1. **Title of the module**  
   Advanced IT Tools for Chemists – GSKCHEM7

2. **School or partner institution which will be responsible for management of the module**  
   GSK

3. **The level of the module (Level 4, Level 5, Level 6 or Level 7)**  
   HE Level 4 / NQF Level 7

4. **The number of credits and the ECTS value which the module represents**  
   5 credits

5. **Which term(s) the module is to be taught in (or other teaching pattern)**  
   Autumn

6. **Prerequisite and co-requisite modules**  
   IT tools for chemists

7. **The programmes of study to which the module contributes**  
   This is an optional module for the Postgraduate Certificate in Professional Development.

8. **The intended subject specific learning outcomes.**  
   **On successfully completing the module students will be able to:**
   
   8.1 Use a combination of IT tools to retrieve and combine various data types, including chemical, structural and biological data, from multiple information sources.
   
   8.2 Use IT tools to analyse complex data sets, assess critically data quality within these sets, and to generate structural activity relationships.
   
   8.3 Demonstrate the ability to communicate and report the output from an SAR analysis project

9. **The intended generic learning outcomes.**  
   **On successfully completing the module students will be able to:**
   
   9.1 Demonstrate the ability to retrieve efficiently and combine various data types from multiple information sources (A3, A4, A5, A7, B1b, B1c, B1d, B1e, B1h, Cn, Co, Cs, Ct)
   
   9.2 Demonstrate the ability to assess critically data quality within complex data sets (A3, A4, A5, A7, B1b, B1c, B1d, B1e, B1g, B1h, Cn, Co, Cq, Cs, Ct)
   
   9.3 Demonstrate the ability to analyse complex data sets and to generate appropriate structure activity relationships (A3, A4, A5, A7, B1b, B1c, B1d, B1e, B1g, B1h, Cn, Co, Cq, Cs, Ct)
   
   9.4 Demonstrate the ability to communicate and report the output from an SAR analysis project (A3, A4, A5, A7, B1e, B1f, B1g, B1h, Cm, Cq, Cs)

10. **A synopsis of the curriculum**  
    This module provides a framework of learning and training in computational packages for Research and Development chemists who have completed the IT tools for chemists module, and who wish to develop specialist skills in data analysis within a particular programme. The aims of the module are to develop advanced informatics techniques for the analysis of complex data-sets. The derived structure activity relationships and ideas generated will have broad impact upon medicinal chemistry programmes. This module provides tools that allow chemists to exert a major strategic influence on ongoing research programmes.
11. Reading list (Indicative list, current at time of publication. Reading lists will be published annually)

Training manuals or reference guides are available for each software package.

12. Learning and teaching methods

Attendance at a classroom training session entitled “Using IT tools to aid compound design” is expected. In addition, for the IT tools studied, the student will be expected to attend the appropriate training sessions available, these include online learning and face-to-face training sessions. In addition, the students will be trained by their supervisor and “lead users” for each specific IT tool. The remaining hours are amassed through “on the job” training and practice within the laboratory setting.

Learning hours: 50

13. Assessment methods

- Within an agreed timeframe (e.g. 6-12 months after module completion), the participant should be able to utilise these computational packages with accuracy and dexterity, as judged by the supervisor’s line manager. The IT Module Leader(s) will advise the line manager, if required. The assessment and recommendation will be ratified by the departmental head.

- Participants will provide a portfolio of work generated using the specific computational packages. This portfolio – in some combination of printed and electronic formats - will demonstrate expert abilities by the participant within the applications and provide supporting evidence for the high quality, accuracy and impact of the work.

The supervisor’s line manager will provide written justification regarding their assessment. The departmental head will review, discuss with the supervisor’s line manager, and ultimately ratify the recommendations.

The External Examiner will have access to:

- Examples where the knowledge acquired has been applied in the workplace, including:
  - Data files and related report/presentation demonstrating the skill level of the participant in the use and application of the computational packages to current research
- The line manager’s and departmental head’s assessment summaries

14. Map of module learning outcomes (sections 8 & 9) to learning and teaching methods (section12) and methods of assessment (section 13)

<table>
<thead>
<tr>
<th>Module learning outcome</th>
<th>8.1-8.5</th>
<th>9.1-9.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Learning/teaching method</td>
<td>Hours allocated</td>
<td></td>
</tr>
<tr>
<td>Private Study</td>
<td>40</td>
<td>X</td>
</tr>
<tr>
<td>Classroom session and Face-to-face training</td>
<td>10</td>
<td>X</td>
</tr>
</tbody>
</table>
15. Inclusive module design

GSK recognises and has embedded the expectations of current equality legislation, by ensuring that the module is as accessible as possible by design. Additional alternative arrangements for students with Inclusive Learning Plans (ILPs)/declared disabilities will be made on an individual basis, in consultation with the relevant policies and support services.

The inclusive practices in the guidance (see Annex B Appendix A) have been considered in order to support all students in the following areas:

a) Accessible resources and curriculum

b) Learning, teaching and assessment methods

16. Campus(es) or centre(s) where module will be delivered

GSK Stevenage

17. Internationalisation

The capability of IT tools, and their application to scientific research by multidisciplinary scientists across the globe, are rapidly advancing. Mastery of the subject-specific learning outcomes will equip students to apply the IT tools studied in this module in a wide range of international contexts. A proportion of the IT tools studied are widely available across the globe, and additionally the skills learnt in this module can be readily applied to the use of alternative IT tools in the wider scientific community. GSK is large multi-national healthcare organisation which enables students to appreciate the international aspects and benefits of scientific research and development.

18. Partner College/Validated Institution

GSK Stevenage

19. University School responsible for the programme

Physical Sciences