

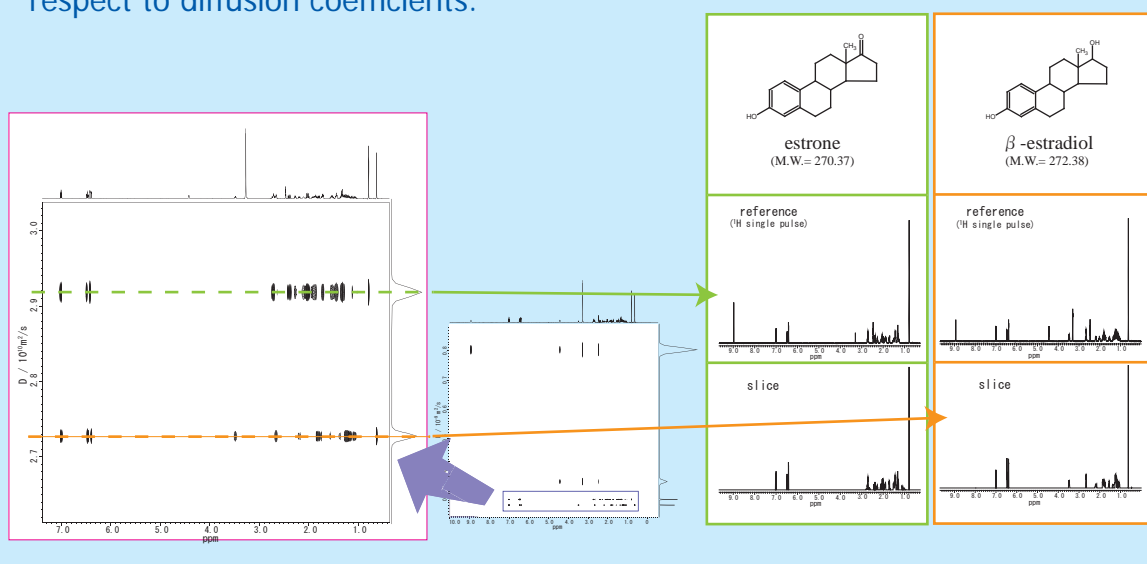
Excellent performance of DOSY processing

JEOL Delta software has high separation capability of DOSY (Diffusion Ordered Spectroscopy) spectra, which is realized by "Maxima" and "Scale" functions. "Maxima" function helps to robustly detect resonance peaks in a series of DOSY spectral data. "Scale" function reduces the distribution of diffusion coefficients evaluated from the peak intensities. These functions of Delta processing, together with high hardware ability of ECA/ECX spectrometers, demonstrate excellent performance in DOSY experiments. This Note shows three examples of DOSY spectra.

Example #1: Estrone and estradiol

NMR spectra of estrone and β -estradiol in a mixture sample are successfully separated by DOSY. Although these estrogens have similar molecular structures, a small difference of their molecular weights of 2 is sufficient to separate their spectra with respect to diffusion coefficients.

Spectrometer: JNM-ECX400
Probe: TH5AT/FG2
Solvent: DMSO-d₆
Method: BPP-STE-LED
Scans: 32
Diffusion time (Δ): 200ms
Gradient pulse width (δ): 2.6ms
Gradient strength (G): 10-330mT/m (16steps)
Software: Delta ver.4.3.4
DOSY algorithm: SPLine MODEL

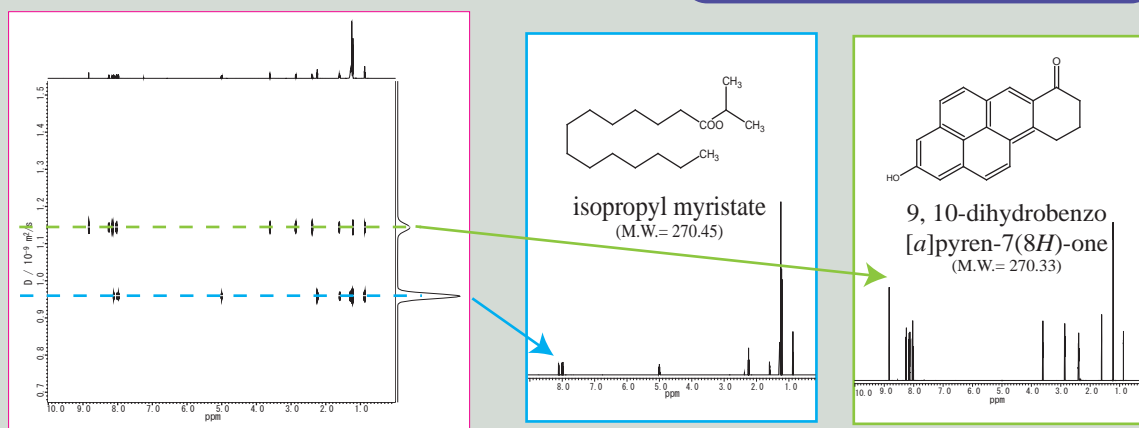


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Example #2: Compounds having almost the same molecular weight

Although isopropyl myristate and dihydrobenzo pyren have almost the same molecular weight, their geometrical shapes and interactions with solvent may differ, giving separated spectra.

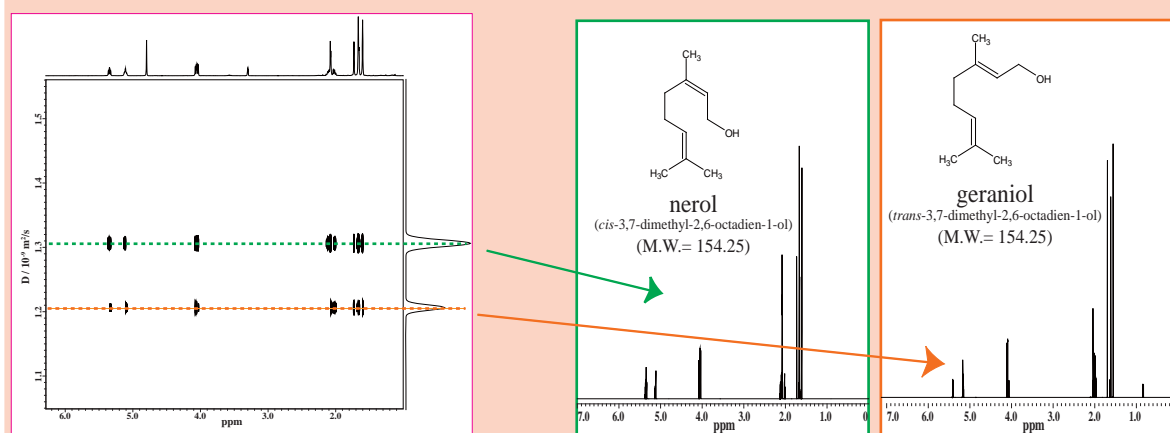
Spectrometer: JNM-ECA700
 Probe: TH5AT/FG2
 Solvent: CDCl₃
 Method: BPP-STE-LED
 Scans: 32
 Diffusion time (Δ): 200ms
 Gradient pulse width (δ): 1.4ms
 Gradient strength (G): 10-300mT/m (16steps)
 Software: Delta ver.4.3.4
 DOSY algorithm: SPLine MODel



Example #3: *cis* and *trans* isomers

A mixture sample of *cis* and *trans* isomers, nerol and geraniol, is separated by DOSY. These isomers have different effective volumes, leading to different diffusion coefficients.

Spectrometer: JNM-ECAX400
 Probe: TH5AT/FG2
 Solvent: Methanol-d₆
 Method: BPP-STE-LED
 Scans: 64
 Diffusion time (Δ): 100ms
 Gradient pulse width (δ): 1.8ms
 Gradient strength (G): 10-300mT/m (32steps)
 Software: Delta ver.4.3.5
 DOSY algorithm: SPLine MODel



(2/2)