**Equipment (Sciex X5OOR QTOF)**

completed by responsible coordinator of equipment

**Equipment: Sciex X500R QTOF HR mass spectrometer**

**No. of Equipment:** TUL14 (pod tímto číslem bude přístroj zařazen)

**Responsible coordinator: doc. RNDr. Michal Řezanka**

**Name of Institution: Technická univerzita v Liberci, Ústav pro nanomateriály, pokročilé technologie a inovace**

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**Equipment Description**

***A QTOF type HRMS mass spectrometer coupled to an HPLC chromatograph. Suitable for screening and trace determination of pollutants (e. g. pesticides) and their metabolites, pharmaceuticals and biomolecules. Use of libraries and in silico fragmentation software allows for the identification of unknowns.***

**Specification of expertise relevant to NanoEnviCz workpackages:**

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| --- |
| **WP3 SYNTHESIS AND DESIGN OF NEW MULTIFUNCTIONAL NANOMATERIALS FOR ENVIRONMENT PROTECTION** |
| Conceptually new nanostructured materials with the potential for application in innovative technologies | ✓ |
| Computer aided nanomaterials design | ✓ |
| Low dimensional materials and their composites (carbon dots, nanotubes, graphene derivatives) | 🗶 |
| Nanofibers | ✓ |
| Magnetic hybrids | 🗶 |
| Metal and metal oxide NPs | 🗶 |
| Redox active nanomaterials | ✓ |
| Nanomaterials for biomedical applications | ✓ |
|  |
| **WP4 HETEROGENEOUS CATALYSIS FOR ENVIRONMENTAL PROTECTION** |
| Nanomaterials for catalytic degradation of pollutants in water, soil and air | ✓ |
| Nanostructured heterogeneous catalysts for abatement of pollutants from industrial processes and automotive transport | ✓ |
| New “clean” catalytic processes for chemical production | ✓ |
|  |
| **WP5 NOVEL NANOMATERIALS AND TECHNOLOGIES FOR SUSTAINABLE PRODUCTION** |
| Processes and technology for sustainable energy and chemical production | ✓ |
| Catalytic processes for transformation of natural gas to liquids | ✓ |
| Nanomaterials for utilization of renewables; Magnetically separable green catalysts | ✓ |
|  |
| **WP6 EFFECTIVE PHOTOCATALYTIC TECHNOLOGIES** |
| Mastering nanomaterials for photocatalysis | ✓ |
| Effective photocatalytic processes | ✓ |
| Photovoltaic paints | 🗶 |
| Functional surfaces for environmental protection | ✓ |
| Hybrid materials combining photocatalysts and heterogeneous catalysts | ✓ |
| Thin photocatalytic films for direct solar splitting of water | 🗶 |
|  |
| **WP7 NANOTECHNOLOGY FOR TRAPPING AND CHEMICAL DEGRADATION OF POLLUTANTS** |
| Nanomaterials for sorption | ✓ |
| Natural based nanomaterials produced by “green” technology | ✓ |
| Reactive sorbents for degradation of pesticides and highly toxic agents | ✓ |
| Degradation of chemical warfare agents | ✓ |
| Analysis of filtering capabilities of nanomaterials | ✓ |
| Elimination of radionuclides contamination | 🗶 |
| Modified nanofiber filters; Advanced antimicrobial filters/membranes | ✓ |
| Nanoiron for groundwater and waste water treatment | ✓ |
| Nano-trapping of heavy metals | 🗶 |
|  |
| **WP8 SENSING AND MONITORING OF POLLUTANTS** |
| Efficient sensing of pollutants | ✓ |
| Biosensing by new devises | 🗶 |
| Application of new sensors in monitoring of pollutants | ✓ |
| Magnetic sensors; Magnetically assisted SERS sensors  | 🗶 |
| Advanced electrochemical sensors | 🗶 |
| Graphene based nanosensors | 🗶 |
|  |
| **WP9 TOXICITY AND RISKS OF NANOMATERIALS** |
| Health risks  | ✓ |
| Environmental risks | ✓ |
| „In vitro“ and „in vivo“ toxicity tests – cytotoxicity, genotoxicity, interactions with membrane | 🗶 |
| RNA gene expression changes and protein expression changes | ✓ |
| Complete eco/aquatoxicity ecotoxicity evaluation | 🗶 |
| Toxicity against bacteria and fungi | ✓ |

**Detailed description of expertise**

**Please, specify the main research topics connected with equipment**:

**Quantifying the release of pharmaceuticals from nanofibrous materials used in medical applications. Identification of degradation products of active ingredients formed during the spinning process. Determining the efficacy of catalysts, photocatalyst and sorbents for the removal of pollutants. Characterisation of precursors to hybrid nanomaterials.**

**Please, specify the secondary research topics connected with equipment**:

**Estimation of the efficacy of catalysts and identification of side products. Identification of markers indicating stress caused by nanoparticle toxicity.**

**Keywords describing research area:**

HPLC, MS, HRMS, API, Nanofibers, Pollutant, Pesticide, Catalyst, Degradation, Marker, Toxicity

**Competence**

**Relevance for applied and industrial research:**

The instrument is suitable for the trace determination of pollutants enabling the determination of efficacy of catalysts, oxidants sorbents and other treatment processes for their removal. It can also be used for the accurate of precursors and products in organic syntheses.

**Relevance for fundamental studies:**

The instrument can be used in metabolomic studies or in elucidation of the degradation mechanisms of pollutants.

**Comments**