

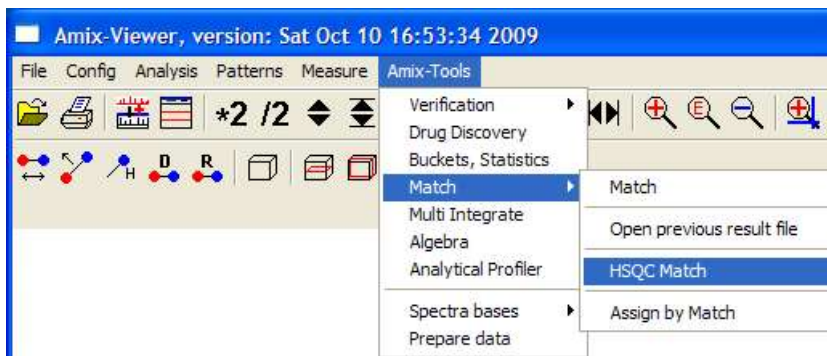
New HSQC Match – HowTo

Summary

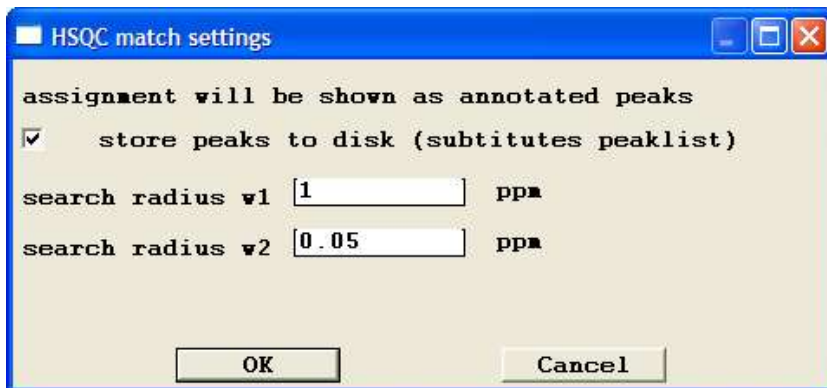
- Overcomes intensity distribution problem (mixture, reference)
- Shows singlet matches with yellow color
- Available for single spectra only
- Noise level: uses visible peaks only
- Simple algorithm: e.g. does not take identical ^{13}C shifts into account
- Result: as peaklist and match result file
- Integration in AMIX (e.g. 3.9.3) -> Peter Neidig has to decide, at the moment he is not available, no connection to the internet.

Step by step

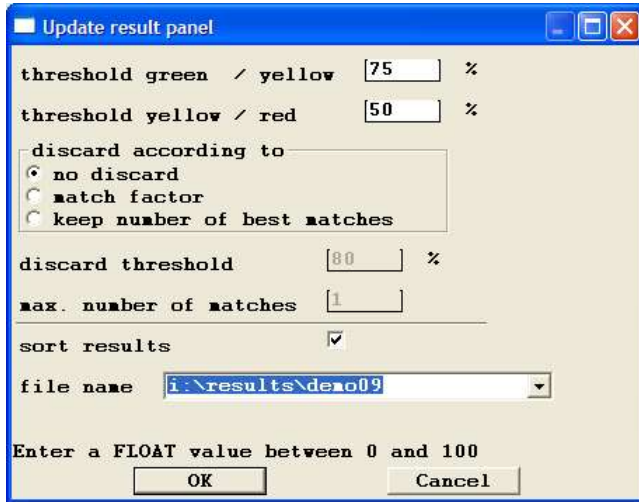
1. Load spectrum
2. Scale to noise level: only visible peaks are used
3. AmixTools -> Match -> HSQC match



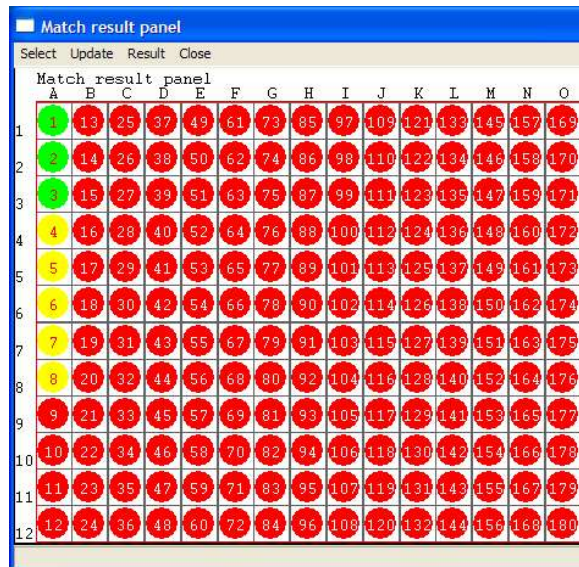
4. Select spectra to match
5. Select search radius + store as peaklist?



6. Result: Singlets found: 0.50, compound found 1.0. Select 75% and 50% as match thresholds to get this result visualized. Suggestion: use "sort results"



7. Panel display



8. Spectrum display

