

Antec Industrieweg 12 2382 NV Zoeterwoude The Netherlands

ROXY EC system

Installation requirements

210.7050, Edition 4, 2012





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Symbols

The following pictogram is used in this installation guide:



Caution, calls attention to a procedure, which, if not correctly executed, could result in damage to the equipment or personal injury. Do not proceed beyond a "CAUTION" sign until the indicated conditions are fully understood and met.

General precautions



LC equipments should be used by trained laboratory personnel only. Use proper eye and skin protection when working with solvents. Additional safety requirements or protection may be necessary depending on the chemicals used in combination with this equipment. Make sure that you understand the hazards associated with the chemicals used and take appropriate measures with regards to safety and protection.

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General information

In this document the requirements are listed for the installation of the $ROXY^{TM}$ EC system (p/n 210.0070) for use upfront mass spectrometry (MS). The $ROXY^{TM}$ EC system hyphenated with electrospray (ESI)-MS is a dedicated system to simulate oxidative metabolism of drugs and xenobiotics.

This document summarizes all relevant conditions, chemicals and consumables that are required at the customer site for a successful installation of the system. Furthermore, the guideline for a standard system check based on the oxidation of Amodiaquin (for application details please read the application note nr. 210.004: "Oxidative Metabolism of Amodiaquin using ROXY[™] EC system") is included in this document.

This document should be send to the customer well in advance of the installation date in order to be able to take the necessary actions. The customer must arrange these necessities before the start of the installation.

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Fig. 1. Photograph of the ROXY EC system.

Computer requirements

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Hardware

The minimal PC hardware requirements for the installation of the ROXYTM EC system in combination with the DialogueTM for ROXY software are listed in the table below:

Operating System	Microsoft Windows XP/2000/Vista/7 [#]
USB	2 free USB port (USB 2.0)*
Drives	CD-ROM or DVD-ROM
Adobe PDF reader	To read electronic versions of the user ma- nuals
Internet explorer 7.0 or other + internet connection	Accessing the Antec support websites, for up- dates of software, manuals, troubleshooting.
MS Office (Excel)*	Analysis of Dialogue data in Excel

[#] An US / European Microsoft[®] Windows[™] version is recommended. The Windows operating system should be updated with the latest Service Packs (SP).

* Necessary for the installation of USB-RS232 converter (with two com ports for syringe pump and ROXY[™] Potentiostat) and license dongle.

Installation precautions

Installation can only be performed by PC users with administrator rights. No screensavers, (USB) hibernate mode, or hard disk shut down (energy saving) should be active.

Mass spectrometer requirements

The mass spectrometer (MS) can be controlled by the ROXY EC or EC/LC system by contact-closure. The end-user should make sure that all required preparations with respect to the MS are accomplished:

An open-ended IO cable or screw terminal connector should be available on the MS side to connect the ROXY trigger cable.

The MS software should be configured in slave mode to be able to start acquisition controlled via contact closure by means of the Dialogue software.

ROXY EC system should be connected via grounded connection.



Conntact your MS manufacturer for details how to establish contactclosure trigger connection and the grounded connection with the ion source.

Laboratory facilities

For the preparation of the LC solutions and standards, access to the proper facilities is a prerequisite (microbalance, pH meter and relevant pH standards, analytical pipettes, pipette tips, tubes, glassware such as measuring cylinders, etc.).

System consumables

Apart from the items provided with the ReactorCell kit (e.g. polishing slurry and polishing disk), the following consumables are necessary for cleaning of a ReactorCell with GC electrode:

- Soft paper tissue.
- A squeeze bottle with deionized water.
- A squeeze bottle with ethanol/methanol.

Chemicals

General

- All relevant chemicals should be available at the lab at the moment of installation to make the mobile phase and the standards, *etc*.
- For EC/MS only chemicals of sufficient specific quality should be used. Note that chemicals that are highly pure (for UV detection) may contain electrochemically active impurities! For example, HPLC grade water (for UV detection) is not recommended for EC detection; use deionized water with a resistivity of 18 megohm-cm.
- See the appendix for detailed descriptions of the chemicals that are use in the Antec R&D laboratory.

Solutions

At the start of the installation the following solutions are necessary. These solutions should be arranged/prepared in advance by the customer.

- About 250mL of mobile phase (20mM ammonium formate (pH 7.4 adjusted with ammonium hydroxide) in 50% acetonitrile)
- The standards solution (10µM Amodiaquin), diluted from stock solutions (1mM) in mobile phase)

The solution of amodiaquin can be stored for longer time in the 4°C.

Table 1. Composition of the stock solutions used for analysis of Amodiaquin.

Stock solution	Composition	Remarks
Mobile phase	20mM ammonium formate (final concentration) 50% acetonitrile pH 7.4	For analysis of amodiaquin
1mM Amodiaquin (stock solution)	Amodiaquin Mobile phase	Should be prepared direct- ly before analysis

The standard should be diluted in the mobile phase to the following concentration:

• 10µM Amodiaquin



The solutions of amodiaquin in ammonium formate and acetonitrile can be used for evaluation of both the ReactorCell and μ -PrepCell.

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APPENDIX

A list of chemicals is shown below as a guideline for the purchase of chemicals at the customer site. The listed brands/purities are not necessarily the best chemicals, but the applications were evaluated/developed at the Antec R&D laboratory using these specific brands/purities. If for any reason alternative chemicals need to be purchased use the following guidelines:

- The chemicals should have at least the same purity or better then the chemicals listed in the table below
- Do not purchase ultra dry grade or anhydrous chemicals

Table 2. Brands and purities of chemicals used for application development at Antec.

Component	Purity	Brand	Order no:	Mw	kg/L
Amodiaquin dihydro- chloride dihydrate		Fluka	A2799	464.81	
Ammonium formate	Puriss p.a., for mass spectroscopy	Fluka	70221-25G-F	63.06	
Acetonitrile	HPLC grade, 99.9%	Acros	268260025	41.05	D:0.781
Ammonium hydroxide	Puriss p.a., additive for LC/MS	Fluka	44273	35.05	D:0.9
Water	TOC <10ppb and deionis	sed, resistiv	ity >18 MOhm-ci	m (Barnstea	ad Easypure II)

Manufacturers

Fluka	http://www.sigmaaldrich.com
Fisher Scientific	http://www.fishersci.com
Barnstead	http://www.thermoscientific.com