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Electronic Supplementary Information

A ^{19}F NMR Probe for the Detection of β-galactosidase: Simple Structure with Low Molecular Weight of 274.2, "Turn-on" Signal without the Background, and Good Performance applicable in Cancer Cell Line

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1. Calculation of the probe

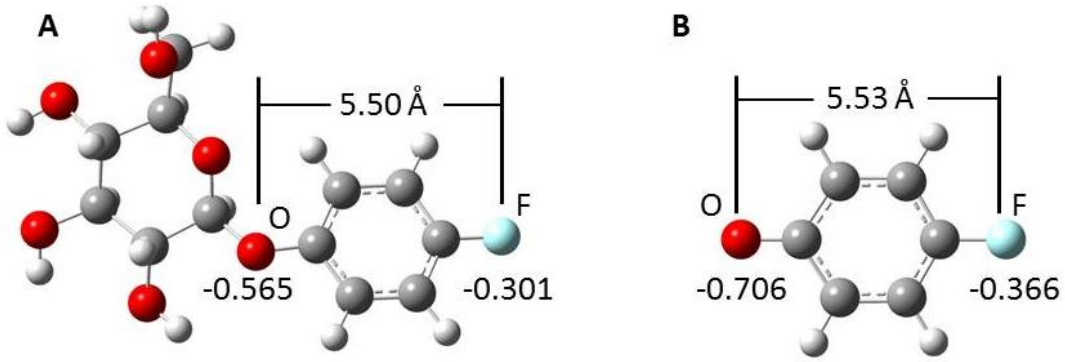

Figure S1. Mulliken charge of the fluorine and oxygen atoms and F-O distances in FB-βGal (A) and FB (B).

2. NMR and MS spectra

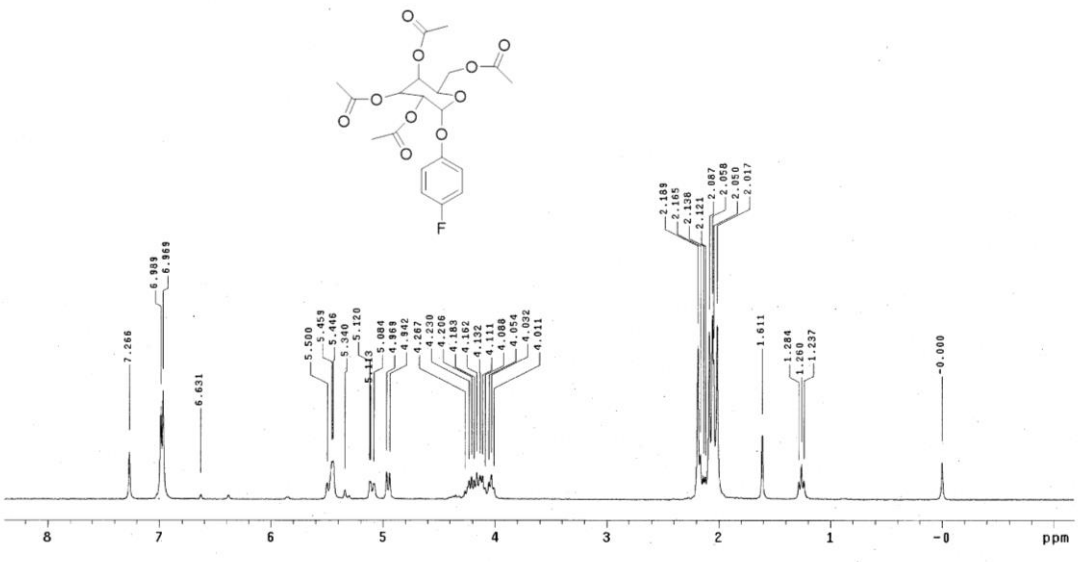

Figure S2. ^{1}H NMR spectrum of FB-βGalAc in 100% CD_2Cl_2 at 25 ℃.

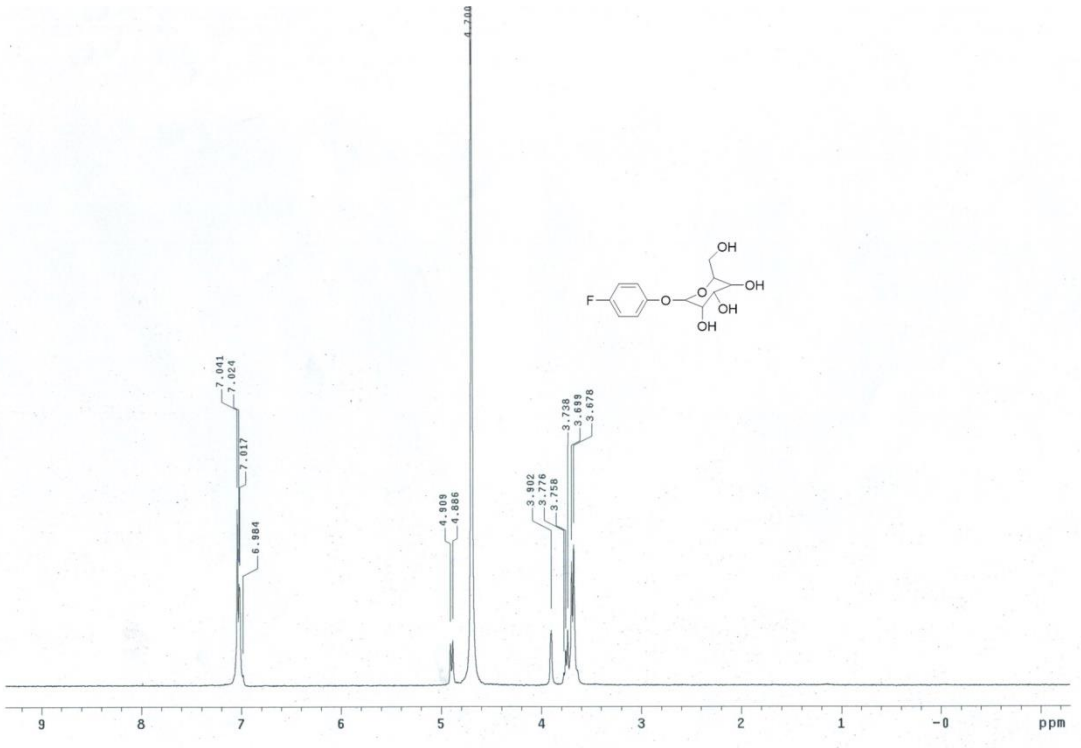

Figure S3. ^{1}H NMR spectrum of FB-βGal in 100% D_2O at 25 ℃.

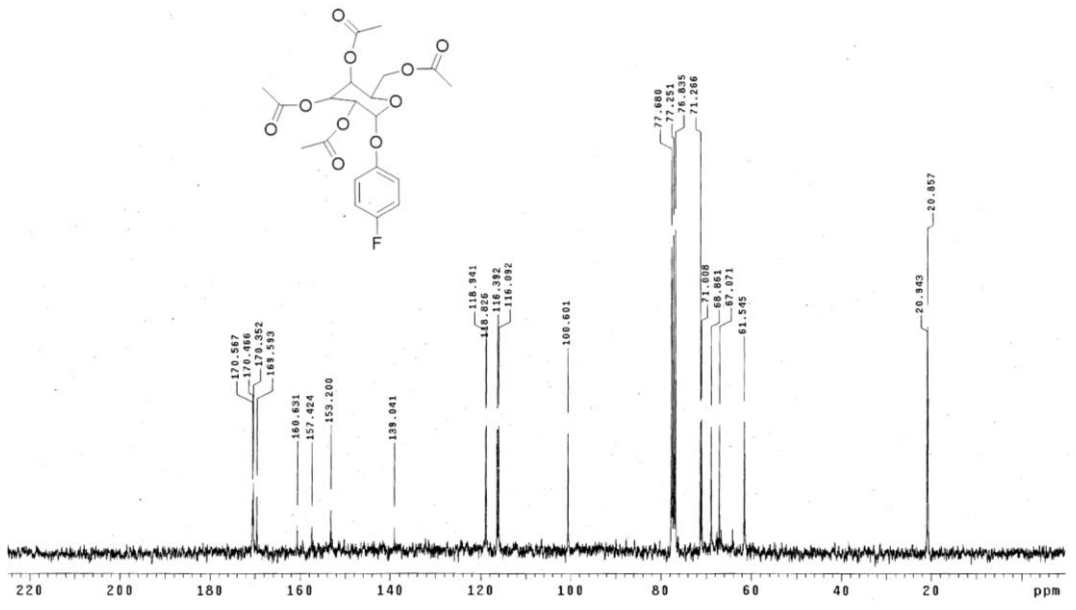

Figure S4. ^{13}C NMR spectrum of FB-βGalAc in 100% CD_2Cl_2 at 25 ℃.

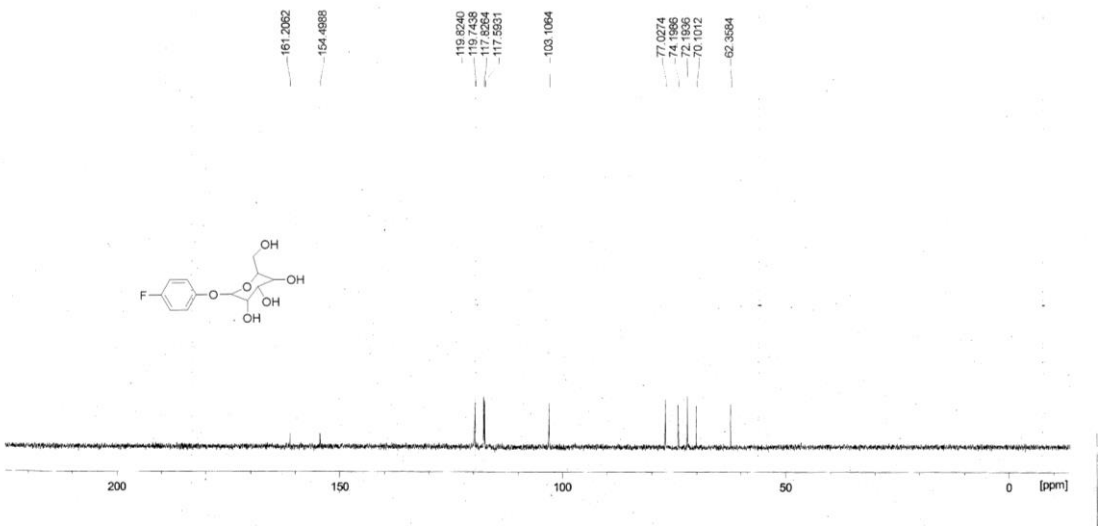

Figure S5. ^{13}C NMR spectrum of FB-βGal in 100% D_2O at 25 ℃.

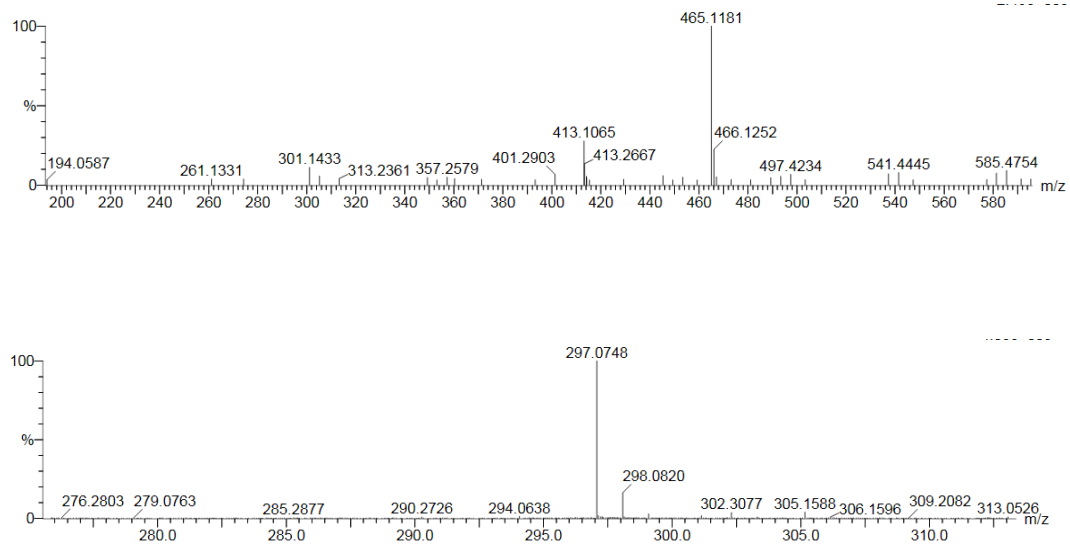

Figure S6. Mass analysis of FB-βGal and FB.

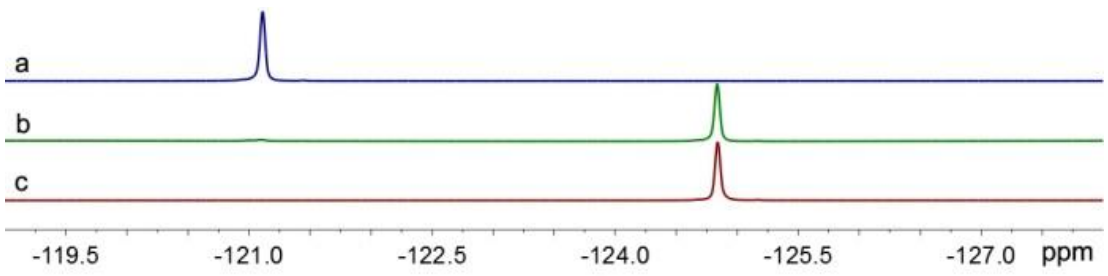

Figure S7. ^{19}F NMR spectra of (a) FB-βGal, (b) after the addition of βgal to the solution containing FB-βGal, and (c) FB.

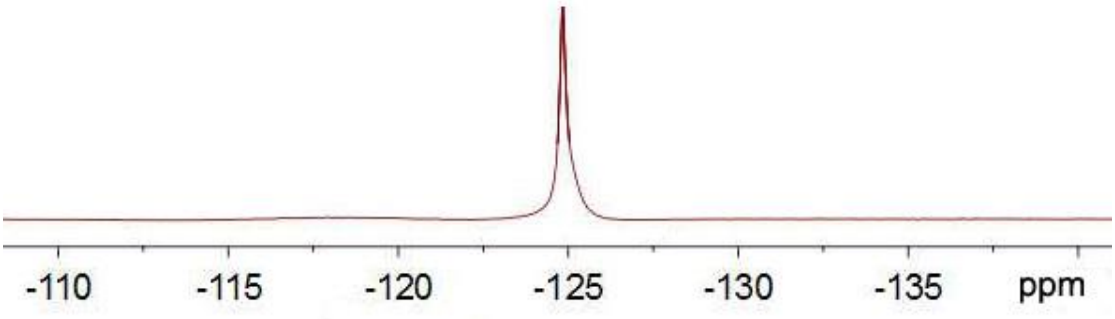

Figure S8. ^{19}F NMR spectrum which was obtained after the addition of FB-βGal at a very low concentration of 3.65×10^{-6} M in E.Coli overexpressedβ-gal within 2 minutes.

3. Toxicity test

Table S1. Toxicity text of FB-βGal to Hela cells and OVCAR-3 cells by MTT methods.

	1	2	3
Mdium DMEM	**0.098**	**0.116**	**0.099**
HeLa cells	**2.662**	**2.629**	**2.645**
HeLa cells + probe (2 mM)	**2.611**	**2.651**	**2.703**
HeLa cells + probe (4 mM)	**2.684**	**2.692**	**2,785**
Mdium 1640	**0.069**	**0.070**	**0.063**
OVCAR-3 cells	**2.196**	**2.151**	**2.148**
OVCAR-3 cells + probe (2mM)	**2.152**	**2.170**	**2.123**
OVCAR-3 cells + probe (4mM)	**2.190**	**2.224**	**2.164**

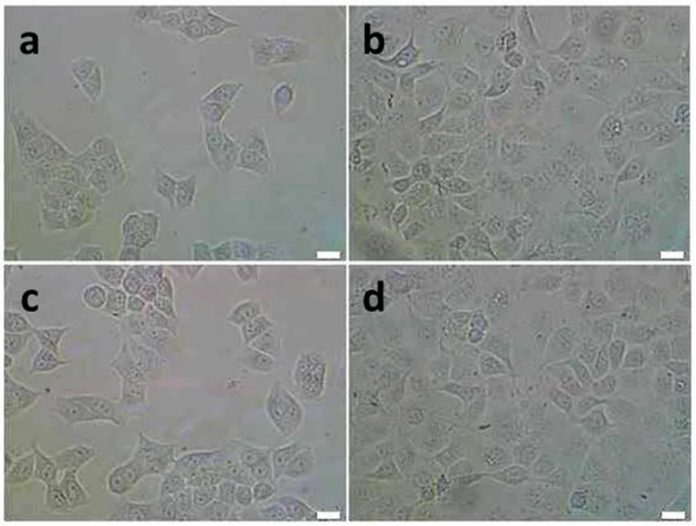

Figure S9. Images taken under daylight (a) HeLa cells (b) OVCAR-3 cells (c) HeLa cells incubated with FB-βGal (4nM) for 6 hours (d) OVCAR-3 cells incubated with FB-βGal (4 nM) for 6 hours. Scale bar: 20 μm.

4. Derivations of formulas

For ^{19}F NMR spectrum, the integral are the same when the F atoms are the same per mole. And derivations of these formulas are based on the assumption that the probe and β-gal reacted with the same amount .So

$$\frac{I_a}{C_0V\text{-}CV} = \frac{I_b}{CV}$$

The volume was always 500 μL. So

$$C= \frac{I_b C_0}{I_a+I_b}$$

The ratio value of the integral at -124.8 ppm to that at -121.1 ppm is

$$n= \frac{I_b}{I_a}$$

The equation becomes:

$$C= \frac{nC_0}{1+n}$$