Electronic Supplementary Information

A. Experimental details of compounds 2, 3, and 5-14

5,5'-[Benzene-1,4-diyl-di(ethyne-2,1-diyl)]diuracil (2a). 5-Iodouracil (1.13 g, 4.7 mmol), 1,4-diethynylbenzene (0.28 g, 2.2 mmol), TTPd (54.7 mg, 0.05 mmol) and CuI (18.0 mg, 0.09 mmol) in TEA (1.2 cm^3) and DMF (10 cm^3) were used. Crystallization from DMF yielded the compound as a yellow powder (0.59 g, 77 %); mp > 300 °C (dec.).

5,5'-[Biphenyl-4,4'-diyl-di(ethyne-2,1-diyl)]diuracil (2b). 5-Iodouracil (1.13 g, 4.7 mmol) and compound **17** (0.45 g, 2.2 mmol) were used (catalyst and solvent correspond to **2a**). Crystallization from DMF yielded the compound as a yellow powder (0.57 g, 62 %); mp > 300 °C (dec.).

5,5'-[Ethyne-1,2-diyl-bis(benzene-4,1-diyl-ethyne-2,1-diyl)]diuracil (2c). 5-Iodouracil (1.13 g, 4.7 mmol) and 4,4'-diethynyltolane (0.45 g, 2.2 mmol) were used (catalyst and solvent correspond to **2a**). The compound was obtained as a yellow powder after recrystallization from DMF (0.90 g, 91 %); mp > 300 °C (dec.).

8,8'-[Benzene-1,4-diyl-di(ethyne-2,1-diyl)]diadenosine (3a). 8-Bromoadenosine (1.00 g, 2.9 mmol), 1,4-diethynylbenzene (0.18 g, 1.4 mmol), BTPdCl (20.3 mg, 0.03 mmol) and CuI (11.0 mg, 0.06 mmol) in TEA (1.2 cm^3) and DMF (25 cm^3) were used. In modification of the general procedure, the reaction mixture was stirred at 110 °C for 7 h, then allowed to cool down to room temperature, and toluene (25 cm^3) was added. The precipitate was washed as described. For purification the crude product was redissolved in hot DMF, precipitated with toluene, collected and washed as before to yield the compound as a brown powder (0.67 g, 73 %); mp > 300 °C (dec.).

8,8'-[Biphenyl-4,4'-diyl-di(ethyne-2,1-diyl)]diadenosine (3b). 8-Bromoadenosine (1.00 g, 2.9 mmol) and compound **17** (0.28 g, 1.4 mmol) (catalyst, solvent and modified conditions correspond to **3a**) were used to yield the compound as a brown powder (0.66 g, 64 %); mp > 300 °C (dec.).

8,8'-[Ethyne-1,2-diyl-bis(benzene-4,1-diyl-ethyne-2,1-diyl)]diadenosine (3c). 8-Bromoadenosine (1.00 g, 2.9 mmol) and 4,4'-diethynyltolane (0.31 g, 1.4 mmol) (catalyst, solvent and modified

conditions correspond to **3a**) were used to obtain the compound as a brown powder (0.94 g, 89 %); mp > 300 °C (dec.).

8,8'-[Benzene-1,4-diyl-di(ethyne-2,1-diyl)]diguanosine (5a). 8-Bromoguanosine (1.46 g, 4.0 mmol), 1,4-diethynylbenzene (0.25 g, 2.0 mmol), TTPd (0.46 g, 0.4 mmol) and CuI (0.15 g, 0.8 mmol) in TEA (1.11 cm^3) and DMF (30 cm^3) were used. In variation of the general procedure, the reaction mixture was stirred for 16 h at 70 °C, then allowed to cool down to room temperature and dichloromethane (30 cm^3) was added. The precipitate was filtered off, stirred in boiling water (300 cm^3), separated and washed with water (5 × 50 cm^3). The solid was stirred in ethyl acetate (200 cm^3) and washed with ethyl acetate (4 × 50 cm^3) followed by dichloromethane (4 × 50 cm^3) and finally diethyl ether (4 × 50 cm^3). The compound was obtained as an orange-yellow powder (1.34 g, 97 %); mp > 300 °C.

8,8'-[Biphenyl-4,4'-diyl-di(ethyne-2,1-diyl)]diguanosine (5b). 8-Bromoguanosine (1.46 g, 4.0 mmol) and compound **17** (0.41 g, 2.0 mmol) (catalyst, solvent and modified conditions correspond to **5a**) were used to yield the compound as an orange-yellow powder (1.41 g, 92 %); mp > 300 °C.

8,8'-[Ethyne-1,2-diyl-bis(benzene-4,1-diyl-ethyne-2,1-diyl)]diguanosine (5c). 8-Bromo-guanosine (1.46 g, 4.0 mmol) and 4,4'-diethynyltolane (0.45 g, 2.0 mmol) (catalyst, solvent and modified conditions correspond to **5a**) were used to yield the compound as an orange-brown powder (1.53 g, 97 %); mp > 300 °C.

8,8'-[Benzene-1,4-diyl-di(ethyne-2,1-diyl)]bis(2',3',5'-tri-*O*-acetylguanosine) (6a). 8-Bromo-2',3',5'-tri-*O*-acetylguanosine (0.98 g, 2.0 mmol), 1,4-diethynylbenzene (0.13 g, 1.0 mmol), TTPd (231.1 mg, 0.2 mmol) and CuI (76.2 mg, 0.4 mmol) in TEA (0.56 cm^3) and DMF (25 cm^3) were used. In variation of the general procedure, the mixture was stirred for 8 h at 50 °C. The solvent was evaporated and the residue stirred in boiling water (200 cm^3). The collected solid was washed with water (5 × 50 cm^3), then stirred in ethyl acetate (200 cm^3), separated and washed with ethyl acetate (5 × 50 cm^3) and diethyl ether (5 × 50 cm^3) to afford the compound as an orange powder (0.80 g, 85 %); mp 270 °C (dec.).

8,8'-[Biphenyl-4,4'-diyl-di(ethyne-2,1-diyl)]bis(2',3',5'-tri-*O*-acetylguanosine) (6b). 8-Bromo-2',3',5'-tri-*O*-acetylguanosine (0.98 g, 2.0 mmol) and compound **17** (0.20 g, 1.0 mmol) (catalyst, solvent and modified conditions correspond to **6a**) were used to yield the compound as an orange powder (0.73 g, 72 %); mp 220 °C (dec.).

8,8'-[Ethyne-1,2-diyl-bis(benzene-4,1-diyl-ethyne-2,1-diyl)]bis(2',3',5'-tri-*O*-acetyl-guanosine) (6c). 8-Bromo-2',3',5'-tri-*O*-acetylguanosine (0.98 g, 2.0 mmol) and 4,4'-diethynyl-tolane (0.23 g, 1.0 mmol) (catalyst, solvent and modified conditions correspond to **6a**) were used to yield the compound as an orange powder (0.90 g, 87 %); mp 240 °C (dec.).

1,4-Bis{[2-*i*-butyramido-6-oxo-9-(2',3',5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-8-yl]-ethynyl}benzene (7a). 8-Bromo-2-*i*-butyramido-9-(2'3'5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-6-one (1.28 g, 2.0 mmol), 1,4-diethynylbenzene (0.13 g, 1.0 mmol), TTPd (231.1 mg, 0.2 mmol) and CuI (76.2 mg, 0.4 mmol) in TEA (0.56 cm^3) and toluene (25 cm^3) were used. In modification of the general procedure, the mixture was stirred for 5 h at 50 °C. The solvent was evaporated and the residue stirred in boiling water (200 cm^3), then collected, washed with water (5 × 50 cm^3) and dried. Purification by column chromatography (SiO_2, eluent: diethyl ether, then CH_2CH_2/MeOH, 9:1) yielded the compound as an orange-brown powder (1.18 g, 90 %); mp 215 °C (dec.).

4,4'-Bis{[2-*i*-butyramido-6-oxo-9-(2',3',5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-8-yl]-ethynyl}biphenyl (7b). 8-Bromo-2-*i*-butyramido-9-(2'3'5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-6-one (1.28 g, 2.0 mmol) and compound **17** (0.20 g, 1.0 mmol) were used with catalyst, solvent and modified conditions corresponding to **7a**, except the reaction time of 8 h and the eluent of chromatography which was diethyl ether/MeOH (gradient 98:2 – 25:75) to yield the compound as a yellow-orange powder (0.83 g, 63 %); mp 145 – 150 °C.

4,4'-Bis{[2-*i*-butyramido-6-oxo-9-(2',3',5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-8-yl]-ethynyl}tolane (7c). 8-bromo-2-*i*-butyramido-9-(2'3'5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-6-one (1.28 g, 2.0 mmol) and 4,4'-diethynyltolane (0.23 g, 1.0 mmol) were used with catalyst, solvent and modified conditions corresponding to **7a**, except the reaction time of 8 h and the eluent of chromatography which was *n*-hexane/ethyl acetate (1:2) to yield the compound as a yellow powder (0.69 g, 51 %); mp 145 – 148 °C.

1-[(6-Amino-9-*β*-D-ribofuranosyl-purine-8-yl)ethynyl]-4-[(2,4-dioxo-1*H*,3*H*-pyrimidine-5-yl)-ethynyl]benzene (8). 8-Bromoadenosine (0.32 g, 0.92 mmol), compound **15** (0.18 g, 0.73 mmol), TTPd (8.5 mg, 0.0073 mmol) and CuI (2.8 mg, 0.015 mmol) in TEA (1.2 cm^3) and DMF (20 cm^3) were used. In modification of the general procedure, the reaction mixture was stirred at 50 °C for 11 h to yield the compound as a brown powder (0.1 g, 27 %); mp > 300 °C (dec.).

8,8',8'',8'''-[Methanetetrayl-tetrakis(benzene-4,1-diyl-ethyne-2,1-diyl)]tetrauracil (9). 5-Iodouracil (2.20 g, 10.3 mmol), compound **19** (0.92 g, 2.2 mmol), TTPd (109.4 mg, 0.10 mmol) and CuI (36.0 mg, 0.18 mmol) in TEA (2.4 cm^3) and DMF (10 cm^3) were used to yield the compound as a yellow powder (1.50 g, 79 %); mp > 300 °C (dec.).

8,8',8'',8'''-[Methanetetrayl-tetrakis(benzene-4,1-diyl-ethyne-2,1-diyl)]tetraadenosine (10). 8-Bromoadenosine (2.5 g, 7.2 mmol), compound **19** (0.71 g, 1.7 mmol), BTPdCl (50.3 mg, 0.07 mmol) and CuI (27.3 mg, 0.14 mmol) in TEA (3.0 cm^3) and DMF (50 cm^3) were used. In modification of the general procedure, the mixture was stirred at 110 °C for 19 h to yield the compound as a brown powder (2.08 g, 83 %); mp > 300 °C (dec.).

8,8',8'',8'''-[Methanetetrayl-tetrakis(benzene-4,1-diyl-ethyne-2,1-diyl)]tetraguanosine (11). 8-Bromoguanosine (0.72 g, 2.0 mmol), compound **19** (0.21 g, 0.5 mmol), TTPd (231.1 mg, 0.2 mmol) and CuI (76.2 mg, 0.4 mmol) in TEA (0.56 cm^3) and DMF (25 cm^3) (modified conditions correspond to **5a**) were used to yield the compound as an orange powder (0.71 g, 95 %); mp > 300 °C.

8,8',8'',8'''-[Methanetetrayl-tetrakis(benzene-4,1-diyl-ethyne-2,1-diyl)]tetrakis(2',3',5'-tri-*O*-acetylguanosine) (12). 8-Bromo-2',3',5'-tri-*O*-acetylguanosine (0.98 g, 2.0 mmol), compound **19** (0.21 g, 0.5 mmol) (catalyst, solvent and modified conditions correspond to **6a**, except the reaction time being 19 h) were used to yield the compound as an orange-brown powder (0.99 g, 97 %); mp 266 °C (dec.).

Tetrakis{4-[(2-*i*-butyramido-6-oxo-9-(2',3',5'-tri-O-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-8-yl)ethynyl]phenyl}methane (13). 8-Bromo-2-*i*-butyramido-9-(2'3'5'-tri-*O*-*i*-butyryl-*β*-D-ribofuranosyl)-1*H*-purine-6-one (1.28 g, 2.0 mmol) and compound **19** (0.21 g, 0.5 mmol) (catalyst and solvent correspond to **7a**) were used. In modification of the general procedure the mixture was stirred for 20 h at 50 °C. The solvent was removed and the residue extracted with chloroform (3 × 100 cm^3). Evaporation of the solvent yielded the compound as a light green powder (1.92 g, 96 %); mp 106 – 111 °C.

4-(2,4-Dioxo-1*H*,3*H*-pyrimidine-5-yl)-1-[(trimethylsilyl)ethynyl]benzene (14). 5-Iodouracil (1.35 g, 5.7 mmol), 4-ethynyl-1-(trimethylsilylethynyl)benzene (1.14 g, 5.7 mmol), TTPd (65.7 mg, 0.06 mmol) and CuI (216 mg, 0.33 mmol) in TEA (3.0 cm^3) and DMF (30 cm^3) were used. In

modification of the general procedure the reaction time was extended to 21 h. From the collected precipitate which had formed, the symmetrical coupling product of the used ethynyl starting compound was isolated (0.36 g; mp 228 – 232 °C). Partial evaporation of the mother liquor and use of the purification steps described for **2a** yielded the compound **14** as a yellow powder (0.87 g, 50 %); mp 292 – 300 °C (dec.).

B. Spectroscopic data of the synthesized compounds

1: IR (KBr) ν_{max}/cm^{-1} = 3090, 3051 2983, 2926, 2840, 2227, 2152, 1781, 1709, 1663, 1617, 1506, 1428, 1331, 1228, 1156, 1110, 996, 839, 792, 739; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.97 (s, 2 H, CH), 11.51 (br s, 4 H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 75.46, 76.59, 95.68, 148.19, 150.29, 162.62.

2a: IR (KBr) ν_{max}/cm^{-1} = 3234, 3074, 2976, 2914, 2836, 2800, 2722, 2221, 1698, 1631, 1491, 1440, 1305, 1222, 1186, 1103, 995, 840, 788, 767; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.46 (s, 4H, ArH), 7.93 (s, 2H, CH), 11.42, 11.46 (2 × s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 84.88, 91.26, 96.71, 122.48, 131.30, 146.11, 150.42, 162.39; *m/z* (EI) calcd for $C_{18}H_{10}N_4O$: 346.07, found: 346.07 $[M]^+$.

2b: IR (KBr) ν_{max}/cm^{-1} = 3233, 3069, 2972, 2908, 2840, 2726, 2216, 1973, 1713, 1674, 1627, 1488, 1438, 1403, 1310, 1224, 1189, 1003, 821, 785, 767; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.55 (d, 4H, ArH, J = 7.6 Hz), 7.77 (d, 4H, ArH, J = 8.4 Hz), 7.94 (s, 2H, CH), 11.41, 11.46 (2 × br s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 83.90, 91.47, 96.91, 122.11, 126.84, 131.72, 138.82, 145.96, 150.46, 162.49; *m/z* (EI) calcd for $C_{24}H_{14}N_4O_4$: 422.10, found: 422.10 $[M]^+$.

2c: IR (KBr) ν_{max}/cm^{-1} = 3236, 3108, 3072, 2969, 2919, 2837, 2805, 2716, 2212, 1977, 1714, 1684, 1627, 1511, 1495, 1432, 1303, 1221, 1181, 1106, 989, 839, 785, 764; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.49 (d, 4H, ArH, J = 8.0 Hz), 7.57 (d, 4H, ArH, J = 7.6 Hz), 7.89 (s, 2H, CH), 11.36 (br s, 4H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 85.20, 90.83, 91.22, 96.66, 121.83, 123.09, 131.33, 131.71, 146.20, 150.40, 162.36; *m/z* (EI) calcd for $C_{26}H_{14}N_4O_4$: 446.10, found: 446.10 $[M]^+$, 450.13 $[M+4H]^+$.

3a: IR (KBr) ν_{max}/cm^{-1} = 3317, 3172, 2919, 2862, 2212, 1638, 1599, 1574, 1488, 1442, 1406, 1367, 1324, 1299, 1256, 1089, 1046, 985, 835, 796; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.57, 3.71 (2 × m, 2H, $C_{5'}H$), 4.04 (d, 2H, $C_{4'}H$), 4.23 (s, 2H, $C_{3'}H$), 5.03 (m, 2H, $C_{2'}H$), 5.29 (d, 2H, $C_{3'}OH$), 5.52

(d, 2H, $C_{5'}OH$), 5.57 (m, 2H, $C_{2'}OH$), 6.08 (d, 2H, $C_{1'}H$, J = 6.8 Hz), 7.75 (br s, 4H, NH_2), 7.81 (s, 4H, ArH), 8.21 (s, 2H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 62.20, 70.99, 71.90, 81.06, 86.82, 89.52, 93.50, 119.83, 121.63, 132.44, 133.00, 148.71, 153.67, 156.28; *m/z* (ESI) calcd for $C_{30}H_{28}N_{10}O_8$: 656.21, found: 657.22 $[M+H]^+$, 1313.43 $[2M+H]^+$, 1642.54 $[5M+4H]^{2+}$.

3b: IR (KBr) ν_{max}/cm^{-1} = 2930, 2869, 2212, 1645, 1599, 1570, 1510, 1449, 1413, 1370, 1331, 1299, 1260, 1124, 1085, 1049, 1003, 821, 796; ^{1}H NMR (400 MHz, DMSO-d_6) δ =3.58, 3.72 (2 × br s, 2H, $C_{5'}H$), 4.05 (br s, 2H, $C_{4'}H$), 4.24 (br s, 2H, $C_{3'}H$), 5.05 (br s, 2H, $C_{2'}H$), 5.28 (d, 2H, $C_{3'}OH$), 5.51, 5.56 (br s, 4H, $C_{5'}OH$, $C_{2'}OH$), 6.10 (br s, 2H, $C_{1'}H$), 7.70 (br s, 4H, NH_2), 7.81 (d, 4H, ArH, J = 8.0 Hz), 7.92 (d, 4H, ArH, J = 8.0 Hz), 8.21 (s, 2H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 62.23, 71.02, 71.86, 79.65, 86.77, 89.52, 94.17, 119.70, 127.42, 132.66, 133.21, 133.36, 140.45, 148.69, 153.51, 156.22; *m/z* (ESI) calcd for $C_{36}H_{32}N_{10}O_8$: 732.24, found: 733.25 $[M+H]^+$, 771.20 $[M+K]^+$, 1465.49 $[2M+H]^+$, 1504.45 $[2M+K]^+$.

3c: IR (KBr) ν_{max}/cm^{-1} = 3187, 2926, 2869, 2212, 1645, 1599, 1574, 1524, 1492, 1449, 1410, 1370, 1331, 1303, 1260, 1124, 1092, 1049, 842, 796; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.57, 3.71 (2 × br s, 2H, $C_{5'}H$), 4.04 (br s, 2H, $C_{4'}H$), 4.23 (br s, 2H, $C_{3'}H$), 5.03 (br s, 2H, $C_{2'}H$), 5.32 (br s, 2H, $C_{3'}OH$), 5.54, 5.62 (br s, 4H, $C_{5'}OH$, $C_{2'}OH$), 6.08 (br d, 2H, $C_{1'}H$), 7.75 (br s, 12H, NH_2, ArH), 8.20 (s, 2H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 62.25, 71.05, 71.92, 80.53, 86.87, 89.60, 91.56, 93.82, 119.84, 120.47, 123.68, 132.14, 132.31, 133.22, 148.70, 153.61, 156.28; *m/z* (EI) calcd for $C_{38}H_{32}N_{10}O_8$: 756.24, found: 757.25 $[M+H]^+$.

4: IR (KBr) ν_{max}/cm^{-1} = 3319, 3162, 3047, 2873, 2773, 2216, 1641, 1592, 1527, 1488, 1356, 1328, 1296, 835, 800; ^{1}H NMR (500 MHz, DMSO-d_6) δ = 7.49 (s, 4H, NH_2), 7.79 (s, 4H, ArH); 8.22 (s, 2H, CH), 13.70 (s, 2H, NH); ^{13}C NMR (125 MHz, DMSO-d_6) δ = 83.13, 89.90, 119.77, 121.81, 132.33, 133.12, 150.25, 153.73, 155.84; *m/z* (EI) calcd for $C_{20}H_{12}N_{10}$: 392.40, found: 392.0 $[M]^+$.

5a: IR (KBr) ν_{max}/cm^{-1} = 3328, 3222, 2930, 2861, 2212, 1634, 1595, 1567, 1535, 1470, 1438, 1360, 1288, 1231, 1189, 1081, 1046, 835, 782, 693; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.53 (dd, 2H, $C_{5'}H$, J = 6.0 Hz, J = 11.6 Hz), 3.64 – 3.67 (m, 2H, $C_{5'}H$), 3.89 (d, 2H, $C_{4'}H$, J = 3.2 Hz), 4.16 (s, 2H, $C_{3'}H$), 4.95, 4.96 (2 × s, 4H, $C_{5'}OH$, $C_{2'}H$), 5.14 (d, 2H, $C_{3'}OH$, J = 4.4 Hz), 5.49 (d, 2H, $C_{2'}OH$, J = 6.0 Hz), 5.89 (d, 2H, $C_{1'}H$, J = 6.4 Hz), 6.64 (s, 4H, NH_2), 7.73 (s, 4H, ArH), 10.82 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 62.01, 70.51, 71.08, 82.07, 85.76, 88.37, 92.03, 117.85, 121.71, 129.11, 132.04, 133.00, 151.32, 154.17, 156.13; *m/z* (ESI) calcd for $C_{30}H_{28}N_{10}O_{10}$: 688.20, found: 689.21 $[M+H]^+$.

5b: IR (KBr) ν_{max}/cm^{-1} = 3219, 2926, 2869, 2209, 1688, 1627, 1592, 1567, 1535, 1470, 1438, 1360, 1288, 1231, 1185, 1081, 1046, 1003, 864, 825, 785, 696, 525; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.56 (s, 2H, C_5'H), 3.66 (s, 2H, C_5'H), 3.90 (s, 2H, C_4'H), 4.18 (s, 2H, C_3'H), 4.98 (s, 4H, C_2'H, C_5'OH), 5.16 (s, 2H, C_3'OH), 5.51 (s, 2H, C_2'OH), 5.92 (d, 2H, C_1'H, J = 6.0 Hz), 6.65 (s, 4H, NH_2), 7.75, 7.90 (2 × d, 4H, ArH), 10.88 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 62.38, 70.89, 71.35, 81.04, 86.05, 88.66, 92.82, 118.00, 120.51, 127.62, 129.05, 129.70, 132.62, 133.52, 140.30, 151.57, 154.49, 156.53; *m/z* (MALDI) calcd for $C_{36}H_{32}N_{10}O_{10}$: 764.23, found: 765.3 $[M+H]^+$, 787.3 $[M+Na]^+$, 803.3 $[M+K]^+$.

5c: IR (KBr) ν_{max}/cm^{-1} = 3204, 2922, 2869, 2205, 1681, 1631, 1595, 1563, 1527, 1478, 1435, 1403, 1360, 1285, 1228, 1185, 1078, 1042, 939, 914, 835, 782, 693; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.54 (s, 2H, C_5'H), 3.65 (s, 2H, C_5'H), 3.89 (s, 2H, C_4'H), 4.17 (s, 2H, C_3'H), 4.98 (s, 4H, C_3'OH, C_5'OH), 5.16 (s, 2H, C_2'OH), 5.50 (d, 2H, C_2'H, J = 5.2 Hz), 5.89 (d, 2H, C_1'H, J = 6.0 Hz), 6.64 (s, 4H, NH_2), 7.70 (s, 8H, ArH), 10.91 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 61.91, 70.42, 70.93, 81.54, 85.66, 88.31, 91.25, 92.04, 117.70, 120.89, 123.01, 129.11, 131.77, 131.90, 132.72, 151.13, 154.00, 156.00; *m/z* (MALDI) calcd for $C_{38}H_{32}N_{10}O_{10}$: 788.23, found: 789.2 $[M+H]^+$, 811.2 $[M+Na]^+$.

6a: IR (KBr) ν_{max}/cm^{-1} = 2933, 2216, 1749, 1684, 1631, 1588, 1531, 1470, 1438, 1367, 1242, 1099, 1046, 935, 900, 839, 792, 693; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 1.94, 2.10, 2.13 (3 × s, 6H, CH_3), 4.19 – 4.23 (m, 2H, C_5'H), 4.37 – 4.46 (m, 4H, C_4'H, C_5'H), 5.67 (t, 2H, C_3'H, J = 6.0 Hz), 6.00 (t, 2H, C_2'H, J = 4.6 Hz), 6.11 (d, 2H, C_1'H, J = 3.6 Hz), 6.72 (s, 4H, NH_2]), 7.63 – 7.78 (m, 4H, ArH), 10.98 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 20.20, 20.22, 20.31, 62.73, 69.78, 71.59, 78.92, 81.05, 86.54, 92.74, 117.58, 121.48, 128.46, 132.03, 132.88, 150.97, 154.36, 155.94, 169.38, 169.46, 168.98; *m/z* (MALDI) calcd for $C_{42}H_{40}N_{10}O_{16}$: 940.26, found: 963.3 $[M+Na]^+$, 979.2 $[M+K]^+$.

6b: IR (KBr) ν_{max}/cm^{-1} = 3036, 2930, 2212, 1749, 1681, 1634, 1592, 1531, 1478, 1431, 1374, 1242, 1096, 1049, 1003, 935, 900, 825, 784, 696; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 1.95, 2.09, 2.13 (3 × s, 6H, CH_3), 4.22 (dd, 2H, C_5'H, J = 6.0 Hz, J = 11.2 Hz), 4.38 – 4.65 (m, 4H, C_4'H, C_5'H), 5.68 (t, 2H, C_3'H, J = 6.4 Hz), 6.03 (t, 2H, C_2'H, J = 5.0 Hz), 6.12 (d, 2H, C_1'H, J =4.0 Hz), 6.73 (s, 4H, NH_2), 7.63 – 7.91 (m, 8H, ArH), 10.99 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 20.22, 20.25, 20.34, 62.74, 69.79, 71.53, 78.94, 79.72, 86.49, 93.23, 117.44, 119.86, 126.88, 127.22,

128.69, 132.36, 133.13, 140.03, 150.97, 154.33, 155.97, 169.40, 169.46, 170.01; *m/z* (MALDI) calcd for $C_{48}H_{44}N_{10}O_{16}$: 1016.29, found: 1039.4 $[M+Na]^+$, 1055.3 $[M+K]^+$.

6c: IR (KBr) ν_{max}/cm^{-1} = 3361, 3215, 2930, 2209, 1748, 1692, 1627, 1585, 1527, 1481, 1438, 1368, 1235, 1097, 1049, 932, 900, 839, 783, 693, 648; ^1H NMR (400 MHz, DMSO-d_6) δ = 1.95, 2.10, 2.13 (3 × s, 6H, CH_3), 4.21 (dd, 2H, C_5'H, J = 5.2 Hz, J = 11.2 Hz), 4.39 – 4.46 (m, 4H, C_4'H, C_5'H), 5.67 (t, 2H, C_3'H, J = 6.0 Hz), 6.01 (t, 2H, C_2'H, J = 4.8 Hz), 6.12 (d, 2H, C_1'H, J = 4.0 Hz), 6.75 (s, 4H, NH_2), 7.70 – 7.76 (m, 8H, ArH), 11.01 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 20.21, 20.24, 20.33, 62.74, 69.79, 71.58, 78.95, 80.65, 86.54, 91.38, 92.93, 117.52, 120.67, 123.23, 128.54, 131.88, 131.93, 131.96, 132.77, 150.95, 154.35, 155.95, 169.39, 169.46, 170.00; *m/z* (MALDI) calcd for $C_{50}H_{44}N_{10}O_{16}$: 1040.29, found: 1063.3 $[M+Na]^+$.

7a: IR (KBr) ν_{max}/cm^{-1} = 3197, 2976, 2933, 2876, 2220, 1742, 1717, 1693, 1610, 1560, 1463, 1438, 1388, 1353, 1249, 1189, 1153, 1124, 1103, 935, 914, 835, 782, 753, 728, 700, 589, 543; ^1H NMR (400 MHz, $CDCl_3$) δ = 1.10 – 1.34 (m, 48H, CH_3), 2.49 – 2.80 (m, 8H, CH), 4.52 – 4.58 (m, 4H, C_4'H, C_5'H), 4.68 (dd, 2H, C_5'H, J = 8.0 Hz, J = 13.6 Hz), 5.95 (t, 2H, C_3'H, J = 4.6 Hz), 6.08 (t, 2H, C_2'H, J = 4.8 Hz), 6.27 (d, 2H, C_1'H, J = 4.8 Hz), 7.45 – 7.70 (m, 4H, ArH), 9.33 (s, 2H, NH), 12.12 (s, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 18.68, 18.75, 18.82, 18.91, 33.72, 33.90, 33.94, 36.52, 62.89, 70.91, 72.66, 79.96, 87.89, 94.72, 122.21, 122.23, 128.57, 132.06, 132.76, 147.30, 148.31, 154.54, 175.43, 175.94, 177.89, 179.03; *m/z* (ESI) calcd for $C_{62}H_{70}N_{10}O_{18}$: 1248.53; found: 1250.03 $[2M+2H]^{2+}$, 1874.77 $[3M+2H]^{2+}$, 1666.73 $[4M+3H]^{3+}$.

7b: IR (KBr) ν_{max}/cm^{-1} = 3204, 3055, 2972, 2933, 2873, 2217, 1740, 1713, 1688, 1606, 1556, 1467, 1435, 1388, 1350, 1249, 1192, 1156, 1121, 1096, 1007, 932, 828, 785, 746, 721, 693, 543; ^1H NMR (400 MHz, $CDCl_3$) δ = 1.11 – 1.33 (m, 48H, CH_3), 2.49 – 2.82 (m, 8H, CH), 4.54 – 4.56 (m, 4H, C_4'H, C_5'H), 4.65 – 4.69 (dd, 2H, C_5'H, J = 7.2 Hz, J = 13.6 Hz), 5.95 (t, 2H, C_3'H, J = 4.2 Hz), 6.11 (t, 2H, C_2'H, J = 4.6 Hz), 6.31 (d, 2H, C_1'H, J = 4.8 Hz), 7.45 – 7.73 (m, 8H, ArH), 9.30 (s, 2H, NH), 12.08 (s, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 18.68, 18.72, 18.77, 18.91, 33.71, 33.89, 33.93, 36.48, 62.92, 70.93, 72.58, 78.60, 79.90, 87.76, 94.98, 120.44, 122.35, 127.17, 128.42, 128.54, 132.02, 132.57, 141.21, 147.28, 148.12, 154.66, 175.39, 175.90, 177.86, 178.97; *m/z* (MALDI) calcd for $C_{68}H_{80}N_{10}O_{18}$: 1324.57, found: 1347.7 $[M+Na]^+$, 1363.7 $[M+K]^+$.

7c: IR (KBr) ν_{max}/cm^{-1} = 3204, 3044, 2972, 2930, 2863, 2212, 1745, 1717, 1695, 1610, 1560, 1517, 1467, 1431, 1392, 1349, 1253, 1189, 1156, 1103, 1049, 953, 928, 910, 839, 782, 753, 725, 696, 543; ^1H NMR (400 MHz, $CDCl_3$) δ = 1.11 – 1.33 (m, 48H, CH_3), 2.51 – 2.81 (m, 8H, CH), 4.53 –

4.58 (m, 4H, $C_{4'}H$, $C_{5'}H$), 4.65 – 4.68 (dd, 2H, $C_{5'}H$, J = 6.0 Hz, J = 13.6 Hz), 5.94 (t, 2H, $C_{3'}H$, J = 4.4 Hz), 6.08 (t, 2H, $C_{2'}H$, J = 4.8 Hz), 6.29 (d, 2H, $C_{1'}H$, J = 4.8 Hz), 7.56 (br s, 8H, ArH), 9.34 (s, 2H, NH), 12.10 (s, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 18.62, 18.81, 33.60, 33.78, 33.83, 36.39, 62.82, 70.83, 72.52, 79.28, 79.79, 87.66, 91.39, 94.66, 120.80, 122.30, 124.21, 128.63, 131.56, 131.66, 131.80, 132.85, 147.20, 148.05, 154.56, 175.28, 175.79, 177.76, 178.88; *m/z* (MALDI) calcd for $C_{70}H_{80}N_{10}O_{18}$: 1348.57, found: 1371.7 $[M+Na]^+$.

8: IR (KBr) ν_{max}/cm^{-1} = 3229, 3087, 2965, 2926, 2819, 2209, 1713, 1626, 1594, 1496, 1339, 1306, 1224, 1185, 1101, 988, 835, 795; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.69, 3.72 (2 × d, 1H, $C_{5'}H$, J = 3.6 Hz), 4.03 (d, 1H, $C_{4'}H$, J = 2.0 Hz), 4.22 (m, 1H, $C_{3'}H$), 5.02 (t, 1H, $C_{2'}H$, J = 5.8 Hz), 5.20 – 5.70 (br s, 3H, $C_{3'}OH$, $C_{5'}OH$, $C_{2'}OH$), 6.06 (d, 1H, $C_{1'}H$, J = 6.8 Hz), 7.44 (d, 1H, ArH, J = 7.6 Hz), 7.51 (d, 1H, ArH, J = 7.6 Hz), 7.60 (d, 1H, ArH, J = 8.0 Hz), 7.67 (d, 1H, ArH, J = 8.0 Hz), 7.72 (d, 1H, NH_2, J = 7.6 Hz), 7.79 (d, 1H, NH_2, J = 8.4 Hz), 7.92 (s, 1H, CH), 8.18 (s, 1H, CH), 10.79 (br s, 1H, NH); *m/z* (EI) calcd for $C_{24}H_{19}N_7O_6$: 501.14, found: 502.15 $[M+H]^+$.

9: IR (KBr) ν_{max}/cm^{-1} = 3083, 3051, 2880, 2205, 1664, 1629, 1573, 1498, 1438, 1399, 1314, 1227, 1162, 1116, 1006, 824, 781; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.19 – 7.63 (m, 16H, ArH), 7.80 (br s, 4H, CH), 12.20 (br s, 8H, NH); *m/z* (MALDI) calcd for $C_{49}H_{28}N_8O_8$: 856.79, found: 857.31 $[M]^+$.

10: IR (KBr) ν_{max}/cm^{-1} = 3329, 3197, 2919, 2865, 2212, 1638, 1595, 1570, 1488, 1453, 1410, 1370, 1331, 1299, 1256, 1089, 1049, 984, 825, 797; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.55, 3.71 (2 × m, 4H, $C_{5'}H$), 4.00 (s, 4H, $C_{4'}H$), 4.21 (s, 4H, $C_{3'}H$), 5.01 (m, 4H, $C_{2'}H$), 5.21 (d, 4H, $C_{3'}OH$), 5.44 (d, 2H, $C_{5'}OH$), 5.53 (m, 4H, $C_{2'}OH$), 6.03 (d, 4H, $C_{1'}H$), 7.37 (m, 8H, ArH), 7.67 – 7.72 (s, 16H, ArH, NH_2), 8.18 (s, 4H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 62.19, 70.97, 71.77, 78.92, 86.76, 89.51, 93.86, 118.29, 119.67, 130.94, 131.96, 133.29, 147.11, 148.63, 153.48, 156.20; *m/z* (MALDI) calcd for $C_{73}H_{64}N_{20}O_{16}$: 1476.48 found: 1477.63 $[M+H]^+$.

11: IR (KBr) ν_{max}/cm^{-1} = 3364, 3208, 2923, 2866, 2208, 1692, 1631, 1587, 1565, 1527, 1477, 1435, 1404, 1363, 1285, 1185, 1084, 1043, 943, 916, 824, 781, 745, 693 ; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.54 (d, 4H, $C_{5'}H$, J = 5.2 Hz), 3.63 – 3.69 (m, 4H, $C_{5'}H$), 3.86 (d, 4H, $C_{4'}H$, J = 4.0 Hz), 4.15 (d, 4H, $C_{3'}H$, J = 4.0 Hz), 4.93 – 4.98 (m, 8H, $C_{3'}OH$, $C_{5'}OH$), 5.16 (d, 4H, $C_{2'}OH$, J = 4.4 Hz), 5.44 (d, 4H, $C_{2'}H$, J = 6.4 Hz), 5.86 (d, 4H, $C_{1'}H$, J = 7.2 Hz), 6.59 (s, 8H, NH_2), 7.33 (d, 8H, ArH, J = 8.4 Hz), 7.65 (d, 8H, ArH, J = 8.0 Hz), 10.86 (s, 4H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ =

62.03, 64.87, 70.50, 70.98, 79.98, 85.72, 88.46, 92.25, 117.66, 118.84, 128.72, 130.92, 131.56, 146.65,151.18, 154.04, 156.04; *m/z* calcd for $C_{73}H_{64}N_{20}O_{20}$: 1540.46.

12: IR (KBr) ν_{max}/cm^{-1} = 2933, 2211, 1746, 1685, 1628, 1587, 1527, 1480, 1432, 1369, 1239, 1093, 1049, 938, 824, 783, 691; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 1.90, 2.07, 2.11 (3 × s, 12H, CH_3), 4.21 (dd, 4H, C_5'H, J = 6.0 Hz, J = 10.8 Hz), 4.35 – 4.43 (m, 8H, C_4'H, C_5'H), 5.64 (t, 4H, C_3'H, J = 5.8 Hz), 6.01 (t, 4H, C_2'H, J = 4.8 Hz), 6.06 (s, 4H, C_1'H), 6.73 (s, 8H, NH_2), 7.34 (d, 8H, ArH, J = 7.6 Hz), 7.69 (d, 8H, ArH, J = 7.2 Hz), 10.99 (s, 4H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 20.18, 20.23, 20.28, 62.69, 64.85, 69.72, 71.37, 78.95, 79.26, 86.40, 92.94, 117.36, 118.50, 128.67, 130.80, 131.60, 146.74, 150.92, 154.29, 155.93, 169.38, 169.43, 169.96; *m/z* (MALDI) calcd for $C_{97}H_{88}N_{20}O_{32}$: 2045.59; found: 2067.7 $[M+Na]^+$, 2084.7 $[M+K]^+$.

13: IR (KBr) ν_{max}/cm^{-1} = 3193, 3056, 2974, 2933, 2873, 2214, 1742, 1717, 1689, 1606, 1556, 1467, 1435, 1388, 1353, 1252, 1192, 1154, 1119, 1100, 824, 748, 723, 698, 542; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.09 – 1.31 (m, 96H, CH_3), 2.49 – 2.68 (m, 16H, CH), 4.44 – 4.50 (m, 8H, C_4'H, C_5'H), 4.60 – 4.68 (m, 4H, C_5'H), 5.93 – 6.00 (m, 4H, C_3'H), 6.05 – 6.15 (m, 4H, C_2'H), 6.23 (d, 4H, C_1'H, J = 4.4 Hz), 7.56 (m, 16H, ArH), 9.31 (s, 4H, NH), 12.06 (s, 4H, NH); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 18.71, 18.83, 33.64, 33.78, 33.84, 36.44, 62.68, 70.63, 72.63, 79.66, 80.11, 87.79, 94.49, 119.40, 122.21, 128.49, 130.80, 131.86, 146.83, 147.23, 148.11, 154.62, 175.37, 175.88, 177.61, 178.91; *m/z* (MALDI) calcd for $C_{137}H_{160}N_{20}O_{36}$: 2662.13, found: 2685.43 $[M+Na]^+$.

14: IR (KBr) ν_{max}/cm^{-1} = 3069, 2955, 2898, 2823, 2220, 2159, 1719, 1688, 1627, 1492, 1435, 1313, 1256, 1228, 867, 846, 760; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 0.24 (s, 9H, CH_3), 7.43 (d, 2H, ArH, J = 8.4 Hz), 7.47 (d, 2H, ArH, J = 8.0 Hz) 7.90 (d, 1H, CH, J = 6.0 Hz), 11.37 – 11.42 (m, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = - 0.13 , 85.19, 91.14, 96.43, 96.67, 104.68, 121.94, 123.17, 131.25, 131.92, 146.21, 150.44, 162.40.

15: IR (KBr) ν_{max}/cm^{-1} = 3290, 3033, 2972, 2798, 2205, 2184, 2102, 1699, 1631, 1560, 1502, 1460, 1342, 1313, 835, 796; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 3.51 (s, 1H, C≡CH), 4.23 (s, 1H, OH), 7.31 (d, 2H, ArH, J = 8.0 Hz), 7.40 (d, 2H, ArH, J = 8.4 Hz), 7.81 (s, 1H, CH), 9.56 (s, 1H, NH); ^{1}H NMR (400 MHz, DMSO-d_6+ D_2O) δ = 7.40 (s, 4H, ArH); 7.85 (s, 1H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 79.19, 81.69, 83.46, 90.01, 92.48, 119.32, 125.60, 130.11, 131.78, 159.79, 163.57, 165.22.

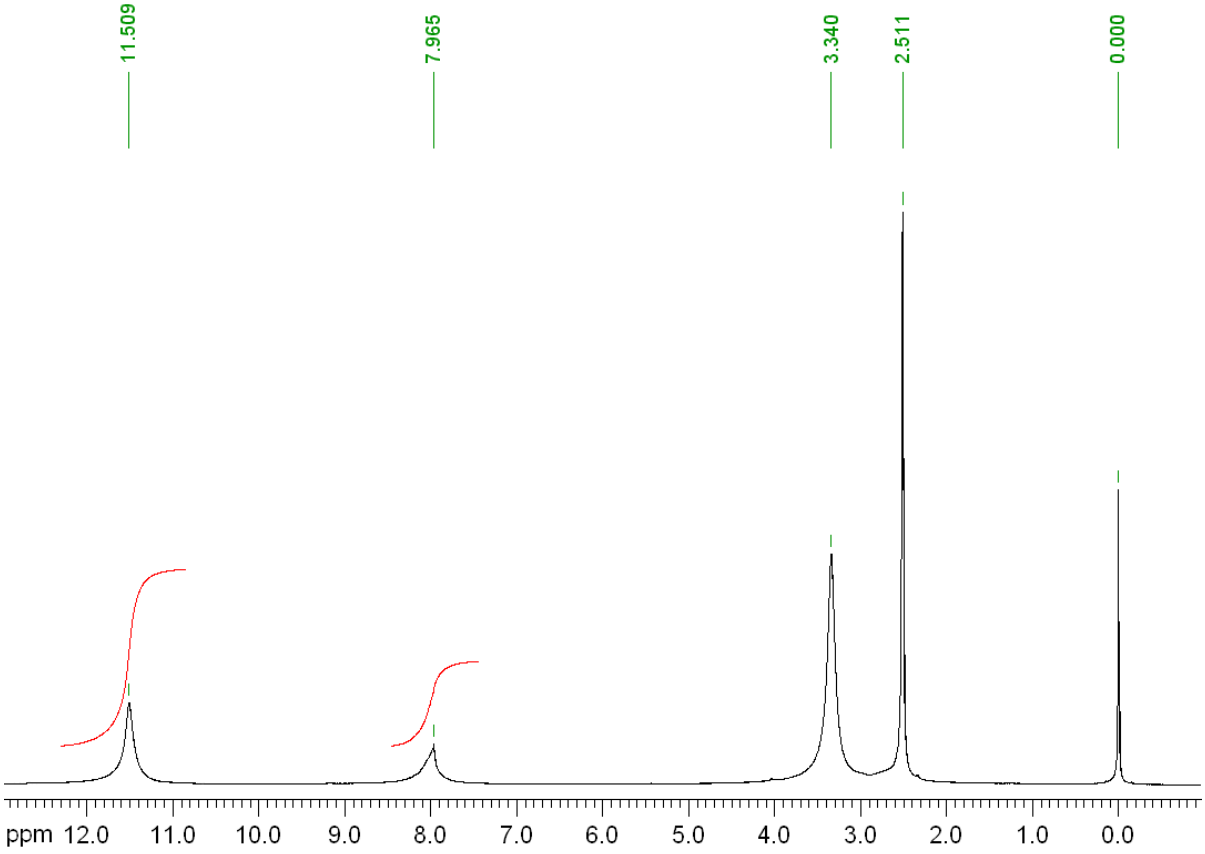
16: IR (KBr) ν_{max}/cm^{-1} = 3040, 2987, 2873, 2230, 1634, 1495, 1378, 1360, 1278, 1160, 967, 910, 825; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 1.49 (s, 12H, CH_3), 5.51 (s, 2H, OH), 7.48 (d, 4H, ArH, J = 8.4 Hz), 7.70 (d, 4H, ArH, J = 8.0 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 31.68, 63.74, 80.21, 97.22, 122.12, 126.74, 131.92, 138.72; *m/z* (EI) calcd for $C_{22}H_{22}O_2$: 318.16, found: 318 $[M]^+$.
17: IR (KBr) ν_{max}/cm^{-1} = 3290, 3269, 3030, 2109, 1606, 1492, 1392, 1249, 1110, 1007, 857, 824, 682, 660, 650, 635; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 4.27 (s, 2H, C≡CH), 7.58 (d, 4H, ArH, J = 8.0 Hz), 7.72 (d, 4H, ArH, J = 8.0 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 81.73, 83.24, 121.26, 126.89, 132.36, 139.41; *m/z* (EI) calcd for $C_{16}H_{10}$: 202.08, found: 202 $[M]^+$.

18: IR (KBr) ν_{max}/cm^{-1} = 3082, 3031, 2977, 2930, 2866, 2230, 1632, 1565, 1549, 1502, 1454, 1363, 1277, 1195, 1163, 1021, 964, 907, 824, 802; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 1.43 (s, 24H, CH_3), 5.46 (s, 4H, OH), 7.03 (d, 8H, ArH, J = 8.4 Hz), 7.34 (d, 8H, ArH, J = 8.4 Hz); ^{13}C NMR (100 MHz, DMSO-d_6) δ = 31.62, 63.00, 63.62, 79.93, 96.61, 120.81, 130.59, 130. 81, 145.29; *m/z* (ESI) calcd for $C_{45}H_{44}O_4$: 648.32, found: 666.3 $[M+NH_4]^+$.

19: IR (KBr) ν_{max}/cm^{-1} = 3281, 3113, 3085, 3063, 3031, 2917, 2851, 2110, 1932, 1603, 1559, 1496, 1407, 1255, 1017, 827; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 3.06 (s, 4H, C≡CH), 7.12 (d, 8H, ArH, J = 8.0 Hz), 7.39 (d, 8H, ArH, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 64.82, 77.62, 83.18, 120.33, 130.76, 131.66, 146.21; *m/z* (EI) calcd for $C_{33}H_{20}$: 416.16, found: 416 $[M]^+$.

C. ^{1}H-NMR-spectra of selected key compounds corresponding to the different structural types

1: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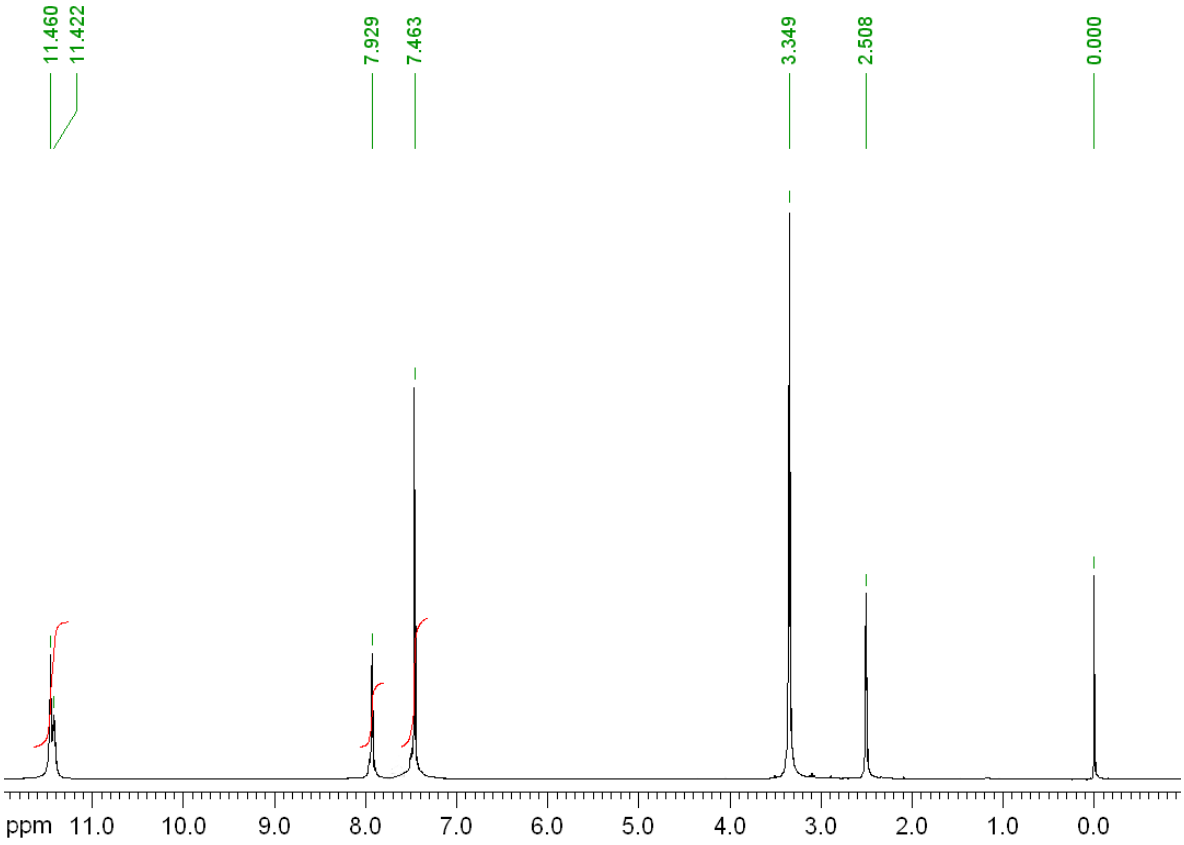
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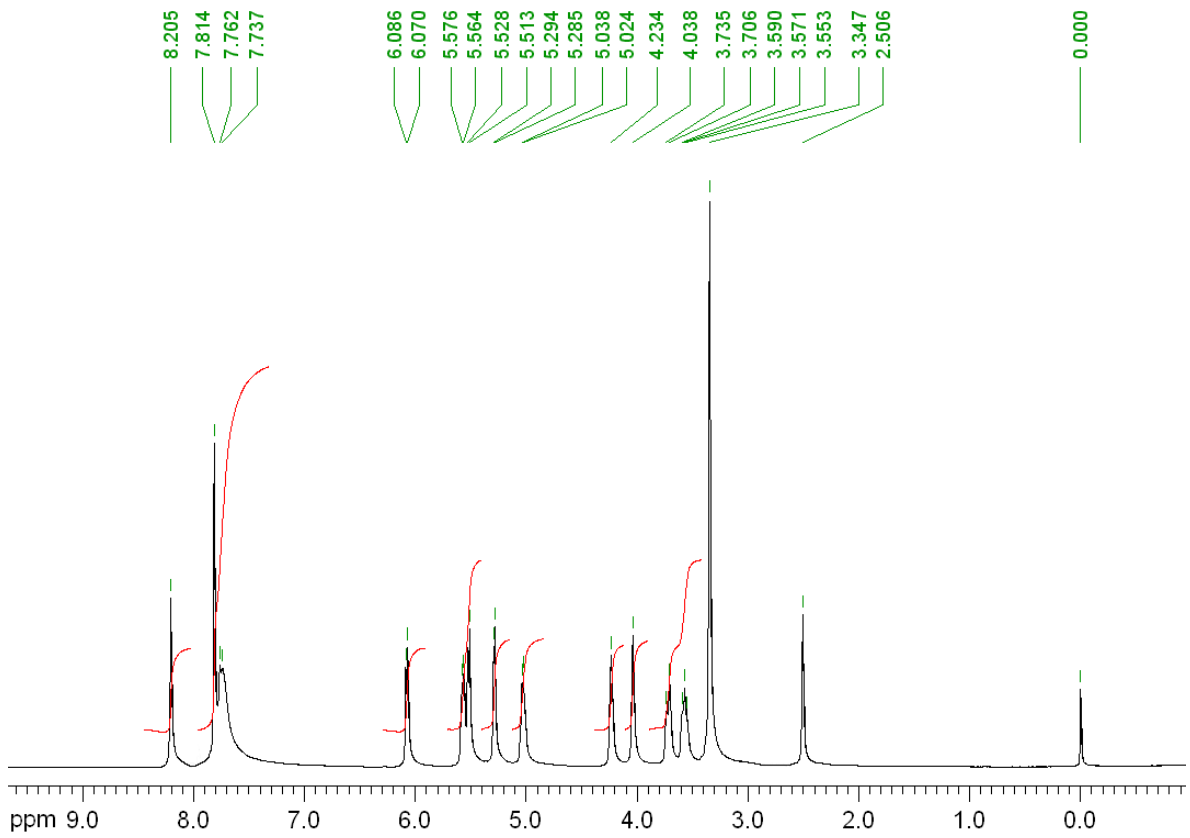
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3.590
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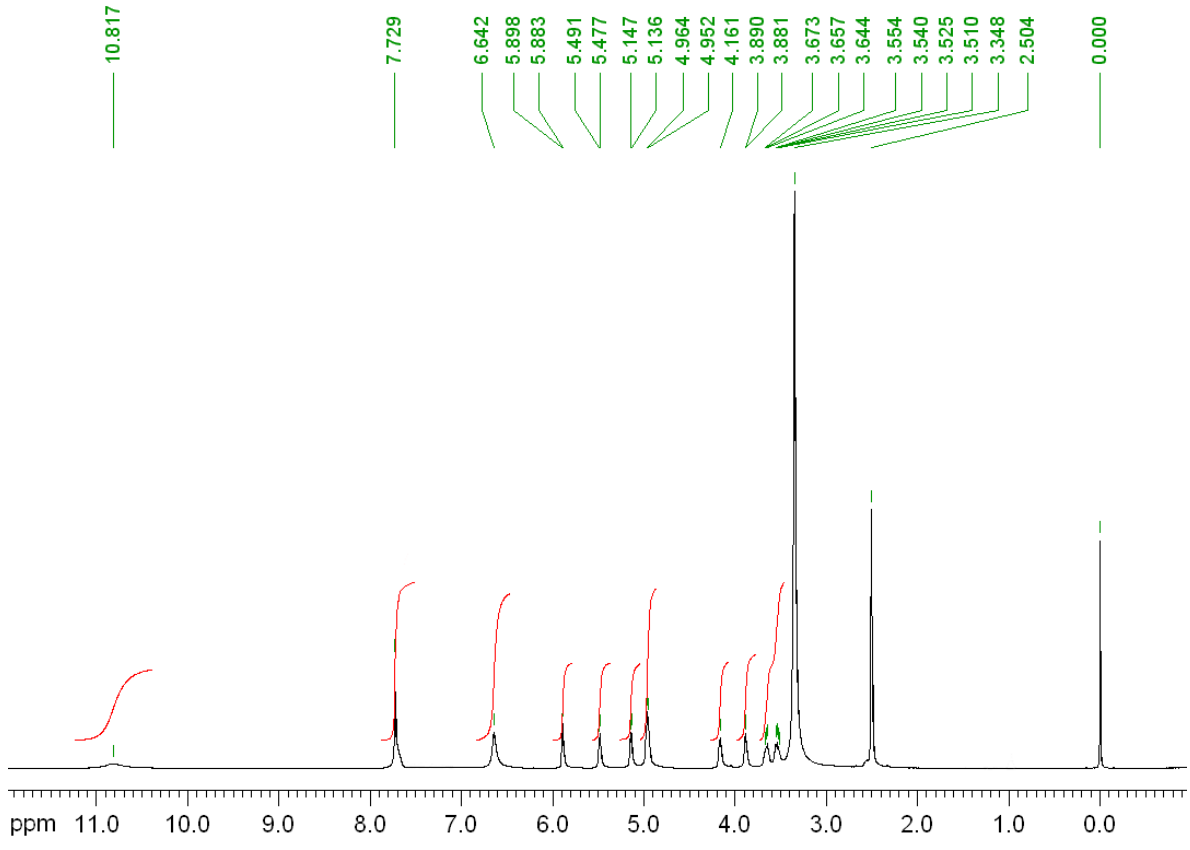
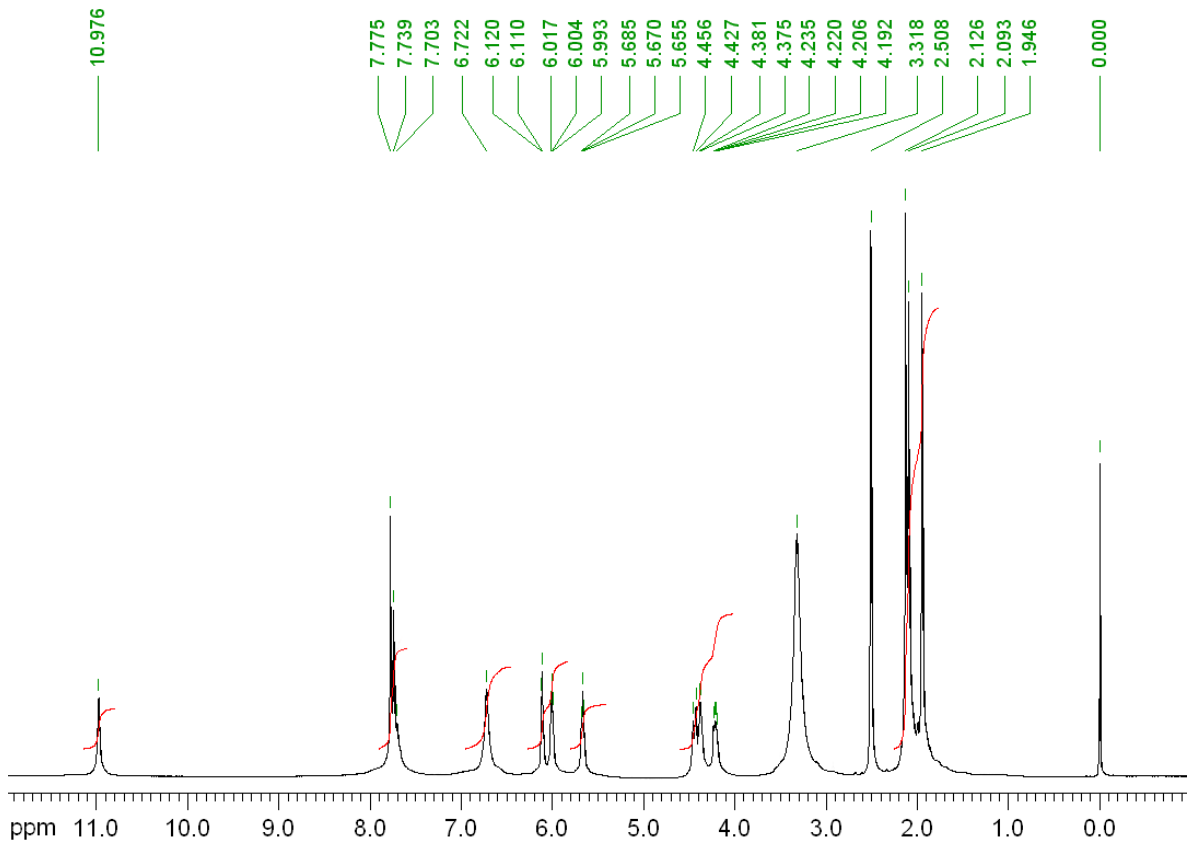
3.347
2.506
0.000
ppm 9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

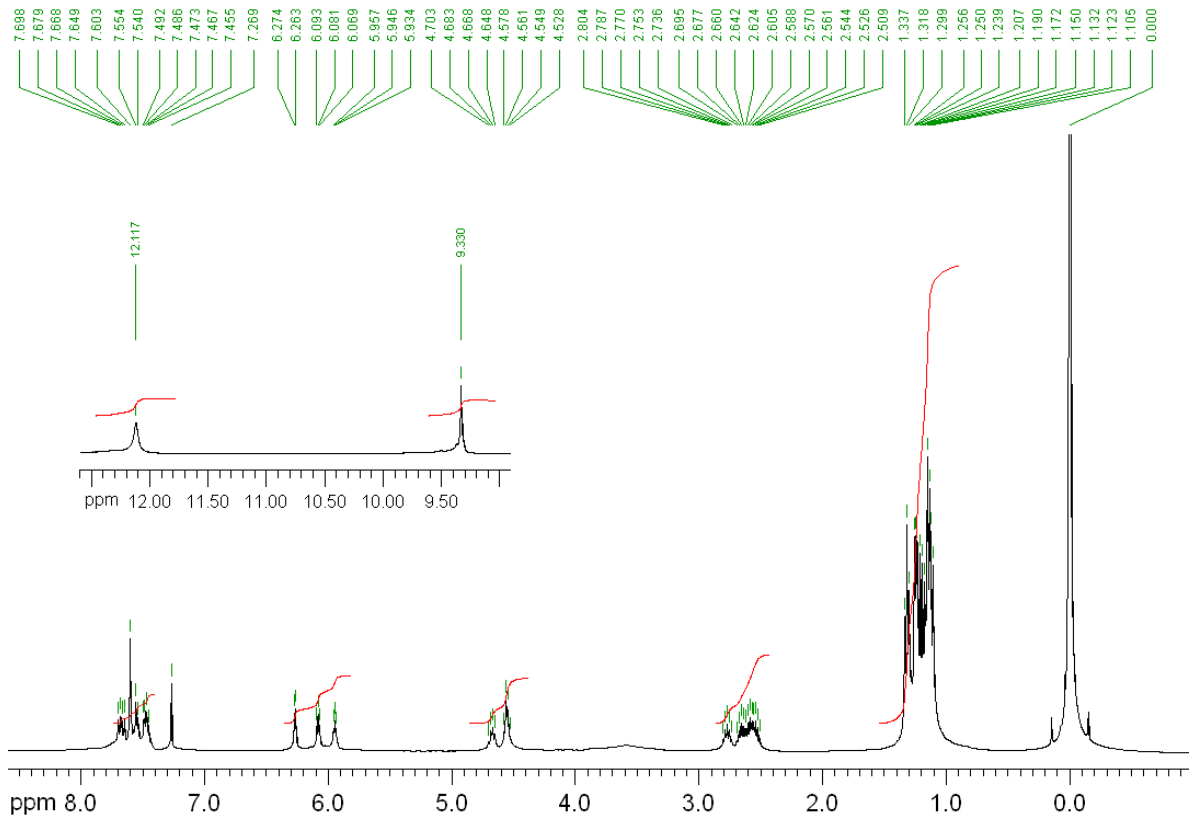
5a:


10.817
7.729
6.642
5.898
5.883
5.491
5.477
5.147
5.136
4.964
4.952
4.161
3.890
3.881
3.673
3.657
3.644
3.554
3.540
3.525
3.510
3.348
2.504
0.000
ppm 11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

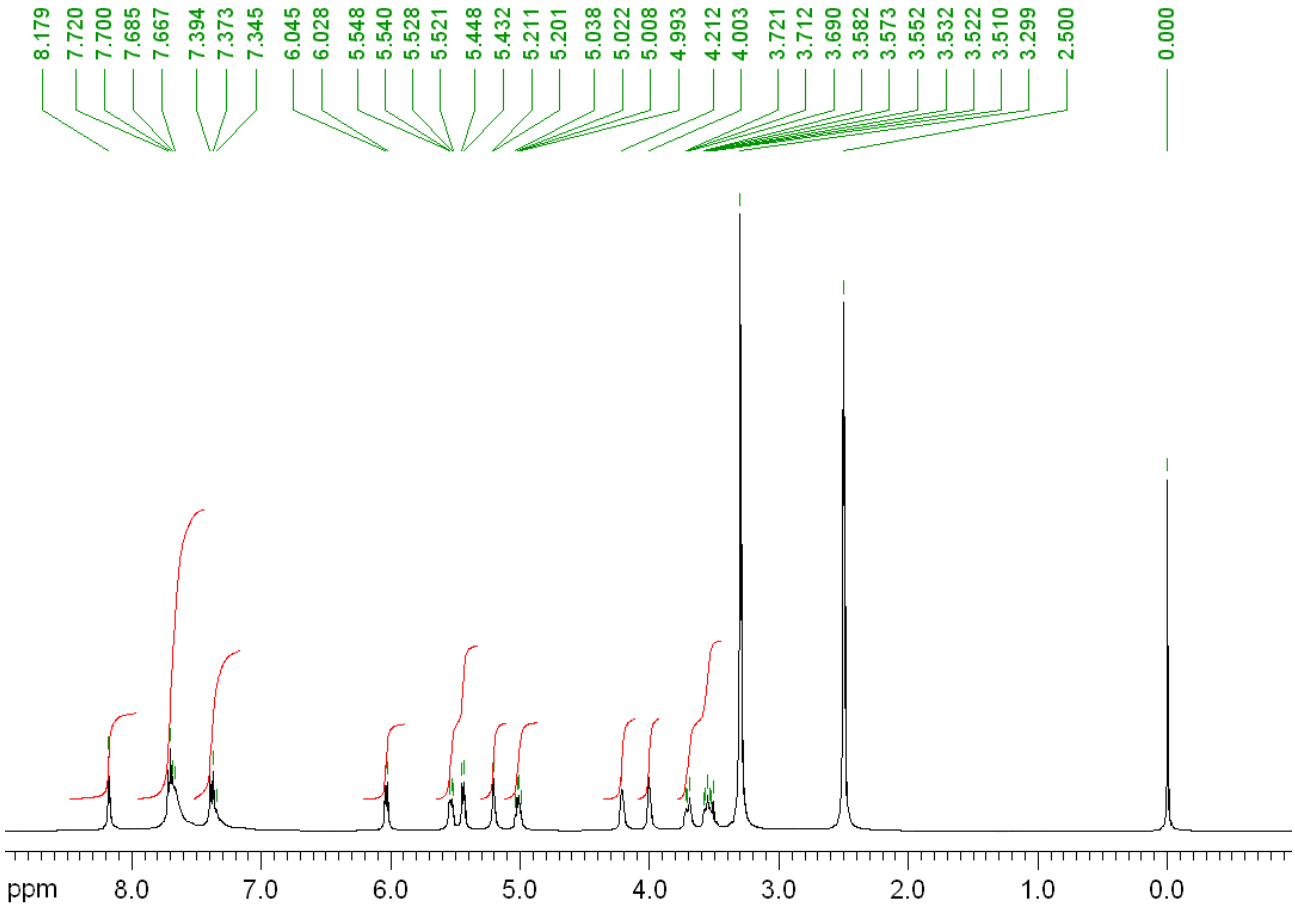
6a:


10.976
7.775
7.739
7.703
6.722
6.120
6.110
6.017
6.004
5.993
5.685
5.670
5.655
4.456
4.427
4.381
4.375
4.235
4.220
4.206
4.192
3.318
2.508
2.126
2.093
1.946
0.000
ppm 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

7a:


7.698
7.679
7.668
7.649
7.603
7.554
7.540
7.492
7.486
7.473
7.467
7.455
7.269
6.274
6.263
6.093
6.081
6.069
5.957
5.946
5.934
4.703
4.683
4.668
4.648
4.578
4.561
4.549
4.528
2.804
2.787
2.770
2.753
2.736
2.695
2.677
2.660
2.642
2.624
2.605
2.588
2.570
2.561
2.544
2.526
2.509
1.337
1.318
1.299
1.256
1.250
1.239
1.207
1.190
1.172
1.150
1.132
1.123
1.105
0.000
12.117
9.330
ppm 12.00 11.50 11.00 10.50 10.00 9.50
ppm 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

10:


8.179
7.720
7.700
7.685
7.667
7.394
7.373
7.345
6.045
6.028
5.548
5.540
5.528
5.521
5.448
5.432
5.211
5.201
5.038
5.022
5.008
4.993
4.212
4.003
3.721
3.712
3.690
3.582
3.573
3.552
3.532
3.522
3.510
3.299
2.500
0.000
ppm
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

D. Distances and angles of hydrogen bond type interactions of compound 1 · 2 DMSO

Atoms involved	Symmetry	Distances / Å		Angle / °
		D···A	H···A	D-H···A
N1-H1···O5	-*x*, -*y*+1, -*z*+1	2.808 (3)	1.94	166
N2-H2···O5	*x*, -*y*+1/2, *z*+1/2	2.871 (3)	1.91	177
N3-H3···O6	*x*, *y*+1, *z*	2.768 (3)	1.78	171
N4-H4···O6	-*x*+1, *y*+3/2, -*z*+1/2	2.843 (3)	1.92	171
C1-H5···O1	-*x*,+1/2+*y*, 3/2-*z*	3.259 (3)	2.38	153.5
C15-H15B···O2	1-*x*, -1/2+*y*, 1/2-*z*	3.216 (3)	2.34	148.7
C12-H12···O3	1-*x*, -1/2+*y*, 1/2-*z*	3.192 (3)	2.25	171.3
C13-H13B···O4	*x*, 3/2-*y*, -1/2+*z*	3.208 (3)	2.27	159.9
C16-H16A···O3	*x*, 3/2-*y*, -1/2+*z*	3.529 (4)	2.62	154.5
C15-H15A···$\pi_{C7\text{-}C8}$	1-*x*, 1-*y*, 1-*z*	3.829 (3)	2.86	171.9
C16-H16B···$\pi_{C5\text{-}C6}$	1-*x*, -1/2+*y*, 1/2-*z*	3.692 (3)	2.82	148.0