comparing the profile for the chemical synthesis against a reference profile, which reference profile is the analytical data recorded over time for a reference chemical synthesis,

wherein the chemical synthesis and the reference chemical synthesis share at least the same reagents and method steps for the same intended product, such as the chemical synthesis and the reference chemical synthesis sharing the same instruction set.

A chemical synthesis may comprise one or more consecutive chemical reaction steps. A reactionware may be provided for the chemical reactions, and this may include multiple reaction vessels which are fluidically connected.

In a second aspect of the invention there is provided an apparatus for use in the method of validating a chemical synthesis, the apparatus comprising a chemical synthesiser, an analytical unit and a control unit, wherein:

the chemical synthesiser comprises a reactionware for the performance of chemical reactions, which reactionware is optionally also provided with one or more modules for work-up and purification, and further comprising reagents, optionally together with solvents and catalysts, for use in the chemical synthesis;

the analytical unit is adapted for measuring analytical data from the reactionware over time, and for reporting analytical data to the control unit; and

the control unit is for receiving analytical data from the analytical unit over time, and is adapted to construct a profile from the analytical data, and the control unit further holding a reference profile for comparison against the profile constructed from the analytical data.

The present invention also provides for the chemical synthesiser itself to operate autonomously. Thus, the apparatus may include a suitably programmed robotic system that is capable of comparative assessment of a synthesis profile against an appropriate reference profiles, and is suitably programmed to react as needed once such comparisons have been made. The apparatus may also be suitably programmed to collect the analytical data, and to create a profile against which comparisons may be made to the reference profile.

The apparatus may also include an autonomous synthesiser which undertakes the chemical synthesis

The analytical data for the profile may be generated throughout the chemical synthesis. Thus, analytical data may be generated for each chemical reaction in the chemical synthesis. Additionally, the analytical data may be generated during the reaction itself, but may also be generated during the initial setting of the reaction mixture, and also the work-up of a reaction, including purification. In this way, a comparison of the profile against that of the reference profile is truly indicative of the similarities in the chemical syntheses.

The analytical data may be recorded at high frequency or continuously. Modern analytical techniques all data generation in this way, and provide a greater number of data points for

the control unit is for receiving analytical data from the analytical unit over time, and is adapted to construct a profile from the analytical data, and the control unit further holding a reference profile for comparison against the profile constructed from the analytical data.

The apparatus may be a robotic chemical synthesiser for autonomous performance of the chemical synthesis, and for autonomous control of the analytical device.

In a further aspect there is provided a method for generating a reference profile, the method comprising the steps of:

performing a chemical synthesis in a chemical synthesiser;

recording analytical data during the chemical synthesis, and developing a reference profile for the analytical data recorded over time; and

providing the reference profile together with the instruction set for the chemical synthesis, wherein the instruction set is for the performance of the chemical synthesis using a reactionware, the instruction set optionally also for the preliminary generation of the reactionware for the chemical synthesis.

In a further aspect of the invention there is provided a method for preparing an apparatus that is a reaction system for performance of a reaction, including the steps of generating a code for the reaction, generating a virtual reaction platform to that code, and generating the physical reactionware for the reaction from the virtual platform.

The apparatus of the invention, and for use in the methods of the invention may be provided as a portable platform. Thus, the scale of the components of the apparatus are such as to allow movement of the apparatus between locations. In this way, the apparatus may be moved to locations where it is needed, or where it is desirable to have ready and immediate access to the product of the chemical synthesis.

The apparatus of the invention is suitable for use outside of the traditional laboratory environment, and allows for the production of target products in locations that would otherwise not be suitable for the preparation of chemical products. It is in such environments that it is particularly desirable to have validation of the chemical synthesis and the target product through the use of a profile compared with an approved reference profile. Alternative methods of analysis, and analytical equipment generally, may not be available to the operator, and therefore the profile from the chemical synthesis serves as the only characterisation of that synthesis, and the only means by which to guarantee the process and its products.