



Molecule Profiler software

Gain better insights on
impurities and biotransformations

Achieve accurate and flexible processing



Molecule Profiler software delivers highly accurate and flexible workflows for determining impurities and biotransformations for a wide variety of therapeutic molecules—from small molecules to synthetic peptides and oligonucleotides and lipids used for drug delivery.

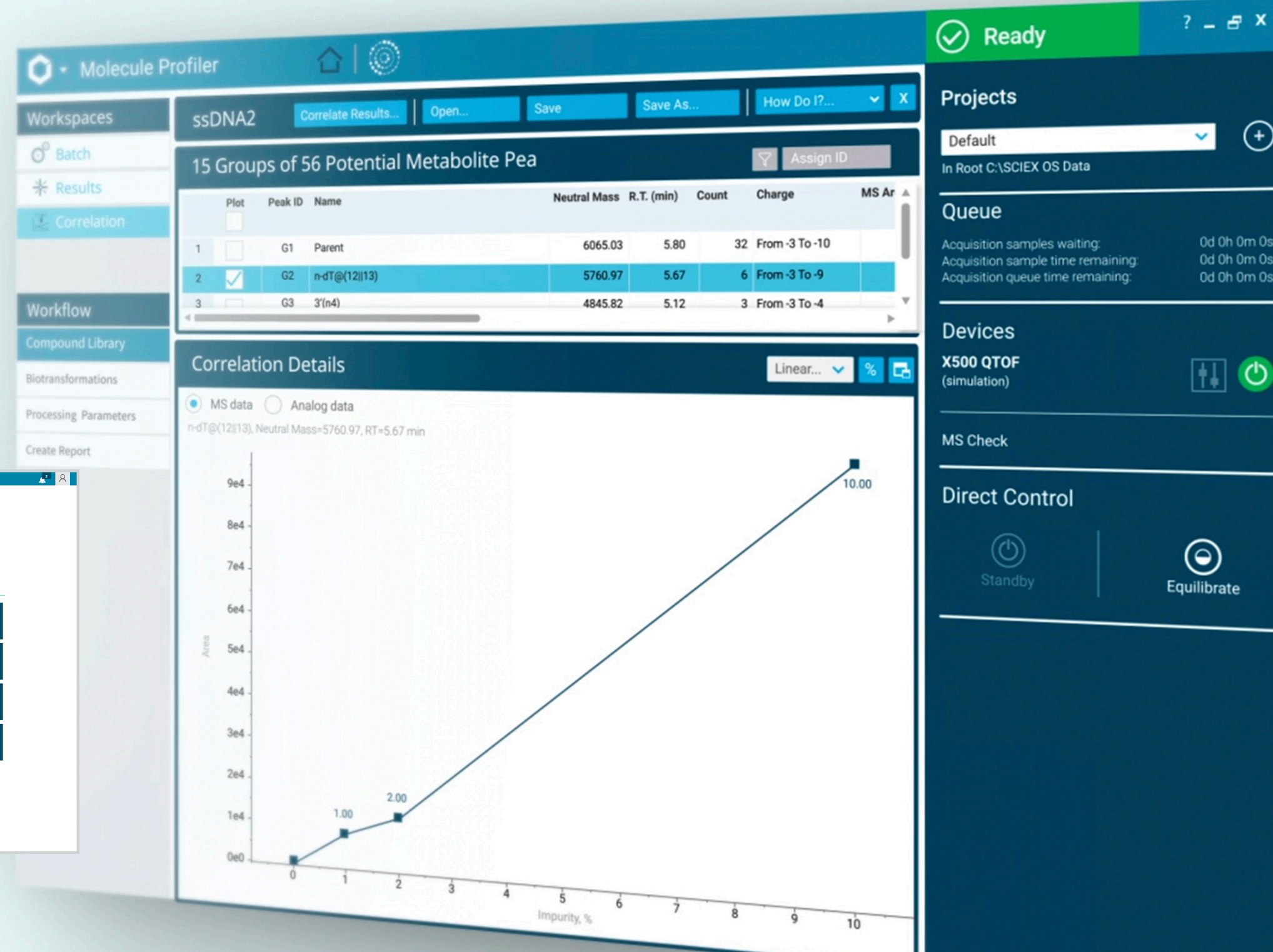
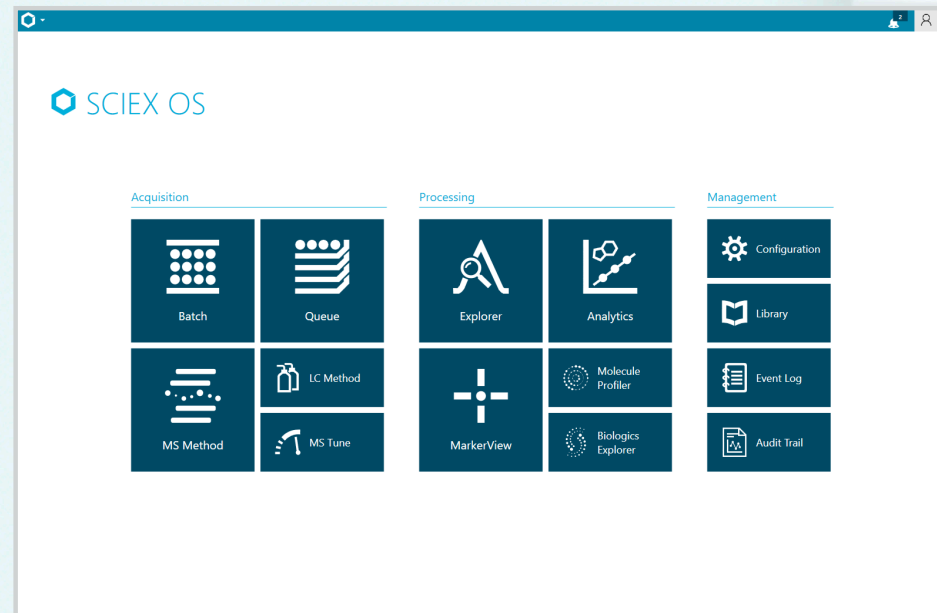


Discover the ease of integration

Having many different software products generally requires you to jump around from application to application, which can take time and increase training requirements.

Molecule Profiler software is seamlessly integrated with SCIEX OS software. You can efficiently perform multiple tasks alongside other functions without the need to transfer data between different programs.

With Molecule Profiler software, you can also easily navigate between the impurity and metabolite discovery functions and the highly customizable quantitative workflows of the Analytics module within SCIEX OS software.



Experience flexibility across molecule types

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

You can now use a single tool to provide insights about impurities and biotransformations across molecular classes, including lipids, therapeutic oligonucleotides, small molecule drugs, peptide therapeutics and even antibody-drug conjugates.

New Save Delete

Compound Information

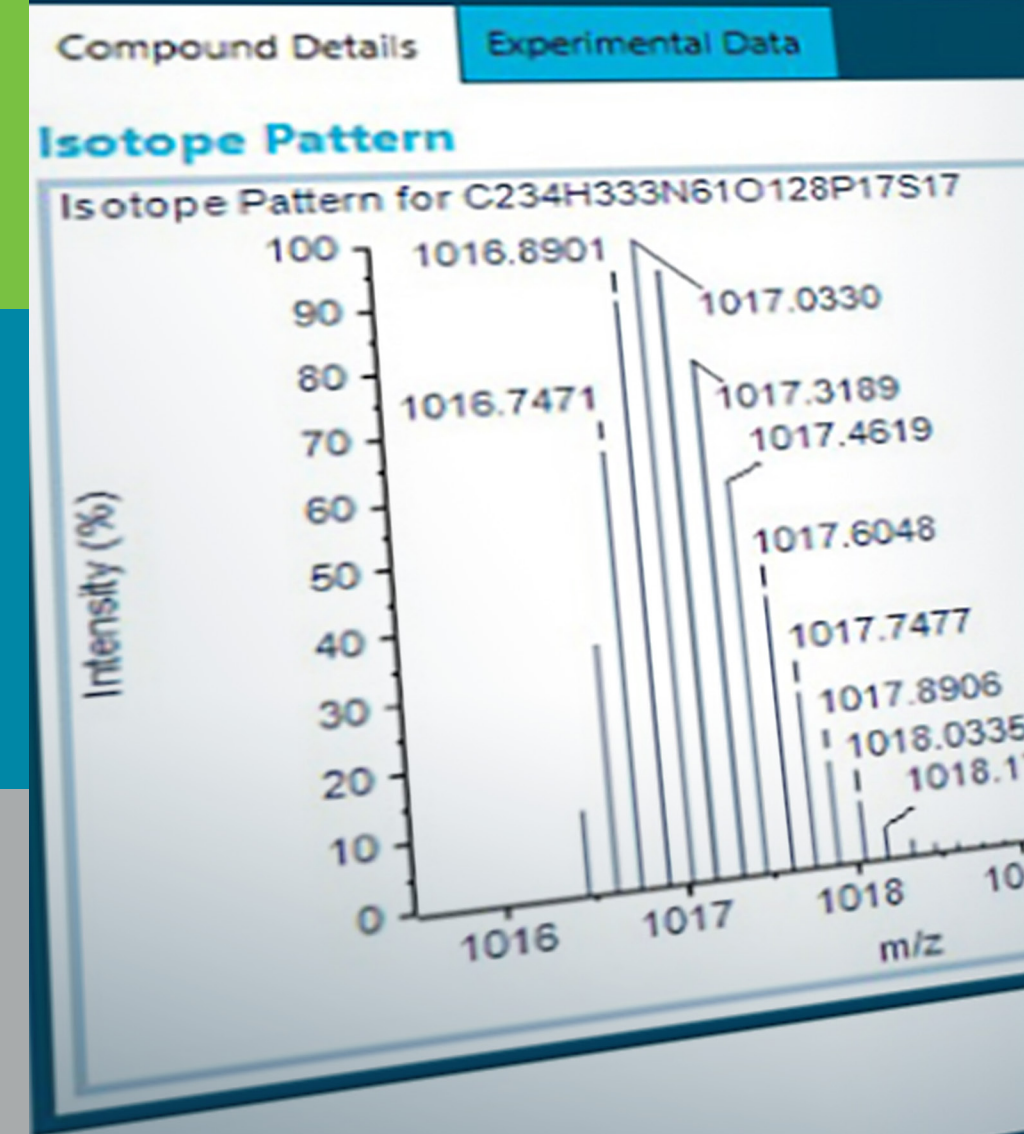
Compound name:

Chemical formula:

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

Adduct: [M-7H]7-
m/z: 1016.4608
Compound class:

Compound Information

Compound name:

Chemical formula:

Polarity: Positive Negative

Structure

Compound Information

Compound name:

Chemical formula:

Polarity: Positive Negative

Sequence

1-20	FPRPGGGGNG DFEEIPEEYL
------	-----------------------

Compound Details Experimental Data

Isotope Pattern

Isotope Pattern for C43H80NO2

m/z	Intensity (%)
642.6184	100
643.6217	~60
644.6250	~15
645.6282	~10
649.6405	~10
654.6558	~5

Adduct: [M+H]⁺
m/z: 642.6184
Compound class:
CAS number:
Comments:

Compound Details Experimental Data

Isotope Pattern

Isotope Pattern for C98H140N24O33

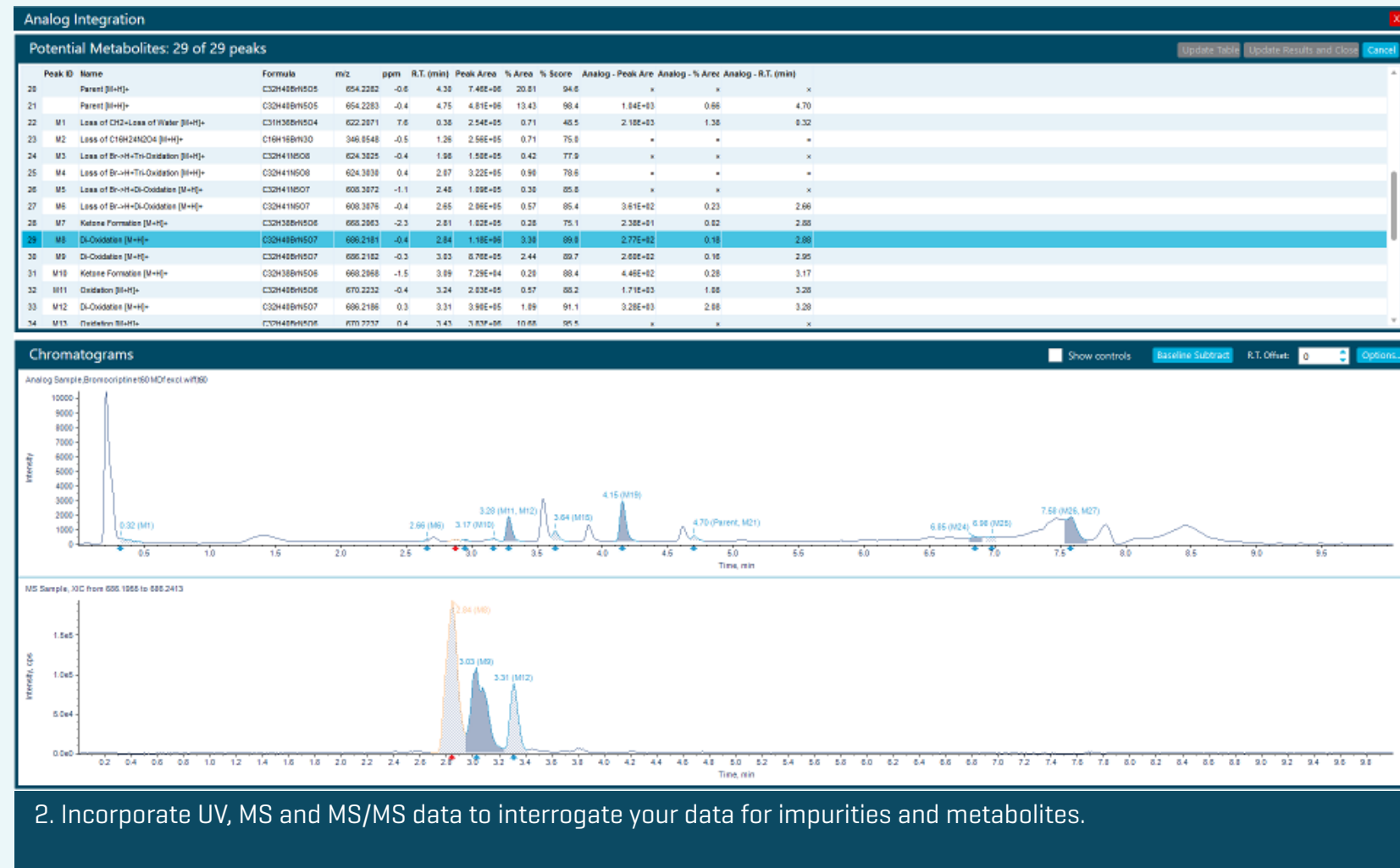
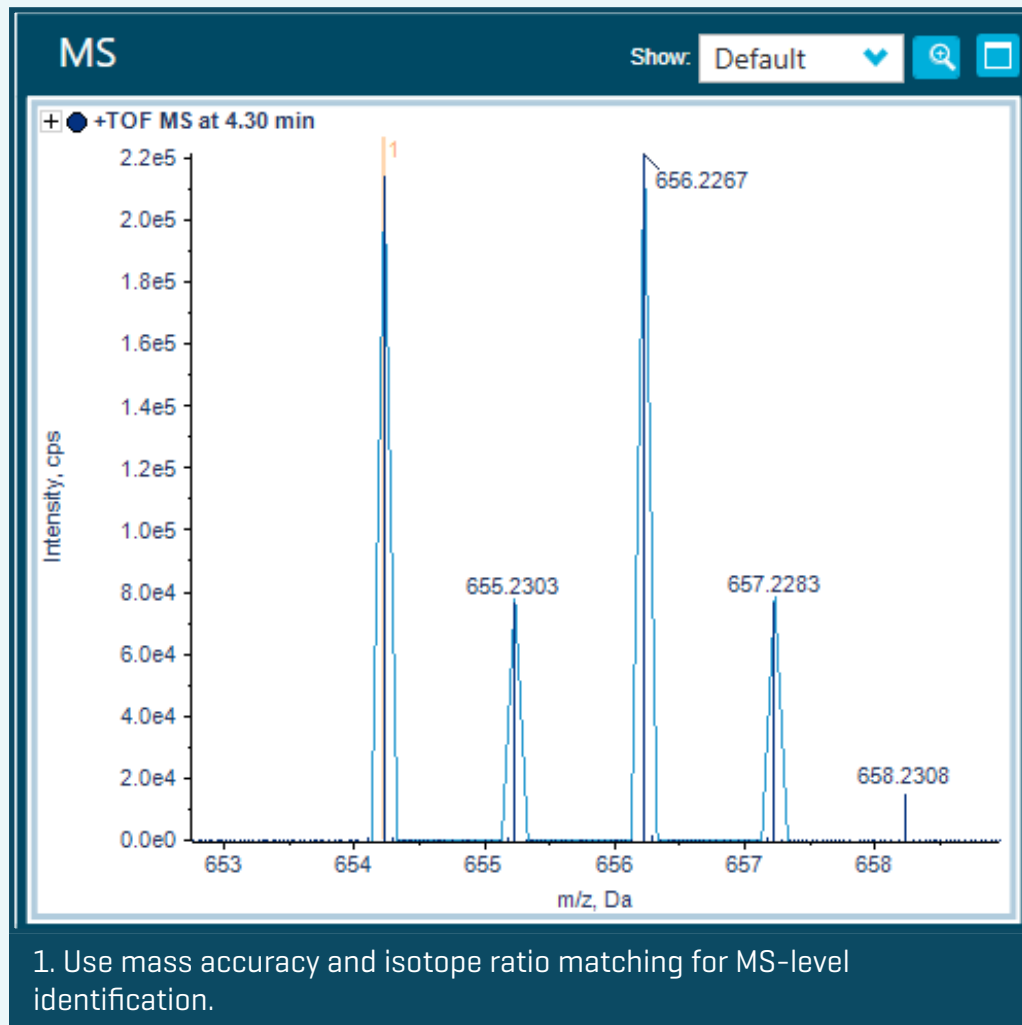
m/z	Intensity (%)
1090.5002	100
1091.0016	~95
1091.5030	~85
1092.0044	~45
1093.0070	~15
1101.0266	~5

Adduct: [M+2H]²⁺
m/z: 1090.5002
Compound class:
CAS number:
Comments:

Increase confidence through MS/MS

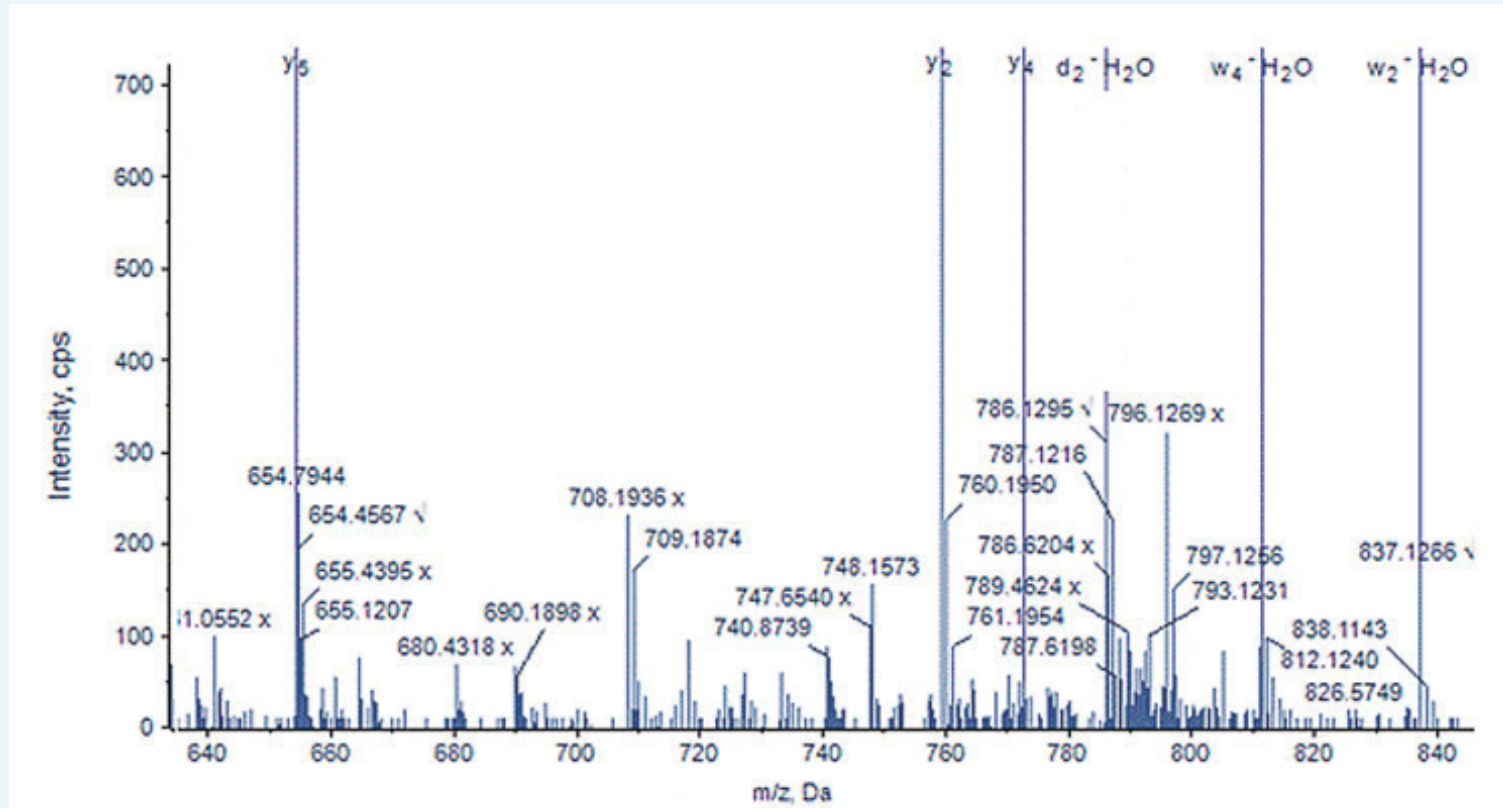
Many impurities and biotransformations result in isoelemental species that an MS-only workflow cannot solve.

With the ability to incorporate UV, MS and MS/MS information, you can get clear and unambiguous results that give you complete confidence.



Increase confidence through MS/MS

Analyze MS/MS spectra efficiently with customizable search criteria and gain detailed insights into fragment ion spectra.



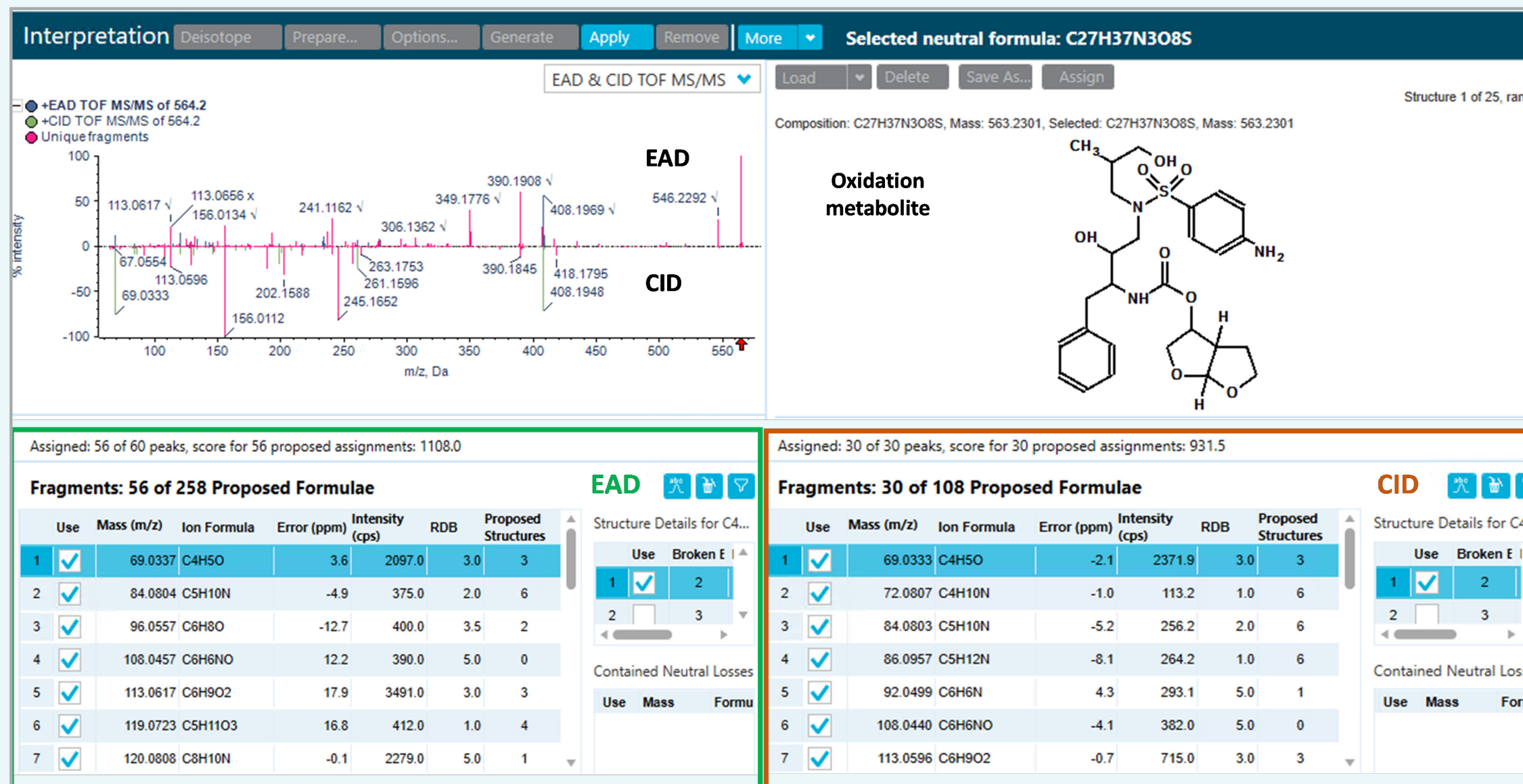
3. Easily customize your search criteria to match MS/MS spectra against in-silico generated impurities or metabolite fragments.

The screenshot shows the Molecule Profiler software interface. At the top, it displays "Potential Metabolites: 21 of 21 Peaks". Below this is a table with columns: Report, Peak ID, Name, Formula, Assigned, Neutral Mass, Average Mass, m/z, Charge, ppm, R.T. (min), Peak Area, % Area, % Score, and MS/MS Spectra. The selected metabolite is M14, with the name "Loss of CH₂+Glucuronidation (M+H)⁺" and formula C₃₂H₄₄N₂O₁₀. Below the table is the "Interpretation" view, which includes a plot of "EAD TOF MS/MS of 617.3" and a chemical structure of the parent compound. The structure is a complex molecule with multiple rings and functional groups. The interface also shows a table of "Fragments: 55 of 212 Proposed Formulae" and a "Structure Details for C₄H₉N" section.

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

Small molecule metabolite identification with speed and ease

Automate your metabolite identification with confident metabolite structure assignments using both collision-induced dissociation (CID) and electron activated dissociation (EAD) data, saving time and money in your laboratory.



Sample/Controls	Additional MS/MS Data	Folder	Processing Parameters	Apply
1 MS Sample: MetID Pioglitazone CID 0min.wiff2 Pioglitazone 0min	MS Sample: MetID Pioglitazone EAD 0min.wiff2 Pioglitazone 0min	Default	Pioglitazone	Pioglitazone_0
2 MS Sample: MetID Pioglitazone CID 30min.wiff2 Pioglitazone 30min	MS Sample: MetID Pioglitazone EAD 30min.wiff2 Pioglitazone 30min	Default	Pioglitazone	Pioglitazone_30
3 MS Sample: MetID Pioglitazone CID 60min.wiff2 Pioglitazone 60min	MS Sample: MetID Pioglitazone EAD 60min.wiff2 Pioglitazone 60min	Default	Pioglitazone	Pioglitazone_60
4 MS Sample: MetID Pioglitazone CID 90min.wiff2 Pioglitazone 90min	MS Sample: MetID Pioglitazone EAD 90min.wiff2 Pioglitazone 90min	Default	Pioglitazone	Pioglitazone_90
5 MS Sample: MetID Pioglitazone CID 120min.wiff2 Pioglitazone 120min	MS Sample: MetID Pioglitazone EAD 120min.wiff2 Pioglitazone 120min	Default	Pioglitazone	Pioglitazone_120
6 MS Sample: MetID Pioglitazone CID 240min.wiff2 Pioglitazone 240min	MS Sample: MetID Pioglitazone EAD 240min.wiff2 Pioglitazone 240min	Default	Pioglitazone	Pioglitazone_240
7				
8				
9				
10				
11				
12				

Get answers faster

Larger and more complex molecules such as lipids, oligonucleotides and peptides can produce very complex MS/MS data.

The powerful MS/MS engine in Molecule Profiler software can reduce the time it takes to get answers from days 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.

Explore structural depth with confidence in lipids

Lipid raw materials and lipid nanoparticles [LNPs] must be fully characterized to differentiate impurities, such as oxidation from ionizable lipids, which can affect product safety and efficacy.

With the ability to automatically process EAD and CID data, you can streamline workflows to get reliable answers faster and ensure the quality of the nucleic acid, including mRNA, in LNPs.

Interpretation Deisotope Prepare... Options... Generate Apply Remove More Selected neutral formula

+EAD TOF MS/MS of 658.6

Intensity, cps

61.0515

59.0472 60.0427 62.0597 62.9765 63.9595 65.0244 65.0374

m/z, Da

Assigned: 44 of 60 peaks, score for 44 proposed assign...

Composition: C₄₃H₇₉NO₃, Mass: 657.6060, Selected: C₂H₉NO, Mass: 60.0449

Structure 1 of 26, rank = 1

Use Mass (m/z) Ion Formula E

Use	Mass (m/z)	Ion Formula	E
<input checked="" type="checkbox"/>	61.0515	C ₂ H ₇ NO	
<input checked="" type="checkbox"/>	114.0905	C ₆ H ₁₂ NO	
<input checked="" type="checkbox"/>	87.0433	C ₄ H ₇ O ₂	
<input checked="" type="checkbox"/>	97.1001	C ₇ H ₁₃	
<input checked="" type="checkbox"/>	108.1000	C ₈ H ₁₃	
<input checked="" type="checkbox"/>	95.0545	C ₇ H ₁₁	
<input checked="" type="checkbox"/>	86.0956	C ₈ H ₁₂ N	

Parent Structure Structure Candidates

Rank	Relative Evidence	Apply to Results
1	No structure	<input type="checkbox"/>
2	1	<input checked="" type="checkbox"/>
3	2	<input type="checkbox"/>
4	3	<input type="checkbox"/>
5	3	<input type="checkbox"/>
6	4	<input type="checkbox"/>

Interpretation Deisotope Prepare... Options... Generate Apply Remove More Selected neutral formula

+EAD TOF MS/MS of 658.6

Intensity, cps

148.0956

141.0880 142 144 146 148 150

m/z, Da

Assigned: 44 of 60 peaks, score for 44 proposed assign...

Composition: C₄₃H₇₉NO₃, Mass: 657.6060, Selected: C₆H₁₂NO₂, Mass: 148.0917

Structure 1 of 26, rank = 1

Use Mass (m/z) Ion Formula E

Use	Mass (m/z)	Ion Formula	E
<input checked="" type="checkbox"/>	148.0956	C ₆ H ₁₂ NO ₂	
<input checked="" type="checkbox"/>	132.1009	C ₆ H ₁₄ NO ₂	
<input checked="" type="checkbox"/>	130.0840	C ₆ H ₁₂ NO ₂	
<input checked="" type="checkbox"/>	61.0515	C ₂ H ₇ NO	
<input checked="" type="checkbox"/>	114.0905	C ₆ H ₁₂ NO	
<input checked="" type="checkbox"/>	87.0433	C ₄ H ₇ O ₂	
<input checked="" type="checkbox"/>	97.1001	C ₇ H ₁₃	

Parent Structure Structure Candidates

Rank	Relative Evidence	Apply to Results
1	No structure	<input type="checkbox"/>
2	1	<input checked="" type="checkbox"/>
3	2	<input type="checkbox"/>
4	3	<input type="checkbox"/>
5	3	<input type="checkbox"/>
6	4	<input type="checkbox"/>

Interpretation Deisotope Prepare... Options... Generate Apply Remove More Selected neutral formula

+EAD TOF MS/MS of 658.6

Intensity, cps

61.0515

59.0472 60.0427 62.0597 62.9765 63.9595 65.0244 65.0374

m/z, Da

Assigned: 44 of 60 peaks, score for 44 proposed assign...

Composition: C₄₃H₇₉NO₃, Mass: 657.6060, Selected: C₄₃H₇₈NO₂, Mass: 640.6033

Structure 1 of 26, rank = 1

Use Mass (m/z) Ion Formula E

Use	Mass (m/z)	Ion Formula	E
<input checked="" type="checkbox"/>	641.6083	C ₄₃ H ₇₉ NO ₂	
<input checked="" type="checkbox"/>	639.5930	C ₄₃ H ₇₇ NO ₂	
<input checked="" type="checkbox"/>	148.0958	C ₆ H ₁₄ NO ₃	
<input checked="" type="checkbox"/>	132.1009	C ₆ H ₁₄ NO ₂	
<input checked="" type="checkbox"/>	130.0840	C ₆ H ₁₂ NO ₂	
<input checked="" type="checkbox"/>	61.0515	C ₂ H ₇ NO	
<input checked="" type="checkbox"/>	114.0905	C ₆ H ₁₂ NO	
<input checked="" type="checkbox"/>	87.0433	C ₄ H ₇ O ₂	

Parent Structure Structure Candidates

Rank	Relative Evidence	Apply to Results
1	No structure	<input type="checkbox"/>
2	1	<input checked="" type="checkbox"/>
3	2	<input type="checkbox"/>
4	3	<input type="checkbox"/>
5	3	<input type="checkbox"/>
6	4	<input type="checkbox"/>

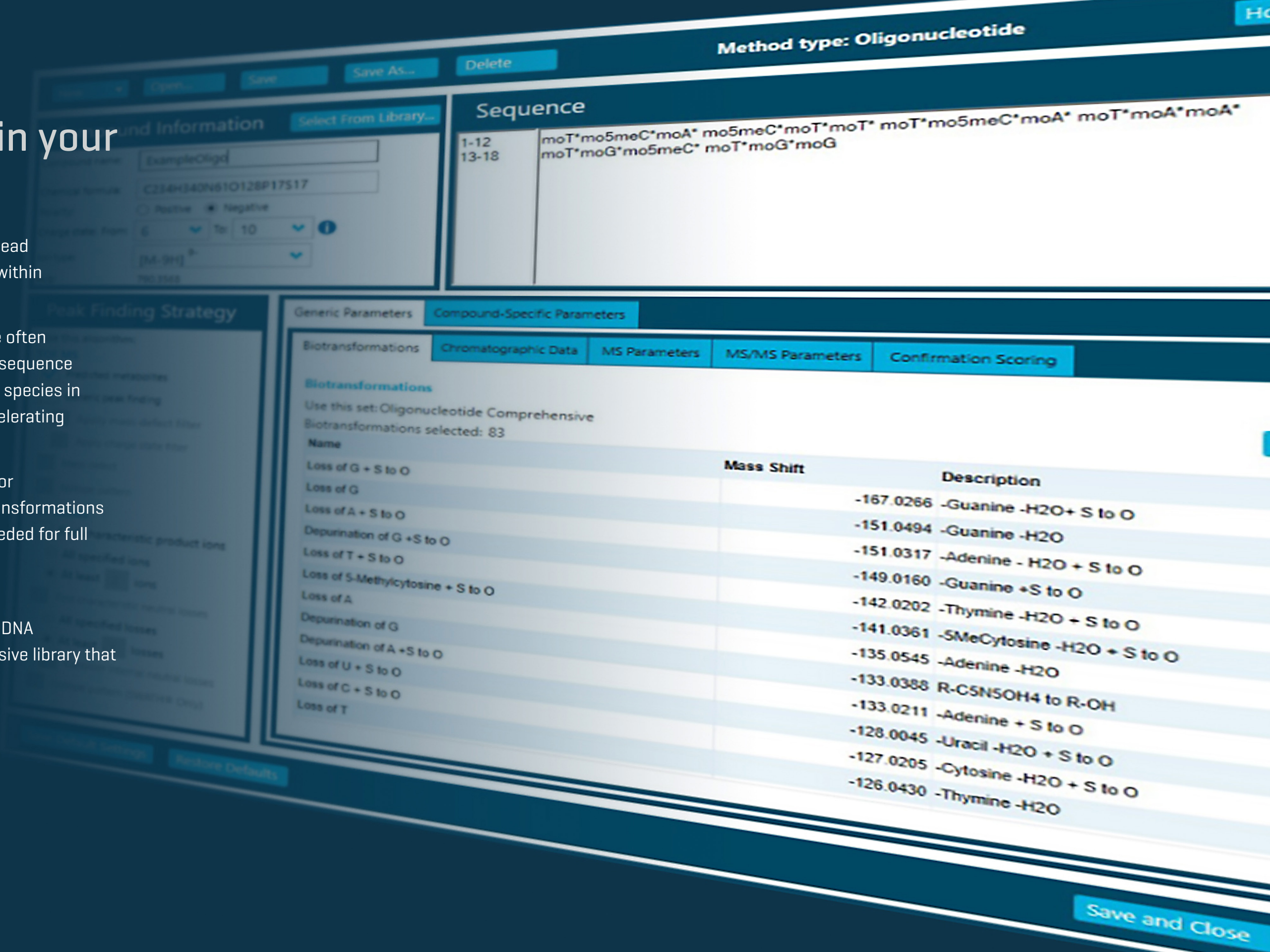
Gain confidence in your oligonucleotides

Side reactions during synthesis can lead to enormous numbers of impurities within oligonucleotide products.

Furthermore, biotransformations are often complex given the high variability of sequence modifications. Quick identification of species in a product or sample is crucial to accelerating development.

Choose from off-the-shelf libraries for oligonucleotide impurities and biotransformations to get a head start and amend as needed for full flexibility.

SCIEX has partnered with Integrated DNA Technologies to create a comprehensive library that helps ensure your sequence is right.



Molecule Profiler software is compatible with SCIEX accurate mass spectrometers



ZenoTOF 7600 system

This accurate mass spectrometer provides comprehensive data with innovations that have never been seen in an accurate mass system. The introduction of electron activated dissociation (EAD) fragmentation and the Zeno trap paved the way for precise and accurate MS and MS/MS data.



X500B and X500R QTOF systems

With simple workflows, robust hardware, sensitivity and precision, the X500B and X500R QTOF systems are the first LC-MS/MS systems designed for both characterization and quantitation.

SCIEX Now support network

SCIEX Now

- Manage your instruments
- Submit and manage support cases, track status and view history
- Access online training courses and articles
- Manage software licenses linked to your registered instruments
- View and report critical instrument statistics when connected to the StatusScope remote monitoring service
- Be a part of the SCIEX community by submitting questions and comments
- Receive notifications from SCIEX with content based on your preferences

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SCIEX Now Learning Hub

- SCIEX Now Learning Hub success programs provide LC-MS and capillary electrophoresis [CE] training customized to meet your exact needs
- With a selection of training methods and certifications available, you can build a mass spectrometry program that is most suited to your lab and users
- Starting with a clear understanding of your desired learning outcomes, we aim to help you improve lab productivity and consistency by designing and delivering a program that is focused on knowledge advancement and retention

Find out more →

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