FlashNote

How confident are you about your compound IDs?

The ultimate goal in metabolomics or phenomics workflows is to quickly pinpoint and confidently identify regulated metabolites ("biomarkers"), usually in large cohorts of complex samples.

Bruker´s MetaboScape enables an intuitive graphical feedback of the achieved "Annotation Quality". This scoring now includes the collisional cross section (CCS) values to boost confidence in compound identification enabled by 4D LC-TIMS-MS/MS analyses.

Challenge

Are you sure about your compound annotations? And how long did it take you to get to that level of confidence?

Solution

MetaboScape offers a sophisticated but intuitive rating system to give a direct feedback on the quality of compound annotations. All relevant parameters like e.g. the mass accuracy or the matching of isotopic patterns are provided as a visual output using the Annotation Quality Scoring icon.

Confidence at a glimpse!

The Annotation Quality Scoring gives direct feedback on the quality of your identification results – at a glimpse! Forget about tediously browsing through complex tables with cryptic types of scoring. And start trusting in the identifications done automatically in MetaboScape!

Prof. Lloyd Sumner
University of Missouri, Columbia, MO, USA

„MetaboScape AQ scoring provides rapid and intuitive visual feedback related to metabolite identifications that we highly trust. The AQ concept has been recently complemented with collisional cross section values. This allows us to incorporate very reproducible CCS value measurements from the timsTOF Pro as additional and orthogonal parameters into our metabolite identification workflow. Metabolite identifications based upon multiple orthogonal data is well aligned with the recommended reporting standards from the Metabolomics community and AQ graphic simplifies the reporting of the annotation confidence level e.g. for publications."

Authors: Ulrike Schweiger-Hufnagel, Aiko Barsch, Sven Meyer; Bruker Daltonik, Bremen

Annotation quality (AQ) symbol

For the quick and reliable de-replication of compounds in 4D metabolomics workflows, several approaches can be used. E.g. the matching of CCS values or the similarity of MS/MS spectra to spectral libraries. In MetaboScape, each annotated bucket (compound) will be labelled with a so-called AQ icon. It gives a visual and therefore very direct feedback on up to five quality parameters:

- **A** Precursor mass accuracy
- **B** Retention time fit
- **C** Isotopic pattern quality
- **D** MS/MS spectra matching
- **E** CCS values

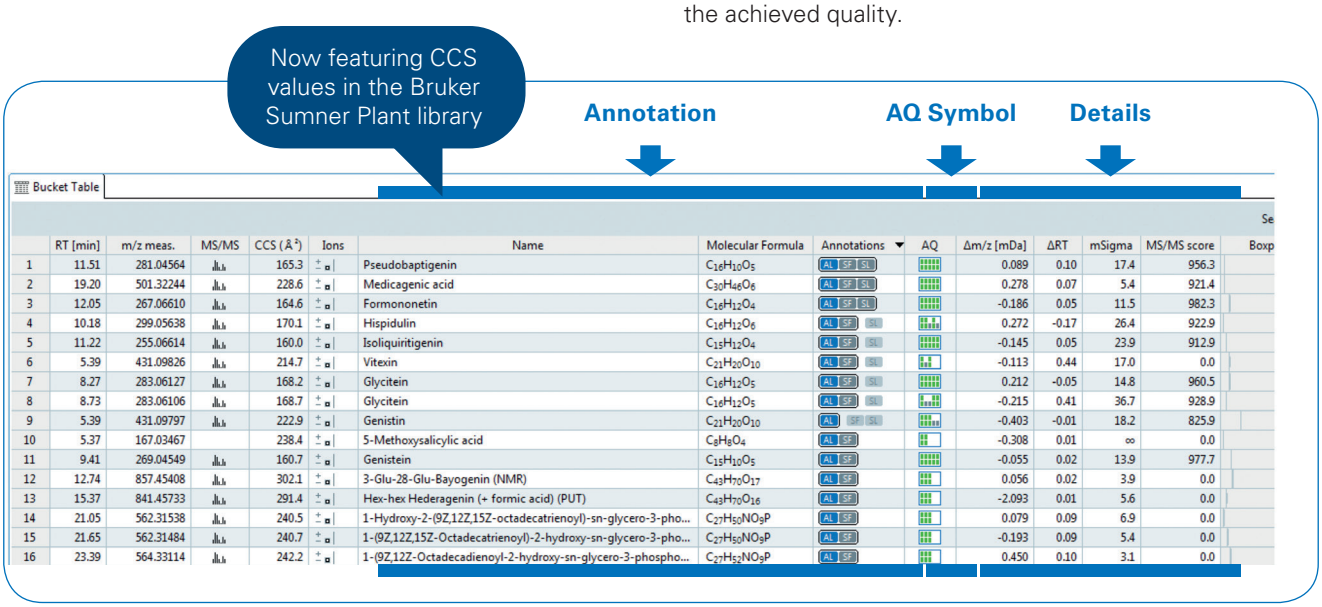
The quality achieved for each parameter is visualized by colored bars:

- Two green bars represent an excellent matching
- A moderate match is displayed by one grey bar (exemplified above for B)
- A blank column shows that either the value is not available or it didn't match

The underlying rating criteria are defined by the user. As a basis for the identification, personal Analyte Lists with a minimal input of a name and a respective formula can be used. All further input like retention times, MS/MS spectra or CCS values are optional and each can provide additional confidence in compound assignment.

Furthermore, there are several MS/MS spectral libraries supported in MetaboScape, either free of charge or commercially available: e.g. the MassBank of North America (MoNA), the LipidBlast library, the Bruker HMDB Metabolite Library.

After annotating features with an Analyte List or a MS/MS library, the bucket table shows the annotation together with the achieved quality.



	RT [min]	m/z meas.	MS/MS	CCS (Å²)	Ions	Name	Molecular Formula	Annotations	AQ	Δm/z [mDa]	ΔRT	mSigma	MS/MS score	Boxp
1	11.51	281.04564		165.3		Pseudobaptigenin	$C_{16}H_{10}O_5$	AL SF SL		0.089	0.10	17.4	956.3	
2	19.20	501.32244		228.6		Medicagenic acid	$C_{30}H_{46}O_6$	AL SF SL		0.278	0.07	5.4	921.4	
3	12.05	267.06610		164.6		Formononetin	$C_{16}H_{12}O_4$	AL SF SL		-0.186	0.05	11.5	982.3	
4	10.18	299.05638		170.1		Hispidulin	$C_{16}H_{12}O_6$	AL SF SL		0.272	-0.17	26.4	922.9	
5	11.22	255.06614		160.0		Isoliquiritigenin	$C_{15}H_{12}O_4$	AL SF SL		-0.145	0.05	23.9	912.9	
6	5.39	431.09826		214.7		Vitexin	$C_{21}H_{20}O_{10}$	AL SF SL		-0.113	0.44	17.0	0.0	
7	8.27	283.06127		168.2		Glycitein	$C_{16}H_{12}O_5$	AL SF SL		0.212	-0.05	14.8	960.5	
8	8.73	283.06106		168.7		Glycitein	$C_{16}H_{12}O_5$	AL SF SL		-0.215	0.41	36.7	928.9	
9	5.39	431.09797		222.9		Genistin	$C_{21}H_{20}O_{10}$	AL SF SL		-0.403	-0.01	18.2	825.9	
10	5.37	167.03467		238.4		5-Methoxysalicylic acid	$C_8H_8O_4$	AL SF		-0.308	0.01	∞	0.0	
11	9.41	269.04549		160.7		Genistein	$C_{15}H_{10}O_5$	AL SF		-0.055	0.02	13.9	977.7	
12	12.74	857.45408		302.1		3-Glu-28-Glu-Bayogenin (NMR)	$C_{43}H_{70}O_{17}$	AL SF		0.056	0.02	3.9	0.0	
13	15.37	841.45733		291.4		Hex-hex Hederagenin (+ formic acid) (PUT)	$C_{43}H_{70}O_{16}$	AL SF		-2.093	0.01	5.6	0.0	
14	21.05	562.31538		240.5		1-Hydroxy-2-(9Z,12Z,15Z-octadecatrienoyl)-sn-glycero-3-pho...	$C_{27}H_{50}NO_9P$	AL SF		0.079	0.09	6.9	0.0	
15	21.65	562.31484		240.7		1-(9Z,12Z,15Z-Octadecatrienoyl)-2-hydroxy-sn-glycero-3-pho...	$C_{27}H_{50}NO_9P$	AL SF		-0.193	0.09	5.4	0.0	
16	23.39	564.33114		242.2		1-(9Z,12Z-Octadecadienoyl-2-hydroxy-sn-glycero-3-phospho...	$C_{27}H_{52}NO_9P$	AL SF		0.450	0.10	3.1	0.0	

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