

- i. CIF IUCr Crystallographic Information Framework
 - ii. CML Chemical Markup Language
 - iii. SMILES -- Simplified Molecular Input Line Entry Specification
 - iv. InChi -- IUPAC International Chemical Identifier
3. Chemical Databases and Data Mining
- i. Cambridge Structural Database CCDC CSD
 - ii. Crystallographic Open Database COD
 - iii. Protein Data Bank PDB Ligand Explorer
 - iv. ChempSpider
4. Molecular Drawing and Interactive Visualization
- i. ChemDraw
 - ii. MarvinSketch
 - iii. ORTEP
 - iv. Chimera, RasMol, PyMol
5. Computer-Aided Drug Design Tools
- i. Molecular Modeling Tools
 - ii. Structural Homology Modeling Tools
 - iii. Docking Tools and Screening Tools
6. Building a Ligand
- i. Building ab initio
 - ii. Building from similar ligands
 - iii. Building with a known macromolecular target
 - iv. Building without a known macromolecular target
 - v. Computational assessment of activity and toxicity and drugability.

References:

1. **Leach, A. R.; Gillet, V. J. (2007)**, An introduction to Chemoinformatics, **Springer**.
2. **Gasteiger, J.; Engel, T. (2003)**, Chemoinformatics: A text-book. **Wiley-VCH**.
3. **Gupta, S. P. (2011)**, QSAR & Molecular Modeling. **Anamaya Pub.**
4. **Gasteiger, J.** Handbook of cheminformatics: from data to knowledge in 4 volumes, **Wiley**.

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DISCIPLINE SPECIFIC ELECTIVE 10

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		

CHEMICAL PATENT ANALYTICS & IP STRATEGY	4	2	0	2	12th Class: Physics, Chemistry, Mathematics	-
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Course Objectives:

- Develop expertise in chemical patent analysis, drafting, and intellectual property (IP) strategy.
- Provide hands-on training in patent search methodologies, analytics, and database navigation.
- Foster understanding of IP commercialization, technology transfer, and portfolio management in the chemical industry.

Learning Outcomes:

By the end of this course, students will be able to learn:

- Analyze chemical patent systems, including Indian and global frameworks (USPTO, EPO, PCT).
- Conduct patent searches, patentability, freedom-to-operate (FTO) analyses, and landscape studies using AI and databases.
- Draft patent claims, specifications, and drawings for chemical inventions.
- Apply IP strategies for commercialization, licensing, and competitive intelligence.

THEORY COMPONENT-

UNIT 1: Chemical Patent Fundamentals

(8 Hours)

Introduction to Chemical Patents: Anatomy of patent: Patent number, inventors, assignee, dates, title, abstract, background, summary, claims, description, drawing, embodiment, etc. Types of chemical patents: Composition, process, formulation, use patents, special considerations for biotechnology patents, differences between product and process patents in chemistry

Indian Patent System for Chemicals: Section 3(d) and its implications for pharma patents, compulsory licensing case studies (Bayer vs Natco), traditional knowledge protection (Turmeric, Neem cases)

Global Patent Systems: PCT filing for chemical inventions, USPTO and EPO requirements for chemical patents, Patent term extensions for agrochemicals

Patentability Criteria: Novelty assessment for chemical compounds, inventive step in process chemistry, industrial applicability requirements

UNIT 2: Patent Search & Analysis

(8 Hours)

Search Methodologies: Keyword strategies for chemical searches, classification systems (IPC, CPC for chemistry), structure-based searching (Markush, SMILES, InChI)

Database Navigation: WIPO Patentscope deep dive, USPTO chemical patent search techniques, specialized chemistry databases (SciFinder, Reaxys), Google patent, Lens.org, FreePatentOnline, Derwent Innovation, PatSnap, Orbit Intelligence (Questel), PatBase, Reaxys, and SciFinder

Analytical Techniques: Citation analysis for identifying key patents, patent family mapping, competitive intelligence through assignee analysis

Freedom-to-Operate Analysis: Risk assessment methodology, case study: generic drug entry strategies

UNIT 3: Patent Drafting for Chemists (8 Hours)

Claim Drafting Strategies: Composition claims vs process claims, Markush language for chemical structures, dependent claim strategies

Specification Writing: Detailed description requirements, examples and embodiments, data presentation best practices

Special Cases: Polymorph patents, formulation patents, biotech sequence listings

Drawings and Diagrams: Chemical structure drawings, Process flow diagrams, spectra presentation

UNIT 4: IP Commercialization (6 Hours)

Technology Transfer: University-industry collaborations, licensing strategies, startup formation

Portfolio Management: Patent valuation methods, maintenance decision making, defensive publishing, case Studies: Novartis Glivec case, agrochemical patent strategies. green chemistry patents,

PRACTICAL COMPONENT (60 Hours)

1. Basic Excel Training (May use AI tools as well)

Essential formulas:

VLOOKUP (for patent family matching)

COUNTIF (for assignee analysis)

Pivot Tables (for technology trend analysis)

Conditional Formatting (highlighting key patents)

Data cleaning techniques for patent exports

2. Database Navigation and Export

WIPO Patentscope, USPTO, Espacenet, Google Patent, Lens.org, FreePatentsOnline

Non-Patent Literature data bases (Google Scholar, Science direct, Scopus, Scopus AI)

3. Novelty Search (Invention from any recent patent application)

Task: Identify prior art for a given invention

Tools: Any freely available data base including AI tools

Deliverable: Excel report with key patents ranked by relevance and novelty assessment summary

5. FTO Search (Provide an invention from any recent granted patent)

Task: Analyze freedom-to-operate for a provided invention

Tools: Any freely available data base including AI tools

Deliverable: Risk assessment matrix in Excel

6. Invalidity Search (Provide a recent granted patent)

Task: Find invalidating prior art for a granted patent

Tools: Any freely available data base including AI tools

Deliverable: Evidence chart in Excel

7. Claim Drafting (Provide an Invention disclosure from a patent)

8. Group project + viva presentation on landscape study

Task: Any topic in a particular interval (2020 to 2025) and convert landscape study into PowerPoint

Tools: Any freely available data base including AI tools, excel, and PPT

Deliverable: Pivot table showing: Top assignees and Technology evolution

Requirements: Technology trends slides, competitor analysis.

RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES

1. WIPO, WIPO Patent Drafting Manual (2023) – World Intellectual Property Organization (<https://www.wipo.int/edocs/pubdocs/en/wipo-pub-867-23-en-wipo-patent-drafting-manual.pdf>)
2. Sampat BN, Shadlen KC. Indian pharmaceutical patent prosecution: The changing role of Section 3(d). PLoS One. 2018 Apr 2;13(4):e0194714. doi: 10.1371/journal.pone.0194714. PMID: 29608604; PMCID: PMC5880378.
3. WIPO, Guidelines for Preparing Patent Landscape Reports(2015)-World Intellectual Property Organization (https://www.wipo.int/edocs/pubdocs/en/wipo_pub_946.pdf)
4. WIPO, Patent Cooperation Treaty(PCT)- Regulations under the PCT (as in force from July 1, 2024) (<https://www.wipo.int/edocs/pubdocs/en/wipo-pub-274-2024-en-patent-cooperation-treaty-pct.pdf>)
5. WIPO, Guide to the International Patent Classification (2025)-World Intellectual Property Organization (<https://www.wipo.int/edocs/pubdocs/en/wipo-guide-ipc-2025-en-guide-to-the-international-patent-classification-2025.pdf>)
6. WIPO, Inventing the Future-An Introduction to Patents for Small and Medium-sized Enterprises (2018)- World Intellectual Property Organization (<https://www.wipo.int/edocs/pubdocs/en/wipo-pub-917-1-en-inventing-the-future.pdf>)
7. WIPO, Identifying Inventions in the Public Domain-A Guide for Inventors and Entrepreneurs (2020)- World Intellectual Property Organization (https://www.wipo.int/edocs/pubdocs/en/wipo_pub_1062.pdf)
8. <https://www.uspto.gov/patents/basics>

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