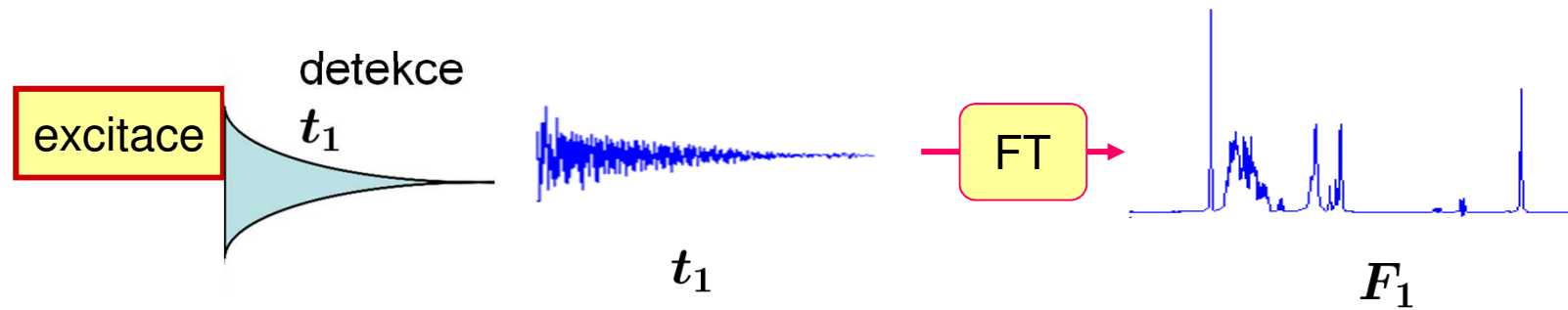


2D spektroskopie

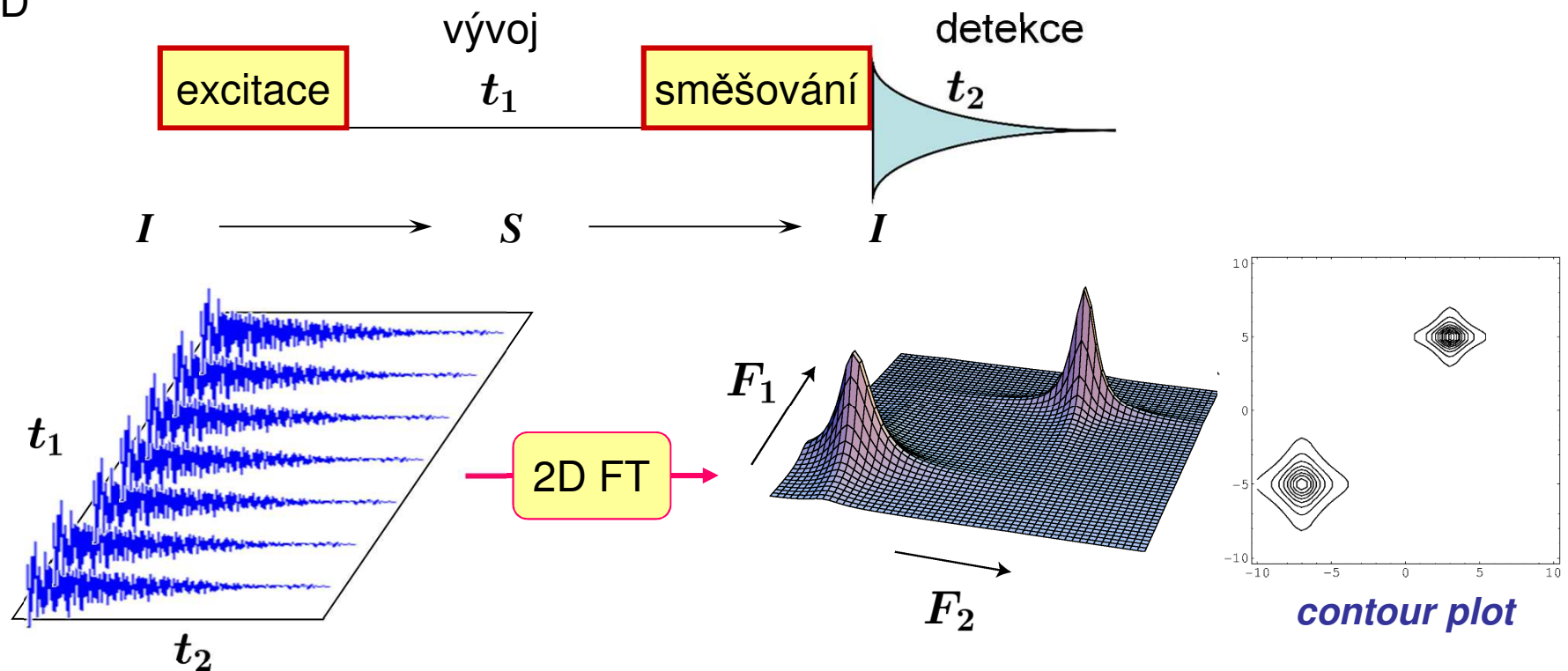
Použití experimentů COSY, HSQC/HMQC, HMBC
a NOESY

Princip 2D experimentů

1D



2D



Základní 2D experimenty

Homonukleární

COSY, NOESY

Heteronukleární

HSQC, HMQC, HMBC

Informace o spojení chemickými vazbami

COSY, HSQC, HMQC, HMBC

J interakce

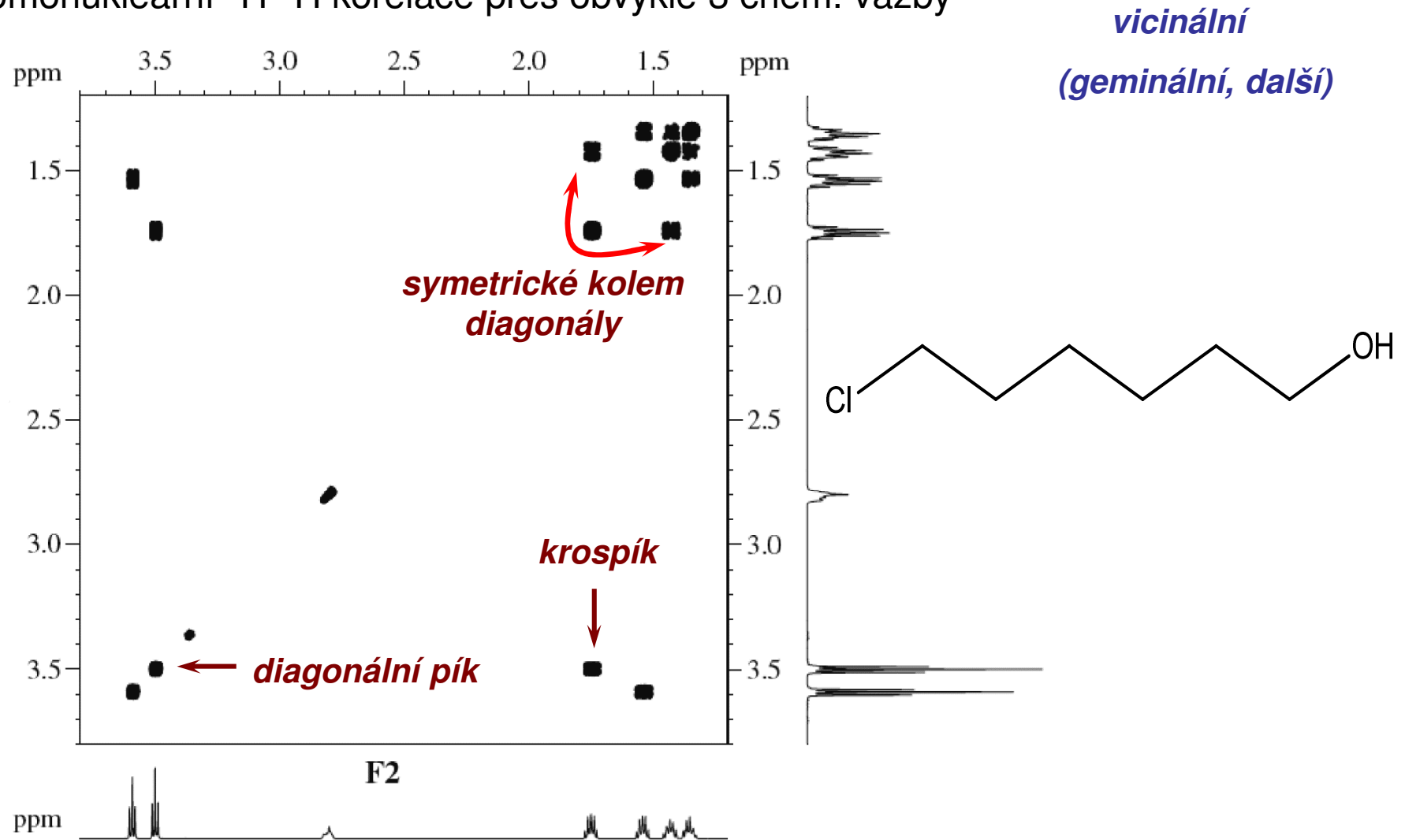
Informace o blízkosti v prostoru

NOESY

***přímá dipól-dipólová
interakce***

Experiment COSY

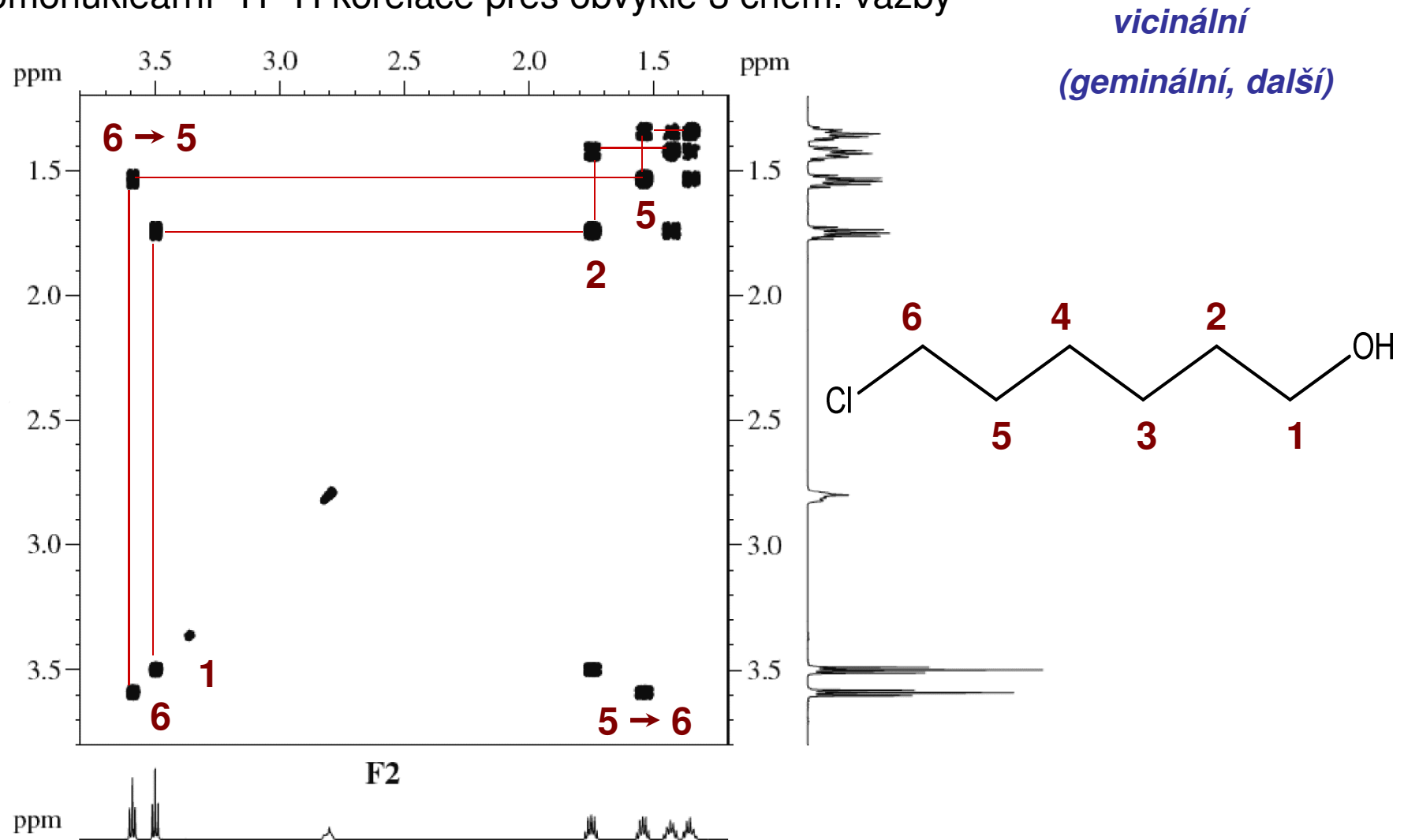
homonukleární ^1H - ^1H korelace přes obvykle 3 chem. vazby



krospík = existuje J vazba mezi danými vodíky, vidíme jen „přímé sousedy“

Experiment COSY

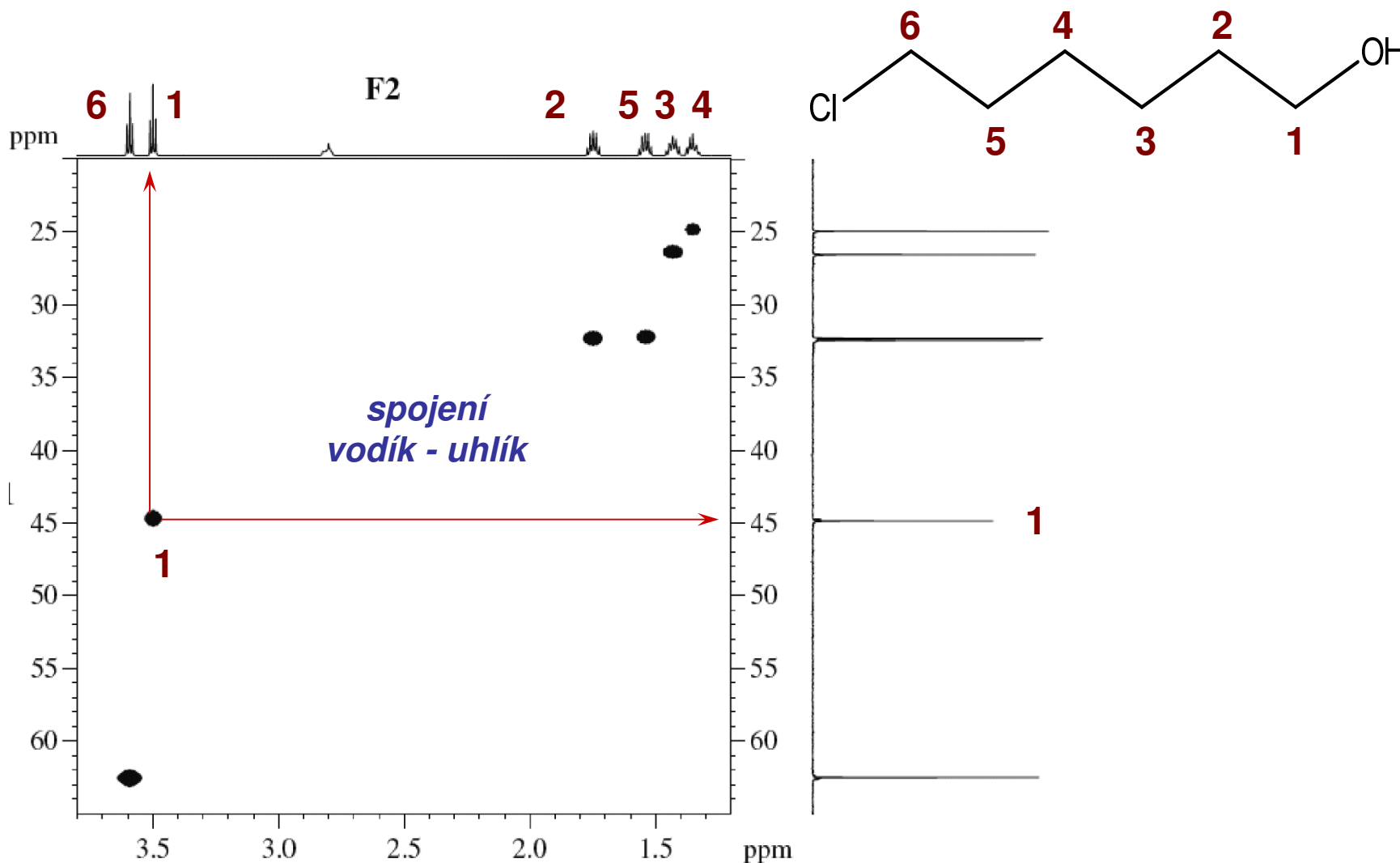
homonukleární ^1H - ^1H korelace přes obvykle 3 chem. vazby



krospík = existuje J vazba mezi danými vodíky, vidíme jen „přímé sousedy“

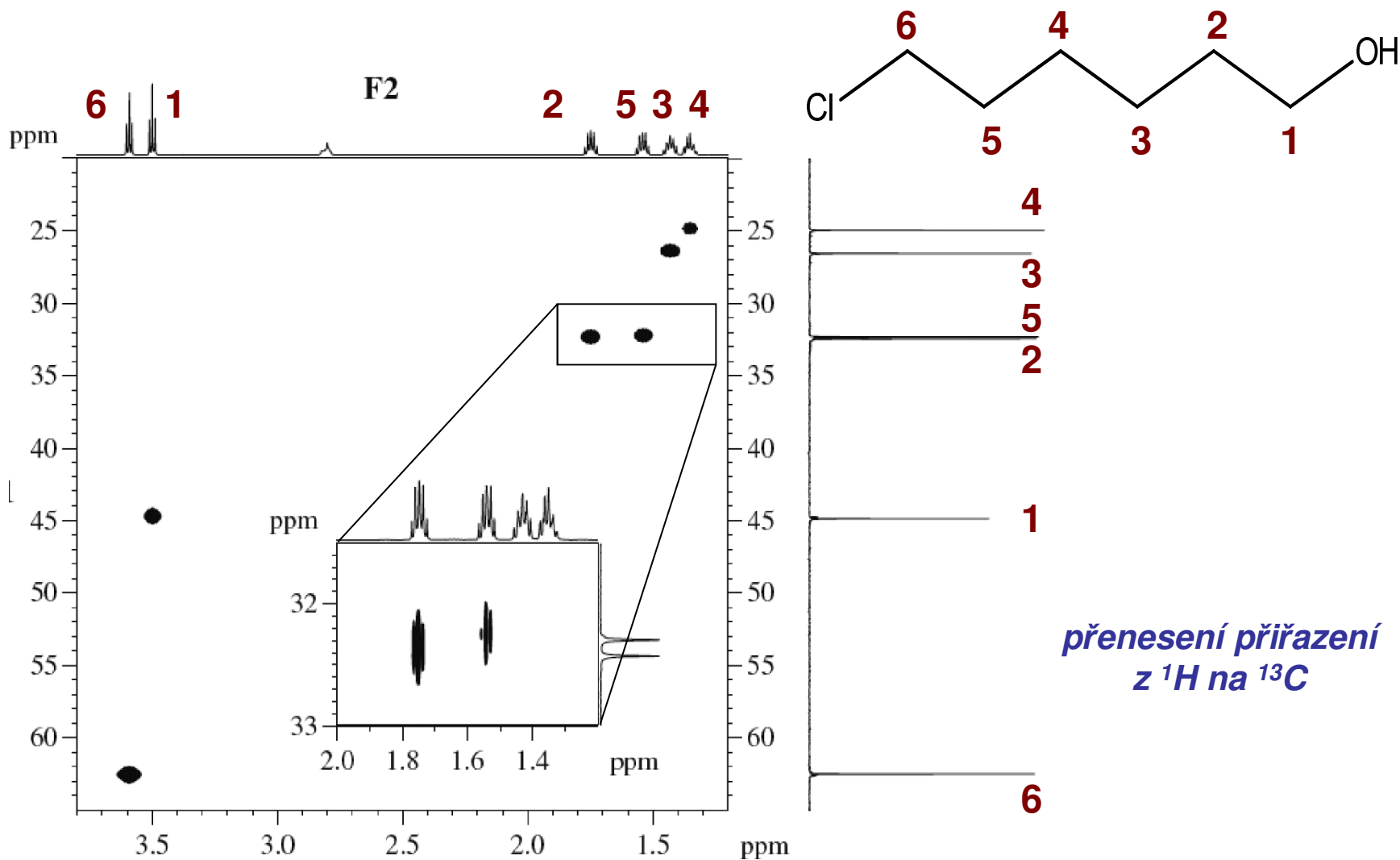
Experimenty HSQC a HMQC

heteronukleární ^1H - ^{13}C korelace přes jednu chem. vazbu



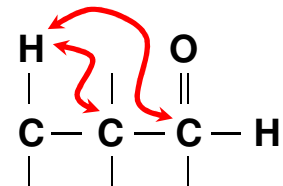
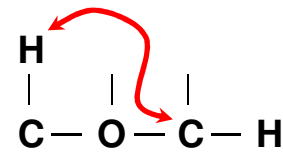
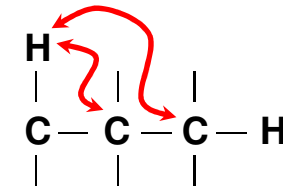
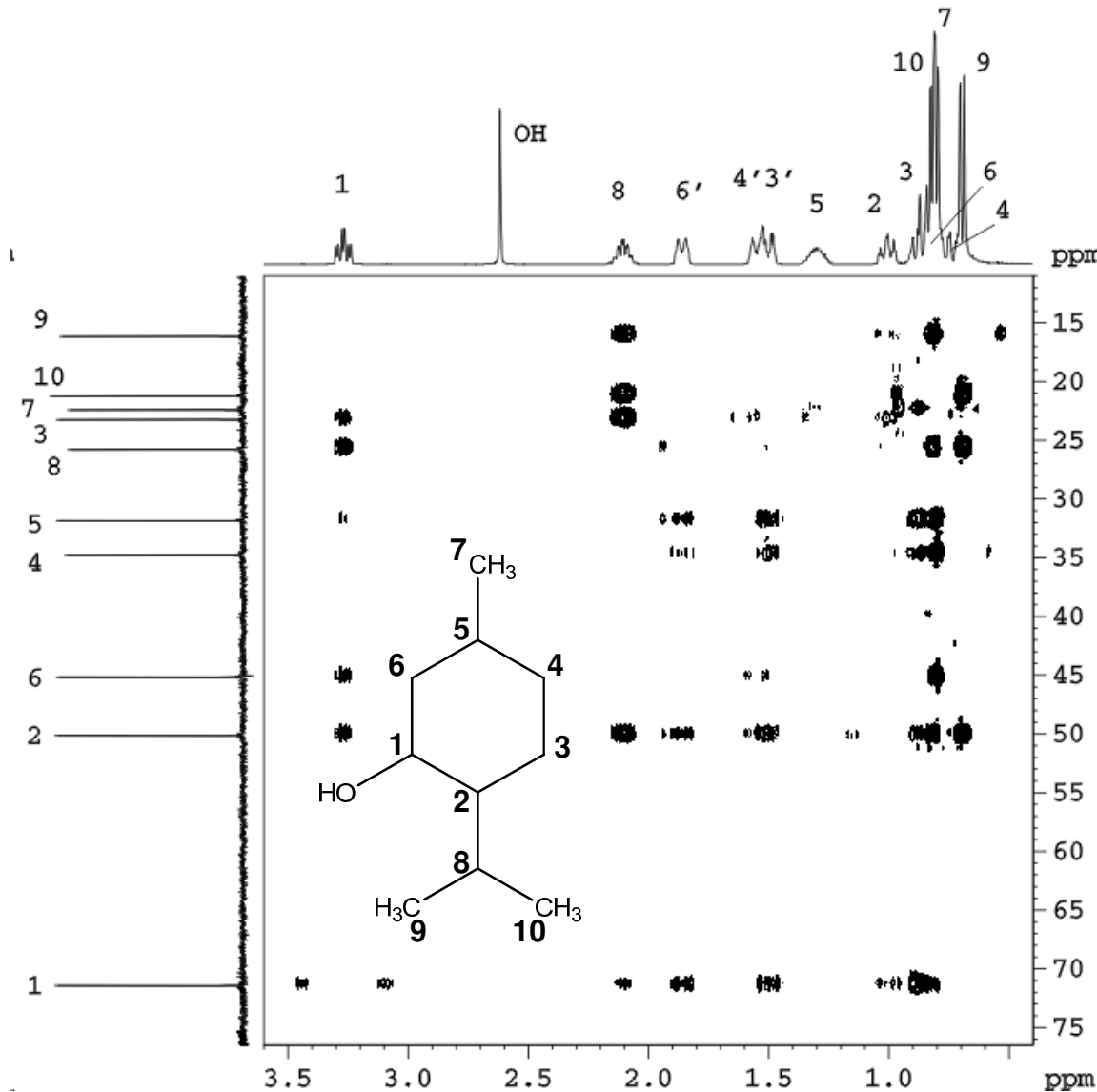
Experimenty HSQC a HMQC

heteronukleární ^1H - ^{13}C korelace přes jednu chem. vazbu



Experiment HMBC

heteronukleární ^1H - ^{13}C korelace přes „2 a více“ chem. vazeb

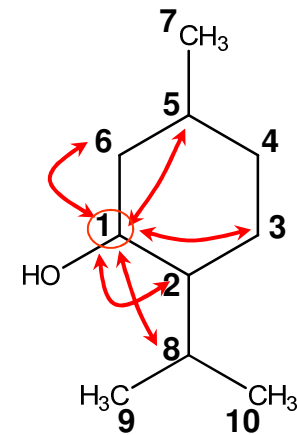
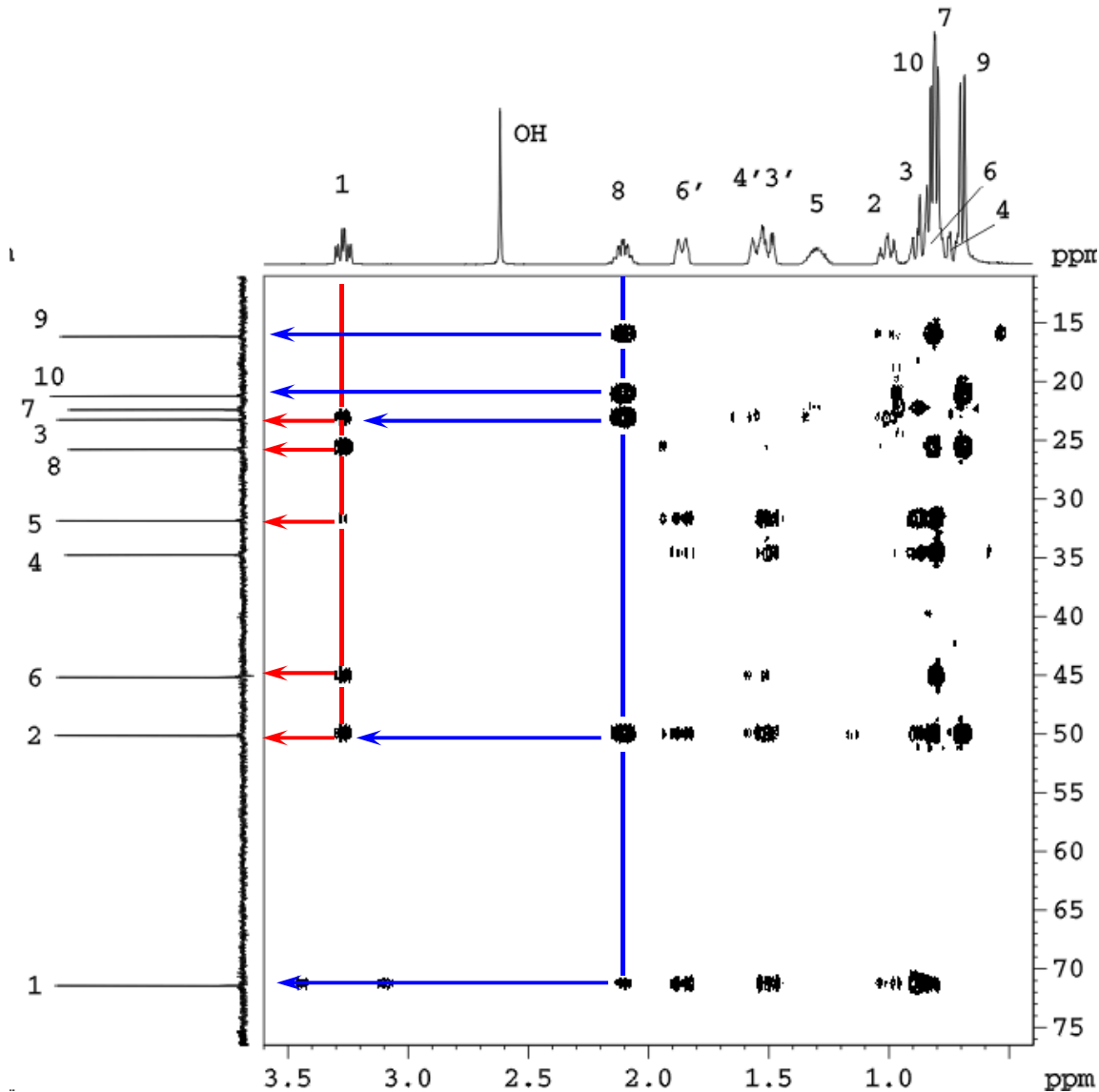


*vodík vidí sousední uhlíky,
vidí skrz hetero-atomy*

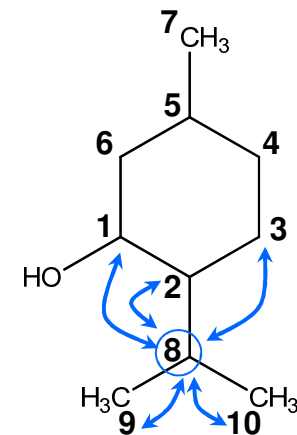
*přiřazení kvarterních ^{13}C
ověření propojení*

Experiment HMBC

heteronukleární ^1H - ^{13}C korelace přes „2 a více“ chem. vazeb

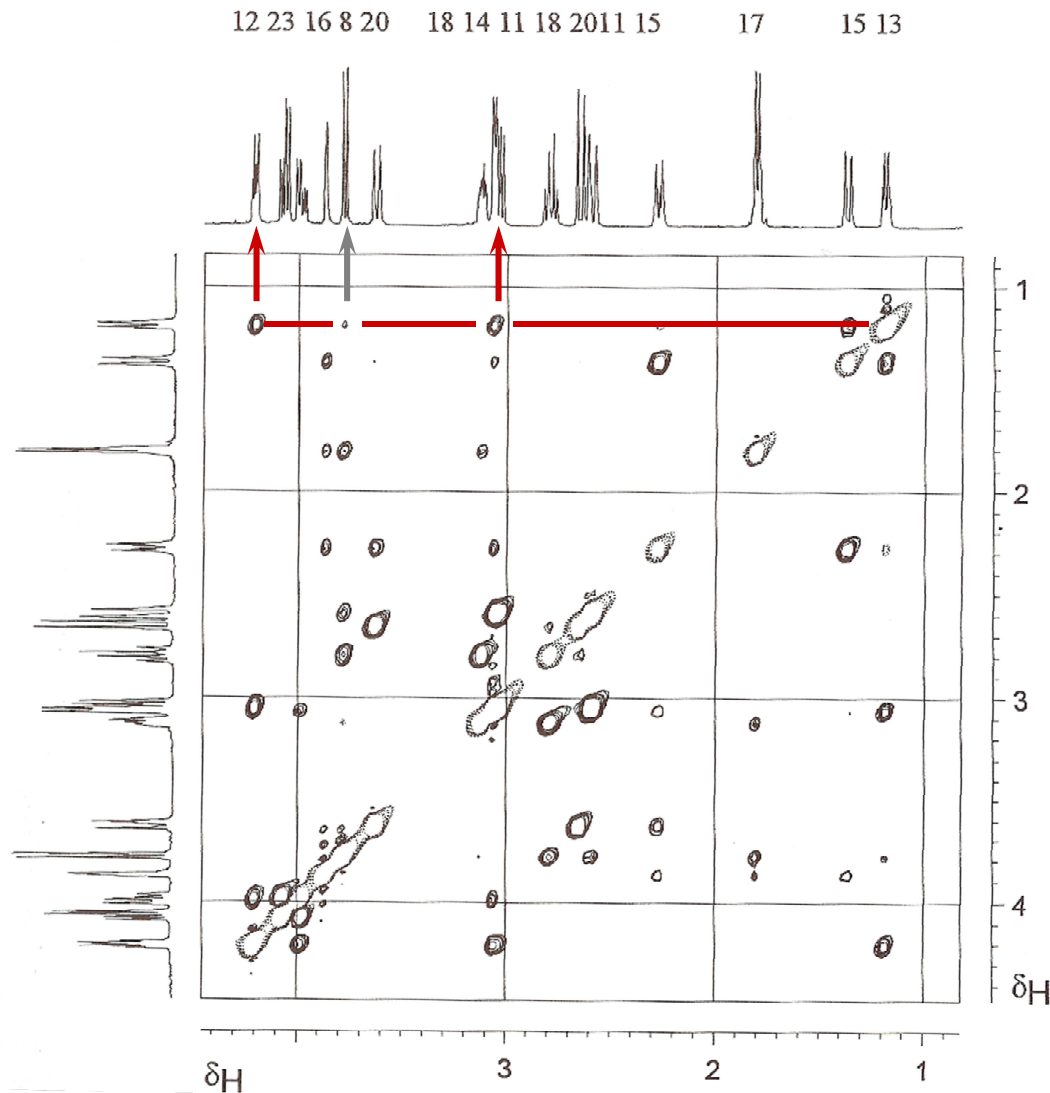


menthol

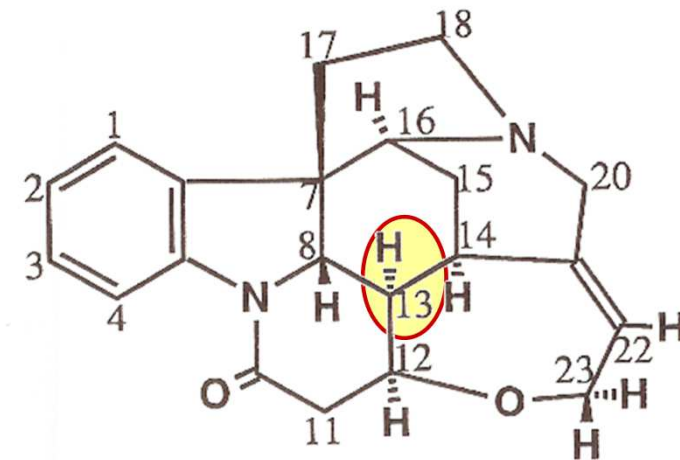


Experiment NOESY

homonukleární ^1H - ^1H korelace přes prostor



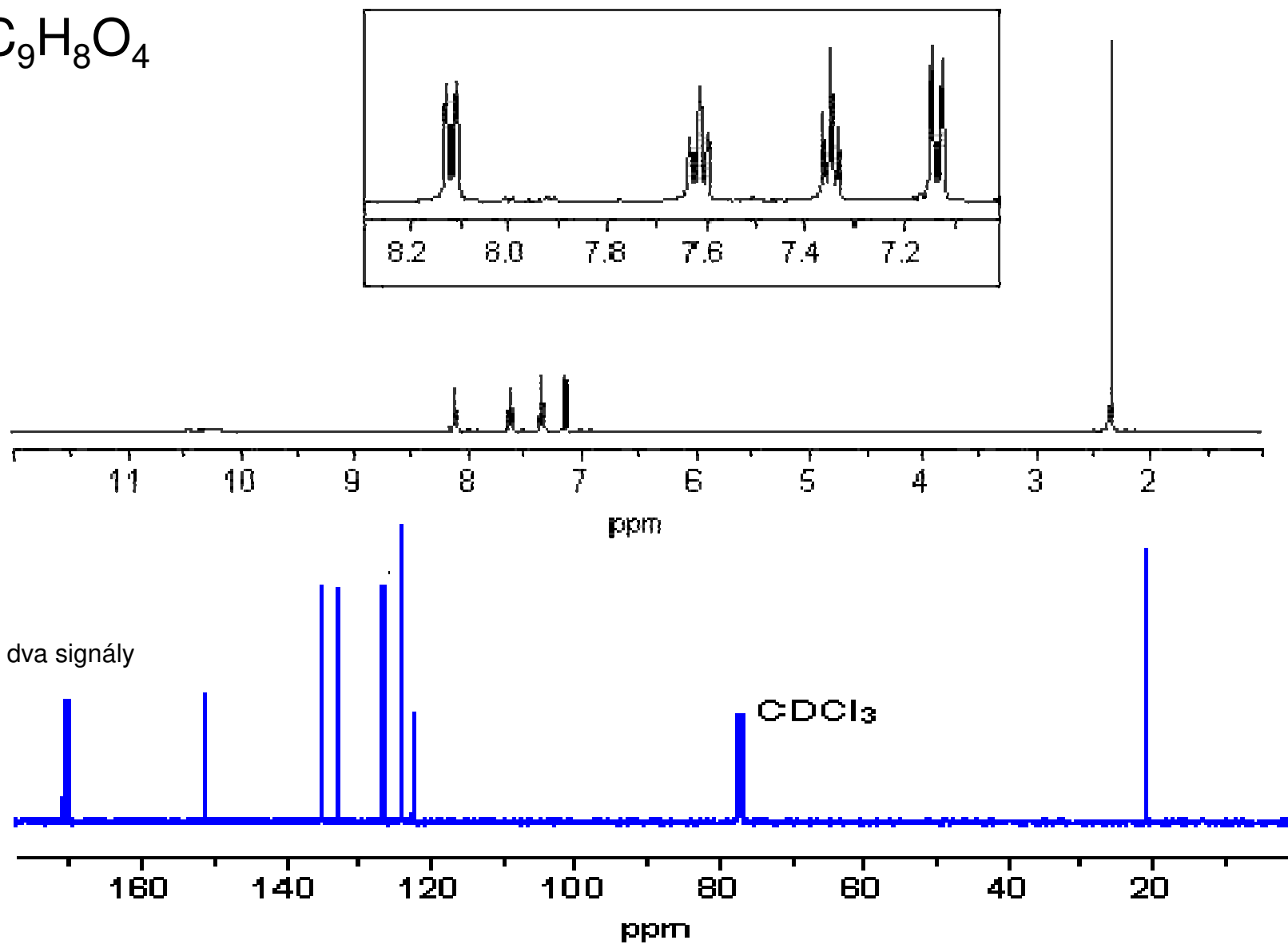
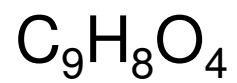
*krospík -
- dané vodíky jsou si blízké v prostoru
(do cca 5 Angströmů)*



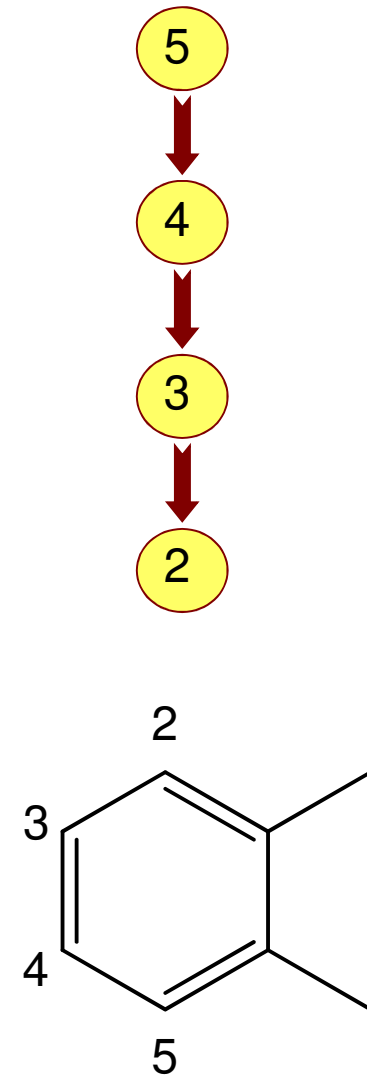
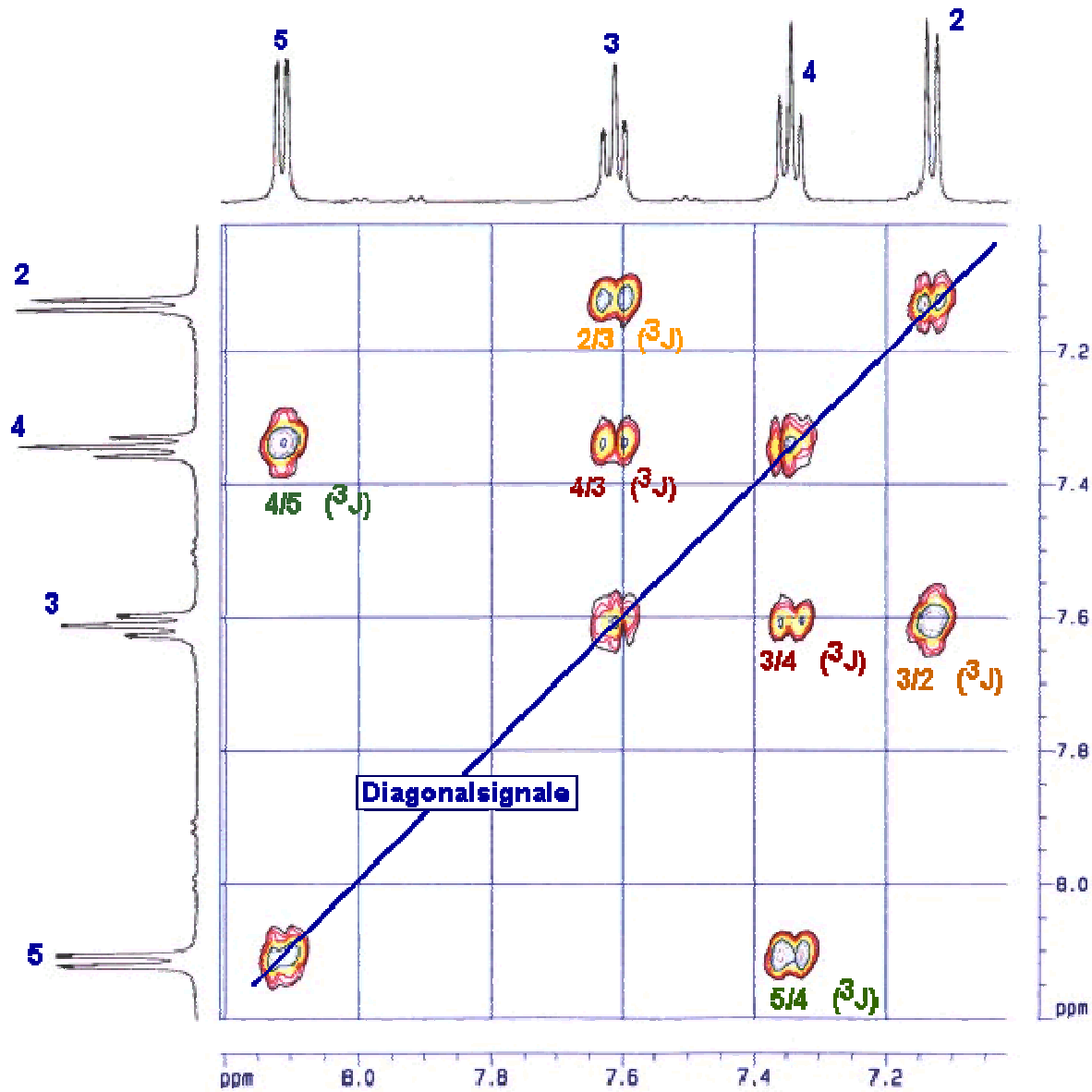
**13 „vidí“ 12 a 14,
„nevidí“ 8**

určení prostorového uspořádání

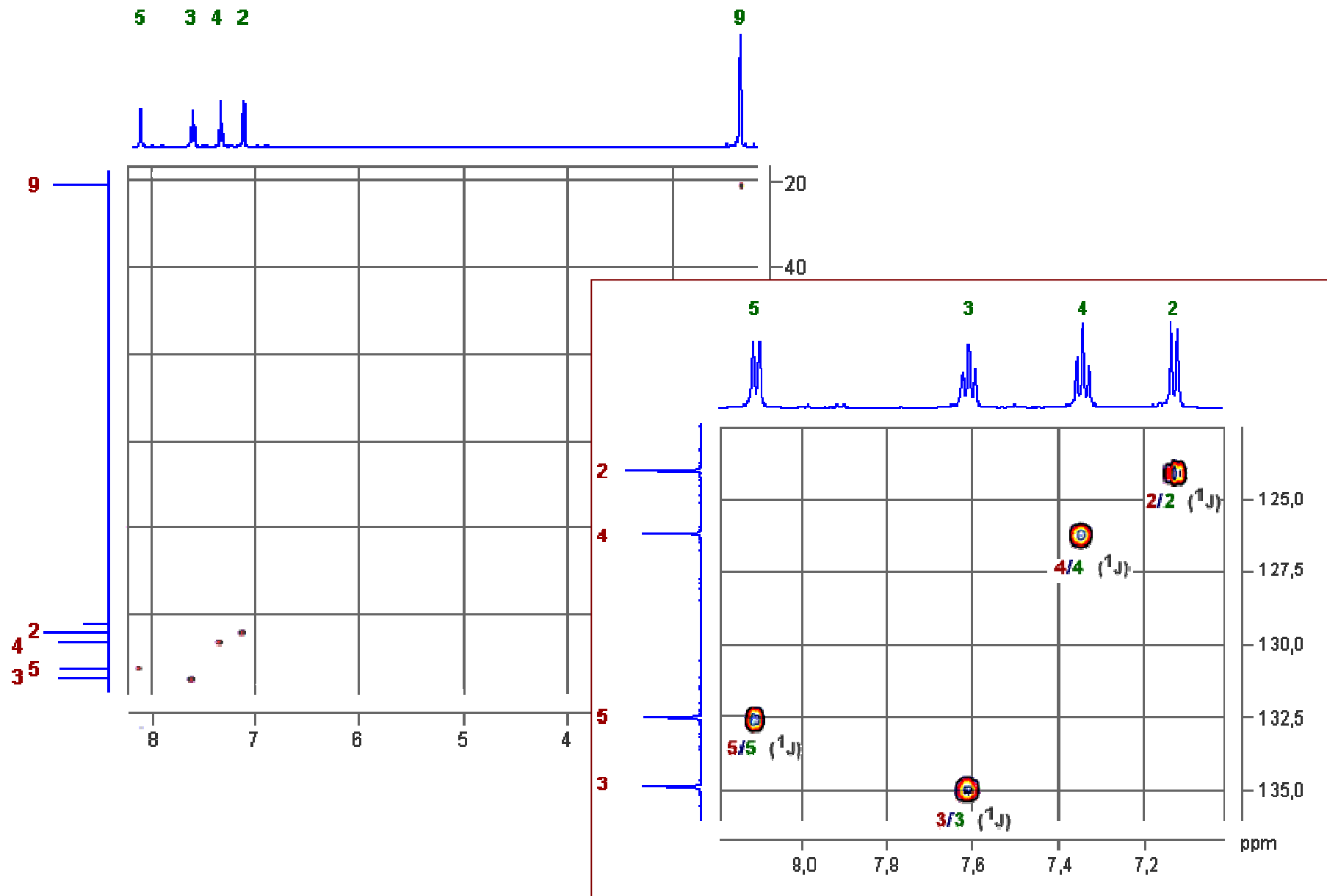
Příklad



Experiment COSY

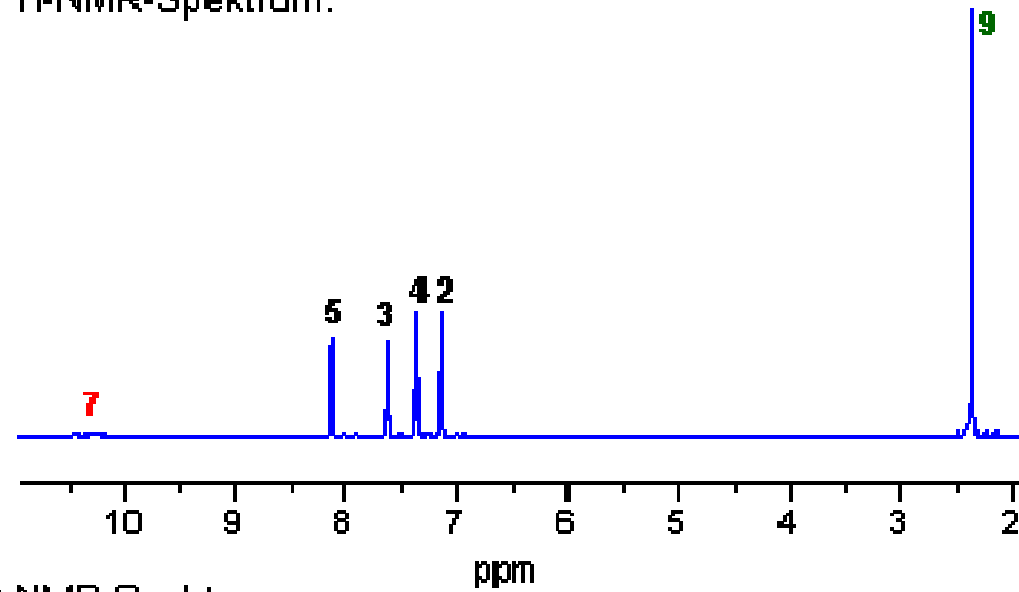


Experiment HMQC

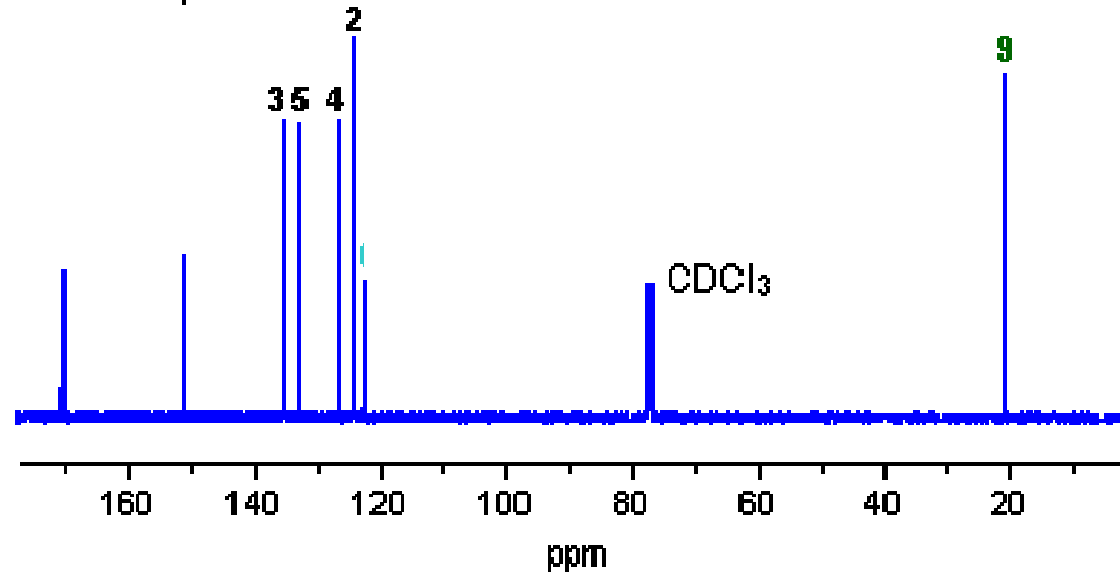


Mezivýsledek

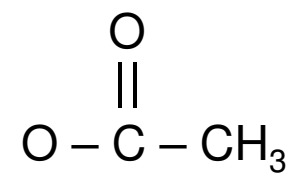
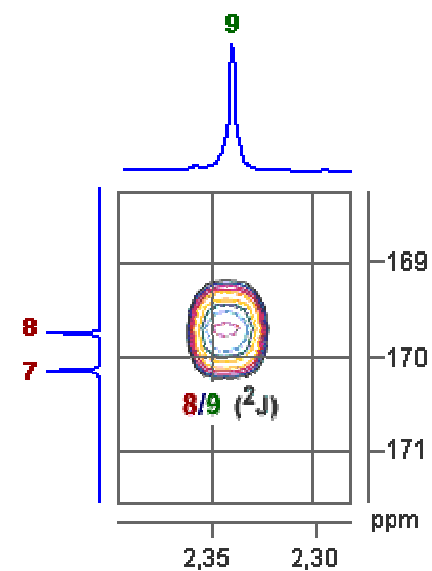
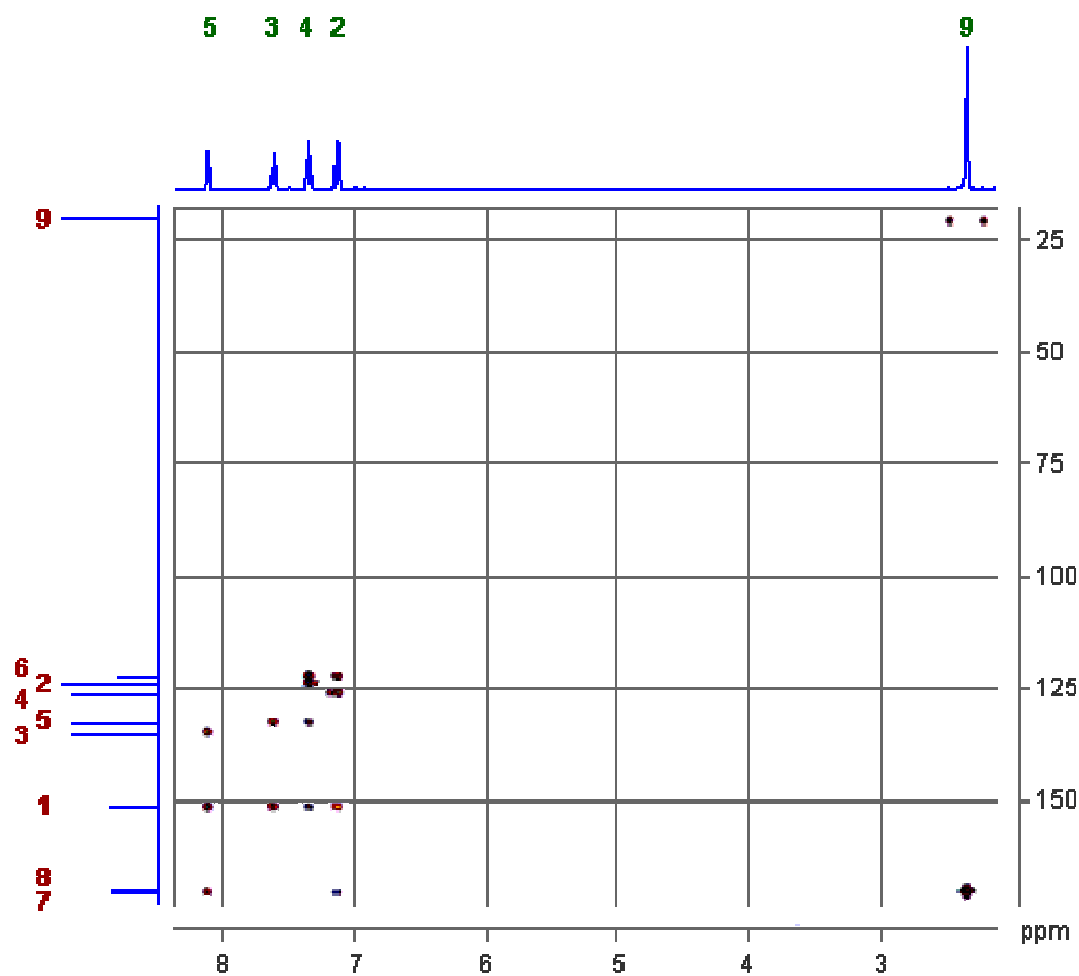
H-NMR-Spektrum:



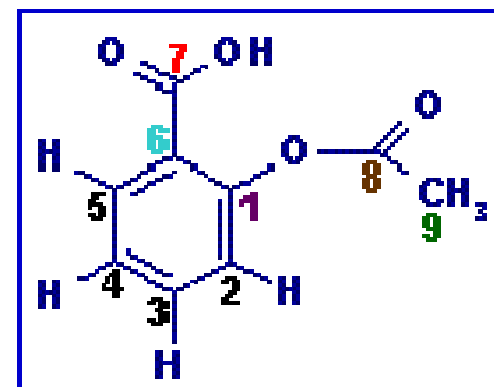
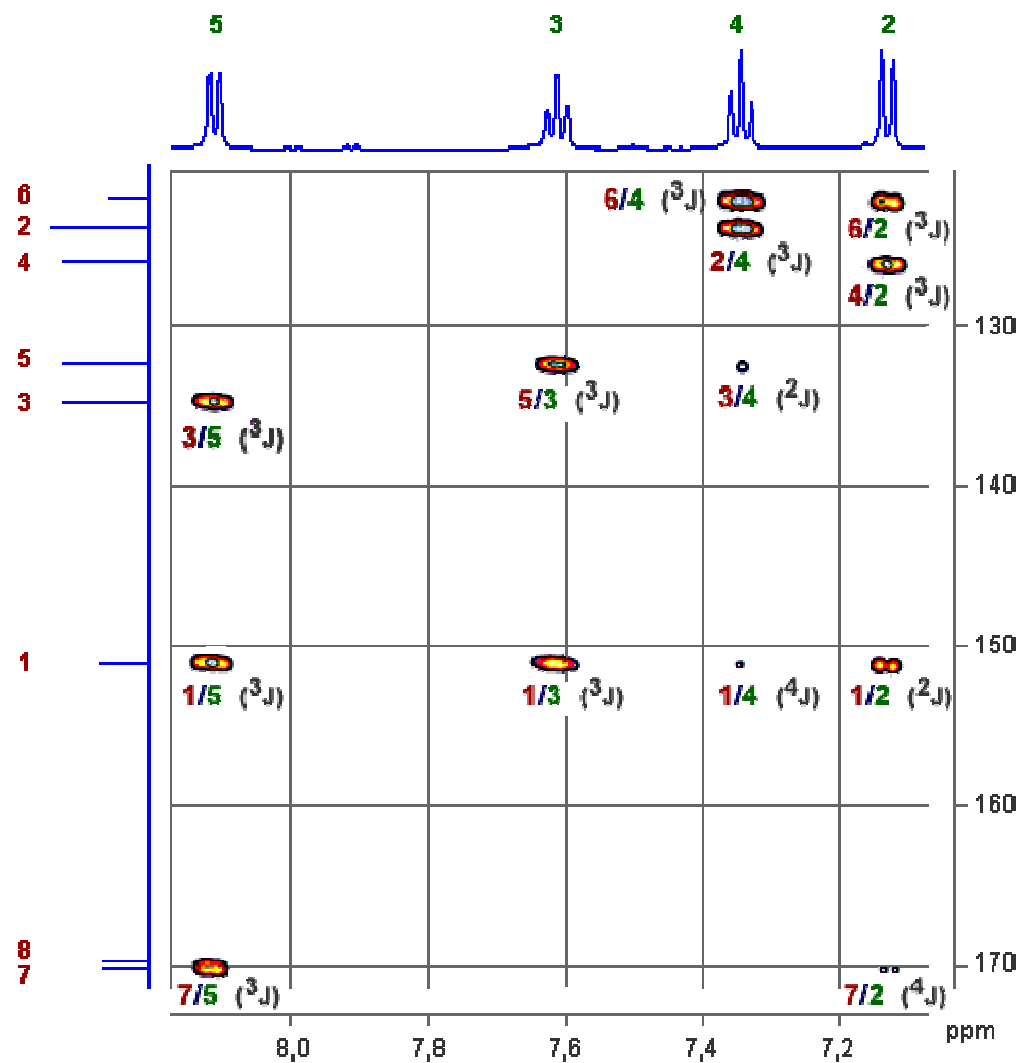
C-NMR-Spektrum:



Experiment HMBC



Experiment HMBC



Kyselina acetylsalicylová