## Measuring methods available and examples of their applications

## 2D HSQC (Heteronuclear Single-Quantum Correlation spectroscopy)

The 2D HSQC experiment permits to obtain a 2D heteronuclear chemical shift correlation map between directly-bonded <sup>1</sup>H and X-heteronuclei (usually <sup>13</sup>C or <sup>15</sup>N). It is widely used because it is based on proton-detection, offering high sensitivity.

HSQC detects correlations between nuclei of two different types which are separated by one bond. This method gives one peak per pair of coupled nuclei, whose two coordinates are the chemical shifts of the two coupled atoms. HSQC works by transferring magnetization from the proton to the other nucleus (the heteroatom) using the <u>INEPT</u> pulse sequence.



Fig. 1. Strychnine nitrate in DMSO-D6, <sup>1</sup>H-<sup>13</sup>C-HSQC phase-sensitive experiment with assignment. Spectrometer: AVANCE III HD 700, Probehead: 5 mm Inverse Broadband with z-Gradients, Experiment time: 14 min



Fig. 2. Vinorelbin tartrate , 20 mM in DMSO-d6 gradient HSQC, Spectrometer: AVANCE III 500, Probehead: 5 mm CPPBBO (Prodigy) with z gradients, Experiment time: 50 min

## 2D HSQC multiplicity edited

The **2D multiplicity-edited HSQC experiment** is a simple and popular modification of the <u>gradient</u> <u>enhanced 2D HSQC experiment</u> in which carbon multiplicity can be directly extracted from the resulting spectra in addition to the conventional heteronuclear correlations by simple analysis of the cross-peaks sign.



Fig. 3. Strychnine nitrate in DMSO-D6, phase-sensitive 2D <sup>1</sup>H-<sup>13</sup>C-HSQC multiplicity- edited experiment with assignment. Spectrometer: AVANCE III HD 700, Probehead: 5 mm Inverse Broadband with z-Gradients, Experiment time: 14 min