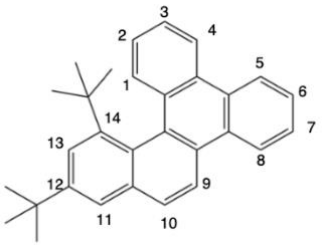
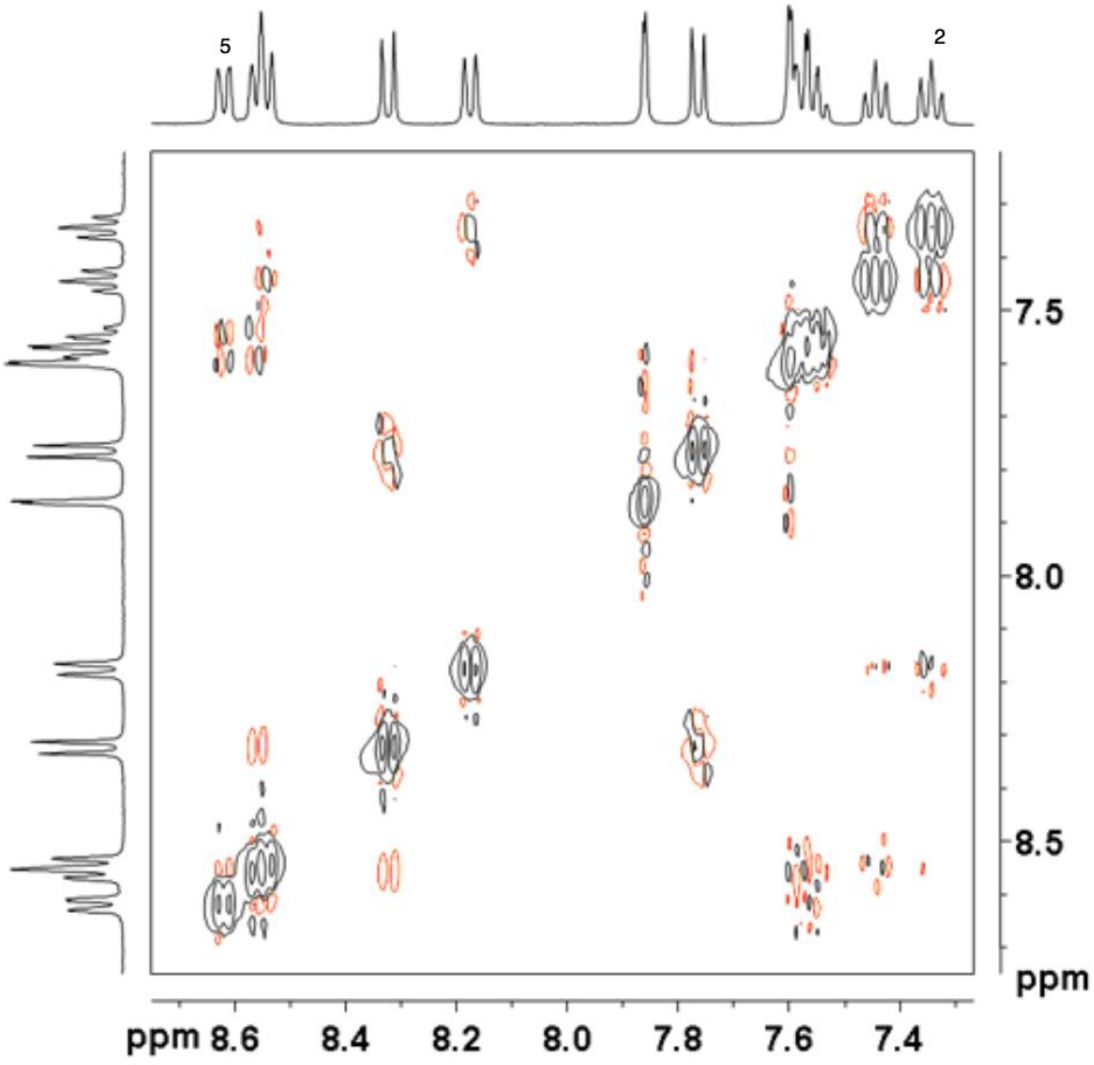
CH-314 Structural Analysis
ruben.rodriguezmadrid@epfl.ch
ray.cowen@epfl.ch

Jigsaw 4B

2D NMR: NOESY and EXSY

1. The 2D NOESY (Nuclear Overhauser Effect SpectroscopY) experiment gives information on through-space interactions, which can be used to identify protons which are close in space. Below, you have the aromatic region of the ^{1}H 2D NOESY spectrum of 12,14-di^{t}butylbenzo[g]chrysene. Assign the different aromatic ^{1}H peaks.





2. [Week 3 Slides 71−80] Consider the EXSY spectrum of a symmetrical 2 spin (A and B) system. The intensity of the four peaks are given by the following equations:

$$I_{AA}(\tau_m) = \frac{1}{2}[1 + \exp(-2k\tau_m)]\exp(-\tau_m/T_1)M_{A0}$$
$$I_{BB}(\tau_m) = \frac{1}{2}[1 + \exp(-2k\tau_m)]\exp(-\tau_m/T_1)M_{B0}$$
$$I_{AB}(\tau_m) = \frac{1}{2}[1 - \exp(-2k\tau_m)]\exp(-\tau_m/T_1)M_{B0}$$
$$I_{BA}(\tau_m) = \frac{1}{2}[1 - \exp(-2k\tau_m)]\exp(-\tau_m/T_1)M_{A0}$$

   a. Draw the 2D EXSY spectrum, taking into account the relative intensity of diagonal and cross peaks, at the following values of $k\tau_m$:

i. $k\tau_m = 0$ ii. $k\tau_m \ll 1$ iii. $k\tau_m \approx 2$ iiv. $k\tau_m \gg 2$

   b. For each plot in (a), explain what is happening to the peak intensity and why.

   c. 2D exchange spectroscopy is used to determine exchange in which motion regime? Explain why.