Analysis of Water by Time of Flight Mass Spectrometry

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Abstract

In this experiment we took water samples from the bay near the battleship Texas to determine the presence of contaminants in the water. We employed an Agilent Time of Flight mass spectrometer to identify these contaminants utilizing accurate mass

Introduction

The Battleship Texas was launched in 1912. It was the last of the Dreadnaught class of ships. The Texas served in both World Wars I and II. She is now located at the San Joaquin battle site memorial. She has been moored in this location since 1980.

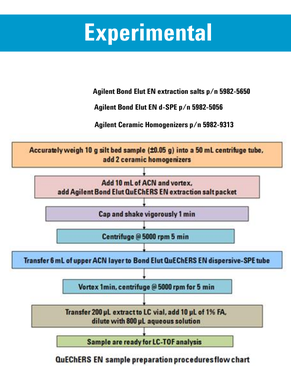
Accurate Mass provides positive identification for compounds of interest by determining the mass to the 4th decimal place rather than just unit mass. This level of mass accuracy is obtained because of the high resolution of the instrument.

To prepare the water samples taken directly from the bay, we used Agilent QuEChERS. Not only does this type of extraction help to keep the instrument clean, it more importantly helps to eliminate ion suppression.

The Agilent 1290 UHPLC was used to introduce the samples into the Time of Flight mass spectrometer. Chromatographic separation with the 1290 facilitates fast, high resolution using Agilent sub 2 micron packing material.

The TOF data give us the ability to search databases to find compounds matches. If a compound is not in a database, we are able to use the ring and double bond information, plus the formula to propose identification such as we did with the Benzaldehyde.

Experimental



QuEChERS EN sample preparation procedures flow chart

HPLC Parameters

Mobile Phase A H2O + 0.1% Formic Acid
Mobile Phase B MeOH +)1% Formic Acid
Flow 0.5 ml/min
Gradient 5% B to 95% B over 10 minutes
Injection volume 1 ul with a 60 sec ACN/IPA/H2O wash
Column temperature 40 degrees C
Diode Array Detector 254nm with a bandwidth off 4 and Reference off
Flow cell 10mmpath 1.8 ul volume collecting all spectra

Column Zorbax Eclipse Plus 2.1 x 100mm 1.8 ul particle size

Agilent 1290 UHPLC system

Time of Flight Parameters

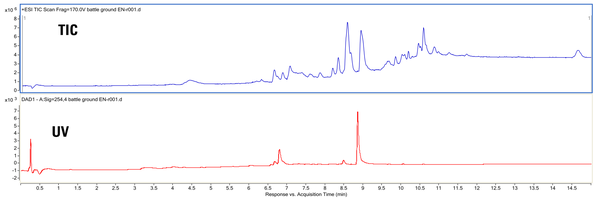
Positive mode
Agilent Jet Stream
Gas temperature 350 degrees C
Drying gas 10 l/min
Nebulizer 60 degrees C
Sheath gas temperature 350 degrees
Sheath gas flow 11 l/min
V cap 3500
Mass range 110 to 1100
Reference Masses 121.050873 & 922.009798

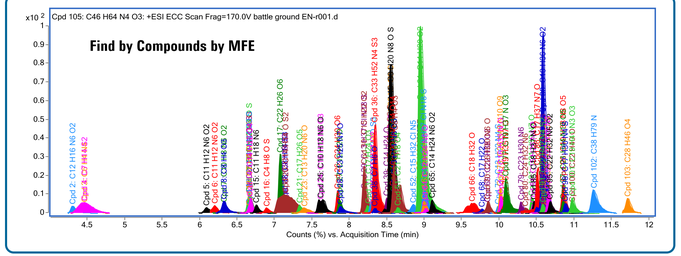
Software

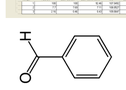
Mass Hunter Data Acquisition
Mass Hunter Qualitative Analysis
Molecular Feature Extractor
Personal Compound Data Library

G6230AA Accurate Mass TOF LC/MS
Agilent Jet Stream

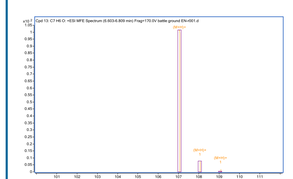
Results and Discussion





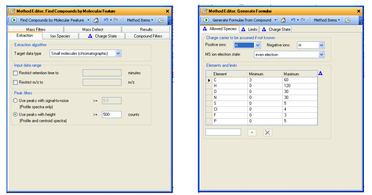


Benzaldehyde

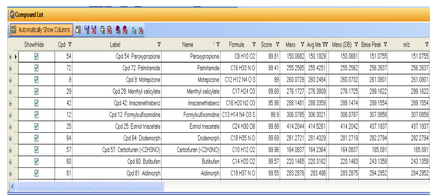


Isotopic Fidelity of Benzaldehyde

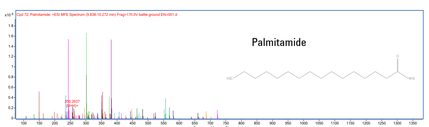
You choose your possible elements in Molecular Formula Generator



Then running Molecular Formula Generator the compound Formulas and the match score will be displayed



The results from a database search. This shows the structure and the isotopic pattern of each identified compound



Compounds found by searches of METLIN, Agilent Tox and Forensic databases

Palmitamide	C16 H33 N O	98.92	255.2565
Motapizone	C12 H12 N4 O S	94.26	260.0728
Formylsulfisomidine	C13 H14 N4 O3 S	95.49	306.0785
Butibufen	C14 H20 O2	98.68	220.1466
Saccharopine	C11 H20 N2 O6	81.19	276.1327
Purine	C5 H4 N4	52.56	120.0436
Oleamide	C18 H35 N O	99.09	281.2721
N-Hexadecyl-L-hydroxyproline	C21 H41 N O3	85.13	355.3083
N-(3-Indolylacetyl)-L-isoleucine	C16 H20 N2 O3	79.15	288.148
methyl 8-[2-(2-formyl-vinyl)-3-hydroxy-5-oxo-cyclopentyl]-octanoate	C17 H26 O5	91.27	310.1782
Met Trp Phe	C25 H30 N4 O4 S	92.93	482.1983
Met His Lys	C17 H30 N6 O4 S	90.38	414.2045
Lys Cys His	C15 H26 N6 O4 S	90.94	386.1733
hydrocinnamic acid	C9 H10 O2	95.91	150.0682
GPA(10:0/10:0)	C23 H45 O8 P	83.37	480.2842
cyclandelate	C17 H24 O3	84.93	276.173
5,8-tetradecadienal	C14 H24 O	99.32	208.1827
4,7,10,13-hexadecatetraenoic acid	C16 H24 O2	86.33	248.1777
3E,13Z-octadecadien-1-ol	C18 H34 O	98.82	266.2608
2-Phenylbutyric acid	C10 H12 O2	47.6	164.0837
20-oxo-heneicosanoic acid	C21 H40 O3	84.15	340.2972
10,10-dimethyl-5Z,8Z,11Z-eicosatrienoic acid	C22 H38 O2	95.48	334.2872

Conclusion

Utilizing Agilent's Time of Flight accurate mass, high resolution, superior isotopic fidelity and the unique features of Mass Hunter software, such as Molecular Feature Extractor and Molecular Formula Generator, we were able to identify over 100 compounds found in the samples.