TraceFinder Software
Software for Targeted and
Non-Targeted Analyses

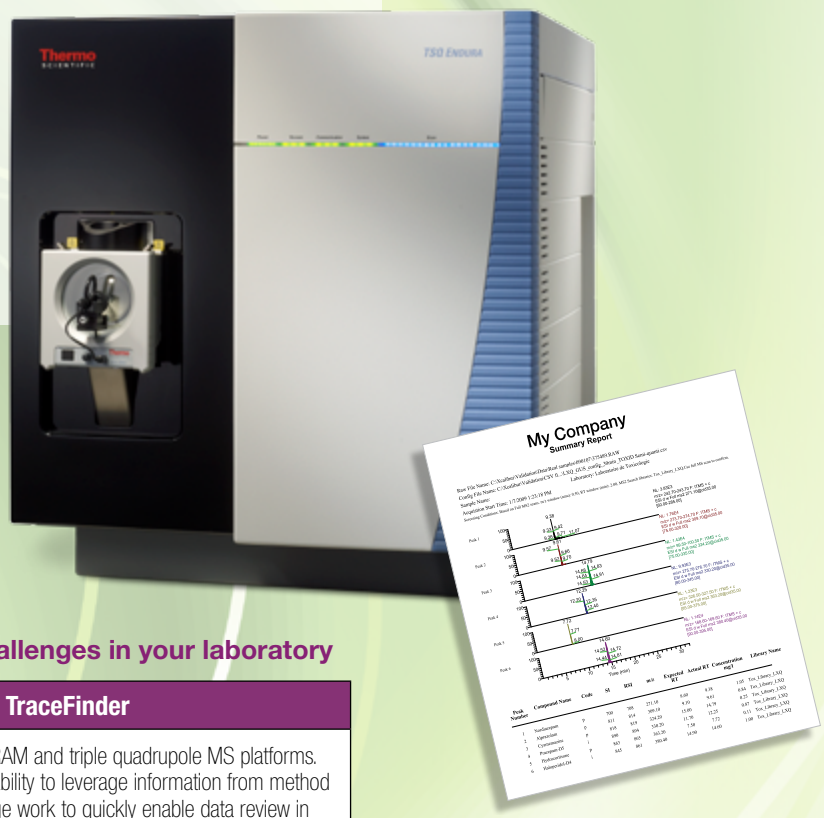
Comprehensive, Fast, Flexible
Mass Spectrometry Software

Thermo
SCIENTIFIC

Achieve unprecedented simplicity and

TraceFinder software is the solution

Thermo Scientific™ TraceFinder™ software makes the challenging steps of targeted and untargeted analysis simple, fast and productive. It is the only software that can be used to develop methods, acquire and process data, and generate reports with the full portfolio of Thermo Scientific quantitative mass spectrometers. Tracefinder software integrates the full range of popular front end chromatography systems, providing laboratories with the suite of features required to address their analytical demands. Now, regardless of the MS expertise of the user, the analytical requirements of every laboratory can be addressed with one software solution.



TraceFinder empowers you to tackle the everyday challenges in your laboratory

Challenge	TraceFinder
Maintain or increase laboratory productivity	One software for both HRAM and triple quadrupole MS platforms. Scientists now have the ability to leverage information from method development in early stage work to quickly enable data review in routine quantitative analysis.
Customizable reporting templates	Customized templates and automatic generation of reports save time and organizational resources.
Efficient method development regardless of expertise	Method development wizard, comprehensive database, and the ability to address critical parameters for all molecule types enable development of sensitive, robust, and reproducible quantitation methods.

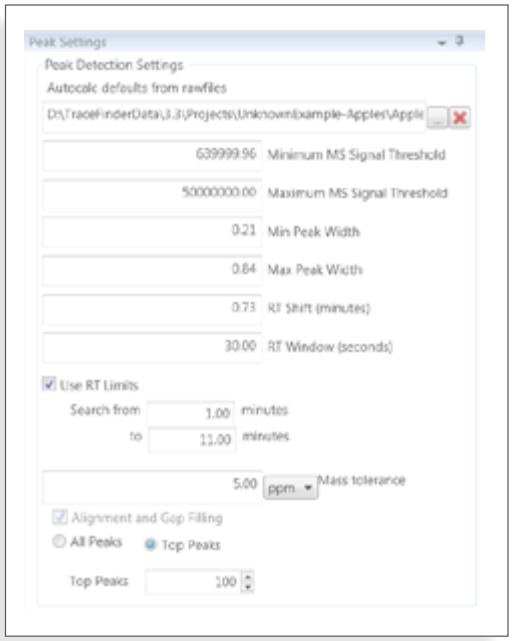
Comprehensive data review allows for rapid data quality determination.

speed

Ensure increased productivity

TraceFinder software simplifies every step of routine mass spectrometry (MS) quantitation and targeted workflows, saving time and increasing productivity. From data acquisition to data processing, review and reporting, TraceFinder empowers you to streamline your processes and get answers faster.

- 4 click workflow from analysis to reports
- Comprehensive method development for screening and quantitative workflows
- Automated and manual flagging are reflected in final reports
- Template driven design to simplify routine workflows
- Automatic method creation with Method Forge™



Experience extraordinary power and fl

TraceFinder software speeds up each step in the analysis of routine MS quantification and screening workflows. Once a method is defined, data acquisition is an easy four-click process that can be monitored in real-time. Data review is fast with comprehensive flagging, and enables association of a sample set with a previous calibration. When needed, the software makes it easy to edit results, and the edits are dynamically reflected in the final report. Customized nomenclature for environmental testing, food safety, clinical research and forensic toxicology applications is available.

Comprehensive method development

TraceFinder software enables the development of better, and more robust methods in a shorter amount of time. Powerful tools enable method developers to meet the demands of advanced users, and address regulatory requirements and existing laboratory protocols.

- Method templates for data processing
- Batch templates use previously defined methods for rapid data acquisition, processing and reporting
- Compound databases (CDB) for selected reaction monitoring (SRM) and high-resolution accurate mass (HRAM) workflows
- Customizable report templates
- User-defined flags for nearly every parameter
- Method association with any previously saved calibration
- Method Forge tool to upload a raw data file and detect peaks via a library search

Four-click data acquisition

Submitting sample batches and initiating analyses is performed in four simple steps:

1. Select the appropriate batch template.
2. Review the selected batch template.
3. If needed, choose a system start-up and shut-down method, or extend a historical calibration curve.
4. Submit the samples.

Increased efficiency with compound databases

The CDB retains all instrument parameters for targeted analysis allowing the method developer to select compounds and develop methods rapidly. New analytes and all corresponding instrument parameters can be readily added to the CDB.

Comprehensive flagging facilitates the technician's role in reviewing data.

exibility
with comprehensive method development

Potent method creation

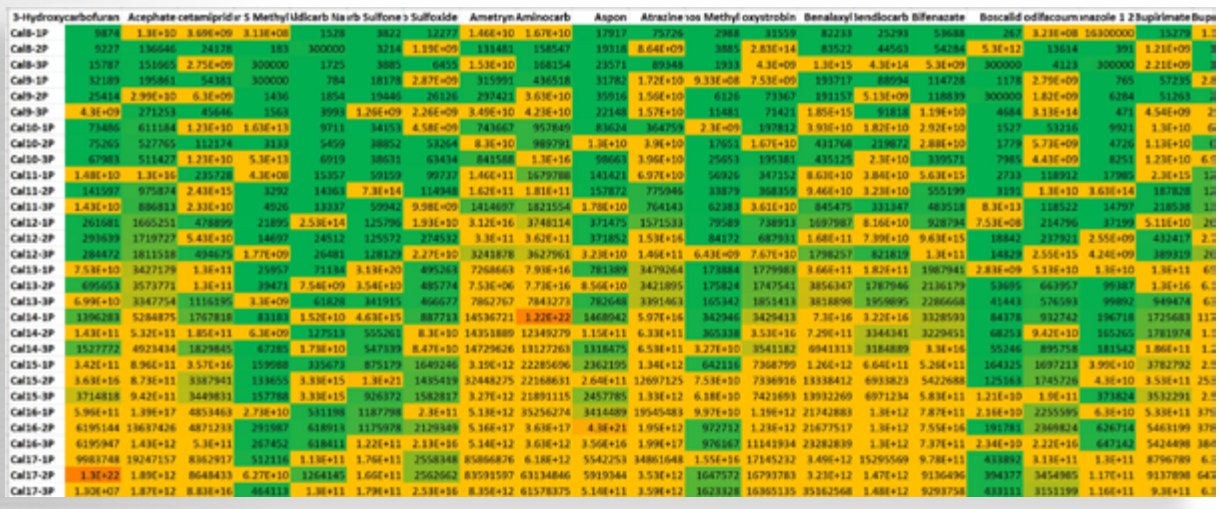
Multiple confirmation criteria and reporting is streamlined with automatic predefined criteria for identification of targeted molecules to include ion ratios, library searches, isotopic distributions, and defined fragmentation patterns. Identification criteria are automatically reported in the customizable report templates. Depending on laboratory requirements, the software offers multiple resources for identification.

TraceFinder software provides user-defined flags for almost every parameter, and the flags chosen are reflected in data review and reports.

Simplified screening

Screening capabilities draw from proven Thermo Scientific screening software, making TraceFinder an easy-to-use tool that substantially simplifies MS/MS targeted screening workflows. The software supports SRM, HRAM, and MS/MS workflows, and uses the widely accepted NIST spectra library and mzVault with mzCloud libraries software for compound identification.

Rich data review capabilities in untargeted screening highlights important information.



	3-Hydroxycarbofuran	Acephate	cetamiprid	Imidacloprid	5 Methyl Uldicarb	Na	rb Sulfone	Sulfoxide	Ametryn	Aminocarb	Aspon	Atrazine	ios Methyl	oxystrobin	Benalaxyl	lendiocarb	Bifenazate	Boscalid	odifacoum	nazole 1 2	Bupirimate	Bupi
Cal8-1P	9874	1.3E+10	3.69E+09	3.13E+08	1528	3822	12272	1.46E+10	1.67E+10	17917	75726	2968	91558	82233	25293	53688	367	3.23E+08	16300000		15279	1.1
Cal8-2P	9227	136646	24178	183	300000	3214	1.19E+09	131481	158547	19318	8.64E+09	3885	2.83E+14	83522	44563	54284	5.3E+12	13614	391	1.21E+09	3	
Cal8-3P	15787	151665	2.75E+09	300000	1725	3885	6455	1.53E+10	168154	23571	89348	1933	4.3E+09	1.3E+15	4.3E+14	5.3E+09	300000	4123	300000	2.21E+09	3	
Cal9-1P	32189	195861	54381	300000	784	18178	2.87E+09	315991	436518	31782	1.72E+10	9.33E+08	7.53E+09	193717	88994	114728	1178	2.79E+09	765	57235	2.8	
Cal9-2P	25414	2.99E+10	6.3E+09	1436	1854	19446	26126	297421	3.63E+10	35916	1.56E+10	6126	73367	191157	5.13E+09	118839	300000	1.82E+09	6284	51263	2	
Cal9-3P	4.3E+09	271253	45646	1563	3993	1.26E+09	2.26E+09	3.49E+10	4.23E+10	22148	1.57E+10	11481	71421	1.85E+15	91818	1.19E+10	4684	3.13E+14	471	4.54E+09	2	
Cal10-1P	73486	611184	1.23E+10	1.63E+13	9711	34153	4.58E+09	743667	957849	83624	364759	2.3E+09	197812	3.93E+10	1.82E+10	2.92E+10	1527	53216	9921	1.3E+10	6	
Cal10-2P	75265	527765	112174	3133	5459	38852	53264	8.3E+10	989791	1.3E+10	3.9E+10	17651	1.67E+10	431768	219872	2.88E+10	1771	5.73E+09	4726	1.13E+10	6	
Cal10-3P	67983	511427	1.23E+10	5.3E+13	6919	38631	63434	841588	1.3E+16	58663	3.96E+10	25653	195381	435125	2.3E+10	330571	7981	4.43E+09	8251	1.23E+10	6.9	
Cal11-1P	1.48E+10	1.3E+16	235728	4.3E+08	15357	50159	99737	1.46E+11	1.67978E	141421	6.97E+10	56926	347152	8.63E+10	3.84E+10	5.63E+15	2733	118912	17960	2.3E+15	12	
Cal11-2P	141597	975874	2.43E+15	3292	14363	7.3E+14	114948	1.62E+11	1.81E+11	157872	775946	33879	368359	9.46E+10	3.23E+10	555199	3191	1.3E+10	3.63E+14	187828	12	
Cal11-3P	1.43E+10	886813	2.33E+10	4926	13337	59942	9.98E+09	1414697	1821554	1.78E+10	764143	62383	3.61E+10	845475	331347	483518	8.3E+13	118522	14797	218538	13	
Cal12-1P	261681	1665251	478899	21895	2.53E+14	125796	1.93E+10	3.12E+16	3748114	371475	1571533	79589	738913	1697987	8.16E+10	928794	7.53E+08	214796	37199	5.11E+10	20	
Cal12-2P	293639	1719727	5.43E+10	14697	24512	125572	274532	3.3E+11	3.62E+11	371852	1.53E+16	84172	687931	1.68E+11	7.39E+10	9.63E+15	18842	237921	2.55E+09	432417	2.2	
Cal12-3P	284472	1811518	434675	1.77E+09	26481	128129	2.27E+10	3241878	3627961	3.23E+10	1.46E+11	6.43E+09	7.67E+10	1798257	821819	1.3E+15	14829	2.55E+15	4.24E+09	389319	26	
Cal13-1P	7.53E+10	3427179	1.3E+11	25957	31184	3.18E+20	495263	7268663	7.93E+16	781389	3479264	173884	1729983	3.66E+11	5.82E+11	1987941	2.83E+09	5.13E+10	1.3E+10	1.3E+11	65	
Cal13-2P	695653	3573771	1.3E+11	39471	7.54E+09	3.54E+10	485774	7.53E+06	7.73E+16	8.56E+10	3421895	175824	1747541	3856347	1787946	2136179	53695	663957	99387	1.3E+16	6.3	
Cal13-3P	6.99E+10	3347754	1116395	3.3E+09	61828	341915	466677	7862767	7843273	782648	3391463	165342	1855413	3818898	1959895	2286668	41443	576593	99892	949474	63	
Cal14-1P	1396283	5284875	1767818	83183	1.52E+10	4.63E+15	887713	14536721	1.22E+22	1468942	5.97E+16	342946	3429413	7.3E+16	3.22E+16	3328593	84378	932742	196718	1725683	113	
Cal14-2P	1.43E+11	5.32E+13	1.85E+11	6.3E+09	127513	555263	8.3E+10	14351889	12349279	1.15E+11	6.3E+11	865338	3.53E+16	7.29E+11	3344341	3229451	68251	9.42E+10	165265	1781978	1.1	
Cal14-3P	1527772	4923434	1829845	67285	1.79E+10	547339	8.47E+10	14729626	13127263	1318475	6.5E+11	3.27E+10	3541182	6941313	3184889	3.3E+16	55246	895758	181542	1.86E+11	1.2	
Cal15-1P	3.42E+11	8.96E+11	3.57E+16	159988	335673	875179	1649246	3.19E+12	22285696	2362195	1.34E+12	662118	7368799	1.26E+12	6.64E+11	5.26E+11	164325	1697213	3.99E+10	3782792	2.5	
Cal15-2P	3.63E+16	8.73E+11	3387941	133655	3.33E+15	1.3E+21	1435419	32448275	22168631	2.64E+11	12697125	7.53E+10	7336916	13338412	6933823	5422688	125163	1745726	4.3E+10	3.53E+11	253	
Cal15-3P	3714818	9.42E+11	3449831	157788	3.33E+15	926372	1582817	3.27E+12	21891115	2457785	1.33E+12	6.18E+10	7421693	13932269	6971234	5.83E+11	1.21E+10	1.9E+11	373824	3532291	2.5	
Cal16-1P	5.96E+11	1.39E+17	4853463	2.73E+10	531198	1187798	2.3E+11	5.13E+12	35256274	3414489	19545483	9.97E+10	1.19E+12	21742883	1.3E+12	7.87E+11	2.56E+10	2255595	6.3E+10	5.33E+13	379	
Cal16-2P	6195144	13637426	4871233	291987	618913	1175978	2129349	5.16E+17	3.63E+17	4.3E+21	1.95E+12	972712	1.23E+12	21677517	1.3E+12	7.55E+16	191781	2369824	626714	5463199	378	
Cal16-3P	6195947	1.43E+12	5.3E+11	267452	618411	1.22E+11	2.13E+16	5.14E+12	3.63E+12	3.56E+16	1.99E+17	976167	11141934	23282839	1.3E+12	7.37E+11	2.34E+10	2.22E+16	647142	5424498	384	
Cal17-1P	9983748	19247157	8362917	512316	1.13E+11	1.76E+11	2558348	85866876	6.18E+12	5542253	34861648	1.55E+16	17145232	3.49E+12	15295569	9.78E+11	433892	3.13E+11	1.3E+11	8796789	6.3	
Cal17-2P	1.3E+22	1.89E+12	8648433	6.27E+10	1264145	1.66E+11	2562662	83591597	63134846	5919344	3.53E+12	1647572	16793783	3.23E+12	1.47E+12	9136496	394377	3454985	1.17E+11	9137898	647	
Cal17-3P	1.30E+07	1.87E+12	8.83E+16	464113	1.3E+11	1.79E+11	2.53E+16	8.35E+12	61578375	5.14E+11	3.59E+12	1623328	16365135	35162568	1.48E+12	9293758	433111	3151199	1.16E+11	9.3E+11	6.3	

The heat map reporting templates allow for the quick evaluation of the presence of components and their relative abundance across the sample set.

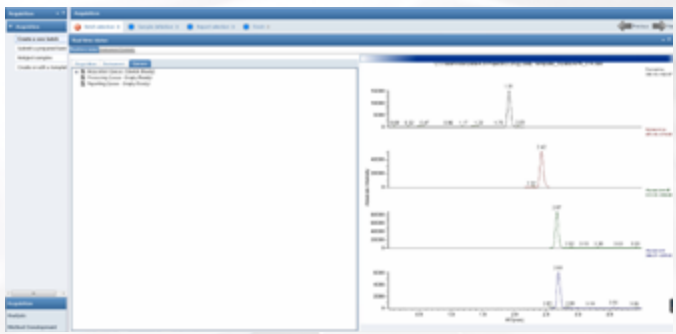
Simple, full-featured data

TraceFinder software offers simple, yet exceptionally feature-rich data review capabilities. The intuitive, workflow-driven arrangements of the software windows simplify your role in reviewing data, and views can be customized to streamline daily tasks. You can quickly and easily observe the data processing status, view compound-related flags to locate compounds which need attention, and take appropriate steps to correct any problems.

To address compound-related difficulties, it's easy to perform compound specific edits such as manual peak rejection and integration, and to change peak-detection parameters. Feedback is immediate, as data is reprocessed and presented in the same software screen and in the final report automatically.

Save time and samples with intelligent sequencing

The Intelligent Sequencing module helps you take complete advantage of the powerful flagging system. It contains parameters that can be configured by sample type to enable actions on flagged results in real-time. Intelligent sequencing allows for real-time rejection of samples, insertion of blanks, and halting of sample sequences in which data has fallen outside of predefined criteria, saving you time and valuable sample resources.



Submitting sample batches and initiating analyses is straightforward.The Real Time Viewer offers immediate access to system status and queues.

review — maximizing laboratory throughput

Data reporting

- Automated reporting and numerous report templates.
- A large number of predefined and customizable report templates to meet a variety of regulatory requirements.
- Changes to the data processing method can immediately be seen in the report view – without manual intervention.
- If desired, save time and paper by choosing only to print reports for compounds above the LOD, LOQ or LOR.

Optimized flagging for targeted screening analysis.

User rights ensure increased security for audit trail

To protect the integrity of analytical data, the software includes a rights-based secure user login system and dual method hierarchy that limits access to methods and data. In addition, an e-signature and audit trails are available, which support the guidelines indicated in 21 CFR Part 11.

	3-Hydroxycarbofuran	Acephate	cetamiprid	ir S Methyl	Aldicarb	Na rb Sulfone	b Sulfoxide	Ametryn	Aminocarb	Aspon	Atrazine	ios Methyl	oxystrobin	Benalaxyl	lendiocarb	Bifenazate	Boscalid	odifacoum	nazole 1 2	Bupirimate	Bup
Cal7-1P	2.534	2.429	2.392	2	1.225	2.411	2.145	2.437	2.395	2.634	2.455	2.425	2.257	2.444	2.18	2.622	2.435	2.56	2	2.662	
Cal7-2P	2.332	2.42	2.538	2	2	2	2.568	2.438	2.517	2.487	2.361	2.114	2.286	2.446	2.224	2.532	2.522	2	2.473	2.714	
Cal7-3P	2.479	2.77	2.276	2	2	2.157	2.159	2.525	2.488	2.547	2.525	2.857	2.263	2.424	2.248	2.437	2	2.22	2.543	2.452	
Cal8-1P	2.793	2.286	1.629	3.243	2.889	2.654	1.226	2.942	2.957	1.229	1.212	2.659	2.174	1.226	2.368	1.296	2.528	2.444	2.529	2.766	
Cal8-2P	2.748	2.65	1.281	-1.353	2	2.564	1.171	2.851	2.928	1.113	1.158	2.887	2.155	1.221	2.62	1.129	2.823	1.328	2.623	2.618	
Cal8-3P	1.222	2.853	1.224	2	1.226	2.663	2.658	2.972	2.964	1.366	1.198	2.392	2.221	1.249	2.572	1.236	2	2.522	2	1.287	
Cal9-1P	2.335	1.45	2.382	2	2.373	2.785	2.755	2.233	2.545	1.856	2.335	2.27	2.427	2.333	1.224	2.41	1.667	2.547	2.827	2.739	
Cal9-2P	1.867	2.848	2.657	2.528	1.115	2.974	2.511	1.914	2.298	2.123	2.115	1.456	2.397	2.323	2.729	2.499	2	1.722	3.525	2.458	
Cal9-3P	2.894	2.473	2.225	2.719	2.6	1.955	2.179	2.245	2.467	1.281	2.128	2.819	2.386	2.231	1.241	2.524	6.161	2.811	2.662	2.182	
Cal10-1P	5.188	7.143	5.268	2.773	6.577	5.175	4.377	4.778	5.644	4.968	4.993	5.145	1.262	4.696	2.431	6.262	2.113	4.715	5.323	5.128	
Cal10-2P	5.311	5.988	4.886	3.28	3.619	5.882	5.287	5.159	5.835	6.265	5.341	4.395	2.897	5.187	2.931	6.181	2.434	5.246	2.756	5.271	
Cal10-3P	4.828	5.763	5.347	5.937	4.634	5.849	6.258	5.428	5.98	5.876	5.424	6.449	1.249	5.227	2.756	7.316	12.437	3.928	4.497	5.754	
Cal11-1P	12.359	12.927	12.314	4.534	12.512	8.96	9.551	9.419	12	8.476	9.618	14.586	1.866	12.385	5.11	12.237	3.654	12.418	9.333	9.546	
Cal11-2P	9.896	12.262	12.539	3.318	9.818	12.64	11.227	12.425	12.819	9.482	12.723	8.572	1.981	11.431	4.298	12.125	4.241	9.256	18.422	8.946	
Cal11-3P	9.796	11.221	12.211	5.781	9.123	9.279	9.557	9.128	12.865	12.724	12.558	16.225	1.941	12.225	4.413	12.514	12.547	12.383	7.744	12.42	
Cal12-1P	18.2	22.276	21.321	31.617	17.257	19.316	18.523	22.226	22.936	22.879	22.238	22.596	4.222	22.798	12.986	22.719	9.815	18.94	19.229	24.772	
Cal12-2P	22.411	23.288	24.17	22.597	16.911	19.28	27.224	19.821	22.123	22.923	21.298	21.823	3.721	22.529	9.926	21.456	24.829	21.233	13.121	22.858	
Cal12-3P	19.776	24.463	22.229	25.197	18.29	19.686	22.127	21.232	22.165	19.633	22.373	16.468	4.157	22.267	11.261	23.798	19.448	22.598	21.661	18.731	
Cal13-1P	52.251	52.33	49.618	37.876	49.862	52.382	52.812	48.258	51.44	52.596	52.54	46.739	9.884	46.578	25.344	47.275	37.829	46.958	56.312	51.583	
Cal13-2P	48.257	52.859	49.457	58.916	52.873	58.456	49.741	49.85	52.142	55.95	49.652	47.298	9.695	49.358	24.825	51.327	75.116	62.728	51.628	51.85	
Cal13-3P	48.496	48.974	52.377	44.513	43.236	56.225	47.6	52.138	52.966	52.686	49.182	44.288	12.299	48.839	27.38	55.496	56.636	53.627	51.922	47.443	
Cal14-1P	96.942	85.526	88.777	129.421	128.574	79.247	122.164	99.814	85.931	125.769	91.35	99.522	19.931	97.121	47.264	87.86	126.526	93.299	127.54	91.916	
Cal14-2P	99.349	86.246	93.881	93.216	92.56	99.969	89.226	98.444	87.166	78.521	97.268	127.235	22.439	121.787	49.355	84.469	98.469	94.246	88.721	95.411	
Cal14-3P	126.1	78.256	92.571	123.322	122.236	98.153	94.484	121.247	94.245	92.438	122.799	94.112	22.65	96.225	46.68	78.429	77.526	88.674	98.361	122.537	
Cal15-1P	238.538	2	2	264.183	252.285	224.145	2	245.671	2	222.974	265.271	231.946	49.762	225.61	119.959	195.73	2	226.247	256.66	282.589	
Cal15-2P	251.397	212.186	241.846	216.198	246.163	2	226.698	251.166	2	2	241.41	339.217	49.468	254.226	128.878	2	214.224	242.716	262.619	239.834	
Cal15-3P	259.466	2	256.985	262.295	246.122	242.585	2	253.374	2	249.672	251.725	217.428	52.254	291.544	132.288	2	224.591	2	234.112	242.971	

Highly customizable reports allow for fast decision making.

TraceFinder

Reliably create, review and report scientific data

Discover the power of TraceFinder software to help you create, review and report scientific data and increase the efficiency of your team. Use TraceFinder software to easily acquire data, perform routine data review, and automatically report results on the fly. TraceFinder allows your laboratory to standardize on a single platform across all your Thermo Fisher Scientific mass spectrometry and chromatography products.

System requirements

- 3.0GHz or faster processor
- Internet Explorer 11
- 8GB of RAM (16GB recommended)
- 5GB of available hard-disk space (solid state hard drive recommended)
- 1024x576 screen resolution (1920x1080 recommended)
- DVD drive
- Video hardware acceleration (optional)

Software

- Microsoft® Windows® 7 SP1 Professional (64-bit only) English only
- Microsoft®.NET Framework 4.5.1
- Adobe® Reader® 10.1

Thermo Scientific software (minimum versions listed):

- Xcalibur 4.0
- Foundation 3.1 SP1
- mzVault 1.0 SP1
- Thermo FreeStyle 1.1 SP1
- Thermo LC Devices 3.0 or later
- Thermo Exactive Series 2.7
- TSQ Endura and Quantiva 1.2 or later
- Fusion 1.2 SP1 or later
- Aria MX 2.2 or later
- SII for Xcalibur 1.1 or later
- GC Devices 3.2 or later
- ISQ 3.2 SP1 or later
- TSQ 8000 3.2 or later
- LTQ Series 2.7 SP4 or later
- TSQ 2.5 or later

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