

Exploration of conformational flexibility and hydrogen bonding of xylosides in different solvents, as a model system for enzyme active site interactions

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Table S1. $^3J_{\text{HH}}$ coupling constants for compound **1** in different solvents, given in Hz.

| Solvent | $J_{1,2}$ | $J_{2,3}$ | $J_{3,4}$ | $J_{4,5\text{pro-R}}$ | $J_{4,5\text{pro-S}}$ | $J_{5\text{pro-R},5\text{pro-S}}$ |
|--------------------------------------|-----------|-----------|-----------|-----------------------|-----------------------|-----------------------------------|
| Dimethyl sulfoxide- d_6 | 7.325 | 8.906 | 8.661 | 5.343 | 10.243 | -11.208 |
| Methanol- d_4 | 7.492 | 9.104 | 8.803 | 5.355 | 10.125 | -11.454 |
| <i>N,N</i> -Dimethylformamide- d_7 | 7.406 | 8.885 | 8.723 | 5.294 | 10.068 | -11.257 |
| Pyridine- d_5 | 7.449 | 8.897 | 8.525 | 5.284 | 10.06 | -11.254 |
| Acetone- d_6 | 7.094 | 8.941 | 8.272 | 5.127 | 9.670 | -11.369 |
| Nitromethane- d_3 | 7.146 | 8.679 | 8.682 | 5.102 | 9.648 | -11.475 |
| Tetrahydrofuran- d_8 | 7.169 | 8.620 | 8.276 | 5.161 | 9.639 | -11.300 |
| Aniline- d_7 | 7.133 | 8.687 | 8.468 | 5.078 | 9.580 | -11.484 |
| Phenol- d_6 | 7.080 | 8.797 | 8.483 | 5.057 | 9.504 | -11.745 |
| Dichloromethane- d_2 | 6.576 | 8.172 | 7.945 | 4.718 | 8.787 | -11.716 |
| Chloroform- d | 6.224 | 7.786 | 7.634 | 4.501 | 8.268 | -11.880 |
| Toluene- d_8 | 5.736 | 7.514 | 7.290 | 3.973 | 7.850 | -11.859 |
| Chlorobenzene- d_5 | 6.135 | 7.665 | 7.522 | 4.474 | 8.092 | -11.745 |
| Benzene- d_6 | 5.803 | 7.354 | 7.191 | 4.163 | 7.716 | -11.786 |

Table S2. δ_{H} and δ_{C} references of intrinsic solvent signals.^a

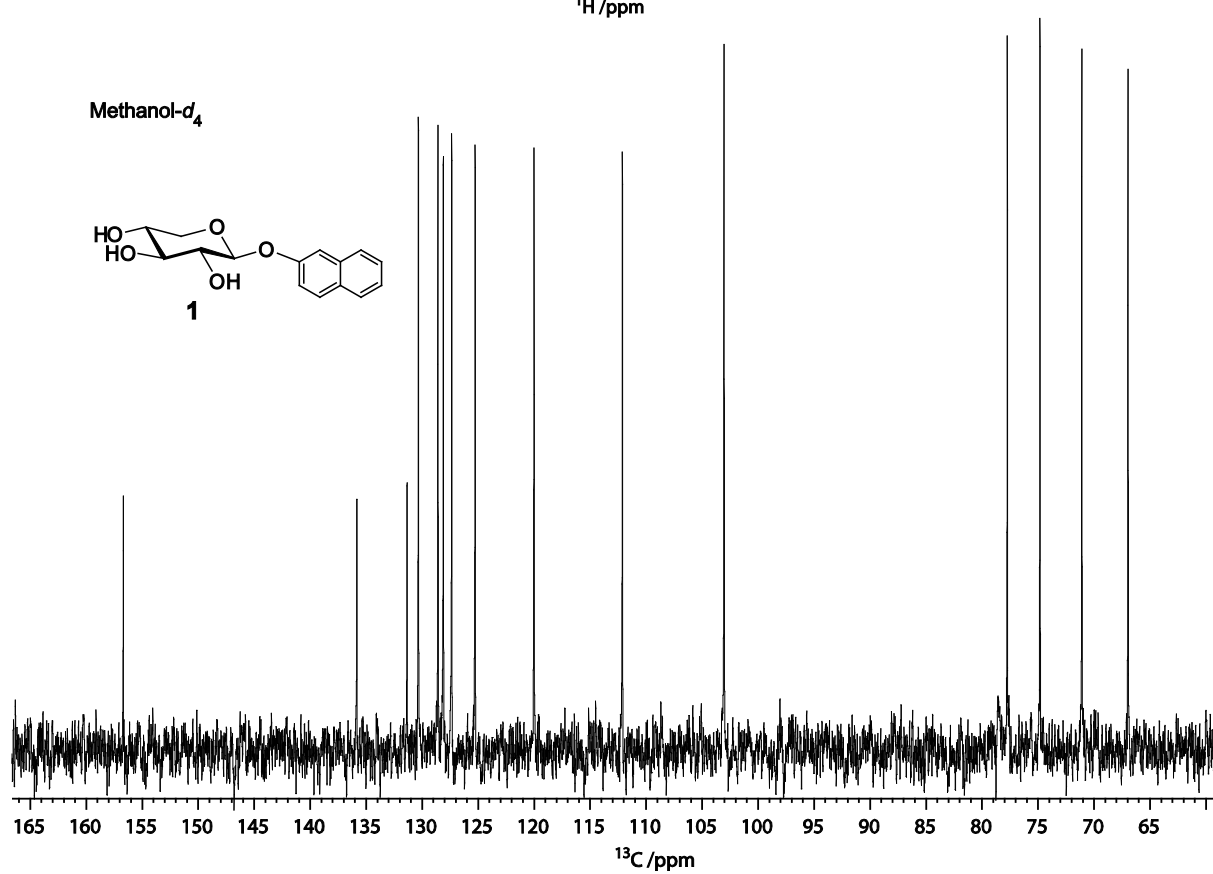
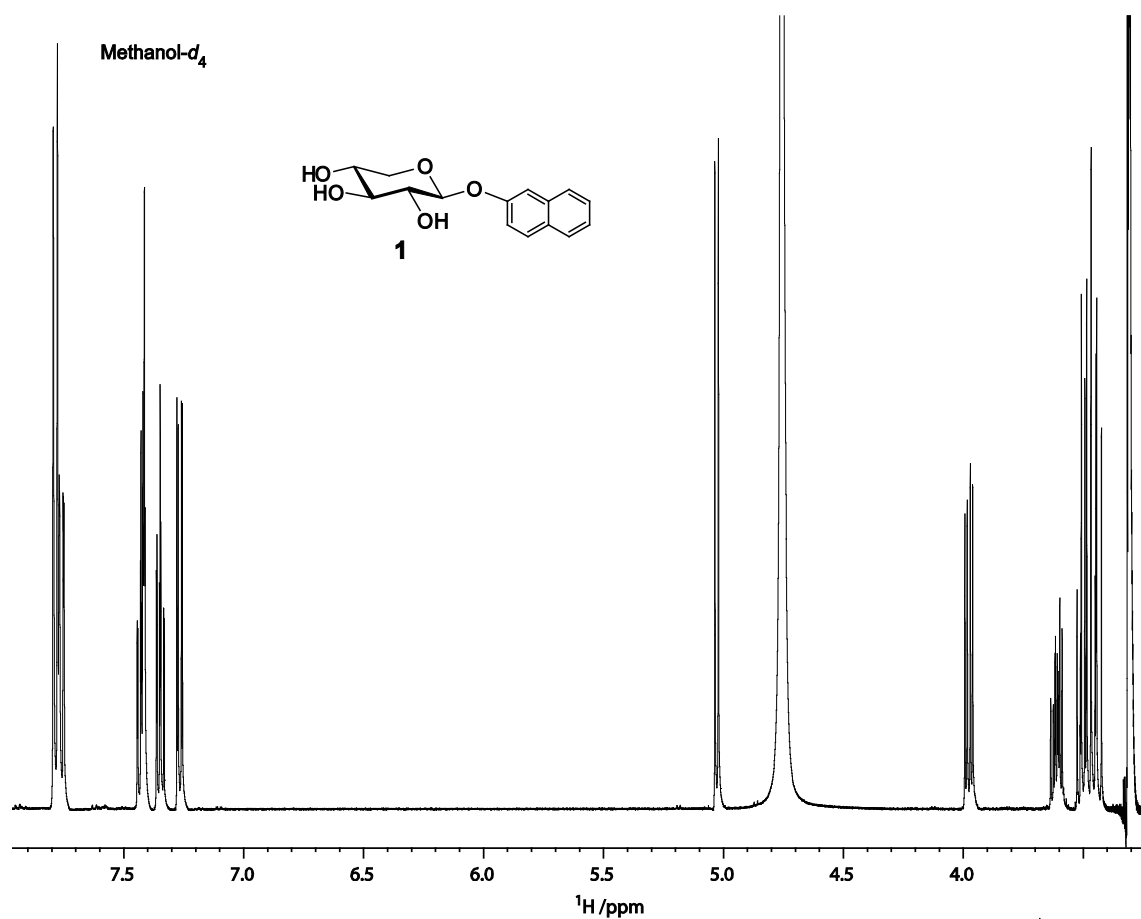
| Solvent | ¹ H | ¹³ C |
|--|----------------|-----------------|
| Dimethyl sulfoxide- <i>d</i> ₆ | 2.50 | 39.52 |
| Methanol- <i>d</i> ₄ | 3.31 | 49.00 |
| <i>N,N</i> -Dimethylformamide- <i>d</i> ₇ | 2.91 | 30.10 |
| Pyridine- <i>d</i> ₅ | 8.71 | 123.50 |
| Acetone- <i>d</i> ₆ | 2.05 | 29.84 |
| Nitromethane- <i>d</i> ₃ | 4.33 | |
| Tetrahydrofuran- <i>d</i> ₈ | 3.58 | 67.40 |
| Aniline- <i>d</i> ₇ | 6.64 | 115.07 |
| Phenol- <i>d</i> ₆ | 7.24 | |
| Dichloromethane- <i>d</i> ₂ | 5.32 | 53.80 |
| Chloroform- <i>d</i> | 7.26 | 77.16 |
| Toluene- <i>d</i> ₈ | 7.09 | |
| Chlorobenzene- <i>d</i> ₅ | 7.14 | |
| Benzene-<i>d</i>₆ | 7.16 | 128.06 |

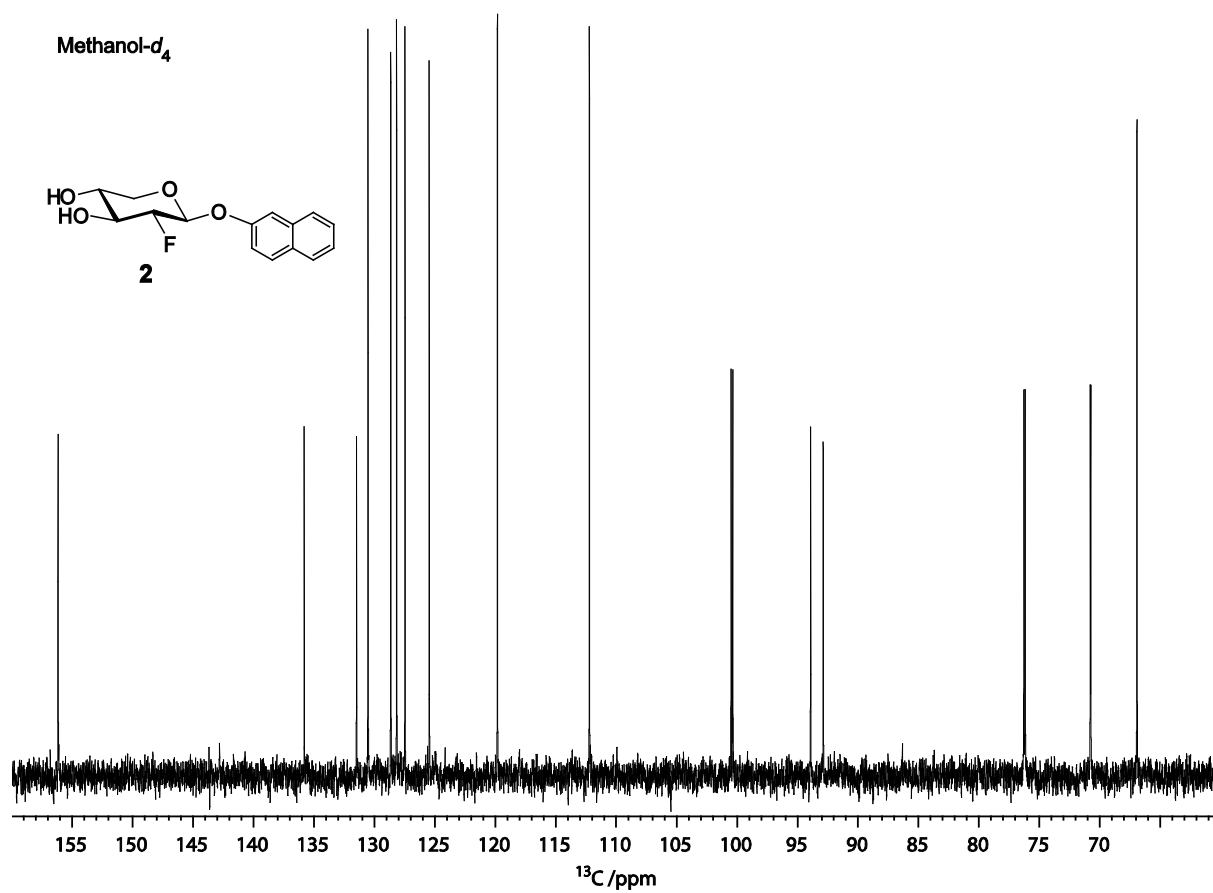
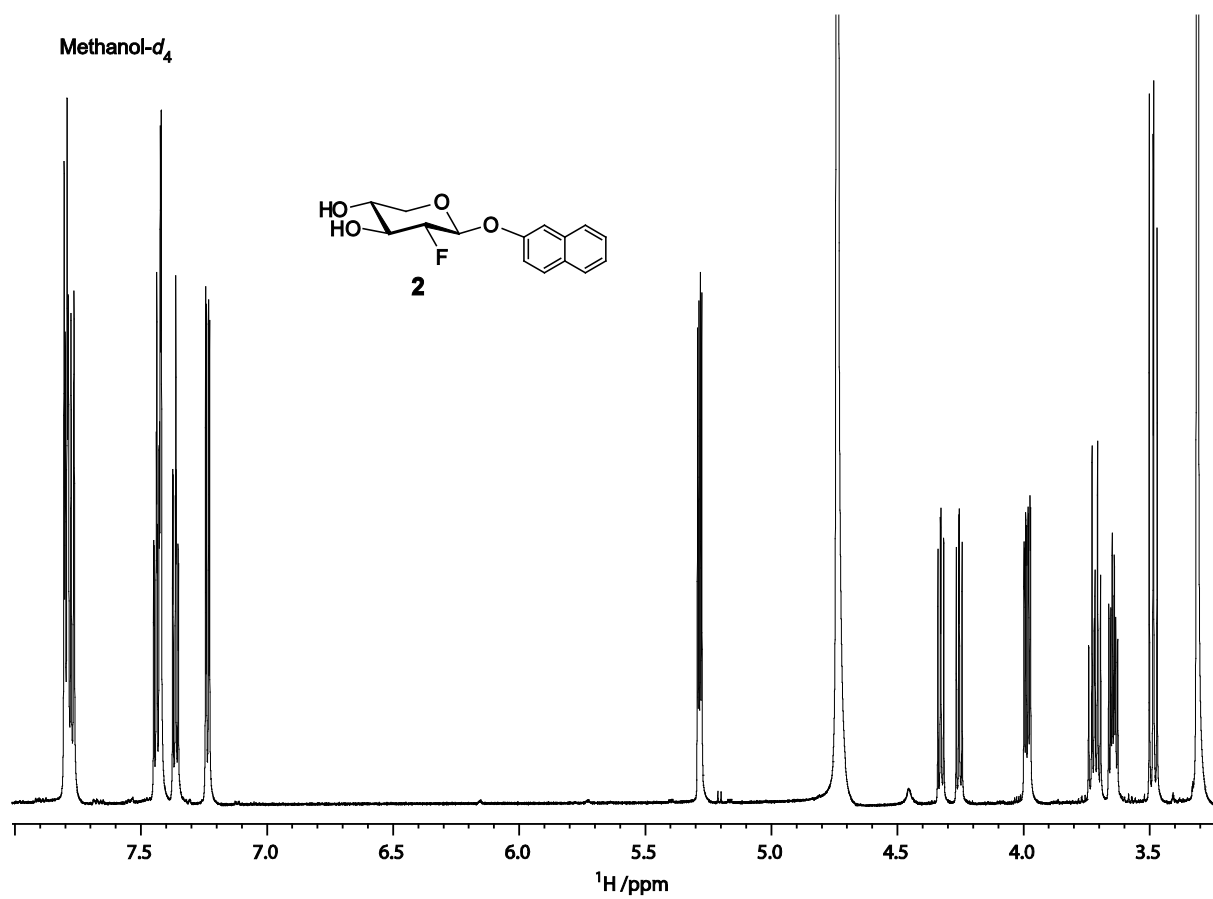
^aData obtained from three sources:

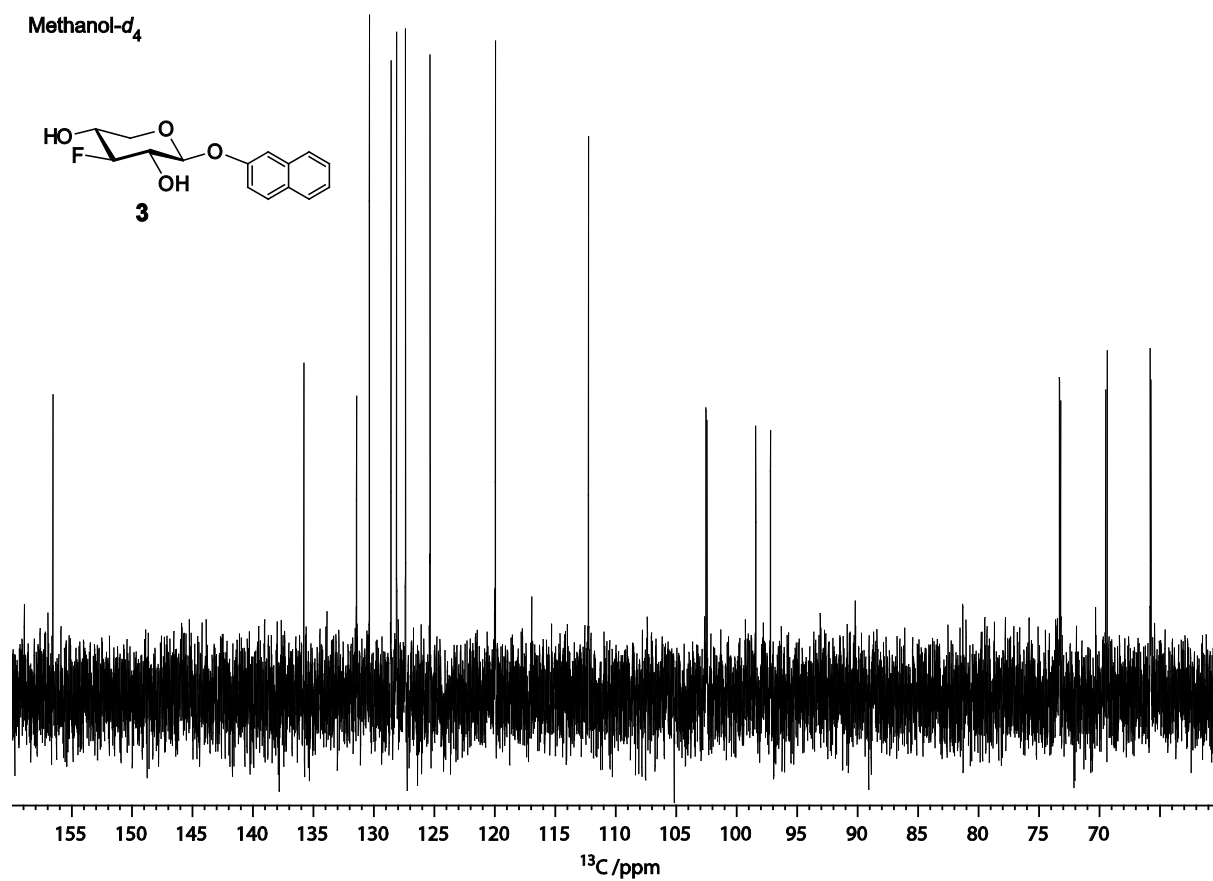
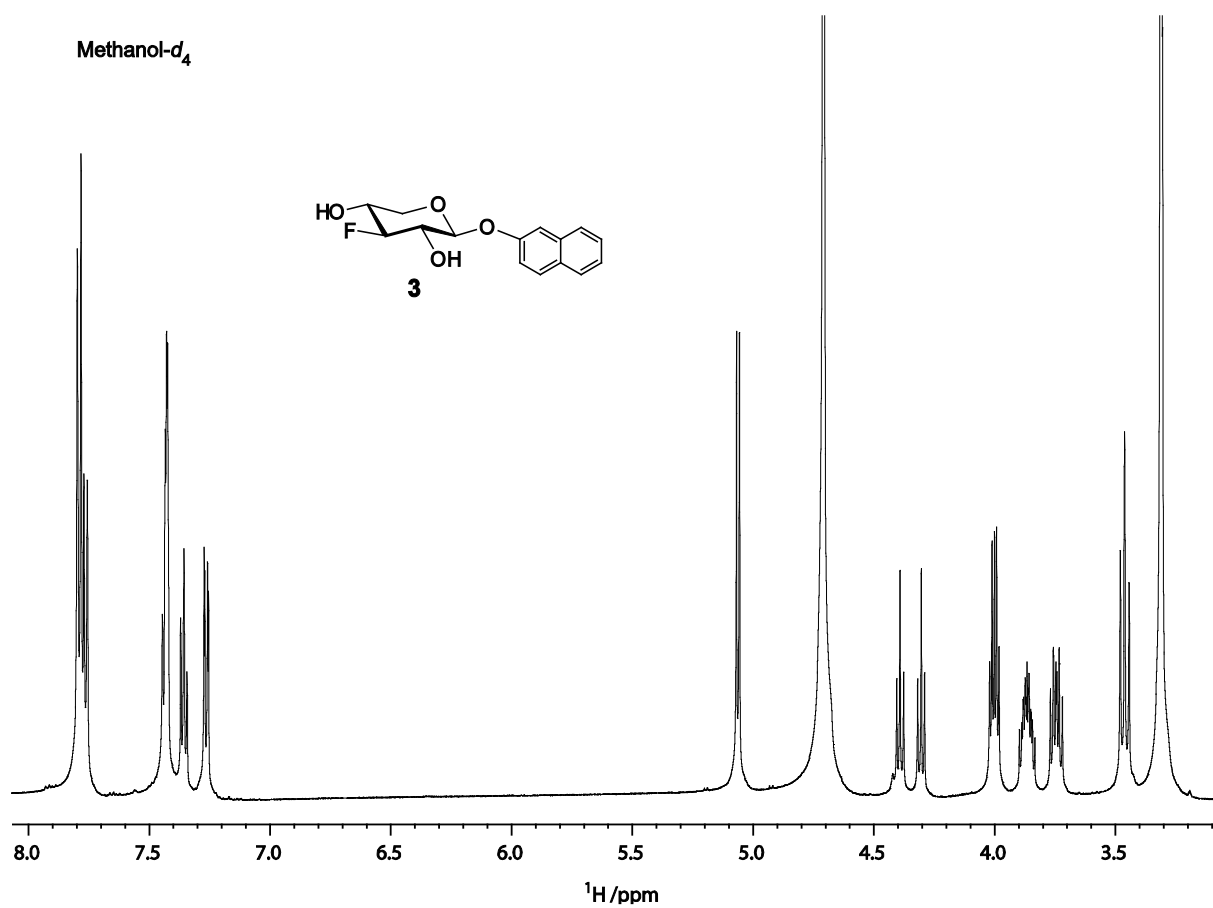
- Fulmer, G.R.; Miller, A.J.M.; Sherden, N.H.; Gottlieb, H.E.; Nudelman, A.; Stoltz, B.M.; Bercaw, J.E.; Goldberg, K.I. *Organometallics*, **2010**, *29*, 2176 – 2179.

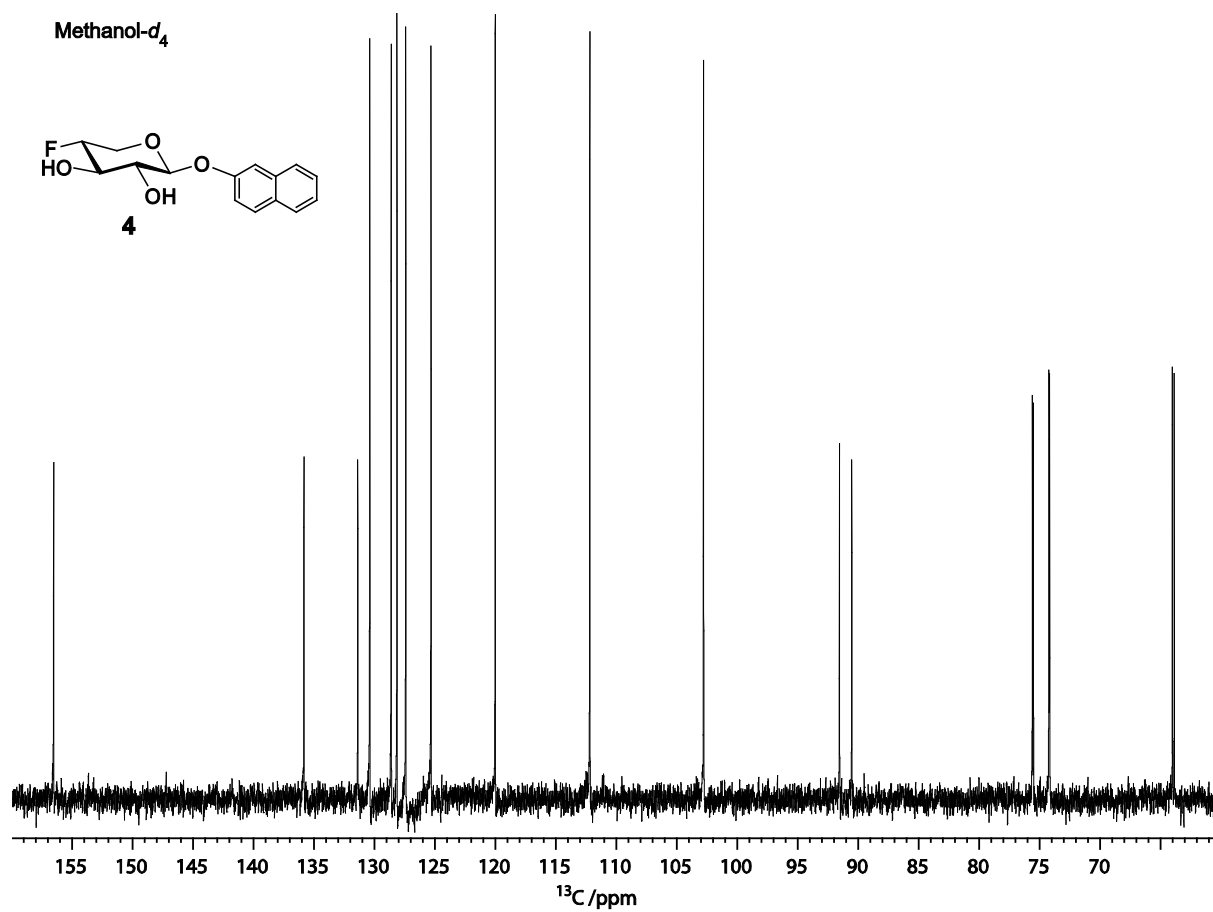
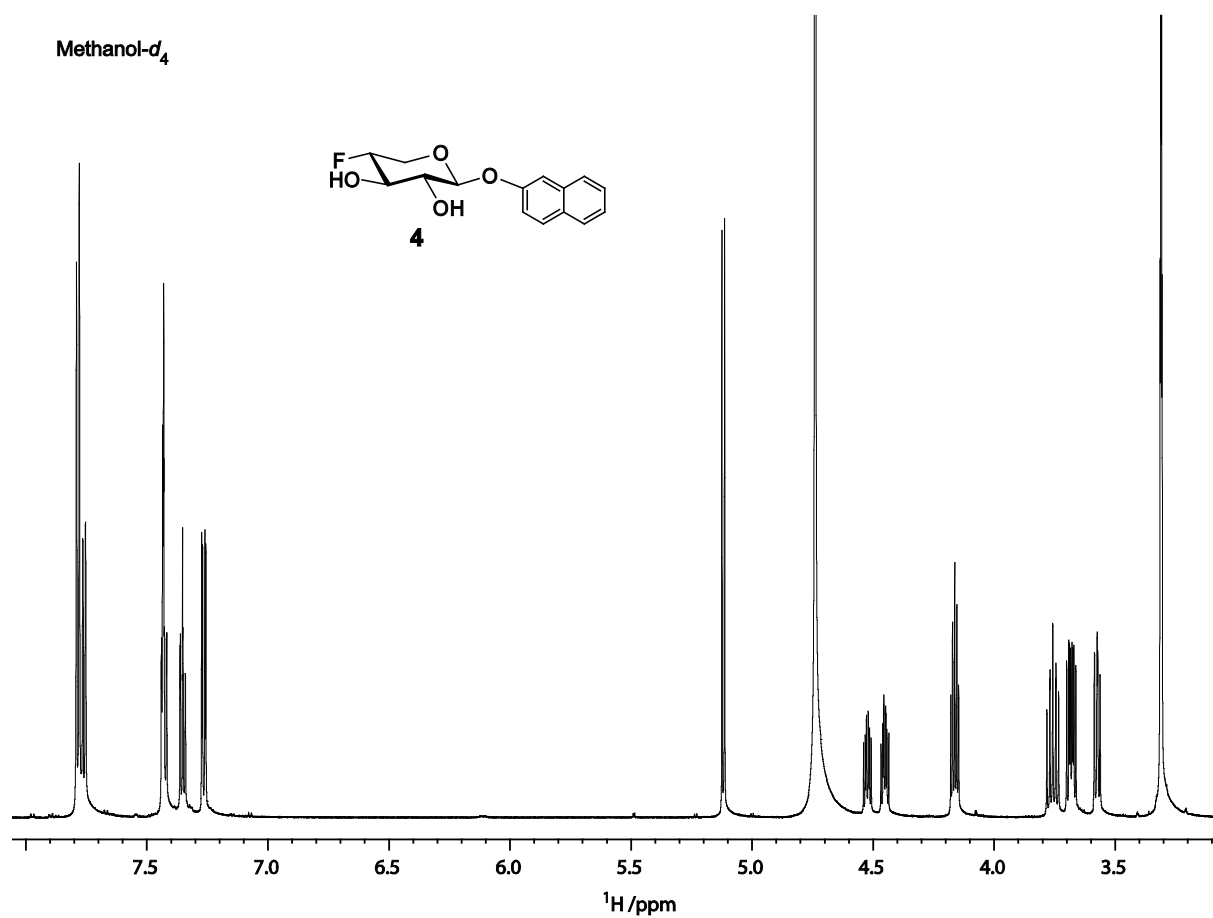
- Isotec Inc.

- http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi, accessed February 2012.

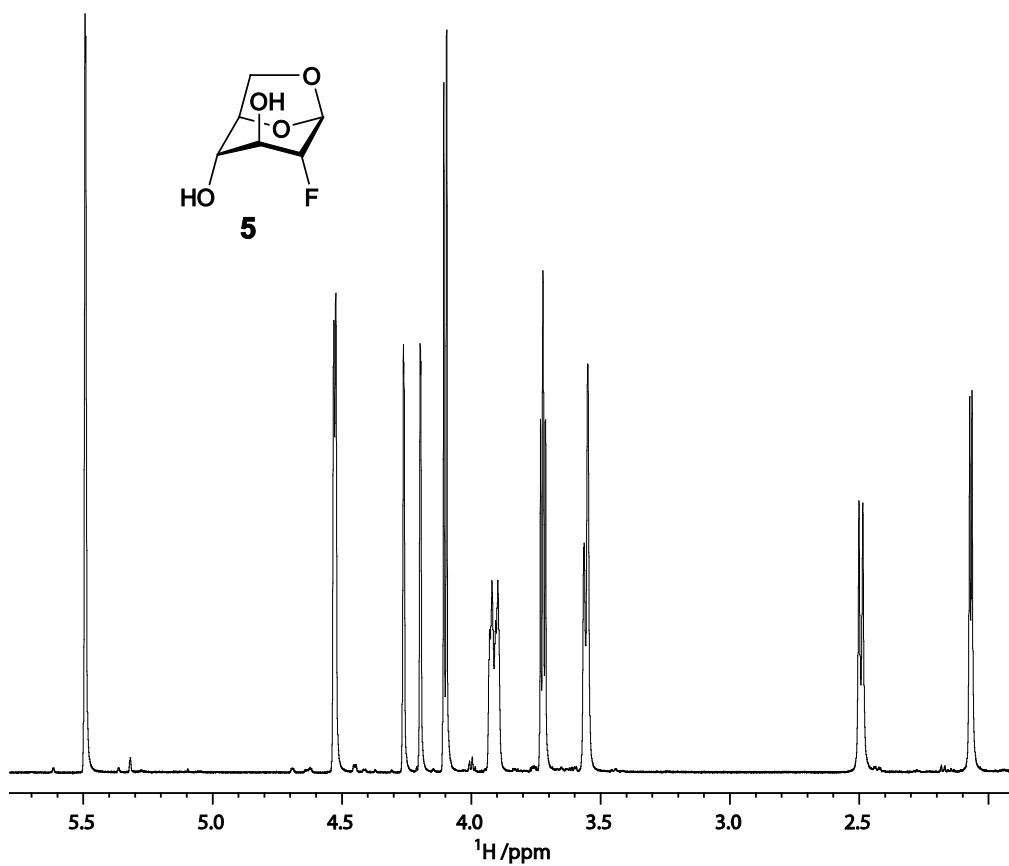








Chloroform-*d*



Chloroform-*d*

