

Explanation of substance ranking

Details of identification (ranking)

Apo-Ident compares the measured spectrum with the other samples saved in the spectral reference library. A maximum of 20 results of the highest consistency may be displayed in the ranking table. In order to view the ranking table, please click the hyperlink **<Value>** in the result section of the user interface.

Result

Name: **Glucose monohydrate**

NIRS Result: **Match**

Value: **99.9%** (Limits 98% to 100%)

Validation: Available

A table will then be displayed which provides all the identification criteria. If you select the button **<Show as PDF>**, you will get the displayed table in PDF format and you may print and file it together with the test report.

At the first position (rank 1) the reference substance with the **highest consistency with the sample** will be displayed. If the criteria for the identification of the substance are met, it will be displayed in **green**.

Thereafter, the nearest reference substances follow in **red**. These are not directly considered in the evaluation of the measured spectrum of the sample. Please note that the name in the ranked list (classification) may differ from the substance name for substances which are summarised in groups. The group name will then be displayed (e.g. "triglycerides").

Ranking	Classification	Sample ID	Significance	Confidence	Correlation	Distance	Value
1	Glucose monohydrate	20031	0.9992	0.9992	0.9999	2.7	99.92%
2	Potassium tartrate hemihydrate	20999	0.9558	0.9076	0.9955	22.3	0.00%
3	Potassium tartrate hemihydrate	21440	0.9373	0.8063	0.9964	26.2	0.00%
4	Lactose monohydrate	20029	0.9309	0.9238	0.9905	30.3	0.00%
5	Levothyroxine sodium	21820SI	0.8920	0.7375	0.4612	41.5	0.00%
6	Borax	20179	0.8762	0.6258	0.8753	51.5	0.00%
7	Arginine	20391	0.8716	0.7486	0.8530	46.8	0.00%
8	Allantoin	20079	0.8561	0.5706	0.7040	63.1	0.00%
9	Levothyroxine sodium	21708	0.8496	0.4669	0.5237	68.3	0.00%
10	Aciclovir	21677	0.8481	0.8602	0.9089	33.0	0.00%
11	Levothyroxine sodium	21708SI	0.8421	0.1656	0.4582	73.1	0.00%
12	Calcium orotate dihydrate	20418	0.8417	0.2483	0.9431	74.8	0.00%
13	D-(+)-Mannose	21035	0.8379	0.3894	0.9617	75.4	0.00%
14	Potassium sodium tartrate tetrahydrate	20782	0.8349	0.2741	0.9798	75.2	0.00%
15	Glucose, anhydrous	20982	0.8280	0.4188	0.9749	57.1	0.00%
16	Tannin	20018	0.8279	0.2466	0.9345	85.7	0.00%
17	Starch	20181	0.8264	0.2812	0.9077	70.9	0.00%
18	Potassium sodium tartrate tetrahydrate	21801	0.8252	0.2044	0.9795	81.0	0.00%
19	Magnesium orotate dihydrate	20429	0.8236	0.0260	0.8795	95.5	0.00%
20	Morphine sulfate	21184SI	0.8220	0.3040	0.1360	100.9	0.00%

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This figure supports the confirmability and validation of the identification results by the user.

You can find an explanation of the particular terms on the next page.

Explanation of Terms

Name	Explanation	Valuation
Ranking	Determined degree of consistency of the measurement compared against the reference samples deposited in the database	
Classification	Substance or substance group clearly distinguishable by <i>Apo-Ident</i> ; A substance group represents several substances which are not distinguishable by <i>Apo-Ident</i> but are available for measurement (e.g. "triglycerides"). For a clear identification further tests are generally necessary	Indication green = identified red = not identified
Sample ID	Identification number of reference samples given by <i>HiperScan GmbH</i> to the spectra of substances which define the basis of the <i>Apo-Ident</i> library; Detailed information for all reference samples may be taken from the validation documentation	
Significance	Measure for the distance of the measurement result regarding to the mean value of the reference measurements of a sample or classification	The greater the value (maximum 1), the closer the spectrum of the sample lies to stored reference values.
Confidence	Outlier evaluation	The higher the value (maximum 1) the nearer the measured spectrum of the sample fits to the stored reference spectra.
Correlation	Statistical measure for the similarity between the back-projection of the mean of the stored reference spectra and the back-projection of the measured spectrum of the sample.	The higher the value (maximum 1) the greater the correlation of the back-projection.
Distance	Distance measure between the mean of the stored spectra of a reference sample and the measured spectrum as a function of the principal component space (Mahalanobis distance)	The smaller the value, the closer is the spectrum of the sample to the stored reference values.
Value	Uses the minimum of significance, confidence and correlation. Any rank after rank 1 forces evaluation to zero.	The greater the value (maximum 100 %), the closer the sample is to the stored reference values. The defined minimum value for an identification is 98 %.
Specificity (only for substance class of PhytoComm)	The specificity of a classification is the true negativ rate. Only if all false samples are rejected, specifity is 100 %.	
Recognition rate (only for substance class of PhytoComm)	This is the true positiv rate. It defines the amount of correctly classified spectra in the validation run.	

If you have any questions, please contact your local distributor or us:



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