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1. Experimental Details and Compound Data

1.1 General Information

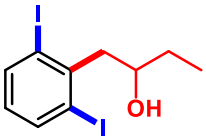
All commercial reagents and chromatography solvents were used as obtained unless otherwise stated. Ethanol, toluene, ethyl acetate, hexanes, anhydrous sodium sulfate (Na_2SO_4, BDH). Anhydrous solvents were distilled over appropriate drying agents prior to use. Analytical thin layer chromatography (TLC) was performed on Merck silica gel 60 F_{254}. Merck Silica gel 60 (0.063 - 0.2 mm) was used for column chromatography. Visualization of TLC was accomplished with UV light (254 nm). NMR spectra were recorded on a Bruker-Avance 400 MHz spectrometer. The residual solvent protons (^1H) or the solvent carbon (^{13}C) were used as internal standards. ^1H-NMR data are presented as follows: chemical shift in ppm (δ) downfield from trimethylsilane (multiplicity, integration, coupling constant). The following abbreviations are used in reporting NMR data: s, singlet; bs, broad singlet; d, doublet; t, triplet; q, quartet; dq, doublet of quartets; dd, doublet of doublets; m, mutiplet. High resolution mass spectra were recorded using Chemical Ionization (CI) and Electrospray ionization (ESI) techniques.

1.2 General procedure for Metal-Iodine Exchange reaction of 5-substituted-1,2,3-triiodoarenes

In a flame-dried round bottom flask, isopropylmagnesium chloride (2M in THF, 1.2 equiv., 0.39 mL, 0.79 mmol) was added to a solution of 1,2,3-triiodoarene (0.66 mmol, 1.0 equiv.) in THF (6.5 mL) at – 78 °C. The mixture was stirred at that temperature for 2 h and then, the oxirane (1.1 equiv.) was added slowly. The solution was slowly warmed to room temperature and stirred overnight. Saturated NH_4Cl was added and the resulting mixture was stirred for

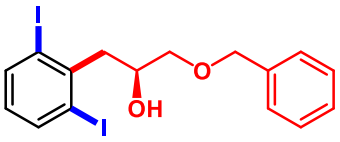
30 min at room temperature. The aqueous layer was extracted with Et_2O (2 X 50 mL). Organic layers were combined and washed with brine, dried with Na_2SO_4, filtered and then the solvent was evaporated under reduced pressure. The crude product was purified by chromatography (5% EtOAc/hexane) to yield the pure desired product.

1.2.1 Synthesis of 1-(2,6-diiodophenyl)butan-2-ol (7a)



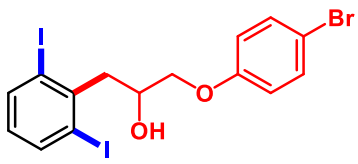
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**66%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.85 (d, 2H, *J* = 7.8 Hz), 6.54 (t, 1H, *J* = 7.8 Hz), 3.97 (bs, 1H), 3.26-3.29 (m, 2H), 1.64-1.70 (m, 2H), 1.44 (d, 1H, *J* = 5.8 Hz), 1.05 (t, 3H, *J* = 7.3 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 143.4, 140.5, 129.9, 100.7, 73.5, 52.5, 30.7, 10.3. **HRMS** (ESI) m/z for $C_{10}H_{12}I_2NaO$ $[M+Na]^+$: calcd. 424.8875; found, 424.8869.

1.2.2 Synthesis of (S)-1-(benzyloxy)-3-(2,6-diiodophenyl)propan-2-ol (7b)



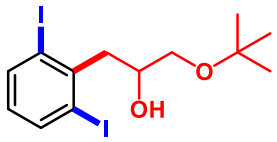
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**70%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.85 (d, 2H, *J* = 7.8 Hz),7.26-7.38 (m, 5H), 6.54 (t, 1H, *J* = 7.8 Hz), 4.61 (s, 2H) 4.23-4.28 (m, 1H), 3.61 (d, 2H, *J* = 4.7Hz), 3.45 (dd, 1H, *J* = 8.1 Hz, J = 13.9 Hz), 3.23 (dd, 1H, *J* = 5.6 Hz, *J* = 13.9 Hz), 2.40 (d, 1H, *J* = 4.0 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 142.8, 140.5, 138.1, 129.9, 128.6, 127.9, 127.8, 100.7, 73.9, 73.6, 70.8, 49.2. **HRMS** (ESI) m/z for $C_{16}H_{16}I_2NaO_2$ $[M+Na]^+$: calcd. 516.9137; found, 516.9131.

1.2.3 Synthesis of 1-(4-bromophenoxy)-3-(2,6-diiodophenyl)propan-2-ol (7c)



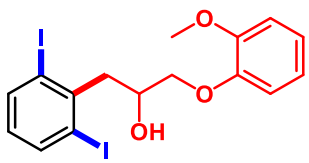
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**58%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.87 (d, 2H, *J* = 7.9 Hz), 7.38 (d, 2H, *J* = 8.8 Hz), 6.81 (d, 2H, *J* = 8.8 Hz), 6.54 (dd, 1H, *J* = 7.9Hz, *J* = 7.8 Hz), 4.42 (bs, 1H) 4.01-4.09 (m, 2H), 3.54 (dd, 1H, *J* = 7.8 Hz, *J* = 14.0 Hz), 3.38 (dd, 1H, *J* = 6.3 Hz, *J* = 13.9 Hz), 2.34 (d, 1H, *J* = 5.5 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ:157.8, 142.2, 140.7, 132.5, 130.2, 116.5, 113.5, 100.7, 71.7, 70.4, 49.2. **M.p**: 94-96 °C. **HRMS** (ESI) m/z for $C_{15}H_{13}BrI_2NaO_2$ $[M+Na]^+$: calcd. 580.8086; found, 580.8078.

1.2.4 Synthesis of 1-(tert-butoxy)-3-(2,6-diiodophenyl)propan-2-ol (7d)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**69%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.85 (d, 2H, *J* = 7.9 Hz), 6.51 (dd, 1H, *J* = 7.9 Hz, *J* = 7.8 Hz), 4.08-4.15 (m, 1H), 3.41-3.48 (m, 3H), 3.15 (dd, 1H, *J* = 5.8 Hz, J = 13.9 Hz), 2.50 (d, 1H, J = 5.0 Hz), 1.22 (s, 9H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 143.1, 140.5, 129.8, 100.7, 73.5, 70.9, 65.5, 49.3, 27.8. **HRMS** (ESI) m/z for $C_{13}H_{18}I_2NaO_2$ $[M+Na]^+$: calcd. 482.9294; found, 482.9287.

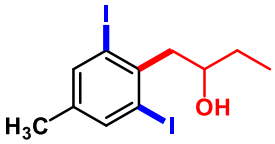
1.2.5 Synthesis of 1-(2,6-diiodophenyl)-3-(2-methoxyphenoxy)propan-2-ol (7e)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**60%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ:7.86 (d, 2H, *J* = 7.8 Hz), 6.88-6.95 (m, 4H), 6.54 (t, 1H, *J* = 7.8 Hz), 4.44 (bs, 1H) 4.11-4.16 (m, 2H), 3.85 (s, 3H), 3.54 (dd, 1H, *J* = 7.5 Hz, J = 13.6 Hz), 3.34 (dd, 1H, *J* = 6.2 Hz, *J* = 13.6 Hz), 2.97(d, 1H, *J* = 4.0 Hz). δ_C (100

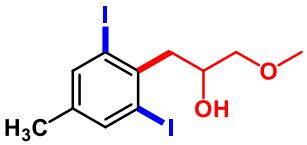
MHz, *d*-$CDCl_3$) δ: 150.1, 148.5, 142.6, 140.6, 130.1, 122.3, 121.2, 115.5, 112.3, 100.7, 74.1, 70.5, 56.1, 49.1. **M.p**: 130-132 °C. **HRMS** (ESI) m/z for $C_{16}H_{16}I_2NaO_3$ $[M+Na]^+$: calcd. 532.9087; found, 532.9084.

1.2.6 Synthesis of 1-(2,6-diiodo-4-methylphenyl)butan-2-ol (7f)



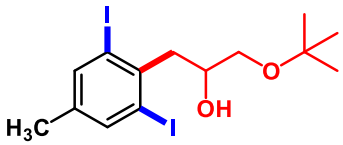
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**52%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.43(s, 2H), 3.92-3.97 (m, 1H), 3.19-3.27 (m, 2H), 2.21 (s, 3H), 1.62-1.69 (m, 2H), 1.45 (d, 1H, *J* = 5.7 Hz), 1.04 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 141.1, 140.2, 140.1, 100.3, 73.6, 51.9, 30.6, 19.7, 10.3. **HRMS** (ESI) m/z for $C_{11}H_{14}I_2NaO$ $[M+Na]^+$: calcd. 438.9032; found, 438.9023.

1.2.7 Synthesis of 1-(2,6-diiodo-4-methylphenyl)-3-methoxypropan-2-ol (7g)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**64%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.69 (s, 2H), 4.16-4.20 (m, 1H), 3.45-3.50 (m, 2H), 3.42 (s, 3H), 3.35 (dd, 1H, *J* = 8.0 Hz, *J* = 14.0 Hz), 3.18 (dd, 1H, *J* = 5.6 Hz, *J* = 14.0 Hz), 2.31 (d, 1H, *J* = 5.0 Hz), 2.21 (s, 3H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 141.2, 140.2, 139.6, 100.1, 76.2, 70.8, 59.3, 48.5, 19.7. **M.p**: 93-95 °C**. HRMS** (ESI) m/z for $C_{11}H_{14}I_2NaO_2$ $[M+Na]^+$: calcd. 454.8981; found, 454.8977.

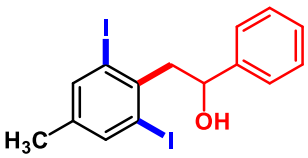
1.2.8 Synthesis of 1-(tert-butoxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7h)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**74%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.68 (s, 2H), 4.07-4.11

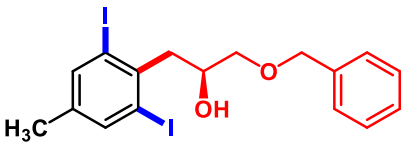
(m, 1H), 3.36-3.45 (m, 3H), 3.14 (dd, 1H, *J* = 6.0 Hz, *J* = 13.9 Hz), 2.48 (d, 1H, *J* = 4.8 Hz), 2.21 (s, 3H), 1.21 (s, 9H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 141.1, 139.9, 139.9, 100.2, 73.4, 71.0, 65.5, 48.7, 27.8, 19.7. **HRMS** (ESI) m/z for $C_{14}H_{20}I_2NaO_2$ $[M+Na]^+$: calcd. 496.9450; found, 496.9442.

1.2.9 Synthesis of 2-(2,6-diiodo-4-methylphenyl)-1-phenylethan-1-ol (7i)



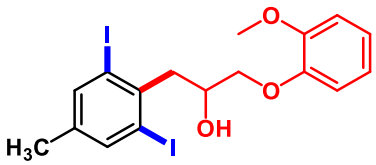
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**30%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.78 (bs, 2H), 7.26-7.38 (m, 5H), 5.30-5.36 (m, 1H), 3.31 (dd, 1H, *J* = 13.8 Hz, *J* = 10.0 Hz), 3.11 (dd, 1H, *J* = 4.7 Hz, *J* = 13.8 Hz), 2.45 (d, 1H, *J* = 6.6Hz), 2.24 (s, 3H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 140.9, 139.9, 137.6, 129.8, 129.2, 128.7, 127.6, 126.9, 81.9, 41.1, 19.7. **HRMS** (ESI) m/z for $C_{15}H_{14}I_2NaO$ $[M+Na]^+$: calcd. 486.9032; found, 486.9027.

1.2.10 Synthesis of (S)-1-(benzyloxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7j)



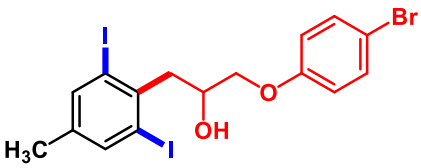
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**57%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.43(s, 2H), 7.26-7.37 (m, 5H), 4.60 (s, 2H), 4.20-4.25 (m, 1H), 3.40 (dd, 1H, J = 8.1 Hz, J = 14.0 Hz) 3.21 (dd, 1H, J = 5.8 Hz, J = 14.0 Hz), 2.36 (d, 1H, J = 5.2Hz), 2.22 (s, 3H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 141.1, 140.2, 139.6, 138.2, 128.6, 127.9, 100.1, 73.9, 73.6, 70.9, 48.6, 19.7. **HRMS** (ESI) m/z for $C_{17}H_{18}I_2NaO_2$ $[M+Na]^+$: calcd. 530.9294; found, 530.9289.

1.2.11 Synthesis of 1-(2,6-diiodo-4-methylphenyl)-3-(2-methoxyphenoxy) propan-2-ol (7k)



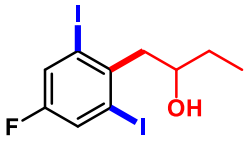
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**62%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.70 (s, 2H), 6.88-6.95 (m, 4H), 4.38-4.45 (m, 1H), 4.10-4.12 (m, 2H), 3.86 (s, 3H), 3.49 (dd, 1H, J = 7.4 Hz, J = 14.0 Hz) 3.31 (dd, 1H, J = 6.6 Hz, J = 14.0 Hz), 2.88 (d, 1H, J = 4.4 Hz), 2.22 (s, 3H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 150.1, 148.5, 141.2, 140.3, 139.3, 122.3, 121.2, 115.4, 112.6, 100.2, 74.1, 70.5, 56.1, 48.5, 19.7. **M.p**: 124-126 °C. **HRMS** (ESI) m/z for $C_{17}H_{18}I_2NaO_3$ $[M+Na]^+$: calcd. 546.9243; found, 546.9239.

1.2.12 Synthesis of 1-(4-bromophenoxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7l)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**60%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.71 (s, 2H), 7.37 (d, 2H, J = 8.8 Hz), 6.81 (d, 2H, *J* = 8.8 Hz), 4.40 (bs, 1H), 3.99-4.08 (m, 2H), 3.46 (dd, 1H, *J* = 7.6 Hz, *J* = 14.0 Hz), 3.34 (dd, 1H, *J* = 6.5 Hz, *J* = 14.1 Hz), 2.32 (d, 1H, *J* = 5.5 Hz), 2.23 (s, 3H). δ_C (100 MHz, *d*-$CDCl_3$) δ:157.8, 141.3, 140.5, 139.0, 132.5, 116.6, 113.5, 100.2, 71.7, 70.5, 48.6, 19.7. **M.p**: 140-142 °C**. HRMS** (ESI) m/z for $C_{16}H_{15}BrI_2NaO_2$ $[M+Na]^+$: calcd. 594.8242; found, 594.8238.

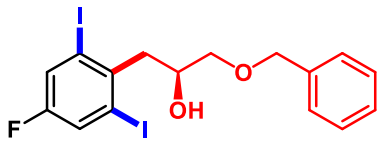
1.2.13 Synthesis of 1-(4-fluoro-2,6-diiodophenyl)butan-2-ol (7m)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**64%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.62(d, 2H, *J* = 7.5 Hz), 3.94 (bs, 1H),

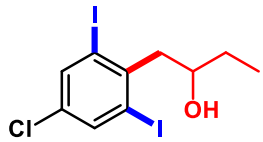
3.22-3.32 (m, 2H), 1.64-1.69 (m, 2H), 1.46 (d, 1H, *J* = 6.0 Hz), 1.04 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 160.9, 158.4, 139.5, 139.5, 127.6, 127.4, 98.6, 98.6, 73.6, 51.3, 30.7, 10.3. **HRMS** (ESI) m/z for $C_{10}H_{11}FI_2NaO$ $[M+Na]^+$: calcd. 442.8781; found, 442.8778.

1.2.14 Synthesis of (S)-1-(benzyloxy)-3-(4-fluoro-2,6-diiodophenyl)propan-2-ol (7n)



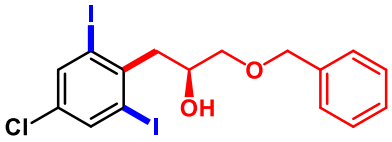
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**60%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.62 (d, 2H, *J* = 7.6 Hz), 7.29-7.36 (m, 5H), 4.61 (s, 2H), 4.10-4.23 (m, 1H), 3.59-3.61 (m, 2H), 3.42 (dd, 1H, *J* = 8.3 Hz, *J* = 14.2 Hz), 3.21 (dd, 1H, *J* = 5.5 Hz, *J* = 14.2 Hz), 2.40 (d, 1H, *J* = 4.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 160.9, 158.4, 139.0, 138.9, 138.0, 128.6, 127.9, 127.9, 127.6, 127.4, 99.6, 99.5, 73.9, 73.6, 70.8, 48.0. **HRMS** (ESI) m/z for $C_{16}H_{15}FI_2NaO_2$ $[M+Na]^+$: calcd. 534.9043; found, 534.9040.

1.2.15 Synthesis of 1-(4-chloro-2,6-diiodophenyl)butan-2-ol (7o)



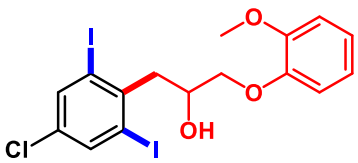
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**63%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.86 (s, 2H), 3.93 (bs, 1H), 3.20-3.32 (m, 2H), 1.59-1.71 (m, 2H), 1.40 (d, 1H, *J* = 6.2 Hz), 1.05 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 142.2, 139.7, 133.3, 99.6, 73.5, 51.8, 30.8, 10.3. **HRMS** (ESI) m/z for $C_{10}H_{11}ClI_2NaO$ $[M+Na]^+$: calcd. 458.8485; found, 458.8477.

1.2.16 Synthesis of (S)-1-(benzyloxy)-3-(4-chloro-2,6-diiodophenyl)propan-2-ol (7p)



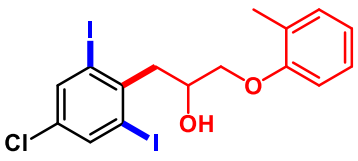
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**53%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.86 (s, 2H), 7.26-7.37 (m, 5H), 4.60 (s, 2H) 4.17-4.22 (m, 1H), 3.58-3.61 (m, 2H), 3.43 (dd, 1H, *J* = 8.3 Hz, J = 14.0 Hz), 3.21 (dd, 1H, *J* = 5.4 Hz, *J* = 14.0 Hz), 2.37 (d, 1H, *J* = 5.5 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 141.6, 139.7, 138.0, 133.4, 128.6, 127.9, 127.9, 99.6, 73.8, 73.6, 70.7, 48.4. **M.p**: 79-81 °C. **HRMS** (ESI) m/z for $C_{16}H_{15}ClI_2NaO_2$ $[M+Na]^+$: calcd. 550.8748; found, 550.8741.

1.2.17 Synthesis of 1-(4-chloro-2,6-diiodophenyl)-3-(2-methoxyphenoxy) propan-2-ol (7q)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**59%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.87 (s, 2H), 6.91-6.70 (m, 4H), 4.35-4.42 (m, 1H), 4.10 (d, 2H, *J* = 4.9 Hz), 3.85 (s, 3H), 3.52 (dd, 1H, *J* = 6.1 Hz, J = 14.0 Hz), 3.31 (dd, 1H, *J* = 6.1 Hz, *J* = 14.0 Hz), 3.0 (d, 1H, *J* = 4.8 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 150.1, 148.4, 141.4, 139.7, 133.4, 122.5, 121.2, 115.6, 112.3, 74.1, 70.3, 56.0, 48.3. **M.p**: 134-136 °C. **HRMS** (ESI) m/z for $C_{16}H_{15}ClI_2NaO_3$ $[M+Na]^+$: calcd. 566.8697; found, 566.8689.

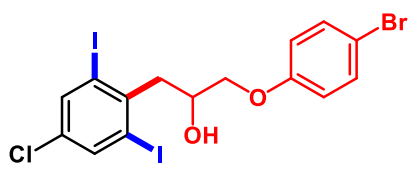
1.2.18 Synthesis of 1-(4-chloro-2,6-diiodophenyl)-3-(o-tolyloxy)propan-2-ol (7r)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid

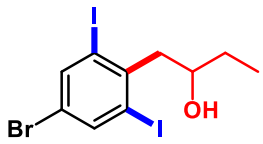
(**69%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.88 (s, 2H), 7.14-7.17 (m, 2H), 6.80-6.90 (m, 2H), 4.40 (bs, 1H), 4.10 (s, 2H), 3.63 (dd, 1H, *J* = 9.2 Hz, *J* = 13.8 Hz), 3.35 (dd, 1H, *J* = 9.6 Hz, *J* = 13.7 Hz), 2.35 (d, 1H, J = 6.20 Hz), 2.29(s, 3H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 156.6, 141.3, 139.8, 133.6, 130.9, 127.1, 126.8, 121.1, 111.1, 99.7, 71.2, 70.5, 48.5, 16.7, 16.7. **M.p**: 114-116 °C. **HRMS** (ESI) m/z for $C_{16}H_{15}ClI_2NaO_2$ $[M+Na]^+$: calcd. 550.8748; found, 550.8739.

1.2.19 Synthesis of 1-(4-bromophenoxy)-3-(4-chloro-2,6-diiodophenyl)propan-2-ol (7s)



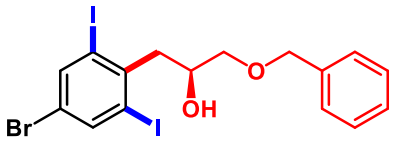
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**51%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.88 (s, 2H), 7.38 (d, 2H, *J* = 8.9 Hz), 6.80 (d, 2H, J = 8.9 Hz), 4.34-4.40 (m, 1H), 4.02-4.04 (m, 2H), 3.52 (dd, 1H, *J* = 8.0 Hz, J = 14.1 Hz), 3.34 (dd, 1H, *J* = 5.9 Hz, *J* = 14.0 Hz), 2.33 (d, 1H, *J* = 5.8 Hz). δ_C (100 MHz, *d*-$CDCl_3$)δ: 157.7, 141.0, 139.8, 133.7, 132.5, 116.5, 99.6, 71.6, 70.2, 48.4. **M.p**: 130-132 °C. **HRMS** (ESI) m/z for $C_{15}H_{12}BrClI_2NaO_2$ $[M+Na]^+$: calcd. 614.7696; found, 614.7691.

1.2.20 Synthesis of 1-(4-bromo-2,6-diiodophenyl)butan-2-ol (7t)



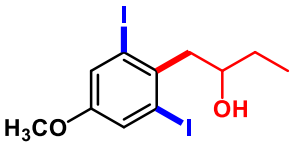
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**63%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 8.00 (s, 2H), 3.90-3.98 (m, 1H), 3.18-3.30 (m, 2H), 1.63-1.71 (m, 2H), 1.40 (d, 1H, *J* = 8.0Hz), 1.04 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 142.7, 142.3, 121.1, 100.3, 73.4, 51.9, 30.8, 10.3. **HRMS** (ESI) m/z for $C_{10}H_{11}BrI_2NaO$ $[M+Na]^+$: calcd. 502.7980; found, 502.7972.

1.2.21 Synthesis of (S)-1-(benzyloxy)-3-(4-bromo-2,6-diiodophenyl)propan-2-ol (7u)



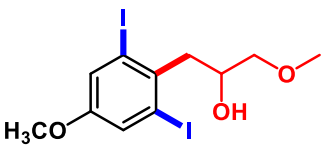
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**59%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 8.00 (s, 2H), 7.30-7.36 (m, 5H), 4.60 (s, 2H), 4.17-4.20 (m, 1H), 3.56-3.62 (m, 2H), 3.41 (dd, 1H, *J* = 8.4 Hz, *J* = 14.0 Hz), 3.18 (dd, 1H, *J* = 5.4 Hz, *J* = 13.9 Hz), 2.36 (d, 1H, *J* = 5.5 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 142.3, 142.1, 138.0, 128.6, 127.9, 127.9, 121.2, 100.2, 48.6. **M.p**: 84-86 °C. **HRMS** (ESI) m/z for $C_{16}H_{15}BrI_2NaO_2$ $[M+Na]^+$: calcd. 594.8242; found, 594.8235.

1.2.22 Synthesis of 1-(2,6-diiodo-4-methoxyphenyl)butan-2-ol (7v)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**46 %** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.43(s, 2H) 3.94-3.90 (m, 1H), 3.75 (s, 3H), 3.23-3.21 (m, 2H), 1.69-1.60 (m, 2H), 1.41 (bs, 1H), 1.04 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 158.3, 135.3, 126.3, 99.5, 73.7, 55.9, 51.3, 30.5, 10.3. **HRMS** (ESI) m/z for $C_{11}H_{14}I_2NaO_2$ $[M+Na]^+$: calcd. 454.8981; found, 454.8978.

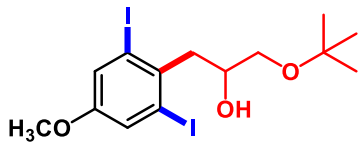
1.2.23 Synthesis of 1-(2,6-diiodo-4-methoxyphenyl)-3-methoxypropan-2-ol (7w)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**71 %** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.42(s, 2H), 4.10 (bs, 1H), 3.74 (s, 3H), 3.47 (d, 2H, J = 4.4 Hz), 3.41 (s, 3H), 3.35 (dd, 1H, *J* = 8.0 Hz, *J* = 14.3Hz), 3.17

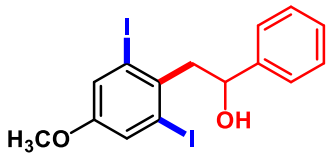
(dd, 1H, *J* = 5.9 Hz, *J* = 14.2Hz), 2.31 (d, 1H, J = 4.8 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 158.4, 134.7, 126.3, 99.4, 76.2, 70.9, 59.3, 55.8, 47.9. **M.p**: 104-106 °C. **HRMS** (ESI) m/z for $C_{11}H_{14}I_2NaO_3$ $[M+Na]^+$: calcd. 470.8930; found, 470.8927.

1.2.24 Synthesis of 1-(tert-butoxy)-3-(2,6-diiodo-4-methoxyphenyl)propan-2-ol (7x)



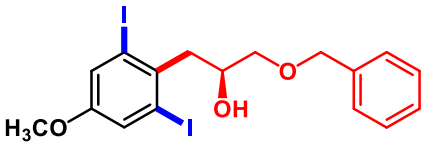
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**67%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.43(s, 2H), 4.00-4.10 (m, 1H), 3.74 (s, 3H), 3.42 (d, 2H, J = 5.3 Hz), 3.34-3.40 (m, 1H), 3.12 (dd, 1H, *J* = 6.1 Hz, *J* = 14.2Hz), 2.50 (d, 1H, *J* = 4.7 Hz), 1.21 (s, 9H). δ_C (100 MHz, *d*-$CDCl_3$) δ: 158.2, 134.9, 126.2, 99.4, 73.4, 71.1, 65.4, 55.8, 47.9, 27.7. **HRMS** (ESI) m/z for $C_{14}H_{20}I_2NaO_3$ $[M+Na]^+$: calcd. 512.9400; found, 512.9396.

1.2.25 Synthesis of 2-(2,6-diiodo-4-methoxyphenyl)-1-phenylethan-1-ol (7y)



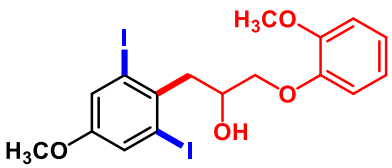
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**25** % yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.50-7.35 (m, 6H), 7.31 (d, 1H, *J* = 7.3Hz), 5.13-5.10 (m, 1H), 3.77 (s, 3H), 3.38 (dd, 1H, *J* = 4.3 Hz, *J* = 14.3 Hz), 3.57 (dd, 1H, *J* = 9.6 Hz, *J* = 14.3 Hz) 1.90 (d, 1H, *J* = 4.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 158.5, 143.9, 134.5, 128.6, 127.9, 126.3, 125.9, 99.7, 74.3, 55.9, 53.5. **HRMS** (ESI) m/z for $C_{15}H_{14}I_2NaO_2$ $[M+Na]^+$: calcd. 502.8981; found, 502.8975.

1.2.26 Synthesis of (S)-1-(benzyloxy)-3-(2,6-diiodo-4-methoxyphenyl)propan-2-ol (7z)



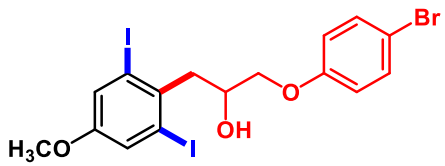
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**55%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.42(s, 2H), 7.36-7.26 (m, 5H), 4.63-4.57 (m, 2H), 4.22-4.18 (m, 1H), 3.74 (s, 3H), 3.60 (d, 2H, *J* = 4.9Hz), 3.38 (dd, 1H, *J* = 8.0 Hz, *J* = 14.2Hz), 3.20 (dd, 1H, *J* = 5.8 Hz, *J* = 14.2Hz), 2.36 (d, 1H, *J* = 4.0 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ:158.4, 138.2, 134.7, 128.6, 127.9, 126.3, 99.4, 73.9, 73.6, 71.1, 55.8, 47.9. **HRMS** (ESI) m/z for $C_{17}H_{18}I_2NaO_3$ $[M+Na]^+$: calcd. 546.9243; found, 546.9239.

1.2.27 Synthesis of 1-(2,6-diiodo-4-methoxyphenyl)-3-(2-methoxyphenoxy) propan-2-ol (7aa)



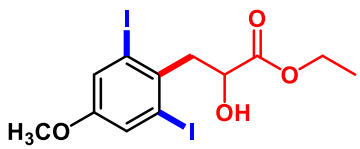
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**50%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.43(s, 2H), 6.80-6.98 (m, 4H), 4.38 (bs, 1H), 4.09-4.20 (m, 2H), 3.86 (s, 3H), 3.75 (s, 3H), 3.47 (dd, 1H, *J* = 7.4 Hz, *J* = 14.2Hz), 3.30 (dd, 1H, *J* = 6.7 Hz, *J* = 14.2Hz), 2.91 (d, 1H, *J* = 4.2 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 158.5, 150.1, 148.5, 134.4, 126.4, 122.3, 121.2, 115.4, 112.3, 99.4, 74.1, 70.6, 56.1, 55.9, 47.9. **M.p**: 105-107 °C. **HRMS** (ESI) m/z for $C_{17}H_{18}I_2NaO_4$ $[M+Na]^+$: calcd. 562.9192; found, 562.9189.

1.2.28 Synthesis of 1-(4-bromophenoxy)-3-(2,6-diiodo-4-methoxyphenyl) propan-2-ol (7ab)



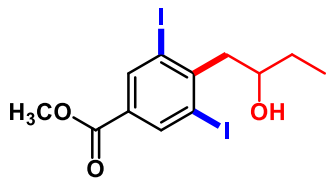
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**57%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.44 (s, 2H), 7.37 (d, 2H, *J* = 8.8 Hz), 6.80 (d, 2H, *J* = 8.9 Hz), 4.34-4.40 (m, 1H), 3.98-4.06 (m, 2H), 3.75 (s, 3H), 3.46 (dd, 1H, *J* = 7.6 Hz, *J* = 14.2 Hz), 3.33 (dd, 1H, *J* = 6.5 Hz, *J* = 14.2 Hz), 2.33 (d, 1H, *J* = 4.0Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ:158.6, 157.8, 134.1, 132.5, 126.4, 116.6, 113.5, 99.4, 71.7, 70.6, 55.9, 47.9. **M.p**: 135-137 °C. **HRMS** (ESI) m/z for $C_{16}H_{15}BrI_2NaO_3$ $[M+Na]^+$: calcd. 610.8192; found, 610.8188.

1.2.29 Synthesis of ethyl 3-(2,6-diiodo-4-methoxyphenyl)-2-hydroxypropanoate (7ac)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**52%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.43(s, 2H), 4.52 (dt, 1H, *J* = 7.3 Hz, J = 7.0 Hz), 4.25-4.28 (m, 2H), 3.75 (s, 3H), 3.40-3.48 (m, 2H), 2.77 (d, 1H, J = 7.4 Hz), 1.25 (dd, 3H, *J* = 7.2 Hz, J = 7.1 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 174.4, 158.6, 133.3, 126.2, 99.5, 70.1, 62.3, 55.9, 49.3, 14.2. **HRMS** (ESI) m/z for $C_{12}H_{14}I_2NaO_4$ $[M+Na]^+$: calcd. 498.8879; found, 498.8875.

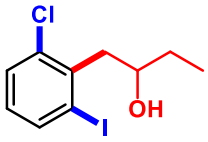
1.2.30 Synthesis of methyl 4-(2-hydroxybutyl)-3,5-diiodobenzoate (7ad)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as white solid (**82%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 8.49 (s, 2H), 3.69-4.03 (m,

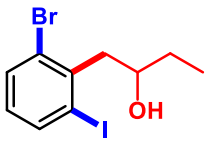
1H), 3.90 (s, 3H), 3.27-3.40 (m, 2H), 1.65-1.73 (m, 2H), 1.40 (d, 1H, *J* = 6.5 Hz), 1.05 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 164.1, 148.5, 141.3, 131.2, 99.9, 73.4, 52.7, 52.6, 30.9, 10.2. **M.p**: 110-112 °C. **HRMS** (ESI) m/z for $C_{12}H_{14}I_2NaO_3$ $[M+Na]^+$: calcd. 482.8930; found, 482.8921.

1.2.31 Synthesis of 1-(2-chloro-6-iodophenyl)butan-2-ol (7ae)



The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**68%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.76 (d, 1H, J = 7.9 Hz), 7.36 (d, 1H, J = 7.9 Hz), 6.84 (t, 1H, *J* = 7.9 Hz), 3.96 (bs, 1H), 3.13-3.23 (m, 2H), 1.61-1.70 (m, 2H), 1.47 (d, 1H, *J* = 4.0 Hz), 1.04 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ: 139.6, 138.8, 134.5, 130.2, 129.2, 102.5, 73.2, 45.8, 30.7, 10.2. **HRMS** (ESI) m/z for $C_{10}H_{12}ClINaO$ $[M+Na]^+$: calcd. 332.9519; found, 332.9514.

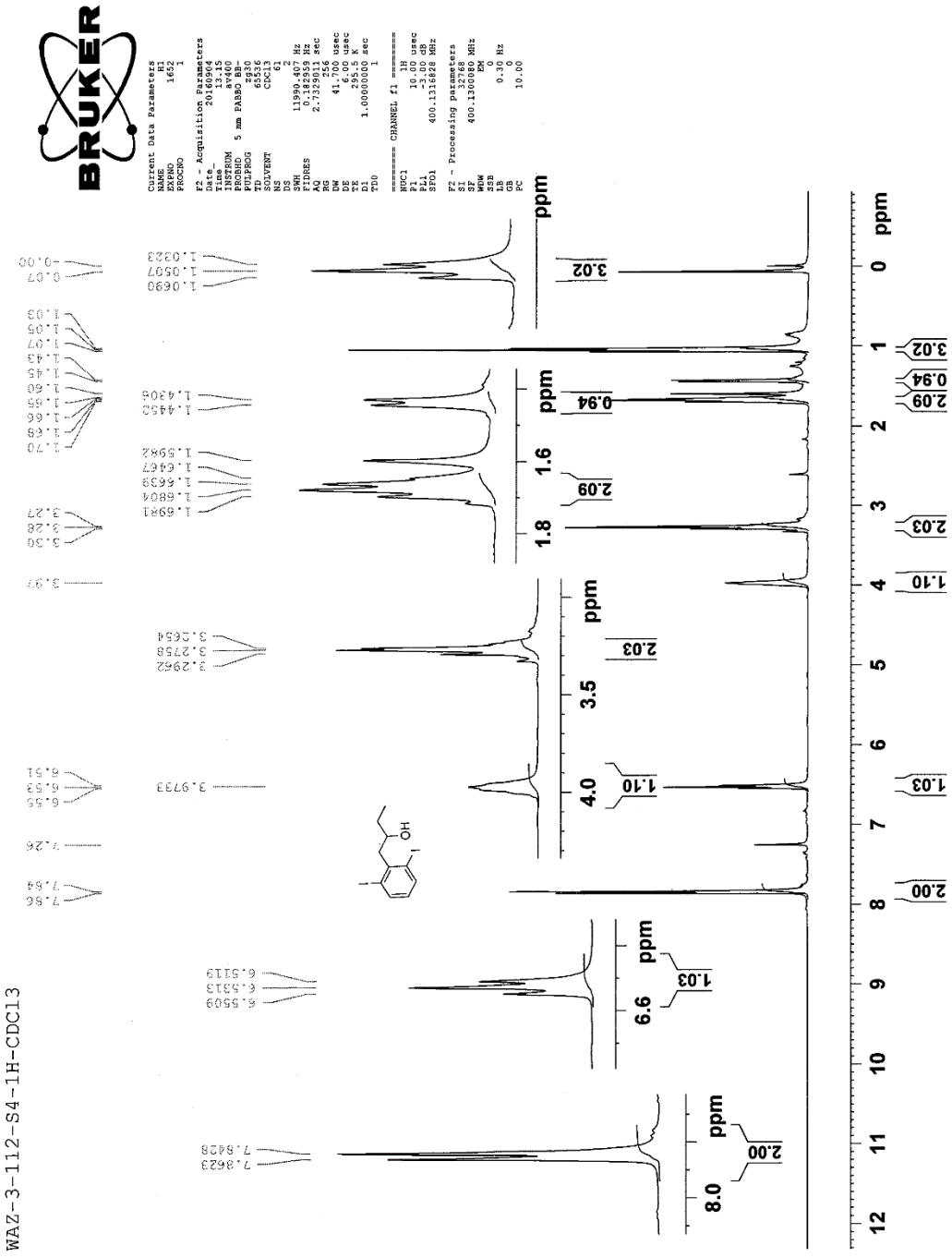
1.2.32 Synthesis of 1-(2-bromo-6-iodophenyl)butan-2-ol (7af)



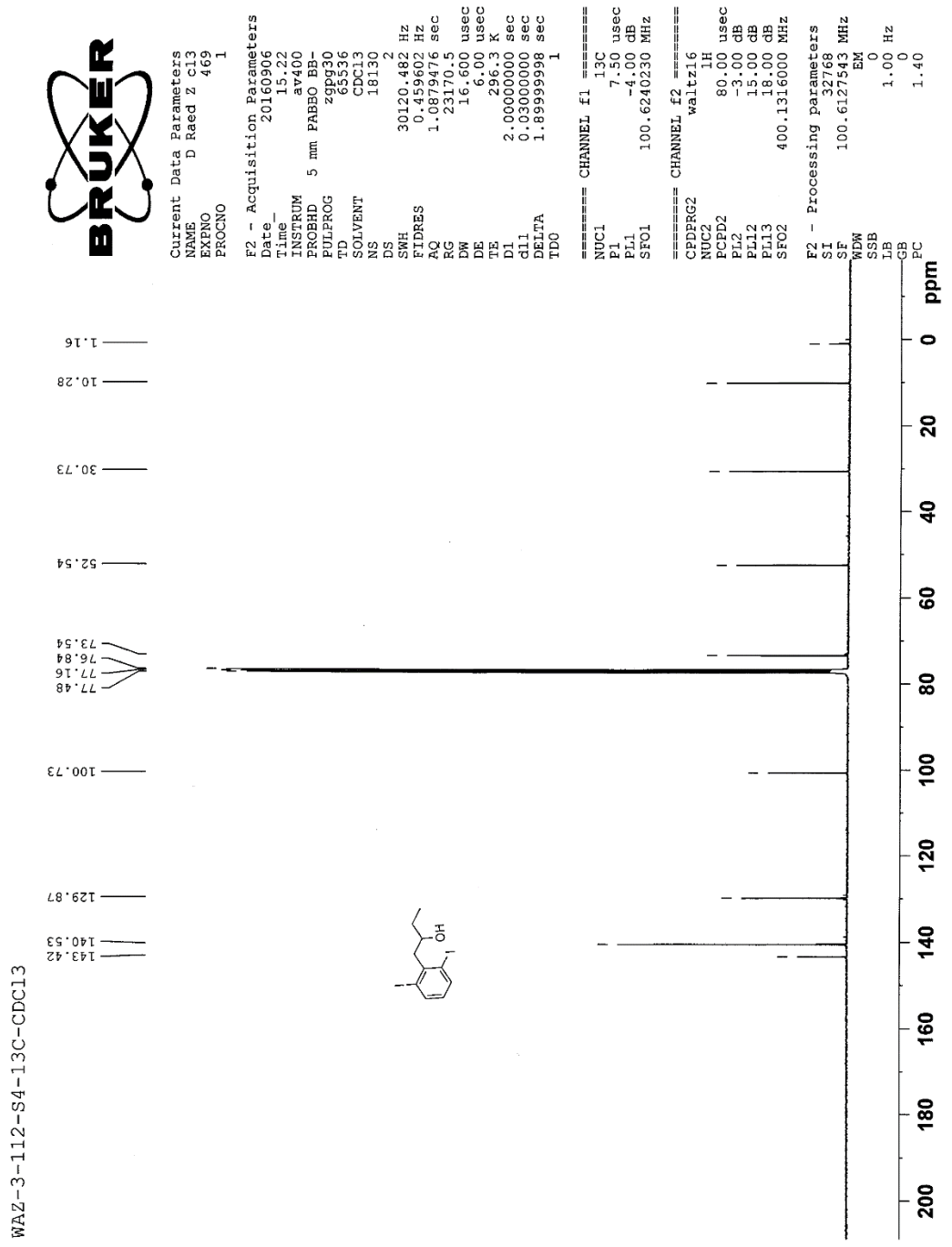
The title compound was prepared using the general procedure for Metal-Iodine Exchange reaction and isolated as colorless oil (**77%** yields). δ_H (400MHz, *d*-$CDCl_3$) δ: 7.81 (d, 1H, J = 7.9 Hz), 7.55 (d, 1H, J = 7.9 Hz), 6.75 (t, 1H, *J* = 7.9 Hz), 3.96-4.01 (m, 1H), 3.18-3.29 (m, 2H), 1.61-1.71 (m, 2H), 1.47 (d, 1H, *J* = 5.9 Hz), 1.04 (t, 3H, *J* = 7.4 Hz). δ_C (100 MHz, *d*-$CDCl_3$) δ:140.9, 139.5, 133.6, 129.5, 124.7, 102.2, 73.3, 48.2, 30.7, 10.3. **HRMS** (ESI) m/z for $C_{10}H_{12}BrINaO$ $[M+H]^+$: calcd. 376.9014; found, 376.9010.

1.3 NMR Spectra for New Compounds

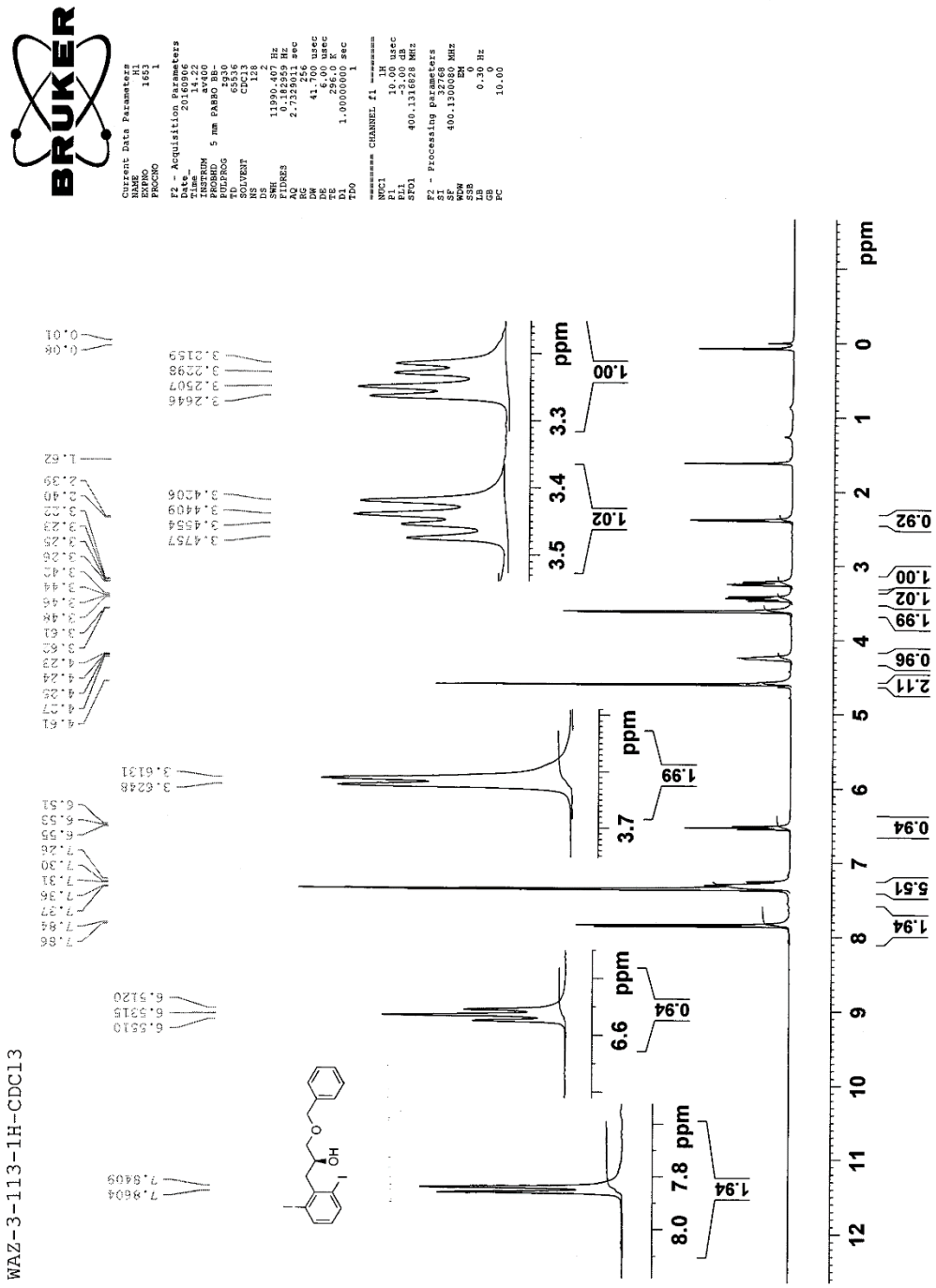
1.3.1 ^{1}H-NMR of 1-(2,6-diiodophenyl)butan-2-ol (7a) in d-$CDCl_3$ at 25 °C.



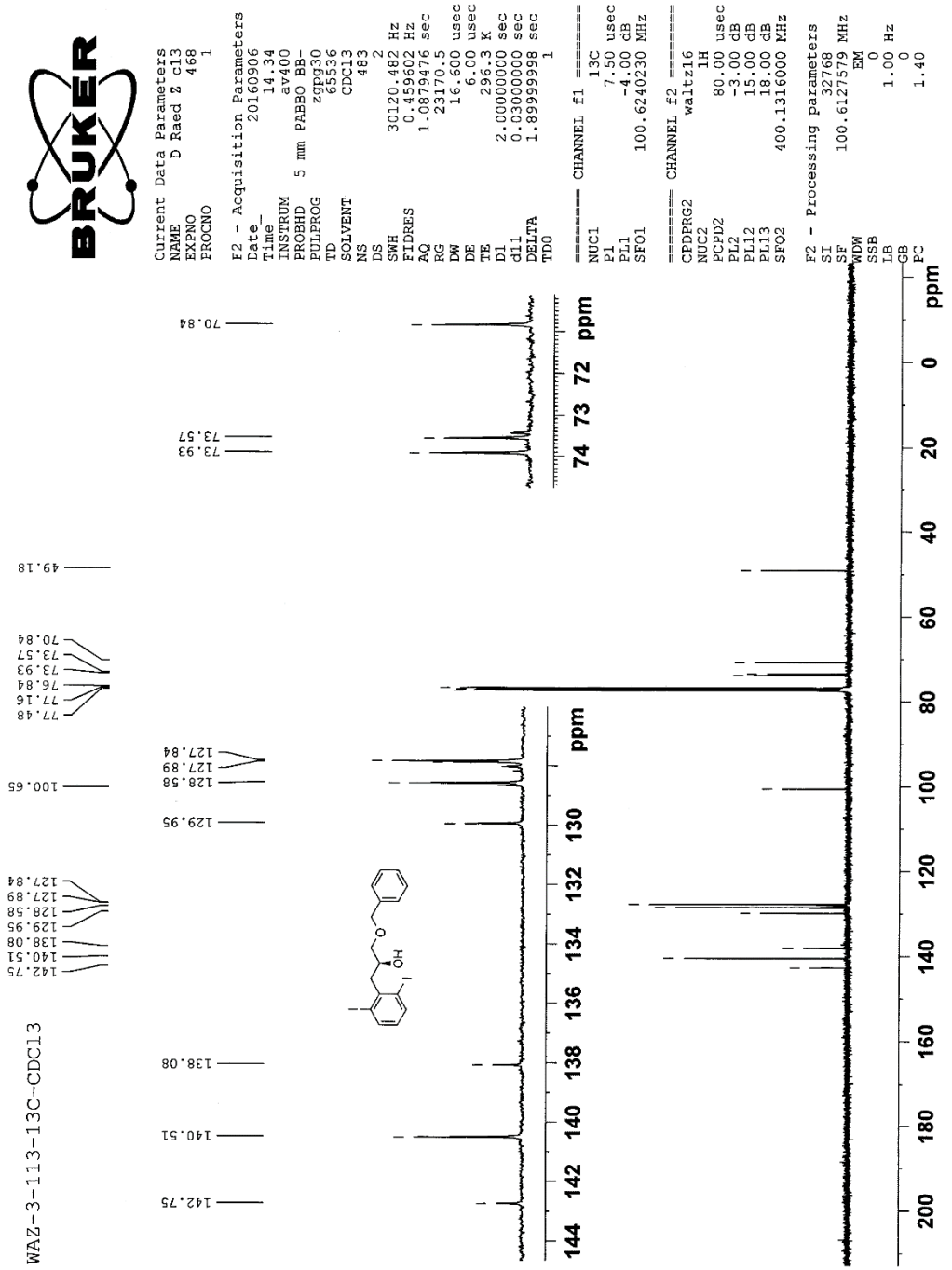
1.3.2 ^{13}C-NMR of 1-(2,6-diiodophenyl)butan-2-ol (7a) in d-CDCl$_3$ at 25 °C.



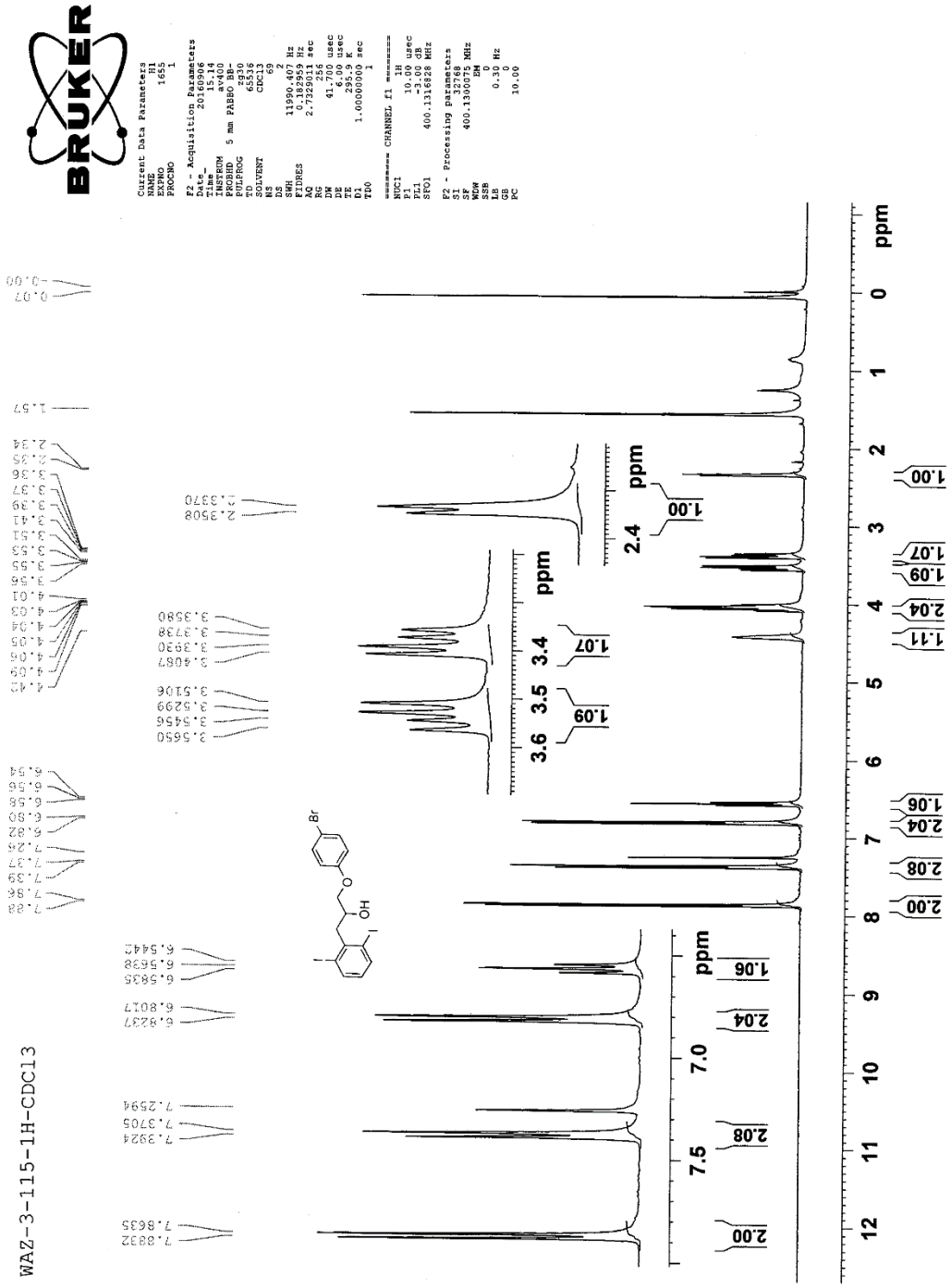
1.3.3 ^{1}H-NMR of (S)-1-(benzyloxy)-3-(2,6-diiodophenyl)propan-2-ol (7b) in d-$CDCl_3$ at 25 °C.



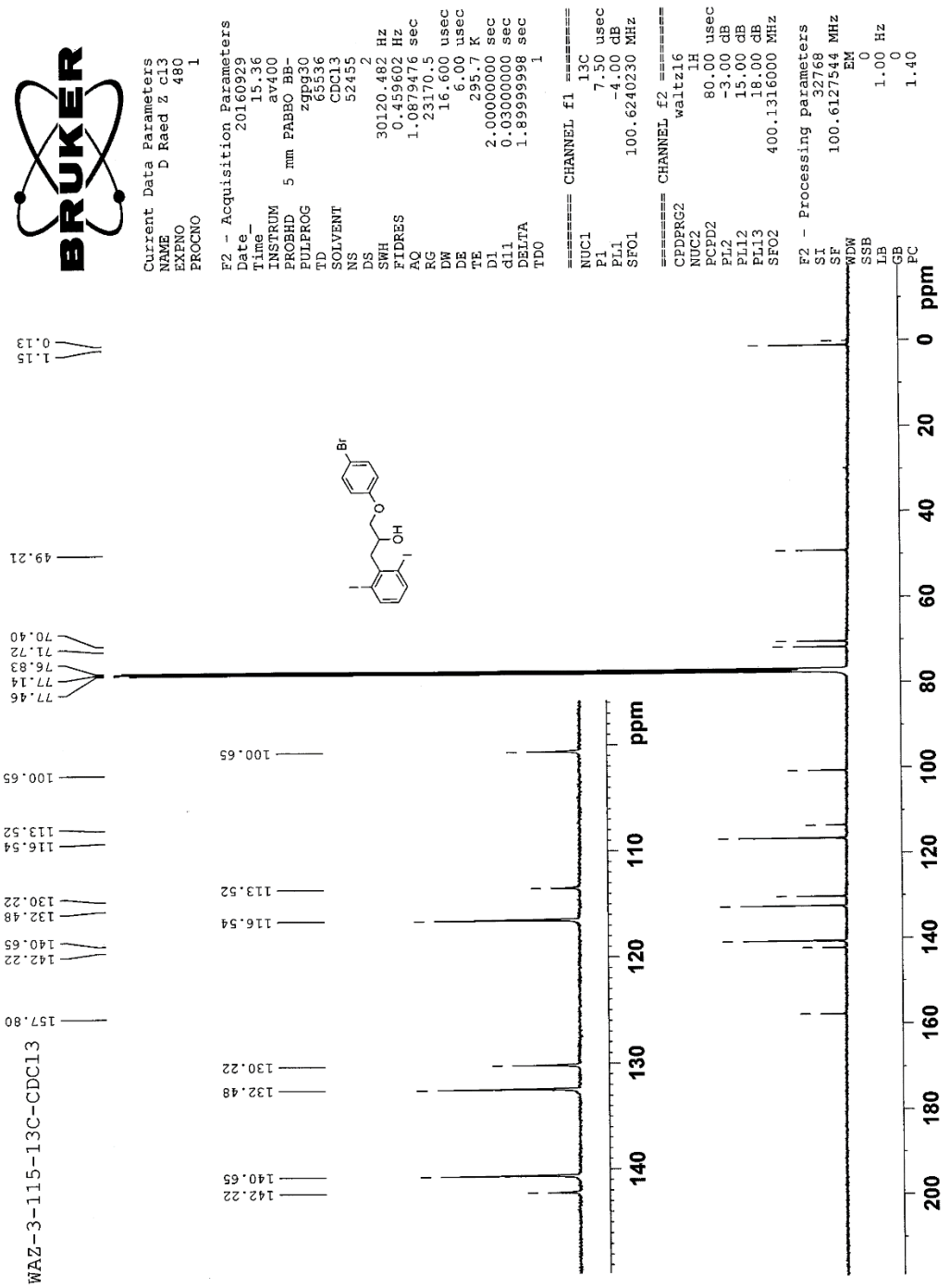
1.3.4 ^{13}C-NMR of (S)-1-(benzyloxy)-3-(2,6-diiodophenyl)propan-2-ol (7b) in d-$CDCl_3$ at 25 °C.



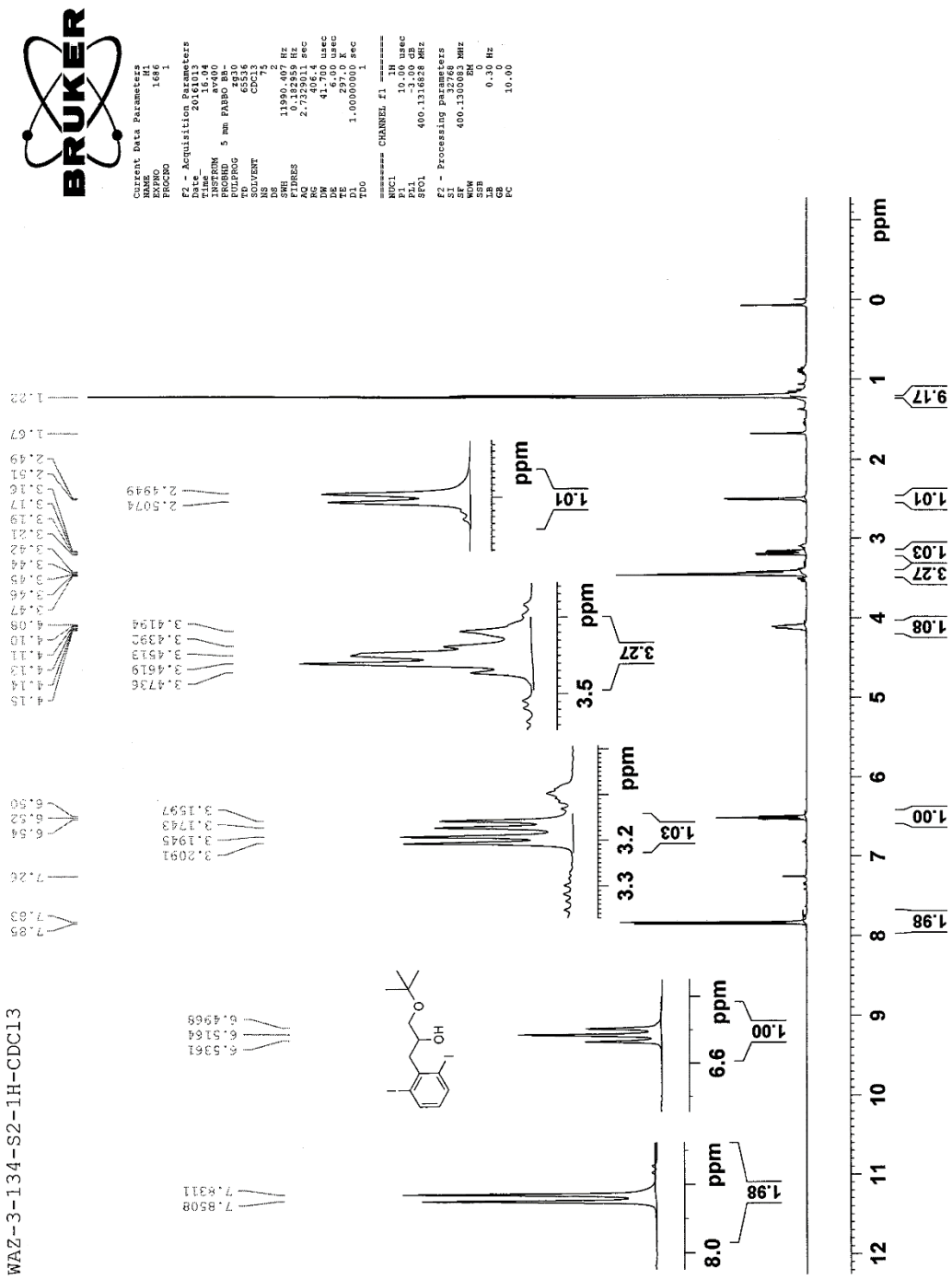
1.3.5 ^{1}H-NMR of 1-(4-bromophenoxy)-3-(2,6-diiodophenyl)propan-2-ol (7c) in d-$CDCl_3$ at 25 °C.



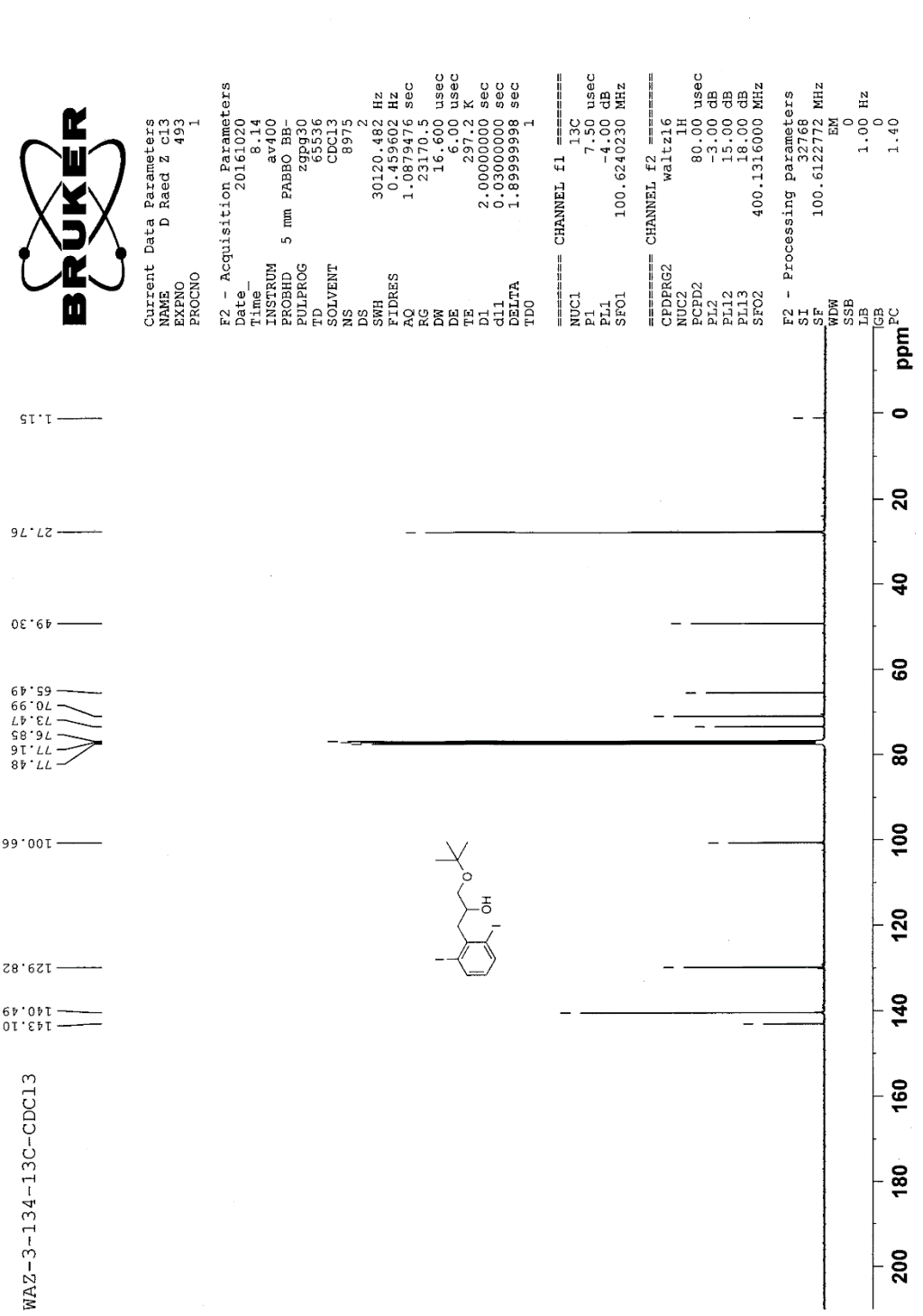
1.3.6 ^{13}C-NMR of 1-(4-bromophenoxy)-3-(2,6-diiodophenyl)propan-2-ol (7c) in d-$CDCl_3$ at 25 °C.



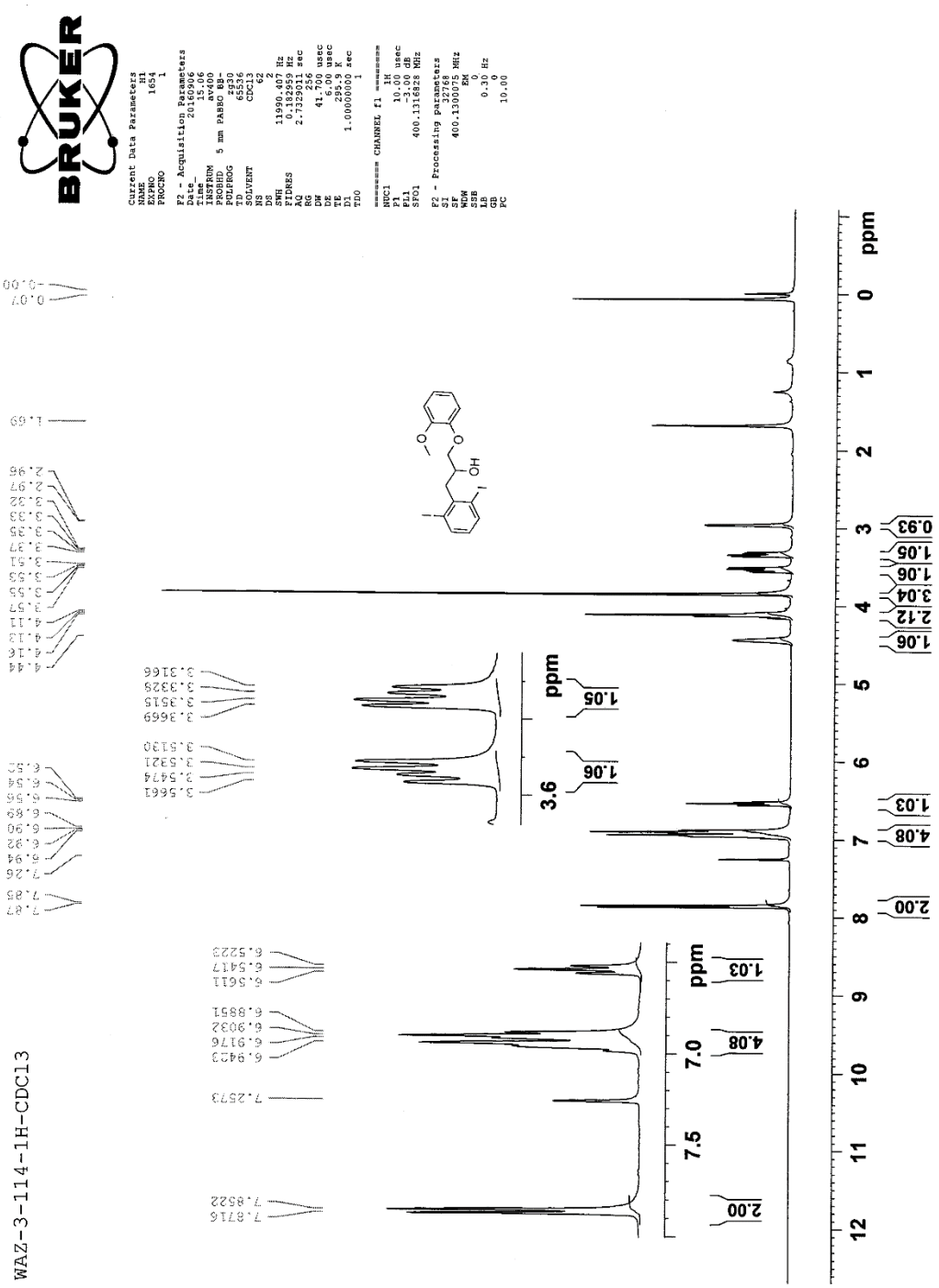
1.3.7 ^{1}H-NMR of 1-(tert-butoxy)-3-(2,6-diiodophenyl)propan-2-ol (7d) in d-$CDCl_3$ at 25 °C.



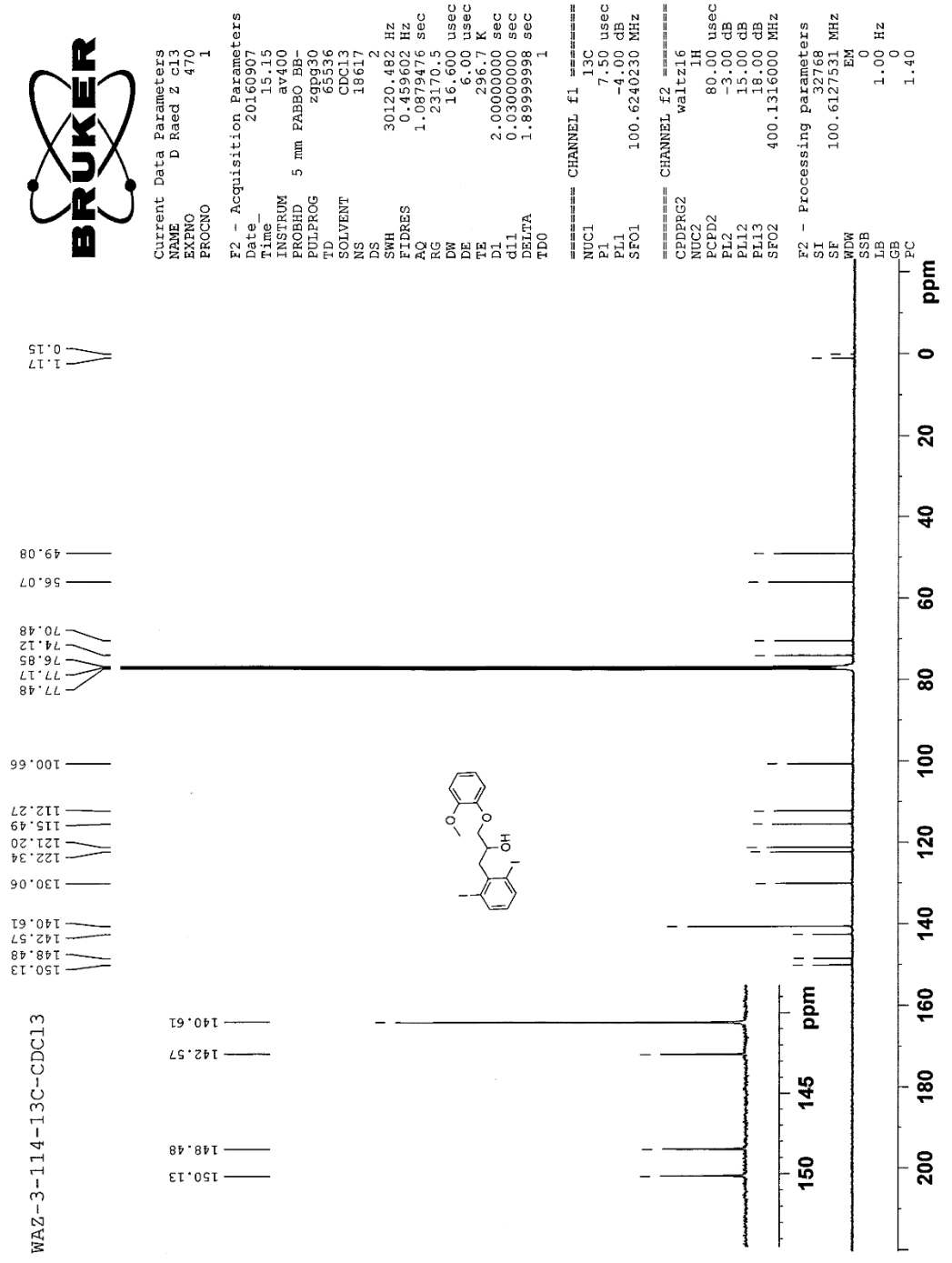
1.3.8 ^{13}C-NMR of 1-(tert-butoxy)-3-(2,6-diiodophenyl)propan-2-ol (7d) in d-$CDCl_3$ at 25 °C.



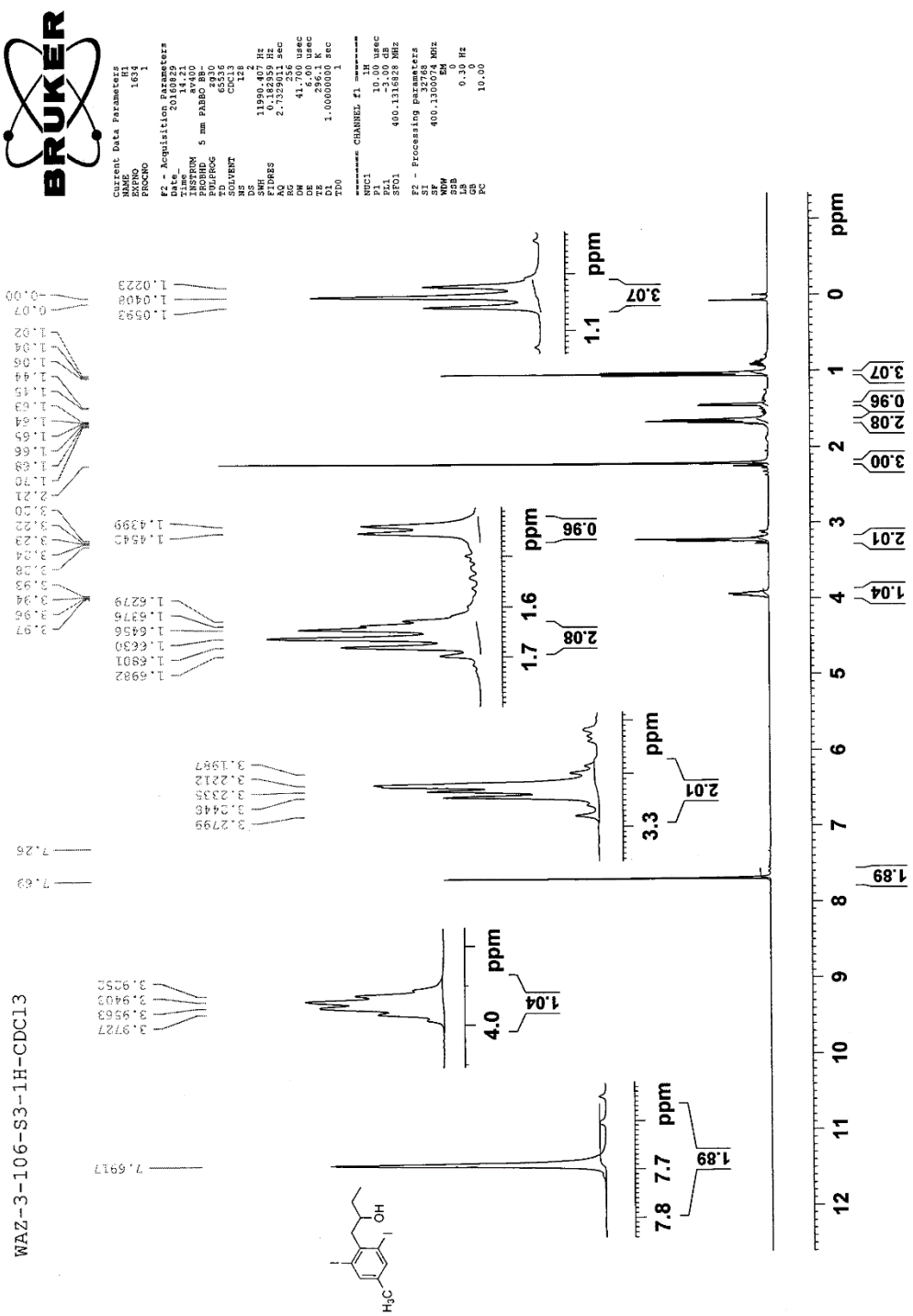
1.3.9 ^{1}H-NMR of 1-(2,6-diiodophenyl)-3-(2-methoxyphenoxy)propan-2-ol (7e) in d-CDCl$_3$ at 25 °C.



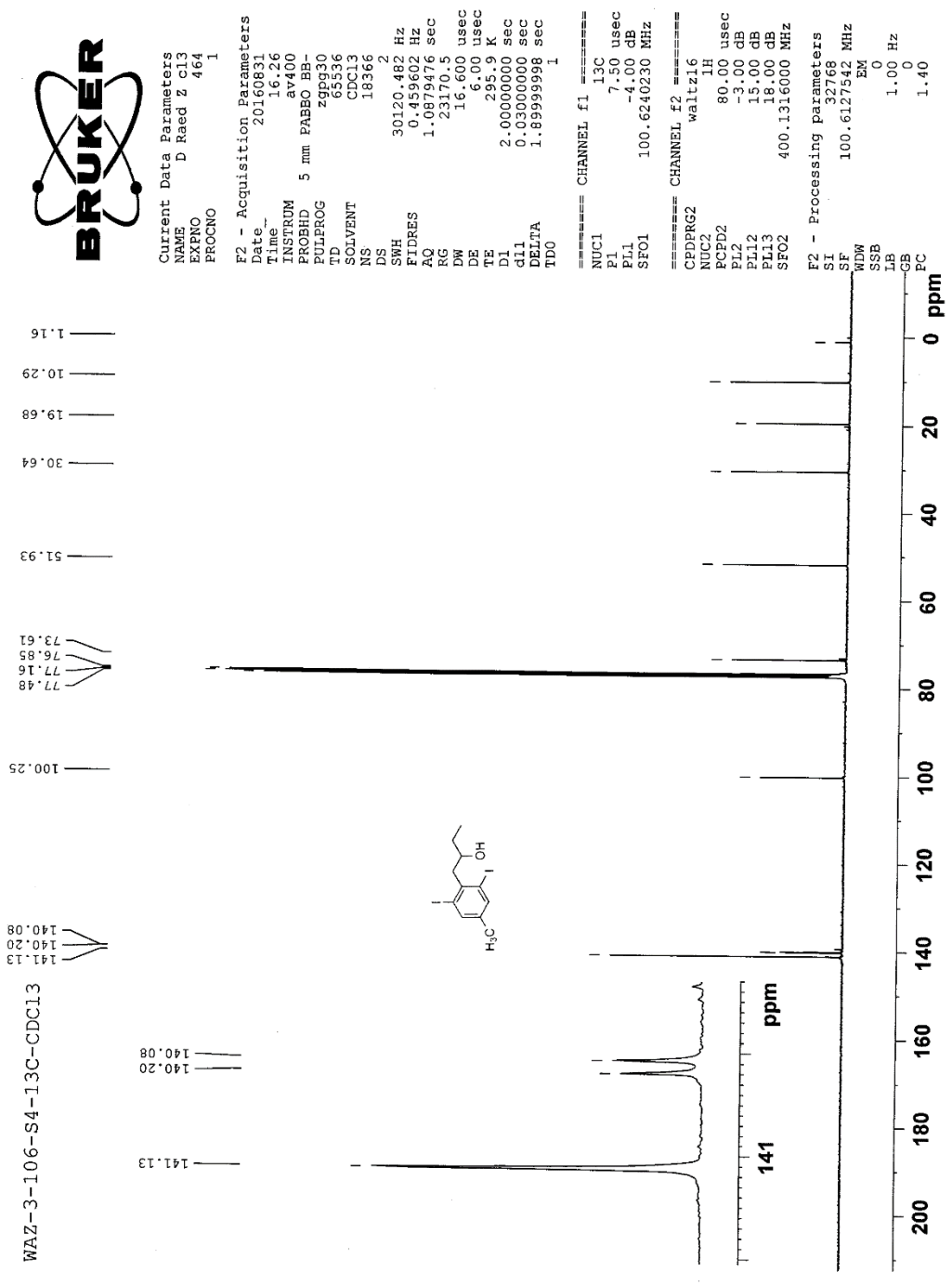
1.3.10 ^{13}C-NMR of 1-(2,6-diiodophenyl)-3-(2-methoxyphenoxy)propan-2-ol (7e) in d-CDCl$_3$ at 25 °C.



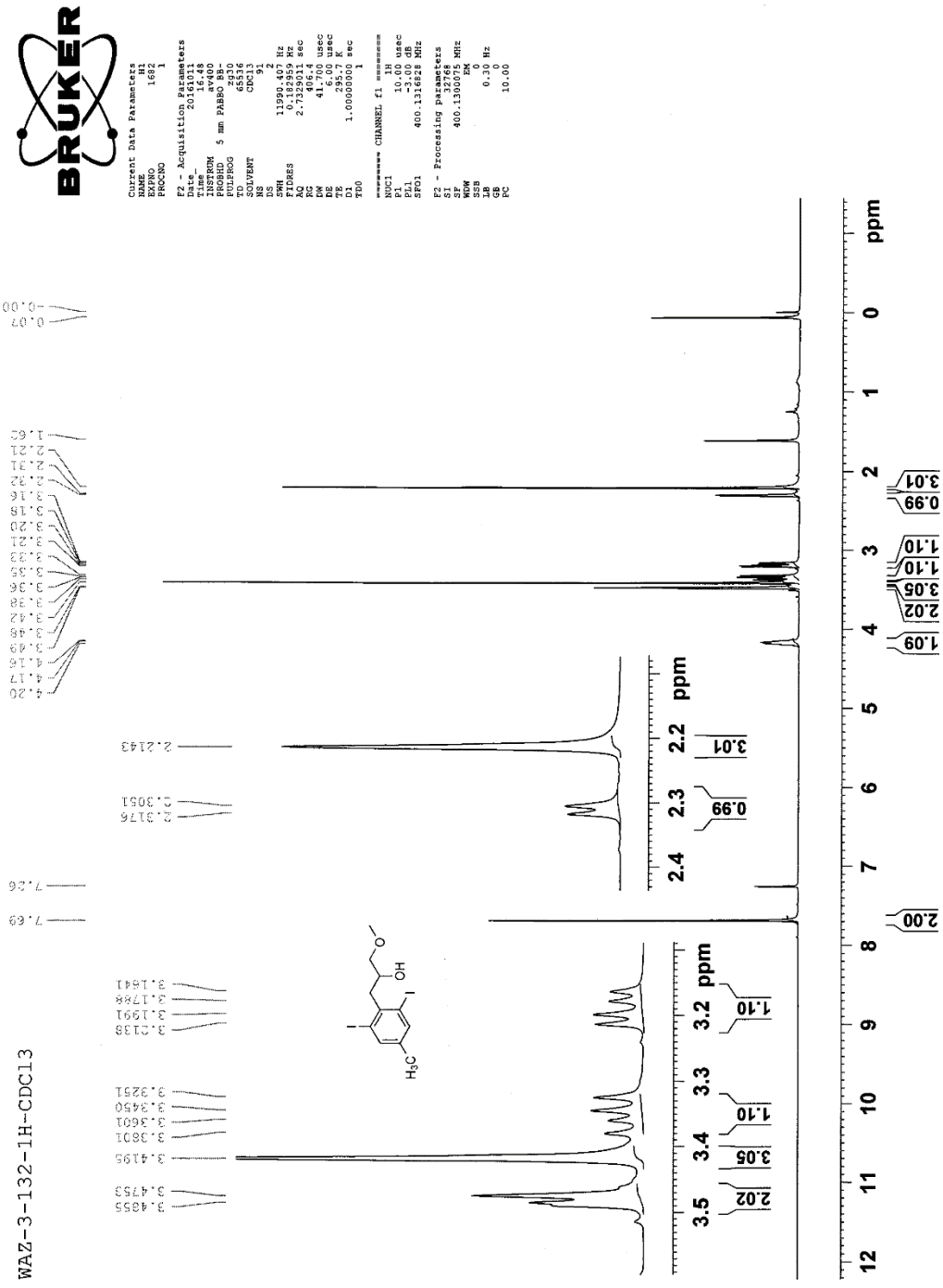
1.3.11 ^{1}H-NMR of 1-(2,6-diiodo-4-methylphenyl)butan-2-ol (7f) in d-CDCl$_3$ at 25 °C.



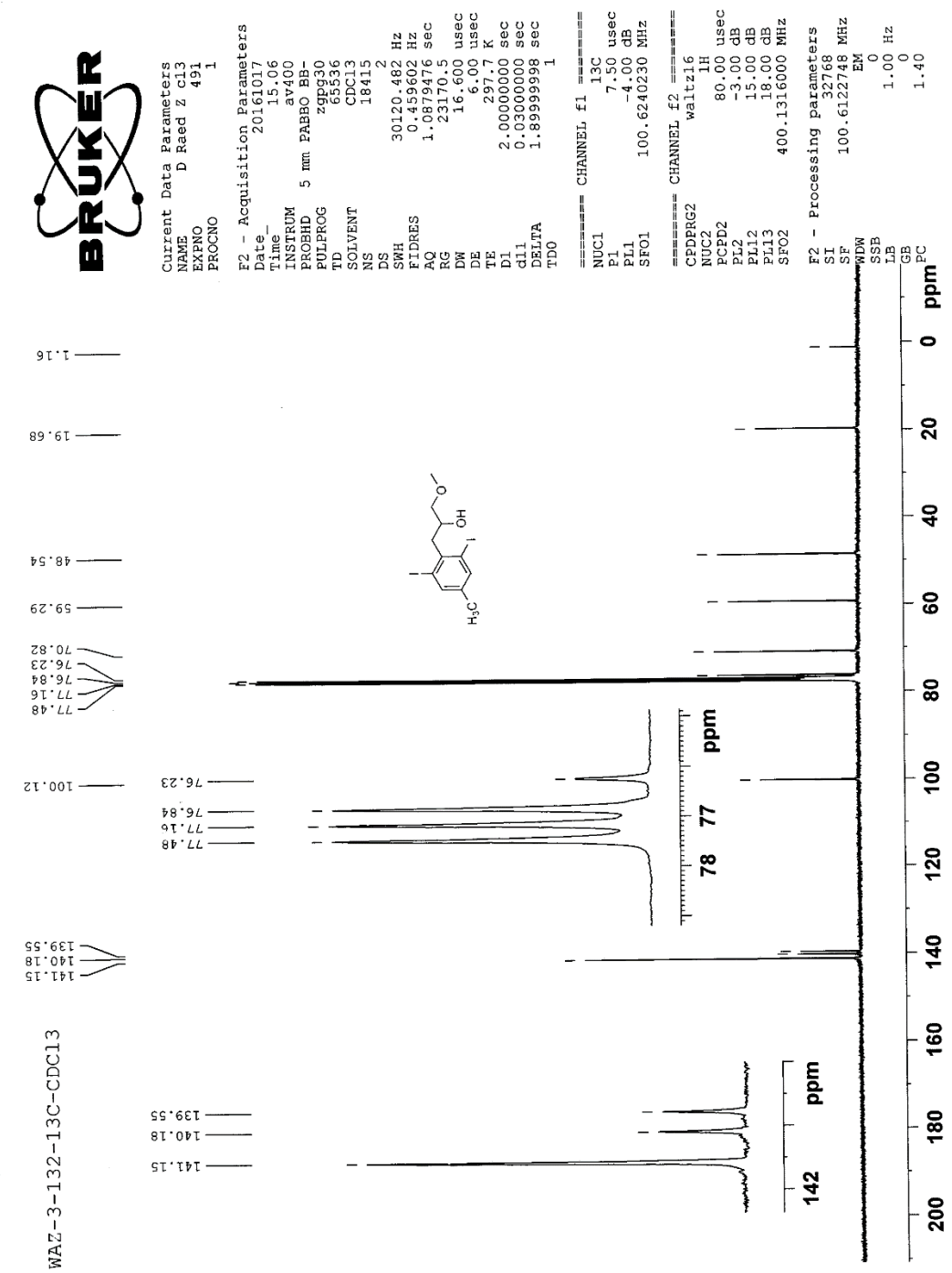
1.3.12 ^{13}C-NMR of 1-(2,6-diiodo-4-methylphenyl)butan-2-ol (7f) in d-CDCl$_3$ at 25 °C.



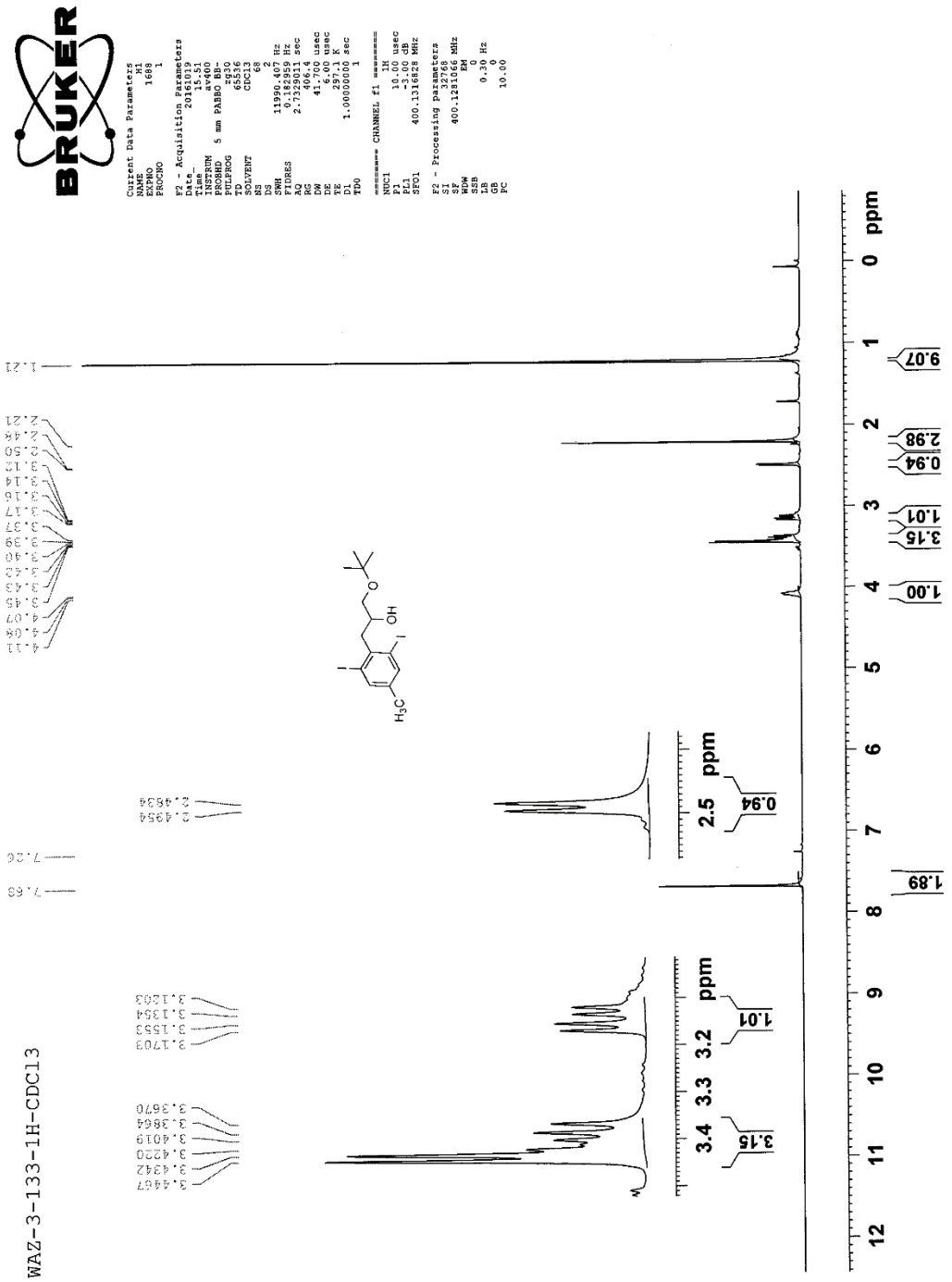
1.3.13 ^{1}H-NMR of 1-(2,6-diiodo-4-methylphenyl)-3-methoxypropan-2-ol (7g) in d-$CDCl_3$ at 25 °C.



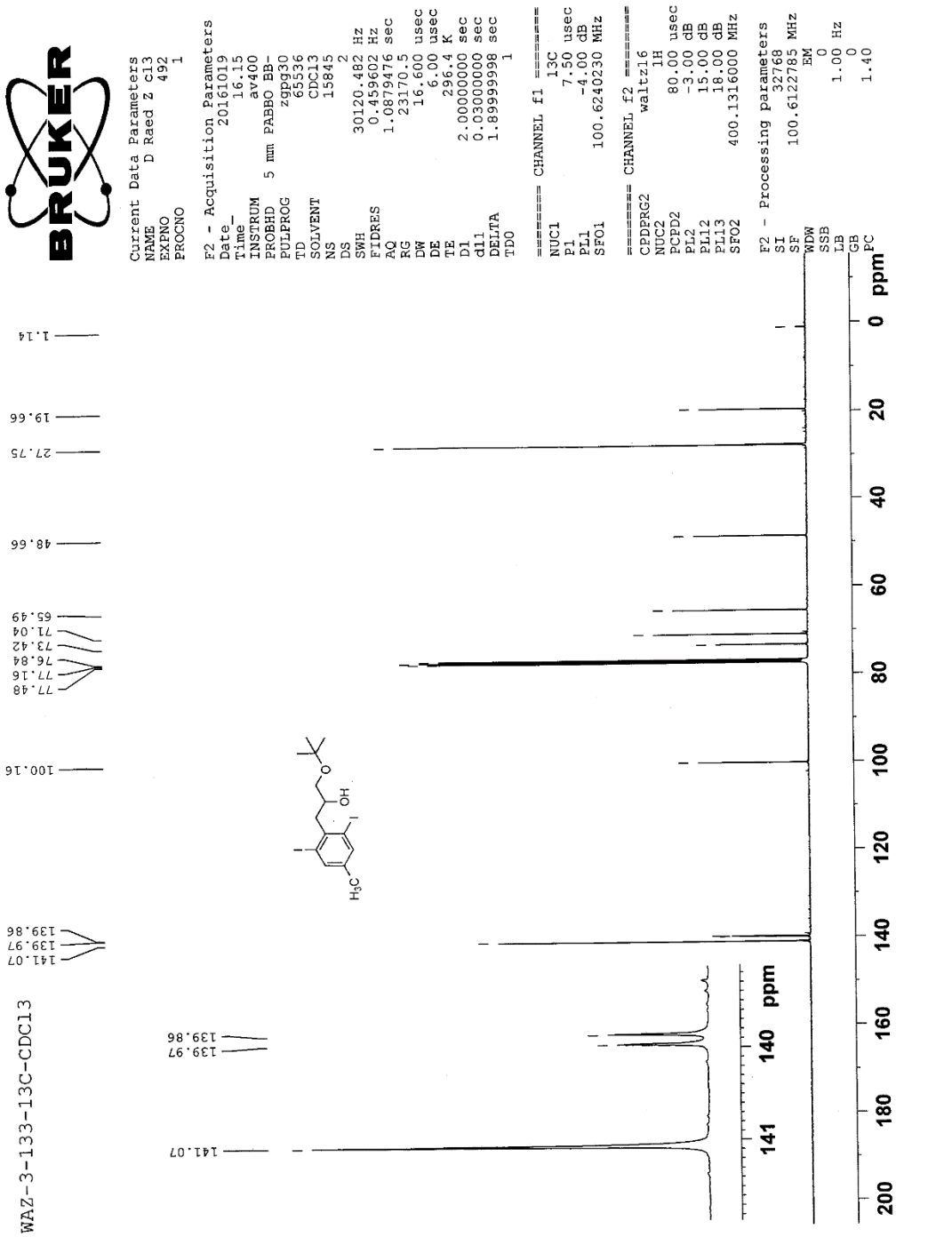
1.3.14 ^{13}C-NMR of 1-(2,6-diiodo-4-methylphenyl)-3-methoxypropan-2-ol (7g) in d-$CDCl_3$ at 25 °C.



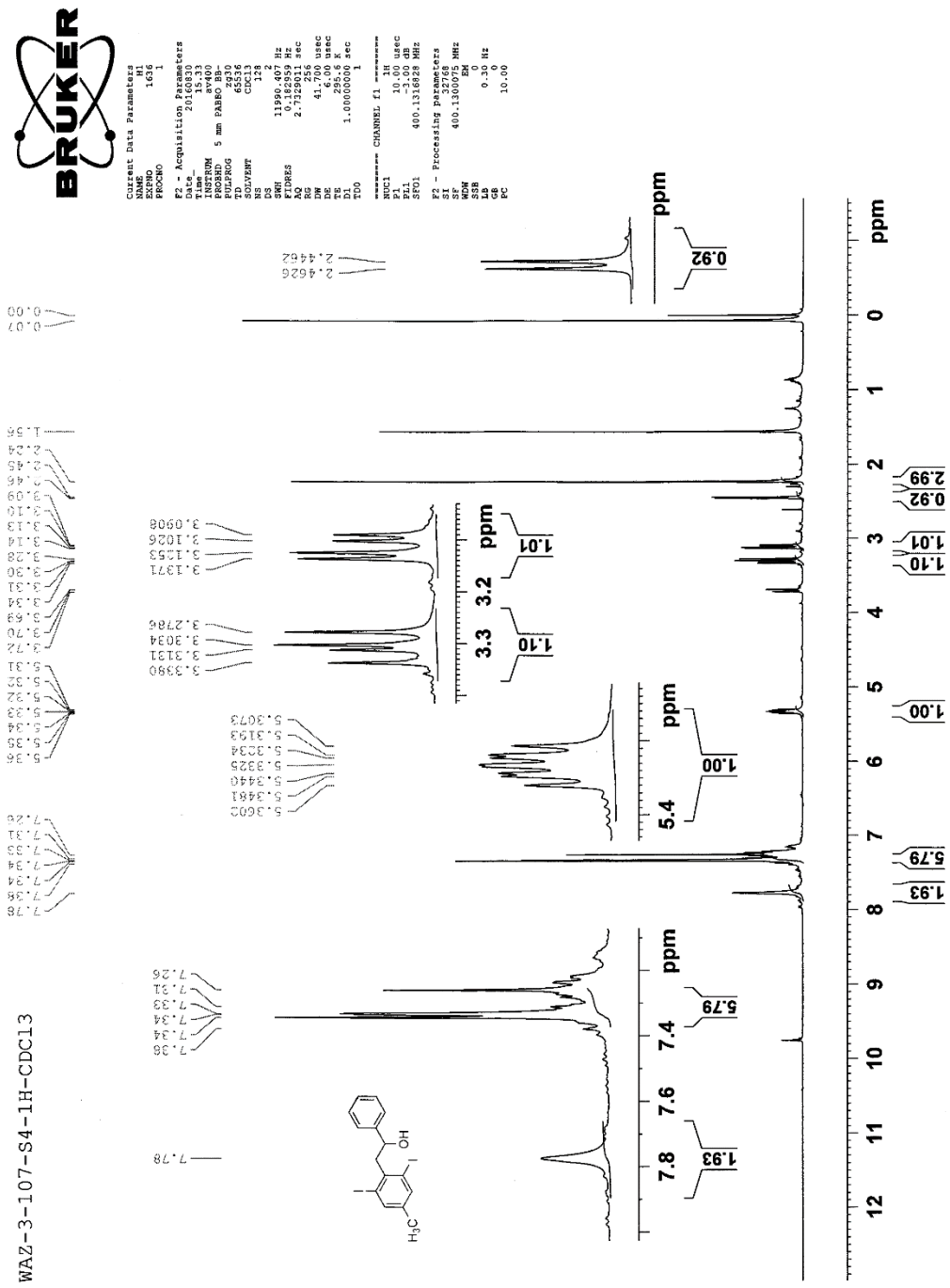
1.3.15 ^{1}H-NMR of 1-(tert-butoxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7h) in d-CDCl$_3$ at 25 °C.



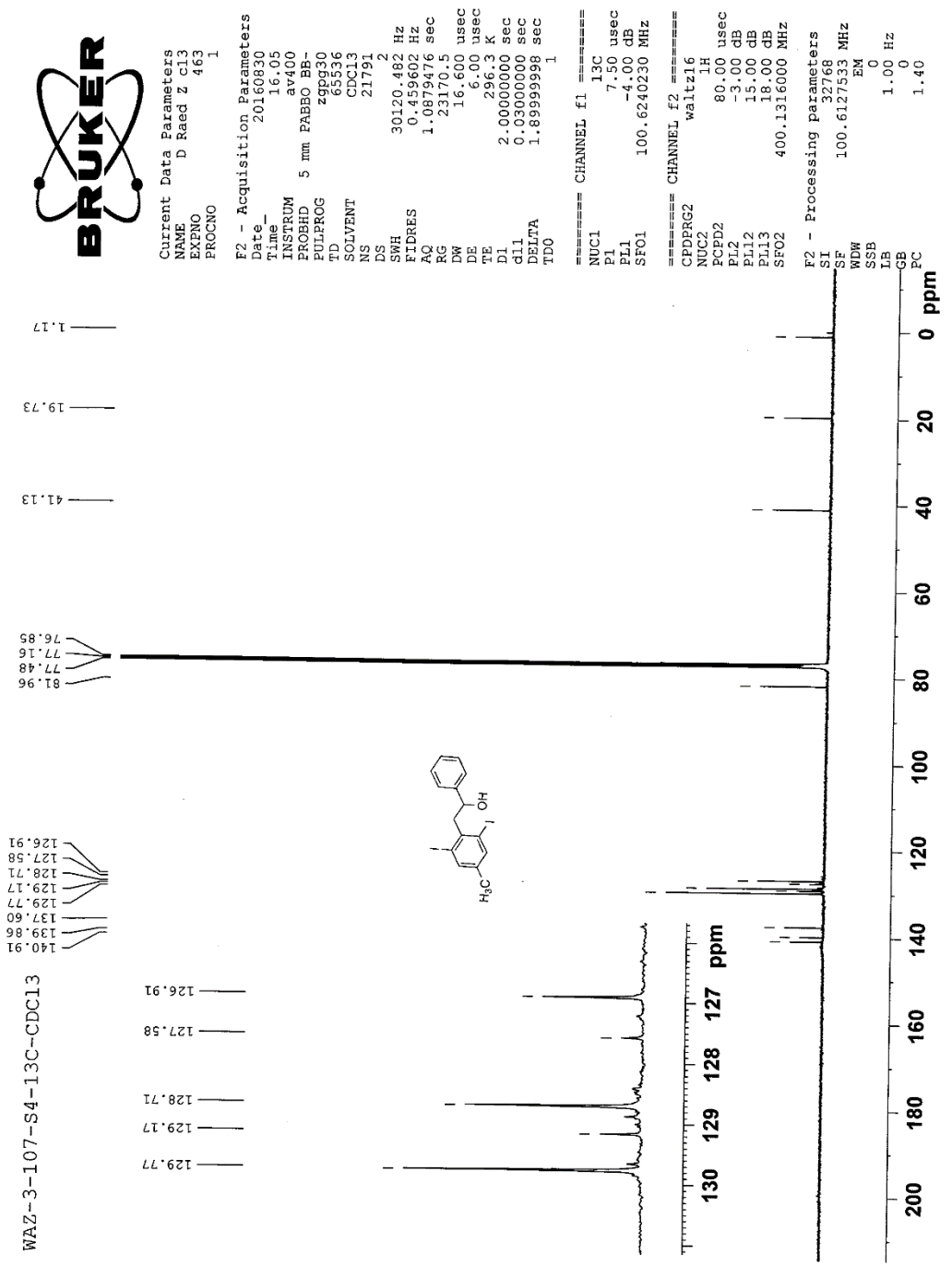
1.3.16 ^{13}C-NMR of 1-(tert-butoxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7h) in d-$CDCl_3$ at 25 °C.



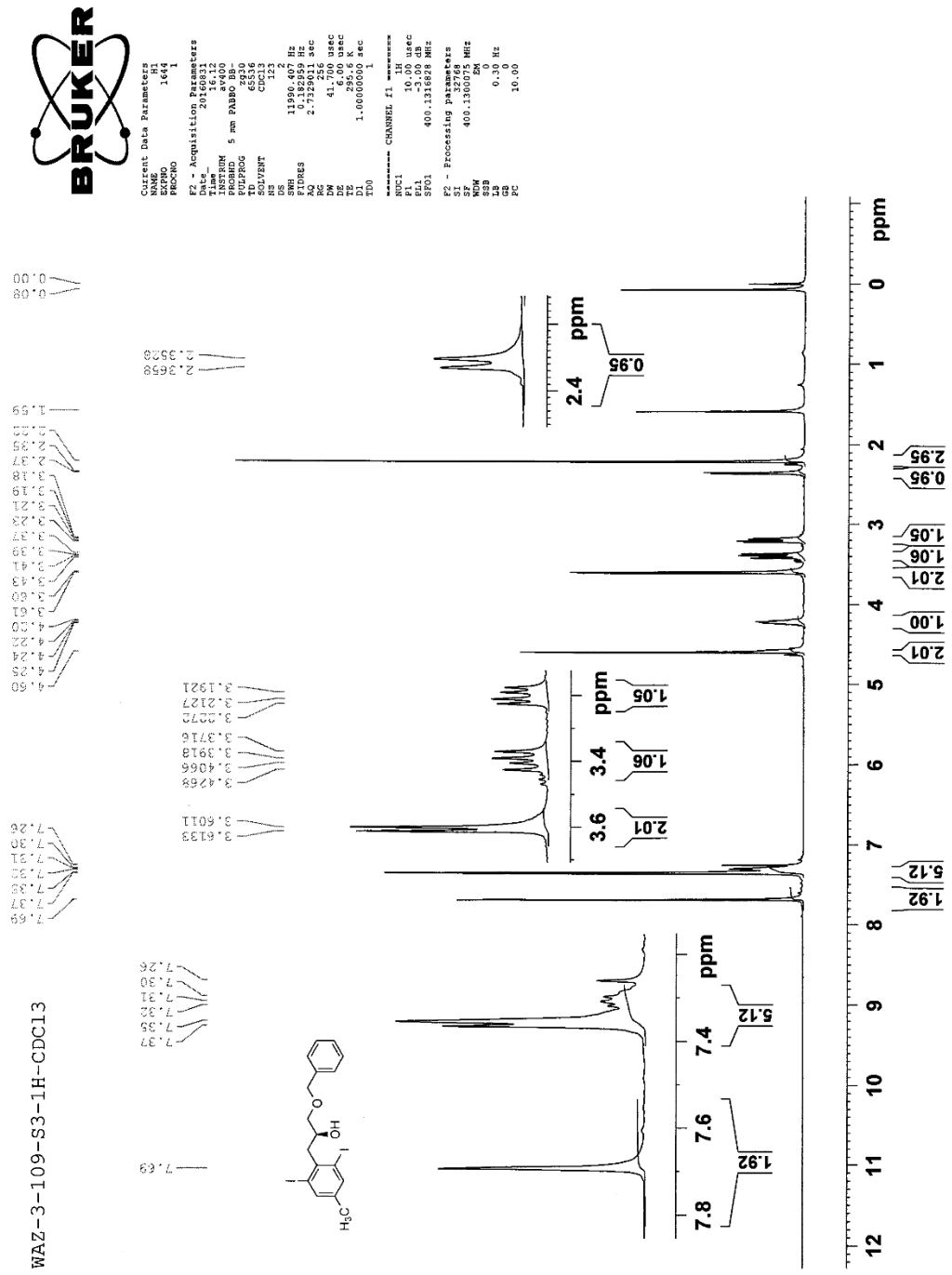
1.3.17 ^{1}H-NMR of 2-(2,6-diiodo-4-methylphenyl)-1-phenylethan-1-ol (7i) in d-$CDCl_3$ at 25 °C.



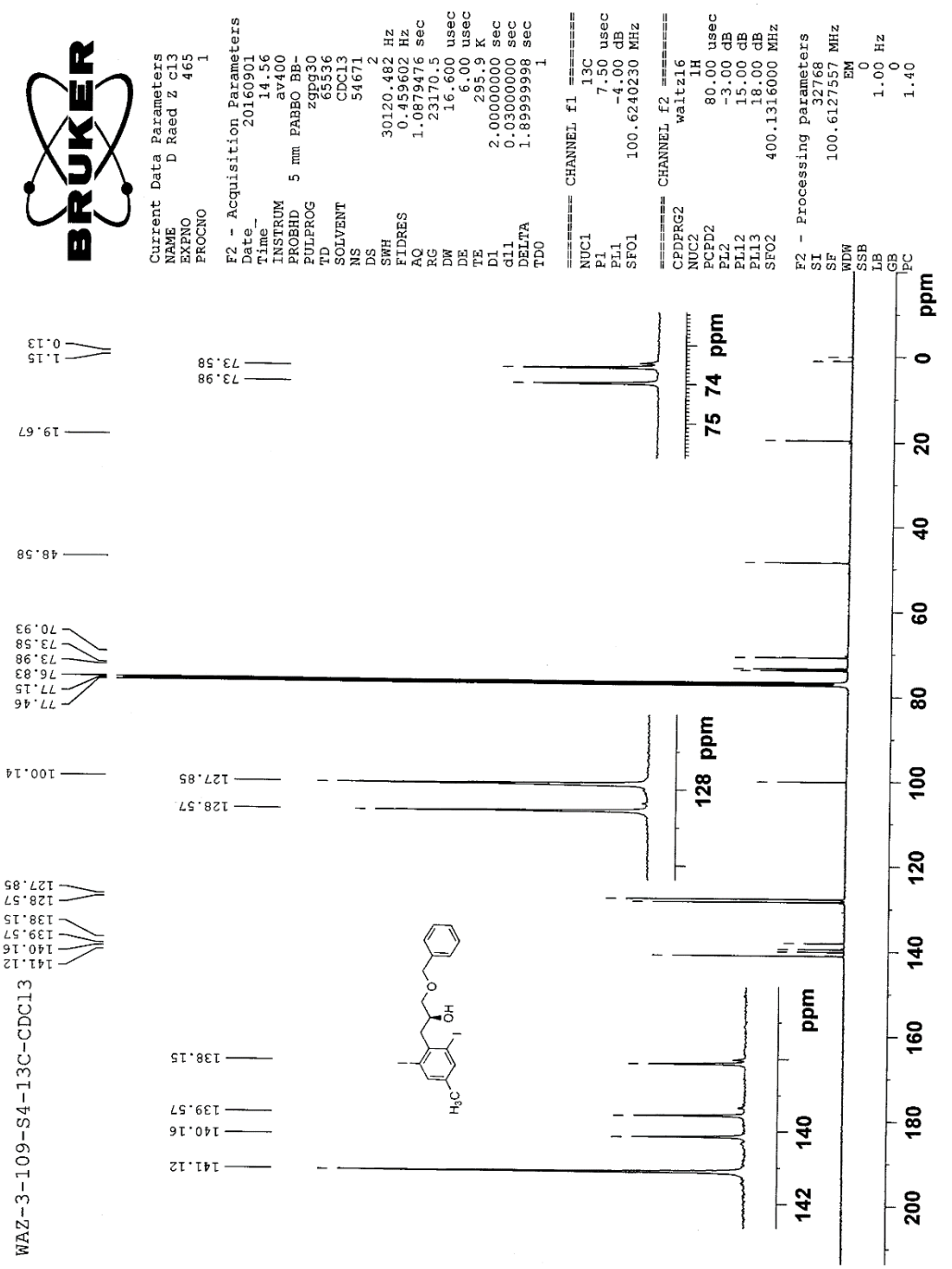
1.3.18 ^{13}C-NMR of 2-(2,6-diiodo-4-methylphenyl)-1-phenylethan-1-ol (7i) in d-$CDCl_3$ at 25 °C.



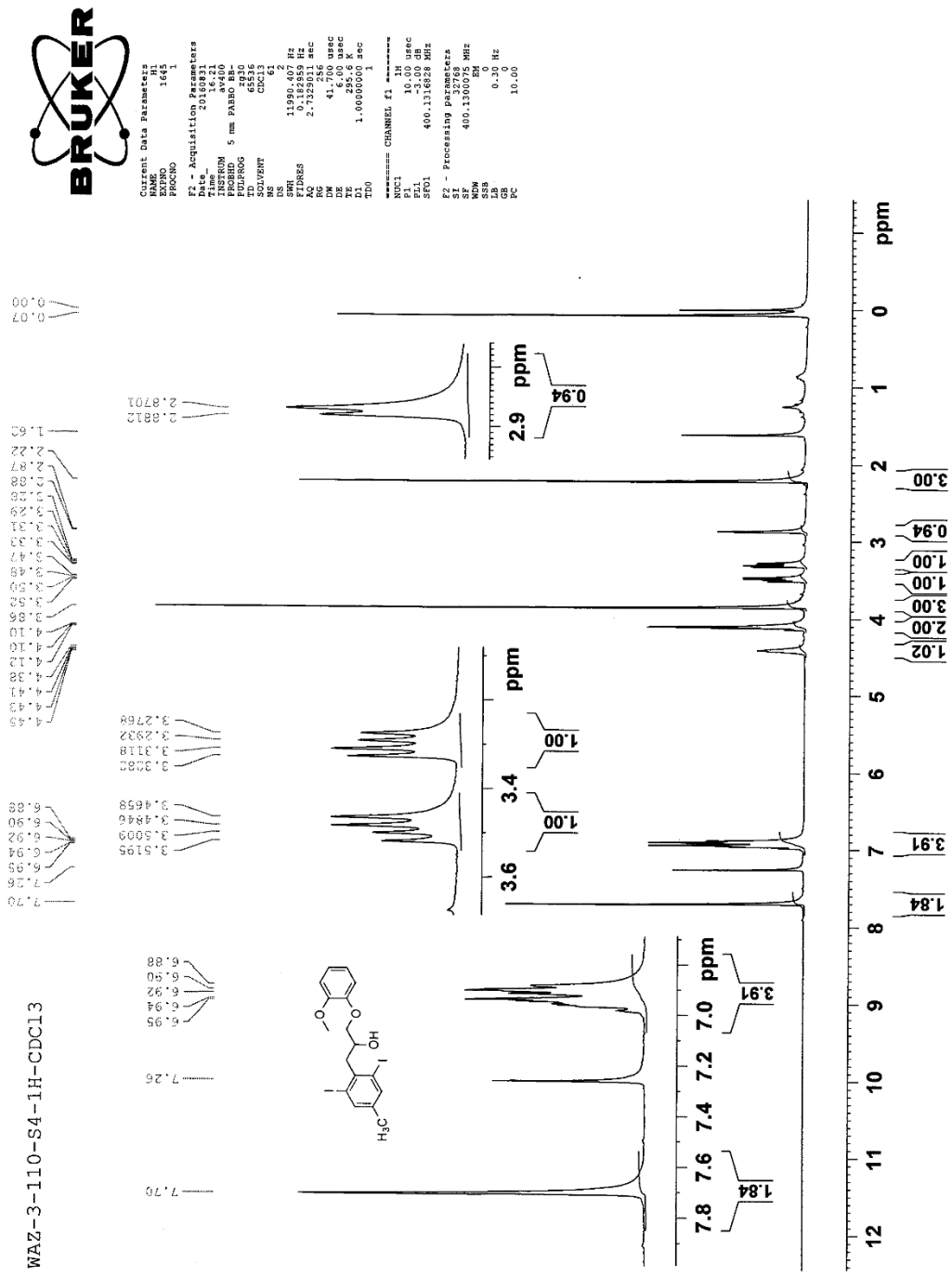
1.3.19 ^{1}H-NMR of (S)-1-(benzyloxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7j) in d-CDCl$_3$ at 25 °C.



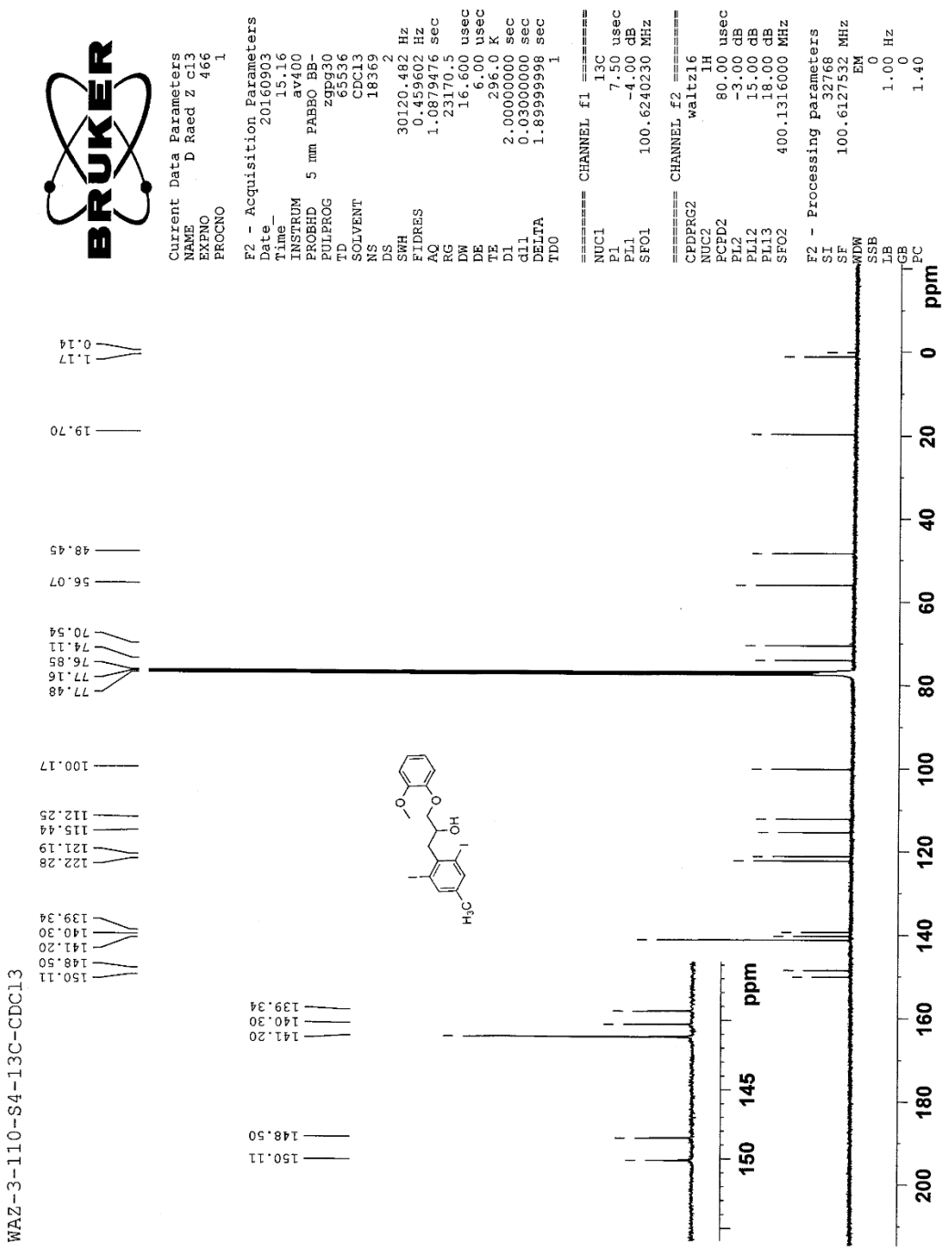
1.3.20 ^{13}C-NMR of (S)-1-(benzyloxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7j) in d-CDCl$_3$ at 25 °C.



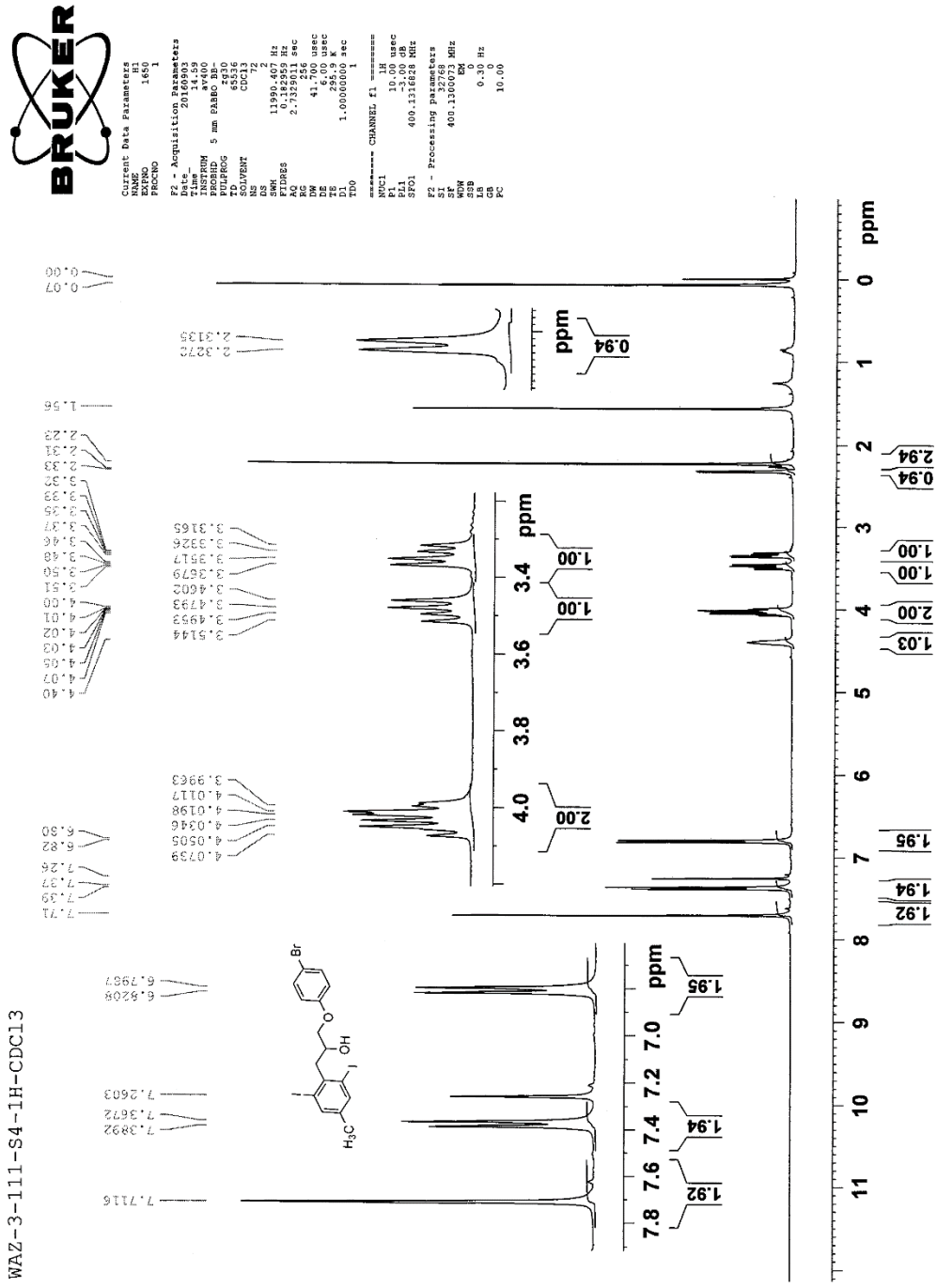
1.3.21 ^{1}H-NMR of 1-(2,6-diiodo-4-methylphenyl)-3-(2-methoxyphenoxy) propan-2-ol (7k) in d-CDCl$_3$ at 25 °C.



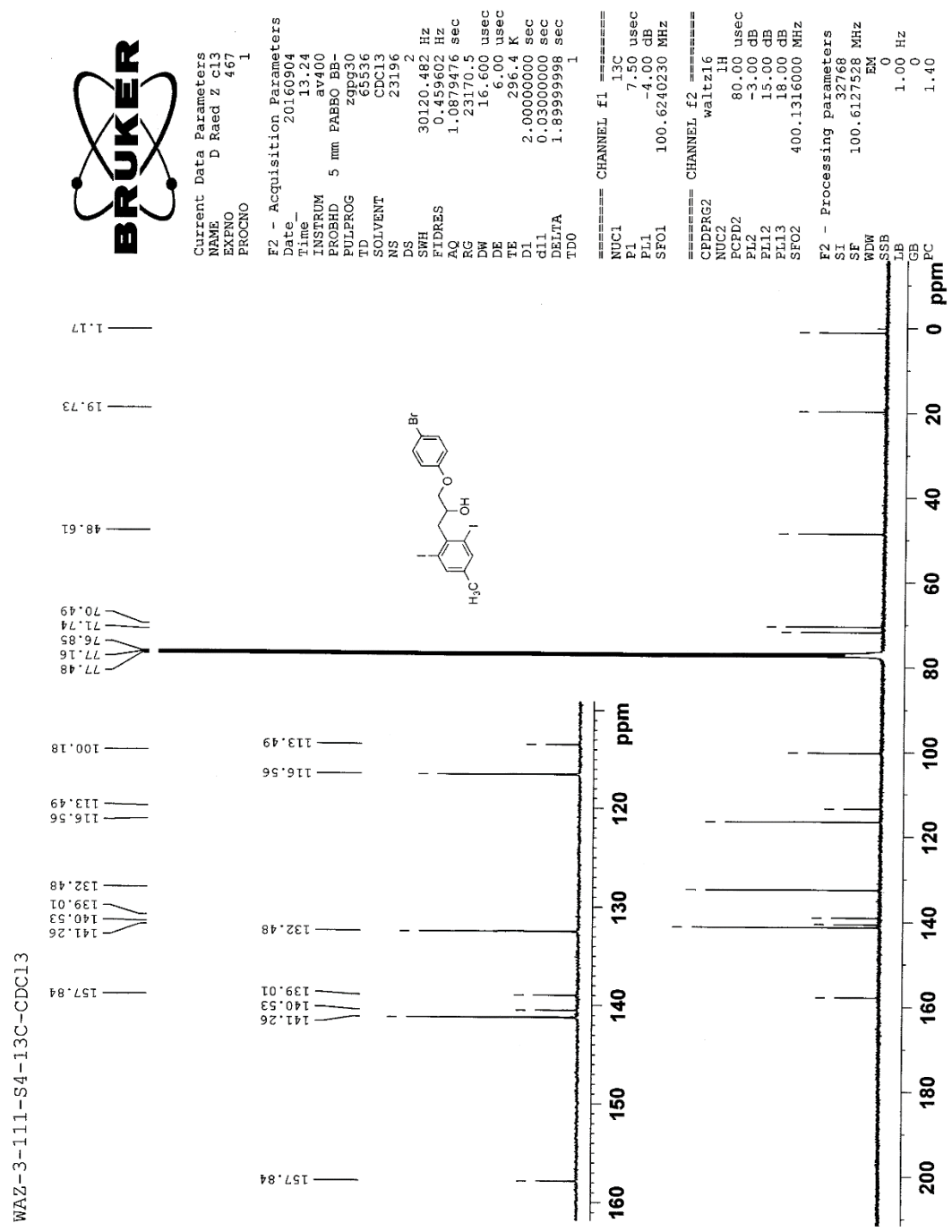
1.3.22 ^{13}C-NMR of 1-(2,6-diiodo-4-methylphenyl)-3-(2-methoxyphenoxy) propan-2-ol (7k) in d-CDCl$_3$ at 25 °C.



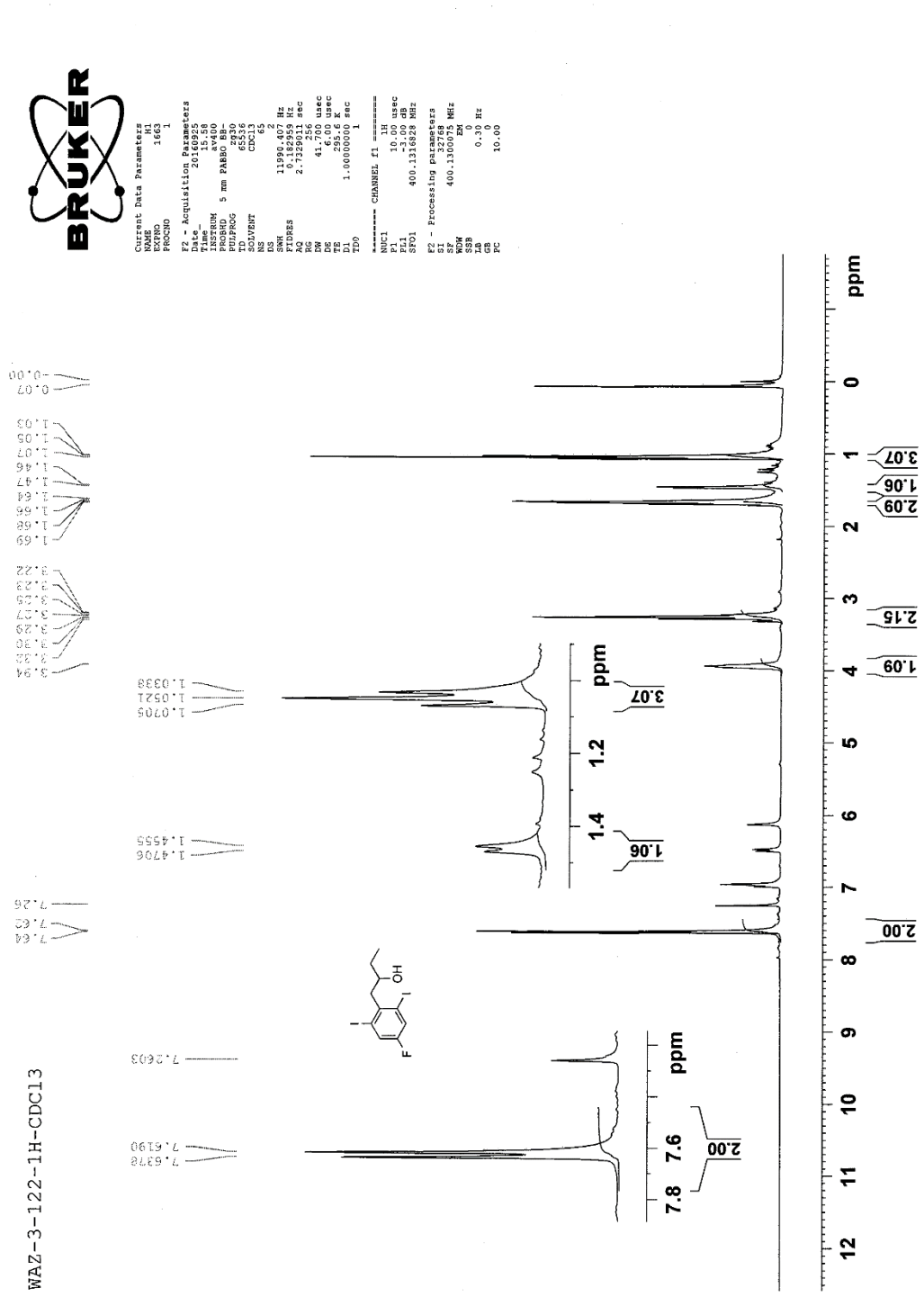
1.3.23 ^{1}H-NMR of 1-(4-bromophenoxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7l) in d-CDCl$_3$ at 25 °C.



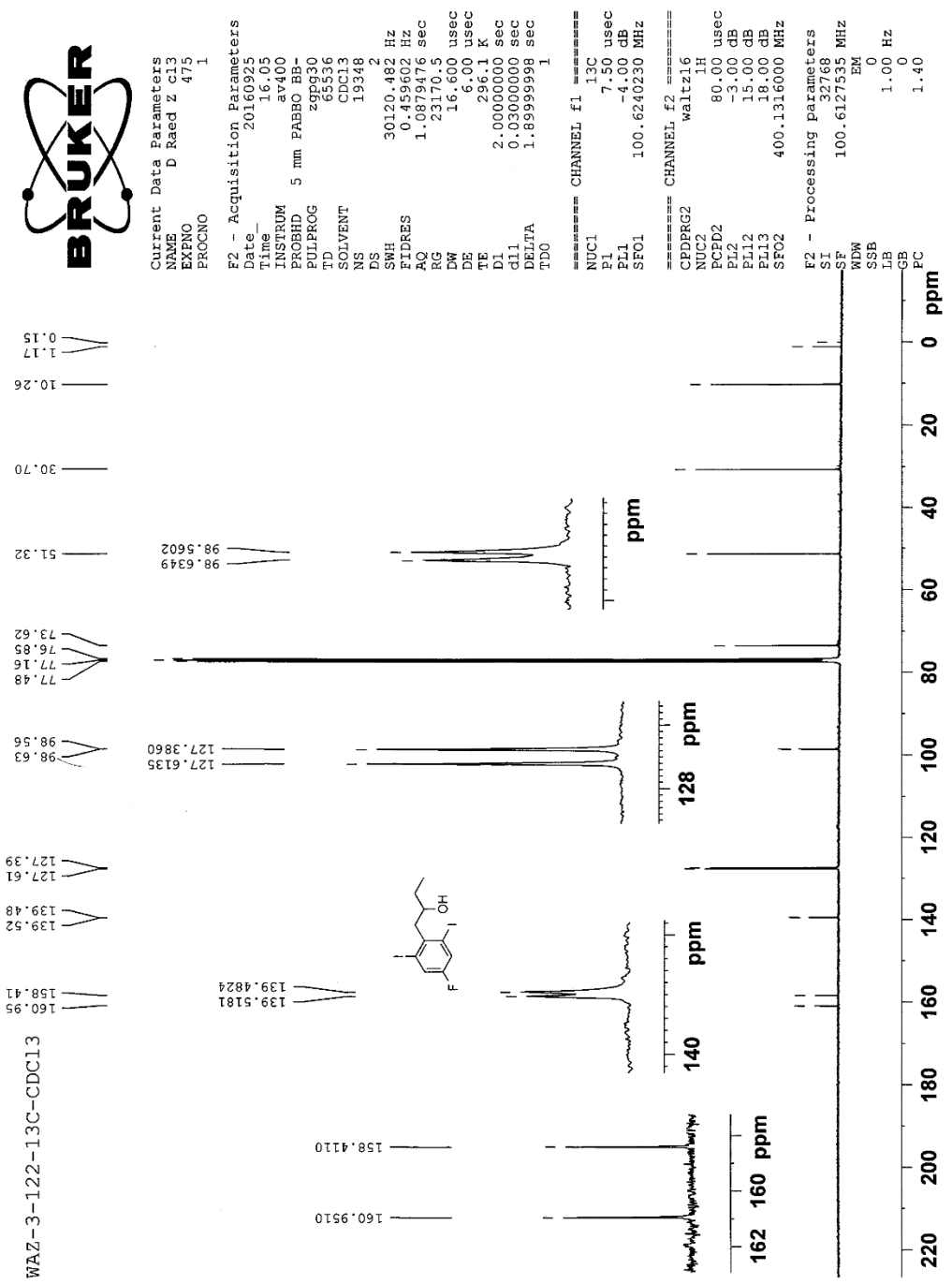
1.3.24 ^{13}C-NMR of 1-(4-bromophenoxy)-3-(2,6-diiodo-4-methylphenyl)propan-2-ol (7l) in d-CDCl$_3$ at 25 °C.



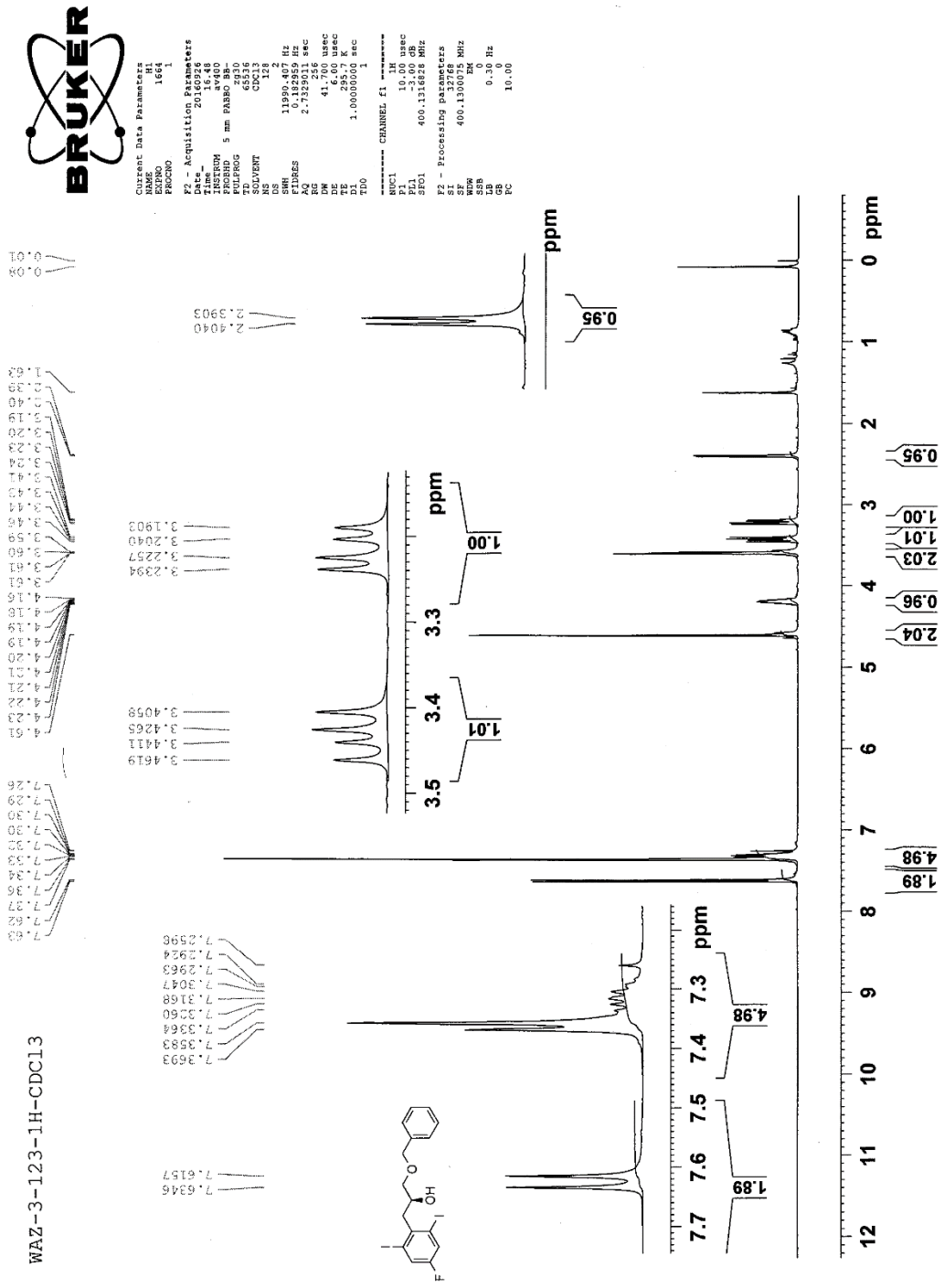
1.3.25 ^{1}H-NMR of 1-(4-fluoro-2,6-diiodophenyl)butan-2-ol (7m) in d-CDCl$_3$ at 25 °C.



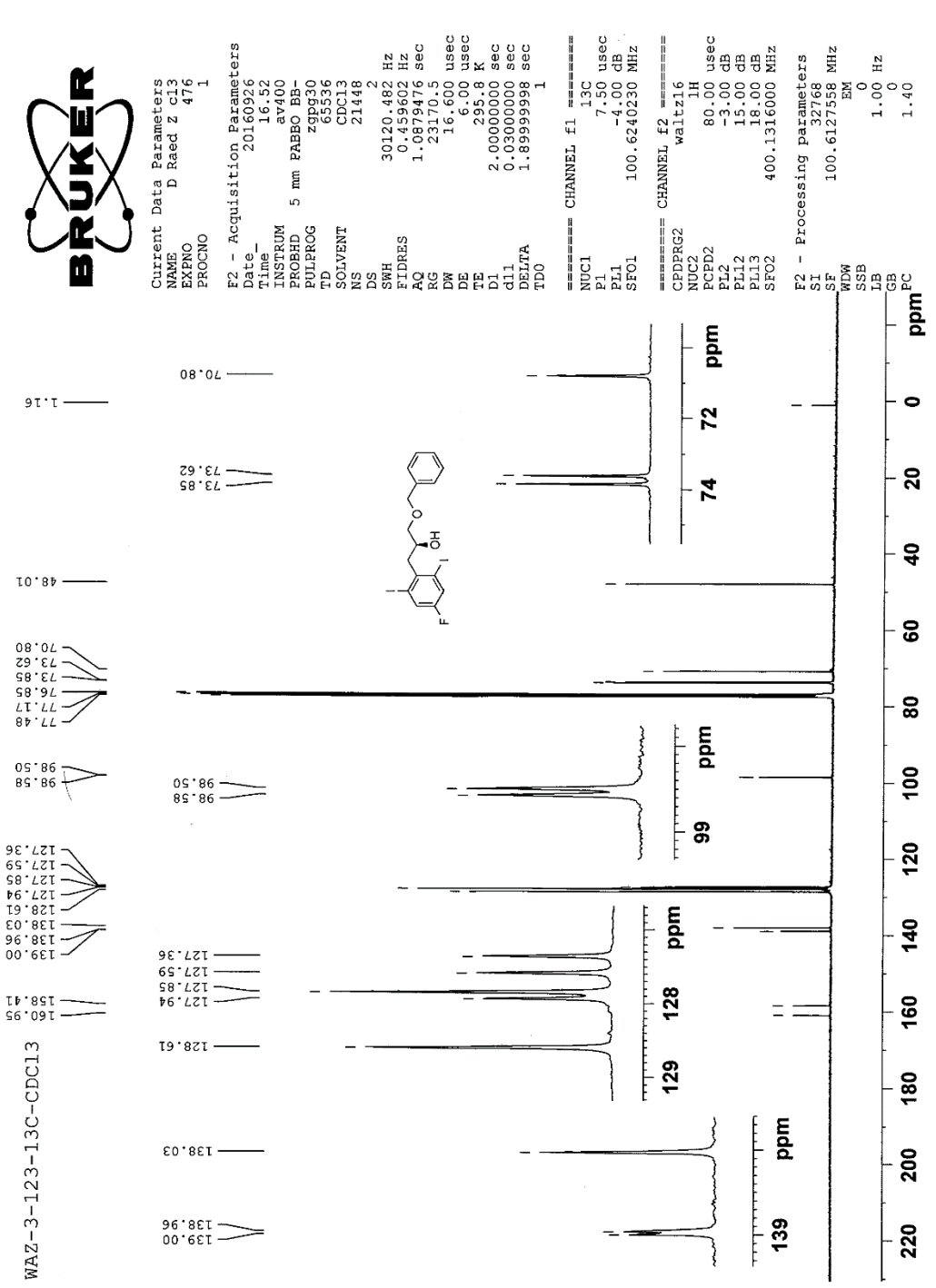
1.3.26 ^{13}C-NMR of 1-(4-fluoro-2,6-diiodophenyl)butan-2-ol (7m) in d-CDCl$_3$ at 25 °C.



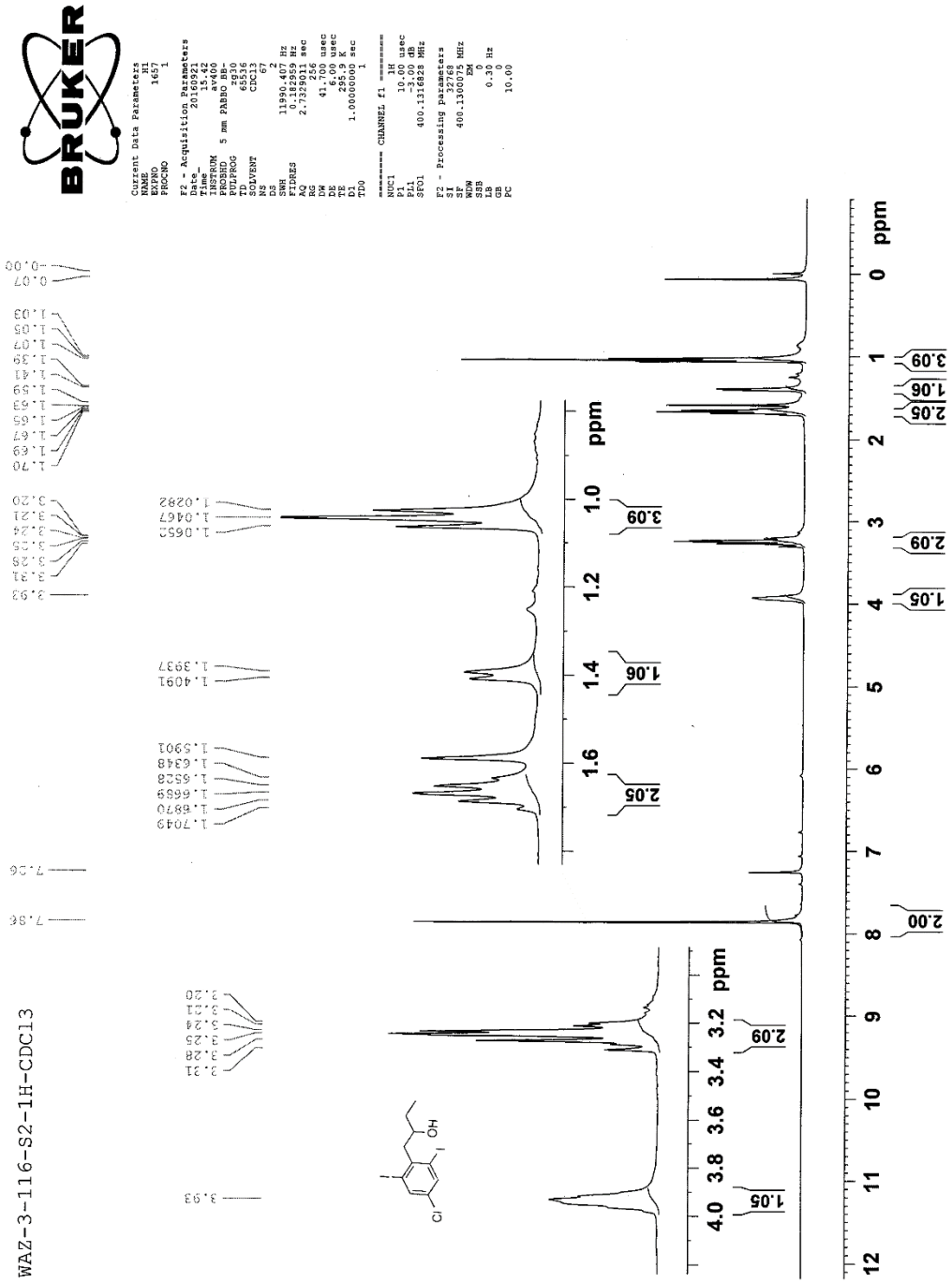
1.3.27 ^{1}H-NMR of (S)-1-(benzyloxy)-3-(4-fluoro-2,6-diiodophenyl)propan-2-ol (7n) in d-CDCl$_3$ at 25 °C.



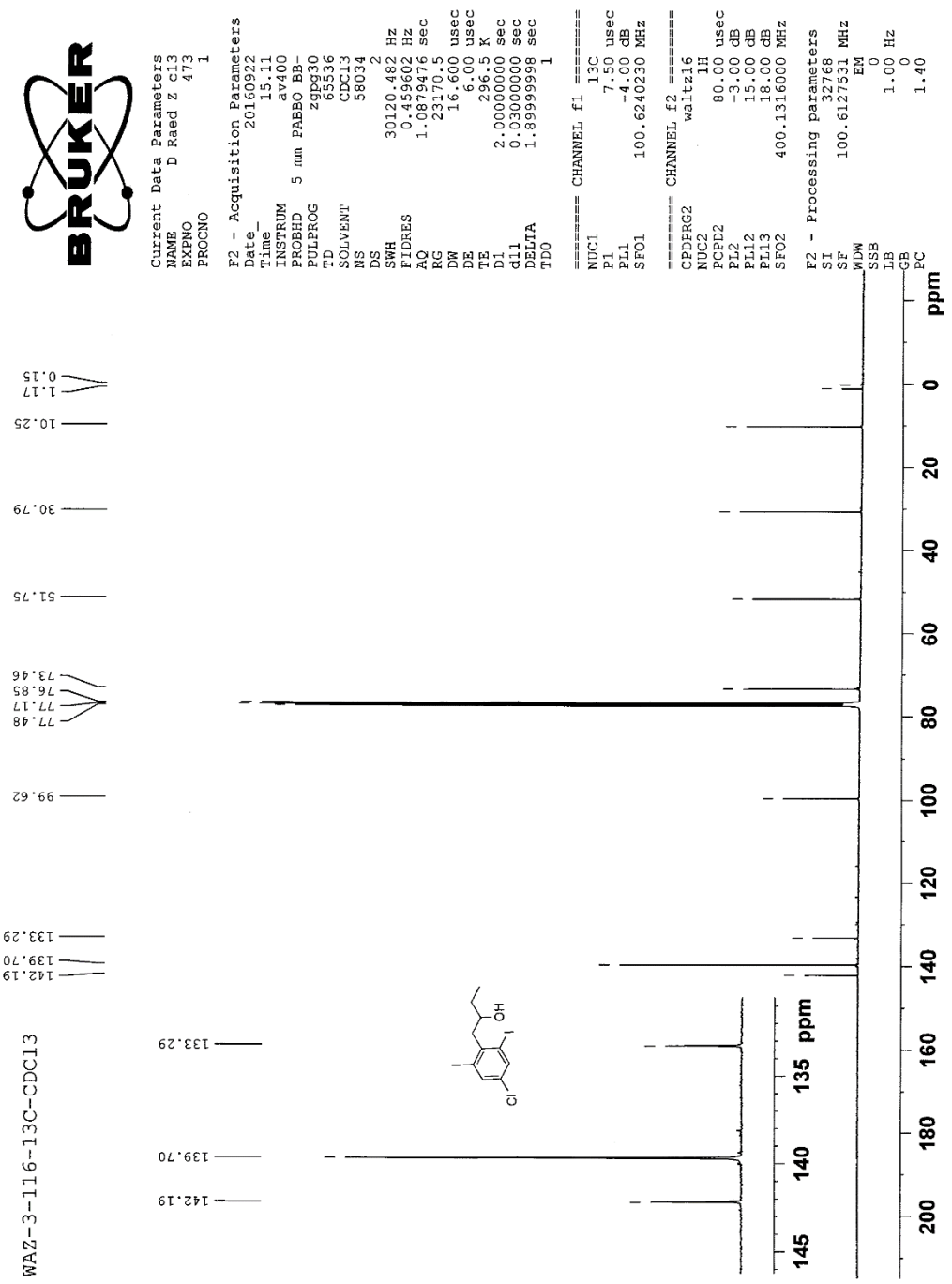
1.3.28 ^{13}C-NMR of (S)-1-(benzyloxy)-3-(4-fluoro-2,6-diiodophenyl)propan-2-ol (7n) in d-$CDCl_3$ at 25 °C.



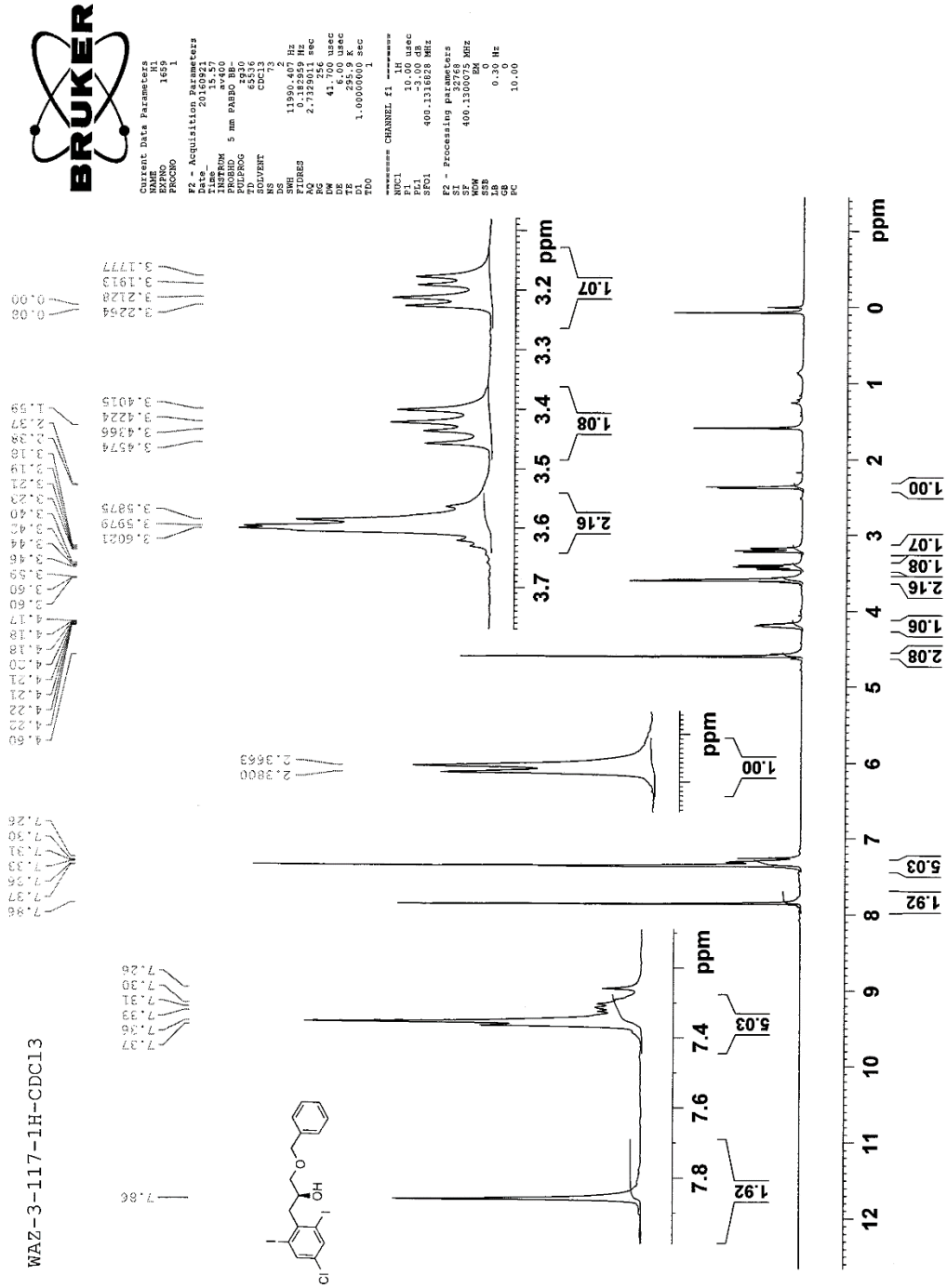
1.3.29 ^{1}H-NMR of 1-(4-chloro-2,6-diiodophenyl)butan-2-ol (7o) in d-CDCl$_3$ at 25 °C.



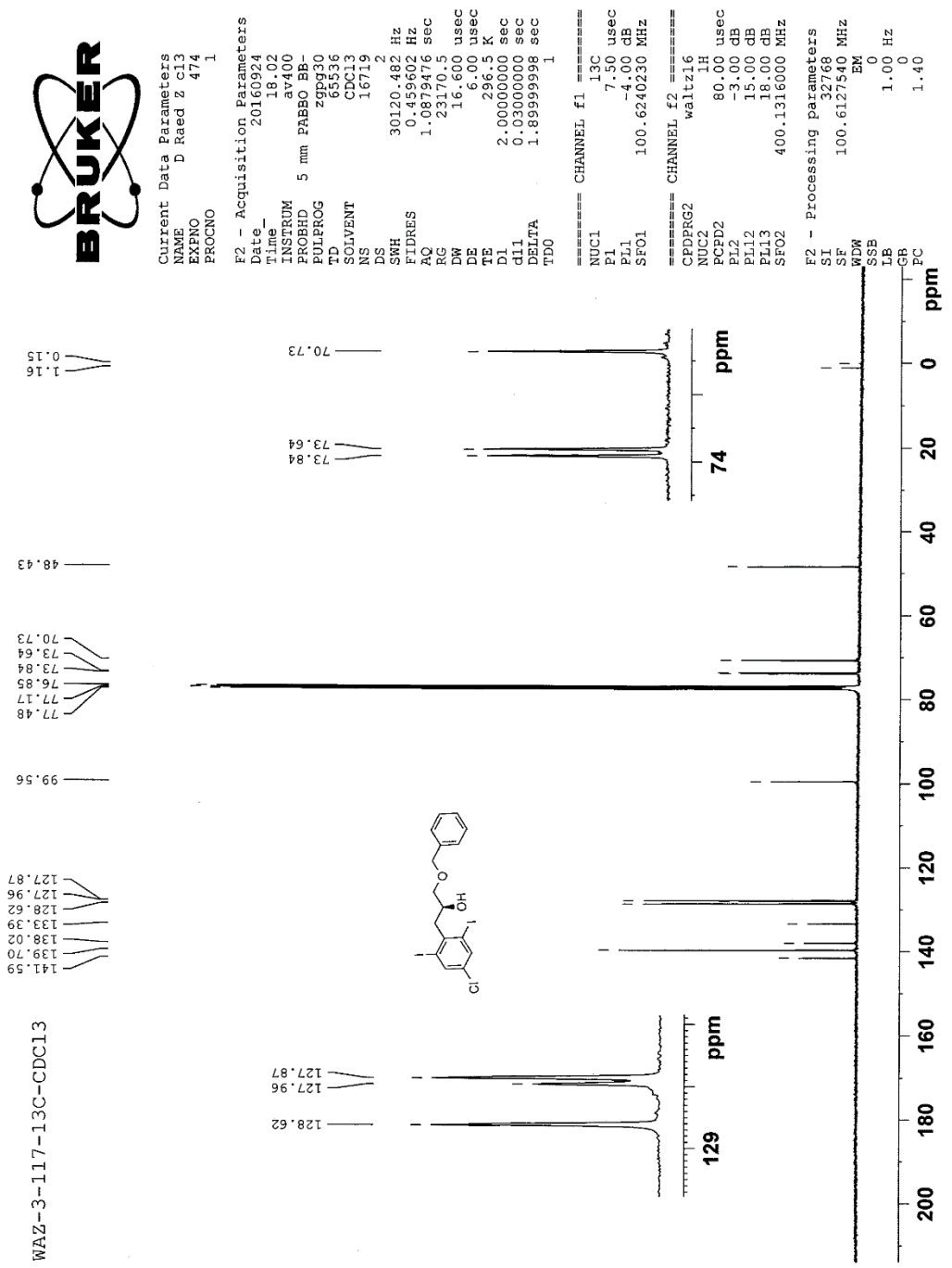
1.3.30 ^{13}C-NMR of 1-(4-chloro-2,6-diiodophenyl)butan-2-ol (7o) in d-CDCl$_3$ at 25 °C.



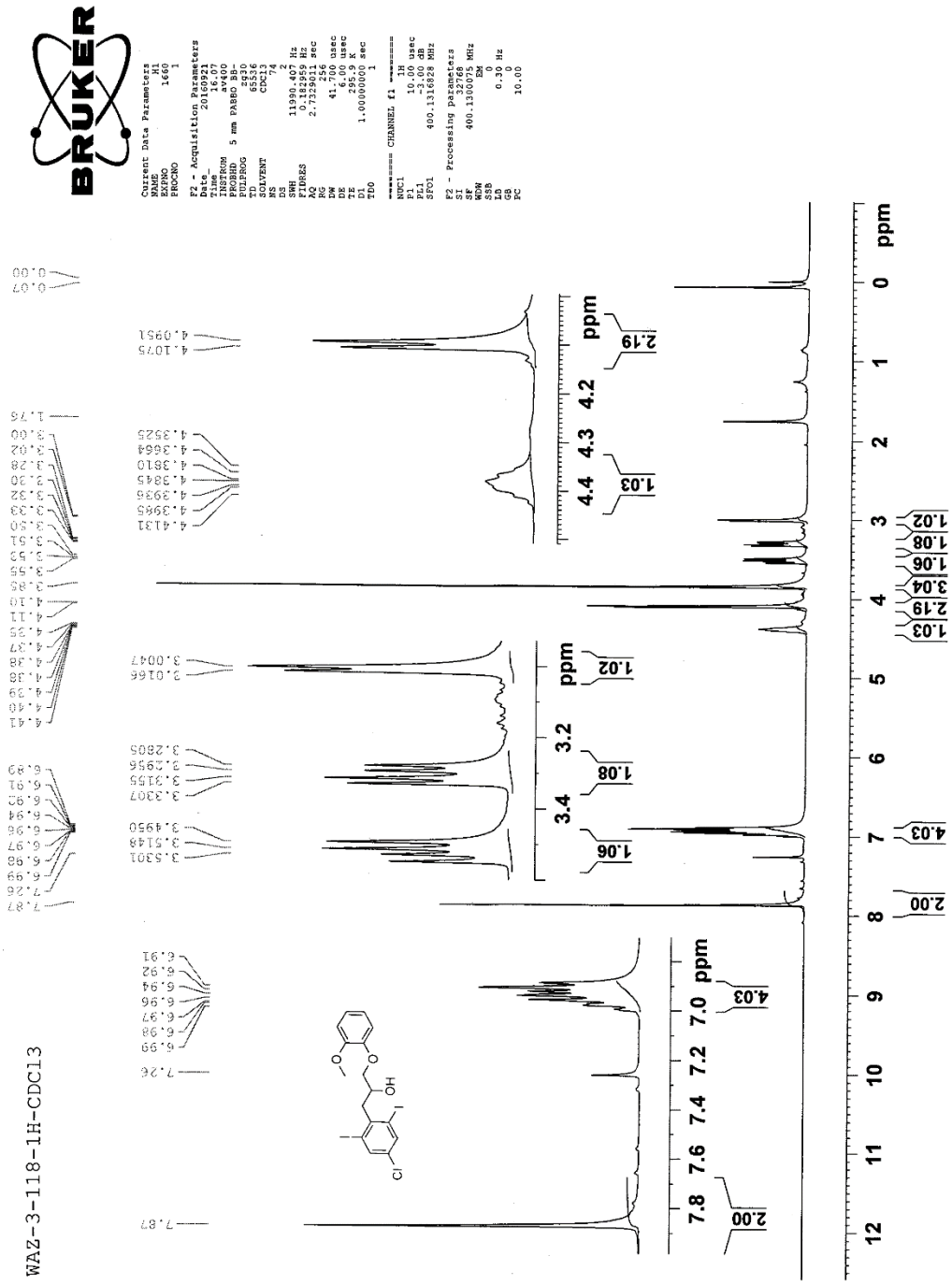
1.3.31 ^{1}H-NMR of (S)-1-(benzyloxy)-3-(4-chloro-2,6-diiodophenyl)propan-2-ol (7p) in d-CDCl$_3$ at 25 °C.



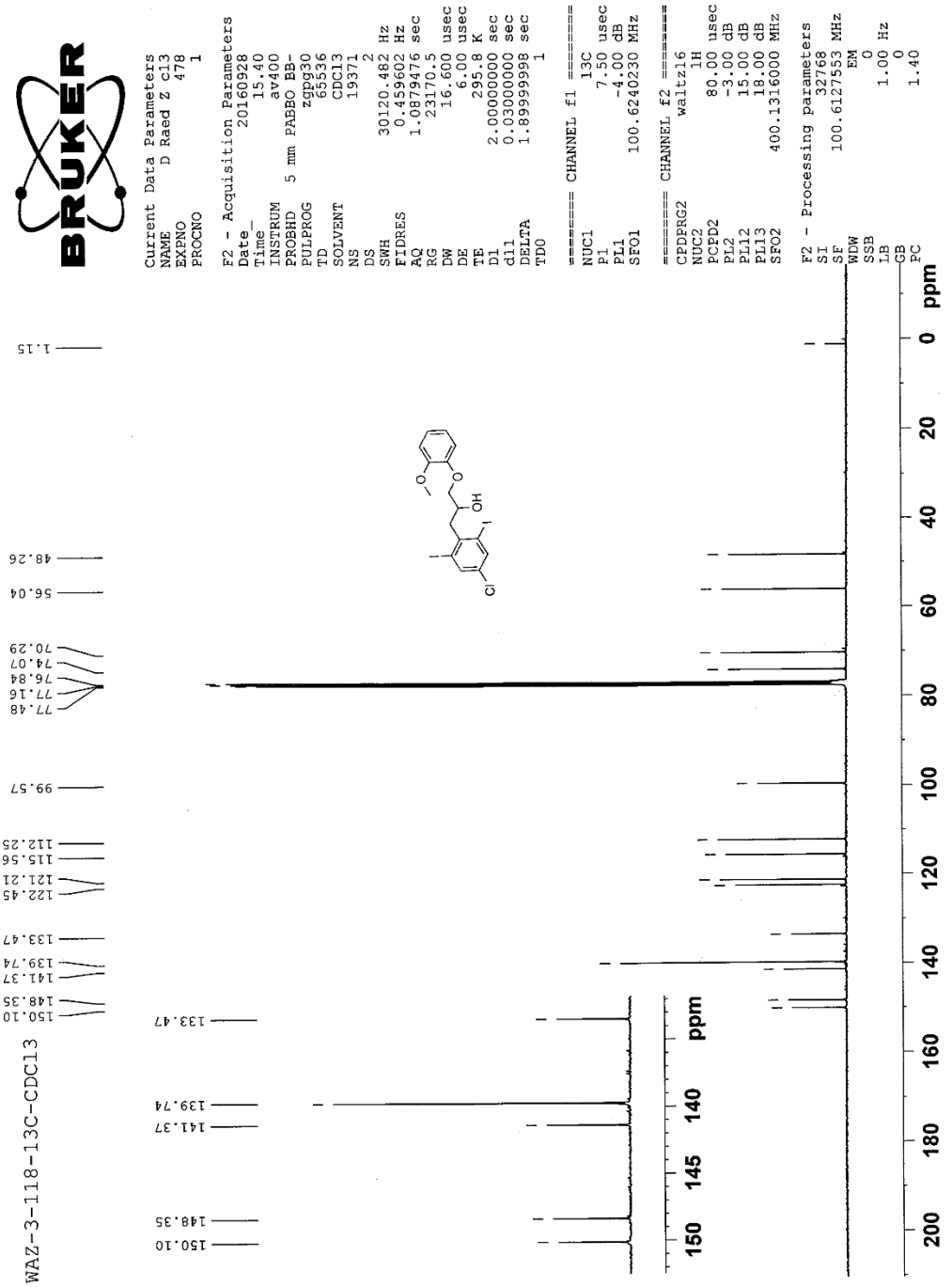
1.3.32 ^{13}C-NMR of (S)-1-(benzyloxy)-3-(4-chloro-2,6-diiodophenyl)propan-2-ol (7p) in d-$CDCl_3$ at 25 °C.



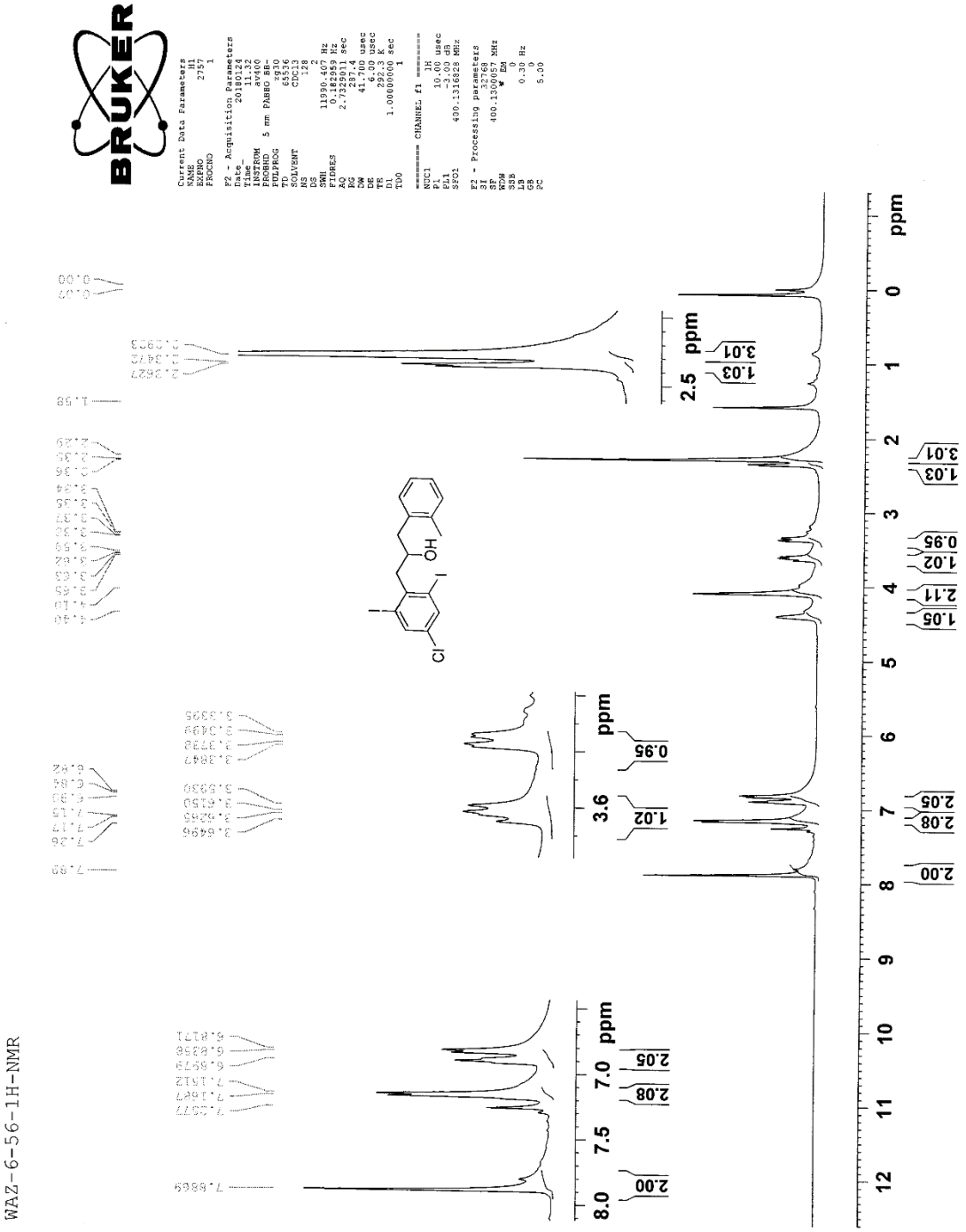
1.3.33 ^{1}H-NMR of 1-(4-chloro-2,6-diiodophenyl)-3-(2-methoxyphenoxy) propan-2-ol (7q) in d-CDCl$_3$ at 25 °C.



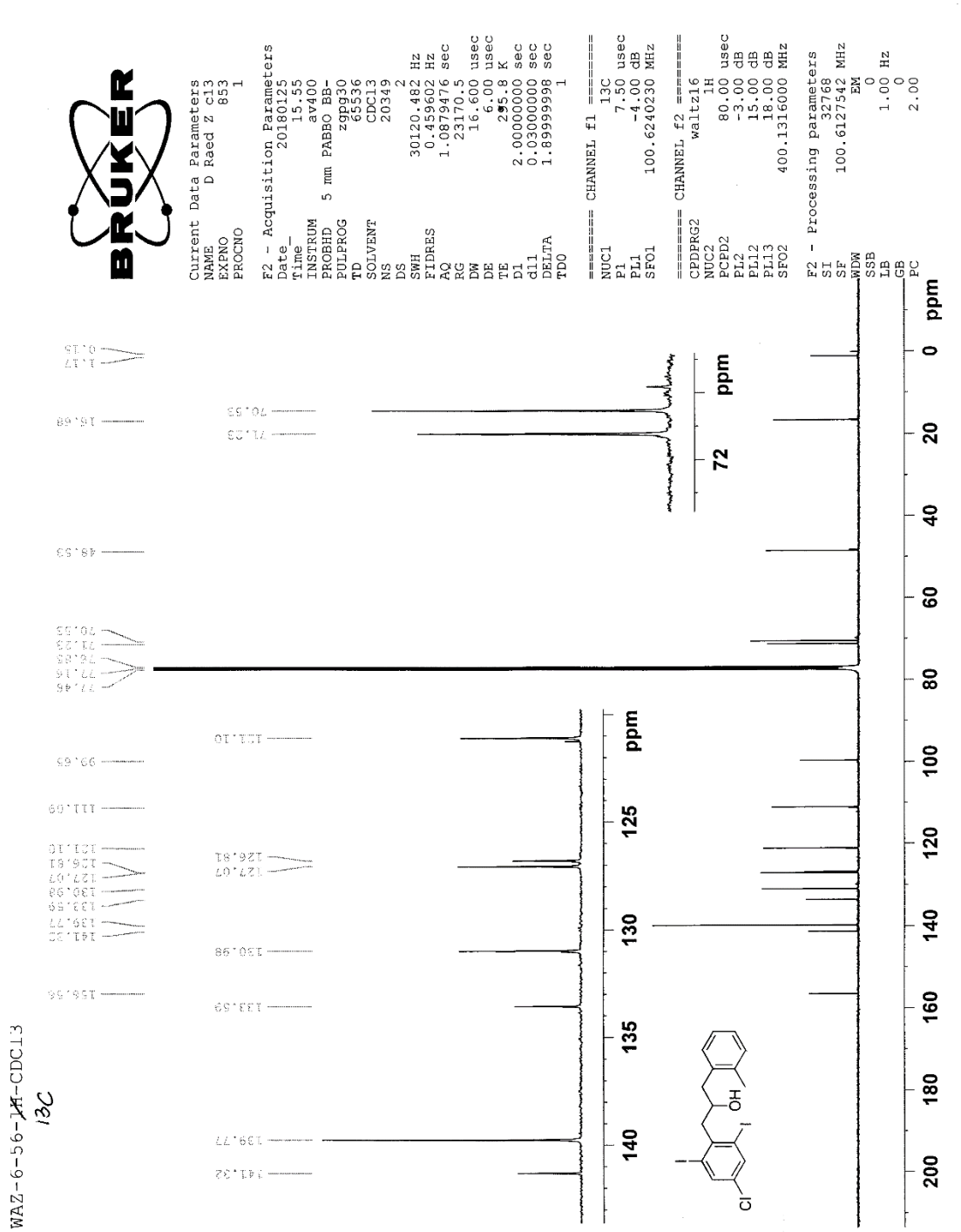
1.3.34 ^{13}C-NMR of 1-(4-chloro-2,6-diiodophenyl)-3-(2-methoxyphenoxy) propan-2-ol (7q) in d-CDCl$_3$ at 25 °C.



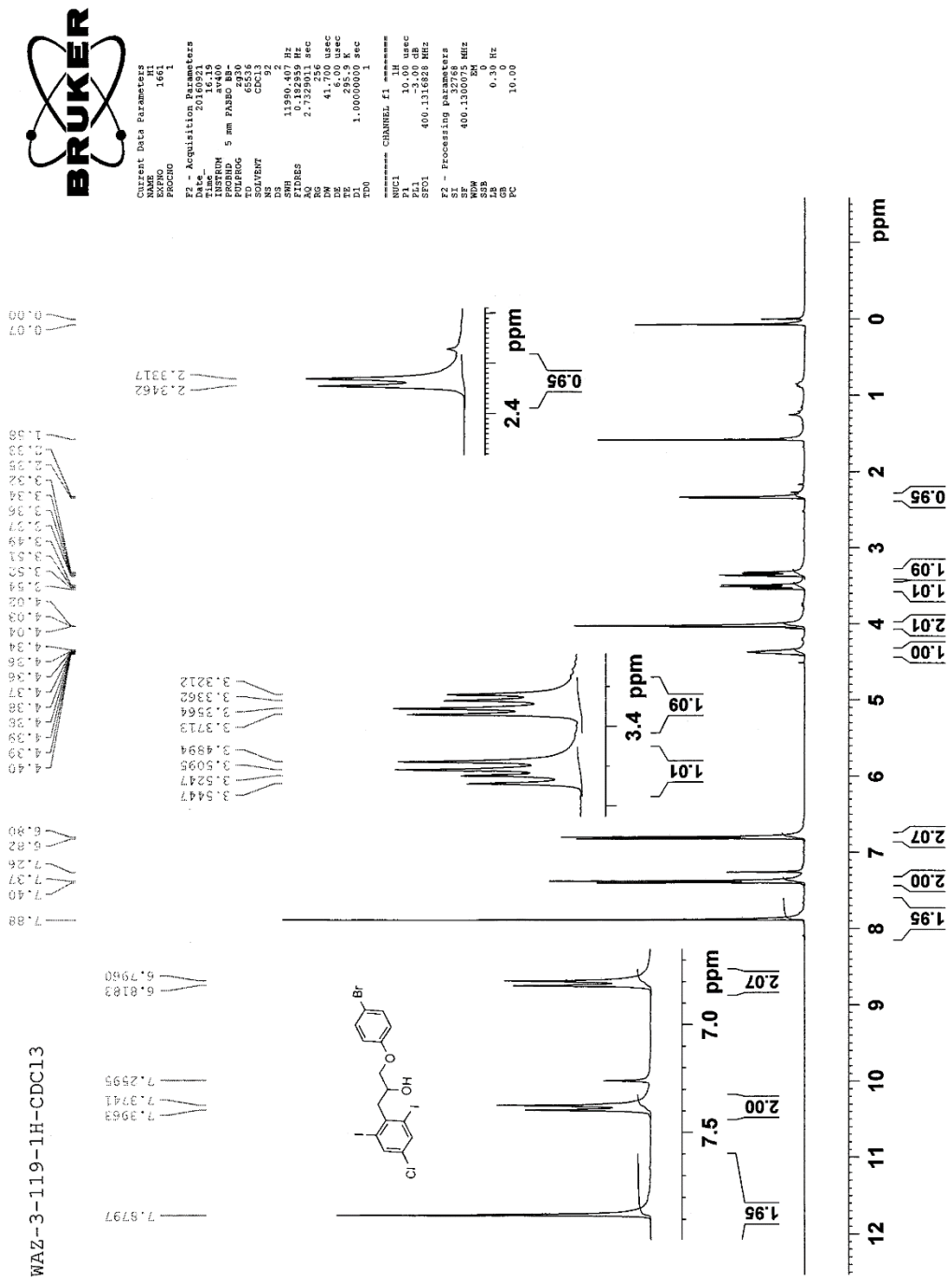
1.3.35 ^{1}H-NMR of 1-(4-chloro-2,6-diiodophenyl)-3-(o-tolyloxy)propan-2-ol (7r) in d-CDCl$_3$ at 25 °C.



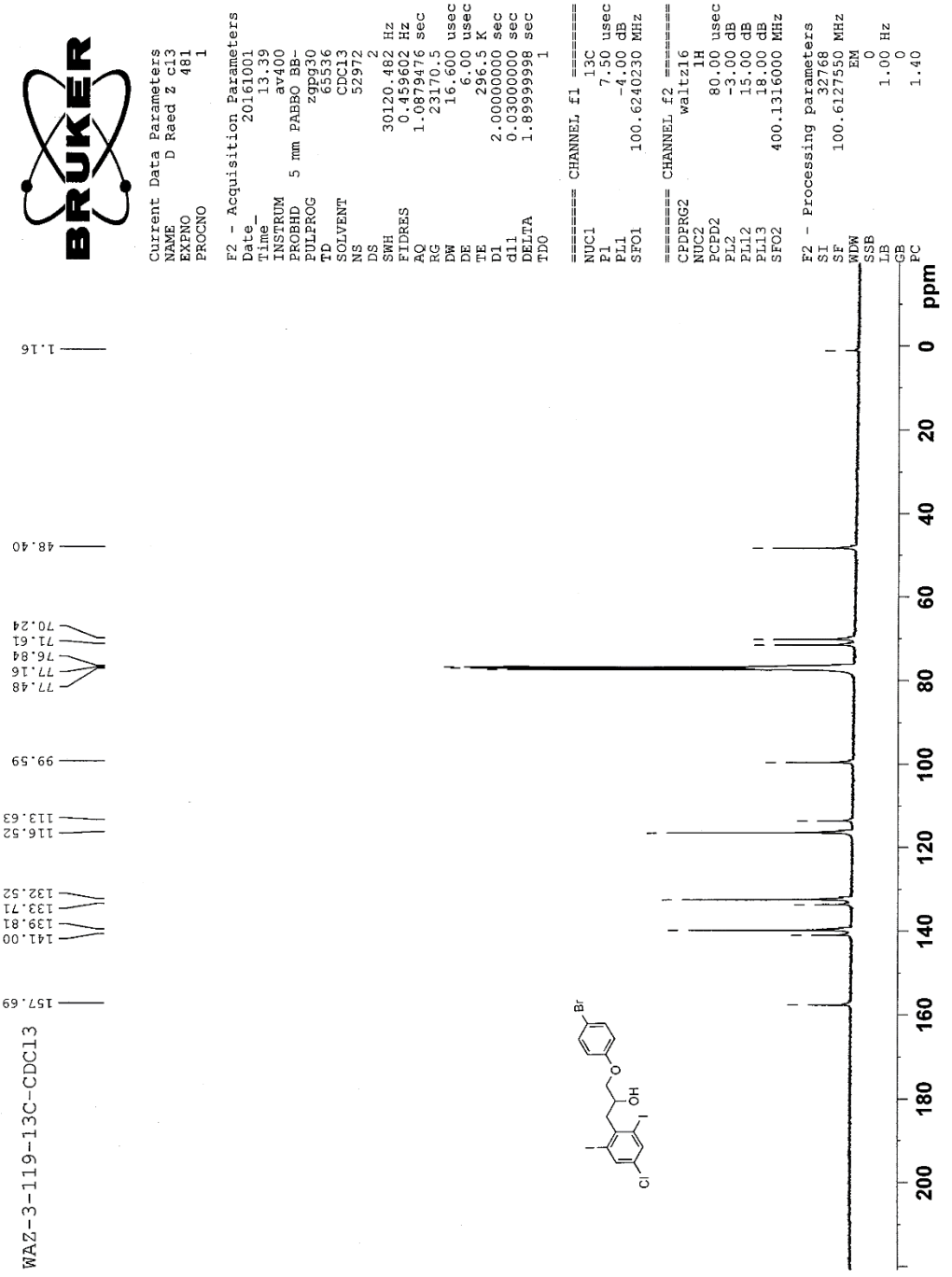
1.3.36 ^{13}C-NMR of 1-(4-chloro-2,6-diiodophenyl)-3-(o-tolyloxy)propan-2-ol (7r) in d-CDCl$_3$ at 25 °C.



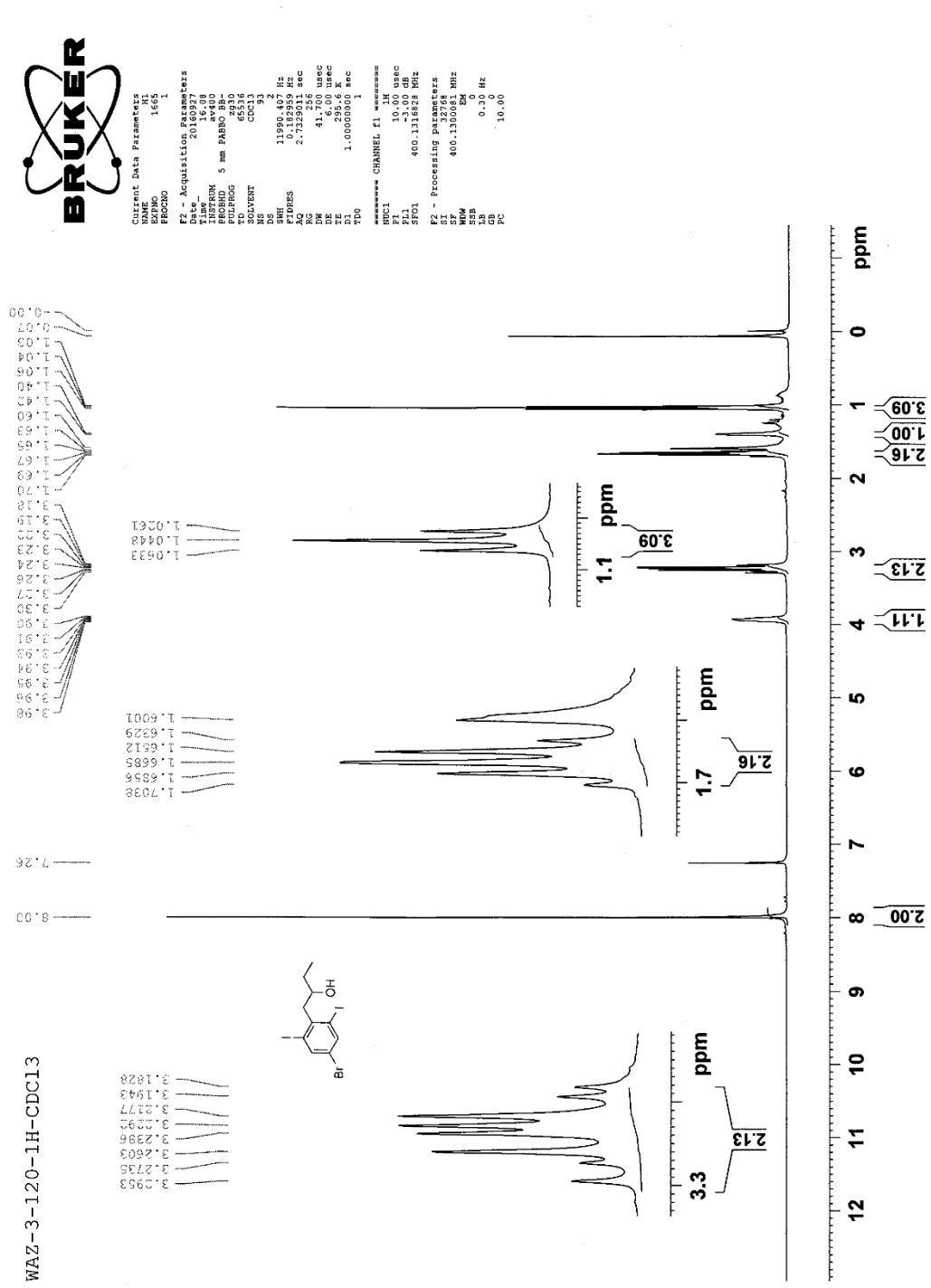
1.3.37 ^{1}H-NMR of 1-(4-bromophenoxy)-3-(4-chloro-2,6-diiodophenyl)propan-2-ol (7s) in d-CDCl$_3$ at 25 °C.



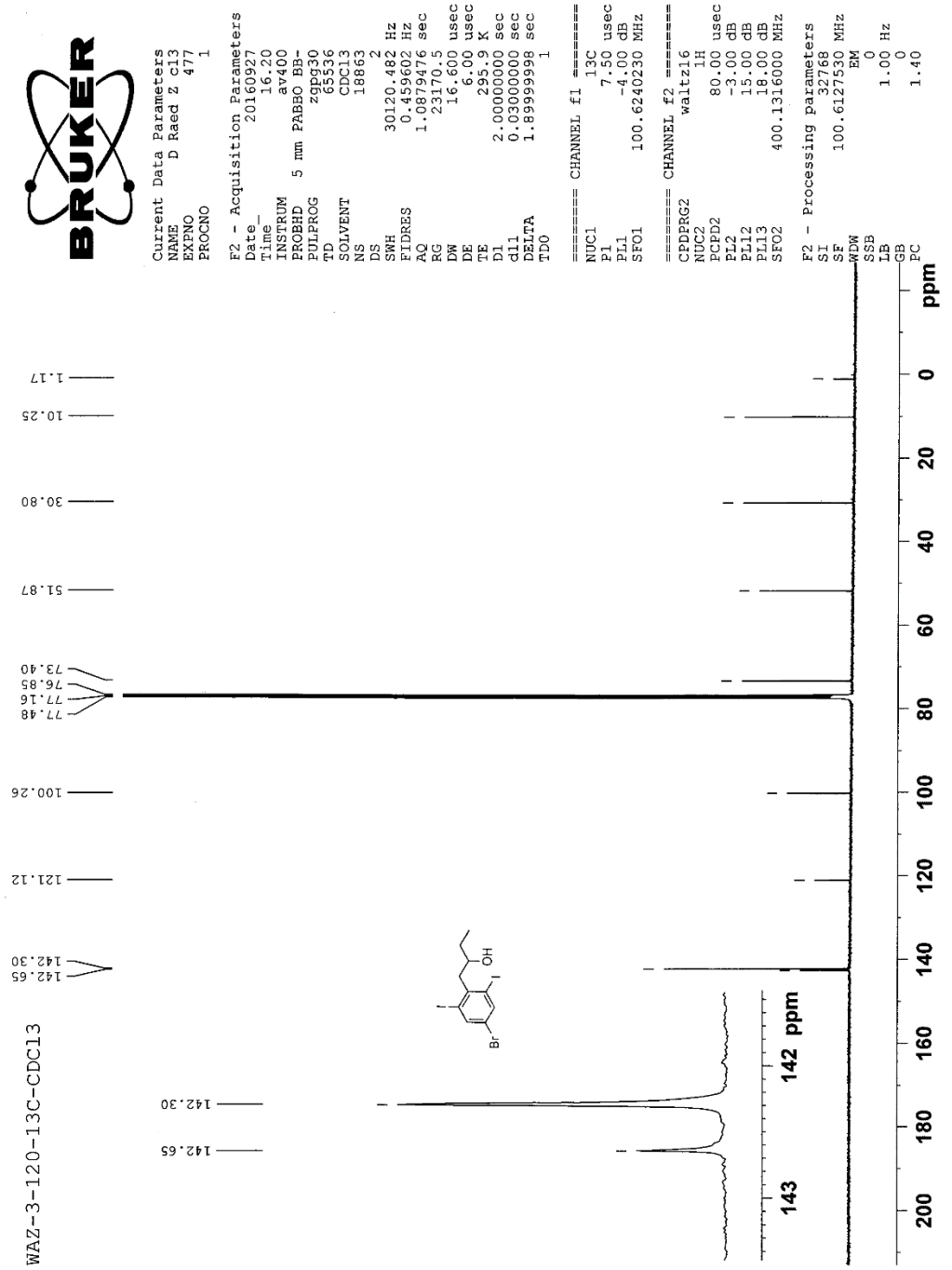
1.3.38 ^{13}C-NMR of 1-(4-bromophenoxy)-3-(4-chloro-2,6-diiodophenyl)propan-2-ol (7s) in d-CDCl$_3$ at 25 °C.



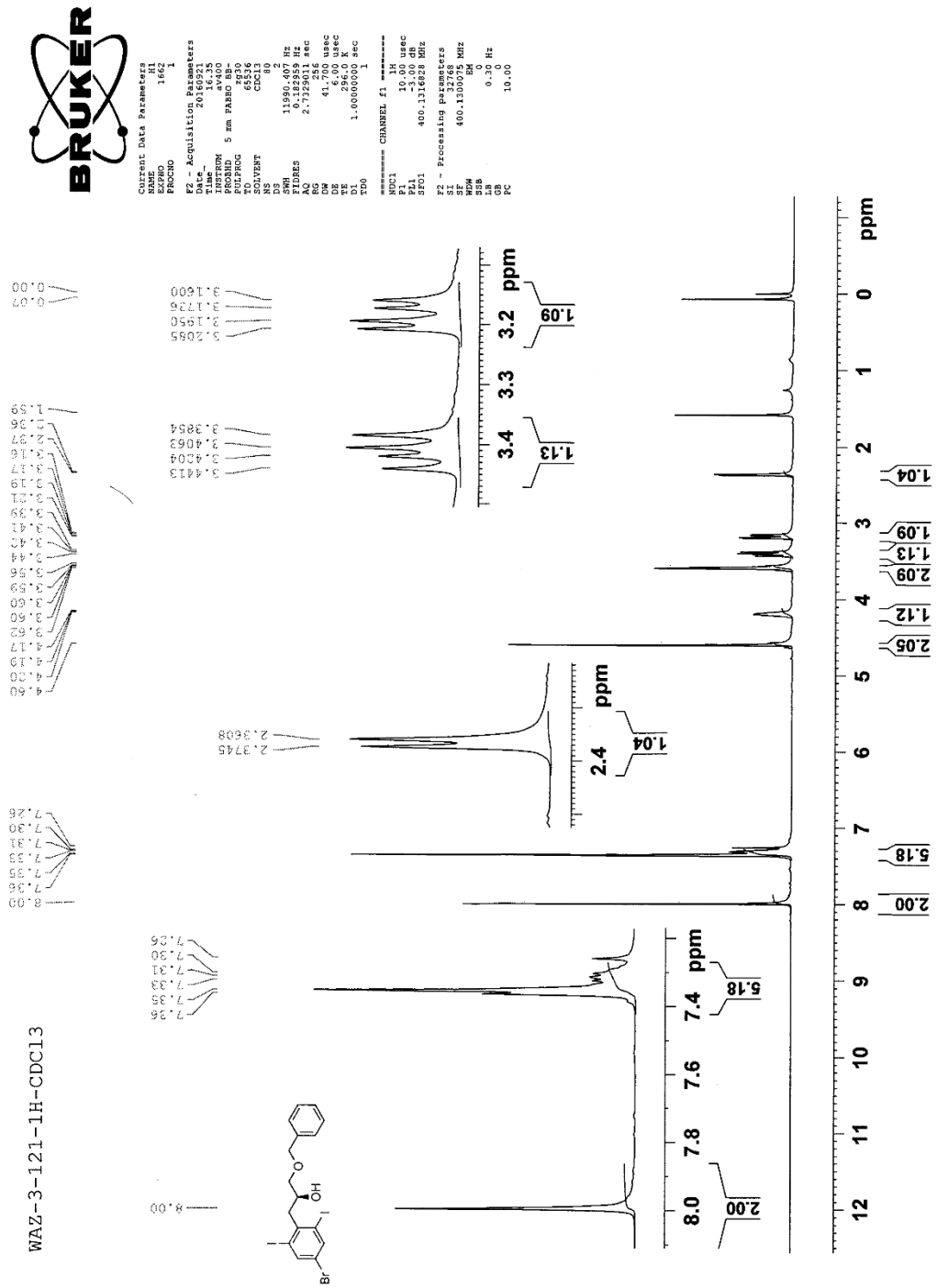
1.3.39 ^{1}H-NMR of 1-(4-bromo-2,6-diiodophenyl)butan-2-ol (7t) in d-CDCl$_3$ at 25 °C.



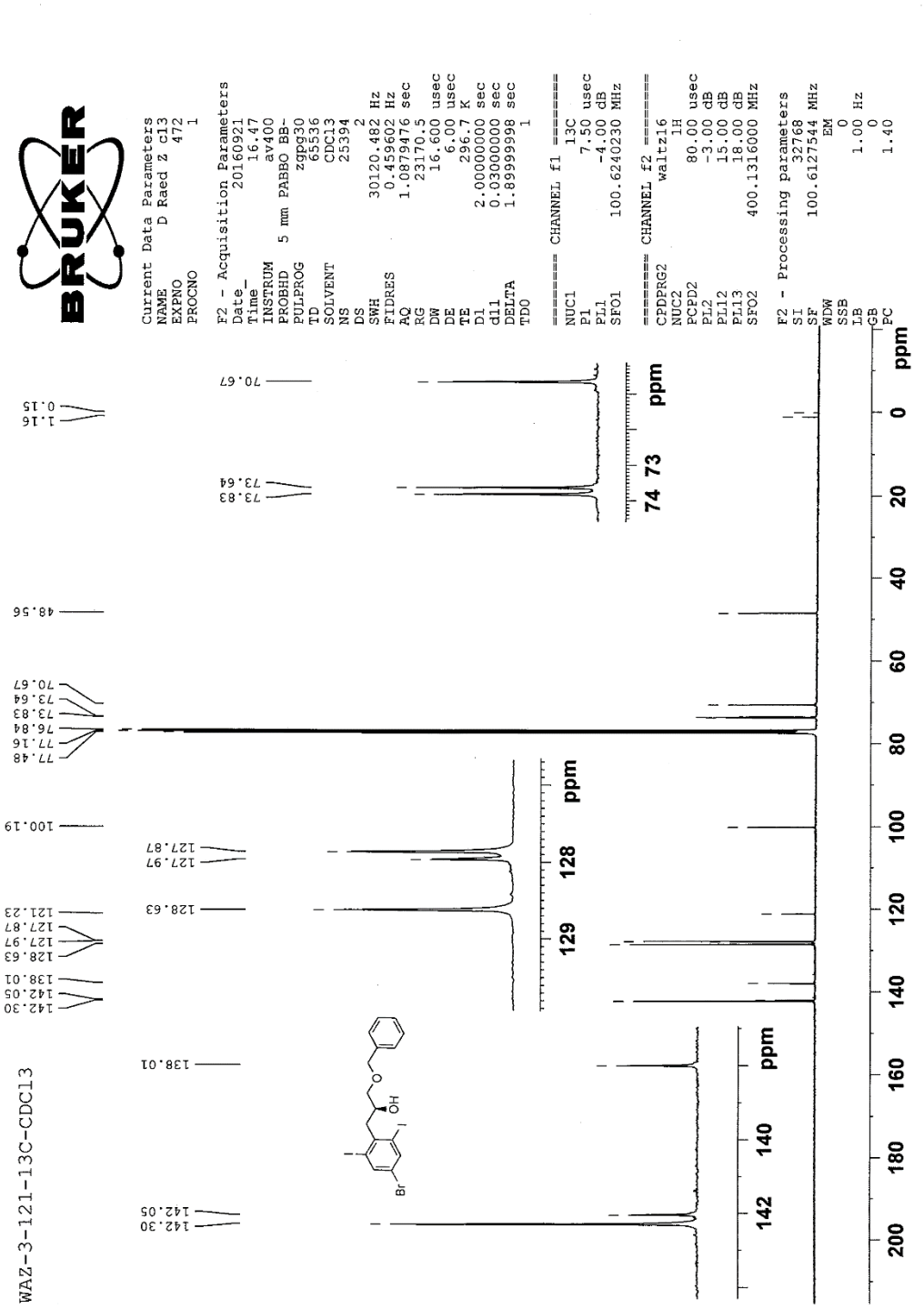
1.3.40 ^{13}C-NMR of 1-(4-bromo-2,6-diiodophenyl)butan-2-ol (7t) in d-CDCl$_3$ at 25 °C.



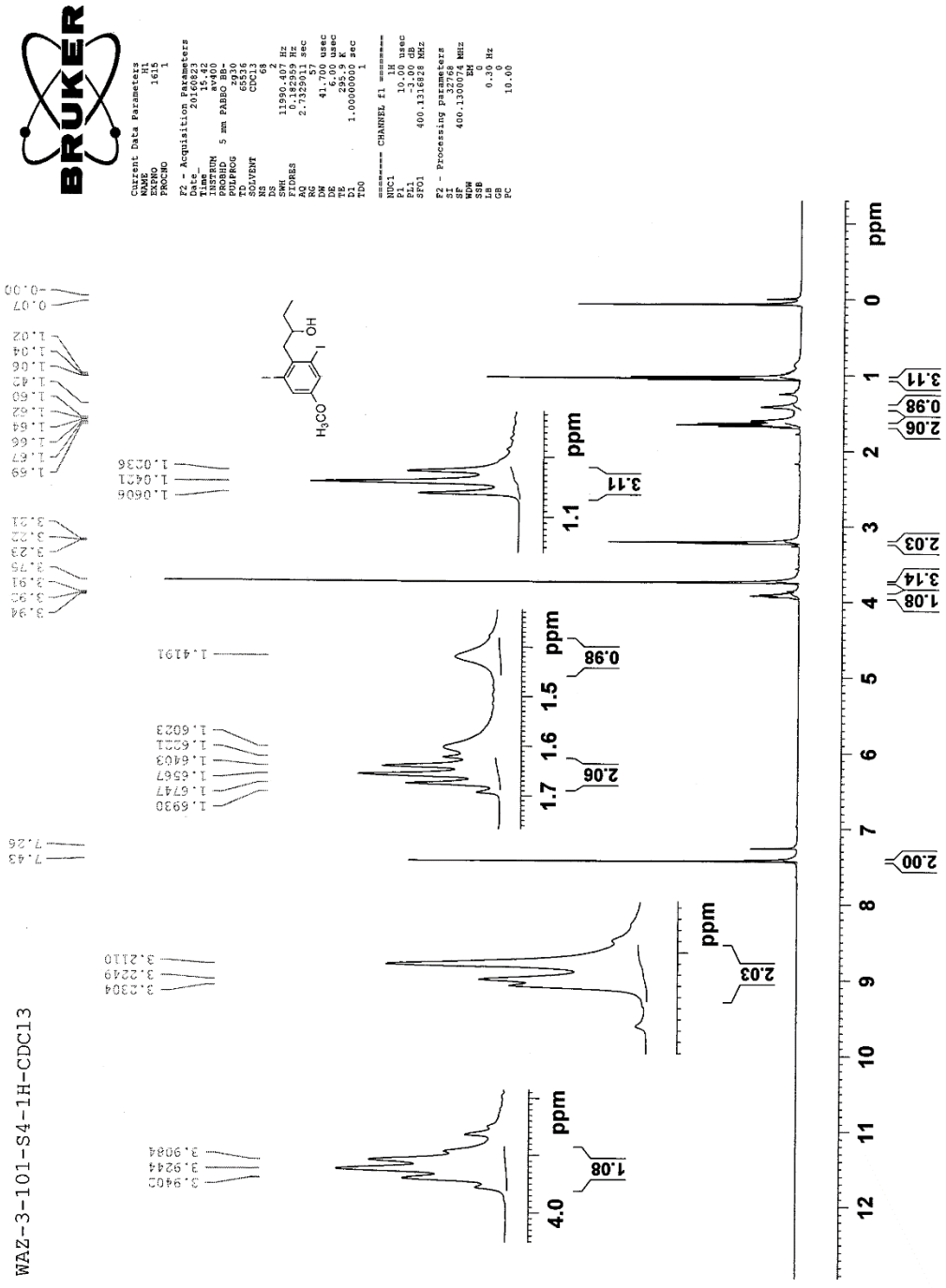
1.3.41 ^{1}H-NMR of (S)-1-(benzyloxy)-3-(4-bromo-2,6-diiodophenyl)propan-2-ol (7u) in d-$CDCl_3$ at 25 °C.



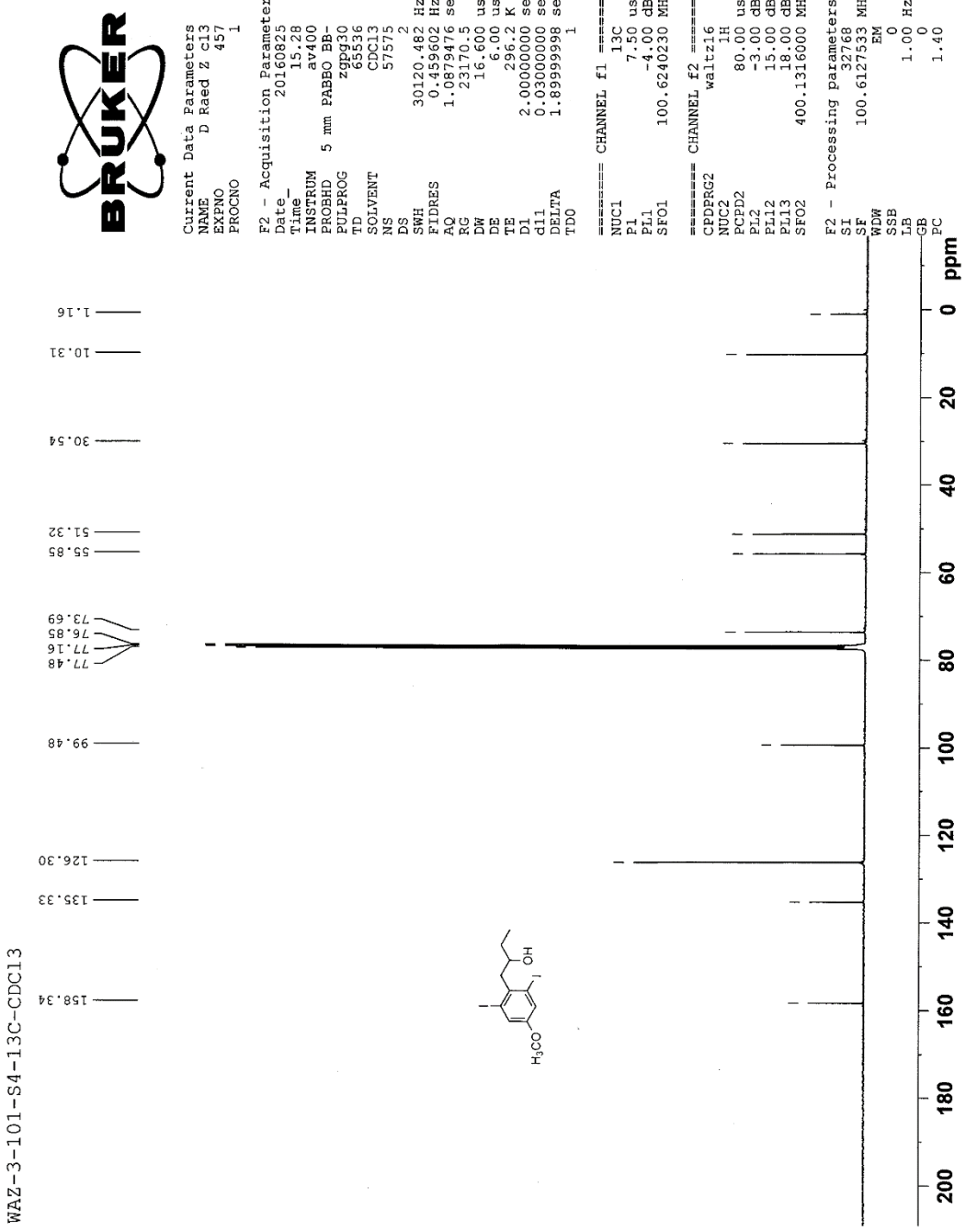
1.3.42 ^{13}C-NMR of (S)-1-(benzyloxy)-3-(4-bromo-2,6-diiodophenyl)propan-2-ol (7u) in d-$CDCl_3$ at 25 °C.



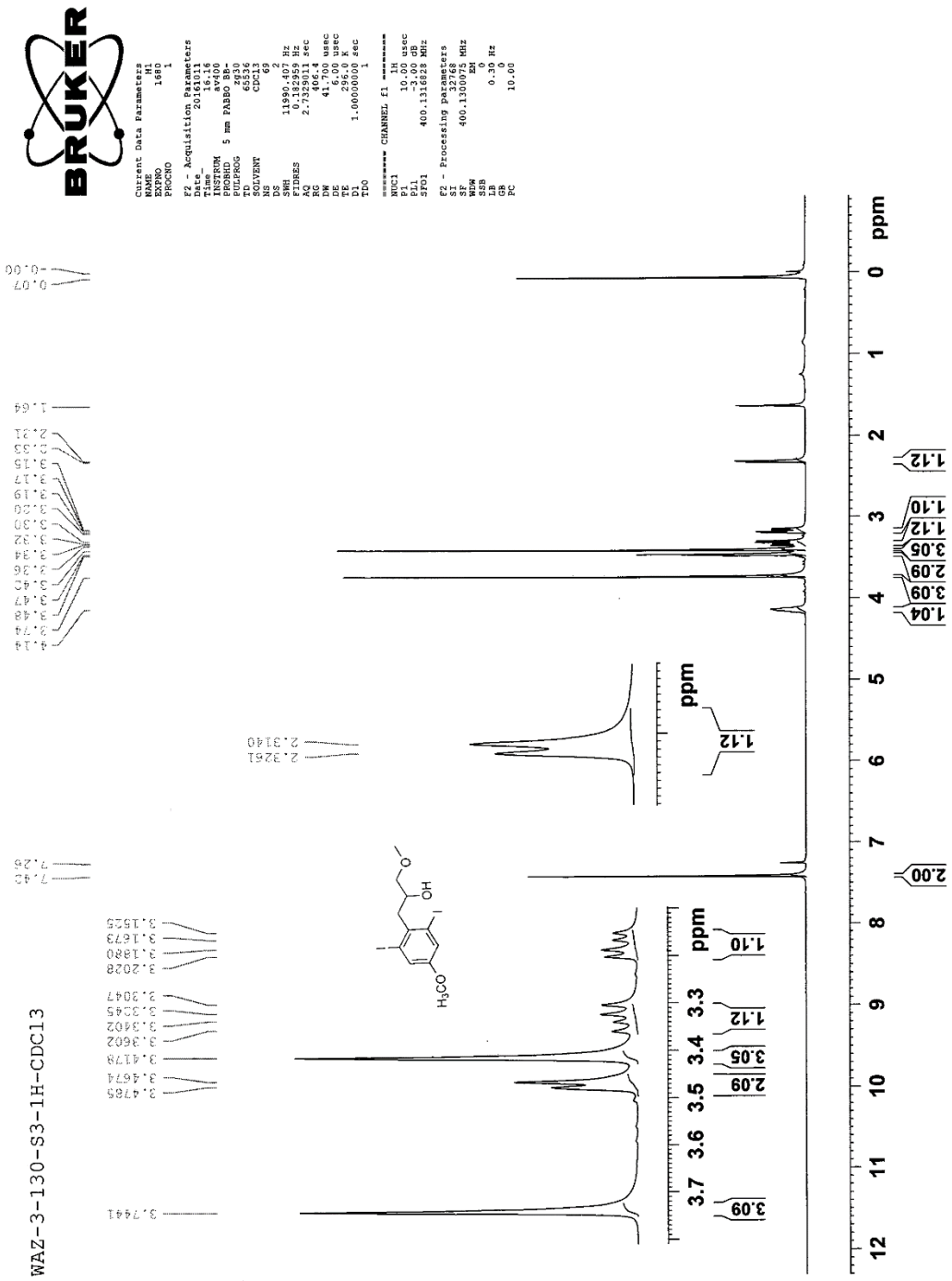
1.3.43 ^{1}H-NMR of 1-(2,6-diiodo-4-methoxyphenyl)butan-2-ol (7v) in d-CDCl$_3$ at 25 °C.



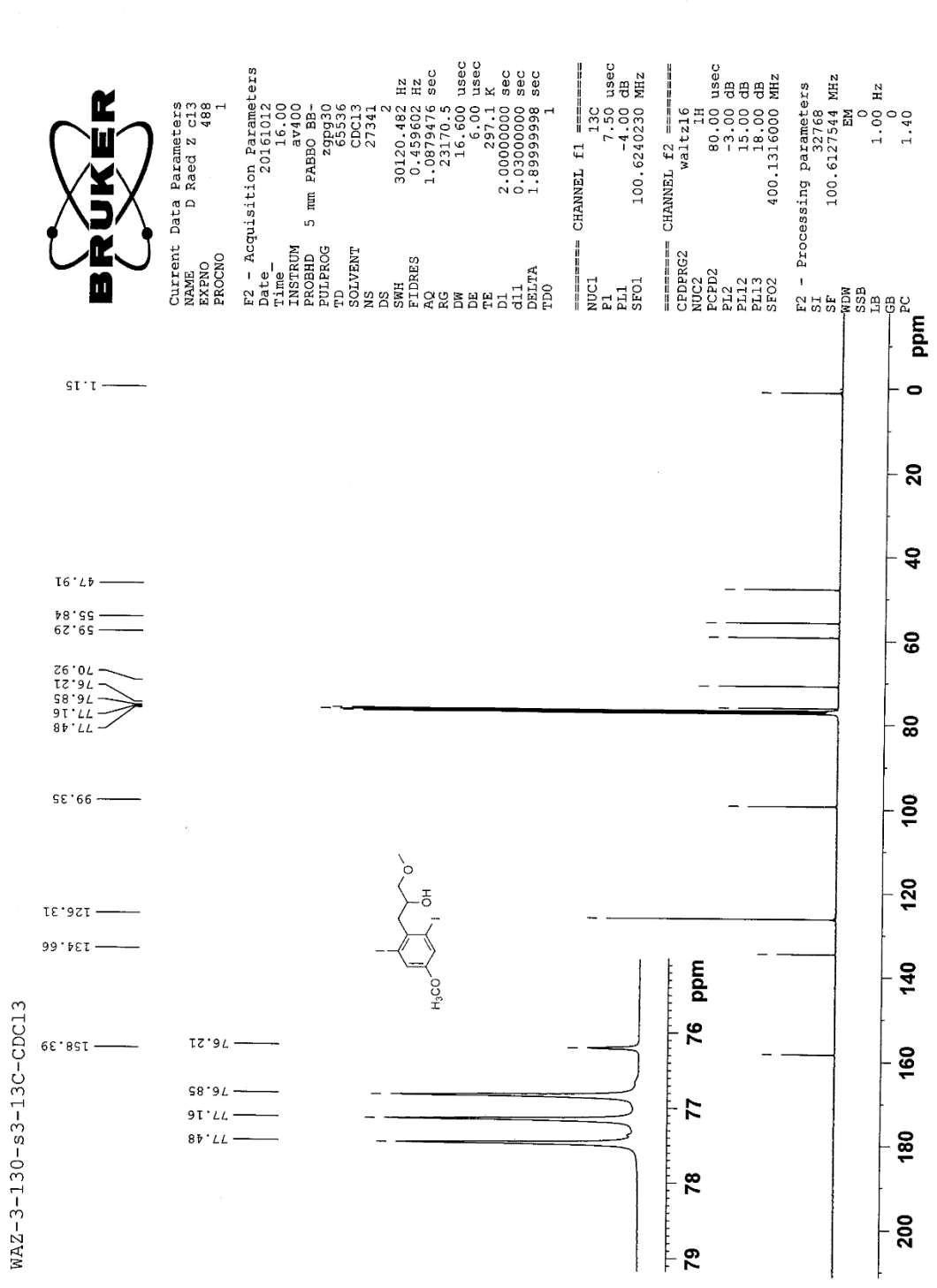
1.3.44 ^{13}C-NMR of 1-(2,6-diiodo-4-methoxyphenyl)butan-2-ol (7v) in d-CDCl$_3$ at 25 °C.



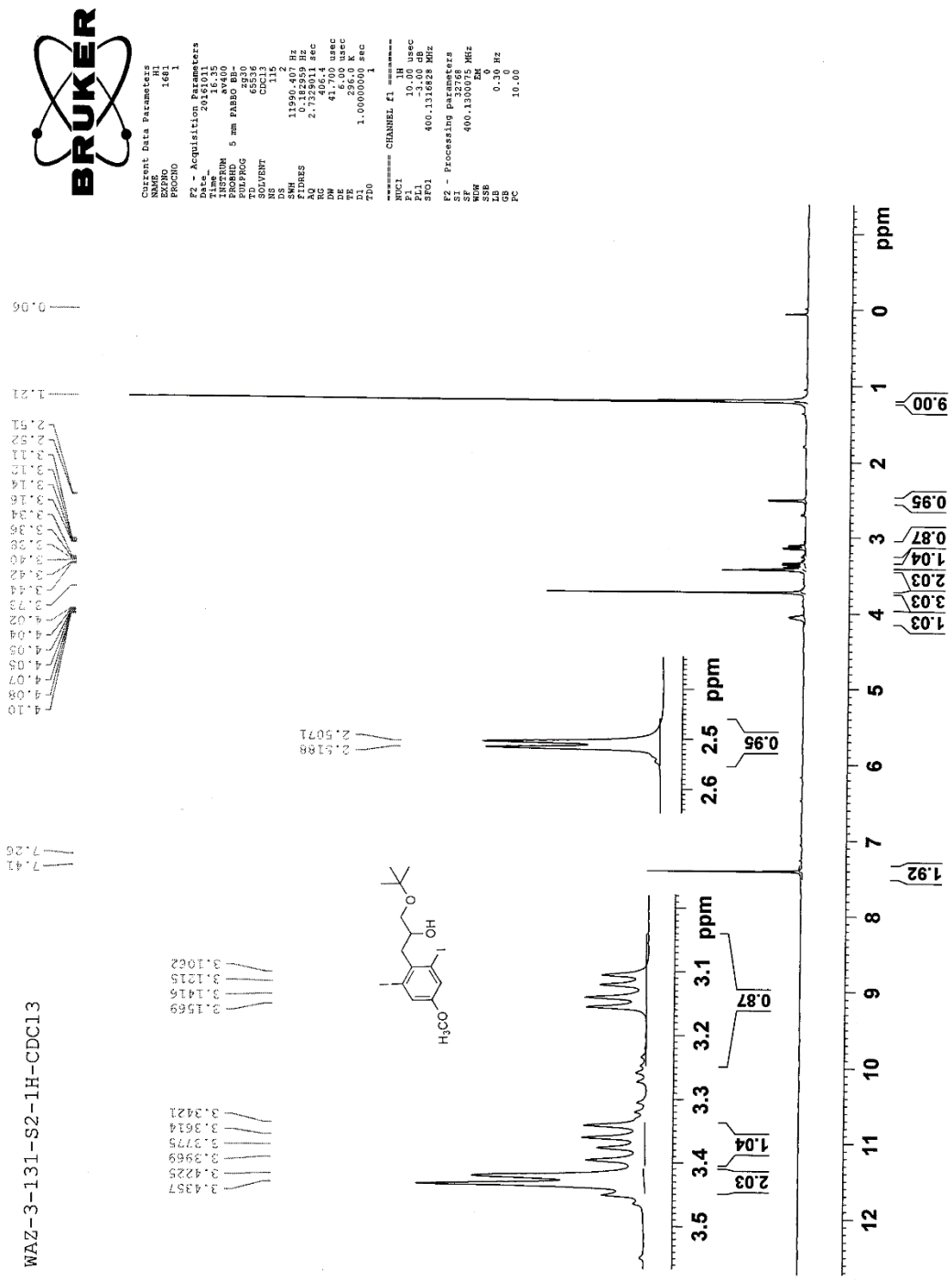
1.3.45 ^{1}H-NMR of 1-(2,6-diiodo-4-methoxyphenyl)-3-methoxypropan-2-ol (7w) in d-CDCl$_3$ at 25 °C.



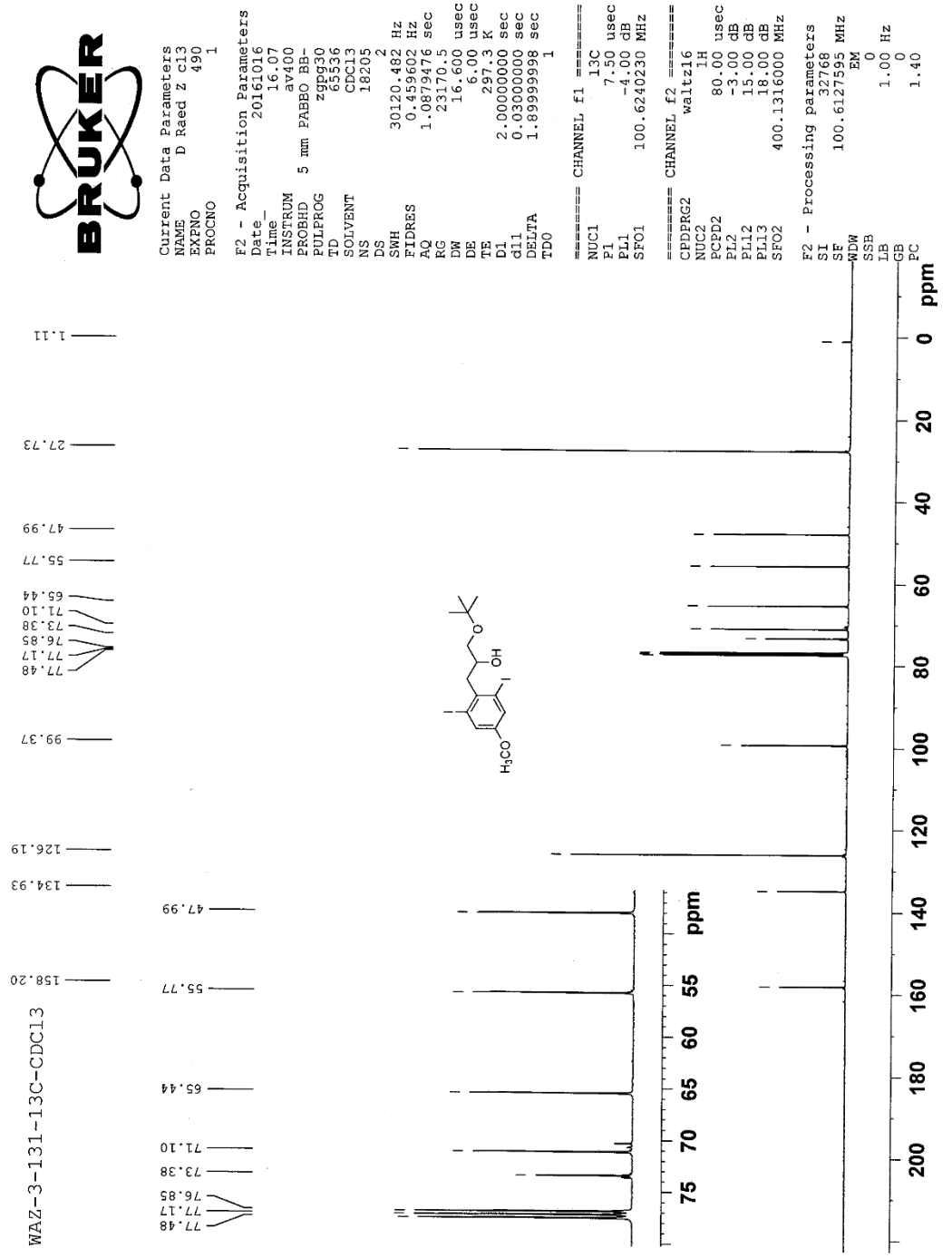
1.3.46 ^{13}C-NMR of 1-(2,6-diiodo-4-methoxyphenyl)-3-methoxypropan-2-ol (7w) in d-CDCl$_3$ at 25 °C.



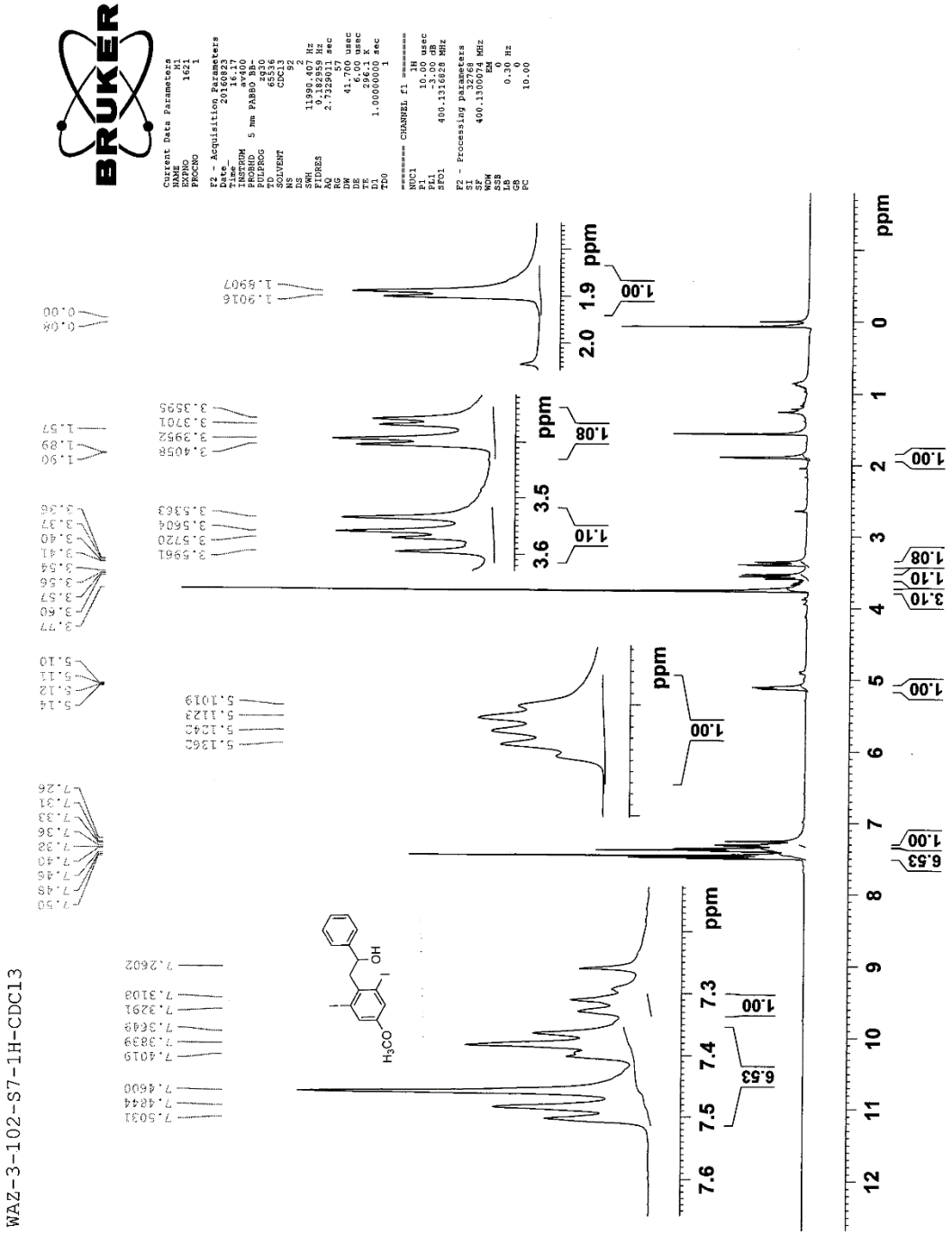
1.3.47 ^{1}H-NMR of 1-(tert-butoxy)-3-(2,6-diiodo-4-methoxyphenyl)propan-2-ol (7x) in d-CDCl$_3$ at 25 °C.



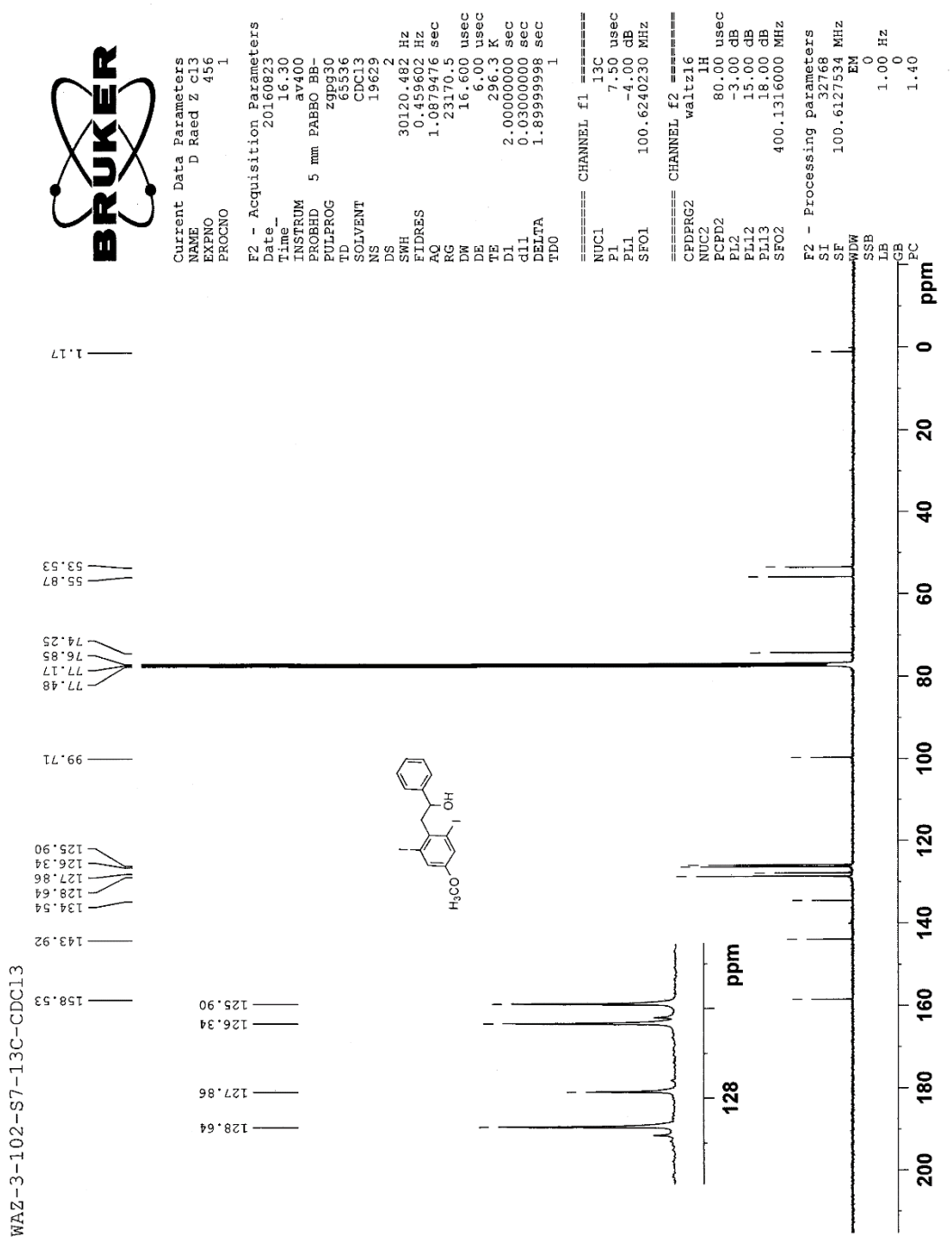
1.3.48 ^{13}C-NMR of 1-(tert-butoxy)-3-(2,6-diiodo-4-methoxyphenyl)propan-2-ol (7x) in d-CDCl$_3$ at 25 °C.



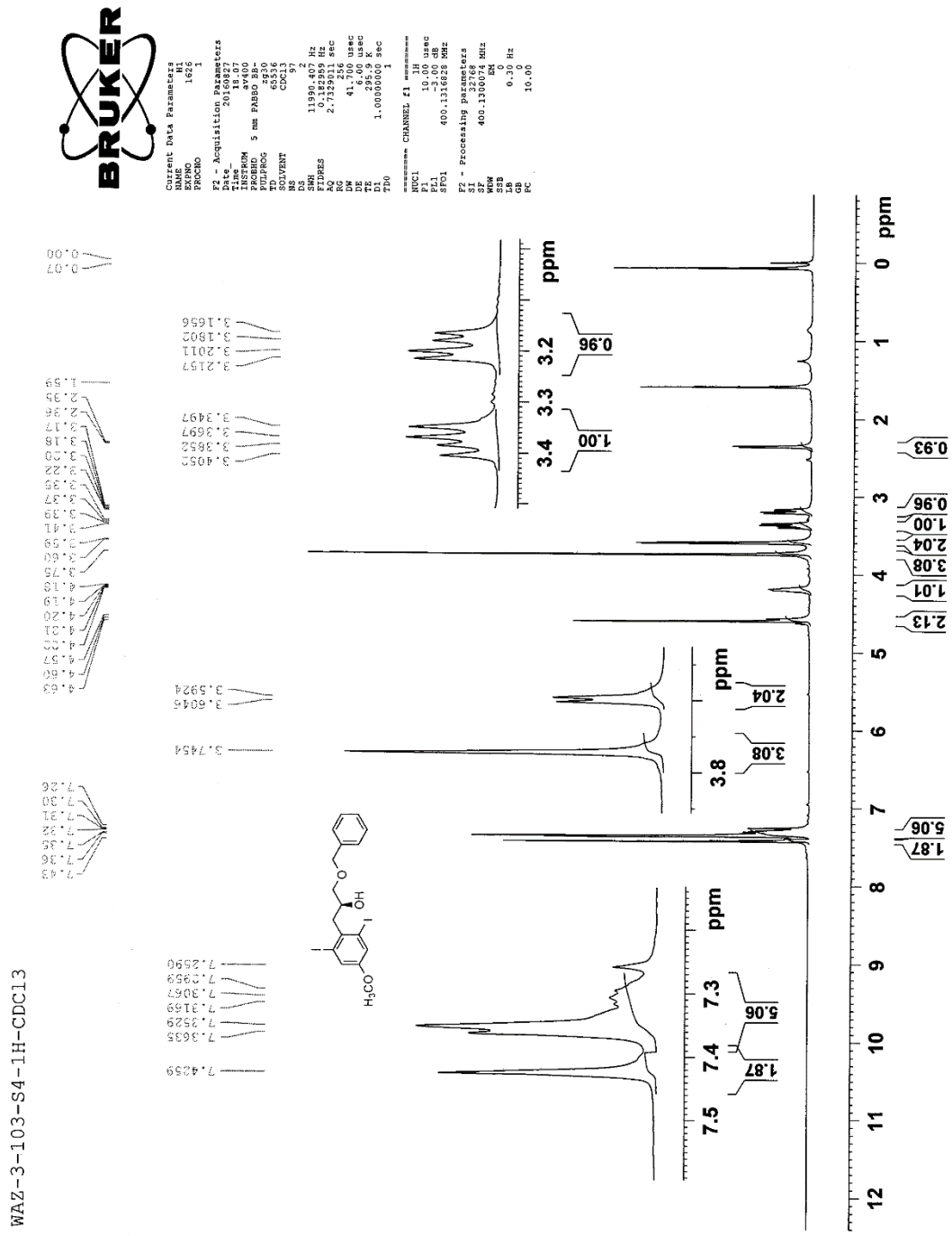
1.3.49 ^{1}H-NMR of 2-(2,6-diiodo-4-methoxyphenyl)-1-phenylethan-1-ol (7y) in d-$CDCl_3$ at 25 °C.



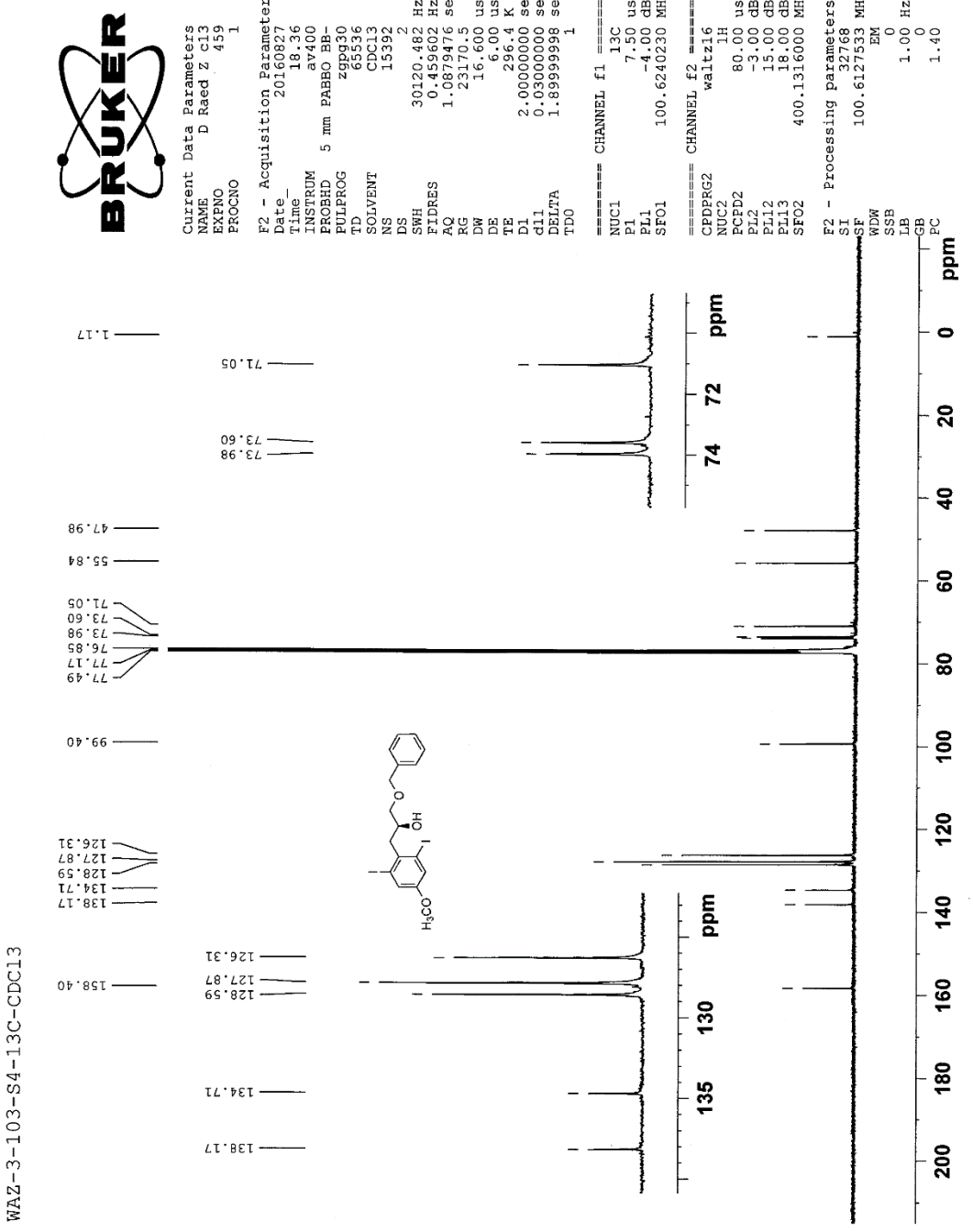
1.3.50 ^{13}C-NMR of 2-(2,6-diiodo-4-methoxyphenyl)-1-phenylethan-1-ol (7y) in d-$CDCl_3$ at 25 °C.



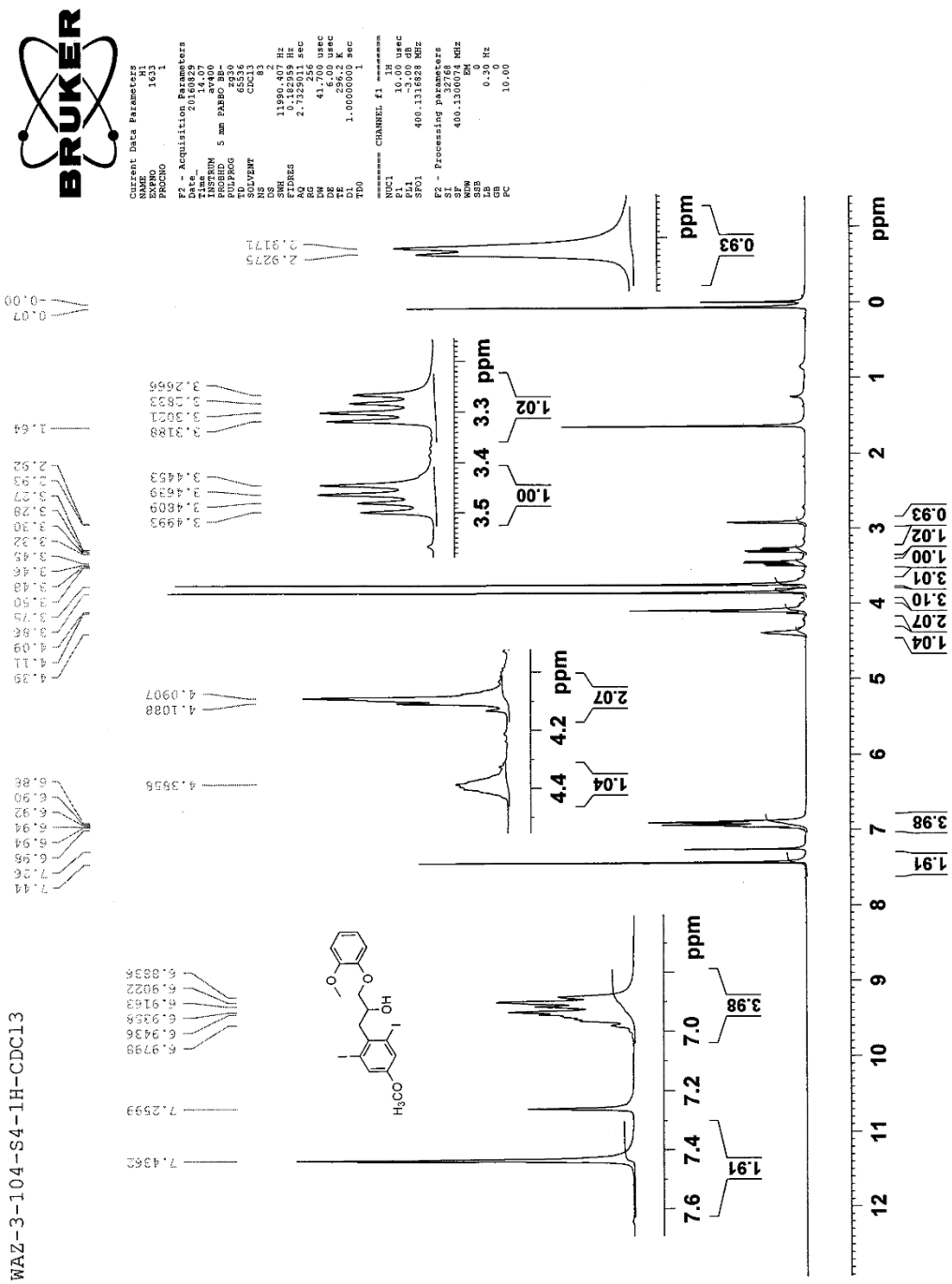
1.3.51 ^{1}H-NMR of (S)-1-(benzyloxy)-3-(2,6-diiodo-4-methoxyphenyl)propan-2-ol (7z) in d-CDCl$_3$ at 25 °C.



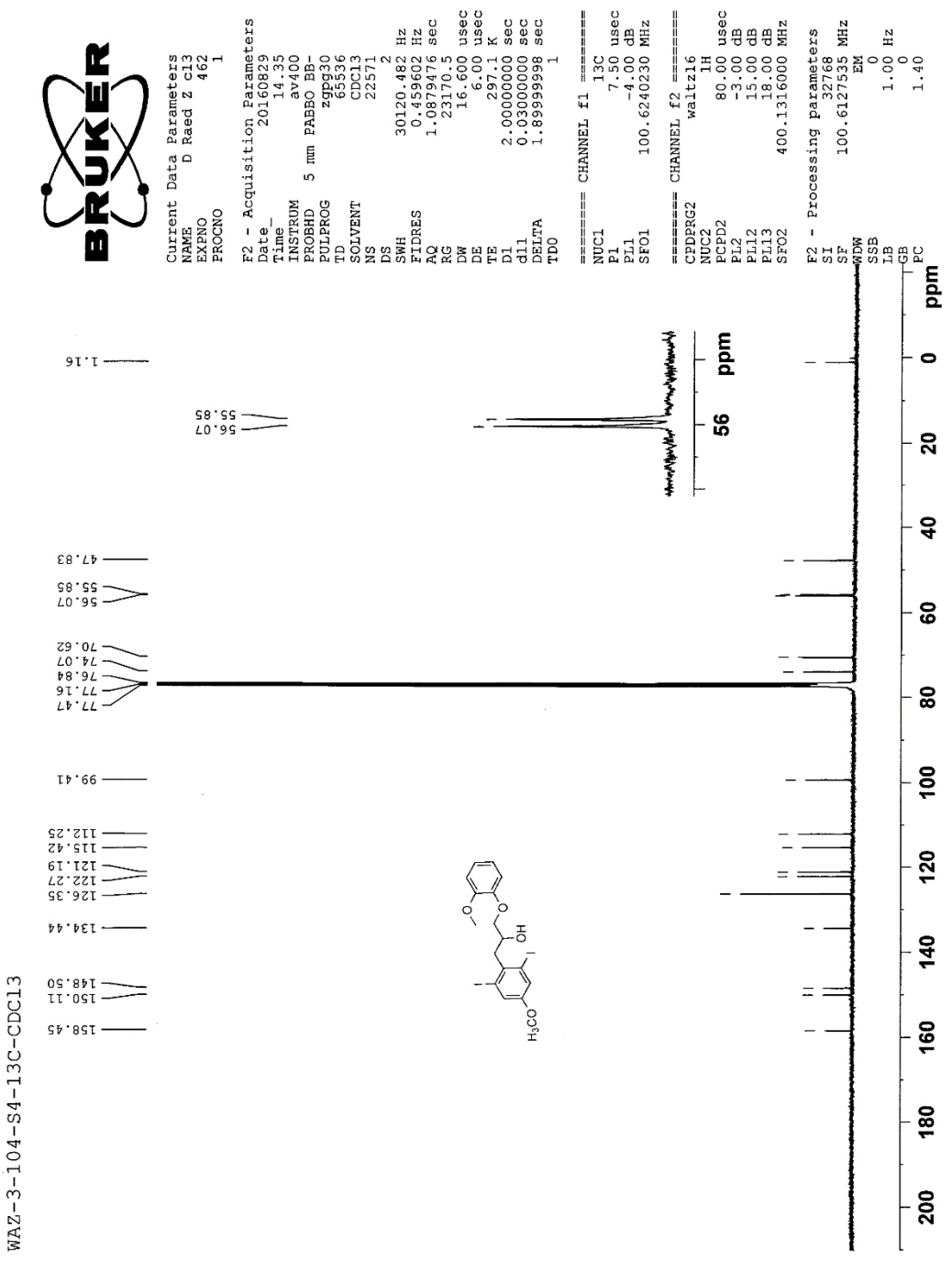
1.3.52 ^{13}C-NMR of (S)-1-(benzyloxy)-3-(2,6-diiodo-4-methoxyphenyl)propan-2-ol (7z) in d-CDCl$_3$ at 25 °C.



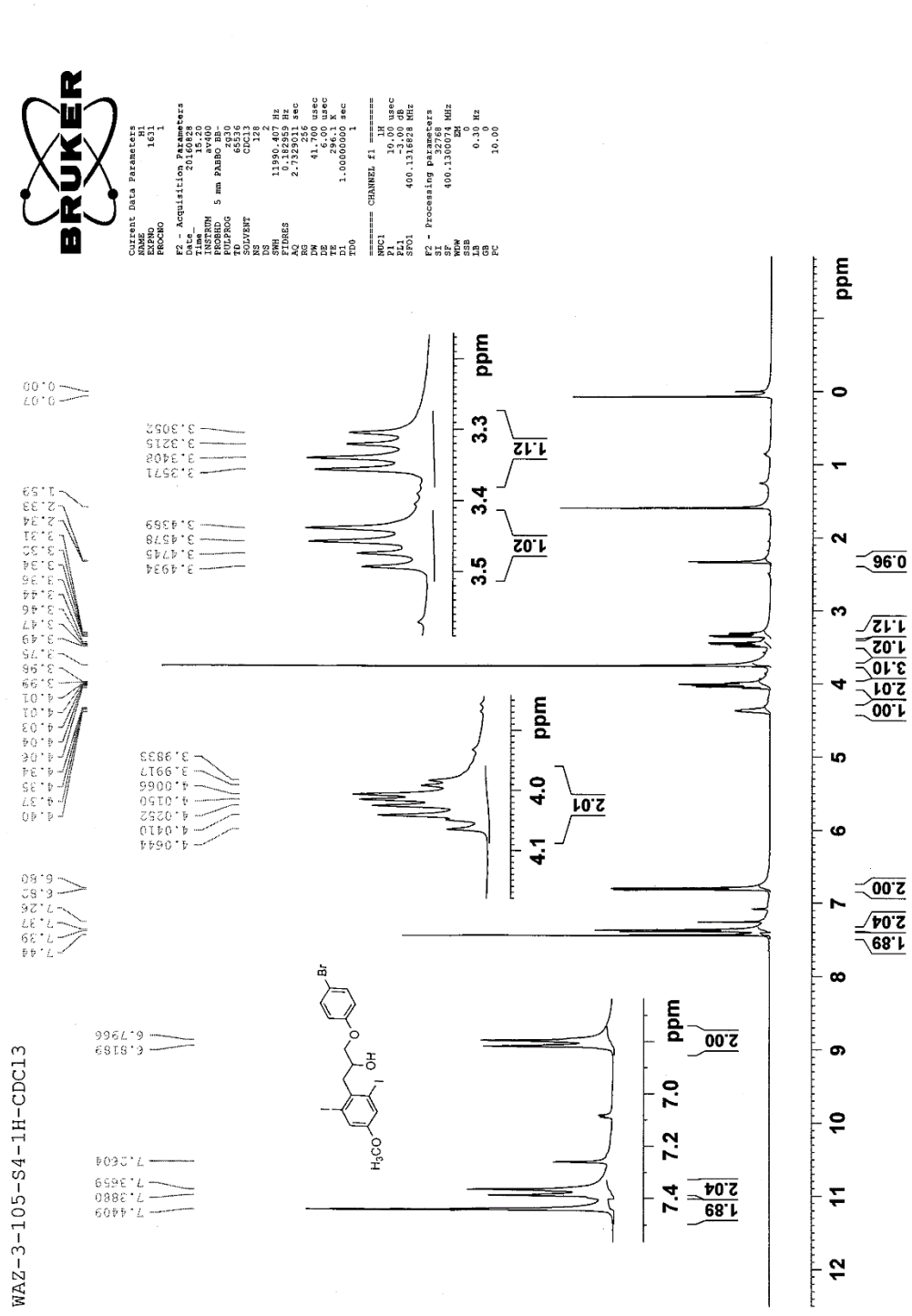
1.3.53 ^{1}H-NMR of 1-(2,6-diiodo-4-methoxyphenyl)-3-(2-methoxyphenoxy) propan-2-ol (7aa) in d-CDCl$_3$ at 25 °C.



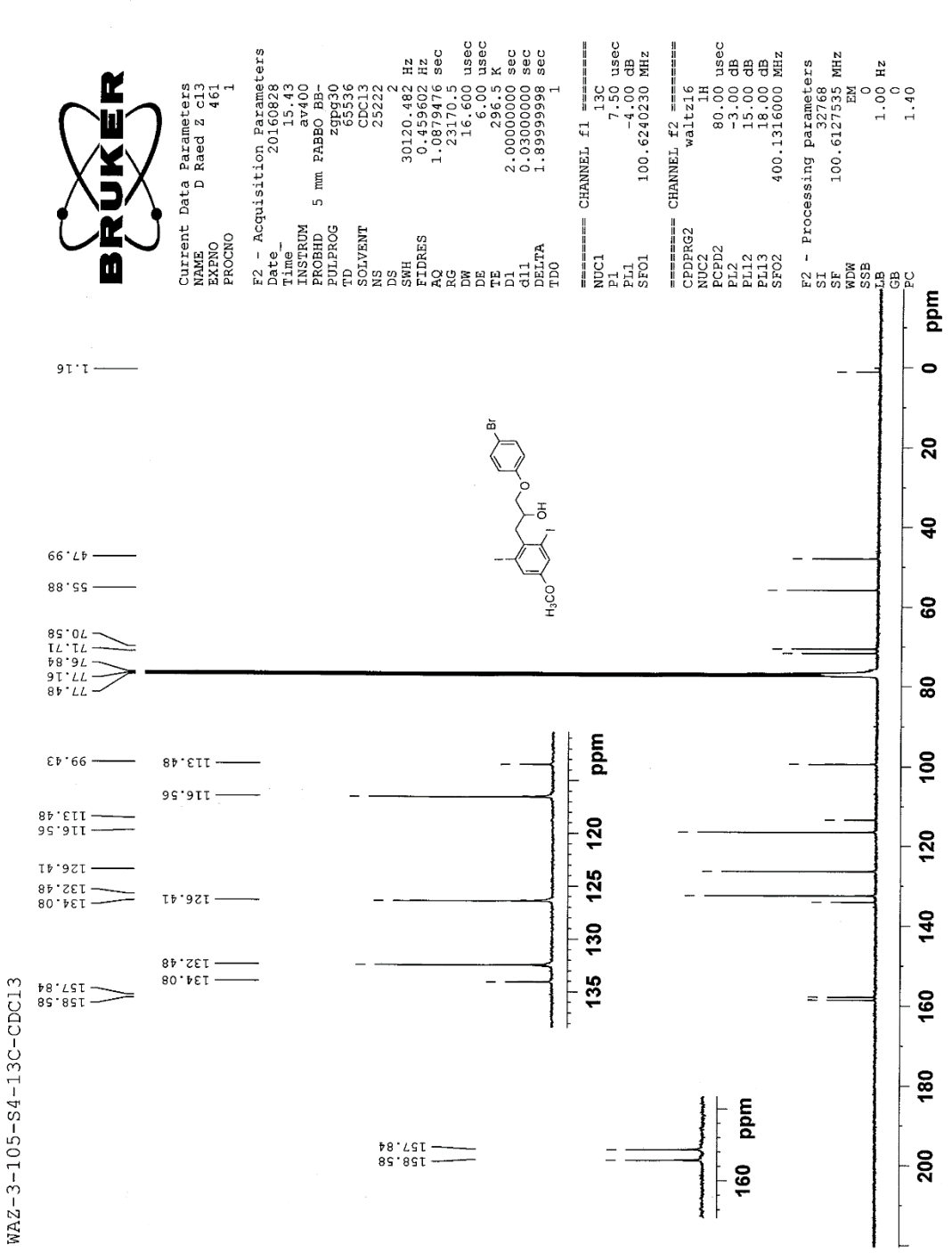
1.3.54 ^{13}C-NMR of 1-(2,6-diiodo-4-methoxyphenyl)-3-(2-methoxyphenoxy) propan-2-ol (7aa) in d-$CDCl_3$ at 25 °C.



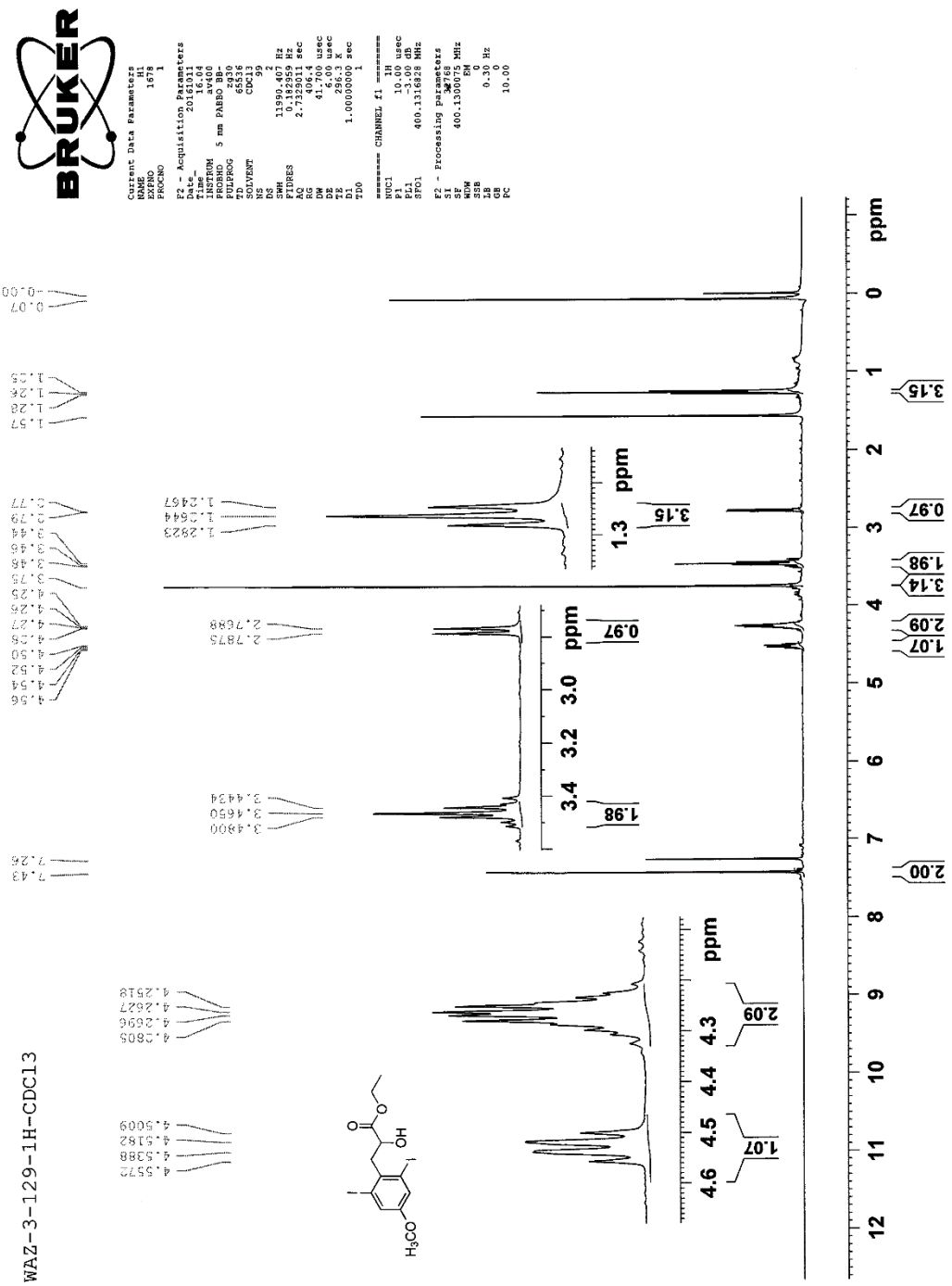
1.3.55 ^{1}H-NMR of 1-(4-bromophenoxy)-3-(2,6-diiodo-4-methoxyphenyl) propan-2-ol (7ab) in d-CDCl$_3$ at 25 °C.



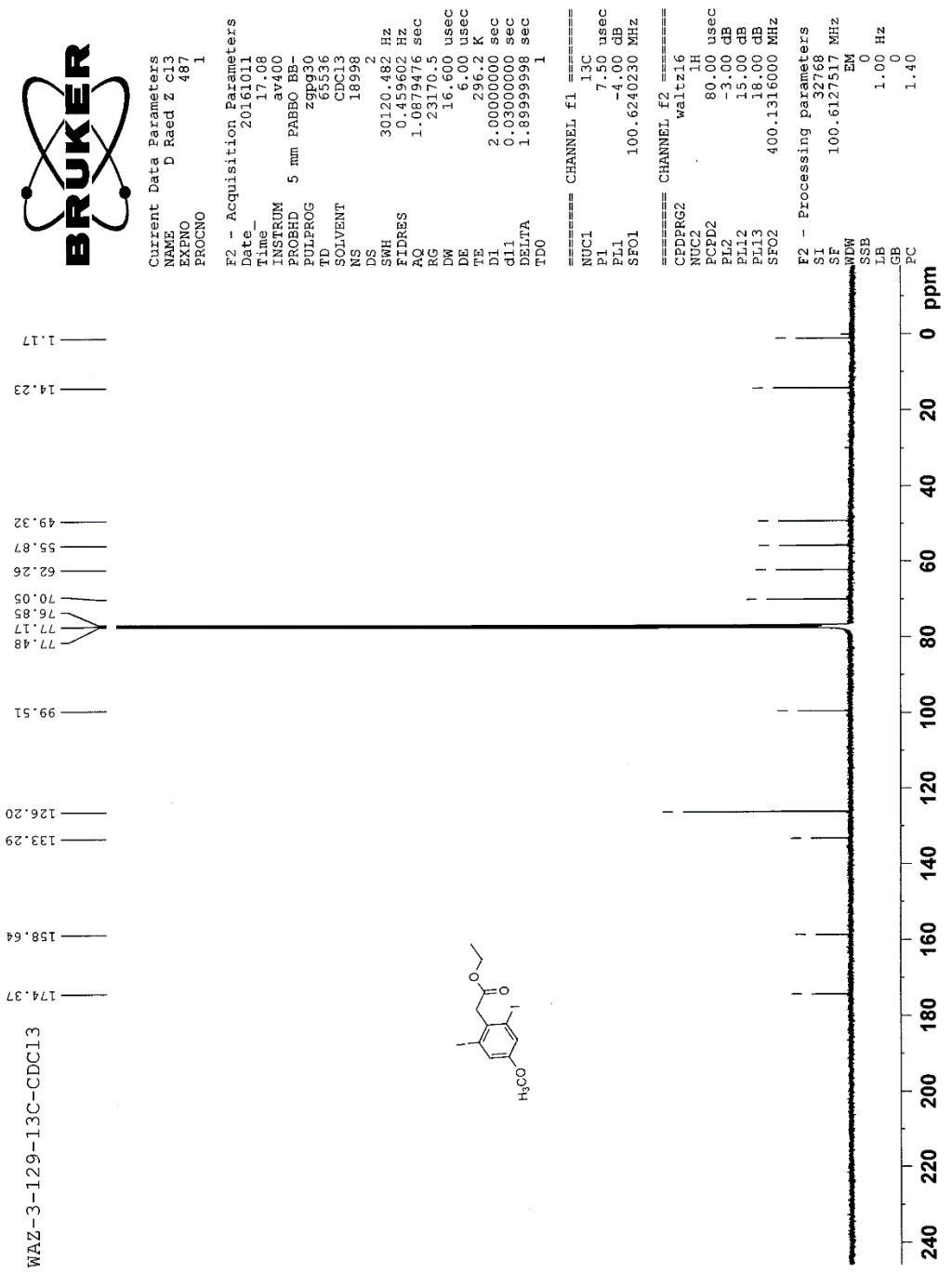
1.3.56 ^{13}C-NMR of 1-(4-bromophenoxy)-3-(2,6-diiodo-4-methoxyphenyl) propan-2-ol (7ab) in d-$CDCl_3$ at 25 °C.



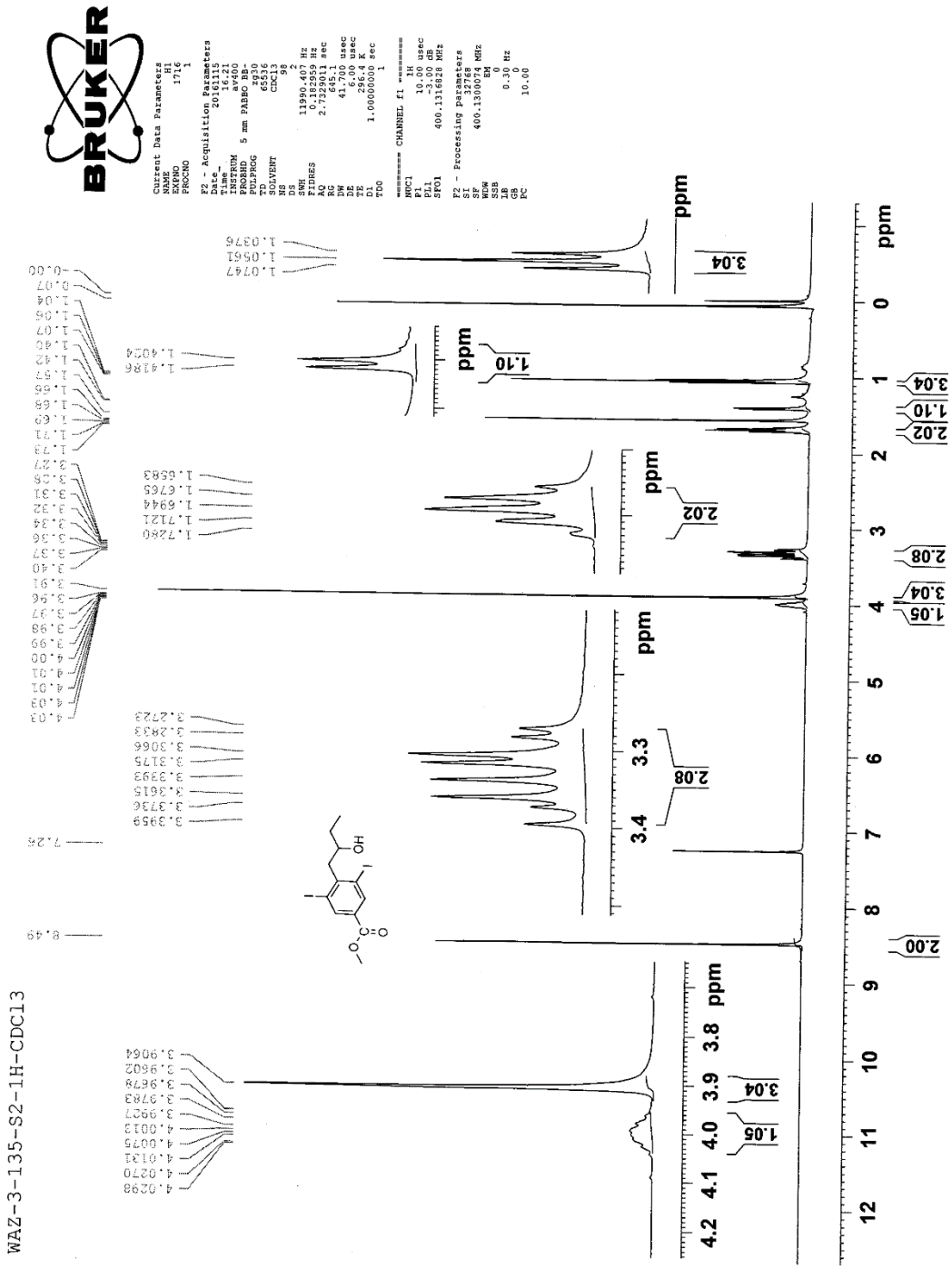
1.3.57 ^{1}H-NMR of ethyl 3-(2,6-diiodo-4-methoxyphenyl)-2-hydroxypropanoate (7ac) in d-CDCl$_3$ at 25 °C.



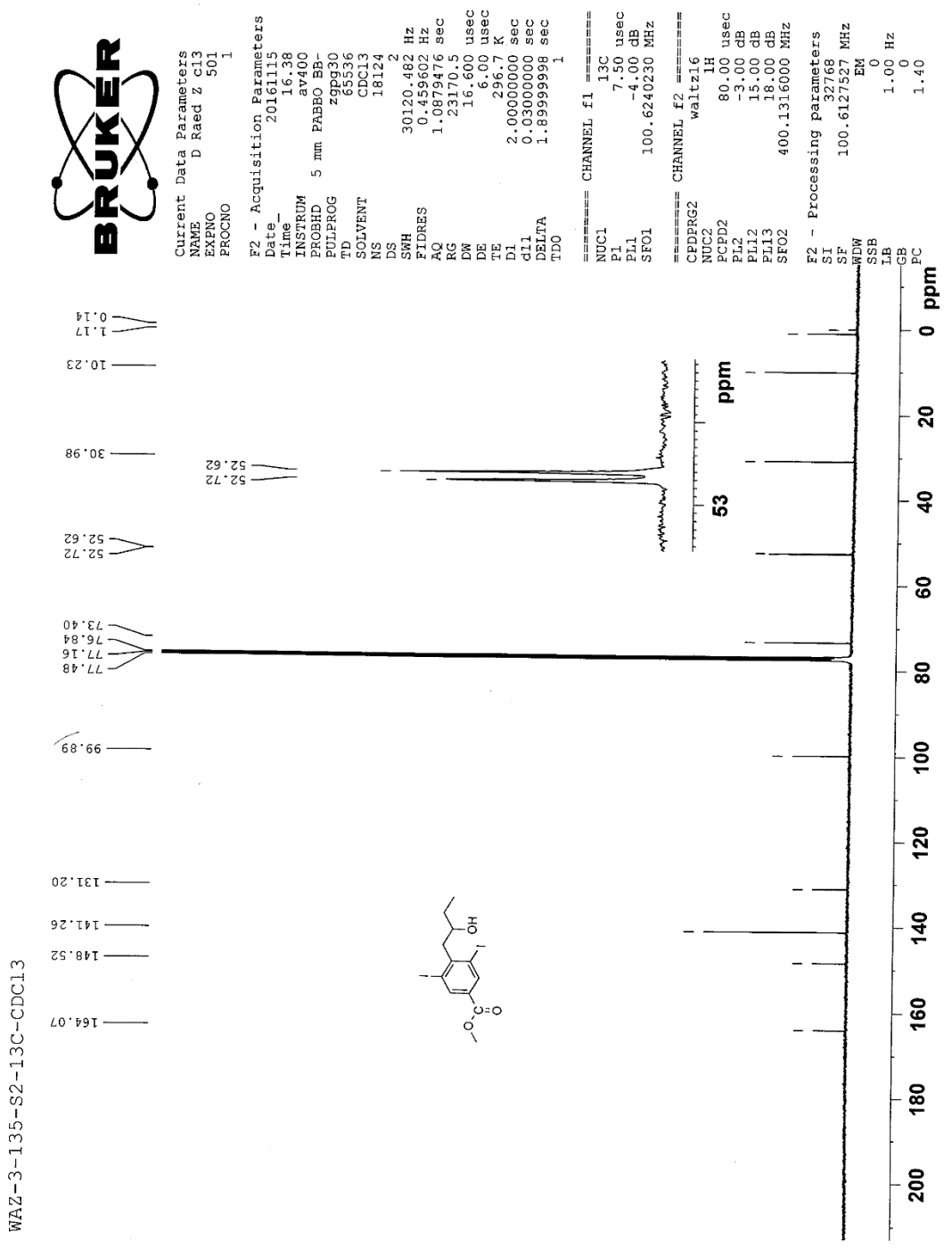
1.3.58 ^{13}C-NMR of ethyl 3-(2,6-diiodo-4-methoxyphenyl)-2-hydroxypropanoate (7ac) in d-CDCl$_3$ at 25 °C.



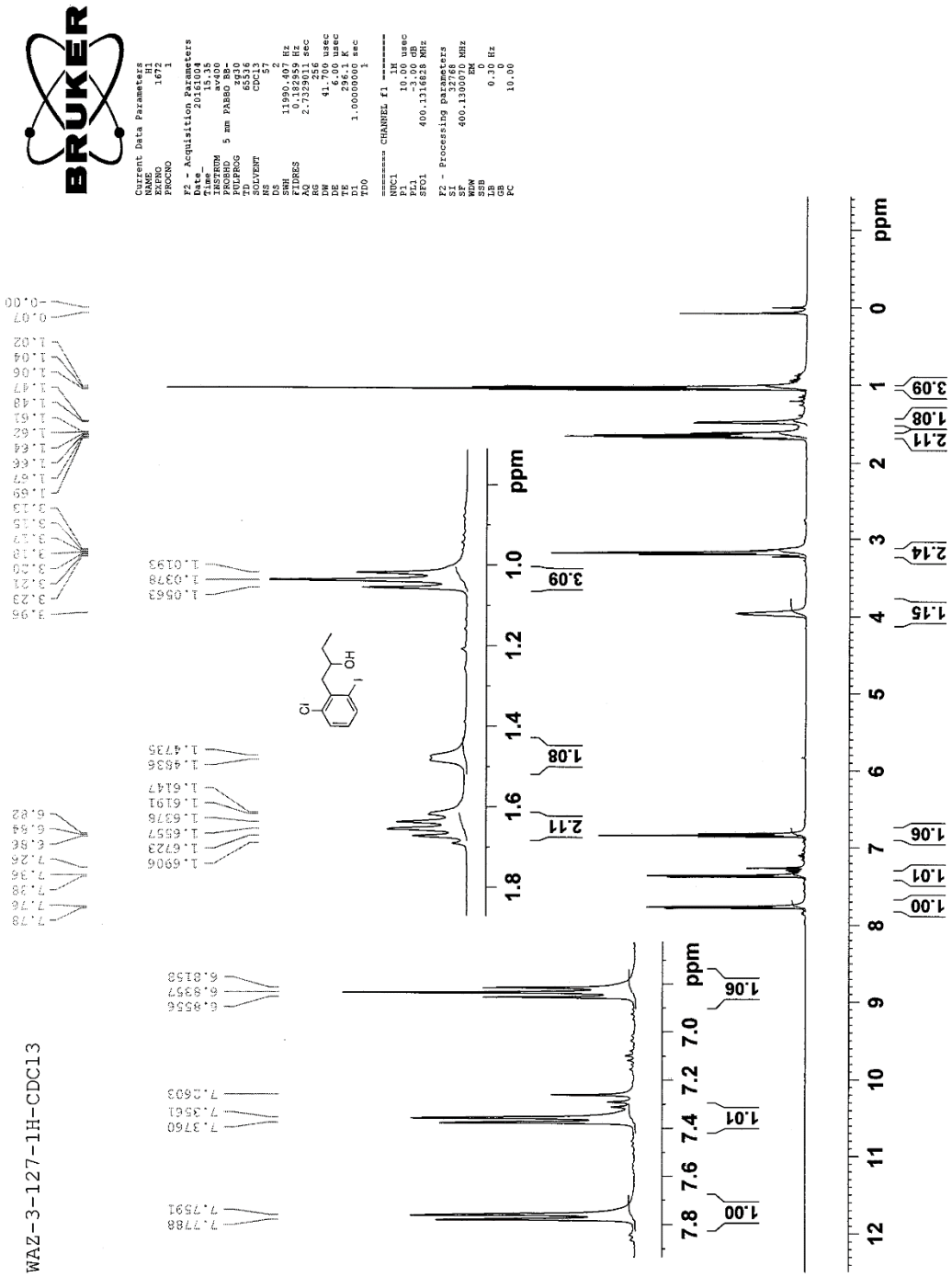
1.3.59 ^{1}H-NMR of methyl 4-(2-hydroxybutyl)-3,5-diiodobenzoate (7ad) in d-$CDCl_3$ at 25 °C.



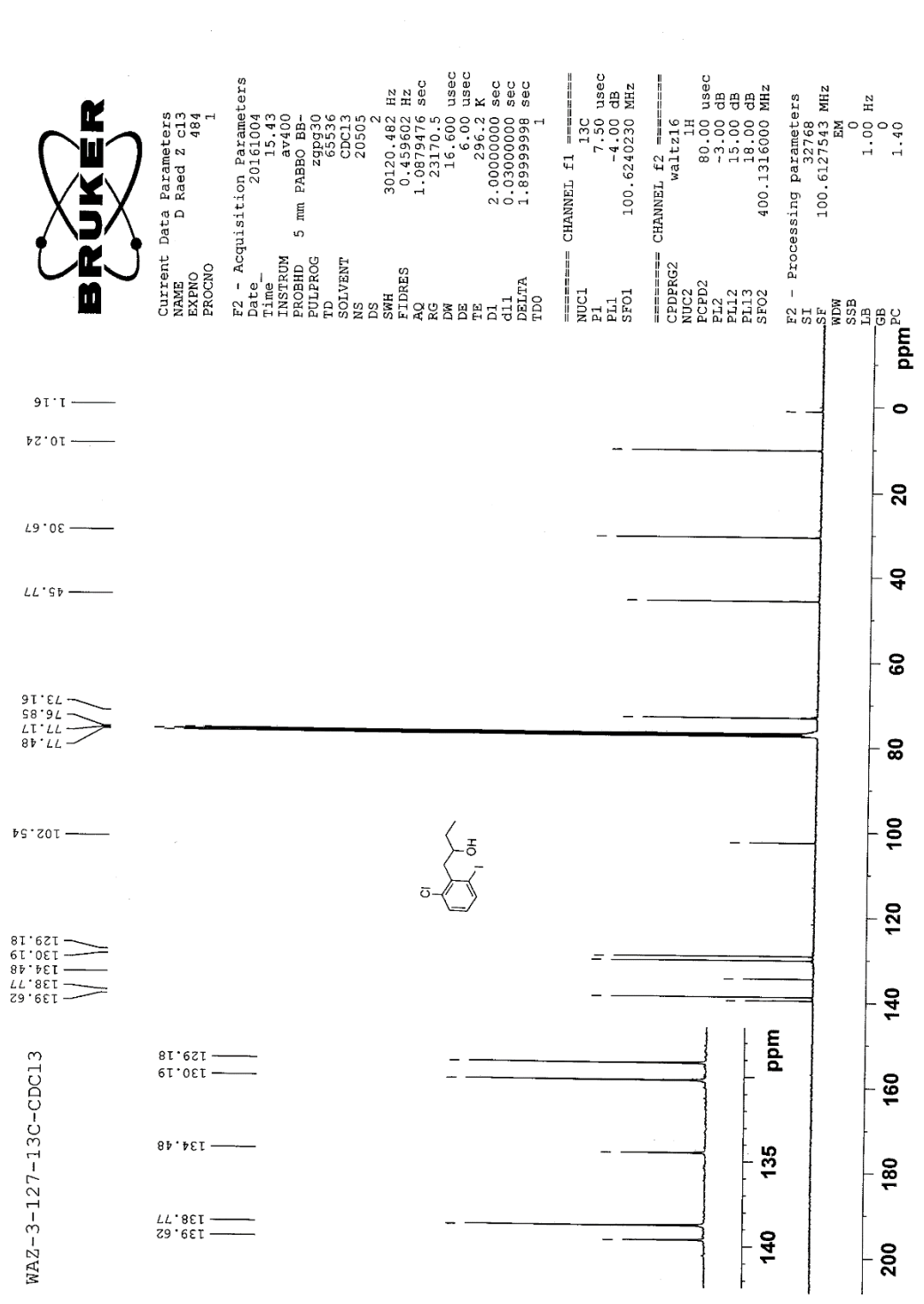
1.3.60 ^{13}C-NMR of methyl 4-(2-hydroxybutyl)-3,5-diiodobenzoate (7ad) in d-$CDCl_3$ at 25 °C.



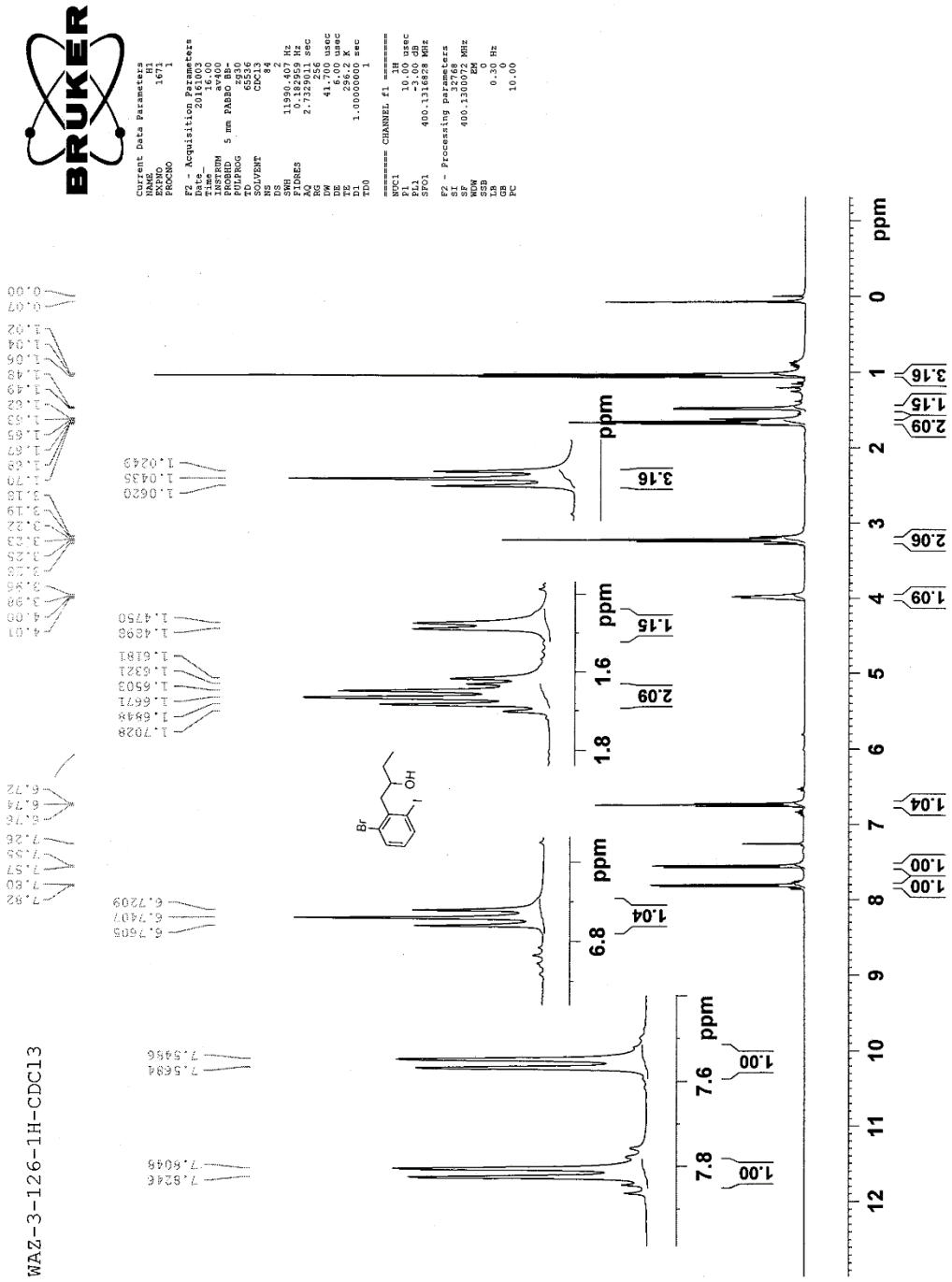
1.3.61 ^{1}H-NMR of 1-(2-chloro-6-iodophenyl)butan-2-ol (7ae) in d-CDCl$_3$ at 25 °C.



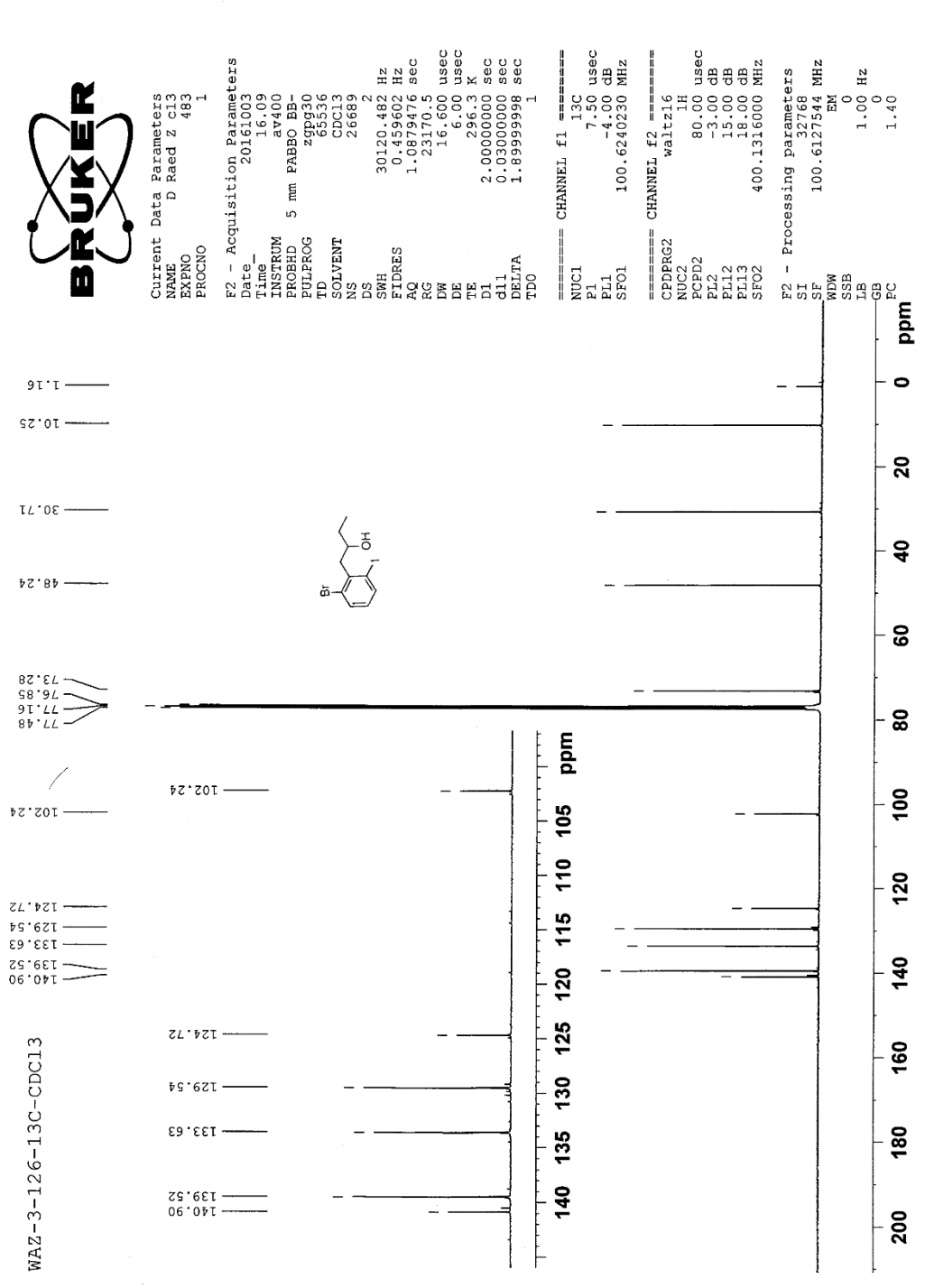
1.3.62 ^{13}C-NMR of 1-(2-chloro-6-iodophenyl)butan-2-ol (7ae) in d-CDCl$_3$ at 25 °C.



1.3.63 ^{1}H-NMR of 1-(2-bromo-6-iodophenyl)butan-2-ol (7af) in d-CDCl$_3$ at 25 °C.



1.3.64 ^{13}C-NMR of 1-(2-bromo-6-iodophenyl)butan-2-ol (7af) in d-CDCl$_3$ at 25 °C.



1.5.1 X-ray data of 1-(2,6-diiodo-4-methylphenyl)-3-methoxypropan-2-ol (**7g**)

STRUCTURE REPORT

XCL Code: JUS1619 **Date:** 23 January 2017

Compound: 1-(2,6-Diiodo-4-methylphenyl)-3-methoxypropan-2-ol
Formula: $C_{11}H_{14}I_2O_2$

Supervisor: R. M. Al-Zoubi, Jordan University of Science and Technology
Crystallographer: R. McDonald

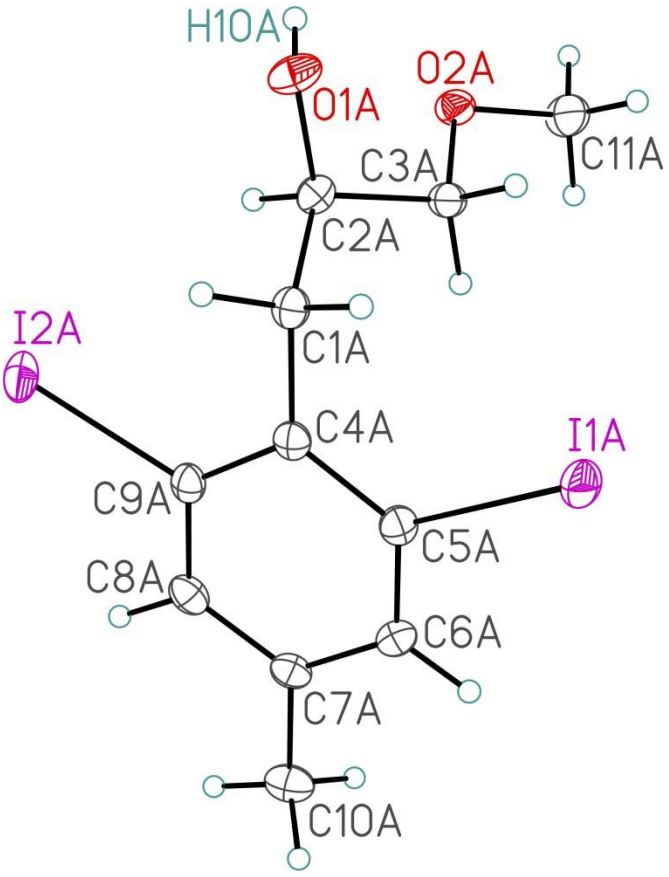
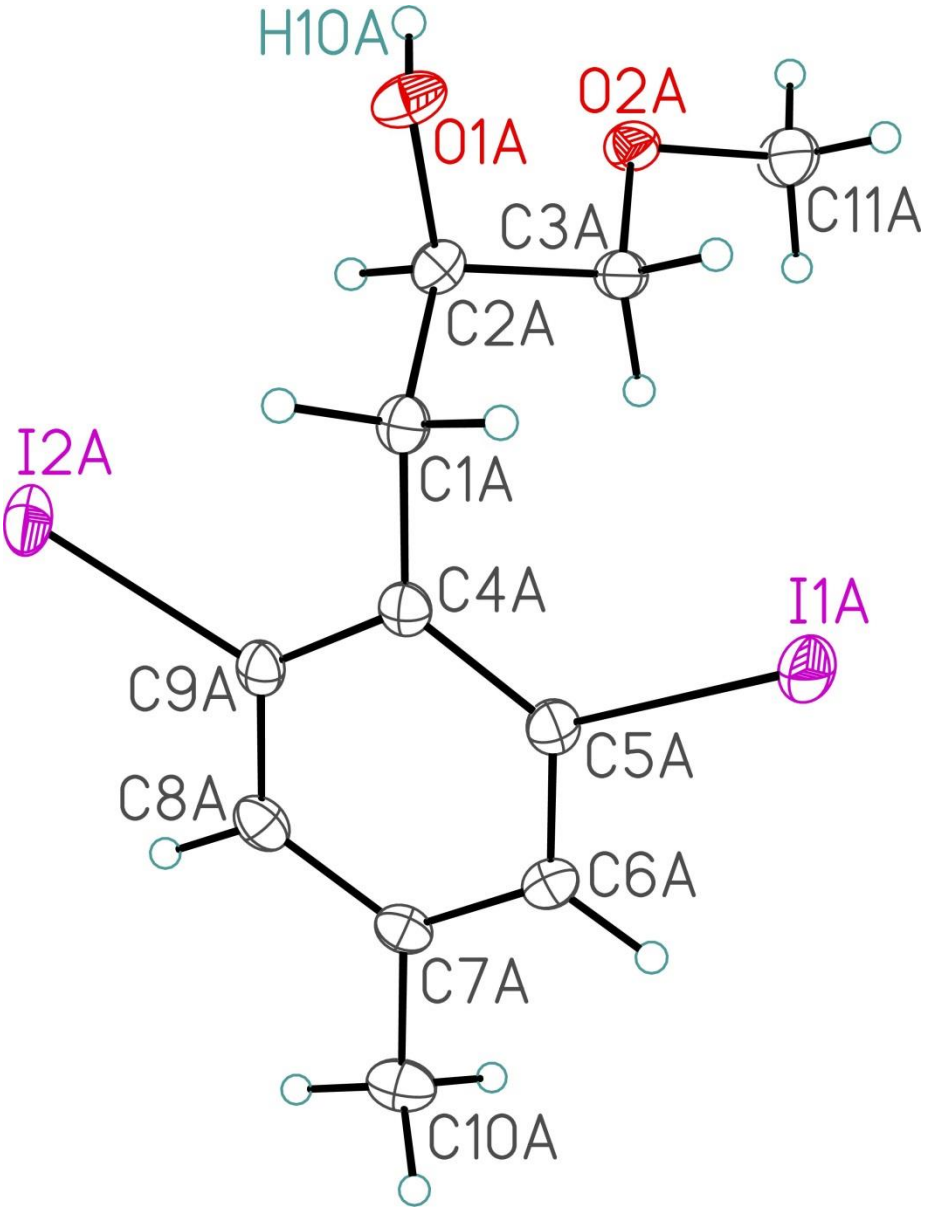


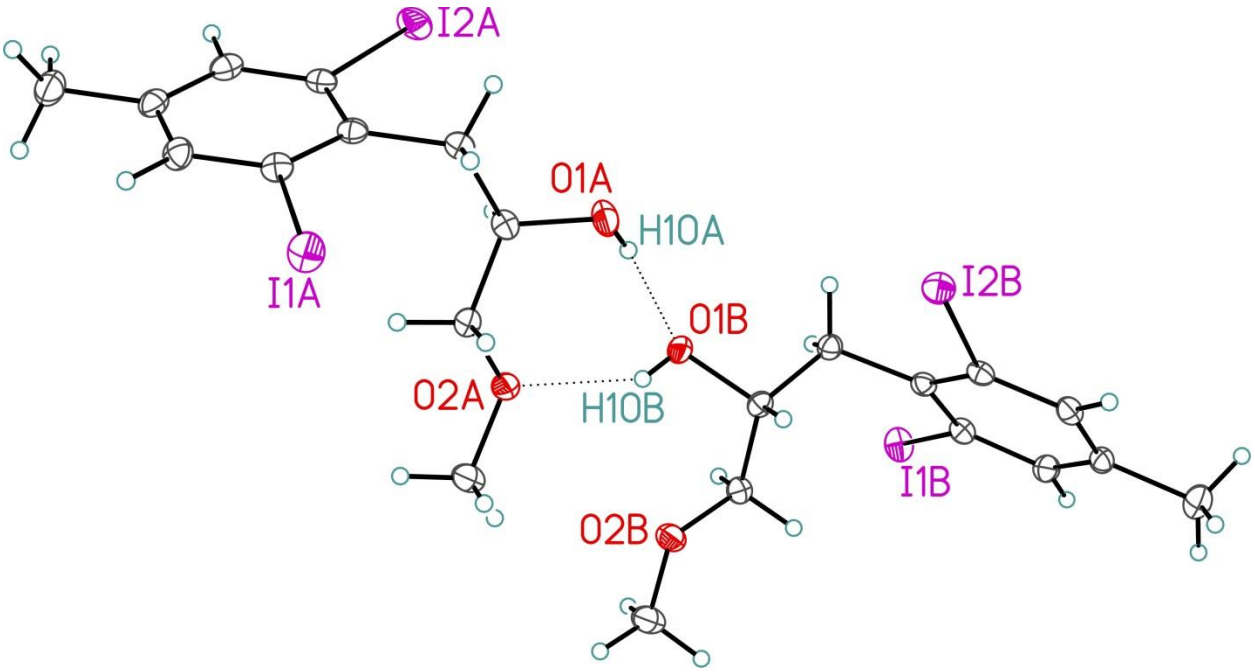
Figure Legends

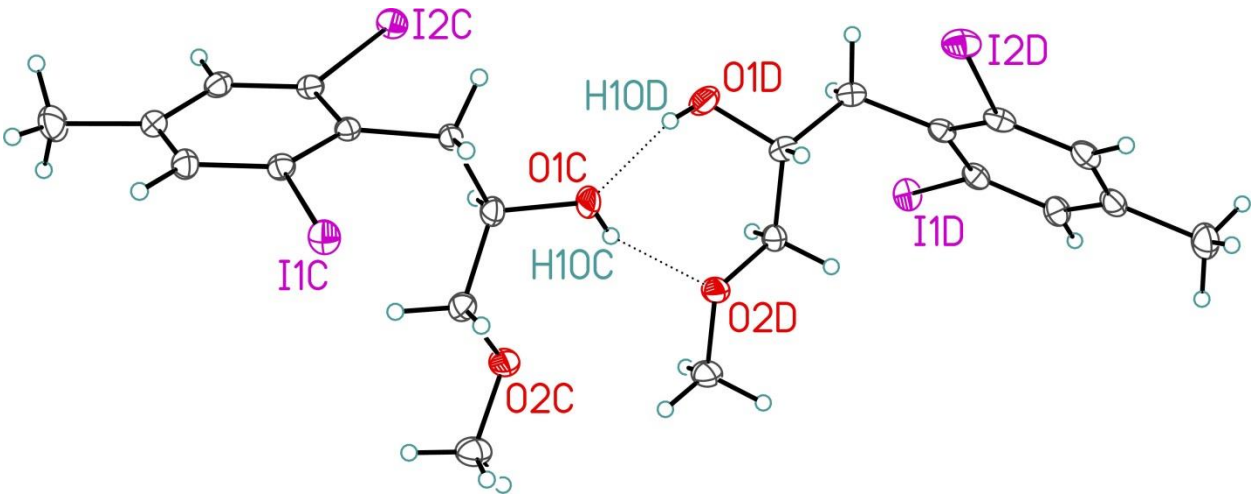
Figure 1. Perspective view of one of the four crystallographically-independent molecules of 1-(2,6-diiodo-4-methylphenyl)-3-methoxypropan-2-ol (molecule A) showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 30% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters.

Figure 2. Illustration of hydrogren-bonded interactions (dotted lines) between adjacent but crystallographically-independent molecules (molecules A and B) in the unit cell lattice. Note that the two molecules are not related by any crystallographic symmetry operations, and neither of these molecules in turn is related by symmetry to the independent molecules C and D (see Figure 3).

Figure 3. Illustration of hydrogren-bonded interactions (dotted lines) between adjacent but crystallographically-independent molecules (molecules C and D) in the unit cell lattice. Note that the two molecules are not related by any crystallographic symmetry operations, and neither of these molecules in turn is related by symmetry to the independent molecules A and B (see Figure 2).


H10A
O1A
O2A
C11A
C3A
C2A
C1A
I2A
C4A
I1A
C9A
C5A
C8A
C6A
C7A
C10A


I2A
O1A
H10A
I1A
O1B
I2B
O2A
H10B
I1B
O2B


I2C
H10D
O1D
I2D
O1C
I1D
I1C
H10C
O2D
O2C

List of Tables

Table 1. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{11}H_{14}I_2O_2$
formula weight	432.02
crystal dimensions (mm)	0.32 × 0.21 × 0.11
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	19.9273 (8)
b (Å)	8.4314 (3)
c (Å)	33.0097 (13)
β (deg)	107.2020 (5)
V (Å^3)	5298.0 (4)
Z	16
ρ_{calcd} (g cm^{-3})	2.167
μ (mm^{-1})	4.729
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (15 s exposures)
data collection 2θ limit (deg)	56.66
total data collected	48427 (-26 ≤ h ≤ 26, -10 ≤ k ≤ 11, -43 ≤ l ≤ 44)
independent reflections	13041 (R_{int} = 0.0244)
number of observed reflections (*NO*)	11132 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT-2014*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2014*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.6964–0.3616
data/restraints/parameters	13041 / 0 / 561
goodness-of-fit (S)[e] [all data]	1.045
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0246
wR_2 [all data]	0.0592
largest difference peak and hole	0.798 and –1.050 e Å^{-3}

[a]Obtained from least-squares refinement of 9803 reflections with 4.98° < 2θ < 53.70°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *A71*, 3–8.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *C71*, 3–8.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0269P)^2 + 3.2851P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

(a) Molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
I1A	0.13147(2)	0.31000(3)	0.00139(2)	0.03884(5)*
I2A	0.02734(2)	-0.03393(3)	0.13643(2)	0.03985(6)*
O1A	0.23704(11)	0.1923(3)	0.15605(7)	0.0363(5)*
O2A	0.18646(11)	0.5179(2)	0.14993(6)	0.0314(4)*
C1A	0.14615(14)	0.1240(3)	0.09479(8)	0.0271(6)*
C2A	0.16904(14)	0.2439(3)	0.13101(8)	0.0271(6)*
C3A	0.17104(14)	0.4105(3)	0.11491(8)	0.0272(6)*
C4A	0.07134(14)	0.1427(3)	0.06648(8)	0.0256(6)*
C5A	0.05390(15)	0.2173(3)	0.02672(8)	0.0273(6)*
C6A	-0.01509(15)	0.2354(4)	0.00138(9)	0.0313(6)*
C7A	-0.07089(15)	0.1786(3)	0.01469(9)	0.0293(6)*
C8A	-0.05540(15)	0.1019(3)	0.05326(9)	0.0307(6)*
C9A	0.01406(15)	0.0861(3)	0.07847(8)	0.0268(6)*
C10A	-0.14618(16)	0.1969(4)	-0.01230(10)	0.0412(8)*
C11A	0.18541(19)	0.6774(4)	0.13557(11)	0.0443(8)*
H1OA	0.2467(19)	0.242(4)	0.1767(11)	0.043(11)

(b) Molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
I1B	0.38848(2)	0.54103(3)	0.38479(2)	0.03626(5)*
I2B	0.47347(2)	0.17131(2)	0.24723(2)	0.03291(5)*
O1B	0.27477(11)	0.4060(3)	0.22605(6)	0.0296(4)*
O2B	0.30744(11)	0.7255(2)	0.22782(6)	0.0333(5)*
C1B	0.36352(13)	0.3521(3)	0.29051(8)	0.0250(5)*
C2B	0.34024(14)	0.4657(3)	0.25272(8)	0.0241(5)*
C3B	0.33112(15)	0.6343(3)	0.26571(8)	0.0274(6)*
C4B	0.43927(13)	0.3740(3)	0.31607(8)	0.0233(5)*
C5B	0.46116(14)	0.4548(3)	0.35473(8)	0.0246(5)*
C6B	0.53140(15)	0.4811(3)	0.37680(8)	0.0283(6)*
C7B	0.58379(14)	0.4225(3)	0.36121(8)	0.0259(6)*
C8B	0.56485(14)	0.3370(3)	0.32360(8)	0.0265(6)*
C9B	0.49422(14)	0.3140(3)	0.30203(8)	0.0230(5)*
C10B	0.66084(15)	0.4493(4)	0.38475(10)	0.0378(7)*
C11B	0.29863(18)	0.8879(4)	0.23608(11)	0.0406(7)*
H1OB	0.2605(19)	0.465(4)	0.2093(11)	0.045(11)

Table 2. Atomic Coordinates and Displacement Parameters (continued)

(c) Molecule C

Atom	*x*	*y*	*z*	U_{eq}, Å^2
I1C	0.15514(2)	0.26110(2)	0.25370(2)	0.03148(5)*
I2C	0.02430(2)	-0.04087(2)	0.38174(2)	0.03538(5)*
O1C	0.23834(12)	0.1627(3)	0.40966(7)	0.0388(5)*
O2C	0.19837(12)	0.4836(2)	0.40391(6)	0.0377(5)*
C1C	0.15222(13)	0.0965(3)	0.34600(8)	0.0233(5)*
C2C	0.17309(15)	0.2186(3)	0.38195(8)	0.0293(6)*
C3C	0.18038(15)	0.3848(3)	0.36710(9)	0.0318(6)*
C4C	0.08040(13)	0.1248(3)	0.31557(8)	0.0221(5)*
C5C	0.06954(14)	0.1972(3)	0.27590(8)	0.0246(5)*
C6C	0.00338(15)	0.2319(3)	0.24931(9)	0.0299(6)*
C7C	-0.05642(15)	0.1966(3)	0.26112(9)	0.0302(6)*
C8C	-0.04773(14)	0.1198(3)	0.29948(9)	0.0277(6)*
C9C	0.01900(14)	0.0845(3)	0.32568(8)	0.0241(5)*
C10C	-0.12837(16)	0.2390(4)	0.23303(11)	0.0455(8)*
C11C	0.19881(19)	0.6458(4)	0.39327(11)	0.0429(8)*
H1OC	0.253(2)	0.217(5)	0.4266(12)	0.057(13)

(d) Molecule D

Atom	*x*	*y*	*z*	U_{eq}, Å^2
I1D	0.37374(2)	0.08056(3)	0.63409(2)	0.03588(5)*
I2D	0.47517(2)	-0.26087(2)	0.49809(2)	0.03929(6)*
O1D	0.26487(12)	-0.0389(3)	0.48073(8)	0.0405(5)*
O2D	0.31751(11)	0.2836(2)	0.48436(6)	0.0337(5)*
C1D	0.35821(15)	-0.1071(3)	0.54122(9)	0.0290(6)*
C2D	0.33379(15)	0.0106(3)	0.50450(9)	0.0281(6)*
C3D	0.33416(15)	0.1796(3)	0.51993(8)	0.0283(6)*
C4D	0.43310(14)	-0.0831(3)	0.56834(8)	0.0263(6)*
C5D	0.45118(15)	-0.0057(3)	0.60763(9)	0.0282(6)*
C6D	0.52017(16)	0.0207(4)	0.63178(9)	0.0323(6)*
C7D	0.57542(15)	-0.0320(3)	0.61752(9)	0.0318(6)*
C8D	0.55980(15)	-0.1133(3)	0.57940(9)	0.0311(6)*
C9D	0.49038(15)	-0.1366(3)	0.55545(9)	0.0289(6)*
C10D	0.65110(17)	-0.0056(4)	0.64304(10)	0.0442(8)*
C11D	0.31891(19)	0.4447(4)	0.49690(10)	0.0445(8)*
H1OD	0.254(2)	0.005(5)	0.4597(12)	0.056(13)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3. Selected Interatomic Distances (Å)

(a) Molecule A

Atom1	Atom2	Distance	Atom1	Atom2	Distance
I1A	C5A	2.113(3)	C4A	C5A	1.403(4)
I2A	C9A	2.111(3)	C4A	C9A	1.398(4)
O1A	C2A	1.430(3)	C5A	C6A	1.390(4)
O2A	C3A	1.428(3)	C6A	C7A	1.396(4)
O2A	C11A	1.424(4)	C7A	C8A	1.379(4)
C1A	C2A	1.529(4)	C7A	C10A	1.509(4)
C1A	C4A	1.515(4)	C8A	C9A	1.395(4)
C2A	C3A	1.507(4)			

(b) Molecule B

Atom1	Atom2	Distance	Atom1	Atom2	Distance
I1B	C5B	2.112(3)	C4B	C5B	1.397(4)
I2B	C9B	2.109(3)	C4B	C9B	1.404(3)
O1B	C2B	1.432(3)	C5B	C6B	1.391(4)
O2B	C3B	1.425(3)	C6B	C7B	1.385(4)
O2B	C11B	1.417(4)	C7B	C8B	1.388(4)
C1B	C2B	1.532(4)	C7B	C10B	1.519(4)
C1B	C4B	1.507(4)	C8B	C9B	1.390(4)
C2B	C3B	1.511(4)			

(c) Molecule C

Atom1	Atom2	Distance	Atom1	Atom2	Distance
I1C	C5C	2.116(3)	C4C	C5C	1.402(3)
I2C	C9C	2.107(3)	C4C	C9C	1.402(3)
O1C	C2C	1.430(3)	C5C	C6C	1.382(4)
O2C	C3C	1.429(3)	C6C	C7C	1.391(4)
O2C	C11C	1.413(4)	C7C	C8C	1.387(4)
C1C	C2C	1.533(4)	C7C	C10C	1.502(4)
C1C	C4C	1.505(3)	C8C	C9C	1.387(4)
C2C	C3C	1.505(4)			

(d) Molecule D

Atom1	Atom2	Distance	Atom1	Atom2	Distance
I1D	C5D	2.114(3)	C4D	C5D	1.401(4)
I2D	C9D	2.106(3)	C4D	C9D	1.405(4)
O1D	C2D	1.428(4)	C5D	C6D	1.388(4)
O2D	C3D	1.424(3)	C6D	C7D	1.392(4)
O2D	C11D	1.418(4)	C7D	C8D	1.385(4)
C1D	C2D	1.531(4)	C7D	C10D	1.511(4)
C1D	C4D	1.510(4)	C8D	C9D	1.389(4)
C2D	C3D	1.513(4)			

Table 4. Selected Interatomic Angles (deg)

(a) Molecule A

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C3A	O2A	C11A	110.5(2)	I1A	C5A	C6A	115.5(2)
C2A	C1A	C4A	115.2(2)	C4A	C5A	C6A	122.6(3)
O1A	C2A	C1A	105.3(2)	C5A	C6A	C7A	120.7(3)
O1A	C2A	C3A	111.6(2)	C6A	C7A	C8A	118.0(3)
C1A	C2A	C3A	112.0(2)	C6A	C7A	C10A	121.6(3)
O2A	C3A	C2A	109.1(2)	C8A	C7A	C10A	120.3(3)
C1A	C4A	C5A	123.3(2)	C7A	C8A	C9A	120.5(3)
C1A	C4A	C9A	121.8(2)	I2A	C9A	C4A	121.7(2)
C5A	C4A	C9A	114.9(2)	I2A	C9A	C8A	115.0(2)
I1A	C5A	C4A	121.9(2)	C4A	C9A	C8A	123.2(3)

(b) Molecule B

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C3B	O2B	C11B	112.4(2)	I1B	C5B	C6B	114.98(19)
C2B	C1B	C4B	113.0(2)	C4B	C5B	C6B	123.4(2)
O1B	C2B	C1B	106.4(2)	C5B	C6B	C7B	120.0(3)
O1B	C2B	C3B	109.9(2)	C6B	C7B	C8B	118.8(2)
C1B	C2B	C3B	112.9(2)	C6B	C7B	C10B	121.1(3)
O2B	C3B	C2B	107.2(2)	C8B	C7B	C10B	120.1(2)
C1B	C4B	C5B	124.2(2)	C7B	C8B	C9B	119.8(2)
C1B	C4B	C9B	121.4(2)	I2B	C9B	C4B	120.98(19)
C5B	C4B	C9B	114.4(2)	I2B	C9B	C8B	115.52(19)
I1B	C5B	C4B	121.63(19)	C4B	C9B	C8B	123.4(2)

(c) Molecule C

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C3C	O2C	C11C	111.8(2)	I1C	C5C	C6C	116.2(2)
C2C	C1C	C4C	113.4(2)	C4C	C5C	C6C	122.7(2)
O1C	C2C	C1C	105.1(2)	C5C	C6C	C7C	120.8(3)
O1C	C2C	C3C	111.0(2)	C6C	C7C	C8C	118.0(3)
C1C	C2C	C3C	113.8(2)	C6C	C7C	C10C	121.1(3)
O2C	C3C	C2C	106.9(2)	C8C	C7C	C10C	120.9(3)
C1C	C4C	C5C	123.1(2)	C7C	C8C	C9C	120.5(3)
C1C	C4C	C9C	121.8(2)	I2C	C9C	C4C	120.68(19)
C5C	C4C	C9C	115.0(2)	I2C	C9C	C8C	116.41(19)
I1C	C5C	C4C	121.11(19)	C4C	C9C	C8C	122.9(2)

Table 4. Selected Interatomic Angles (continued)

(d) Molecule D

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C3D	O2D	C11D	111.7(2)	I1D	C5D	C6D	115.3(2)
C2D	C1D	C4D	114.2(2)	C4D	C5D	C6D	123.1(3)
O1D	C2D	C1D	105.9(2)	C5D	C6D	C7D	120.2(3)
O1D	C2D	C3D	111.6(2)	C6D	C7D	C8D	118.5(3)
C1D	C2D	C3D	112.0(2)	C6D	C7D	C10D	121.6(3)
O2D	C3D	C2D	109.0(2)	C8D	C7D	C10D	119.9(3)
C1D	C4D	C5D	123.4(2)	C7D	C8D	C9D	120.4(3)
C1D	C4D	C9D	121.8(3)	I2D	C9D	C4D	121.2(2)
C5D	C4D	C9D	114.9(3)	I2D	C9D	C8D	115.9(2)
I1D	C5D	C4D	121.6(2)	C4D	C9D	C8D	122.9(3)

Table 5. Hydrogen-Bonded Interactions

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (deg)
O1A–H1OA···O1B	0.78(3)	2.08(4)	2.850(3)	171(4)
O1B–H1OB···O2A	0.74(4)	2.12(4)	2.772(3)	147(4)
O1C–H1OC···O2D	0.71(4)	2.04(4)	2.703(3)	155(4)
O1D–H1OD···O1C	0.76(4)	2.07(4)	2.818(3)	168(4)

Table 6. Torsional Angles (deg)

(a) Molecule A

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11A	O2A	C3A	C2A	-177.2(2)	C1A	C4A	C9A	C8A	179.7(3)
C4A	C1A	C2A	O1A	173.2(2)	C5A	C4A	C9A	I2A	178.92(19)
C4A	C1A	C2A	C3A	-65.4(3)	C5A	C4A	C9A	C8A	-0.1(4)
C2A	C1A	C4A	C5A	100.3(3)	I1A	C5A	C6A	C7A	179.9(2)
C2A	C1A	C4A	C9A	-79.5(3)	C4A	C5A	C6A	C7A	-0.2(4)
O1A	C2A	C3A	O2A	-67.5(3)	C5A	C6A	C7A	C8A	-1.1(4)
C1A	C2A	C3A	O2A	174.8(2)	C5A	C6A	C7A	C10A	-180.0(3)
C1A	C4A	C5A	I1A	0.9(4)	C6A	C7A	C8A	C9A	1.7(4)
C1A	C4A	C5A	C6A	-179.1(3)	C10A	C7A	C8A	C9A	-179.4(3)
C9A	C4A	C5A	I1A	-179.25(19)	C7A	C8A	C9A	I2A	179.8(2)
C9A	C4A	C5A	C6A	0.8(4)	C7A	C8A	C9A	C4A	-1.1(4)
C1A	C4A	C9A	I2A	-1.2(4)					

(b) Molecule B

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11B	O2B	C3B	C2B	-178.5(2)	C1B	C4B	C9B	C8B	177.2(2)
C4B	C1B	C2B	O1B	165.9(2)	C5B	C4B	C9B	I2B	174.68(18)
C4B	C1B	C2B	C3B	-73.4(3)	C5B	C4B	C9B	C8B	-2.3(4)
C2B	C1B	C4B	C5B	101.9(3)	I1B	C5B	C6B	C7B	176.6(2)
C2B	C1B	C4B	C9B	-77.6(3)	C4B	C5B	C6B	C7B	-1.8(4)
O1B	C2B	C3B	O2B	-59.5(3)	C5B	C6B	C7B	C8B	-0.3(4)
C1B	C2B	C3B	O2B	-178.2(2)	C5B	C6B	C7B	C10B	-179.8(3)
C1B	C4B	C5B	I1B	5.2(4)	C6B	C7B	C8B	C9B	1.0(4)
C1B	C4B	C5B	C6B	-176.5(3)	C10B	C7B	C8B	C9B	-179.5(3)
C9B	C4B	C5B	I1B	-175.32(18)	C7B	C8B	C9B	I2B	-176.8(2)
C9B	C4B	C5B	C6B	3.0(4)	C7B	C8B	C9B	C4B	0.4(4)
C1B	C4B	C9B	I2B	-5.8(3)					

(c) Molecule C

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11C	O2C	C3C	C2C	-173.3(2)	C9C	C4C	C5C	I1C	-178.12(18)
C4C	C1C	C2C	O1C	173.8(2)	C9C	C4C	C5C	C6C	2.3(4)
C4C	C1C	C2C	C3C	-64.6(3)	C1C	C4C	C9C	I2C	-6.6(3)
C2C	C1C	C4C	C5C	100.9(3)	C1C	C4C	C9C	C8C	175.2(2)
C2C	C1C	C4C	C9C	-77.0(3)	C5C	C4C	C9C	I2C	175.30(18)
O1C	C2C	C3C	O2C	-62.9(3)	C5C	C4C	C9C	C8C	-2.9(4)
C1C	C2C	C3C	O2C	178.8(2)	I1C	C5C	C6C	C7C	-179.2(2)
C1C	C4C	C5C	I1C	3.8(4)	C4C	C5C	C6C	C7C	0.4(4)
C1C	C4C	C5C	C6C	-175.8(3)	C5C	C6C	C7C	C8C	-2.7(4)

Table 6. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C5C	C6C	C7C	C10C	177.9(3)	C7C	C8C	C9C	I2C	-177.5(2)
C6C	C7C	C8C	C9C	2.1(4)	C7C	C8C	C9C	C4C	0.7(4)
C10C	C7C	C8C	C9C	-178.4(3)					

(d) Molecule D

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11D	O2D	C3D	C2D	-178.4(2)	C1D	C4D	C9D	C8D	178.7(3)
C4D	C1D	C2D	O1D	175.2(2)	C5D	C4D	C9D	I2D	178.53(19)
C4D	C1D	C2D	C3D	-62.9(3)	C5D	C4D	C9D	C8D	-0.8(4)
C2D	C1D	C4D	C5D	100.6(3)	I1D	C5D	C6D	C7D	179.6(2)
C2D	C1D	C4D	C9D	-78.8(3)	C4D	C5D	C6D	C7D	-0.7(4)
O1D	C2D	C3D	O2D	-66.9(3)	C5D	C6D	C7D	C8D	-1.2(4)
C1D	C2D	C3D	O2D	174.5(2)	C5D	C6D	C7D	C10D	-179.9(3)
C1D	C4D	C5D	I1D	1.9(4)	C6D	C7D	C8D	C9D	2.1(4)
C1D	C4D	C5D	C6D	-177.8(3)	C10D	C7D	C8D	C9D	-179.3(3)
C9D	C4D	C5D	I1D	-178.67(19)	C7D	C8D	C9D	I2D	179.6(2)
C9D	C4D	C5D	C6D	1.6(4)	C7D	C8D	C9D	C4D	-1.1(4)
C1D	C4D	C9D	I2D	-2.0(4)					

Table 7. Anisotropic Displacement Parameters (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1A	0.03830(11)	0.05088(13)	0.03132(10)	0.00538(9)	0.01641(9)	-0.00416(9)
I2A	0.04497(12)	0.03570(11)	0.04251(12)	0.01357(9)	0.01855(10)	-0.00039(9)
O1A	0.0365(12)	0.0379(13)	0.0287(11)	-0.0012(10)	0.0009(9)	0.0134(10)
O2A	0.0355(11)	0.0247(10)	0.0289(10)	-0.0013(8)	0.0017(9)	-0.0009(9)
C1A	0.0301(14)	0.0235(14)	0.0290(14)	0.0007(11)	0.0107(12)	0.0020(11)
C2A	0.0285(14)	0.0281(15)	0.0250(13)	0.0016(11)	0.0084(11)	0.0039(11)
C3A	0.0256(13)	0.0281(15)	0.0260(13)	-0.0007(11)	0.0049(11)	-0.0006(11)
C4A	0.0309(14)	0.0209(13)	0.0261(13)	-0.0042(10)	0.0103(11)	-0.0004(11)
C5A	0.0318(15)	0.0274(14)	0.0255(13)	-0.0035(11)	0.0127(12)	-0.0013(12)
C6A	0.0344(16)	0.0355(17)	0.0228(13)	-0.0014(12)	0.0066(12)	-0.0022(13)
C7A	0.0290(14)	0.0276(15)	0.0304(14)	-0.0074(12)	0.0073(12)	-0.0025(12)
C8A	0.0308(15)	0.0268(15)	0.0365(15)	-0.0081(12)	0.0133(12)	-0.0043(12)
C9A	0.0344(15)	0.0198(13)	0.0281(13)	-0.0017(11)	0.0119(12)	-0.0011(11)
C10A	0.0315(16)	0.0444(19)	0.0421(18)	-0.0074(15)	0.0023(14)	-0.0001(14)
C11A	0.054(2)	0.0265(16)	0.0436(18)	0.0044(14)	0.0007(16)	-0.0013(15)
I1B	0.03690(11)	0.04505(12)	0.02971(10)	-0.00424(8)	0.01430(8)	0.00938(9)
I2B	0.03692(11)	0.03092(10)	0.03188(10)	-0.00898(8)	0.01169(8)	0.00246(8)
O1B	0.0276(10)	0.0300(11)	0.0254(10)	0.0027(9)	-0.0011(8)	-0.0049(9)
O2B	0.0423(12)	0.0255(11)	0.0283(10)	0.0017(8)	0.0046(9)	0.0011(9)
C1B	0.0222(13)	0.0253(14)	0.0278(13)	-0.0008(11)	0.0077(11)	-0.0006(11)
C2B	0.0237(13)	0.0266(14)	0.0218(12)	-0.0018(10)	0.0063(10)	-0.0027(11)
C3B	0.0278(14)	0.0272(14)	0.0256(13)	0.0018(11)	0.0055(11)	0.0002(11)
C4B	0.0252(13)	0.0210(13)	0.0248(13)	0.0036(10)	0.0091(11)	-0.0004(10)
C5B	0.0279(14)	0.0243(14)	0.0231(13)	0.0006(10)	0.0101(11)	0.0035(11)
C6B	0.0311(15)	0.0291(15)	0.0226(13)	-0.0006(11)	0.0045(11)	-0.0012(12)
C7B	0.0235(13)	0.0265(14)	0.0262(13)	0.0055(11)	0.0051(11)	0.0000(11)
C8B	0.0263(13)	0.0264(14)	0.0285(13)	0.0056(11)	0.0108(11)	0.0043(11)
C9B	0.0298(14)	0.0195(13)	0.0206(12)	0.0013(10)	0.0091(11)	0.0020(10)
C10B	0.0300(15)	0.0461(19)	0.0345(16)	0.0001(14)	0.0055(13)	-0.0033(14)
C11B	0.0484(19)	0.0272(16)	0.0450(18)	0.0042(14)	0.0117(15)	0.0001(14)
I1C	0.03049(10)	0.03862(11)	0.02809(9)	0.00459(8)	0.01289(8)	-0.00062(8)
I2C	0.03839(11)	0.03674(11)	0.03336(10)	0.00887(8)	0.01422(8)	-0.00466(8)
O1C	0.0394(13)	0.0350(13)	0.0290(11)	-0.0045(10)	-0.0098(10)	0.0048(10)
O2C	0.0459(13)	0.0266(11)	0.0351(11)	-0.0064(9)	0.0032(10)	0.0011(9)
C1C	0.0234(13)	0.0231(13)	0.0222(12)	0.0002(10)	0.0048(10)	0.0021(10)
C2C	0.0281(14)	0.0317(15)	0.0239(13)	-0.0003(11)	0.0013(11)	0.0022(12)
C3C	0.0304(15)	0.0304(16)	0.0319(15)	-0.0035(12)	0.0052(12)	-0.0001(12)
C4C	0.0243(13)	0.0194(13)	0.0222(12)	-0.0019(10)	0.0061(10)	-0.0002(10)
C5C	0.0258(13)	0.0244(14)	0.0242(13)	-0.0008(10)	0.0083(11)	-0.0018(11)
C6C	0.0294(14)	0.0320(15)	0.0260(13)	0.0027(12)	0.0045(11)	-0.0011(12)

Table 7. Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C7C	0.0281(14)	0.0252(14)	0.0327(15)	0.0000(12)	0.0018(12)	-0.0015(11)
C8C	0.0235(13)	0.0258(14)	0.0338(14)	-0.0046(12)	0.0087(11)	-0.0028(11)
C9C	0.0290(14)	0.0220(13)	0.0221(12)	-0.0011(10)	0.0088(11)	-0.0033(11)
C10C	0.0275(16)	0.046(2)	0.058(2)	0.0139(17)	0.0040(15)	0.0059(14)
C11C	0.047(2)	0.0302(17)	0.053(2)	-0.0051(15)	0.0178(16)	-0.0002(14)
I1D	0.03691(11)	0.04433(12)	0.03025(10)	-0.00184(8)	0.01585(8)	0.00659(9)
I2D	0.04881(13)	0.03061(11)	0.04615(12)	-0.01048(9)	0.02594(10)	-0.00152(9)
O1D	0.0395(13)	0.0405(14)	0.0343(12)	-0.0008(11)	-0.0002(10)	-0.0153(10)
O2D	0.0414(12)	0.0254(11)	0.0283(10)	0.0008(8)	0.0008(9)	-0.0026(9)
C1D	0.0332(15)	0.0241(14)	0.0317(14)	-0.0018(11)	0.0127(12)	-0.0042(12)
C2D	0.0307(15)	0.0277(14)	0.0266(13)	-0.0020(11)	0.0096(12)	-0.0059(12)
C3D	0.0295(14)	0.0279(15)	0.0245(13)	0.0017(11)	0.0036(11)	0.0007(12)
C4D	0.0310(14)	0.0208(13)	0.0294(14)	0.0048(11)	0.0125(12)	0.0008(11)
C5D	0.0336(15)	0.0261(14)	0.0280(14)	0.0041(11)	0.0138(12)	0.0052(12)
C6D	0.0342(16)	0.0351(16)	0.0269(14)	0.0046(12)	0.0080(12)	0.0041(13)
C7D	0.0325(15)	0.0272(15)	0.0358(15)	0.0095(12)	0.0102(13)	0.0059(12)
C8D	0.0333(15)	0.0266(15)	0.0387(16)	0.0068(12)	0.0186(13)	0.0074(12)
C9D	0.0394(16)	0.0201(13)	0.0326(14)	0.0027(11)	0.0189(13)	0.0015(12)
C10D	0.0358(17)	0.052(2)	0.0403(18)	0.0110(16)	0.0042(14)	0.0048(15)
C11D	0.056(2)	0.0272(17)	0.0384(17)	-0.0022(13)	-0.0046(15)	-0.0052(15)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	0.1782	0.1329	0.0770	0.033
H1B	0.1516	0.0159	0.1071	0.033
H2A	0.1358	0.2394	0.1485	0.032
H3A	0.2075	0.4189	0.1001	0.033
H3B	0.1251	0.4376	0.0945	0.033
H6A	-0.0243	0.2870	-0.0253	0.038
H8A	-0.0923	0.0595	0.0627	0.037
H10A	-0.1775	0.1524	0.0027	0.049
H10B	-0.1531	0.1405	-0.0392	0.049
H10C	-0.1568	0.3096	-0.0180	0.049
H11A	0.1961	0.7494	0.1600	0.053
H11B	0.2207	0.6905	0.1205	0.053
H11C	0.1388	0.7021	0.1164	0.053
H1C	0.3334	0.3689	0.3092	0.030
H1D	0.3566	0.2416	0.2800	0.030
H2B	0.3757	0.4638	0.2367	0.029
H3C	0.2962	0.6384	0.2817	0.033
H3D	0.3763	0.6764	0.2840	0.033
H6B	0.5434	0.5394	0.4026	0.034
H8B	0.6000	0.2943	0.3126	0.032
H10D	0.6657	0.5450	0.4022	0.045
H10E	0.6873	0.4623	0.3643	0.045
H10F	0.6791	0.3577	0.4030	0.045
H11D	0.2823	0.9458	0.2092	0.049
H11E	0.2638	0.8983	0.2516	0.049
H11F	0.3436	0.9321	0.2532	0.049
H1E	0.1873	0.0989	0.3301	0.028
H1F	0.1534	-0.0106	0.3585	0.028
H2C	0.1371	0.2182	0.3976	0.035
H3E	0.2176	0.3892	0.3528	0.038
H3F	0.1356	0.4204	0.3468	0.038
H6C	-0.0013	0.2804	0.2226	0.036
H8C	-0.0878	0.0911	0.3079	0.033
H10G	-0.1605	0.1502	0.2321	0.055
H10H	-0.1261	0.2615	0.2043	0.055
H10I	-0.1455	0.3331	0.2444	0.055
H11G	0.2113	0.7097	0.4192	0.052
H11H	0.2333	0.6635	0.3779	0.052
H11I	0.1521	0.6767	0.3753	0.052
H1G	0.3268	-0.0981	0.5594	0.035

Table 8. Derived Parameters for Hydrogen Atoms (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1H	0.3534	-0.2160	0.5295	0.035
H2D	0.3656	0.0026	0.4861	0.034
H3G	0.2992	0.1917	0.5357	0.034
H3H	0.3811	0.2061	0.5393	0.034
H6D	0.5297	0.0749	0.6581	0.039
H8D	0.5967	-0.1533	0.5696	0.037
H10J	0.6814	-0.0204	0.6247	0.053
H10K	0.6642	-0.0818	0.6665	0.053
H10L	0.6567	0.1025	0.6544	0.053
H11J	0.3072	0.5127	0.4717	0.053
H11K	0.2845	0.4614	0.5124	0.053
H11L	0.3660	0.4714	0.5152	0.053

1.5.2 X-ray data of 1-(2,6-diiodo-4-methylphenyl)-3-(2-methoxyphenoxy)propan-2-ol (**7k**)

STRUCTURE REPORT

XCL Code: JUS1617 **Date:** 23 January 2017

Compound: 1-(2,6-Diiodo-4-methylphenyl)-3-(2-methoxyphenoxy)propan-2-ol
Formula: $C_{17}H_{18}I_2O_3$

Supervisor: R. M. Al-Zoubi, Jordan University of Science and Technology
Crystallographer: R. McDonald

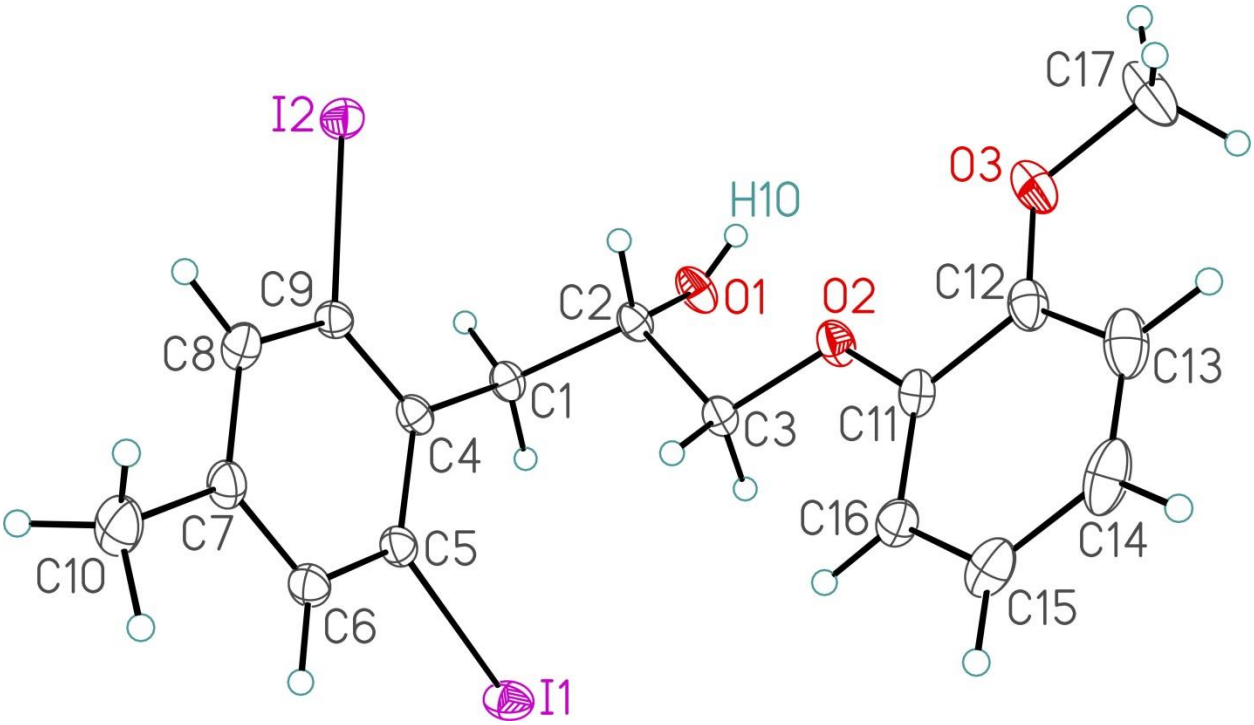
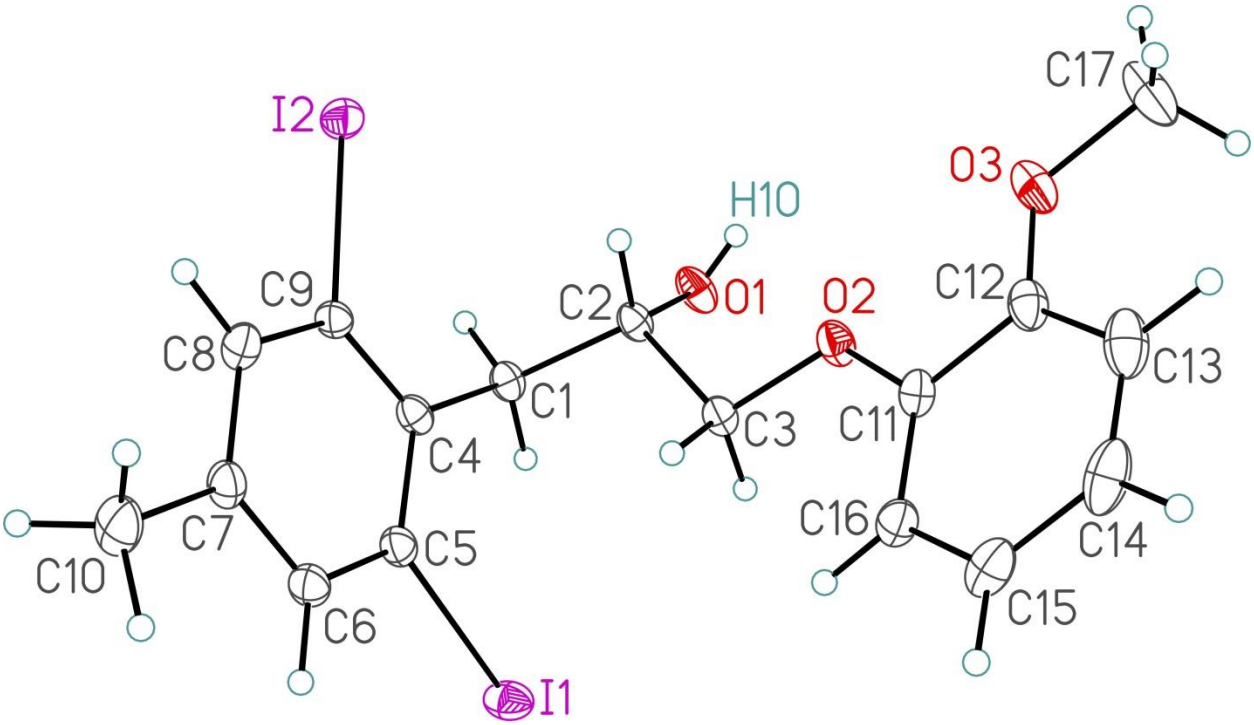
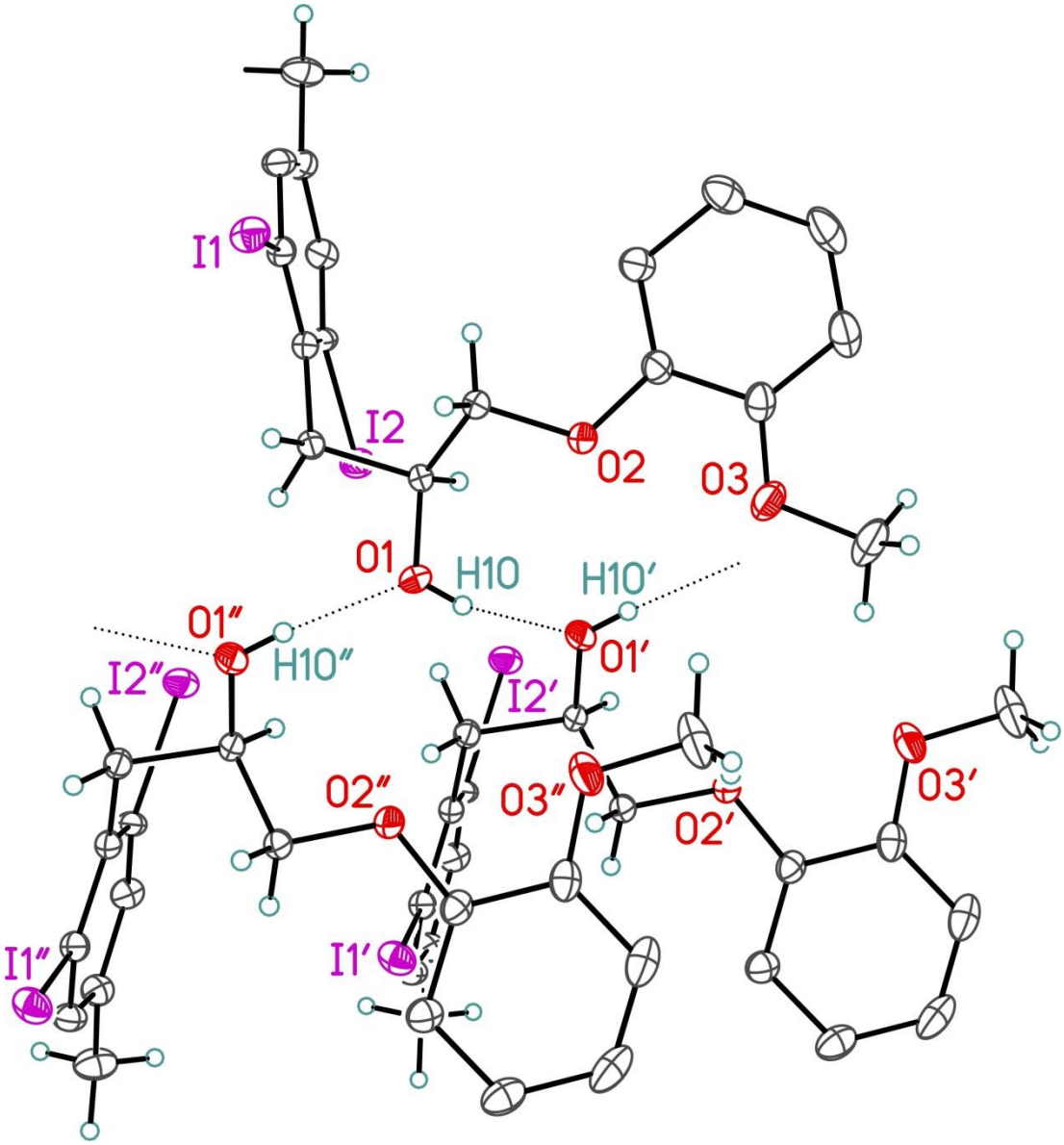


Figure Legends

Figure 1. Perspective view of the 1-(2,6-diiodo-4-methylphenyl)-3-(2-methoxyphenoxy)-propan-2-ol molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 30% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters.

Figure 2. Illustration of hydrogen-bonded contacts (dotted lines) between adjacent molecules in the crystal lattice. Primed atoms are related to unprimed ones via the crystallographic rotational-translational symmetry operation (x, $^{1}/_{2}–y$, $^{1}/_{2}+z$). Double-primed atoms are related to unprimed ones via the crystallographic rotational-translational symmetry operation (x, $^{1}/_{2}–y$, $^{-1}/_{2}+z$). The chain propagates in a direction parallel to the crystal unit cell's c axis.


C17
I2
O3
H10
C9
C2
O1
O2
C12
C8
C1
C3
C11
C13
C4
C7
C5
C16
C14
C10
C6
C15
I1


I1
I2
O2
O3
O1
H10
H10′
O1″
H10″
O1′
I2″
I2′
O2″
O3″
O2′
O3′
I1″
I1′

List of Tables

Table 1. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{17}H_{18}I_2O_3$
formula weight	524.11
crystal dimensions (mm)	0.31 × 0.10 × 0.04
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	10.6792 (4)
b (Å)	29.0562 (9)
c (Å)	5.62368 (19)
β (deg)	92.355 (2)
V (Å^3)	1743.54 (10)
Z	4
ρ_{calcd} (g cm^{-3})	1.997
μ (mm^{-1})	28.41
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω and ϕ scans (1.0°) (5 s exposures)
data collection 2θ limit (deg)	148.18
total data collected	11975 (-13 ≤ h ≤ 12, -36 ≤ k ≤ 36, -6 ≤ l ≤ 6)
independent reflections	3517 (R_{int} = 0.0502)
number of observed reflections (*NO*)	3075 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT-2014*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2014*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	1.0000–0.4831
data/restraints/parameters	3517 / 0 / 204
goodness-of-fit (S)[e] [all data]	1.023
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0310
wR_2 [all data]	0.0834
largest difference peak and hole	1.066 and –1.399 e Å^{-3}

[a]Obtained from least-squares refinement of 9976 reflections with 6.08° < 2θ < 148.00°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *A71*, 3–8.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *C71*, 3–8.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0501P)^2]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	*x*	*y*	*z*	U_{eq}, Å^2
I1	0.13498(3)	0.08465(2)	-0.52957(5)	0.03591(10)*
I2	-0.16250(2)	0.19914(2)	0.17704(5)	0.03350(9)*
O1	0.2094(3)	0.23473(10)	-0.1249(6)	0.0352(7)*
O2	0.3423(3)	0.16776(10)	0.1542(5)	0.0314(6)*
O3	0.4729(3)	0.19215(12)	0.5218(6)	0.0426(8)*
C1	0.0513(4)	0.18029(13)	-0.2347(7)	0.0256(7)*
C2	0.1567(4)	0.19207(13)	-0.0512(7)	0.0248(7)*
C3	0.2574(4)	0.15537(13)	-0.0384(7)	0.0252(7)*
C4	-0.0224(4)	0.13768(13)	-0.1705(7)	0.0253(7)*
C5	-0.0023(4)	0.09441(14)	-0.2745(7)	0.0273(8)*
C6	-0.0661(4)	0.05514(14)	-0.2126(8)	0.0309(8)*
C7	-0.1554(4)	0.05655(15)	-0.0388(8)	0.0305(8)*
C8	-0.1801(4)	0.09896(15)	0.0646(8)	0.0305(8)*
C9	-0.1152(4)	0.13797(12)	-0.0039(7)	0.0253(7)*
C10	-0.2220(4)	0.01336(16)	0.0364(10)	0.0431(11)*
C11	0.4170(4)	0.13413(14)	0.2523(8)	0.0287(8)*
C12	0.4873(4)	0.14749(16)	0.4560(8)	0.0330(9)*
C13	0.5633(4)	0.1153(2)	0.5766(9)	0.0446(12)*
C14	0.5672(5)	0.0705(2)	0.4951(11)	0.0507(14)*
C15	0.4989(4)	0.05721(17)	0.2931(10)	0.0412(11)*
C16	0.4242(4)	0.08934(15)	0.1669(8)	0.0321(9)*
C17	0.5473(6)	0.2087(2)	0.7215(9)	0.0554(15)*
H1O	0.233(5)	0.2464(19)	-0.017(10)	0.031(14)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3. Selected Interatomic Distances (Å)

Atom1	Atom2	Distance	Atom1	Atom2	Distance
I1	C5	2.112(4)	C5	C6	1.381(6)
I2	C9	2.119(4)	C6	C7	1.394(6)
O1	C2	1.430(5)	C7	C8	1.392(6)
O2	C3	1.429(4)	C7	C10	1.511(6)
O2	C11	1.364(5)	C8	C9	1.391(5)
O3	C12	1.360(6)	C11	C12	1.398(6)
O3	C17	1.432(6)	C11	C16	1.391(6)
C1	C2	1.534(5)	C12	C13	1.395(6)
C1	C4	1.519(5)	C13	C14	1.382(8)
C2	C3	1.515(5)	C14	C15	1.380(8)
C4	C5	1.407(5)	C15	C16	1.402(6)
C4	C9	1.391(6)			

Table 4. Selected Interatomic Angles (deg)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C3	O2	C11	117.9(3)	C8	C7	C10	121.3(4)
C12	O3	C17	117.9(4)	C7	C8	C9	120.0(4)
C2	C1	C4	113.3(3)	I2	C9	C4	121.3(3)
O1	C2	C1	106.6(3)	I2	C9	C8	114.8(3)
O1	C2	C3	109.7(3)	C4	C9	C8	123.9(4)
C1	C2	C3	112.0(3)	O2	C11	C12	114.7(4)
O2	C3	C2	106.6(3)	O2	C11	C16	124.8(4)
C1	C4	C5	122.7(4)	C12	C11	C16	120.5(4)
C1	C4	C9	123.1(3)	O3	C12	C11	115.2(4)
C5	C4	C9	114.2(4)	O3	C12	C13	125.2(4)
I1	C5	C4	121.6(3)	C11	C12	C13	119.6(5)
I1	C5	C6	115.1(3)	C12	C13	C14	119.7(5)
C4	C5	C6	123.3(4)	C13	C14	C15	121.0(5)
C5	C6	C7	120.7(4)	C14	C15	C16	120.1(5)
C6	C7	C8	117.7(4)	C11	C16	C15	119.1(4)
C6	C7	C10	121.0(4)				

Table 5. Hydrogen-Bonded Interactions

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (deg)
O1–H1O···O1[a]	0.73(6)	2.29(6)	2.9485(18)	150(6)

[a]At *x*, 1/2–*y*, 1/2+*z*.

Table 6. Torsional Angles (deg)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11	O2	C3	C2	159.5(3)	I1	C5	C6	C7	177.3(3)
C3	O2	C11	C12	-173.2(3)	C4	C5	C6	C7	-0.3(6)
C3	O2	C11	C16	5.4(6)	C5	C6	C7	C8	1.7(6)
C17	O3	C12	C11	-176.7(4)	C5	C6	C7	C10	-177.6(4)
C17	O3	C12	C13	4.3(7)	C6	C7	C8	C9	-0.9(6)
C4	C1	C2	O1	-175.0(3)	C10	C7	C8	C9	178.4(4)
C4	C1	C2	C3	65.1(4)	C7	C8	C9	I2	-178.9(3)
C2	C1	C4	C5	-100.8(4)	C7	C8	C9	C4	-1.4(7)
C2	C1	C4	C9	79.0(5)	O2	C11	C12	O3	-1.6(5)
O1	C2	C3	O2	67.9(4)	O2	C11	C12	C13	177.5(4)
C1	C2	C3	O2	-174.0(3)	C16	C11	C12	O3	179.8(4)
C1	C4	C5	I1	0.6(5)	C16	C11	C12	C13	-1.2(6)
C1	C4	C5	C6	178.0(4)	O2	C11	C16	C15	-176.0(4)
C9	C4	C5	I1	-179.2(3)	C12	C11	C16	C15	2.5(6)
C9	C4	C5	C6	-1.8(6)	O3	C12	C13	C14	178.2(5)
C1	C4	C9	I2	0.1(5)	C11	C12	C13	C14	-0.8(7)
C1	C4	C9	C8	-177.2(4)	C12	C13	C14	C15	1.3(8)
C5	C4	C9	I2	180.0(3)	C13	C14	C15	C16	0.1(7)
C5	C4	C9	C8	2.6(6)	C14	C15	C16	C11	-2.0(7)

Table 7. Anisotropic Displacement Parameters (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	0.04579(17)	0.03350(15)	0.02917(15)	-0.00375(10)	0.01044(11)	-0.00345(11)
I2	0.03196(14)	0.02755(14)	0.04114(17)	-0.00503(10)	0.00350(11)	0.00278(10)
O1	0.0429(17)	0.0235(14)	0.0381(18)	0.0017(13)	-0.0106(14)	-0.0095(13)
O2	0.0310(14)	0.0260(14)	0.0363(16)	0.0002(12)	-0.0105(12)	-0.0003(11)
O3	0.0429(18)	0.0454(18)	0.0386(18)	-0.0054(15)	-0.0078(14)	-0.0130(15)
C1	0.0264(17)	0.0248(18)	0.0253(19)	0.0031(14)	-0.0032(14)	-0.0029(15)
C2	0.0277(17)	0.0215(17)	0.0244(19)	0.0020(14)	-0.0067(14)	-0.0003(14)
C3	0.0255(17)	0.0232(17)	0.0266(19)	0.0006(14)	-0.0043(14)	-0.0019(14)
C4	0.0269(17)	0.0224(17)	0.0261(19)	0.0009(14)	-0.0055(14)	-0.0010(14)
C5	0.0252(17)	0.0261(18)	0.030(2)	-0.0015(15)	-0.0042(15)	0.0003(15)
C6	0.0294(18)	0.0225(18)	0.041(2)	-0.0022(16)	-0.0010(17)	-0.0003(15)
C7	0.0256(18)	0.028(2)	0.038(2)	0.0016(17)	0.0006(16)	-0.0051(16)
C8	0.0243(17)	0.030(2)	0.037(2)	0.0033(17)	0.0030(16)	-0.0005(16)
C9	0.0252(17)	0.0181(16)	0.032(2)	-0.0026(14)	-0.0010(15)	0.0011(14)
C10	0.036(2)	0.028(2)	0.066(3)	0.006(2)	0.009(2)	-0.0068(18)
C11	0.0211(17)	0.0311(19)	0.034(2)	0.0040(16)	-0.0009(15)	-0.0021(15)
C12	0.0270(18)	0.045(2)	0.027(2)	0.0053(18)	-0.0004(16)	-0.0058(18)
C13	0.033(2)	0.061(3)	0.039(3)	0.019(2)	-0.0066(19)	-0.007(2)
C14	0.030(2)	0.057(3)	0.064(4)	0.027(3)	-0.004(2)	0.008(2)
C15	0.031(2)	0.038(2)	0.056(3)	0.010(2)	0.006(2)	0.0057(19)
C16	0.0262(18)	0.031(2)	0.039(2)	0.0017(17)	0.0021(16)	0.0001(16)
C17	0.060(3)	0.073(4)	0.032(3)	0.000(2)	-0.008(2)	-0.036(3)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	-0.0068	0.2068	-0.2498	0.031
H1B	0.0881	0.1754	-0.3916	0.031
H2	0.1208	0.1959	0.1090	0.030
H3A	0.2200	0.1248	-0.0094	0.030
H3B	0.3018	0.1541	-0.1894	0.030
H6	-0.0489	0.0268	-0.2894	0.037
H8	-0.2413	0.1013	0.1820	0.037
H10A	-0.3082	0.0136	-0.0304	0.052
H10B	-0.2231	0.0122	0.2104	0.052
H10C	-0.1779	-0.0137	-0.0221	0.052
H13	0.6121	0.1242	0.7140	0.054
H14	0.6177	0.0485	0.5795	0.061
H15	0.5026	0.0263	0.2394	0.049
H16	0.3790	0.0806	0.0250	0.039
H17A	0.5277	0.2411	0.7494	0.067
H17B	0.5287	0.1906	0.8630	0.067
H17C	0.6363	0.2055	0.6889	0.067