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# Elemental analysis applications compendium

Your samples, our experience





## Introduction

To understand the elemental composition of a sample and draw conclusion on product quality, Elemental Analysis (EA) utilizes carbon, hydrogen, nitrogen, sulfur and oxygen, which help determine the structure of an unknown compound, as well as to evaluate the structure and purity of a synthesized compound.

Being approved by official methods, ASTM among others, Elemental Analysis is the technique of choice for the quantitative determination, by oxidation and pyrolysis, of CHNS/O content in samples. When coupled to detectors (for example a Flame Photometric Detector (FPD) or to an Isotope Ratio Mass Spectrometry) Elemental Analysis enables to access a wealth of information from a sample.

The analytical technique provides reliable analysis of elemental content for a variety of application fields:

- **Organic chemistry and pharmaceuticals:** for quality control analysis of fine chemicals, organometallic compounds, refractory compounds, food supplements, halogen-compounds etc.
- **Petrochemistry and energy:** for the characterization of refined fuels, biofuels, biomass fuel, gasoline, coal, pet-coke, and lubricants.
- **Environmental:** for the determination of elemental content of compost, water, particulate matter in water and air, waste material.
- Agronomy and marine science: for the characterization of soil, leaves, plants, fertilizers, sediments, rocks, particulate matter in water, water, algae, plankton etc.
- **Material characterization:** for quality assessment of rubbers, polymers, plastic, paper, carbon fiber, graphene, lubricants, metals etc.
- Food and feed quality: for the analysis of protein content for compliance with labeling and other food and feed manufacturers requirements.

This Elemental Analysis Compendium will guide you through CHNS/O analysis performed using the Thermo Scientific<sup>™</sup> Flash*Smart*<sup>™</sup> Elemental Analyzer, which helps laboratories in their quantitative determinations of samples in a variety of application fields.

### Application contents

- 1 Organic chemistry and pharmaceuticals
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### Chapter 1 Organic chemistry and pharmaceuticals

The chemical characterization of organic compounds plays a very important role in pharmaceuticals synthesis, separation, purification and structural identification, both for research and quality control purposes. The elemental composition of the organic compound is periodically monitored because the raw materials are required to undergo rigorous quality control assessment. Therefore, quality control processes in pharmaceutical applications need to be supported by a technique ensuring compliance with existing regulations, while being automated and providing fast and accurate results.

This chapter presents applications on pharmaceutical samples performed with the Thermo Scientific<sup>™</sup> Flash*Smart*<sup>™</sup> Elemental Analyzer, which is based on the dynamic combustion method (modified Dumas method).

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- AN42162 CHN determination in fluorine-compounds
- AN42192 CHNS determination of pharmaceutical products
- AN42266 Accurate and precise sulfur analysis

- AN42306 CHNS/O characterization of pharmaceutical products
- AN42346 CHNS determination of organic liquids and fuels

#### Chapter 2 Petrochemistry and energy

Elemental determinations are important in Quality Assurance and Quality Control (QA/QC) testing for the petrochemical and energy sector. It quantifies the CHNS/O content for the characterization of the products and their properties (such as providing the data in compliance with Heat Values and the  $CO_2$  Emission Trade).

Elemental Analysis can be used with solid, liquid, volatile, viscous and gas samples that must be carefully monitored for their quality and for their commercial value.

For example, nitrogen-compounds are used as additives in lubricants and petrochemical companies need to evaluate these additives so they can assess quality of the final products.

The ASTM (American Standard and Testing Methods) define methods and guidelines for the analysis of petrochemical and lubricant products.

This chapter presents applications of the Flash*Smart* Elemental Analyzer for the CHNS/O analysis in petrochemical and lubricants products for quality controls and monitoring purposes. For Trace Sulfur analysis the Flash*Smart* EA can be coupled to Flame Photometric Detector (FPD).

The dedicated Eager*Smart* Data Handling Software calculates automatically the Heat Values and the CO<sub>2</sub> Emission Trade.



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- AN42152 CHNS/O determination of diesel and bio-diesel
- AN42182 CHNS/O determination in carbon
- AN42216 CHNS determination of lubricants and oils
- AN42218: CHNS/O determination in coals
- AN42222 Total oxygen determination in gasoline
- AN42238 CHNS/O characterization of carbon black compliance with ASTM D5373 Method
- AN42251 CHNS/O characterization of biomass and bio-fuels

- AN42253 CHN characterization of coals using argon as carrier gas
- AN42263 fully automated double channel analysis for petrochemical applications
- AN42266 Accurate and precise sulfur analysis
- AN42346 CHNS determination of organic liquids and fuels
- AN42485 Nitrogen determination of lubricants using a single reactor
- TN42287 Nitrogen determination of lubricants with different pure organic calibration standards

#### Chapter 3 Environmental

In recent years the demand for the characterization of environmental samples has increased.

Among the applications, the detection of pollution markers (for example with the quantification of sulfur in leaves) and the characterization of compost (for the definition of its use) are of great monitoring interest.

For the evaluation of the Heat Values of the alternative energy sources and composts and for the evaluation of the  $CO_2$  Emission Trade, laboratories need an automated system, allowing direct comparisons.

Environmental laboratories need to analyze materials with percentage and trace level (ppm) concentrations with an automated analytical approach, enabling also accurate measurements and routine analysis.

This chapter presents applications on environmental samples performed with the Thermo Scientific Flash*Smart* Elemental Analyzer.





- AN42197 CHNS/O characterization of compost
- AN42202 Nitrogen determination in soils and plants using argon as carrier gas
- AN42219 NC determination in soils and plants using argon as carrier gas
- AN42244 NC determination of soils and plants with a single reactor

- AN42252 CHN characterization of soils and plants using argon as carrier gas
- AN42266 Accurate and precise sulfur analysis
- AN42305 CHNS/O characterization of particulate matter in water and air (filters)
- AN42342 N, NC, CHNS/O and TOC characterization of sewage sludge

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#### Chapter 4 Agronomy and marine science

Elemental characterization for agricultural purposes give information useful for determining agronomy management plans. The determination of nitrogen and carbon, Total Carbon, Total Organic Carbon (TOC) and sulfur enables to characterize soils, leaves, plants, crops and other materials and to set up fertilization plans.

Nitrogen, carbon and TOC determinations give also information on the deficiency or excess of nutritional elements in soils and plants.

Sulfur is an essential component of living matter and the lack of sulfur in vegetables, for example, affects their growth and the quality of proteins through the synthesis of amino acids such as methionine, cysteine and cystine, and in the synthesis of vitamins.

Similarly, carbon, hydrogen, nitrogen and sulfur are basic building blocks that are analyzed for marine science. Fluctuations in the concentration ratio and/or content of carbon, nitrogen and sulfur define the origin of marine samples, the depositional environment and the diagenetic alteration of the source materials. The typical materials studied in marine science are sediments, plankton and algae. This chapter presents applications on agricultural and marine samples performed with the Thermo Scientific Flash*Smart* Elemental Analyzer.



- AN42198 NCS characterization of fertilizers
- AN42202 Nitrogen determination in soils and plants using argon as carrier gas
- AN42219 NC determination in soils and plants using argon as carrier gas
- AN42187 Low sulfur determination in geological and agronomy samples
- AN42244 NC determination of soils and plants with a single reactor
- AN42252 CHN characterization of soils and plants using argon as carrier gas

- AN42264 High accuracy of nitrogen, carbon and sulfur analysis for agronomy applications
- AN42266 Accurate and precise sulfur analysis
- AN42304 CHNS/O determination of marine samples
- AN42305 CHNS/O characterization of particulate matter in water and air (filters)
- AN42499 CHNS/O characterization of solid and liquid fertilizers
- AN42515 CHNS characterization of rocks
- TN42285 NC determination of high weight soil samples by single and double reactor

#### Chapter 5 Material characterization

The development and production of materials require rigorous quality control of raw products, additives, stabilizers. For the QA/QC of the material itself and of the intermediate and final products, nitrogen, carbon, hydrogen, sulfur and oxygen are analyzed. For example, for plastics and polymers the determination of nitrogen and sulfur is crucial to identify the polymerization reaction. For carbon fibers and graphene, carbon presence is important to define the quality of the final product.

Elemental Analysis is used for several applications in the R&D and production of new materials because the percentage of the elemental content allows the final use of the materials to be predicted.

In many applications, the manufacturers need an analytical solution providing accurate measurements and routine robust analysis.

This Elemental Analysis Compendium chapter presents examples of analysis on different materials performed with the Thermo Scientific Flash*Smart* Elemental Analyzer.

- AN42183 CHNS/O characterization of rubbers and tires
- AN42230 CHNS/O characterization of polymers and plastics
- AN42231 NCS characterization of paper
- AN42216 CHNS determination of lubricants and oils
- AN42266 Accurate and precise sulfur analysis

- AN42278 CHN determination of graphene
- AN42279 CHNS determination of carbon fibers
- AN42485 Nitrogen determination of lubricants using a single reactor
- TN42287 Nitrogen determination of lubricants with different pure organic calibration standards

#### Chapter 6 Food and animal feed

The nutritional composition of food and animal feed is regularly analyzed by manufacturers to comply with official regulations.

Official Methods regarding processed and raw products require a series of tests aimed at determining product quality and at preventing fraud. One of the tests is the determination of protein content in food and animal feed. The exact determination of the protein content, through the determination of nitrogen content, is fundamental to define the nutritional features of animal feed and for the safety of final food products intended for human consumption.Official regulations establish the protein content and labeling requirements, which enable consumers to perform price and quality comparisons based on % protein declarations.

The Kjeldahl Method is the classical technique for this analysis, even though it is recognized not to meet modern laboratories requirements. For this reason, the use of an automated technique allowing fast analysis with excellent reproducibility, which avoids the need of handling toxic chemicals, is required. An alternative to the classical Kjeldahl method is the Dumas (combustion) method, which is comparatively quicker, cheaper, easier to perform, safer and more environmental friendly. The Dumas method is approved by AACC, AOAC, AOCS, ASBC, IDF, IFFO and ISO.

This chapter presents applications on Food and Animal Feed samples performed with the Thermo Scientific Flash*Smart* Elemental Analyzer, which is based on the dynamic combustion method (modified Dumas method).



- AN42157 Nitrogen/Protein determination of cereals and beans
- AN42186 Sulfur determination in food
- AN42196 CHNS determination of food and animal feed
- AN42200 Nitrogen determination of high-protein content in animal feed using argon as carrier gas
- AN42201 Nitrogen/Protein determination of flours
- AN42217 NC determination in flours using argon as carrier gas
- AN42242 Nitrogen/Protein determination of dairy products
- AN42243 Nitrogen determination of high-protein content in food and animal feed
- AN42255 Nitrogen/Protein determination of infant food using argon as carrier gas
- AN42262 Nitrogen/Protein determination in food and animal feed by combustion method (Dumas)
- AN42266 Accurate and precise sulfur analysis
- AN42490 Nitrogen and simultaneous CHNS determination of Indian tea

- AN42297 Nitrogen/Protein and sulfur determination in soy and fish Asian sauces
- AN42303 Nitrogen/Protein and sulfur determination of Dried Baker's Yeast
- AN42336 Nitrogen/Protein and CHNS determination of insect-based food and animal feed
- AN42341 Nitrogen/Protein and CHNS determination of spirulina algae
- AN42478 Nitrogen/Protein by single reactor and sulfur determination of food and animal feed
- AN42481 Nitrogen/Protein and sulfur determination in brewery industry
- AN42497 Nitrogen/Protein determination of animal feed reference materials
- AN42514 Nitrogen/Protein determination in starch
- TN42504 High productivity Nitrogen/Protein and CHNS analysis with MultiValve Control Module

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#### Questions and answers

SN42260 What do "Flash" and "Smart" mean in the Thermo Scientific Flash*Smart* Analyzer?

SN42259 Why the gas chromatographic separation method used in the Thermo Scientific Flash*Smart* Elemental Analyzer is the most reliable for elemental analysis?

SN42269 How can you reduce helium consumption on the Thermo Scientific Flash*Smart* Elemental Analyzer?

SN42238 How can the oxygen injection be optimized in the Thermo Scientific Flash*Smart* Elemental Analyzer?

SN42283 How Nitrogen/Protein determination performed with Elemental Analysis can be used for quality and labeling purposes of food and animal feed?

SN42237 Which official methods are fulfilled by the FlashSmart Elemental Analyzer?

SN42296 What software features enable high productivity in elemental analysis?

SN42335 How can you validate your Elemental Analyzer?

SN42344 How can I get more from my EA and EA-IRMS systems?

SN000181 How flexible is Flash*Smart* Elemental Analyzer to meet your growing analytical needs?

SN42282 How many configurations are available on the Flash EA Series?

How to increase productivity of your elemental analysis? TN42256 High productivity of CHNS/O analysis TN42257 High productivity of CHN/O analysis TN42265 High productivity of CHNS/CHNS analysis TN42504 High productivity of Nitrogen/Protein analysis

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#### Conclusions

Elemental Analysis is a very versatile technique, which is able to deal with different samples and applications. Whether you are focused on QA/QC of lubricants or petrochemical products or N/Protein analysis of food and feed samples or you need to determine the quality of a material or pharmaceutical product, Elemental Analysis enables you to characterize your samples through the quantification of carbon, hydrogen, nitrogen, sulfur and oxygen.

Being recognized by Official Methods, Elemental Analysis enables compliant analyses in a variety of applications.

The Flash*Smart* EA enables your laboratory to meet existing regulations and have the flexibility of dealing with growing analytical demands.

Utilizing the Dumas (combustion) method, it offers efficiency and features that a modern lab requires, meeting demand on usability and throughput.

Your sample, our experience.

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