



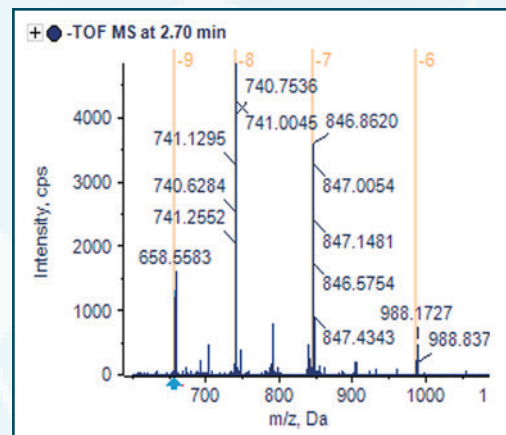
Molecule Profiler software

**Achieve better insights on
biotransformation and impurities**

Accurate and flexible workflow



Molecule Profiler software delivers highly accurate and flexible workflows for determining impurities and biotransformations for a wide variety of therapeutic molecules.



Acquire LC-HRMS/MS data

Potential Metabolites: 103 of 103 Peaks

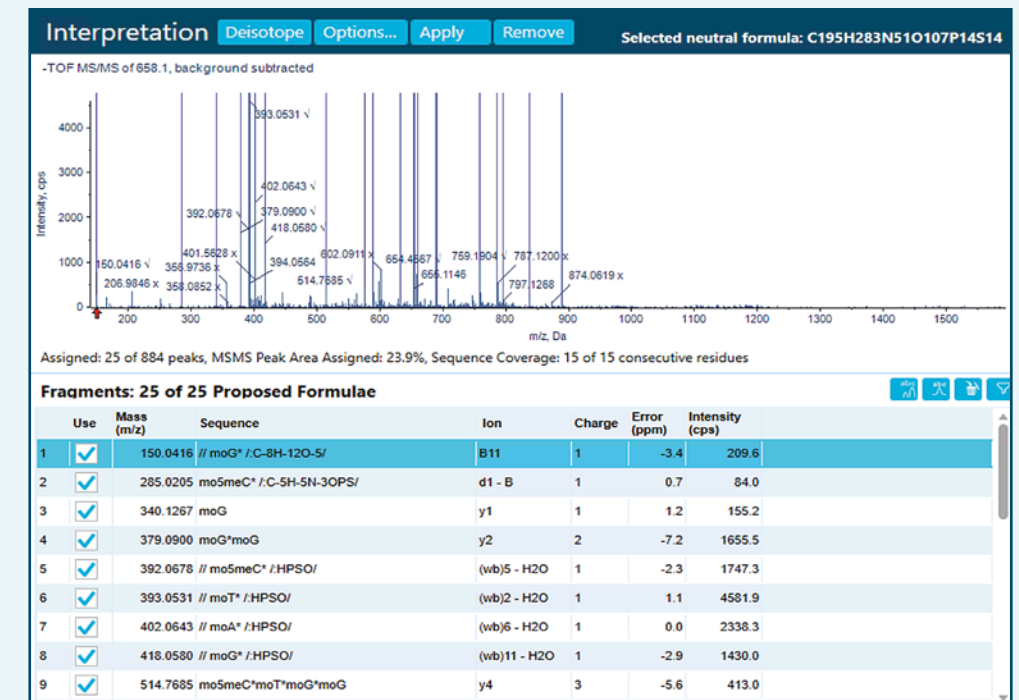
Report	Peak ID	Name	Formula	Neutral Mass	Average Mass	m/z	Charge
1	M16-3	S ⁽ⁿ⁻²⁾ [M-6H] ⁶⁻	C208H301N56O113P15S15	6335.13	6339.30	1054.8474	-6
2	M27-3	Desulfurization [M-7H] ⁷⁻	C234H340N61O129P17S16	7106.29	7110.96	1014.1770	-7
3	M4-3	S ⁽ⁿ⁻³⁾ [M-6H] ⁶⁻	C195H283N51O107P14S14	5932.08	5935.87	987.6720	-6
4	M16-2	S ⁽ⁿ⁻²⁾ [M-7H] ⁷⁻	C208H301N56O113P15S15	6335.14	6339.22	904.0120	-7
5		Parent [M-8H] ⁸⁻	C234H340N61O128P17S17	7122.29	7126.95	889.2784	-8
6	M23-1	Di-Desulfurization [M-8H] ⁸⁻	C234H340N61O130P17S15	7090.32	7095.05	885.2822	-8
7		Parent [M-9H] ⁹⁻	C234H340N61O128P17S17	7122.29	7127.13	790.3580	-9
8	M29	S ⁽ⁿ⁻³⁾ [M-8H] ⁸⁻	C195H283N51O107P14S14	5932.07	5935.85	740.5014	-8
9	M27-1	Desulfurization [M-10H] ¹⁰⁻	C234H340N61O129P17S16	7106.30	7110.96	709.6230	-10
10	M16	S ⁽ⁿ⁻²⁾ [M-9H] ⁹⁻	C208H301N56O113P15S15	6335.15	6339.20	702.8804	-9
11	M4	S ⁽ⁿ⁻³⁾ [M-9H] ⁹⁻	C195H283N51O107P14S14	5932.08	5935.89	658.1124	-9
12	M16-1	S ⁽ⁿ⁻²⁾ [M-10H] ¹⁰⁻	C208H301N56O113P15S15	6335.13	6339.21	632.5059	-10
13	M27	Desulfurization [M-9H] ⁹⁻	C234H340N61O129P17S16	7106.31	7110.84	788.5831	-9
14		Parent [M-7H] ⁷⁻	C234H340N61O128P17S17	7122.29	7127.02	1016.4631	-7
15		Parent [M-9H] ⁹⁻	C234H340N61O128P17S17	7122.31	7127.07	790.3601	-9
16		Parent [M-8H] ⁸⁻	C234H340N61O128P17S17	7122.27	7126.99	889.2770	-8

Identify potential metabolite based on TOF-MS

7 Groups of 27 Potential Metabolite Peak

Group ID	Name	Formula	Neutral Mass	Charge
1	G1	Parent	C234H340N61O128P17S17	7122.30 From -6 To -10
2	G2	Desulfurization	C234H340N61O129P17S16	7106.31 From -6 To -10
3	G3	S ⁽ⁿ⁻¹⁾	C221H321N59O120P16S16	6728.21 From -6 To -10
4	G4	S ⁽ⁿ⁻³⁾	C195H283N51O107P14S14	5932.08 From -6 To -9
5	G5	S ⁽ⁿ⁻²⁾	C208H301N56O113P15S15	6335.14 From -6 To -10
6	G6	S ⁽ⁿ⁻³⁾ +Desulfurization	C195H283N51O108P14S13	5916.07 From -7 To -8
7	G7	S ⁽ⁿ⁻¹⁾ +Desulfurization	C221H321N59O121P16S15	6712.19 From -8 To -9

Group charge states for relative quantification



Assign metabolite structures based on automated fragment ion assignment

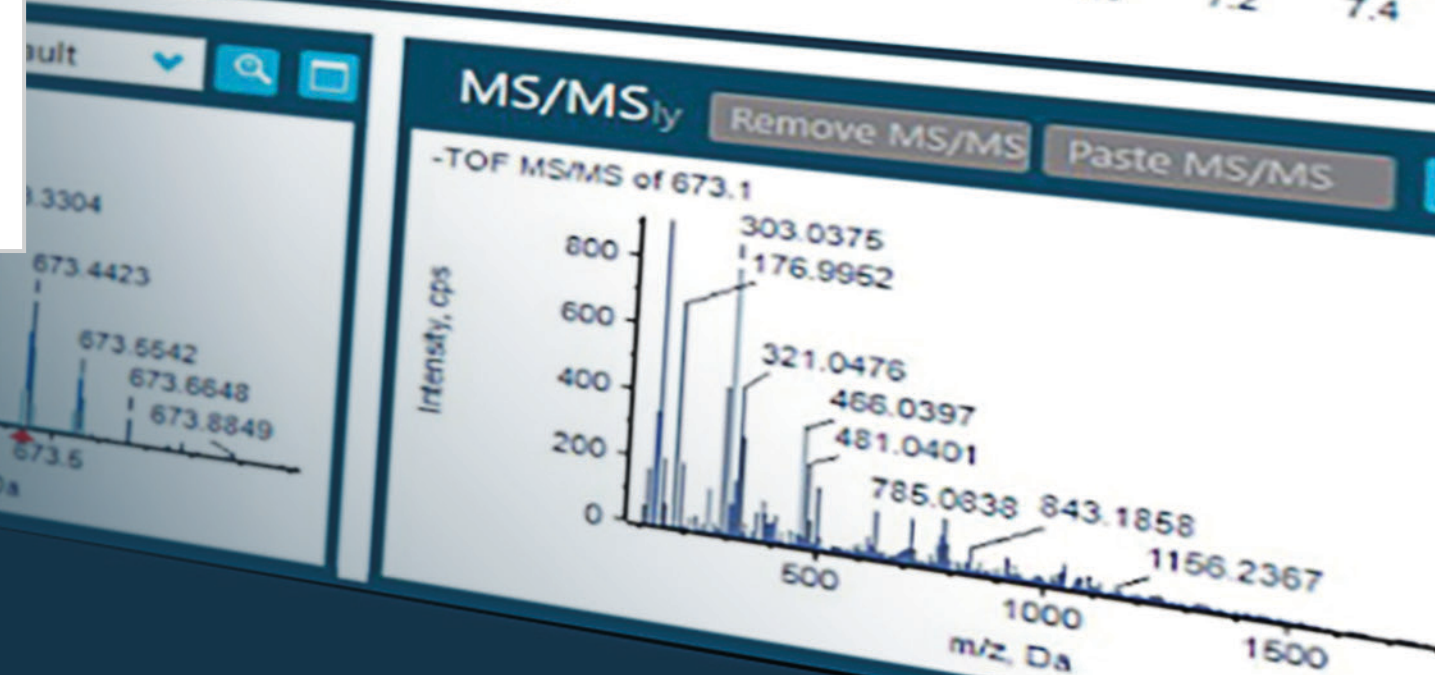
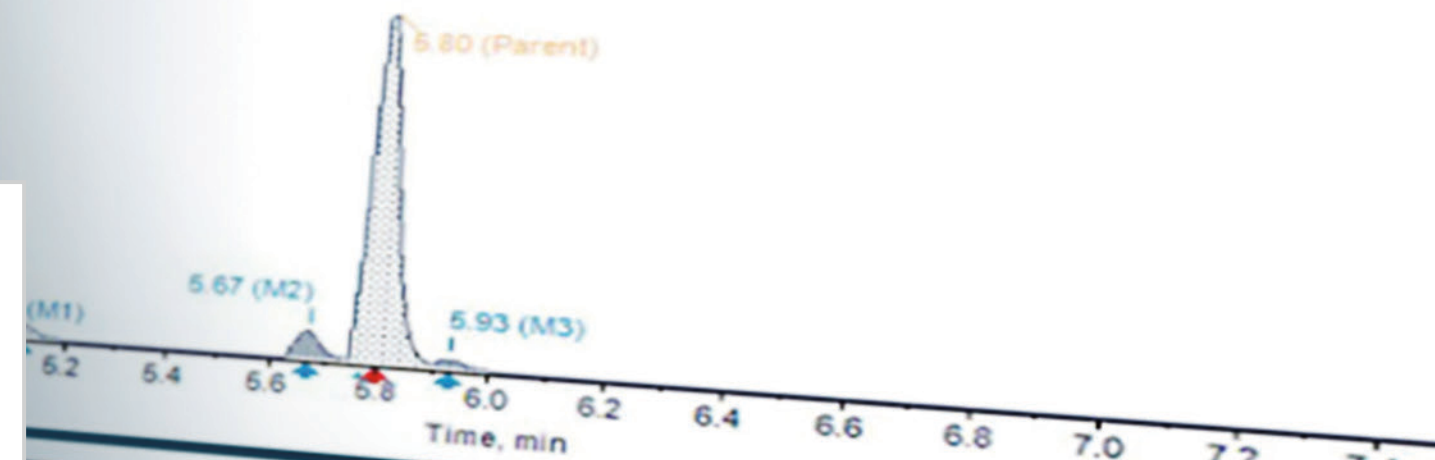
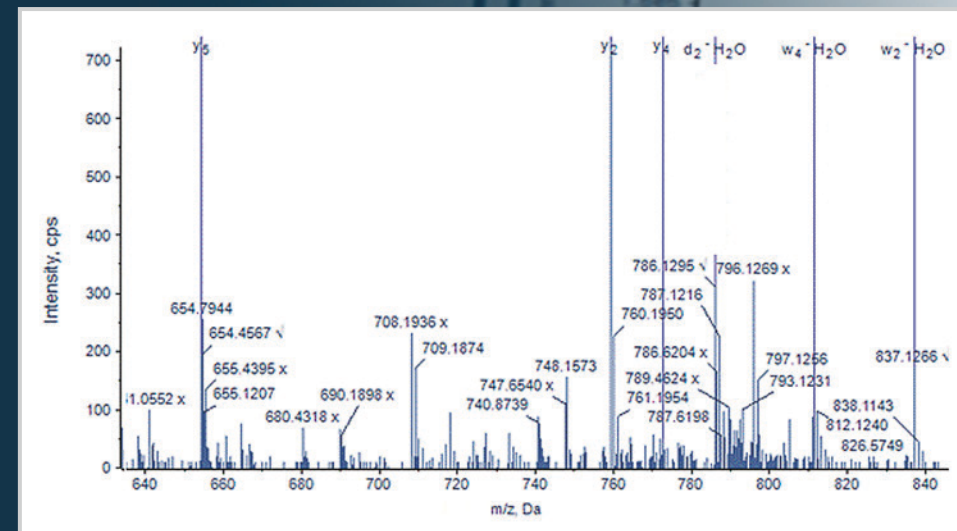
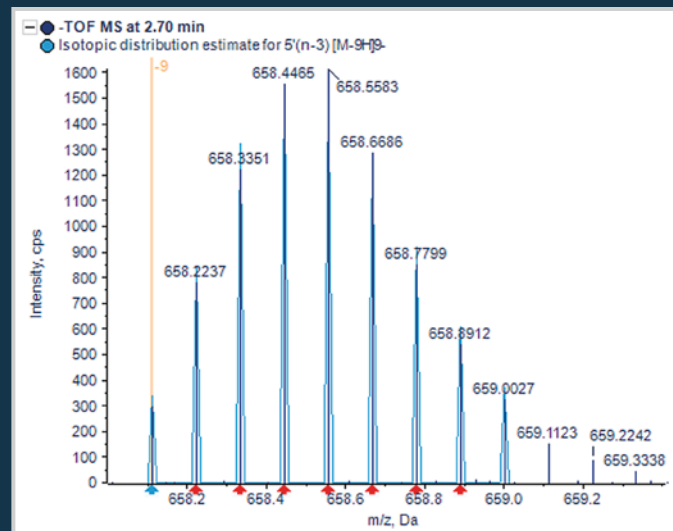
Confidence through MS/MS

Many impurities and biotransformations result in isoelemental species that an MS-only workflow just cannot solve.

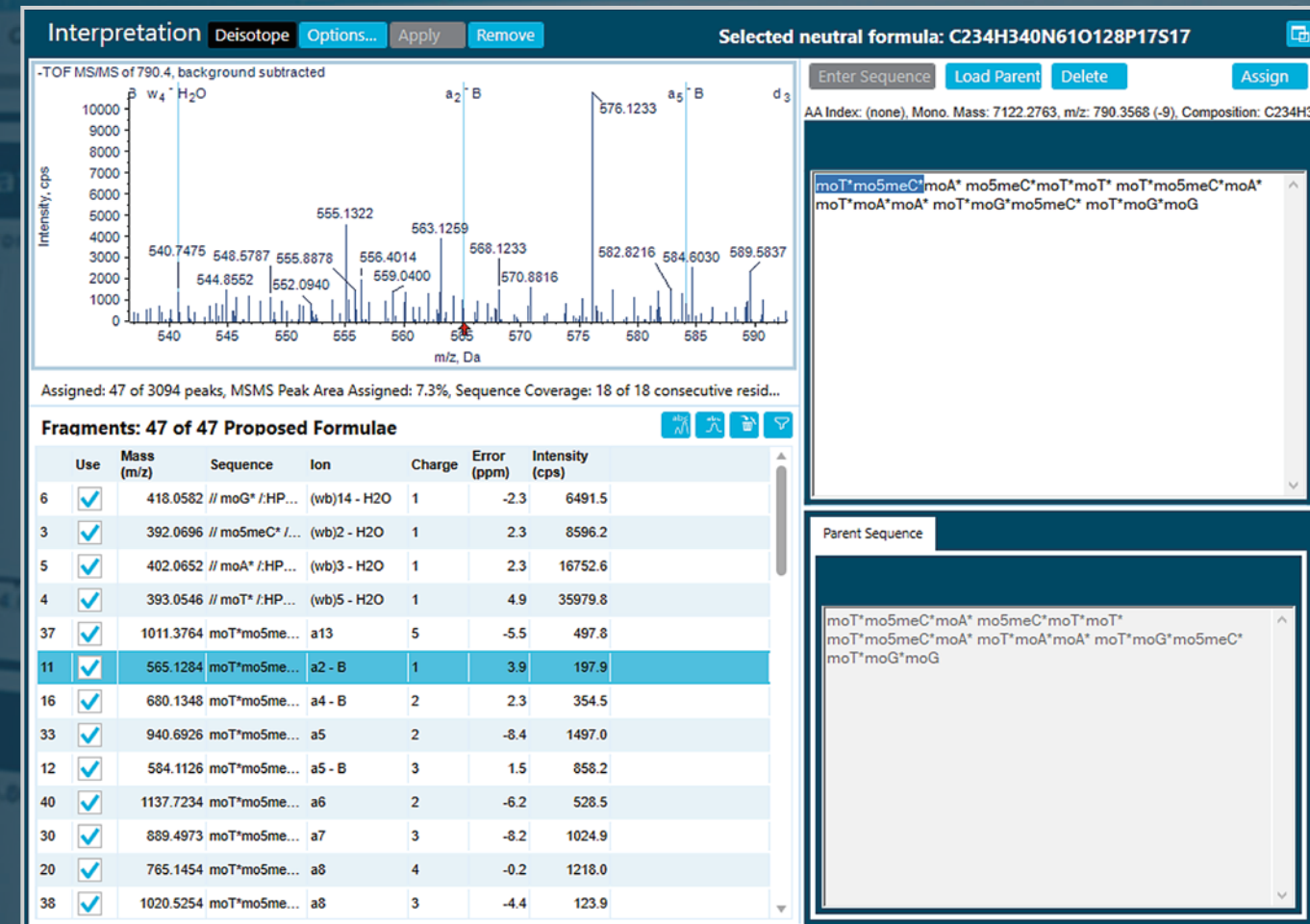
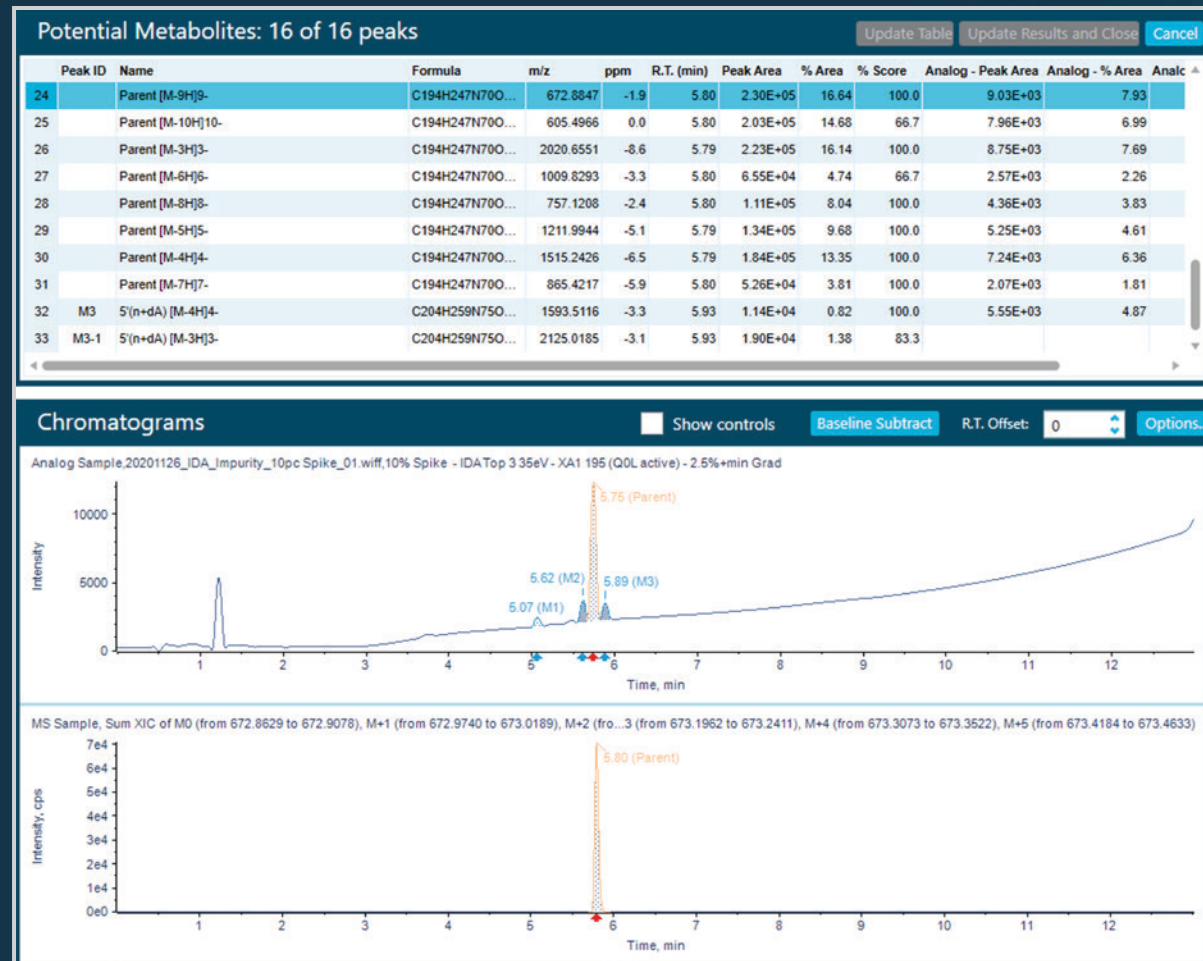
Molecule Profiler incorporates UV, MS and MS/MS information to provide clear and unambiguous results that give you complete confidence.

Use a variety of tools for identification at the MS level including mass accuracy and isotope ratio matching.

Easily customize your search tolerances to match MS/MS fragment spectra against *in-silico* generated full-length, impurity or metabolite spectra.



Confidence through MS/MS



Molecule Profiler software gives you the flexibility to incorporate UV, MS or MS/MS data into your interrogation of metabolites or impurities.

Easily switch between the results view and the interpretation view to get highly detailed information on your fragment ion spectra.

Flexibility across molecule types

Why have a separate piece of software for every type of molecule you develop?

Molecule Profiler is a single software to provide insights about biotransformations and impurities across molecular classes including: therapeutic oligonucleotides, small molecule drugs, peptide therapeutics and even antibody-drug conjugates.

New Save Delete

Compound Information

Compound name: ExampleOligo

Chemical formula: C234H340N61O128P17S17

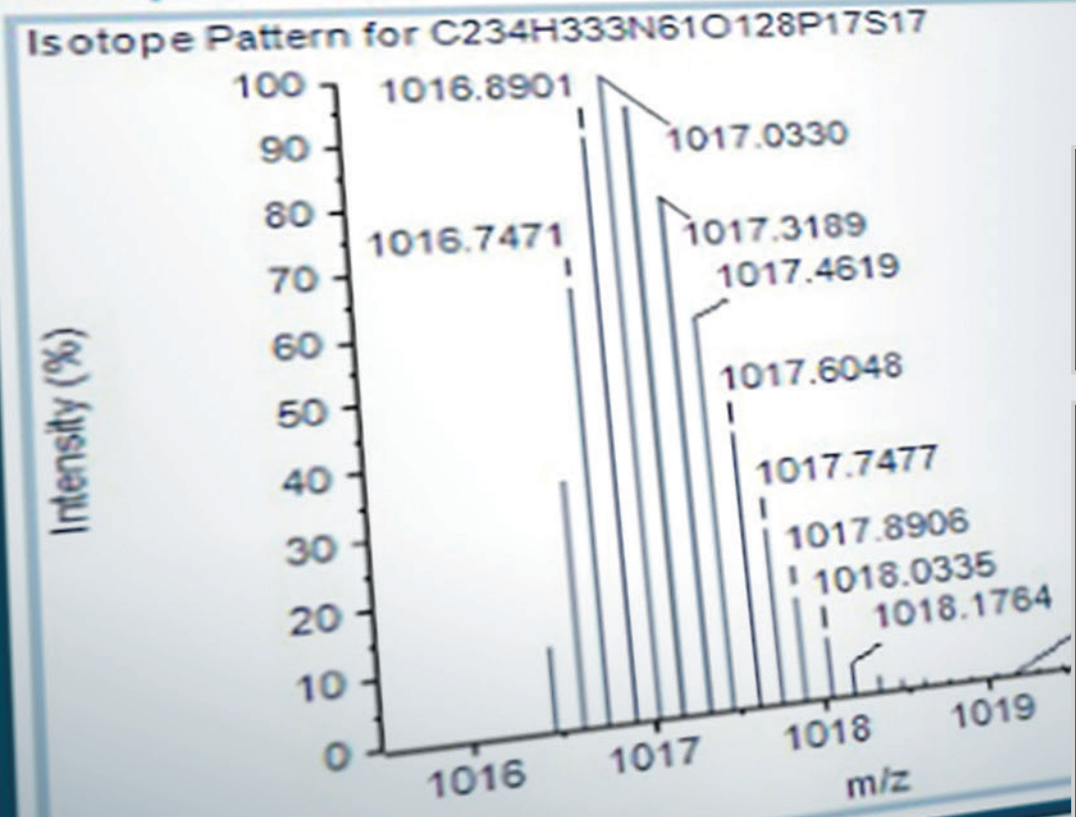
Polarity: Positive Negative

Sequence

1-9	moT*mo5meC*moA* mo5meC*moT*moT* moT*mo5meC*moA*
10-18	moT*moA*moA* moT*moG*mo5meC* moT*moG*moG

Compound Details Experimental Data

Isotope Pattern



Adduct: [M-7H]7-

m/z: 1016.4608

Compound class:

Compound Information

Compound name: Clozapine

Chemical formula: C18H19N4Cl

Polarity: Positive Negative

Structure

Open Structure... Clear

Compound Information

Compound name: Bivalirudin

Chemical formula: C98H138N24O33

Polarity: Positive Negative

Sequence

1-20	FPRPGGGGNG DFEEIPEEYL
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Compound Details Experimental Data

Isotope Pattern

Isotope Pattern for C18H20ClN4

m/z	Intensity (%)
327.1371	100
329.1347	~45
328.1401	~35
330.1373	~25
331.1401	~15

Adduct: [M+H]⁺

m/z: 327.1371

Compound class:

CAS number:

Comments:

Compound Details Experimental Data

Isotope Pattern

Isotope Pattern for C98H140N24O33

m/z	Intensity (%)
1090.5002	100
1091.0016	~95
1091.5030	~85
1092.0044	~75
1092.5057	~65
1093.0070	~55
1101.0266	~15

Adduct: [M+2H]²⁺

m/z: 1090.5002

Compound class:

CAS number:

Comments:

MS Sample:	Folder	Processing Parameters
MyOligo Biotrans t=0	Default	Predicted_a...
MyOligo Biotrans t=5	Default	Predicted_a...
MyOligo Biotrans t=10	Default	Predicted_a...
MyOligo Biotrans t=15	Default	Predicted_a...
MyOligo Biotrans t=20	Default	Predicted_a...
MyOligo Biotrans t=25	Default	Predicted_a...
MyOligo Biotrans t=30	Default	Predicted_a...
MyOligo Biotrans t=35	Default	Predicted_a...
MyOligo Biotrans t=40	Default	Predicted_a...
MyOligo Biotrans t=45	Default	Predicted_a...

Get to an answer, faster

Larger and more complex therapeutics like oligonucleotides and peptides can produce very complex MS/MS data.

The powerful MS/MS engine in Molecule Profiler can reduce the time to an answer from days down to hours.

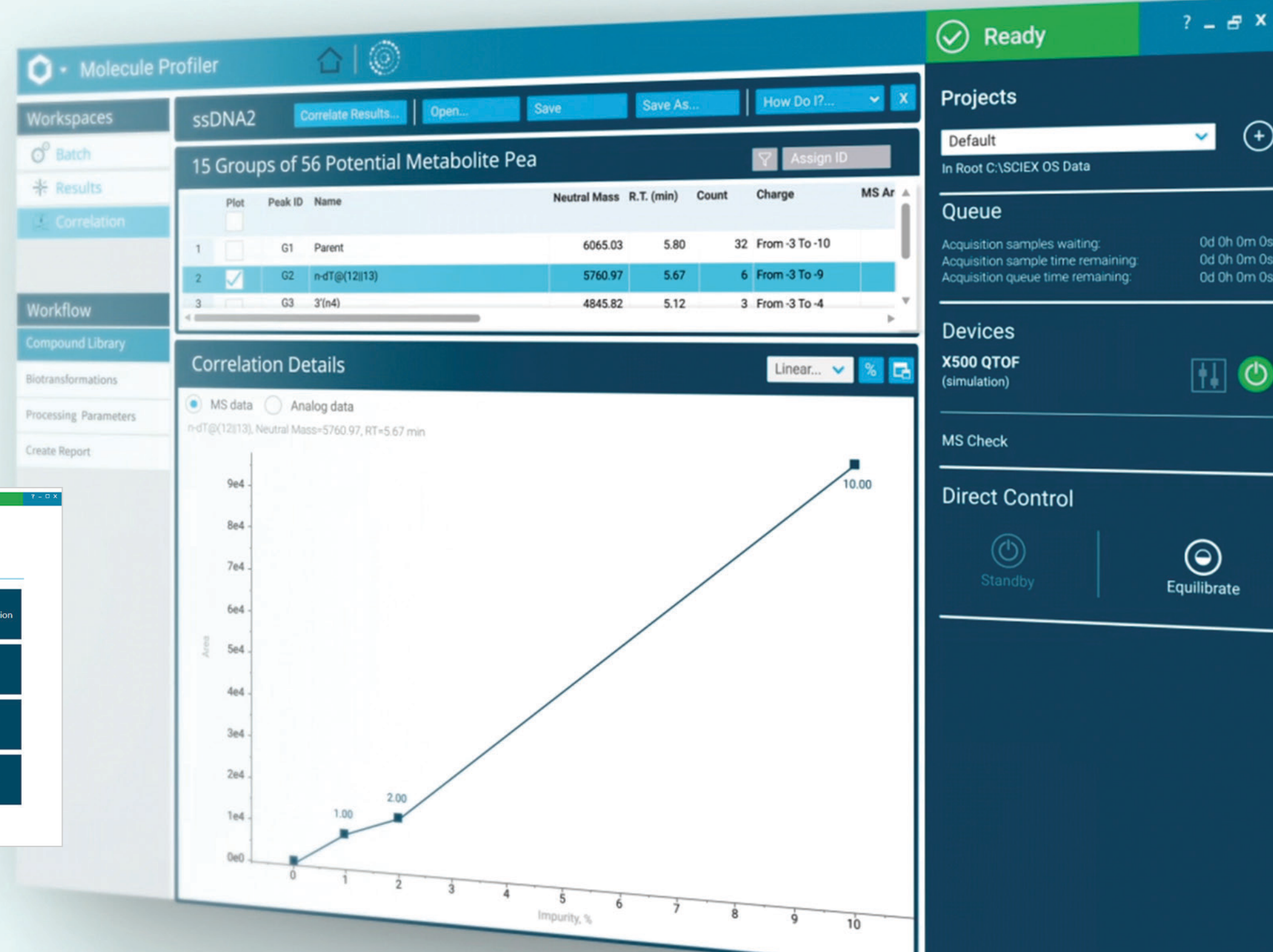
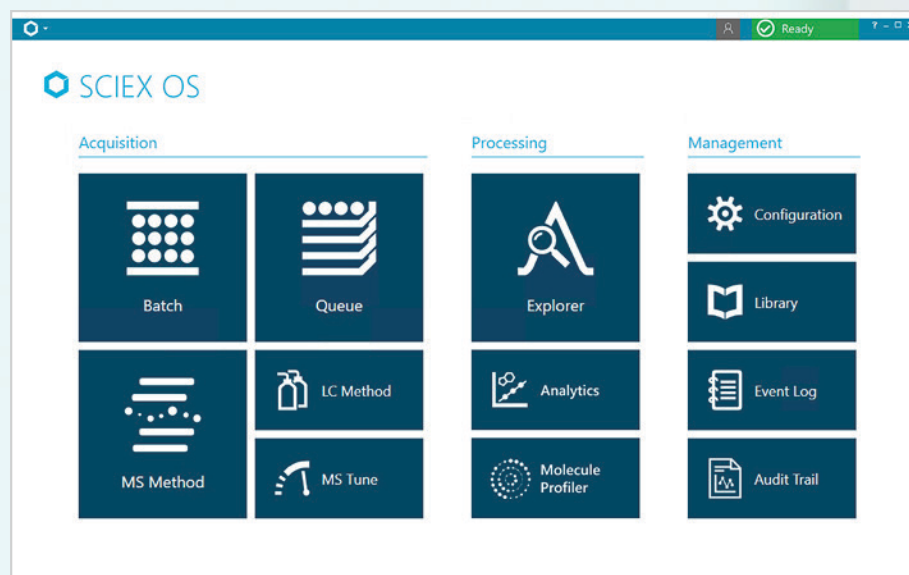
Easily build processing queues with the ability to choose multiple processing methods and controls. Each result analysis can be completed in just a few minutes.

Integrated for ease

Having many different software products generally requires you to jump around from app to app.

Molecule Profiler is fully integrated as part of SCIEX OS, and has the same look and feel. Easily multitask with other functions in SCIEX OS. And, there is no need to move data around.

Molecule Profiler software is an application within SCIEX OS software. There is no need to move data files around since all acquired data are easily accessible within the SCIEX OS framework between different applications. It is also easy to navigate between the impurity and metabolite discovery functions of Molecule Profiler to the highly customizable quantitative workflows of Analytics.



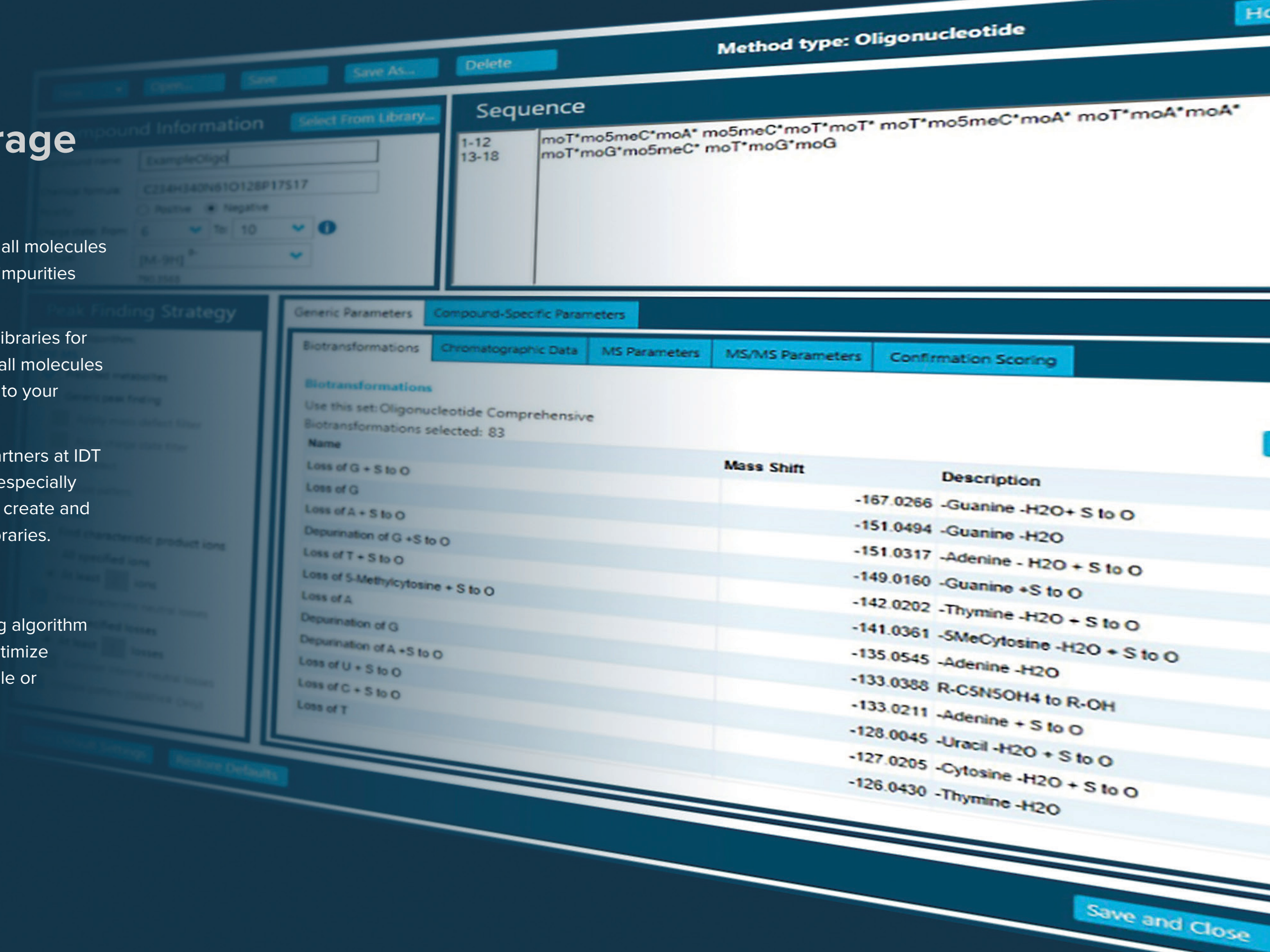
Complete coverage

Oligonucleotides, peptides and small molecules can have an enormous number of impurities and biotransformations.

Molecule Profiler has off-the-shelf libraries for oligonucleotides, peptides and small molecules with thousands of entries targeted to your molecule type.

SCIEX has also worked with our partners at IDT to create a comprehensive library especially for oligonucleotides. You can even create and edit your own biotransformation libraries.

You can customize the peak finding algorithm and library search algorithms to optimize your search for a particular molecule or molecule class.





ZenoTOF 7600 system

This mass spectrometer gives richer, more comprehensive data with new innovations that have never been seen in an accurate mass system. EAD fragmentation and the Zeno trap pave the way for precise and accurate MS and MS/MS data.



TripleTOF 6600+ system

This high-performance accurate mass solution offers a combination of qualitative and quantitative analysis and advanced workflow capabilities. Optimized for large-scale quantitative mass spectrometry, the TripleTOF 6600+ system offers sensitive and robust performance.

SCIEX Now support network

The destination for all your support needs



Molecule Profiler software

Achieve better insights on biotransformation and impurities

Learn more about what Molecule Profiler Software can do for you!



Start your path to success now: sciex.com/sciexnow



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