

Electronic Supplementary Information

A Cp*CoI₂ dimer as a precursor for cationic Co(III)-catalysis: application to C-H phosphoramidation of indoles

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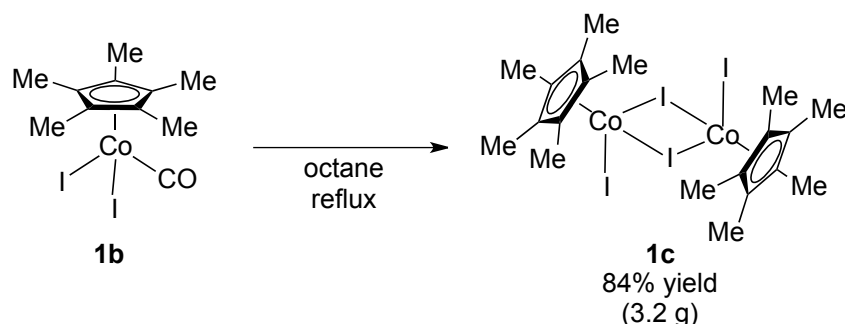
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General: Infrared (IR) spectra were recorded on a JASCO FT/IR 410 Fourier transform infrared spectrophotometer. NMR spectra were recorded on JEOL JNM-ECX500 spectrometers, operating at 500 MHz for ¹H NMR and 125 MHz for ¹³C NMR or JNM-ECS400 spectrometers, operating at 400 MHz for ¹H NMR, 100 MHz for ¹³C NMR and 158 MHz for ³¹P NMR. All spectra were obtained at ambient temperature. The chemical shifts (δ) were recorded in parts per million (ppm). The coupling constants (*J*) were shown in Hertz (Hz). Chemical shifts in CDCl₃ were reported the residual CHCl₃ (7.24 ppm for ¹H NMR, 77.0 ppm for ¹³C NMR). ESI mass spectra for HRMS were measured on a JEOL JMS-T100LC AccuTOF spectrometer. 1,4-dioxane(Super Dehydrated) was purchased from Wako Ltd. and used without purification. 1-(Pyrimidin-2-yl)-1H-indole derivatives **2** were prepared by following the same procedure as described in the literature.^[S1,S2] DPPA **3a** was purchased from Tokyo Chemical Industry Co., Ltd. and used without purification. Bis(4-methoxyphenyl)phosphoroazidate were prepared by following the same procedure as described in the literature.^[S3]

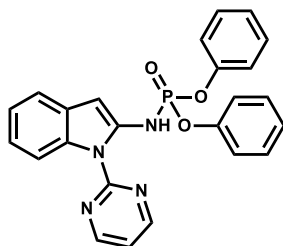
Preparation of [Cp*CoI₂]₂ catalyst: ^[S4]



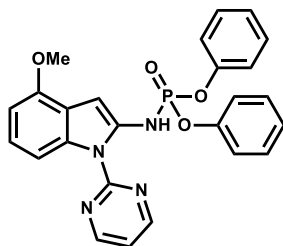
To a round-bottomed flask was charged with *n*-octane (50 mL) and [Cp*Co(CO)I₂] (4.0 g). The mixture was heated to reflux under argon for 12 h. After cooling to room temperature, the solid precipitate was collected in a sintered- glass filtration funnel, washed with pentane, and dried under high vacuum to afford [Cp*CoI₂]₂ (3.2 g, 84%) as a black powder. ¹H NMR (500 MHz, CDCl₃) δ 1.76 (s, 30H).

General Procedure of Co-catalyzed C-H Amidation of Indoles:

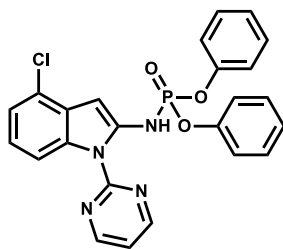
To a dried screw-capped vial were added indole **2** (0.80 mmol), phosphoryl azide **3** (0.40 mmol), [Cp*CoI₂]₂ (17.6 mg, 20 μmol), AgSbF₆ (27.2 mg, 80 μmol), and 1,4-dioxane (0.20 mL) under Ar atmosphere. The vial was capped, and the mixture was heated at 60 °C for 36 h with stirring. The resulting mixture was cooled to room temperature, and directly purified by silica gel column chromatography (hexane:ethyl acetate = 1:1 for all compounds) to give product **4**.

**Diphenyl (1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4aa):**

colorless solid; IR (KBr) ν 3052, 2917, 1615, 1423, 1283, 1185, 951, 781, 687 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 10.31 (d, *J* = 12.1 Hz, 1H), 8.55 -8.49 (m, 3H), 7.43 -7.39 (m, 1H), 7.22 -7.16 (m, 8H), 7.16 -7.09 (m, 2H), 7.09 -7.02 (m, 2H), 6.92 (t, *J* = 4.9 Hz, 1H), 6.45 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 158.3, 157.5, 150.2 (d, *J* = 6.3 Hz), 136.4 (d, *J* = 7.2 Hz), 133.0, 129.7, 129.3, 125.4, 123.0, 121.8, 120.4 (d, *J* = 5.4 Hz), 119.0, 116.2, 115.9, 91.9; ³¹P NMR (158 MHz, CDCl₃) δ -9.01; HRMS (ESI): *m/z* calculated for C₂₄H₁₉N₄NaO₃P⁺ [*M*+Na⁺]: 465.1087, found: 465.1089.

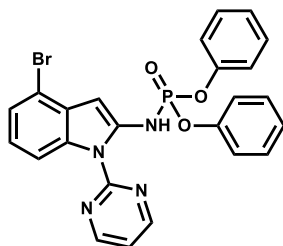
**Diphenyl (4-methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ba):**

colorless solid; IR (KBr) ν 3067, 2955, 1568, 1367, 1270, 1194, 1014, 963, 689 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 10.17 (d, *J* = 12.1 Hz, 1H), 8.58 (d, *J* = 4.9 Hz, 2H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.26 -7.19 (m, 8H), 7.12 -7.07 (m, 3H), 6.97 (t, *J* = 4.9 Hz, 1H), 6.67 (d, *J* = 7.6 Hz, 1H), 6.62 (s, 1H), 3.91 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 158.4, 157.5, 151.7, 150.2 (d, *J* = 6.3 Hz), 134.9 (d, *J* = 6.3 Hz), 134.0, 129.7, 125.3 (d, *J* = 1.8 Hz), 122.5, 120.5 (d, *J* = 5.4 Hz), 119.3, 116.3, 109.1, 103.7, 89.3, 55.4; ³¹P NMR (158 MHz, CDCl₃) δ -8.80; HRMS (ESI): *m/z* calculated for C₂₅H₂₁N₄NaO₄P⁺ [*M*+Na⁺]: 495.1193, found: 495.1183.



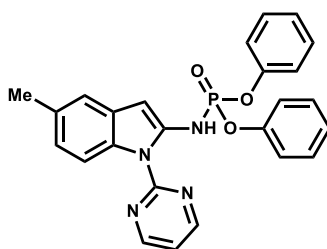
Diphenyl (4-chloro-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ca):

colorless solid; IR (KBr) ν 3081, 2909, 1567, 1428, 1279, 1193, 1024, 954, 765 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 10.47 (d, $J = 12.1$ Hz, 1H), 8.67 (d, $J = 4.6$ Hz, 2H), 8.54 (d, $J = 8.6$ Hz, 1H), 7.37 -7.29 (m, 8H), 7.28 -7.23 (m, 1H), 7.21 -7.16 (m, 2H), 7.15 -7.09 (m, 2H), 6.64 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.2, 157.6, 150.2 (d, $J = 7.2$ Hz), 137.3 (d, $J = 7.2$ Hz), 133.5, 129.8, 128.1, 125.5, 124.1, 122.9, 122.3, 120.4 (d, $J = 4.8$ Hz), 116.7, 114.5, 89.9; ^{31}P NMR (158 MHz, CDCl_3) δ -9.45; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{ClN}_4\text{NaO}_3\text{P}^+$ $[\text{M}+\text{Na}^+]$: 499.0697, found: 499.0689.



Diphenyl (4-bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4da):

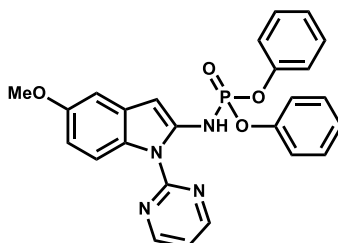
colorless solid; IR (KBr) ν 3039, 2914, 1567, 1447, 1280, 1192, 1020, 902, 757 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.37 (d, $J = 12.1$ Hz, 1H), 8.57 (d, $J = 4.9$ Hz, 2H), 8.49 (d, $J = 8.5$ Hz, 1H), 7.31 (d, $J = 8.1$ Hz, 1H), 7.25 -7.17 (m, 8H), 7.11 -7.05 (m, 2H), 7.02 (t, $J = 4.9$ Hz, 1H), 6.97 (dd, $J = 8.5, 8.1$ Hz, 1H), 6.50 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.2, 157.6, 150.2 (d, $J = 7.2$ Hz), 137.3 (d, $J = 7.2$ Hz), 133.1, 129.9, 129.8, 125.9, 125.5, 122.6, 120.4 (d, $J = 4.5$ Hz), 116.7, 115.1, 112.7, 91.7; ^{31}P NMR (158 MHz, CDCl_3) δ -9.51; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{BrN}_4\text{NaO}_3\text{P}^+$ $[\text{M}+\text{Na}^+]$: 543.0192, found: 543.0198.



Diphenyl (5-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ea):

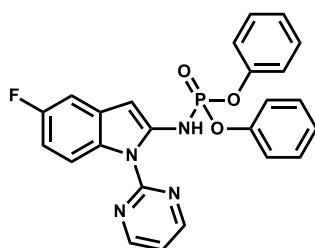
colorless solid; IR (KBr) ν 3041, 2915, 1561, 1480, 1274, 1012, 957, 788, 615 cm^{-1} ;

^1H NMR (400 MHz, CDCl_3) δ 10.36 (d, $J = 12.6$ Hz, 1H), 8.51 (d, $J = 4.9$ Hz, 2H), 8.41 (d, $J = 8.5$ Hz, 1H), 7.23 -7.14 (m, 9H), 7.09 -7.02 (m, 2H), 6.96 -6.89 (m, 2H), 6.37 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.4, 157.4, 150.2 (d, $J = 7.2$ Hz), 136.5 (d, $J = 7.2$ Hz), 132.5, 131.1, 129.7, 129.5, 125.4, 123.0, 120.4 (d, $J = 4.5$ Hz), 119.1, 116.0, 115.7, 91.7, 21.3; ^{31}P NMR (158 MHz, CDCl_3) δ -8.98; HRMS (ESI): m/z calculated for $\text{C}_{25}\text{H}_{21}\text{N}_4\text{NaO}_3\text{P}^+ [\text{M}+\text{Na}^+]$: 479.1243, found: 479.1237.



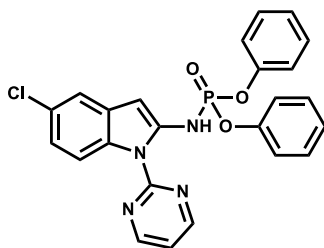
Diphenyl (5-methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4fa):

yellow solid; IR (KBr) ν 3062, 2995, 1582, 1424, 1212, 1089, 936, 779, 691 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.44 (d, $J = 12.1$ Hz, 1H), 8.52 (d, $J = 4.9$ Hz, 2H), 8.45 (d, $J = 9.0$ Hz, 1H), 7.23 -7.15 (m, 8H), 7.09 -7.04 (m, 2H), 6.94 -6.89 (m, 2H), 6.73 -6.70 (m, 1H), 6.39 (s, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.3, 157.4, 156.1, 150.2 (d, $J = 6.3$ Hz), 137.2 (d, $J = 7.2$ Hz), 130.3, 129.7, 127.5, 125.4, 120.4 (d, $J = 4.5$ Hz), 117.0, 116.0, 109.7, 102.2, 91.8, 55.5; ^{31}P NMR (158 MHz, CDCl_3) δ -9.05; HRMS (ESI): m/z calculated for $\text{C}_{25}\text{H}_{21}\text{N}_4\text{NaO}_4\text{P}^+ [\text{M}+\text{Na}^+]$: 495.1193, found: 495.1197.



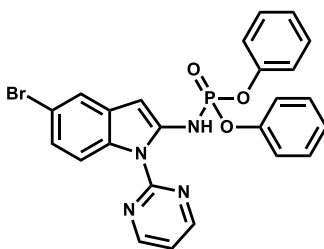
Diphenyl (5-fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ga):

yellow solid; IR (KBr) ν 3063, 2923, 1597, 1495, 1285, 1200, 1024, 905, 767 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.45 (d, $J = 12.1$ Hz, 1H), 8.56 (d, $J = 4.9$ Hz, 2H), 8.51 (dd, $J = 9.2, 4.5$ Hz, 1H), 7.25 -7.16 (m, 8H), 7.10 -7.04 (m, 3H), 6.99 (t, $J = 4.9$ Hz, 1H), 6.82 (ddd, $J = 9.2, 9.2, 2.7$ Hz, 1H), 6.40 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.6 (d, $J = 237.4$ Hz), 158.2, 157.5, 150.1 (d, $J = 6.3$ Hz), 138.0 (d, $J = 7.2$ Hz), 130.4 (d, $J = 9.9$ Hz), 129.8, 129.2, 125.4 (d, $J = 1.8$ Hz), 120.4 (d, $J = 4.5$ Hz), 117.1 (d, $J = 9.0$ Hz), 116.4, 109.0 (d, $J = 24.3$ Hz), 104.6 (d, $J = 24.3$ Hz), 91.6 (d, $J = 3.6$ Hz); ^{31}P NMR (158 MHz, CDCl_3) δ -9.31; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{FN}_4\text{NaO}_3\text{P}^+ [\text{M}+\text{Na}^+]$: 483.0993, found: 483.0987.



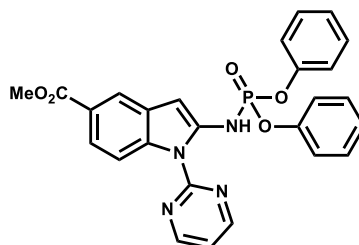
Diphenyl (5-chloro-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ha):

colorless solid; IR (KBr) ν 3062, 2927, 1565, 1498, 1256, 1071, 983, 764, 652 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 10.42 (d, $J = 12.1$ Hz, 1H), 8.55 (d, $J = 4.6$ Hz, 2H), 8.47 (d, $J = 8.6$ Hz, 1H), 7.36 (d, $J = 2.3$ Hz, 1H), 7.24 - 7.16 (m, 8H), 7.10 - 7.03 (m, 3H), 6.99 (t, $J = 4.6$ Hz, 1H), 6.37 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.2, 157.6, 150.1 (d, $J = 6.0$ Hz), 137.8 (d, $J = 7.2$ Hz), 131.3, 130.7, 129.8, 128.5, 125.5, 121.7, 120.4 (d, $J = 4.8$ Hz), 118.4, 117.2, 116.5, 91.1; ^{31}P NMR (158 MHz, CDCl_3) δ -9.36; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{ClN}_4\text{NaO}_3\text{P}^+$ [$\text{M}+\text{Na}^+$] : 499.0697, found: 499.0710.



Diphenyl (5-bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ia):

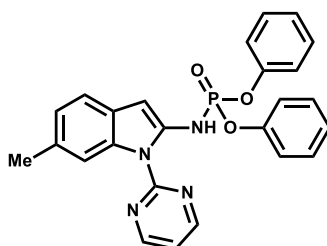
colorless solid; IR (KBr) ν 3042, 2924, 1582, 1492, 1276, 1163, 954, 771, 690 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.42 (d, $J = 12.1$ Hz, 1H), 8.55 (d, $J = 4.9$ Hz, 2H), 8.41 (d, $J = 9.0$ Hz, 1H), 7.51 (s, 1H), 7.25 - 7.15 (m, 9H), 7.10 - 7.04 (m, 2H), 6.99 (t, $J = 4.9$ Hz, 1H), 6.37 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.2, 157.5, 150.1 (d, $J = 6.3$ Hz), 137.7 (d, $J = 7.2$ Hz), 131.6, 131.1, 129.8, 125.5 (d, $J = 1.8$ Hz), 124.4, 121.4, 120.3 (d, $J = 4.5$ Hz), 117.6, 116.5, 116.3, 90.9; ^{31}P NMR (158 MHz, CDCl_3) δ -9.39; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{BrN}_4\text{NaO}_3\text{P}^+$ [$\text{M}+\text{Na}^+$] : 543.0192, found: 543.0199.



Methyl 2-((diphenoxyposphoryl)amino)-1-(pyrimidin-2-yl)-1H-indole-5-carboxylate (4ja):

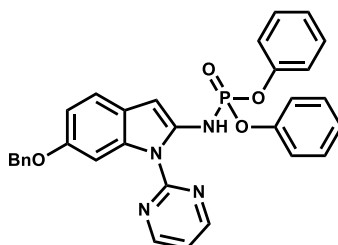
colorless solid; IR (KBr) ν 3057, 2953, 1704, 1564, 1491, 1292, 970, 767, 652 cm^{-1} ;

^1H NMR (400 MHz, CDCl_3) δ 10.28 (d, $J = 12.1$ Hz, 1H), 8.60 -8.53 (m, 3H), 8.13 (d, $J = 1.8$ Hz, 1H), 7.81 (dd, $J = 9.0, 1.8$ Hz, 1H), 7.25 -7.16 (m, 8H), 7.09 -7.05 (m, 2H), 7.03 (t, $J = 4.9$ Hz, 1H), 6.50 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.6, 158.1, 157.7, 150.1 (d, $J = 7.2$ Hz), 137.6 (d, $J = 7.2$ Hz), 135.7, 129.8, 129.0, 125.5, 124.8, 123.3, 120.9, 120.3 (d, $J = 4.5$ Hz), 116.9, 115.6, 92.0, 51.9; ^{31}P NMR (158 MHz, CDCl_3) δ -9.36; HRMS (ESI): m/z calculated for $\text{C}_{26}\text{H}_{21}\text{N}_4\text{NaO}_5\text{P}^+$ $[\text{M}+\text{Na}^+]$: 523.1142, found: 523.1125.



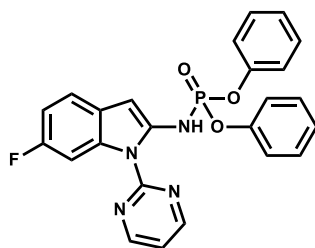
Diphenyl (6-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ka):

colorless solid; IR (KBr) ν 3063, 2915, 1577, 1428, 1284, 1185, 954, 813, 691 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.17 (d, $J = 12.6$ Hz, 1H), 8.55 (d, $J = 4.9$ Hz, 2H), 8.35 (s, 1H), 7.30 (d, $J = 7.6$ Hz, 1H), 7.22 -7.14 (m, 8H), 7.08 -7.03 (m, 2H), 7.00 -6.97 (m, 1H), 6.94 (t, $J = 4.9$ Hz, 1H), 6.41 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.3, 157.5, 150.2 (d, $J = 7.2$ Hz), 135.7 (d, $J = 7.2$ Hz), 133.3, 131.7, 129.7, 126.9, 125.3, 124.3, 120.5 (d, $J = 4.5$ Hz), 118.7, 116.1, 116.0, 92.1, 22.0; ^{31}P NMR (158 MHz, CDCl_3) δ -8.80; HRMS (ESI): m/z calculated for $\text{C}_{25}\text{H}_{21}\text{N}_4\text{NaO}_3\text{P}^+$ $[\text{M}+\text{Na}^+]$: 479.1243, found: 479.1241.



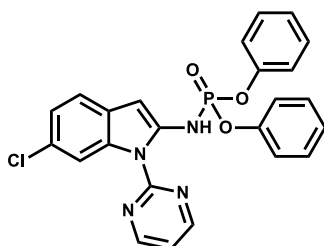
Diphenyl (6-(benzyloxy)-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate(4la):

yellow solid; IR (KBr) ν 3061, 2905, 1578, 1416, 1281, 1158, 953, 775, 695 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3) δ 10.12 (d, $J = 14.1$ Hz, 1H), 8.52 (d, $J = 4.6$ Hz, 2H), 8.30 (d, $J = 2.3$ Hz, 1H), 7.41 (brd, $J = 7.5$ Hz, 2H), 7.32 -7.27 (m, 3H), 7.25 -7.16 (m, 9H), 7.08 -7.02 (m, 2H), 6.94 (t, $J = 4.6$ Hz, 1H), 6.88 (dd, $J = 8.6, 2.3$ Hz, 1H), 6.38 (s, 1H), 5.05 (s, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.3, 157.5, 155.2, 150.2 (d, $J = 7.2$ Hz), 137.5, 135.4 (d, $J = 6.0$ Hz), 133.8, 129.7, 128.5, 127.8, 127.6, 125.3, 123.3, 120.4 (d, $J = 4.8$ Hz), 119.2, 116.1, 111.5, 103.3, 92.1, 70.8; ^{31}P NMR (158 MHz, CDCl_3) δ -8.83; HRMS (ESI): m/z calculated for $\text{C}_{31}\text{H}_{25}\text{N}_4\text{NaO}_4\text{P}^+$ $[\text{M}+\text{Na}^+]$: 571.1506, found: 571.1531.



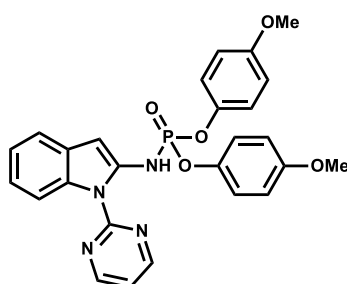
Diphenyl (6-fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ma):

colorless solid; IR (KBr) ν 3065, 2911, 1577, 1496, 1283, 1197, 969, 809, 687 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.22 (d, $J = 12.1$ Hz, 1H), 8.56 (d, $J = 4.9$ Hz, 2H), 8.35 (dd, $J = 11.2, 2.2$ Hz, 1H), 7.33 -7.28 (m, 1H), 7.24 -7.16 (m, 8H), 7.09 -7.04 (m, 2H), 6.99 (t, $J = 4.9$ Hz, 1H), 6.94 -6.88 (m, 1H), 6.41 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.3 (d, $J = 234.7$ Hz), 158.2, 157.6, 150.2 (d, $J = 6.3$ Hz), 136.7 (d, $J = 3.6$ Hz), 136.6 (d, $J = 3.6$ Hz), 132.9 (d, $J = 12.6$ Hz), 129.7, 125.4, 120.4 (d, $J = 4.5$ Hz), 119.2 (d, $J = 9.9$ Hz), 116.5, 110.8 (d, $J = 23.4$ Hz), 103.8 (d, $J = 29.7$ Hz), 91.7; ^{31}P NMR (158 MHz, CDCl_3) δ -9.11; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{FN}_4\text{NaO}_3\text{P}^+[\text{M}+\text{Na}^+]$: 483.0993, found: 483.0976.



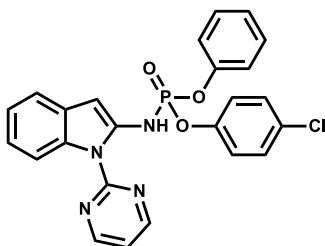
Diphenyl (6-chloro-1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4na):

colorless solid; IR (KBr) ν 3054, 2919, 1577, 1496, 1281, 1194, 953, 770, 689 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.31 (d, $J = 12.1$ Hz, 1H), 8.61 (d, $J = 1.8$ Hz, 1H), 8.57 (d, $J = 4.9$ Hz, 2H), 7.31 (d, $J = 8.5$ Hz, 1H), 7.24 -7.16 (m, 8H), 7.14 -7.11 (m, 1H), 7.10 -7.05 (m, 2H), 7.01 (t, $J = 4.9$ Hz, 1H), 6.41 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.2, 157.6, 150.1 (d, $J = 7.2$ Hz), 137.1 (d, $J = 7.2$ Hz), 133.2, 129.8, 127.8, 127.3, 125.4, 123.4, 120.4 (d, $J = 4.5$ Hz), 119.5, 116.6, 116.3, 91.6; ^{31}P NMR (158 MHz, CDCl_3) δ -9.22; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{ClN}_4\text{NaO}_3\text{P}^+[\text{M}+\text{Na}^+]$: 499.0697, found: 499.0694.



Bis(4-methoxyphenyl) (1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ab):

colorless solid; IR (KBr) ν 3080, 2935, 1600, 1457, 1285, 1184, 955, 828, 743 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.18 (d, $J = 12.1$ Hz, 1H), 8.56-8.52 (m, 3H), 7.42 (dd, $J = 6.3, 1.8$ Hz, 1H), 7.17-7.07 (m, 6H), 6.95 (t, $J = 4.9$ Hz, 1H), 6.72-6.67 (m, 4H), 6.43 (s, 1H), 3.64 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.4, 157.5, 156.9, 143.7 (d, $J = 6.3$ Hz), 136.6 (d, $J = 6.3$ Hz), 133.0, 129.3, 123.0, 121.8, 121.3 (d, $J = 4.5$ Hz), 119.0, 116.2, 115.9, 114.6, 91.9, 55.5; ^{31}P NMR (158 MHz, CDCl_3) δ -7.80; HRMS (ESI): m/z calculated for $\text{C}_{26}\text{H}_{23}\text{N}_4\text{NaO}_5\text{P}^+$ $[\text{M}+\text{Na}^+]$: 525.1298, found: 525.1319.

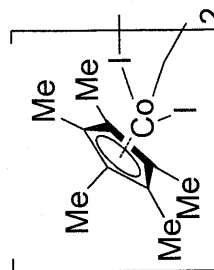


4-chlorophenyl phenyl (1-(pyrimidin-2-yl)-1H-indol-2-yl)phosphoramidate (4ac): yellow oil; IR (neat) ν 3057, 1583, 1485, 1427, 1352, 1190, 944, 747 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.32 (d, $J = 12.1$ Hz, 1H), 8.59-8.45 (m, 3H), 7.45-7.36 (m, 1H), 7.25-7.01 (m, 11H), 6.90 (td, $J = 4.9, 1.3$ Hz, 1H), 6.41 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 158.3, 157.4, 150.0 (d, $J = 7.2$ Hz), 148.6 (d, $J = 7.2$ Hz), 136.1 (d, $J = 7.2$ Hz), 133.0, 130.7, 129.7, 129.7, 129.1, 125.5, 123.1, 122.0, 121.8 (d, $J = 3.6$ Hz), 120.3 (d, $J = 4.8$ Hz), 119.0, 116.2, 116.0, 92.1; ^{31}P NMR (158 MHz, CDCl_3) δ -8.87; HRMS (ESI): m/z calculated for $\text{C}_{24}\text{H}_{18}\text{ClN}_4\text{NaO}_3\text{P}^+$ $[\text{M}+\text{Na}^+]$: 499.0697, found: 499.0686.

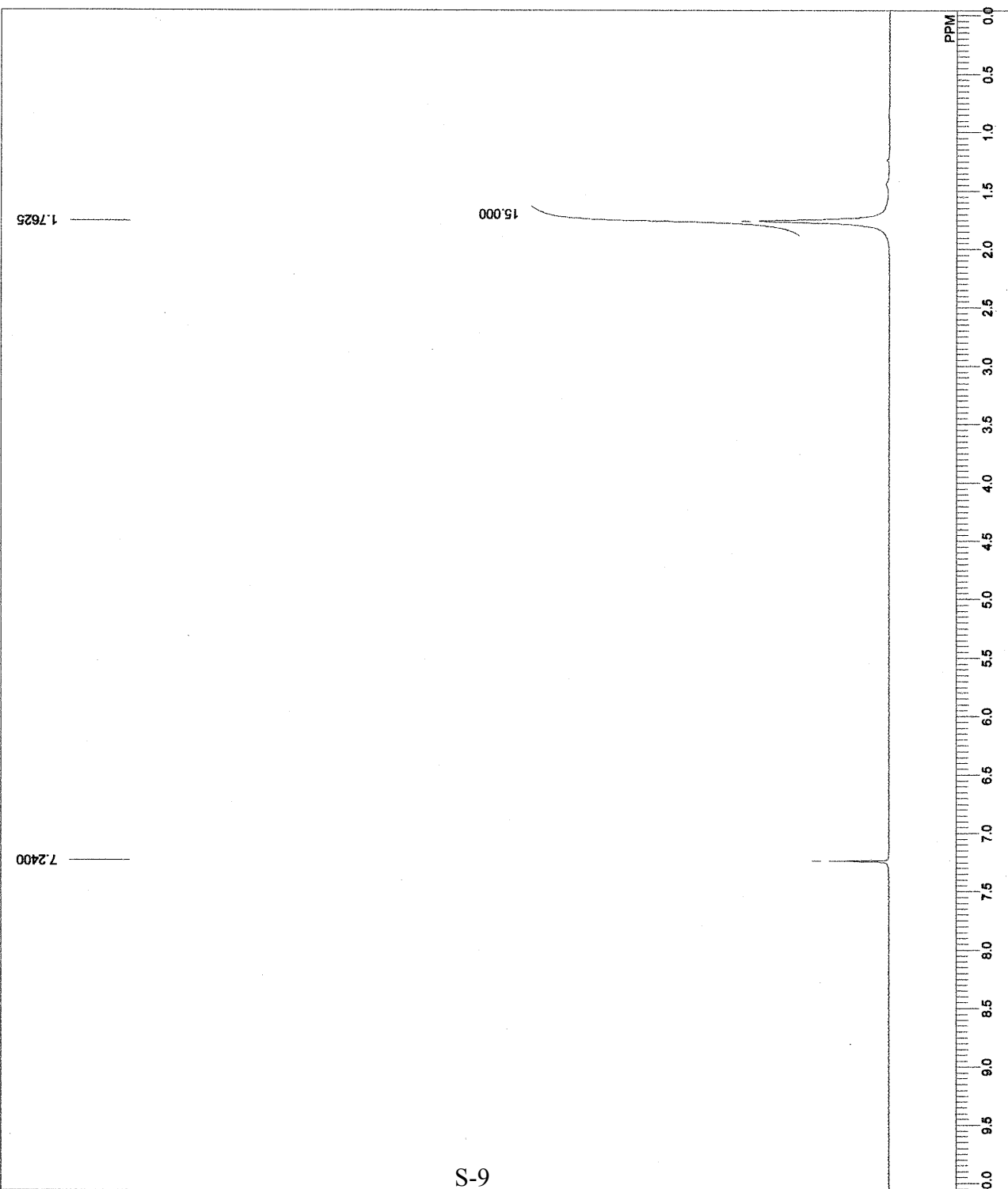
Reference:

- [S1] L. Ackermann, A. V. Lygin. *Org. Lett.* **2011**, 13, 3332.
- [S2] J. Shi, B. Zhou, Y. Yang, Y. Li. *Org. Biomol. Chem.* 2012, 10, 8953.
- [S3] S. H. Kim, D. Y. Jung, S. Chang. *J. Org. Chem.*, **2007**, 72, 9769.
- [S4] S. A. Frith, J. Spencer. *Inorganic Syntheses*. **1990**, 28, 273.
- [S5] W. Li, L. Weng, G. Jin. *Inorg. Chem. Commun.* **2004**, 7, 1174.

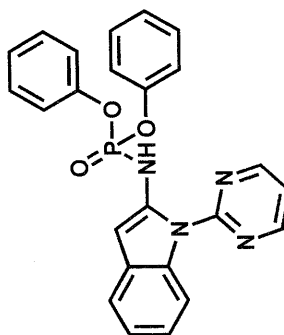
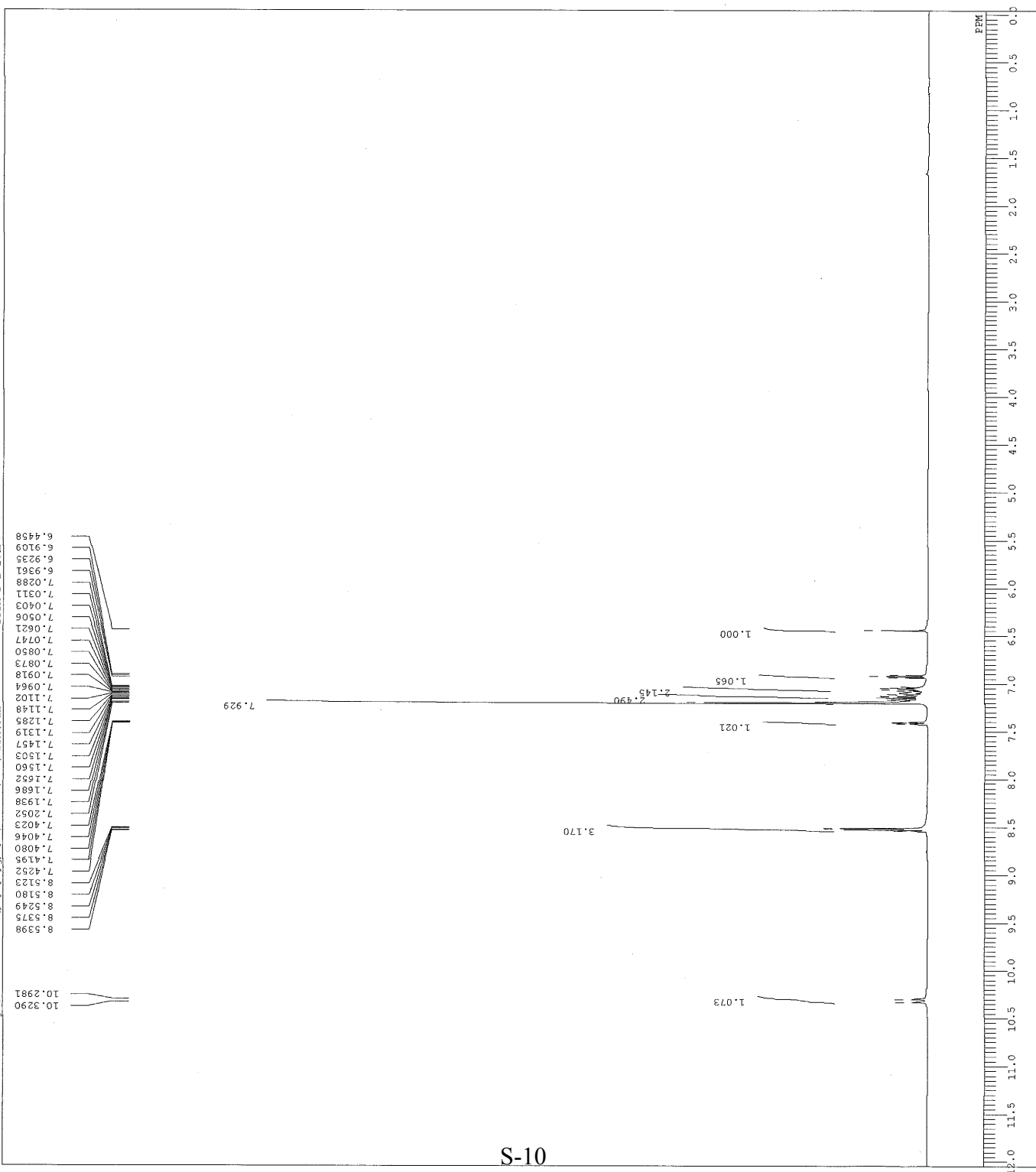
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 PD 5.55 usec
 PW1 1H
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 CTEMP CDCL3
 SLVNT 7.24 ppm
 EXREF 0.12 Hz
 BF 40
 RGAIN



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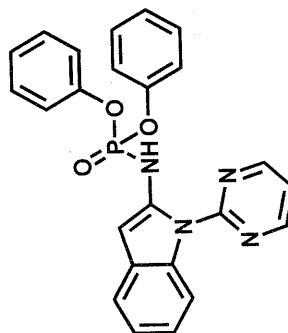
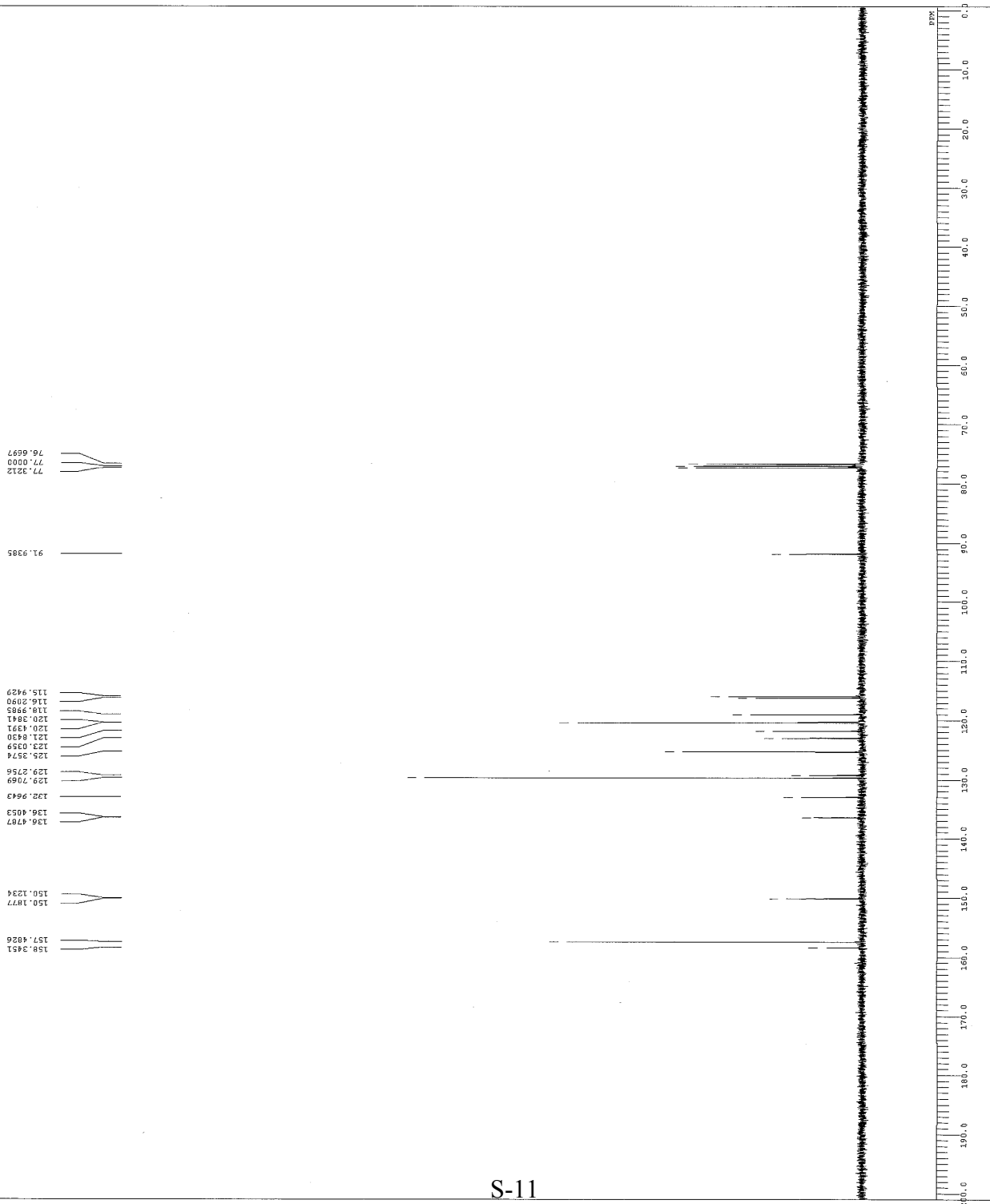


4aa

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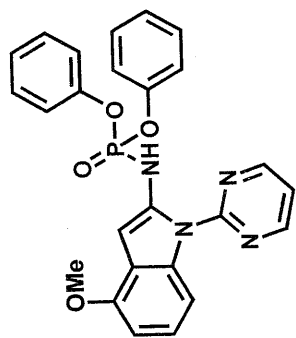
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101.32 MHz
8.74 Hz
26514 Hz
POINT
23686.69 Hz
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PREQ 2.0000 sec
PD 3.00 usec
FID 1
PULP 1
PRG 1
NAME IN
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SLOWP CDOL3 77.60 ppm
INSTR BRUKER
PROB 0.12 Hz
RGAIN 60

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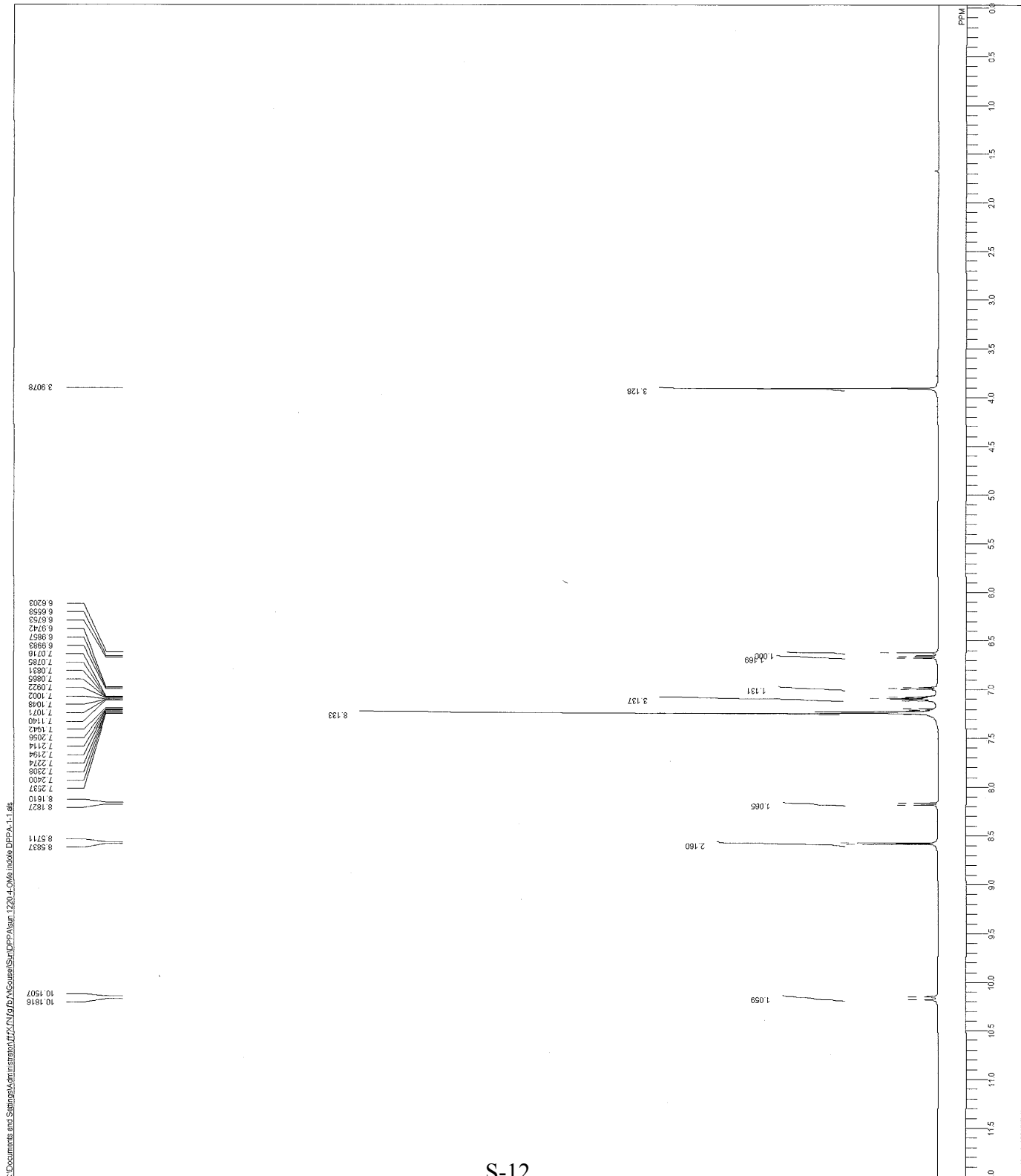


4aa

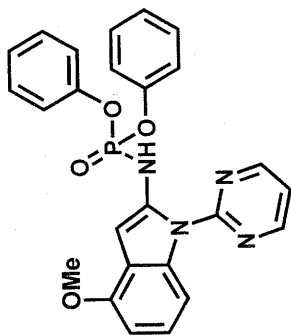
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 P0 5.00 sec
 P01 5.00 sec
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 CTEMP 21.4 c
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 BF 0.12 Hz
 RGAIN 30



4ba



sun 1220 4-OMe indole DPPA-2.1.xls



4ba

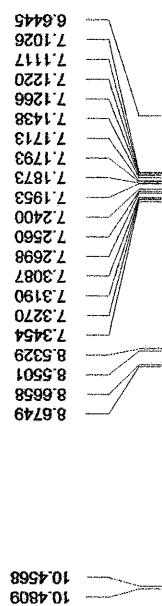
sun 1224 4-Cl Indole DPPA-1-1.als

DFILE
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DATIM
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EXMOD
OBFREQ
OBSET
OBFIN
POINT
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SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

2013-12-24 23:36:54

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proton.jpg
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6.01 Hz
16384
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1H
21.2 c
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0.12 Hz
34

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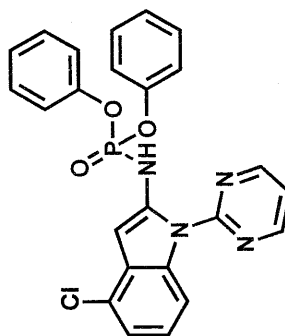
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1.000

2.117

1.079

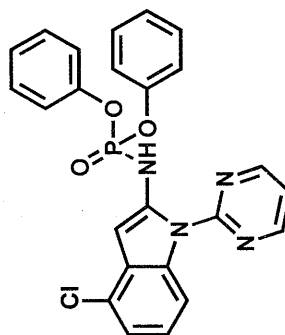


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 RGAIN 60

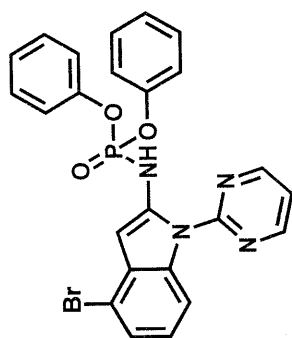
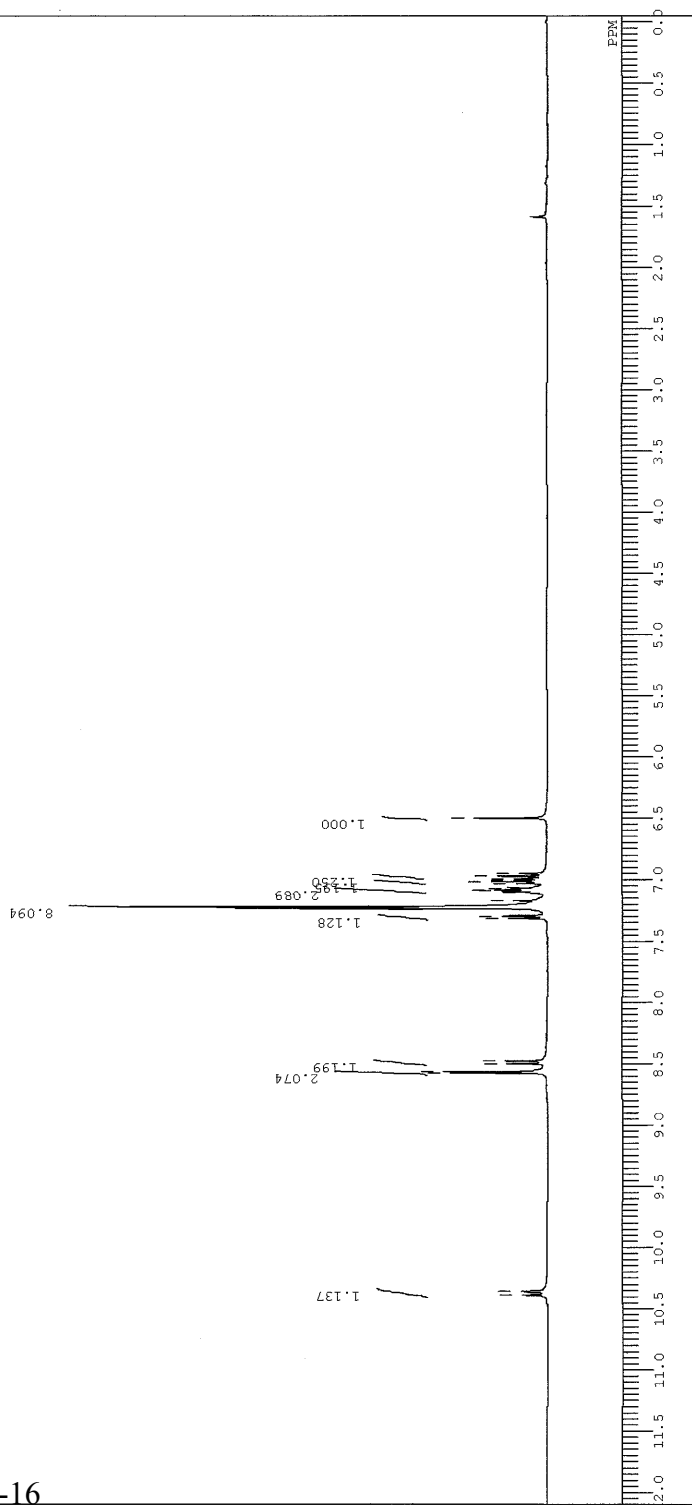
C:\Documents and Settings\user\1\My Documents\1224 4-Cl indole DPPA-2-1.als

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 133.5241
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 122.8507
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 120.4375
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 116.7271
 114.5428
 89.9244
 77.2575
 77.0000
 76.7520



4ca

t	n (alpha=0.001)	n (alpha=0.002)	n (alpha=0.005)	n (alpha=0.01)	n (alpha=0.02)
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20	-	5.0	2.5	1.5	1.2
30	-	7.5	3.5	1.8	1.3
40	-	8.5	4.0	2.0	1.4
50	-	9.0	4.2	2.1	1.5
60	-	9.2	4.3	2.2	1.6
70	-	9.3	4.4	2.3	1.7
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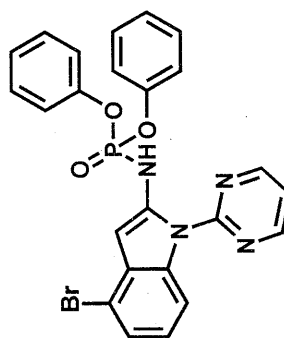


4da

S-17

Mass spectrum plot showing relative intensity (0.0 to 100.0) versus mass-to-charge ratio (m/z, 20.0 to 240.0). The base peak is at m/z 77.3303. Other significant peaks are labeled with their m/z values.

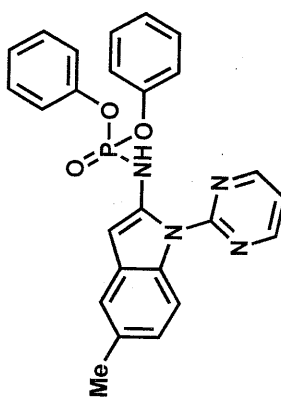
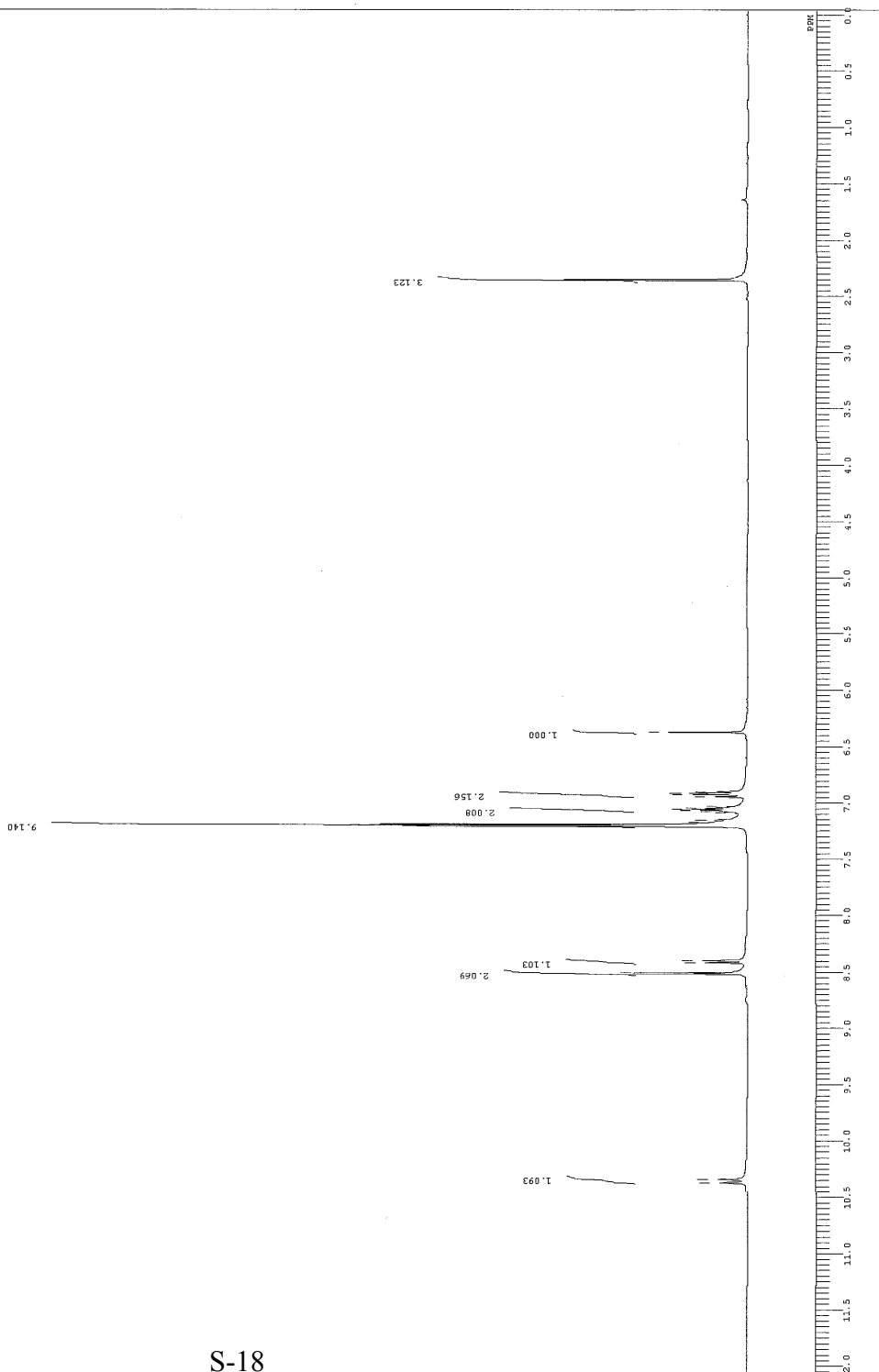
m/z	Relative Intensity (%)
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157.6190	~5
150.1957	~5
150.1223	~5
137.3128	~10
137.2394	~5
133.1470	~5
129.9446	~5
129.7978	~5
125.9256	~5
125.4760	~5
122.6315	~5
120.4476	~5
120.4018	~5
116.7406	~5
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112.6665	~5
91.6997	~10
77.3303	100
77.0000	~5
76.6788	~5



4da

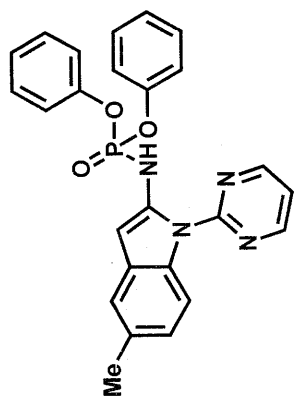
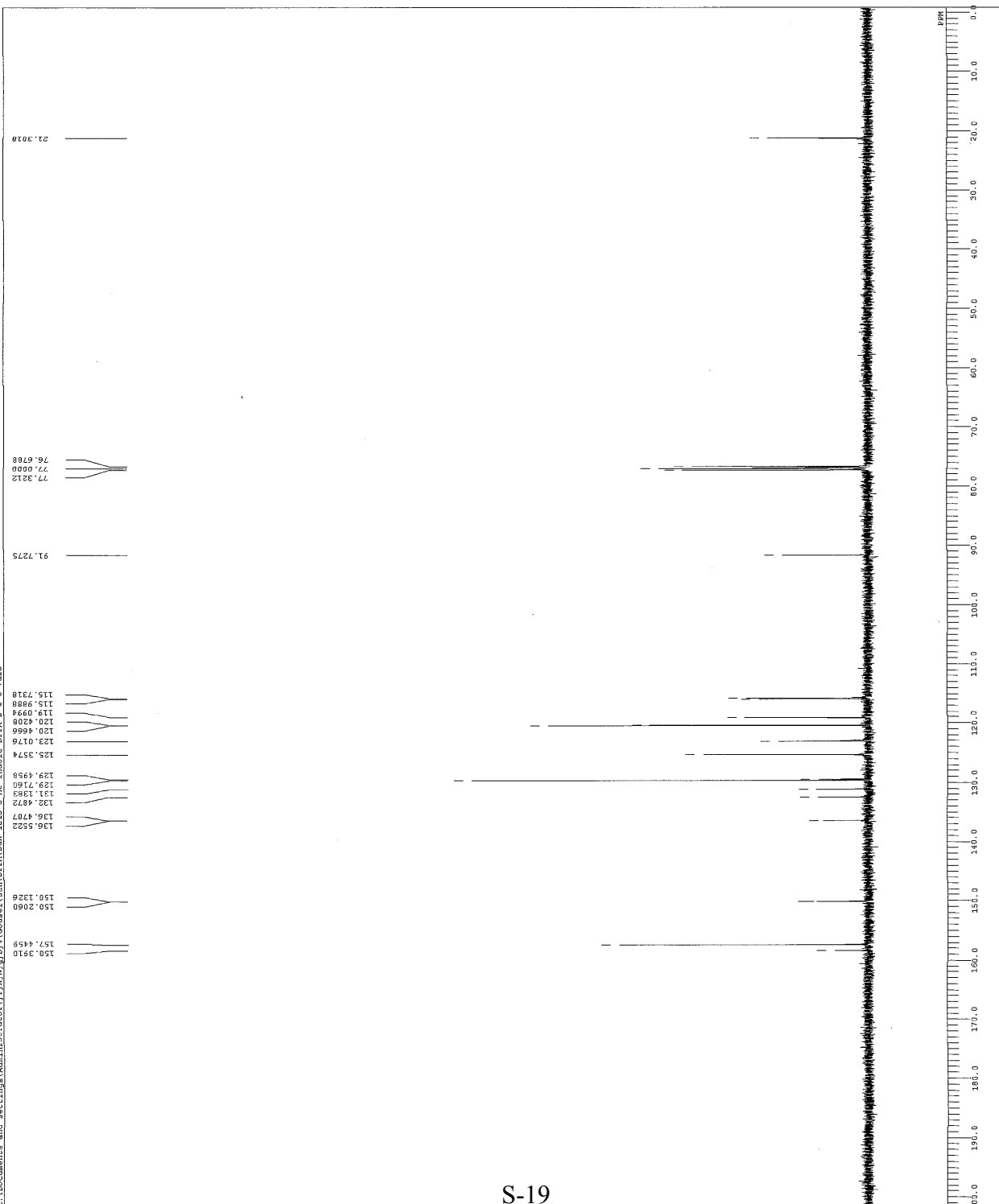
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0.3724
0.3403



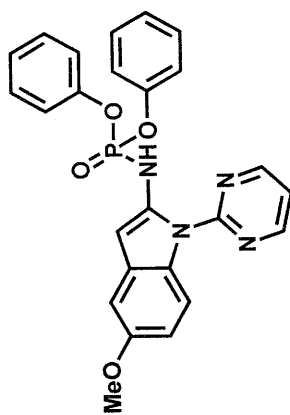
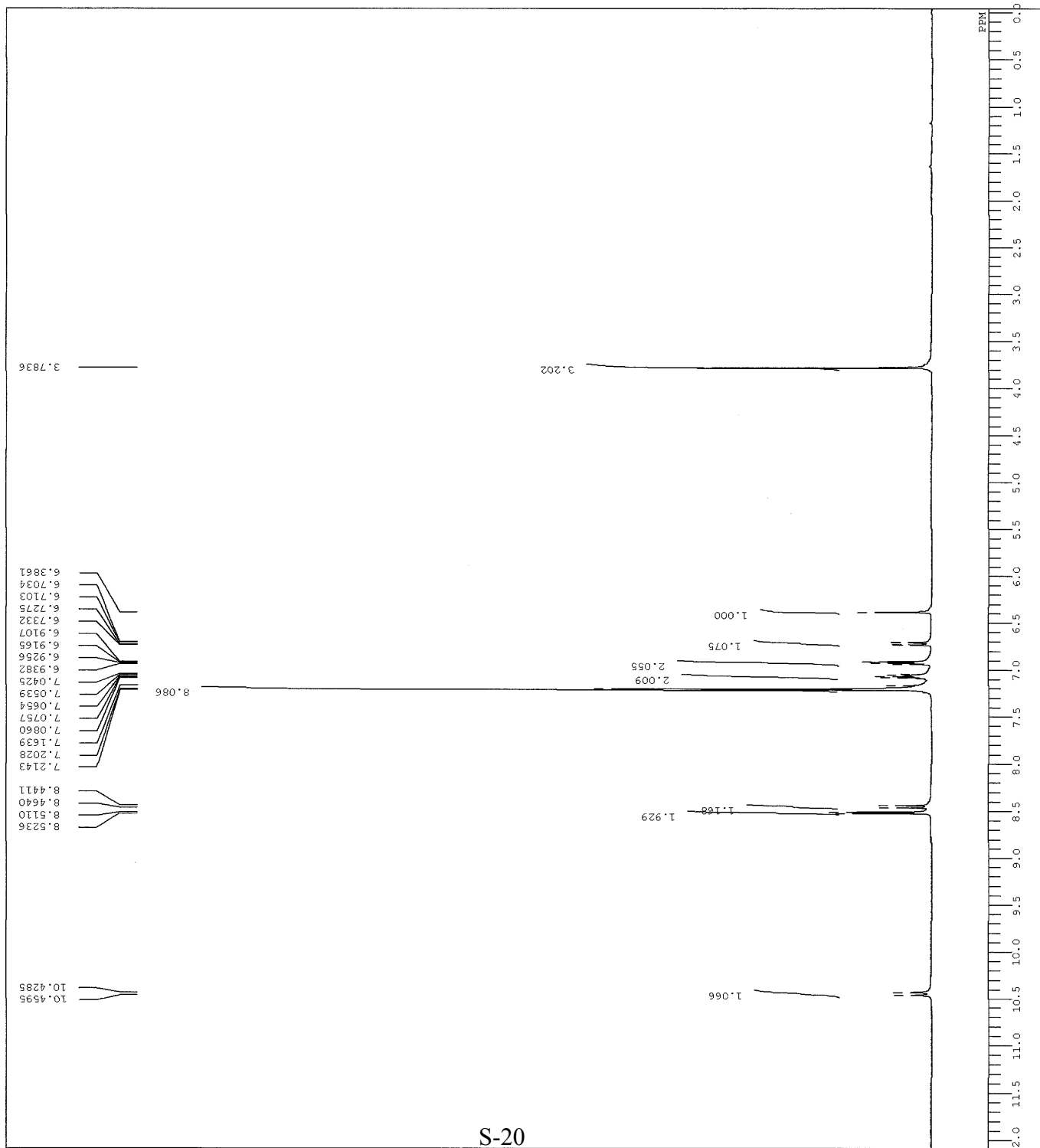
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 CEST2_ 8.74 KHz
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 SCANS_ 125
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 DELT_ 2.310 sec
 PR1_ 3.310 sec
 IRNUC_ 1H
 CTEMP_ 21.7 c
 EXREF_ CDCl3 77.00 ppm
 BP_ 0.12 Hz
 RGAIN_ 50



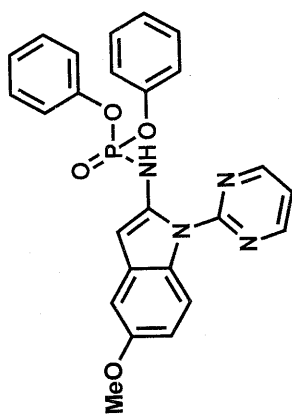
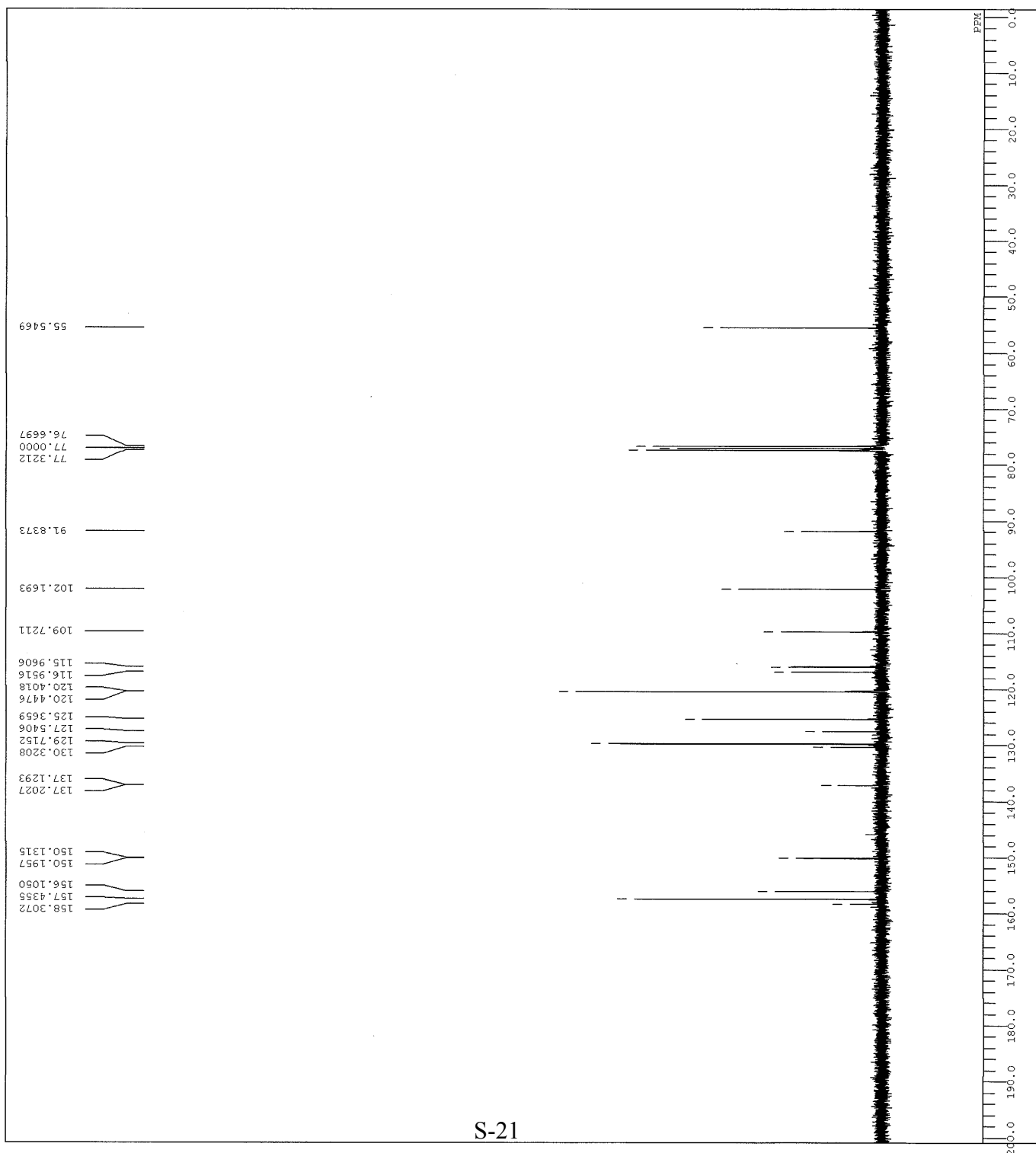
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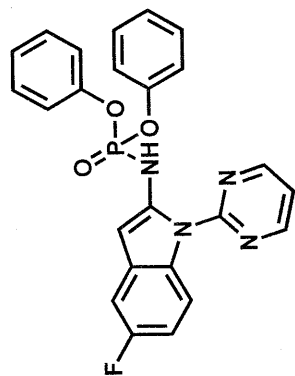
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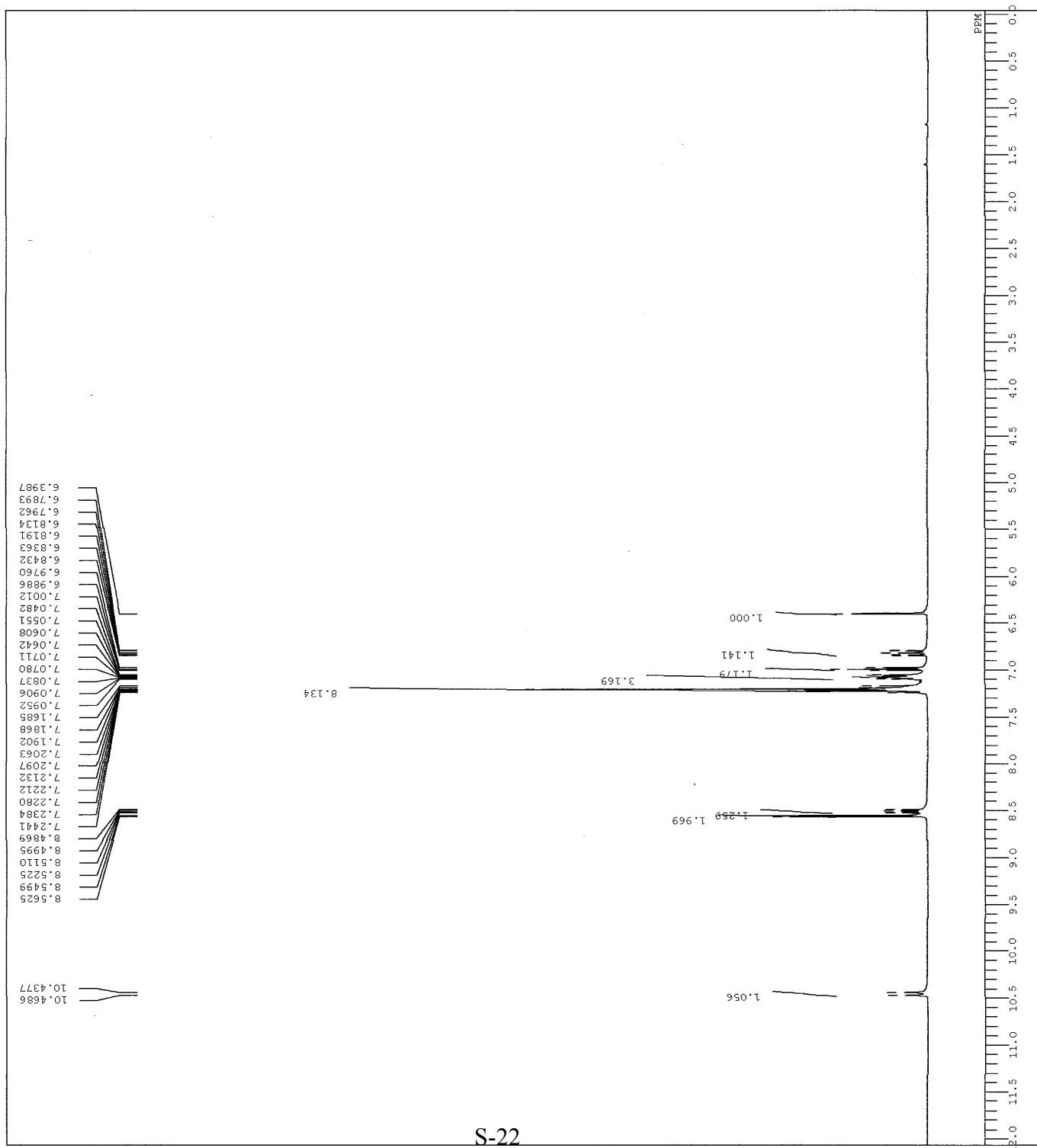


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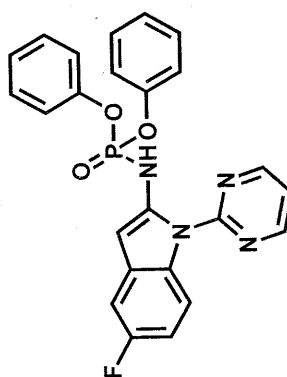
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 INUC 21.2 C
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 RGAIN



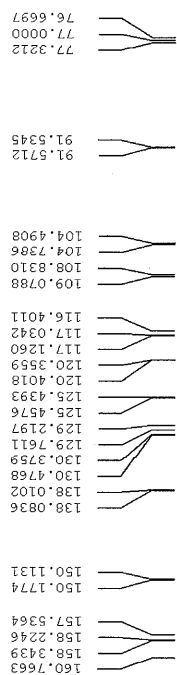
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 PW1 3.00 ussc
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4ga



sun 1224 5-Cl indole DPPA-1-1.als

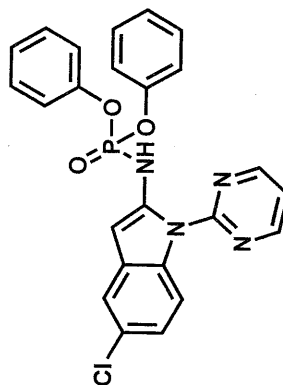
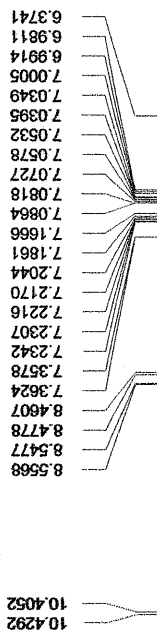
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 POINT
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 EXREF
 BF
 RGAIN

2013-12-24 23:22:24

1H
 proton, jxp

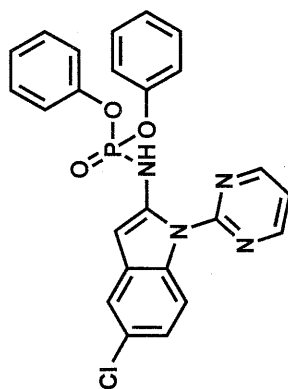
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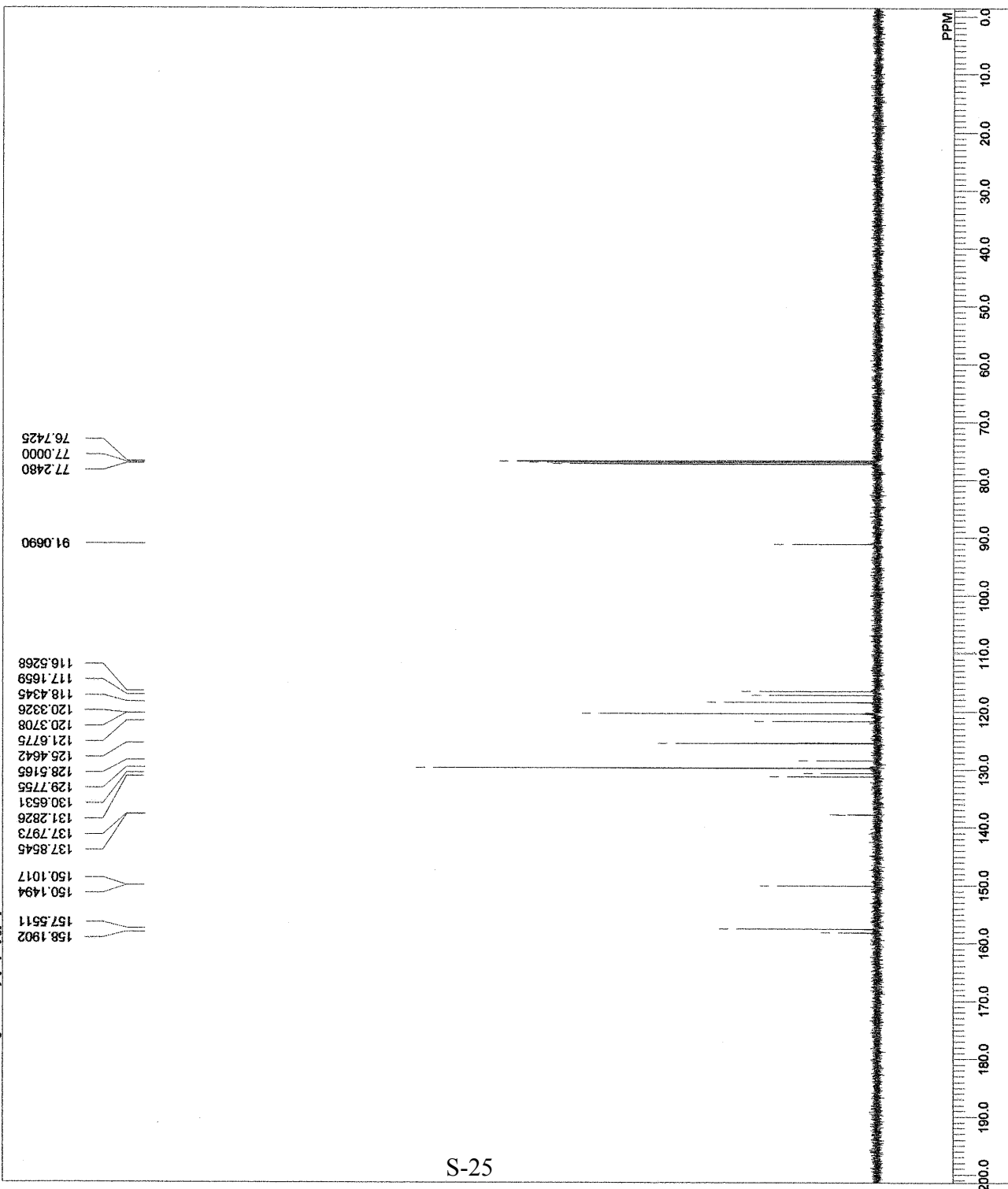
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 CTEMP 21.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



4ha

C:\Documents and Settings\user1\fffx\N/g/b/v/Gouseisun\IDPPA\sun 1224 5-Cl indole DPPA-2-1.als

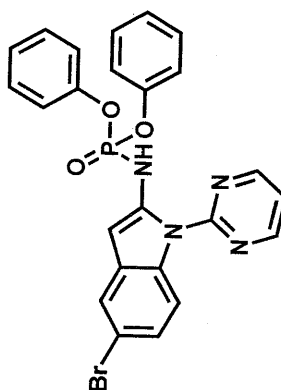
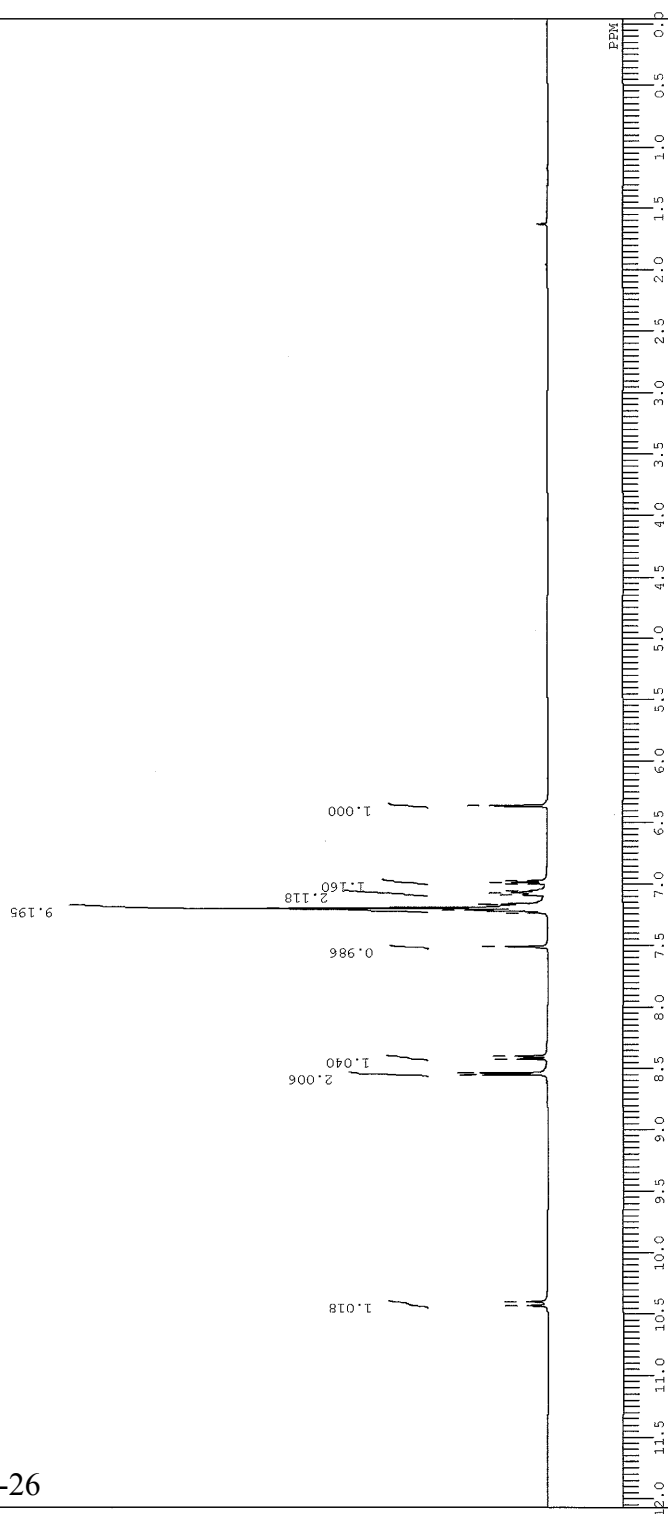


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 ACQTM 2.2282 sec
 PD 5.0000 sec
 PW1 5.25 usec
 IRNUC 1H
 CTMP 21.6 c
 SLVT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 30

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 6.9875
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 7.0711
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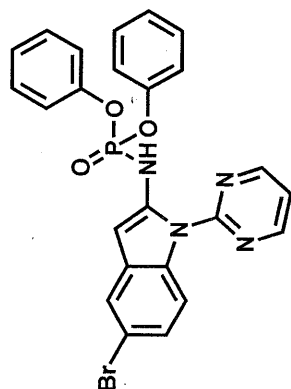
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S-26

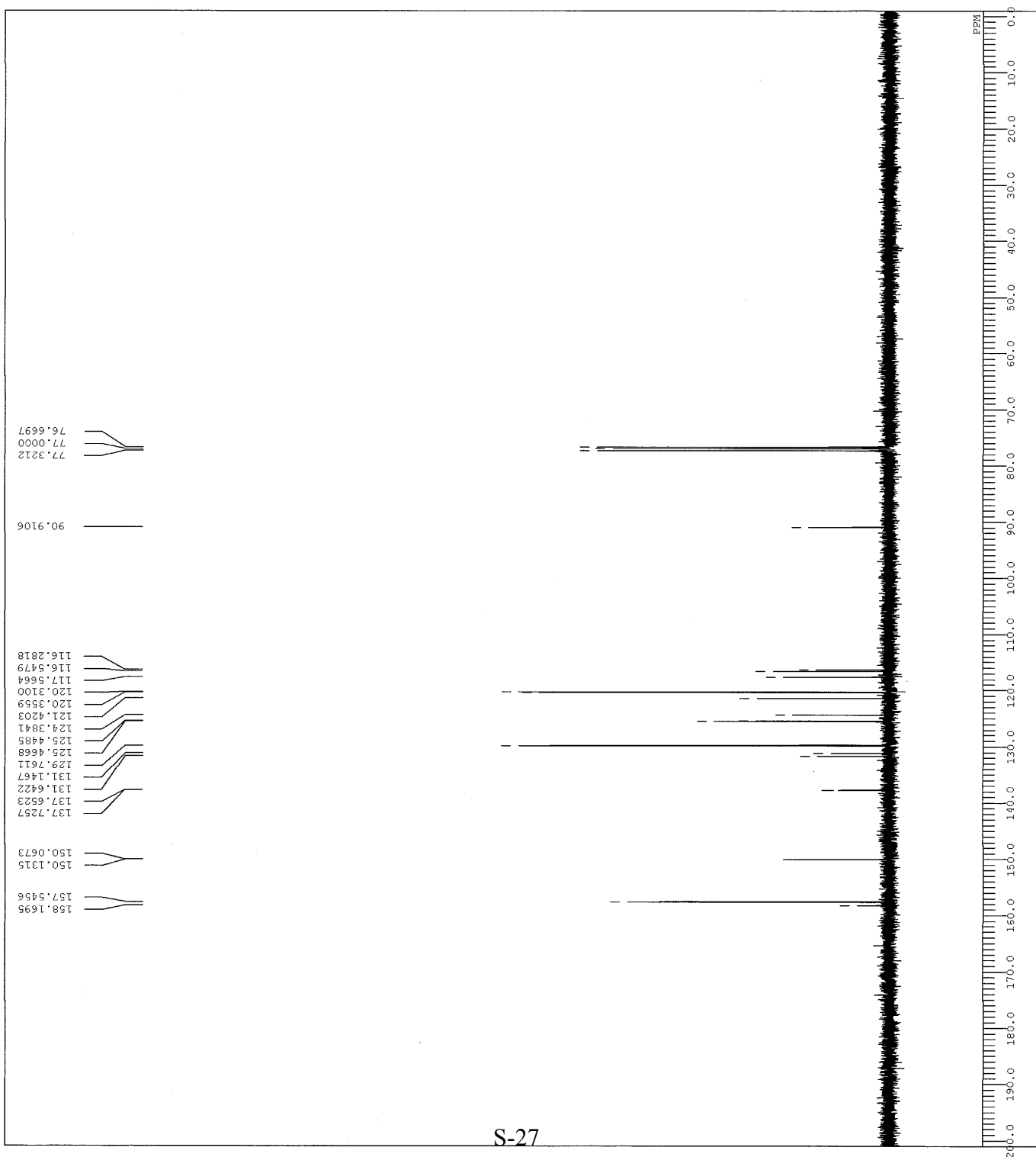


4ia

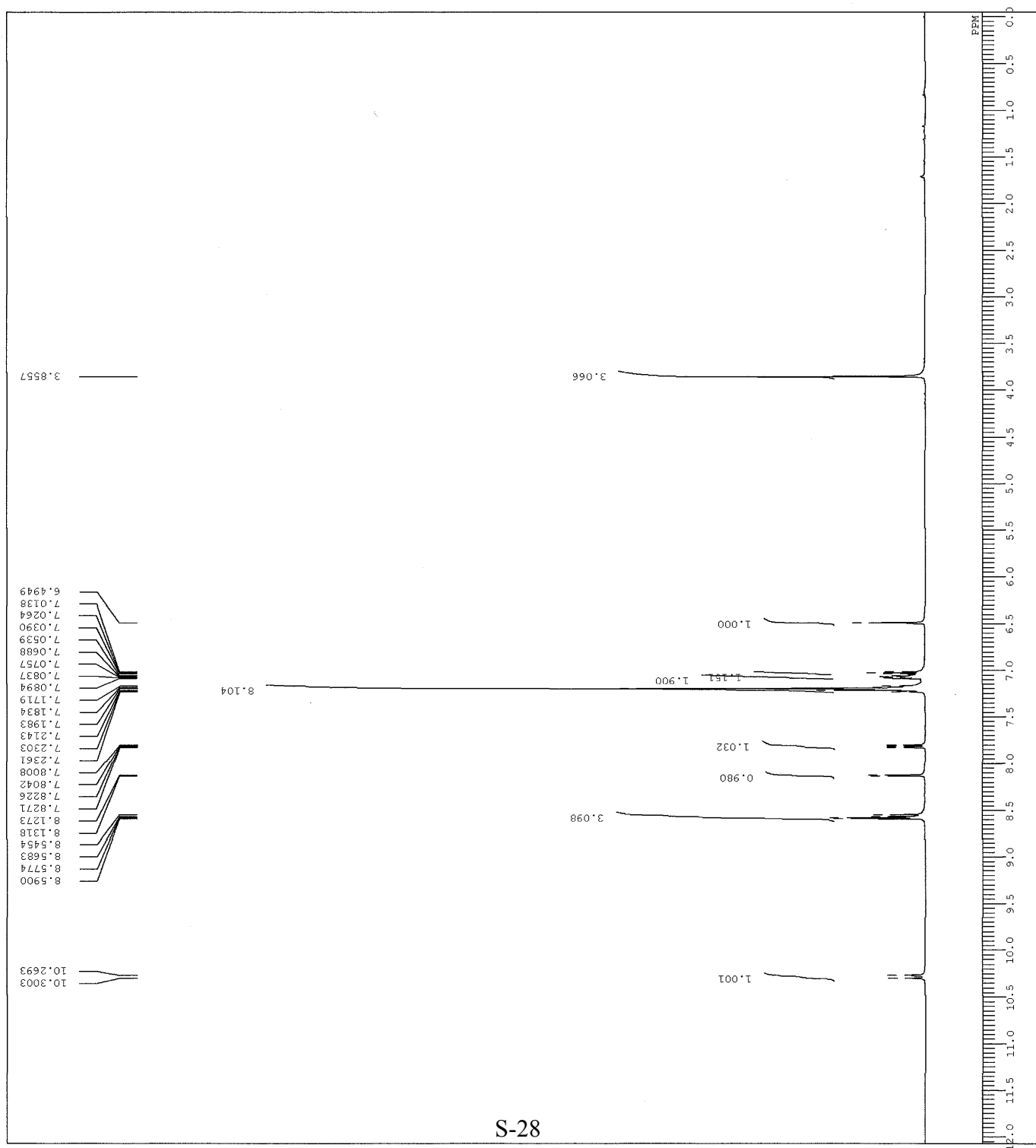
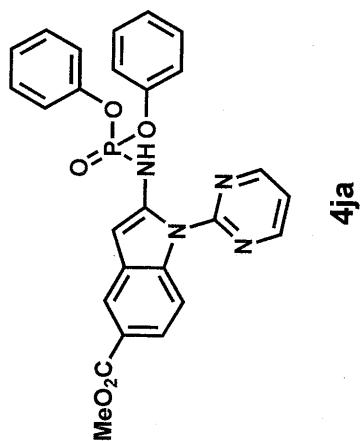
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 OBNUC 13C
 EXMOD carbon-jxp
 OBFREQ 98.52 MHz
 OBSSET 4.64 kHz
 OBFIN 8.74 Hz
 POINT 32767
 FREQU 29620.85 Hz
 SCANS 96
 ACQTM 1.1062 sec
 PD 2.0000 sec
 Fw1 3.00 usec
 IRNUC 1H
 CTMP 21.6 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



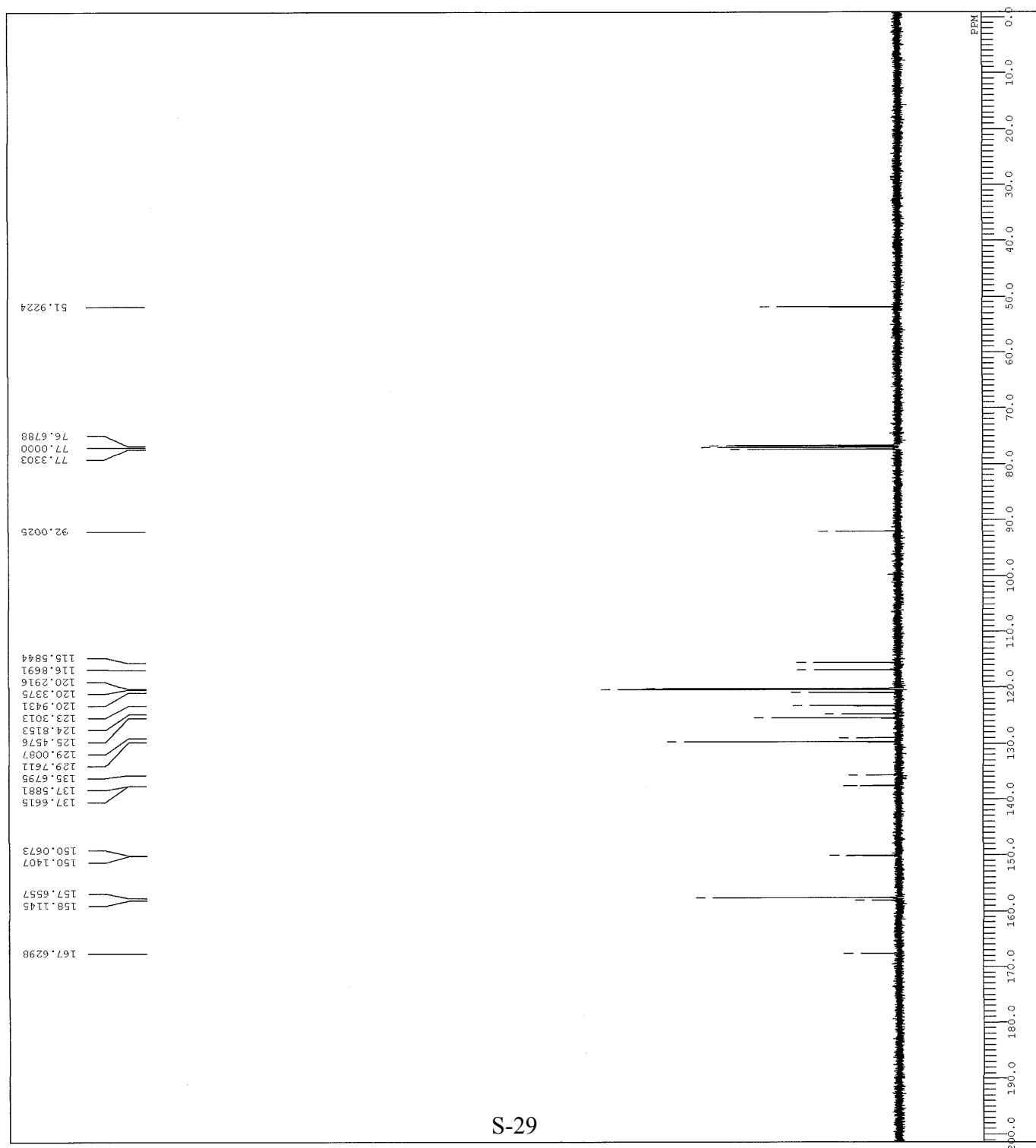
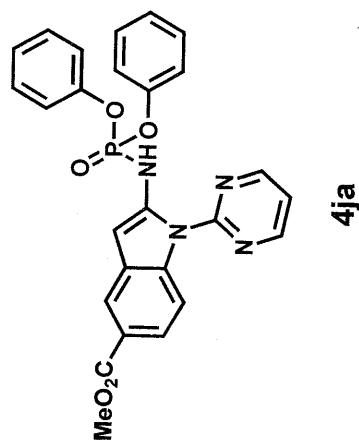
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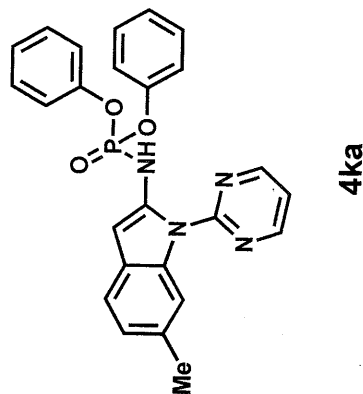
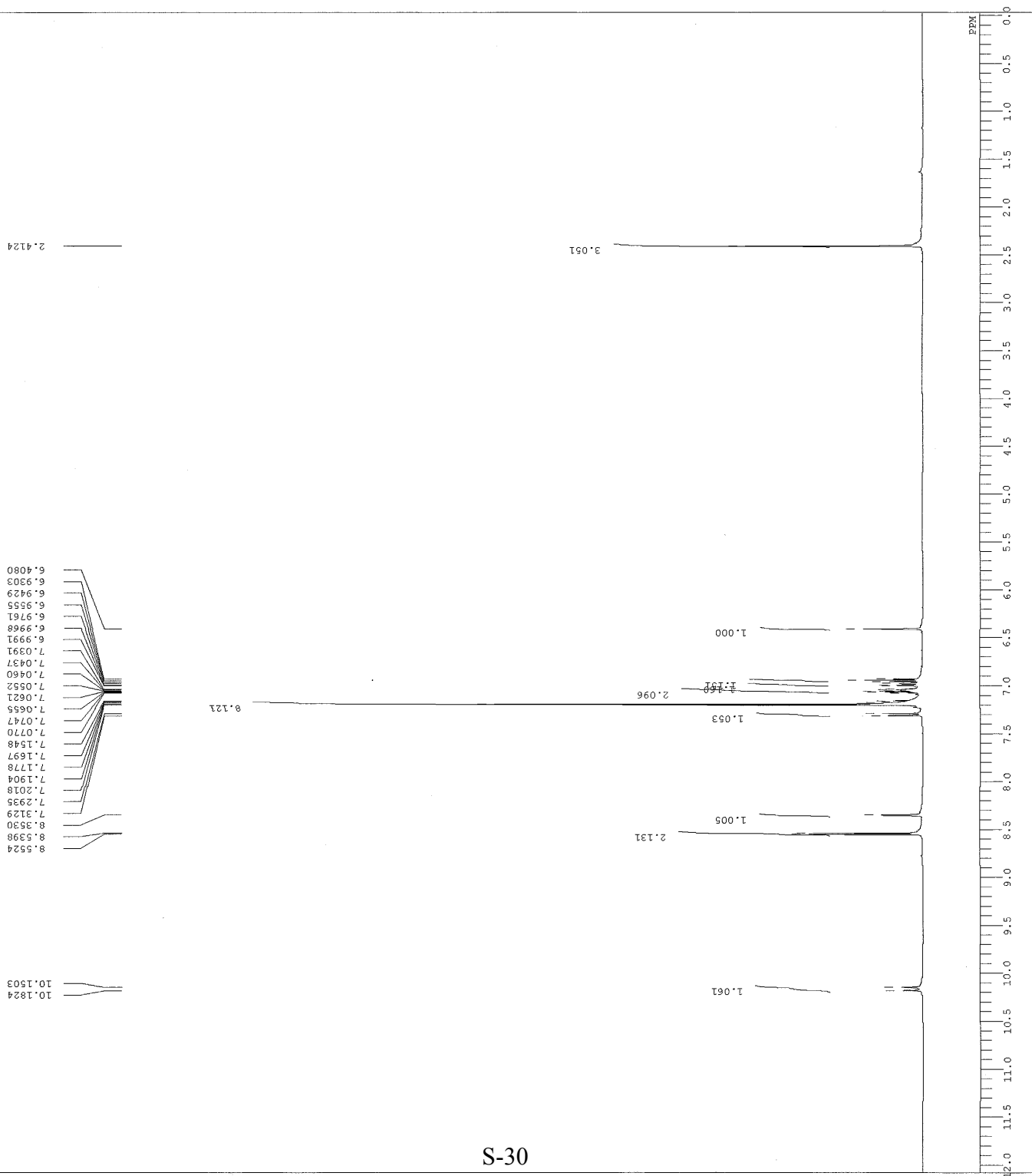
DP113 sun 1220 5-CO2Me indole DPPA-2-1.als
 COMMT 20-12-2013 09:28:30
 DATIM
 OBNUC 1H
 EXMOD proton,3kp
 OFFRQ 391.78 MHz
 OSET 6.51 KHz
 OFIN 3.34 Hz
 POINT 16384
 FREQU 7352.94 Hz
 SCANS 8
 ACQTM 2.2282 sec
 PD 5.0000 sec
 FW 5.25 usec
 INUC 1H 21.2 c
 CTEMP CDCL3 0.00 ppm
 EXREF 0.12 Hz
 BF 23
 RGAIN



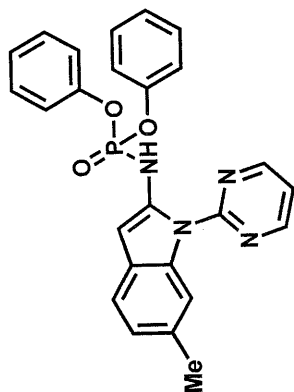
DFIL3 sun 1220 5-CO2Me indole DPFA-3-1.jdf
 CONNT 20-12-2013 09:31:13
 DATIM 13C
 OBNUC carbon-13p
 EXMOD 98.52 MHz
 OBFREQ 4.64 KHz
 OBSET 8.74 Hz
 OBFIN 32767
 POINT 29620.85 Hz
 FREQU 117
 SCANS 1.1062 sec
 ACQTM 2.0000 sec
 PD 3.00 usec
 PW1 1H
 IRNUC 21.2 c
 CTMP
 SLVNT CDCL3
 EXREF 77.00 DPM
 BF 0.12 Hz
 RGAIN 60



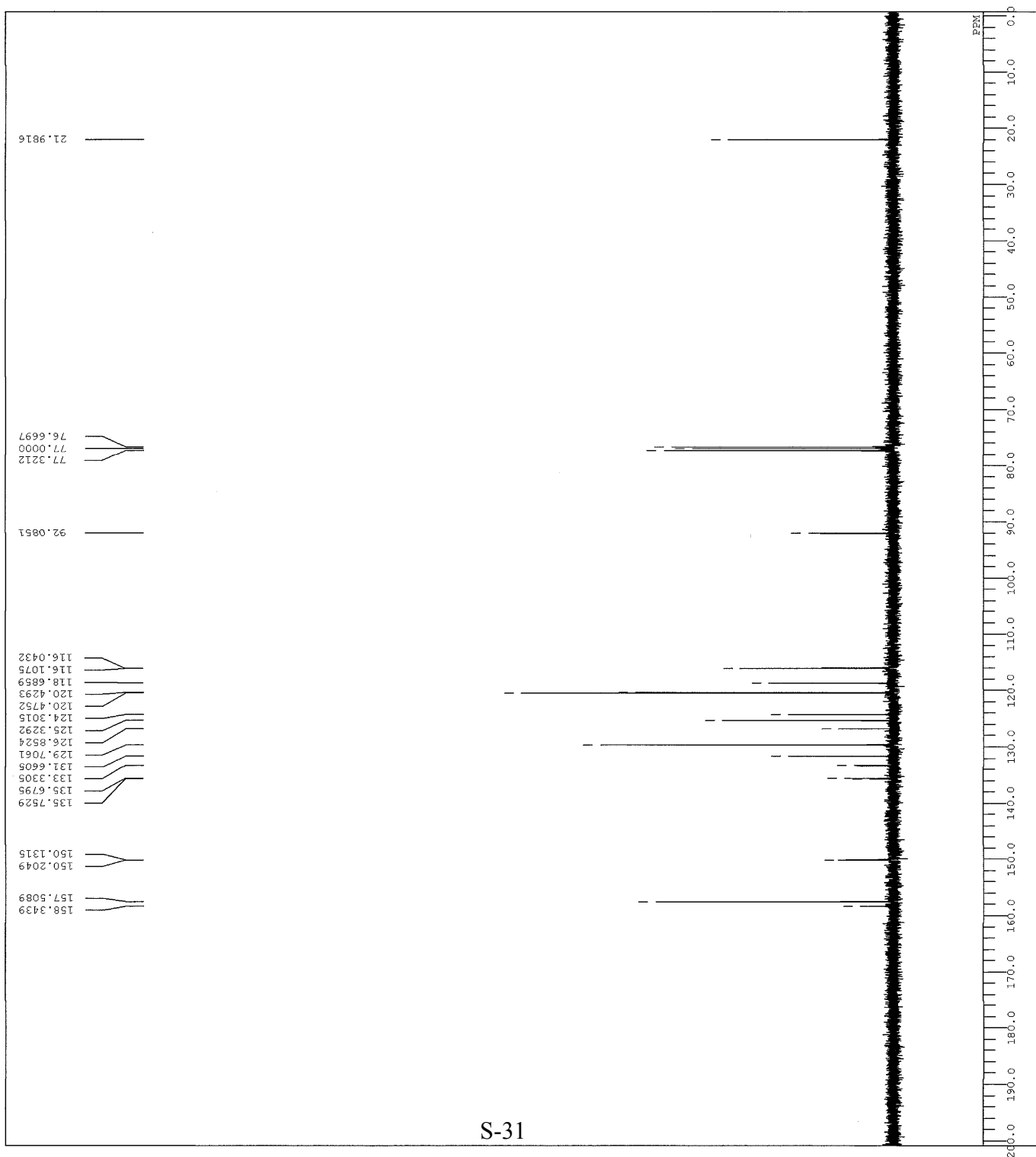
DFIL sun 1217 6-Me indole DPpa-1-1.als
 COMMT 18-12-2013 00:00:11
 DATIM 1H
 OBNUC 1H
 EXMOD proton.jxp
 OFFRQ 391.78 MHz
 OBSET 8.51 KHz
 OFFIN 3.34 Hz
 POINT 13107
 FREQU 5862.35 Hz
 SCANS 8
 ACQTH 2.2282 sec
 FID 5.0000 sec
 FID 5.25 usec
 TNUC 1H
 CTMP 21.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 28



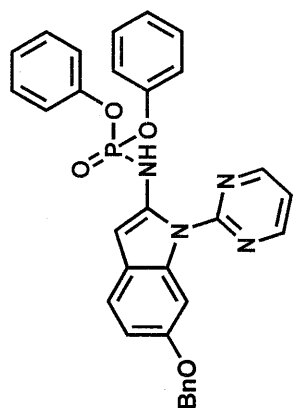
DFILE sun 1217 6-Me indole DPPA-2-1.als
 COMMT
 DATIM 18-12-2013 00:01:53
 OBNUC 13C
 EXMOD carbon.jpg
 OFRQ 98.52 MHz
 OBSET 4.64 KHz
 OFFIN 8.74 Hz
 POINT 32767
 FREQU 29620.85 Hz
 SCANS 69
 ACQTM 1.1062 sec
 PD 2.0000 sec
 PW1 3.00 usec
 INUC 1H
 CTEMP 21.4 c
 SLVNT CDCl3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



4ka

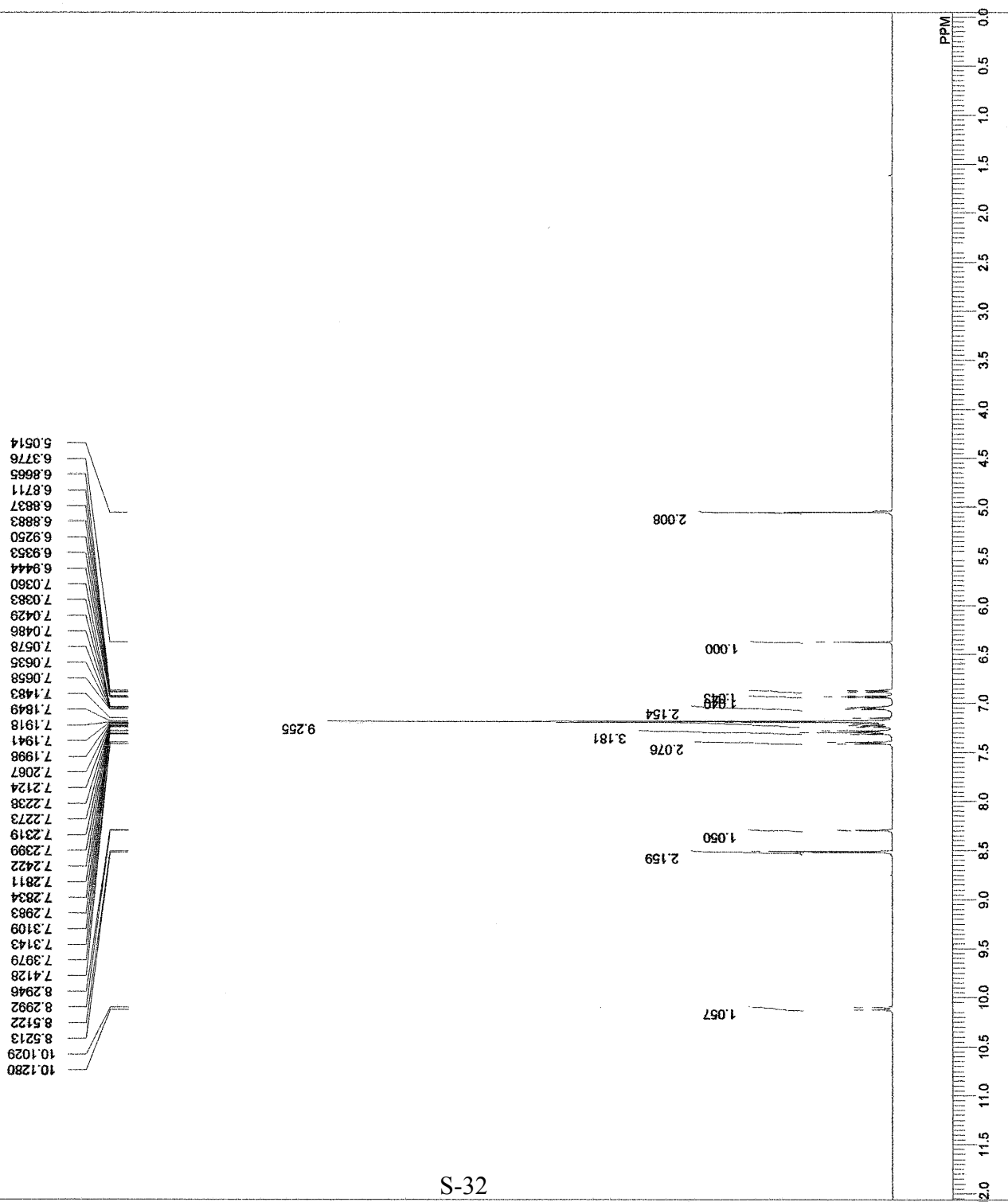


DFILE sun 1224 6-OBn indole DPPA-1-1.als
 COMNT
 DATIM 2013-12-24 23:49:46
 OBNUC 1H
 EXMOD proton.jpg
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.55 usec
 1H 21.3 c
 ODCL3
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 30



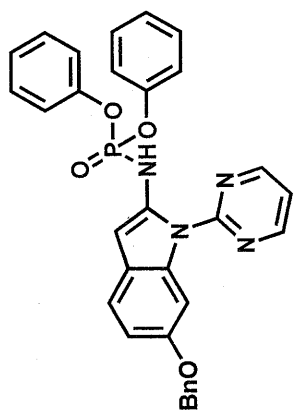
4la

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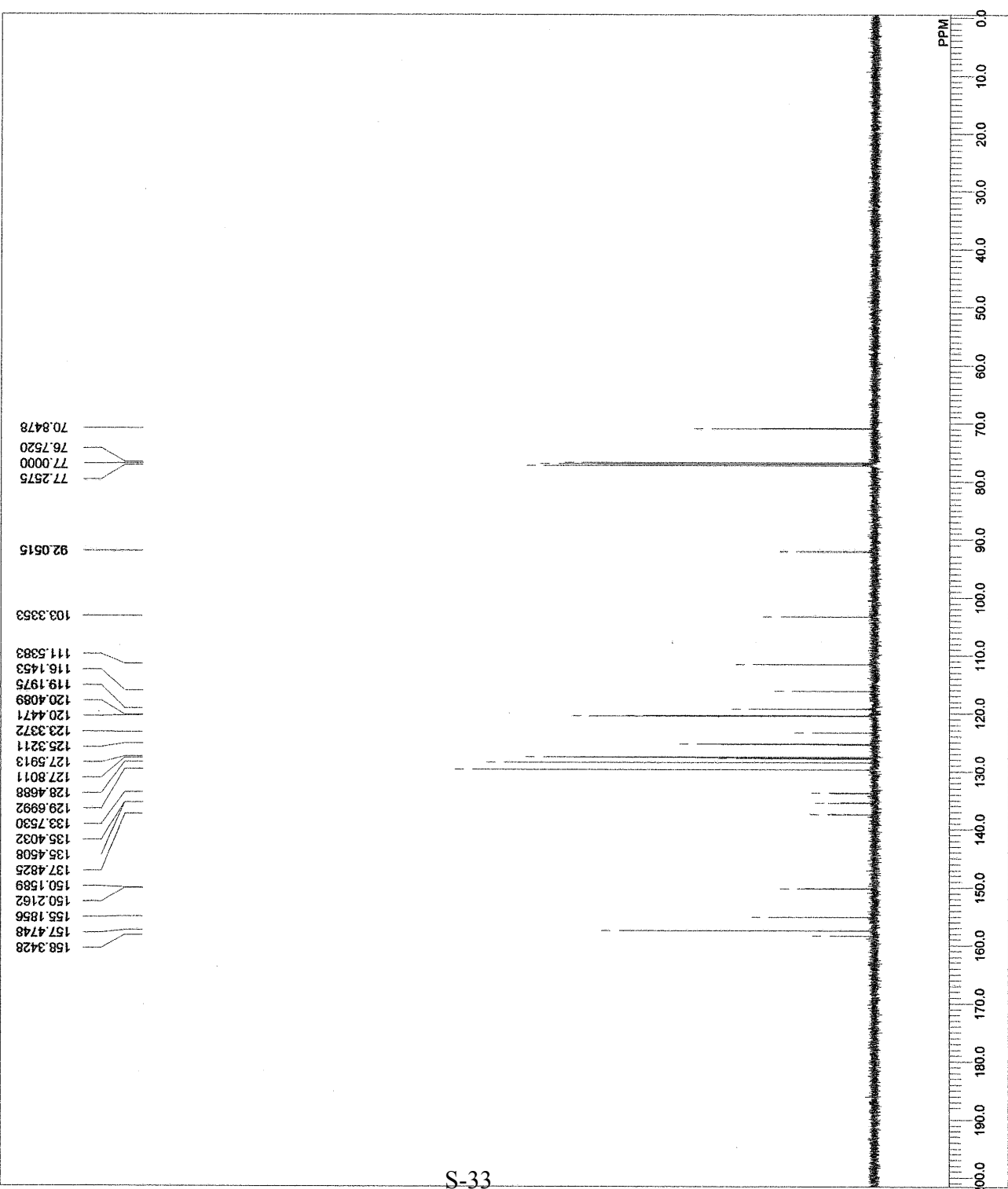
sun 1224 6-OBn indole DPPA-2-1.als

DFILE COMNT
DATIM 2013-12-24 23:51:26
OBNUC 13C
EXMOD carbon.jpg
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32767
FREQU 39308.18 Hz
SCANS 111
ACQTM 0.8336 sec
PD 3.0000 sec
PW1 3.40 usac
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60

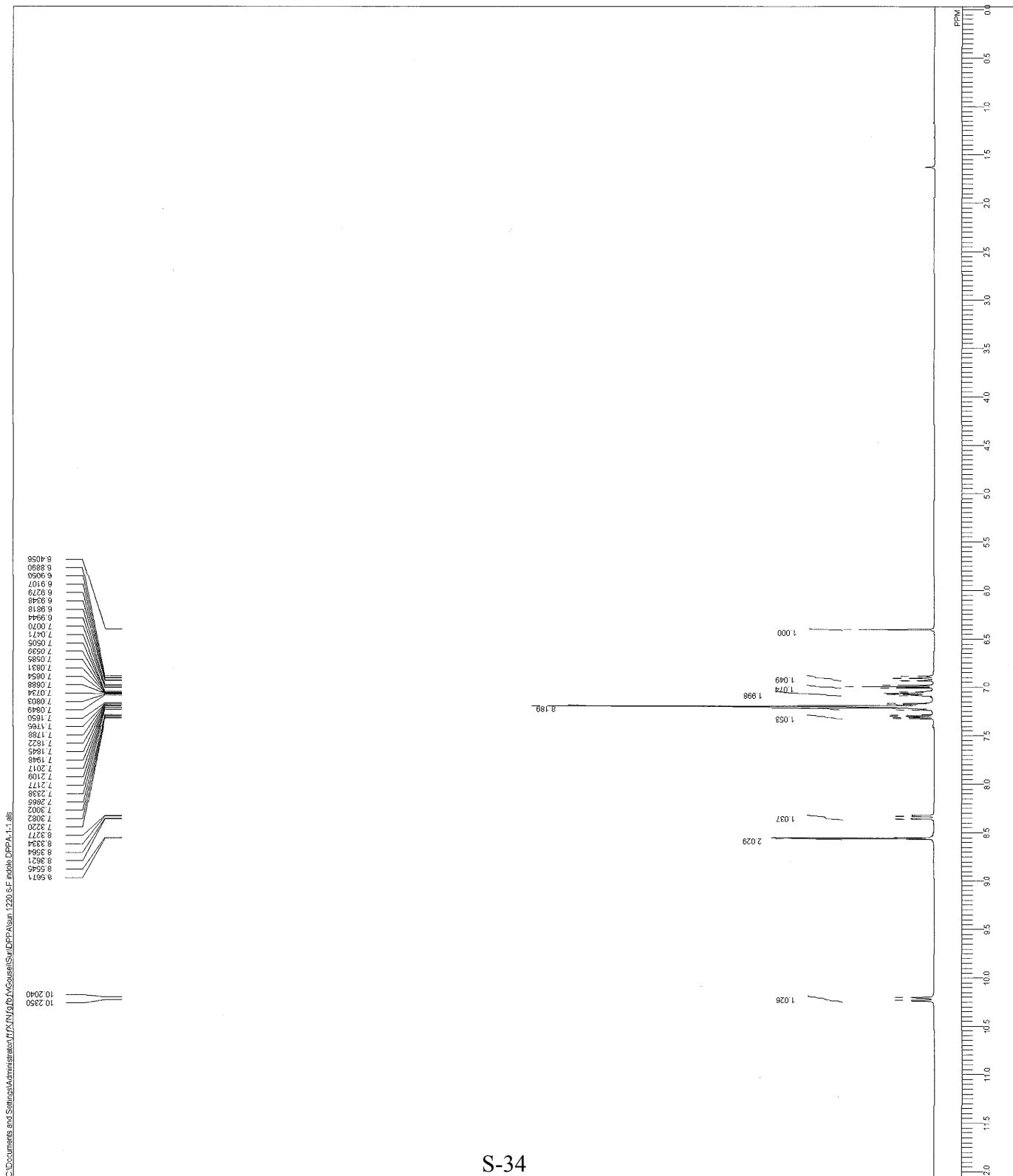


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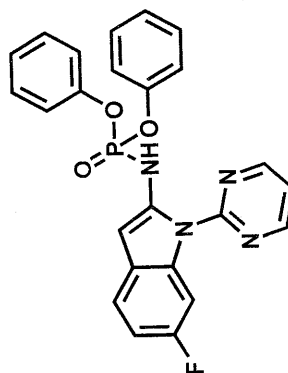
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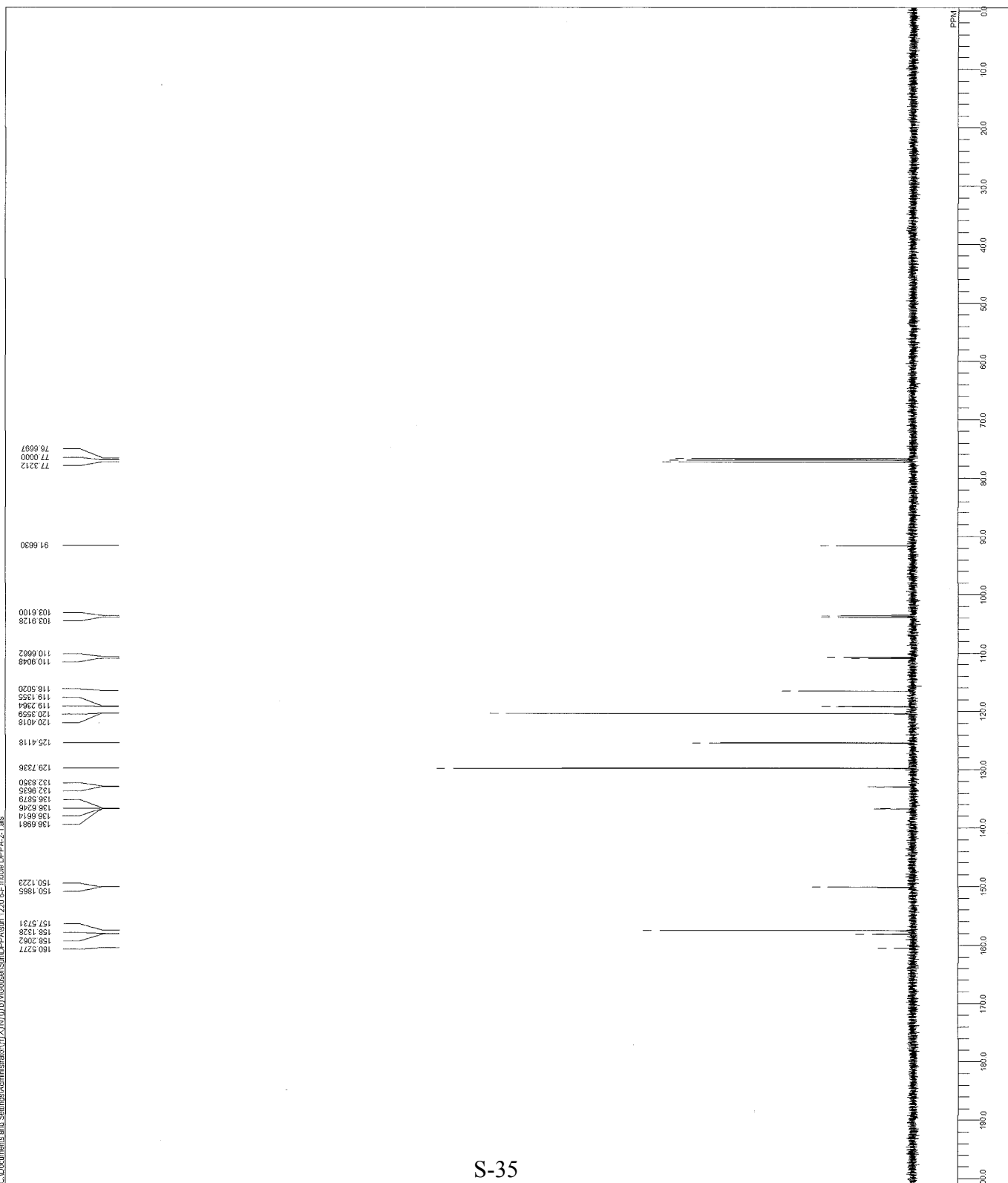
sun 1220 6-F indole DPPA-1-1.mh
 2012-2013 23:38:27
 CONVT
 CNUC 1H
 EMOD
 CNUC 1H
 OBSY 851 MHz
 OBSY 851 MHz
 OBSY 3.34 Hz
 OBSY 16354
 POINT 733.84 Hz
 SCANS 8
 ACQTM 2.2282 sec
 FID 2.2282 sec
 PM1 2.2282 sec
 PM1 2.2282 sec
 IRNUC 1H
 CTEMP 21.5 c
 NUC1 COC
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 30



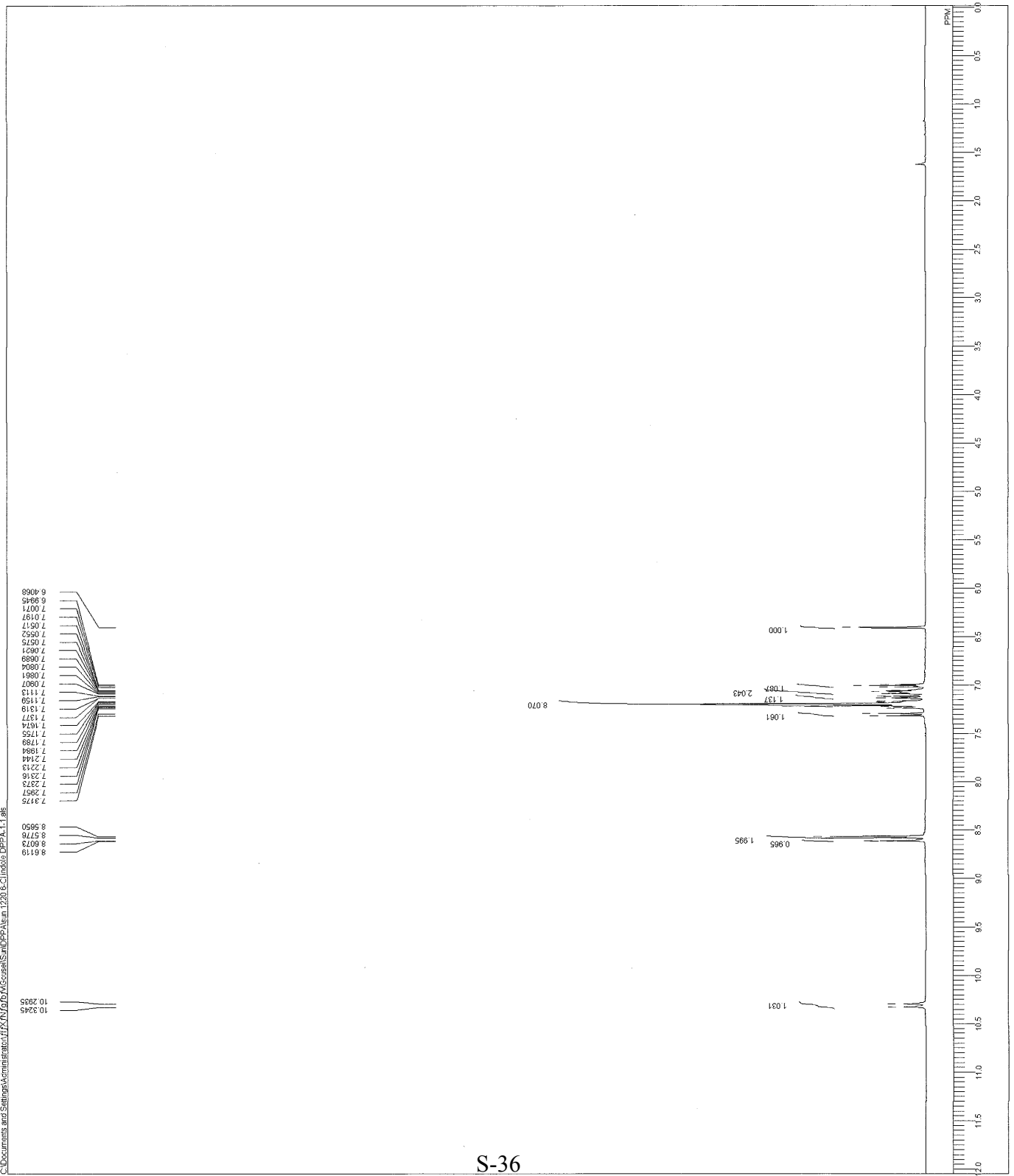
DPFA
 CONTC 38.12.2013 23:41:13
 DATE 13
 EXMO carbon 130
 OBRQ 98.52 MHz
 OBRQ 400 MHz
 OBRQ 8.74 Hz
 POINT 32787
 PREDS 2887.85 Hz
 SCD 121
 ACOTM 1.1062 sec
 PD 2.0000 sec
 INVC 5.0000 sec
 INVC 1H
 CTMP 216 c
 CO 13
 SUNIT 72.00 ppm
 BF 0.12 Hz
 RGAN 80



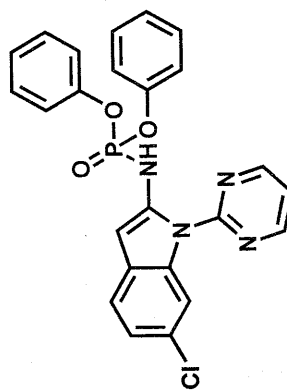
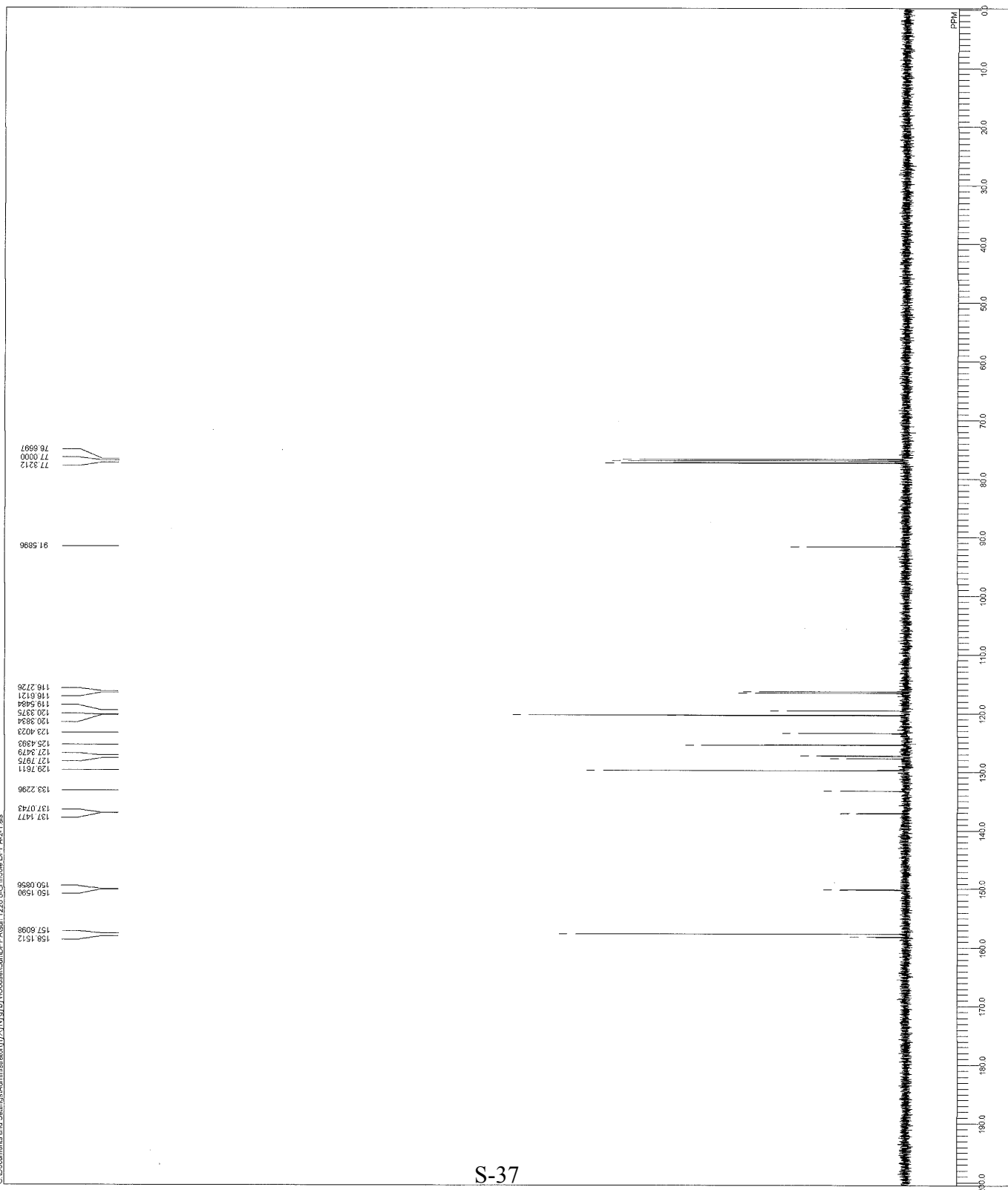
4ma



OFLE sun 1220 6-Cl indole DPPA-1.1.xls
 DATE 20-12-2013 23:21:31
 OBNUC 1H
 PULPROG zgpg30
 CDECO 101.78 MHz
 OBSSET 8.51 KHz
 OBRN 334 Hz
 FREQ 500.135 MHz
 SCANS 6
 ACQ 27.29 sec
 PCOTM 5.000 sec
 PVI 5.25 msec
 IRNUC 1H
 C13 21.3 c
 CDCL3
 EXREF 0.00 ppm
 RF 0.10 Hz
 RGAIN 30

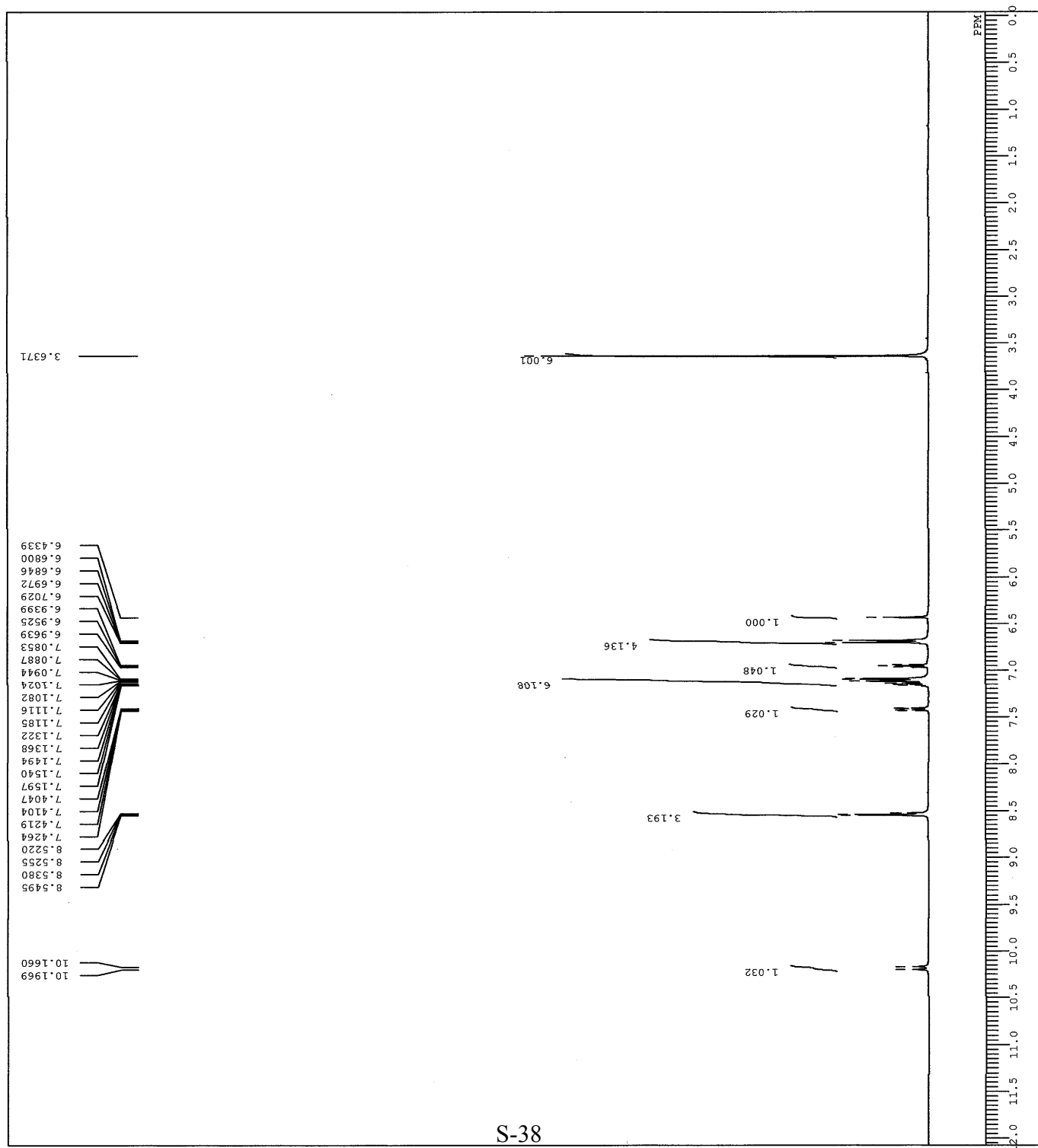
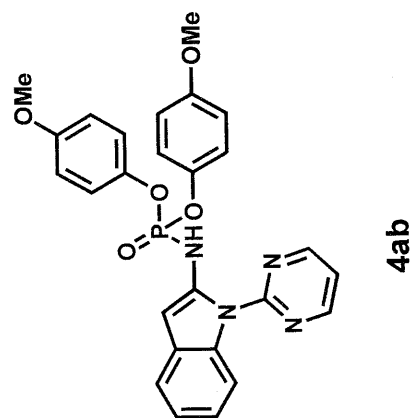


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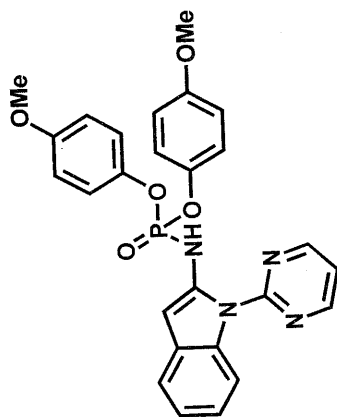


4na

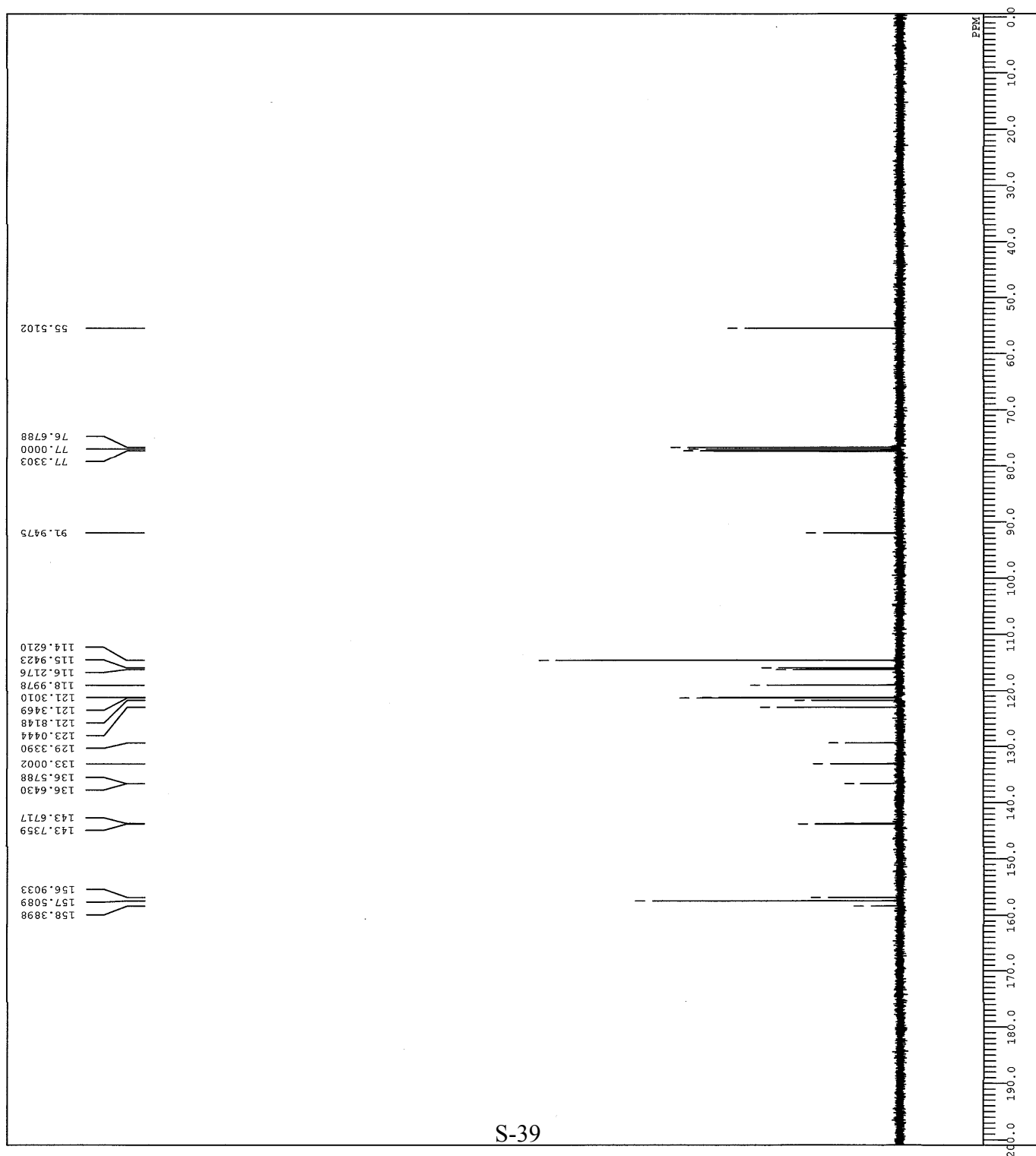
DF1LE sun 0113 indole (4-OMeO)2P(O)-1-1.als
 COMNT 13-01-2014 21:57:18
 DATIM 1H
 OBNUC 1H
 EXMOD proton.jxp
 OBFRO 391.78 MHz
 OBSER 8.51 KHz
 OBFIN 3.34 Hz
 POINT 16384
 FREQU 7348.62 Hz
 SCANS 12
 ACQTM 2.2295 sec
 PD 5.0000 sec
 PW1 5.25 usec
 IRTUC 1H
 CTEMP 25.0 C
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 30



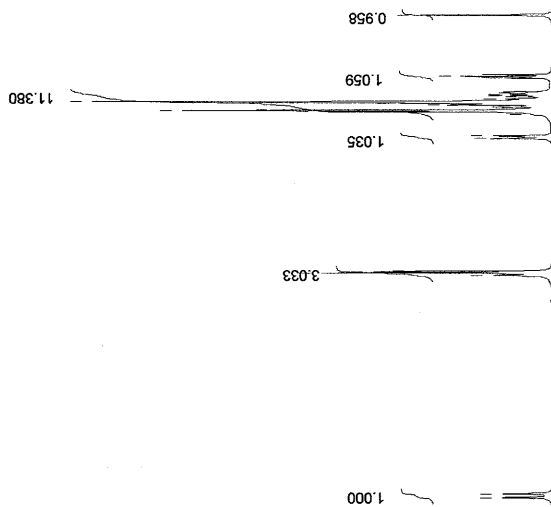
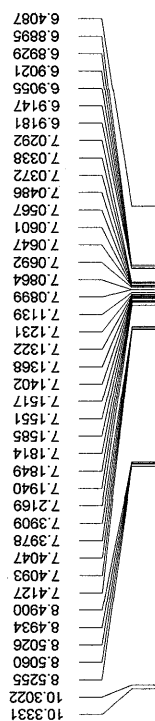
DF1LE sun 0113 indole (4-OMeO)2P(O)-2-1.als
 COMNT
 DATIM 13-01-2014 21:59:58
 OBNUC 13C
 EXMOD carbon.jxp
 OBFRQ 98.52 MHz
 OBSET 4.64 KHz
 OBFIN 8.74 Hz
 POINT 32767
 FREQU 29620.85 Hz
 SCANS 155
 ACQTM 1.1062 sec
 PD 2.0000 sec
 PW1 3.00 usec
 IIRNUC 1H
 CTEMP 25.0 C
 SINT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



4ab

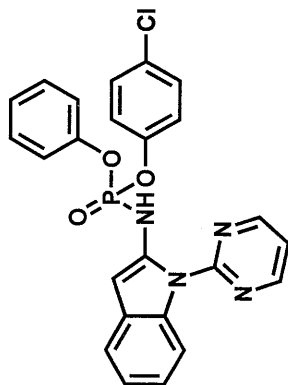


DFILE sun 0127 indole N3 P=O OPh Op-CIPh-1-1.jdf
 COMNT 27-01-2015 18:13:29
 DATIM 1H
 OBNUC proton.jxp
 EXMOD 391.78 MHz
 OBFREQ 8.51 KHz
 OBSET 3.34 Hz
 OBFIN 16384
 POINT 7348.62 Hz
 FREQU 8
 SCANS 2.2295 sec
 ACQTM 5.0000 sec
 PD 6.50 usec
 PW1 1H
 IRLUC 460.0 c
 CTEMP CDCL3
 SLVNT 0.00 ppm
 EXREF 0.12 Hz
 BF 26
 RGAIN



DFILE sun 0127 indole N3 P=O OPb Op-ClPh-I-
 COMNT 2015-01-27 18:09:19
 DATIM 13C
 EXMOD carbon.jxp
 OBFREQ 125.77 MHz
 OBSSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32767
 FREQU 39308.18 Hz
 SCANS 216
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.40 usec
 IRNUC 1H
 CTMP 23.7 c
 SLVNT CDCl3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60

158.2570
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 150.0254
 149.9682
 148.6423
 148.5851
 136.1376
 136.0804
 132.9518
 130.7008
 129.7469
 129.6611
 129.0983
 125.4738
 123.0701
 121.9637
 121.8110
 121.7824
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 119.0068
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 115.9831
 92.0706



4ac

