

ECHIBIOTEB : Reunion d'avancement

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CIRSEE



conditions experimentales

✓ Paramètres d'analyse

➤ Conditions analytiques

➤ ASE

➤ Mélange Méthanol/acétone (90:10)

✓ Analyse du chromatogramme ; faire une bibliothèque de composés d'intérêt.

➤ S/N >25

➤ Similarité >700, puis examen de tous les inconnus

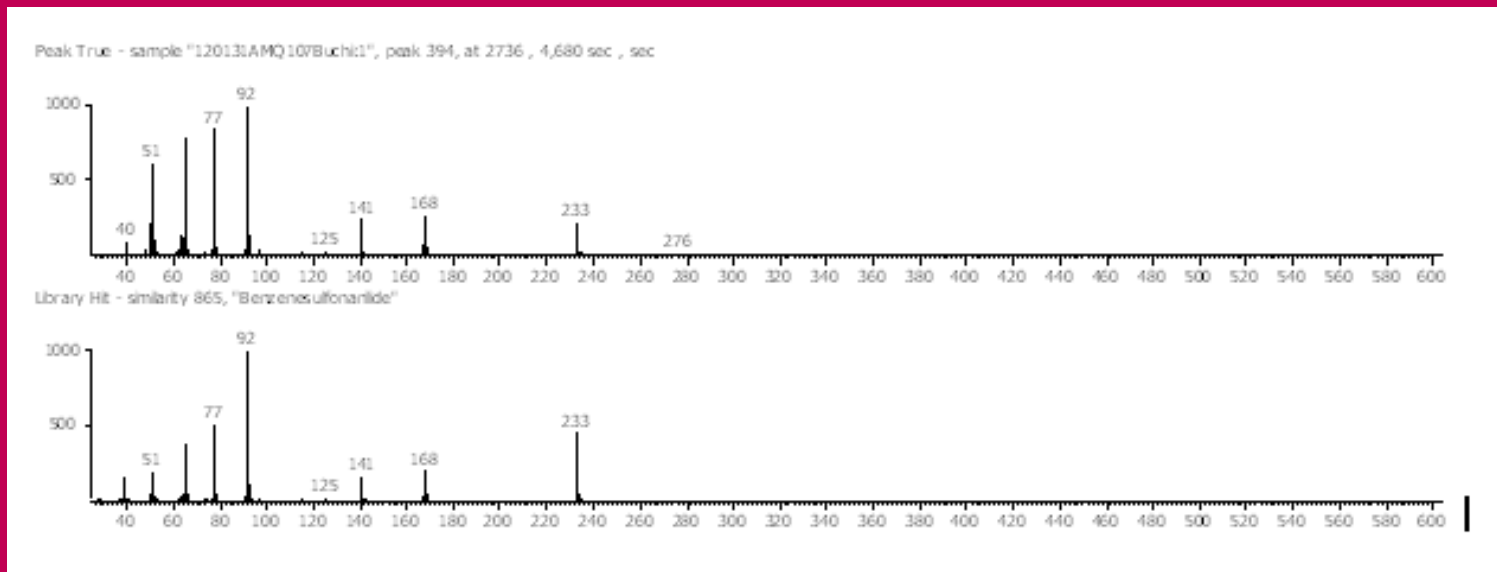
Pour un chromatogramme on vérifie environ 1500-1800 pics.

➤ Boues AMQ 69, 70 et 75

➤ Eaux AMQ 100, 101, 107, 108

Classification des spectres

- **Spectres jugés parfaits : tous les fragments spécifiques sont présents, y compris ceux de faible intensité. Identification très probable, à l'isomère près**
- **Spectres nécessitant une amélioration : manque quelques fragments ou quelques fragments en trop. Besoin d'un pic plus intense pour trancher.**



* +2,6-Diisopropyl-naphthalene	2,4-DIPN	pesticide /plant growth regulator
* 1-Methyldecahydronaphthalene	trans decaline	aromatic hydrocarbon
* 70 3-Pyridinecarboxamide	nicotinamide	coenzyme NAD / water soluble B group vitamin
* 75 2-Furancarboxaldehyde, 5-(hydroxymethyl)-	5 hydroxymethylfurfural	Antioxidant (cancerigene)
* 75 3-Acetamidofuran		Furan
* 75 5,7-Octadien-2-one, 3-acetyl-		ketone
* 75 9,12-Octadecadienoic acid, methyl ester	Linoleic acid methyl ester	unsaturated fatty acid methyl ester (FAME)
* 75 Acetic acid		carboxylic acid (organic acid)
* 75 Bumetrizole		protection contre les UV. (cosmetique)
* 75 C4 Benzene Benzene, 1-methyl-2-(1-methylethyl)-		aromatic hydrocarbon
* 75 Pyridine, 2-methyl-		Pyridine
* 75Acetamide		amide
* 75Levoglucofenone		produit de pyrolyse de cellulose
* acid, methyl ester	methyl hexanoate	carboxylic acid
* Amide 6,8-Dichlorooctanamide		amide
* benzoique acide Heptanediamide, N,N'-di-benzoyloxy-		amide???
* Chloré Benzene, (trichloromethyl)-	trichloromethylbenzene	halogenated benzene derivative
* DEHP 1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester		Plastifiant
* hexadecadiene Z-1,9-Tetradecadiene	9,10-tetradecenol	fatty alcohol
* Musk Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-		musc
* Musk tonailde galaxolide		musc
* sterol (Ergost-8(14)-en-3-ol, (3á)-)		sterol
* sterol 7-Oxo-5-cholesten-3beta-yl benzoate		sterol
* Sterol Androstan-17-one, 16,16-dimethyl-, (5à)-		sterol
* Sterol Androstan-17-one, 16,16-dimethyl-, (5à)-		sterol
* sterol Cholesta-4,6-dien-3-ol, (3á)-		sterol
* sterol Ergost-5-en-3-ol, acetate, (3á,24R)-	Campesterol acetate???	sterol
*(ethyl aniline)		precursor to indole
*??Galaxolide lactone??	CAS does not match compound	musc / metabolite of Galaxolide
*1,2-Benzothiazole		aromatic heterocyclic compound
*1-Hexanol, 2-ethyl-		alcohol
*1H-Indole, 2-methyl-		aromatic heterocyclic compound
*1H-Pyrrole, 2,3-dimethyl-		aromatic heterocyclic compound
*1H-Pyrrole, 3-methyl-		aromatic heterocyclic compound
*1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-		aromatic heterocyclic compound
*1-Methyldecahydronaphthalene		polycyclic aromatic hydrocarbon
*1-Propanol, 2,3-dichloro-, phosphate (3:1)		phosphate
*2(1H)Naphthalenone, 3,5,6,7,8,8a-hexahydro-4,8a-dimethyl-6-(1-methylethenyl)-		polycyclic ketone
*2(1H)-Naphthalenone, octahydro-8a-methyl-, cis-		polycyclic ketone
*2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	Dihydroactinidiolide	volatile terpene
*2-(Methylthio)phenyl isothiocyanate		isothiocyanate
*2,2,6,6-Tetramethyl-4-piperidone		Piperidine derivative

*2,5-Pyrrolidinedione, 3-ethyl-3-methyl-	Ethosuximide	imide	
*2-Hexanol, 2-methyl- (exemple alcool)		alcohol	
*2H-Indol-2-one, 1,3-dihydro-		aromatic heterocyclic compound	
*2H-Pyran-2-one, tetrahydro-		Ketone	
*2-Methyl-6-propylpyridine		pyridine	
*2-Nonanone		Ketone	
*2-Pentanone, 4-methoxy-4-methyl-		ketone	
*2-Piperidinone		Piperidine derivative	
*2-Propanol, 1-chloro-, phosphate (3:1)		phosphate	
*3,5-Heptadien-2-one, 6-methyl-, (E)-		ketone	
*3-Acetamidofuran		Furan	
*3-Hexanol, 3-methyl-		alcohol	
*3-Hexen-2-one		Ketone	
*3-Penten-2-one, 4-methyl-		Ketone	
*4(H)-Pyridine, N-acetyl-		Pyridine	
*4,8,12,16-Tetramethylheptadecan-4-olide	2(3H)-Furanone, dihydro-5-methyl-5-(4,8,12,16-tetramethylheptadecan-4-ylidene)-	heterocyclic compound - furanone	
*4-Iodophenylacetonitrile		nitrile	
*4-Piperidinone, 2,2,6,6-tetramethyl-	tempidon	analgesic drug	
*4-tert-Butylphenyl acetate		acetate	
*5-Hepten-2-one, 6-methyl-		Ketone	
*7 OXabicyclo 221 hept5 en 2 one		cyclic ketone ???	
*70 Benzene, (1-methoxy-1-methylethyl)-	Methyl cumyl ether	ether	
*70 Benzeneacetic acid, 3-hydroxy-	3-Hydroxyphenylacetic acid	carboxylic acid	
*70 Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-		heterocyclic compound	
*75 BHT	Butylhydroxytoluene	phenolic	
*75 1,4:3,6-Dianhydro-à-d-glucopyranose		glucose-cyclic pyranose configuration/sugar/anhydrohexose	
*75 1,6-Anhydro-à-D-glucopyranose (levoglucosan)		glucose-cyclic pyranose configuration/sugar/anhydrohexose	
*75 1H-Indole, 2-methyl-		aromatic heterocyclic compound	
*75 2(1H)-Quinolinone, 3,4-dimethyl-		pharmaceutical	
*75 2(5H)-Furanone		heterocyclic compound	
*75 2,5-Pyrrolidinedione	Butanimide	amide	
*75 2-Pentanone		ketone/additif alimentaire aromatisant	
*75 3-Pyridinecarboxamide	Nicotinamide	water soluble B group vitamin	
*75 3-Pyridinecarboxylic acid	nicotinic acid/niacin	water soluble B group vitamin	
*75 4-Piperidinone, 2,2,6,6-tetramethyl-		amine	
*75 Benzenepropanoic acid, methyl ester		ester	
*75 Cyclopropane, 1,1,2,2-tetramethyl-		branched alkane	
*75 Hexanal	hexanaldehyde	aldehyde	
*75 Indole		aromatic heterocyclic compound	
*75 Pyridine, 1-acetyl-1,2,3,4-tetrahydro-		heterocyclic compound	

*75 Toluène		Aromatic hydrocarbon	
*75 Propane, 2,2-dimethoxy-		alkylating reagent	
*7-Hexadecenoic acid, methyl ester, (Z)-		carboxylic acid methyl ester	
*9(11)-Dehydroergosterol tosylate		sterol	
*Acetamide	ethanamide	amide	
*Acetamide:2		solvant et stabilisant en synthèse orga	
*Acetic acid		carboxylic acid (organic acid)	
*Acetophenone	Phenyl methyl ketone	ketone-additif de cigarettes	
*Alcene C8		alkene	
*amide			
*Amide			
*Amide 9-Octadecenamide, (Z)-	Oleamide	amide of the fatty acid oleic acid. Endogenous substance	
*Aniline	phenylamine	primary amine	
*Aromadendrene (hemi terpène)		sesquiterpenoid hydrocarbon	
*Benzaldehyde, 4-hydroxy-		aldehyde	
*Benzene		Aromatic hydrocarbon	
*Benzene, (1-butylhexyl)-		Branched aromatic hydrocarbon	
*Benzene, (1-pentylheptyl)-		Branched aromatic hydrocarbon	
*Benzene, (1-propylnonyl)-		Branched aromatic hydrocarbon	
*Benzene, (iodomethyl)-	Benzyl iodide	benzyl hydrocarbon	
*Benzenemethanol, à,à-dimethyl-	2-Phenyl-2-propanol	phenyl alcohol	
*Benzenepropanenitrile, à-phenyl-	isothiocyanatodiphenylmethane	isothiocyanate	
*Benzoic acid, methyl ester	Methyl benzoate	benzoate/ester of benzoic acid	
*Benzophenone	diphenyl ketone	Ketone-Anti UV	
*Benzyl chloride		aromatic hydrocarbon (toluene derivative)	
*Bicyclo[4.1.0]heptane, 7-(1-methylethylidene)-		Cycloalkane	
*Boldenone		anabolic steroid/veterinary equine	
*BPA		Phenol	
*Butane		alkane	
*Butanoic acid, 2-methyl-, methyl ester	Methyl 2-methylbutyrate	carboxylic acid methyl ester	
*Butanoic acid, methyl ester	Methyl butanoate	carboxylic acid methyl ester	
*Butyrolactone	Dihydro-2(3H)-furanone	furan	
*C13 benzene(+)-N-Benzyl-alpha-methyl-N-nitrosobenzylamine	benzimidazole thiophene analogue,30	pharmaceutical product	
*Carbonic acid, dimethyl ester	Dimethyl carbonate	alkyl carbonate	
*Cetone C5	2-pentanone	ketone	
*Cholest-3-ene, (5à)-		sterol	
*Cholest-5-en-3-ol (3à)-, propanoate		sterol	
*Cholesta-4,6-dien-3-ol, (3à)-		sterol	
*Cholesta-4,6-dien-3-one		sterol	
*Cholestan-3-ol	5β-Coprostanol	stanol	

*cis-Decalin, 2-syn-methyl-	2-Methyldecahydronaphthalene	polycyclic aromatic hydrocarbon	
*Cyclohexane, (2-ethyl-1-methylbutylidene)-		cycloalkene	
*Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8-hexa	Galaxolide	musk	
*Cycloundecene, 1-methyl- (cyclo alcène)	2-Undecyne	alkyne	
*decene, (E)-		Alkene	
*Dibutyl phthalate		Plastifiant	
*dichloro benzène		Aromatic hydrocarbon	
*Diethyl Phthalate		Plastifiant	
*dimethyl naphtalène		polycyclic aromatic hydrocarbon	
*Dimethyl sulfone		sulfone	
*Dimethyl trisulfide		trisulphide	
*Dioxide soufre	sulphur dioxide	dioxide	
*Dodecanamide		amide	
*Dodecanoic acid	Lauric acid	Fatty acid (saturated)	
*Dodecanoic acid:2			
*ester d'acide Octanoic acid, methyl ester	Caprylic acid methyl ester	saturated fatty acid methyl ester (FAME)	
*Formamide, (2-acetylphenyl)-		ketone-amide	
*Furan, 2-pentyl-		furan	
*Geosmine		Taste and odour	
*Glycerin	Glycerol	hydroxyl alcohol	
*Heptadecanoic acid	margaric acid	Fatty acid (saturated)	
*Heptanoic acid	enanthic acid	Fatty acid (saturated)	
*Hexadecanal aldehydes		aldehyde	
*Hexadecane, 1,1-dimethoxy-		acetal	
*Hexane, 3,3,4,4-tetrafluoro-		fluoroalkane	
*Indan-1,3-diol monopropionate		polycyclic carboxylate	
*Indigo		Blue dye	
*m-Cymene, 5-tert-butyl-(C8 benzene)		aromatic hydrocarbon	
*Methyl propionate		ester	
*N-(3-Oxobutyl)-2-methylazetidine		ketone amine	
*naphthalene		polycyclic aromatic hydrocarbon	
*Naphthalene, 2-methoxy-		polycyclic aromatic hydrocarbon	
*Nonanal	Nonaldehyde	Aldehyde	
*Nonanamide		Amide	
*n-tertadecanoique acid	Palmitic acid	Fatty acid (saturated)	

*Oleic Acid C18	Octadecenoic acid	Fatty acid (unsaturated)	
*Oleic diethanolamide		amide of the fatty acid oleic acid. Endogenous substance	
*Pentadecanoic acid		Fatty acid (saturated)	
*Phenanthrene, tetradecahydro-		cyclic hydrocarbon	
*Phenol		Phenol	
*Phenol, 3-methoxy-2,5,6-trimethyl-		Phenol	
*Phenol, 3-methyl-	m-cresol	Phenol	
*Phthalate Phthalic acid, neopentyl octyl ester		Phthalate ester	
*Phthalate Phthalic acid, neopentyl octyl ester			
*Pregnane		Steroid hormone	
*Propane, 2,2-dimethoxy-	2,2-dimethoxypropane	acetal	
*p-Xylene		Volatile hydrocarbon	
*Pyrene		polycyclic aromatic hydrocarbon	
*Pyrene, hexadecahydro-	Perhydropyrene	hydrocarbon	
*Pyridine, 2,3,5-trimethyl-		Pyridine	
*Pyridine, 2,3-dimethyl-		Pyridine	
*Pyridine, 2-ethyl-4,6-dimethyl-		Pyridine	
*Pyridine, 2-methyl-		Pyridine	
*Pyridine, 3,5-dimethyl-		Pyridine	
*Pyrимidine, 2-methyl-		branched pyrimidine	
*Pyrrole, 1-methyl-3-(1,1-dimethylethyl)-		branched heterocyclic aromatic hydrocarbon	
*Silane, dimethoxydimethyl-		Silane	
*Silane, tetra(methoxy)-		Silane	
*Sterol Cholestan-3 α -ol acetate	5 β -Cholest-3-ene	Cholestene	
*Sterol Cholestan-3 α -ol acetate			
*Tetradecanoic acid, 12-methyl-, methyl ester	12-methyl Myristic acid methyl ester	saturated branched fatty acid methyl ester (FAME)	
*Tetrasulfide, dimethyl	Dimethyl tetrasulphide	tetrasulphide	
*Thiocyanic acid, methyl ester	methyl thiocyanate	alkyl thiocyanate	
*Thiophene, 2,4-dimethyl-		heterocyclic branched/thiophene	
*Toluène	methylbenzene	Volatile hydrocarbon	
*Triclosan		fongicide et bactéricide	
*Tridecanoic acid	Tridecylic acid	Fatty acid (saturated)	
*tridecene (c13)		isomeric olefin hydrocarbon	
*Vitamin E		fat-soluble vitamin/anti oxidant	
*Vitamin E acetate		acetate of vitamin E	

Suite du screening

- **Examen d'échantillons supplémentaires (3 boues, 8 eaux)**
- **Nettoyer la liste ci-dessus pour faire apparaître les composés les plus intéressants**
- **Etablir liste similaire pour l'eau**
- **Sélectionner liste restreinte (30-50) pour travail plus quantitatif.**