



MSChromSearch 3.0

Software for chromatogram comparisons

Axel Semrau®

Users are regularly faced with the task of comparing chromatograms from GC/MS systems or analog detectors. Currently this is usually done visually and is thereby rather subjective. In addition, it is almost impossible to deal with larger numbers of complex chromatograms based on visual comparison.

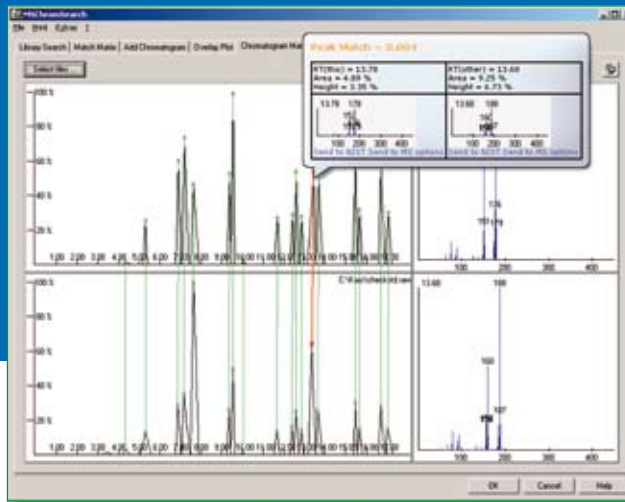
This is exactly where MSChromSearch comes in: MSChromSearch compares a chromatogram with a library of other chromatograms, similar to a library search in a mass spectrum library. The user can select between mass spectra, retention times, retention indices, and/or peak intensity data. From the selected data a "fit value" is calculated as a measure for the match between two chromatograms. Chromatograms that were found are listed in the form of a hit list based on the fit value. MSChromSearch enables comparison of a chromatogram with several hundred chromatograms within a very short time.

In addition, two chromatograms from different data systems can be compared in detail in order to obtain information about interrelationships or deviations.

The software can be used in pyrolysis applications for identification of organic solids, for comparison of volatile components to determine the cause of a fire or in quality control for good/poor comparison of samples.

MSChromSearch saves a tremendous amount of time (just think how long a visual comparison of several hundred chromatograms would take), and offers an objective numerical value for the match between two chromatograms.

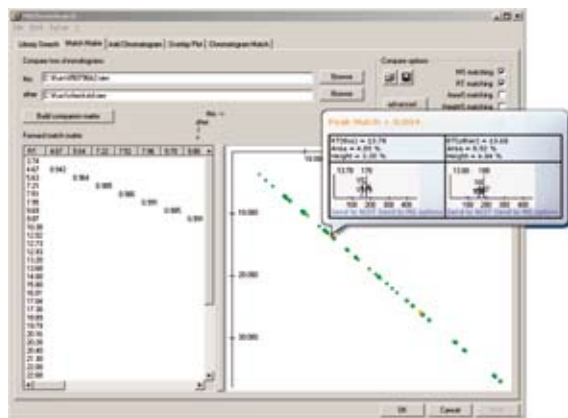
MS chromatogram comparison fast, efficient, easy



MSChromSearch software enables fully automatic comparison of chromatograms.

New useful functions have been added in Version 3.0:

- ✓ New module for reading Agilent Chemstation files
- ✓ New overlay module enables superposition of any number of chromatograms from different data systems
- ✓ New "Chromatogram Match" module offers detailed comparison of two chromatograms and their spectrums and a NIST search option
- ✓ Chromatogram search in subfolders allows building structured chromatogram libraries
- ✓ Comprehensive Online help
- ✓ Mass spectrum import from NIST and other programs
- ✓ Inclusion of LC/MS chromatograms
- ✓ With MSChromSearch 3.0 retention indices can now also be used for comparison



Comparative matrix of two chromatograms with one highly differing peak (Peak Match)

List of results with numerical values for the dimension of conformance

Name	RT	Area	Height
A1 1-Butanol	13.78	4.89	3.38
A2 2-Butanol	13.68	9.25	4.73
A3 1-Pentanol	13.58	13.61	6.08
A4 2-Pentanol	13.48	17.96	8.42
A5 1-Hexanol	13.38	22.31	10.76
A6 2-Hexanol	13.28	26.66	13.10
A7 1-Heptanol	13.18	31.01	15.44
A8 2-Heptanol	13.08	35.36	17.78
A9 1-Octanol	12.98	39.71	20.12
A10 2-Octanol	12.88	44.06	22.46
A11 1-Nonanol	12.78	48.41	24.80
A12 2-Nonanol	12.68	52.76	27.14
A13 1-Decanol	12.58	57.11	29.48
A14 2-Decanol	12.48	61.46	31.82
A15 1-Undecanol	12.38	65.81	34.16
A16 2-Undecanol	12.28	70.16	36.50
A17 1-Dodecanol	12.18	74.51	38.84
A18 2-Dodecanol	12.08	78.86	41.18
A19 1-Tridecanol	11.98	83.21	43.52
A20 2-Tridecanol	11.88	87.56	45.86
A21 1-Tetradecanol	11.78	91.91	48.20
A22 2-Tetradecanol	11.68	96.26	50.54
A23 1-Pentadecanol	11.58	100.61	52.88
A24 2-Pentadecanol	11.48	104.96	55.22
A25 1-Hexadecanol	11.38	109.31	57.56
A26 2-Hexadecanol	11.28	113.66	59.90
A27 1-Heptadecanol	11.18	118.01	62.24
A28 2-Heptadecanol	11.08	122.36	64.58
A29 1-Octadecanol	10.98	126.71	66.92
A30 2-Octadecanol	10.88	131.06	69.26
A31 1-Nonadecanol	10.78	135.41	71.60
A32 2-Nonadecanol	10.68	139.76	73.94
A33 1-Eicosanol	10.58	144.11	76.28
A34 2-Eicosanol	10.48	148.46	78.62
A35 1-Henicosanol	10.38	152.81	80.96
A36 2-Henicosanol	10.28	157.16	83.30
A37 1-Triacontanol	10.18	161.51	85.64
A38 2-Triacontanol	10.08	165.86	87.98
A39 1-Tetracosanol	9.98	170.21	90.32
A40 2-Tetracosanol	9.88	174.56	92.66
A41 1-Pentacosanol	9.78	178.91	95.00
A42 2-Pentacosanol	9.68	183.26	97.34
A43 1-Hexacosanol	9.58	187.61	99.68
A44 2-Hexacosanol	9.48	191.96	102.02
A45 1-Heptacosanol	9.38	196.31	104.36
A46 2-Heptacosanol	9.28	200.66	106.70
A47 1-Octacosanol	9.18	205.01	109.04
A48 2-Octacosanol	9.08	209.36	111.38
A49 1-Nonacosanol	8.98	213.71	113.72
A50 2-Nonacosanol	8.88	218.06	116.06
A51 1-Triacontanol	8.78	222.41	118.40
A52 2-Triacontanol	8.68	226.76	120.74
A53 1-Tetracosanol	8.58	231.11	123.08
A54 2-Tetracosanol	8.48	235.46	125.42
A55 1-Pentacosanol	8.38	239.81	127.76
A56 2-Pentacosanol	8.28	244.16	130.10
A57 1-Hexacosanol	8.18	248.51	132.44
A58 2-Hexacosanol	8.08	252.86	134.78
A59 1-Heptacosanol	7.98	257.21	137.12
A60 2-Heptacosanol	7.88	261.56	139.46
A61 1-Octacosanol	7.78	265.91	141.80
A62 2-Octacosanol	7.68	270.26	144.14
A63 1-Nonacosanol	7.58	274.61	146.48
A64 2-Nonacosanol	7.48	278.96	148.82
A65 1-Triacontanol	7.38	283.31	151.16
A66 2-Triacontanol	7.28	287.66	153.50
A67 1-Tetracosanol	7.18	292.01	155.84
A68 2-Tetracosanol	7.08	296.36	158.18
A69 1-Pentacosanol	6.98	300.71	160.52
A70 2-Pentacosanol	6.88	305.06	162.86
A71 1-Hexacosanol	6.78	309.41	165.20
A72 2-Hexacosanol	6.68	313.76	167.54
A73 1-Heptacosanol	6.58	318.11	169.88
A74 2-Heptacosanol	6.48	322.46	172.22
A75 1-Octacosanol	6.38	326.81	174.56
A76 2-Octacosanol	6.28	331.16	176.90
A77 1-Nonacosanol	6.18	335.51	179.24
A78 2-Nonacosanol	6.08	339.86	181.58
A79 1-Triacontanol	5.98	344.21	183.92
A80 2-Triacontanol	5.88	348.56	186.26
A81 1-Tetracosanol	5.78	352.91	188.60
A82 2-Tetracosanol	5.68	357.26	190.94
A83 1-Pentacosanol	5.58	361.61	193.28
A84 2-Pentacosanol	5.48	365.96	195.62
A85 1-Hexacosanol	5.38	370.31	197.96
A86 2-Hexacosanol	5.28	374.66	200.30
A87 1-Heptacosanol	5.18	379.01	202.64
A88 2-Heptacosanol	5.08	383.36	204.98
A89 1-Octacosanol	4.98	387.71	207.32
A90 2-Octacosanol	4.88	392.06	209.66
A91 1-Nonacosanol	4.78	396.41	212.00
A92 2-Nonacosanol	4.68	400.76	214.34
A93 1-Triacontanol	4.58	405.11	216.68
A94 2-Triacontanol	4.48	409.46	219.02
A95 1-Tetracosanol	4.38	413.81	221.36
A96 2-Tetracosanol	4.28	418.16	223.70
A97 1-Pentacosanol	4.18	422.51	226.04
A98 2-Pentacosanol	4.08	426.86	228.38
A99 1-Hexacosanol	3.98	431.21	230.72
A100 2-Hexacosanol	3.88	435.56	233.06

MSChromSearch is a product of Axel Semrau®



Please contact us for more information or a web presentation!



Axel Semrau®

About Axel Semrau®

Axel Semrau GmbH & Co. KG is one of the largest German dealers for analytical equipment. Axel Semrau® develops own products and trades with laboratory hardware. The Development and configuration of software for chemical analysis and laboratories is one of the main strengths of the company. Software products like **MSChromSearch** for fast comparisons of MS chromatograms and CHRONOS-ISS, a new software to control PAL autosampler from CTC Analytics are distributed worldwide.

Information request

To: Axel Semrau GmbH & Co. KG

Fax: +49 (0) 2339 / 6030 or

E-Mail: info@axelsemrau.de

Information MSChromSearch

- Please send me more information concerning MSChromSearch.
- I am interested in a web presentation.
- I am interested in a demo version of MSChromSearch.
- Please send me information concerning CHRONOS-ISS (New software to control PAL autosampler from CTC Analytics).
- I need an offer.
- Please call me.

Further comments or questions:

Your address details:

Title, name: _____

Company: _____

Department: _____

Street: _____

City: _____

Country: _____

E-Mail: _____

Phone: _____

Homepage: _____



**Free demoverison
for 8 weeks!**

**Use our special offer and
download your
demoverison under**

**www.mschromsearch.de
⇒ ⇒ **download****

**or contact us!
info@axelsemrau.de**