



Figure 1. Principle of operation of the HPLC-UV/MS-SPE-NMR instrument: 1) separation of the sample was performed by reversed-phase HPLC, 2) chromatographic peaks were detected using a photodiode array detector in-line with an ion trap mass spectrometer and the peaks of interest trapped on solid-phase extraction (SPE) cartridges after dilution of the HPLC eluate with water, 3) the loaded SPE cartridges were nitrogen dried and the analytes transferred to a 600 MHz NMR spectrometer using CD_3CN .

Abbreviation List

MeOH	methanol
XAD-2	chromatography resin
LH-20	chromatography resin
LC	liquid chromatography
RP	reverse-phase
RT	retention time
UV	ultra violet
MW	molecular weight
MS	mass spectrometry
APCI	Atmospheric pressure chemical ionization
ESI	electrospray ionisation
MS/MS	tandem mass spectrometry
m/z	mass-to-charge ratio
NMR	nuclear magnetic resonance
SPE	solid phase extraction

CD ₃ CN	deuterated acetonitrile
Hz	Hertz
MHz	mega hertz
ppm	parts per million
δ_{H}	proton chemical shift
δ_{C}	carbon chemical shift
J	coupling constant
m	multiplicity
COSY	¹ H- ¹ H Correlation SpectroscopY experiment
HSQC	Heteronuclear Single Quantum Correlation experiment
HMBC	Heteronuclear Multiple Bond Correlation experiment
TOCSY	TOtal Correlation SpectroscopY experiment
NOESY	multiple presaturation 1D Nuclear Overhauser Effect SpectroscopY

