

WILEY-VCH WILEY

Spectra Lab Desktop version Quick-start Guide

Powered by KnowItAll®



Desktop version Quick-start Guide

Welcome. This guide is to get you started with Wiley Spectra Lab. With millions of spectra and advanced spectroscopy software, Wiley Spectra Lab gives you the best chance of identifying unknown compounds with high confidence in the results. If you should require further assistance or would like a full demonstration of the capabilities of Wiley Spectra Lab, please <u>email us</u> and we will be happy to assist you.

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ID Expert[™] (IR/Raman)

Open Wiley Spectra Lab by double-clicking on the "Know-it-All" icon on your desktop.



Select ID Expert in the left-hand toolbar and you'll immediately be asked for a data file.



Select the appropriate file and click "open". ID Expert will recognize if the file is an IR or Raman spectrum and begin to search for a match in the databases. The results will be displayed in the results window. A score of over 90% and ideally over 95% is a good match.

Search Status	1-	Compor	nent	Results	Functio	onal Groups
1-Component Results: Top Hit: 99.1%	×	Score V	Info	Name		Chemical Structure
2-Component Results: Click to Continue Searching	1	99.09	Ō	2-NAPHTHYL	ACRYLATE	
Functional Groups:	2	80.45	١	BISPHENOL A DIACRYLATE		
10 Functional Groups Found	3	71.45	٩	METHACRYLIC	C ACID, 2,3- L ESTER	No Change and



On the top toolbar, you can change the view to Offset/Overlay/Stacked View, box zoom, and scale.



If the search finishes without finding a reasonable 1-component hit, it will then run a 2-component, then 3-component and so on. If no hit is found, make sure "Optimized Corrections" is enabled for the appropriate technique in the "Optimized Corrections" tab under File->Settings.

	Settings
	General Optimized Corrections Databases
	Iechnique: IR Raman
ID Expert - KnowItAll® Informatics Syst	✓ Enabled
<u>File Edit View License H</u> elp	✓ <u>B</u> aseline
Open Spectrum Ctrl+O	Vertical Clipping
	✓ Intensity Distortion
Create PDF Report	✓ <u>H</u> orizontal Offset
Cattings	Vertical Offset
Settings	☑ ATR Correction Adjustment
Exit Alt+F4	ATR Correction Polarization

ID Expert[™] (IR/Raman)

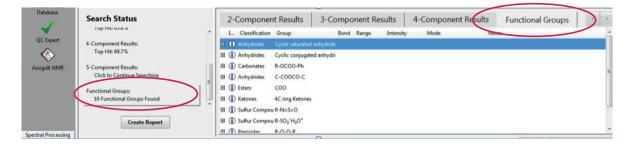
Optimized corrections is a feature unique to Spectra Lab that automatically and instantly performs multiple data and spectral corrections, which would otherwise require lengthy, manual data processing by an expert in each technique. To see which corrections are performed on any spectrum, click the "i" button.



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If no hit is found in any search, the "Functional Groups" analysis will suggest which functional groups could be present to help with further analysis through other techniques.



If a yellow question mark appears in the "Query Status" area, Spectra Lab is telling us there is a problem with one or more components of the spectrum.

Checklist	St	atus	Fix?
Baseline	2	١	
Voise		١	
Contaminants		١	
Fechnique		٦	ATR-IR

Click the "i" icon to see what the problem is

Baseline Analys	sis Status: Uncertain
Area difference between the original spectrum and - 8.9% he wake above is the percentage of the area difference obtained the original spectrum and a baseline control of version areas used to determine whether or not a baseline control on a necessary.	a baseline-corrected version of the original spectrum:
	4000 3500 3000 2500 2000 1500 1000 500

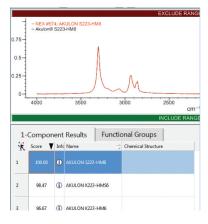
Then check "Fix" to use have Spectra Lab correct the problem. ID Expert then restarts the query with the corrected spectrum.

Deformulation Expert[™](IR)

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Deformulation Expert is used to examine the components of a formulated product by IR spectroscopy. Open a spectrum in ID Expert and let the spectral search run. This will match the IR spectrum of the complete product.



Transfer the query to Deformulation Expert by clicking "Transfer to: Deformulation Expert"

🙇 ID Expert - KnowItAll® Informatics System, Wiley Spectra Lab Edition	
File Edit View License Help	
💠 👻 🚽 🔻 Transfer to: 🗞 Report 🕅 🖧 Deformulation Expert 🚳 Searchit 🆓 Mixture Analysis 🐨 Minelt Database 🖌 QC Expert 🚫 Processit IR 🔇 Analyzelt IR 🔇 Analyzelt	Polymer IR
Basics ID Expert	
Data 🖉 🖻 🖻 🕅 🕅 🖓 🖟 + 🛄 🖳 🕙 👒 🛣 🌆 \leftrightarrow λ 🚧 🛄 🚛 🖽 🦄 🛄 🖬 🕼	

The deformulation analysis will then show the breakdown of the components of the sample.

New Search	1-	Compo	onent	Results	2-Component	Results		
	×	Score	▼ Info	Weight 🗦	Name 🚽	Chemical Structure	Spectrum	<auto> (IR/ATR-IR)</auto>
Search Status								
1-Component Results: Top Hit: 73.9%	^ 1	98.81		N.A.	Composite Spectrum		_hr_	Mulu
2-Component Results: Top Hit: 98.8%	E		١	0.57	POLY(HEXAMETHYLENEA DIPAMIDE)		_lm_	Mun
3-Component Results:	-		١	0.43	MAGNESIUM SILICATE, HYDRATE			lu
Create Report				N.A.	Residual Spectrum			

QC Expert[™](IR)

One-Time Configuration

Your copy of Wiley Spectra Lab needs to have an Administrator account configured. Perform these steps before running any samples.



After loading QC Expert for the first time, you will get a "There are no users defined for this application" message. Click "OK", add your digital signature and password, make sure "Administrative Privileges" is checked then click "OK".

Add New Digital Sign	ature 💌
Digital Signature:	
$\left(\right)$	Administrative Privileges
<u>P</u> assword:	
Confirm Password:	
	OK Cancel

Add the relevant details and verify. Then add any user accounts in the same way but uncheck "Administrative Privileges".



Setting a Reference Spectrum

To select the reference database, click File->Settings and select the one you want to use on the "Reference/Validation Databases" tab, then click "OK".

✓ QC Expert - KnowitA Eile Edit View Lice Eile Edit View Lice Eile Edit View Lice Eile Edit View Lice Sample Spect	nse <u>H</u> elp ≷ + 	. @ <	Settings Genefal Reference/Validation Databases Iechnique: IR • Available for Searching:
Checklist	Status		
Baseline			
Noise			Reference - Unlicensed ATR-IR - Controlle

To select a reference spectrum, click "Select Reference Spectrum".

Select Reference Spectrum

QC Expert[™](IR)

Login as administrator then search for the desired spectrum in the reference database. Set the algorithm, match threshold, and proximity warning parameters in the lower left, then click "OK".

Technique:	IR			•]		
<u>Filter</u> :	DEET						
Name		7 L	ot Number	1	CAS Registry Num;		
					134-62-3	Sigma-Aldrich Company LLC., Supelco	Multi-Techniq Demo Databas Bio-Rad Sadtle
<u>C</u> ompariso	n Algorithm:	Correl	lation		•		
-	n Algorithm:		lation		•		

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Running a sample

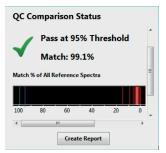
To run a sample, click on "New Comparison" and if the sample is ATR-IR or NIR, this can be indicated. Click "OK" and the analysis will run.

ample Specti	rum Status			Recent Places		known Sample 5021961.irf	29/07/2016 12:00	IRF File
Checklist	Status	Fix?		inceciar inces		of Unknown Sample 8675309.irf of Unknown Sample 1282013.irf	29/07/2016 12:00 29/07/2016 12:00	IRF File IRF File
	Status					of Unknown Sample 09071995.irf	29/07/2016 12:00	IRF File
Baseline					Akulon S22	3-HM8.irf	29/07/2016 12:00	IRF File
Noise				Desktop	DEET.SPA		29/07/2016 12:00	SPA File
Contaminants					Epichlorohy	drin Sample Spectrum.irf	29/07/2016 12:00	IRF File
					Raman Spe	ctrum of Mint Candy.wdf	29/07/2016 12:00	WDF File
Technique		· · · ·		Libraries	📄 Raman Spe	ctrum of Plastic.l6s	29/07/2016 12:00	L6S File
				Computer ZWEILI5238	•			Þ
) New Comparise	on			File name:		- (<u>O</u> pen
					Files of type:	All Files (*.*)	•	Cancel
QC Compariso	n Status		Name	Imported spe	ctrum in ATD-ID	Imported spectrum is Near	TD .	
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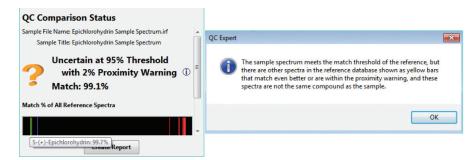
QC Expert[™](IR)

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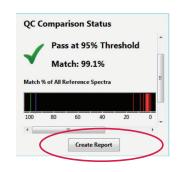
The "QC comparison status" will then show "pass" "fail" if the sample and reference spectra match or don't match.



"Proximity warning" is displayed if the sample and reference spectra match but the sample spectrum also matches another spectrum that isn't the chosen reference spectrum. Click "i" for more information. Hovering over the colored bars will display the names of the spectra that are within the proximity warning parameter.



To create a digitally-signed report Click on "create report", select your name from the "digital signatures" drop-down, enter the password, fill out the sample information, then click "OK".



SearchIt[™] & MineIt[™] for GCMS

Open Wiley Spectra Lab by double-clicking on the "Know-it-All" icon on your desktop.





Select Searchlt in the left-hand toolbar.

Set "Limit Spectral Technique" to MS then click "Remove All" then "Add All". This activates only the MS databases for the search.

Jatabases					
Available for Searching:					
	Limit to spectral technique:	All	-		Refresh Advanced
All	Name	All	ode	Location	
Local	118 NMR - Wolfgang Robi	e Near IR		<latest version=""></latest>	
Networks	13C NMR - AIST SDBS	1H NMR		<latest version=""></latest>	
Reference - Licensed	13C NMR - Bio-Rad Sadtler	11B NMR		<latest version=""></latest>	
- Reference - Unlicensed	13C NMR - Flavors & Fragr	15N NMR		<latest version=""></latest>	
- User	13C NMR - Natural Produc			<latest version=""></latest>	
- Hit List	13C NMR - NIOSH Pocket	19F NMR		<latest version=""></latest>	
	13C NMR - Organic Comp	31P NMR		<latest version=""></latest>	
< >	•	UV-Vis		m	
		Raman MS			Remove Remove

Click the "Open Spectrum or Structure" button on the top SearchIt toolbar to open the spectrum file, select the desired file then click "Open".

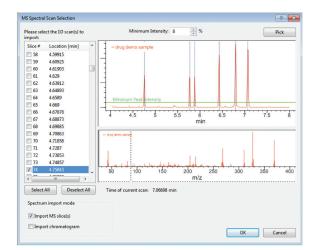
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iii ID France	Search Open Spectrum or Structure rame Basic: Databases

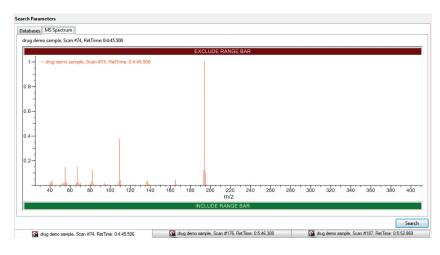
SearchIt[™] & Minelt[™] for GCMS

The GCMS chromatogram or total ion chromatogram (TIC) is shown. Set the minimum peak intensity by dragging the green bar up or down to include or exclude peaks.

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Click "OK" to import all the MS slices. Select the MS slice that you want to identify and click "Search" to start the search.



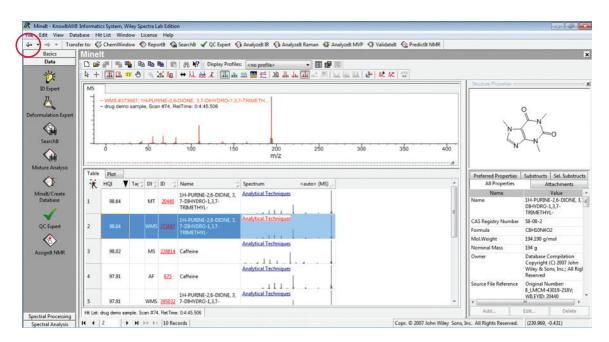


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SearchIt[™] & Minelt[™] for GCMS

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Hits are ranked according to hit quality index (HQI) and spectrum information including synonyms for the selected matching spectrum is displayed on the right.

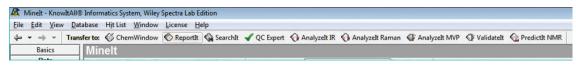


To identify the next MS slice, click the "back" button on the top left, select the spectrum and click "Search" to start the search.

On the top toolbar, you can change the view to Offset/Overlay/Stacked View, box zoom, and scale.

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To make a report, click "Transfer to: ReportIt" on the top toolbar.



SearchIt[™] & Minelt[™] for GCMS

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Select a Report Template			-2
ease select one of these temp		10.	
Title Landscape	File Path C:\Users\Public\Documents\Bi	BIO FAD Indefinition	Date Time And a Karm
Landscape with peak list Mixture Analysis Portrait Portrait Portrait with peak list Spectrum Landscape Spectrum Portrait	Cr\Users/Public\Documents/Bi Cr\Users/Public\Documents/Bi Cr\Users/Public\Documents/Bi Cr\Users/Public\Documents/Bi Cr\Users/Public\Documents/Bi Cr\Users/Public\Documents/Bi	CA1 + VHR (PM) CA1 + VH	

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Double-click on "Title here" on the top left to enter a title and double click on "Date/Time" or "Analyst Name" on the top right to enter the corresponding details.

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BIO RAD Bio-Rad Laboratories Informatics Division	Date/Time: Analyst Name:
Title Here	
1 - WMS #373687; 1H-PURINE-2,6-DIONE; 3,7-DIHYDRO-1,3,7-TRIME - drug demo sample, Scan #74, RetTime: 0.4:45.505	THVL-
0.8	N N
0.6	2 Lyco
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0 50 100 150	2do 250 3do 350 4do m/z
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Opener, y₂, n. L Synonyme	13.7 YHARTYIC 5. SOLIYOON HHPURIKE 2.8 DIOILE # 1.3.7 YHARTYIC 5.0 OHYOON HHPURIKE 2.8 DIOILE (COMPUTER GENERATED 1.3.7 TANKITYIC 5.0 DIOINE HHPURIKE 2.8 DIOILE (COMPUTER GENERATED 1.3.7 TANKITYIC 7.3 DIVIYOON HHPURIKE 2.8 DIOILE (COMPUTER GENERATED 1.4.7 TANKITYIC 7.5 DIVIYOON HHPURIKE 2.8 DIVIX 7.5 TANKITYIC 7.5 TANK

Report templates can be customized, including the layout, by clicking "Edit Report Templates" in the "File" menu in the main "Minelt" window.

ile	Edit View Database	Hit List	Window	License
	New Database			Ctrl+N
	Open Database			Ctrl+0
	Open Hit List			
	Close		Ct	rl+W/F4
	Close All			
	Import			Ctrl+I
	Batch Import			
	Import Attachment(s)			
	Export			
	Save Hit List As			
	Edit Report Templates			
	Preferences			

SearchIt[™] & MineIt[™] for NMR

Open Wiley Spectra Lab by double-clicking on the "Know-it-All" icon on your desktop

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Select SearchIt in the left-hand toolbar.

Set "Limit Spectral Technique" to the appropriate NMR technique then click "Remove All" then "Add All". This activates only the NMR databases for the search.

Databases						
Available for Searching:						
	Limit to spectral technique:				Refresh Adva	anced.
All	Name	All IR	ode	Location		
Local	11B NMR - Wolfgang Robie			<latest version=""></latest>		
Networks		1H NMR		<latest version=""></latest>		
Reference - Licensed	13C NMR - Bio-Rad Sadtler	11B NMR 13C NMR		<latest version=""></latest>		
Reference - Unlicensec	13C NMR - Flavors & Fragra	15N NMR		<latest version=""></latest>		
User	13C NMR - Natural Product			<latest version=""></latest>		
- Hit List	13C NMR - NIOSH Pocket C	19F NMR		<latest version=""></latest>		
	13C NMR - Organic Compo	31P NMR		<latest version=""></latest>		
4 III +		UV-Vis	-	.111		

Click the "Open Spectrum or Structure" button on the top SearchIt toolbar to open the spectrum file, select the desired file then click "Open".

🧟 SearchIt - KnowIt	All® Informatics System, Wiley Spectra Lab Edi
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·	Search Open Spectrum or Structure ram
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Searchlt[™] & Minelt[™] for NMR

To process the spectrum, click "Transfer to ProcessIt NMR"

🧟 SearchIt - Kn	owItAll® Informatics System, Wiley Spectra Lab Edition
<u>File Edit Viev</u>	v <u>L</u> icense <u>H</u> elp
$\leftrightarrow \star \rightarrow \star$	Transfer to: 🔇 Reportit 💊 Mixture Analysis 🕥 Minelt Database 🖌 QC Expert 🚫 Processit NMR
Basics	Searchit



To apply processing macros, click "Macro" and either create or edit a macro or apply an existing one. For 13C NMR, the in-built "C13ProcessSample" can be used for minor spectral corrections.

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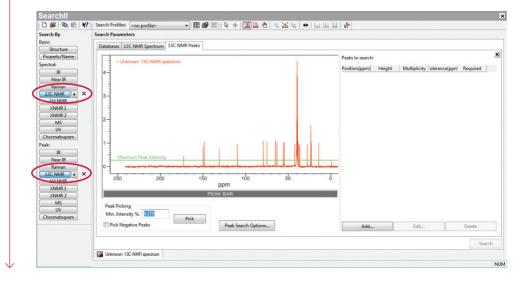
A ProcessIt NMR - KnowItAll® Inform	atics System, Wiley Spectra Lab Edition
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Spectral Processing	H1ProcessSample
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When processing is complete, click "SearchIt and Save" on the top toolbar.

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← ▾ → ▾ Return to: SearchIt and Save	SearchIt and Discard
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On the "SearchIt" screen, click the corresponding technique under "Peak" on the left-hand side, then click the corresponding technique under "Spectral" in the menu above to deselect it. Set the minimum peak intensity by either typing the value into the "Min. Intensity" box or by dragging the green line to the desired position, then click "Pick" to pick the peaks.



Searchlt[™] & Minelt[™] for NMR

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Search By	Search Parameters									
Basic:	Databases 13C NMR Peaks									
t Structure					a 0000 0					×
Property/Name	- Unknown 13C-NMR spectrum				Peaks to search	6				-
Spectral:					Position(ppm)	Height	Multiplicity	olerance(ppm	Required	
I Expert IR	4-				14.22	1.01	unknown	2.00	No	
Near IR	1				22.73	1.05	unknown	2.00	No	
Raman 13C NMR					23.62	1.76	unknown	2.00	No	
13C NMR 1H NMR	3-				27.65	0.94	unknown	2.00	No	
XNMR1					36.44	0.93	unknown	2.00	No	
XNMR 2					37.46	0.96	unknown	2.00	No	
ilysis MS	2-1				38.95	1.89	unknown	2.00	No	
UV					39.23	3.80	unknown	2.00	No	
Chromatogram					39.51	4.48	unknown	2.00	No	=
ate Peak	1-1				39.79	3.90	unknown	2.00	No	
e IR			1 11		40.07	2.02	unknown	2.00	No	
Near IR	Minimum Peak Intensity				40.35	0.72	unknown	2.00	No	
Raman	0-			المراجعة المساطنيات	42.32	0.96	unknown	2.00	No	
rt 13C NMR +	250 200	150	100		54.71	1.04	unknown	2.00	No	
1H NMR	250 200	150 ppm	100	50	0 55.85	1.04	unknown	2.00	No	
XNMR1				_	65.06	1.03	unknown	2.00	No	
MR XNMR 2		PEAK BAR			75.06	1.06	unknown	2.00	No	
MS	Peak Picking				79.28	1.09	unknown	2.00	No	
UV	Min. Intensity %: 6.175				109.71	0.96	unknown	2.00	No	
Chromatogram	P	ick			130.88	0.77	unknown	2.00	No	-
	Pick Negative Peaks	Peal	k Search Options		Add		Edit		Delete	

Hits are ranked according to hit quality index (HQI) and spectrum information including synonyms for the selected matching spectrum is displayed on the right.

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	×	HQI 🔻 Ta	Í LÍ	45638	Andrographolide		C NMR)			All Properties Name CAS Registry Number	Attachments Value Andrographolide 5508-58-7	
	×	HQI 🔻 Ta	NO	45638	Andrographolide	Analytical Techniques	C NMR)		E	All Properties Name CAS Registry Number Formula	Attachments Value Andrographolide 5508-58-7 C20H30O5	
	×	HQI V Ta	NO	45638	Andrographolide	Analytical Techniques	C NMR)		×	All Properties Name CAS Registry Number Formula Instrument Name	Attachments Value Andrographolide 5508-58-7 C20H30O5 Varian CFT-20	\$
	×	HQI V Ta	NO	45638 20592	Andrographolide ANDROGRAPHOLID;COM POUND=#1 ENT-14-BETA-HYDROXY-	Analytical Techniques			×	All Properties Name CAS Registry Number Formula	Attachments Value Andrographolide 5508-58-7 C20H30O5	s
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	×	HQI V Ta 76.88 76.88	WRX	45638 20592 150940	Andrographolide ANDROGRAPHOLID;COM POUND=1 ENT-14-BETA-HYDROXY- 8(7),12-LABDADIEN-16, 15-OLIDE-3- BETA.19-	Analytical Techniques Analytical Techniques			, H	All Properties Name CAS Registry Number Formula Instrument Name	Attachments Value Andrographolide 5508-58-7 C20H30O5 Varian CFT-20 A. Patra, A.K. Mitra, S. Biswas, Org. Magn.	s
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	K 1 2 3	HQI V Ta 76.88 76.88	WRX	45638 20592 150940	Andrographolide ANDROGRAPHOLID;COM POUND-91 ENT_14-BETA-HVDROXY- 8(7),12-LABDADIEN-16, 15-OLIDE-3- BETA,19- ANDROGRAPHOLIDE-3-12- ADDROGRAPHOLIDE-3-12- BICAHYDRO-6-	Analytical Techniques Analytical Techniques				All Properties Name CAS Registry Number Formula Instrument Name Literature Reference Mol.Weight	Attachments Value Andrographolide 5508-58-7 C20H3005 Varian CFT-20 A. Patra, A.K. Mitra, S. Biswas, Org. Magn. Resonance 16, 75 (198 350.455 g/mol DMSO-D6 Chemical Concepts. A	s
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