

compute dialogue (single)

SIRIUS - Molecular Formula Identification

General Instrument: Q-TOF

MS2 mass accuracy (ppm): 10

Fix formula for detected lipid:

Possible Adducts:

- [M + H]⁺
- [M + K]⁺
- [M + Na]⁺
- [M]⁺
- [M + H3N + H]⁺
- [M - H2O + K]⁺

all none

compute dialogue (all)

SIRIUS - Molecular Formula Identification

General Instrument: Q-TOF

MS2 mass accuracy (ppm): 10

Fix formula for detected lipid:

Fallback Adducts:

- [M + H]⁺
- [M + K]⁺
- [M + Na]⁺
- [M]⁺
- [M + H3N + H]⁺
- [M - H2O + K]⁺

all none enforce

importing full LCMS runs

feature detection/alignment & adduct/ion detection

[M+H]⁺
415.21 m/z
11.22 min

[M+H3N+H]⁺
432.24 m/z
11.22 min

[M+Na]⁺
437.19 m/z
11.22 min

feature list

582605990820353196

Det. Adduct [M + H]⁺
Precursor 415,211 Da
RT 11,22 min
Confidence (A) 0.237

582605991340450690

Det. Adduct [M + H3N + H]⁺
Precursor 432,237 Da
RT 11,22 min
Confidence (A) 0.257

582605991520806766

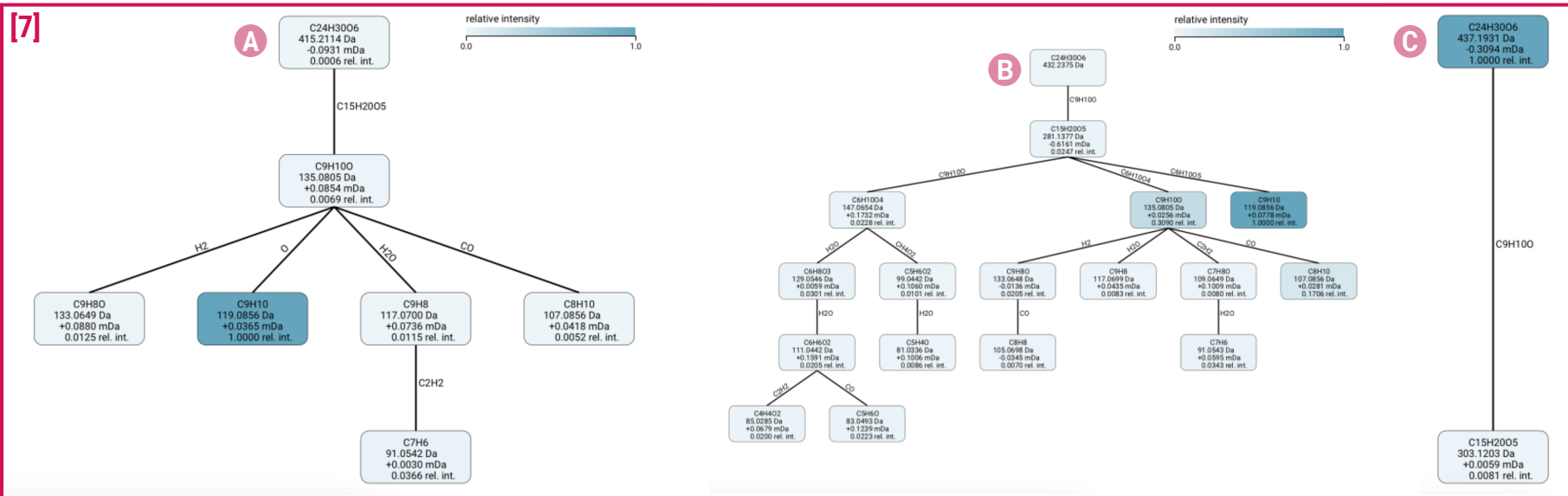
Det. Adduct [M + Na]⁺
Precursor 437,193 Da
RT 11,22 min
Confidence (A)

Formulas view

Rank	Molecular Formula	Adduct	Sirius Score	Isotope Score	Tree Score	Explained Peaks
1	C24H30O6	[M + H] ⁺	97,954%	6,560	21,974	6/6
2	C25H26N4O2	[M + H] ⁺	1,735%	5,561	18,939	6/6
3	C20H26N6O4	[M + H] ⁺	0,311%	4,389	18,392	6/6
4	C23H25F3N4	[M + H] ⁺	0,001%	5,859	10,798	3/6

Rank	Molecular Formula	Adduct	Sirius Score	Isotope Score	Tree Score	Explained Peaks
1	C24H30O6	[M + H3N + H] ⁺	99,993%	6,392	55,594	16/22
2	C20H26N6O4	[M + H3N + H] ⁺	0,007%	0,000	52,412	16/22
3	C25H26N4O2	[M + H3N + H] ⁺	0,000%	5,302	40,396	16/22
4	C23H25F3N4	[M + H3N + H] ⁺	0,000%	0,000	12,190	10/22

Rank	Molecular Formula	Adduct	Sirius Score	Isotope Score	Tree Score	Explained Peaks
1	C24H30O6	[M + Na] ⁺	97,615%	6,539	5,126	1/9
2	C25H26N4O2	[M + Na] ⁺	1,665%	5,464	2,129	1/9
3	C23H25F3N4	[M + Na] ⁺	0,367%	5,848	0,234	0/9
4	C20H26N6O4	[M + Na] ⁺	0,353%	4,382	1,660	1/9



Compound Classes view

LC-MS Formulas Predicted Fingerprints Compound Classes Structures De Novo Structures Substructure Annotations Library Matches

A C24H30O6 + H⁺ (SIRIUS 97.954%)

Main Classes: Organic compounds > Superclass (Benzeneoids) > Class (Phenol ethers) > Subclass (Anisoles)

Description: This compound belongs to the class Anisoles, which describes organic compounds containing a methoxybenzene or a derivative thereof.

B C24H30O6 + H3N + H⁺ (SIRIUS 99.993%)

Main Classes: Organic compounds > Superclass (Benzeneoids) > Class (Benzene and substituted derivatives)

Description: This compound belongs to the class Benzene and substituted derivatives, which describes aromatic compounds containing one monocyclic ring system consisting of benzene.

Structures view

LC-MS Formulas Predicted Fingerprints Compound Classes Structures De Novo Structures Substructure Annotations Library Matches

SMARTS filter: Type to search

A Bis-(3,4-dimethylbenzylidene)sorbitol (C24H30O6)

Substructures: [Progress bar]

Sources: DSSTox, NORMAN, PubChem, train

B Bis-(3,4-dimethylbenzylidene)sorbitol (C24H30O6)

Substructures: [Progress bar]

Sources: DSSTox, NORMAN, PubChem, train