Supplementary Information

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

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Figure S11: $^1$H NMR spectrum of 2-O-tert-butyldimethylsilyl-4,6-bis-O-pyrenoyl-mylo-inositol-1,3,5-orthoformate (6) in CDCl$_3$. 

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Figure S12. $^{13}$C NMR spectrum of 2-O-tert-butyldimethylsilyl-4,6-bis-O-pyrenoyl-1,3,5-inositol-1,3,5-orthoformate (6) in CDCl$_3$. 

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Figure SI 3: 1H 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-myoinositol-1,3,5-orthoformate (7) in CDCl$_3$
**Figure S1 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-myoinositol-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$_2$O.
Figure SI 8. $^{13}$C NMR spectrum of 4,6-bis-O-pyrenoyl-myoinositol (8) in DMSO-d$_6$/D$_2$O
**Figure SI 9**: $^1$H COSY spectrum of 4,6-bis-O-pyrenoyl-myoinositol (8) in DMSO-d$_6$/D$_2$O
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 S1 12: $^1$H NMR spectrum of 2-O-tert-butyldimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-myoinositol-1,3,5-orthoacetate (10) in CDCl$_3$
Figure S1 13: $^{13}$C NMR spectrum of 2-O-tert-butyldimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-myoinositol-1,3,5-orthoacetate (10) in CDCl$_3$
Figure SI 14: $^1$H NOESY spectrum of 2-O-tert-butylidimethylsilyl-4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-myoinositol-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-myoinositol (11) in DMSO-d$_6$
Figure 15b. $^{1}H$ NMR spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-\textit{myo}-inositol (11) in DMSO-\textsubscript{d6} / D\textsubscript{2}O.
Figure S1.16: $^{13}$C NMR spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-myoinositol (11) in DMSO-$d_6$/D$_2$O.

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**Figure SI 17:** $^1$H NOESY spectrum of 4-O-[4-(dimethylamino)benzoyl]-6-O-pyrenoyl-myoinositol 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 cross-peaks 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.