

Supporting Information File 1
for
Synthesis and biological evaluation of new
glycoconjugated LDH inhibitors as anticancer agents

Felicia D'Andrea^{1,*}, Giulia Vagelli², Carlotta Granchi¹, Lorenzo Guazzelli¹,
Tiziano Tuccinardi¹, Giulio Poli¹, Dalila Iacopini², Filippo Minutolo¹ and
Valeria Di Bussolo^{2,*}

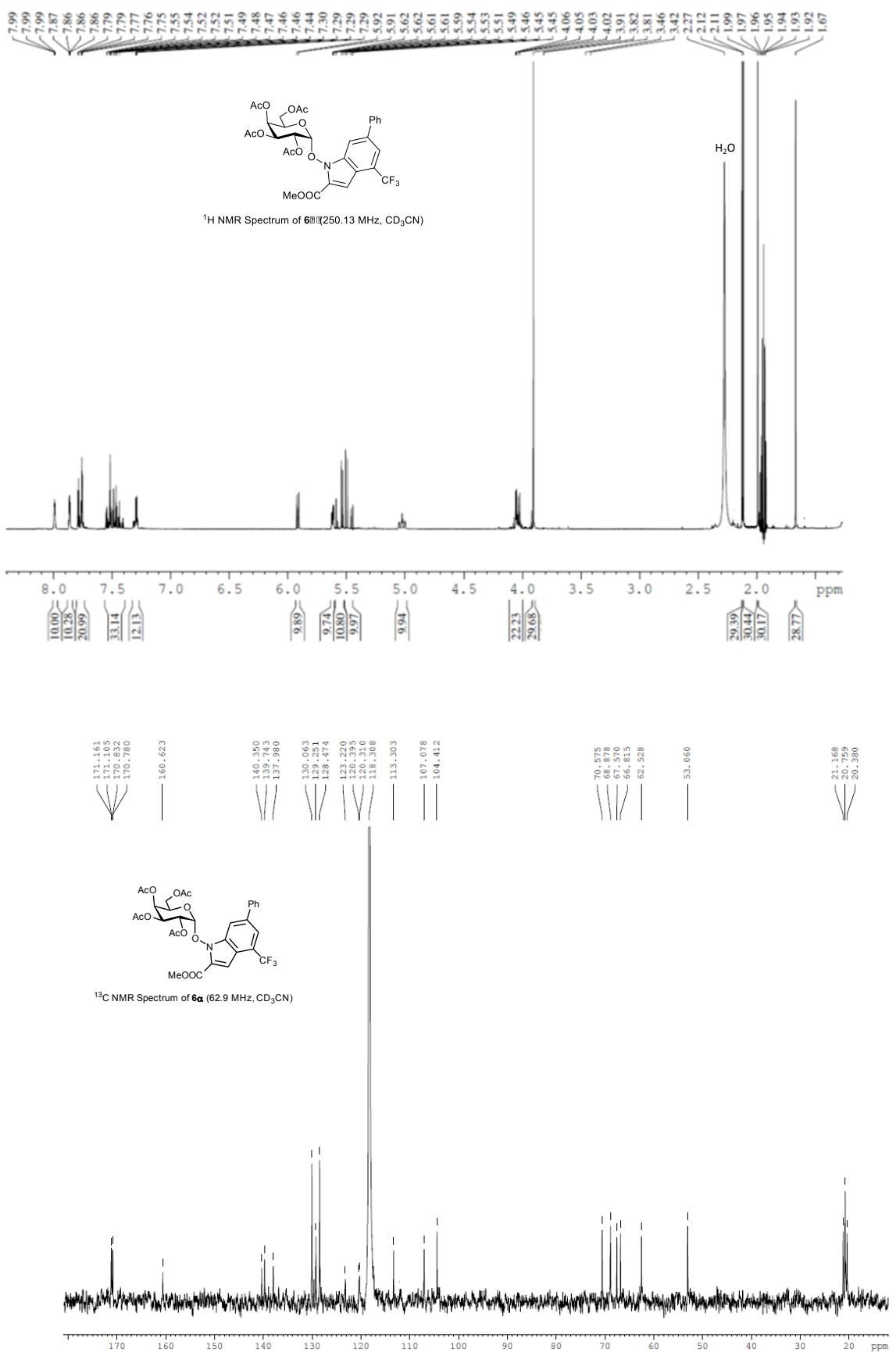
¹Dipartimento di Farmacia, Università di Pisa, Via Bonanno 33, 56126 Pisa, Italy;

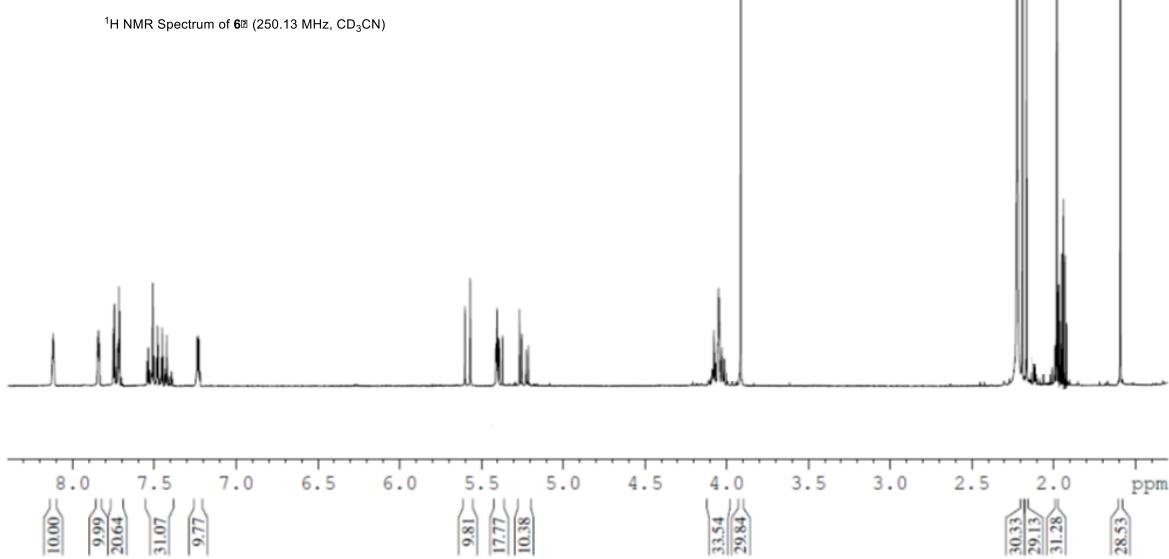
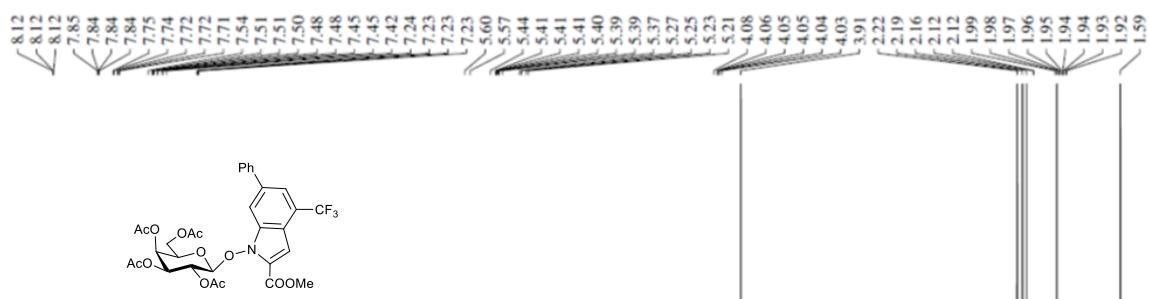
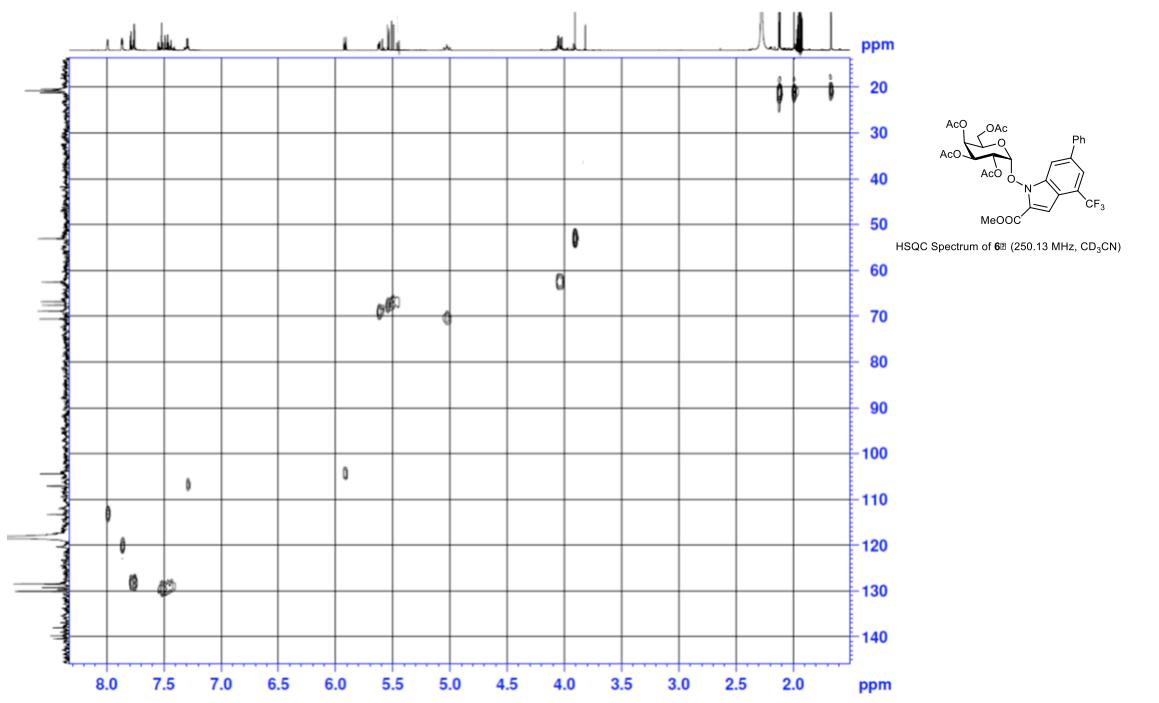
²Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Via G. Moruzzi 3, 56124 Pisa, Italy

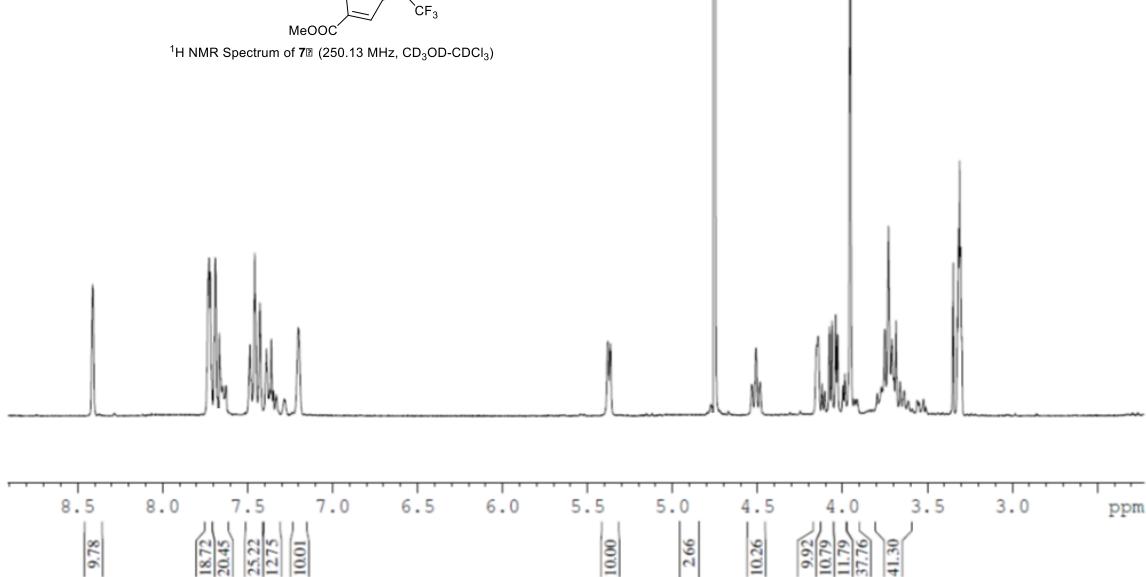
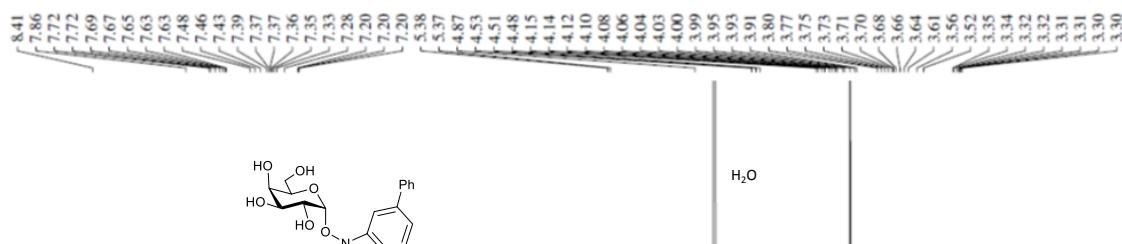
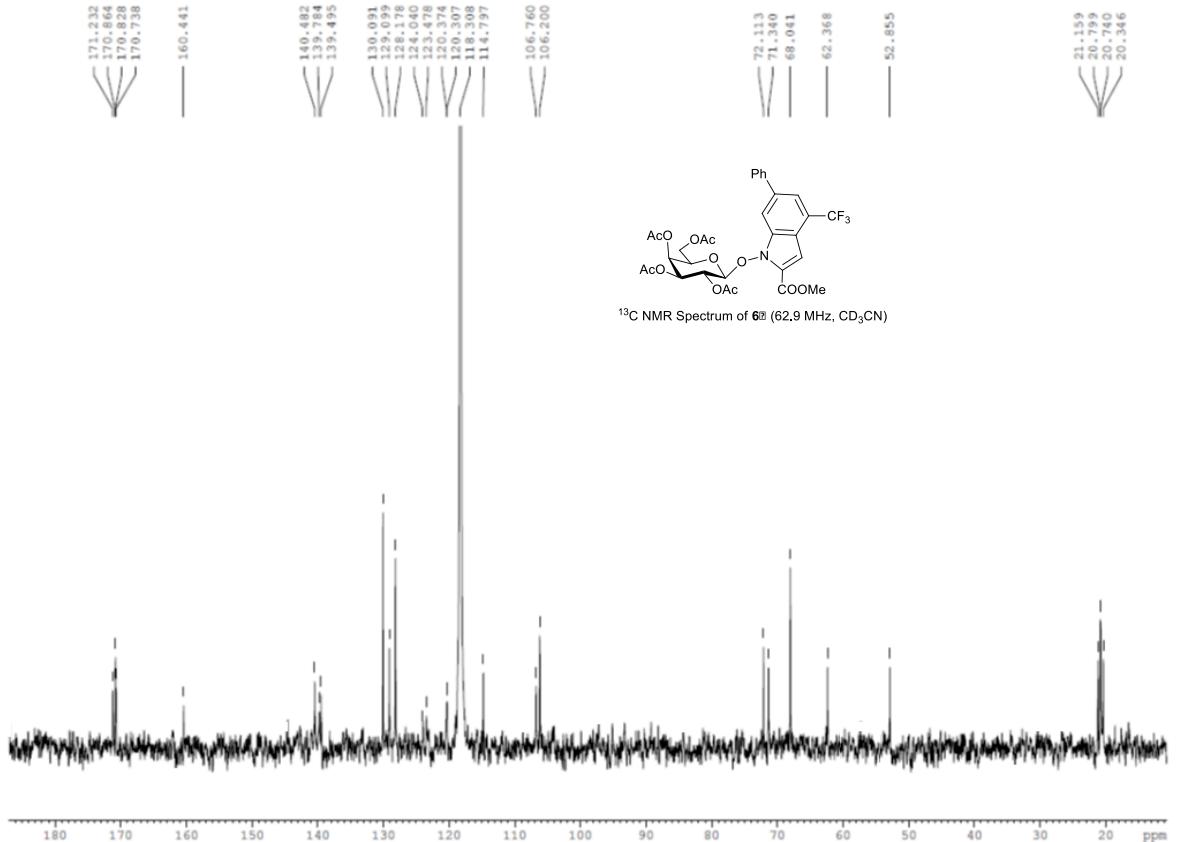
*Corresponding authors: felicia.dandrea@unipi.it, valeria.dibussolo@unipi.it.

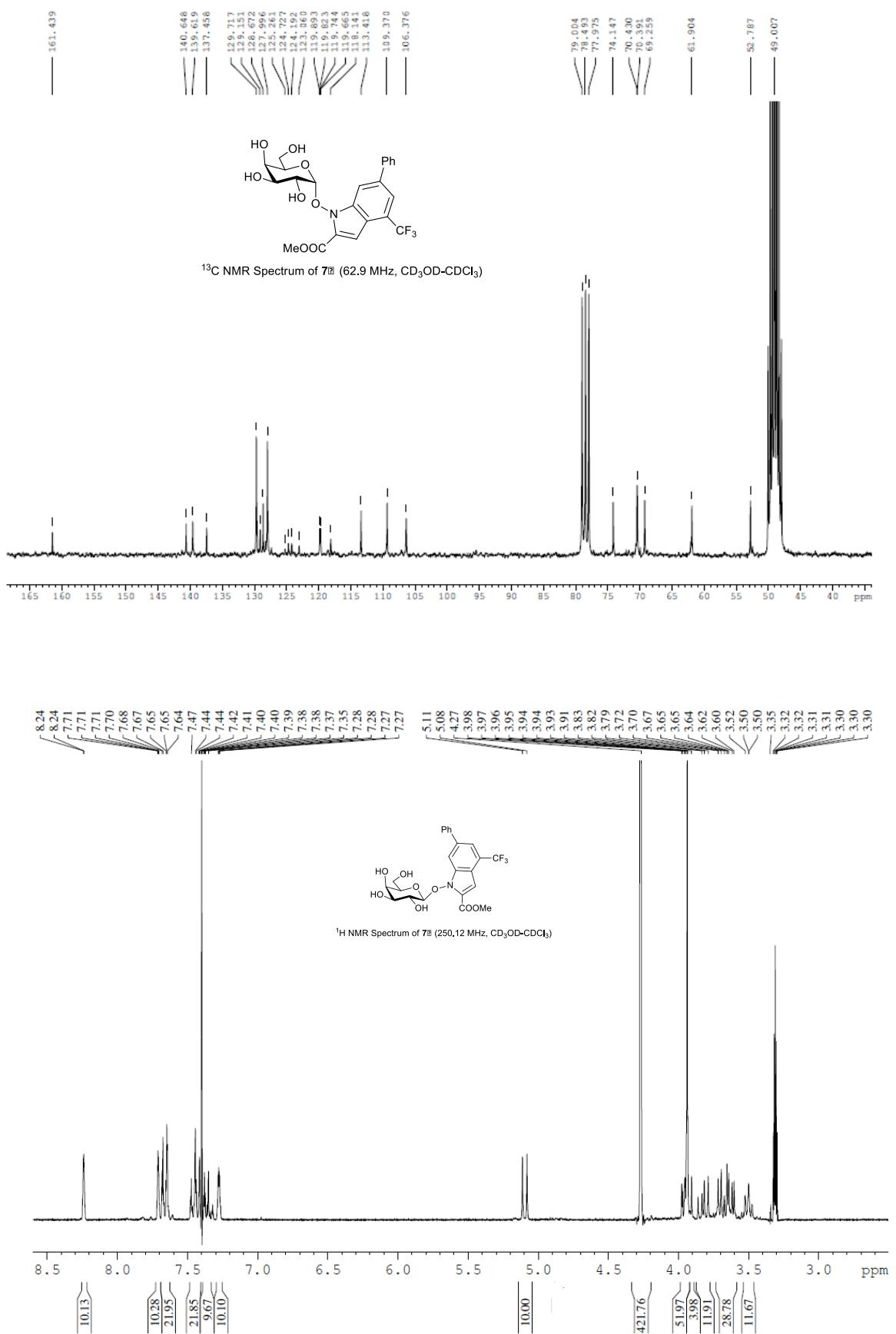
Contents

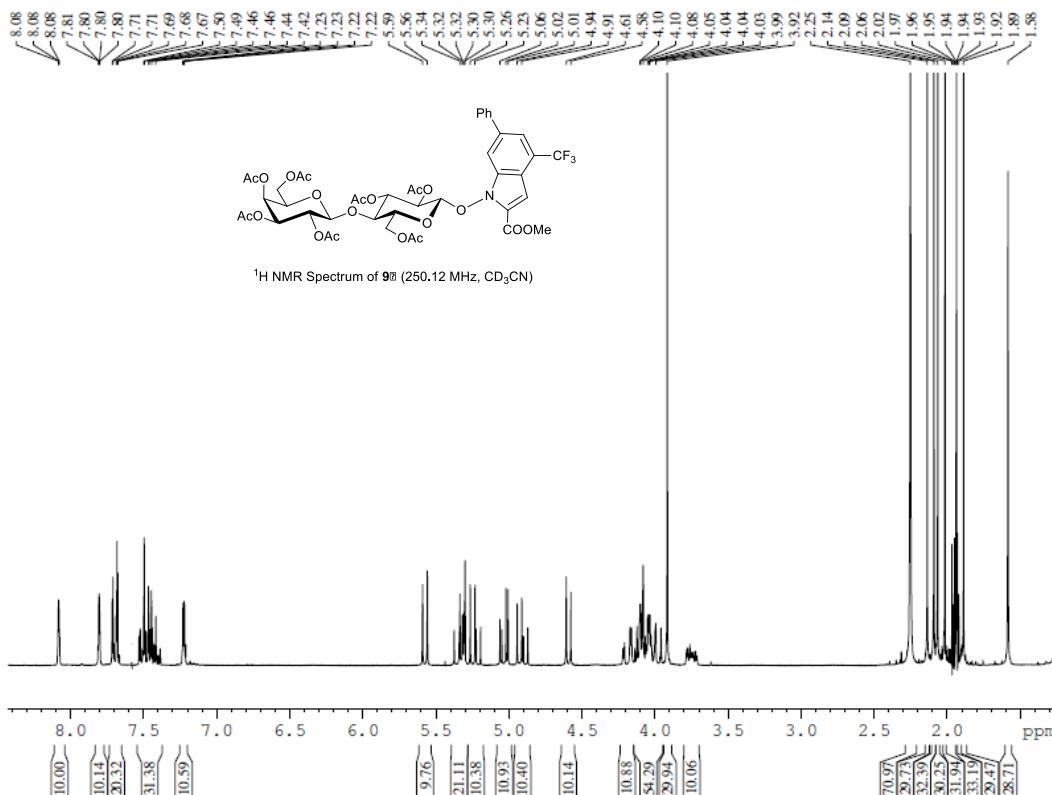
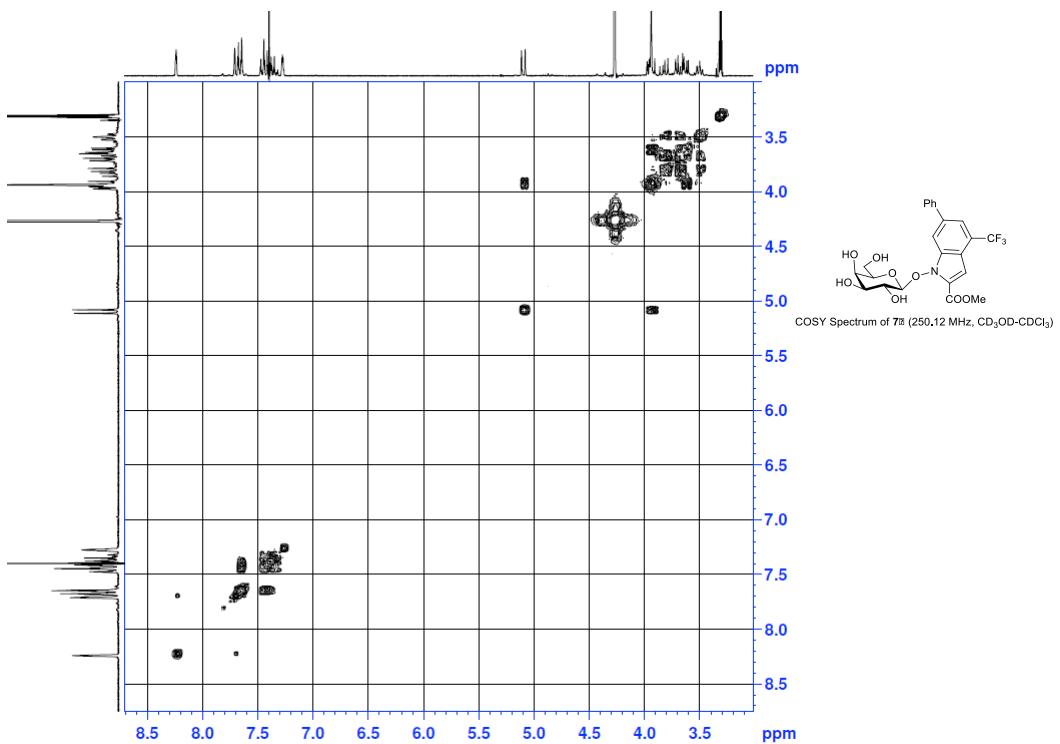
¹ H-, ¹³ C NMR, and HSQC spectrum of 6α	S2-S3
¹ H- and ¹³ C NMR spectrum of 6β	S3-S4
¹ H- and ¹³ C NMR spectrum of 7α	S4-S5
¹ H NMR and COSY spectrum of 7β	S5-S6
¹ H-, ¹³ C NMR, COSY and HSQC spectrum of 9β	S6-S8
¹ H- and ¹³ C NMR spectrum of 10β	S8-S9
¹ H- and ¹³ C NMR spectrum of 12	S9-S10
¹ H-, ¹³ C NMR and HSQC spectrum of 13	S10-S11
¹ H-, ¹³ C-NMR, COSY and HSQC spectrum of 16	S12-S13
¹ H- and ¹³ C-NMR, COSY and HSQC spectrum of 17	S14-S15
¹ H-, ¹³ C-NMR and HSQC spectrum of 18	S16-S17
¹ H-, ¹³ C-NMR and COSY spectrum of 19	S17-S18
¹ H-, ¹³ C-NMR and HSQC spectrum of 21	S19-S20
¹ H-, ¹³ C-NMR, COSY and HSQC spectrum of 22	S20-S22
¹ H-, ¹³ C-NMR and COSY spectrum of 23	S22-S23
Binding disposition of 7β , 10β , 13 , 18 , 19 , 23 into <i>h</i> LDH5 (Fig. S1-S3)	S24-S25

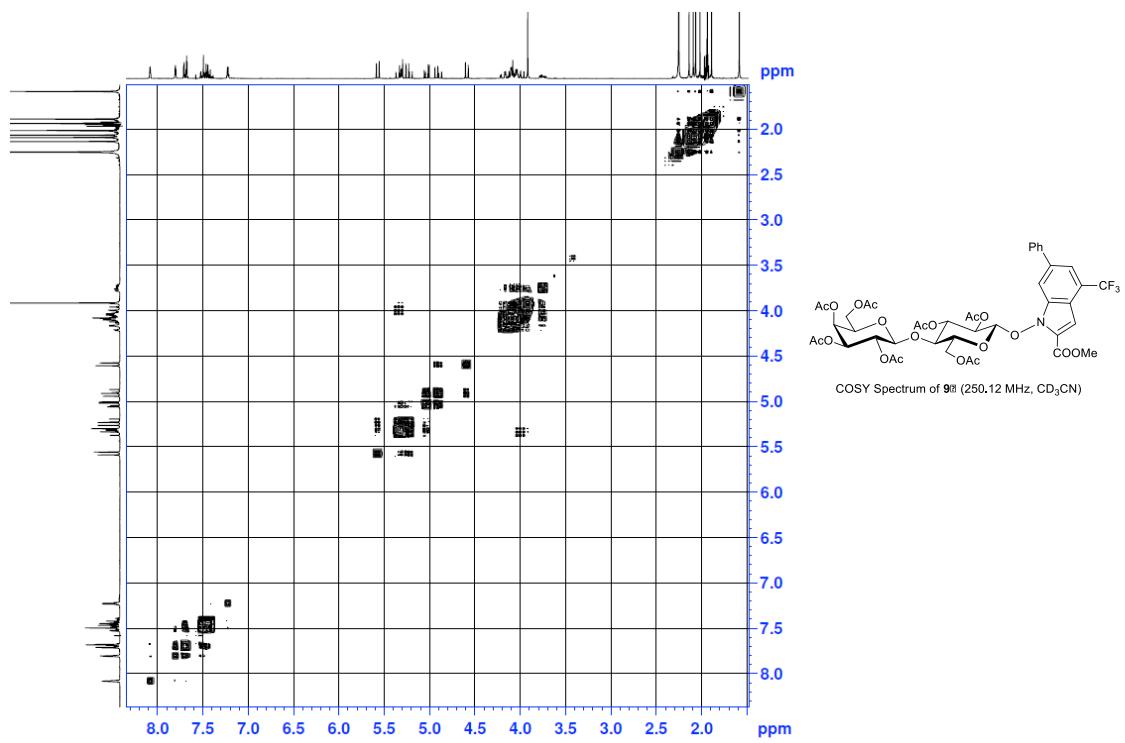
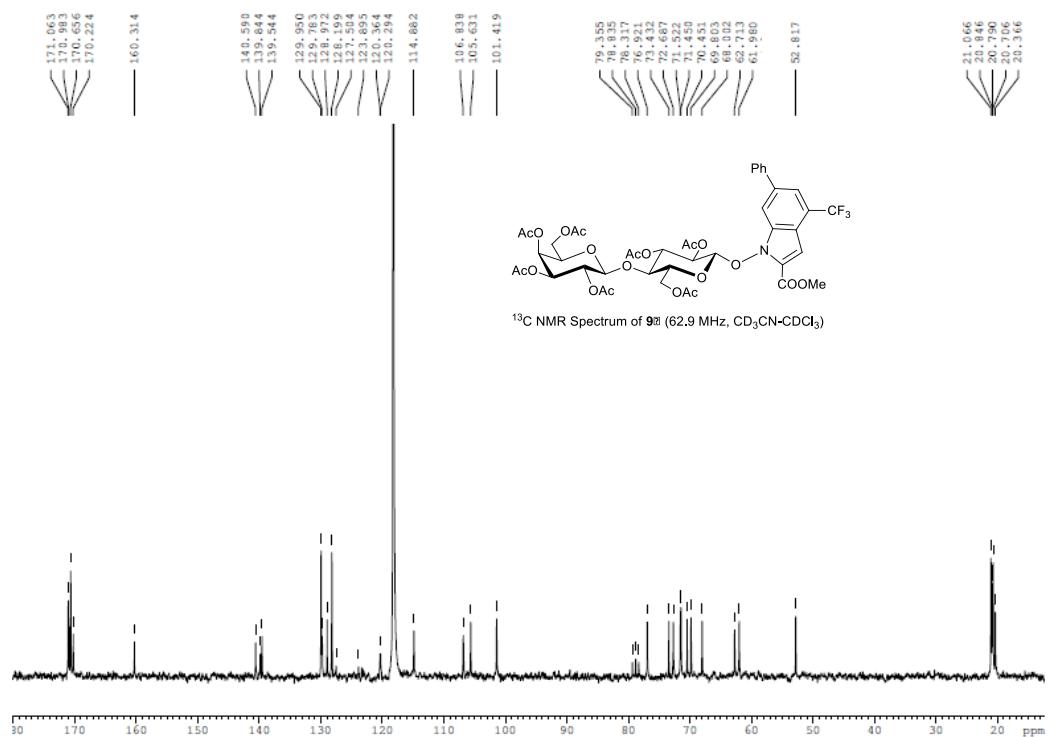


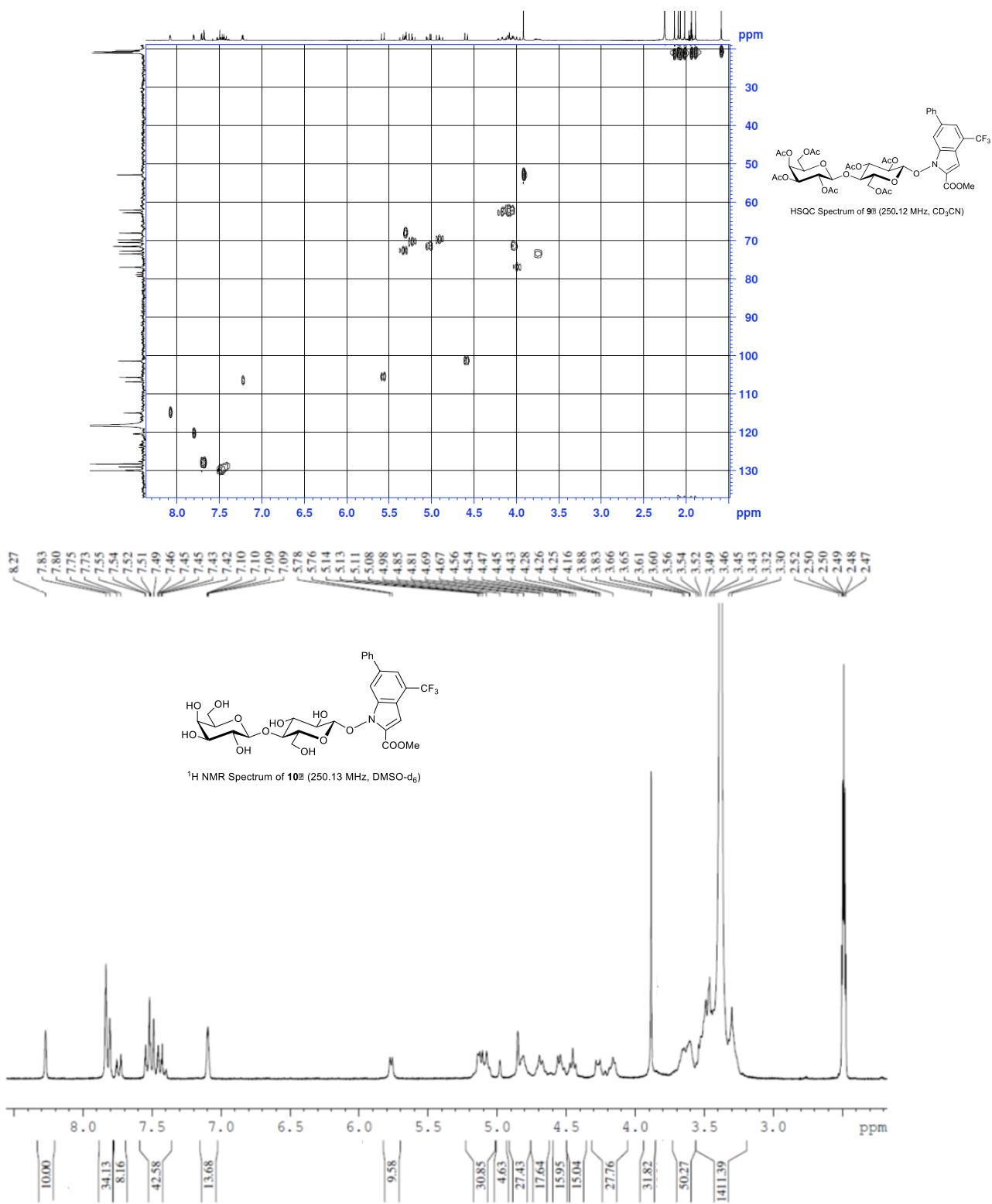


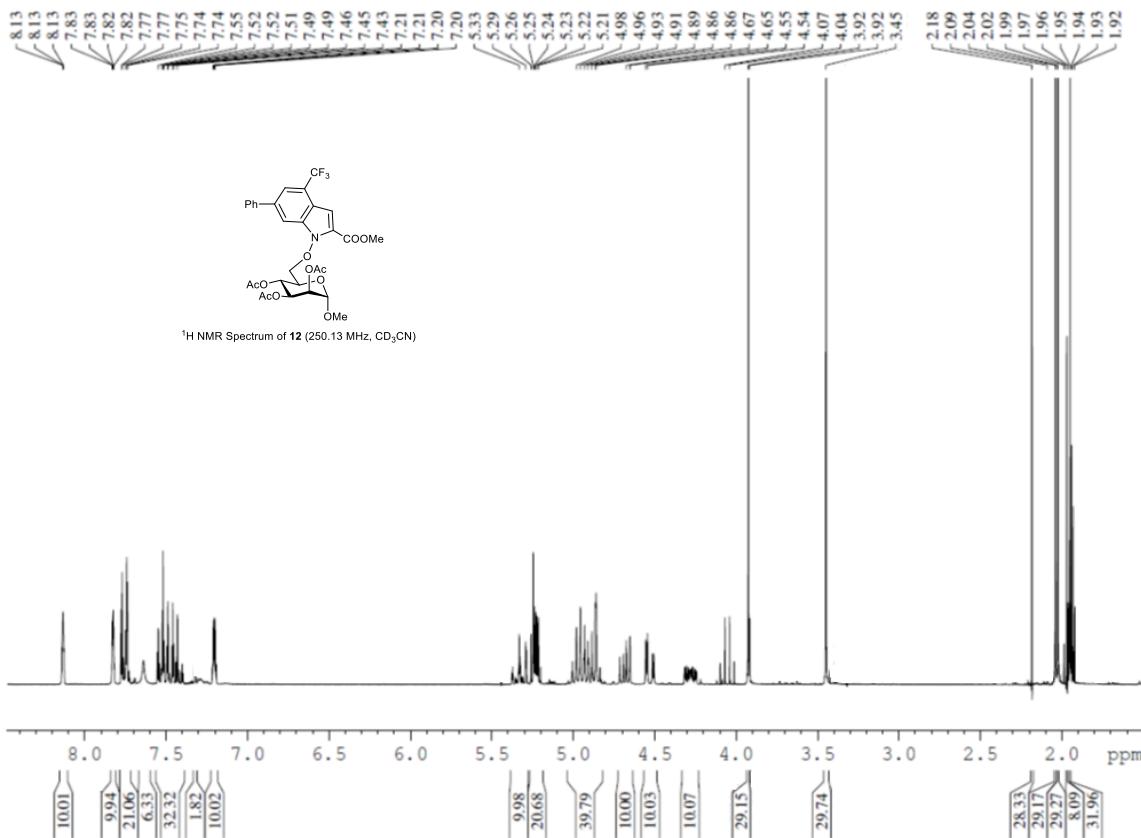
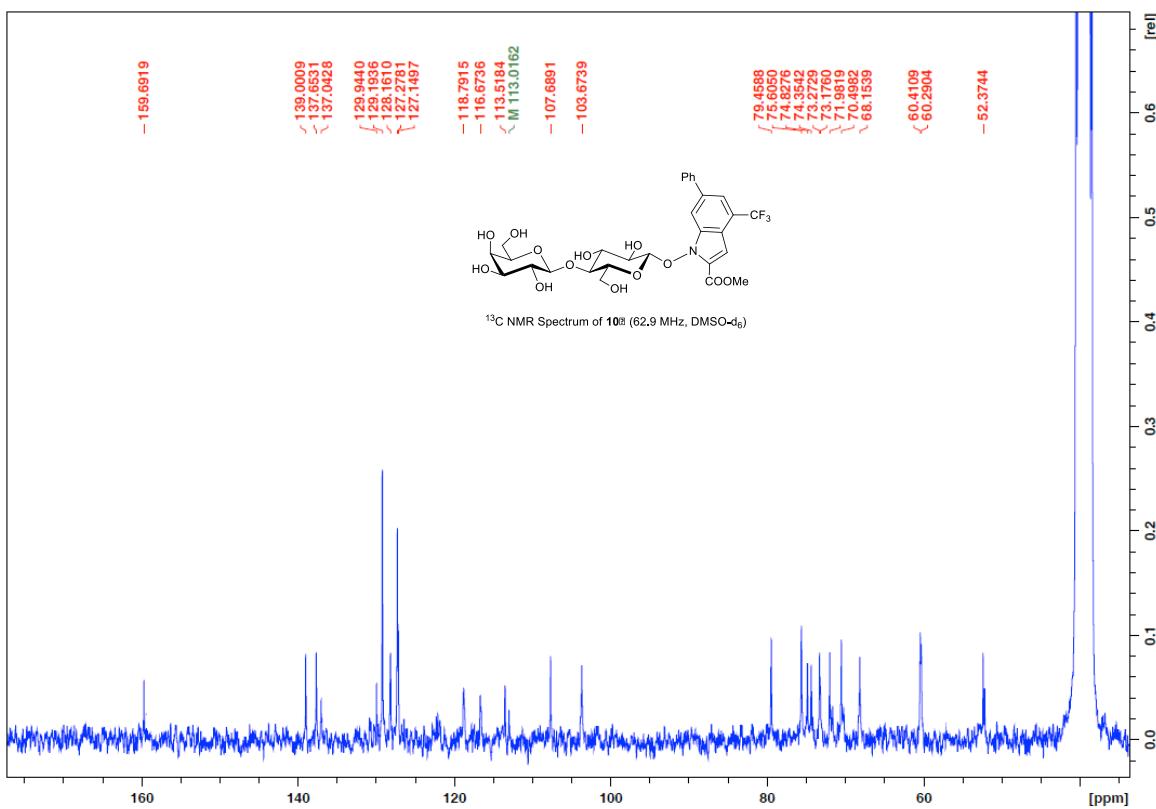


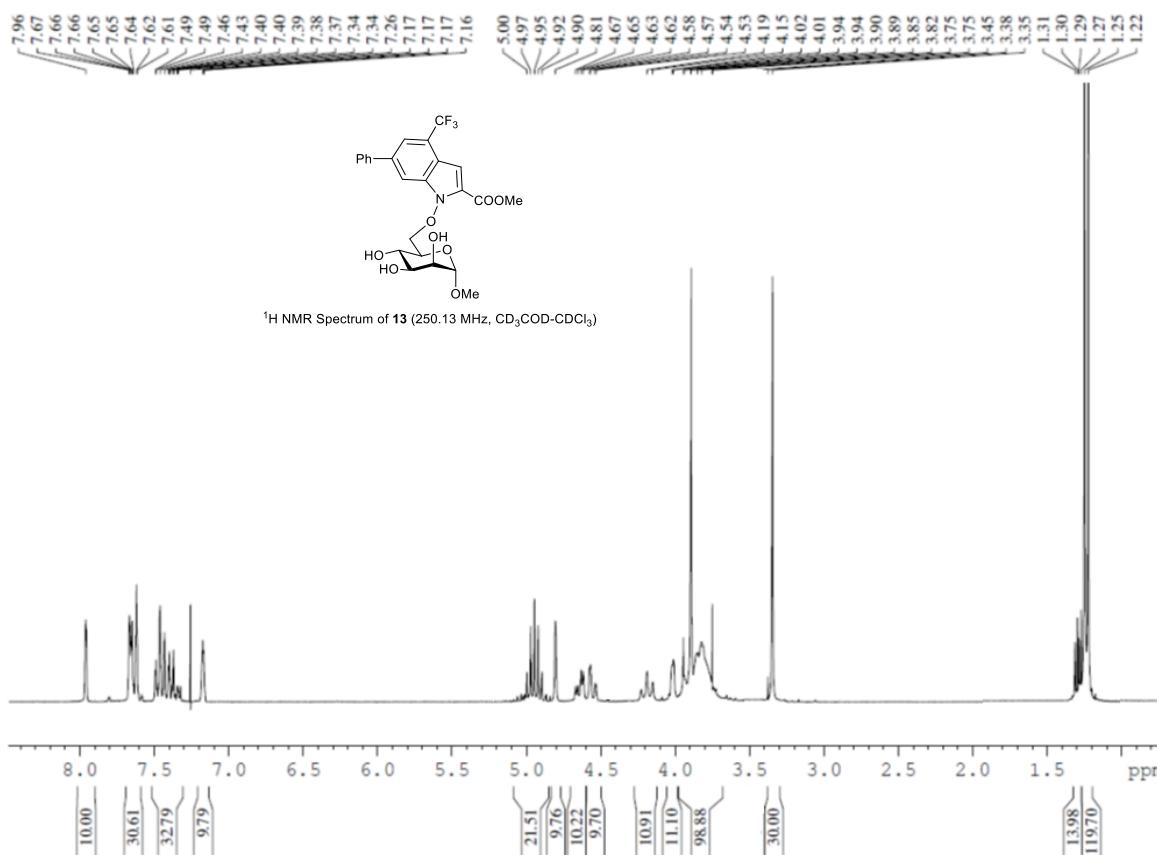
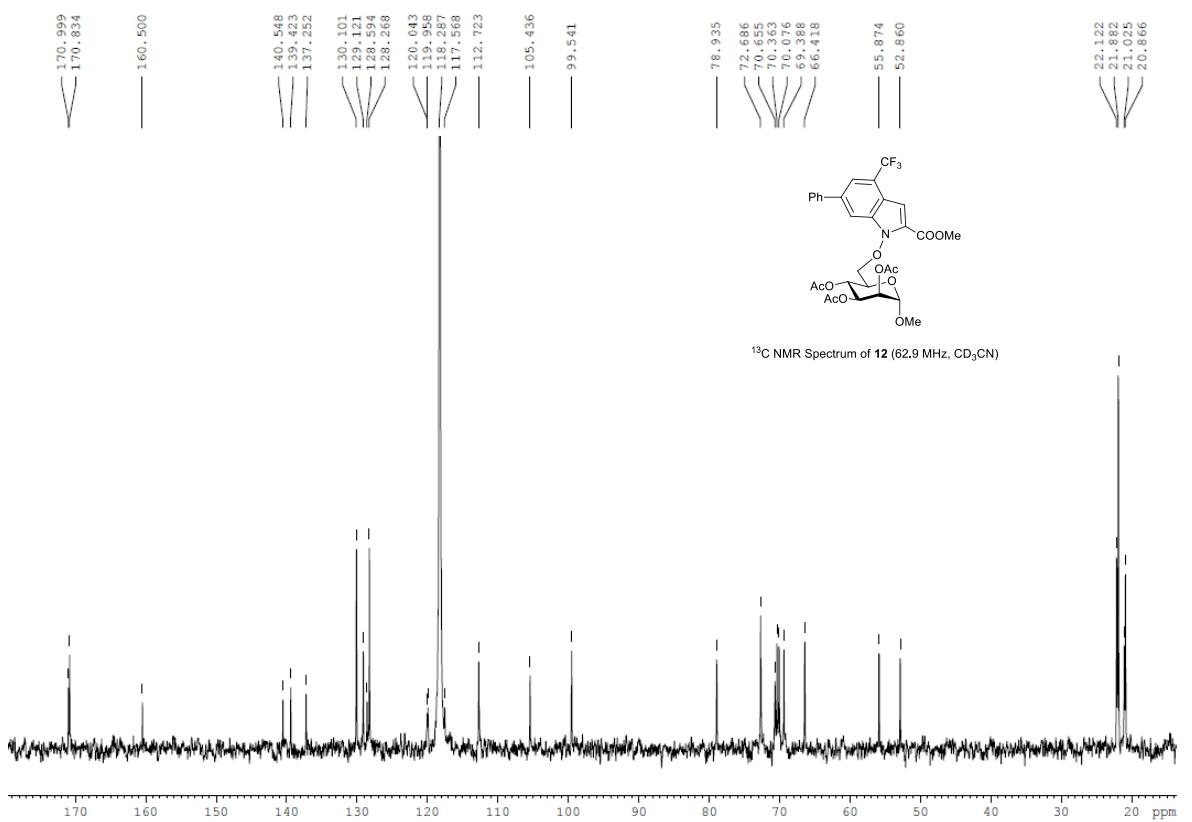


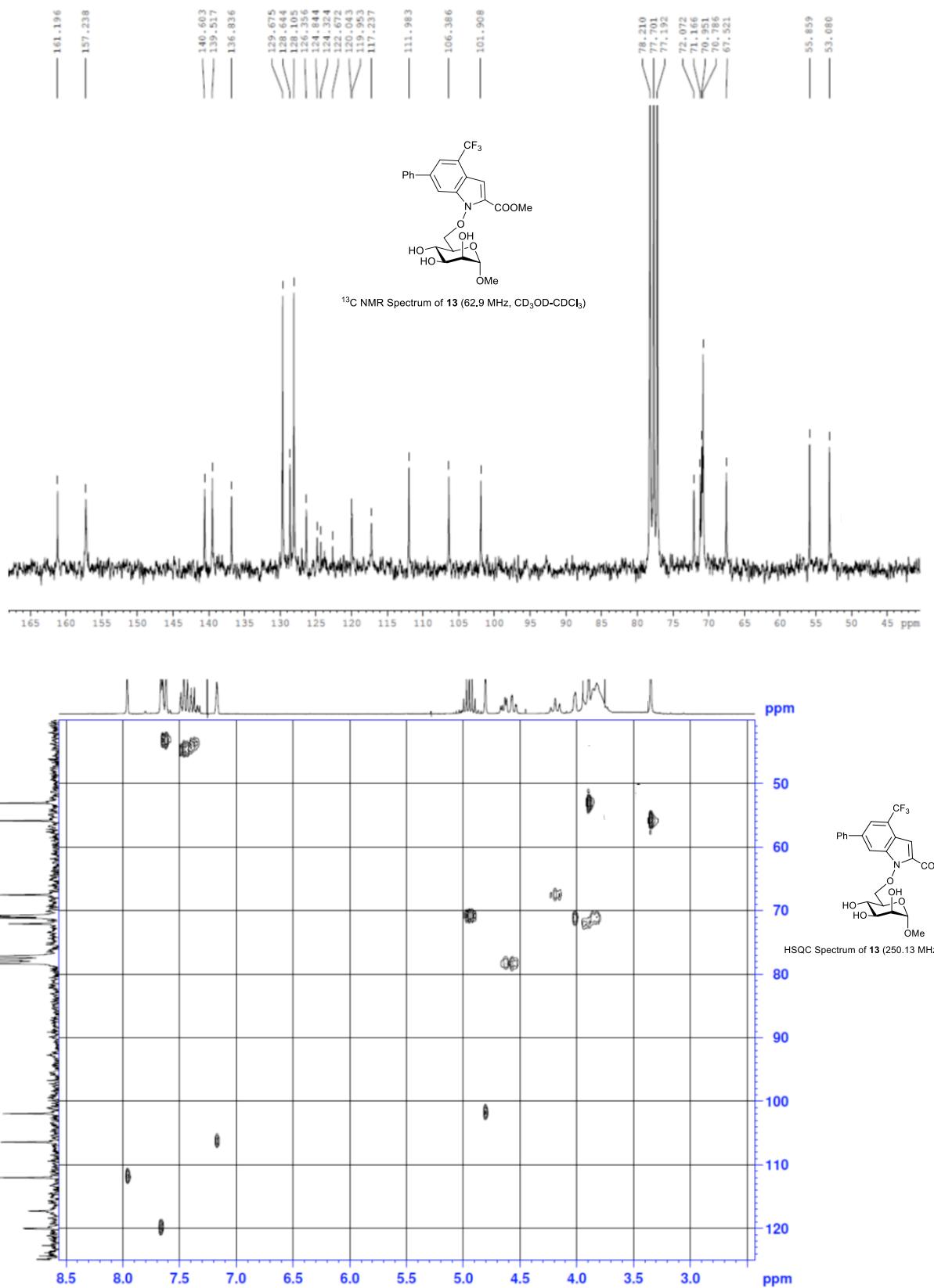


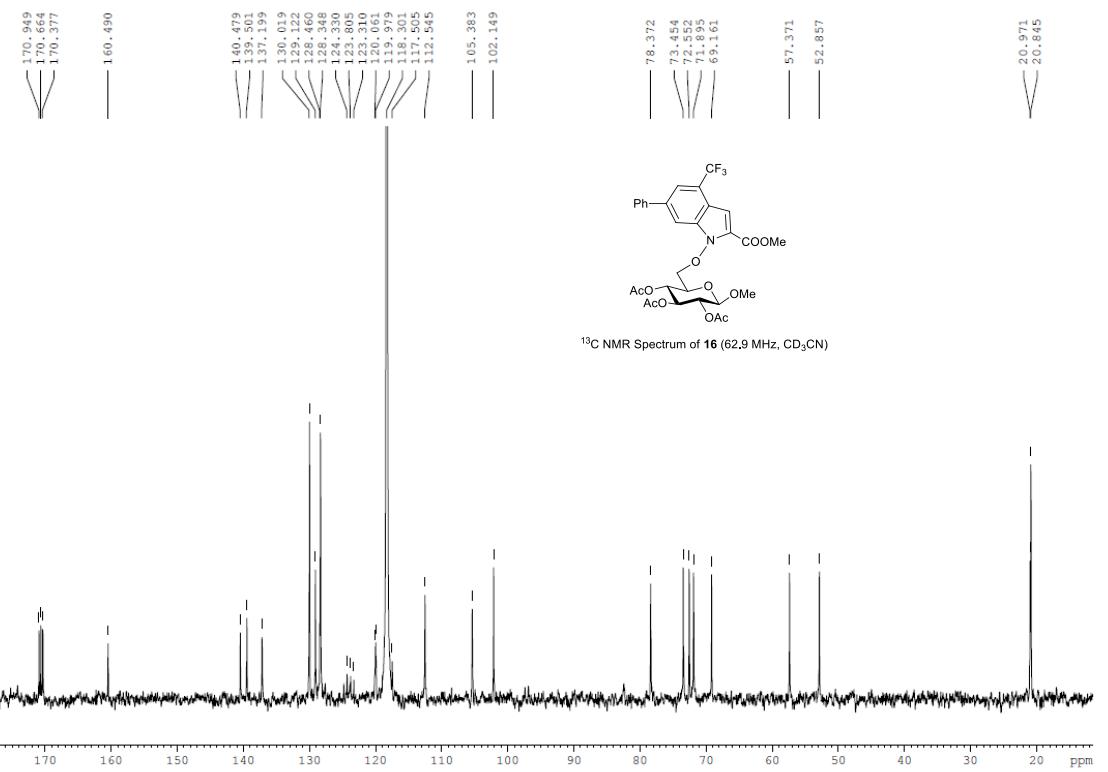
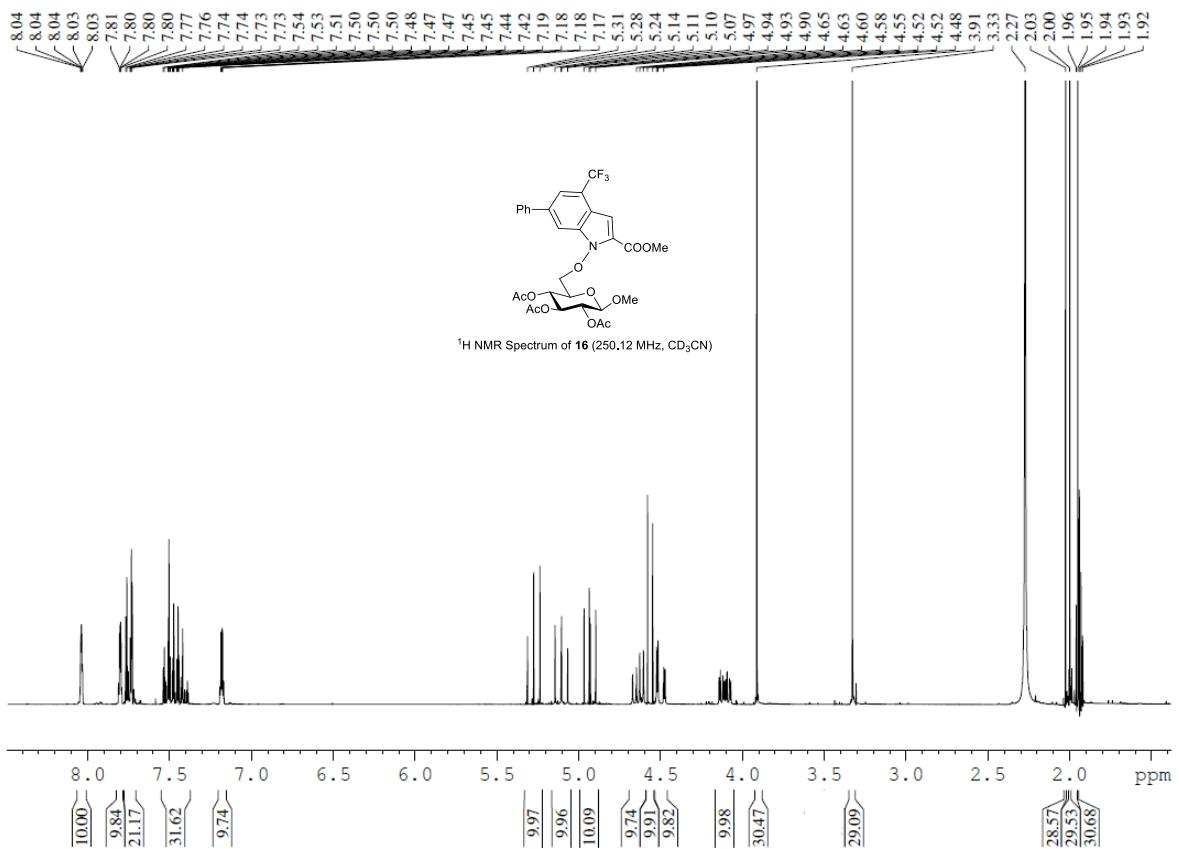


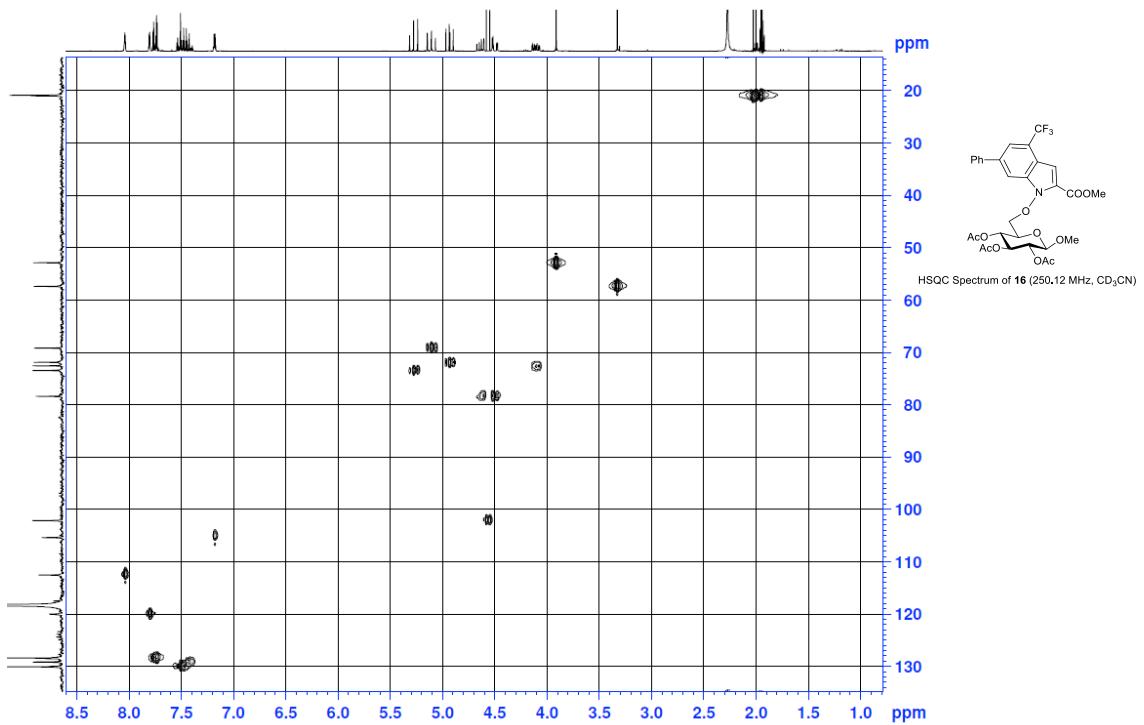
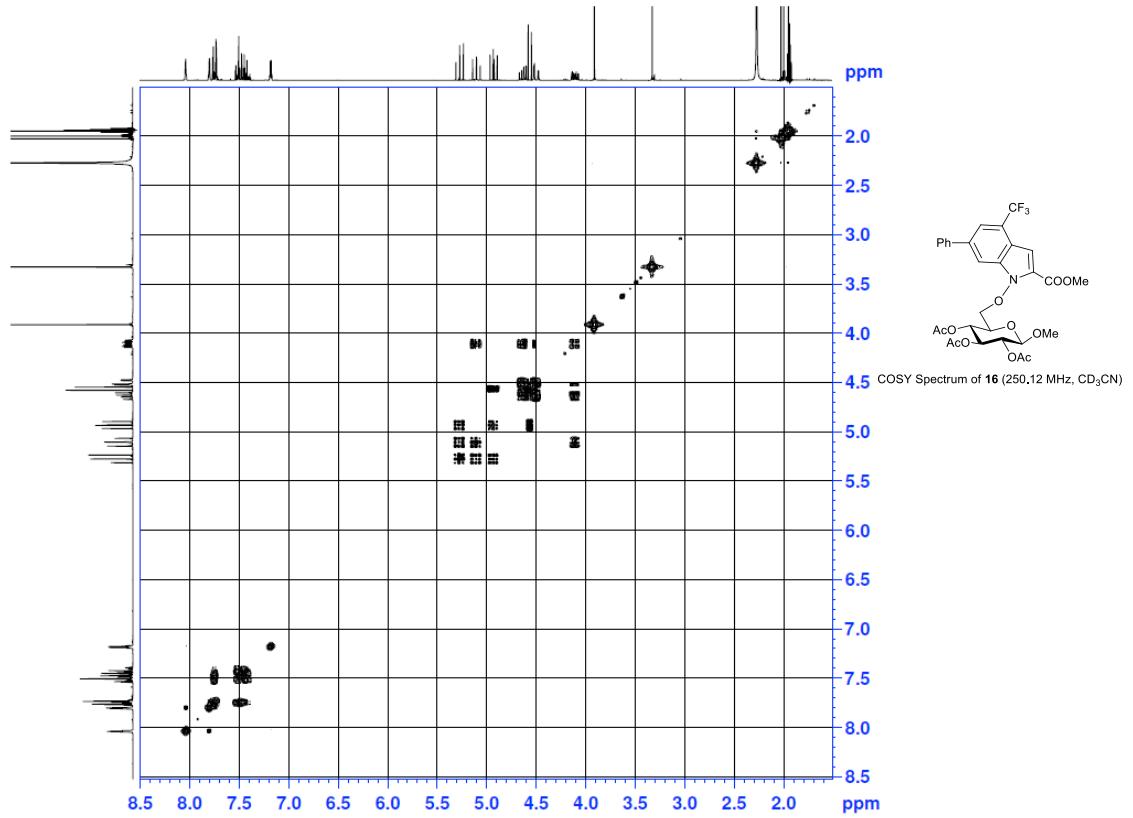


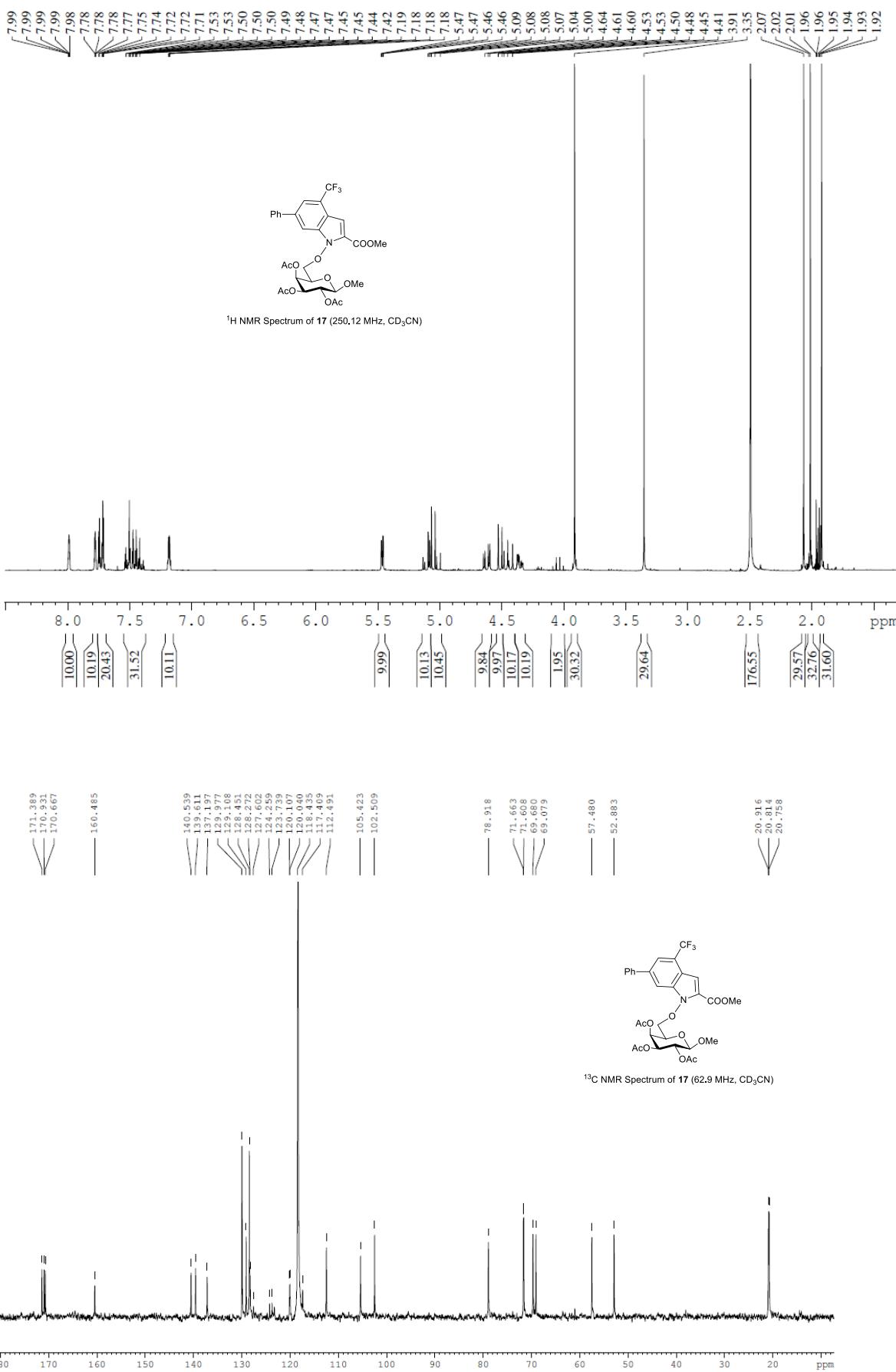


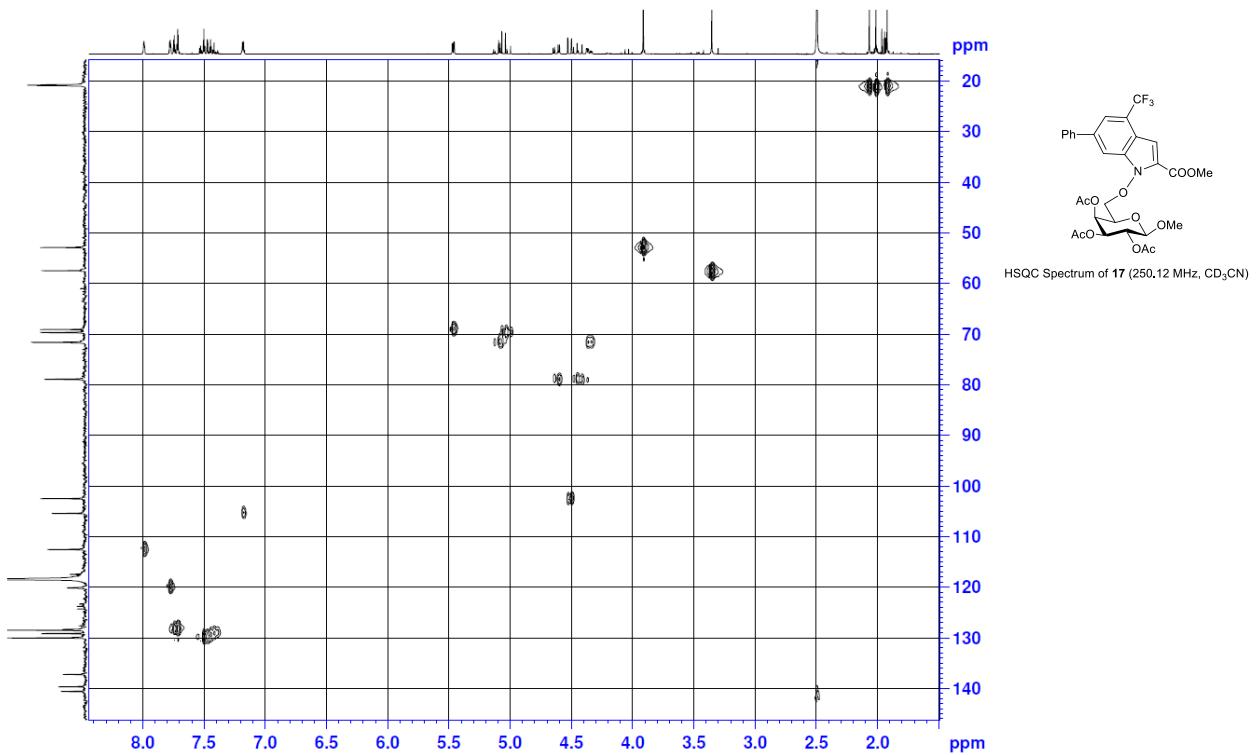
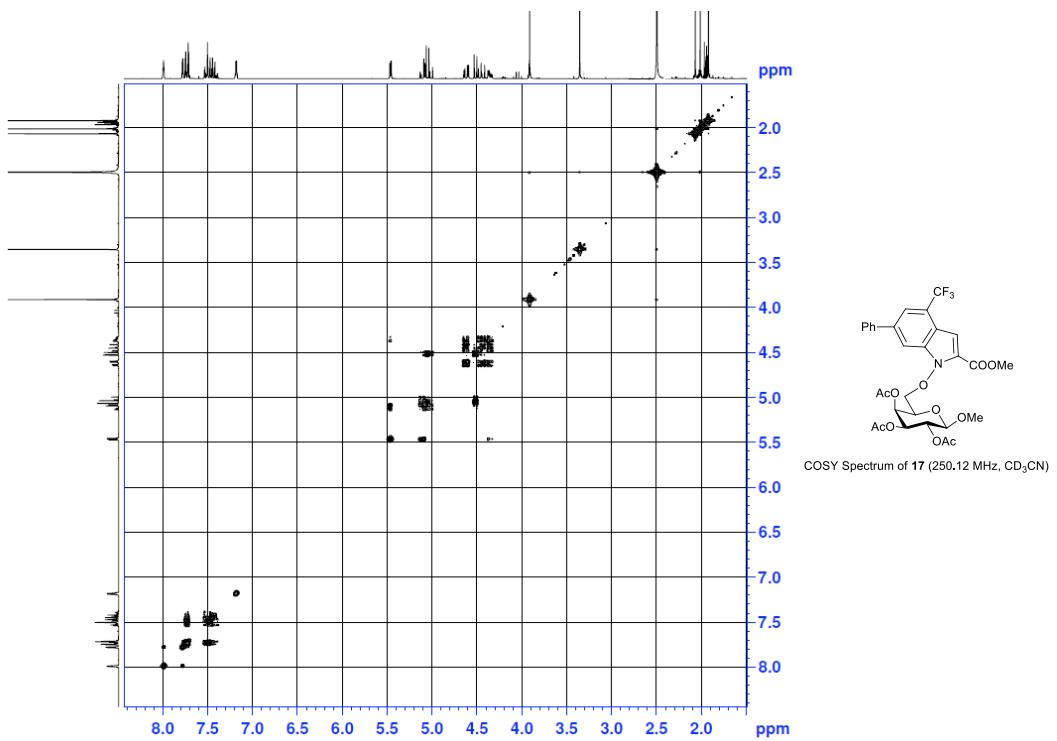


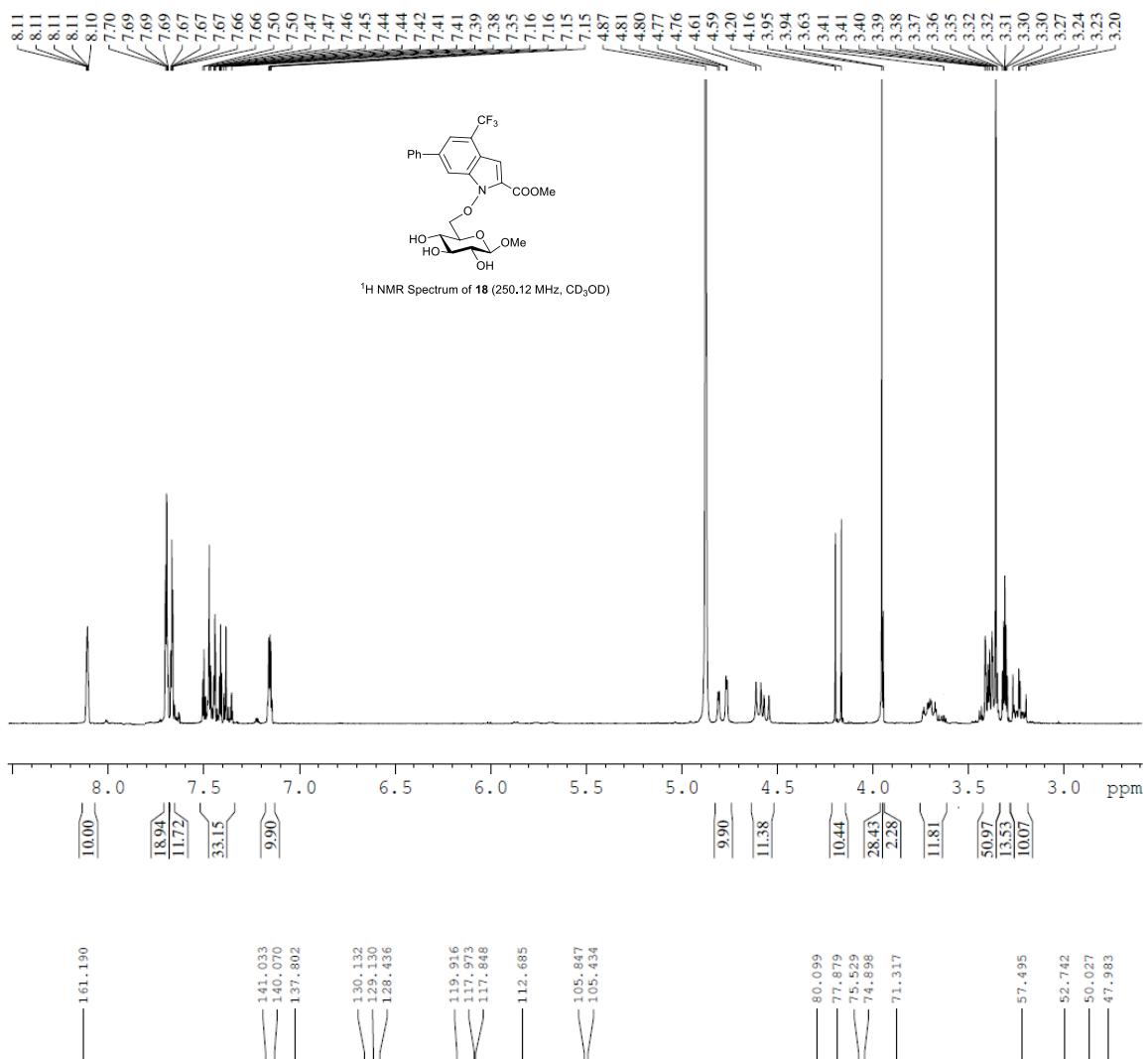




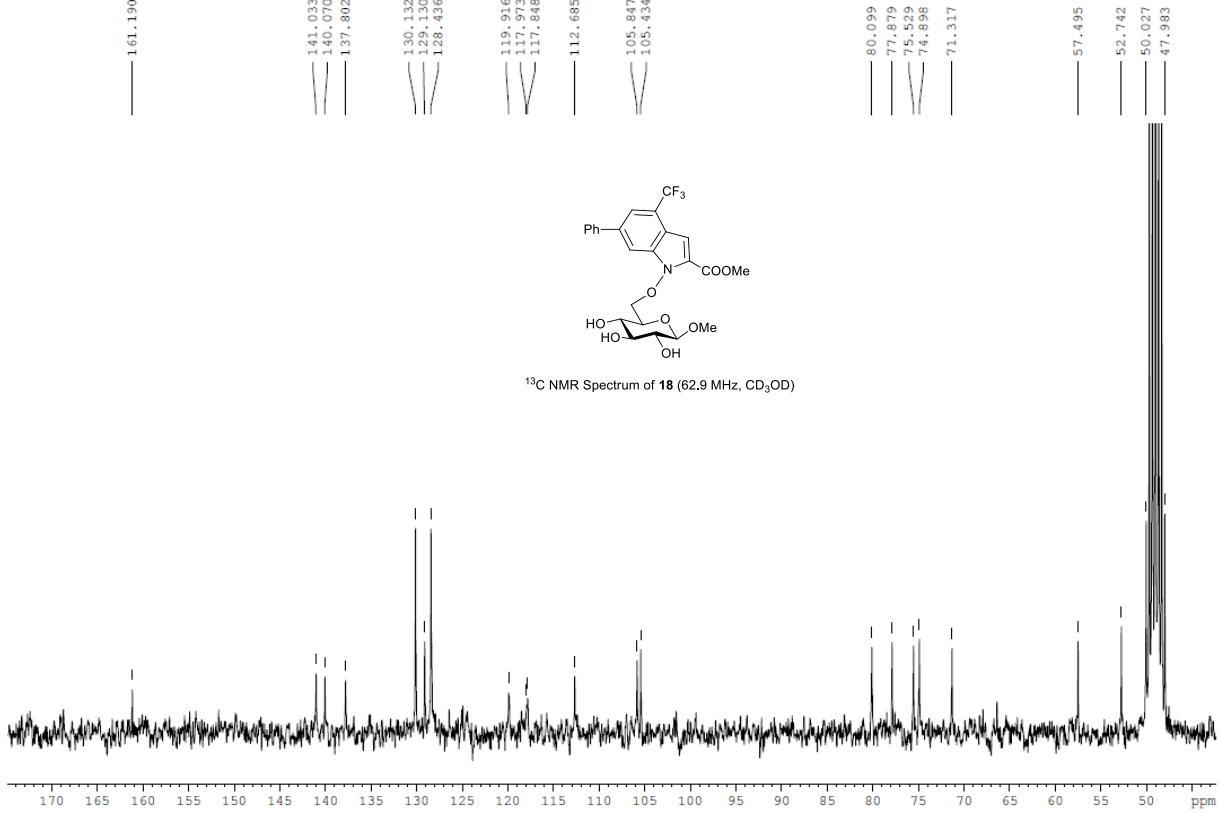


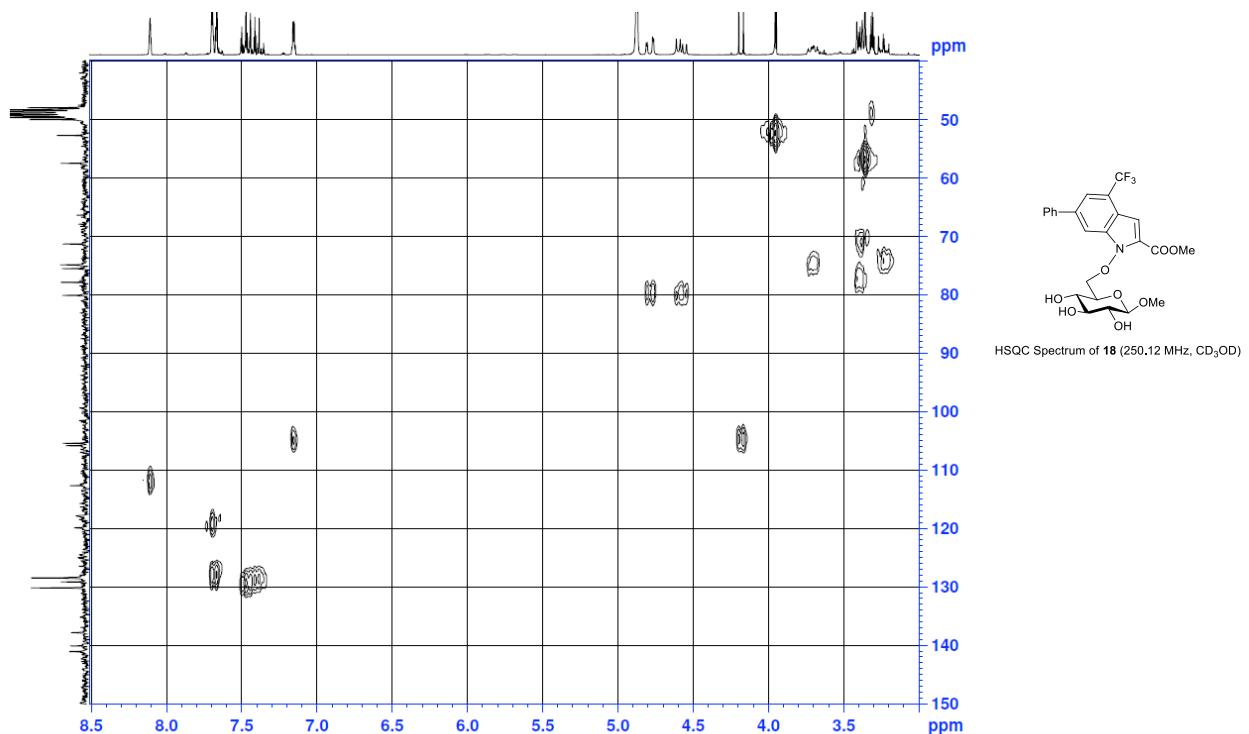




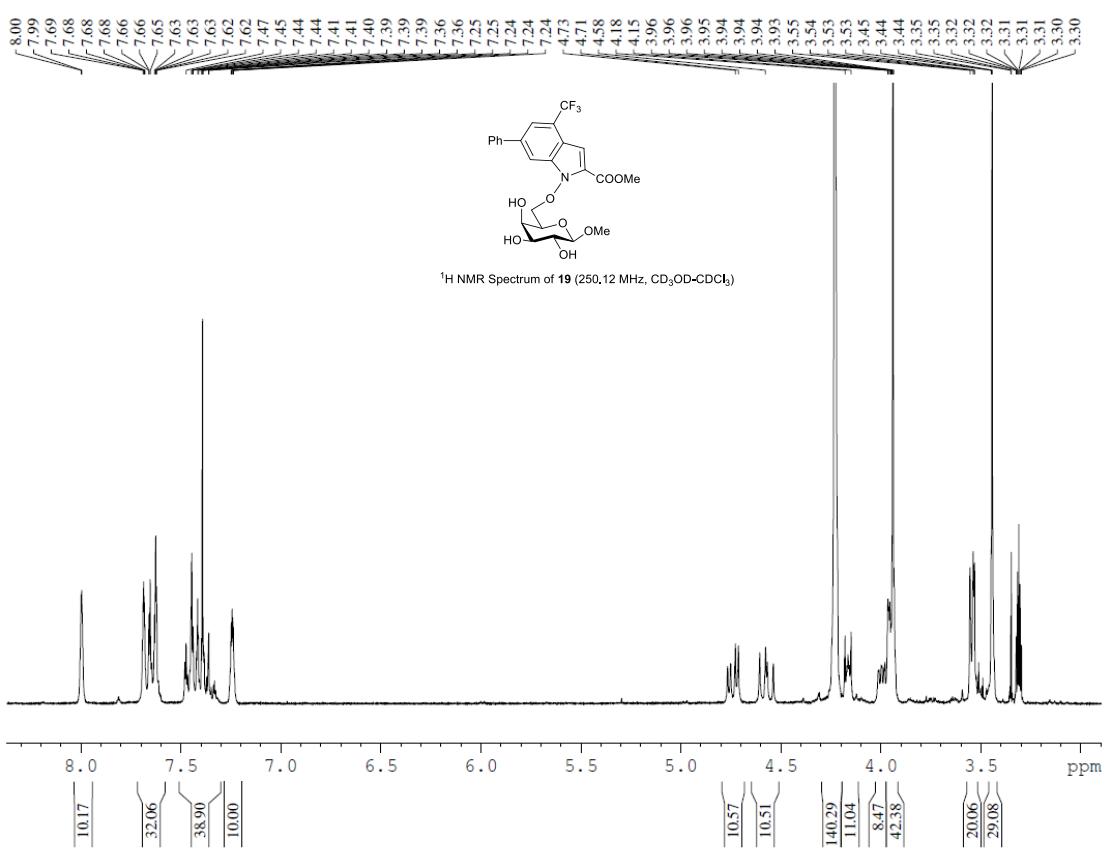


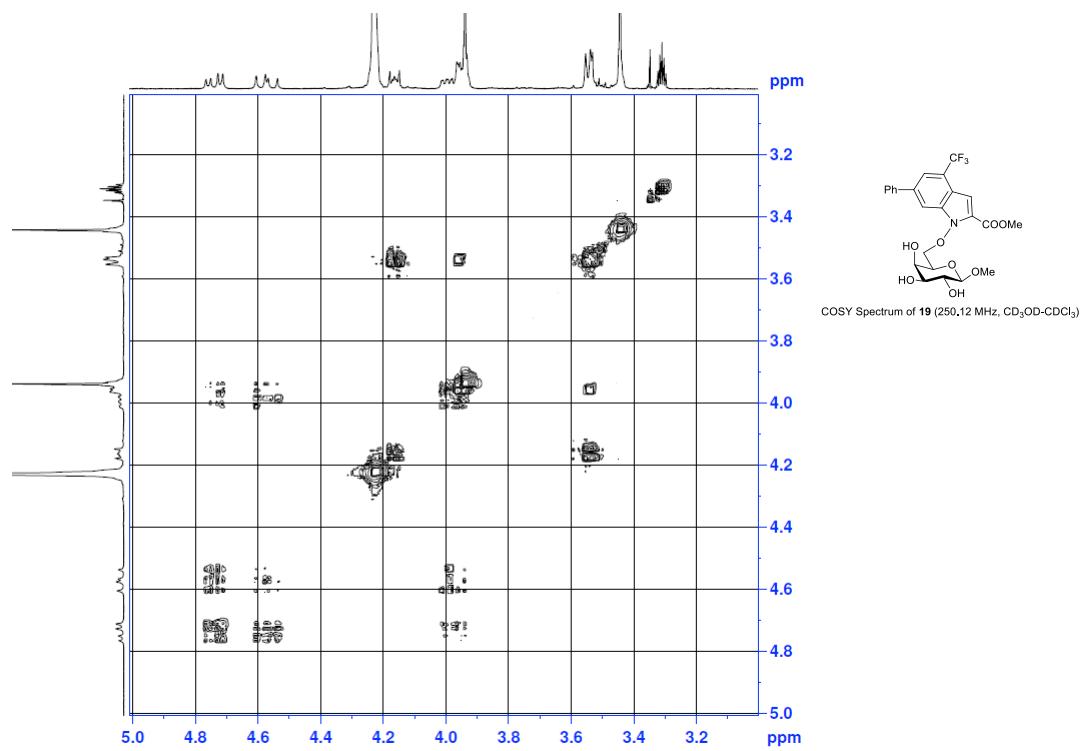
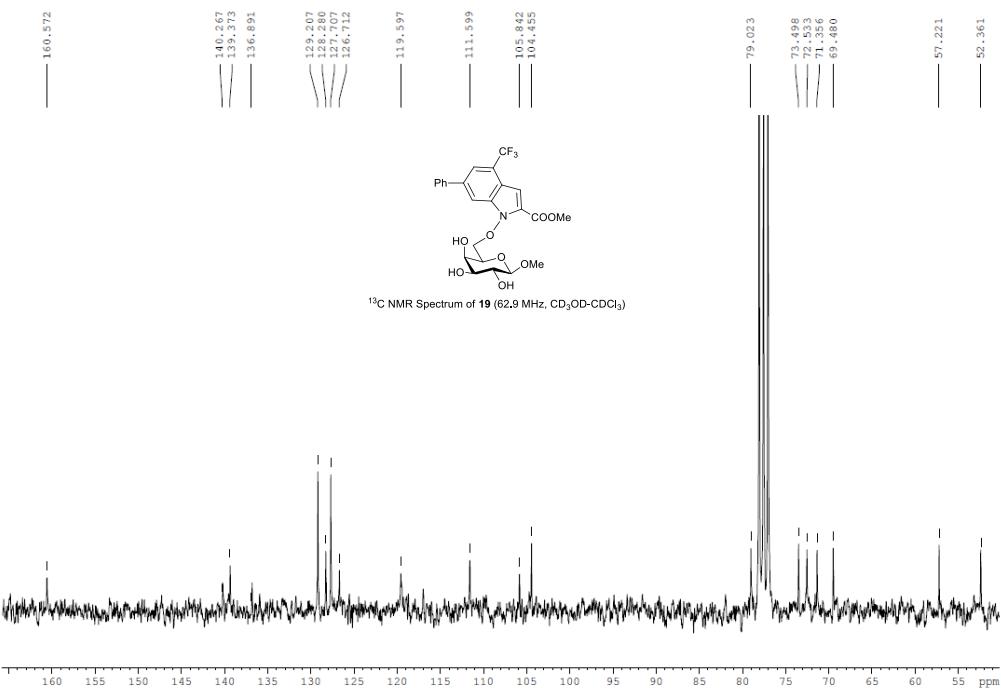
¹H NMR Spectrum of **18** (250.12 MHz, CD₃OD)

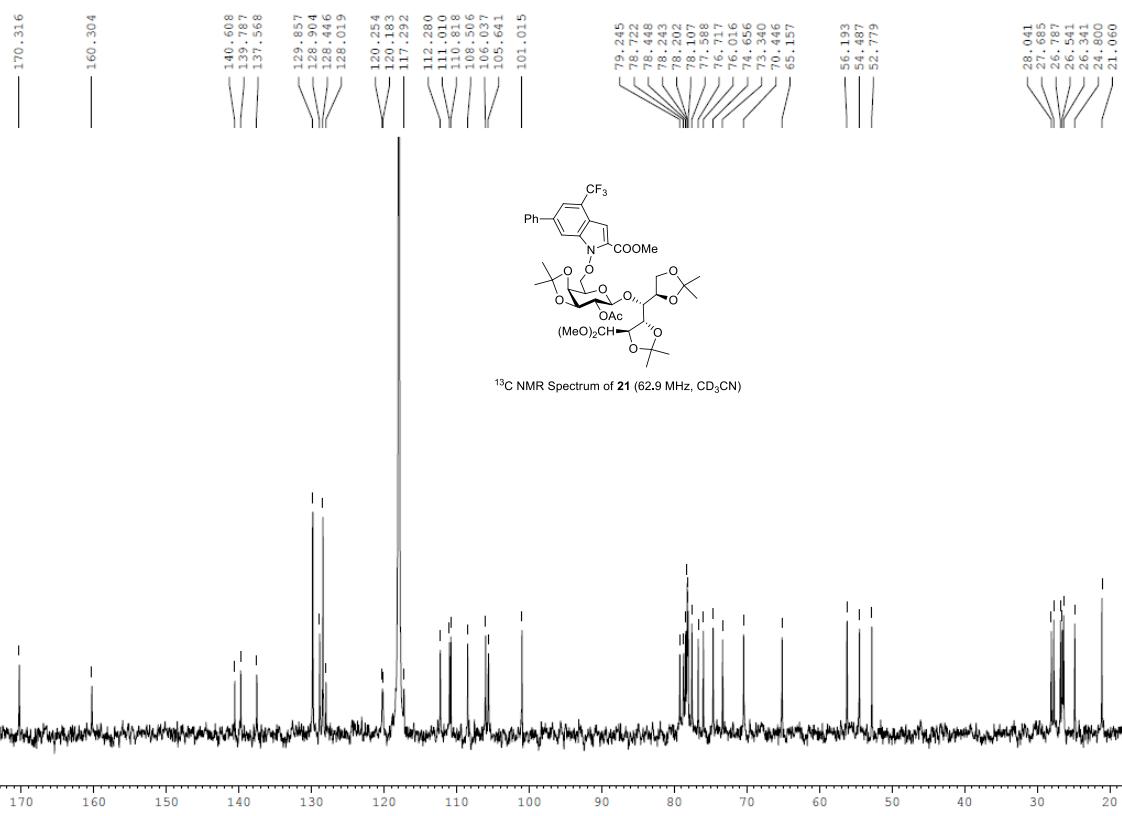
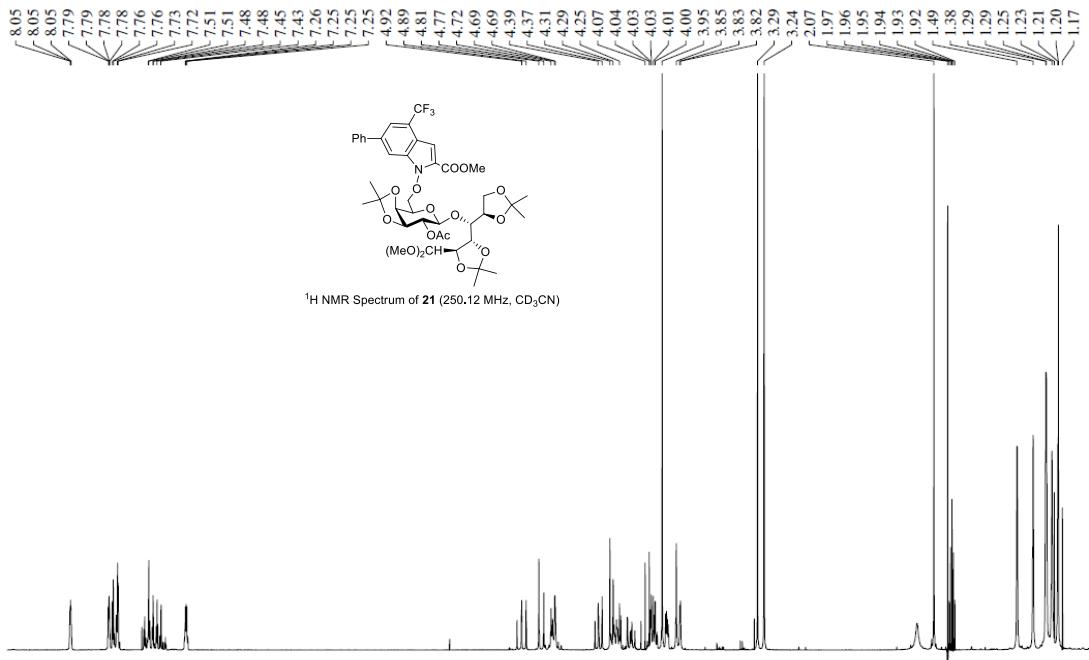


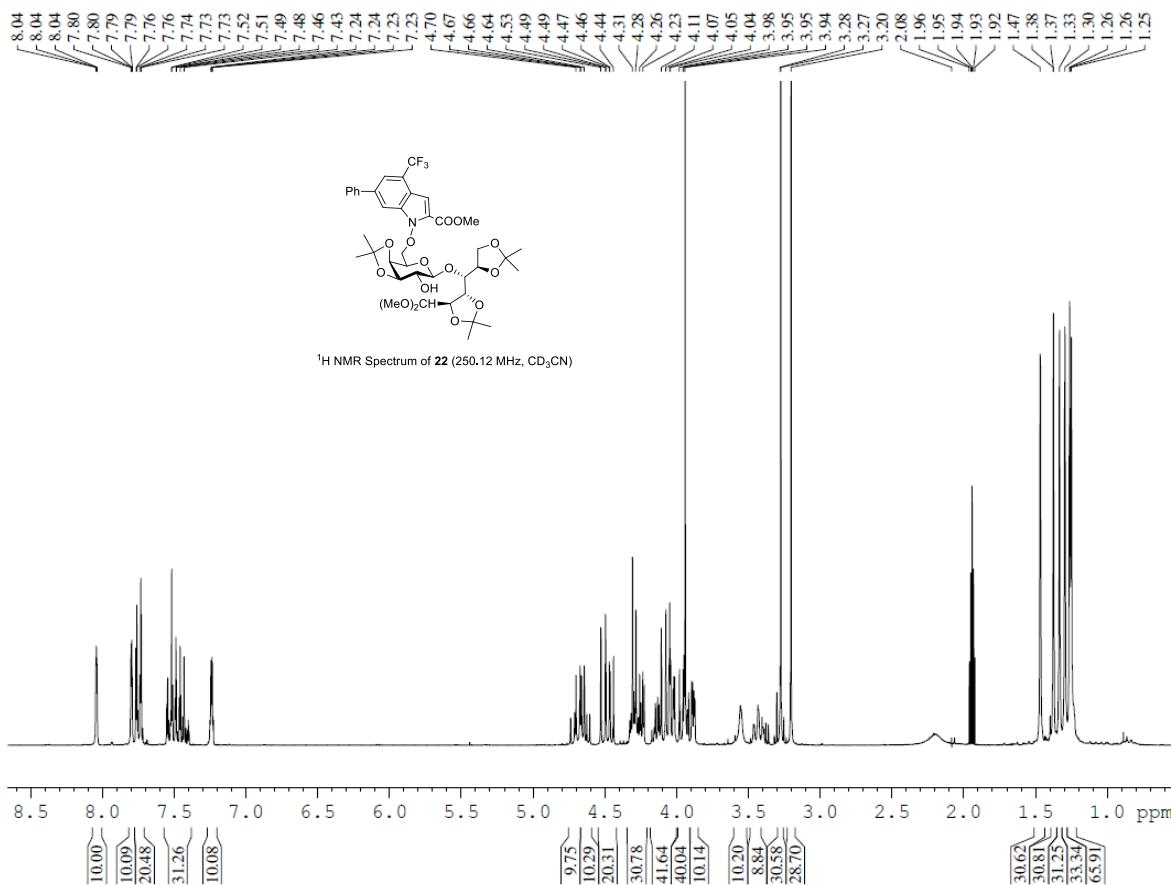
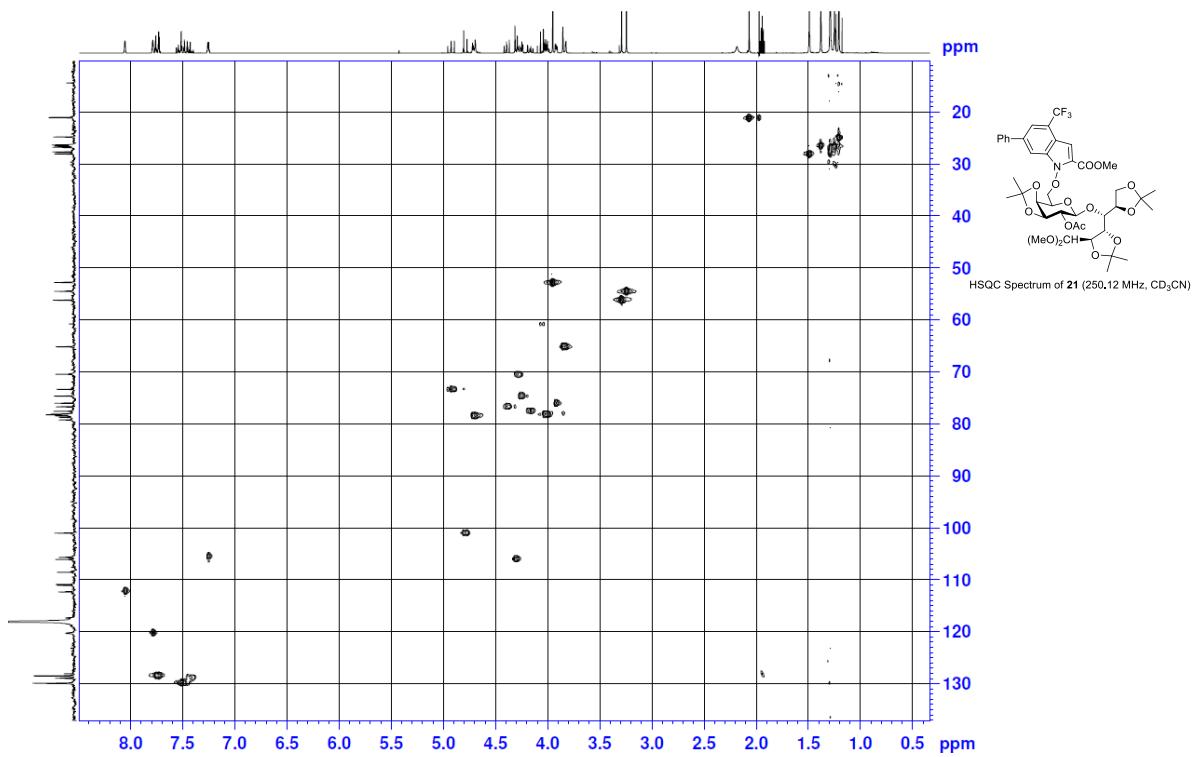


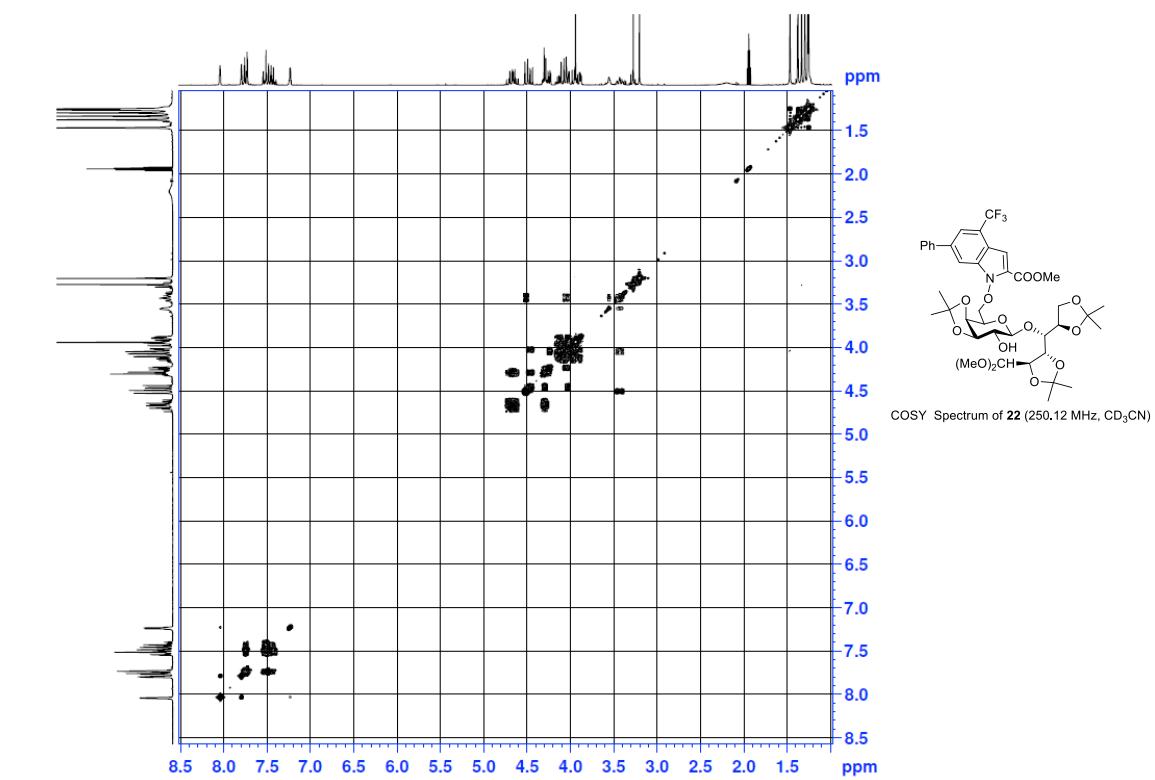
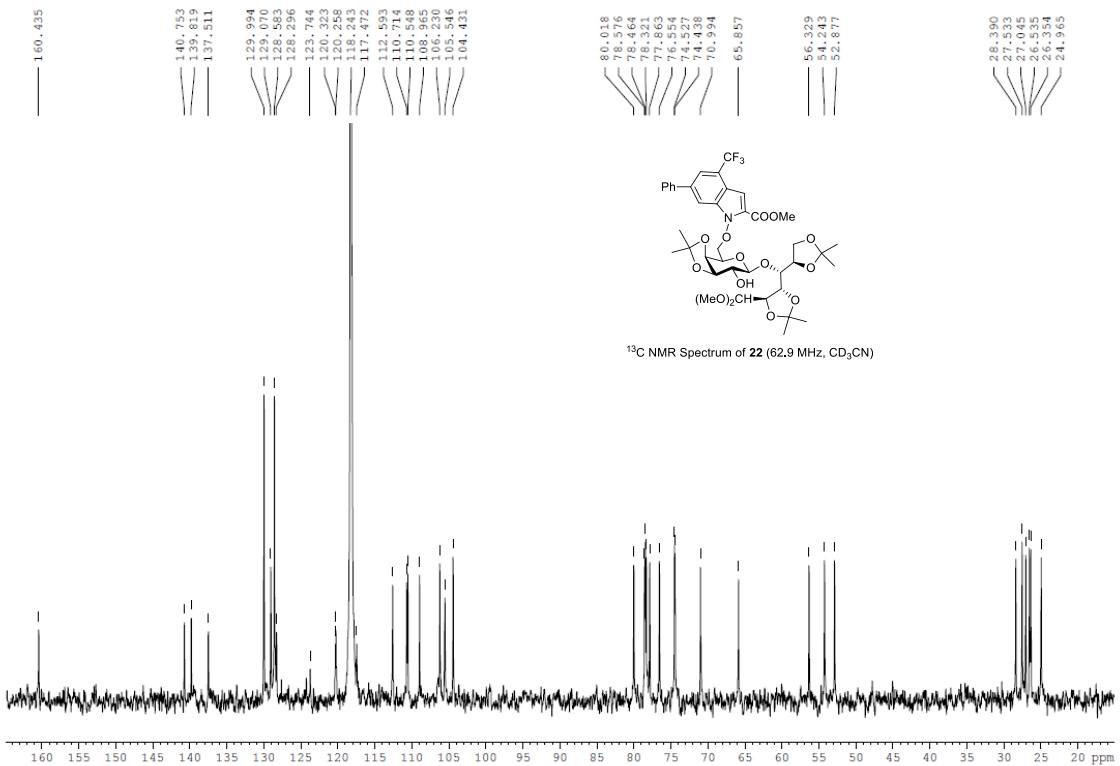
HSQC Spectrum of **18** (250.12 MHz, CD_3OD)

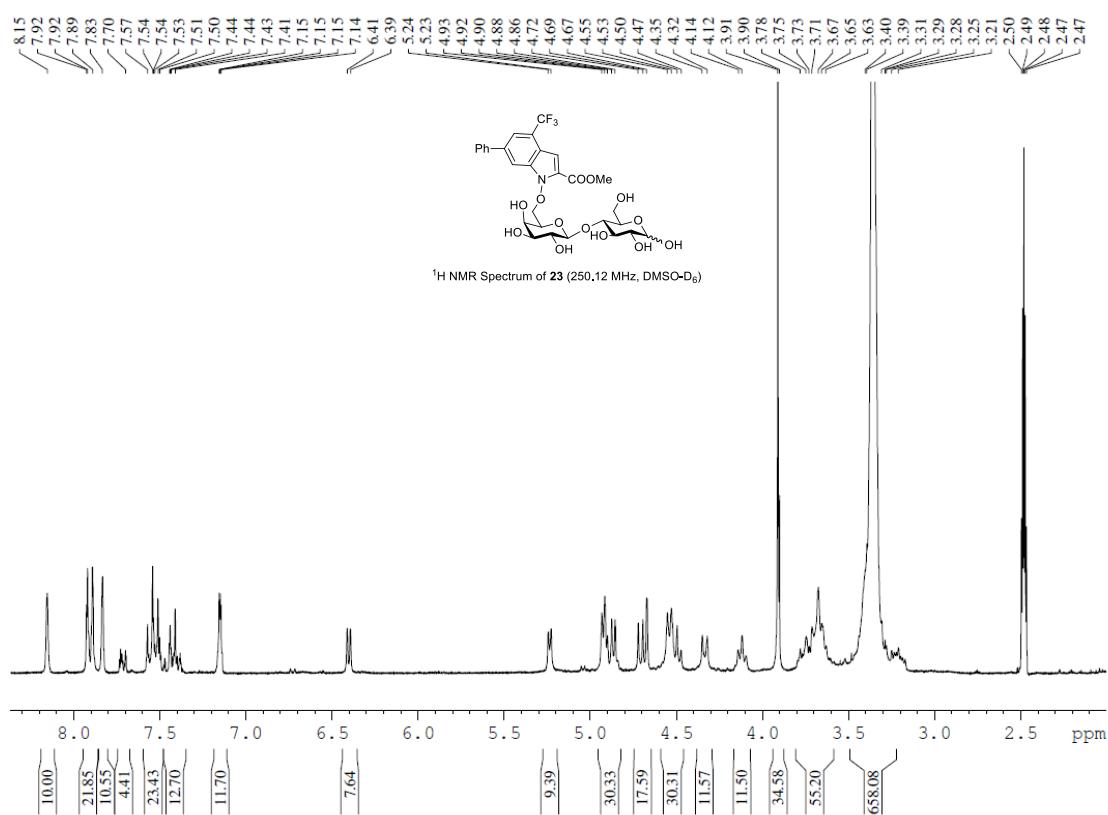
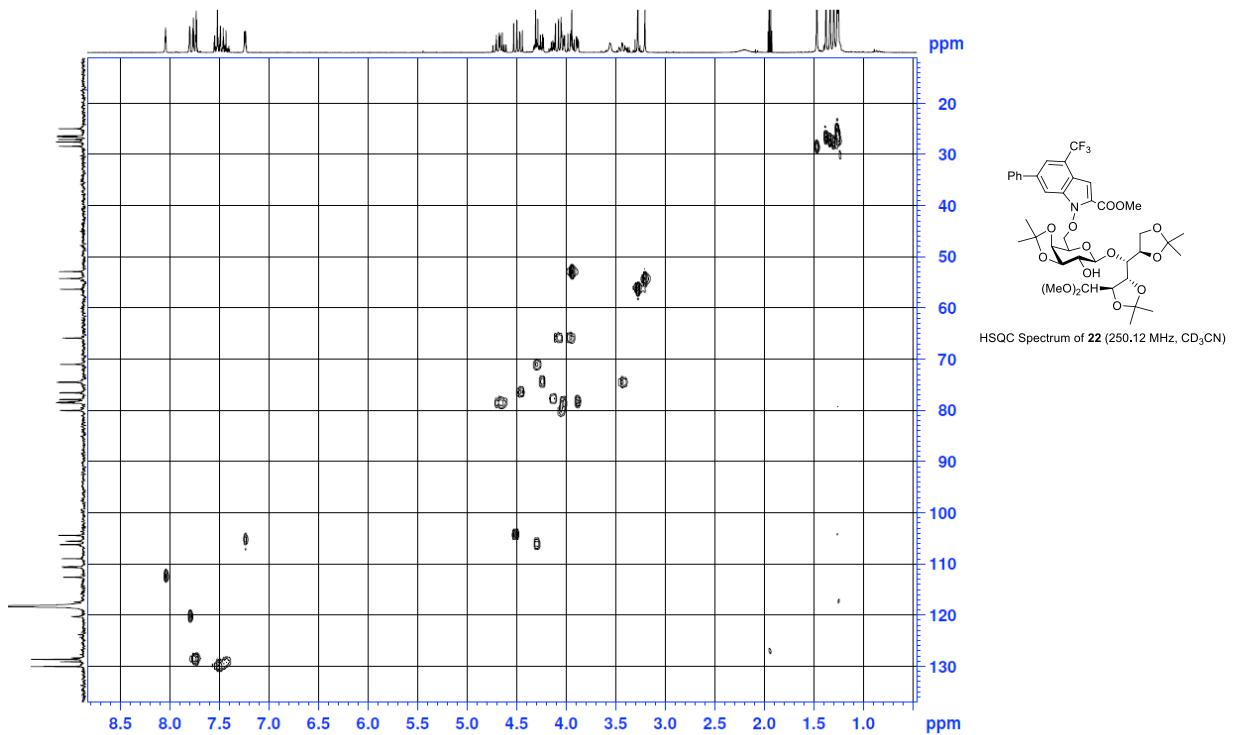


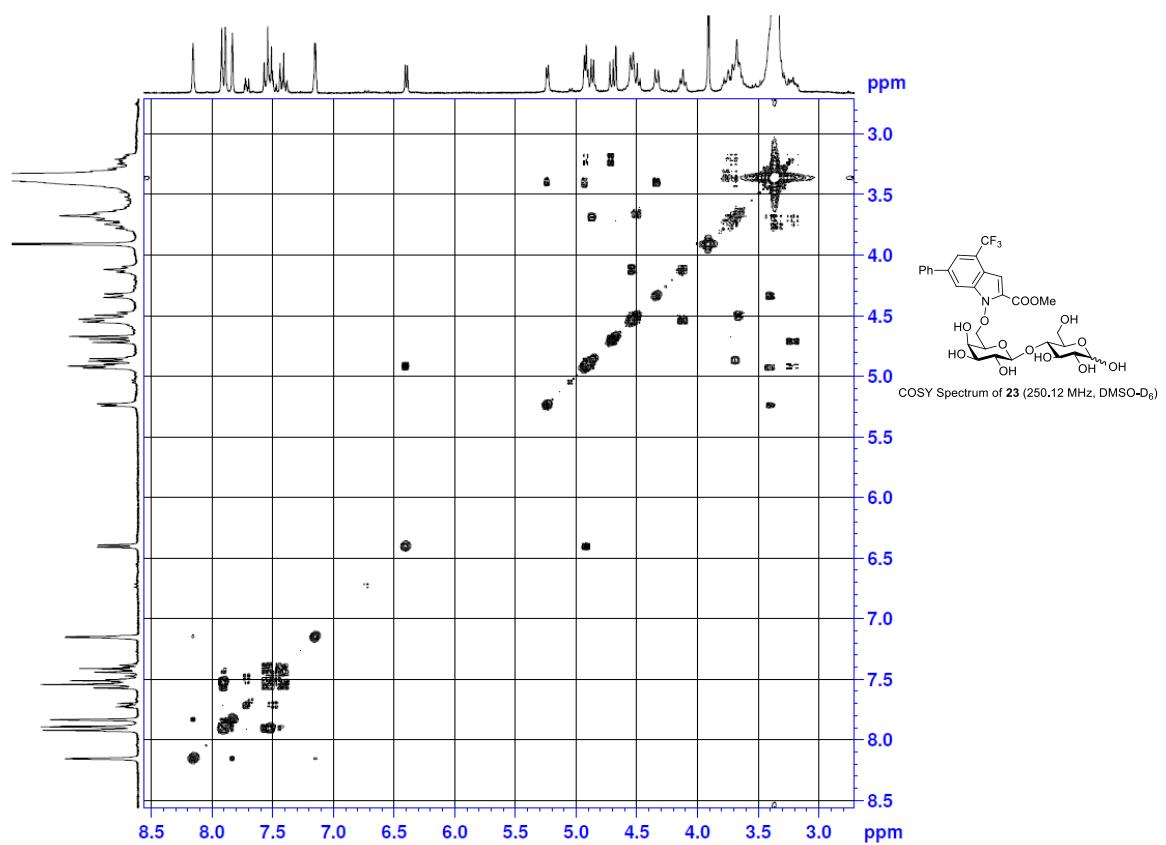
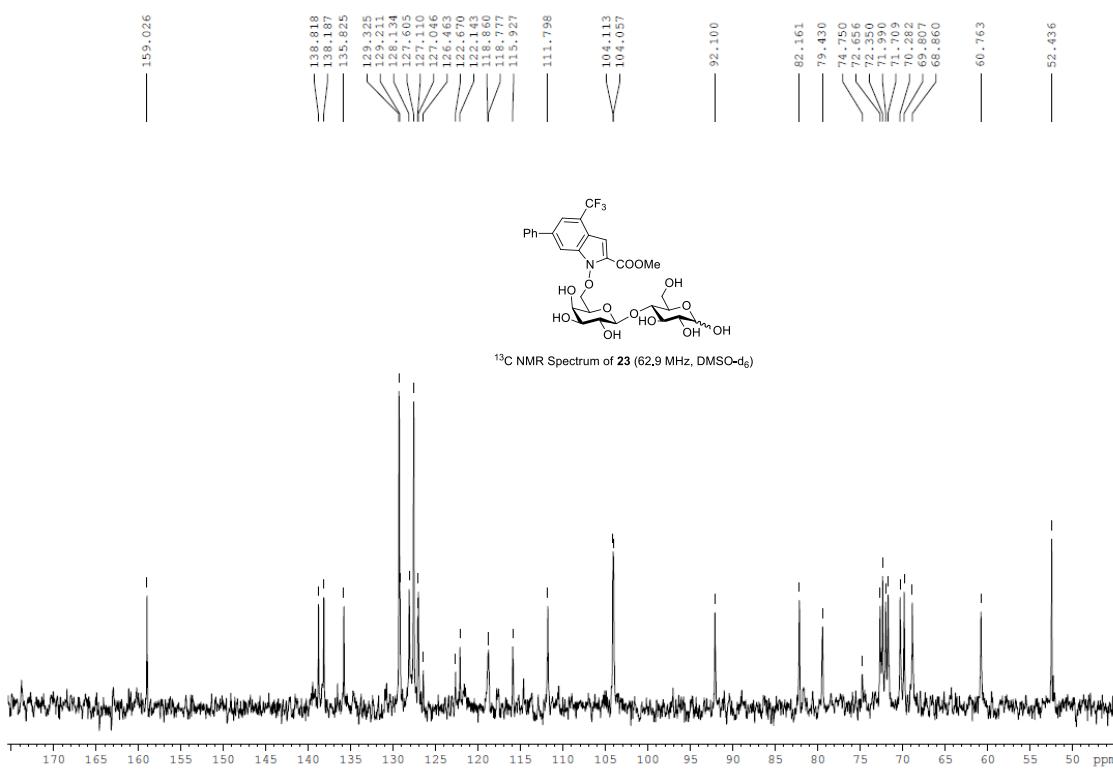












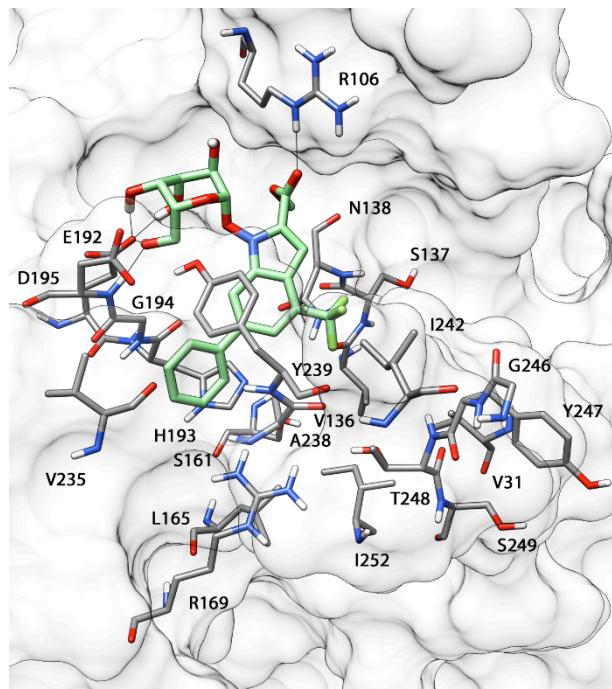


Figure S1. Binding disposition of **7 β** into *hLDH5*.

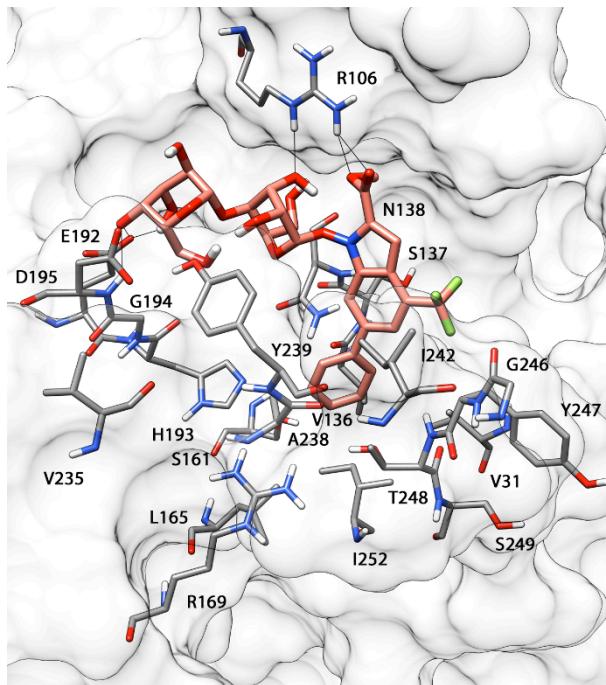


Figure S2. Binding disposition of **10 β** into *hLDH5*.

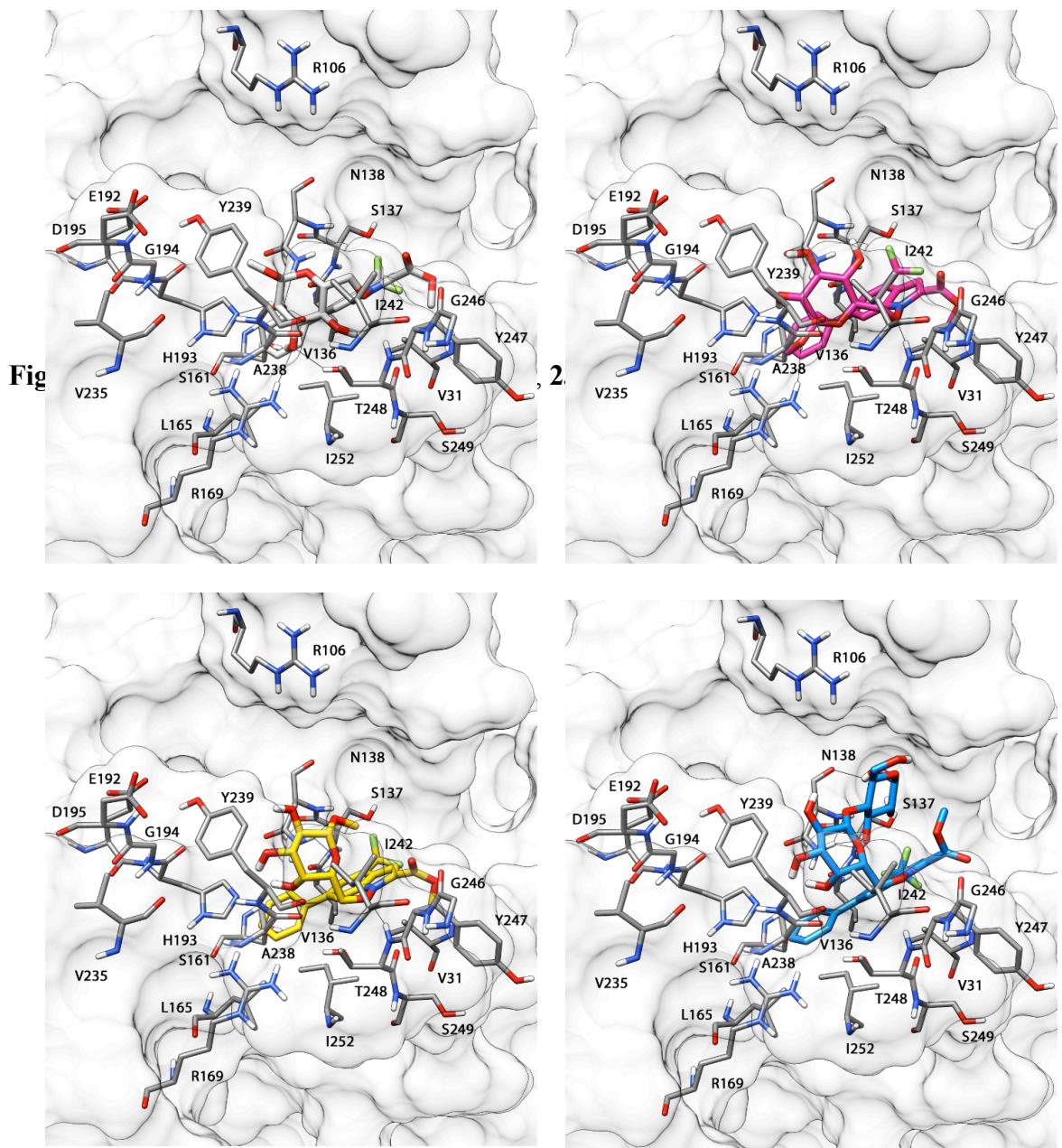


Figure S3. Binding disposition of **13**, **18**, **19** and **23** into *hLDH5*.