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Use the X-ray Diffraction in Forensic Science as a Device for Phase Analysis
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Phase identification, material comparison and quantification are basic tasks in a forensic science. Importance of XRD phase analysis in forensic science lies namely in: analysis of relatively small-volume samples, relatively non-destructive (probative value is preserved), exact phase analysis (unlike other instrumental chemical methods), quantitative analysis (in majority of cases), conclusive for a court. However, XRD analysis is not a very popular technique in forensic science community and is routinely used in only a few specialized laboratories (e.g. FBI (USA), BKA (Germany), FSS (England), NFI (Netherlands), central laboratories in Poland, Ukraine and Russia, laboratories in Japan and Australia). XRD analysis is currently employed at ICP in 7 main areas: Soils –EDS/WDS, XRF, FTIR, etc. are not able to perform exact determination of phases, namely alumosilicates. Explosives and post-blast residues – direct determination of inorganic components. Pigments and paints – phases of artworks, car paints, lacquer systems of tools, building industry and some printing colours. Type and origin of goods – customs and financial frauds, counterfeit, money laundering, etc. Unknown substances, poisons and contaminants - industrial accidents and leakage, threatening and extortionate letters, etc. Degraded skeletal remains – burnt, damaged or unusual fragments undeterminable by standard anthropological techniques. Quantitative drug analyses – higher precision of quantitative analysis compared with FTIR and GC. XRD is faster and its preparation is simpler.
Keywords: forensic microanalysis, powder diffraction, phase analysis

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Resolving Ambiguous Side-chain Orientations of Asparagine and Glutamine
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The electron densities obtained from proteins are sometimes insufficient to distinguish certain atom types. Prominent examples are the oxygen and nitrogen atoms in the side chains of Glutamine (GLN) and Asparagine (ASN) and the nitrogens in the imidazole ring of Histidine (HIS). Assignments of these atom types is often achieved indirectly by using information in the neighborhood of such atoms. This is often unreliable and it is known [1] that approximately 15% of these assignments are incorrect.

We derive a mean force heavy atom potential [2] from a set of highly resolved PDB [3] protein chains. Ambiguous residues in this set are evaluated using the potential and in case of an unfavorably high interaction energy the reverse orientation is taken. This procedure is iterated till convergence. The final potential function is then used for assigning the correct side-chain orientation of ambiguous amino acids in an arbitrary PDB file. A comparison to expert curated assignments [4] shows sensitivity and selectivity values higher than 90% for ASN and GLN. A web service is available athttp://services.came.sbg.ac.at/flipper.

[1] Hooft R.W.W, et al., *Proteins*, 1996, **26**, 363. [2] Sippl M.J., *Proteins*, 1993, **17**, 355. [3] Berman H.M., et al, *Nucleic Acids Res*., 2000, **28**, 235. [4] Word J.M., et al, *J. Mol. Biol.*, 1999, **285**, 1735.
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