ChemOffice v22.0 Suite of Products

Version 22.0 New Features	系统	ChemDraw Professional	ChemOffice	ChemOffice+ Cloud Standard*
Atom/Bong Grab Hotkey/ 新增抓取快捷键g	Win/Mac	●	●	●
3D Rotation Shortcut/ 3D旋转快捷键Shift+Alt+箭头	Win/Mac	●	●	●
Open CIF Files/ 打开CIF格式文件	Win/Mac	●	●	●
Toggle CIF Files Hydrogens/ 打开CIF文件切换氢原子	Win/Mac	●	●	●
Hydrogen Bond Tool/ 新增氢键工具	Win/Mac	●	●	●
Millipore Sigma Synthia Add-in/ 提供Synthia接口（逆合成软件，需是该软件的订阅者	Win/Mac	●	●	●
HELM Cartoon Representation/ 单体动画展示（多颜色）	Win/Mac	●	●	●
HELM Library Improvements/ HELM库功能增强	Win/Mac	●	●	●
Support for Ambiguous FASTA/HELM Monomers/ 快速粘贴单体或FASTA序列到CD	Win/Mac	●	●	●
DNA/RNA Sequence Numbering Improvements/ 脱氧核糖核酸与核糖核酸序列计数	Win/Mac	●	●	●
Ring Fill Color Transfer to 3MF model **/ 3MF格式模型支持环内颜色填充 **	Win/Mac		●	●
3MF Export Settings for 3D Printing/ 3MF格式模型支持3D打印设置	Win/Mac		●	●
pic2mol Image to Structure Add-in/ Pic2mol接口（支持图片转化为可编辑结构式到CD，需是该软件的订阅者）	Win/Mac		●	●
ChemOffice+ ***/ 云模块功能增强***	Win/Mac			●
Dedicated Tenant in multi-tenant Cloud Environment/ 专用户名	Win/Mac			●
ChemDraw JS for internal development/ 将ChemDraw作为绘制工具嵌入到内部网站，且生物聚合物序列多颜色展示功能可在JS中实现	Win/Mac			●
**ChemOffice+ Features ** **	**系统**	**ChemDraw Professional**	**ChemOffice**	**ChemOffice+ Cloud Standard***
Browse & Drill-down into ChemDraw Files (.cdx, .cdxml)/ 浏览和直接拖拽ChemDraw文件	Win/Mac			●
Browse & Drill-down ChemDraw Files embedded in MS Word/ 浏览和拖拽出嵌入在Word文档中的ChemDraw文件	Win/Mac			●
Browse & Drill-down ChemDraw Files embedded in MS Powerpoint/ 浏览和拖拽出嵌入在PPT中的ChemDraw文件	Win/Mac			●
Browse ChemDraw For Excel Files/ 浏览使用ChemDraw For Excel模块生成的Excel文件	Win			●
Create Collection from .csv files/从csv格式文件中采集整理结构式	Win/Mac			●
Create collection from SMILES text file/ 从SMILES文本文件中采集整理结构式数据	Win/Mac			●
Browse .mol & .sdf Files/ 浏览.mol & .sdf格式文件	Win/Mac			●
View .sdf Files properties/ 查看 .sdf 文件属性	Win/Mac			●
Copy Embedded Chemical Structures to the Clipboard/ 将嵌入的化学结构复制到剪贴板	Win/Mac			●
Create Collection of Chemical Structures/ 多文件中采集化学结构式	Win/Mac			●
Adding Properties to Collections/ 为采集到的结构式添加属性	Win/Mac			●
Editing Properties of Collections/ 给采集到的结构式编辑属性	Win/Mac			●
Saving Collection Layout as a Template/采集样式保存成模板	Win/Mac			●
Batch-Editing of Multiple Chemical Structures in Collections/ 在采集到的结构式进行中批量编辑	Win/Mac			●
Structure-searching inside Cloud-hosted MS Office documents/ 在云端MS Office 文件中进行结构式搜索	Win/Mac			●
Searching across Signals Notebook (SNB) Experiments****/ 在SNB电子实验记录本中进行跨实验搜索****	Win/Mac			●
Create Collection of Reactions from SNB Experiments/ 在SNB电子实验记录本中采集反应式	Win/Mac			●

ChemOffice+ Features ** Continued	系统	ChemDraw Professional	ChemOffice	ChemOffice+ Cloud Standard*
Export Collections to SD Files (v2000, v3000)/ 将采集到的结构式整理导出为SD文件(v2000, v3000)	Win/Mac			●
Create Powerpoint Reaction Report Slide from SNB Experiments****/ 从SNB电子实验记录本中创建反应报告PPT****	Win/Mac			●
Create Powerpoint Molecule Report Slide from Collection/ 从Collection中直接创建分子报告PPT	Win/Mac			●
Recent Additions	**系统**	**ChemDraw Professional**	**ChemOffice**	**ChemOffice+ Cloud Standard***
Magic Hotkeys Enhancements/ 热键增强	Win/Mac	●	●	●
Shortcuts Enhancements/ 快捷键增强	Win/Mac	●	●	●
Join function improvements/ 增强的合并连接键功能	Win/Mac	●	●	●
Smart Copy/Paste (SMILES, InChI, HELM)/只能复制黏贴，支持SMILES, InChI, HELM格式	Win/Mac	●	●	●
Aromatic Cycle Display Toggle and Preferences/ 芳香环显示切换键和属性设置	Win/Mac	●	●	●
Stereochemistry handling improvements/增强立体化学处理能力	Win/Mac	●	●	●
Improved Polymer Brackets (Average MW)/ 改进的聚合物括号功能(显示平均分子量)	Win/Mac	●	●	●
Atom/Bond Color Highlighting/ 原子和键的颜色高亮标记	Win/Mac	●	●	●
Ring-Fill Coloring/ 环内颜色填充	Win/Mac	●	●	●
Search into SciFinder-n/直接连接到SciFinder-n数据库搜索	Win/Mac	●	●	●
Search into Reaxys/ 可直接连接到Reaxys数据库搜索	Win/Mac	●	●	●
Improved HELM Monomer Toolbar/ 改进的单体工具栏	Win/Mac	●	●	●
HELM Monomer versioning Support/ 给HELM单体标注版本	Win/Mac	●	●	●
Copy as 3D-printable object (.3MF)**/ 复制为可3D打印对象**	Win/Mac	●	●	●
Atom/Bond Color Highlight Transfer to 3MF/3MF格式模型支持原子和键的颜色高亮	Win/Mac	●	●	●
Google Patents/Scholar Add-in/ 提供直接连接到谷歌浏览器进行查询的接口	Win/Mac		●	●
PubChem GHS Safety Add-in/ 提供直接连接到PubChem数据库(该数据库可免费下载)的接口进行安全信息查询	Win/Mac		●	●
ChemDraw Add-ins SDK/ 自定义接口	Win/Mac		●	●
ChemDraw Add-ins Dynamic Download/ 自定义接口	Win/Mac		●	●
Support for Add-ins Token-based Authentication/ 支持认证	Win/Mac		●	●
Shared HELM Libraries/ HELM共享	Win/Mac		●	●
Includes	**系统**	**ChemDraw Professional**	**ChemOffice**	**ChemOffice+ Cloud Standard***
Read and Save as .cdx / .cdxml Files/ 打开和保存为 .cdx / .cdxml格式文件	Win/Mac	●	●	●
Read and Save as .rxn Files (v2000, v3000)/ 打开和保存为 .rxn (v2000, v3000)格式文件	Win/Mac	●	●	●
Read and Save as .skc Files/ 打开和保存为 .skc格式文件	Win/Mac	●	●	●
Read and Save as .mol Files (v2000, v3000)/ 打开和保存为 .mol (v2000, v3000)格式文件	Win/Mac	●	●	●
Read and Save as .sdf Files (v2000, v3000)/ 打开和保存为 .sdf (v2000, v3000)格式文件	Win/Mac	●	●	●
Read and Save as .rdf Files (v2000, v3000)/ 打开和保存为.rdf (v2000, v3000)格式文件	Win/Mac	●	●	●
Save ChemDraw Style Sheet/ 保存为ChemDraw样张(模板)	Win/Mac	●	●	●
Structure Clean-up/ 结构式整理	Win/Mac	●	●	●
Reaction Clean-up/ 反应式整理	Win/Mac	●	●	●
Magic Hotkeys/ 魔法热键	Win/Mac	●	●	●
Chemical Bonds Tools/ 化学键绘制工具	Win/Mac	●	●	●
Text Tool/ 文字工具	Win/Mac	●	●	●
3D Perspective Tool/ 3D透视工具	Win/Mac	●	●	●
Chemical Rings Tools/ 化学环绘制工具	Win/Mac	●	●	●

Includes Continued	系统	ChemDraw Professional	ChemOffice	ChemOffice+ Cloud Standard*
Arrow Tool/ 箭头绘制工具	Win/Mac	●	●	●
Orbitals Tool/轨道绘制工具	Win/Mac	●	●	●
Brackets Tool/括号绘制工具	Win/Mac	●	●	●
Pen Tools/ 画笔工具	Win/Mac	●	●	●
Shapes Tool/ 形状绘制工具	Win/Mac	●	●	●
Chemical Polymers Tools/ 化学聚合物工具	Win/Mac	●	●	●
Mass Fragmentation Tools/ 裂解切割工具，使用质量碎片工具在一个或多个键之间拖动光标，释放鼠标键时穿过的键会断裂	Win/Mac	●	●	●
Thin Layer Chromatography Tool/ 薄层色谱工具	Win/Mac	●	●	●
Gel Electrophoresis Tool/ 凝胶电工具泳	Win/Mac	●	●	●
Insert OLE Object in ChemDraw/ 插入OLE对象，可将Excel, Word等文件插入，双击可启动。	Win	●	●	●
Copy ChemDraw Structures as OLE Object/ 复制结构式作为OLE对象	Win	●	●	●
Show Stereochemistry/ 显示立体化学abs, or1, &1	Win/Mac	●	●	●
Relative Stereochemistry (ISIS compatibility)/ 相对立体化学（ISIS兼容性）	Win/Mac	●	●	●
Reaction Interpretation/ 反应解析，用颜色标记出反应物，生成物和中间物	Win/Mac	●	●	●
Reaction Mapping/ 反应映射	Win/Mac	●	●	●
Calculate MW/ 分子质量计算	Win/Mac	●	●	●
Calculate Exact Mass/ 精确分子量计算	Win/Mac	●	●	●
Calculate Chemical Formula/ 化学公式计算	Win/Mac	●	●	●
Calculate Elemental Analysis/ 元素分析	Win/Mac	●	●	●
Calculate m/z 质荷比	Win/Mac	●	●	●
Copy/Paste as CDXML/ 复制粘贴为CDXML文件格式	Win/Mac	●	●	●
Copy/Paste as SMILES/支持复制粘贴 SMILES(code形式)	Win/Mac	●	●	●
Copy/Paste as SYBYL (SLN)/复制粘贴为SYBYL (SLN)	Win/Mac	●	●	●
Copy/Paste as InChI/ 支持复制粘贴InChI（code形式）	Win/Mac	●	●	●
Copy/Paste as Mol File / Mol3000/支持复制粘贴摩尔文件	Win/Mac	●	●	●
pKa 酸度系数/ Log P 油水分配系数/ Log S 计算	Win/Mac	●	●	●
Atom List Generic Structures (Enumeration)/ 原子列表枚举	Win/Mac	●	●	●
tPSA/ 基于碎片贡献的极性表面积计算	Win/Mac	●	●	●
Variable Attachment Generic Structures (Enumeration)/ 根据化学逻辑把具有可变结合点的化合物可能的类型全部展开	Win/Mac	●	●	●
Label Repeating Units Generic Structures (Enumeration)/ 把一个标签类型的重复单元，根据标记数量全部枚举展开	Win/Mac	●	●	●
Polymer Repeating Units Generic Structures (Enumeration)/ 把一个聚合物的重复单元，根据标记数量全部枚举展开	Win/Mac	●	●	●
Chemical Structures Templates/ 化学结构式绘制模板	Win/Mac	●	●	●
Laboratory Equipment Templates/ 实验室设备绘制模板	Win/Mac	●	●	●
Analyze/Check Structures结构分析	Win/Mac	●	●	●
Expand/Contract Labels 展开/收起标签	Win/Mac	●	●	●
Define/Use Nicknames 定义/使用别称	Win/Mac	●	●	●
Document Metadata/Tagging 文档标签	Win/Mac	●	●	●
MulCple ChemDraw Items Folder/多个ChemDraw项目文件夹	Win/Mac	●	●	●
Multicenter Attachments/ 多中心附件	Win/Mac	●	●	●
Save as JPEG image/ 保存为JPEG图片格式	Win/Mac	●	●	●
Save as PNG image/ 保存为PNG图片格式	Win/Mac	●	●	●
Save as TIFF image/ 保存为标签图像文件格式	Win/Mac	●	●	●
Save as Scalable Vector Graphics (SVG)/存为可缩放矢量图形	Win/Mac	●	●	●
Save as Encapsulated Post Script (EPS)/ 保存为EPS图片格式，一种被封装的PostScript格式	Win/Mac	●	●	●
Name-to-Structure / Structure-to-Name 名称结构式互换	Win/Mac	●	●	●
Predict 1H NMR/ 核磁光谱氢谱预测	Win/Mac	●	●	●

Includes Continued	系统	ChemDraw Professional	ChemOffice	ChemOffice+ Cloud Standard*
Predict 13C NMR/ 核磁光谱碳谱预测	Win/Mac	●	●	●
Search SciFinder/ 可直接连接到SciFinder数据库搜索	Win/Mac	●	●	●
Search SciFinder-n/ 直接连接到SciFinder-n数据库搜索	Win/Mac	●	●	●
Search Reaxys/ 可直接连接到Reaxys数据库搜索	Win/Mac	●	●	●
Reaction Stoichiometry Grid/ 反应式化学计量网格	Win/Mac	●	●	●
R-Group Table Generic Structures (Enumeration)/ R-Group表泛结构式展开（枚举）	Win/Mac	●	●	●
BioDraw Toolbar/ 生物绘制工具栏	Win/Mac	●	●	●
cLogP/ 有机化合物的疏水常数计算	Win/Mac	●	●	●
HELM Toolbar/ HELM 工具栏	Win/Mac	●	●	●
Copy/Paste as HELM/ 支持复制粘贴HELM	Win/Mac	●	●	●
Copy/Paste as FASTA Peptide/复制粘贴FASTA文件中的肽	Win/Mac	●	●	●
Copy/Paste as FASTA DNA/RNA/ 支持复制粘贴FASTA文件中的脱氧核糖核酸与核糖核酸	Win/Mac	●	●	●
Support for HELM notation/ 支持HELM注释	Win/Mac	●	●	●
CAS RN to Structure from ChemACX.com/ 支持从CAS number直接转换成结构式	Win/Mac	●	●	●
Enhanced Stereochemistry Support/ 高级立体化学	Win/Mac	●	●	●
ChemDraw for Excel/ 与微软Excel兼容使用	Win	●	●	●
CombiChem for Excel/ CombiChem与微软Excel兼容	Win	●	●	●
Name-to-Structure / Structure-to-Name for ChemDraw for Excel/ 在Excel中进行名称结构互换	Win	●	●	●
Chem3D Professional/ 3D组件pro版	Win	●	●	●
ChemFinder Standard/ 数据库建库组件标准版	Win	●	●	●
ChemScript 编程	Win	●	●	●
PubChem GHS Safety Add-in/ 提供直接连接到PubChem数据库(该数据库可免费下载)的接口进行安全信息查询	Win/Mac		●	●
Google Scholar / Google Patents Add-in/ 提供直接连接到谷歌浏览器进行查询的接口	Win/Mac		●	●
Save as 3D-printable object (.3MF)/ 保存为支持3D打印对象	Win/Mac		●	●
Copy as 3D-printable object (.3MF)**/ 复制为可3D打印对象**	Win/Mac		●	●
Transfer Atom/Bond Color Highlights to 3D-printable object/ 3D状态下的原子/键的颜色高亮	Win/Mac		●	●
ChemACX Explorer 化学品比价数据库	Win/Mac		●	●
Custom ChemDraw Add-ins SDK/ ChemDraw 自定义接口	Win/Mac		●	●
Support for Token-based Authentication of Add-ins/ 自定义开发，支持令牌的身份验证	Win/Mac		●	●
Shared HELM Libraries/ HELM共享	Win/Mac		●	●
Mnova ChemDraw Edition/ Mnova一维计算	Win/Mac		●	●
Chem3D Ultra/ 3D组件Ultra版	Win		●	●
Chem3D Interface to Conflex/提供直接连接到Conflex的接口	Win		●	●
Chem3D Interface to Autodock/ 提供直连到Autodock的接口	Win		●	●
Chem3D Interface to GAMESS 2020/ 提供直接连接到GAMESS(该数据库可免费下载)的接口进行3D计算	Win		●	●
Chem3D Interface to Gaussian 16W/ 提供直接连接到Gaussian 的接口进行3D计算	Win		●	●
Chem3D Interface to MOPAC 2016/ 提供直接连接到MOPAC （该数据库高校用户免费下载）的接口进行3D计算	Win		●	●
ChemFinder Ultra/ 数据库建库组件Ultra版	Win		●	●
ChemFinder for Oracle/ ChemFinder链接Oracle数据库	Win		●	●
Explorer Window View in ChemFinder Ultra/ ChemFinder Ultra中的浏览窗口显示	Win		●	●
BioViz in ChemFinder Ultra/支持该模块中的BioViz散点图	Win		●	●
Compound Profiles in ChemDraw Finder Ultra/ ChemDraw Finder Ultra中的化合物信息显示	Win		●	●

Includes Continued	系统	ChemDraw Professional	ChemOffice	ChemOffice+ Cloud Standard*
Clustering in ChemFinder Ultra/ ChemFinder Ultra中的集群	Win		●	●
Combine ChemFinder Query Hit Lists/ 合并查询名单	Win		●	●
ChemFinder Exports to MS Word/Excel/ ChemFinder 数据导出为MS Word/Excel格式	Win		●	●
ClogP/CMR for ChemDraw for Excel/Chem3D/ 与Excel合作批量计算ClogP和CMR	Win	●	●	●
Molecular Networks (pKa/Log P/Log S) for ChemDraw for Excel/Chem3D/ 与Excel合作批量计算pKa/Log P/Log S	Win	●	●	●
Molecular Topology for ChemDraw for Excel/Chem3D/分子拓扑	Win	●	●	●
ChemProp Std Properties for ChemDraw for Excel/Chem3D/提供ChemProp Std模块包含的批量计算功能	Win	●	●	●
ChemProp Pro Properties for ChemDraw for Excel/Chem3D/提供ChemProp Pro模块包含的批量计算功能	Win		●	●
IUPAC-based Atom Numbering/ 基于IUPAC命名的原子量自动计数	Win/Mac	●	●	●
Metallocene hotkeys/ 茂金属热键	Win/Mac	●	●	●
3D Clean-up Enhancements/ 3D 结构整理增强	Win/Mac	●	●	●
ChemACX Explorer/ ChemACX化学品比价数据库	Win/Mac		●	●

带星功能注释：

* 最小起定量5用户

** 在PPT中粘贴.3MF对象需同时是MS Office365的订阅用户

*** ChemOffice+ 是一款云应用模块，预计每季度自动升级

**** 该功能需要Signals Notebook权限

ChemDraw/ChemOffice 补充说明

	ChemDraw Professional	ChemOffice
ChemFinder Standard	●	●
ChemFinder Ultra		●
Chem3D Pro	●	●
Chem3D Ultra		●
ChemPropPro in ChemDraw for Excel		●

ChemFinder Standard 和 ChemFinder Ultra功能对比	ChemFinder Standard	ChemFinder Ultra
打开/浏览数据库文件	●	●
文件导入/导出	●	支持更多格式
新建数据库		●
编辑现有数据库		●
三维检索		●
支持BioViz散点图		●
Compound Profiles / 化合物信息显示		●
与微软办公软件兼容使用		●
ChemFinder for Oracle/ 支持Oracle数据库连接		●
Clustering/ 集群		●
Explorer Window View/ 浏览窗口显示		●
Combine ChemFinder Query Hit Lists/ 合并查询名单		●

Chem3D Pro 和 Chem3D Ultra功能对比	Chem3D Pro	Chem3D Ultra
3D 立体显示	●	●
MM2 最小能量计算	●	●
MMFF94 高分子计算		●
Gaussian 计算接口（Chem3D通过Gaussian计算红外、紫外）		●
GAMESS 计算接口 （Chem3D通过GAMESS计算核磁、红外）		●
Conflex 计算接口		●
Autodock 计算接口		●
MOPAC 计算接口		●

ChemPropPro模块, 在 ChemDraw for Excel 中对如下数值的批量计算	ChemDraw Professional	ChemOffice
Boiling Point 沸点		●
LogP 油水分配系数		●
Critical Volume 临界体积		●
Critical Pressure 临界压力值		●
Critical Temperature 临界温度		●
GIBBS Free Energy GIBBS自由能		●
Heat of Formation 生成热		●
Henry Law Constant 亨利定律常数		●
Ideal Gas Thermal Capacity 理想气体热容量		●
Melting Point 熔点		●
Mol Refractivity 摩尔折射率		●
Vapor Pressure 饱和蒸汽压		●
Water Solubility 水溶性		●