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Workflow for the identification of 'unknown' substances in feed and food

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Background

Regularly biological effects or instrumental signals are observed in food or feed samples that cannot be explained by the presence of a chemical substance that is included in targeted analysis. It is desirable to further identify those signals or effects, thus facilitating risk-based monitoring. This poster presents a workflow for identification of unknown compounds responsible for observed effects or signals. The workflow is based on multi-disciplinary approaches. These include analytical chemistry (mass spectrometry, NMR), biochemistry (biosensors, DNA analysis), physical chemistry (microscopy) and knowledge of bioactive compounds. The workflow was assessed using an artificial (left) and a real case (right).

Workflow

The starting point of the search for 'unknowns' in the workflow can be threefold: (a) an observed effect in a bioassay and (b) a case from the field, for example negative health effects, (c) a suspect signal in a chemical analysis, e.g. high resolution mass spectrometry. Every case starts with a case manager, assembling a multidisciplinary team to solve the case. An interactive scheme, of which figure 1 shows a 2D impression, helps the team to make decisions and provides information. Every button (marked with a letter) provides practical information. The information consists for instance of operational procedures, articles, expert names etc. Every step (click) made in the scheme is documented in a standard report format. When closing a case, a report is created showing the applied approach, expert discussion, results and evaluation of the approach. A structured report will facilitate to solve cases in the future more efficient.
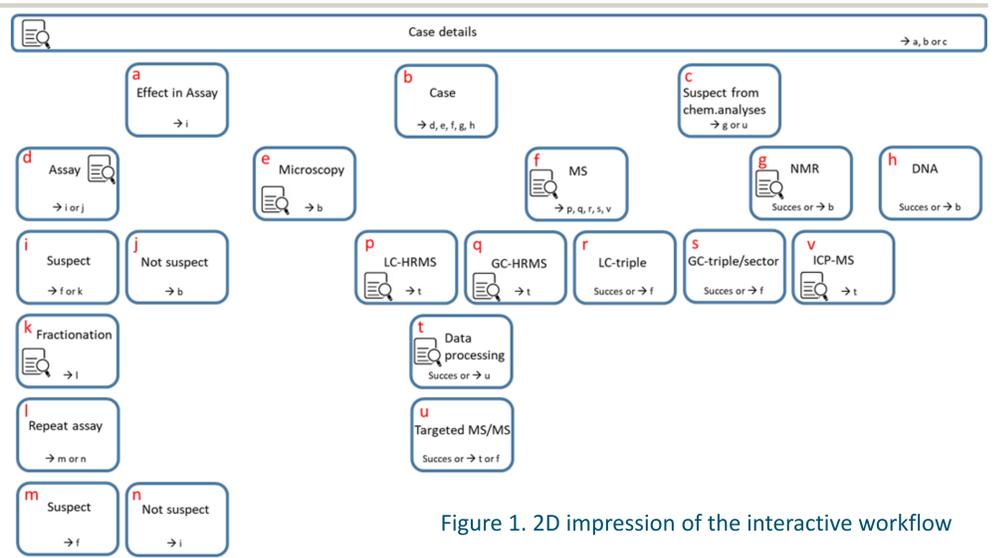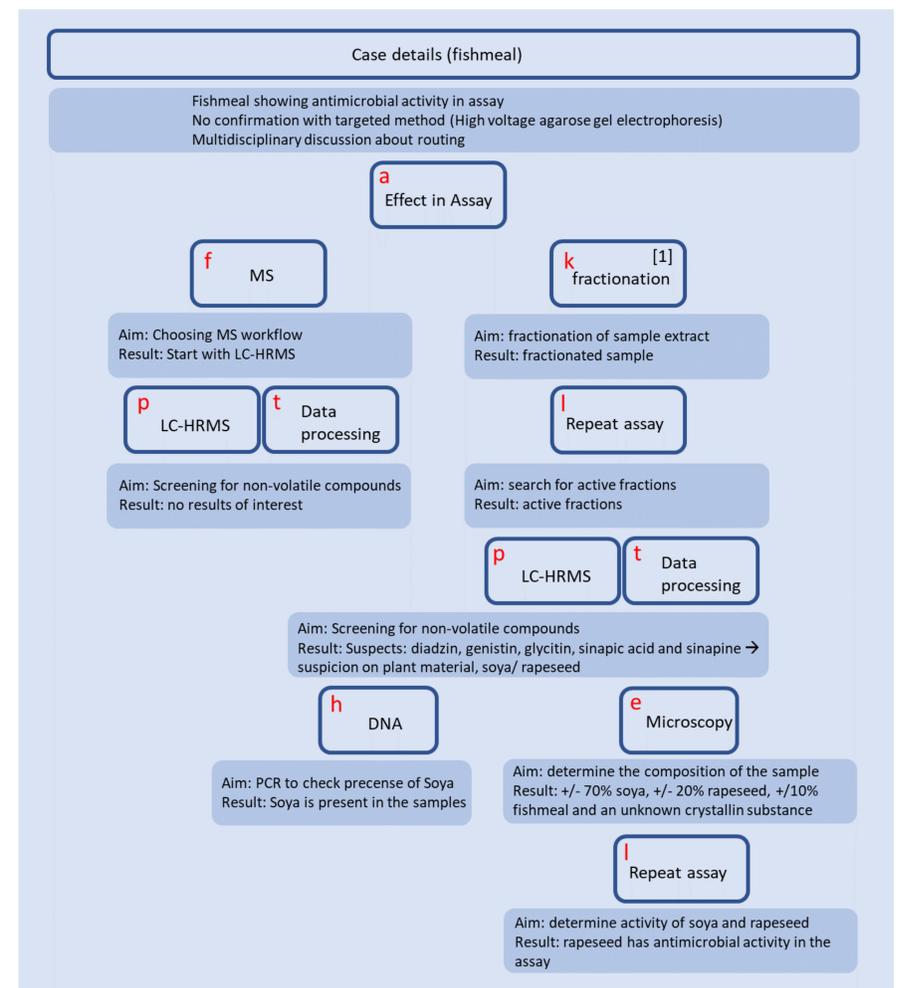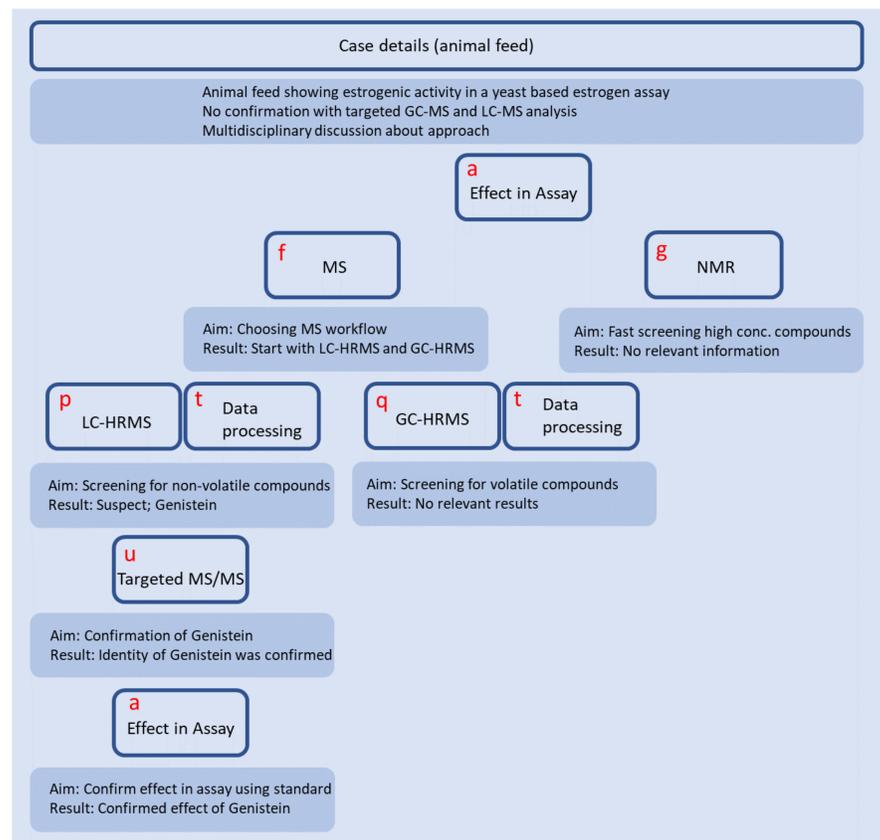

Figure 1. 2D impression of the interactive workflow

Assessment of the workflow

The followed approach of two cases is shown below. The first case (left) is an artificial case (animal feed). The second case (right) is a real case (fishmeal). The artificial case is successfully finished. The real case yielded the detection of an until-then unknown fraud case.

Conclusions

The identity of the 'unknown' substance in the artificial case was successfully confirmed. It was confirmed that a large fraction of the "fishmeal" sample consists of soya and rapeseed (fraud) instead of fish. It was confirmed that the antimicrobial activity shown in the assay can be explained by the presence of rapeseed. We experienced that the success rate of identification of the unknown substance increases when multidisciplinary research is applied in which biochemistry, analytical chemistry and physical chemistry are combined.