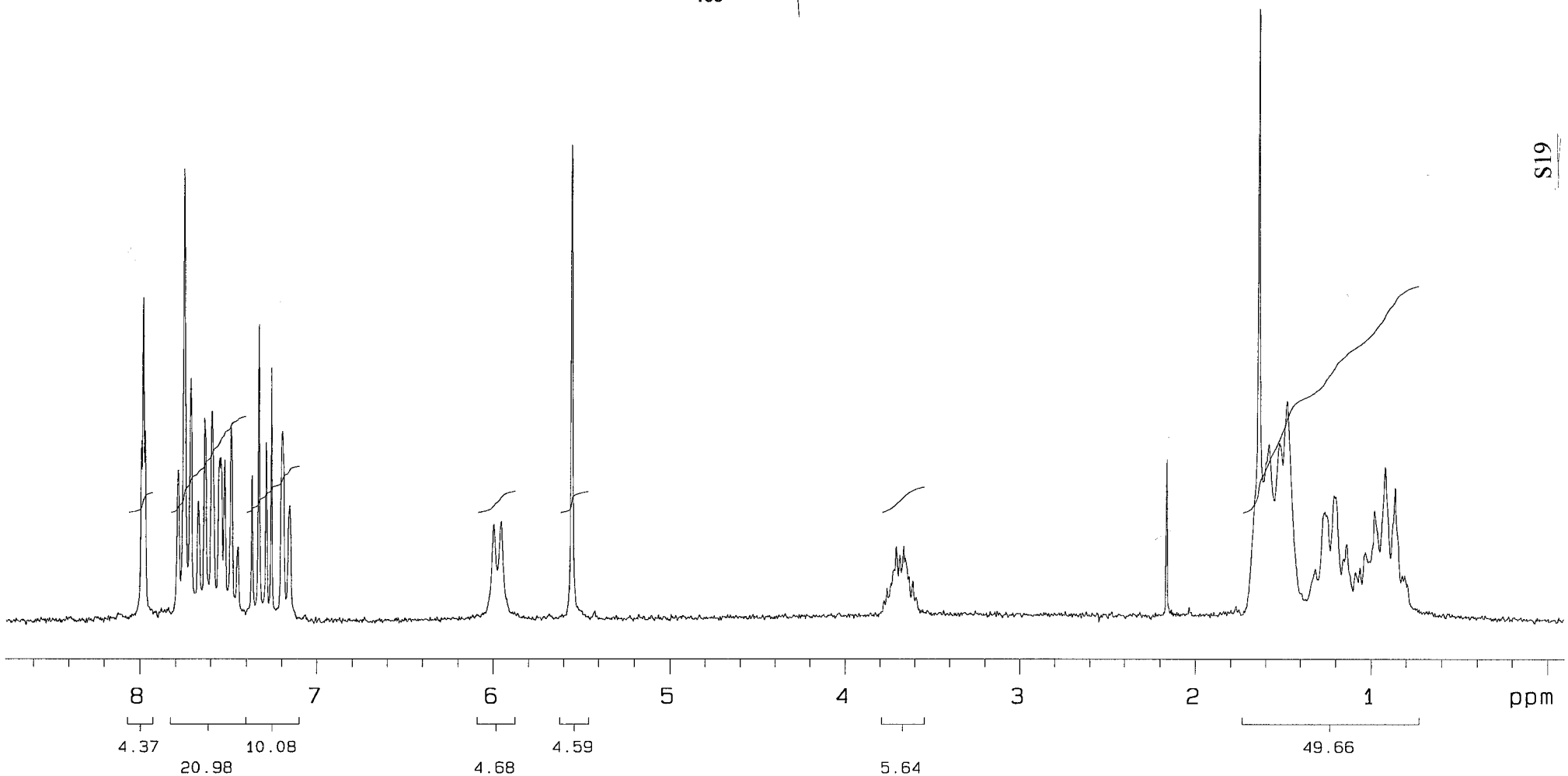
5.16 5.38 34.35 19.24 12.67 5.90 17.30

prodotto bianco

Pulse Sequence: s2pul

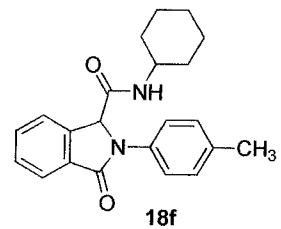


18c



prodotto bianco con metile

Pulse Sequence: s2pul

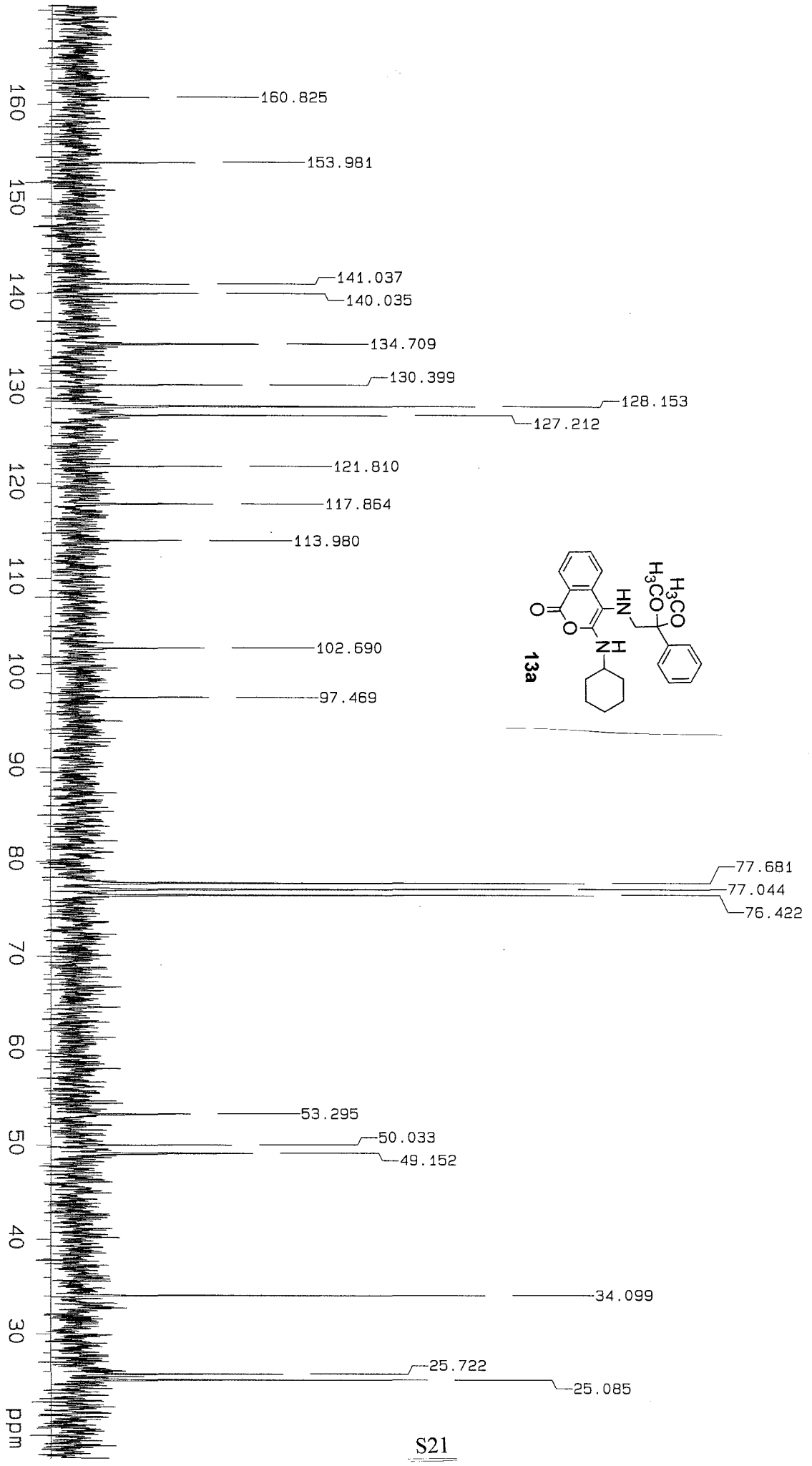


18f

S20

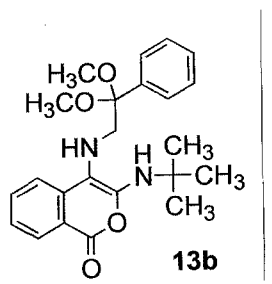
8 7 6 5 4 3 2 1 ppm

22.93 9.00 4.42 3.85 5.10 10.28 44.43

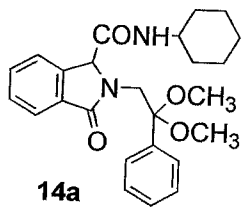

160.825
153.981
141.037
140.035
134.709
130.399
128.153
127.212
121.810
117.864
113.980
102.690
97.469
77.681
77.044
76.422
53.295
50.033
49.152
34.099
25.722
25.085
ppm
13a

13C OBSERVE

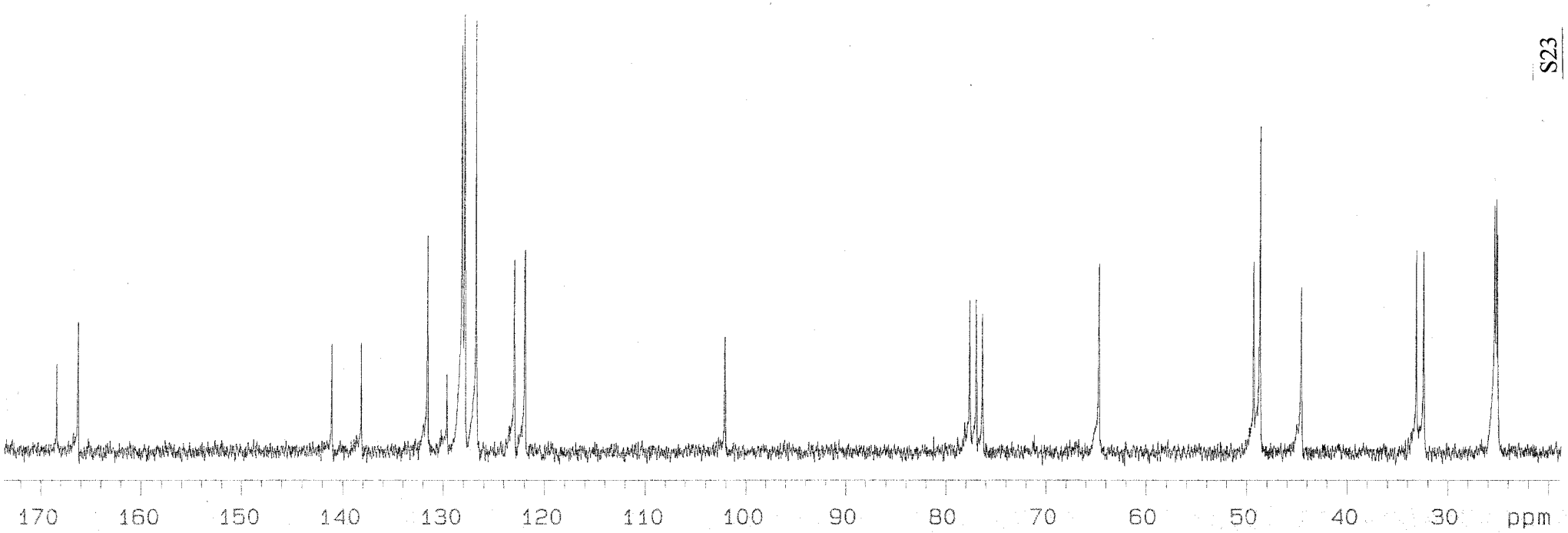
Pulse Sequence: s2pul



13b

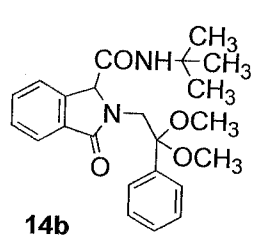

CONH
N
O
OCH3
OCH3

14a


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

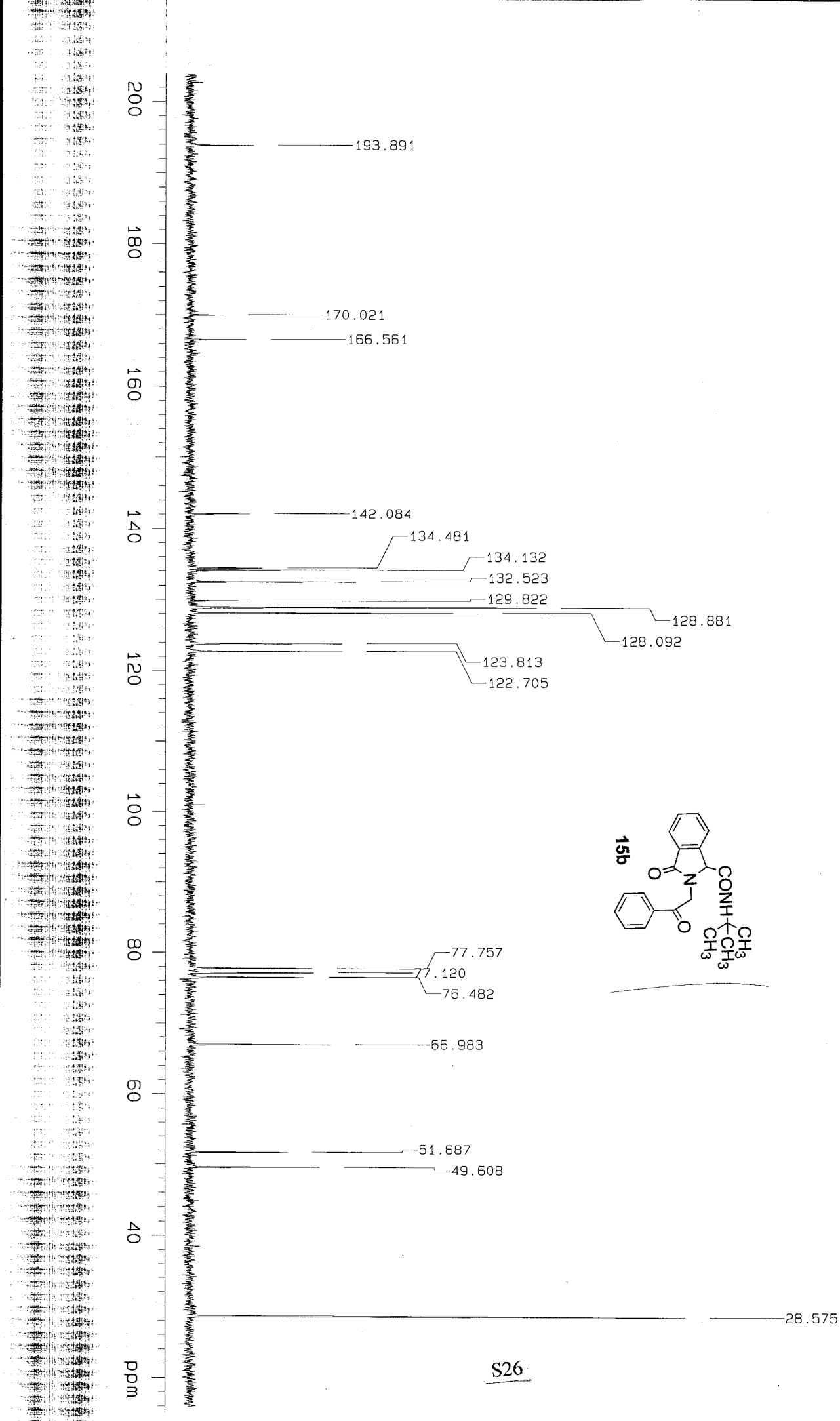
13C OBSERVE

Pulse Sequence: s2pul



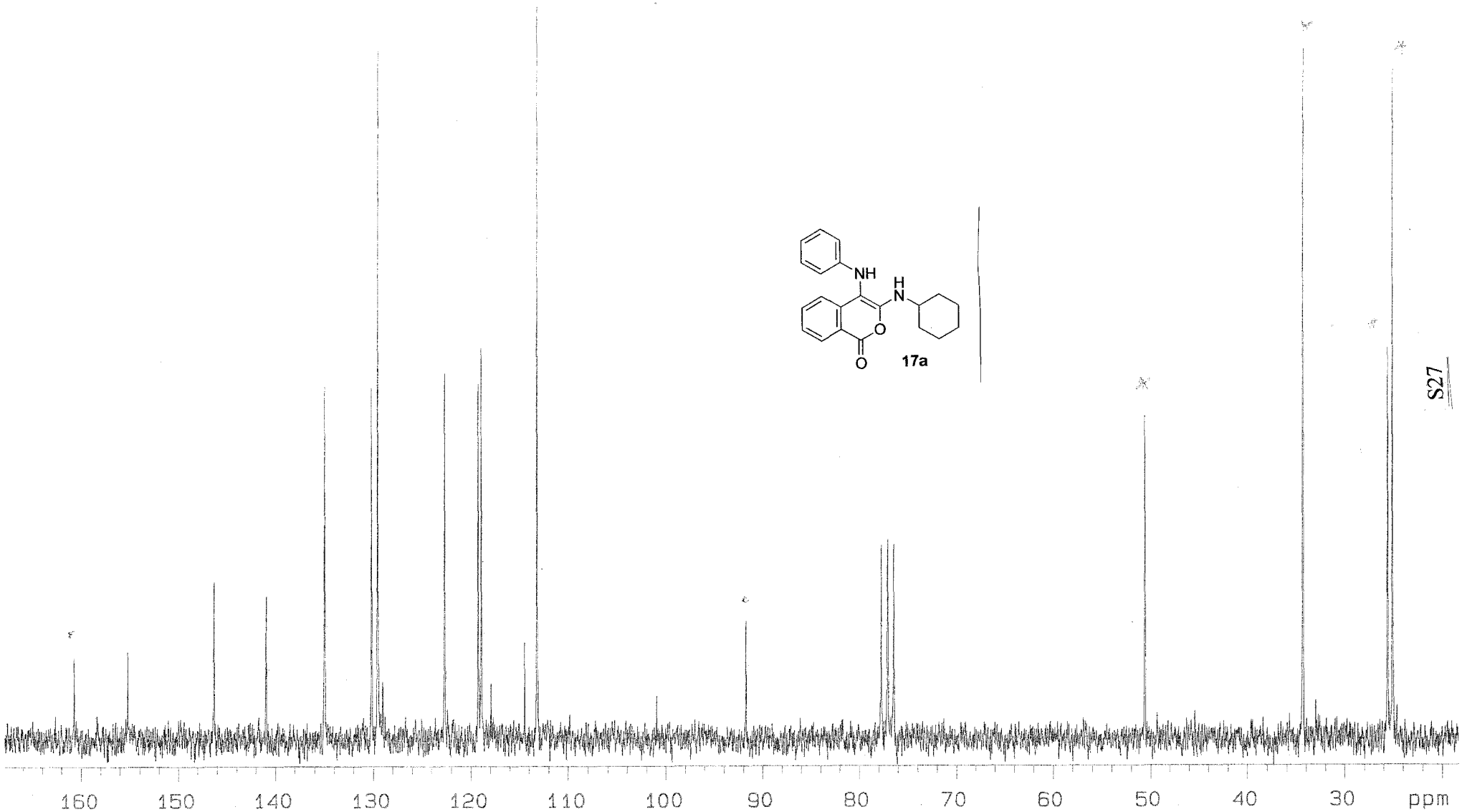
14b

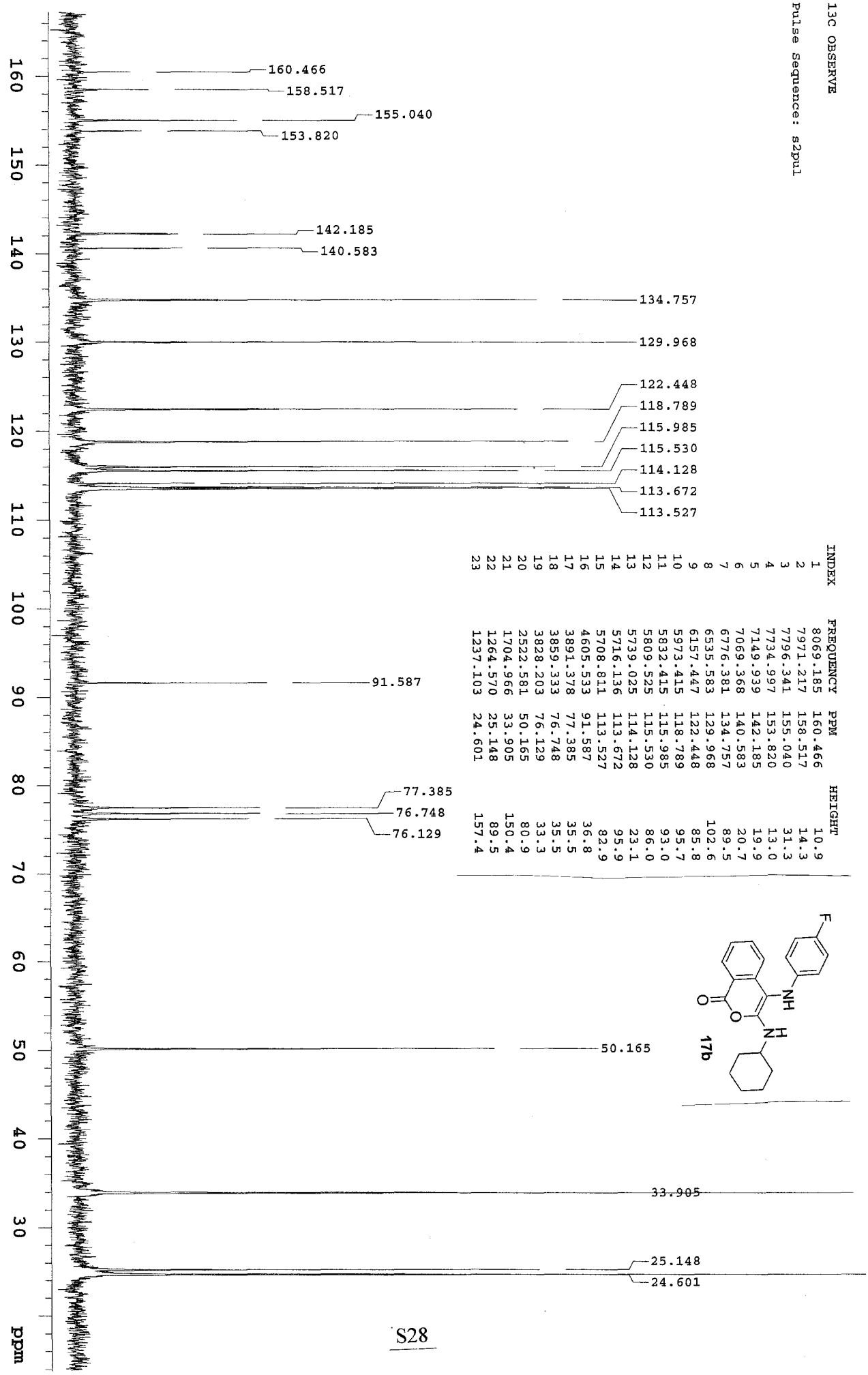
15a


SM_tert_butile deprotetto
Pulse Sequence: s2pul
193.891
170.021
166.561
142.084
134.481
134.132
132.523
129.822
128.881
128.092
123.813
122.705
77.757
77.120
76.482
66.983
51.687
49.608
28.575
200
180
160
140
120
100
80
60
40
ppm
15b
O
N
O
CONH
CH3
CH3
CH3

13C OBSERVE

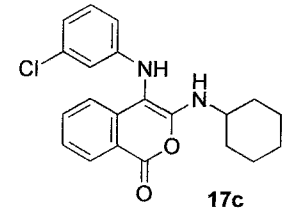
Pulse Sequence: s2pul




13C OBSERVE
Pulse Sequence: s2pul
160.466
158.517
155.040
153.820
142.185
140.583
134.757
129.968
122.448
118.789
115.985
115.530
114.128
113.672
113.527
91.587
77.385
76.748
76.129
50.165
33.905
25.148
24.601
INDEX FREQUENCY PPM HEIGHT
1 8069.185 160.466 10.9
2 7971.217 158.517 14.3
3 7796.341 155.040 31.3
4 7734.997 153.820 13.0
5 7149.939 142.185 19.9
6 7069.368 140.583 20.7
7 6776.381 134.757 89.5
8 6535.583 129.968 102.6
9 6157.447 122.448 85.8
10 5973.415 118.789 95.7
11 5832.415 115.985 93.0
12 5809.525 115.530 86.0
13 5739.025 114.128 23.1
14 5716.136 113.672 95.9
15 5708.811 113.527 82.9
16 4605.533 91.587 36.8
17 3891.378 77.385 35.5
18 3859.333 76.748 33.3
19 3828.203 76.129 80.9
20 2522.581 50.165 150.4
21 1704.966 33.905 89.5
22 1264.570 25.148 157.4
23 1237.103 24.601
F
NH
O
O
N
H
17b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

SM_Giallo_metacloro novembre2009

Pulse Sequence: s2pul

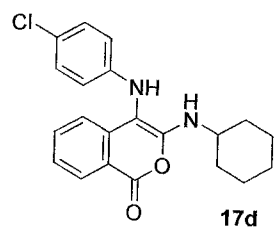


17c

160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

paracloro derivato settembre 2009 C13

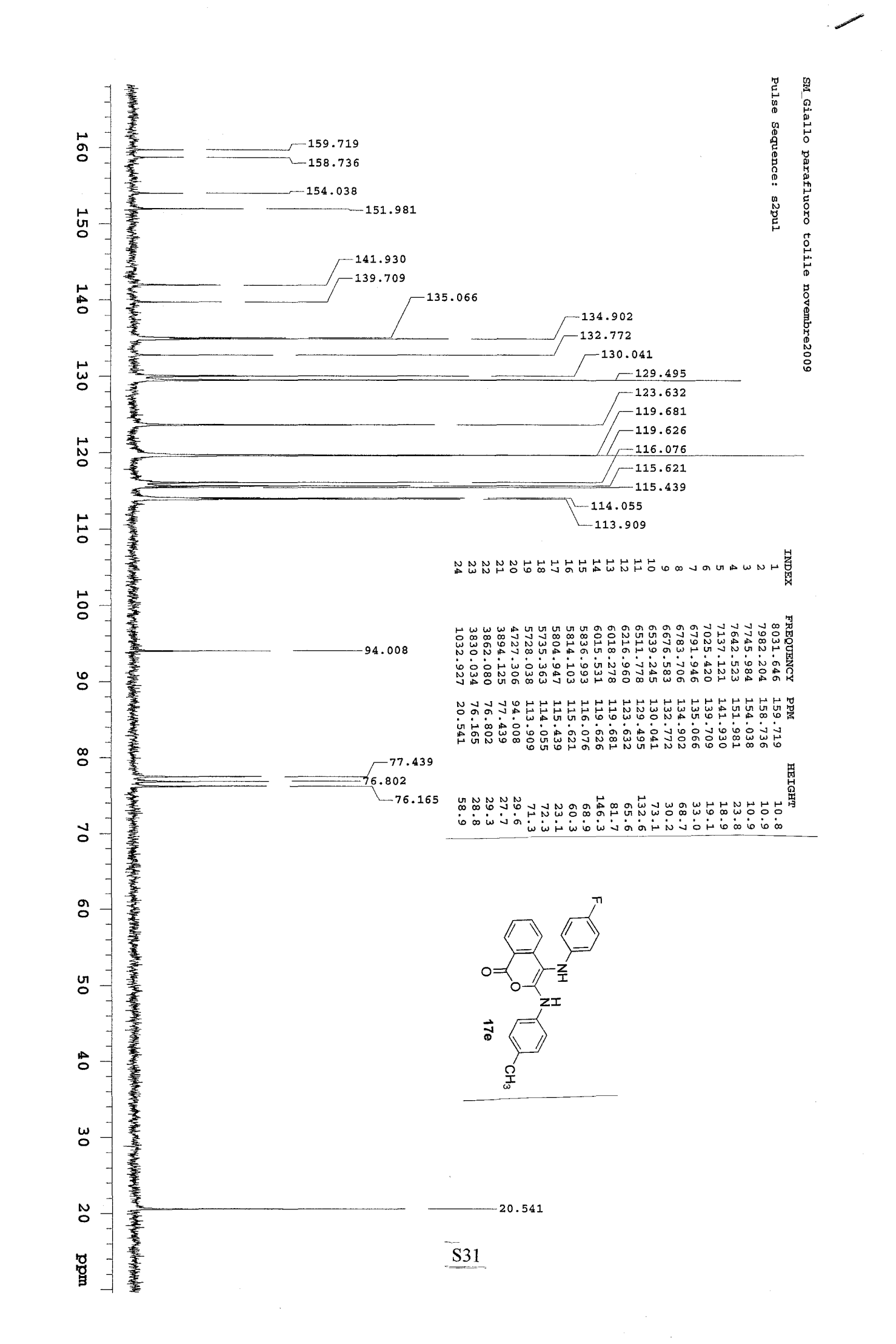
Pulse Sequence: s2pul

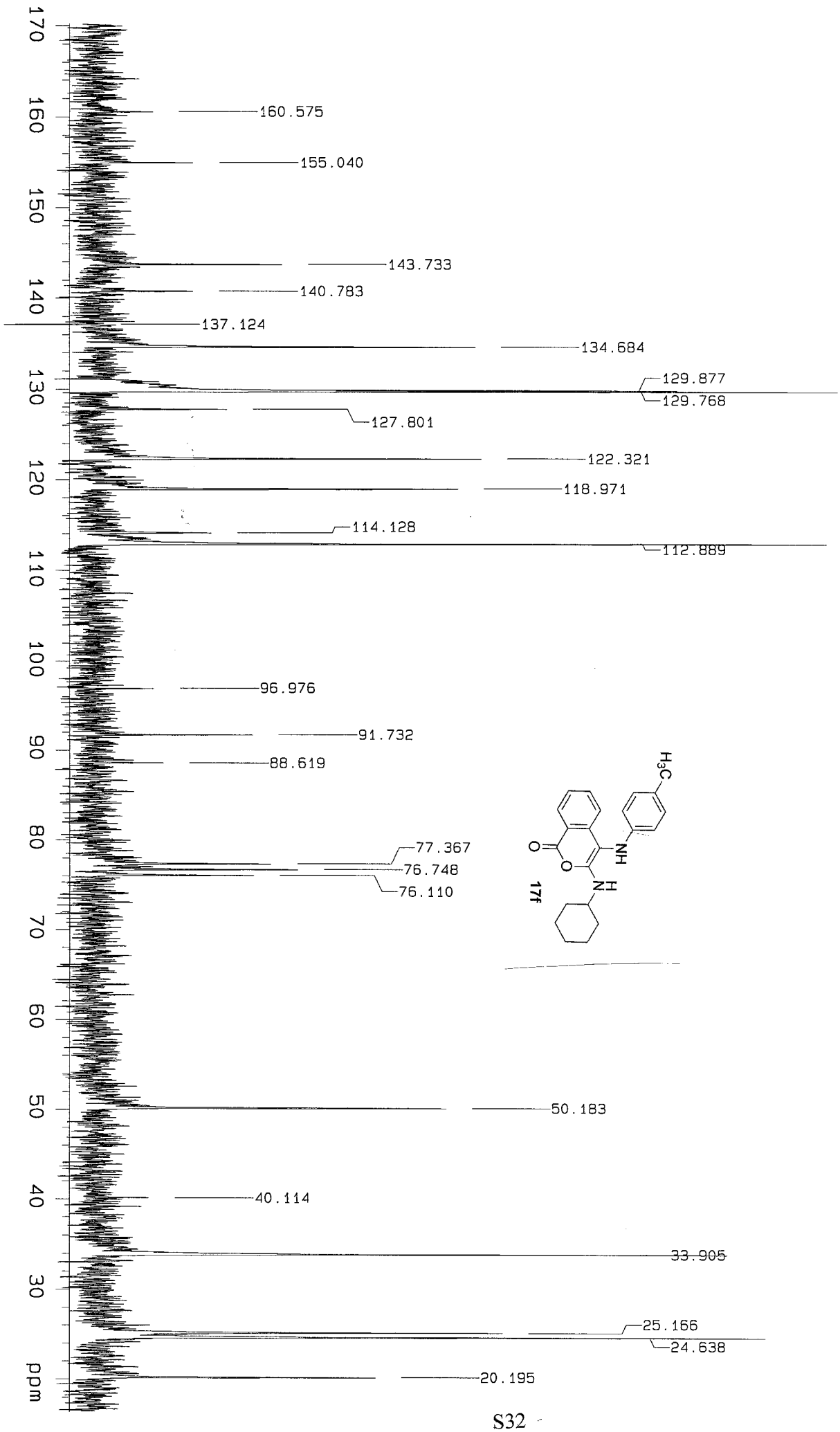


17d

S30

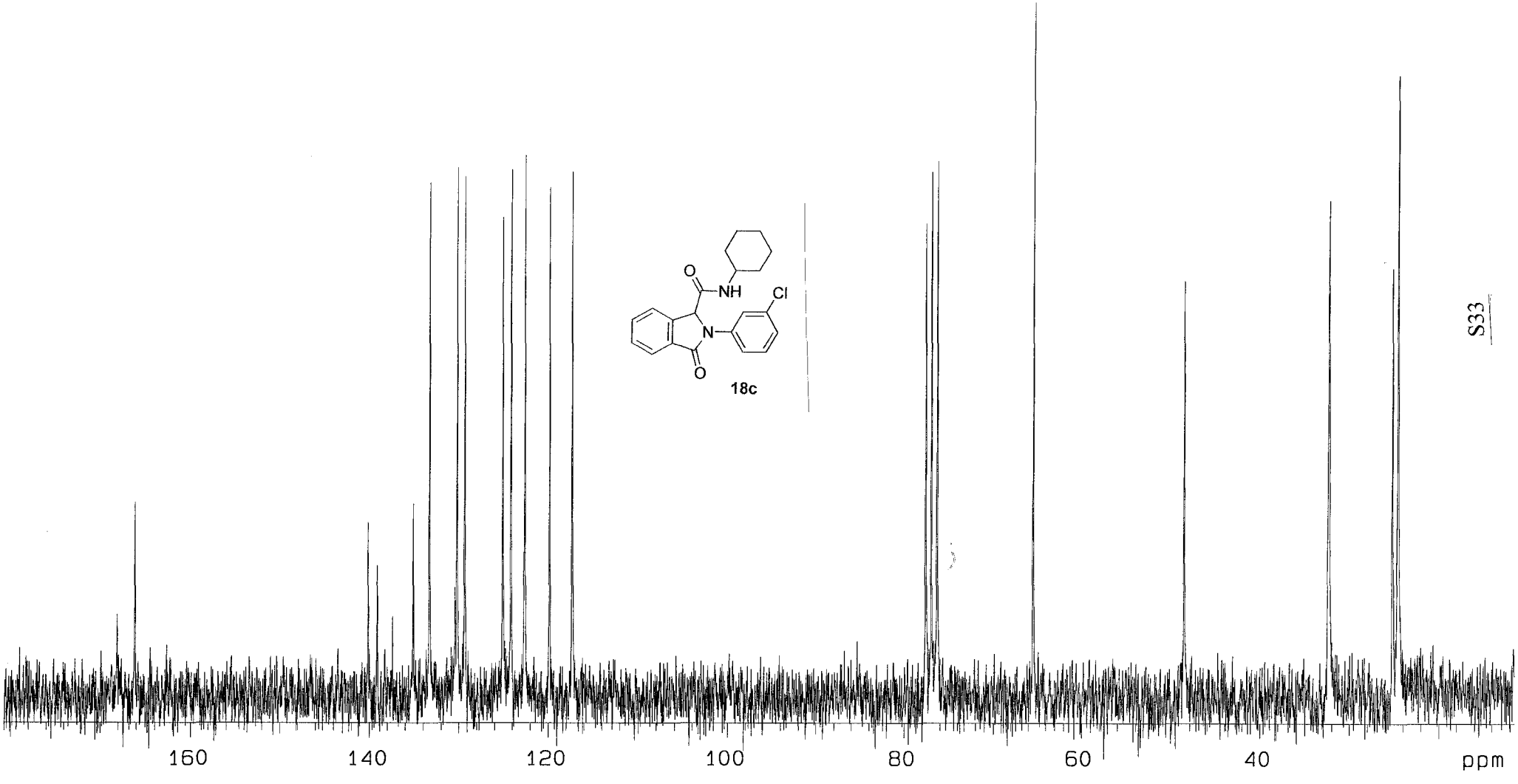
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm


SM_Giallo parafluoro tolile novembre2009
Pulse Sequence: s2pul
159.719
158.736
154.038
151.981
141.930
139.709
135.066
134.902
132.772
130.041
129.495
123.632
119.681
119.626
116.076
115.621
115.439
114.055
113.909
94.008
77.439
76.802
76.165
20.541
INDEX FREQUENCY PPM HEIGHT
1 8031.646 159.719 10.8
2 7982.204 158.736 10.9
3 7745.984 154.038 10.9
4 7642.523 151.981 23.8
5 7137.121 141.930 18.9
6 7025.420 139.709 19.1
7 6791.946 135.066 33.0
8 6783.706 134.902 68.7
9 6676.583 132.772 30.2
10 6539.245 130.041 73.1
11 6511.778 129.495 132.6
12 6216.960 123.632 65.6
13 6018.278 119.681 81.7
14 6015.531 119.626 146.3
15 5836.993 116.076 68.9
16 5814.103 115.621 60.3
17 5804.947 115.439 23.1
18 5735.363 114.055 72.3
19 5728.038 113.909 71.3
20 4727.306 94.008 29.6
21 3894.125 77.439 27.7
22 3862.080 76.802 29.3
23 3830.034 76.165 28.8
24 1032.927 20.541 58.9
F
NH
O
O
N
H
17e
CH3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


160.575
155.040
143.733
140.783
137.124
134.684
129.877
129.768
127.801
122.321
118.971
114.128
112.889
96.976
91.732
88.619
77.367
76.748
76.110
50.183
40.114
33.905
25.166
24.638
20.195
ppm
H3C
NH
O
O
NH
17f

cg 44 fraz 1 ossasel isopr 12.06.09

Pulse Sequence: s2pul

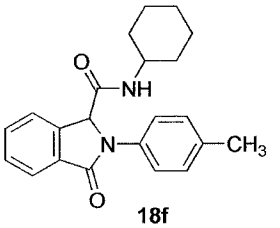


18c

S33

13C OBSERVE
Pulse Sequence: s2pul

INDEX	FREQUENCY	PPM	HEIGHT
1	8440.963	167.881	12.1
2	8373.057	166.530	27.8
3	7053.854	140.293	28.6
4	6801.306	135.270	22.4
5	6785.283	134.951	27.8
6	6674.650	132.751	73.0
7	6583.092	130.930	20.3
8	6527.394	129.822	142.7
9	6492.297	129.124	74.9
10	6234.407	123.995	73.0
11	6166.502	122.645	73.4
12	6042.898	120.186	142.3
13	3908.826	77.742	81.7
14	3876.781	77.105	80.3
15	3844.735	76.467	82.1
16	3298.437	65.602	72.0
17	2443.130	48.591	66.4
18	1632.076	32.460	131.1
19	1275.761	25.373	76.4
20	1242.953	24.721	82.2
21	1239.901	24.660	74.7
22	1060.599	21.094	44.3



18f