Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Material

Development of highly sensitive and selective molecules for detection of spermidine and spermine.

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X-Ray crystallographic analysis of [21·2MeOH].

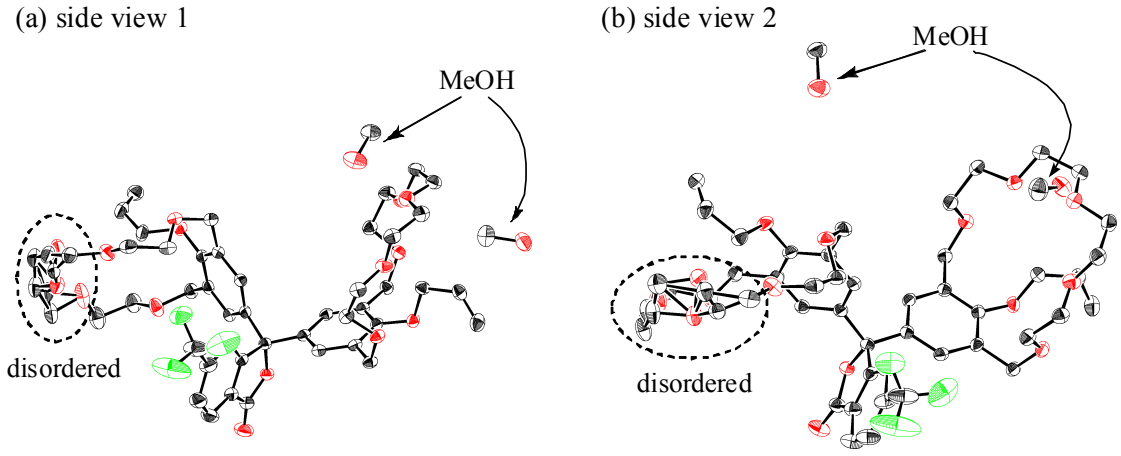
The intensity data were collected on a Rigaku/MSC Mercury CCD diffractometer with graphite monochromated MoKα radiation (λ = 0.71069 Å). Single crystals suitable for X-ray analysis were obtained by slow recrystallization from MeOH at room temperature. A colorless crystal (0.10 × 0.10 × 0.02 mm^3) of [**21**·2MeOH**]** was mounted on a glass fiber. The structure was solved by a direct method (SIR-97[S1]) and refined by full-matrix least-squares procedures on F^2 for all reflections (SHELXL-97[S2]). Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 669857. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk.).

Crystal data for **21**·2MeOH: C49H65F3O16, M = 967.01, monoclinic, a = 16.2859(2), b = 18.5760(4), c = 17.0941(3) Å , b = 107.1049(8) °, V = 4942.68(15) $Å^3$, space group $P21/a$ (#14), Z = 4, D = 1.300 g/cm^3, Mo-Ka (λ = 0.71070 Å, T = 93 K), measured reflections = 42593. Structure solution by SIR-97, refinement by full-matrix least-squares using all reflections (SHELXL-97), R = 0.0475 [|Fo | > 2r(Fo)], Rw = 0.119 (all reflections), GOF = 1.061.

S1. Altomare, A., Burla, M., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A., Polidori, G. & Spagna, R. 1999 *J. Appl. Cryst.* **32**, 115-119.

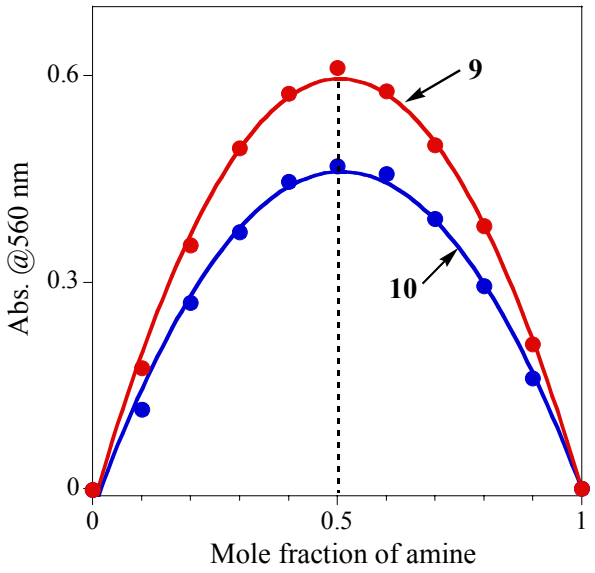
S2. Sheldrick, G.M. 1997 SHELX-97, Program for the Refinement of Crystal Structures; University of Göttingen, Germany.

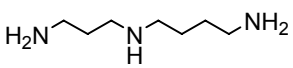
Figure S1. Structure of compound **21**·2MeOH.



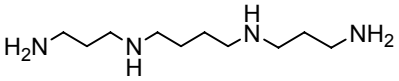
Displacement ellipsoids are scaled to the 50% probability level.

Figure S2. Job's plot between host **5** and spermidine (**9**) and spermine (**10**).





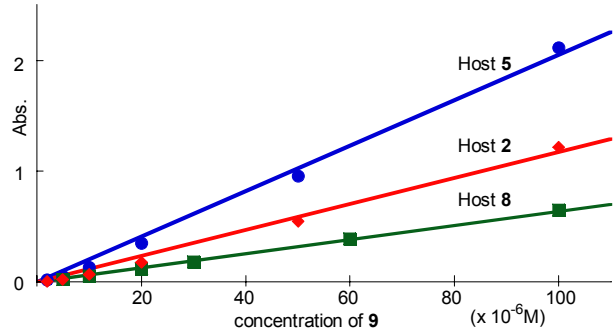
Spermidine (**9**)



Spermine (**10**)

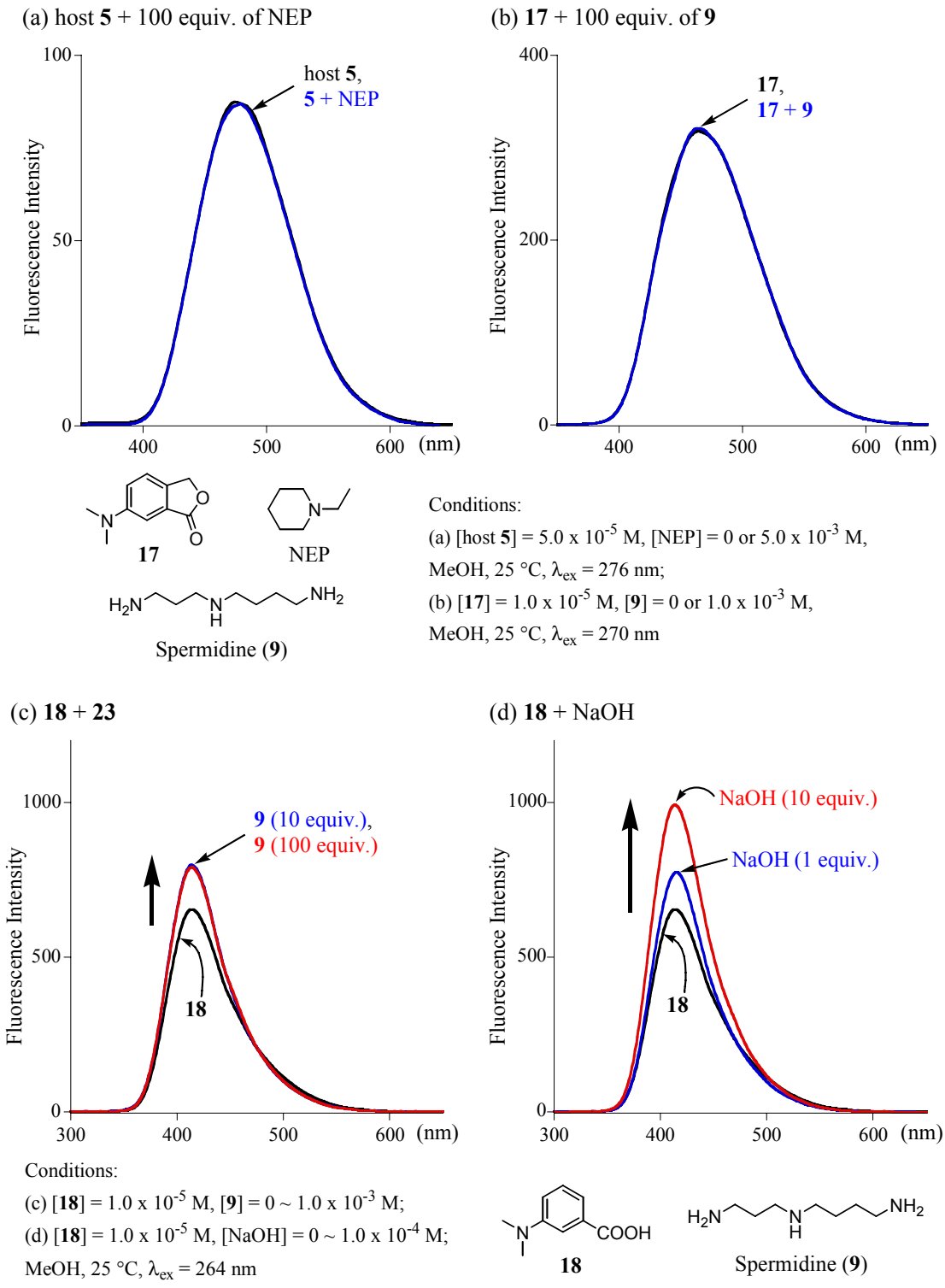
Conditions:
[host **5**] + [amine] = 2.5 x 10^{-4} M,
MeOH, 25 °C

Figure S3. Detection sensitivities of hosts **2**, **5**, and **8**.



Conditions: [host **2**] = 5.0 x 10^{-4} M, [host **5**] = 1.0 x 10^{-3} M, [host **8**] = 2.0 x 10^{-4} M, 25 °C, Methanol, light path length = 1 cm.

Figure S4. Fluorescence spectra of host **5** and spermidine (**9**).



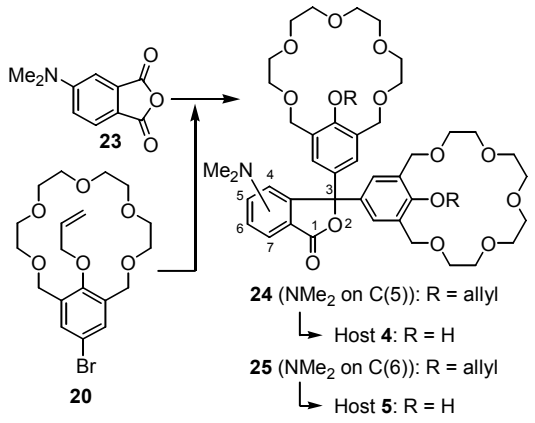
Experimental Section

Generals:

All solvents and reagents were purchased commercially and used without further purification unless otherwise mentioned. Air and moisture sensitive reactions were conducted in heat gun-dried glassware sealed with rubber septa under a positive pressure of nitrogen or argon. Dry tetrahydrofuran (THF), *N*, *N*-dimethyformaminde (DMF) and acetic anhydride (Ac_2O) were freshly distilled just before use from sodium benzophenone ketyl (THF), P_2O_5 (DMF) or CaH_2 (Ac_2O). Molecular sieves were activated for 2 minutes (500 W) by kitchen microwave (Panasonic, NE-AT70) followed by cooling *in vacuo*, and these operation were repeated twice.

Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm silica gel 60 F_{254} (0.25 mm, Merck) and were visualized by one or a combination of the following methods: (a) viewing under UV light, (b) exposure to iodine vapor, (c) exposure to 5% ethanolic phosphomolybdic acid solution, and (d) gentle heating on a hot plate. Preparative thin-layer chromatography (PTLC) separations were carried out on silica gel 60 F_{254} (0.5 mm, Merck). Wakogel C-200 (100-200 mesh, Wako Pure Chemical Industries Ltd.) or Silica Gel 60N (63-210 μm, Kanto Chemical Co., Inc.) was used for column chromatography. Silica Gel 60 Spherical (150-230 mesh, Nacarai tesque) or UltraPure Silica Gel (230−400 mesh, SiliCycle) was used for flash column chromatography. Recyclable HPLC was performed on LC-908 (Japan Analytical Industry Co., Ltd.) equipped with a combination column of both JAIGEL-1H (20 x 600 mm) and JAIGEL-2H (20 x 600 mm): flow, 3.5 ml/min ($CHCl_3$); detection, UV (254 nm) and/or RI (Refractive Index).

Scheme S-1. Synthetic route to hosts **4** and **5**.



Compounds 24 and 25: Compounds **24** and **25** have been synthesized similar to compounds **21** and **22**. Compound **23** is known (Vazquez, M. E.; Rothaman, D. M.; Imperiali, B. *Org. Biomol. Chem.* **2004**, *2*, 1965-1966.)

24: 58% yield, White solid; R_f = 0.27 (EtOAc-EtOH, 10:1); m.p. 79-80 °C (from MeOH); IR (KBr) 3502, 2872, 1749, 1604, 1523, 1477, 1352, 1295, 1252, 1110, 1025, 981, 945 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.8 Hz, 1H), 7.26 (dd, *J* = 12.4, 2.4 Hz, 4H), 6.79 (dd, *J* = 8.8, 2.0 Hz, 1H), 657 (d, *J* = 2.0 Hz, 1H), 6.25-6.12 (m, 2H), 5.50 (dd, *J* = 17.6, 2.0 Hz, 2H), 5.21 (dd, *J* = 10.8, 2.0 Hz, 2H), 4.98-4.91 (m, 4H), 4.49 (ABq, $\Delta\upsilon$ = 316 Hz, J_{AB} = 10.4 Hz, 4H), 3.67-3.35 (m, 32H+6H), 3.07 (s, 6H), 2.03 (s, 2H, D_2O exchangable); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.4, 159.0, 155.0, 154.5, 136.3, 135.8, 132.19, 132.16, 131.6, 131.0, 126.9, 115.2, 113.0, 112.0, 14.8, 90.0, 70.8, 70.3, 70.2, 70.10, 70.07, 69.2, 68.6, 68.4, 40.5; MS (FAB+, NBA) *m/z* (rel. intensity) = 916 $[(M+K)^+$, 10], 900 $[(M+Na)^+$, 100], 878 $[(M+H)^+$, 15]; HRMS (FAB+, NBA) Calcd for $C_{48}H_{64}O_{14}N$ $(M+H)^+$ 878.4327, Found 878.4341; *Anal.* Calcd for $C_{48}H_{63}O_{14}N{\cdot}2.0\ H_2O$: C, 63.07; H, 7.39; N, 1.53. Found: C, 63.21; H, 7.17; N, 1.40.

25: 39% yield, White powder; R_f = 0.35 (EtOAc-EtOH, 10:1); m.p. 86-87 °C (from MeOH); IR (KBr) 3503, 2872, 1765, 1625, 1516, 1474, 1352, 1249, 1110, 1023, 947 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.8 Hz, 1H), 7.23 (dd, *J* = 11.2, 2.4 Hz, 4H), 7.12 (d, *J* = 2.4 Hz, 1H), 7.08 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.25-6.12 (m, 2H), 5.50 (dd, *J* = 17.2, 2.0 Hz, 2H) , 5.21 (dd, *J* = 10.4, 2.0 Hz, 2H), 4.91 (d, *J* = 5.2 Hz, 4H), 4.50 (ABq, $\Delta\upsilon$ = 313 Hz, J_{AB} = 10.4 Hz, 4H), 4.48 (ABq, $\Delta\upsilon$ = 311 Hz, J_{AB} = 10.4 Hz, 4H), 3.66-3.35 (m, 32H), 3.04 (s, 6H), 2.20 (s, 2H, D_2O exchangable); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.9, 158.8, 151.3, 139.8, 136.3, 136.0, 132.22, 132.17, 131.1, 130.9, 126.4, 124.4, 119.1, 115.1, 106.9, 90.9, 70.7, 70.3, 70.2, 70.1, 69.19, 69.17, 68.7, 68.6, 40.6; MS (FAB+, NBA) *m/z* (rel. intensity) = 916 $[(M+K)^+$, 10], 900 $[(M+Na)^+$, 30]; HRMS (FAB+, NBA) Calcd for $C_{48}H_{63}O_{14}NNa$ $(M+Na)^+$ 900.4146, Found 900.4128; *Anal.* Calcd for $C_{48}H_{63}O_{14}N{\cdot}2.0\ H_2O$: C, 63.07;

H, 7.39; N, 1.53. Found: C, 63.26; H, 7.21; N, 1.50.

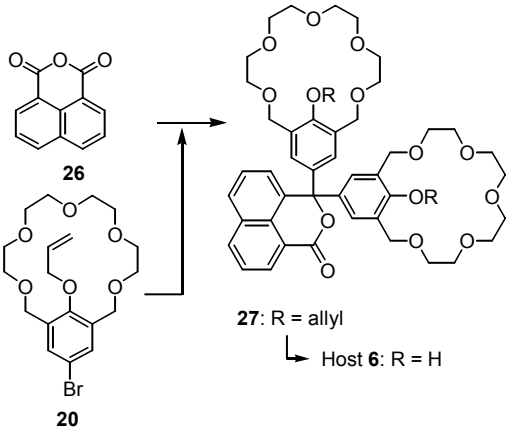
Host 4: Host **4** has been synthesized similar to host **2**.

Host **4**: 90% yield, Pale yellow foam; R_f = 0.32 ($CHCl_3$-MeOH, 10:1); IR (neat) 3350, 2872, 1743, 1604, 1521, 1485, 1355, 1294, 1107 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 2H), 7.69 (d, J = 8.8 Hz, 1H), 7.08 (s, 4H), 6.74 (dd, J = 8.8, 2.0 Hz, 4H), 6.47 (d, J = 2.0 Hz, 1H), 4.58 (AB, $\Delta\upsilon$ = 0 Hz, J_{AB} = 11.2 Hz, 8H), 3.78-3.58 (m, 32H), 3.05 (s, 6H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.4, 156.0, 155.1, 154.3, 132.2, 128.8, 126.8, 124.3, 112.8, 112.2, 104.9, 90.6, 70.6, 70.5, 70.3, 70.0, 69.4, 40.5; MS (FAB+, Glycerol) m/z (rel. intensity) = 842 [$(M+2Na-H)^+$, 10], 836 [$(M+K)^+$, 15], 820 [$(M+Na)^+$, 100], 798 [$(M+H)^+$, 45]; HRMS (FAB+, NBA) Calcd for $C_{42}H_{56}O_{14}N$ $(M+H)^+$ 798.3701, Found 798.3707; *Anal.* Calcd for $C_{48}H_{63}O_{14}N{\cdot}1.0\ H_2O$: C, 61.83; H, 7.04; N, 1.72. Found: C, 61.85; H, 6.82; N, 1.79.

Host 5: Host **5** has been synthesized similar to host **2**.

Host **5**: 90% yield, Pale yellow foam; R_f = 0.33 ($CHCl_3$-MeOH, 10:1); IR (neat) 3344, 2872, 1757, 1686, 1619, 1514, 1485, 1356, 1248, 1107, 943 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 2H), 7.30 (d, J = 8.8 Hz, 1H), 7.08 (d, J = 2.4 Hz, 4H), 7.00 (dd, J = 8.8, 2.4 Hz, 1H), 4.57 (AB, $\Delta\upsilon$ = 0 Hz, J_{AB} = 11.2 Hz, 8H), 3.76-3.58 (m, 32H), 3.02 (s, 6H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 171.0, 156.0, 151.2, 140.1, 132.5, 128.7, 126.4, 124.6, 124.4, 118.8, 106.9, 91.4, 70.62, 70.55, 70.3, 70.0, 69.4, 40.6; MS (FAB+, Glycerol) m/z (rel. intensity) = 820 [$(M+Na)^+$, 10], 798 [$(M+H)^+$, 35], 737 (10), 645 (20), 553 (35), 369 (20); HRMS (FAB+, Glycerol) Calcd for $C_{42}H_{56}O_{14}N$ $(M+H)^+$ 798.3701, Found 798.3696; *Anal.* Calcd for $C_{48}H_{63}O_{14}N{\cdot}2.0\ H_2O$: C, 60.49; H, 7.13; N, 1.68. Found: C, 60.80; H, 6.88; N, 1.66.

Scheme S-2. Synthetic route to host **6**.



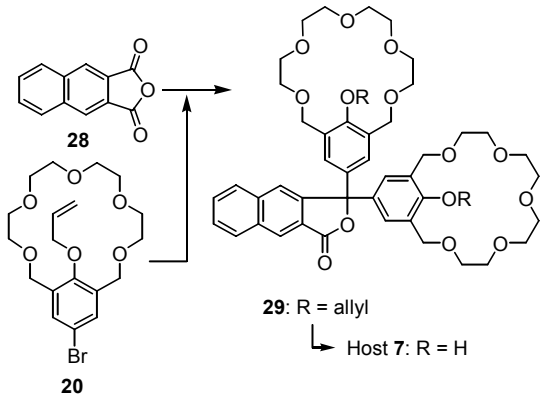
Compound 27: Compound **27** has been synthesized similar to compounds **21** and **22**.

27: 61% yield, White powder; R_f = 0.30 (AcOEt-MeOH, 10:1); m.p. 142-143 °C; IR (KBr) 2360, 1721, 1644, 1585, 1477, 1137, 1110 cm^{-1}; δ 8.42 (d, *J* = 7.3 Hz, 1H), 8.17 (d, *J* = 7.3 Hz, 1H), 7.94 (d, *J* = 7.3 Hz, 1H), 7.67 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.60 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.09 (dd, *J* = 36.2, 2.3 Hz, 4H), 6.24-6.11 (m, 2H), 5.49 (dd, *J* = 17.4, 2.3 Hz, 2H), 5.21 (dd, *J* = 10.5, 2.3 Hz, 2H), 4.94 (d, *J* = 4.1 Hz, 4H), 4.43 (ABq, $\Delta\upsilon$ = 302 Hz, J_{AB} = 10.6 Hz, 4H), 4.44 (ABq, $\Delta\upsilon$ = 329 Hz, J_{AB} = 10.6 Hz, 4H), 3.63-3.30 (m, 32H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 165.2, 159.2, 138.3, 136.7, 134.4, 134.3, 132.7, 132.4, 132.4, 130.4, 128.8, 128.3, 128.2, 126.9, 126.7, 121.7, 115.4, 90.7, 71.2, 70.7, 70.6, 69.7, 69.1, 69.0; MS (FAB+, NBA) *m/z* (rel. intensity) = 907 [$(M+Na)^+$, 100], 465 (30); HRMS (FAB+, NBA) Calcd for $C_{50}H_{60}O_{14}Na$ $(M+Na)^+$ 907.3881, Found 907.3870; *Anal.* Calcd for $C_{50}H_{60}O_{14}$: C, 67.86; H, 6.83. Found: C, 67.89; H, 6.91.

Host 6: Host **6** has been synthesized similar to host **2**.

Host **6**: 44% yield, White powder; R_f = 0.28 ($CHCl_3$-MeOH, 10:1); m.p. 175-176 °C; IR (KBr) 3344, 2870, 1716, 1608, 1486, 1353, 1139, 1108 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 6.9 Hz, 1H), 8.19 (brs, *2*H), 7.64 (d, *J* = 8.2 Hz, 1H), 7.63 (dd, *J* = 8.2, 8.2 Hz, 1H), 7.50 (dd, *J* = 8.2, 8.2 Hz, 1H), 7.09 (d, *J* = 6.9 Hz, 1H), 6.90 (s, 4H), 4.53 (AB, $\Delta\upsilon$ = 0 Hz, J_{AB} = 11.4 Hz, 8H), 3.80-3.59 (m, 32H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 165.4, 156.4, 134.5, 134.2, 132.5, 129.8, 128.6, 128.0, 127.9, 126.6, 126.3, 124.2, 121.6, 90.8, 71.0, 70.9, 70.6, 70.1, 69.7; MS (FAB+, NBA) *m/z* (rel. intensity) = 827 [$(M+Na)^+$, 40], 805 [$(M+H)^+$, 10], 154 (100); HRMS (FAB+, NBA) Calcd for $C_{44}H_{53}O_{14}$ $(M+H)^+$ 805.3436, Found 805.3444; *Anal.* Calcd for $C_{44}H_{52}O_{14}\cdot 0.5\ H_2O$: C, 64.93; H, 6.56. Found: C, 65.10; H, 6.50.

Scheme S-3. Synthetic route to host **7**.



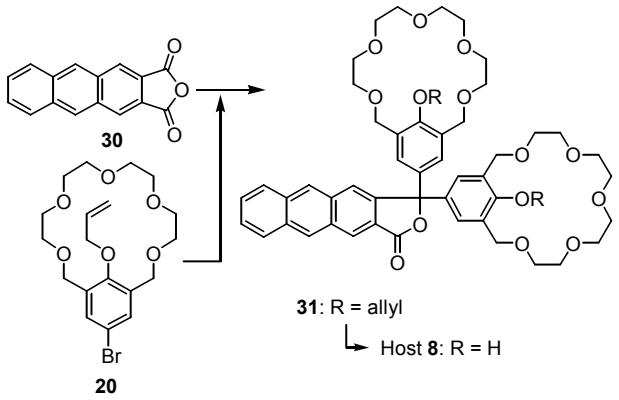
Compound 29: Compound **29** has been synthesized similar to compounds **21** and **22**.

29: 95% yield, White powder, R_f = 0.41 (EtOAc-acetone, 4:1); m.p. 77-78 °C; IR (KBr) 2871, 1766, 1636, 1479, 1351 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.07 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.96 (s, 1H), 7.67 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.61 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.30 (dd, *J* = 15.6, 2.8 Hz, 4H), 6.25-6.12 (m, 2H), 5.50 (dd, *J* = 17.4, 1.8 Hz, 2H), 5.21 (d, *J* = 17.4 Hz, 2H), 4.94 (d, *J* = 5.0 Hz, 4H), 4.87 (dd, *J* = 10.14, 1.8 Hz, 4H),), 4.10 (dd, *J* = 10.14, 2.8 Hz, 4H), 3.70-3.32 (m, 32H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.2, 159.6, 145.3, 136.8, 136.7, 136.1, 133.7, 133.0, 132.9, 131.6, 131.5, 130.3, 129.5, 129.3, 127.9, 127.7, 123.9, 115.5, 91.9, 71.2, 70.7, 70.6, 69.6, 69.2; MS (FAB+, NBA) *m*/*z* (rel. intensity) = 907 [$(M+Na)^+$, 100], 885 [$(M+H)^+$, 30], 499 (25); HRMS (FAB+) Calcd for $C_{50}H_{61}O_{14}$ $(M+H)^+$ 885.4061, Found 885.4059; *Anal.* Calcd for $C_{50}H_{60}O_{14}\cdot H_2O$: C, 66.50; H, 6.92. Found: C, 66.84; H, 6.89.

Host 7: Host **7** has been synthesized similar to host **2**.

Host **7**: 69% yield, White powder; R_f = 0.33 ($CHCl_3$-MeOH, 10:1); m.p. 199-201 °C; IR (KBr) 3339, 2870, 1762, 1609, 1486, 1355 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.4-8.1 (brs, *2*H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.88 (s, 1H), 7.65 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.58 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.12 (s, 4H), 4.58 (AB, $\Delta\upsilon$ = 0 Hz, J_{AB} = 11.0 Hz, 8H), 3.70-3.55 (m, 32H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.3,156.7, 146.5, 136.6, 133.5, 132.5, 130.2, 129.4, 129.2, 129.1, 127.7, 127.5, 125.0, 124.1, 123.7, 92.4, 71.1, 71.0, 70.7, 70.4, 69.9; MS (FAB+, NBA) *m*/*z* (rel. intensity) = 827 [$(M+Na)^+$, 100], 805 [$(M+H)^+$, 15], 307 (60); HRMS (FAB+, Glycerol) Calcd for $C_{44}H_{53}O_{14}$ $(M+H)^+$ 804.3435, Found 804.3424; *Anal.* Calcd for $C_{44}H_{52}O_{14}$: C, 65.66; H, 6.51. Found: C, 65.29; H, 6.67.

Scheme S-4. Synthetic route to host **8**.

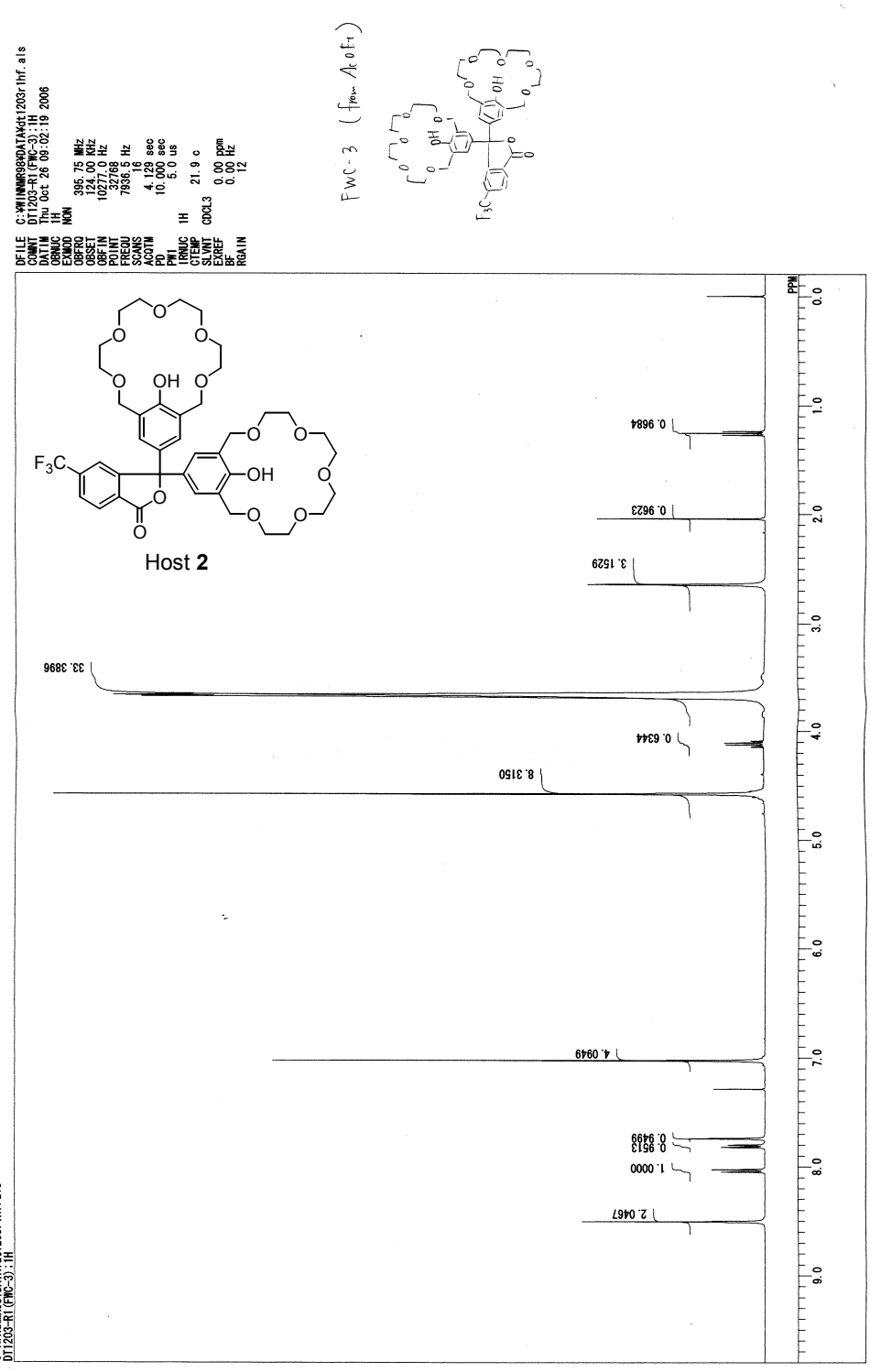


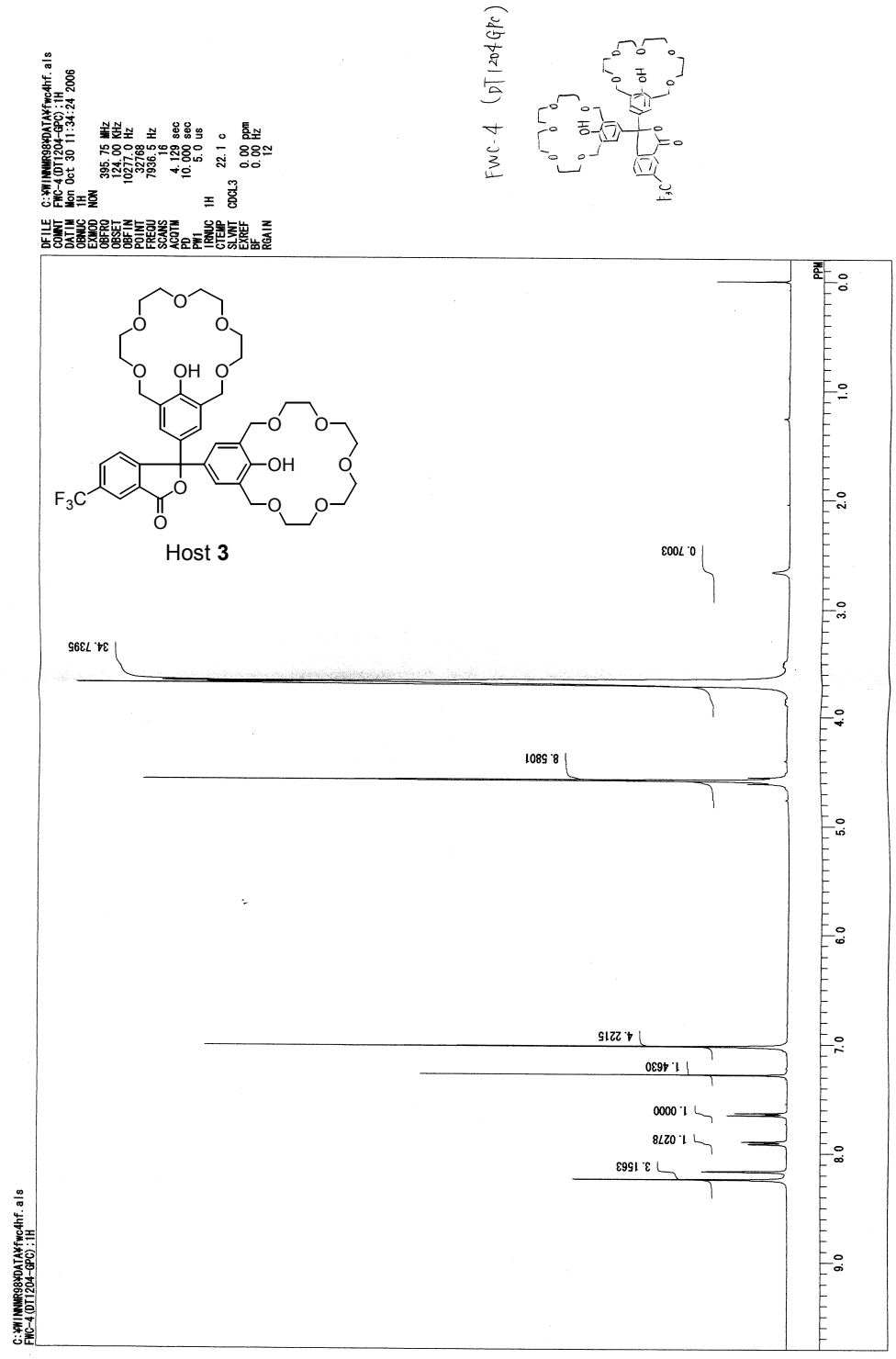
Compound 31: Compound **31** has been synthesized similar to compounds **21** and **22**.

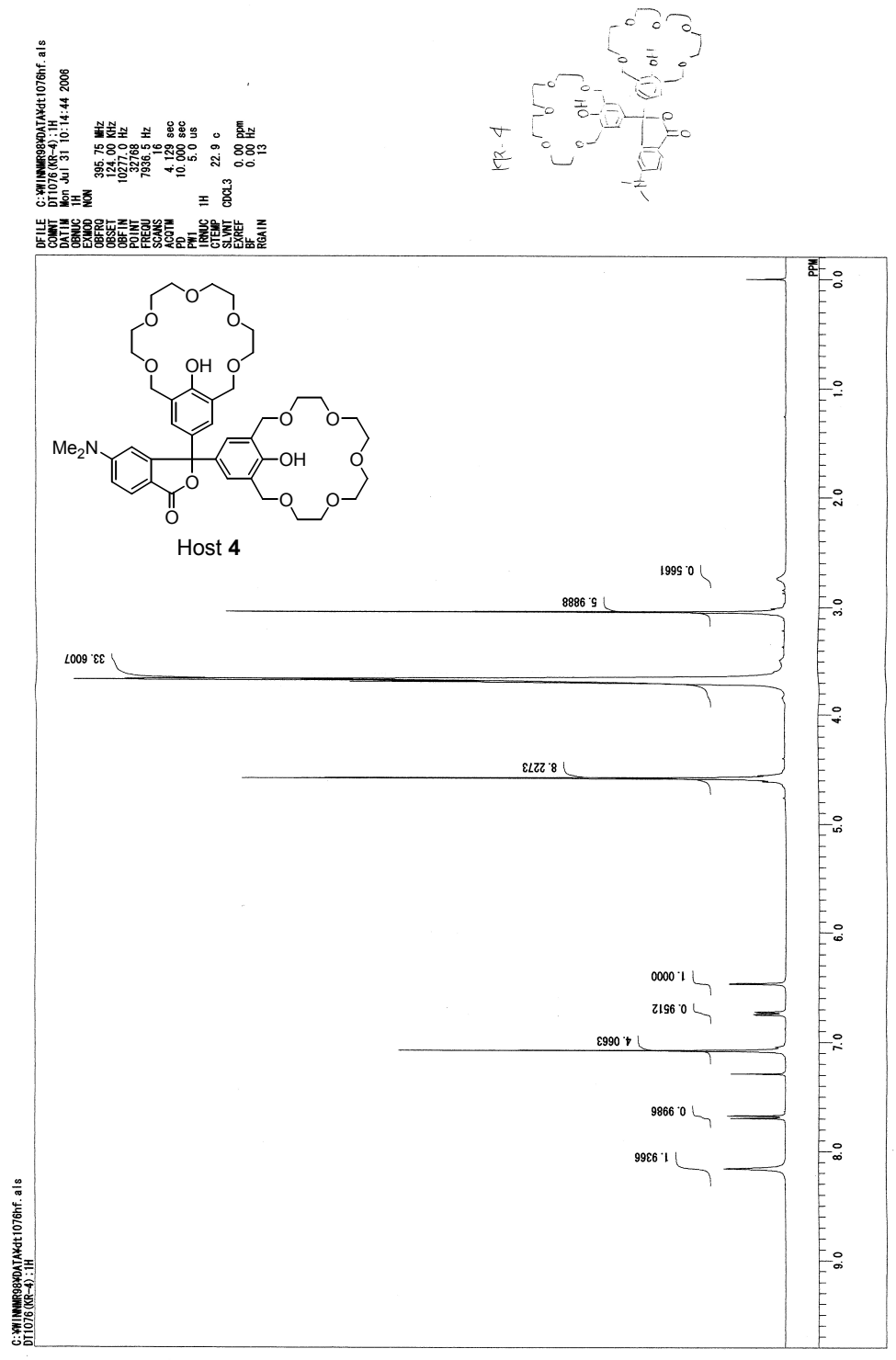
31: 93% yield, pale yellow powder, R_f = 0.33 (EtOAc-MeOH, 10:1); m.p. 90-91 °C; IR (KBr) 2871, 1764, 1638, 1213, 1112 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 8.71 (s, 1H), 8.58 (s, 1H), 8.10 (s, 1H), 8.09-8.01 (m, 2H), 7.59-7.51 (m, 2H), 7.33 (dd, J = 16.0, 2.3 Hz, 4H), 6.23-6.14 (m, 2H), 5.50 (dd, J = 17.4, 2.3 Hz, 2H), 5.21 (dd, J = 10.6, 2.3 Hz, 2H), 4.95 (d, J = 5.0 Hz, 4H), 4.49 (ABq, $\Delta\upsilon$ = 305 Hz, J_{AB} = 10.1 Hz, 4H), 4.49 (ABq, $\Delta\upsilon$ = 309 Hz, J_{AB} = 10.1 Hz, 4H), 3.66-3.33 (m, 32H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.0, 159.6, 144.1, 136.8, 136.3, 133.9, 133.5, 132.9, 132.6, 131.7, 131.5, 131.2, 130.0, 129.3, 128.9, 128.6, 127.9, 127.6, 126.8, 124.1, 123.8, 115.5, 91.9, 71.2, 70.7, 70.6, 70.5, 69.6, 69.2; MS (FAB+, NBA) *m/z* (rel. intensity) = 957 [$(M+Na)^+$, 100], 935 [$(M+H)^+$, 15], 307 (20); HRMS (FAB+) Calcd for $C_{54}H_{63}O_{14}$ $(M+H)^+$ 935.4218, Found 935.4245; *Anal.* Calcd for $C_{54}H_{62}O_{14}\cdot 0.5H_2O$: C, 68.70; H, 6.73. Found: C, 68.92; H, 6.72.

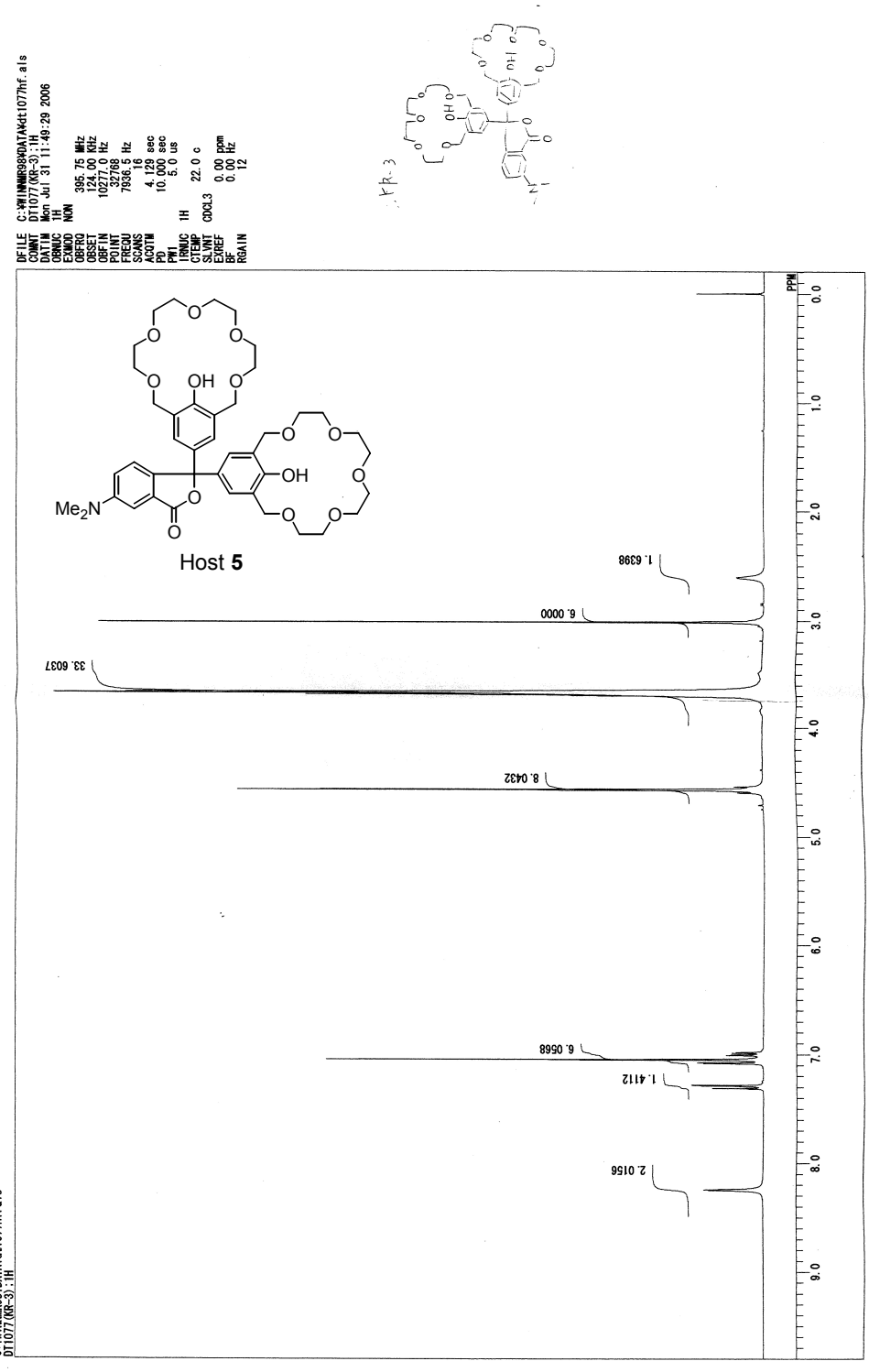
Host 8: Host **8** has been synthesized similar to host **2**.

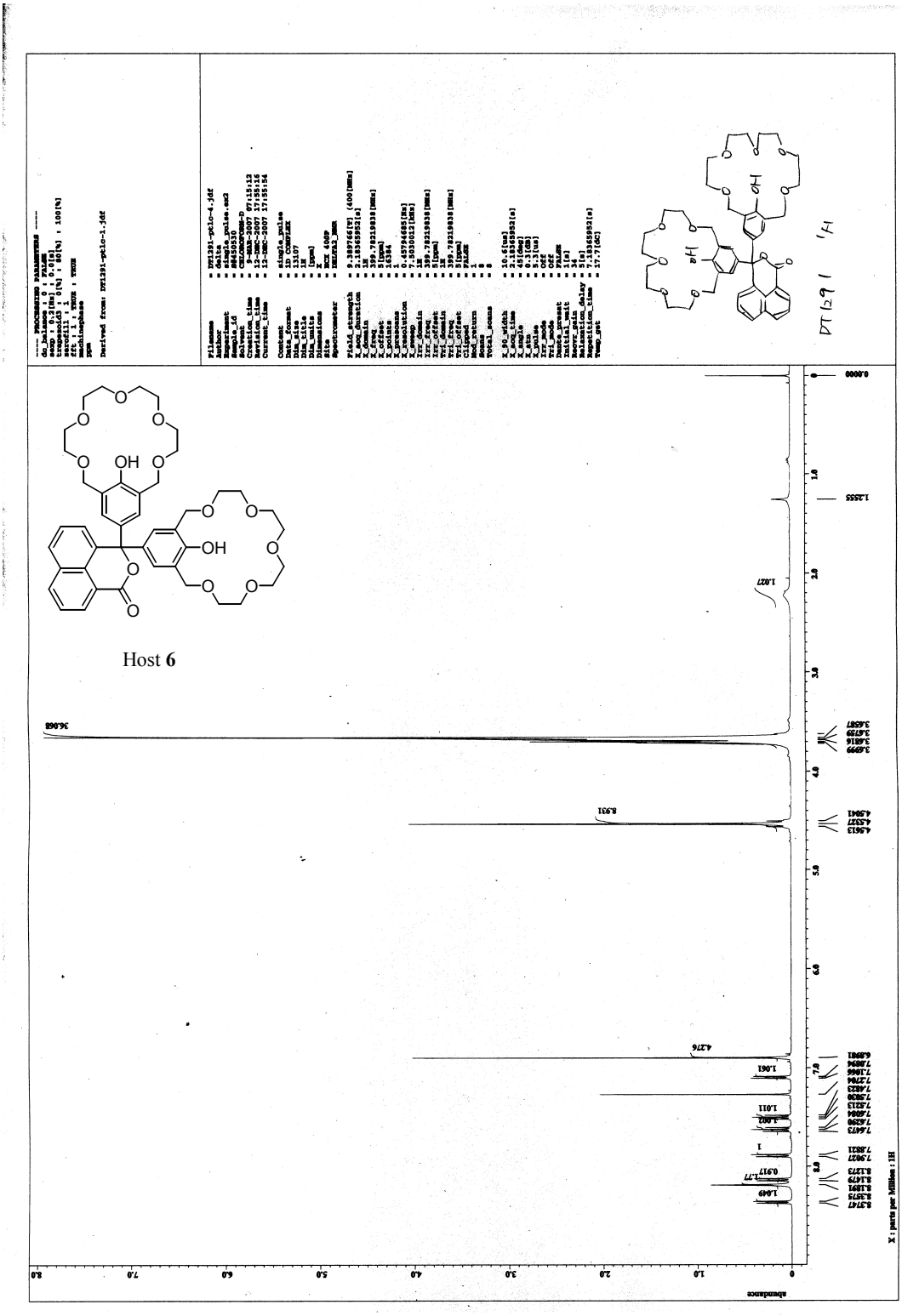
Host **8**: 64% yield, White powder; R_f = 0.30 ($CHCl_3$-MeOH, 10:1); m.p. 191- °C (decomp.); IR (KBr) 3357, 2871, 1761, 1637, 1486, 1355 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.70 (s, 1H), 8.68 (s, 1H), 8.53 (s, 1H), 8.20 (s, 2H, O<u>H</u>), 8.1-8.0 (m, 2H), 8.01 (s, 1H), 7.6-7.5 (m, 2H), 7.15 (s, 4H), 4.58 (AB, $\Delta\upsilon$ = 16 Hz, J_{AB} = 5.5 Hz, 8H), 3.75-3.6 (m, 32H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.1, 157.1, 156.6, 144.3, 133.8, 133.3, 132.7, 132.5, 131.0, 129.8, 129.1, 128.9, 128.8, 128.5, 127.7, 127.5, 126.8, 125.5, 125.0, 123.9, 123.8, 92.4, 71.0, 71.0, 70.8, 70.7, 70.3, 69.9; MS (FAB+, NBA) *m/z* (rel. intensity) = 877 [$(M+Na)^+$, 2], 460 (4) 154 (100); HRMS (FAB+, NBA) Calcd for $C_{48}H_{54}O_{14}Na$ $(M+Na)^+$ 877.3412, Found 877.3391; *Anal.* Calcd for $C_{48}H_{54}O_{14}\cdot 0.15CHCl_3$: C, 66.26; H, 6.25. Found: C, 66.29; H, 6.19.

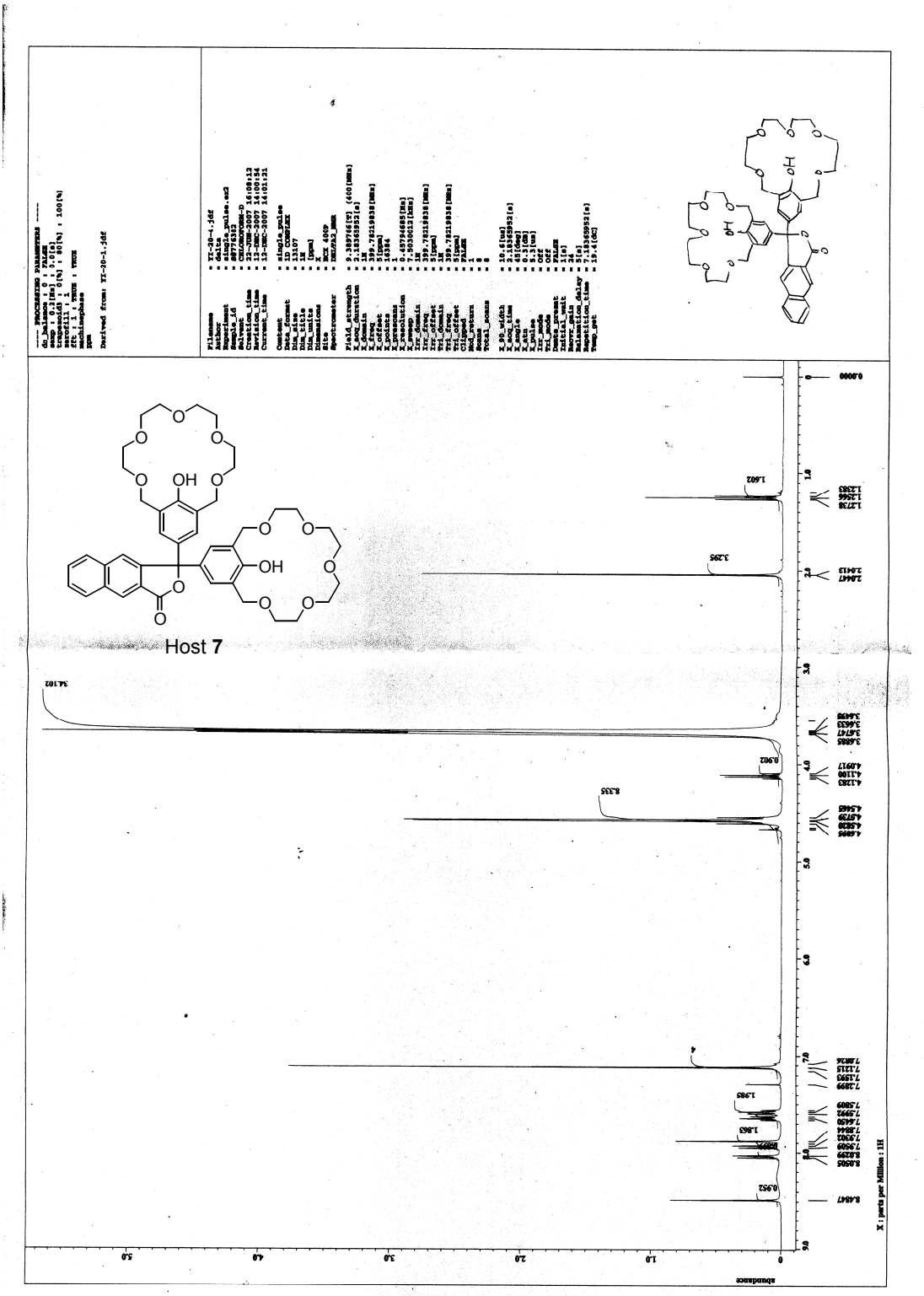

Host 2
0.9684
0.9623
3.1529
33.3896
0.6344
8.3150
4.0949
0.9499
0.9613
1.0000
2.0467
PPM

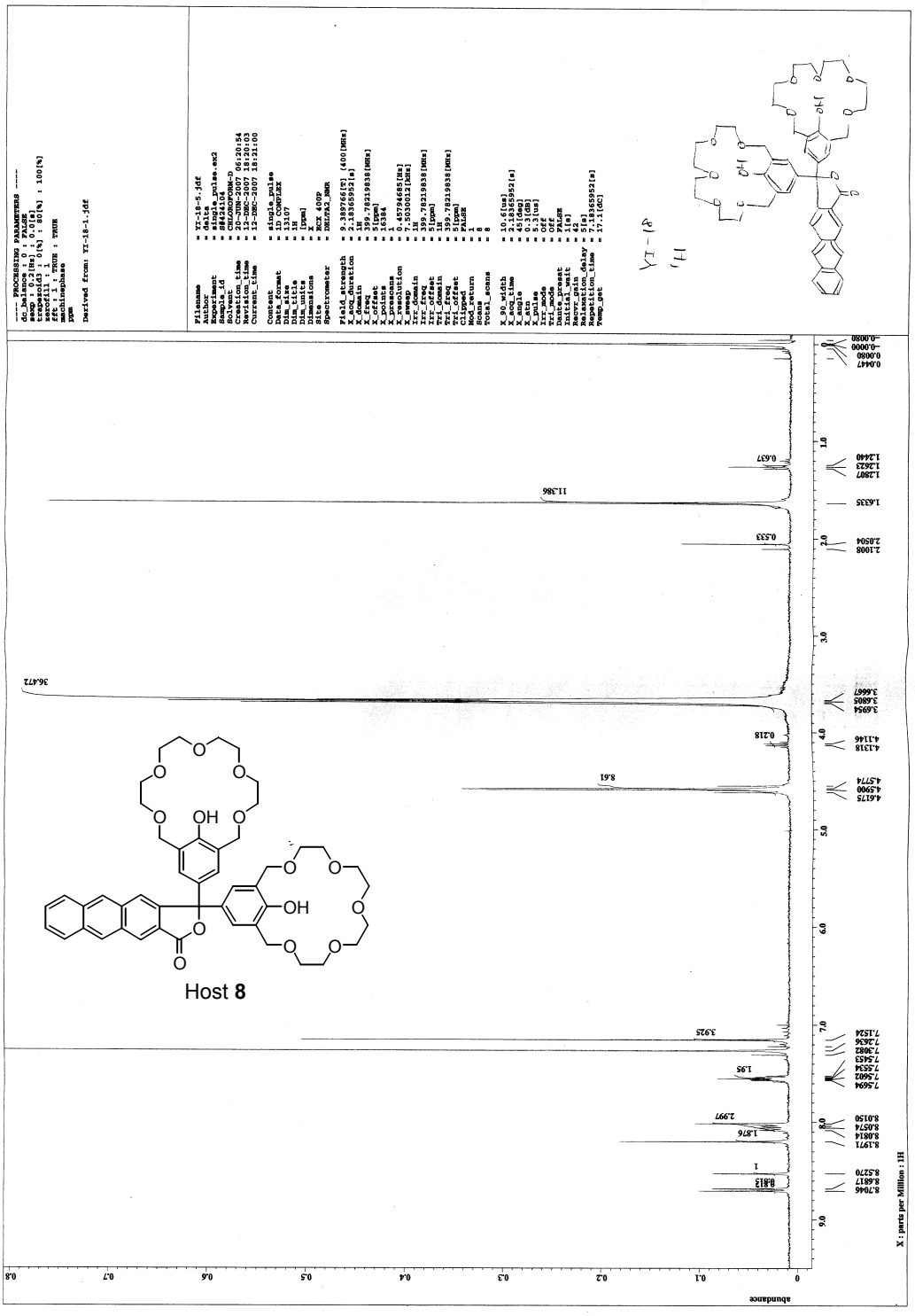

Host 3
FWC-4 (DT1204GPC)
0.7003
34.7395
8.5801
4.2215
1.4630
1.0000
1.0278
3.1563
PPM

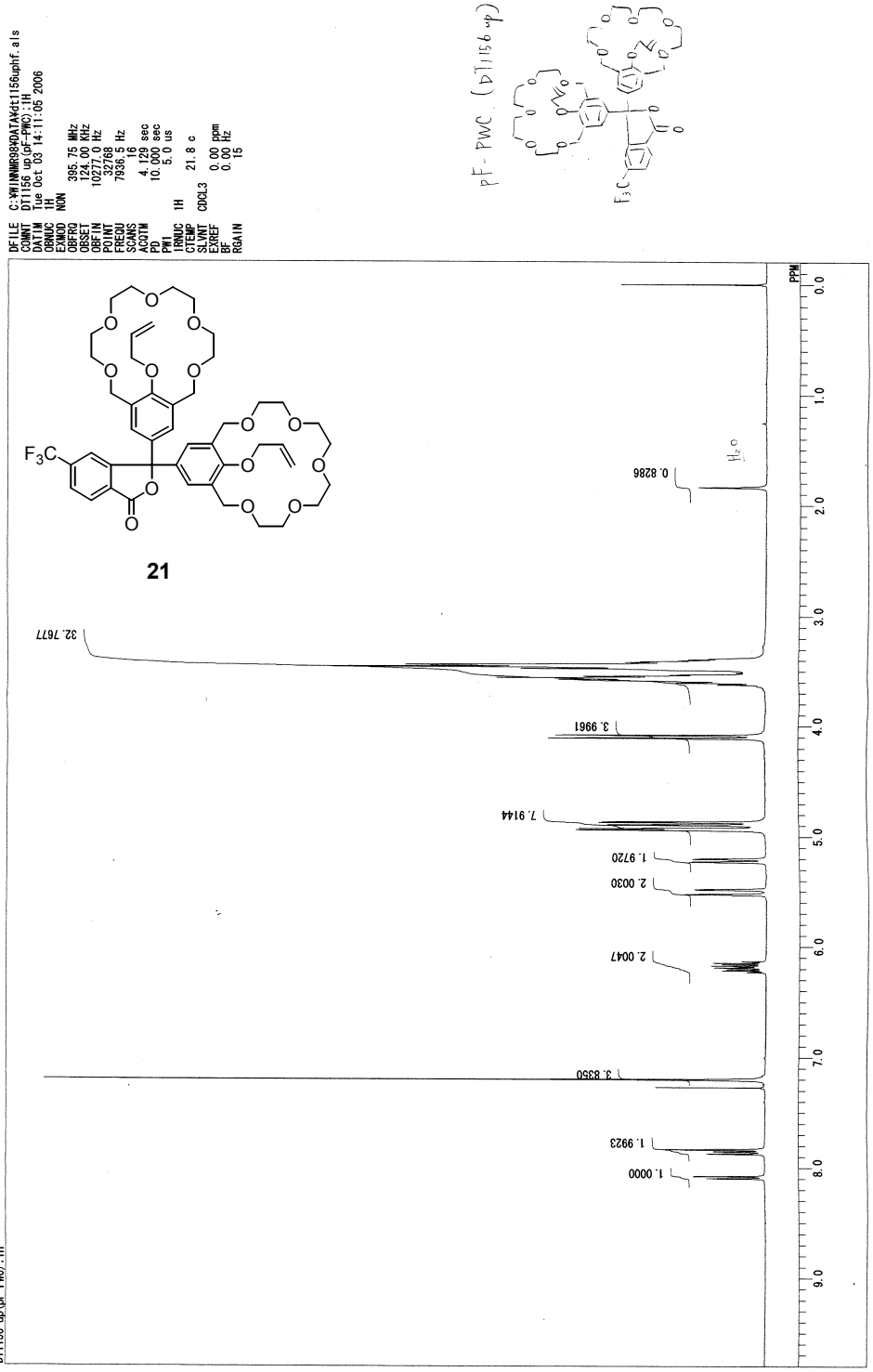

Host 4
Me2N
OH
OH
0.5661
5.9888
33.6007
8.2273
1.0000
0.9512
4.0663
0.9986
1.9366
PPM

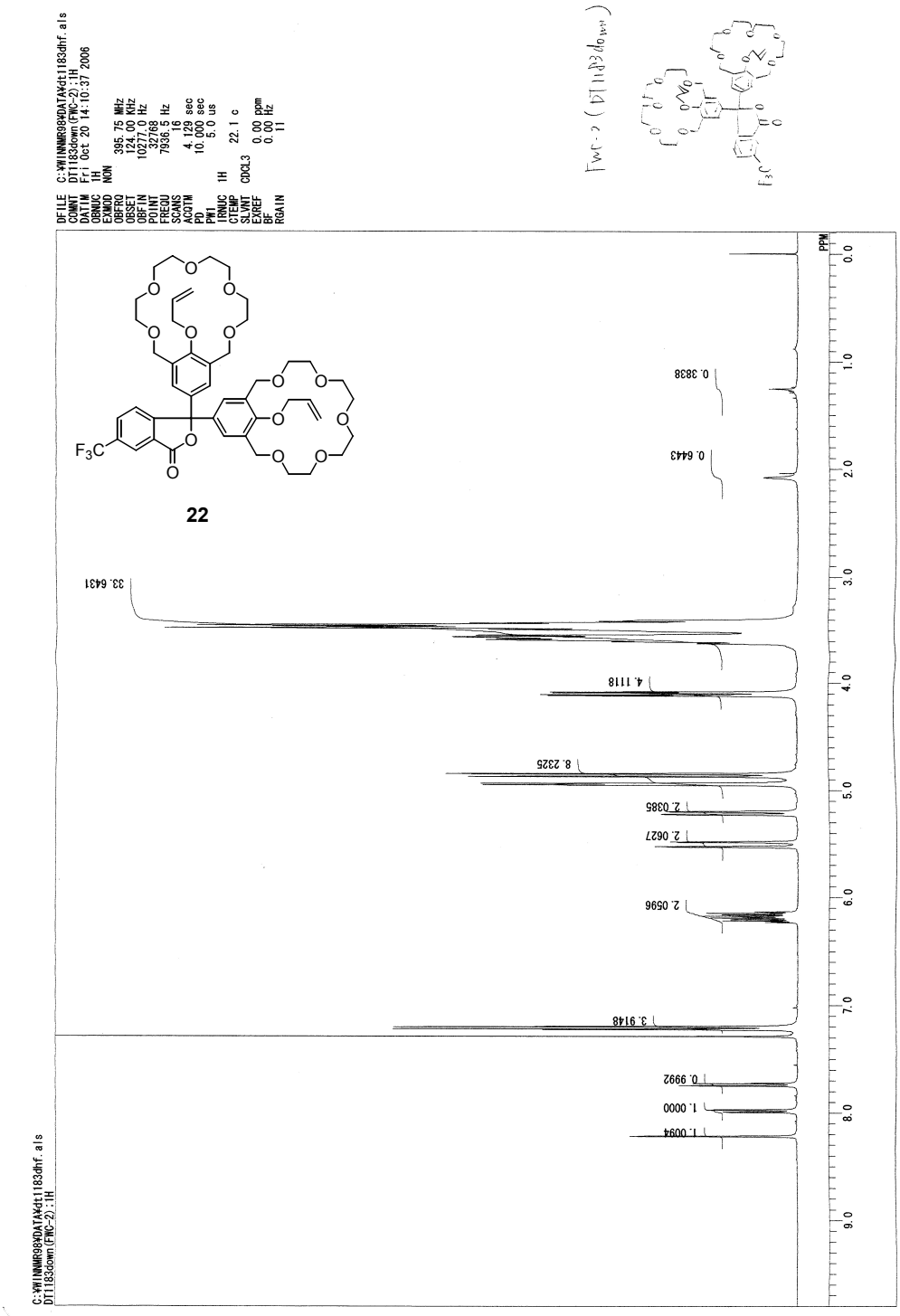

Host 5
Me2N
OH
OH
1.6398
6.0000
33.6037
8.0432
6.0568
1.4112
2.0156
PPM

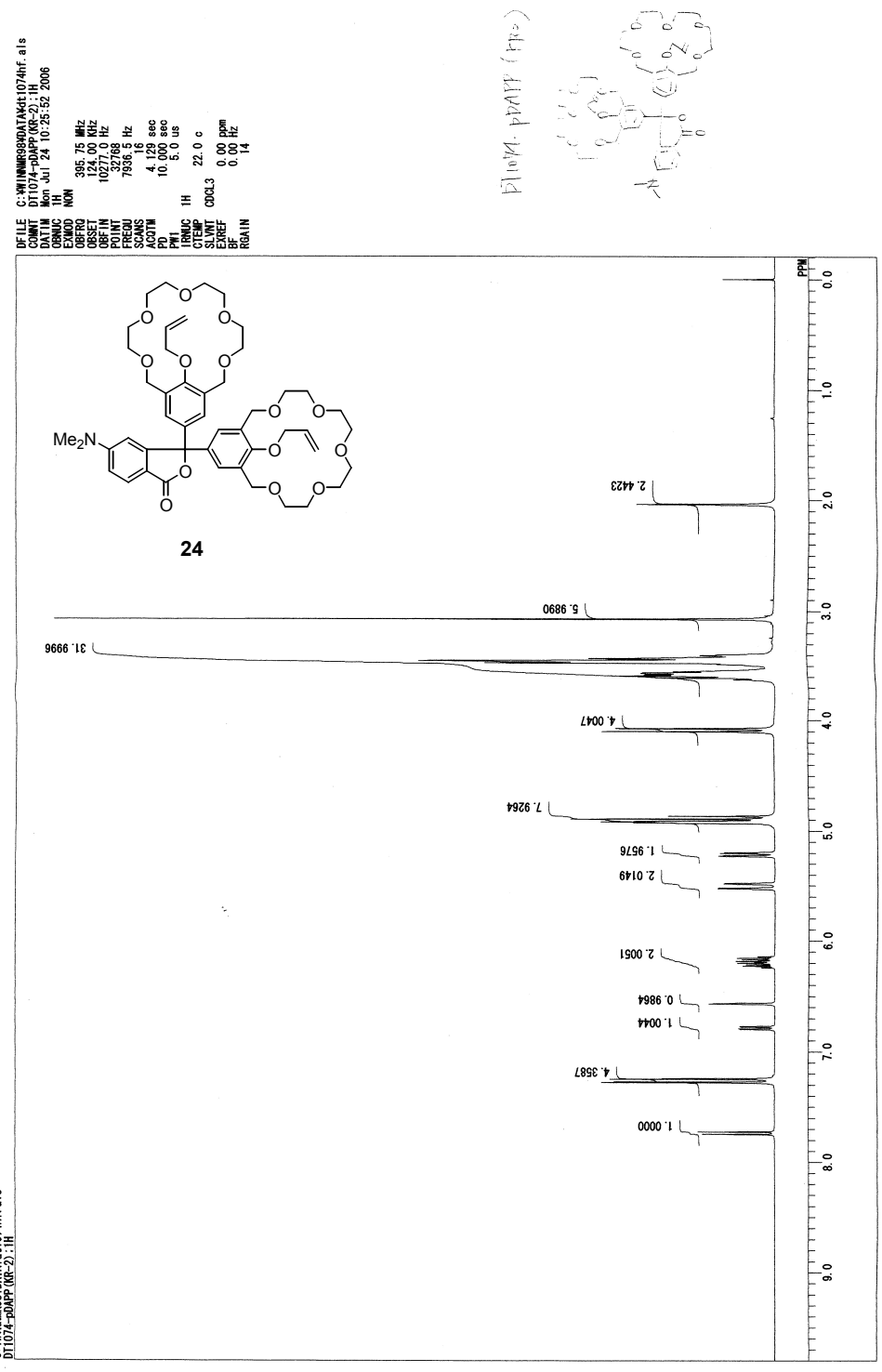

OH
OH
O
Host 6

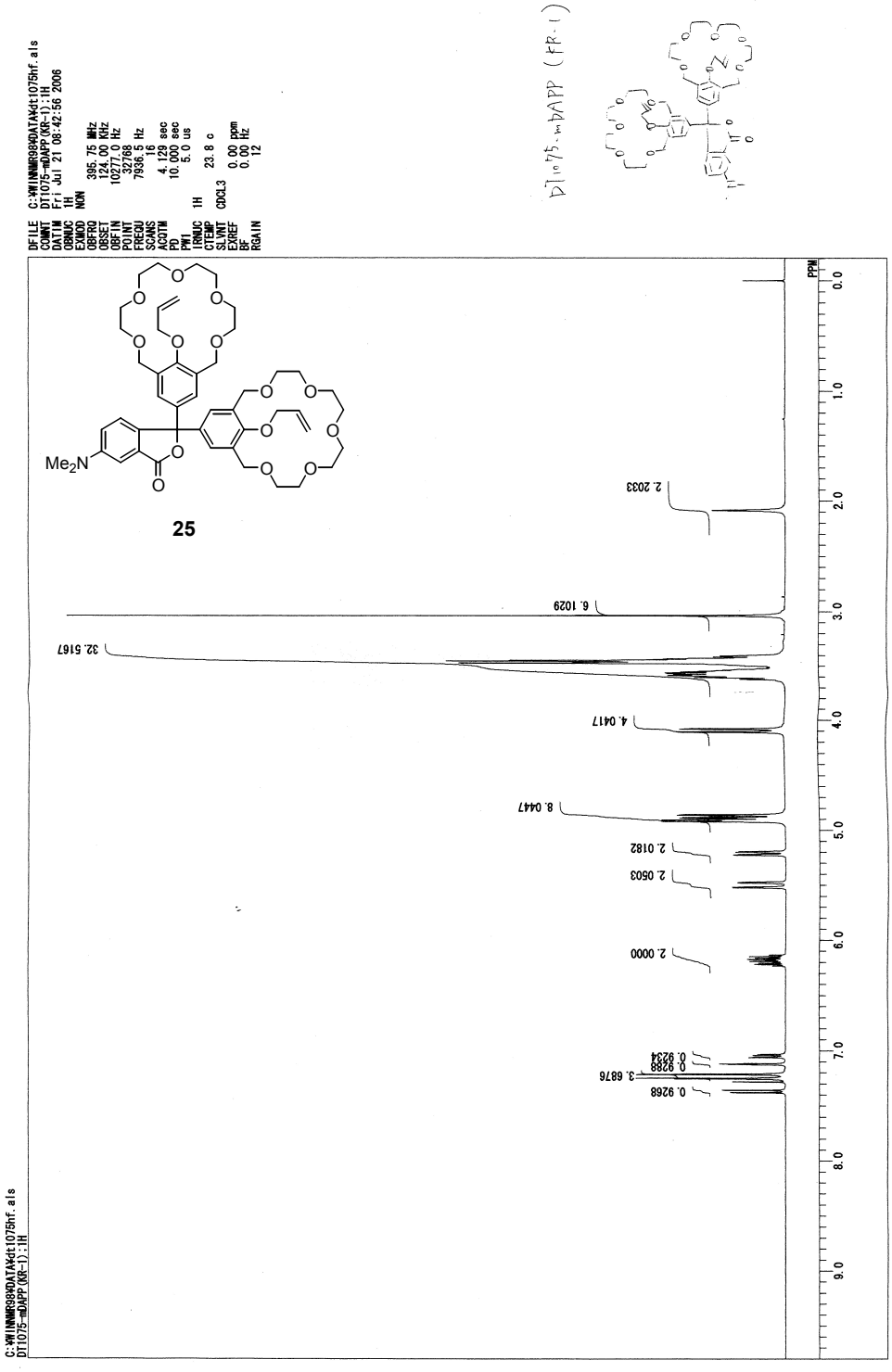

Host 7

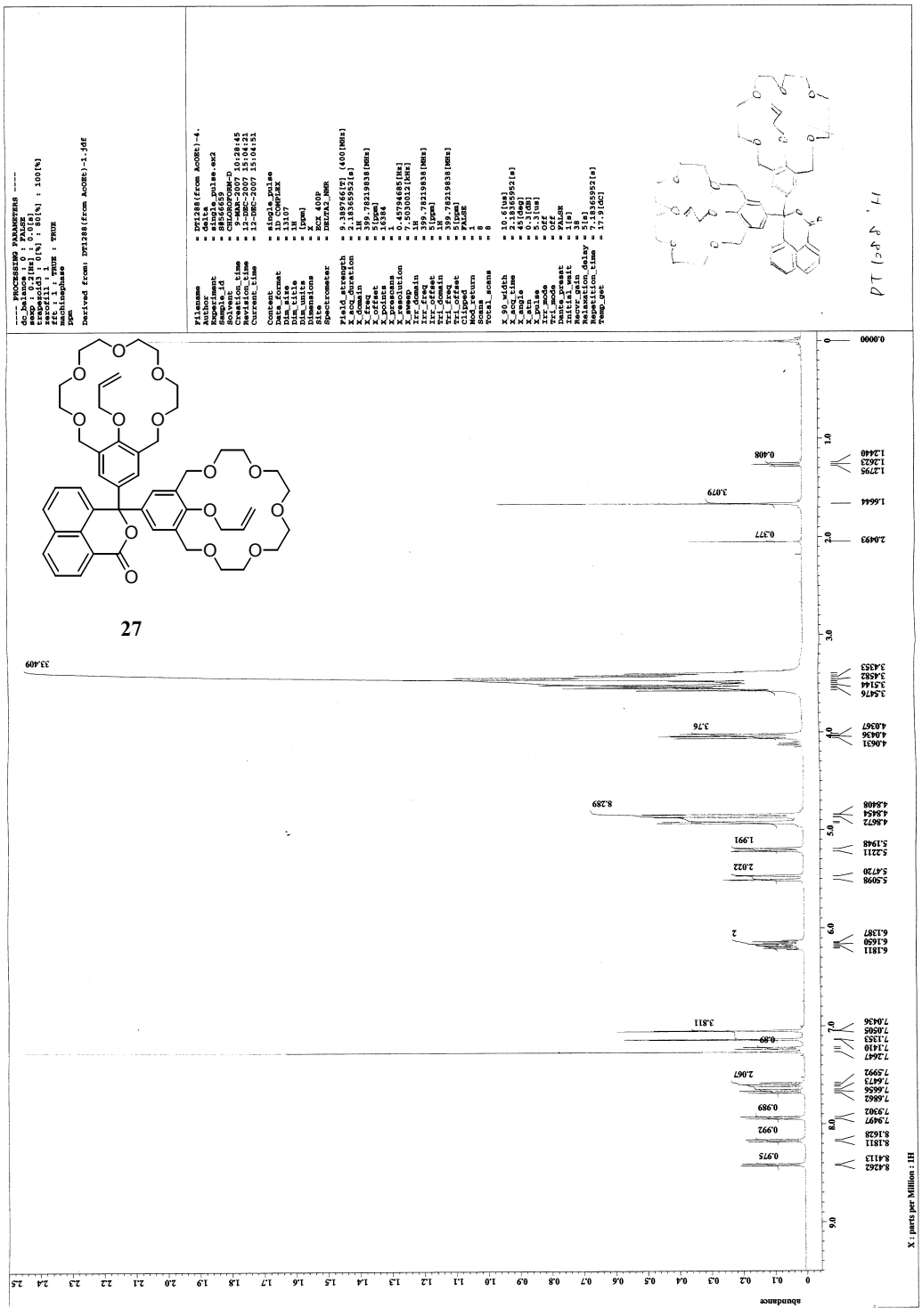

Host 8

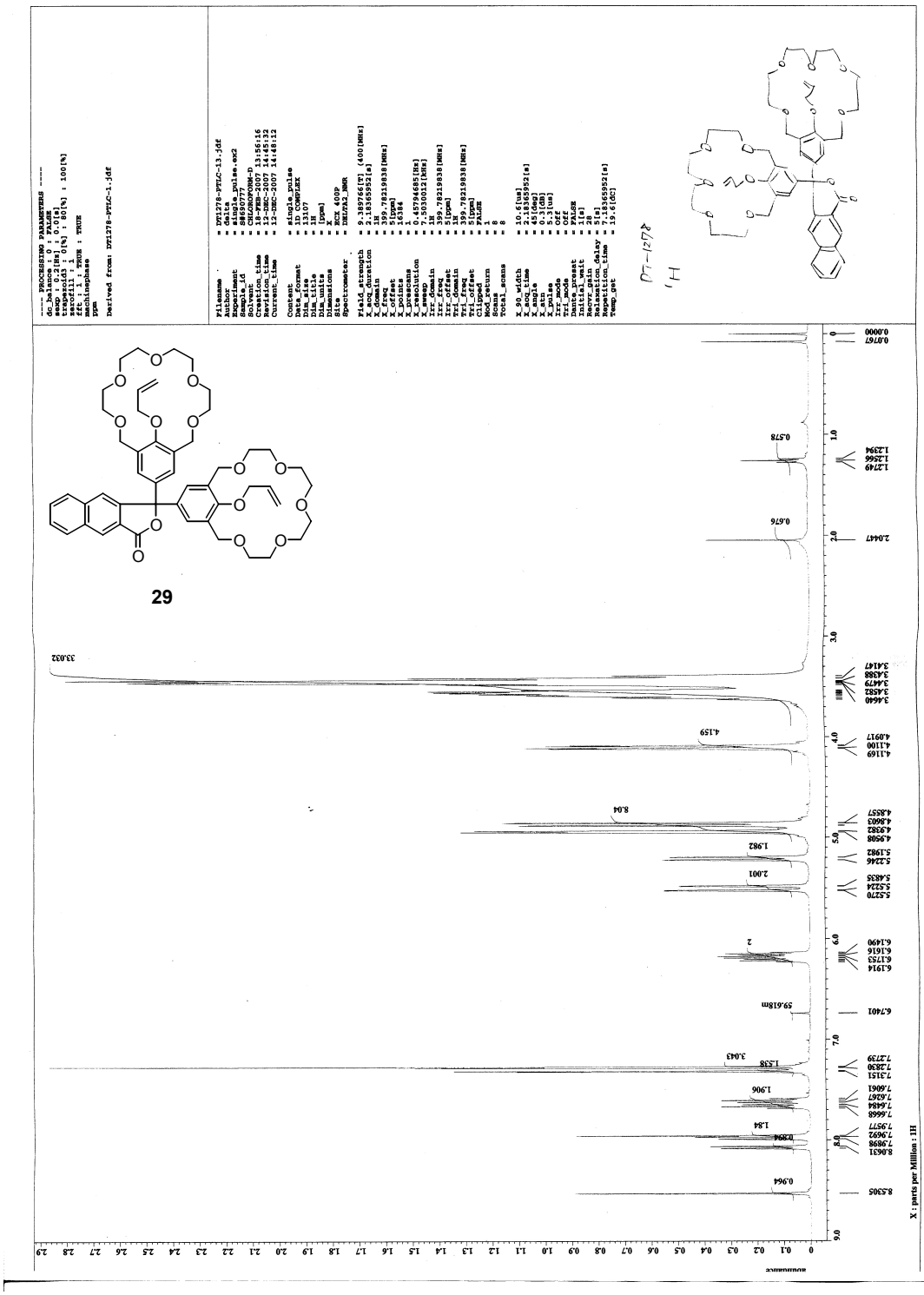

21
PF-PWC (DT1156up)
0.8286
32.7677
3.9961
7.9144
1.9720
2.0030
2.0047
3.8350
1.9923
1.0000
PPM

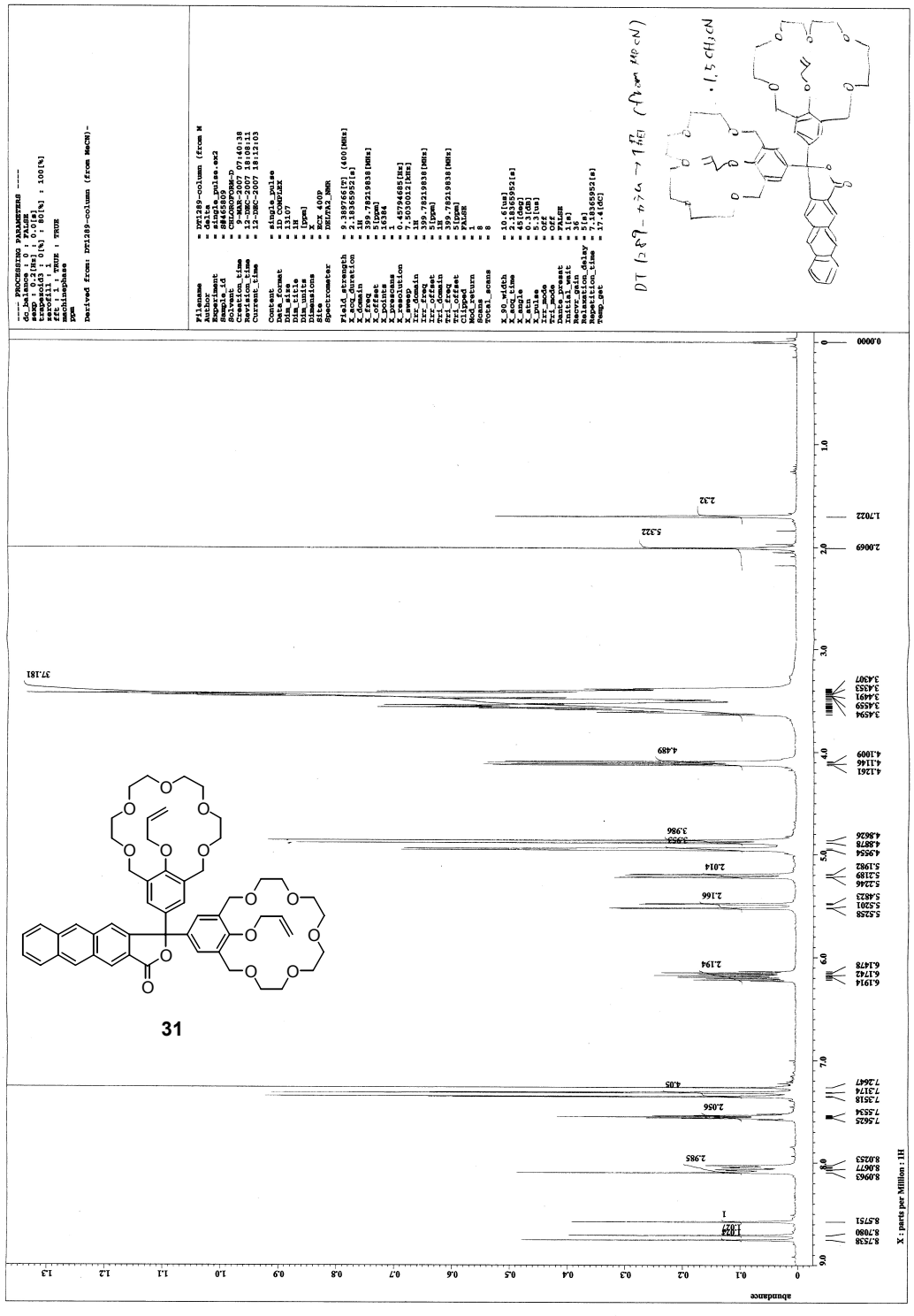

22
0.3838
0.6443
33.6431
4.1118
8.2325
2.0385
2.0627
2.0596
3.9148
0.9992
1.0000
1.0094
PPM


Me2N
24
2.4423
5.9890
31.9996
4.0047
7.9264
1.9576
2.0149
2.0051
0.9864
1.0044
4.3587
1.0000
PPM


DT1075-mDAPP (KR-1)
Me2N
25
2.2033
6.1029
32.5167
4.0417
8.0447
2.0182
2.0503
2.0000
0.9234
0.9288
3.6876
0.9268
PPM


27
X : parts per Million : 1H
abundance


29


31