Bruker Fusion-SV

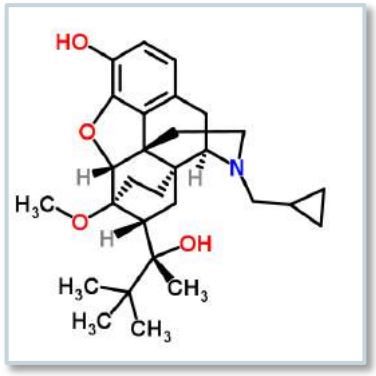
Wenxin Xu, Ph.D.

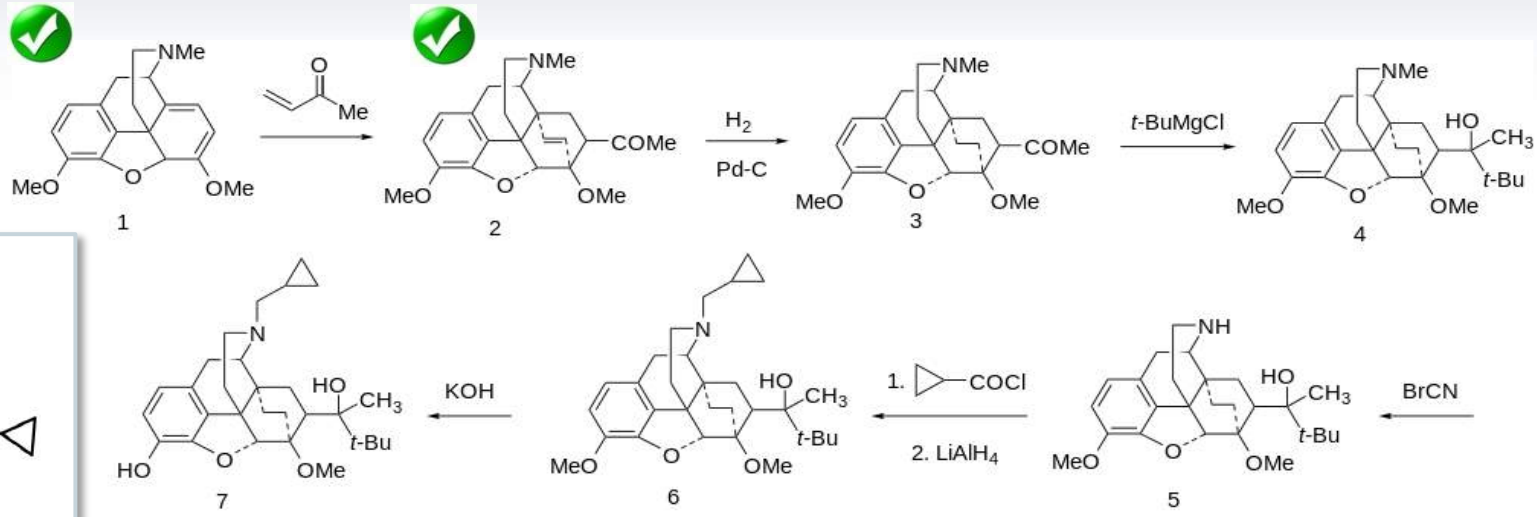
Application

Sep, 2016

Would you like to learn more? Contact a customer service representative.

Chemical Synthesis Control





Anything from:

⇨ quick and dirty check of intermediates of synthetic process

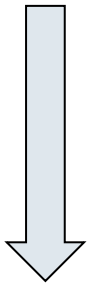
⇨ Verification of final product

⇨ Several analytical technique used

⇨ depends on chemical question and required certainty

Chemists' full verification…

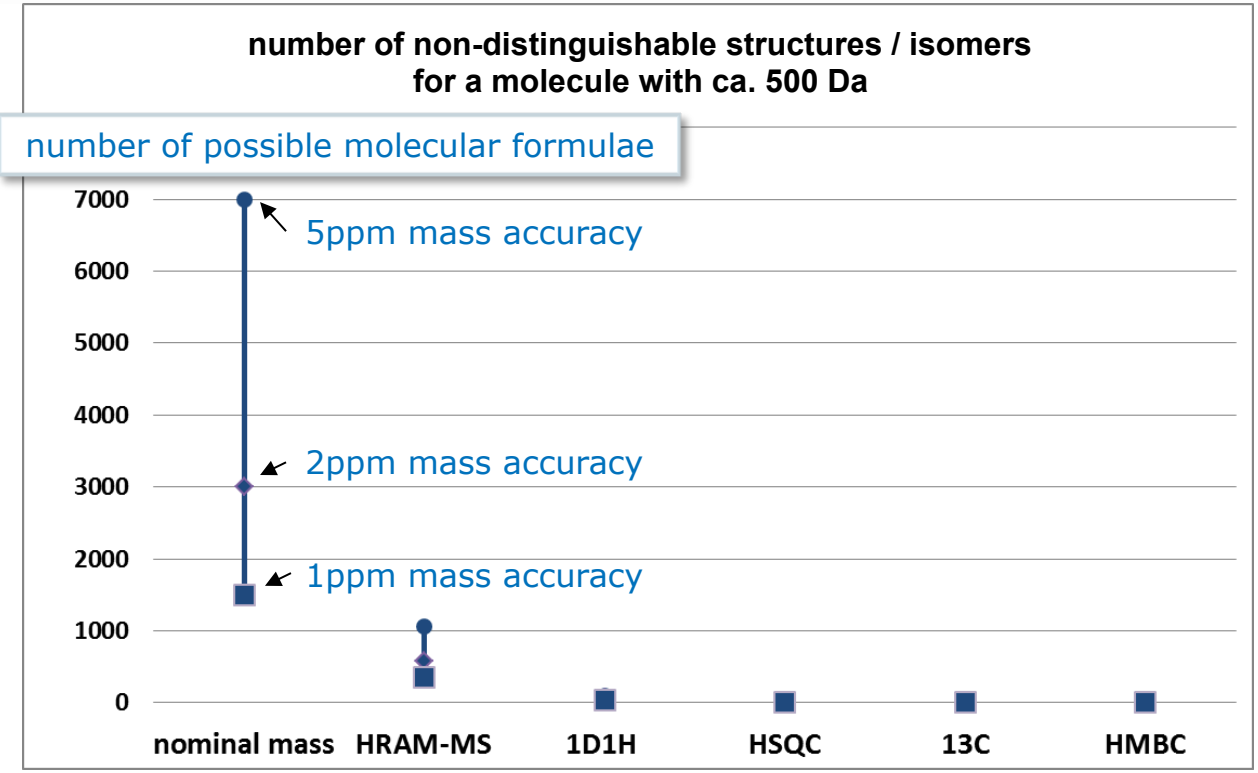
- They want to be sure, **not to file the wrong structure** as a drug candidate
- **Orthogonal data** is needed to minimize the chance for false positives
- MS can do things NMR can not (Cl/Br, S/O …)
  - Nominal mass → leaves 1'000s of potential false positives
  - **HRAM-MS** → verifies the **molecular formula**
- **NMR** can do things MS can not
  - 100's of possible structures per molecular formula → potential false positives
  - 1D ^{1}H
  - HSQC
  - HMBC
  - 13C



Further reduction of potential wrong passes

Structure Verification

MW 467.298

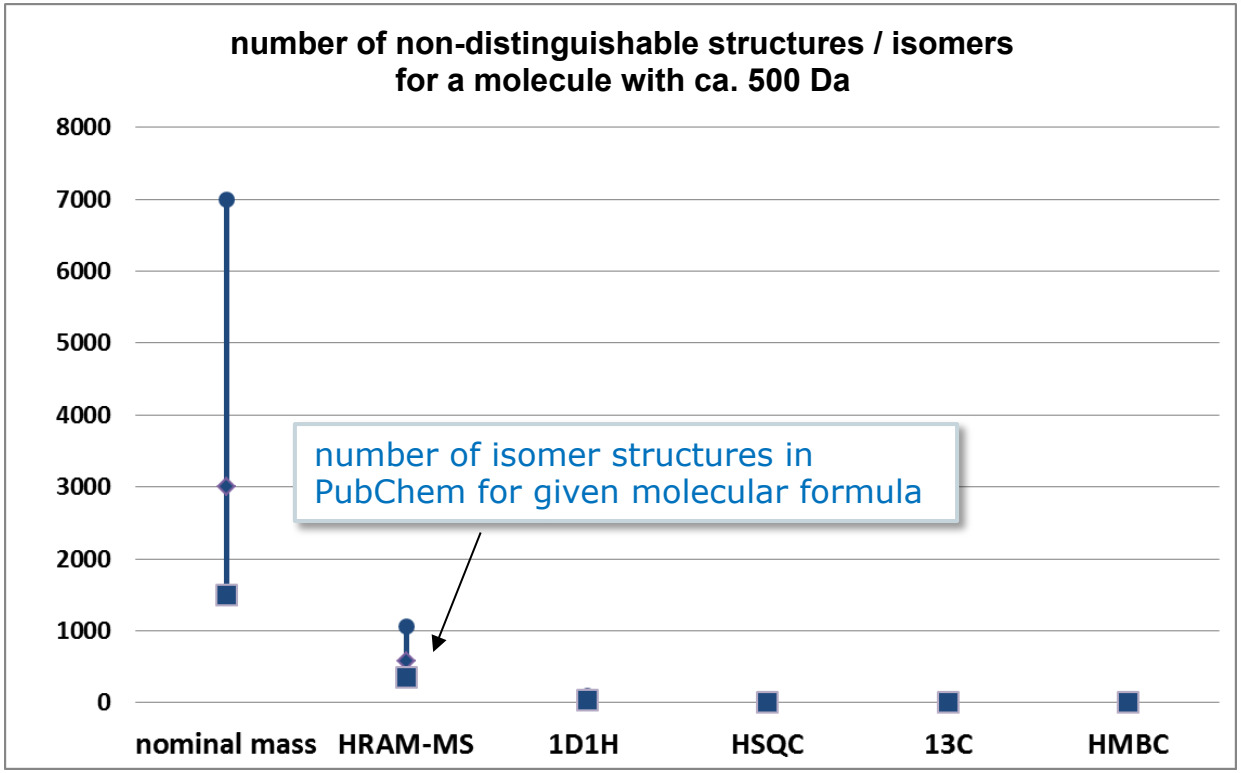


⇨ nominal mass only is not able to rule out 1000s of potentially false positives

Structure Verification

MW 467.298

$C_{20}H_{22}NO_4$



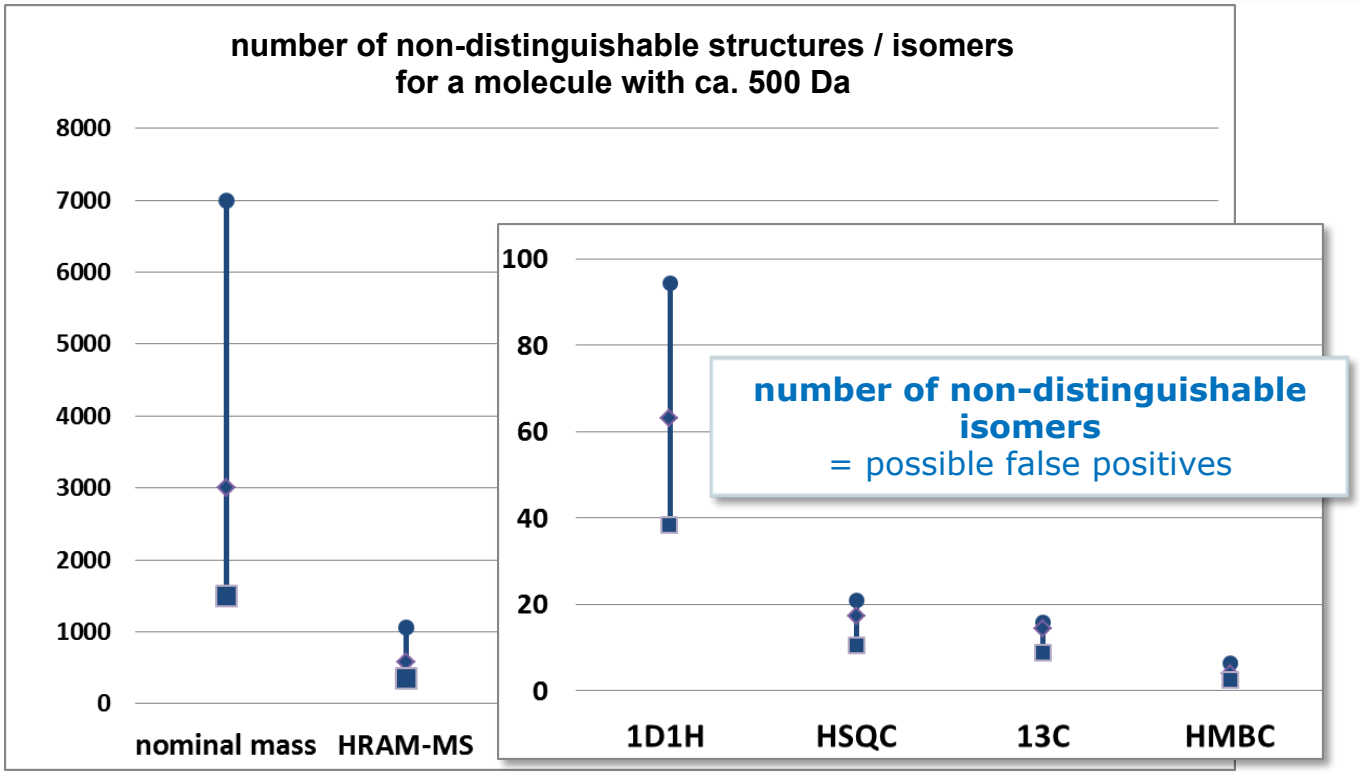
⇨ HRAM-MS verifies the molecular formula

⇨ still several 100 isomers that cannot be ruled out (potential false positives)

Structure Verification

MW 467.298

$C_{20}H_{22}NO_4$



⇨ ^{1}H NMR still leaves many potential isomers that cannot be distinguished

⇨ clever combination of orthogonal information adds confidence

Bruker Fusion-SV

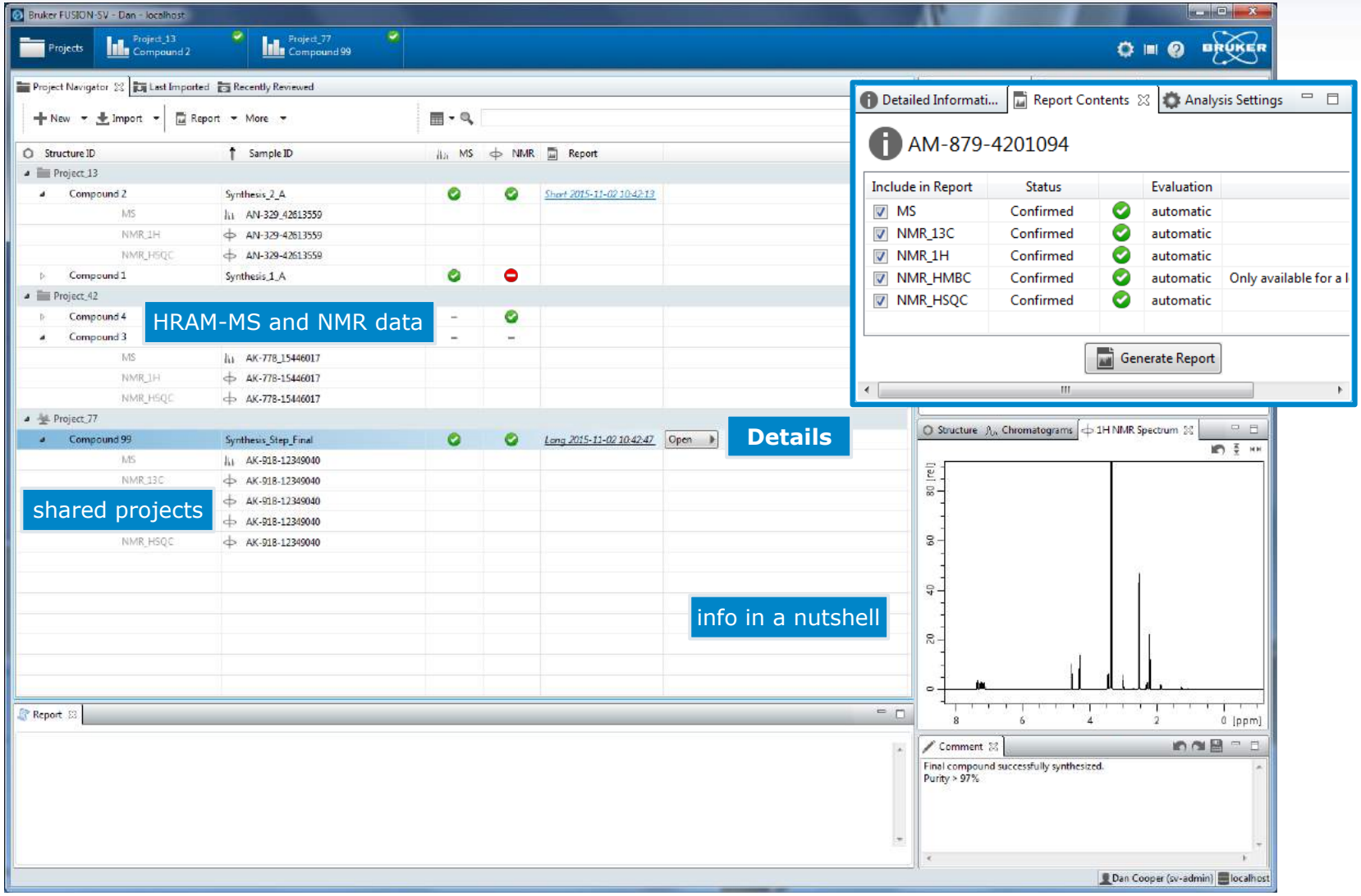
new, fully automatic analysis solution using HRAM-MS and NMR structure verification (SV)

N
HRAM-MS
R

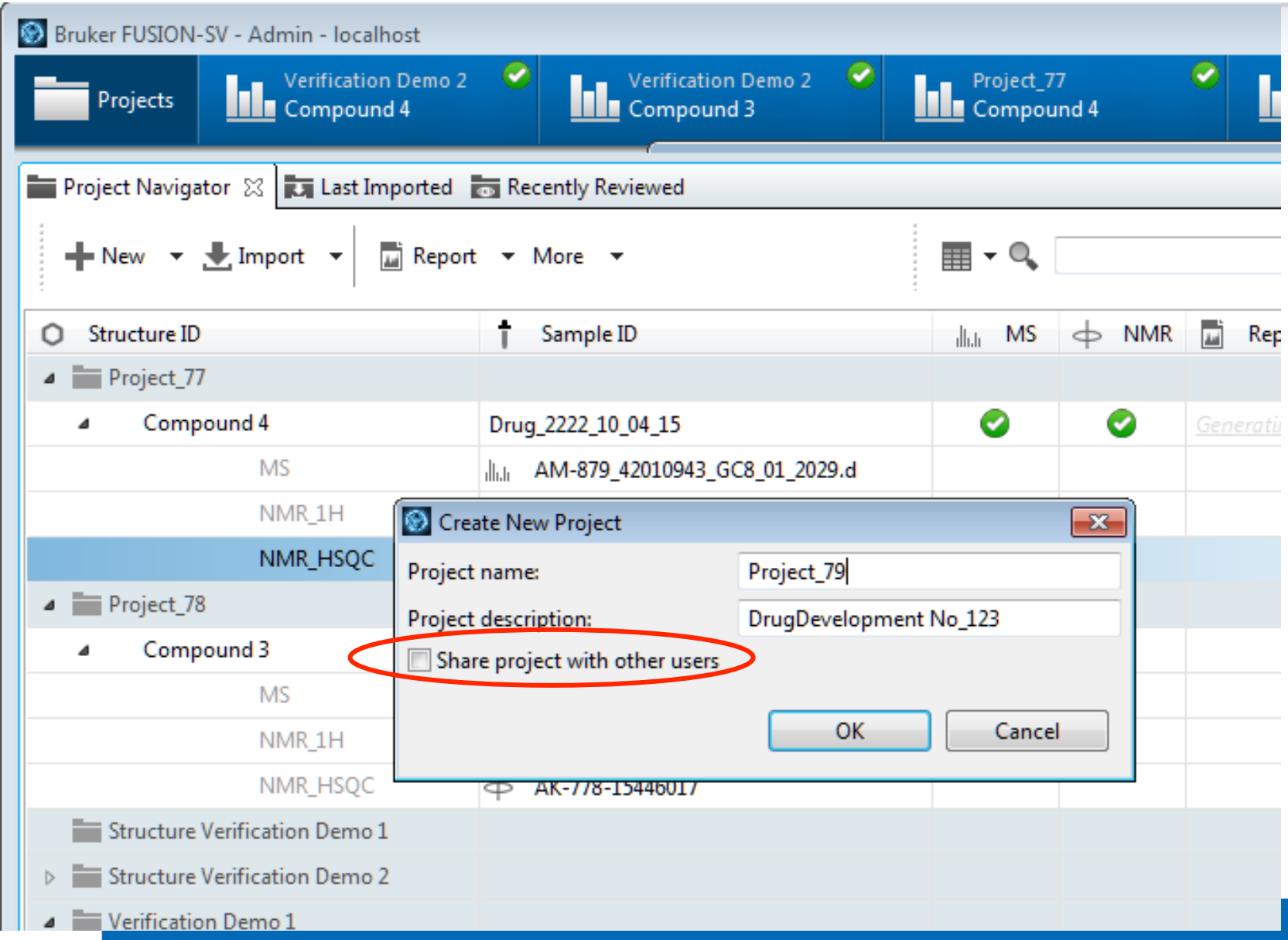
Designed for Chemists

- structure centered
- workflow oriented
- Network embedded

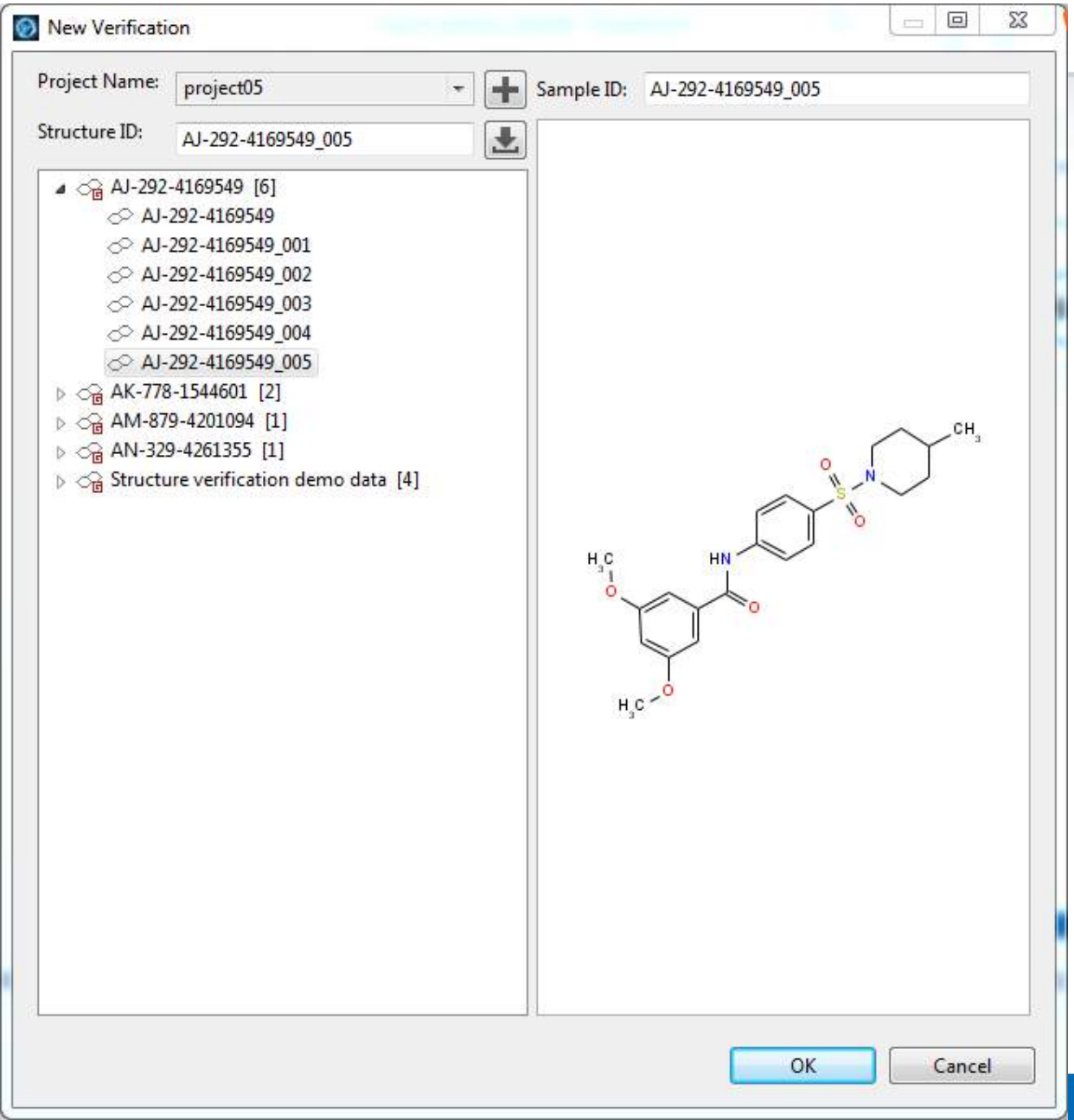
New: Bruker Fusion-SV 1.1



Bruker Fusion-SV 1.1: Workbench

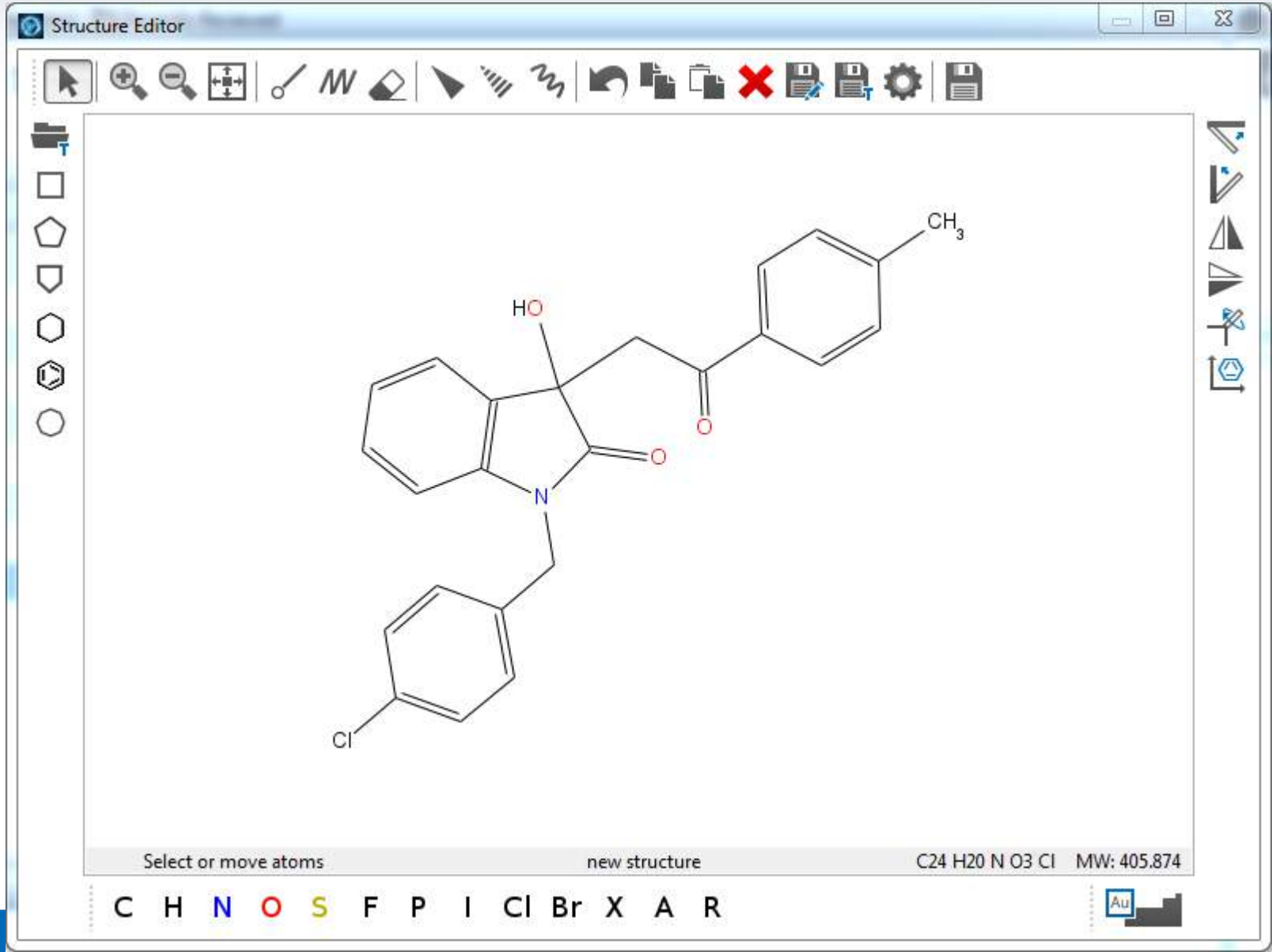


Bruker Fusion-SV 1.1: Workbench

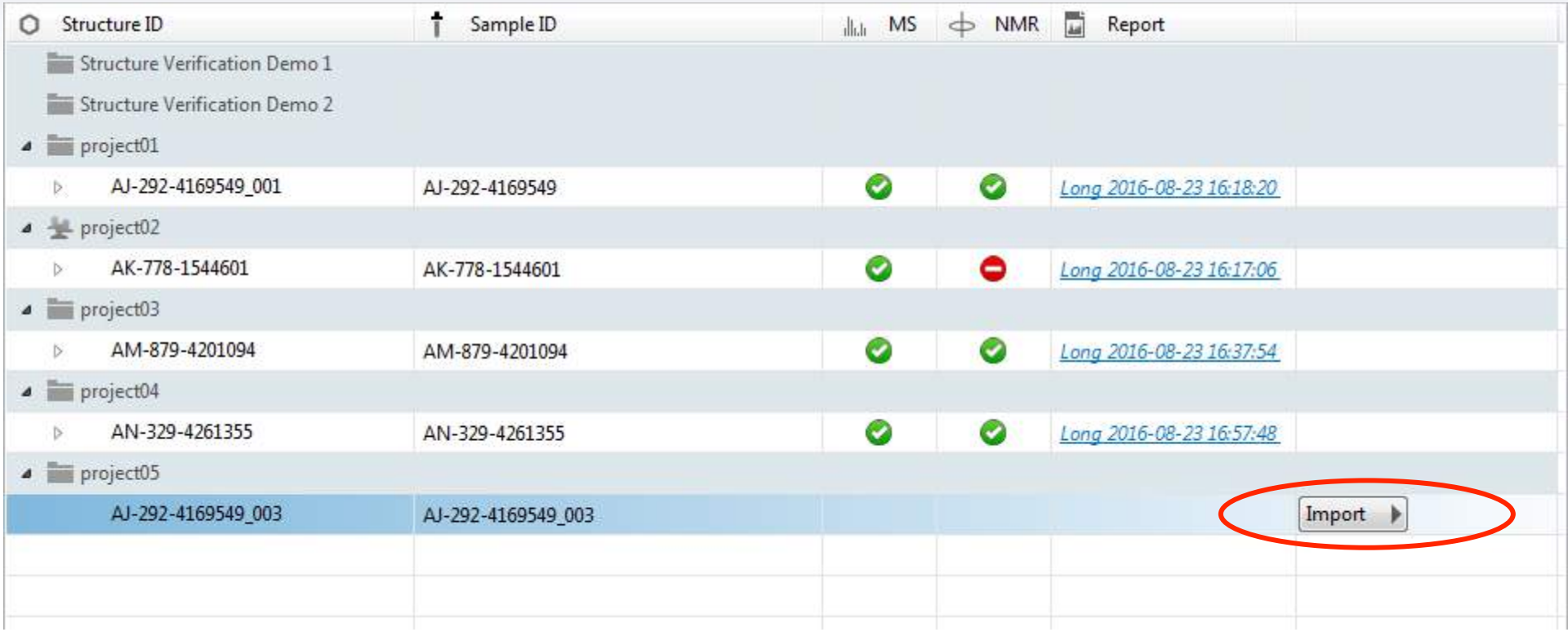


.mol or .sdf

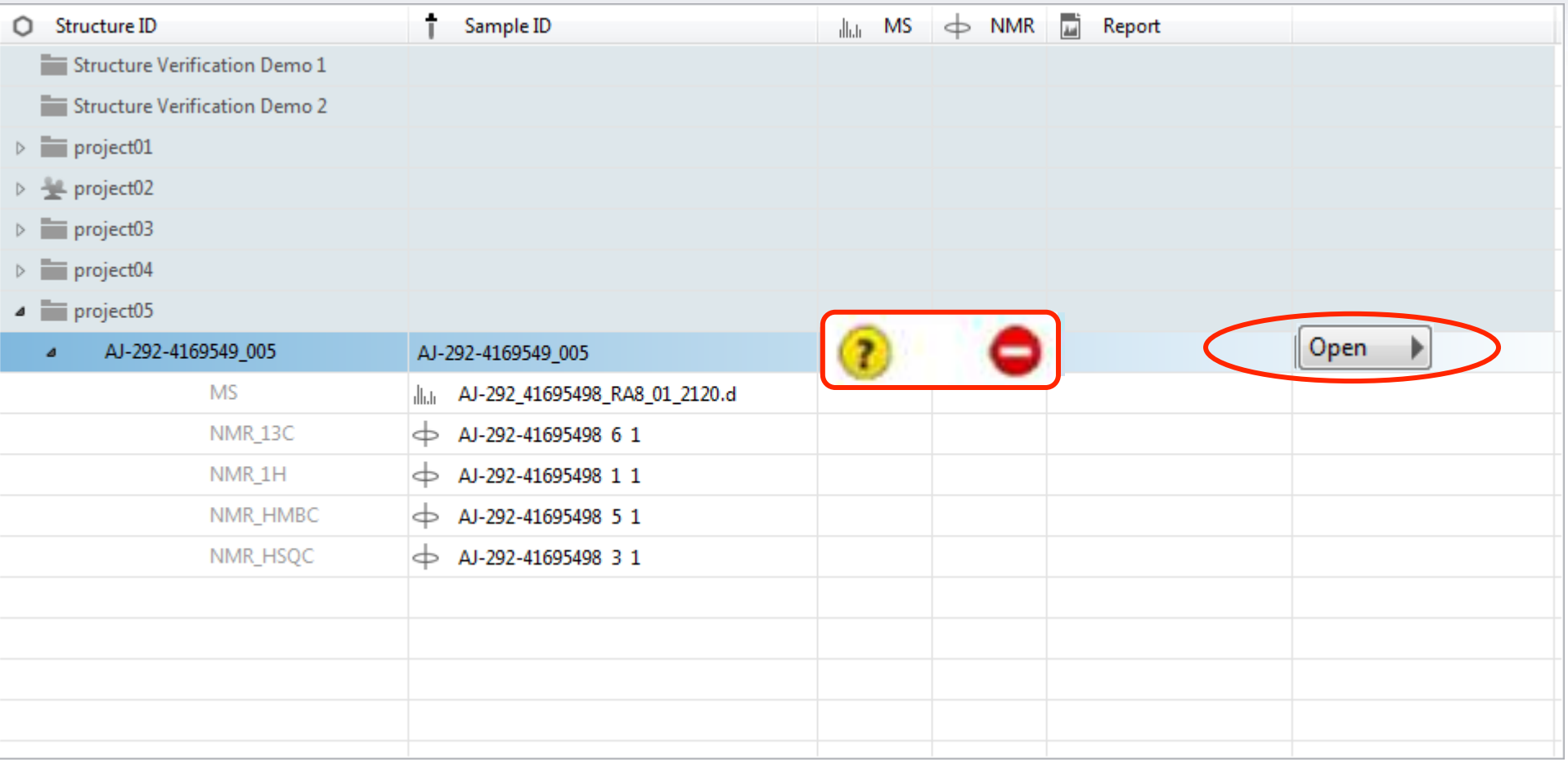
Structure Editor



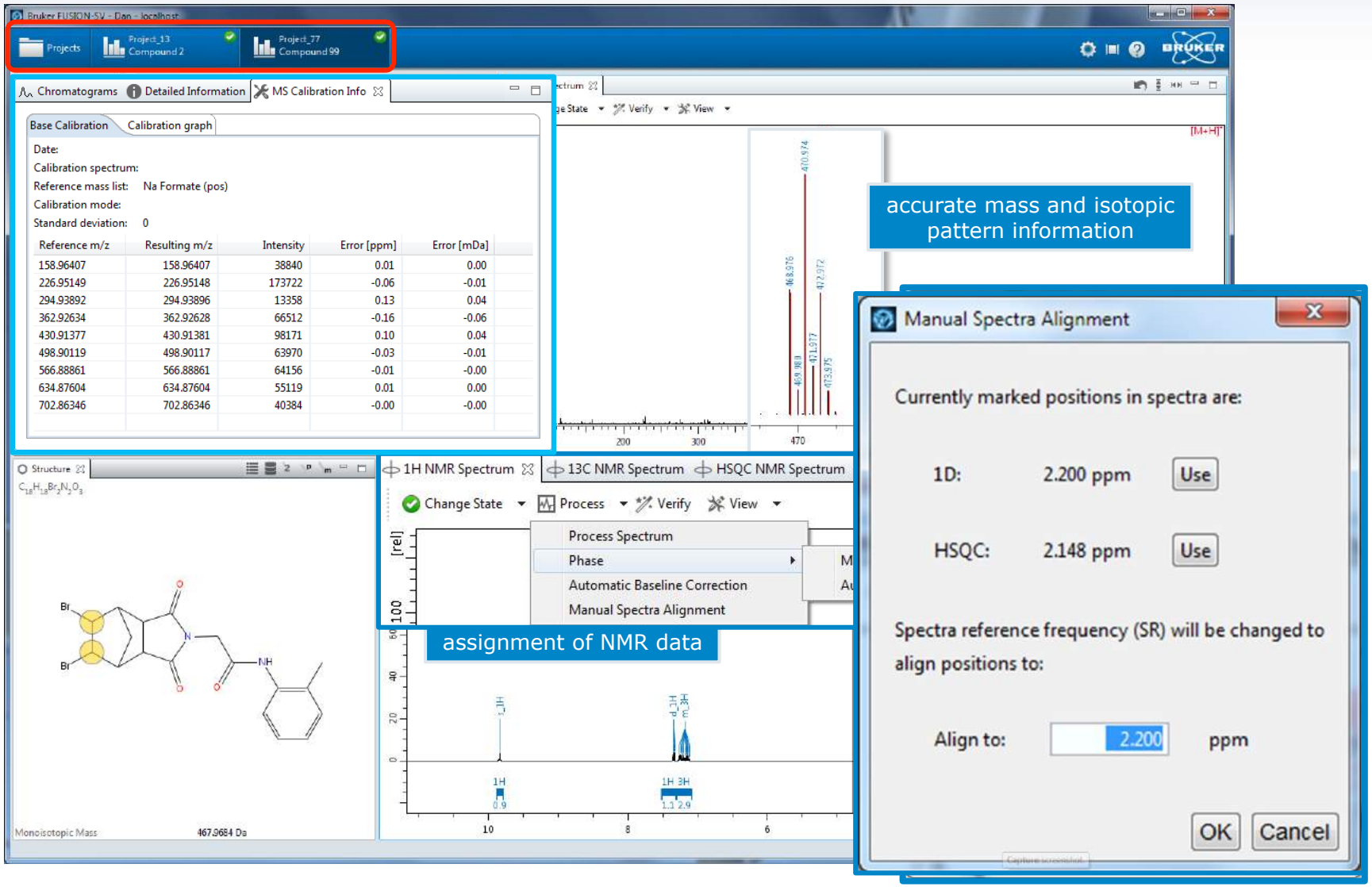
Import MS & NMR data



Verify


Structure ID
Sample ID
MS
NMR
Report
Structure Verification Demo 1
Structure Verification Demo 2
project01
project02
project03
project04
project05
AJ-292-4169549_005
AJ-292-4169549_005
Open
MS
AJ-292_41695498_RA8_01_2120.d
NMR_13C
AJ-292-41695498 6 1
NMR_1H
AJ-292-41695498 1 1
NMR_HMBC
AJ-292-41695498 5 1
NMR_HSQC
AJ-292-41695498 3 1

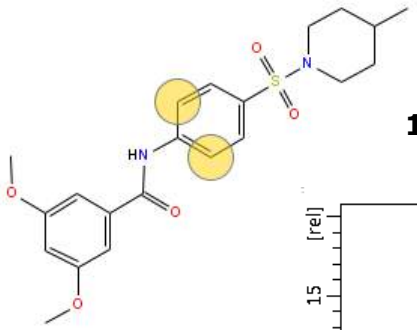
Verification review



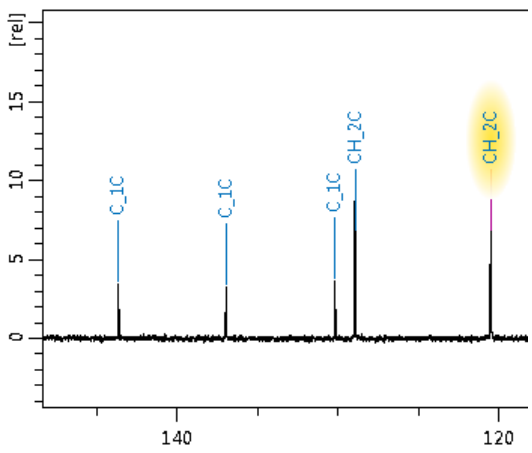
New: Bruker Fusion-SV 1.1

Automatic analysis of combined **1D ^{1}H, HSQC, HMBC and 1D ^{13}C** data for

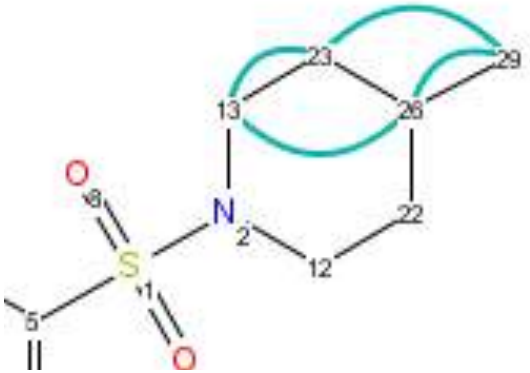
- ⇨ Automatic processing of NUS data (HSQC, HMBC)
- ⇨ Spectra interpretation easily understandable



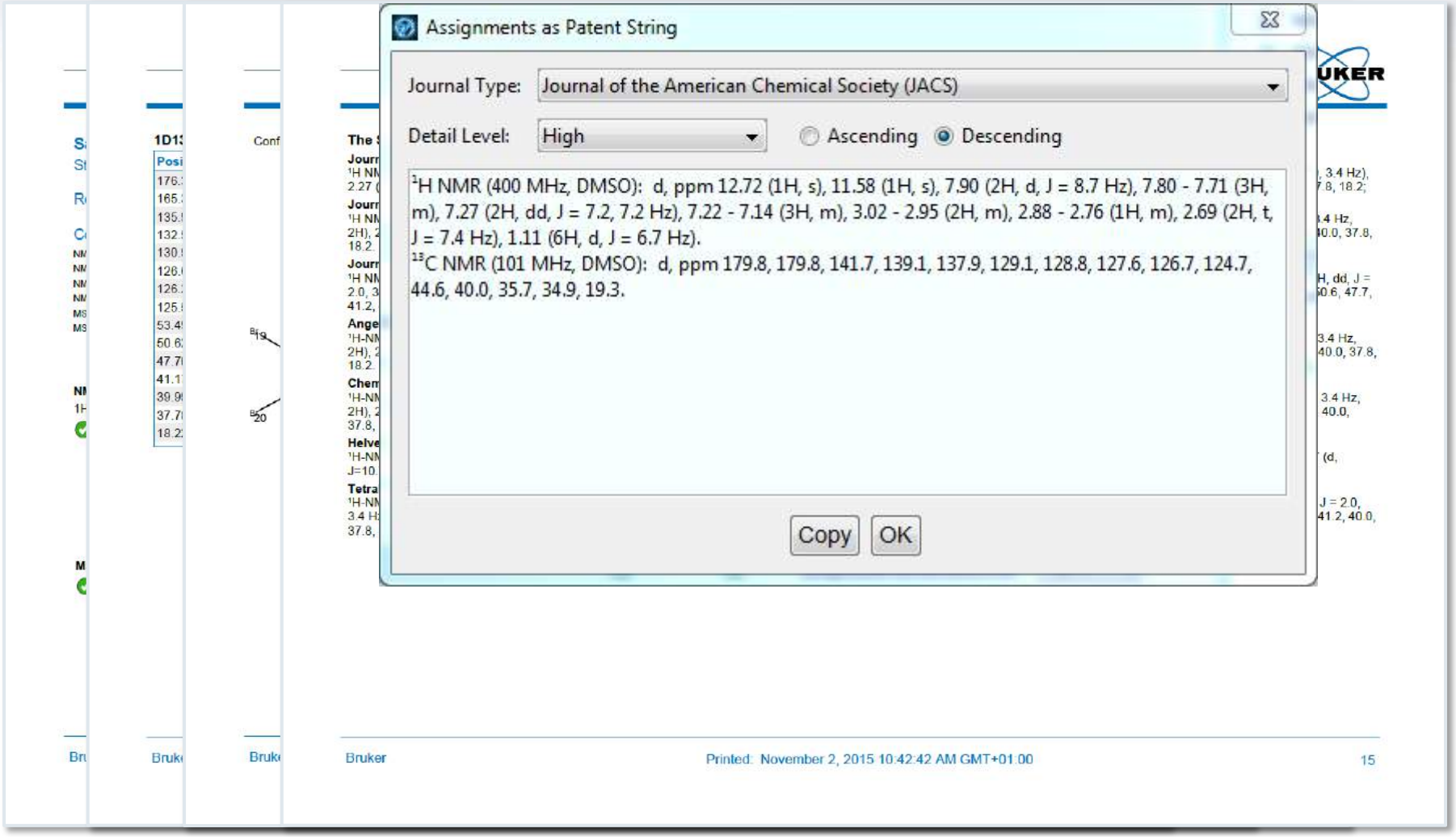
^{13}C assignment



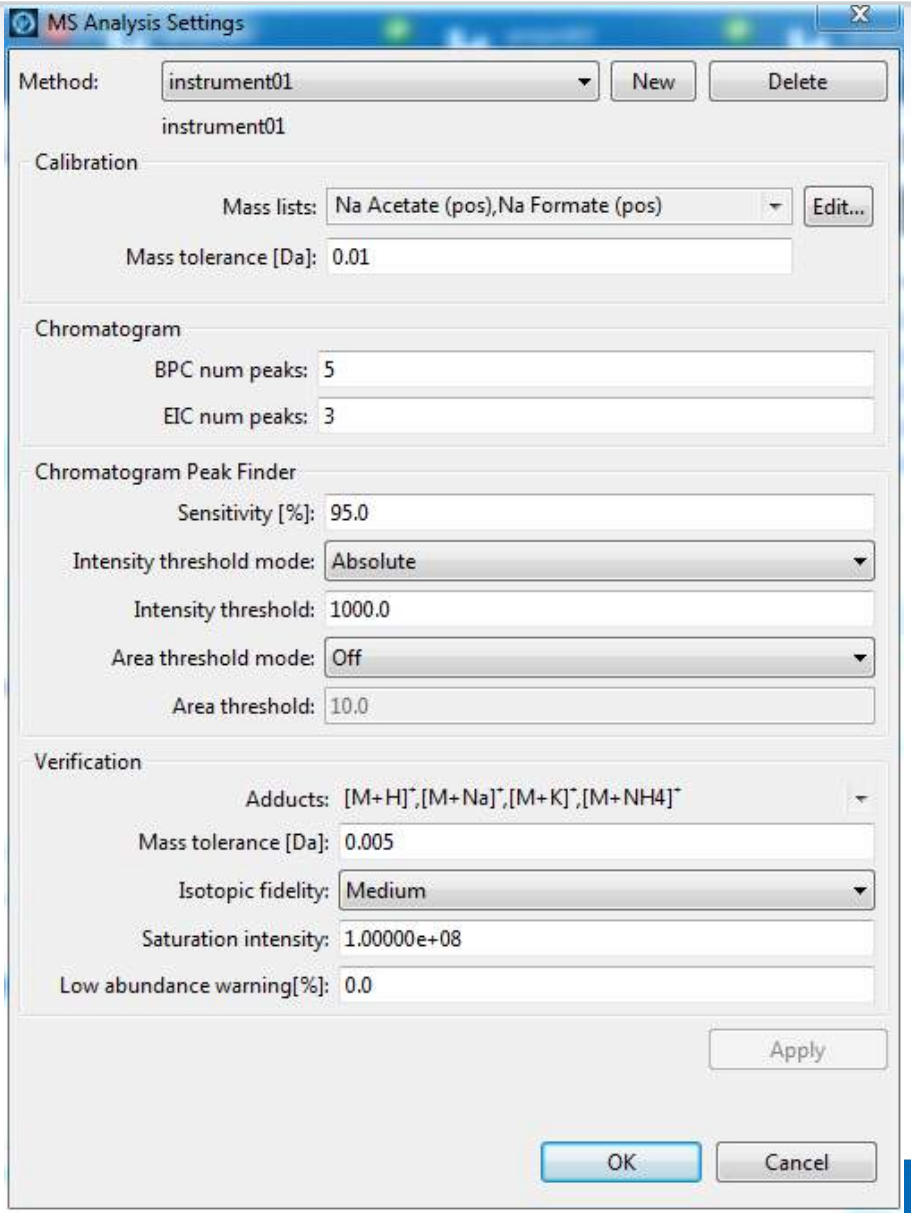
HMBC correlations

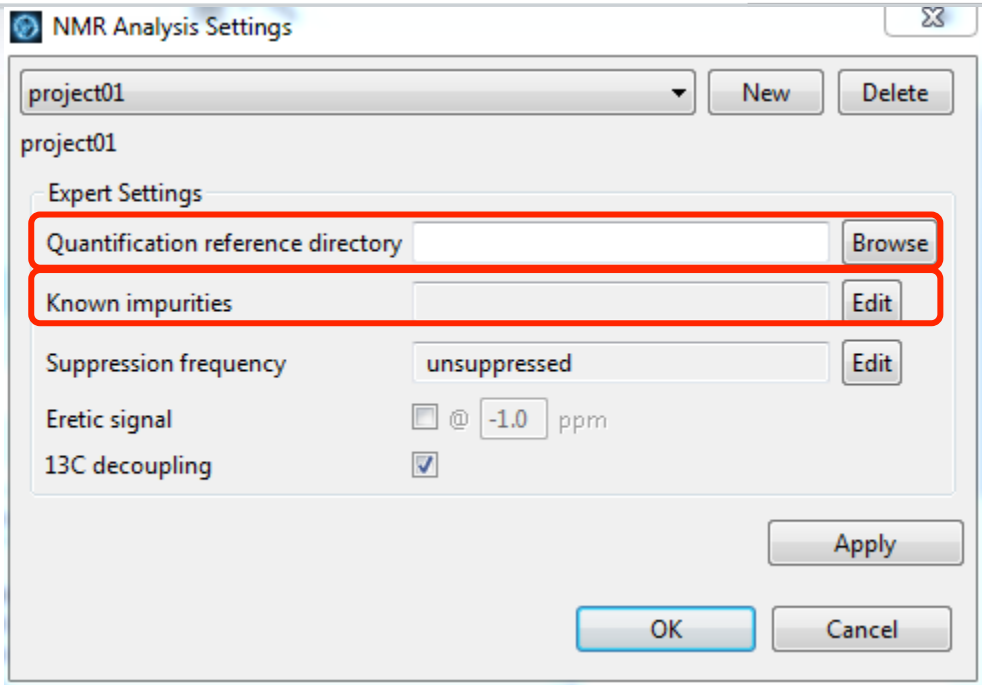


Generate Report

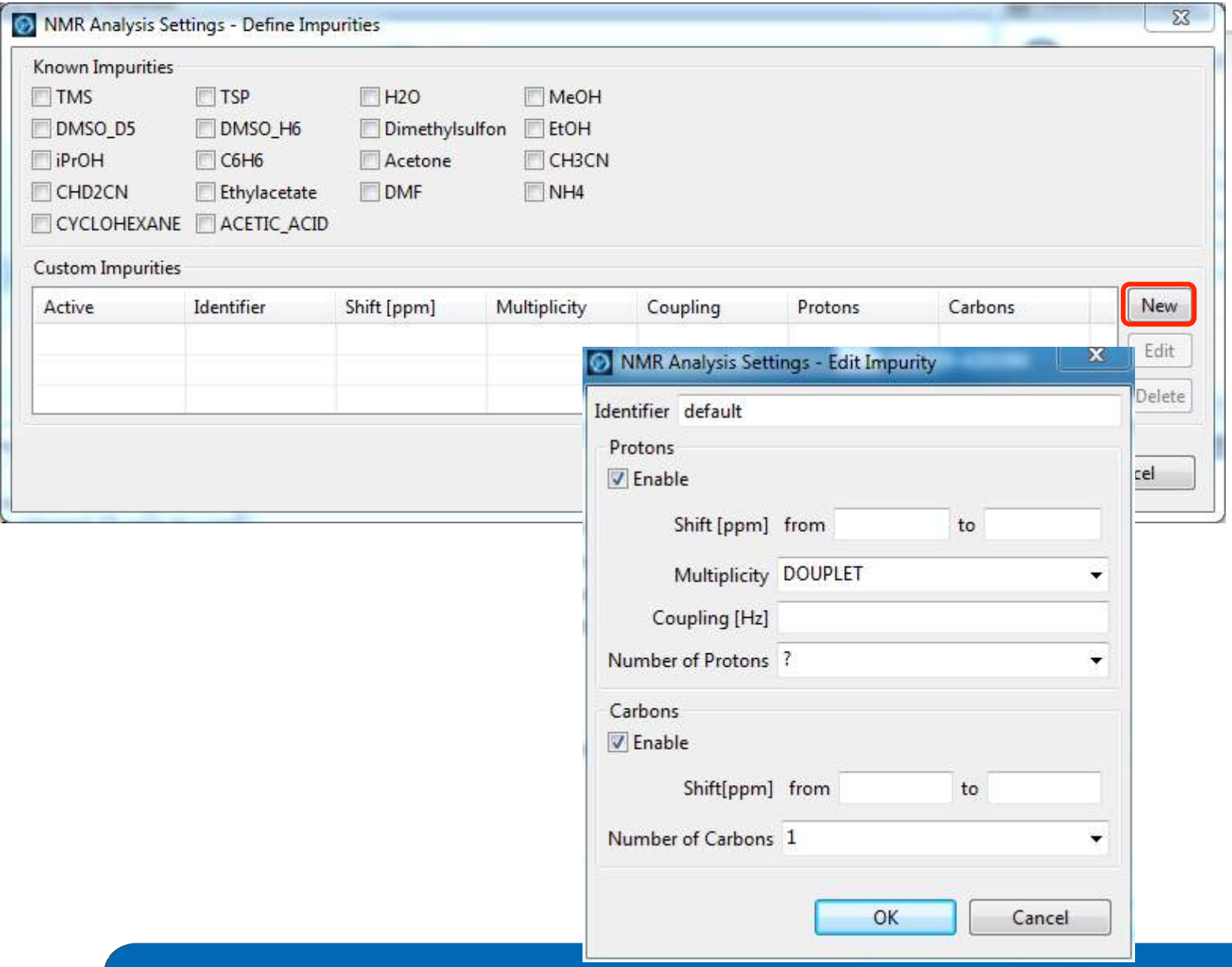


MS & NMR Analysis Settings

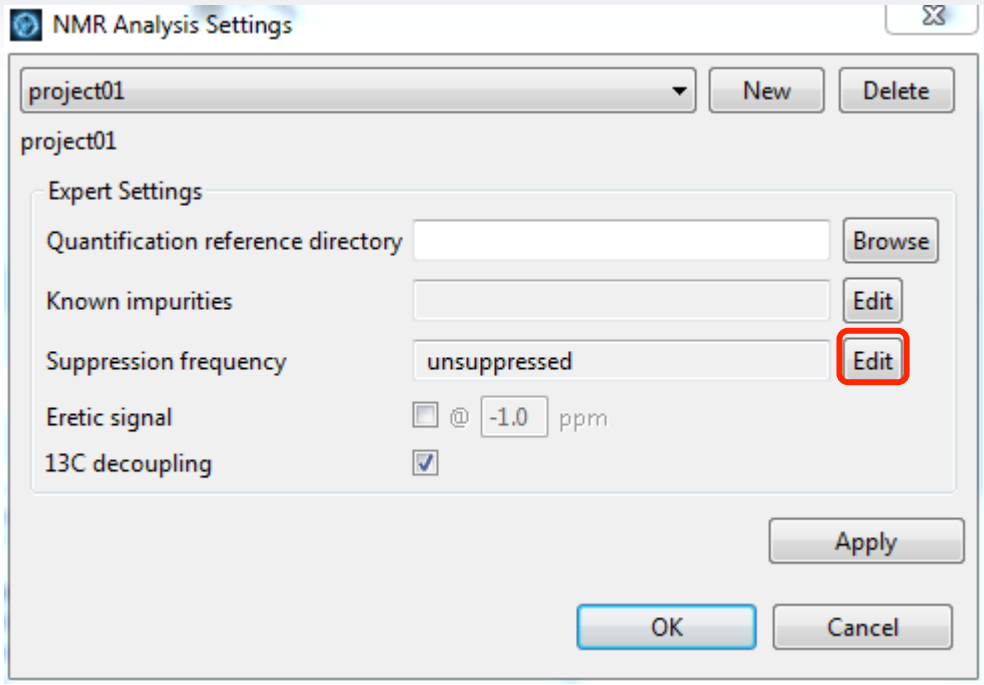


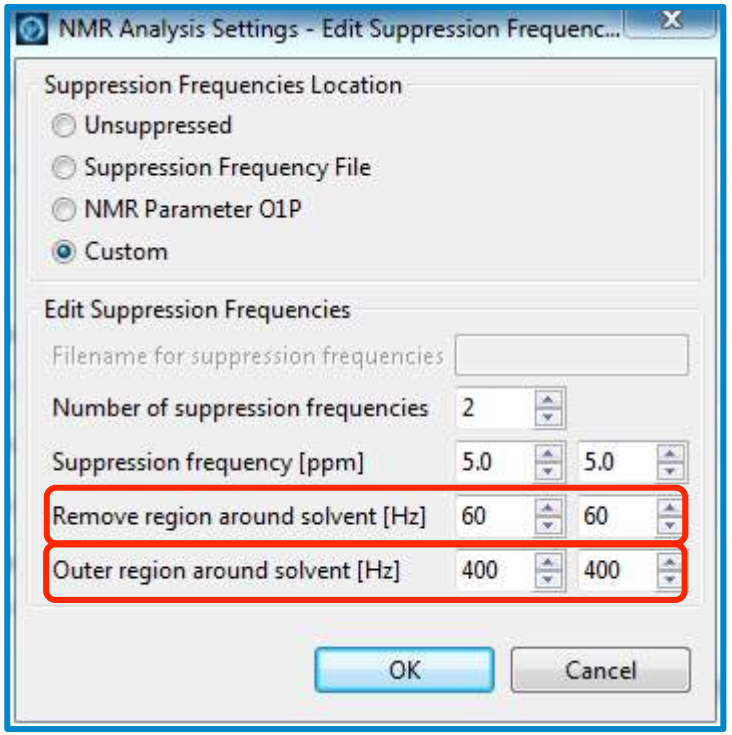


NMR Analysis Settings

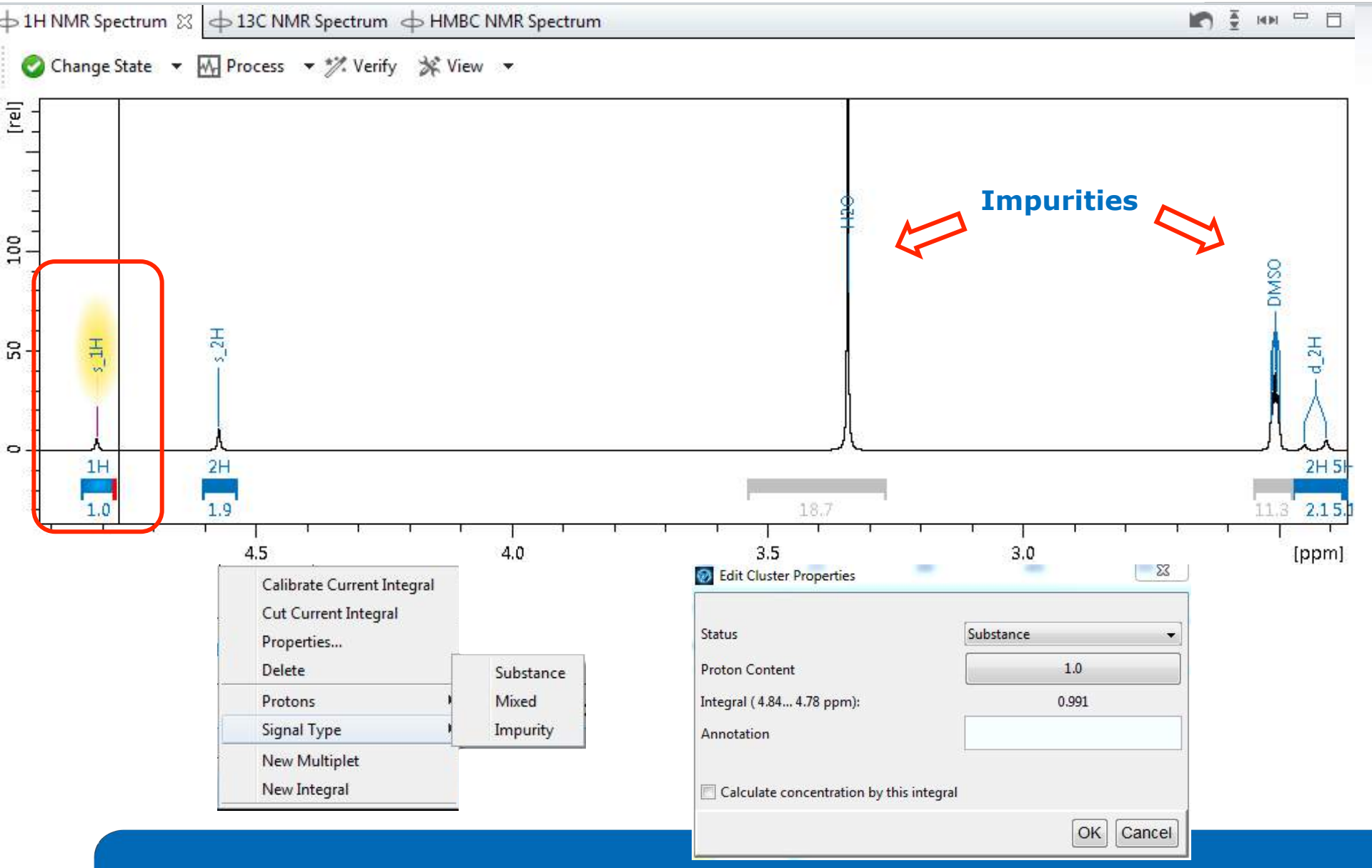


NMR Analysis Settings

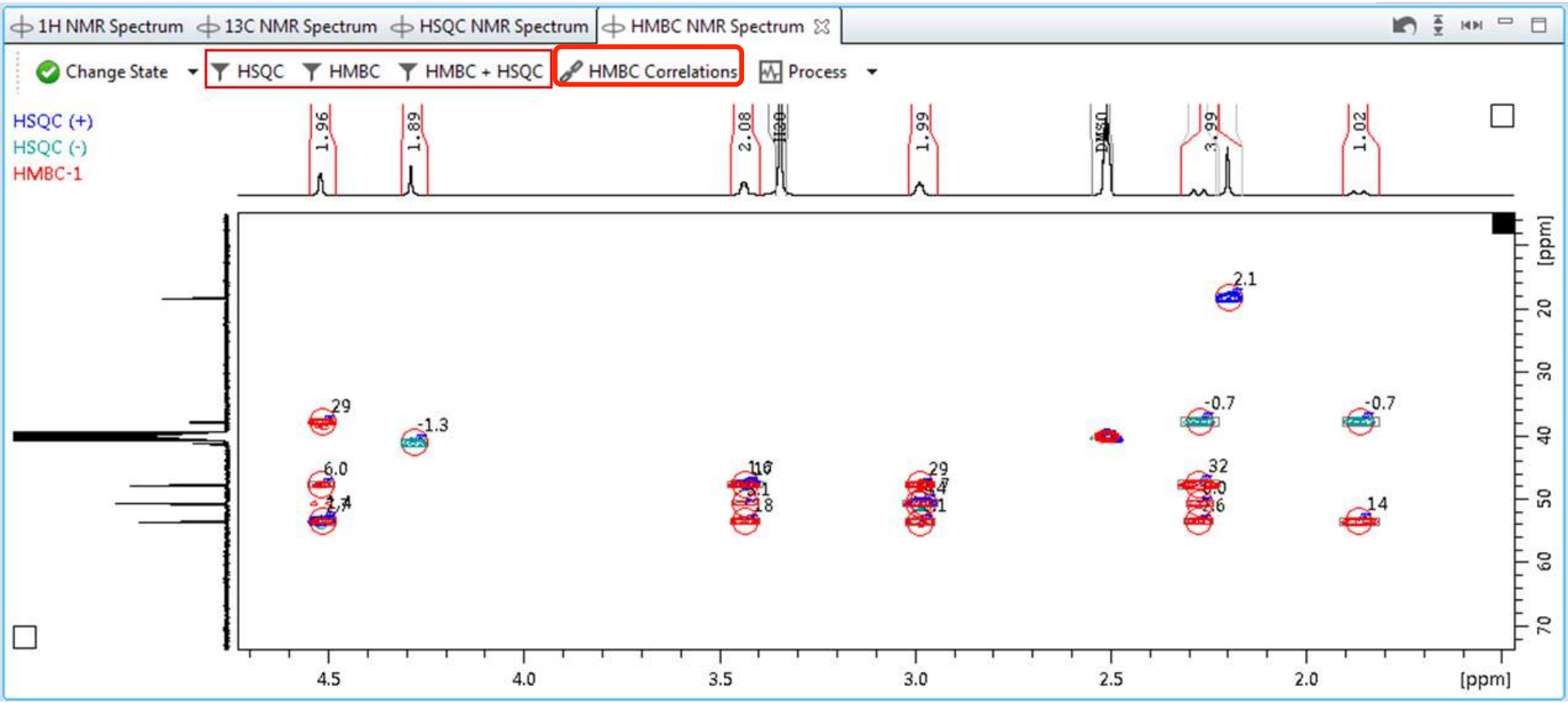




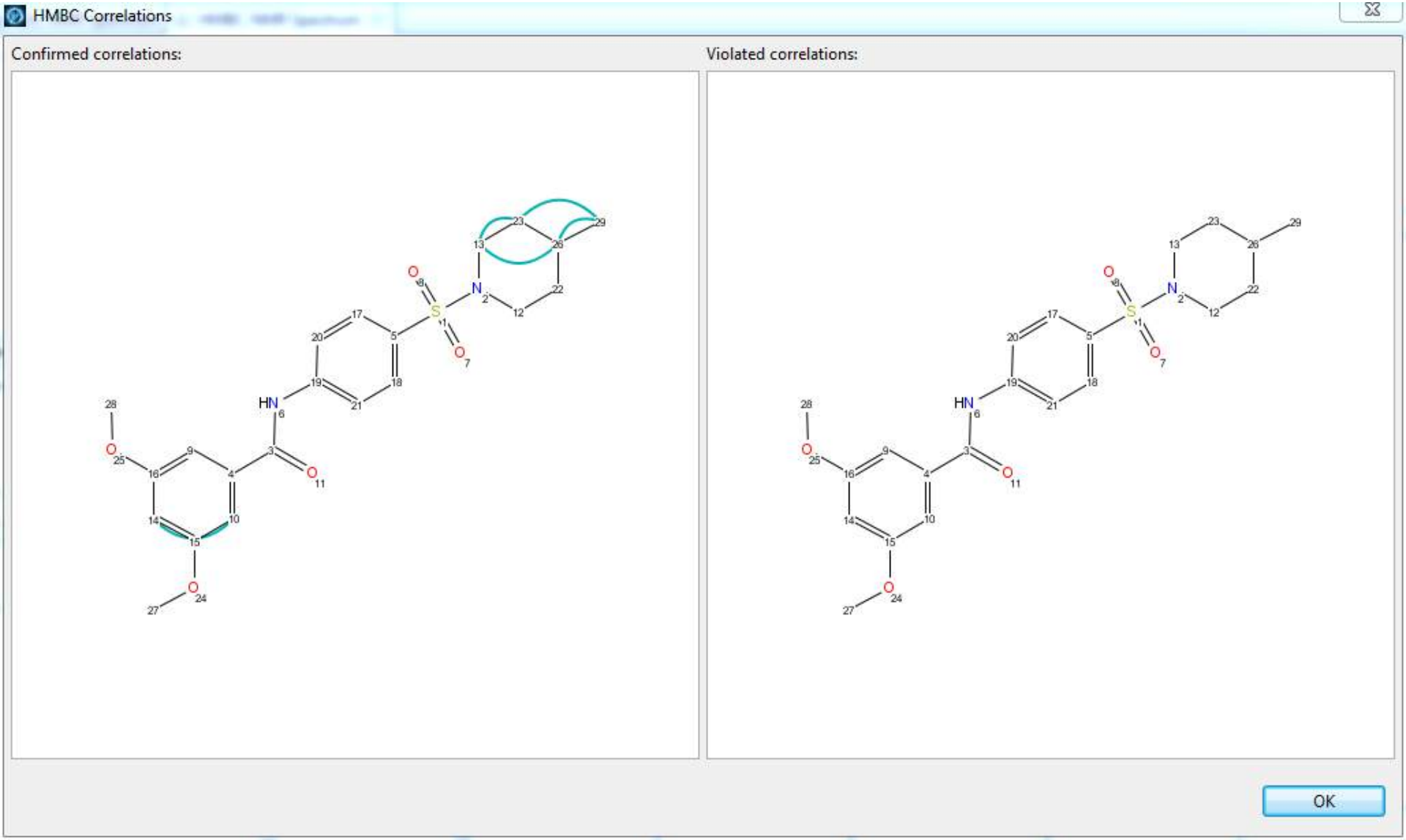
Modifying results from an automated analysis



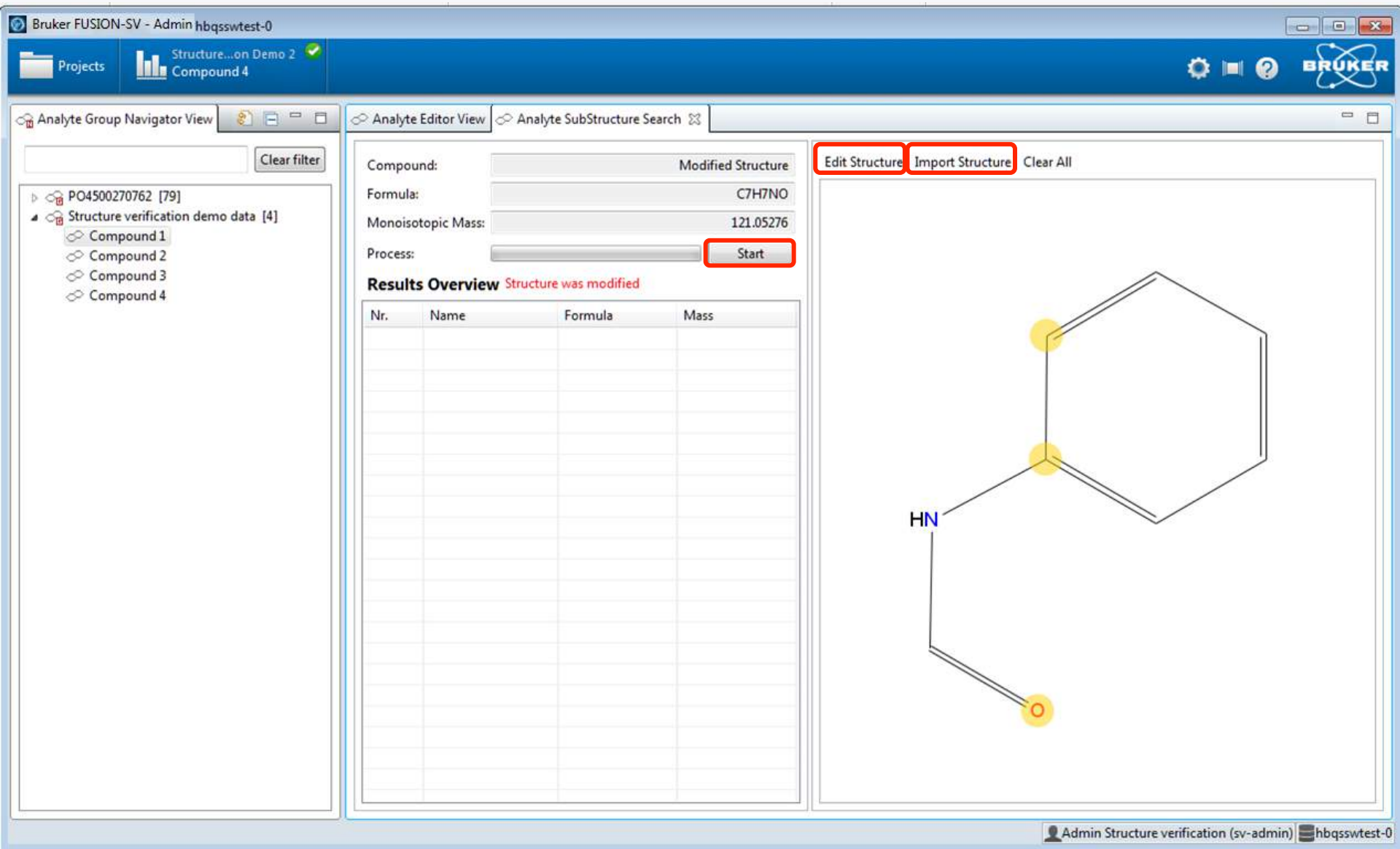
HMBC spectrum



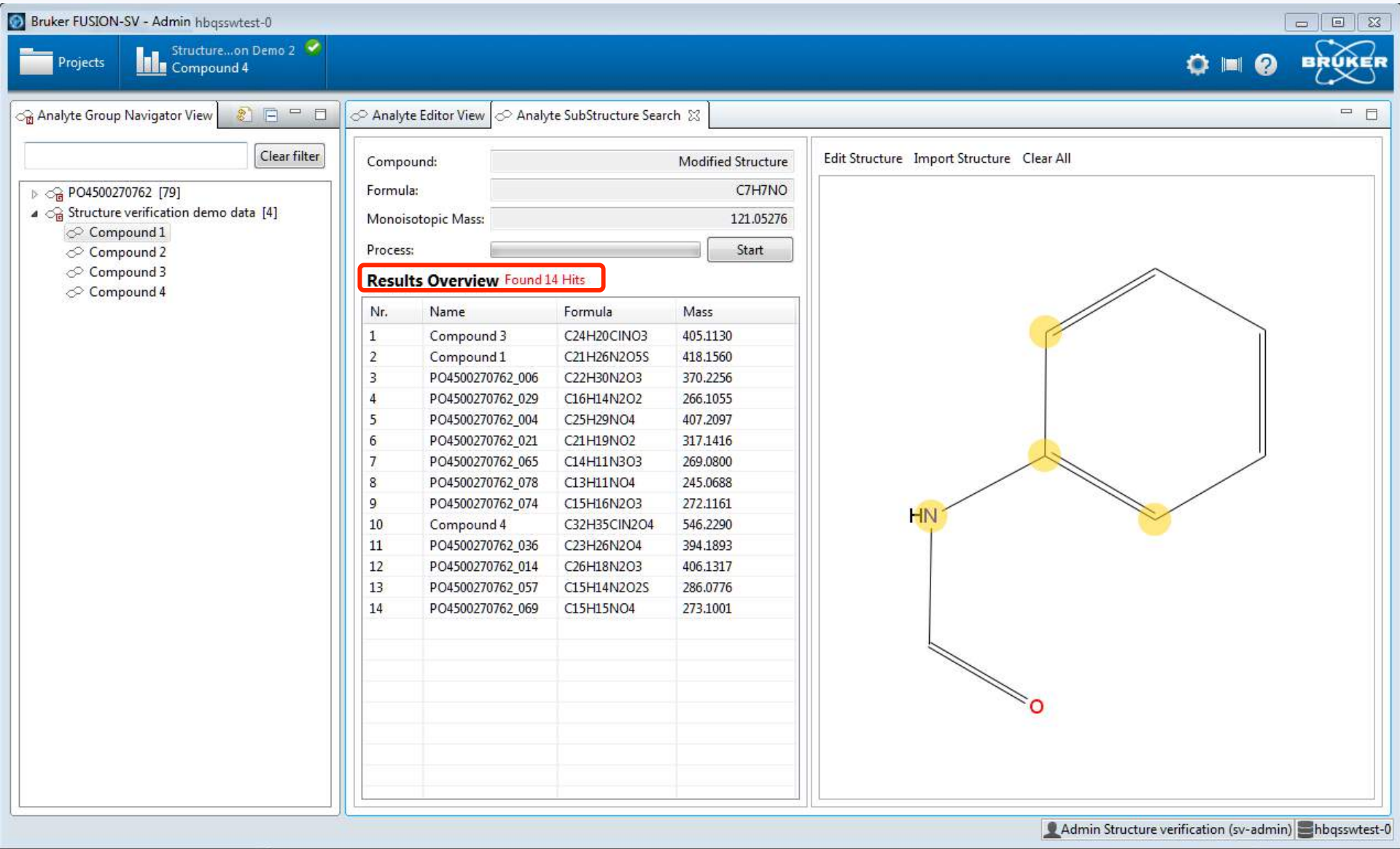
HMBC Correlation



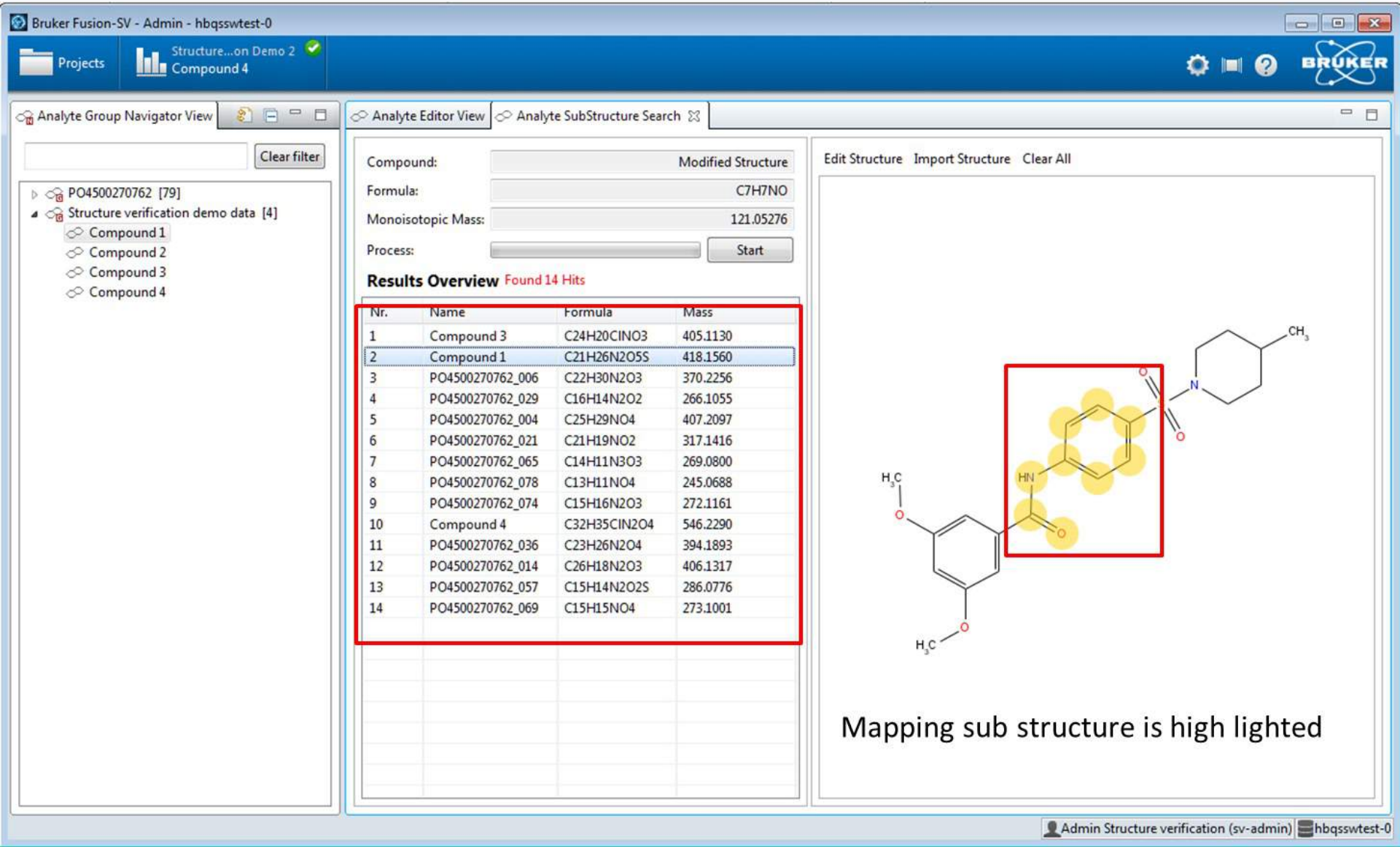
Substructure search



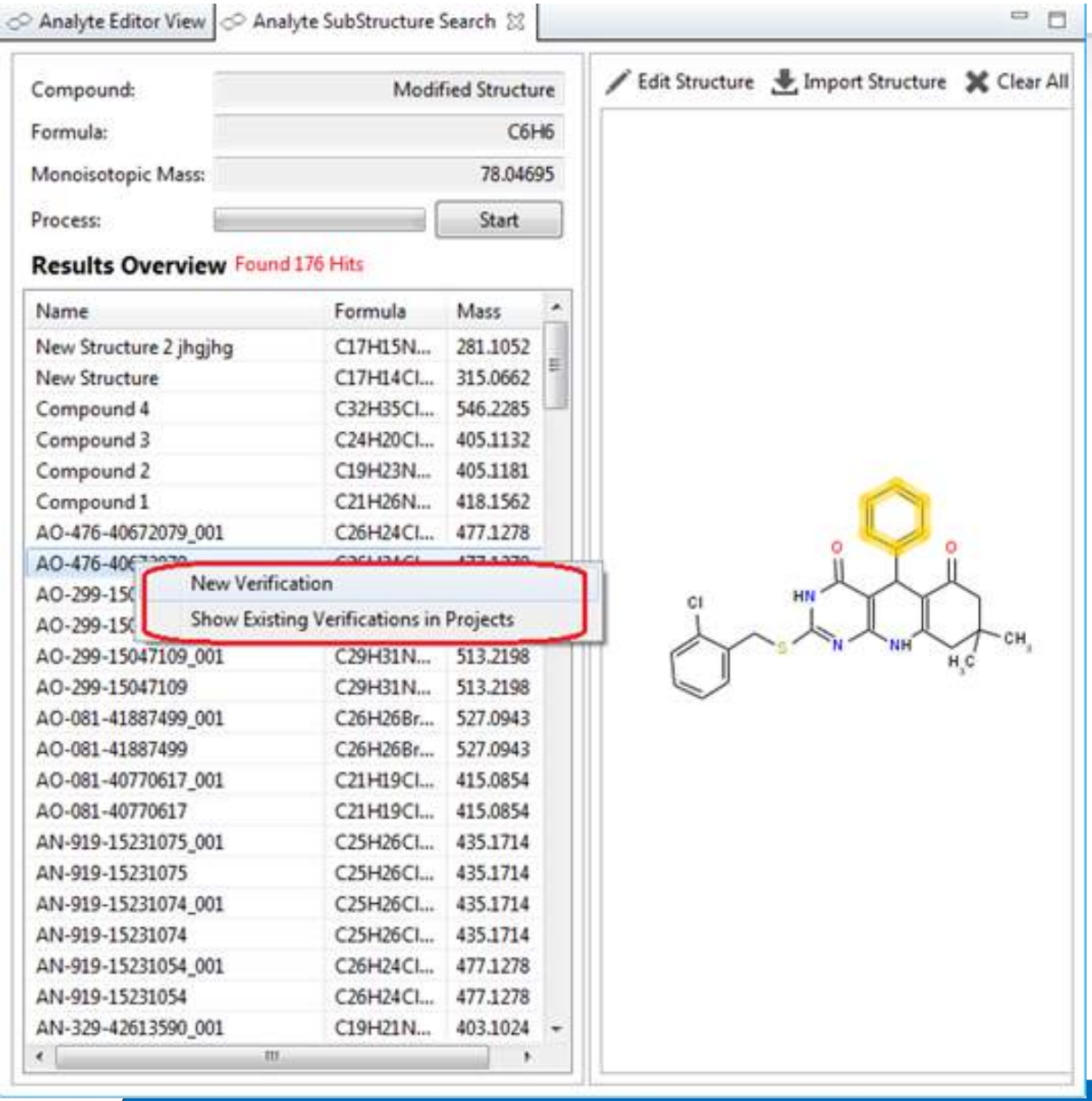
Substructure search



Substructure search

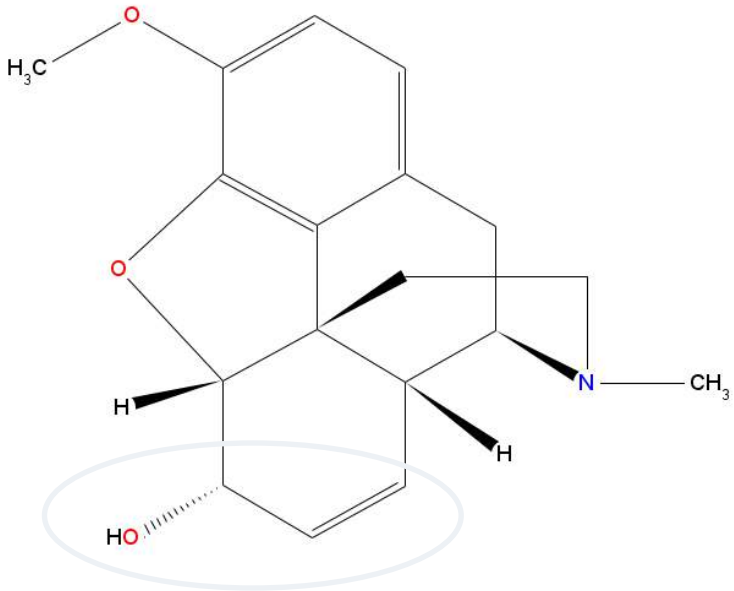


Substructure search

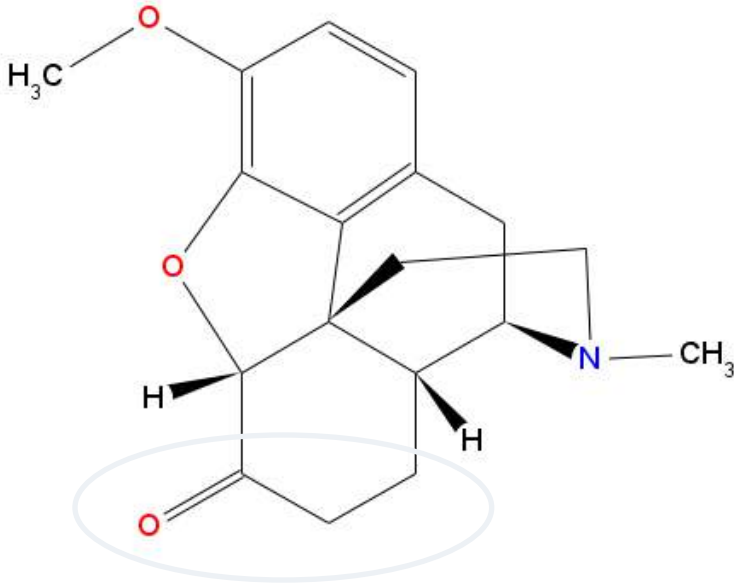


Example

Codeine and Hydrocodone

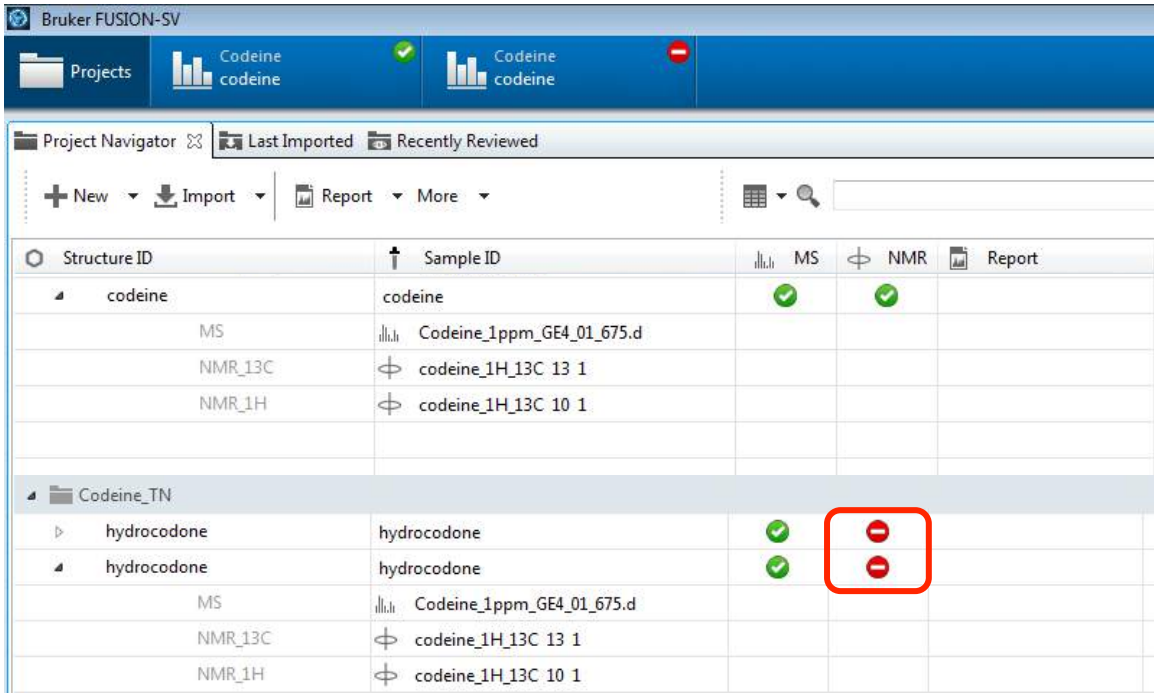


Codeine
$C_{18}H_{21}NO_3$
299.365



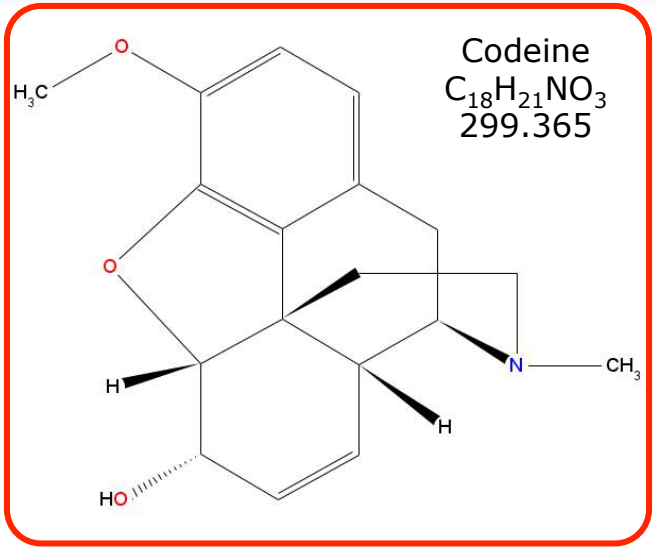
Hydrocodone
$C_{18}H_{21}NO_3$
299.365

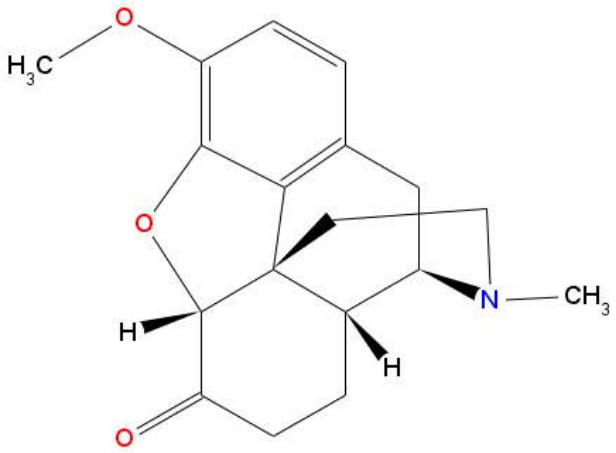
Example
Codeine and Hydrocodone

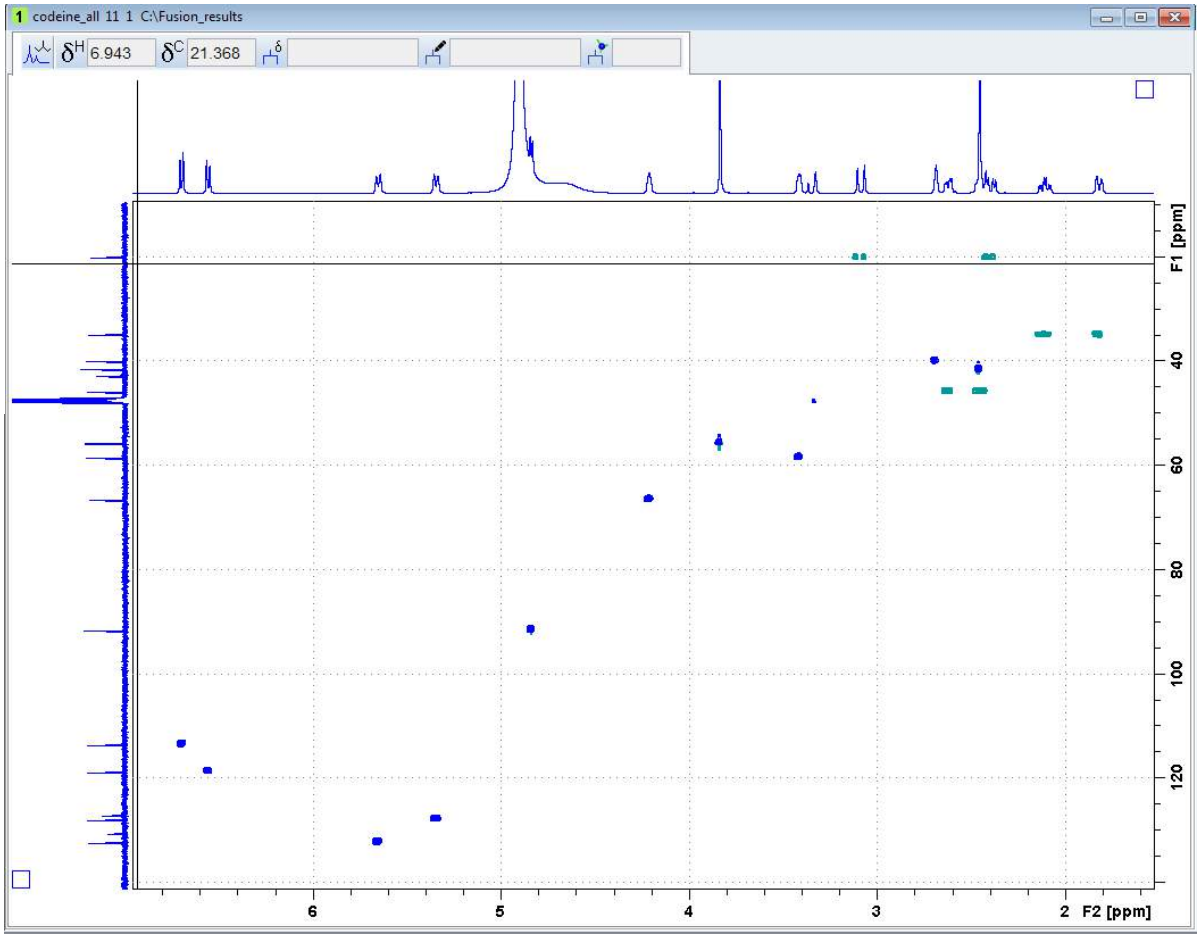


- with the wrong structure FUSION reports NOT OK from NMR

...But from the data we can tell!







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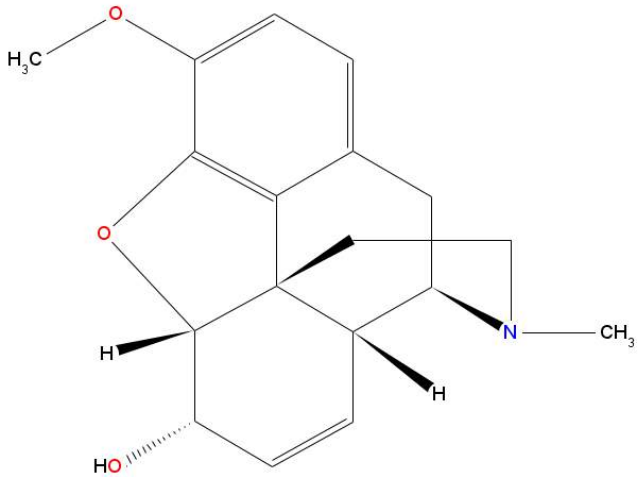
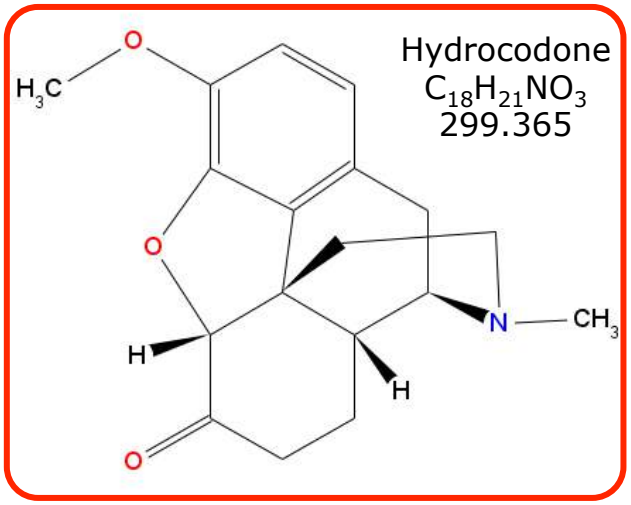
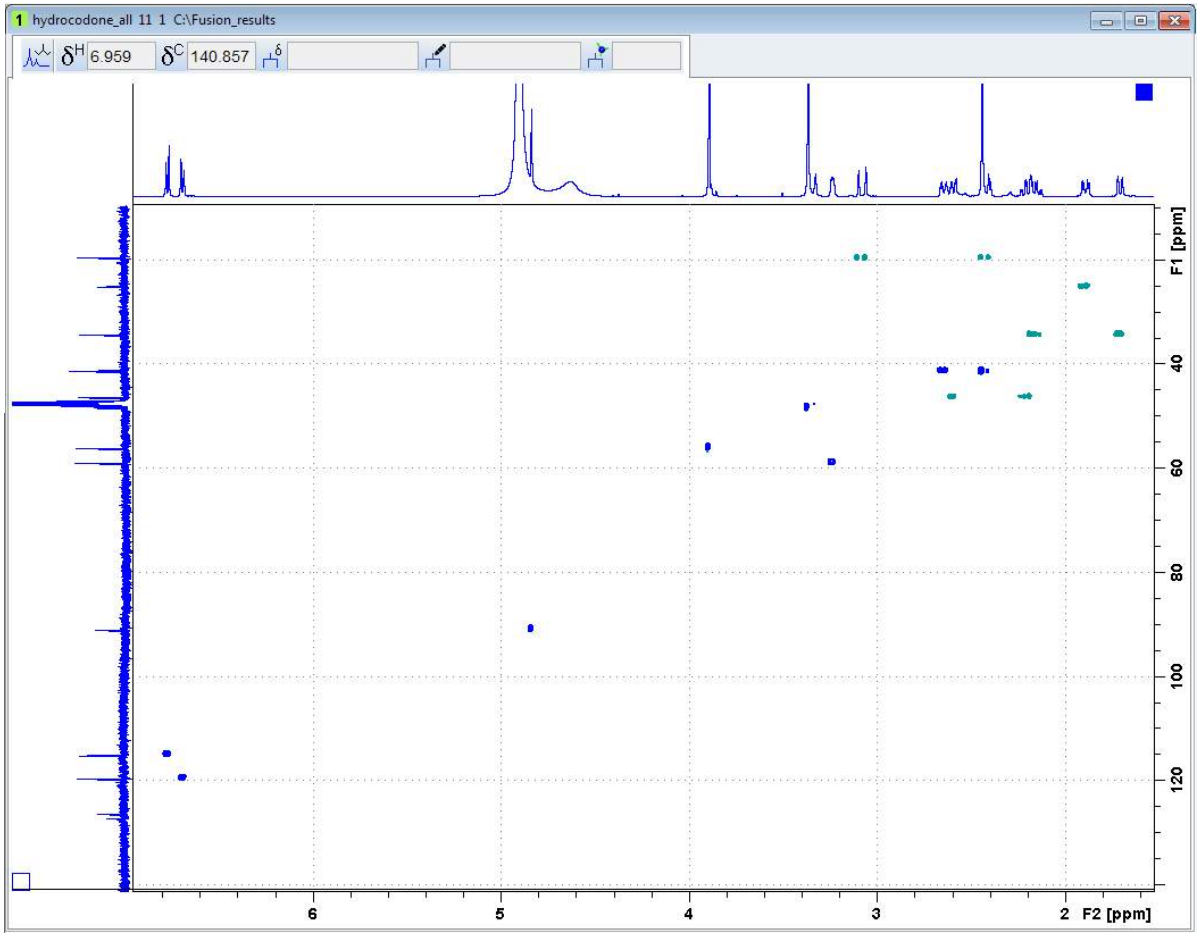
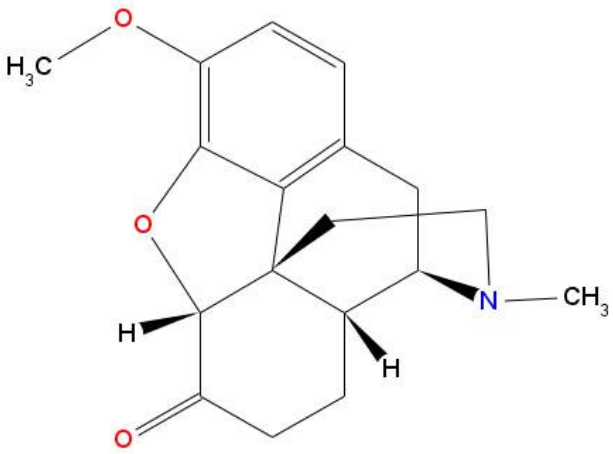


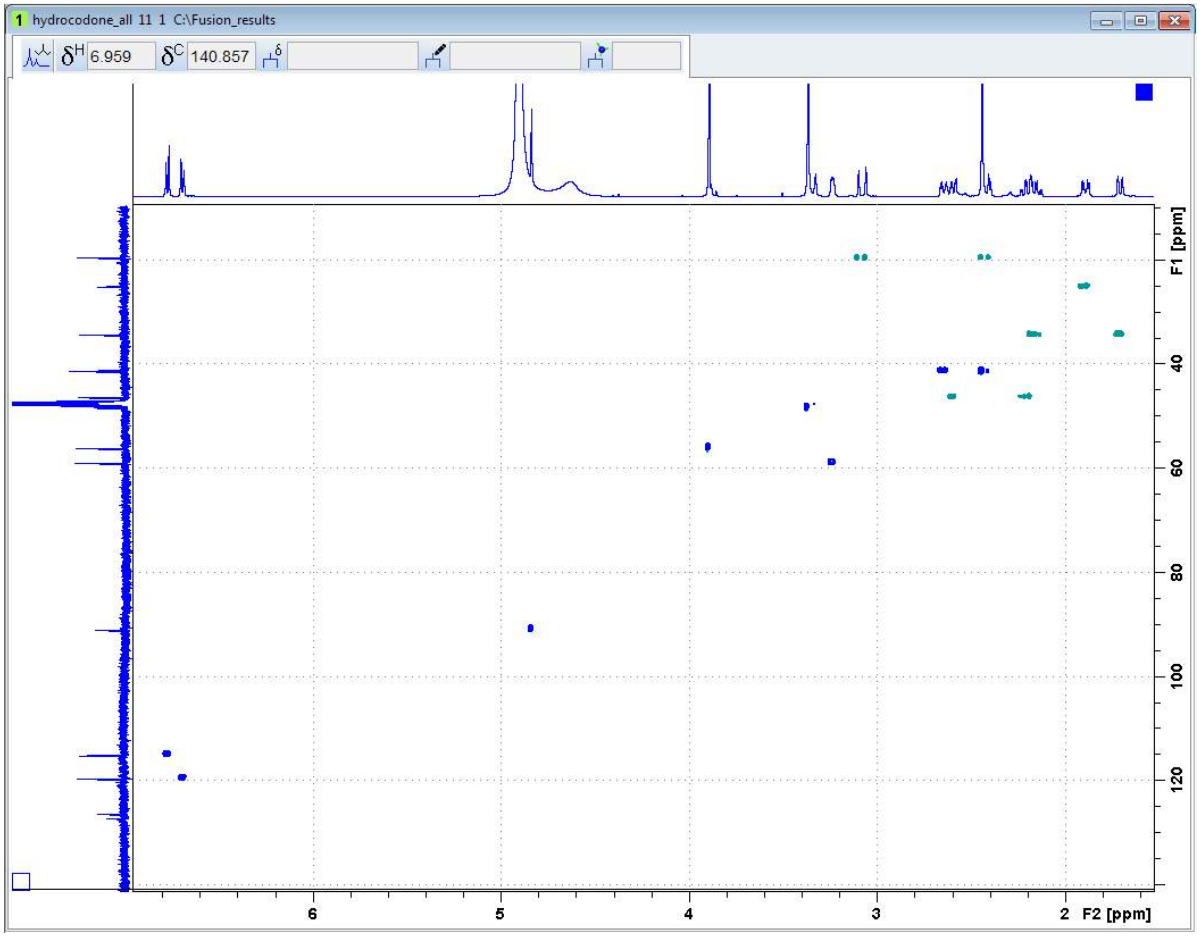




…But from the data we can tell!

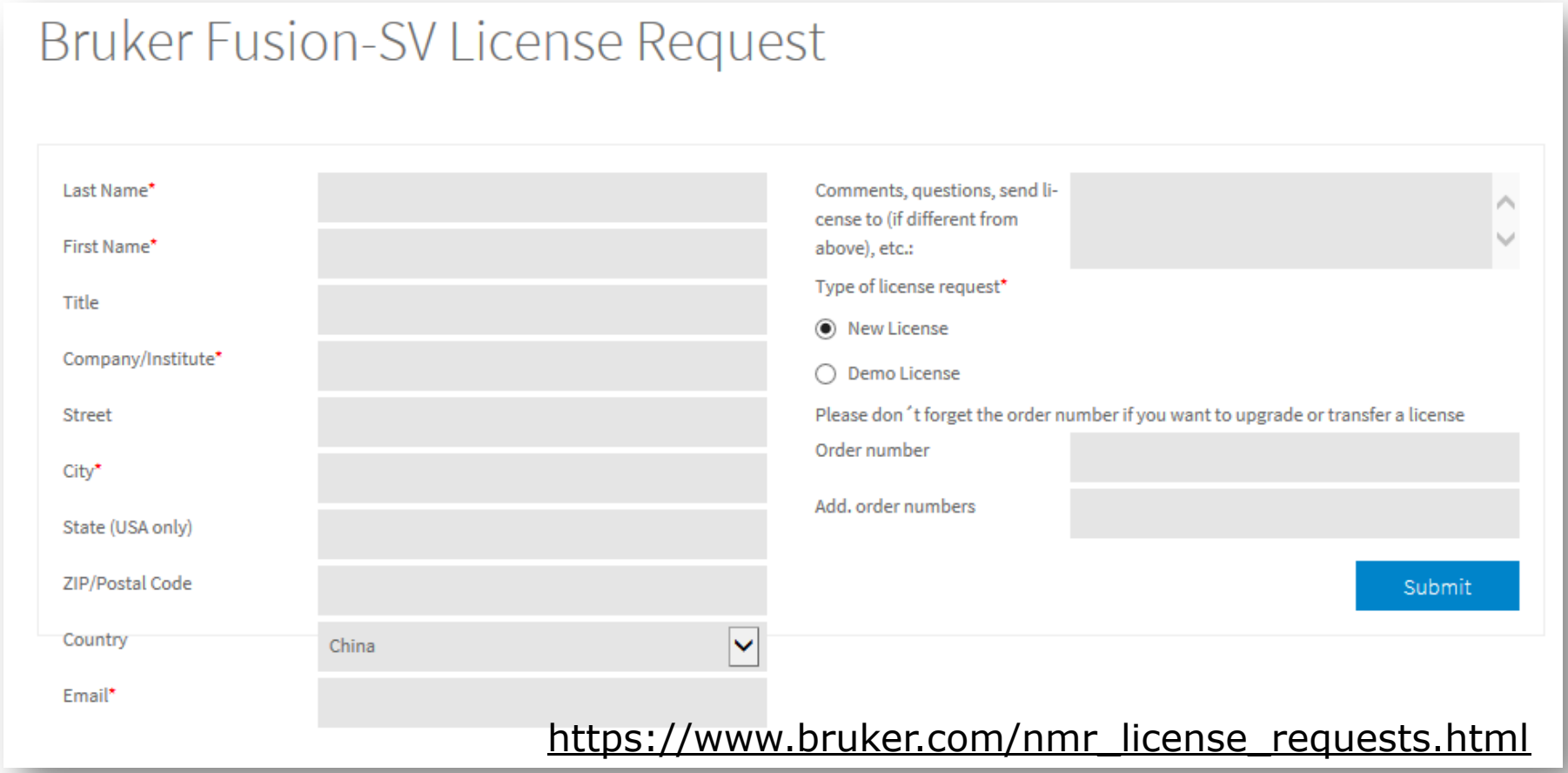
- HSQC of hydrocodone tells us something has happened, and this isn't hydrocodone anymore!





Let's Demo Fusion!

- CMC-assist and FUSION are a black box yes or no
- Be prepared when going through the data to see some incorrect assignments



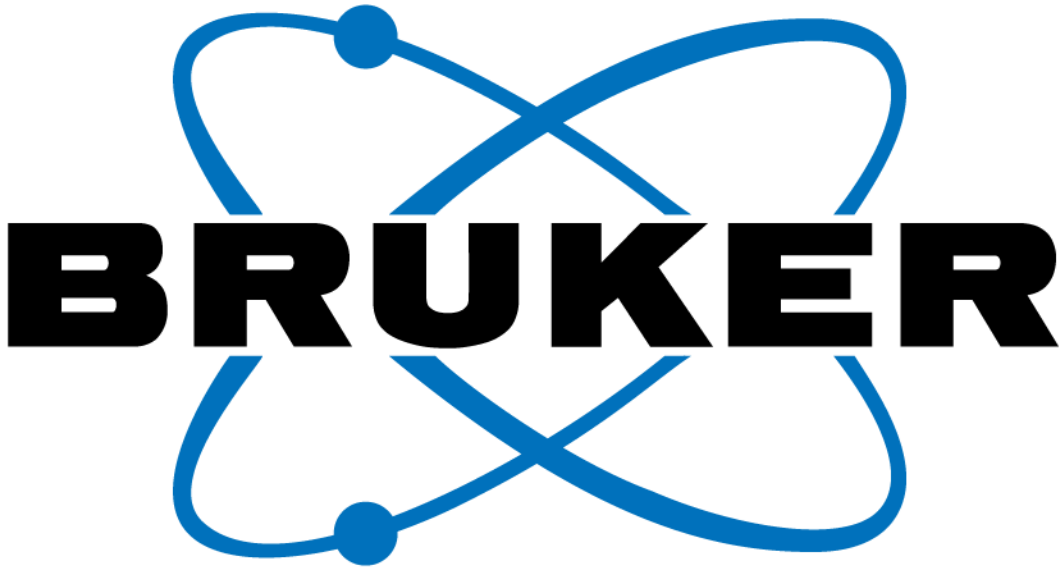
https://www.bruker.com/nmr_license_requests.html

Bruker Fusion-SV: Unique Solution for SV Synthesis Control

full integration HRAM-MS and NMR data (orthogonal techniques)

- significantly increased accuracy and throughput of Structure Verification
- easily useable – also for non-experts
- fully automated data analysis
- proprietary NMR auto-analysis algorithms based on human logic emulation
- unique *Smart Formula*™ for mass accuracy and True Isotopic Pattern (TIP)

⇨ Bruker FUSION-SV coalesces NMR data with HRAM-MS data and yields a combined result



www.bruker.com

Q & A

是否有问题?

请您在 Q&A 面板中提交您的问题

我们做的如何?

当您退出webinar的时候，请填写您对此次webinar的评价，我们非常感谢您的反馈。

Thank you!

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Lu.shan@bruker.com