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## Annex 2: MRTP Use and Health Risk - Toxicology

Product	<i>Marlboro Amber HeatSticks</i> <i>Marlboro Green Menthol HeatSticks</i> <i>Marlboro Blue Menthol HeatSticks</i> <i>IQOS System Holder and Charger</i> <i>IQOS 3.0 System Holder and Charger</i>
FDA STN	MR0000059, MR0000060, MR0000061, MR0000133, MR0000192
Reporting Period	March 1, 2022 to February 28, 2023

### Confidentiality Statement

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## 1. OVERVIEW

As part of the initial product characterization of the *IQOS* System, non-targeted differential screening (NTDS) analyses of the aerosol generated from *Marlboro* Amber *HeatSticks* (MR0000059), *Marlboro* Green Menthol *HeatSticks* (MR0000060), and *Marlboro* Blue Menthol *HeatSticks* (MR0000061) with the *IQOS* System Holder and Charger (MR0000133) were performed to identify compounds which were potentially new, or significantly increased in *IQOS* aerosol relative to 3R4F smoke. A hazard identification protocol was developed to determine the genotoxic and carcinogenic potential of both these inhaled tobacco product constituents and their potentially reactive and toxic metabolites.

The protocol was accepted by FDA on February 24, 2021. PMP SA appointed two Contract Research Organizations (CROs) for the performance of the study (b) (4)

(b) (4) and (b) (4)  
(b) (4) The study was divided in 3 phases:

- The project Phase 1 is intended to determine the genotoxicity and/or carcinogenicity potential of the 80 chemicals (parent compounds) identified as potentially new, or significantly increased in *IQOS* aerosol relative to 3R4F smoke.
- The project Phase 2 is intended to determine the potential metabolites of the 80 chemicals relevant to humans
- The project Phase 3 is intended to determine the genotoxicity and/or carcinogenicity potential of the relevant metabolites.

The phase 1 was completed and reported in the previous reporting period. Phase 2 has been completed and the outcome is presented on the next section. Phase 3 completion is expected by end of Q2 2023.

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## 2. PHASE 2 RESULTS

*In silico* prediction and literature/database search for any mammalian metabolites of the parent compounds were performed. Searches of relevant literature were conducted, and the metabolites identified in published studies and/or Expert group reviews were recorded. Two *in silico* software packages (Meteor Nexus and the OECD (Q)SAR Toolbox) were used to predict likely mammalian metabolites in a range of models as described in Table 1. A human expert assessment was included to ensure the biological relevance of the data, their quality, and their robustness. For each compound, the name of the retrieved metabolites, and the related CAS number when available, is mentioned. In addition, the status (known or predicted metabolite) and the ranking are reported. The ranking refers to the biological relevance and the robustness of the data as described in Table 2. The results are summarized in Table 3. When the software was not able to retrieve the chemical name of the predicted molecule, the SMILES of the molecule was provided instead. From 80 parent compounds, 1659 (thousand six hundred fifty-nine) metabolites were retrieved.

**Table 1: Prediction models**

Software	Models applied
Meteor Nexus 3.1.0	Limited to mammals, using site of metabolism scoring <sup>1</sup> and a molecular mass similarity threshold of at least 70%.
OECD (Q)SAR Toolbox Desktop Client 4.5	A. In vivo rat metabolism simulator B. Observed mammalian metabolism C. Observed rat in vivo metabolism D. Observed rat liver with quantitative data E. Observed rat liver S9 metabolism F. Rat liver S9 metabolism simulator

<sup>1</sup> Site of metabolism scoring is a machine learning system that takes likelihood of a biotransformation, experimental data for similar compounds, and tissue type [presumably site of metabolism] into account.

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**Table 2: Ranking level**

Ranking	Description
1	Known phase I metabolite, described in the literature from established metabolic pathways
2	Metabolite predicted by 2 (two) models or more
3	Metabolite predicted by 1 (one) model only
4	Phase 2 (conjugated) metabolite, known and predicted

**Table 3: Metabolite prediction of the 80 identified chemicals**

CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
100-51-6	Benzyl alcohol	100-52-7	Benzaldehyde	Known	1
		65-85-0	Benzoic acid	Known	1
		19542-77-9	Benzylmercapturic acid	Known	4
		6756-74-7	Benzoyl coenzyme A	Known	4
		495-69-2	Hippuric acid	Known	4
		19237-53-7	Benzoyl glucuronide	Known	4
		5285-02-9	Benzyl $\beta$ -D-glucopyranosiduronic acid	Predicted	4
			Benzyl sulfate	Predicted	4
10267-21-7	Labdane-8,15-diol, (13S)		8-Hydroxylabdan-15-oic acid	Predicted	2
			8-Hydroxylabdan-15-al	Predicted	2
			Labdane-8,13-15-triol	Predicted	3
			8,18-Dihydroxylabdan-15-al	Predicted	3

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			8,17-Dihydroxylabdan-15-oic acid	Predicted	3
			8,17-Dihydroxylabdan-15-al	Predicted	3
			Labdane-8,15-diol 18-carbaldehyde	Predicted	3
			Labdane-8,15,18-triol	Predicted	3
			Labdane-8,15,17-triol	Predicted	3
			Labdane-8,15-diol 16-carbaldehyde	Predicted	3
			Labdane-8,16-diol 15-carbaldehyde	Predicted	3
			Labdane-8,15,16-triol	Predicted	3
			8,13-Dihydroxylabdan-15-oic acid	Predicted	3
			Labdane-8,9-15-triol	Predicted	3
			Glucuronide conjugate of labdane-8,15-diol	Predicted	4
			Labdane-5,8,15-triol	Predicted	3
10458-14-7	Menthone	1490-04-6	Menthol	Known	1
		107551-97-3	Menthol glucuronide	Known	4
		2216-52-6	(+)-Neomenthol	Known	1
			(+)-Neomenthol glucuronide	Known	4
		23283-97-8	(+)-Isomenthol	Known	1

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			(+)-Isomenthol glucuronide	Known	4
		3304-24-3	8-Hydroxymenthone	Known	1
			Glucuronic acid conjugate of 8-hydroxymenthone	Known	4
		721427-57-2	7-Hydroxymenthone	Known	1
			4,5-Dihydroxy-2-(2-hydroxypropan-2-yl)-5-methylcyclohexan-1-one	Predicted	3
			4-Hydroxy-5-(hydroxymethyl)-2-(2-hydroxypropan-2-yl)cyclohexan-1-one	Predicted	3
			5-Hydroxy-2-(2-hydroxypropan-2-yl)-5-methylcyclohexan-1-one	Predicted	2
		155348-06-4	4-(2-Hydroxy-2-propanyl)-1-methyl-1,3-cyclohexanediol	Predicted	2
			4-(2-Hydroxypropan-2-yl)-3-oxocyclohexane-1-carbaldehyde	Predicted	3
			5-(Hydroxymethyl)-2-(2-hydroxypropan-2-yl)cyclohexan-1-one	Predicted	3
		74219-28-6	2-Hydroxy-2-isopropyl-5-methylcyclohexanone	Predicted	2
			4,5-Dihydroxy-5-methyl-2-(propan-2-yl)cyclohexan-1-one	Predicted	3
			4-Hydroxy-2-isopropyl-5-methylcyclohexanone	Predicted	3

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		63865-64-5	5-Hydroxy-2-isopropyl-5-methylcyclohexanone	Predicted	2
		1612-98-2	p-Menthane-1,3-diol; 1-Methyl-4-propan-2-ylcyclohexane-1,3-diol	Predicted	2
			2-(4-Hydroxy-4-methyl-2-oxocyclohexyl)propanoic acid	Predicted	3
			2-(4-Hydroxy-4-methyl-2-oxocyclohexyl)propanal	Predicted	3
			5-Hydroxy-2-(1-hydroxypropan-2-yl)-5-methylcyclohexan-1-one	Predicted	2
			4-Hydroxy-2-(2-hydroxypropan-2-yl)-5-methylcyclohexan-1-one	Predicted	3
		1933756-41-2	4-Methyl-2-oxocyclohexyl]propanoic acid	Predicted	2
			2-(4-Methyl-2-oxocyclohexyl)propanal	Predicted	2
		623531-70-4	2-(1-Hydroxy-2-propanyl)-5-methylcyclohexanone	Predicted	2
		42822-86-6	2-(2-Hydroxy-2-propanyl)-5-methylcyclohexanol; p-Menthane-3,8-diol	Predicted	2
			4,8,8-Trimethyl-7-oxabicyclo[4.2.0]octane	Predicted	3
			3-Oxo-4-(propan-2-yl)cyclohexane-1-carboxylic acid	Predicted	3
			3-Oxo-4-(propan-2-yl)cyclohexane-1-carbaldehyde	Predicted	3

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		721427-57-2	5-(Hydroxymethyl)-2-isopropylcyclohexanone; 7-Hydroxymenthone	Predicted	3
			3-O-Glucuronide conjugate of 8-hydroxymenthol	Predicted	4
			1-(2-Hydroxypropan-2-yl)-4-methylcyclohexane-1,2-diol; 4,8-Dihydroxymenthol	Predicted	3
			2-(2-Hydroxy-4-methylcyclohexyl)propane-1,2-diol; 8,9-Dihydroxymenthol	Predicted	3
			8-O-Glucuronide conjugate of 8-hydroxymenthol	Predicted	4
			2-(1,2-Dihydroxypropan-2-yl)-5-methylcyclohexan-1-one; 8,9-Dihydroxymenthone	Predicted	3
			Glucuronide/glucuronic acid conjugate of 8-hydroxymenthone	Predicted	4
			3-O-Glucuronide conjugate of 1-hydroxymenthol	Predicted	4
			4-(1-Hydroxypropan-2-yl)-1-methylcyclohexane-1,3-diol; 1,9-Dihydroxymenthol	Predicted	3
			4-Methyl-1-(propan-2-yl)cyclohexane-1,2,4-triol; 1,4-Dihydroxymenthol	Predicted	3
			1-O-Glucuronide conjugate of 1-hydroxymenthol	Predicted	4
			9-O-Glucuronide conjugate of 1,9-Dihydroxymenthone	Predicted	4

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			Glucuronide conjugate of 1-hydroxymenthone	Predicted	4
			2-(1-Hydroxypropan-2-yl)-5-methylcyclohexan-1-ol; 9-Hydroxymenthol	Predicted	3
			3-O-Glucuronide conjugate of 9-hydroxymenthol	Predicted	4
			Glucuronide conjugate of 9-hydroxymenthone	Predicted	4
			3-Hydroxy-5-methyl-2-(propan-2-yl)cyclohexan-1-one; 5-Hydroxymenthone	Predicted	3
			5-Methyl-2-(propan-2-yl)cyclohexane-1,3-diol; 5-Hydroxymenthol	Predicted	3
			4-Methyl-1-(propan-2-yl)cyclohexane-1,2-diol; 4-Hydroxymenthol	Predicted	3
			2-Hydroxy-3-methyl-6-(propan-2-yl)cyclohexan-1-one; 2-Hydroxymenthone	Predicted	3
			3-Methyl-6-(propan-2-yl)cyclohexane-1,2-diol; 2-Hydroxymenthol	Predicted	3
105-43-1	3-Methylvaleric acid	116-53-0	2-Methylbutyric acid	Known	1
		72-89-9	Acetyl CoA	Known	1
		67-64-1	Acetone	Known	1
		300-85-6	$\beta$ -Hydroxybutyric acid	Known	1

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		151-11-1	5-Hydroxy-3-methylpentanoic acid	Known	1
		150-96-9	3-Hydroxy-3-methylpentanoic acid	Known	1
		150-97-0	Mevalonic acid	Known	1
		64-18-6	Formic acid	Known	1
		626-51-7	3-Methylglutaric acid; 3-Methylpentanedioic acid	Predicted	2
		1314934-24-1	3-Methyl-5-oxopentanoic acid	Predicted	2
		41654-03-9	4-Hydroxy-3-methylpentanoic acid	Predicted	2
			4-Hydroxy-3-(hydroxymethyl)pentanoic acid	Predicted	3
		636-48-6	2-Ethylsuccinic acid; 2-Ethylbutanedioic acid	Predicted	2
		127194-25-6	3-Formylpentanoic acid	Predicted	2
		81381-86-4	3-(Hydroxymethyl)pentanoic acid	Predicted	2
		503-49-1	3-Hydroxymethylglutaric acid	Predicted	3
			3-(Hydroxymethyl)-5-oxopentanoic acid	Predicted	3
			2-(2-Hydroxyethyl)butanedioic acid	Predicted	3
			3-Formyl-5-hydroxypentanoic acid	Predicted	3
			5-Hydroxy-3-(hydroxymethyl)pentanoic acid	Predicted	3

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			3,4-Dihydroxy-3-methylpentanoic acid	Predicted	3
			2-(3-Methylpentanoylamino)acetic acid	Predicted	3
			3,4,5-Trihydroxy-6-[(3-methylpentanoyl)oxy]oxane-2-carboxylic acid	Predicted	4
			5-Amino-2-(3-methylpentanamido)-5-oxopentanoic acid	Predicted	3
105453-16-5	Germacrene D		2-[(2Z,7E)-8-(Hydroxymethyl)-4-methylidenecyclodeca-2,7-dien-1-yl]propan-2-ol	Predicted	3
			2-[(5Z)-1-Methyl-7-methylidene-11-oxabicyclo[8.1.0]undec-5-en-4-yl]propan-2-ol	Predicted	3
			(2Z,7Z)-2-Methyl-6-methylidene-9-(propan-2-yl)cyclodeca-2,7-dien-1-one	Predicted	2
			(2Z,4Z,9Z)-8-Hydroxy-3,9-dimethyl-6-(propan-2-yl)cyclodeca-2,4,9-trien-1-one	Predicted	3
			(5Z)-5-Methyl-9-methylidene-2-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-en-4-ol	Predicted	3
			(2Z,7Z)-2-Methyl-6-methylidene-9-(propan-2-yl)cyclodeca-2,7-dien-1-ol	Predicted	2
			(4Z,9Z)-9-Methyl-6-(propan-2-yl)-1-oxaspiro[2.9]dodeca-4,9-dien-8-ol	Predicted	3

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			(1E,6Z)-4-Hydroxy-5-methylidene-8-(propan-2-yl)cyclodeca-1,6-diene-1-carboxylic acid	Predicted	3
			(1E,6Z)-5-Methylidene-8-(propan-2-yl)cyclodeca-1,6-diene-1-carboxylic acid	Predicted	2
			5-Methyl-9-methylidene-2-(propan-2-yl)-11-oxabicyclo[8.1.0]undecane-5,6-diol	Predicted	3
			(6Z)-1-Methyl-5-methylidene-8-(propan-2-yl)cyclodec-6-ene-1,2-diol	Predicted	2
			(11Z)-7-Methyl-10-(propan-2-yl)-1-oxaspiro[2.9]dodec-11-ene-6,7-diol	Predicted	3
			(2Z,4Z,9Z)-3,9-Dimethyl-6-(propan-2-yl)cyclodeca-2,4,9-trien-1-one	Predicted	2
			(2E,4Z,9Z)-3-(Hydroxymethyl)-9-methyl-6-(propan-2-yl)cyclodeca-2,4,9-trien-1-one	Predicted	3
			(2Z,4Z,9Z)-3,9-Dimethyl-6-(propan-2-yl)cyclodeca-2,4,9-trien-1-ol	Predicted	3
			(2Z,7Z)-3-Methyl-9-methylidene-6-(propan-2-yl)cyclodeca-2,7-dien-1-ol	Predicted	2
			(3Z,8Z)-8-Methyl-2-methylidene-5-(propan-2-yl)cyclodeca-3,8-dien-1-one	Predicted	2

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			(5Z)-6-Methyl-2-methylidene-9-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-en-3-ol	Predicted	3
			(6Z,11Z)-7-Methyl-10-(propan-2-yl)-1-oxaspiro[2.9]dodeca-6,11-dien-4-ol	Predicted	3
			(6Z)-6-Methyl-10-methylidene-3-(propan-2-yl)cyclodec-6-ene-1,2-diol	Predicted	2
			(5Z)-5-Methyl-9-methylidene-2-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-ene	Predicted	2
			(2Z,7Z)-1-Hydroxy-7-methyl-4-(propan-2-yl)cyclodeca-2,7-diene-1-carbaldehyde	Predicted	3
			(5Z)-2-(Hydroxymethyl)-6-methyl-9-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-en-2-ol	Predicted	3
			(2Z,7Z)-1-(Hydroxymethyl)-7-methyl-4-(propan-2-yl)cyclodeca-2,7-dien-1-ol	Predicted	3
			(9Z)-9-Methyl-6-(propan-2-yl)-1-oxaspiro[2.9]dodec-9-ene-4,5-diol	Predicted	3
			(4Z,9Z)-9-Methyl-6-(propan-2-yl)-1-oxaspiro[2.9]dodeca-4,9-diene	Predicted	3
			(1E,6Z)-4-Hydroxy-5-methylidene-8-(propan-2-yl)cyclodeca-1,6-diene-1-carbaldehyde	Predicted	3
			(1E,6Z)-5-Methylidene-8-(propan-2-yl)cyclodeca-1,6-diene-1-carbaldehyde	Predicted	2

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			(2Z,4Z,9E)-9-(Hydroxymethyl)-3-methyl-6-(propan-2-yl)cyclodeca-2,4,9-trien-1-one	Predicted	3
			(3Z,8E)-8-(Hydroxymethyl)-2-methylidene-5-(propan-2-yl)cyclodeca-3,8-dien-1-ol	Predicted	3
			[(1E,6Z)-5-Methylidene-8-(propan-2-yl)cyclodeca-1,6-dien-1-yl]methanol	Predicted	2
			(5Z)-10-Methyl-4-methylidene-7-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-en-3-ol	Predicted	2
			1-Methyl-7-methylidene-4-(propan-2-yl)-11-oxabicyclo[8.1.0]undecane-5,6-diol	Predicted	3
			(5Z)-1-Methyl-7-methylidene-4-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-ene	Predicted	2
			(5Z)-4-(Hydroxymethyl)-10-methyl-7-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-en-4-ol	Predicted	3
			2-[(2Z,7Z)-8-Methyl-4-methylidenecyclodeca-2,7-dien-1-yl]propanoic acid	Predicted	2
			2-[(2Z,7Z)-8-Methyl-4-methylidenecyclodeca-2,7-dien-1-yl]propanal	Predicted	2
			(2Z,7Z)-9-(1-Hydroxypropan-2-yl)-2-methyl-6-methylidenecyclodeca-2,7-dien-1-ol	Predicted	2

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			(2Z,4Z,9Z)-6-(1-Hydroxypropan-2-yl)-3,9-dimethylcyclodeca-2,4,9-trien-1-one	Predicted	3
			(3Z,8Z)-5-(1-Hydroxypropan-2-yl)-8-methyl-2-methylidenecyclodeca-3,8-dien-1-ol	Predicted	2
			2-[(2Z,7Z)-8-Methyl-4-methylidenecyclodeca-2,7-dien-1-yl]propan-1-ol	Predicted	2
			(3Z,8E)-8-(Hydroxymethyl)-5-(1-hydroxypropan-2-yl)-2-methylidenecyclodeca-3,8-dien-1-ol	Predicted	3
			2-[(5E)-5-(Hydroxymethyl)-9-methylidene-11-oxabicyclo[8.1.0]undec-5-en-2-yl]propan-1-ol	Predicted	3
			2-[(2Z,7E)-8-(Hydroxymethyl)-4-methylidenecyclodeca-2,7-dien-1-yl]propan-1-ol	Predicted	3
			2-[(4Z,9E)-9-(Hydroxymethyl)-1-oxaspiro[2.9]dodeca-4,9-dien-6-yl]propan-1-ol	Predicted	3
			2-[(5Z)-1-(Hydroxymethyl)-7-methylidene-11-oxabicyclo[8.1.0]undec-5-en-4-yl]propan-1-ol	Predicted	3
			2-[(2Z,7E)-8-(Hydroxymethyl)-4-methylidenecyclodeca-2,7-dien-1-yl]propane-1,2-diol	Predicted	3
			(2Z,7Z)-9-(2-hydroxypropan-2-yl)-2-methyl-6-methylidenecyclodeca-2,7-dien-1-ol	Predicted	2

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			2-[(5Z)-5-Methyl-9-methylidene-11-oxabicyclo[8.1.0]undec-5-en-2-yl]propan-2-ol	Predicted	3
			(3Z,8Z)-5-(2-Hydroxypropan-2-yl)-8-methyl-2-methylidenecyclodeca-3,8-dien-1-ol	Predicted	2
			(2Z,7Z)-6-(2-Hydroxypropan-2-yl)-3-methyl-9-methylidenecyclodeca-2,7-dien-1-ol	Predicted	2
			2-[(2Z,7Z)-8-Methyl-4-methylidenecyclodeca-2,7-dien-1-yl]propan-2-ol	Predicted	2
			(2Z,4Z,9Z)-6-(2-Hydroxypropan-2-yl)-3,9-dimethylcyclodeca-2,4,9-trien-1-one	Predicted	3
			2-[(4Z,9Z)-9-Methyl-1-oxaspiro[2.9]dodeca-4,9-dien-6-yl]propan-2-ol	Predicted	3
			(4Z,9Z)-4-Methyl-8-methylidene-1-(propan-2-yl)cyclodeca-4,9-diene-1,3-diol	Predicted	3
			(2Z,7Z)-8-Methyl-4-methylidene-1-(propan-2-yl)cyclodeca-2,7-diene-1,5-diol	Predicted	3
			(2Z,7Z)-8-Methyl-4-methylidene-1-(propan-2-yl)cyclodeca-2,7-dien-1-ol	Predicted	3
			Glucuronide conjugate of (2Z,7Z)-3-Methyl-9-methylidene-6-(propan-2-yl)cyclodeca-2,7-dien-1-ol	Predicted	4

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			(5Z)-6-Methyl-2-methylidene-9-(propan-2-yl)-11-oxabicyclo[8.1.0]undec-5-en-4-ol	Predicted	3
			(6Z)-7-Methyl-3-methylidene-10-(propan-2-yl)cyclodec-6-ene-1,2,5-triol	Predicted	3
			(2Z,7Z)-3-Methyl-9-methylidene-6-(propan-2-yl)cyclodeca-2,7-dien-1-one	Predicted	3
			(2Z,7Z)-6-(1-Hydroxypropan-2-yl)-3-methyl-9-methylidenecyclodeca-2,7-dien-1-ol	Predicted	3
			(3Z,8Z)-4-Methyl-10-methylidene-7-(propan-2-yl)cyclodeca-3,8-diene-1,2-diol	Predicted	3
			2-[(5Z)-5-Methyl-9-methylidene-11-oxabicyclo[8.1.0]undec-5-en-2-yl]propan-1-ol	Predicted	3
			2-[(5Z)-1-Methyl-7-methylidene-11-oxabicyclo[8.1.0]undec-5-en-4-yl]propan-1-ol	Predicted	3
			1-Methyl-8-methylidene-4-(propan-2-yl)-6,12-dioxatricyclo[9.1.0.05,7]dodecane	Predicted	3
			Glucuronide conjugate of 2-[(2Z,7Z)-8-Methyl-4-methylidenecyclodeca-2,7-dien-1-yl]propan-1-ol	Predicted	4
106-33-2	Ethyl dodecanoate (Ethyl laurate)	143-07-7	Lauric acid	Known	1
		64-17-5	Ethyl alcohol	Known	1

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		32459-66-8	11-Hydroxydodecanoic acid	Predicted	2
		64-19-7	Acetic acid	Predicted	2
		1422-27-1	9-Hydroxydecanoic acid	Predicted	3
			10-Hydroxylauric acid	Predicted	3
			10,11-Dihydroxydodecanoic acid	Predicted	3
		114212-45-2	4-Oxodecanedioic acid	Predicted	3
		124-07-2	Caprylic acid (octanoic acid)	Predicted	3
		2388-78-5	11-Oxododecanoic acid	Predicted	3
			12-hydroxy-9-oxododecanoic acid	Predicted	3
		30828-09-2	4-Oxododecanedioic acid	Predicted	3
		334-48-5	Capric acid (decanoic acid)	Predicted	3
			3-Oxodecanedioic acid	Predicted	3
			4-hydroxydecanedioic acid	Predicted	3
			4-hydroxydodecanedioic acid	Predicted	3
		505-95-3	12-Hydroxydodecanoic acid	Predicted	3
		51551-01-0	9,12-dioxododecanoic acid	Predicted	3
		673-85-8	10-Oxododecanoic acid	Predicted	3
		68490-89-1	9-hydroxy-dodecanoic acid	Predicted	3

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		75-07-0	Acetaldehyde	Predicted	2
			9,11-dihydroxydodecanoic acid	Predicted	3
			9-hydroxy-12-oxododecanoic acid	Predicted	3
			9-Oxo-dodecanoic acid	Predicted	3
			ethyl 12-hydroxydodecanoate	Predicted	3
			ethyl 9-hydroxydodecanoate	Predicted	3
			<chem>CC(O)C(=O)CCCCCCCC(O)=O</chem> )	Predicted	3
111-61-5	Stearate, ethyl-	57-11-4	Stearic acid; Octadecanoic acid	Predicted	2
		64-17-5	Ethyl alcohol	Predicted	2
		64-19-7	Acetic acid	Predicted	2
			17-oxooctadecanoic acid	Predicted	3
			15-hydroxyhexadecanoic acid	Predicted	2
		4552-19-6	17-hydroxyoctadecanoic acid	Predicted	2
		57-10-3	Hexadecanoic acid	Predicted	2
		13126-28-8	16-oxooctadecanoic acid	Predicted	3
			15-hydroxyoctadecanoic acid	Predicted	3
			15-oxooctadecanoic acid	Predicted	3
			16-hydroxystearic acid	Predicted	3

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			18-hydroxy-15-oxooctadecanoic acid	Predicted	3
		3155-42-8	18-hydroxyoctadecanoic acid	Predicted	3
			4-hydroxyhexadecanedioic acid	Predicted	3
		544-63-8	Myristic acid	Predicted	3
		75-07-0	Acetaldehyde	Predicted	2
			ethyl 17-hydroxyoctadecanoate	Predicted	3
			ethyl 18-hydroxyoctadecanoate	Predicted	3
			CC(O)C(=O)CCCCCCCCCCCCC CC(O)=O	Predicted	3
			CC(O)C(O)CCCCCCCCCCCCC C(O)=O	Predicted	3
1125-80-0	Isoquinoline, 3-methyl	215237-76-6	3-Methylisoquinolin-5-ol	Predicted	3
		14548-00-6	3-Methylisoquinoline N-oxide	Predicted	2
		3336-53-6	3-methylisoquinolin-4-ol	Predicted	2
		76884-34-9	3-Isoquinolinemethanol	Predicted	2
		1037219-67-2	3-Methylisoquinolin-8-ol	Predicted	3
		63485-73-4	3-Methylisoquinolin-7-ol	Predicted	3
		6624-49-3	Isoquinoline-3-carboxylic Acid	Predicted	2
		696575-22-1	3-Methylisoquinolin-6-ol	Predicted	3

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		7114-80-9	3-methylisoquinolin-1(2H)-one	Predicted	3
		5470-80-4	Isoquinoline-3-carbaldehyde	Predicted	2
116-09-6	1-Hydroxy-2-propanone	127-17-3	Pyruvic acid	Predicted	2
			2-Oxopropyl hydrogen sulfate	Predicted	4
		50-21-5	Lactic acid	Predicted	3
		57-55-6	Propylene glycol	Predicted	2
		598-35-6	2-Hydroxypropanal	Predicted	3
		78-98-8	Methylglyoxal (2-Oxopropanal)	Predicted	2
		64-19-7	Acetic acid	Predicted	3
		75-07-0	Acetaldehyde	Predicted	2
1191-41-9	Ethyl linolenate		Octadeca-9,12,15-trienoic acid	Predicted	2
			18-hydroxyoctadeca-9,12,15-trienoic acid	Predicted	2
			12,13-dihydroxyoctadeca-9,15-dienoic acid	Predicted	3
		13435-77-3	15,16-epoxyoctadeca-9,12-dienoic acid	Predicted	3
		140129-22-2	15,16-dihydroxyoctadeca-9,12-dienoic acid	Predicted	2
		338746-11-5	2-[[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]sulfanyl]acetic acid	Predicted	4

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		503058-67-1	8-[3-[4-(3-ethyloxiran-2-yl)but-2-enyl]oxiran-2-yl]octanoic acid	Predicted	3
		64-17-5	Ethyl alcohol	Predicted	3
		64-19-7	Acetic acid	Predicted	2
		868364-07-2	8-[3-[(3-pent-2-enyloxiran-2-yl)methyl]oxiran-2-yl]octanoic acid	Predicted	3
		868364-08-3	11-[3-[(3-ethyloxiran-2-yl)methyl]oxiran-2-yl]undec-9-enoic acid	Predicted	3
		88159-18-6	11-(3-pent-2-enyloxiran-2-yl)undec-9-enoic acid	Predicted	3
		88199-24-0	8-(3-octa-2,5-dienyloxiran-2-yl)octanoic acid	Predicted	3
			9,10-dihydroxyoctadeca-12,15-dienoic acid	Predicted	3
			hexadeca-7,10,13-trienoic acid	Predicted	2
			octadeca-3,6,9-trienedioic acid	Predicted	3
			17-Hydroxyoctadeca-9,12,15-trienoic acid	Predicted	2
		75-07-0	Acetaldehyde	Predicted	3
			Tetradeca-5,8,11-trienoic acid	Predicted	3
1192-58-1	2-Formyl-1-methylpyrrole	6973-60-0	N-Methylpyrrole-2-carboxylic acid	Known	1
			2-[(1-Methylpyrrole-2-carbonyl)amino]acetic acid	Predicted	3

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			1-Methyl-5-oxo-4,5-dihydro-1H-pyrrole-2-carboxylic acid	Predicted	3
			1-Methyl-5-hydroxy-2-pyrrolicarboxylic acid	Predicted	3
119903-95-6	Bourbonene, beta		1-Methyl-4,9-dihydroxy-5-methylidene-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-5-methylidene-8-(propan-2-ol-2-yl)-9-hydroxytricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-4,10-dihydroxy-5-methylidene-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-5-methylidene-8-(propan-2-ol-2-yl)-10-hydroxytricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-3,4-dihydroxy-5-methylidene-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-3-hydroxy-5-methylidene-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-4-hydroxy-5-(2-oxiranyl)-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-5-methylidene-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-5-hydroxy-5-(hydroxymethyl)-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3

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			1-Methyl-5-(2-oxiranyl)-8-(propan-2-ol-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-3-oxo-5-methyl-8-(propan-2-yl)-9-hydroxytricyclo[5.3.0.0]dec-4-ene	Predicted	3
			1-Methyl-4,9-dihydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-5-methylidene-8-(propan-2-yl)-9-hydroxytricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-3-oxo-5-methyl-8-(propan-2-yl)-10-hydroxytricyclo[5.3.0.0]dec-4-ene	Predicted	3
			1-Methyl-4,10-dihydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-5-methylidene-8-(propan-2-yl)-10-hydroxytricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-3-oxo-5-methyl-8-(propan-2-yl)tricyclo[5.3.0.0]dec-4-ene	Predicted	2
			1-Methyl-3-oxo-5-(hydroxymethyl)-8-(propan-2-yl)tricyclo[5.3.0.0]dec-4-ene	Predicted	3
			1-Methyl-3,4-dihydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-3-hydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	2

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			1-Methyl-4-oxo-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-4-hydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	2
			1-Methyl-4,5-dihydroxy-5-(hydroxymethyl)-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-4-hydroxy-5-(2-oxiranyl)-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-5-hydroxy-8-(propan-2-yl)tricyclo[5.3.0.0]decane-5-carbaldehyde	Predicted	3
			1-Methyl-5-hydroxy-5-(hydroxymethyl)-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-5-(2-oxiranyl)-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			2-(1-Methyl-4-hydroxy-5-methylidenetricyclo[5.3.0.0]decyl) propanoic acid	Predicted	3
			2-(1-Methyl-5-methylidenetricyclo[5.3.0.0]decyl) propanoic acid	Predicted	2
			2-(1-Methyl-4-hydroxy-5-methylidenetricyclo[5.3.0.0]decyl) propanal	Predicted	3
			2-(1-Methyl-5-methylidenetricyclo[5.3.0.0]decyl) propanal	Predicted	2

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			2-(1-Methyl-3-oxo-5-methyltricyclo[5.3.0.0]dec-4-enyl)propan-1-ol	Predicted	3
			2-(1-Methyl-4-hydroxy-5-methylidenetricyclo[5.3.0.0]decyl)propan-1-ol	Predicted	2
			2-(1-Methyl-5-methylidenetricyclo[5.3.0.0]decyl)propan-1-ol	Predicted	2
			2-(1-Methyl-3-oxo-5-methyltricyclo[5.3.0.0]dec-4-enyl)propan-2-ol	Predicted	3
			1-Methyl-4,8-dihydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-5-methylidene-8-hydroxy-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-2,4-dihydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			1-Methyl-2-hydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane	Predicted	3
			[Glucuronide conjugate of 2-(1-methyl-5-methylidenetricyclo[5.3.0.0]decyl)propan-1-ol]	Predicted	4
			2-(3a-methyl-6-methylidenedecahydrocyclobuta[1,2-a:3,4-a']dicyclopenten-1-yl)propane-1,3-diol	Predicted	3

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			[Glucuronide conjugate of 1-methyl-5-methylidene-8-(propan-2-yl)-9-hydroxytricyclo[5.3.0.0]decane]	Predicted	4
			1-(Propan-2-yl)-3a-methyl-6-methylideneoctahydrocyclobuta[1,2-a:3,4-a']dicyclopenten-2(1H)-one	Predicted	3
			[Glucuronide conjugate of 1-methyl-3-hydroxy-5-methylidene-8-(propan-2-yl)tricyclo[5.3.0.0]decane]	Predicted	4
121-32-4	Ethyl Vanillin	5438-38-0	3-Ethoxy-4-hydroxybenzoic acid	Known	1
		64-19-7	Acetic acid	Predicted	3
		64-17-5	Ethyl alcohol	Predicted	3
		99-50-3	Protocatechuic acid; 3,4-Dihydroxybenzoic acid	Predicted	2
		139-85-5	3,4-Dihydroxybenzaldehyde	Predicted	3
			Glucuroethyl vanillin	Known	4
		617-05-0	Ethyl vanillic acid	Known	1
			Glucuronide or sulfate conjugates of ethyl vanillic acid	Known	4
		4912-58-7	Ethyl vanillyl alcohol (2-Ethoxy-4-(hydroxymethyl)phenol)	Known	1
		75-07-0	Acetaldehyde	Predicted	3
			glycine conjugate of vanillic acid ethyl vanilloyl glycine	Known	4

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122-78-1	Phenylacetaldehyde	103-82-2	Phenylacetic acid	Known	1
		500-98-1	Phenylacetyl glycine	Predicted	3
		102-32-9	2-(3,4-Dihydroxyphenyl)acetic acid	Predicted	3
		156-38-7	2-(4-Hydroxyphenyl)acetic acid	Predicted	3
13246-52-1	Ethyl 2,4-dioxohexanoate	64-19-7	Acetic acid	Predicted	2
		64-17-5	Ethyl alcohol	Predicted	2
		75-07-0	Acetaldehyde	Predicted	2
			6-hydroxy-2,4-dioxohexanoic acid	Predicted	2
			5-hydroxy-2,4-dioxohexanoic acid	Predicted	2
		10191-25-0	3-oxopentanoic acid	Predicted	3
			4,5-dihydroxy-2-oxohexanoic acid	Predicted	3
			4,6-dihydroxy-2-oxohexanoic acid	Predicted	3
			4-hydroxy-2-oxohexanoic acid	Predicted	3
		623-38-1	1,3-pentanedione	Predicted	3
			ethyl 2-hydroxy-4-oxohexanoate	Predicted	3
		338746-11-5	2-[[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]sulfanyl]acetic acid	Predicted	4
		4383-93-1	2,4-dioxohexanoic acid	Predicted	2

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
139559-06-1	Isolinderanolide		<chem>CC(=O)C(O)C(=CCCCCCCCCCC</chem> <chem>CCCCC=O)C(O)=O)</chem>	Predicted	3
			<chem>CC(=O)C(O)C(=CCCCCCCCCCC</chem> <chem>CCCCCO)C(O)=O)</chem>	Predicted	3
		64-19-7	Acetic acid	Predicted	2
1490-04-6	Menthol	79466-08-3	Menthol glucuronide	Known	4
			Menthol sulfate conjugate	Known	4
			Hydroxyl menthol glucuronide	Known	4
		42822-86-6	p-Menthane-3,8-diol	Known	1
			p-Menthane-3,9-diol	Known	1
		91006-77-8	3-Hydroxy-p-menthane-7-carboxylic acid	Known	1
			3,8-Oxy-p-menthane-7-carboxylic acid	Known	1
			3,8-Dihydroxy-p-menthane-7-carboxylic acid	Known	1
		625389-64-2	p-Menthane-3,7-diol; 5-(Hydroxymethyl)-2-isopropylcyclohexanol	Known	1
		157230-26-7	3-Hydroxy-p-menthane-9-carboxylic acid	Known	1
			p-Menthane-3,7,8-triol	Known	1
		91739-72-9	(+)-(1S,3S,4R)- trans-p-Menthane-3,8-diol	Known	1

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			(-)-(1R,3R,4S)-trans-p-Menthane-3,8-diol	Known	1
		58506-23-3	p-Menthan-2,8-diol	Known	1
		155348-06-4	4-(2-Hydroxy-2-propanyl)-1-methyl-1,3-cyclohexanediol	Predicted	2
		1612-98-2	p-Menthane-1,3-diol; 1-Methyl-4-(propan-2-yl)cyclohexane-1,3-diol	Predicted	2
		10458-14-7	Isomenthone	Predicted	2
			(8,8-Dimethyl-7-oxabicyclo[4.2.0]octan-4-yl)methanol	Predicted	3
			4,8,8-Trimethyl-7-oxabicyclo[4.2.0]octan-4-ol	Predicted	3
		42822-86-6	2-(2-Hydroxy-2-propanyl)-5-methylcyclohexanol	Predicted	2
			4,8,8-Trimethyl-7-oxabicyclo[4.2.0]octane	Predicted	3
			(4,8-Dimethyl-7-oxabicyclo[4.2.0]octan-8-yl)methanol	Predicted	3
		91006-77-8	3-Hydroxy-4-isopropylcyclohexanecarboxylic acid	Predicted	3
			3-Hydroxy-4-isopropylcyclohexanecarbaldehyde	Predicted	3
			8-Hydroxymenthol glucuronide	Predicted	4

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			1-(2-Hydroxypropan-2-yl)-4-methylcyclohexane-1,2-diol	Predicted	3
			1-Hydroxymenthyl glucuronide	Predicted	4
			4-(1-Hydroxypropan-2-yl)-1-methylcyclohexane-1,3-diol; 1,9-Dihydroxymenthyl	Predicted	3
			4-Methyl-1-(propan-2-yl)cyclohexane-1,2,4-triol; 1,4-Dihydroxymenthyl	Predicted	3
			4-Methyl-1-(propan-2-yl)cyclohexane-1,2-diol; 4-Hydroxymenthyl	Predicted	3
			4-Hydroxymenthyl glucuronide	Predicted	4
			2-(2-Hydroxypropan-2-yl)-5-methylcyclohexan-1-one; 8-Hydroxymenthone	Predicted	3
			5-Hydroxy-5-methyl-2-(propan-2-yl)cyclohexan-1-one; 1-Hydroxymenthone	Predicted	3
			2-(1-Hydroxypropan-2-yl)-5-methylcyclohexan-1-ol; 9-Hydroxymenthyl	Predicted	3
15506-54-4	2-Methylcyclobutane-1,3-dione	1824081-43-7	3-Hydroxy-2-methylcyclobutanone	Predicted	2
			Cyclobutane-1,3-dione-2-carboxylic acid	Predicted	2
			2-(Hydroxymethyl)-cyclobutane-1,3-dione	Predicted	2
			(2,4-Dioxocyclobutyl)methyl hydrogen sulfate	Predicted	4

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			2-Hydroxy-2-methylcyclobutane-1,3-dione	Predicted	2
			2,3-Dihydroxy-2-methylcyclobutanone	Predicted	3
			2,4-Dioxocyclobutane-1-carbaldehyde	Predicted	3
			3-Hydroxycyclobutanone-2-carboxylic acid	Predicted	3
			2-Oxo-4-hydroxycyclobutane-1-carbaldehyde	Predicted	3
			2-(Hydroxymethyl)-3-hydroxycyclobutanone	Predicted	3
1560-82-3	Heneicosane, 2-methyl-		21-Hydroxy-21-methylheneicosanal	Predicted	3
			21-Hydroxy-21-methylheneicosanol	Predicted	3
		646-07-1	4-Methylvaleric acid	Predicted	3
		929-10-2	6-Methylheptanoic acid; Isocaproic acid; Isooctanoic acid	Predicted	3
		26403-17-8	8-Methylnonanoic acid; Isodecanoic acid	Predicted	3
		2724-56-3	10-Methylundecanoic acid	Predicted	3
		2724-57-4	12-Methyltridecanoic acid; Isomyristic acid	Predicted	3
		4669-02-7	14-Methylpentadecanoic acid; Isopalmitic acid	Predicted	3

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		2724-58-5	16-Methylheptadecanoic acid; Isostearic acid	Predicted	3
			2,4-Dihydroxy-20-methylheneicosane	Predicted	3
			4-Hydroxy-20-methylheneicosanal	Predicted	3
			4-Hydroxy-20-methylheneicosanol	Predicted	3
			18-Methylnonadecanoic acid	Predicted	3
			2,3-Dihydroxy-20-methylheneicosane	Predicted	3
			3-Hydroxy-20-methylheneicosanol	Predicted	3
			1,19-Dimethyleicosanol	Predicted	2
			20-Methylheneicosanoic acid	Predicted	2
			20-Methylheneicosanal	Predicted	2
			20-Methylheneicosanol	Predicted	2
			21-Hydroxy-2-methylheneicosanal	Predicted	3
			21-Hydroxy-20-methylheneicosanal	Predicted	3
			2-Methylheneicosan-1,21-diol	Predicted	3
		64-19-7	Acetic acid	Predicted	3
			19-Hydroxy-1,19-dimethyleicosanol	Predicted	2
			20-Hydroxy-2-methylheneicosanal	Predicted	3

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			20-Hydroxy-2-methylheneicosanol	Predicted	2
			20-Methylheneicosan-3-one	Predicted	3
		79-09-4	Propanoic acid	Predicted	3
			19-Hydroxy-2-methylheneicosan-2-ol	Predicted	3
			20-Methylheneicosan-3-ol	Predicted	2
			19-Hydroxy-2-methylheneicosan-1-ol	Predicted	3
			20-Hydroxy-20-methylheneicosan-4-one	Predicted	3
			20-Methylheneicosan-4-one	Predicted	3
			20-(Hydroxymethyl)heneicosan-4-one	Predicted	3
			20-Hydroxy-20-methylheneicosan-4-ol	Predicted	3
			20-Methylheneicosan-4-ol	Predicted	3
			18-Hydroxy-2-methylheneicosanal	Predicted	3
			18-Hydroxy-2-methylheneicosanol	Predicted	3
		646-30-0	Nonadecanoic acid	Predicted	3
			2-Methylheneicosan-2-ol	Predicted	2
			2-Methylheneicosanoic acid	Predicted	2
			2-Methylheneicosanal	Predicted	2

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			2-Methylheneicosanol	Predicted	2
			20-Methylheneicosan-2-one	Predicted	3
			20-Methylheneicosan-1,2-diol	Predicted	3
1560-84-5	Eicosane, 2-methyl-		19-Hydroxy-19-methyleicosanal	Predicted	3
			19-Hydroxy-19-methyleicosanol	Predicted	3
		503-74-2	3-Methylbutanoic acid	Predicted	3
		628-46-6	5-Methylhexanoic acid; Isoenanthic acid	Predicted	3
		26896-18-4	Isononanoic acid	Predicted	3
		1119-63-7	9-Methyldecanoic acid	Predicted	3
		5691-98-1	11-Methyldecanoic acid	Predicted	3
		2485-71-4	13-Methyltetradecanoic acid; 13-Methylmyristic acid	Predicted	3
		1603-03-8	15-Methylhexadecanoic acid; 15-Methylpalmitic acid	Predicted	3
			2,4-Dihydroxy-19-methyleicosane	Predicted	3
			4-Hydroxy-19-methyleicosanal	Predicted	3
			19-Methyleicosan-1,4-diol	Predicted	3
		2724-59-6	17-Methyloctadecanoic acid; 17-Methylstearic acid	Predicted	3
			2,3-Dihydroxy-19-methyleicosane	Predicted	3

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			19-Methyleicosan-1,3-diol	Predicted	3
			Eicosan-2-ol	Predicted	2
		59708-73-5	19-Methyleicosanoic acid; 19-Methylarachidic acid	Predicted	2
			19-Methyleicosanal	Predicted	2
			19-Methyleicosanol	Predicted	2
			20-Hydroxy-2-methyleicosanal	Predicted	3
			20-Hydroxy-19-methyleicosanal	Predicted	3
			19-Methyleicosan-1,20-diol	Predicted	3
		64-19-7	Acetic acid	Predicted	3
			19-Methyleicosan-2,19-diol	Predicted	2
			19-Hydroxy-2-methyleicosanal	Predicted	3
			2-Methyleicosan-1,19-diol	Predicted	2
			19-Methyleicosan-3-one	Predicted	3
		79-09-4	Propanoic acid	Predicted	3
			19-Methyleicosan-3,19-diol	Predicted	3
			19-Methyleicosan-3-ol	Predicted	3
			2-Methyleicosan-1,18-diol	Predicted	3
			19-Hydroxy-19-methyleicosan-4-one	Predicted	3

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			19-Methyleicosan-4-one	Predicted	3
			20-Hydroxy-19-methyleicosan-4-one	Predicted	3
			19-Methyleicosan-4,19-diol	Predicted	3
			19-Methyleicosan-4-ol	Predicted	3
			17-Hydroxy-2-methyleicosanal	Predicted	3
			2-Methyleicosan-1,17-diol	Predicted	3
		57-11-4	Stearic acid; Octadecanoic acid	Predicted	3
			2-Methyleicosan-2-ol	Predicted	2
			2-Methyleicosanoic acid	Predicted	2
			2-Methyleicosanal	Predicted	2
			2-Methyleicosanol	Predicted	2
			19-Methyleicosan-2-one	Predicted	2
179694-78-1	Isopulegone caffeate	32676-16-7	4-Isopropenylcyclohexanecarboxylic acid	Predicted	2
		137886-38-5	4-Isopropenylcyclohexane carbaldehyde	Predicted	2
			(4-Isopropenylcyclohexylmethyl)-3-(3,4-dihydroxyphenyl)propanoate	Predicted	2
		18479-64-6	(4-Isopropenylcyclohexyl)methanol;	Predicted	2

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			(4-Prop-1-en-2-ylcyclohexyl)methanol		
			(4-(2-Hydroxypropanalyl)cyclohexylmethyl)-3-(3,4-dihydroxyphenyl)prop-2-enoate	Predicted	3
			(4-(2-Hydroxypropanolyl)cyclohexylmethyl)-3-(3,4-dihydroxyphenyl)prop-2-enoate	Predicted	3
			(4-(2-Hydroxypropanolyl)cyclohexylmethyl)-3-(3,4-dihydroxyphenyl)propanoate	Predicted	3
		64-19-7	Acetic acid	Predicted	3
			(4-(2-Methyloxiranyl)cyclohexylmethyl)-3-(3,4-dihydroxyphenyl)prop-2-enoate	Predicted	3
			(4-(2-Methyloxiranyl)cyclohexylmethyl)-3-(3,4-dihydroxyphenyl)propanoate	Predicted	3
		331-39-5	Caffeic acid; 3-(3,4-Dihydroxyphenyl)prop-2-enoic acid	Predicted	2
		1078-61-1	3-(3,4-Dihydroxyphenyl)propanoic acid	Predicted	2
		17362-17-3	3-(3-Hydroxyphenyl)propanoic acid	Predicted	3
		99-50-3	Protocatechuic acid; 3,4-Dihydroxybenzoic acid	Predicted	2
			4-Hydroxy-3-methoxybenzoic acid	Predicted	3

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			3-Hydroxy-4-(sulfooxy)benzoic acid	Predicted	4
			(3,4-Dihydroxybenzamido)acetic acid	Predicted	3
			4-Hydroxy-3-(sulfooxy)benzoic acid	Predicted	4
			6-(4-Carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	4
			(2E)-3-[3-Hydroxy-4-(sulfooxy)phenyl]prop-2-enoic acid	Predicted	3
			(2E)-3-(4-Hydroxy-3-methoxyphenyl)prop-2-enoic acid	Predicted	3
			6-{4-[(E)-2-Carboxyethenyl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	4
			3-(3,4-Dihydroxyphenyl)oxirane-2-carboxylic acid	Predicted	3
			[4-(2-Methyloxiran-2-yl)cyclohexyl]methanol	Predicted	3
			2-[4-(Hydroxymethyl)cyclohexyl]propane-1,2-diol	Predicted	3
			3,4,5-Trihydroxy-6-{[4-(2-methyloxiran-2-yl)cyclohexyl]methoxy}oxane-2-carboxylic acid	Predicted	4
			1-(Hydroxymethyl)-4-(2-methyloxiran-2-yl)cyclohexan-1-ol	Predicted	3

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			4-(2-Methyloxiran-2-yl)cyclohexane-1-carboxylic acid	Predicted	3
			4-(Hydroxymethyl)-1-(2-methyloxiran-2-yl)cyclohexan-1-ol	Predicted	3
			3,4,5-Trihydroxy-6-{{[4-(prop-1-en-2-yl)cyclohexyl]methoxy}oxane-2-carboxylic acid	Predicted	4
			2-[4-(Hydroxymethyl)cyclohexyl]prop-2-en-1-ol	Predicted	3
			1-(Hydroxymethyl)-4-(prop-1-en-2-yl)cyclohexan-1-ol	Predicted	3
			4-(Hydroxymethyl)-1-(prop-1-en-2-yl)cyclohexan-1-ol	Predicted	3
			[4-(Prop-1-en-2-yl)cyclohexyl]methyl (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate	Predicted	3
			[4-(Prop-1-en-2-yl)cyclohexyl]methyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate 4-O-glucuronide	Predicted	4
			[4-(Prop-1-en-2-yl)cyclohexyl]methyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate 3-O-glucuronide	Predicted	4
			[4-(Prop-1-en-2-yl)cyclohexyl]methyl (2E)-3-(3-hydroxy-4-methoxyphenyl)prop-2-enoate	Predicted	3
18881-04-4	(S)-cis-Verbenol		4,6,6-Trimethylbicyclo [3.1.1]hept-3-en-2-ol glucuronide11	Known	4

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			[Glucuronide conjugate of verbenol]		
			4-(Hydroxymethyl)-6,6-dimethylbicyclo[3.1.1]hept-3-en-2-ol12; 2-pinene-4,10-diol	Known	1
			2-Hydroxy-4,6,6-trimethylcyclohex-3-ene-1-carboxylic acid	Known	1
			4-Hydroxy-2,6,6-trimethylcyclohex-2-ene-1-carboxylic acid	Known	1
			2-Hydroxy-4-(hydroxymethyl)-6,6-dimethylcyclohex-3-ene-1-carboxylic acid	Known	1
			4-Hydroxy-2-(hydroxymethyl)-6,6-dimethylcyclohex-2-ene-1-carboxylic acid	Known	1
			3,5,5-Trimethylbicyclo[3.1.1]heptan-1,2,4-triol	Predicted	2
			2,7,7-Trimethyl-3-oxatricyclo[4.1.1.0 <sup>2,4</sup> ]octan-5-ol	Predicted	2
		80-57-9	4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one; Verbenone	Predicted	2
			4-Hydroxy-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-carboxylic acid	Predicted	2
		162936-74-5	(1S,4S,5R)-4-Hydroxy-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-carbaldehyde	Predicted	3
		1401068-67-4	4-(Hydroxymethyl)-6,6-dimethylbicyclo[3.1.1]hept-3-en-2-one	Predicted	2

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			2-Pinene-4,10-diol	Predicted	2
			1-Hydroxy-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-one	Predicted	3
			5-Hydroxy-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-one	Predicted	3
			4,6-Dimethylbicyclo[3.1.1]hept-3-en-2-ol-6-carboxylic acid	Predicted	3
			4,6-Dimethylbicyclo[3.1.1]hept-3-en-2-ol-6-carbaldehyde	Predicted	3
			6-(Hydroxymethyl)-4,6-dimethylbicyclo[3.1.1]hept-3-ene-2-ol	Predicted	2
			4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-ol glucuronide	Predicted	4
			4-(Hydroxymethyl)-6,6-dimethylbicyclo[3.1.1]hept-3-en-2-ol 2-O-glucuronide	Predicted	4
			4-(Hydroxymethyl)-6,6-dimethylbicyclo[3.1.1]hept-3-en-2-ol 4-O-glucuronide	Predicted	4
			2-(Hydroxymethyl)-7,7-dimethyl-3-oxatricyclo[4.1.1.0 <sup>2,4</sup> ]octan-5-ol	Predicted	3
			4-(Hydroxymethyl)-6,6-dimethylbicyclo[3.1.1]hept-3-en-2-one 4-O-glucuronide	Predicted	4
			4,6,6-Trimethylbicyclo[3.1.1]hept-3-ene-1,2-diol	Predicted	3

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			4,6,6-Trimethylbicyclo[3.1.1]hept-3-ene-1,2-diol 2-O-glucuronide	Predicted	4
			4-(Hydroxymethyl)-6,6-dimethylbicyclo[3.1.1]hept-3-ene-1,2-diol	Predicted	3
			2,7,7-Trimethyl-3-oxatricyclo[4.1.1.0 <sup>2,4</sup> ]octan-5-ol glucuronide	Predicted	4
20296-29-1	3-Octanol		Glucuronic acid conjugate of 3-octanol	Known	4
			Sulfate conjugate of 3-octanol	Known	4
		106-68-3	3-Octanone	Known	1
		64-19-7	Acetic acid	Predicted	2
		13532-38-2	4-Hydroxyhexanoic acid	Predicted	2
			2,6-Octanediol	Predicted	2
		64165-18-0	6-Hydroxyoctanoic acid	Predicted	2
			6-Hydroxyoctanal	Predicted	2
		4066-76-6	Octane-1,6-diol	Predicted	2
		20653-90-1	2,3-Octanediol	Predicted	2
		14192-27-4	3-Hydroxyoctanoic acid	Predicted	2
		96189-01-4	3-Hydroxyoctanal	Predicted	2
		23433-05-8	1,3-Octanediol	Predicted	2

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			3,4,5-Trihydroxy-6-[(octan-3-yl)oxy]oxane-2-carboxylic acid	Predicted	4
			Octan-3-yl hydrogen sulfate	Predicted	4
2230-87-7	Neomenthyl acetate		Same metabolites as Menthyl acetate (isomer)	Predicted	cf Menthyl acetate
23283-97-8	Isomenthol		Same metabolites as Menthol (isomer)	cf Menthol	cf Menthol
2601-90-3	Oleoylglycine	56-40-6	Glycine	Predicted	2
		2027-47-6	Octadec-9-enoic acid	Predicted	2
		64-19-7	Acetic acid	Predicted	3
		4546-57-0	17-hydroxyoctadec-9-enoic acid	Predicted	2
			hexadec-7-enoic acid	Predicted	2
			18-hydroxyoctadec-9-enoic acid	Predicted	3
		2443-39-2	9,10-Epoxyoctadecanoic acid	Predicted	3
		544-66-1	5-Tetradecenoic acid	Predicted	3
			<chem>CC(O)CCCCCCC=CCCCCCCCC(=O)NCC(O)=O</chem>	Predicted	3
			<chem>OC(=O)CCCCCCCC=CCCCCCC(=O)NCC(O)=O</chem>	Predicted	3
			<chem>OC(=O)CNC(=O)CCCCCCCC=C(=O)CCCCCCCC=O</chem>	Predicted	3
3008-43-3			6-Methyl-cyclohexane-1,2-diol	Known	1

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	Cyclohexane-1,2-dione, 3-methyl		Glucuronide conjugate of 6-methyl-cyclohexane-1,2-diol	Known	4
		1566175-05-0	2,3-Dioxocyclohexane carbaldehyde	Predicted	3
		1584140-73-7	2,3-Dihydroxy-3-methylcyclohexanone	Predicted	3
		1824414-91-6	2,6-Dihydroxy-2-methylcyclohexanone	Predicted	3
		52456-90-3	2-Hydroxy-6-methylcyclohexanone	Predicted	2
			3-(Hydroxymethyl)-cyclohexane-1,2-dione	Predicted	2
			2,3-Dioxocyclohexane-1-carboxylic acid	Predicted	3
			4-Hydroxy-3-methylcyclohexane-1,2-dione	Predicted	3
			3-Hydroxy-6-methylcyclohexane-1,2-dione	Predicted	3
			3,4,5-Trihydroxy-6-[(3-methyl-4,5-dioxocyclohexyl)oxy]oxane-2-carboxylic acid	Predicted	4
			3,4,5-Trihydroxy-6-[(2-methyl-3,4-dioxocyclohexyl)oxy]oxane-2-carboxylic acid	Predicted	4
			3,4,5-Trihydroxy-6-[(4-methyl-2,3-dioxocyclohexyl)oxy]oxane-2-carboxylic acid	Predicted	4

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			6-[(2,3-Dioxocyclohexyl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	4
			3-Hydroxy-3-methylcyclohexane-1,2-dione	Predicted	2
			6-Hydroxy-3-methylcyclohexane-1,2-dione	Predicted	2
			2-Hydroxy-3-methylcyclohexanone	Predicted	2
			3,4-Dihydroxy-3-methylcyclohexane-1,2-dione	Predicted	3
			2,3,4-Trihydroxy-3-methylcyclohexanone	Predicted	3
			3,5-Dihydroxy-3-methylcyclohexane-1,2-dione	Predicted	3
			2,4,6-Trihydroxy-2-methylcyclohexane-1,2-dione	Predicted	3
			2,4-Dihydroxy-3-methylcyclohexanone	Predicted	3
			5-Hydroxy-3-methylcyclohexane-1,2-dione	Predicted	3
			4,6-Dihydroxy-2-methylcyclohexanone	Predicted	3
			Cyclohexane-1,2-dione-3-carboxylic acid	Predicted	3
			2-Hydroxycyclohexanone-3-carbaldehyde	Predicted	3

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			5-Hydroxy-2,3-dioxocyclohexanecarbaldehyde	Predicted	3
			2-Hydroxycyclohexanone-6-carbaldehyde	Predicted	3
			3-(Hydroxymethyl)-4,5-dihydroxycyclohexane-1,2-dione	Predicted	3
			3-(Hydroxymethyl)-4-hydroxycyclohexane-1,2-dione	Predicted	3
			2,4-Dihydroxy-3-(hydroxymethyl)-cyclohexanone	Predicted	3
			3-(Hydroxymethyl)-cyclohexane-1,2,5-trione	Predicted	3
			3-(Hydroxymethyl)-5,5-dihydroxycyclohexane-1,2-dione	Predicted	3
			3-(Hydroxymethyl)-5-hydroxycyclohexane-1,2-dione	Predicted	3
			2,5-Dihydroxy-3-(hydroxymethyl)-cyclohexanone	Predicted	3
			2,4-Dihydroxy-6-(hydroxymethyl)-cyclohexanone	Predicted	3
			3-(Hydroxymethyl)-2-hydroxycyclohexanone	Predicted	3
			2-Hydroxy-6-(hydroxymethyl)-cyclohexanone	Predicted	3
3188-00-9	3(2H)-Furanone, dihydro-2-methyl	29848-44-0	2-methyloxolan-3-ol	Predicted	2
			3-oxoxolane-2-carbaldehyde	Predicted	3

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			3-oxoxolane-2-carboxylic acid	Predicted	2
			3-hydroxyoxolane-2-carbaldehyde	Predicted	3
			3-hydroxyoxolane-2-carboxylic acid	Predicted	3
			2-(hydroxymethyl)oxolan-3-one	Predicted	2
			2-(hydroxymethyl)oxolan-3-ol	Predicted	3
			4-hydroxy-3-oxopentanoic acid	Predicted	3
			4-hydroxy-3-oxopentanal	Predicted	3
			3,4-dihydroxypentanoic acid	Predicted	3
			3,4-dihydroxypentanal	Predicted	3
			<chem>OC2C(OCC1OCCC1=O)OC(C(O)C2O)C(O)=O</chem>	Predicted	3
33691-73-5	2H-Pyran-2-one, tetrahydro-5-hydroxy	60833-12-7	oxane-2,5-dione	Predicted	2
		2889-31-8	2-hydroxypentanedioic acid	Predicted	2
		99419-40-6	4-hydroxy-5-oxopentanoic acid	Predicted	2
			4,5-dihydroxyoxan-2-one	Predicted	3
		66679-29-6	4,5-dihydroxypentanoic acid	Predicted	2
			<chem>OC2C(OC1COC(CC1)=O)OC(C(O)C2O)C(O)=O</chem>	Predicted	3
			<chem>OS(OC1COC(CC1)=O)(=O)=O</chem>	Predicted	3

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3674-21-3	trans-4-Hydroxymethyl-2-methyl-1,3-dioxolane		2-methyl-1,3-dioxolane-4-carboxylic acid	Predicted	2
			2-(hydroxymethyl)-1,3-dioxolan-4-yl]methanol	Predicted	2
		112397-23-6	2-methyl-1,3-dioxolane-4-carbaldehyde	Predicted	2
			2-(hydroxymethyl)-1,3-dioxolane-4-carboxylic acid	Predicted	3
			OS(OCC1OC(OC1)C)(=O)=O	Predicted	3
			OC2C(OCC1OC(OC1)C)OC(C(O)C2O)C(O)=O	Predicted	3
			CC(O)OC(C=O)C(O)=O	Predicted	3
			CC(O)OC(CO)C(O)=O	Predicted	3
			CC(O)OC(CO)C=O	Predicted	3
3856-25-5	Copaene	41610-69-9	(1-methyl-8-propan-2-yl-3-tricyclo[4.4.0.02,7]dec-3-enyl)methanol	Predicted	2
			2-(6,8-dimethyl-3-tricyclo[4.4.0.02,7]dec-8-enyl)propan-2-ol	Predicted	2
			6,8-dimethyl-3-propan-2-yltricyclo[4.4.0.02,7]dec-8-en-3-ol	Predicted	2
			2,8-dimethyl-5-propan-2-yltricyclo[4.4.0.02,7]dec-8-en-4-ol	Predicted	2
			1,5-dimethyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-4-en-3-one	Predicted	3

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			1-methyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-3-ene-3-carbaldehyde	Predicted	3
			1-methyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-3-ene-3-carboxylic acid	Predicted	3
			OC3C1C2C(CCC1(C)C2C(C)=C3)C(C)C	Predicted	3
			OC1C(OC(C(O)C1O)C(O)=O)OC4C2C3C(CCC2(C)C3C(C)=C4)C(C)C	Predicted	3
			CC(C)(O)C1CCC2(C)C3C(O)C4OC4(C)C2C13	Predicted	3
			CC(C)(O)C1CCC2(C)C3CC4OC4(C)C2C13	Predicted	3
			CC(C)(O)C1CCC2(C)C3CC=C(C(O)C2C13	Predicted	3
			CC(C)C1CCC2(C)C3C(O)C=C(C)C2C13	Predicted	3
3857-25-8	2-Furanmethanol, 5-methyl	1883-75-6	5-(hydroxymethyl)furan-2-yl]methanol	Predicted	2
		620-02-0	5-methylfuran-2-carbaldehyde	Predicted	2
		1917-15-3	5-methylfuran-2-carboxylic acid	Predicted	2
		6338-41-6	5-(hydroxymethyl)furan-2-carboxylic acid	Predicted	2
		67-47-0	5-(Hydroxymethyl)furfural	Predicted	3

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		97207-45-9	2-[(5-methylfuran-2-carbonyl)amino]acetic acid	Predicted	3
			CC12OC1C=C(CO)O2	Predicted	3
38877-21-3	2,3-Dihydro-5-hydroxy-6-methyl-4Hpyran-4-one (Dihydromaltol)	178626-85-2	3-Hydroxy-2-methyloxan-4-one	Predicted	3
			5-Hydroxy-6-methyl-4-oxo-3,4-dihydro-2H-pyran-3-yl hydrogen sulfate	Predicted	4
			3,5-Dihydroxy-6-methyl-2,3-dihdropyran-4-one	Predicted	3
			3,4,5-Trihydroxy-6-[(5-hydroxy-6-methyl-4-oxo-3,4-dihydro-2H-pyran-3-yl)oxy]oxane-2-carboxylic acid	Predicted	4
			3,5-Dihydroxy-4-oxohexanal	Predicted	3
			4,5-Dihydroxy-3-oxohexanal	Predicted	3
			2-Methyldihydro-2H-pyran-3,4-dione	Predicted	3
			4-Hydroxy-2-methyloxan-3-one	Predicted	3
			3-Hydroxy-4-oxo-5,6-dihdropyran-2-carbaldehyde	Predicted	3
			2-(Hydroxymethyl)-3-hydroxy-4-oxo-5,6-dihdropyran	Predicted	3
4230-97-1	Octanoic acid, 2-propenyl ester	124-07-2	octanoic acid	Predicted	2
		107-18-6	prop-2-en-1-ol	Predicted	2
		24412-91-7	oxiran-2-ylmethyl octanoate	Predicted	3

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		79-10-7	prop-2-enoic acid	Predicted	2
		107-02-8	prop-2-enal	Predicted	2
		64-19-7	Acetic acid	Predicted	3
		17173-14-7	7-hydroxyoctanoic acid	Predicted	2
		14292-29-6	3-hydroxyhexanedioic acid	Predicted	3
		142-62-1	hexanoic acid	Predicted	3
		17369-50-5	5-hydroxyoctanoic acid	Predicted	3
			2-[[3-(oxiran-2-ylmethoxy)-5-pentylphenoxy]methyl]oxirane	Predicted	3
		26402-26-6	2,3-dihydroxypropyl octanoate	Predicted	3
			2-acetamido-3-(2-carboxyethylsulfanyl)propanoic acid	Predicted	4
		3637-14-7	5-oxooctanoic acid	Predicted	3
			3-oxooctanedioic acid	Predicted	3
		4233-57-2	6-oxooctanoic acid	Predicted	3
			4-hydroxyoctanedioic acid	Predicted	3
			5,7-dihydroxyoctanoic acid	Predicted	3
			5,8-dioxooctanoic acid	Predicted	3
		503-11-7	oxirane-2-carboxylic acid	Predicted	3

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		56-81-5	Glycerol	Predicted	3
			6,8-dihydroxyoctanoic acid	Predicted	3
		64165-18-0	6-hydroxyoctanoic acid	Predicted	3
		689-31-6	3-oxohexanedioic acid	Predicted	3
		849724-26-1	prop-2-enyl 8-hydroxyoctanoate	Predicted	3
			8-hydroxy-6-oxooctanoic acid	Predicted	3
			<chem>CC(O)C(=O)CCCC(O)=O</chem>	Predicted	3
491-07-6	Cyclohexanone, 5-methyl-2-(1methylethyl)-, cis-(D,L-Isomenthone)		Same metabolites as menthone (isomer)	cf menthone	cf menthone
494-90-6	Menthofuran		Menthofuran epoxide	Known	1
		22125-63-9	2-Hydroxyfuran	Known	1
		166584-27-6	(+)-Mintlactone	Known	1
		16434-37-0	(-)-Isomintlactone	Known	1
			8-Pulegone aldehyde	Known	1
		459-80-3	Geranic acid	Known	1
			Neronic acid	Known	1
			5-Methyl-2-cyclohexenene	Known	1
		591-21-3	3-Methylcyclohexanol	Known	1

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		5515-76-4	4-methyl-2-cyclohexenone	Known	1
			4-Hydroxy-4-methyl-2-cyclohexenone	Known	1
		106-44-5	para-Cresol	Known	1
		529-63-5	(6S)-3,6-dimethyl-6,7-dihydro-5H-1-benzofuran-4-one	Predicted	3
			3,6-dimethyl-5,6-dihydro-4H-1-benzofuran-7-one	Predicted	2
			(3-methyl-4,5,6,7-tetrahydro-1-benzofuran-6-yl)methanol	Predicted	3
		137846-35-6	4,5,6,7-tetrahydro-3,6-dimethyl-2-Benzofuranol,(R)-	Predicted	2
		141396-29-4	2-(4-methyl-2-oxocyclohexylidene)propanal	Predicted	2
			2-(2-hydroxy-4-methylcyclohexyl)propanoic acid	Predicted	3
			2-(4-methyl-2-oxocyclohexyl)propanoic acid	Predicted	3
			2-(4-methyl-2-oxocyclohexylidene)propanoic acid	Predicted	3
			3,6-dimethyl-4,5,6,7-tetrahydro-3H-1-benzofuran-2-one	Predicted	3
			3-methyl-4,5,6,7-tetrahydro-1-benzofuran-6-carboxylic acid	Predicted	3
			3,6-dimethyl-4,5,6,7-tetrahydro-1-benzofuran-4-ol	Predicted	3

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497-23-4	2(5H)-Furanone	26099-09-2	but-2-enedioic acid	Predicted	2
		22418-77-5	4-oxobut-2-enoic acid	Predicted	2
		24587-49-3	4-hydroxybut-2-enoic acid	Predicted	2
		19444-84-9	3-hydroxyoxolan-2-one	Predicted	3
		754147-29-0	3,6-dioxabicyclo[3.1.0]hexan-2-one	Predicted	3
		5469-16-9	4-hydroxyoxolan-2-one	Predicted	3
			<chem>OC(C(NC(C)=O)CSC1COC(C1)=O)=O</chem>	Predicted	3
5077-67-8	1-Hydroxy-2-butanone	138320-11-3	1,3-dihydroxybutan-2-one	Predicted	3
		140-86-3	1,4-dihydroxybutan-2-one	Predicted	2
		123-38-6	Propionaldehyde	Predicted	2
		162369-88-2	4-hydroxy-3-oxobutanoic acid	Predicted	3
		600-18-0	2-oxobutanoic acid	Predicted	2
		4417-81-6	2-oxobutanal	Predicted	3
		584-03-2	butane-1,2-diol	Predicted	2
		2134-29-4	3-hydroxypropanal	Predicted	3
		22136-38-5	4-hydroxy-2-oxobutanoic acid	Predicted	3
		28119-61-1	4-hydroxy-2-oxobutanal	Predicted	3
			2-oxobutyl hydrogen sulfate	Predicted	4

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		3068-00-6	butane-1,2,4-triol	Predicted	3
			4-hydroxy-3-oxobutanal	Predicted	3
		503-66-2	3-hydroxypropanoic acid	Predicted	3
		79-09-4	Propanoic acid	Predicted	3
			<chem>OC1C(OCC(CC)=O)OC(C(O)C1O)C(O)=O;</chem>	Predicted	3
53907-91-8	1,4-Dioxane, 2-ethyl-5-methyl		(5-ethyl-1,4-dioxan-2-yl)methanol	Predicted	3
			2-(2-hydroxybutoxy)propanoic acid	Predicted	3
			<chem>OC(C)C1OCC(OC1)C</chem>	Predicted	3
			<chem>CC1COC(CO1)C(C)O</chem>	Predicted	3
			<chem>OC(C1OCC(OC1)CC)=O</chem>	Predicted	3
			<chem>CC1COC(CCO)CO1</chem>	Predicted	3
			<chem>CC1COC(CO1)CC(O)=O</chem>	Predicted	3
			<chem>CC1COC(CO1)CC=O</chem>	Predicted	3
544-35-4	Ethyl linoleate	2197-37-7	octadeca-9,12-dienoic acid	Predicted	2
		64-17-5	Ethyl alcohol	Predicted	3
		64-19-7	Acetic acid	Predicted	2
			11-(3-pentyloxiran-2-yl)undec-9-enoic acid	Predicted	3

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		113972-57-9	8-(3-oct-2-enyloxiran-2-yl)octanoic acid	Predicted	3
			12,13-dihydroxyoctadec-9-enoic acid	Predicted	3
			18-hydroxyoctadeca-9,12-dienoic acid	Predicted	3
		2936-83-6	hexadeca-7,10-dienoic acid	Predicted	3
		338746-11-5	2-[[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]sulfanyl]acetic acid	Predicted	4
		50632-63-8	8-[3-(8-hydroxyoct-2-enyl)oxiran-2-yl]octanoic acid	Predicted	3
		53734-70-6	9,10-dihydroxyoctadec-12-enoic acid	Predicted	3
		75-07-0	Acetaldehyde	Predicted	2
			<chem>CC(O)CCCC=CCC=CCCCCCCCC(O)=O</chem>	Predicted	3
54750-70-8	Anhydro linalool oxide		Hydroxy[2-methyl-5-(prop-1-en-2-yl)oxolan-2-yl]acetaldehyde	Predicted	3
		556775-91-8	1-[2-Methyl-5-(prop-1-en-2-yl)oxolan-2-yl]ethane-1,2-diol	Predicted	2
			2-Methyl-2-(oxiran-2-yl)-5-(prop-1-en-2-yl)oxolane	Predicted	2
			2-(5-Ethenyl-5-methyloxolan-2-yl)-2-hydroxypropanal	Predicted	3
			2-[5-Methyl-5-(oxiran-2-yl)oxolan-2-yl]propane-1,2-diol	Predicted	3

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			2-(5-Ethenyl-5-methyloxolan-2-yl)propane-1,2-diol	Predicted	3
			2-(5-Ethenyl-5-methyloxolan-2-yl)prop-2-enoic acid	Predicted	2
			2-(5-Ethenyl-5-methyloxolan-2-yl)prop-2-enal	Predicted	2
			2-(5-Ethenyl-5-methyloxolan-2-yl)prop-2-en-1-ol	Predicted	2
			1-[2-Methyl-5-(2-methyloxiran-2-yl)oxolan-2-yl]ethane-1,2-diol	Predicted	3
			2-Ethenyl-2-methyl-5-(2-methyloxiran-2-yl)oxolane	Predicted	3
			[2-Ethenyl-5-(prop-1-en-2-yl)oxolan-2-yl]methanol	Predicted	3
			2-Ethenyl-5-(prop-1-en-2-yl)oxolane-2-carboxylic acid	Predicted	3
			2-Ethenyl-5-(prop-1-en-2-yl)oxolane-2-carbaldehyde	Predicted	3
57-55-6	Propylene glycol	598-35-6	Lactaldehyde	Known	1
		127-17-3	Pyruvic acid	Known	1
		64-19-7	Acetic acid	Known	1
		50-21-5	Lactic acid	Known	1
		123-38-6	Propionaldehyde	Known	1
		78-98-8	Methylglyoxal (2-Oxopropanal)	Known	1

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			Phosphate metabolites: propylene glycol phosphate, acetol phosphate, lactaldehyde phosphate, lactyl phosphate	Known	4
			1-hydroxypropan-2-yl hydrogen sulfate	Predicted	4
			2-hydroxypropyl hydrogen sulfate	Predicted	4
		338746-11-5	2-[[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]sulfanyl]acetic acid	Predicted	4
		56-81-5	Glycerol	Predicted	3
		75-07-0	Acetaldehyde	Predicted	3
		116-09-6	1-hydroxypropan-2-one (2-Propanone)	Predicted	3
57-87-4	Ergosterol		17 $\alpha$ ,24-dihydroxyergosterol	Known	1
			20-hydroxy-22,23-epoxy-22,23-dihydroergosterol	Known	1
			22-keto-23-hydroxy-22,23-dihydroergosterol	Known	1
			17-(5,6-Dimethylhept-3-en-2-yl)-10,13-dimethyl-1,2,6,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-3-one	Predicted	2
		23454-50-4	17-(5,6-dimethylhept-3-en-2-yl)-10,13-dimethyl-1,2,4,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-3-one	Predicted	2

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			<chem>CC(C)C(C)(O)C=CC(C)C1C(O)C2C3=CC=C4CC(O)CCC4(C)C3CCC21C</chem>	Predicted	3
			<chem>OCC(C(C)C)C=CC(C)C4CCC2C4(C)CCC3C1(C)CCC(O)CC1=CC=C23</chem>	Predicted	3
			<chem>OC3CCC4(C)C2CCC1(C)C(CCC1C2=CC=C4C3)C(C)C=CC(C(C)C)C(O)=O</chem>	Predicted	3
			<chem>OC3CCC4(C)C2CCC1(C)C(CCC1(O)C(C)C=CC(C)C(C)C)C2=CC=C4C3</chem>	Predicted	3
			<chem>CC(C)C(C)(O)C=CC(C)C1CC(O)C2C3=CC=C4CC(O)CCC4(C)C3CCC12C</chem>	Predicted	3
			<chem>CC(C)C(C)(O)C=CC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC12C</chem>	Predicted	3
			<chem>CC(C)C(C)(O)C=CC(C)C1CCC2C3=CCC4=CC(=O)CCC4(C)C3CC12C</chem>	Predicted	3
			<chem>CC(C)C(C)C(O)C(O)C(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CC12C</chem>	Predicted	3
			<chem>CC(C)C(C)C1OC1C(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC12C</chem>	Predicted	3
581-49-7	Anatabine		1-(6-Carboxy-3,4,5-trihydroxyoxan-2-yl)-3-(1,2,3,6-tetrahydropyridin-2-yl)pyridin-1-ium	Predicted	3
			1-Oxo-3-(1,2,3,6-tetrahydropyridin-2-yl)-1λ-pyridine	Predicted	3

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			4-(Pyridin-3-yl)-7-oxa-3-azabicyclo[4.1.0]heptane	Predicted	3
			3-(1,2,3,6-Tetrahydropyridin-2-yl)pyridine-N-oxide	Predicted	2
			1,4-Dihydro-3-(1,2,3,6-tetrahydropyridin-2-yl)pyridin-4-one	Predicted	2
			3-(1,2,3,6-Tetrahydropyridin-2-yl)pyridin-4-ol	Predicted	2
			3-(1,2,3,6-Tetrahydropyridin-2-yl)pyridin-5-ol	Predicted	2
			3-Amino-3-(1-oxo-1λ-pyridin-3-yl)propanoic acid	Predicted	3
			(2E)-5-Amino-5-(1-oxo-1λ-pyridin-3-yl)pent-2-enoic acid	Predicted	3
			(2E)-5-Amino-5-(1-oxo-1λ-pyridin-3-yl)pent-2-en-1-ol	Predicted	3
			2-(1-Oxo-1λ-pyridin-3-yl)-1,2,3,6-tetrahydropyridin-3-ol	Predicted	3
			4-(1-Oxo-1λ-pyridin-3-yl)-7-oxa-3-azabicyclo[4.1.0]heptane	Predicted	3
			1-Methyl-3-(1,2,3,6-tetrahydropyridin-2-yl)pyridin-1-ium	Predicted	3
			(2E)-5-Amino-5-(pyridin-3-yl)pent-2-enoic acid	Predicted	3
			1,2,3,6-Tetrahydro[2,3'-bipyridin]-3-ol	Predicted	3

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			3-(1-Amino-2-carboxyethyl)-1-(6-carboxy-3,4,5-trihydroxyoxan-2-yl)pyridin-1-ium	Predicted	3
			1-(6-Carboxy-3,4,5-trihydroxyoxan-2-yl)-3-(3-hydroxy-1,2,3,6-tetrahydropyridin-2-yl)pyridin-1-ium	Predicted	3
			1-(6-Carboxy-3,4,5-trihydroxyoxan-2-yl)-3-(7-oxa-3-azabicyclo[4.1.0]heptan-4-yl)pyridin-1-ium	Predicted	3
			3,4,5-Trihydroxy-6-[(1,2,3,6-tetrahydro[2,3'-bipyridin]-3-yl)oxy]oxane-2-carboxylic acid	Predicted	3
			6-(Pyridin-3-yl)piperidine-3,4-diol	Predicted	3
			3,4,5-trihydroxy-6-[[4-hydroxy-6-(pyridin-3-yl)piperidin-3-yl]oxy]oxane-2-carboxylic acid	Predicted	3
			3,4,5-Trihydroxy-6-[[5-hydroxy-2-(pyridin-3-yl)piperidin-4-yl]oxy]oxane-2-carboxylic acid	Predicted	3
			(2E)-5-Amino-5-(pyridin-3-yl)pent-2-en-1-ol	Predicted	3
			3,6-Dihydro[2,3'-bipyridin]-1(2H)-ol	Predicted	3
58319-05-4	cis-sesquisabinene hydrate		6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylheptane-2,3,6-triol	Predicted	3
			6-Hydroxy-6-(4-hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-en-4-one	Predicted	3

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			2-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-6-methylhept-5-ene-2,4-diol	Predicted	3
			5-(2-Hydroxy-6-methylhept-5-en-2-yl)-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	2
			(2E)-6-Hydroxy-6-(4-hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-enal	Predicted	3
			6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-en-4-one	Predicted	3
			(2E)-1-Hydroxy-6-(4-hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-en-4-one	Predicted	3
			5-(4-Hydroxy-6-methylhept-5-en-2-yl)-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	2
			6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylheptane-2,3-diol	Predicted	2
			5-[4-(3,3-Dimethyloxiran-2-yl)butan-2-yl]-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	2
			(2E)-6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-enoic acid	Predicted	3
			(2E)-6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-enal	Predicted	3
			5-[(5E)-7-Hydroxy-6-methylhept-5-en-2-yl]-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	2

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			(2E)-6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-ene-1,6-diol	Predicted	3
			5-[4-(3,3-Dimethyloxiran-2-yl)-2-hydroxybutan-2-yl]-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	3
			5-(1-Hydroxy-6-methylhept-5-en-2-yl)-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	3
			2-Methyl-5-(6-methylhept-5-en-2-yl)bicyclo[3.1.0]hexane-2,3-diol	Predicted	3
			4-Methyl-1-(6-methylhept-5-en-2-yl)bicyclo[3.1.0]hexane-2,4-diol	Predicted	3
			2-(Hydroxymethyl)-5-(6-methylhept-5-en-2-yl)bicyclo[3.1.0]hexan-2-ol	Predicted	3
			2-[4-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)pentylidene]propane-1,3-diol	Predicted	3
			Glucuronide conjugate of 5-[(5Z)-7-hydroxy-6-methylhept-5-en-2-yl]-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	4
			5-{4-[3-(Hydroxymethyl)-3-methyloxiran-2-yl]butan-2-yl}-2-methylbicyclo[3.1.0]hexan-2-ol	Predicted	3
			6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylheptane-1,2,3-triol	Predicted	3
			(2Z)-6-(4-Hydroxy-4-methylbicyclo[3.1.0]hexan-1-yl)-2-methylhept-2-ene-1,4-diol	Predicted	3

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			Glucuronide conjugate of 5-(4-hydroxy-6-methylhept-5-en-2-yl)-2-methylbicyclo [3.1.0]hexan-2-ol	Predicted	4
			Glucuronide conjugate of 2-methyl-5-(6-methylhept-5-en-2-yl)bicyclo[3.1.0]hexan-2-ol	Predicted	4
587-45-1	Tyrosine, 3-hydroxy	51-61-6	Dopamine	Known	1
		102-32-9	3,4-dihydroxyphenylacetic acid	Known	1
		306-08-1	3-methoxy-4-hydroxyphenylacetic acid	Known	1
		7636-26-2	3-Methoxytyrosine	Predicted	3
		4228-66-4	3,4-Dihydroxyphenylpyruvic acid	Predicted	2
		10597-60-1	Hydroxytyrosol	Predicted	3
		1081-71-6	3-(4-hydroxy-3-methoxyphenyl)-2-oxopropanoic acid	Predicted	3
			2-amino-3-(4-hydroxy-3-sulfooxyphenyl)propanoic acid	Predicted	4
			2-amino-3-hydroxy-3-(2,3,4-trihydroxyphenyl)propanoic acid	Predicted	3
		38339-02-5	Dopamine 4-O-Sulfate	Predicted	4
			4-[2-(hydroxyamino)ethyl]benzene-1,2-diol	Predicted	3
		51317-41-0	Dopamine 3-O-Sulfate	Predicted	4
		554-52-9	3-Methoxytyramine	Predicted	3

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		5707-55-1	2-(3,4-dihydroxyphenyl)acetaldehyde	Predicted	3
			6-[2-(3,4-dihydroxyphenyl)acetyl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	3
		99-50-3	Protocatechuic acid; 3,4-Dihydroxybenzoic acid	Predicted	3
		64-19-7	Acetic acid	Predicted	3
		75435-17-5	3,4-Dioxobenzoic acid	Predicted	3
		4430-97-1	L-dopaquinone	Predicted	3
592-20-1	2-Propanone, 1-(acetyloxy)	64-19-7	Acetic acid	Predicted	2
		116-09-6	1-hydroxypropan-2-one (2-Propanone)	Predicted	2
		627-69-0	1,2-Propanediol, 1-acetate	Predicted	2
		50-21-5	Lactic acid	Predicted	3
		56-81-5	Glycerol	Predicted	3
		592-20-1	2-oxopropyl acetate	Predicted	3
		598-35-6	Lactaldehyde	Predicted	3
		75-07-0	Acetaldehyde	Predicted	3
		57-55-6	Propylene glycol	Predicted	2
		127-17-3	Pyruvic acid	Predicted	2
		78-98-8	Methylglyoxal (2-Oxopropanal)	Predicted	2

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611-13-2	Methyl furoate	88-14-2	2-Furoic acid	Known	1
		67-56-1	Methanol	Known	1
		50-00-0	Formaldehyde	Predicted	3
		64-18-6	Formic acid	Predicted	3
		5657-19-2	N-(2-Furoyl)glycine	Predicted	3
61142-76-5	Benzene, 1,2,3,4-tetramethyl-4-(1methylethenyl)		2-Methyl-2-(2,3,4,5-tetramethylphenyl)oxirane	Predicted	2
			1-Isopropenyl-3-(hydroxymethyl)-2,4,5-trimethylbenzene	Predicted	2
			1-Isopropenyl-5-(hydroxymethyl)-2,3,4-trimethylbenzene	Predicted	2
			1-Isopropenyl-2-(hydroxymethyl)-3,4,5-trimethylbenzene	Predicted	2
			1-Isopropenyl-4-(hydroxymethyl)-2,3,5-trimethylbenzene	Predicted	2
			2-(2,3,4,5-Tetramethylphenyl)propan-1,2-diol	Predicted	2
			1-Isopropenyl-2,3,4-trimethylbenzene-5-carboxylic acid	Predicted	2
			1-Isopropenyl-2,3,5-trimethylbenzene-4-carboxylic acid	Predicted	2
			1-Isopropenyl-2,4,5-trimethylbenzene-3-carboxylic acid	Predicted	2
			1-Isopropenyl-3,4,5-trimethylbenzene-2-carboxylic acid	Predicted	2

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			1-Isopropenyl-3,4,5-trimethylbenzene-2-carbaldehyde	Predicted	2
			1-Isopropenyl-2,4,5-trimethylbenzene-3-carbaldehyde	Predicted	2
			1-Isopropenyl-2,3,5-trimethylbenzene-4-carbaldehyde	Predicted	2
			1-Isopropenyl-2,3,4-trimethylbenzene-5-carbaldehyde	Predicted	2
			2-(2,3,4,5-Tetramethylphenyl)prop-2-enoic acid	Predicted	2
			2-(2,3,4,5-Tetramethylphenyl)prop-2-enal	Predicted	2
			2-(2,3,4,5-Tetramethylphenyl)prop-2-en-1-ol	Predicted	2
			2-Hydroxy-2-(2,3,4,5-tetramethylphenyl)propanal	Predicted	2
			3,4,5-Trihydroxy-6-{{[4,5,6-trimethyl-2-(prop-1-en-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			3,4,5-Trihydroxy-6-{{[2,3,5-trimethyl-5-(prop-1-en-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			3,4,5-Trihydroxy-6-{{[2,3,6-trimethyl-5-(prop-1-en-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4

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			3,4,5-Trihydroxy-6-{{[2,3,4-trimethyl-5-(prop-1-en-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			3,4,5-Trihydroxy-6-{{[4,5,6-trimethyl-2-(2-methyloxiran-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			3,4,5-Trihydroxy-6-{{[2,5,6-trimethyl-4-(2-methyloxiran-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			3,4,5-Trihydroxy-6-{{[2,3,6-trimethyl-5-(2-methyloxiran-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			3,4,5-Trihydroxy-6-{{[2,3,4-trimethyl-5-(2-methyloxiran-2-yl)phenyl]methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			2-[2-(Hydroxymethyl)-3,4,5-trimethylphenyl]propane-1,2-diol	Predicted	3
			2-[3-(Hydroxymethyl)-2,4,5-trimethylphenyl]propane-1,2-diol	Predicted	3
			2-[4-(Hydroxymethyl)-2,3,5-trimethylphenyl]propane-1,2-diol	Predicted	3
			2-[5-(Hydroxymethyl)-2,3,4-trimethylphenyl]propane-1,2-diol	Predicted	3

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			2-(2,3,4,5-Tetramethylphenyl)propane-1,2,3-triol	Predicted	3
			6-{{2-(2,3,4,5-Tetramethylphenyl)-1-hydroxypropan-2-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,6-Dimethyl-4-(prop-1-en-2-yl)-1,2-phenylene]dimethanol	Predicted	3
			2,4-Dimethyl-6-(prop-1-en-2-yl)-1,3-phenylene]dimethanol	Predicted	3
			[4-Methyl-6-(prop-1-en-2-yl)benzene-1,2,3-triyl]trimethanol	Predicted	3
			[2,3,4-Trimethyl-6-(2-methyloxiran-2-yl)phenyl]methanol	Predicted	3
			3,4,5-Trihydroxy-6-{{4-(hydroxymethyl)-3-(prop-1-en-2-yl)-5,6-dimethylphenyl}methoxy}oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,4,5-Trihydroxy-6-{{3-(hydroxymethyl)-4-(prop-1-en-2-yl)-2,6-dimethylphenyl}methoxy}oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,4,5-Trihydroxy-6-{{3,6-dimethyl-2-(hydroxymethyl)-5-(prop-1-en-2-yl)phenyl}methoxy}oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4

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			3,4,5-Trihydroxy-6-{{5-(hydroxymethyl)-2-(prop-1-en-2-yl)-4,6-dimethylphenyl}methoxy}oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			2,3,6-Trimethyl-4-(2-methyloxiran-2-yl)phenyl]methanol	Predicted	3
			[3,6-Dimethyl-4-(2-methyloxiran-2-yl)-1,2-phenylene]dimethanol	Predicted	3
			[2,4-Dimethyl-6-(2-methyloxiran-2-yl)-1,3-phenylene]dimethanol	Predicted	3
			3,4,5-Trihydroxy-6-{{2-(hydroxymethyl)-3-(prop-1-en-2-yl)-5,6-dimethylphenyl}methoxy}oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,4-Dimethyl-6-(prop-1-en-2-yl)-1,2-phenylene]dimethanol	Predicted	3
			[3,4-Dimethyl-5-(prop-1-en-2-yl)-1,2-phenylene]dimethanol	Predicted	3
			[2,4-Dimethyl-5-(prop-1-en-2-yl)-1,3-phenylene]dimethanol	Predicted	3
			[4-Methyl-5-(prop-1-en-2-yl)benzene-1,2,3-triyl]trimethanol	Predicted	3
			[2,3-Dimethyl-5-(prop-1-en-2-yl)-1,4-phenylene]dimethanol	Predicted	3
			[3-Methyl-5-(prop-1-en-2-yl)benzene-1,2,4-triyl]trimethanol	Predicted	3

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			[3-Methyl-6-(prop-1-en-2-yl)benzene-1,2,4-triyl]trimethanol	Predicted	3
			3,4,5-Trihydroxy-6-{{2-(hydroxymethyl)-3,4-dimethyl-5-(prop-1-en-2-yl)phenyl}methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,4,5-Trihydroxy-6-{{2-(hydroxymethyl)-3,4-dimethyl-6-(prop-1-en-2-yl)phenyl}methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			2,3,6-Trimethyl-5-(2-methyloxiran-2-yl)phenyl]methanol	Predicted	3
			[3,4-Dimethyl-6-(2-methyloxiran-2-yl)-1,2-phenylene]dimethanol	Predicted	3
			3,4,5-Trihydroxy-6-{{3,6-dimethyl-2-(hydroxymethyl)-4-(prop-1-en-2-yl)phenyl}methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,4,5-Trihydroxy-6-{{2-(hydroxymethyl)-4-(prop-1-en-2-yl)-5,6-dimethylphenyl}methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			3,4,5-Trihydroxy-6-{{2,6-dimethyl-3-(hydroxymethyl)-5-(prop-1-en-2-yl)phenyl}methoxy} oxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4

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			3,4,5-Trihydroxy-6-{{[4-(hydroxymethyl)-2-(prop-1-en-2-yl)-5,6-dimethylphenyl]methoxy}oxane-2-carboxylic acid (Glucuronide conjugate)}	Predicted	4
			[2,3,4-Trimethyl-5-(2-methyloxiran-2-yl)phenyl]methanol	Predicted	3
			3,4-Dimethyl-5-(2-methyloxiran-2-yl)-1,2-phenylene]dimethanol	Predicted	3
			[2,4-Dimethyl-5-(2-methyloxiran-2-yl)-1,3-phenylene]dimethanol	Predicted	3
			[2,3-Dimethyl-5-(2-methyloxiran-2-yl)-1,4-phenylene]dimethanol	Predicted	3
			[2,3,4-Trimethyl-6-(prop-1-en-2-yl)phenyl]methyl hydrogen sulfate	Predicted	4
			[2,3,6-Trimethyl-4-(prop-1-en-2-yl)phenyl]methyl hydrogen sulfate	Predicted	4
			2,3,6-Trimethyl-5-(prop-1-en-2-yl)phenyl]methyl hydrogen sulfate	Predicted	4
			[2,3,4-Trimethyl-5-(prop-1-en-2-yl)phenyl]methyl hydrogen sulfate	Predicted	4
			2-(2,3,4-Trimethyl-5-(hydroxymethyl)phenyl)prop-2-en-1-ol	Predicted	3
			2-(2,3,5-Trimethyl-4-(hydroxymethyl)phenyl)prop-2-en-1-ol	Predicted	3

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			2-(2,4,5-Trimethyl-3-(hydroxymethyl)phenyl)prop-2-en-1-ol	Predicted	3
			2-(3,4,5-Trimethyl-2-(hydroxymethyl)phenyl)prop-2-en-1-ol	Predicted	3
620-02-0	2-Furancarboxaldehyde, 5-methyl- (5-Methylfurfural)	1917-15-3	5-methylfuran-2-carboxylic acid	Known	1
		1193-79-9	5-methylfuryl methylketone	Known	1
		6338-41-6	5-Hydroxymethyl-2-furoic acid	Known	1
		38716-68-6	N-(5-hydroxymethyl-2-furoyl)glycine	Known	4
		3238-40-2	2,5-Furandicarboxylic acid	Known	1
			CoA thioester of 5-methylfuroic acid and related alpha-ketoester	Known	4
		13529-17-4	5-formylfuran-2-carboxylic acid	Predicted	3
		97207-45-9	2-[(5-methylfuran-2-carbonyl)amino]acetic acid	Predicted	3
		67-47-0	5-Hydroxymethylfurfural	Predicted	3
623-05-2	Benzenemethanol, 4-hydroxy-	99-97-6	4-Hydroxybenzoic acid	Known	1
		108-95-2	Phenol	Known	1
		106-44-5	4-Hydroxytoluene	Known	1
			Sulfate conjugate of 4-hydroxybenzoic acid	Known	4

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			Glucuronic acid conjugate of 4-hydroxybenzoic acid	Known	4
			p-Hydroxybenzyl alcohol O-sulfate	Known	4
		123-08-0	4-Hydroxybenzaldehyde	Predicted	2
		123-31-9	Hydroquinone	Predicted	3
		50-00-0	Formaldehyde	Predicted	3
			(4-hydroxybenzamido)acetic acid	Predicted	3
			4-(hydroxymethyl)benzene-1,2-diol	Predicted	3
			4-(hydroxymethyl)phenyl hydrogen sulfate	Predicted	4
628-97-7	Hexadecanoic acid, ethyl ester	57-10-3	Hexadecenoic acid	Predicted	2
			15-hydroxyhexadecanoic acid	Predicted	2
		64-17-5	Ethyl alcohol	Predicted	3
		64-19-7	Acetic acid	Predicted	2
			13-hydroxyhexadecanoic acid	Predicted	3
			13-oxohexadecanoic acid	Predicted	3
			14,15-dihydroxyhexadecanoic acid	Predicted	3
			14-hydroxyhexadecanoic acid	Predicted	3
			14-oxohexadecanoic acid	Predicted	3

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			16-hydroxy-13-oxohexadecanoic acid	Predicted	3
		338746-11-5	2-[[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]sulfanyl]acetic acid	Predicted	4
			3-oxotetradecanedioic acid	Predicted	3
			4-hydroxyhexadecanedioic acid	Predicted	3
		506-13-8	16-hydroxyhexadecanoic acid	Predicted	3
		75-07-0	Acetaldehyde	Predicted	2
			ethyl 13-oxohexadecanoate	Predicted	3
			ethyl 16-hydroxyhexadecanoate	Predicted	3
			<chem>CC(O)C(=O)CCCCCCCCCCCCC(O)=O</chem>	Predicted	3
6387-89-9	Glycidyl acetate	555-62-5	Glycidol	Predicted	3
		56-81-5	Glycerol	Predicted	3
		64-19-7	Acetic acid	Predicted	2
		106-61-6	1-Monoacetin	Predicted	2
		473-81-4	2,3-Dihydroxypropanoic acid	Predicted	2
		89712-14-1	2-Hydroxy-3-oxopropyl acetate	Predicted	2
			3-Acetyloxy-2-hydroxypropanoic acid	Predicted	2
			Hydroxypyruvic acid	Predicted	3

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		503-11-7	Glycidic acid	Predicted	3
		5371-49-3	2-Oxoethyl acetate	Predicted	3
		70909-43-2	3-Acetoxy-2-oxopropanoic acid	Predicted	3
			3-(Acetyloxy)-2-hydroxypropanoic acid	Predicted	3
			2-Acetamido-3-[[3-(acetyloxy)-2-hydroxypropyl]sulfanyl]propanoic acid	Predicted	3
			6-[3-(Acetyloxy)-2-hydroxypropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	3
			3,4,5-Trihydroxy-6-[(oxiran-2-yl)methoxy]oxane-2-carboxylic acid	Predicted	3
			2,3-Dihydroxypropyl acetate	Predicted	3
			6-(2,3-Dihydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	3
			2,3-Dihydroxypropyl hydrogen sulfate	Predicted	4
			6-[(1,3-Dihydroxypropan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	3
			6-[[1-Acetyloxy]-3-hydroxypropan-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	3
			1,3-Dihydroxypropan-2-yl hydrogen sulfate	Predicted	4

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			2-Acetamido-3-[[1-(acetyloxy)-3-hydroxypropan-2-yl]sulfanyl]propanoic acid	Predicted	3
			Oxiran-2-yl)methyl hydrogen sulfate	Predicted	4
6418-46-8	Eicosane, 3-methyl		20-Hydroxy-3-methyleicosanal	Predicted	3
			20-Hydroxy-18-methyleicosanal	Predicted	3
			3-Methyleicosan-1,20-diol	Predicted	3
		64-19-7	Acetic acid	Predicted	3
			19-Hydroxy-18-methyleicosanal	Predicted	3
			3-Methyleicosan-2,20-diol	Predicted	2
			3-Methyleicosan-2,19-diol	Predicted	2
			19-Hydroxy-3-methyleicosanal	Predicted	3
			3-Methyleicosan-1,19-diol	Predicted	2
			3-Methyleicosan-3,19-diol	Predicted	2
			18-Hydroxy-18-methyleicosanal	Predicted	3
			3-Methyleicosan-3,20-diol	Predicted	3
		7416-57-1	10-Methyldodecanoic acid; 10-Methylauric acid	Predicted	3
		5502-94-3	12-Methyltetradecanoic acid; 12-Methylmyristic acid	Predicted	3

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		5918-29-6	14-Methylhexadecanoic acid; 14-Methylpalmitic acid	Predicted	3
			18-Methyleicosan-2,4-diol	Predicted	3
			18-Methyleicosan-1,4-diol	Predicted	3
			18-Methyleicosan-3-one	Predicted	3
		17001-28-4	16-Methyloctadecanoic acid; 16-Methylstearic acid	Predicted	3
			18-Methyleicosan-2,3-diol	Predicted	3
			18-Methyleicosan-3-ol	Predicted	2
			18-Methyleicosan-1,3-diol	Predicted	3
			18-Methyleicosan-2-ol	Predicted	2
		36332-93-1	18-Methyleicosanoic acid; 18-Methylarachidic acid	Predicted	2
			18-Methyl-16-eicosen-1-ol	Predicted	2
			18-Methyleicosanol	Predicted	2
			18-Formyleicosan-2-ol	Predicted	3
			18-Formyleicosan-1-ol	Predicted	3
			18-(Hydroxymethyl)eicosan-2-ol	Predicted	2
			18-(Hydroxymethyl)eicosanal	Predicted	3
			18-(Hydroxymethyl)eicosan-1-ol	Predicted	3

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			3-Methyleicosan-3,18-diol	Predicted	3
			3-Methyleicosan-2,18-diol	Predicted	3
			3-Methyleicosan-1,18-diol	Predicted	3
			18-(Hydroxymethyl)eicosan-3-ol	Predicted	3
			18-Hydroxy-18-methyleicosan-4-one	Predicted	3
			19-Hydroxy-18-methyleicosan-4-one	Predicted	3
			18-Methyleicosan-4-one	Predicted	3
			20-Hydroxy-18-methyleicosan-4-one	Predicted	3
			3-Methyl-eicosan-2,3,17-triol	Predicted	3
			3-Methyleicosan-3,17-diol	Predicted	3
			3-Methyleicosan-1,3,17-triol	Predicted	3
			17-Hydroxy-3-methyleicosan-2-one	Predicted	3
			3-Methyleicosan-2,17-diol	Predicted	3
			18-Methyleicosan-4-ol	Predicted	3
			17-Hydroxy-3-methyleicosanal	Predicted	3
			3-Methyleicosan-1,17-diol	Predicted	3
			18-(Hydroxymethyl)eicosan-4-ol	Predicted	3

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			3-(Hydroxymethyl)eicosan-1,17-diol	Predicted	3
			3-Methyleicosan-2,3-diol	Predicted	3
			3-Methyleicosan-3-ol	Predicted	2
			3-Hydroxy-3-methyleicosanal	Predicted	3
			3-Methyleicosan-1,3-diol	Predicted	3
			3-Methyleicosan-2-ol	Predicted	2
			3-Methyleicosanoic acid	Predicted	2
			3-Methyleicosanal	Predicted	2
			3-Methyleicosanol	Predicted	2
			3-Formyleicosane	Predicted	2
			3-(Hydroxymethyl)eicosane	Predicted	2
			3-Formyleicosan-1-ol	Predicted	3
			3-(Hydroxymethyl)eicosan-2-ol	Predicted	2
			3-(Hydroxymethyl)eicosanal	Predicted	3
			3-(Hydroxymethyl)eicosan-1-ol	Predicted	3
			18-Methyleicosan-2-one	Predicted	2
			3-Methyleicosan-2-one	Predicted	3
		69868-05-9	2-Ethylnonadecanoic acid	Predicted	3

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65-23-6	Pyridoxin	65-23-6	Pyridoxin	Known	1
		82-82-6	4-Pyridoxic acid	Known	1
			Pyridoxal 5'-phosphate	Known	4
		447-05-2	Pyridoxine phosphate	Known	4
		16567-04-7	4,5-Bis(hydroxymethyl)-2-methyl-1-oxidopyridin-1-ium-3-ol	Predicted	2
		29712-70-7	2,4,5-tris(hydroxymethyl)pyridin-3-ol	Predicted	2
		107467-06-1	[4,5-bis(hydroxymethyl)-2-methylpyridin-3-yl] hydrogen sulfate	Predicted	4
		49797-76-4	3-hydroxy-4,5-bis(hydroxymethyl)pyridine-2-carbaldehyde	Predicted	3
		524-07-2	5-Pyridoxic acid	Predicted	2
		6560-46-9	Isopyridoxal	Predicted	2
		66-72-8	Pyridoxal	Predicted	2
			[O-][N+]=2C=C(CO)C(COC1OC(C(O)C(O)C1O)C(O)=O)=C(O)C=2C	Predicted	3
67402-83-9	4(H)-Pyridine, N-acetyl	64-19-7	Acetic acid	Predicted	3
		3337-17-5	1,4-Dihydropyridine	Predicted	3
			1-(4-Hydroxy-1,4-dihydropyridin-1-yl)ethan-1-one	Predicted	2

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			2-(1,4-Dihydropyridin-1-yl)-2-oxoacetaldehyde	Predicted	2
			2-(1,4-Dihydropyridin-1-yl)-2-oxoacetic acid	Predicted	2
			1-(1,4-Dihydropyridin-1-yl)-2-hydroxyethan-1-one	Predicted	2
			1-(2,3,5,6-Tetrahydroxypiperidin-1-yl)ethan-1-one	Predicted	3
			1-{3,4-Dihydroxy-7-oxa-2-azabicyclo[4.1.0]heptan-2-yl}ethan-1-one	Predicted	3
			1-(2,3,4-Trihydroxy-1,2,3,4-tetrahydropyridin-1-yl)ethan-1-one	Predicted	3
			1-{5-Hydroxy-7-oxa-2-azabicyclo[4.1.0]hept-3-en-2-yl}ethan-1-one	Predicted	3
			1-(2,3-Dihydroxy-1,2,3,4-tetrahydropyridin-1-yl)ethan-1-one	Predicted	3
			1-{7-Oxa-2-azabicyclo[4.1.0]hept-3-en-2-yl}ethan-1-one	Predicted	3
			2-(4-Hydroxy-1,4-dihydropyridin-1-yl)-2-oxoacetic acid	Predicted	3
			2-(4-Hydroxy-1,4-dihydropyridin-1-yl)-2-oxoacetaldehyde	Predicted	3
			2-Hydroxy-1-(4-hydroxy-1,4-dihydropyridin-1-yl)ethan-1-one	Predicted	3
6890-88-6			14a-Demethylated eburicol	Known	1

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	Lanost-8-en-3-ol, 24-methylene-, (3beta); Eburicol		Eburicol 23-carbaldehyde	Predicted	3
			22,23-Dihydroxyeburicol	Predicted	3
			20,23-Dihydroxyeburicol	Predicted	3
			23-Hydroxydehydroeburicol	Predicted	3
			23-Hydroxyeburicone	Predicted	3
			23-Hydroxyeburicol	Predicted	2
			23,28-Dihydroxyeburicol	Predicted	3
			Eburicol 22-carbaldehyde	Predicted	3
			20,22-Dihydroxyeburicol	Predicted	3
			22-Hydroxydehydroeburicol	Predicted	3
			7,22-Dihydroxyeburicol	Predicted	3
			22-Hydroxyeburicone	Predicted	3
			11,22-Dihydroxyeburicol	Predicted	3
			22-Hydroxyeburicol	Predicted	2
			22,28-Dihydroxyeburicol	Predicted	3
			16,20-Dihydroxyeburicol	Predicted	3
			15,20-Dihydroxyeburicol	Predicted	3
			20-Hydroxydehydroeburicol	Predicted	3

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			7,20-Dihydroxyeburicol	Predicted	3
			11,20-Dihydroxyeburicol	Predicted	3
			20-Hydroxyeburicol	Predicted	2
			16-Hydroxyeburicol	Predicted	2
			16,28-Dihydroxyeburicol	Predicted	3
			15-Hydroxyeburicol	Predicted	2
			15,28-Dihydroxyeburicol	Predicted	3
			Dehydroeburicol[7,8]oxirene	Predicted	3
			Dehydroeburicone	Predicted	3
			Dehydroeburicol	Predicted	2
			Dehydroeburicol[9,11]oxirene	Predicted	3
			28-Hydroxydehydroeburicol	Predicted	3
			7-Oxoeburicol	Predicted	3
			7-Hydroxyeburicone	Predicted	3
			7-Hydroxyeburicol	Predicted	2
			7,28-Dihydroxyeburicol	Predicted	3
			11-Hydroxyeburicone	Predicted	3
			Eburicone	Predicted	2

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			11-Oxoeburicol	Predicted	3
			11-Hydroxyeburicol	Predicted	2
			Eburicol 28-carbaldehyde	Predicted	3
			11,28-Dihydroxyeburicol	Predicted	3
			28-Hydroxyeburicol	Predicted	2
			24,24-Dihydroxyeburicol	Predicted	3
			20-Hydroxyeburicol[24,24]oxirane	Predicted	3
			22-Hydroxyeburicol[24,24]oxirane	Predicted	3
			23,26-Dihydroxyeburicol	Predicted	3
			Eburicol 26-carbaldehyde	Predicted	3
			16,26-Dihydroxyeburicol	Predicted	3
			15,26-Dihydroxyeburicol	Predicted	3
			26-Hydroxydehydroeburicol	Predicted	3
			7,26-Dihydroxyeburicol	Predicted	3
			11,26-Dihydroxyeburicol	Predicted	3
			26-Hydroxyeburicol	Predicted	2
			Dehydroeburicol[24,24]oxirane	Predicted	3
			7-Hydroxyeburicol[24,24]oxirane	Predicted	3

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			11-Hydroxyeburicol[24,24]oxirane	Predicted	3
			Eburicol[24,24]oxirane	Predicted	3
			22,26-Dihydroxyeburicol	Predicted	3
			Eburicol 27-carboxylic acid	Predicted	3
			17-Hydroxyeburicol	Predicted	3
			Glucuronide conjugate of eburicol	Predicted	4
7786-67-6	Cyclohexanol, 5-methyl-2-(1methylethenyl)-(Menth-8-en-3-ol; Isopulegol)		Glucuronic acid conjugate of isopulegol	Known	4
		29606-79-9	Isopulegone	Known	1
			9-Hydroxyisopulegone	Known	1
		42822-86-6	Citriodiol	Known	1
			5-Methyl-2-(1-hydroxypropan-2-yl)cyclohexanol	Known	1
			2-(2-Hydroxy-4-methylcyclohexyl)propanoic acid	Known	1
			Glutathione conjugate of isopulegol	Known	4
		89-82-7	Pulegone	Known	1
		494-90-6	Menthofuran	Known	1
		529-02-2	Pulegol	Known	1

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			Allylic oxidation to [the] 9-hydroxy derivative” of pulegone	Known	1
			Menthofuran-glutathione conjugate	Known	4
			Phase II conjugates of hydroxylated menthofuran	Known	4
		89-81-6	Piperitone	Known	1
		491-09-8	Piperitenone	Known	1
		10458-14-7	Menthone	Known	1
			4-Methyl-1-(prop-1-ene-2-yl)cyclohexane-1,2-diol	Known	1
			9-Hydroxyisopulegol	Known	1
		193285-32-7	4-Isopropenyl-1-methyl-1,3-cyclohexanediol	Predicted	2
			3-Hydroxy-4-(prop-1-en-2-yl)cyclohexane-1-carboxylic acid	Predicted	2
			3-Hydroxy-4-(prop-1-en-2-yl)cyclohexane-1-carbaldehyde	Predicted	2
			5-(Hydroxymethyl)-2-(prop-1-en-2-yl)cyclohexan-1-ol	Predicted	2
			2-(2,4-Dihydroxy-4-methylcyclohexyl)prop-2-enoic acid	Predicted	3
			2-(2,4-Dihydroxy-4-methylcyclohexyl)prop-2-enal	Predicted	3

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			4-(3-Hydroxyprop-1-en-2-yl)-1-methylcyclohexane-1,3-diol	Predicted	3
			4-(1,2-Dihydroxypropan-2-yl)-1-methylcyclohexane-1,3-diol	Predicted	2
			1-Methyl-4-(2-methyloxiran-2-yl)cyclohexane-1,3-diol	Predicted	2
		38049-02-4	2-Hydroxy-4-methylcyclohexyl]acrylic acid	Predicted	2
			2-Hydroxy-4-methylcyclohexyl]acrylaldehyde	Predicted	2
			2-(3-Hydroxyprop-1-en-2-yl)-5-methylcyclohexan-1-ol [9-hydroxyisopulegol]	Predicted	2
			2-Hydroxy-2-(2-hydroxy-4-methylcyclohexyl)propanal	Predicted	3
		820208-69-3	2-(2-Hydroxy-4-methylcyclohexyl)-1,2-propanediol; p-menthan-3,8,9-triol	Predicted	2
		294634-38-1	5-Methyl-2-(2-methyl-2-oxiranyl)cyclohexanol	Predicted	2
			5-(Hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)cyclohexan-1-one	Predicted	3
			5-(Hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)cyclohexan-1-ol	Predicted	3
			3,4,5-Trihydroxy-6-[2-hydroxy-2-(2-hydroxy-4-methylcyclohexyl)propoxy]oxane-2-carboxylic acid	Predicted	4

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			2-(2-Hydroxy glucuronide-4-methylcyclohexyl)propane-1,2-diol	Predicted	4
			3,4,5-Trihydroxy-6-{{[5-methyl-2-(2-methyloxiran-2-yl)cyclohexyl]oxy}oxane-2-carboxylic acid	Predicted	4
			5-Methyl-2-(2-methyloxiran-2-yl)cyclohexan-1-one	Predicted	3
			4-Methyl-1-(2-methyloxiran-2-yl)cyclohexane-1,2-diol	Predicted	3
			3,4,5-Trihydroxy-6-{{[5-methyl-2-(prop-1-en-2-yl)cyclohexyl]oxy}oxane-2-carboxylic acid	Predicted	4
			4-Methyl-1-(prop-1-en-2-yl)cyclohexane-1,2-diol	Predicted	3
			3,4,5-Trihydroxy-6-{{[2-hydroxy-5-methyl-2-(prop-1-en-2-yl)cyclohexyl]oxy}oxane-2-carboxylic acid	Predicted	4
			3,4,5-Trihydroxy-6-{{[2-(3-hydroxyprop-1-en-2-yl)-5-methylcyclohexyl]oxy}oxane-2-carboxylic acid	Predicted	4
			3,4,5-Trihydroxy-6-{{[5-hydroxy-5-methyl-2-(prop-1-en-2-yl)cyclohexyl]oxy}oxane-2-carboxylic acid	Predicted	4
80933-73-9	Maltozazine		<chem>OC1CC(=O)C=2N3CCCC3OCC1=2</chem>	Predicted	3
			<chem>OC4C(OC1CC(=O)C=2N3CCCC3OCC1=2)OC(C(O)C4O)C(O)=O</chem>	Predicted	3

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			<chem>OC3CC=2COC1N(CCC1)C=2C3=O</chem>	Predicted	3
			<chem>O=C1CCC2OCC3CCC(=O)C=3N21</chem>	Predicted	3
			<chem>OC1CC2OCC3CCC(=O)C=3N2C1=O</chem>	Predicted	3
89-48-5	Menthyl acetate	1490-04-6	Menthol	Known	1
		64-19-7	Acetic acid	Known	1
		155348-06-4	4-(2-Hydroxy-2-propanyl)-1-methyl-1,3-cyclohexanediol	Predicted	3
		1612-98-2	p-Menthane-1,3-diol	Predicted	2
		10458-14-7	Isomenthone	Predicted	2
			(8,8-Dimethyl-7-oxabicyclo[4.2.0]octan-4-yl)methanol	Predicted	3
			4,8,8-Trimethyl-7-oxabicyclo[4.2.0]octan-4-ol	Predicted	3
			2-[2-(Acetyloxy)-4-methylcyclohexyl]propanoic acid	Predicted	2
			5-Methyl-2-(1-oxopropan-2-yl)cyclohexyl acetate	Predicted	2
			2-(1-Hydroxypropan-2-yl)-5-methylcyclohexyl acetate	Predicted	2
		42822-86-6	2-(2-Hydroxy-2-propanyl)-5-methylcyclohexanol	Predicted	2

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			4,8,8-Trimethyl-7-oxabicyclo[4.2.0]octane	Predicted	3
			(4,8-Dimethyl-7-oxabicyclo[4.2.0]octan-8-yl)methanol	Predicted	3
			3-Acetoxy-p-menthan-1-ol	Predicted	2
			3-(Acetyloxy)-4-(propan-2-yl)cyclohexane-1-carboxylic acid	Predicted	3
			5-Formyl-2-(propan-2-yl)cyclohexyl acetate	Predicted	3
			5-(Hydroxymethyl)-2-(propan-2-yl)cyclohexyl acetate	Predicted	3
			Menthol glucuronide	Predicted	4
			8-Hydroxymenthol glucuronide	Predicted	4
			1-Hydroxymenthol glucuronide	Predicted	4
			4-Methyl-1-(propan-2-yl)cyclohexane-1,2-diol; 4-Hydroxymenthol	Predicted	3
			2-(1-Hydroxypropan-2-yl)-5-methylcyclohexan-1-ol; 9-Hydroxymenthol	Predicted	3
			2-(2-Hydroxypropan-2-yl)-5-methylcyclohexyl acetate; 8-Hydroxymenthol acetate	Predicted	3
			2-Hydroxy-5-methyl-2-(propan-2-yl)cyclohexyl acetate; 4-Hydroxymenthol acetate	Predicted	3

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89-81-6	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- (Piperitone)	491-04-3	Piperitol	Known	1
			Glucuronide conjugate of piperitol	Known	4
		43205-82-9	Carvotanacetone	Known	1
		89-83-8	Thymol	Known	1
		490-03-9	Diosphenol	Known	1
			4-(2-Hydroxypropan-2-yl)-3-oxocyclohex-1-ene-1-carboxylic acid	Predicted	3
			4-(2-Hydroxypropan-2-yl)-3-oxocyclohex-1-ene-1-carbaldehyde	Predicted	3
			3-(Hydroxymethyl)-6-(2-hydroxypropan-2-yl)cyclohex-2-en-1-one	Predicted	3
			3-(2-Hydroxypropan-2-yl)-6-methyl-7-oxabicyclo[4.1.0]heptan-2-ol	Predicted	3
		9094217-54-5	5-Isopropyl-2-methyl-2-cyclohexene-1,4-dione	Predicted	3
		78391-96-5	4-Hydroxy-5-isopropyl-2-methyl-2-cyclohexen-1-one	Predicted	3
		141978-04-3	4-Hydroxy-6-isopropyl-3-methyl-2-cyclohexen-1-one	Predicted	2
		4031-55-4	5-Isopropyl-2-methyl-2-cyclohexene-1,4-diol	Predicted	3
			3-Oxo-4-(propan-2-yl)cyclohex-1-ene-1-carboxylic acid	Predicted	2

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		160152-34-1	4-Isopropyl-3-oxo-1-cyclohexene-1-carbaldehyde	Predicted	2
		67252-15-7	3-Hydroxy-4-isopropyl-1-cyclohexene-1-carbaldehyde	Predicted	3
		55955-54-9	3-(Hydroxymethyl)-6-isopropyl-2-cyclohexen-1-one	Predicted	2
			3-(Hydroxymethyl)-6-(propan-2-yl)cyclohex-2-en-1-ol	Predicted	3
			2-(5-Hydroxy-4-methyl-2-oxocyclohex-3-en-1-yl)propanoic acid	Predicted	3
			2-(4-Methyl-2-oxocyclohex-3-en-1-yl)propanoic acid	Predicted	2
			2-(5-Hydroxy-4-methyl-2-oxocyclohex-3-en-1-yl)propanal	Predicted	3
			2-(4-Methyl-2-oxocyclohex-3-en-1-yl)propanal	Predicted	2
			4-Hydroxy-6-(1-hydroxypropan-2-yl)-3-methylcyclohex-2-en-1-one	Predicted	2
		1824572-50-0	6-(1-Hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-one	Predicted	2
			3-(Hydroxymethyl)-6-(1-hydroxypropan-2-yl)cyclohex-2-en-1-one	Predicted	3
			3-(Hydroxymethyl)-6-(1-hydroxypropan-2-yl)cyclohex-2-en-1-ol	Predicted	3

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			6-(1,2-Dihydroxypropan-2-yl)-3-(hydroxymethyl)cyclohex-2-en-1-one	Predicted	3
			5-(2-Hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	Predicted	3
			4-Hydroxy-6-(2-hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-one	Predicted	2
			5-(2-Hydroxy-2-propanyl)-2-methyl-2-cyclohexene-1,4-diol	Predicted	3
		87791-00-2	6-(2-Hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-one	Predicted	2
		6252-34-2	6-(2-Hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-ol	Predicted	3
			4,6-Dihydroxy-3-methyl-6-(propan-2-yl)cyclohex-2-en-1-one	Predicted	3
		1197-72-4	6-Hydroxy-3-methyl-6-(propan-2-yl)cyclohex-2-en-1-one	Predicted	2
			8-Hydroxypiperitone 8-O-glucuronide	Predicted	4
			3-(2-Hydroxypropan-2-yl)-6-methyl-7-oxabicyclo[4.1.0]heptan-2-one	Predicted	3
			6-(1,2-Dihydroxypropan-2-yl)-3-methylcyclohex-2-en-1-one; 8,9-Dihydroxypiperitone	Predicted	3
			4-Hydroxypiperitone-4-O-glucuronide	Predicted	4
		5286-38-4	Piperitone oxide	Predicted	3

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			6-Methyl-3-(propan-2-yl)-7-oxabicyclo[4.1.0]heptan-2-ol	Predicted	3
			6-Methyl-3-(propan-2-yl)-7-oxabicyclo[4.1.0]heptan-2-ol glucuronide	Predicted	4
			1-Methyl-4-(propan-2-yl)cyclohexane-1,2,3-triol; 1,2-Dihydroxymenthol	Predicted	3
			2,3-Dihydroxy-3-methyl-6-(propan-2-yl)cyclohexan-1-one; 1,2-Dihydroxymenthone	Predicted	3
942-43-8	1H-Indene, 2,3-dihydro-1,1,5,6-tetramethyl		(3,3,6-trimethyl-1,2-dihydroinden-5-yl)methanol	Predicted	2
			3,3,5,6-tetramethyl-1,2-dihydroinden-1-ol	Predicted	2
		54789-22-9	1-H-Inden-1-one,2,3-dihydro-3,3,5,6-tetramethyl	Predicted	3
			<chem>OCC1=CC=2CCC(C)(C)C=2C=C1C</chem>	Predicted	3
			<chem>Cc1cc2C(O)C(O)C(C)(C)c2cc1C</chem>	Predicted	3
			<chem>Cc1cc2CC(=O)C(C)(C)c2cc1C</chem>	Predicted	3
96-48-0	Butyrolactone	591-81-1	gamma-Hydroxybutyric acid	Known	1
		110-15-6	Succinic acid	Known	1
		124-38-9	Carbon dioxide	Known	1
		1518-61-2	3,4-Dihydroxybutyric acid	Known	1

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		79-14-1	Glycolic acid	Known	1
		162369-88-2	4-Hydroxy-3-oxobutyric acid	Known	1
		541-50-4	3-Oxobutyric acid	Known	1
		617-65-2	Glutamic acid	Known	1
		256928-74-2	Succinylcarnitine	Known	4
		56-12-2	gamma-Aminobutyric acid (GABA)	Known	1
		1518-62-3	2,4-Dihydroxybutyric acid	Known	1
		1439527-93-1	gamma-Hydroxybutyric acid glucuronide	Known	4
		5469-16-9	4-Hydroxyoxolan-2-one	Predicted	3
		92-29-5	4-Oxobutanoic acid	Predicted	2
			3,4,5-Trihydroxy-6-[(5-oxooxolan-3-yl)oxy]oxane-2-carboxylic acid [Glucuronide conjugate of butyrolactone]	Predicted	4
			(5-Oxooxolan-3-yl) hydrogen sulfate	Predicted	4
96937-49-4	Benzoic acid, 2,5-dihydroxy-methyl		6-[[3-Carboxy-4-(hydroxymethyl)phenyl]methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			6-[[2-Carboxy-4-(hydroxymethyl)phenyl]methoxy]-3,4,5-trihydroxyoxane-2-	Predicted	4

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CAS-Number	Parent chemicals	CAS-Number	Metabolites	Status	Ranking
			carboxylic acid (Glucuronide conjugate)		
			[2,5-Bis(hydroxymethyl)benzamido]acetic acid	Predicted	3
			4-(Hydroxymethyl)phthalic acid	Predicted	2
			2-Formyl-5-(hydroxymethyl)benzoic acid	Predicted	2
			5-Formyl-2-(hydroxymethyl)benzoic acid	Predicted	2
			4-(Hydroxymethyl)isophthalic acid	Predicted	2
			2-Hydroxy-3,6-bis(hydroxymethyl)benzoic acid	Predicted	3
			5-(Hydroxymethyl)-2-[(sulfooxy)methyl]benzoic acid	Predicted	4
			2-(Hydroxymethyl)-5-[(sulfooxy)methyl]benzoic acid	Predicted	4
			6- {[2,5-Bis(hydroxymethyl)benzoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
			6- {[2-Carboxy-3-hydroxy-4-(hydroxymethyl)phenyl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid (Glucuronide conjugate)	Predicted	4
97-99-4	2-Furanmethanol, tetrahydro	16874-33-2	Tetrahydrofuran-2-carboxylic acid	Predicted	2
		7681-84-7	Tetrahydro-2-furancarboxaldehyde	Predicted	2

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			2-hydroxy-5-oxopentanoic acid	Predicted	3
		58534-88-6	5-(Hydroxymethyl)Tetrahydrofuran-3-ol	Predicted	3
		66679-29-6	4,5-dihydroxypentanoic acid	Predicted	3
			oxolan-2-ylmethylhydrogen sulfate	Predicted	4
			OC2C(OCC1OCCC1)OC(C(O)C2O)C(O)=O	Predicted	3
98-55-5	3-Cyclohexene-1-methanol, $\alpha,\alpha,4$ trimethyl- (Terpineol)		Glucuronic acid conjugate of alpha-terpineol	Known	4
		57761-51-0	2-(6-Methyl-7-oxabicyclo[4.1.0]hept-3-yl)-2-propanol	Known	1
		58506-22-2	p-Menthane-1,2,8-triol	Known	1
		5027-76-9	Oleuropeic acid	Known	1
		183996-92-1	Dihydrooleuropeic acid	Known	1
		33746-68-8	4-(2-Hydroxy-2-propanyl)-1-cyclohexene-1-carboxylic acid	Predicted	2
		62014-81-7	4-(2-Hydroxy-2-propanyl)-1-methyl-1,2-cyclohexanediol	Predicted	2
			4-(2-Hydroxypropan-2-yl)-1-methylcyclohexane-1,2,3-triol	Predicted	3
		38223-81-3	4-(2-Hydroxy-2-propanyl)-1-cyclohexene-1-carbaldehyde	Predicted	2

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		5502-74-9	p-Menth-1-ene-7,8-diol; 4-(2-Hydroxy-2-propyl)cyclohexene-1-methanol	Predicted	2
			3-(2-Hydroxypropan-2-yl)-6-methyl-7-oxabicyclo[4.1.0]heptan-2-ol	Predicted	2
		7712-46-1	5-(2-Hydroxy-2-propanyl)-2-methyl-2-cyclohexen-1-one	Predicted	2
		32226-54-3	Sobrerol	Predicted	2
		87791-00-2	6-(2-Hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-one	Predicted	2
		6252-34-2	6-(2-Hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-ol	Predicted	2
		97762-06-6	2-Hydroxymethyl-5-(1-hydroxy-1-isopropyl)-2-cyclohexen-1-one	Predicted	2
			3-(Hydroxymethyl)-6-(2-hydroxypropan-2-yl)cyclohex-2-en-1-one	Predicted	3
			4-Hydroxy-6-(2-hydroxy-2-propanyl)-3-methyl-2-cyclohexen-1-one	Predicted	3
		1823895-38-0	4-Hydroxy-5-(2-hydroxy-2-propanyl)-2-methyl-2-cyclohexen-1-one	Predicted	3
			6-Hydroxy-6-(2-hydroxypropan-2-yl)-3-methylcyclohex-2-en-1-one	Predicted	3
			3-(Hydroxymethyl)-6-(2-hydroxypropan-2-yl)cyclohex-2-en-1-ol	Predicted	3

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			2-(Hydroxymethyl)-5-(2-hydroxypropan-2-yl)cyclohex-2-en-1-ol	Predicted	3
			3,4,5-Trihydroxy-6-{{4-(2-hydroxypropan-2-yl)cyclohex-1-en-1-yl}methoxy}oxane-2-carboxylic acid	Predicted	4
			3,4,5-Trihydroxy-6-({2-[4-(hydroxymethyl)cyclohex-3-en-1-yl]propan-2-yl}oxy)oxane-2-carboxylic acid	Predicted	4
			2-[6-(Hydroxymethyl)-7-oxabicyclo[4.1.0]heptan-3-yl]propan-2-ol	Predicted	3
			4-(Hydroxymethyl)-1-(2-hydroxypropan-2-yl)cyclohex-3-en-1-ol	Predicted	3
			2-[4-(Hydroxymethyl)cyclohex-3-en-1-yl]propane-1,2-diol	Predicted	3
			2-(Hydroxymethyl)-5-(2-hydroxypropan-2-yl)cyclohex-2-en-1-ol 1-O-glucuronide	Predicted	4
			3,4,5-Trihydroxy-6-{{6-hydroxy-4-(1-hydroxypropan-2-yl)cyclohex-1-en-1-yl}methoxy}oxane-2-carboxylic acid	Predicted	4
			2-(Hydroxymethyl)-5-(2-hydroxypropan-2-yl)cyclohex-2-ene-1,4-diol	Predicted	3
			5-(2-Hydroxypropan-2-yl)-2-methylcyclohex-2-en-1-ol 1-O-glucuronide	Predicted	4

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			5-(2-Hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-diol	Predicted	3
			5-(2-Hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-diol 1-O-glucuronide	Predicted	4
			5-(2-Hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-diol 4-O-glucuronide	Predicted	4
			5-(2-Hydroxypropan-2-yl 2-O-glucuronide)-2-methylcyclohex-2-en-1-ol	Predicted	4
			4-(2-Hydroxypropan-2-yl)-1-methyl-7-oxabicyclo[4.1.0]heptan-2-ol	Predicted	3
			2-(5-Hydroxy-4-methylcyclohex-3-en-1-yl)propane-1,2-diol	Predicted	3
			2-[5-Hydroxy-4-(hydroxymethyl)cyclohex-3-en-1-yl]propane-1,2-diol	Predicted	3
			1-(2-Hydroxypropan-2-yl)-4-methylcyclohex-4-ene-1,3-diol	Predicted	3
			3,4,5-Trihydroxy-6-{{[2-(4-methylcyclohex-3-en-1-yl)propan-2-yl]oxy}oxane-2-carboxylic acid	Predicted	4
			3-(Hydroxymethyl)-6-(2-hydroxypropan-2-yl)cyclohex-2-en-1-ol 3-O-glucuronide	Predicted	4
			3-(Hydroxymethyl)-6-(2-hydroxypropan-2-yl)cyclohex-2-en-1-ol 1-O-glucuronide	Predicted	4

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			6-(2-Hydroxypropan-2-yl)-3-methylcyclohex-2-en-1-ol 1-O-glucuronide	Predicted	4
			1-(2-Hydroxypropan-2-yl)-4-methylcyclohex-3-ene-1,2-diol	Predicted	3
			6-(2-Hydroxypropan-2-yl 2-O-glucuronide)-3-methylcyclohex-2-en-1-ol	Predicted	4
			1-(2-Hydroxypropan-2-yl)-4-methylcyclohex-3-en-1-ol	Predicted	3
			4-(Hydroxymethyl)-1-(2-hydroxypropan-2-yl)cyclohex-3-en-1-ol 4-O-glucuronide	Predicted	4
			1-(2-Hydroxypropan-2-yl)-4-methylcyclohex-4-ene-1,3-diol 3-O-glucuronide	Predicted	4
			4-(Hydroxymethyl)-1-(2-hydroxypropan-2-yl)cyclohex-4-ene-1,3-diol	Predicted	3
			1-(2-Hydroxypropan-2-yl 2-O-glucuronide)-4-methylcyclohex-3-en-1-ol	Predicted	4
			2-(4-Methylcyclohex-3-en-1-yl)propane-1,2-diol	Predicted	3
99-49-0	2-Cyclohexen-1-one, 2-methyl-5-(1methylethenyl)- (6,8-P-Menthadien-2-one) / Carvone	83994-34-7	Dihydrocarvonic acid	Known	1
		362483-06-5	Carvonic acid	Known	1
		402593-42-4	Uroterpenolone	Known	1
		99-48-9	Carveol	Known	1

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			Glucuronic acid conjugate of carveol	Known	4
		619-01-2	Dihydrocarveol	Known	1
			Glucuronic acid conjugate of dihydrocarveol	Known	4
			(+)-9-Hydroxycarvone	Known	1
			Glucuronic acid conjugate of (+)-9-hydroxycarvone	Known	4
			1,5-Dimethyl-1,5-hexadien-1,6-dicarboxylic acid	Known	1
		586-23-2	A carbinol, possibly 5-isopropyl-2-methyl-2-cyclohexen-1-ol	Known	1
			Glutathione conjugate of carvone	Known	4
			2-Methyl-5-(prop-1-en-2-yl)cyclohex-2-ene-1,4-dione	Predicted	2
		56423-48-4	4-Hydroxy-5-isopropenyl-2-methyl-2-cyclohexen-1-one	Predicted	2
			3-Hydroxy-6-oxo-4-(prop-1-en-2-yl)cyclohex-1-ene-1-carbaldehyde	Predicted	3
			4-Hydroxy-2-(hydroxymethyl)-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	2
		1823040-77-2	4-Hydroxy-6-isopropenyl-3-methyl-2-cyclohexen-1-one	Predicted	3
			6-Oxo-4-(prop-1-en-2-yl)cyclohex-1-ene-1-carboxylic acid	Predicted	2

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		56081-00-6	4-Isopropenyl-6-oxo-1-cyclohexene-1-carbaldehyde	Predicted	2
		182295-55-0	10-Hydroxycarvone	Predicted	3
			2-(2-Hydroxy-4-methyl-5-oxocyclohex-3-en-1-yl)prop-2-enoic acid	Predicted	3
			2-(2-Hydroxy-4-methyl-5-oxocyclohex-3-en-1-yl)prop-2-enal	Predicted	3
			4-Hydroxy-5-(3-hydroxyprop-1-en-2-yl)-2-methylcyclohex-2-en-1-one	Predicted	2
			5-(1,2-Dihydroxypropan-2-yl)-4-hydroxy-2-methylcyclohex-2-en-1-one	Predicted	2
			4-Hydroxy-2-methyl-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one	Predicted	2
		79763-05-6	2-(4-Methyl-5-oxo-3-cyclohexen-1-yl)acrylaldehyde	Predicted	3
			2-Hydroxy-2-(4-methyl-5-oxocyclohex-3-en-1-yl)propanal	Predicted	3
		81679-70-1	5-(1,2-Dihydroxy-2-propenyl)-2-methyl-2-cyclohexen-1-one	Predicted	3
		294634-40-5; 56423-45-1; 672898-51-0	2-Methyl-5-(2-methyl-2-oxiran-2-yl)-2-cyclohexen-1-one	Predicted	2
			2-(5-Hydroxy-4-methylcyclohex-3-en-1-yl)prop-2-enoic acid	Predicted	3

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			2-(5-Hydroxy-4-methylcyclohex-3-en-1-yl)prop-2-enal	Predicted	3
		1823640-02-3	5-(3-Hydroxy-1-propen-2-yl)-2-methyl-2-cyclohexen-1-ol	Predicted	3
			4-Hydroxy-2-(hydroxymethyl)-5-(3-hydroxyprop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	2
			2-(Hydroxymethyl)-5-(3-hydroxyprop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	2
			2-(Hydroxymethyl)-5-(3-hydroxyprop-1-en-2-yl)cyclohex-2-en-1-ol	Predicted	3
			2-(Hydroxymethyl)-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one	Predicted	3
			2-(Hydroxymethyl)-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one glucuronide	Predicted	4
			4-Hydroxy-2-(hydroxymethyl)-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one	Predicted	3
			5-(1,2-Dihydroxypropan-2-yl)-2-(hydroxymethyl)cyclohex-2-en-1-one	Predicted	3
			4-Hydroxy-2-methyl-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one glucuronide	Predicted	4
			3,4,5-Trihydroxy-6-[2-hydroxy-2-(4-methyl-5-oxocyclohex-3-en-1-yl)propoxy]oxane-2-carboxylic acid	Predicted	4

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			5-Hydroxy-2-methyl-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one	Predicted	3
			5-Hydroxy-2-(hydroxymethyl)-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one	Predicted	3
			4,5-Dihydroxy-2-methyl-5-(2-methyloxiran-2-yl)cyclohex-2-en-1-one	Predicted	3
			1-Methyl-4-(2-methyloxiran-2-yl)-7-oxabicyclo[4.1.0]heptan-2-one	Predicted	3
			2-(Hydroxymethyl glucuronide)-5-(3-hydroxyprop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	4
			2-(Hydroxymethyl)-5-(3-hydroxyprop-1-en-2-yl glucuronide)cyclohex-2-en-1-one	Predicted	4
			3,4,5-Trihydroxy-6-{{[6-oxo-4-(prop-1-en-2-yl)cyclohex-1-en-1-yl]methoxy} oxane-2-carboxylic acid	Predicted	4
			5-Hydroxy-2-(hydroxymethyl)-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	3
			1-(Hydroxymethyl)-4-(prop-1-en-2-yl)-7-oxabicyclo[4.1.0]heptan-2-one	Predicted	3
			4-Hydroxy glucuronide-2-(hydroxymethyl)-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	4
			4-Hydroxy-2-(hydroxymethyl glucuronide)-5-(prop-1-en-2-	Predicted	4

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			yl)cyclohex-2-en-1-one glucuronide		
			4-Hydroxy-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-one glucuronide	Predicted	4
			4,5-Dihydroxy-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	3
			4,5-Dihydroxy-2-(hydroxymethyl)-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	3
			5-Hydroxy-1-methyl-4-(prop-1-en-2-yl)-7-oxabicyclo[4.1.0]heptan-2-one	Predicted	3
			2-Methyl-5-(2-methyloxiran-2-yl)cyclohex-2-ene-1,4-dione	Predicted	3
			4-Hydroxy-5-(3-hydroxyprop-1-en-2-yl glucuronide)-2-methylcyclohex-2-en-1-one	Predicted	4
			5-Hydroxy-5-(3-hydroxyprop-1-en-2-yl)-2-methylcyclohex-2-en-1-one	Predicted	3
			5-Hydroxy-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	3
			1-Methyl-4-(prop-1-en-2-yl)-7-oxabicyclo[4.1.0]heptan-2-one	Predicted	3
			1-Methyl-4-(prop-1-en-2-yl)-7-oxabicyclo[4.1.0]heptan-2-ol	Predicted	3
			6-Hydroxy-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-one	Predicted	3
	12,14-Labdadiene-7,8-diol, (7beta,8alpha,12Z)		(2Z,6E,11E)-8,10-Dihydroxy-2,6,10-trimethyl-13-(propan-2-	Predicted	3

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N/A changed to 57605-80-8	changed to alpha-cembratriene-diol		yl)cyclotetradeca-2,6,11-trien-1-one		
			(2E,6Z,11E)-8,13-Dihydroxy-3,7,13-trimethyl-10-(propan-2-yl)cyclotetradeca-2,6,11-trien-1-one	Predicted	3
			(5Z,9Z)-2,6,10-Trimethyl-13-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-5,9-diene-2,4,11-triol	Predicted	3
			(4E,9Z,13E)-3,9,13-Trimethyl-6-(propan-2-yl)cyclotetradeca-4,9,13-triene-1,3,8-triol	Predicted	2
			(5Z,10Z)-4,10,14-Trimethyl-7-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-5,10-diene-2,4,9-triol	Predicted	3
			(1E,5E,10E)-7,9-Dihydroxy-5,9-dimethyl-12-(propan-2-yl)cyclotetradeca-1,5,10-triene-1-carboxylic acid	Predicted	3
			(5Z,10E)-1,5,9-Trimethyl-12-(propan-2-yl)cyclotetradeca-5,10-diene-1,2,7,9-tetraol	Predicted	3
			(2Z,7E,12Z)-9,11-Dihydroxy-3,9,13-trimethyl-6-(propan-2-yl)cyclotetradeca-2,7,12-trien-1-one	Predicted	3
			(2Z,6Z,11E)-5,13-Dihydroxy-3,7,13-trimethyl-10-(propano-2-yl)cyclotetradeca-2,6,11-trien-1-one	Predicted	3
			(5Z,9Z)-2,6,10-Trimethyl-13-(propan-2-yl)-15-	Predicted	3

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			oxabicyclo[12.1.0]pentadeca-5,9-diene-2,4,8-triol		
			(4Z,8Z,13E)-1,5,9-Trimethyl-12-(propan-2-yl)cyclotetradeca-4,8,13-triene-1,3,7-triol	Predicted	2
			(5Z,10Z)-4,10,14-Trimethyl-7-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-5,10-diene-2,4,12-triol	Predicted	3
			(6E,11Z)-1,5,11-Trimethyl-8-(propan-2-yl)cyclotetradeca-6,11-diene-1,2,3,5-tetrol	Predicted	3
			(2E,6Z,11E)-13-Hydroxy-3,7,13-trimethyl-10-(propan-2-yl)cyclotetradeca-2,6,11-trien-1-one	Predicted	2
			(6E,10Z)-3,7,11-Trimethyl-14-(propan-2-yl)cyclotetradeca-6,10-diene-1,2,3,5-tetrol	Predicted	3
			(5Z,9Z)-2,6,10-Trimethyl-13-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-5,9-diene-2,4-diol	Predicted	3
			(5Z,10Z)-4,10,14-Trimethyl-7-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-5,10-diene-2,4-diol	Predicted	2
			(1E,5E,10E)-7,9-Dihydroxy-5,9-dimethyl-12-(propan-2-yl)cyclotetradeca-1,5,10-triene-1-carbaldehyde	Predicted	3
			(4E,8E,13E)-9-(Hydroxymethyl)-1,5-dimethyl-12-(propan-2-yl)cyclotetradeca-4,8,13-triene-1,3-diol	Predicted	2

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			(4Z,9Z)-4,8,14-Trimethyl-11-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-4,9-diene-2,6,8-triol	Predicted	3
			(4Z,9Z)-4,8,14-Trimethyl-11-(propan-2-yl)-15-oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol	Predicted	2
			2-[(2E,7E,11Z)-4,6-Dihydroxy-4,8,12-trimethylcyclotetradeca-2,7,11-trien-1-yl]propanoic acid	Predicted	2
			2-[(2E,7E,11Z)-4,6-Dihydroxy-4,8,12-trimethylcyclotetradeca-2,7,11-trien-1-yl]propanal	Predicted	3
			(4E,9Z,13E)-3,9,13-Trimethyl-6-(1-hydroxypropan-2-yl)cyclotetradeca-4,9,13-triene-1,3,8-triol	Predicted	3
			(4Z,8Z,13E)-1,5,9-Trimethyl-12-(1-hydroxypropan-2-yl)cyclotetradeca-4,8,13-triene-1,3,7-triol	Predicted	3
			(4E,8Z,13E)-1,5,9-Trimethyl-12-(1-hydroxypropan-2-yl)cyclotetradeca-4,8,13-triene-1,3-diol	Predicted	2
			(4E,8Z,13E)-1,5,9-Trimethyl-12-(propan-2-yl)cyclotetradeca-4,8,13-triene-1,3,6-triol	Predicted	2
			(4E,8Z,13E)-1-(Hydroxymethyl)-5,9-dimethyl-12-(propan-2-yl)cyclotetradeca-4,8,13-triene-1,3-diol	Predicted	2
		1019321-23-3	(4Z,8Z,13E)-5-(Hydroxymethyl)-1,9-dimethyl-12-(propan-2-	Predicted	2

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			yl)cyclotetradeca-4,8,13-triene-1,3-diol		
			(4Z,9Z)-4-(Hydroxymethyl)-11-(propan-2-yl)-8,14-dimethyl-15-oxabicyclo[12.1.0]pentadeca-4,9-diene-6,8-diol	Predicted	3
			(10Z)-12-(Propan-2-yl)-4,9,15-Trimethyl-5,16-dioxatricyclo[13.1.0.0.4,6]hexadec-10-ene-7,9-diol	Predicted	3
			[(1E,6E,11Z)-3,5,14-Trihydroxy-8-(propan-2-yl)-5,11-dimethylcyclotetradeca-1,6,11-trien-1-yl]methanol	Predicted	3
			(5Z,10E)-10-(Hydroxymethyl)-7-(propan-2-yl)-4,14-dimethyl-15-oxabicyclo[12.1.0]pentadeca-5,10-diene-2,4-diol	Predicted	3
			2-(2E,7Z,11E)-4,8,12-Trimethylcyclotetradeca-2,7,11-triene-4,6-diyl]propan-2-ol	Predicted	3
			Glucuronide conjugate of (4Z,8Z,13E)-12-(propan-2-yl)-1,5,9-Trimethylcyclotetradeca-4,8,13-triene-1,3-diol	Predicted	4
102-62-5	1,2,3-Propanetriol, diacetate (1,2-diacetin)	64-19-7	Acetic acid	Predicted	2
		100-78-7	Glyceryl 2-acetate	Predicted	2
		26446-35-5	2,3-dihydroxypropyl acetate	Predicted	2
			2-acetyloxy-3-hydroxypropanoic acid	Predicted	2
		473-81-4	2,3-dihydroxypropanoic acid	Predicted	2

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			(2-acetyloxy-3-oxopropyl) acetate	Predicted	2
			(2-hydroxy-3-oxopropyl) acetate	Predicted	2
			1,3-dihydroxypropan-2-yl hydrogen sulfate	Predicted	4
		1113-60-6	3-hydroxy-2-oxopropanoic acid	Predicted	3
		13831-30-6	2-acetyloxyacetic acid	Predicted	3
			2,3-diacetyloxypropanoic acid	Predicted	2
			2,3-dihydroxypropyl hydrogen sulfate	Predicted	4
			2,3-dioxopropanoic acid	Predicted	3
			2-acetyloxypropanedioic acid	Predicted	3
			3-acetyloxy-2-oxopropanoic acid	Predicted	3
		473-90-5	2-oxopropanedioic acid	Predicted	3
		5371-49-3	2-oxoethyl acetate	Predicted	3
		56-81-5	Glycerol	Predicted	3
		96-26-4	1,3-dihydroxypropan-2-one	Predicted	3
			(1-hydroxy-3-oxopropan-2-yl) acetate	Predicted	2
106-61-6	1,2,3-Propanetriol, 1-acetate (1-monoacetin)	64-19-7	Acetic acid	Known	1
		56-81-5	Glycerol	Known	1

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		13831-30-6	Acetoxyacetic acid	Predicted	3
			3-acetyloxy-2-hydroxypropanoic acid	Predicted	2
		473-81-4	2,3-dihydroxypropanoic acid	Predicted	2
			3-acetyloxy-2-oxopropanoic acid	Predicted	3
			(2-hydroxy-3-oxopropyl) acetate	Predicted	2
		107-21-1	Ethylene glycol	Predicted	3
		1113-60-6	3-hydroxy-2-oxopropanoic acid	Predicted	3
		13831-30-6	2-acetyloxyacetic acid	Predicted	3
		141-46-8	2-Hydroxyacetaldehyde	Predicted	3
		144-62-7	Oxalic acid	Predicted	3
			2,3-dihydroxypropanal	Predicted	2
			2,3-dihydroxypropyl hydrogen sulfate	Predicted	4
			2,3-dioxopropanoic acid	Predicted	3
		298-12-4	Glyoxylic Acid	Predicted	3
		473-90-5	2-oxopropanedioic acid	Predicted	3
		52737-02-7	1-Acetoxy-3-Hydroxy-Acetone	Predicted	3
		5371-49-3	2-oxoethyl acetate	Predicted	3
		79-14-1	Glycolic Acid	Predicted	3

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		80-69-3	2-hydroxypropanedioic acid	Predicted	3
		96-26-4	1,3-Dihydroxyacetone	Predicted	3
		542-59-6	2-Hydroxyethyl acetate	Predicted	3
128-37-0	Butylated hydroxytoluene	88-26-6	2,6-Di-tert-butyl-4-hydroxymethylphenol	Known	1
		1620-98-0	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	Known	1
		1421-49-4	3,5-Di-tert-butyl-4-hydroxybenzoic acid	Known	1
			Glucuronide conjugate of 2,6-di-tert-butyl-4-hydroxymethylphenol	Known	4
			Alternative glucuronide conjugate of 2,6-di-tert-butyl-4-hydroxymethylphenol	Known	4
			Glucuronide conjugate of 3,5-di-tert-butyl-4-hydroxybenzaldehyde and 3,5-di-tert-butyl-4-hydroxybenzoic acid	Known	4
			Alternative glucuronide conjugate of 3,5-di-tert-butyl-4-hydroxybenzaldehyde	Known	4
			Alternative glucuronide conjugate of 3,5-di-tert-butyl-4-hydroxybenzoic acid	Known	4
			Glucuronide conjugate of butylated hydroxytoluene	Known	4
			Glycine conjugate of 3,5-di-tert-butyl-4-hydroxybenzoic acid	Known	4

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			Aldehydes / acids formed via oxidation of the methyl groups of butylated hydroxytoluene	Known	1
			S-(3,5-Di-tert-butyl-4-hydroxybenzyl)-N-acetylcysteine	Known	4
			Alternative N-acetylcysteine conjugate of 2,6-di-tert-butyl-4-hydroxymethylphenol	Known	4
			N-Acetylcysteine conjugate of 3,5-di-tert-butyl-4-hydroxybenzaldehyde	Known	4
			N-Acetylcysteine conjugate of 3,5-di-tert-butyl-4-hydroxybenzoic acid	Known	4
			Sulfate conjugate of 2,6-di-tert-butyl-4-hydroxymethylphenol	Known	4
			Alternative sulfate conjugate of 2,6-di-tert-butyl-4-hydroxymethylphenol	Known	4
			Sulfate conjugate of 3,5-di-tert-butyl-4-hydroxybenzaldehyde	Known	4
			Sulfate conjugate of 3,5-di-tert-butyl-4-hydroxybenzoic acid	Known	4
			Butylated hydroxytoluene dimer	Known	1
		2607-52-5	BHT-quinone methide	Known	1
			2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one	Known	1
		719-22-2	2,6-Di-tert-butyl-1,4-benzoquinone	Known	1

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		16758-24-0	S-(3,5-Di-tert-butyl-4-hydroxybenzyl)-N-acetylcysteine	Predicted	4
25395-31-7	Diacetin (1,3-diacetin)	64-19-7	Acetic acid	Predicted	2
		26446-35-5	2,3-dihydroxypropyl acetate	Predicted	2
		56-81-5	Glycerol	Predicted	3
			3-acetyloxy-2-oxopropanoic acid	Predicted	2
		6946-10-7	1,3-Diacetoxyacetone	Predicted	2
		13831-30-6	Acetoxyacetic acid	Predicted	3
		473-81-4	2,3-dihydroxypropanoic acid	Predicted	2
			(2-hydroxy-3-oxopropyl) acetate	Predicted	2
			1,3-dihydroxypropan-2-yl hydrogen sulfate	Predicted	4
			(3-acetyloxy-2-sulfooxypropyl) acetate	Predicted	4
		1113-60-6	3-hydroxy-2-oxopropanoic acid	Predicted	3
		13831-30-6	2-acetyloxyacetic acid	Predicted	3
			2,3-dihydroxypropyl hydrogen sulfate	Predicted	4
			2,3-dioxopropanoic acid	Predicted	3
			2,3-dioxopropyl acetate	Predicted	3
			3-acetyloxy-2-hydroxypropanoic acid	Predicted	3

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			3-acetyloxy-2-oxopropanoic acid	Predicted	3
		473-90-5	2-oxopropanedioic acid	Predicted	3
		5371-49-3	2-oxoethyl acetate	Predicted	3
		96-26-4	1,3-Dihydroxyacetone	Predicted	3
		52737-02-7	1-acetoxy-3-hydroxyacetone	Predicted	3
28564-83-2	Pyranone		2,3,5-trihydroxy-4-oxohexanal	Predicted	3
			2-methyloxane-3,4,5-trione	Predicted	3
			5-hydroxy-2-methyloxane-3,4-dione	Predicted	3
			5-hydroxy-6-methyloxane-3,4-dione	Predicted	3
		69924-31-8	3,5-dihydroxy-2-methyloxan-4-one	Predicted	3
			<chem>OC2C(OC1COC(C)=C(O)C1=O)OC(C(O)C2O)C(O)=O</chem>	Predicted	3
			<chem>OC1=C(OCC(OS(O)(=O)=O)C1=O)C</chem>	Predicted	3
			<chem>OC1=C(OCC(=O)C1=O)C</chem>	Predicted	3
			<chem>CC1OCC(=O)C(=O)C=1O</chem>	Predicted	3
			<chem>OC1COC(C=O)=C(O)C1=O</chem>	Predicted	3
			<chem>OCC1OCC(=O)C(=O)C=1O</chem>	Predicted	3
			<chem>CC(O)C(O)C(=O)C(O)C=O</chem>	Predicted	3

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487-06-9	5,7-Dimethoxycoumarin	23053-61-4	5-Hydroxy-7-methoxycoumarin	Predicted	2
		3067-10-5	5-Methoxy-7-hydroxycoumarin	Predicted	2
		2732-18-5	5,7-dihydroxy-2Hchromen-2-one	Predicted	2
			2-(2,4,6-trihydroxyphenyl)acetaldehyde	Predicted	3
			3-(2,4,6-trihydroxyphenyl)prop-2-enoic acid	Predicted	3
		486-28-2	6-hydroxy-5,7-dimethoxychromen-2-one	Predicted	3
			5,7,8-trihydroxychromen-2-on	Predicted	3
			5,7-dimethoxy-3,4-dihydrochromen-2-one	Predicted	3
		50656-75-2	5,6-dihydroxy-7-methoxychromen-2-one	Predicted	3
		53269-07-1	7,8-dihydroxy-5-methoxychromen-2-one	Predicted	3
			6,7-dihydroxy-5-methoxychromen-2-one	Predicted	3
		61899-44-3	8-hydroxy-5,7-dimethoxychromen-2-one	Predicted	3
		64-18-6	Formic acid	Predicted	3
		50-00-0	Formaldehyde	Predicted	2
			<chem>COc1cc(O)c(C=CC(O)=O)c(O)c1</chem>	Predicted	3

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			<chem>COc1cc(O)c(C=CC(O)=O)c(OC)c1</chem>	Predicted	3
765-87-7	Cyclohexane, 1,2-dioxo-	1452767-32-6	2,4-Dihydroxycyclohexanone	Predicted	3
		533-60-8	Adipoin 2-Hydroxycyclohexanone	Predicted	2
			4-Hydroxycyclohexane-1,2-dione	Predicted	3
			3-Hydroxycyclohexane-1,2-dione	Predicted	3
			6-[(2,3-Dioxocyclohexyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	Predicted	4
		339319-34-5	2-Hydroxy-2-cyclohexene-1,4-dione	Predicted	3
			2,5-Dihydroxycyclohex-2-en-1-one	Predicted	3
			2,6-Dihydroxycyclohex-2-en-1-one	Predicted	3
			3,4,5-Trihydroxy-6-[(3-hydroxy-2-oxocyclohex-3-en-1-yl)oxy]oxane-2-carboxylic acid	Predicted	4
			2,4-Dihydroxy-2-cyclohexenone	Predicted	3
930-60-9	2-Cyclopentene-1,4-dione		6-Oxabicyclo[3.1.0]hexane-2,4-dione	Predicted	3
			4,5-Dihydroxycyclopentane-1,3-dione	Predicted	3
			2-Acetamido-3-[(2-hydroxy-3,5-dioxocyclopentyl)sulfanyl]propanoic acid	Predicted	4
		59995-49-2	4-Hydroxycyclopentenone	Predicted	3

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			2-Acetamido-3-[(2,4-dioxocyclopentyl)sulfanyl]propanoic acid	Predicted	4
			3,4,5-Trihydroxy-6-[(2-hydroxy-3,5-dioxocyclopentyl)oxy]oxane-2-carboxylic acid	Predicted	4
556-52-5	Glycidol		S-(2,3-Dihydroxypropyl) glutathione	Known	4
		23255-32-5	S-(2,3-Dihydroxypropyl) cysteine	Known	4
		23255-15-4	DHPMA [2,3-dihydroxypropyl mercapturic acid]	Known	4
			Iso-DHPMA	Known	4
		69519-13-7	$\beta$ -Chlorolactaldehyde	Known	1
		1713-85-5	$\beta$ -Chlorolactic acid	Known	1
		96-24-2	3-Monochloro propanediol (3-MCPD, also known as $\alpha$ -chlorohydrin)	Known	1
			3-Phospho- $\alpha$ -chlorohydrin	Known	1
		56-81-5	Glycerol	Known	1
		144-62-7	Oxalic acid	Known	1
		765-34-4	Glycidaldehyde	Known	1
			2-Acetamido-3-thiodiglyceryl propanoic acid	Known	4
		107-21-1	Ethylene glycol	Predicted	3

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		141-46-8	2-Hydroxyacetaldehyde	Predicted	3
		473-81-4	2,3-Dihydroxypropanoic acid	Predicted	2
		503-11-7	Glycidic acid; oxirane-2-carboxylic acid	Predicted	3
		56-82-6	Glyceraldehyde	Predicted	2
		80-69-3	Hydroxypropanedioic acid	Predicted	3
			3,4,5-Trihydroxy-6-[(oxiran-2-yl)methoxy]oxane-2-carboxylic acid [Glucuronide conjugate of (oxiran-2-yl)methanol]	Predicted	4
		96-26-4	1,3-Dihydroxypropan-2-one	Predicted	3
			6-(2,3-Dihydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid [Glucuronide conjugate of propane-1,2,3-triol]	Predicted	4
			2,3-Dihydroxypropyl hydrogen sulfate	Predicted	4
			6-[(1,3-Dihydroxypropan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid [Glucuronide conjugate of propane-1,2,3-triol]	Predicted	4
			(Oxiran-2-yl)methyl hydrogen sulfate	Predicted	4
96-24-2	1,2-Propanediol, 3-chloro	1713-85-5	$\beta$ -Chlorolactic acid	Known	1
		144-62-7	Oxalic acid	Known	1
		473-81-4	2,3-dihydroxypropanoic acid	Predicted	3

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		24423-98-1	1-chloro-3-hydroxypropan-2-one	Predicted	3
		69519-13-7	3-chloro-2-hydroxypropanal	Predicted	2
			(1-chloro-3-hydroxypropan-2-yl) hydrogen sulfate	Predicted	4
			(3-chloro-2-hydroxypropyl) hydrogen sulfate	Predicted	4
		1113-60-6	3-hydroxy-2-oxopropanoic acid	Predicted	3
		3681-17-2	3-chloro-2-oxopropanoic acid	Predicted	3
		56-81-5	Glycerol	Predicted	3
			2-acetamido-3-(2,3-dihydroxypropylsulfanyl)propanoic acid	Predicted	4
		80-69-3	2-hydroxypropanedioic acid	Predicted	3
		96-26-4	1,3-dihydroxyacetone	Predicted	3
		107-07-3	2-chloroethanol	Predicted	3
98-00-0	Furanmethanol	98-01-1	Furfural	Known	1
		88-14-2	2-Furoic acid	Known	1
		539-47-9	2-furanacrylic acid	Known	1
			2-furanacryloylglycine	Known	4
			2-Sulfoxymethylfuran	Known	4
			2-Furoic acid coenzyme A	Known	4

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		5657-19-2	2-furoylglycine	Known	4
			2-furanacryoyl coenzyme A	Known	4
			3-(furan-2-yl)prop-2-enoic acid	Known	1
			Furan-2-ylmethylhydrogen sulfate	Predicted	4
			5-hydroxy-4-oxopent-2-enal	Predicted	3
		129886-80-2	5-hydroxy-2-furanmethanol	Predicted	3
			2,6-dioxabicyclo[3.1.0]hex-3-en-3-ylmethanol	Predicted	3
			<chem>OC2C(OCC=1OC=CC=1)OC(C(O)C2O)C(O)=O</chem>	Predicted	3
98-01-1	Furfural	88-14-2	2-Furoic acid	Known	1
			2-furanacrylic acid	Known	1
			2-furanacryloylglycine	Known	4
			2-Sulfoxymethylfuran	Known	4
			2-Furoic acid coenzyme A	Known	4
		5657-19-2	2-furoylglycine	Known	4
			2-furanacryoyl coenzyme A	Known	4
			Fa-Gly-Oh	Known	4
		539-47-9	3-(2-Furyl)acrylic acid	Predicted	3

### Confidentiality Statement

*Data and information contained in this document are considered to constitute trade secrets and confidential commercial information, and the legal protections provided to such trade secrets and confidential information are hereby claimed under the applicable provisions of United States law. No part of this document may be publicly disclosed without the written consent of Philip Morris Products S.A.*

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After completion of Phase 3 of the project, identified hazards will be reported for each group of compounds (parents and metabolites) and segmented according to the quality and the reliability of data. Any collected data will be integrated into a narrative by human experts to evaluate and discuss all relevant factors associated with the data to help understand the formation of metabolites from parent compounds as well as the potential genotoxicity/carcinogenicity risk of the parent and the metabolite compounds.

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