Deoxyfluorinated N-acetyllactosamines as carbohydrate-based probes for human galectins

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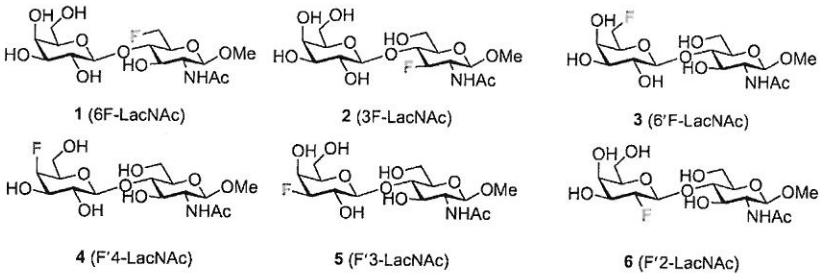
Human galectins (hGals) are carbohydrate-binding proteins playing key roles in a plethora of physiological processes. They are able to modulate immune responses or neoplastic transformation processes via molecular recognition of galactoside-containing glycans.[1] Therefore, the development of their selective inhibitors has become a focus of pharmaceutical research. However, the preparation of inhibitors targeting individual hGals remains challenging as 12 hGals featuring similar substrate specificities have been identified. A deeper understanding of differences between individual hGals could facilitate the development of galectin inhibitors, and deoxyfluorinated carbohydrates are established tools capable of providing such valuable information.[2]

This work is focused on a detailed NMR investigation of human galectins via a complete series of mono-deoxyfluorinated *N*-acetyllactosamine probes **1–6**, which were prepared previously in our laboratory.[3] Advanced ^{19}F NMR T_2-filter technique enabled the identification of hydroxyl groups essential for the interaction with various hGals, and permitted to compare hGals in terms of the importance of these key hydroxyl groups in the recognition events. Furthermore, the library was also investigated by various NMR techniques such as ^{19}F EXSY, STD and ^{15}N CSP to reveal the molecular origin of recognition events.



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