Supplementary Information

Exciplex and excimer molecular probes: detection of conformational flip in a myo-inositol chair

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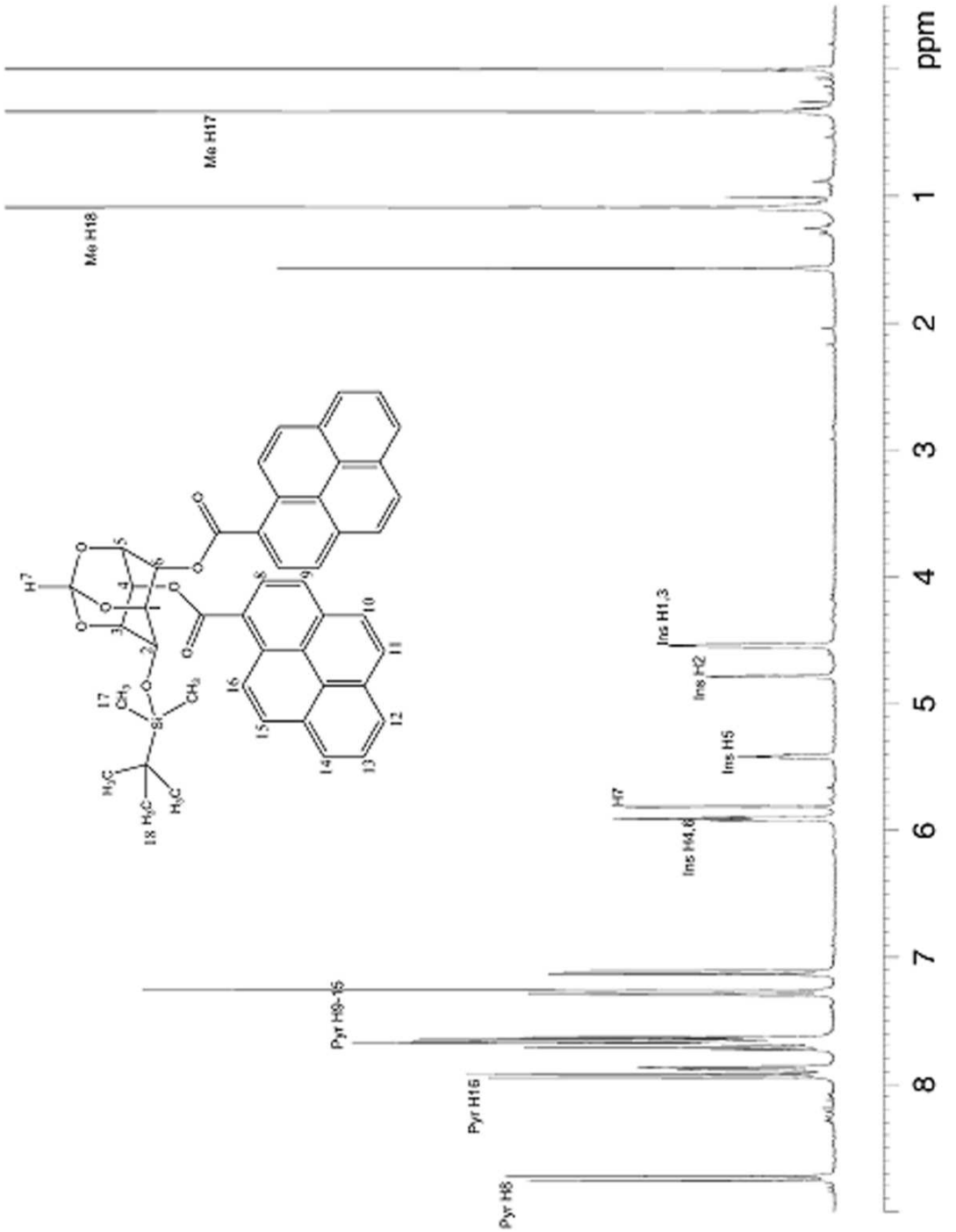

Figure SI 1: ^{1}H NMR spectrum of 2-O-*tert*-butyldimethylsilyl-4,6-bis-O-pyrenoyl-*myo*-inositol-1,3,5-orthoformate (**6**) in $CDCl_3$

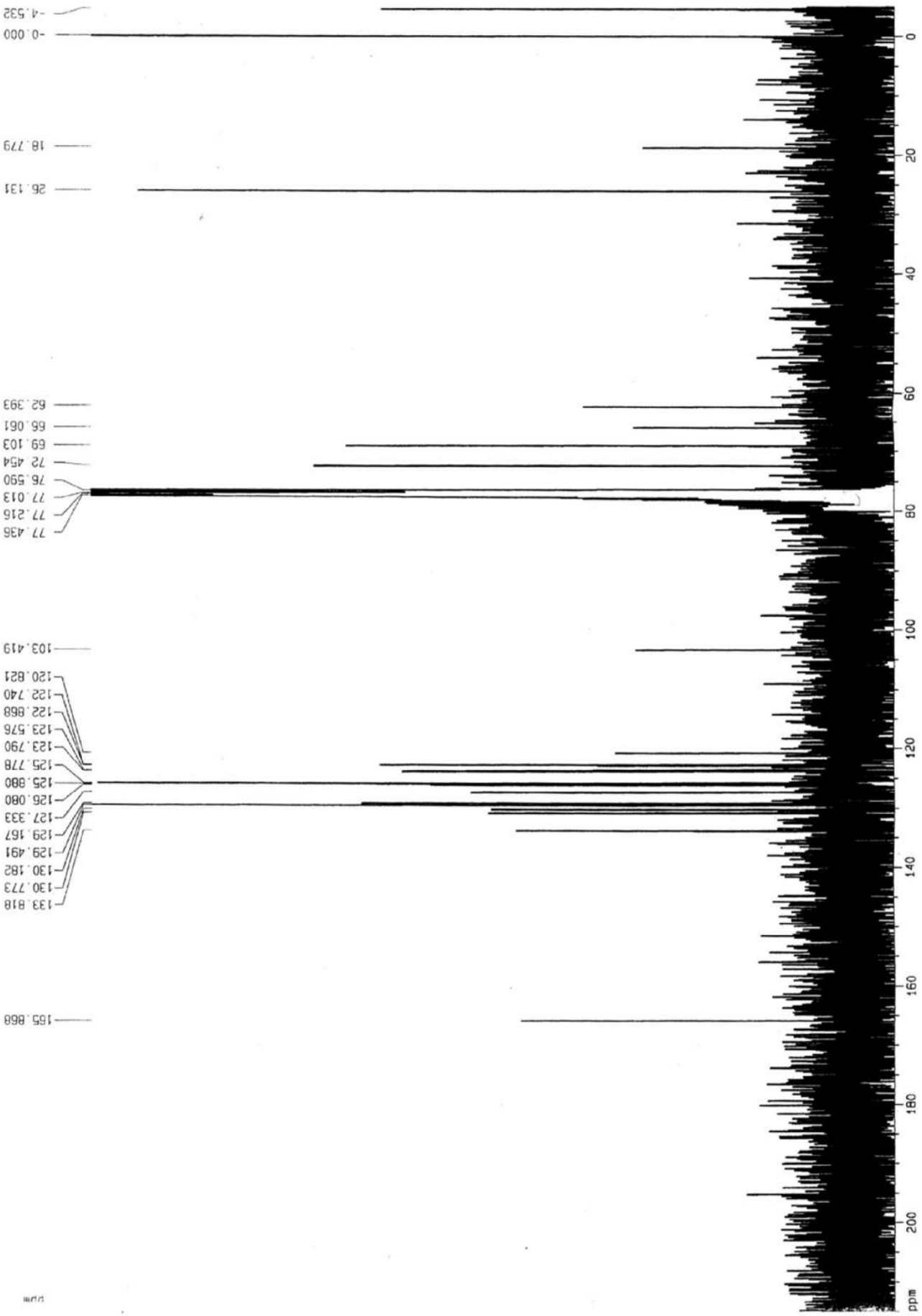

Figure SI 2: ^{13}C NMR spectrum of 2-O-*tert*-butyldimethylsilyl-4,6-bis-O-pyrenoyl-*myo*-inositol-1,3,5-orthoformate (**6**) in $CDCl_3$

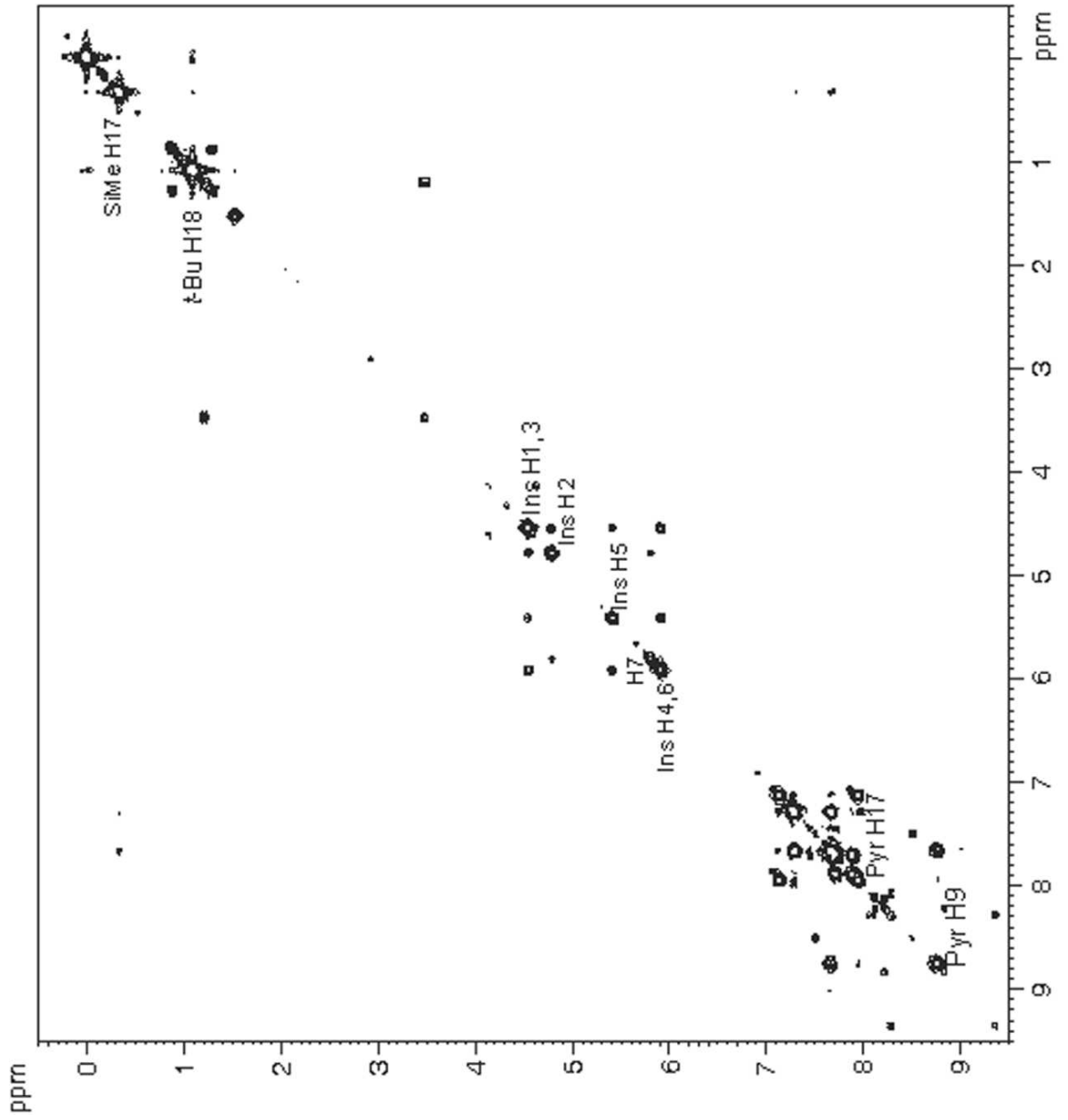

Figure SI 3: ^{1}H COSY spectrum of 2-O-*tert*-butyldimethylsilyl-4,6-bis-O-pyrenoyl-*myo*-inositol-1,3,5-orthoformate (**6**) in $CDCl_3$

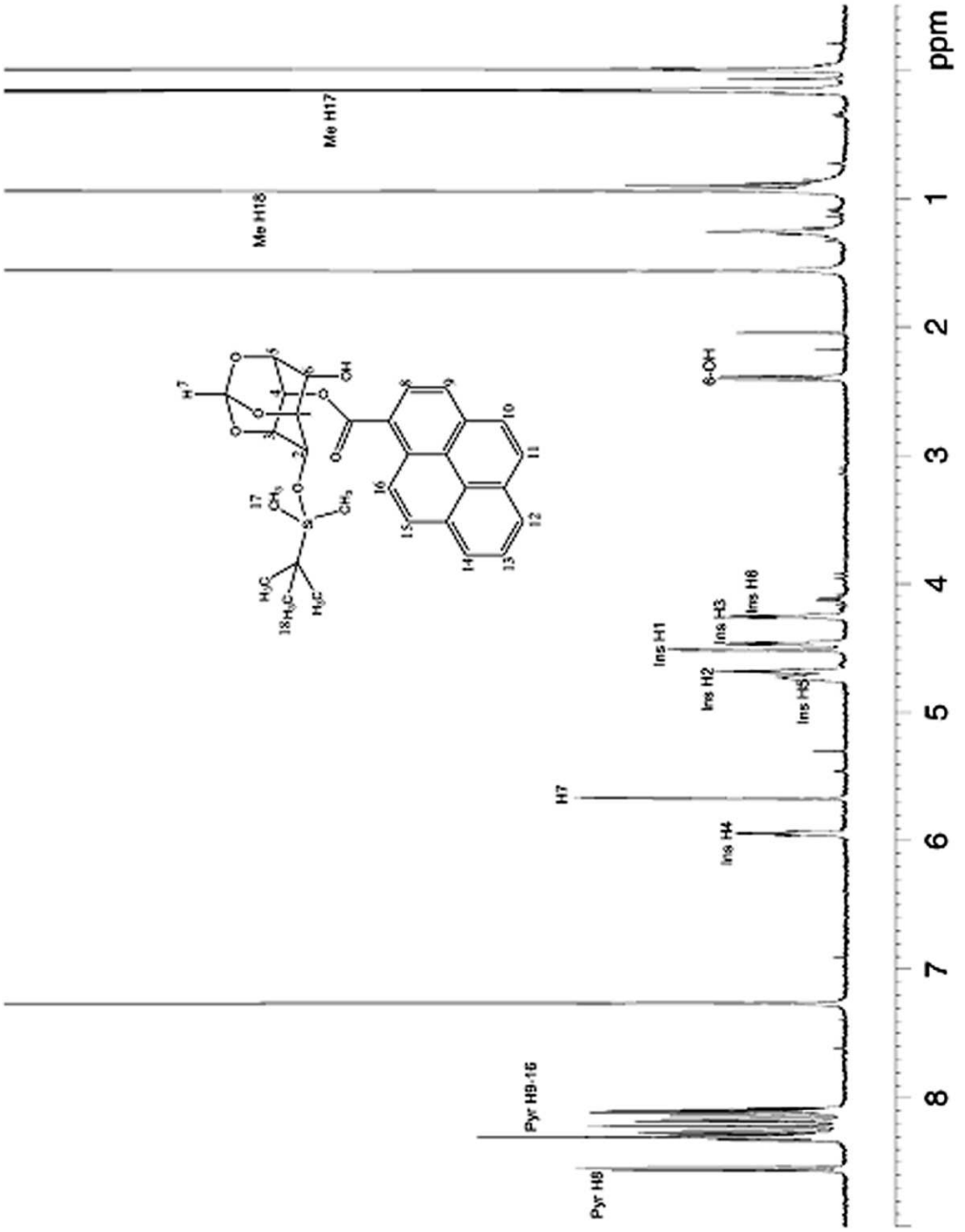

Figure SI 4: ^{1}H spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-pyrenoyl-*myo*-inositol-1,3,5-orthoformate (**7**) in $CDCl_3$

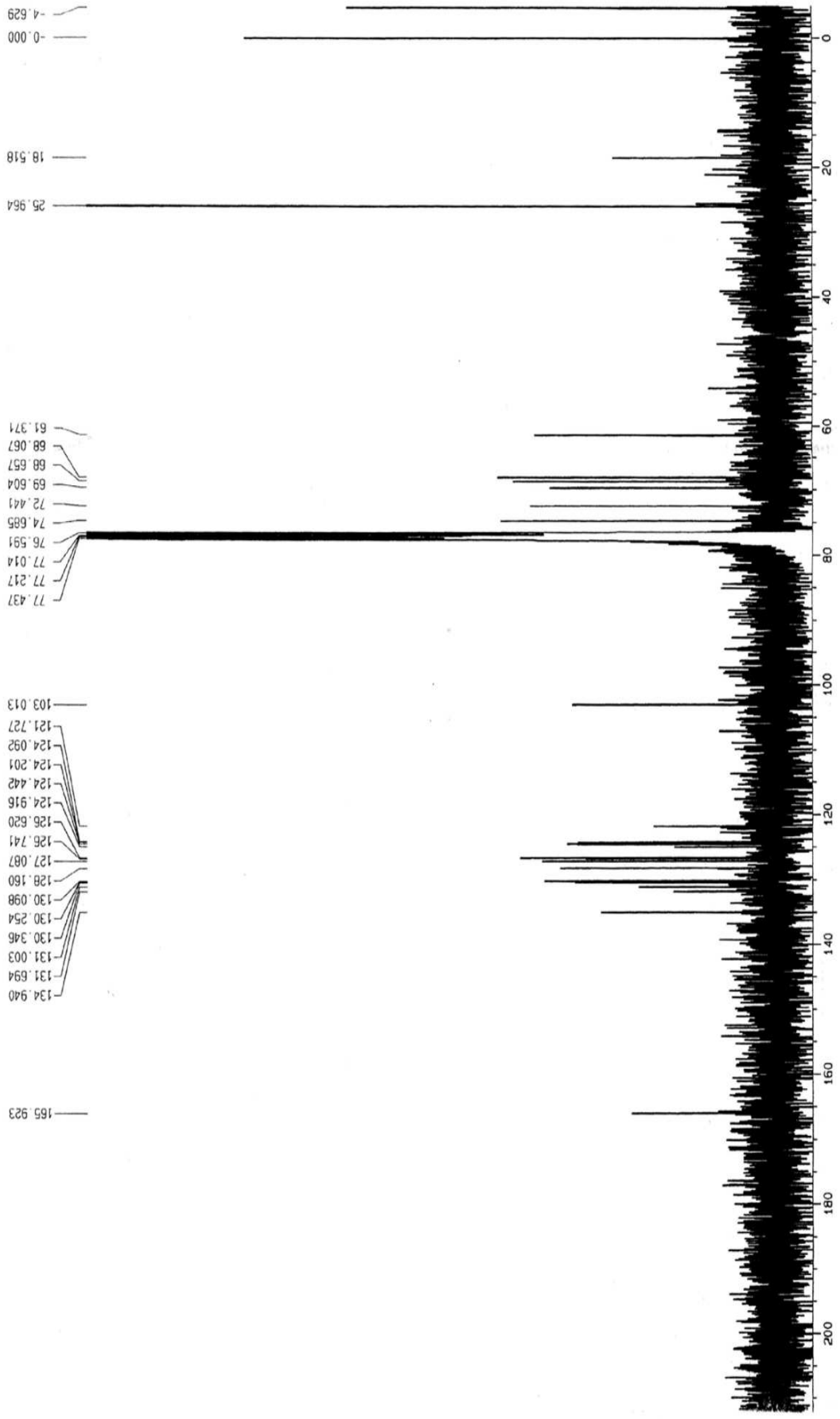

Figure SI 5: ^{13}C NMR spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-pyrenoyl-*myo*-inositol-1,3,5-orthoformate (**7**) in $CDCl_3$

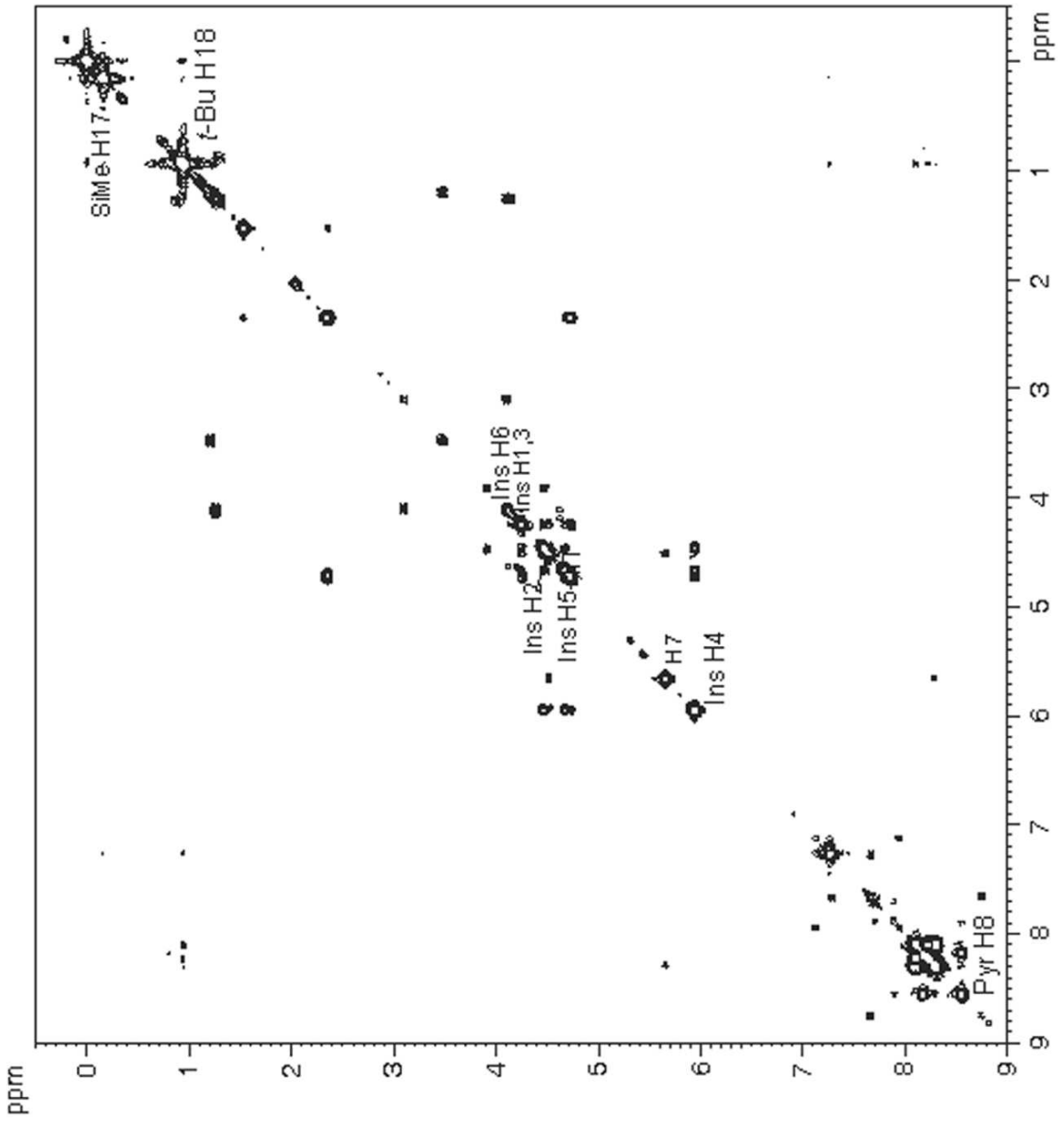

Figure SI 6: ^{1}H COSY spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-pyrenoyl-*myo*-inositol-1,3,5-orthoformate (**7**) in $CDCl_3$

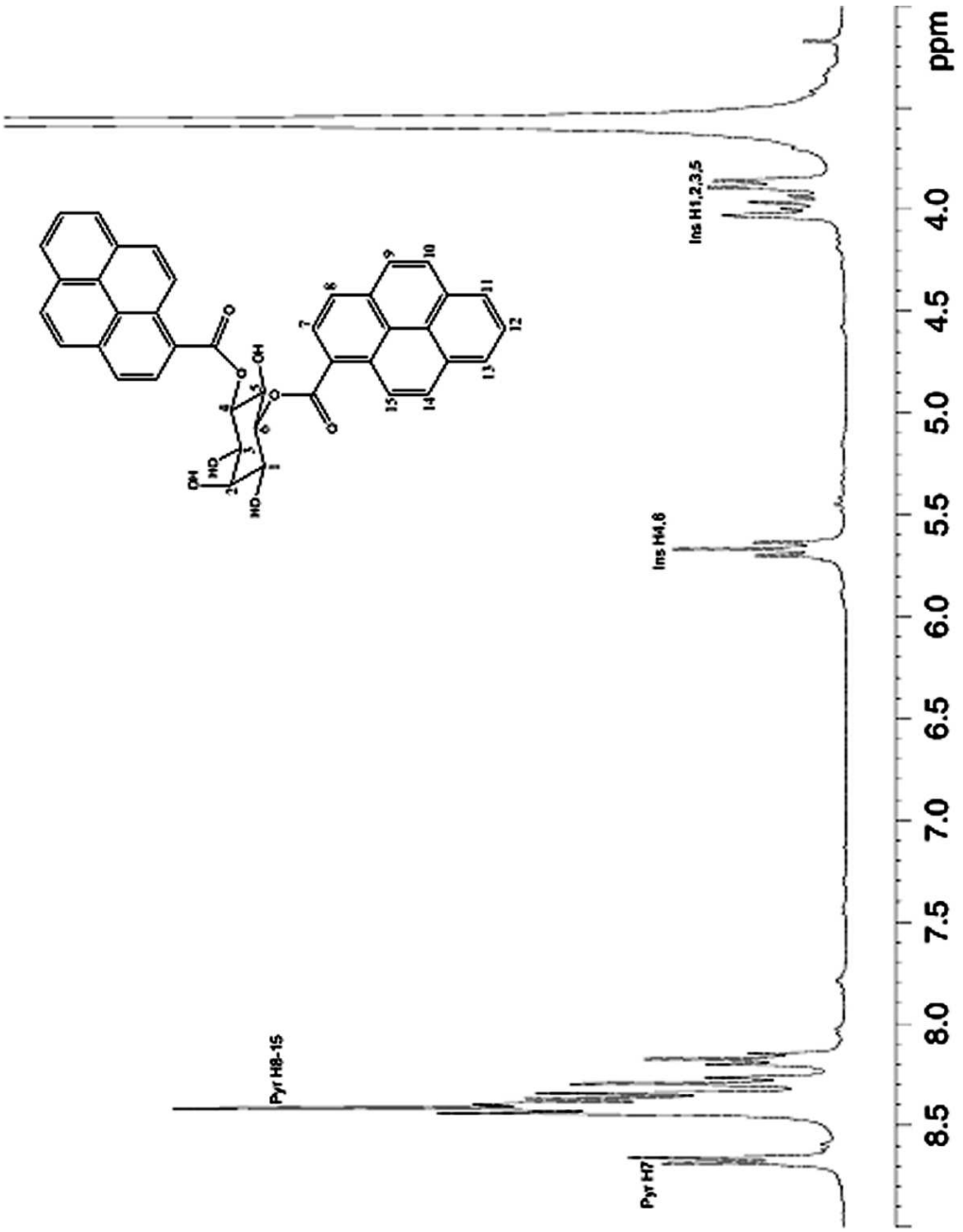

Figure SI 7: ^{1}H NMR spectrum of 4,6-bis-O-pyrenoyl-*myo*-inositol (**8**) in DMSO-d_6/D_2O

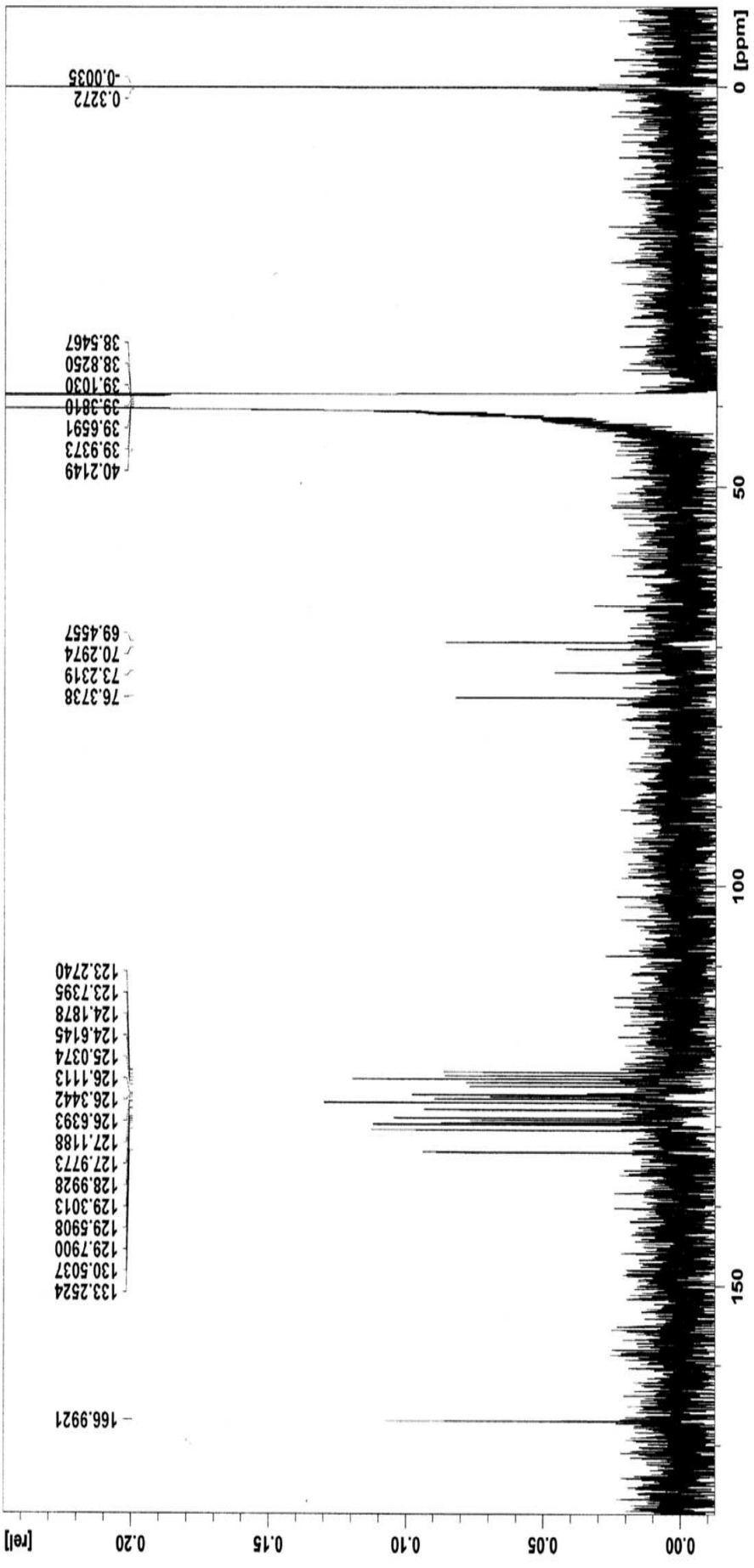

Figure SI 8: ^{13}C NMR spectrum of 4,6-bis-O-pyrenoyl-*myo*-inositol (**8**) in DMSO-d_6/D_2O

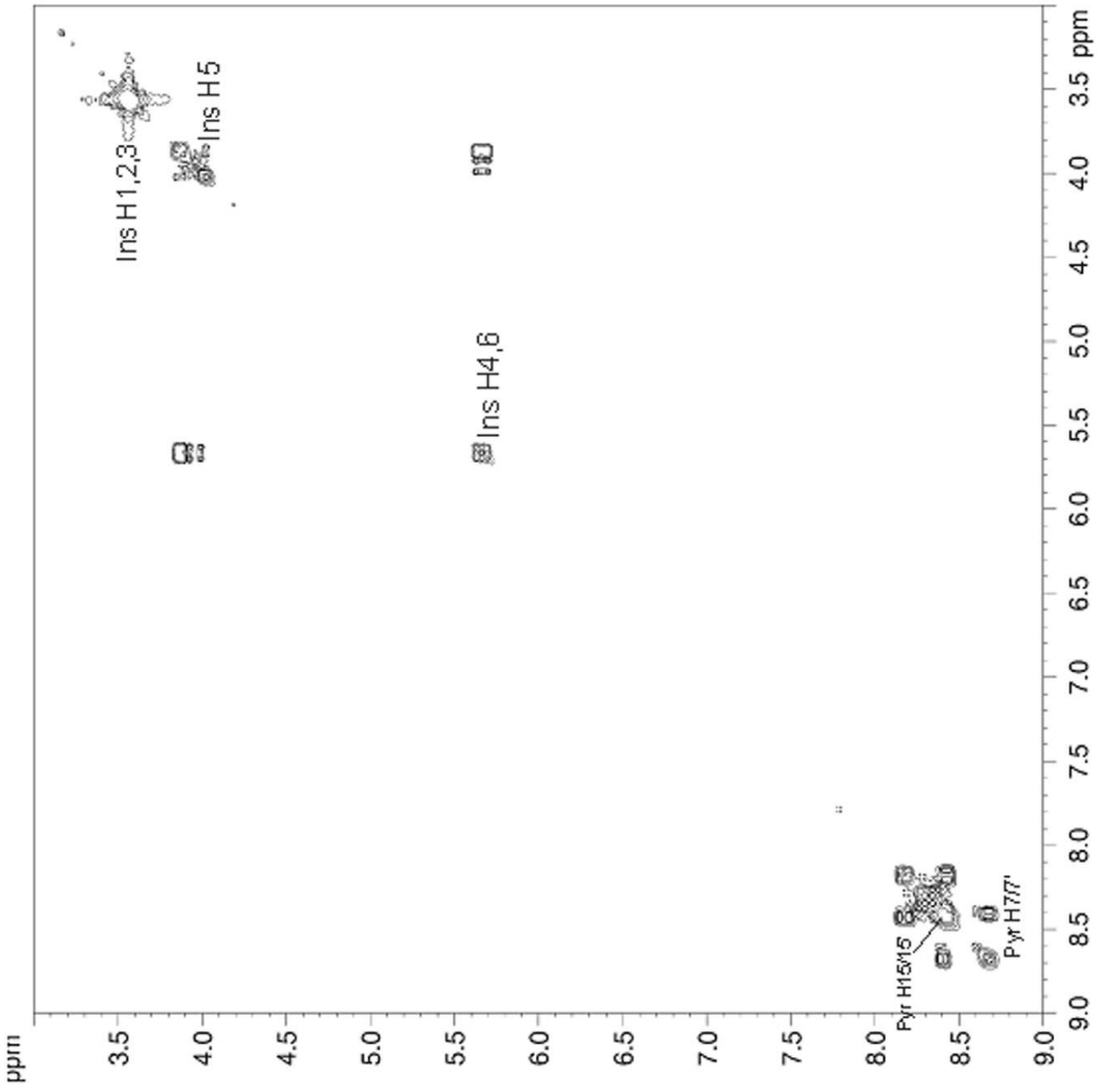

Figure SI 9: ^{1}H COSY spectrum of 4,6-bis-O-pyrenoyl-*myo*-inositol (**8**) in DMSO-d_6/D_2O

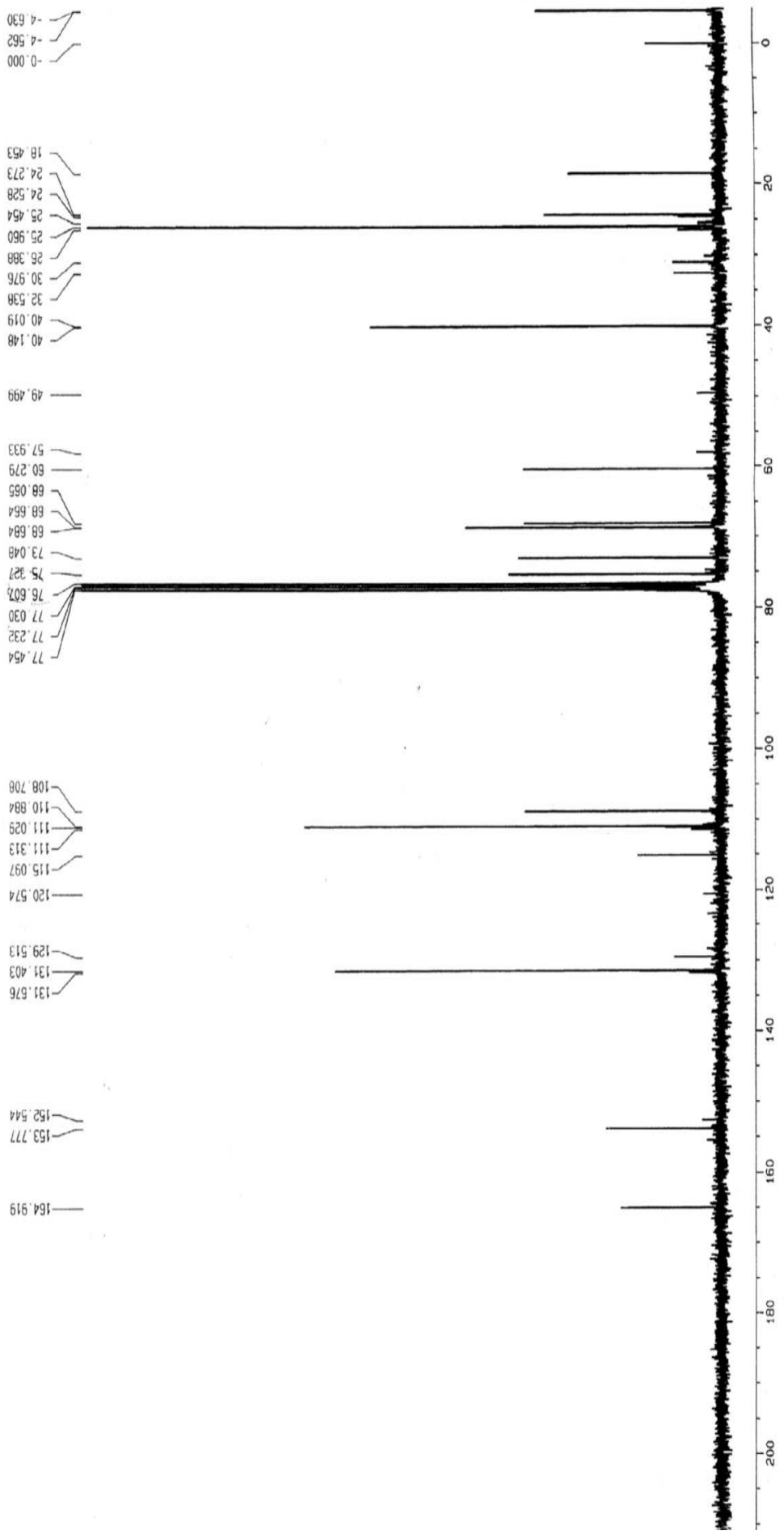

Figure SI 11: ^{13}C NMR spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-*myo*-inositol-1,3,5-orthoacetate (**9**) in $CDCl_3$

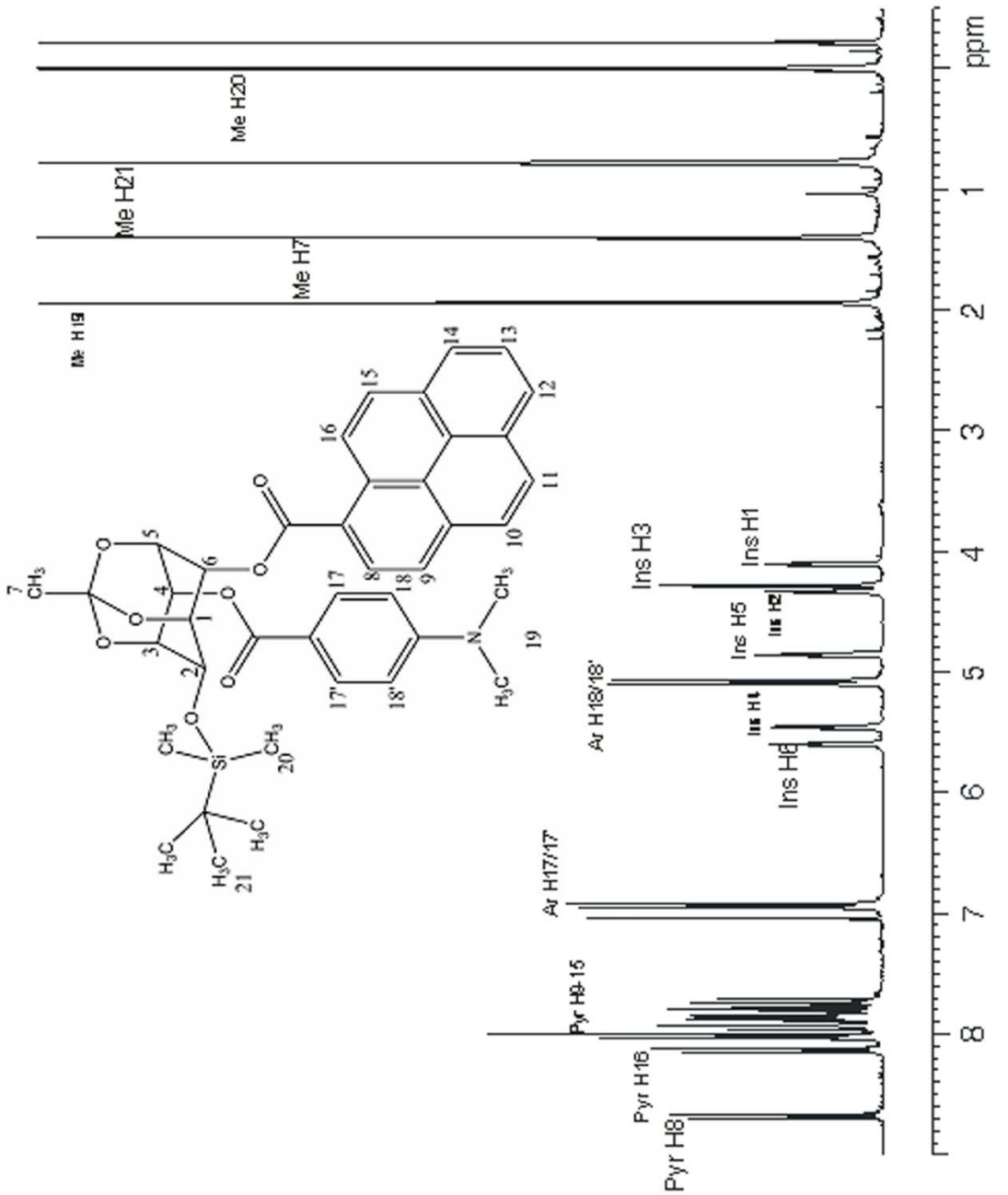

Figure SI 12: ^{1}H NMR spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol-1,3,5-orthoacetate (**10**) in $CDCl_3$

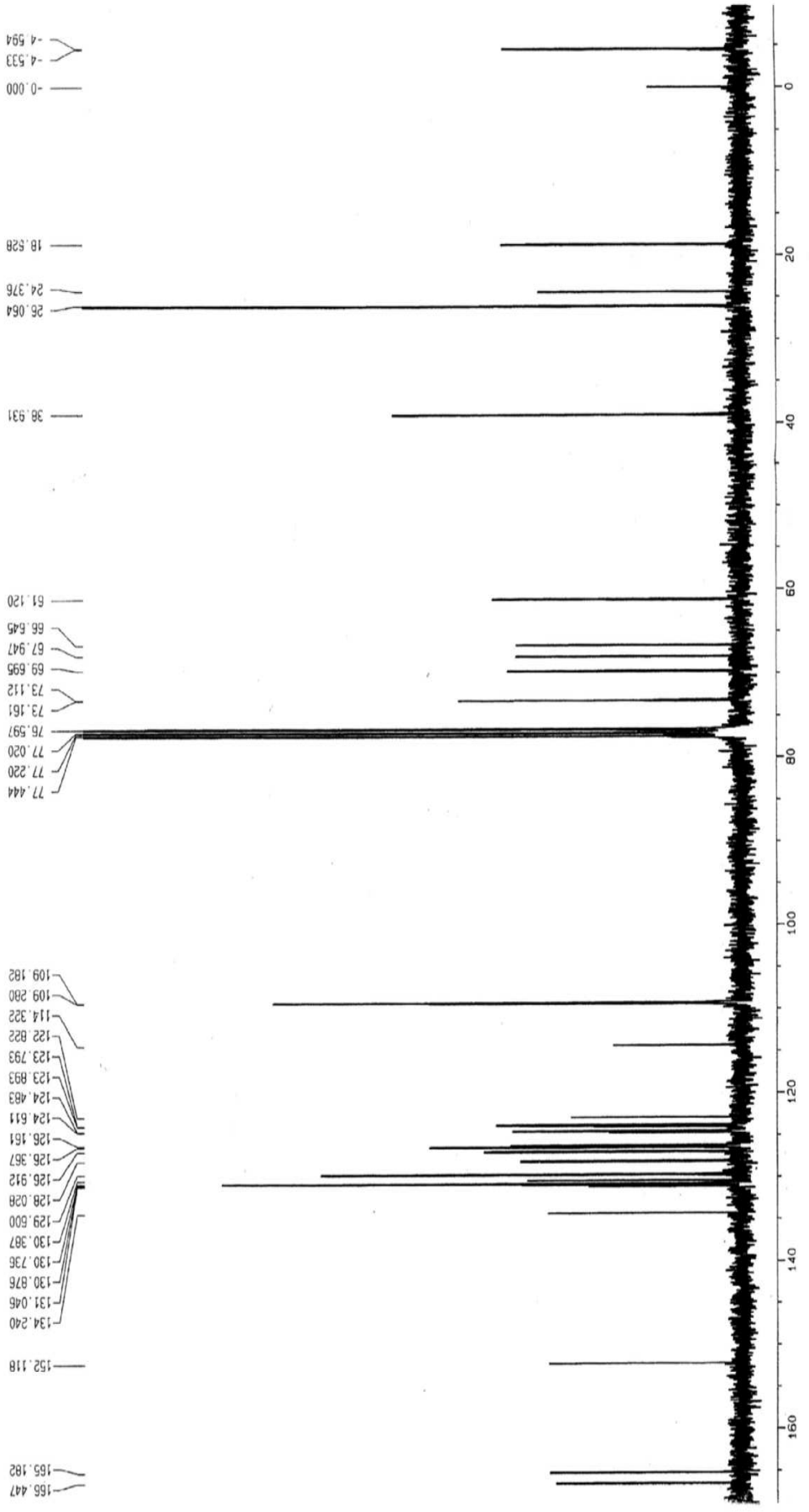

Figure SI 13: ^{13}C NMR spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol-1,3,5-orthoacetate (**10**) in $CDCl_3$

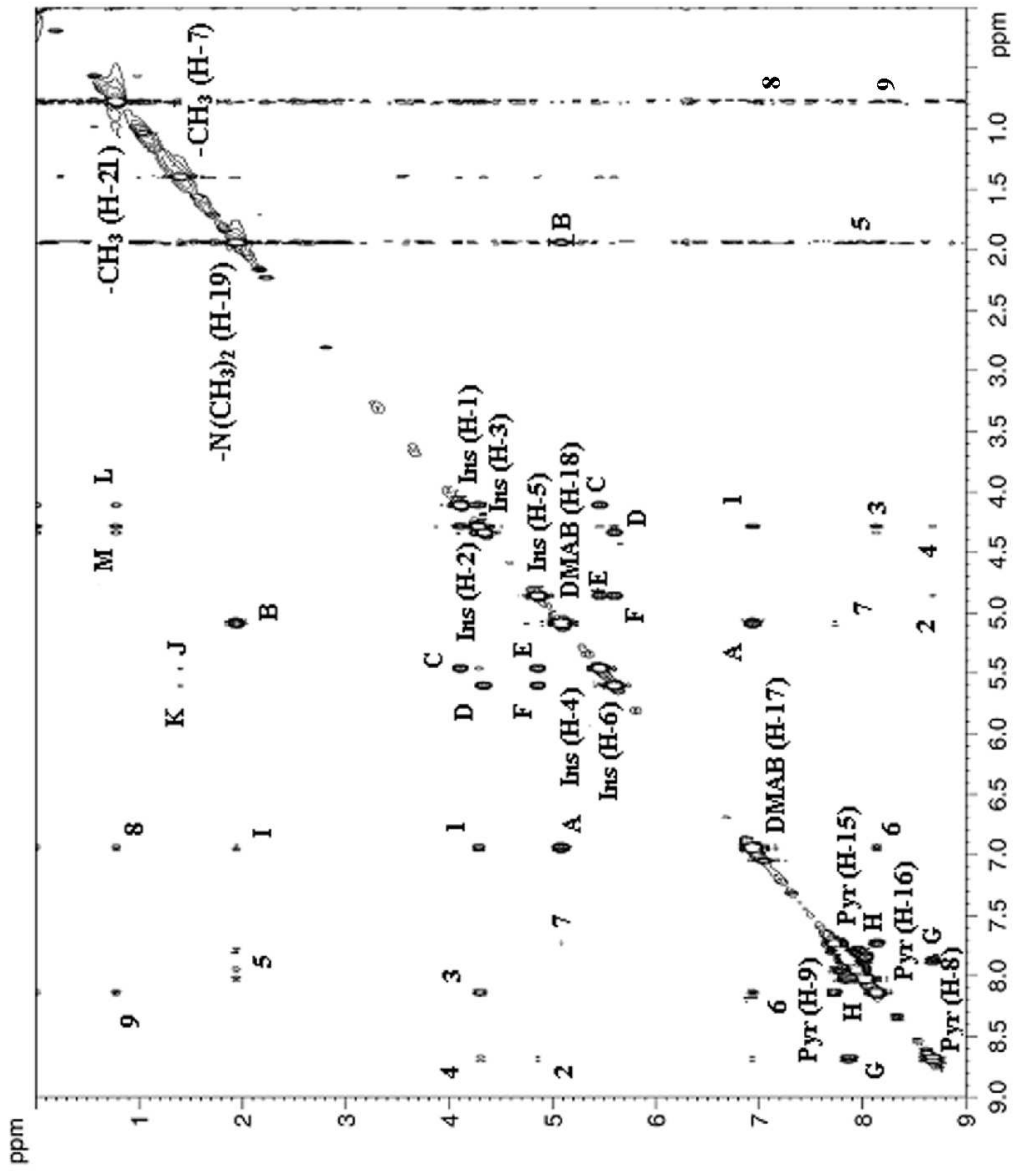

Figure SI 14: ^{1}H NOESY spectrum of 2-O-*tert*-butyldimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol-1,3,5-orthoacetate **10** in $CDCl_3$. The assignments of pyrenoyl (Pyr), inositol (Ins) and 4-(dimethylamino)benzoyl (DMAB) protons are shown by diagonal cross-peak labelling. Off-diagonal cross-peaks labelled by numbers show some NOE-interactions between closely located protons within the Pyr, Ins and DMAB moieties: **A**: DMAB (H-17) - DMAB (H-18); **B**: -N$(CH_3)_2$ (H-19) - DMAB (H-18); **C**: Ins (H-1) - Ins (H-4); **D**: Ins (H-2) - Ins (H-6); **E**: Ins (H-5) - Ins (H-4); **F**: Ins (H-5) - Ins (H-6); **G**: Pyr (H-8) - Pyr (H-9); **H**: Pyr (H-16) - Pyr (H-15), **I**: -NMe_2 (H-19) - DMAB (H-17); **J**: -CH_3 (H-7) – Ins (H-4); **K**: -CH_3 (H-7) – Ins (H-6); **L**: -CH_3 (H-21) – Ins (H-1); **M**: -CH_3 (H-21) – Ins (H-2). Cross-peaks labelled by numerals 1-9 indicate *inter*-partner interactions between pyrenoyl, inositol and DMAB moieties: DMAB (H-17) - Ins (H-2), cross-peak **1**; Pyr (H-8) - Ins (H-5), cross-peak **2**; Pyr (H-16) - Ins (H-2), cross-peak **3**; Pyr (H-8) - Ins (H-2), cross-peak **4**; Pyr (H-9 - H-15) - NMe_2(H-19), cross-peaks **5**; Pyr (H-16) - DMAB (H-17), cross-peak **6;** Pyr (H-15) - DMAB (H-18), cross-peak **7;** DMAB (H-17)- Ins –CH_3(H-21), cross-peak **8**; Pyr(16) - Ins –CH_3(H-21), cross-peak **9.**

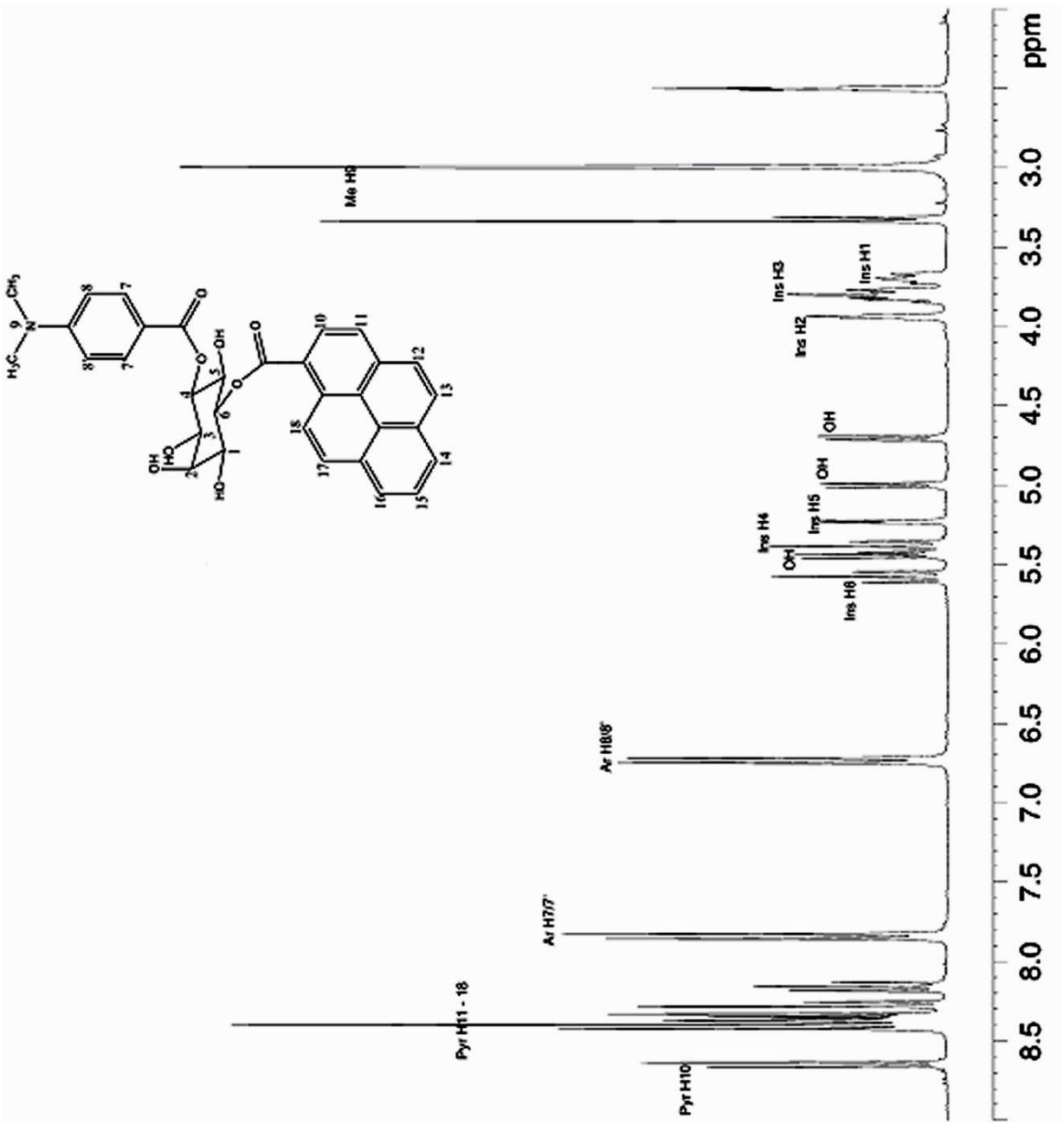

Figure SI 15a: ^{1}H NMR spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol (**11**) in DMSO-d_6

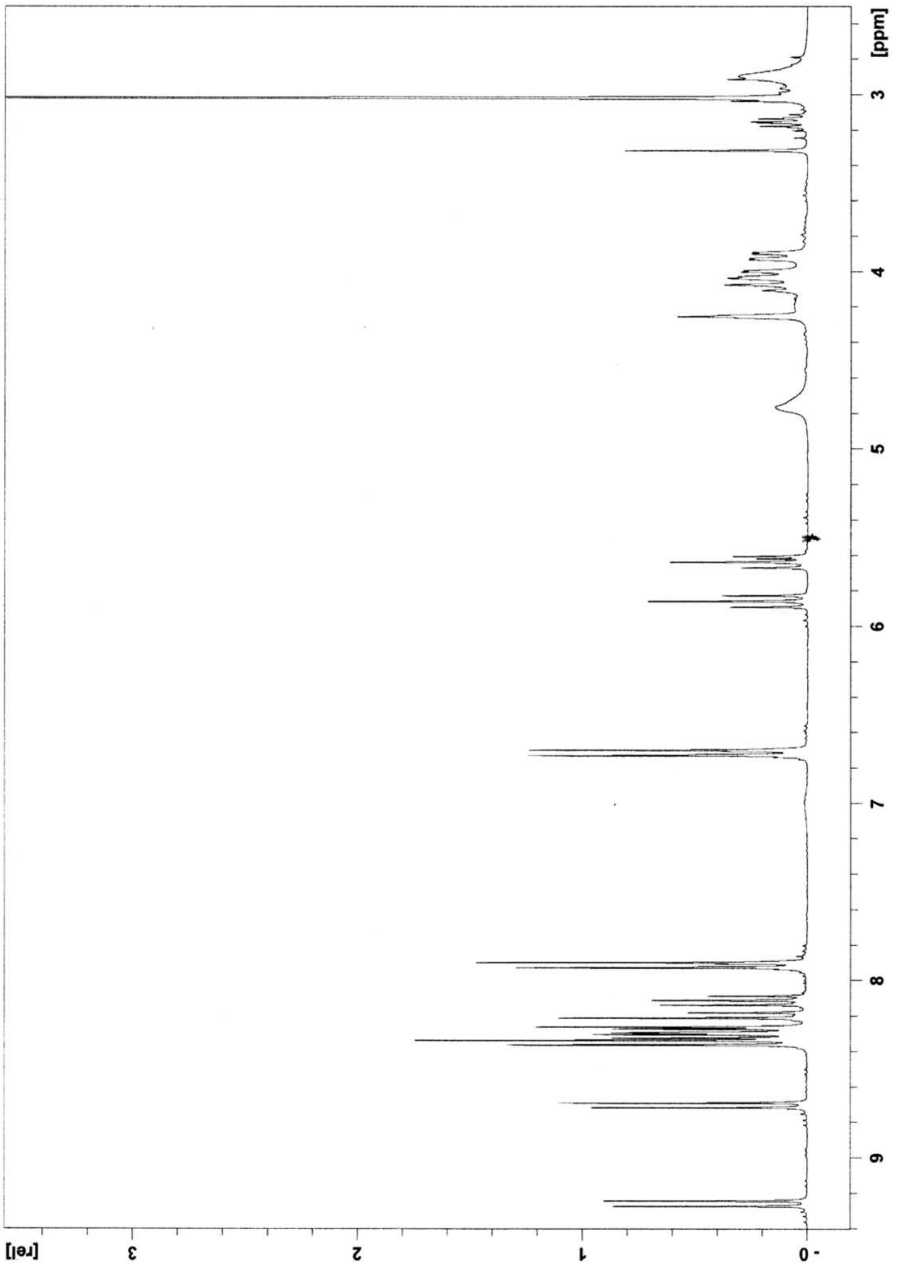

Figure 15b: ^{1}H NMR spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol (**11**) in DMSO-d_6 / D_2O

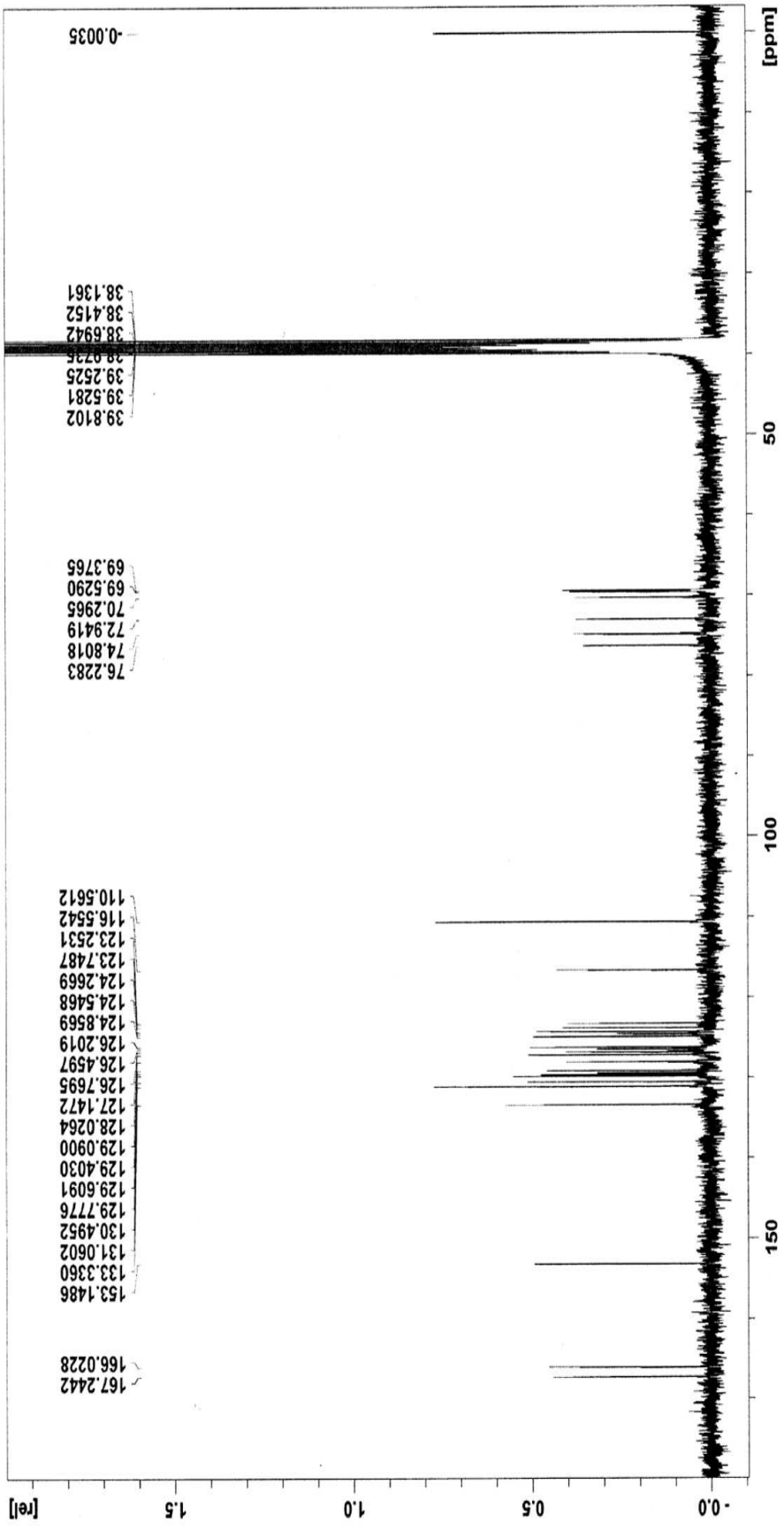

Figure SI 16: ^{13}C NMR spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol (**11**) in DMSO-d_6/D_2O

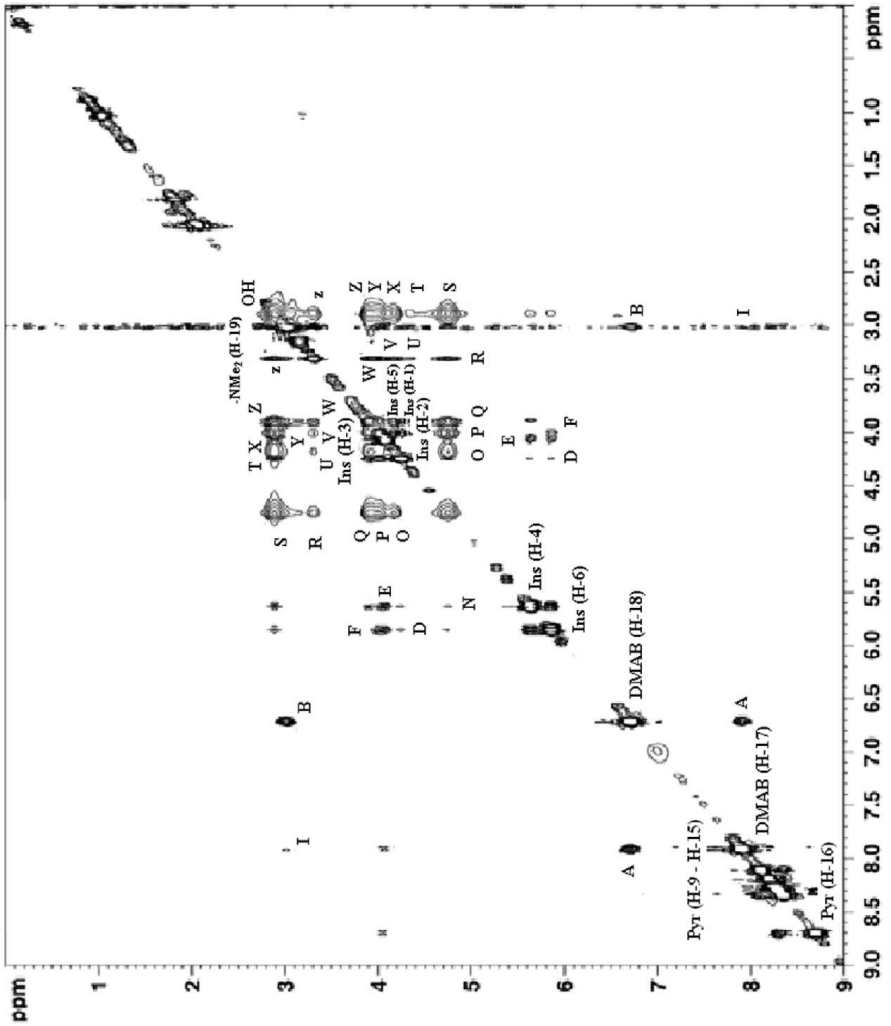

Figure SI 17: ^{1}H NOESY spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-*myo*-inositol **11**. The assignments of pyrenoyl (Pyr), inositol (Ins) and 4-(dimethylamino)benzoyl (DMAB) protons are shown by diagonal cross-peak labelling. Off-diagonal cross-peaks labelled by letters show some NOE-interactions between closely located protons within the Pyr, Ins and DMAB moieties: **A-I** crosspeaks show the same interactions among protons as labelled in Figure 2; **N**: OH – Ins (H-4); **O**: OH- Ins (H-2); **P**: OH – Ins (H-5); **Q**: OH – Ins (H-3); **R**: OH – OH; **S**: OH – OH; **T**: OH-OH, **U**: Ins (H-2) – OH; **V**: Ins (H-3) – OH; **W**: Ins (H-1) – OH; **X**: Ins (H-3)-OH; **Y**: Ins (H-5) – OH; **Z**: Ins (H-1) – OH; **z**: OH – OH.