3D DOSY

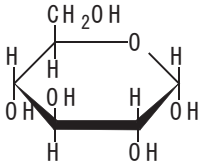
(Three Dimensional Diffusion-Ordered NMR Spectroscopy)

DOSY is a method for separating NMR spectra of mixture samples containing several molecular species by using the difference of diffusion coefficients of the individual species. The method can be extended to "3D-DOSY", where the diffusion coefficient axis is appended to usual 2D spectra, such as COSY, HMQC, and HMBC. The slice data of the 3D spectra with respect to the diffusion coefficient give the 2D spectra of the individual molecular species.

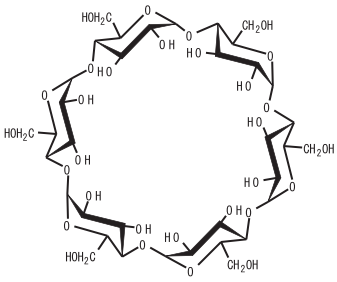
< Measurements for mixture of glucose and α-cyclodextrin >

Sample: Glucose 30mg, α-Cyclodextrin 30mg
Solvent: D_2O 400μl

Glucose
$C_6H_{12}O_6$
M.W.=180.16

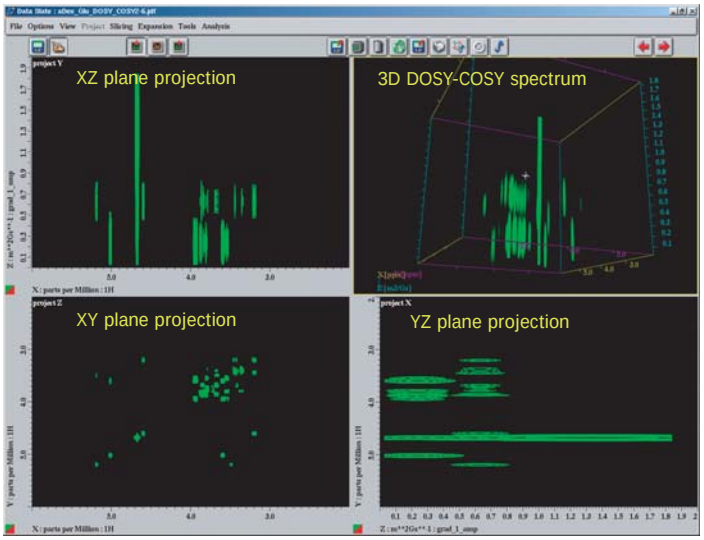


α-Cyclodextrin
$(C_6H_{10}O_5)_6$
M.W.=972.85

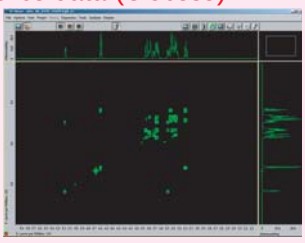


DOSY-COSY (BPP-STE-DOSY-COSY)

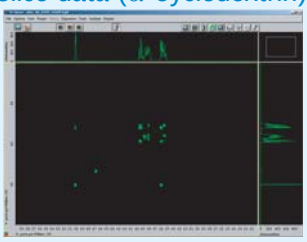
Spectrometer: ECA500, Measurement time: 15hour 50min, Diffusion parameters: δ=1.2ms, Δ=300ms, Field gradient: ~0.32T/m, DOSY process algorithm: SPLMOD



Slice data (Glucose)



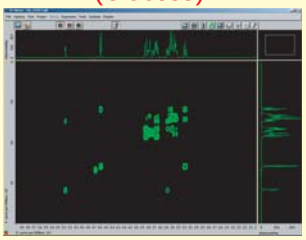
Slice data (α-Cyclodextrin)



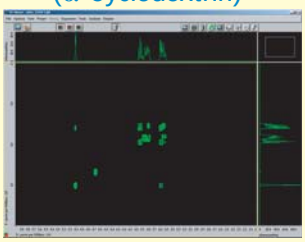
Reference data

Conventional 2D spectra observed for each compound of glucose and α-cyclodextrin

(Glucose)

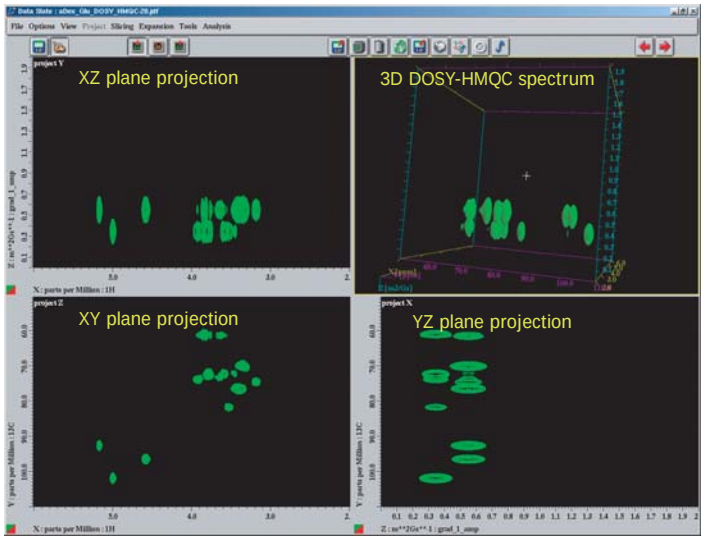


(α-Cyclodextrin)

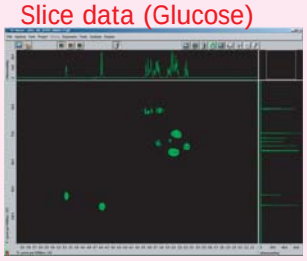


DOSY-HMQC (GC-STE-DOSY-HMQC)

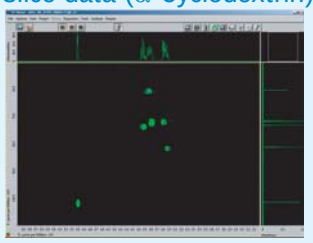
Spectrometer: ECX400, Measurement time: 51hour 51min, Diffusion parameters: δ=1.2ms, Δ=300ms,
Field gradient: ~0.33T/m, DOSY process algorithm: SPLMOD



Slice data (Glucose)

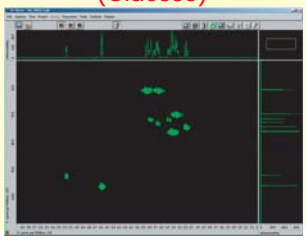


Slice data (α-Cyclodextrin)

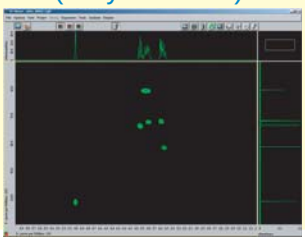


Reference data

(Glucose)

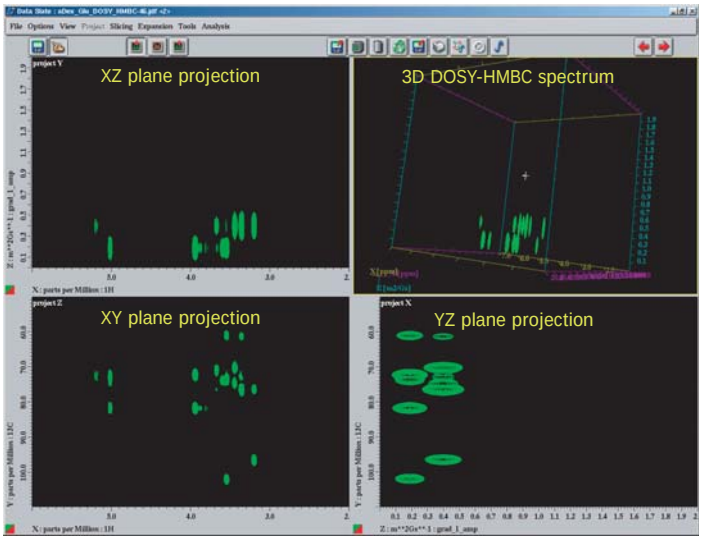


(α-Cyclodextrin)



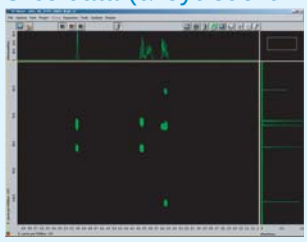
DOSY-HMBC (GC-STE-DOSY-HMBC)

Spectrometer: ECA500, Measurement time: 39hour 7min, Diffusion parameters: δ=1.2ms, Δ=300ms,
Field gradient: ~0.32T/m, DOSY process algorithm: SPLMOD



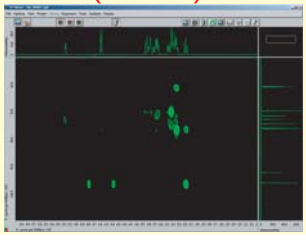
Slice data (Glucose)

Slice data (α-Cyclodextrin)



Reference data

(Glucose)



(α-Cyclodextrin)