Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

代谢产物鉴定

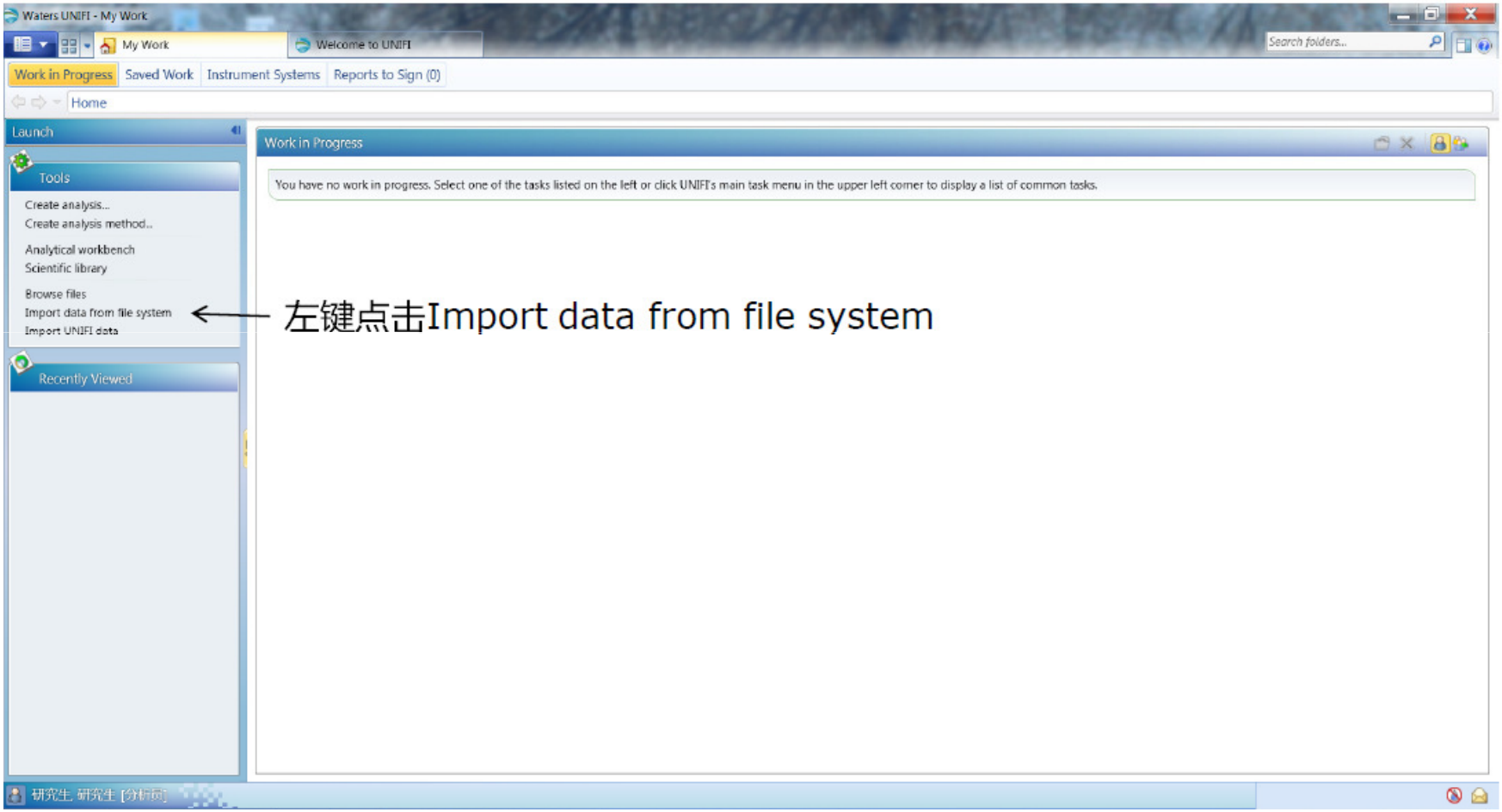
基本流程

Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

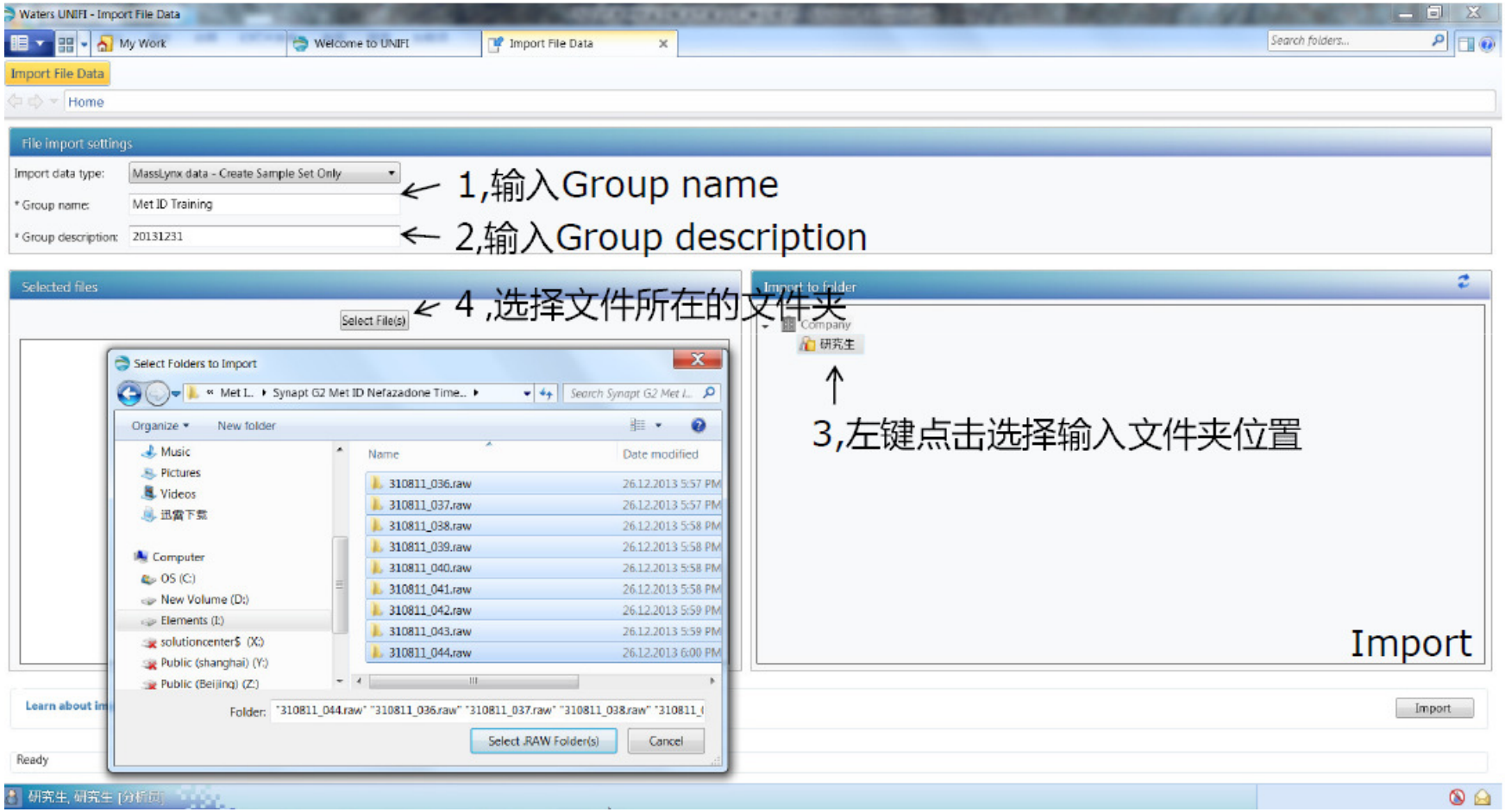
- 导入数据
- 创建分析方法
- 创建分析
- 处理数据
- 浏览结果
- 打印报告

导入masslynx数据

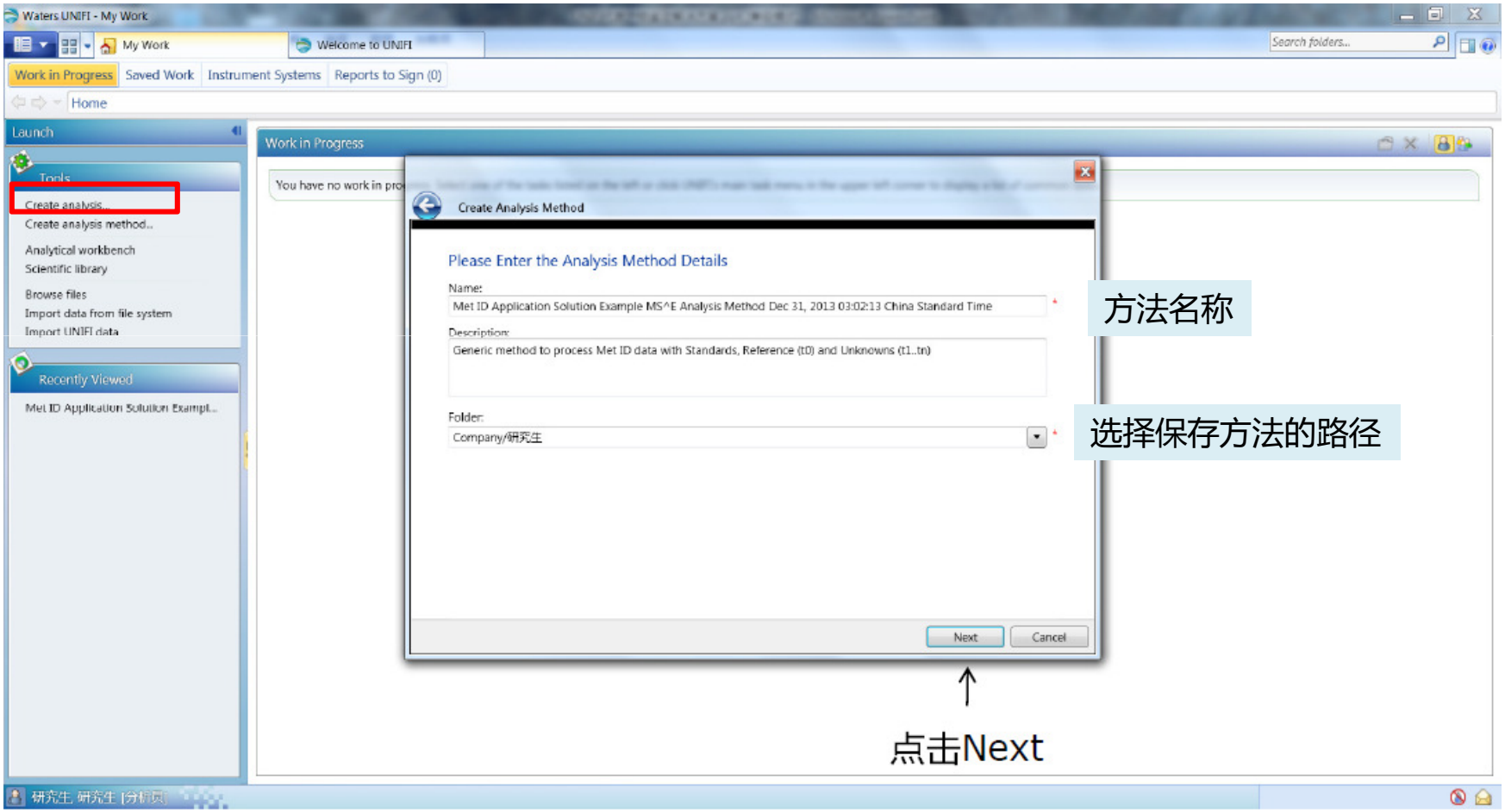
Waters
THE SCIENCE OF WHAT'S POSSIBLE.®



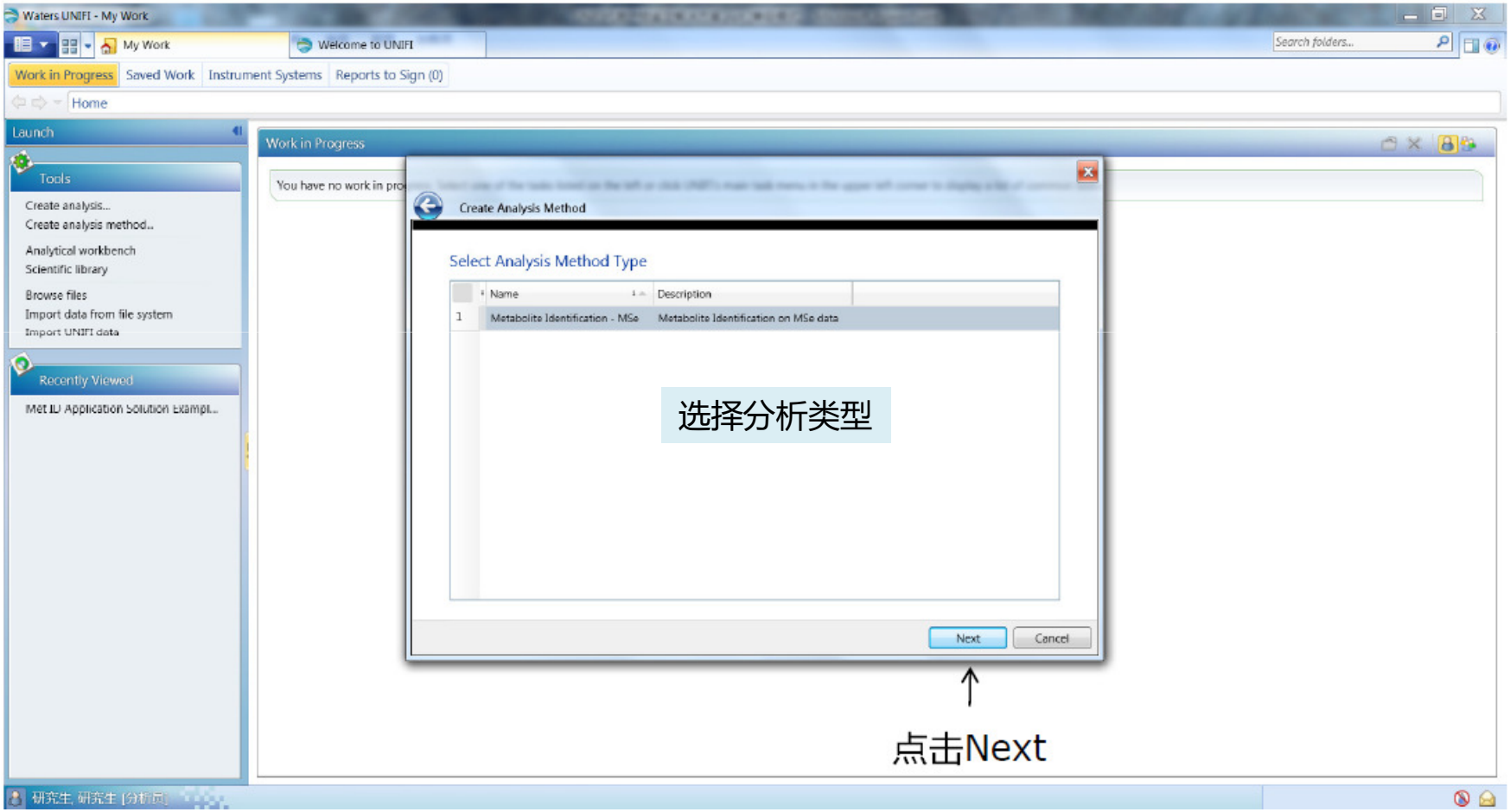
导入masslynx数据



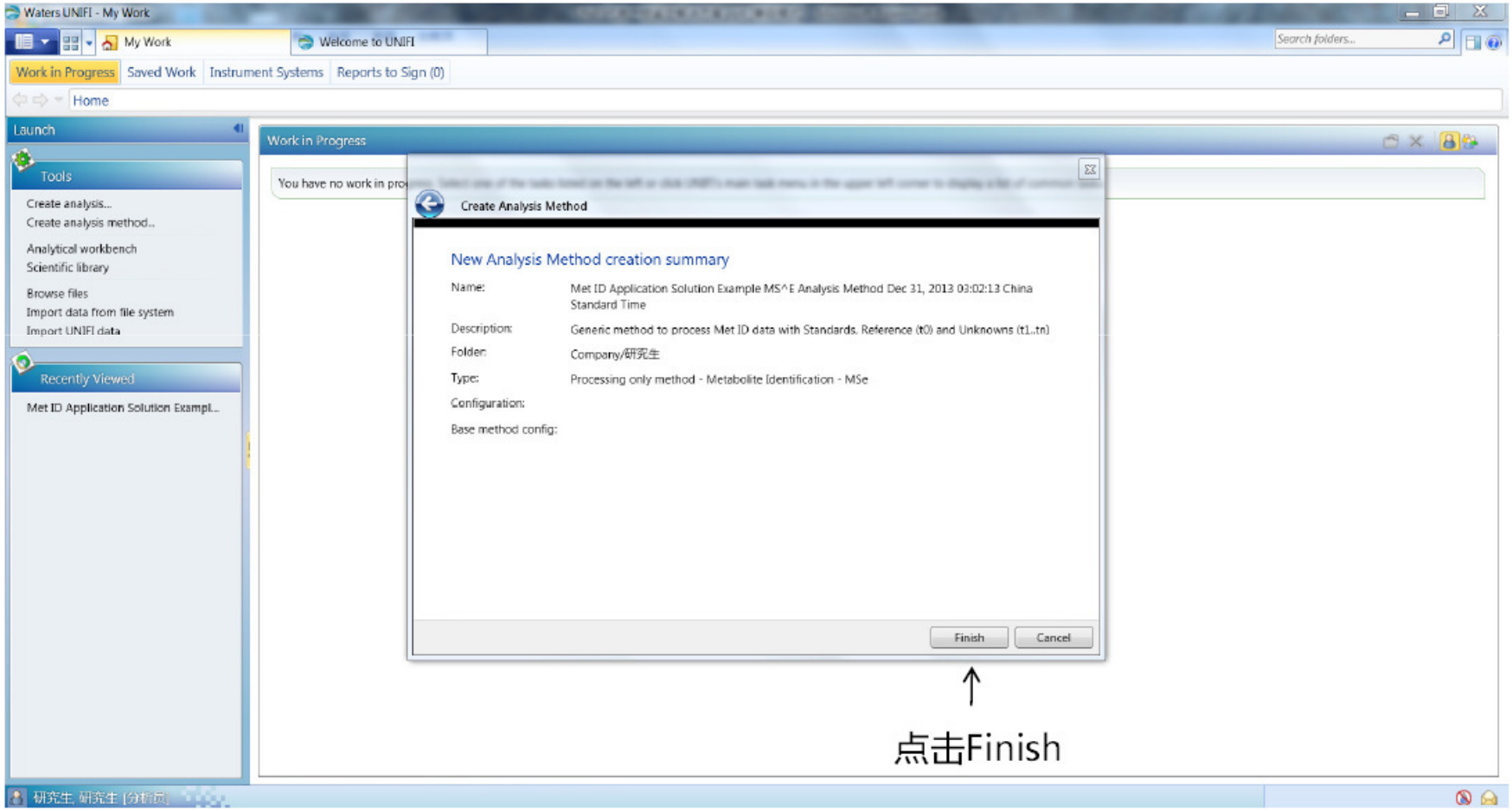
创建分析方法



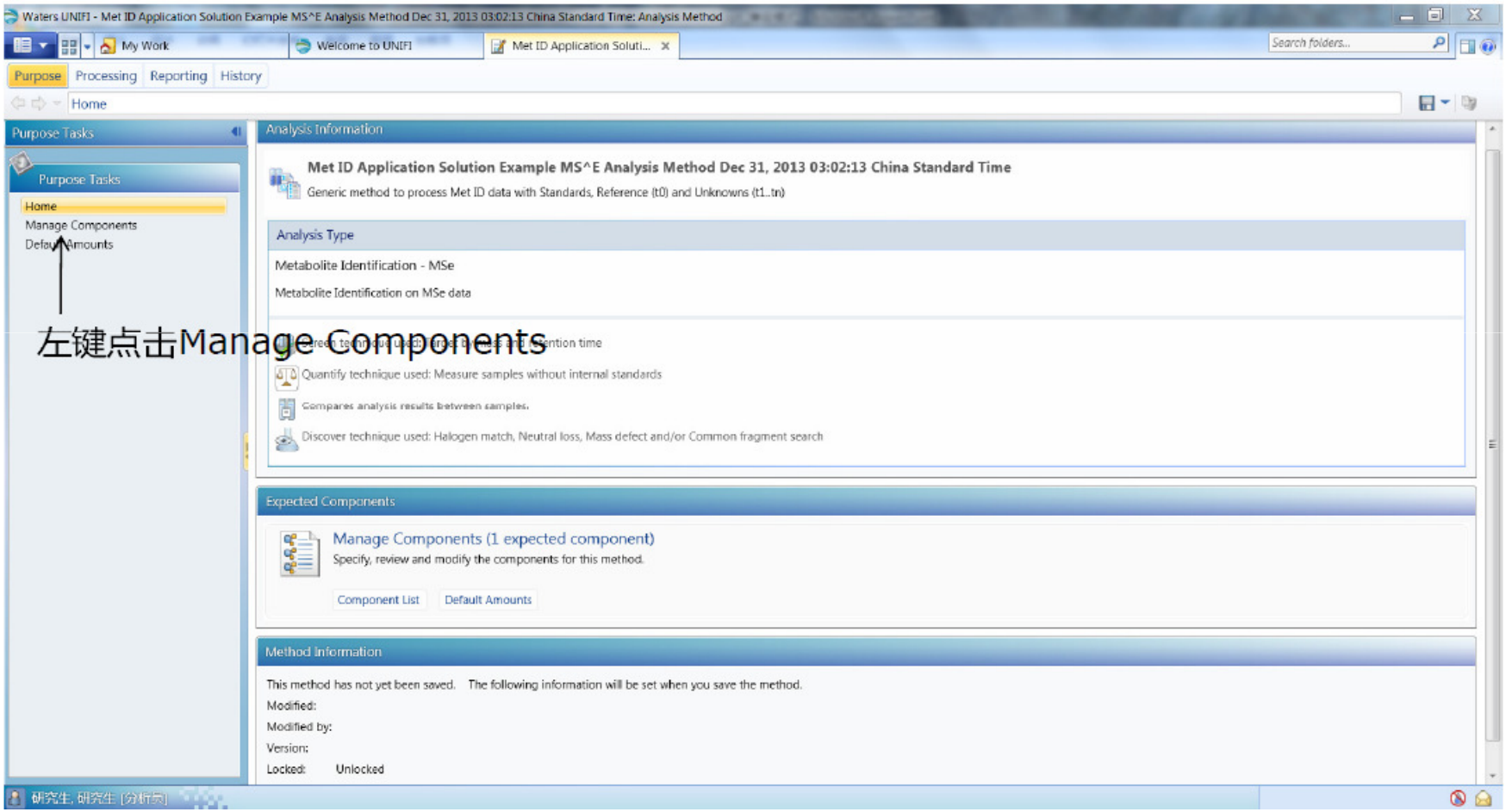
创建分析方法



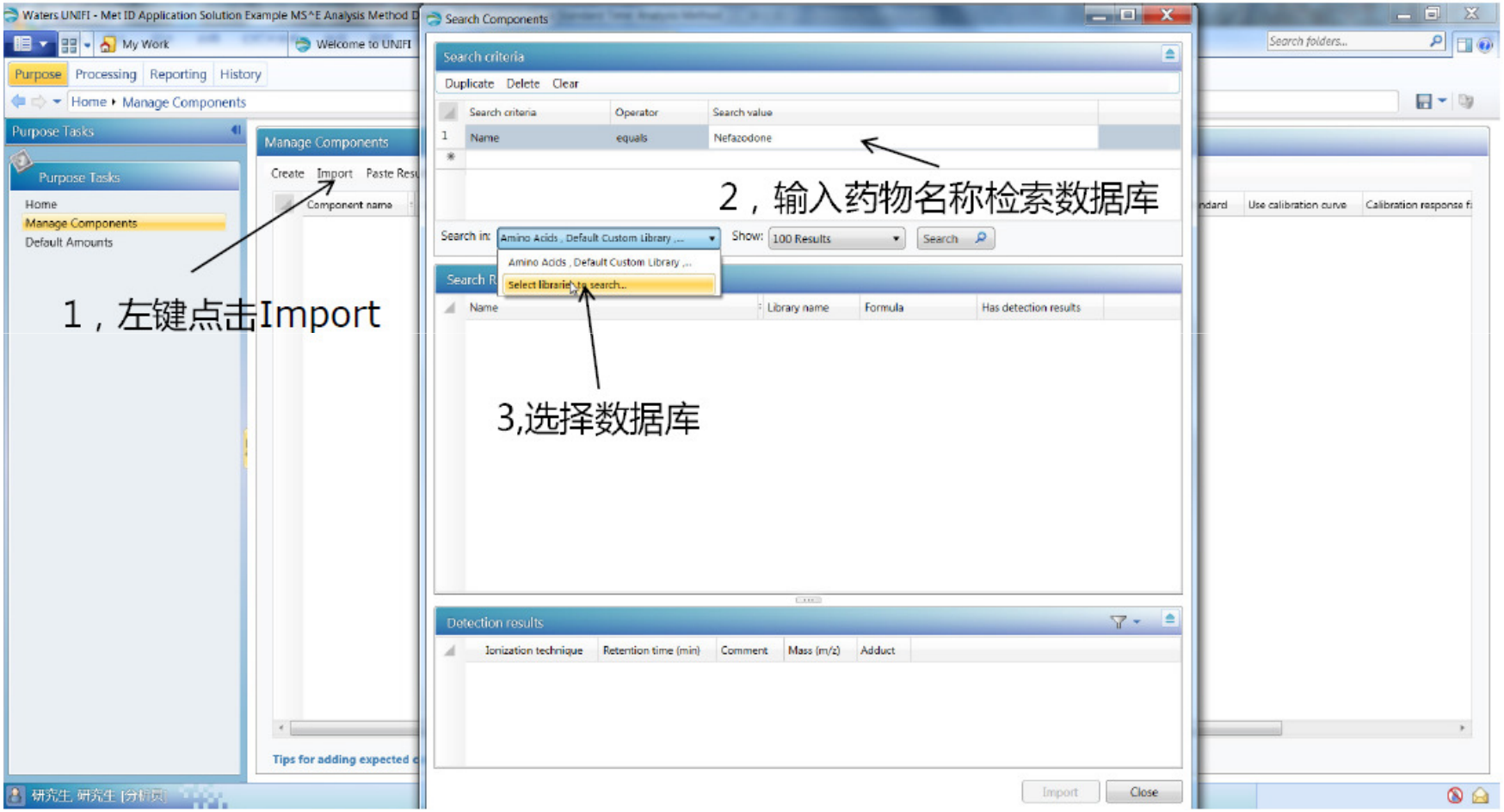
创建分析方法



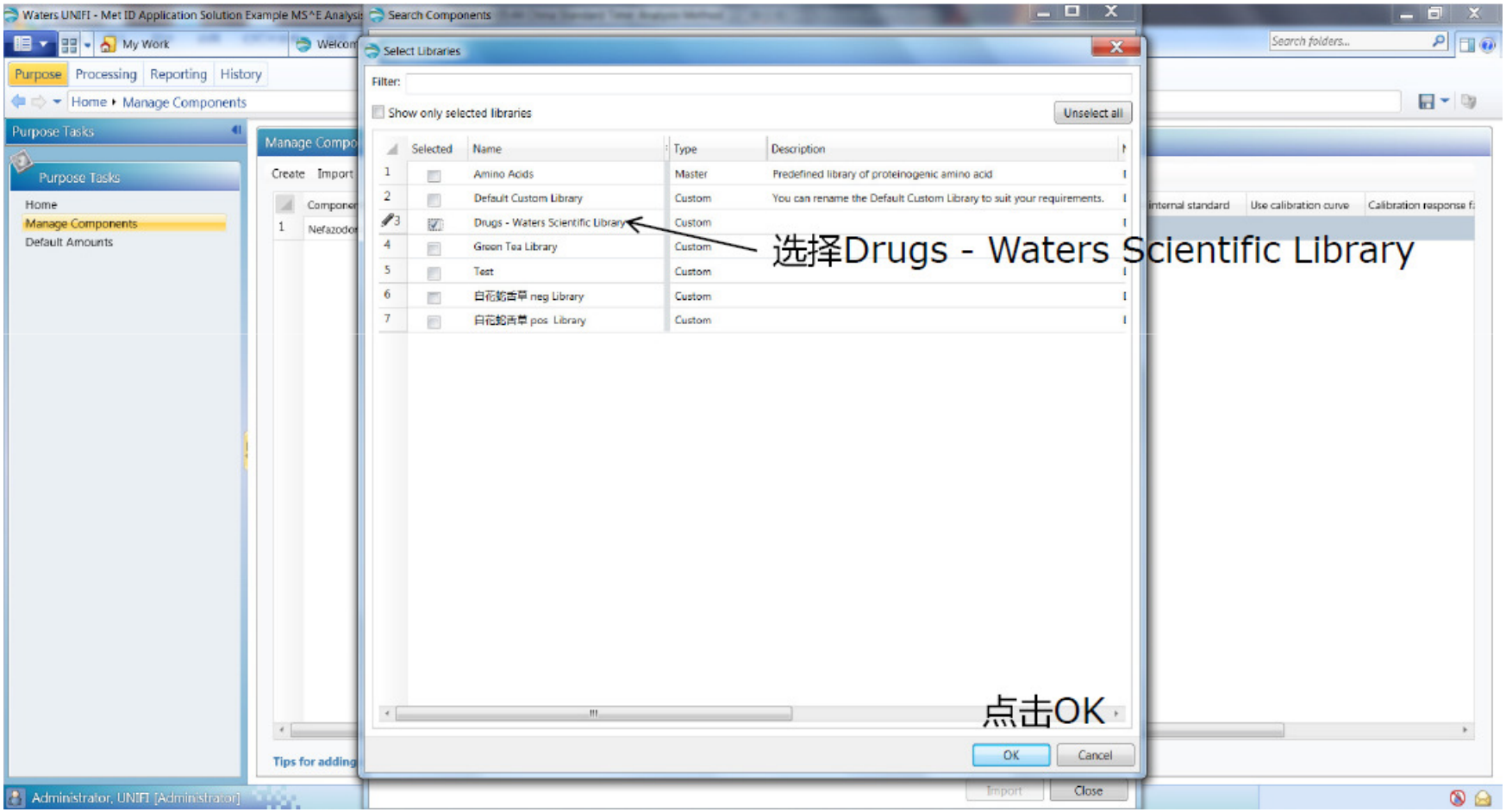
编辑原药信息



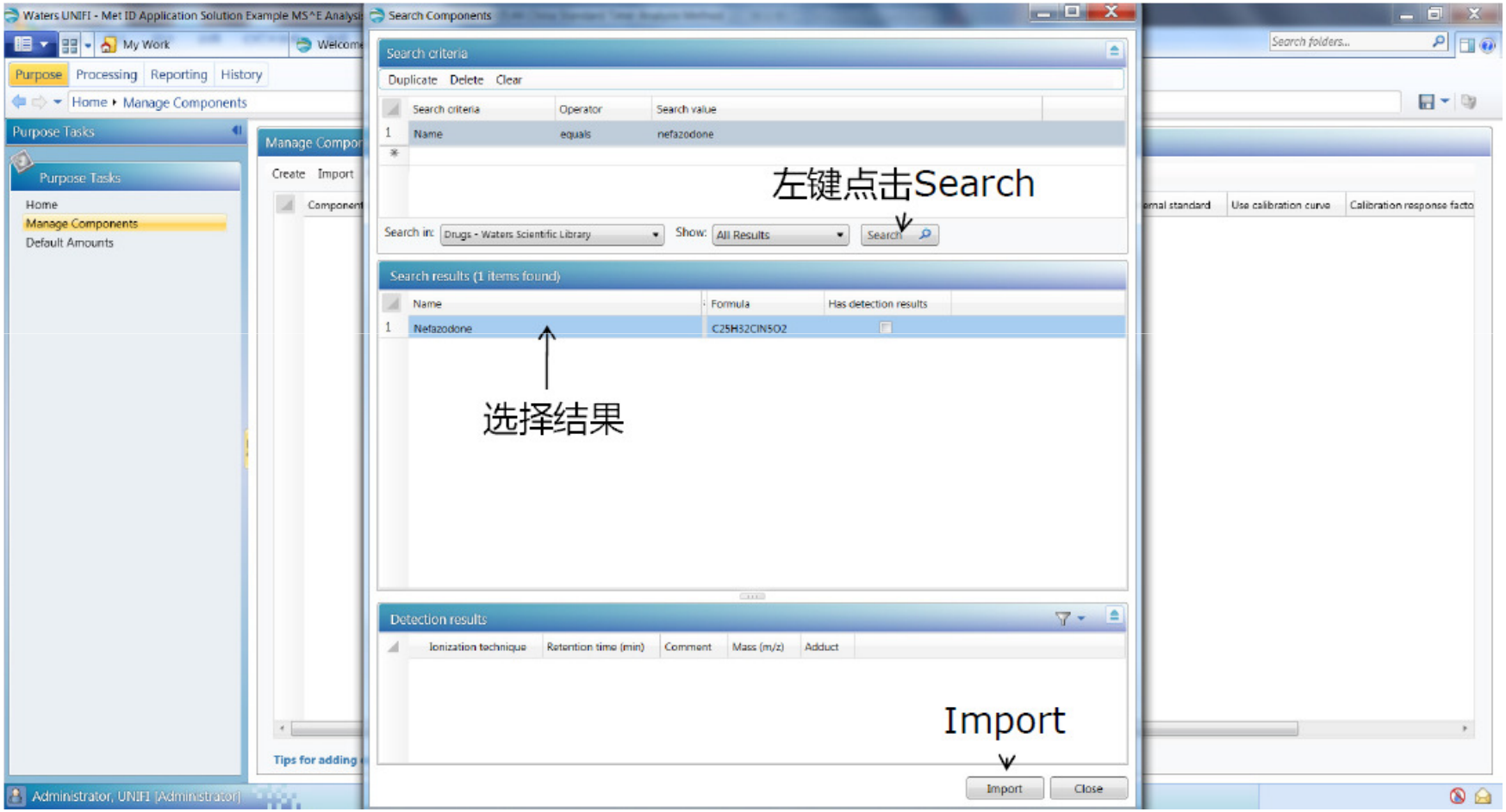
从数据库导入

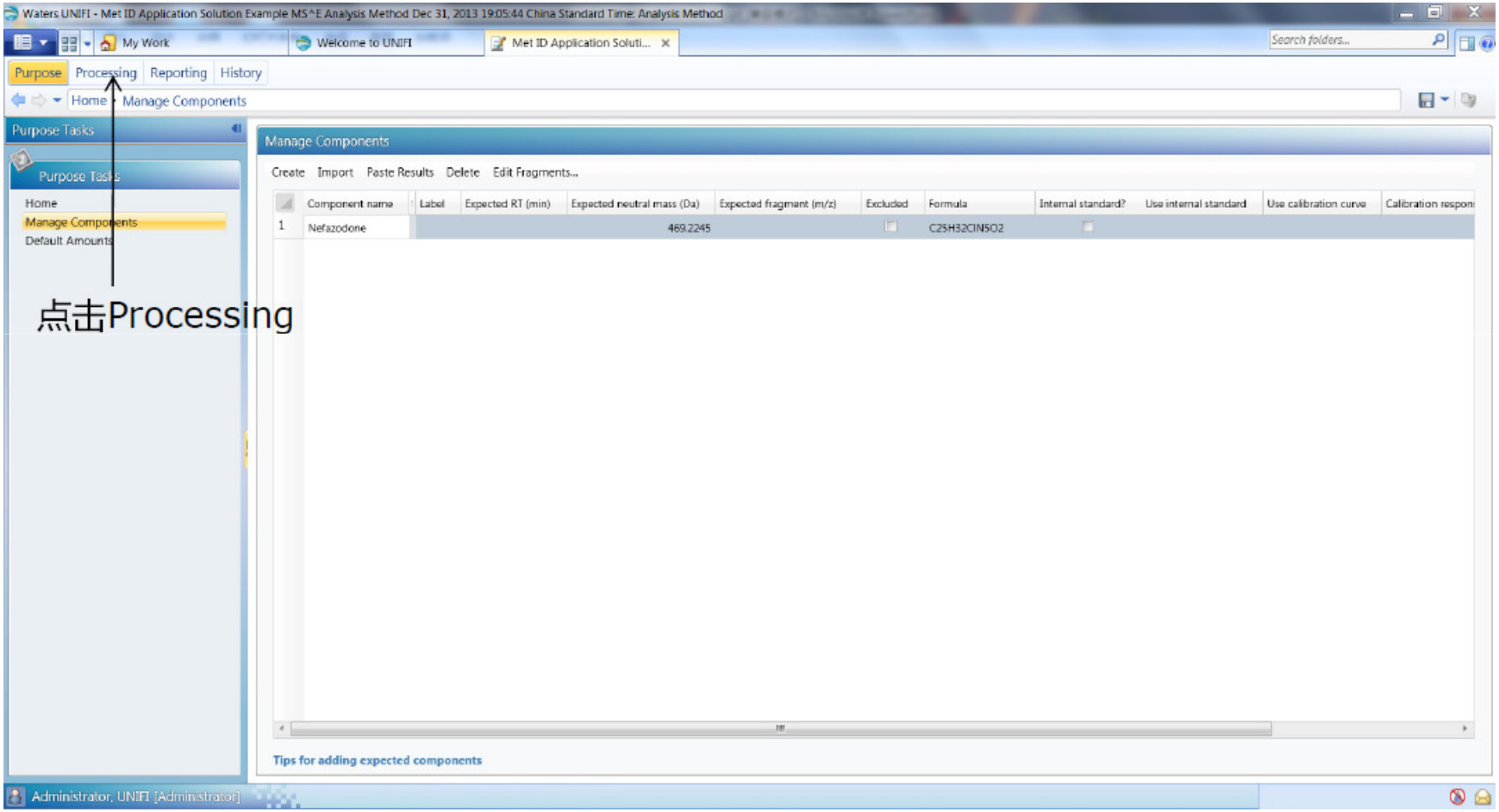


从数据库导入

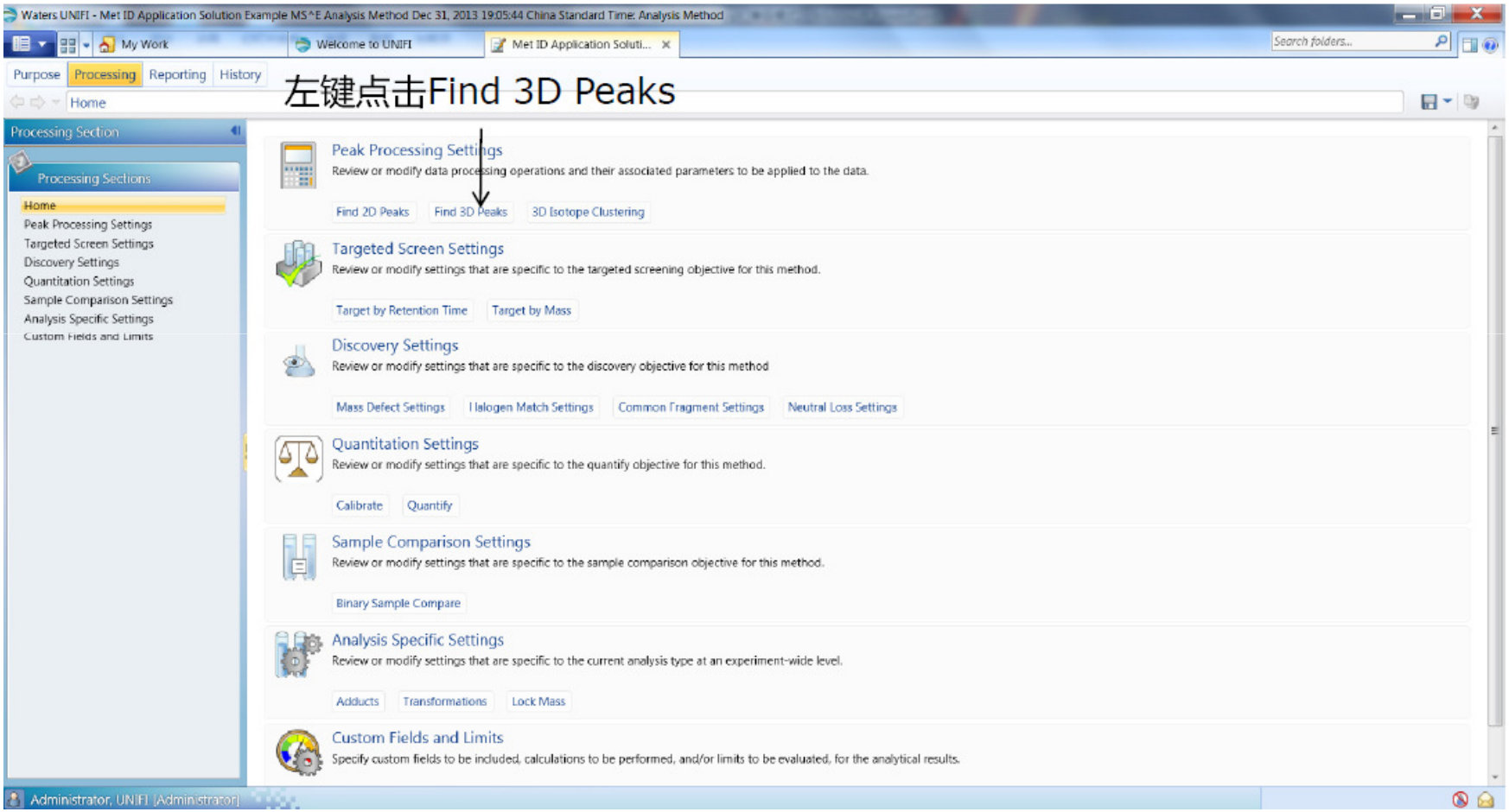


从数据库导入

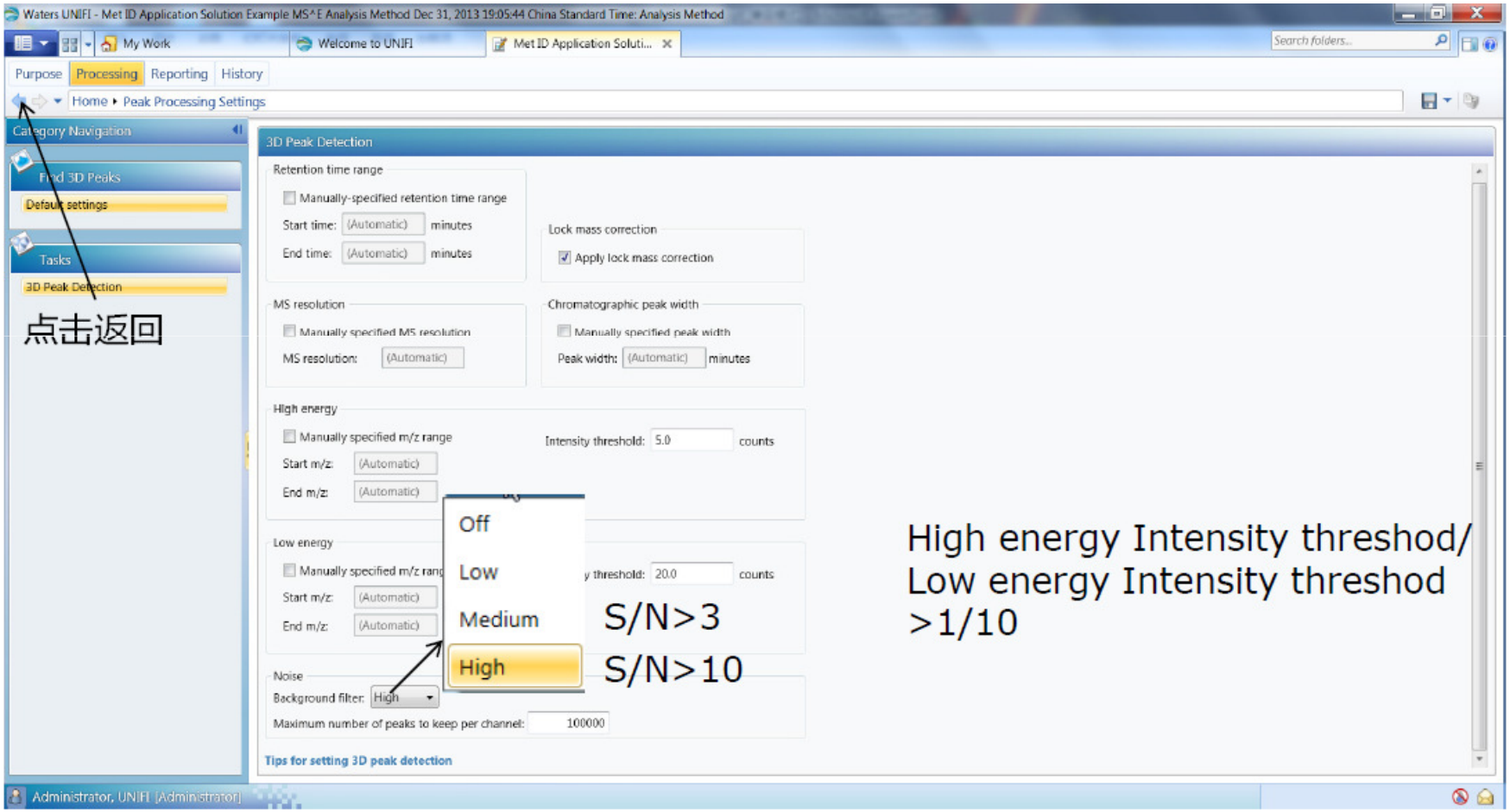




设置峰提取参数

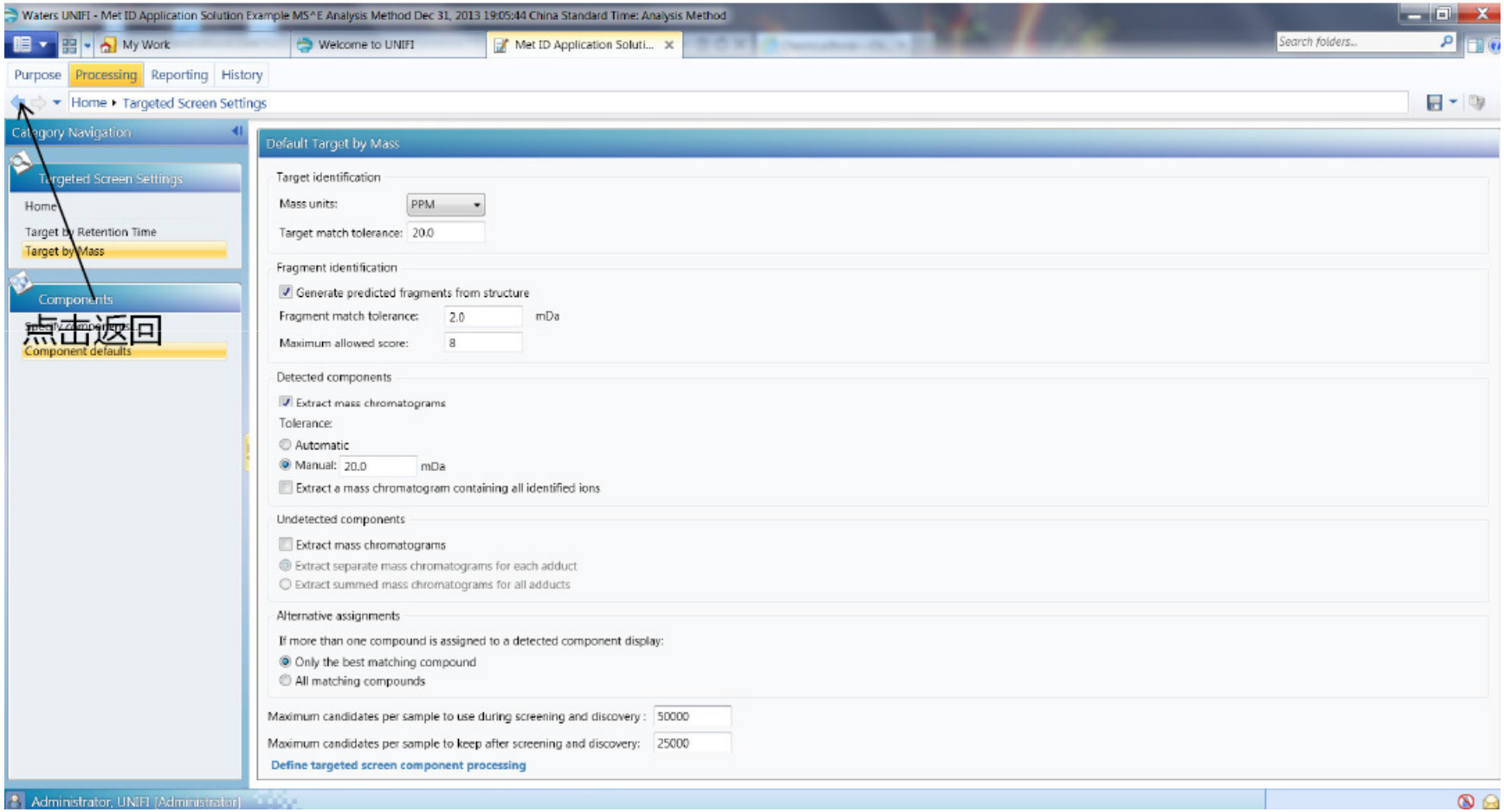


设置峰提取参数

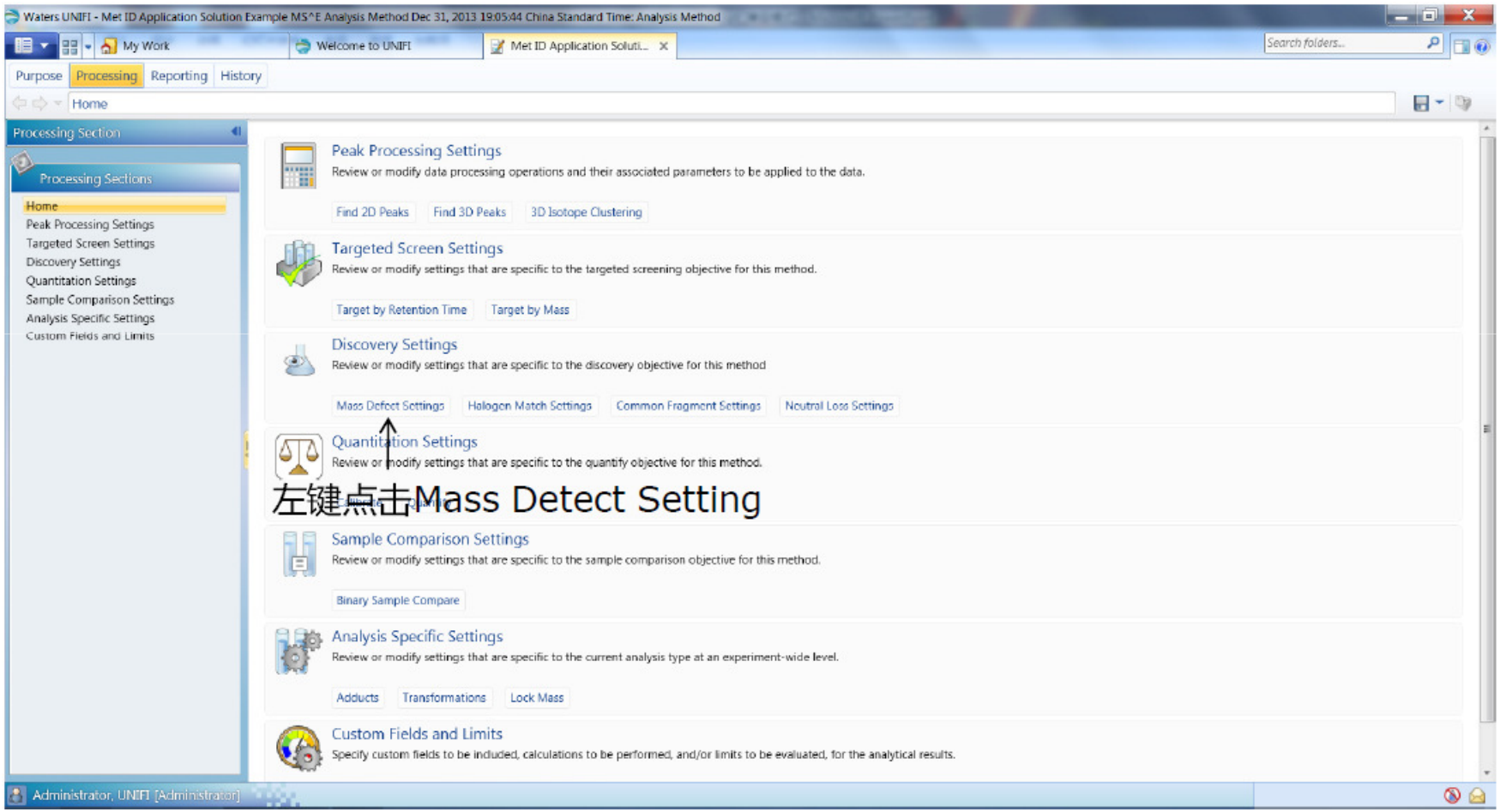


设置质量匹配参数

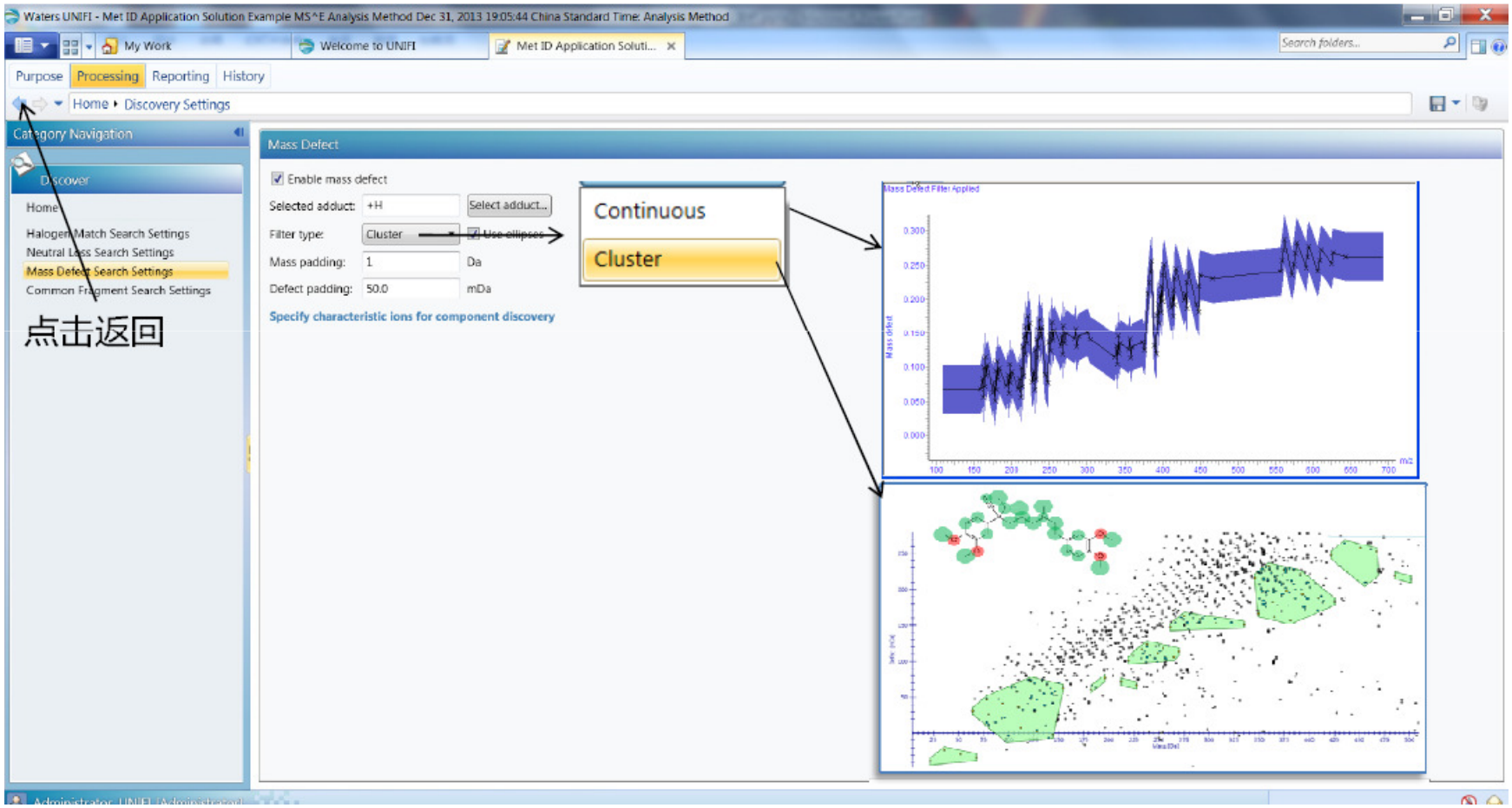
设置质量匹配参数



设置质量亏损（MDF)参数

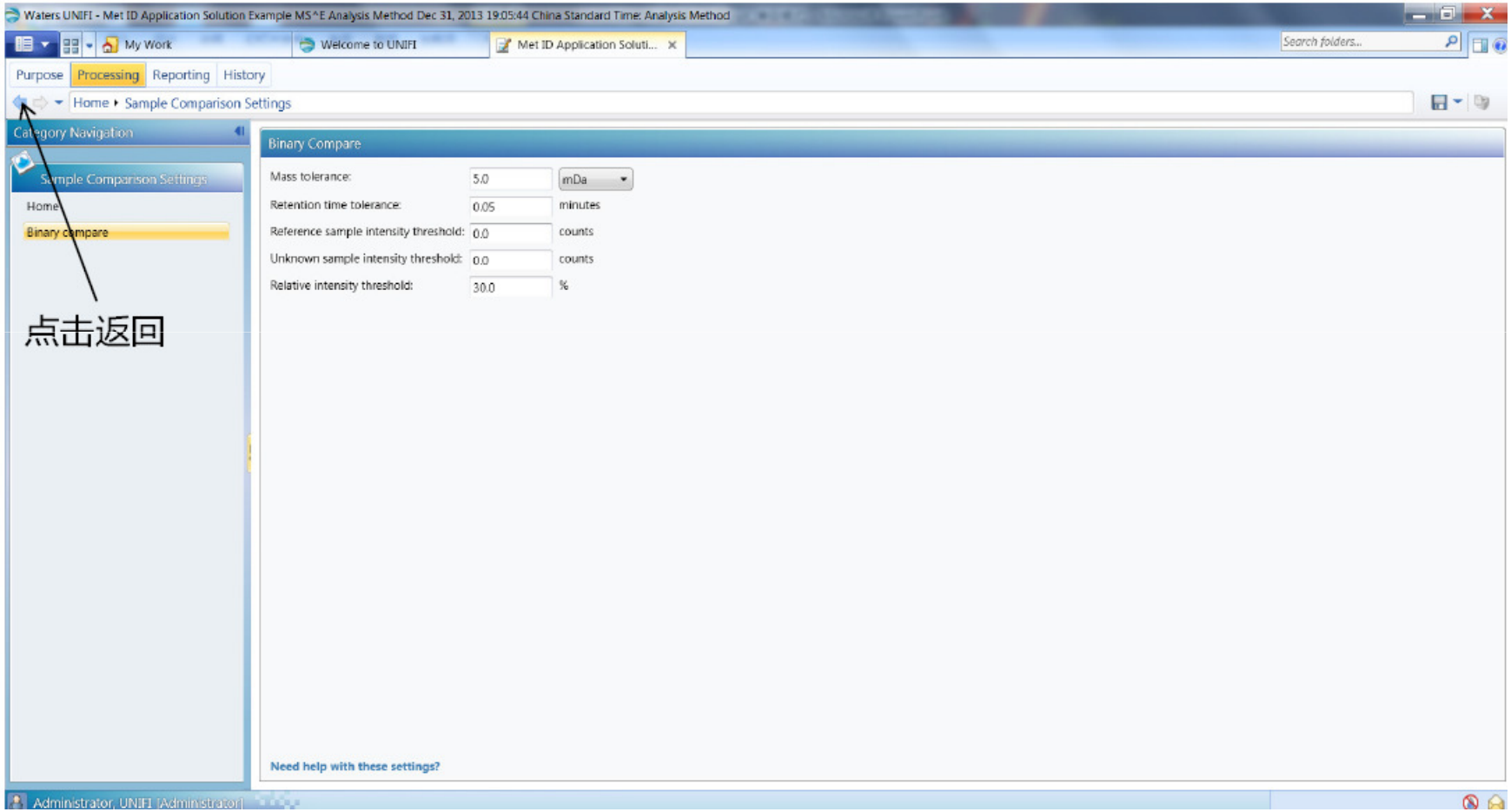


设置质量亏损参数

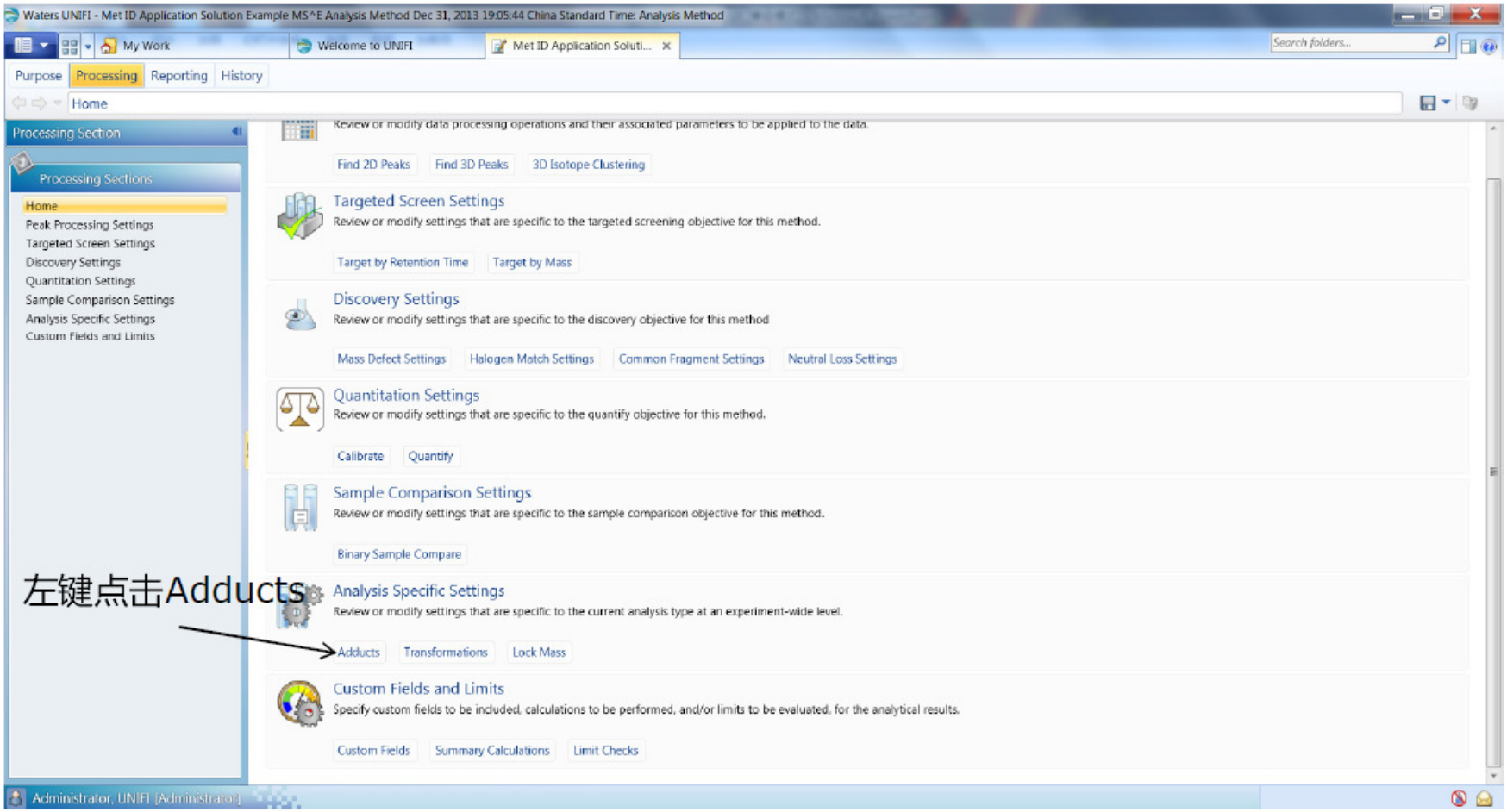


设置二元比较方法

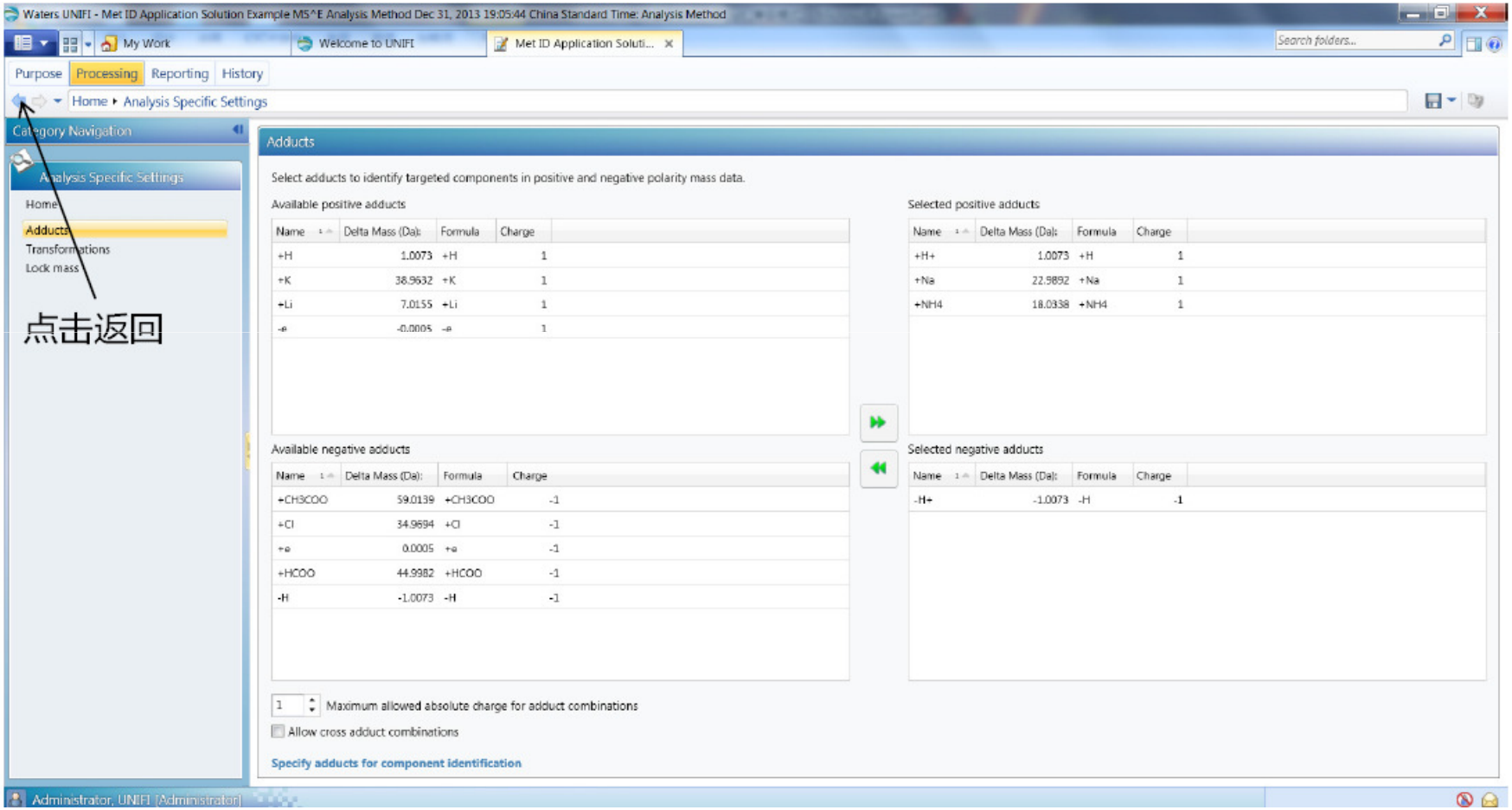
二元比较



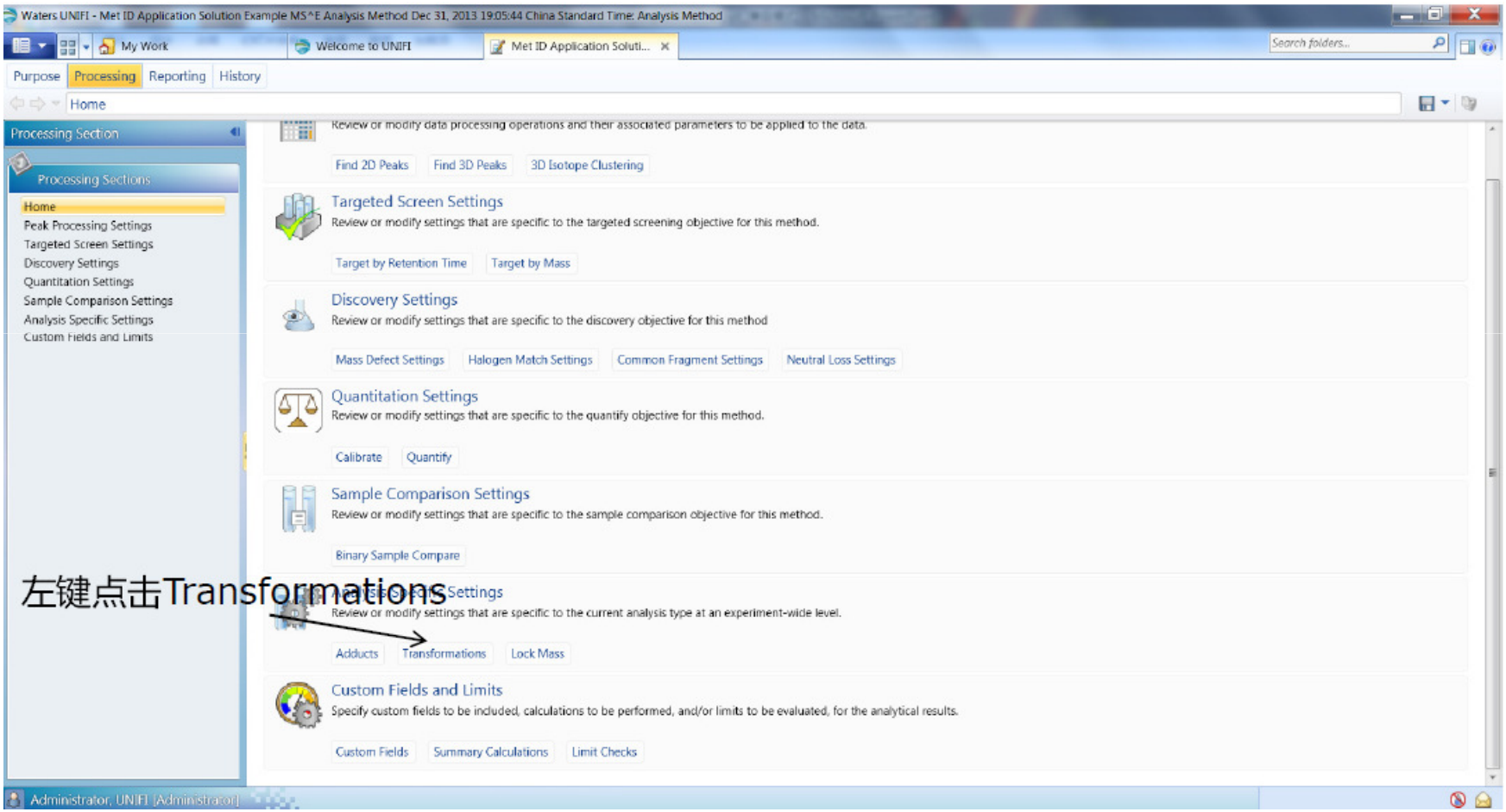
设置加和离子



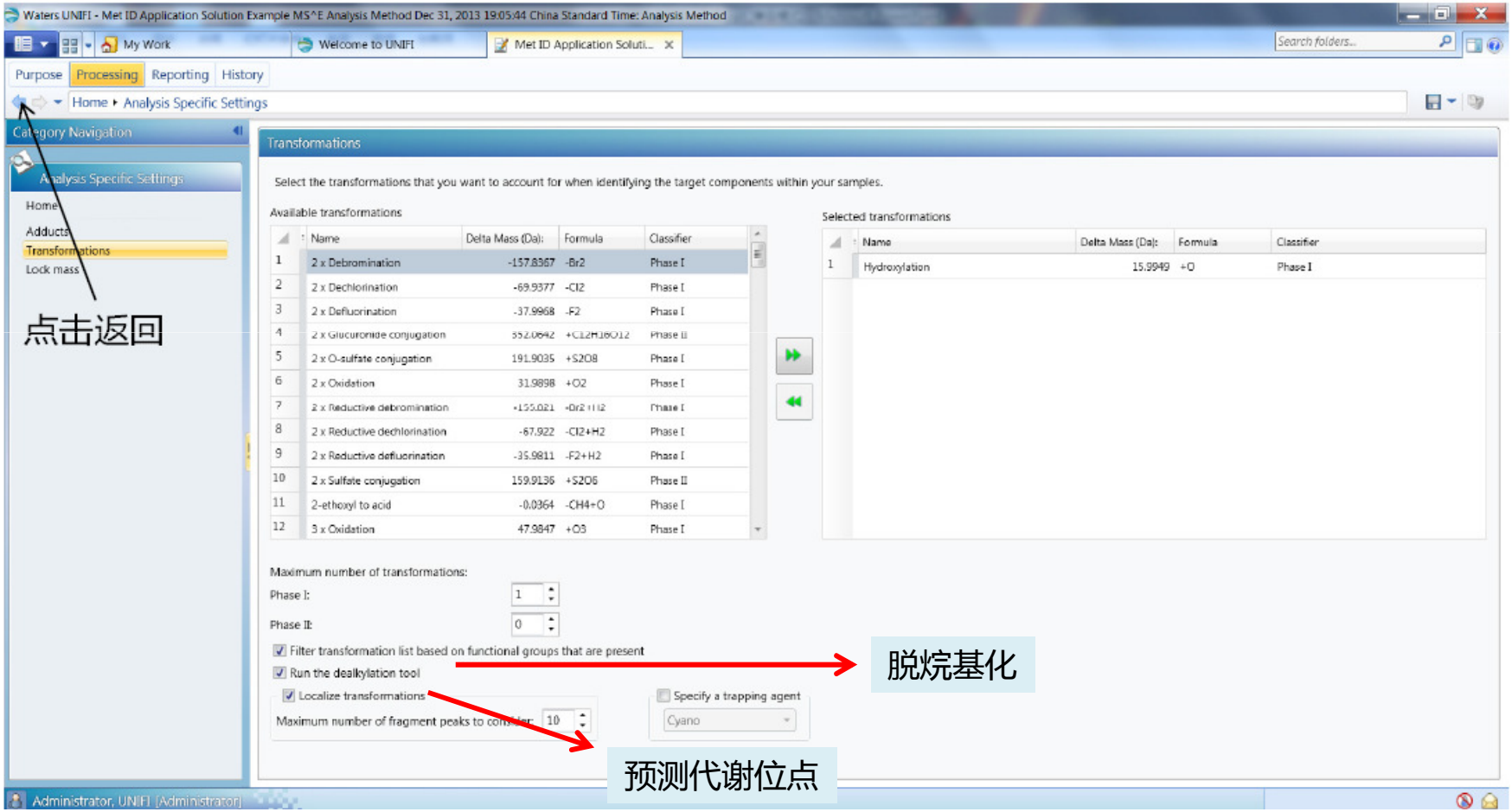
加和离子



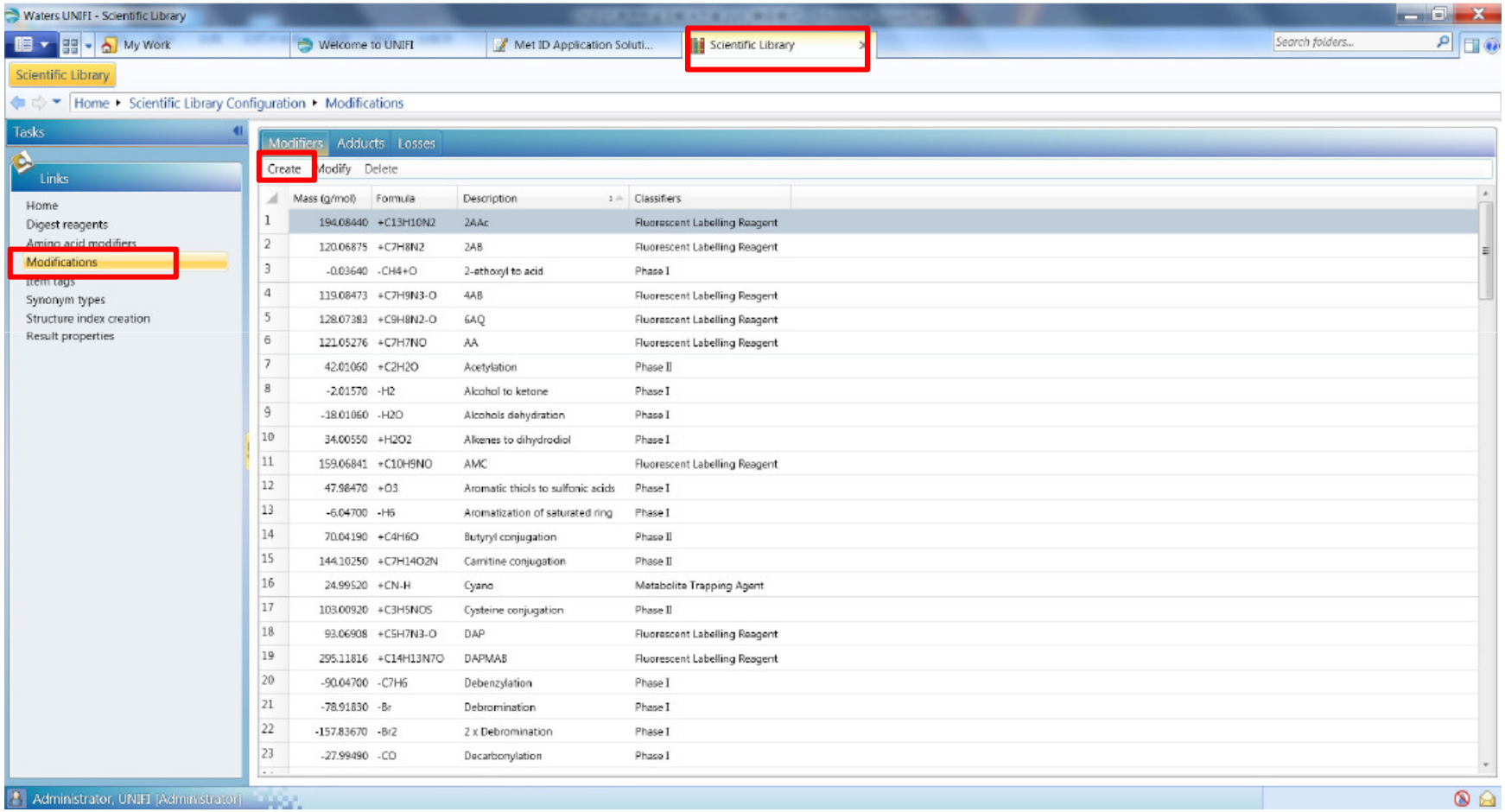
编辑代谢基团



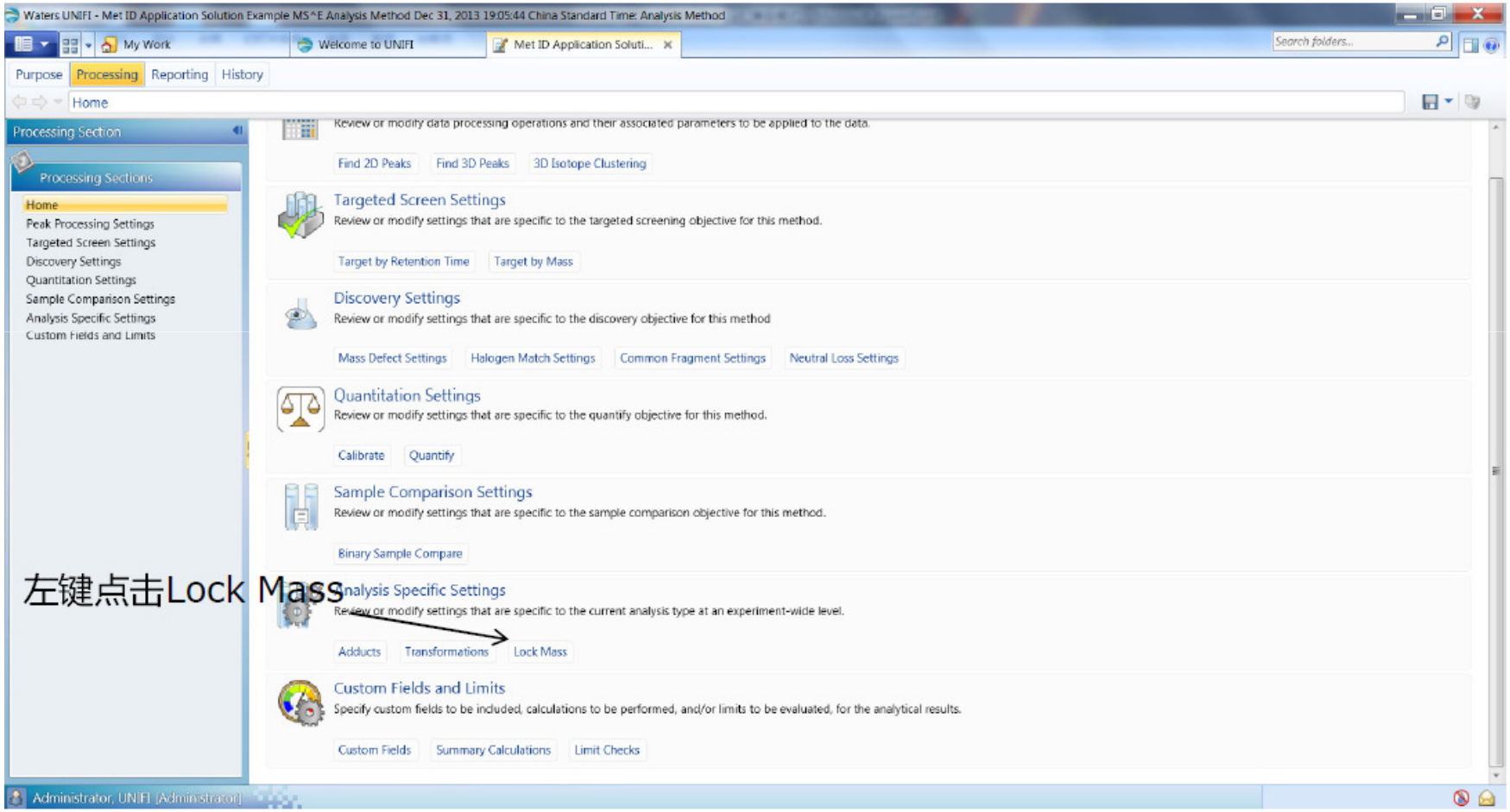
编辑代谢基团



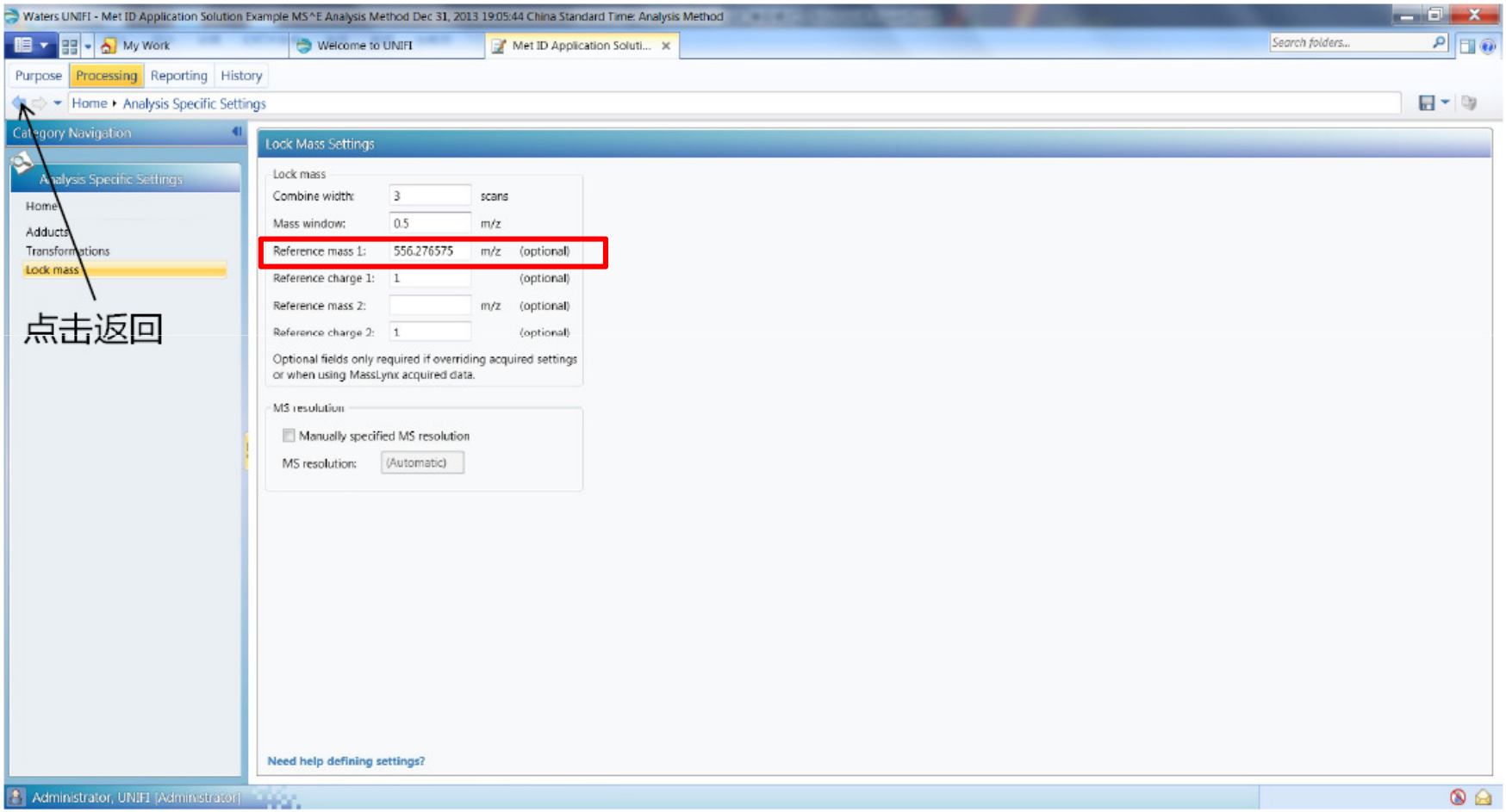
添加代谢基团



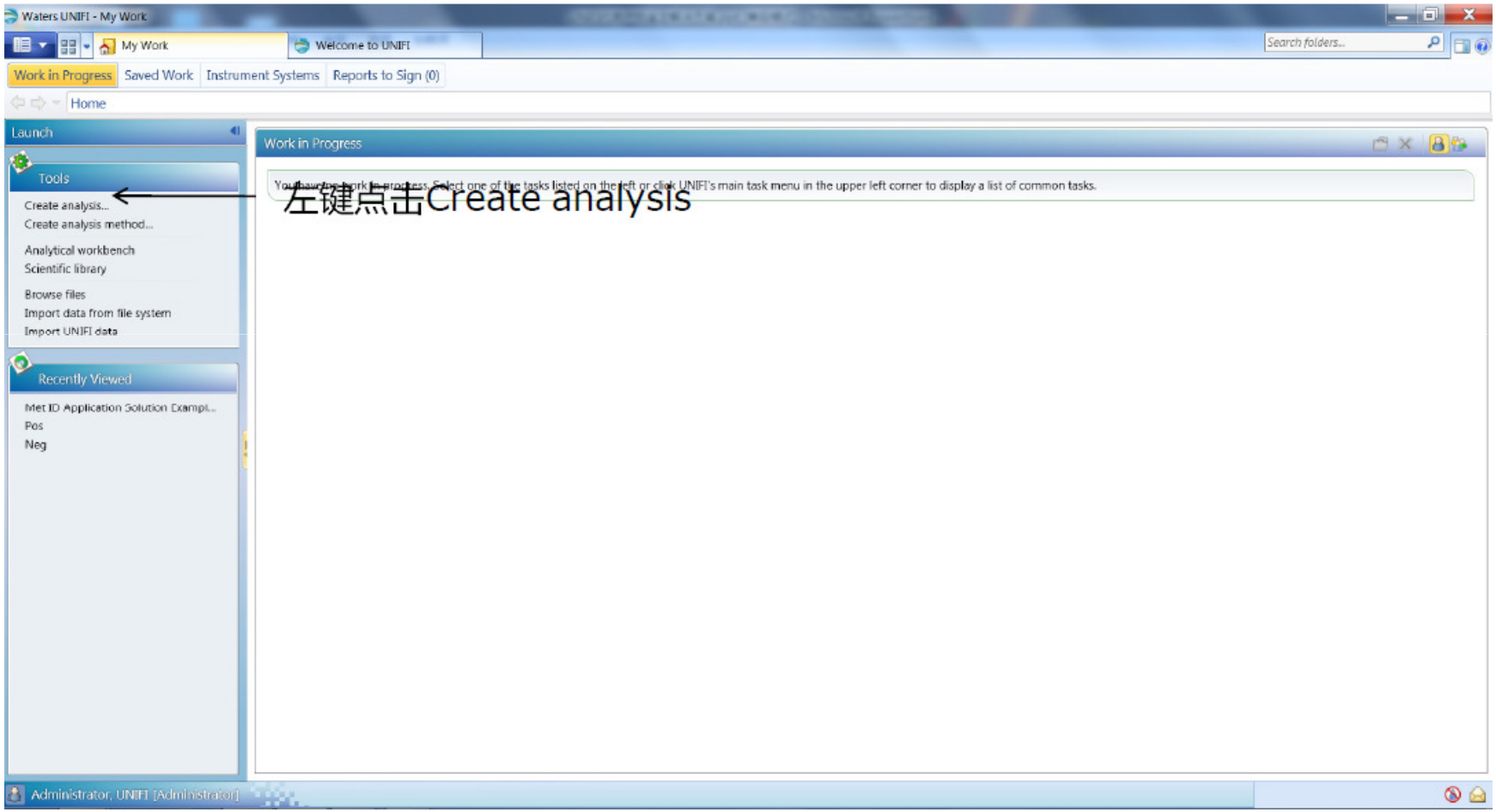
设置lockmass

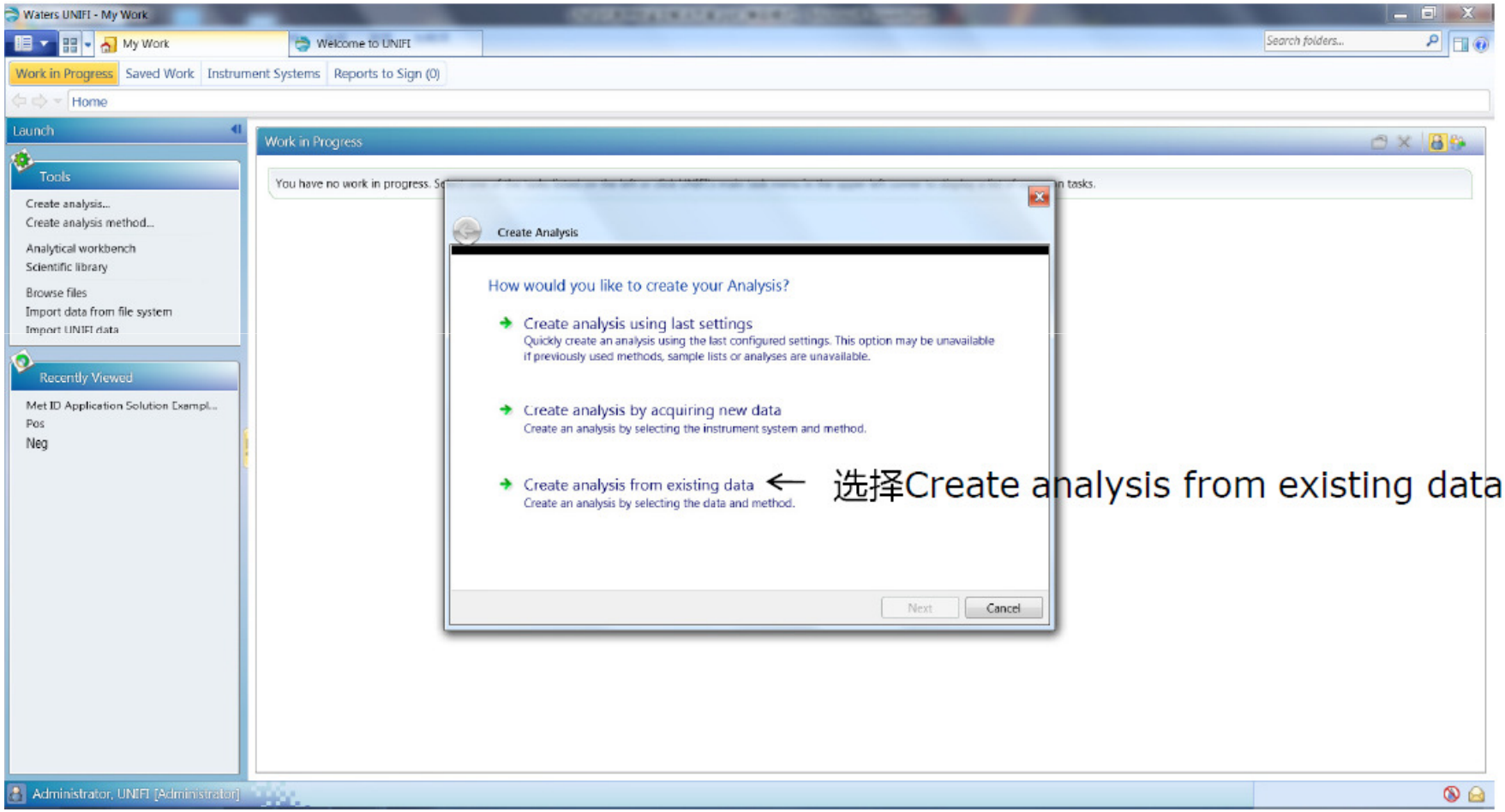


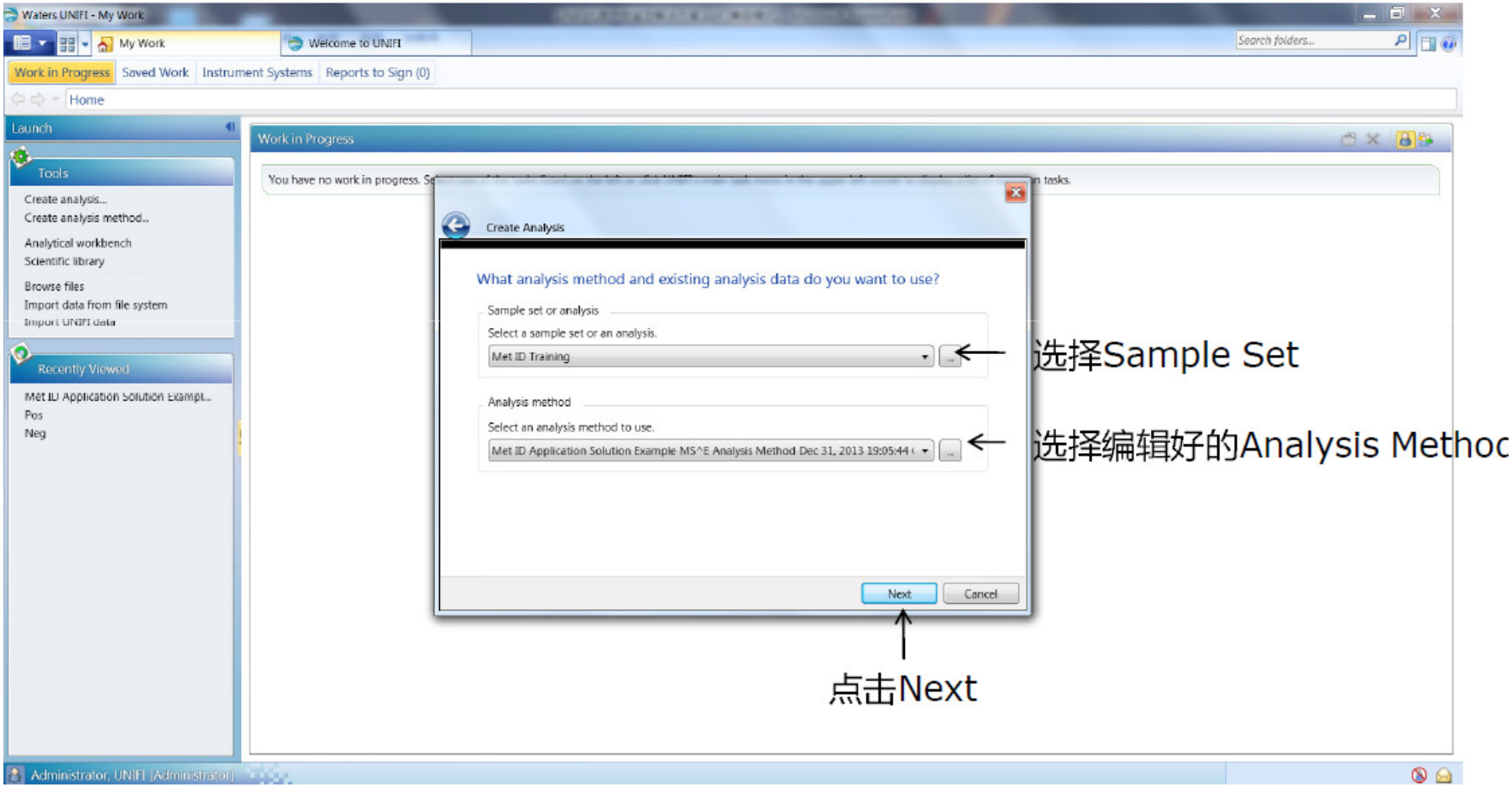
左键点击Lock Mass

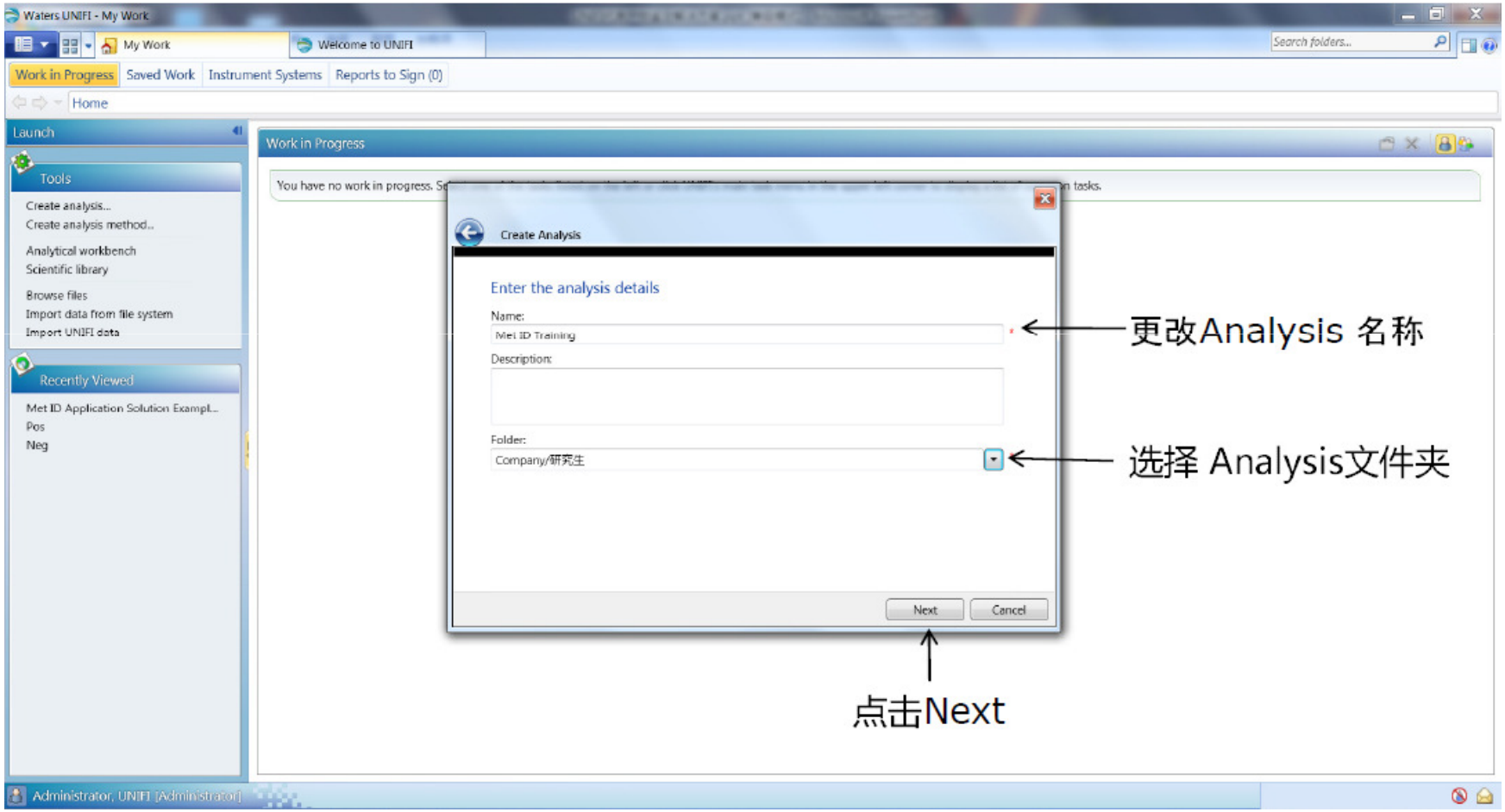


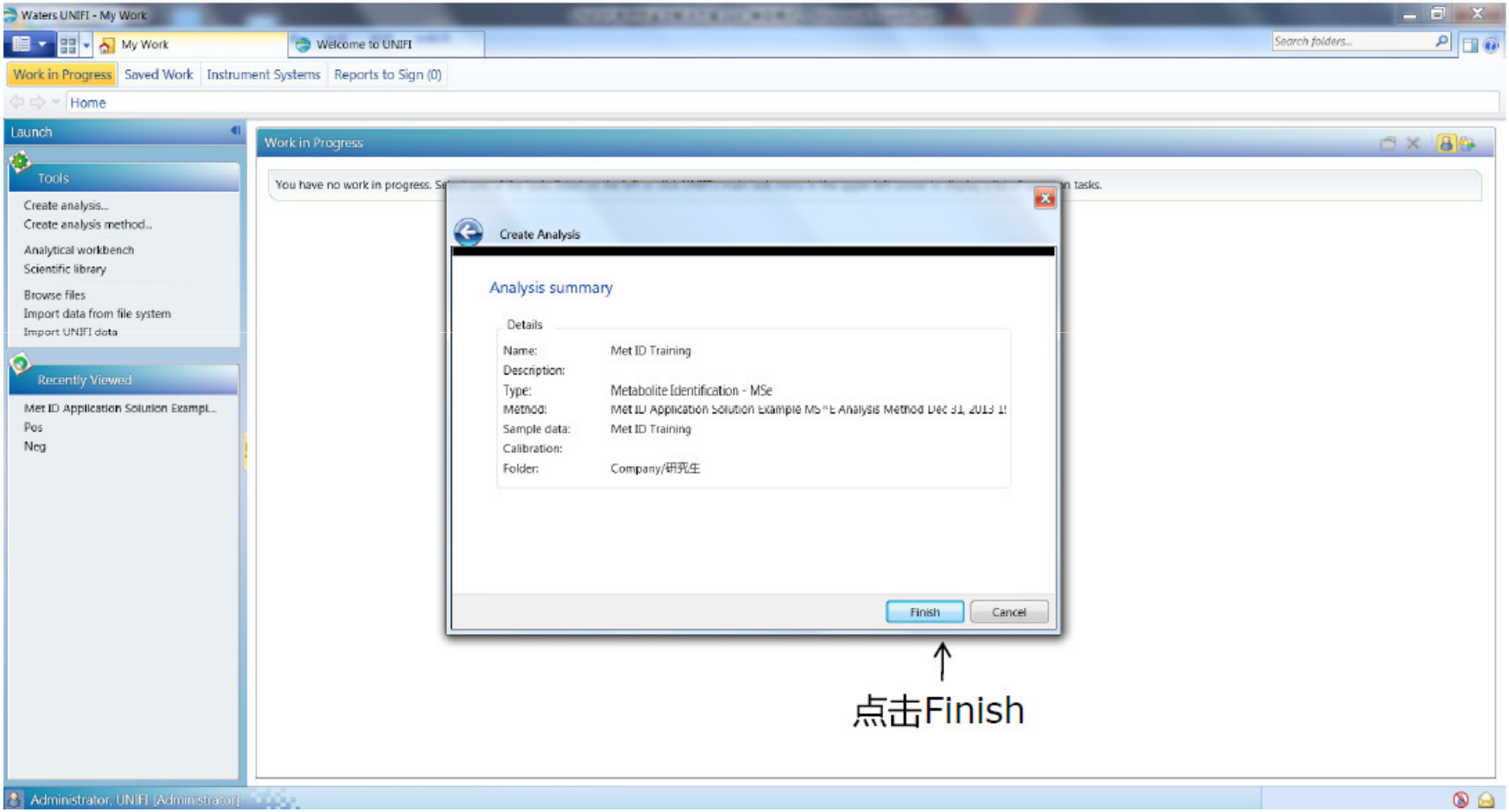
创建分析

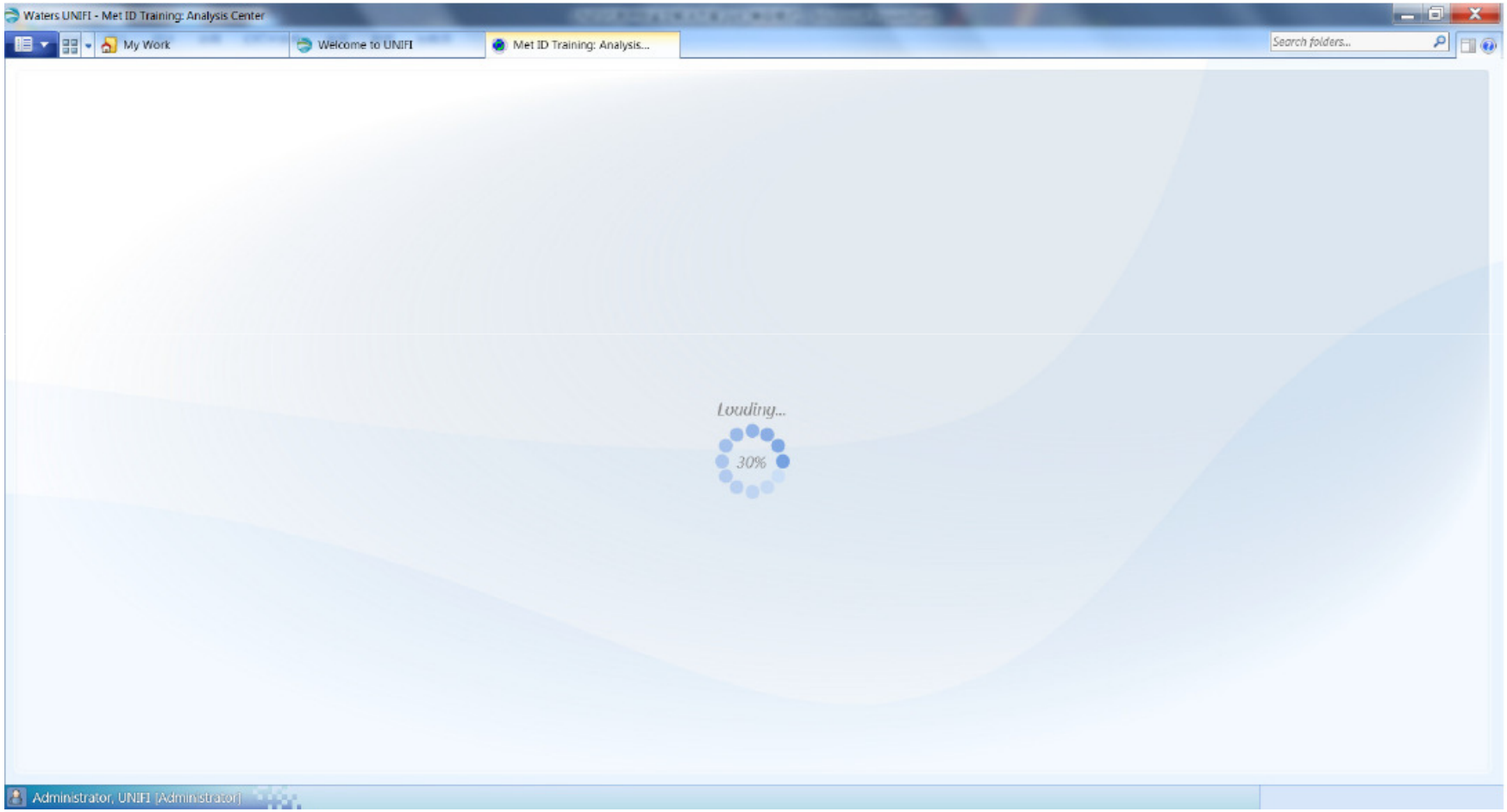




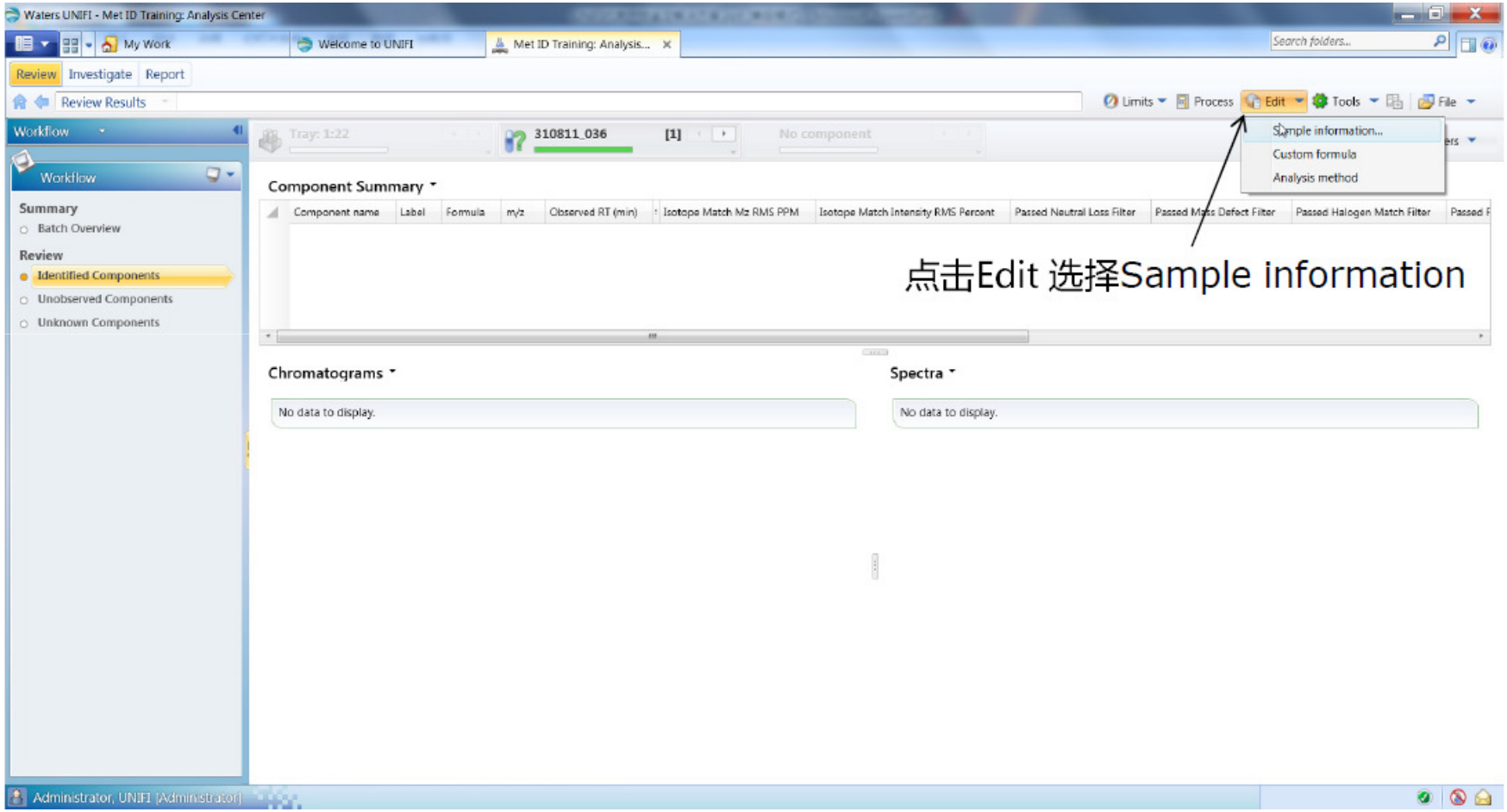


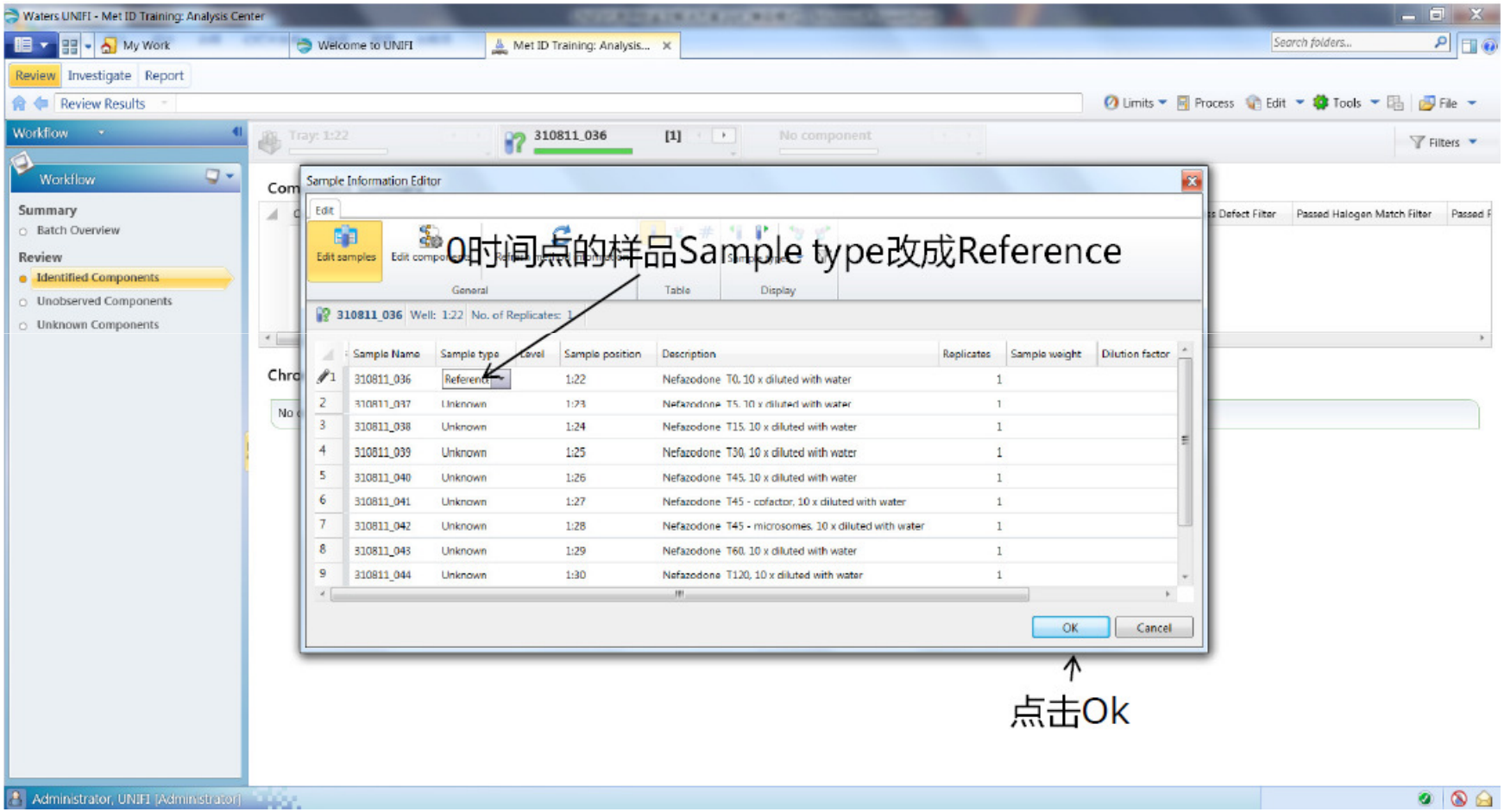




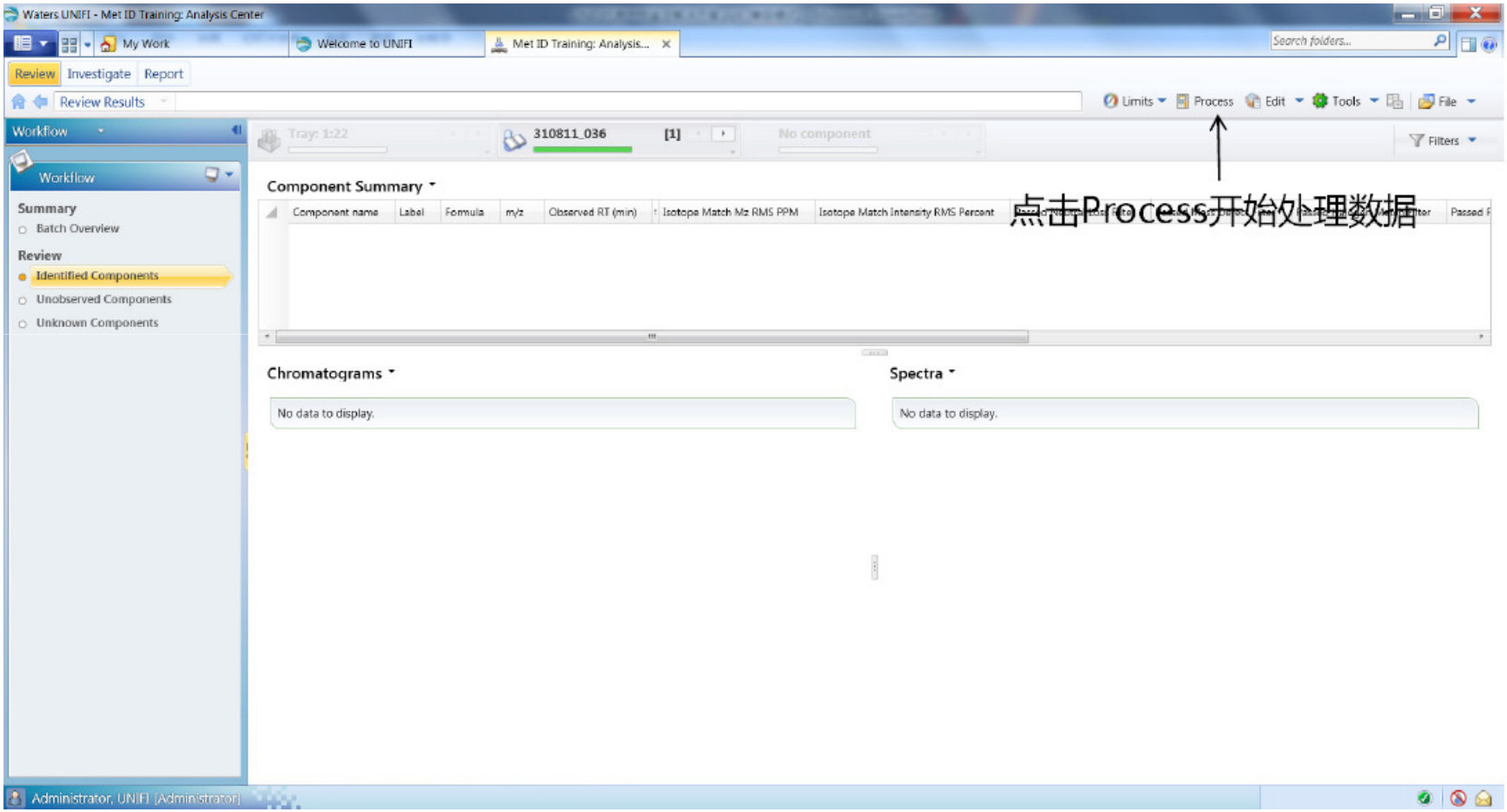


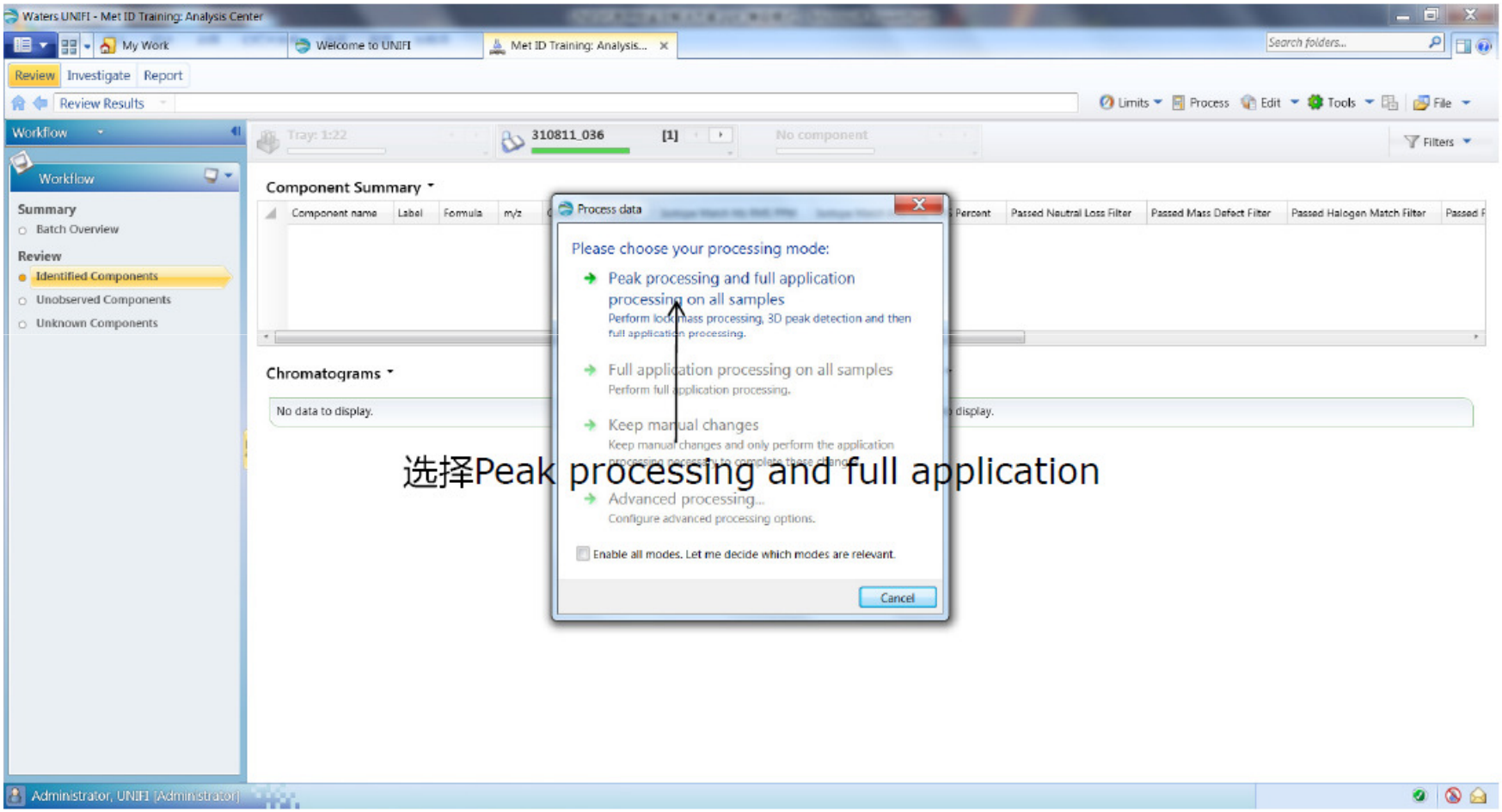
编辑样品信息



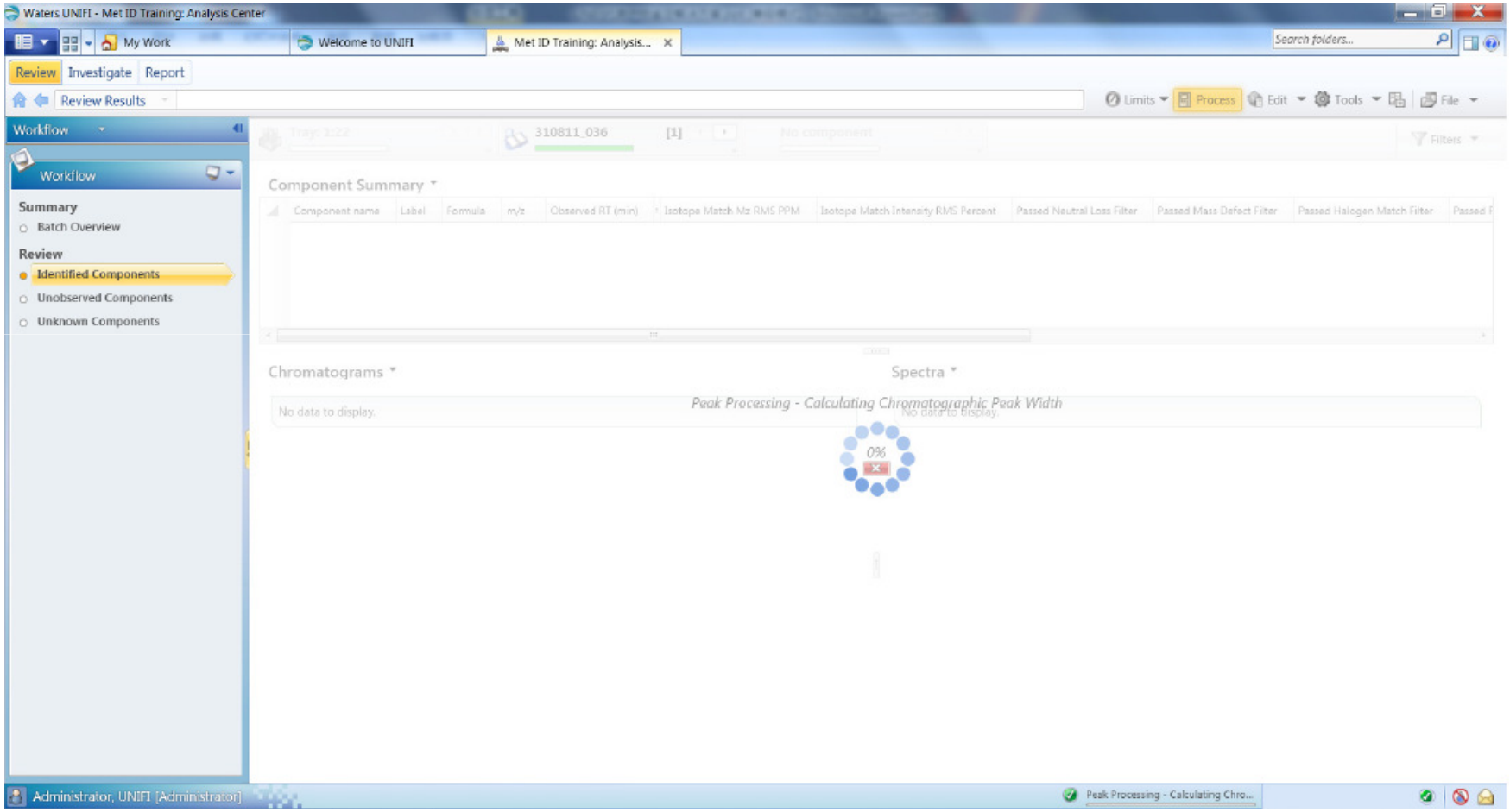


开始处理数据

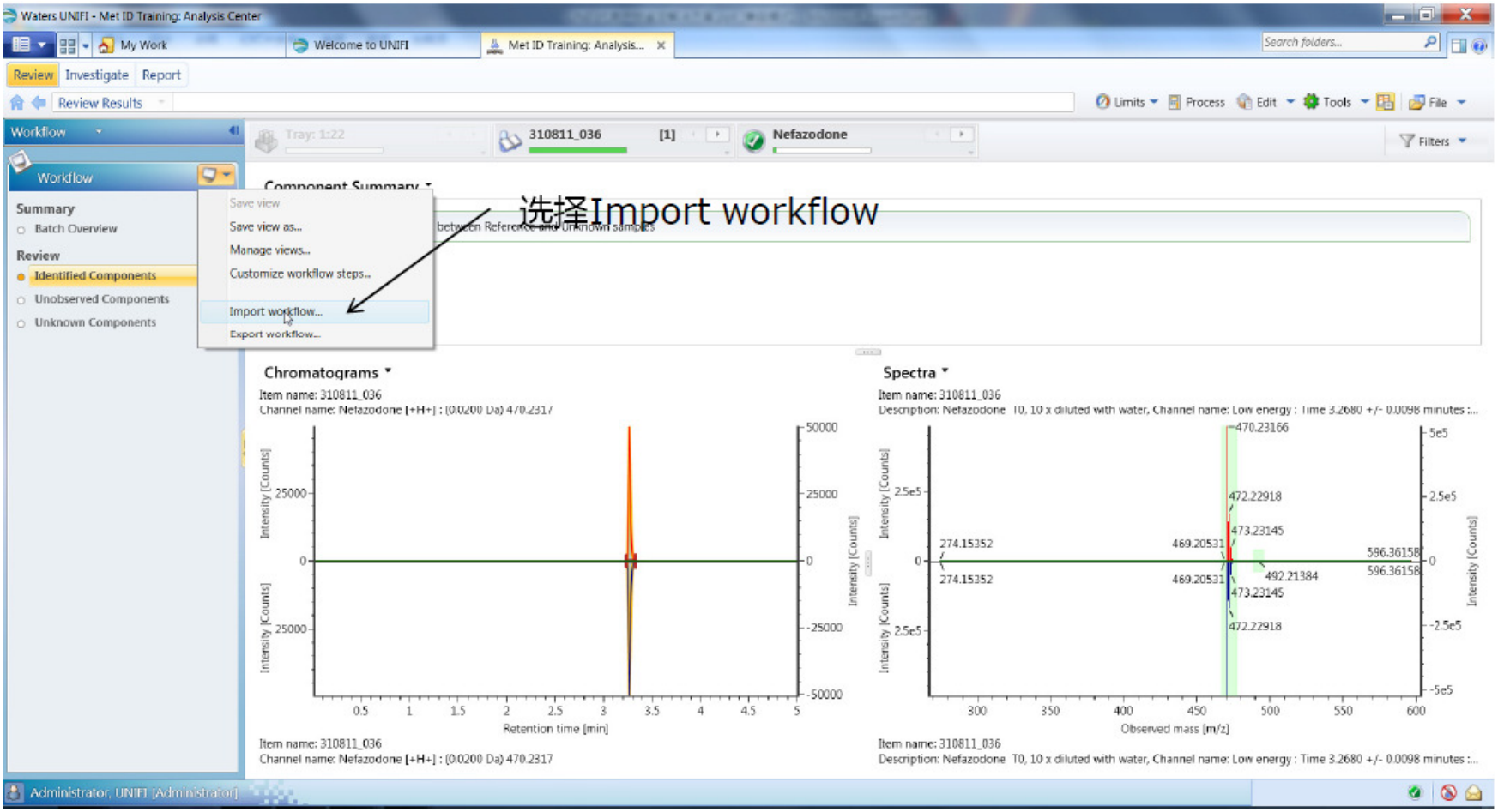


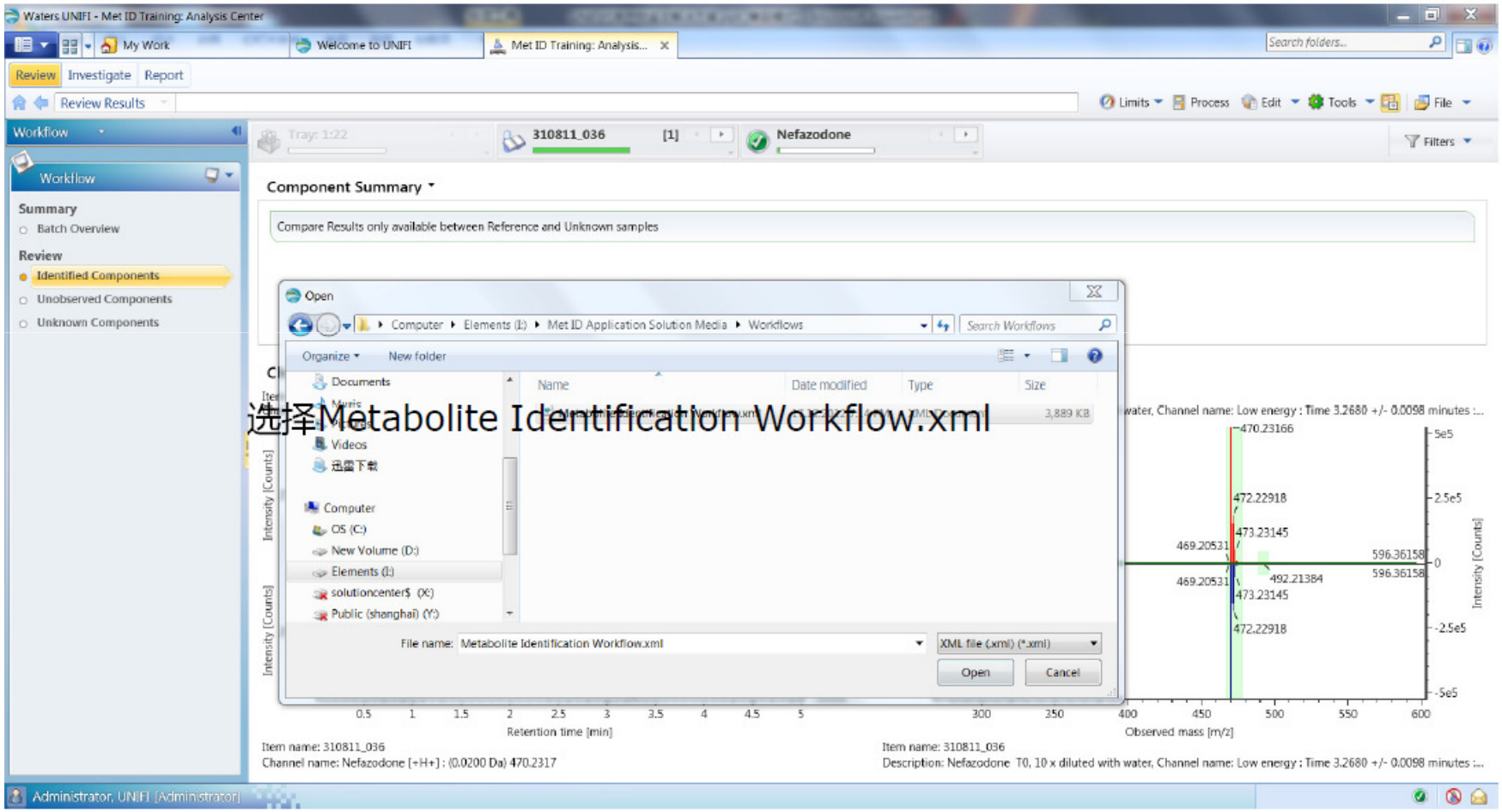


数据开始处理



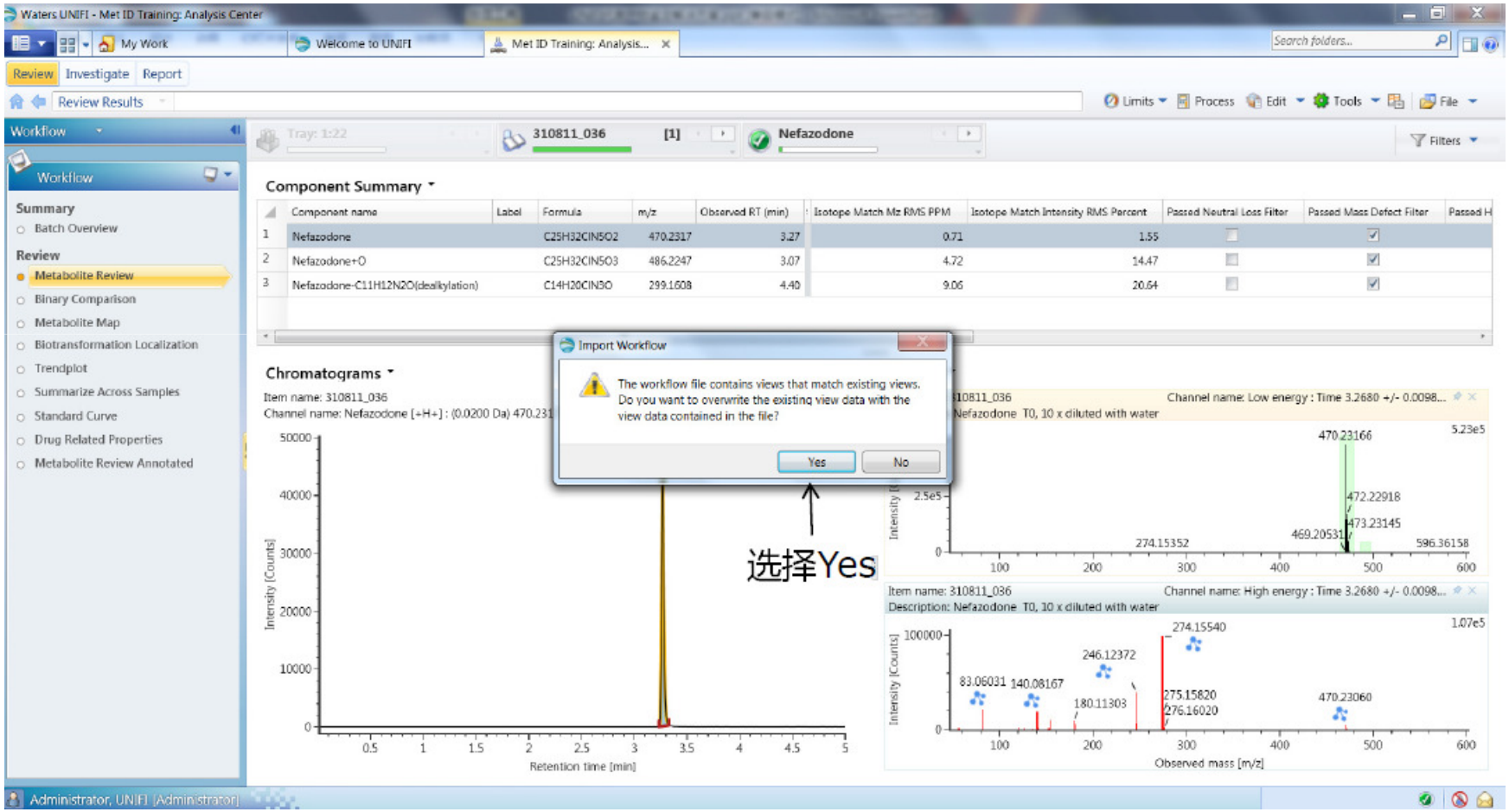
导入workflow



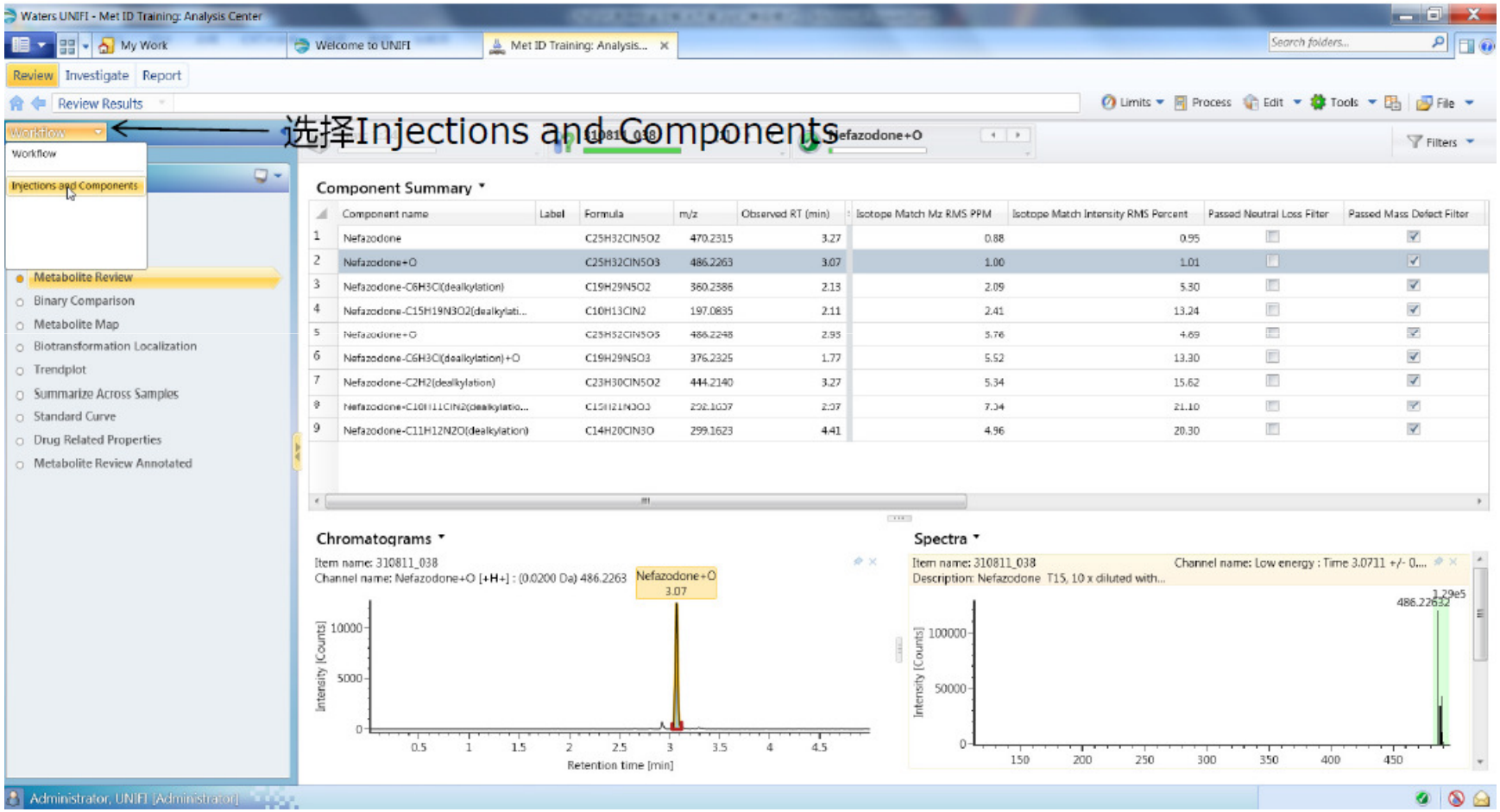


Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

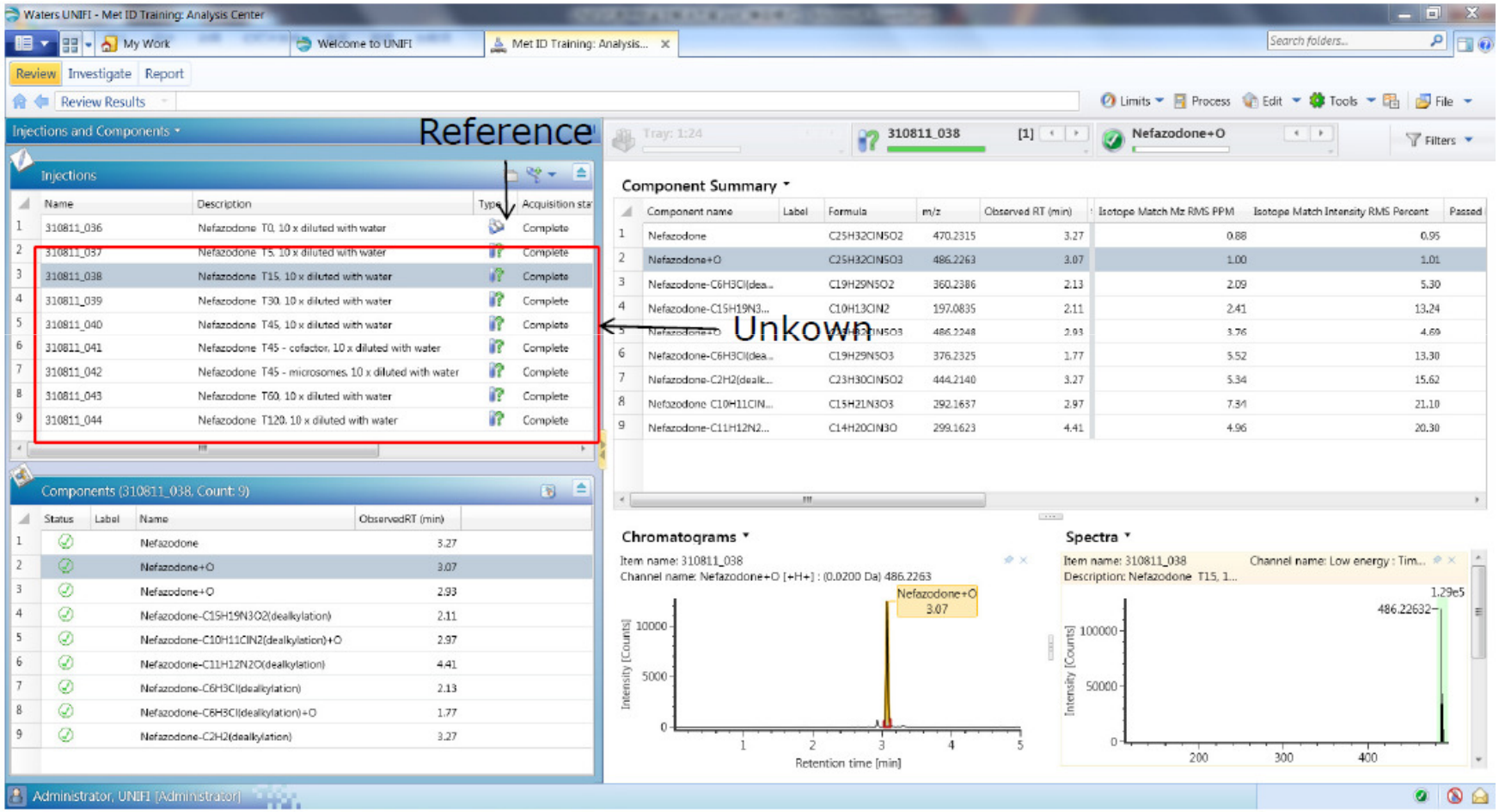


处理结果浏览



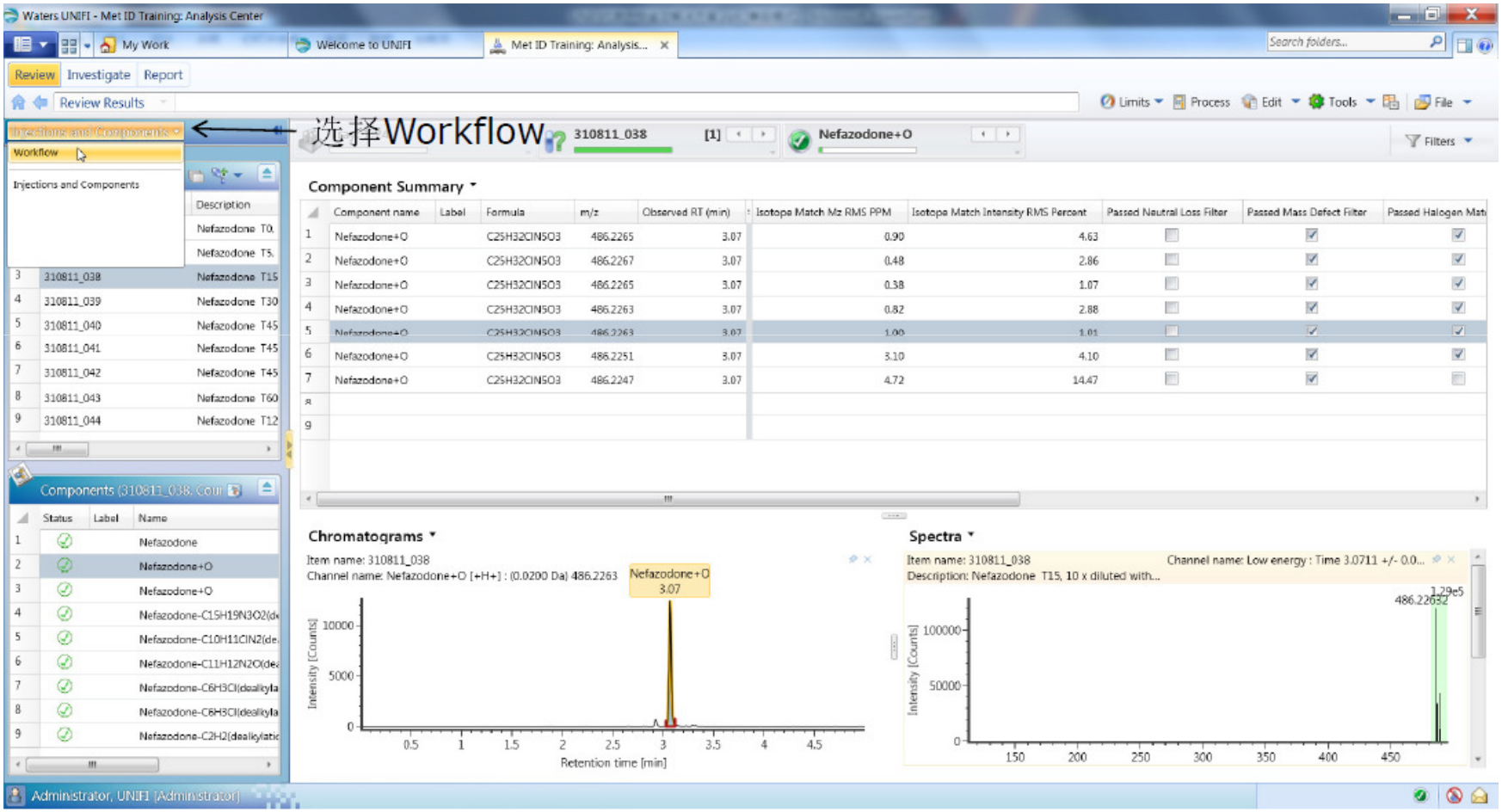
Waters

THE SCIENCE OF WHAT'S POSSIBLE.®



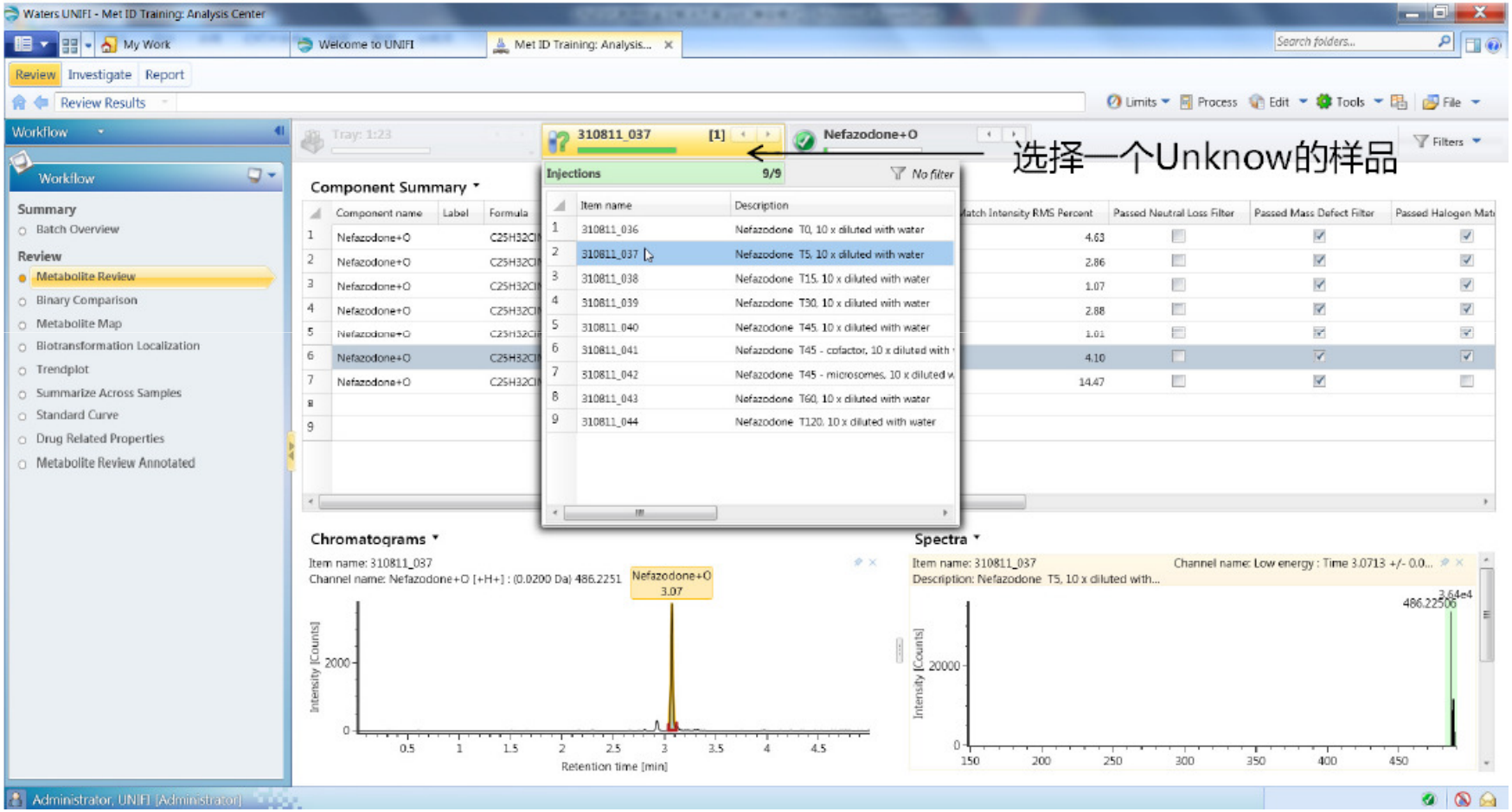
Waters

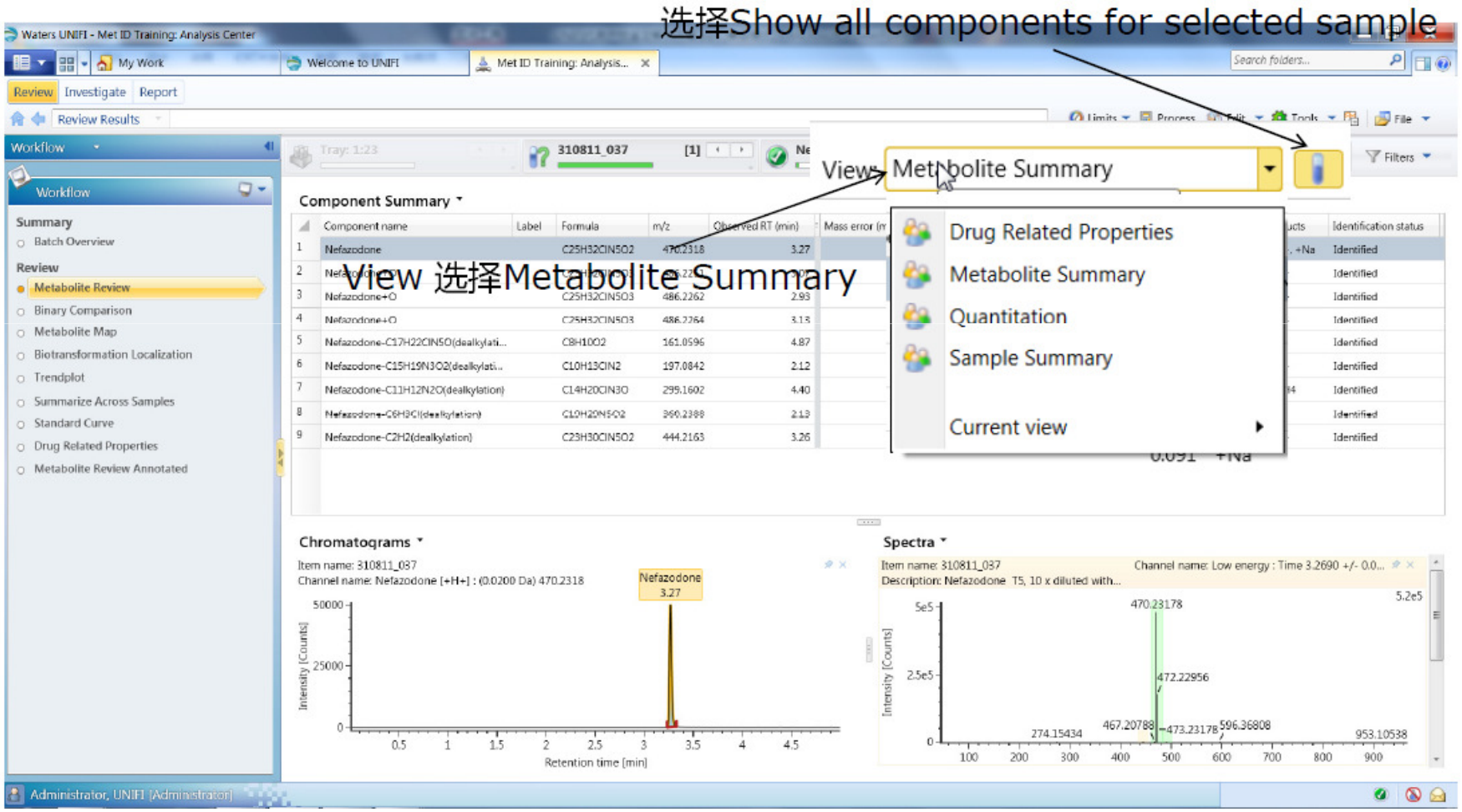
THE SCIENCE OF WHAT'S POSSIBLE.®



Waters

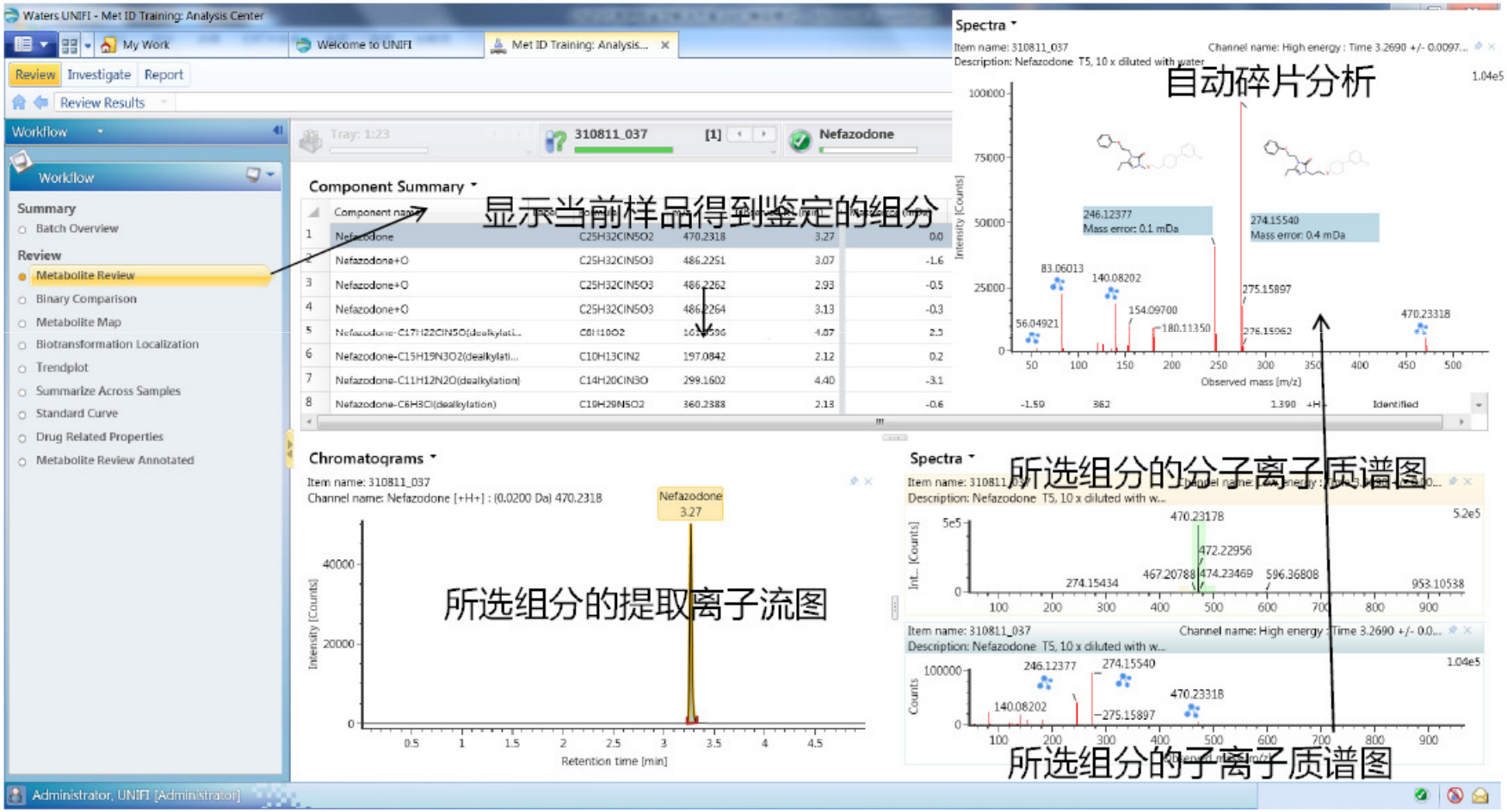
THE SCIENCE OF WHAT'S POSSIBLE.®



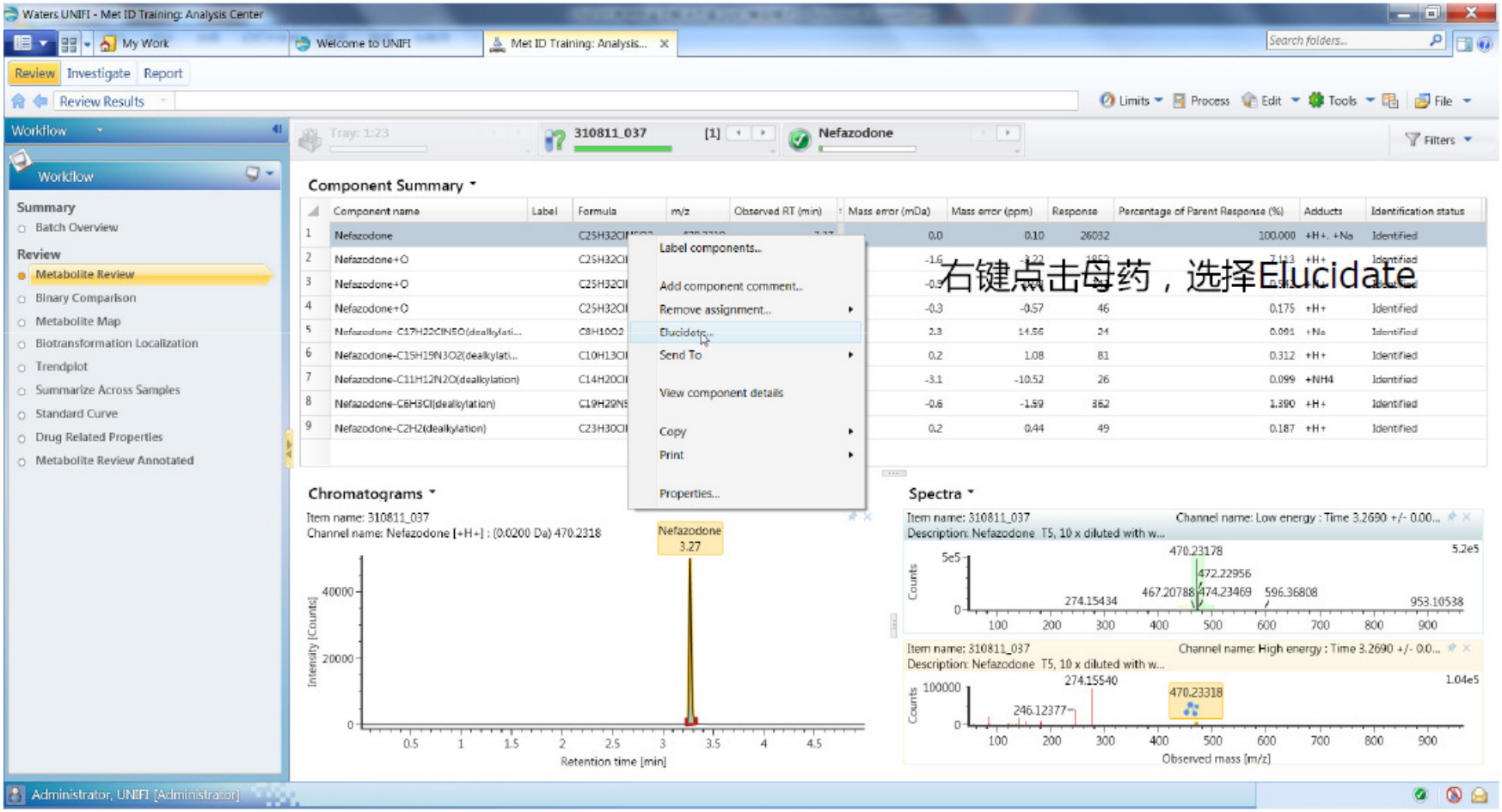


Waters

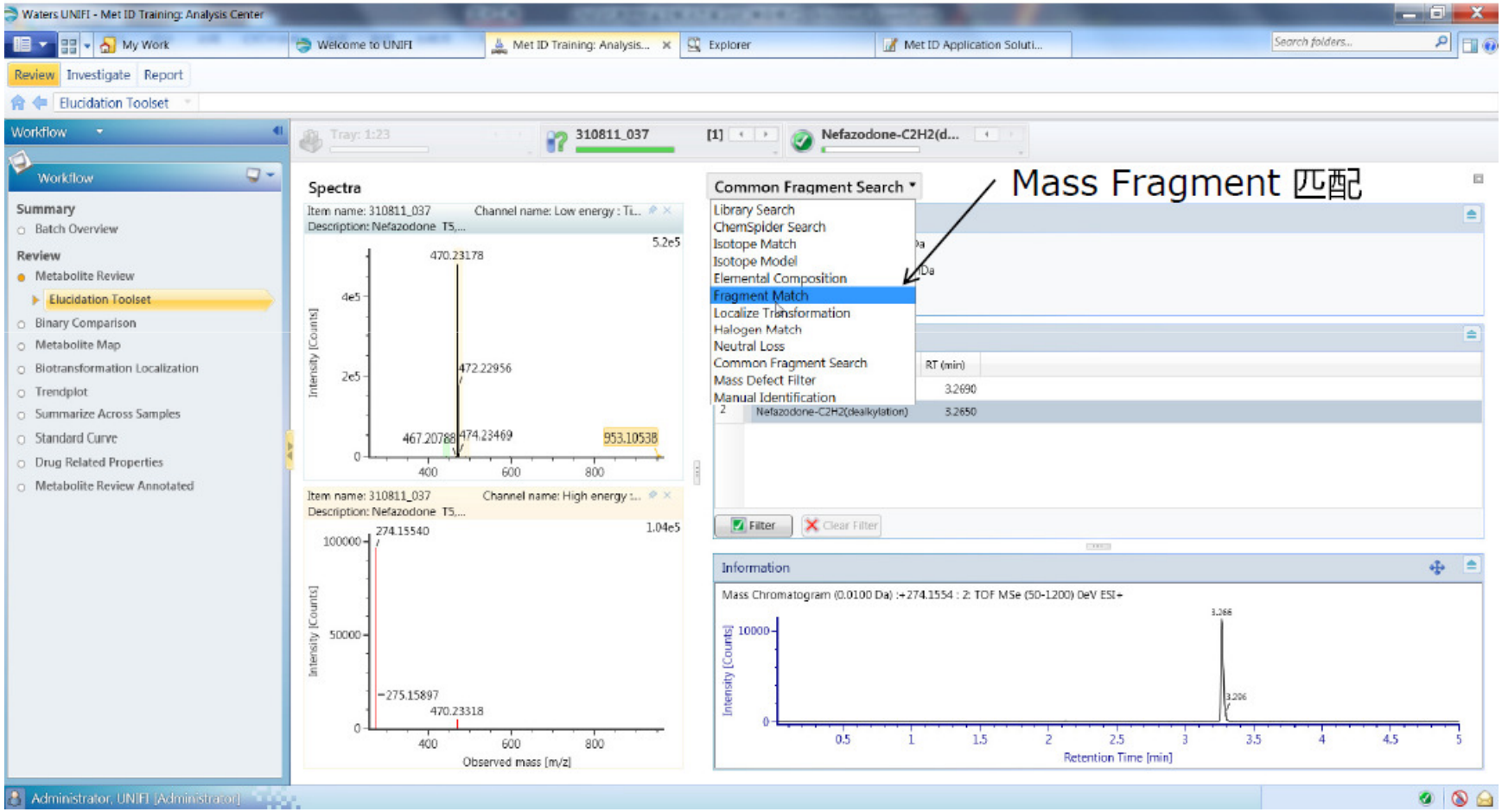
THE SCIENCE OF WHAT'S POSSIBLE.®



考察母药的裂解

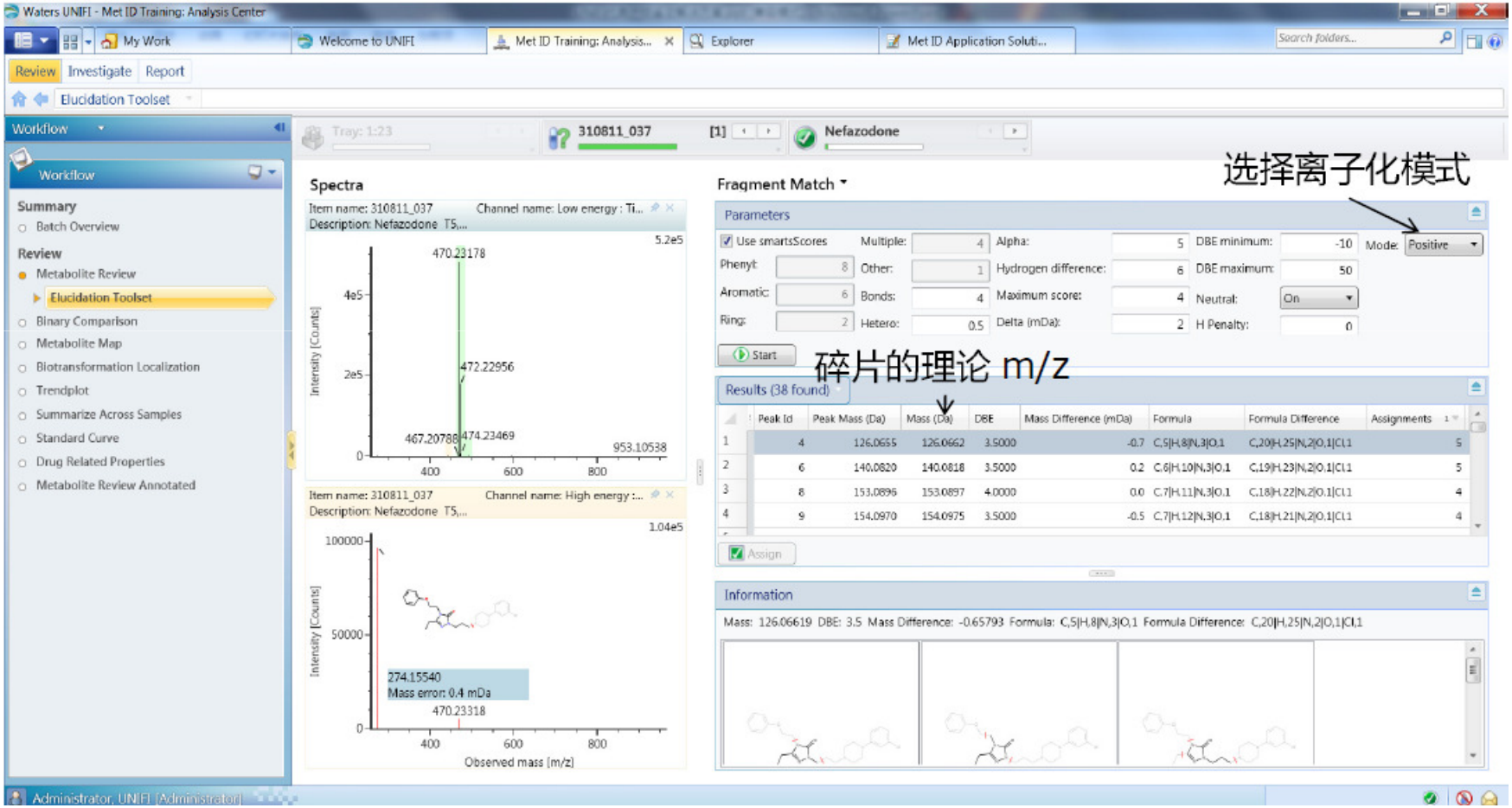


分析母离子（原药）的碎片信息



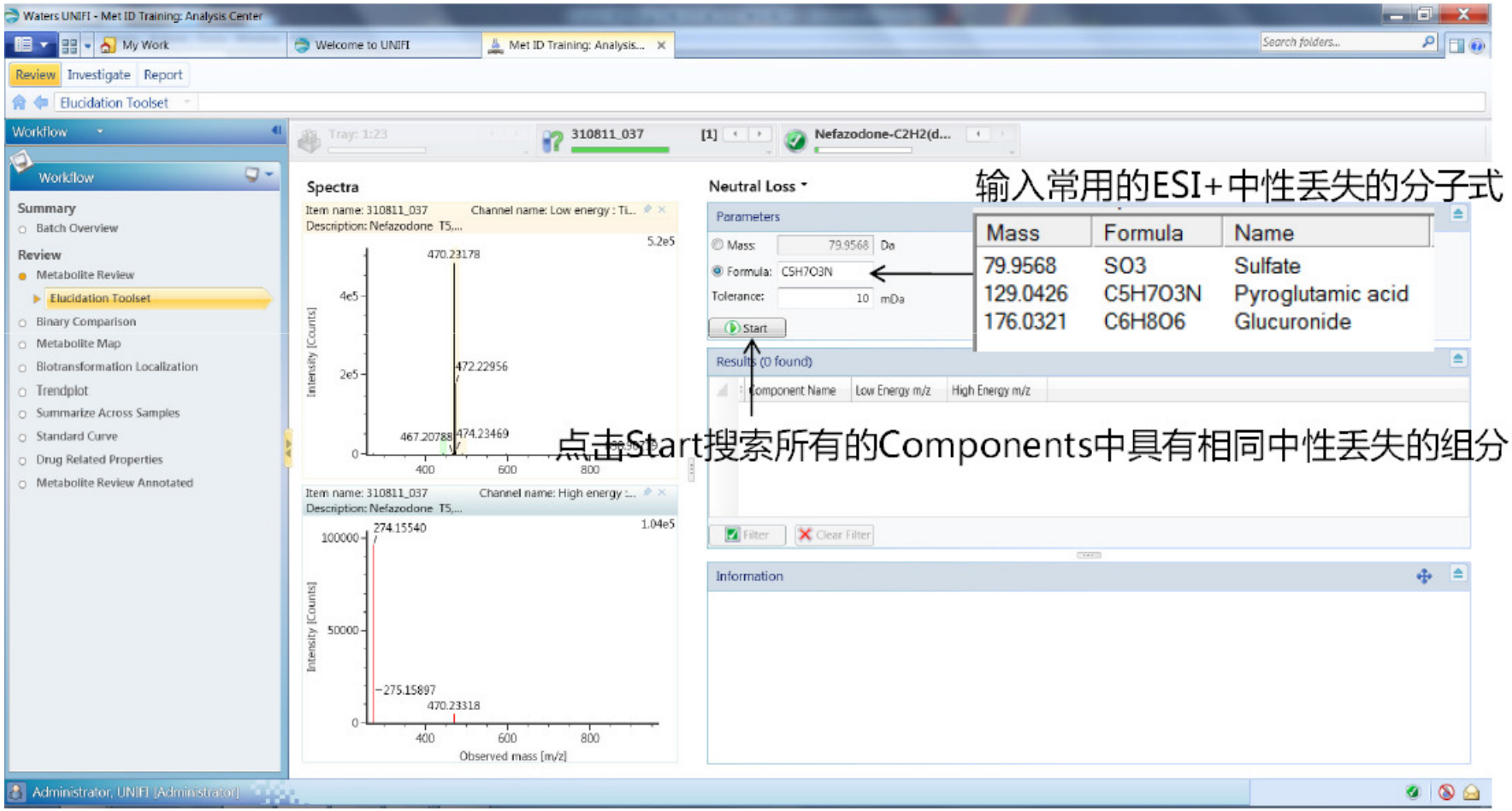
分析母离子的碎片信息

Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

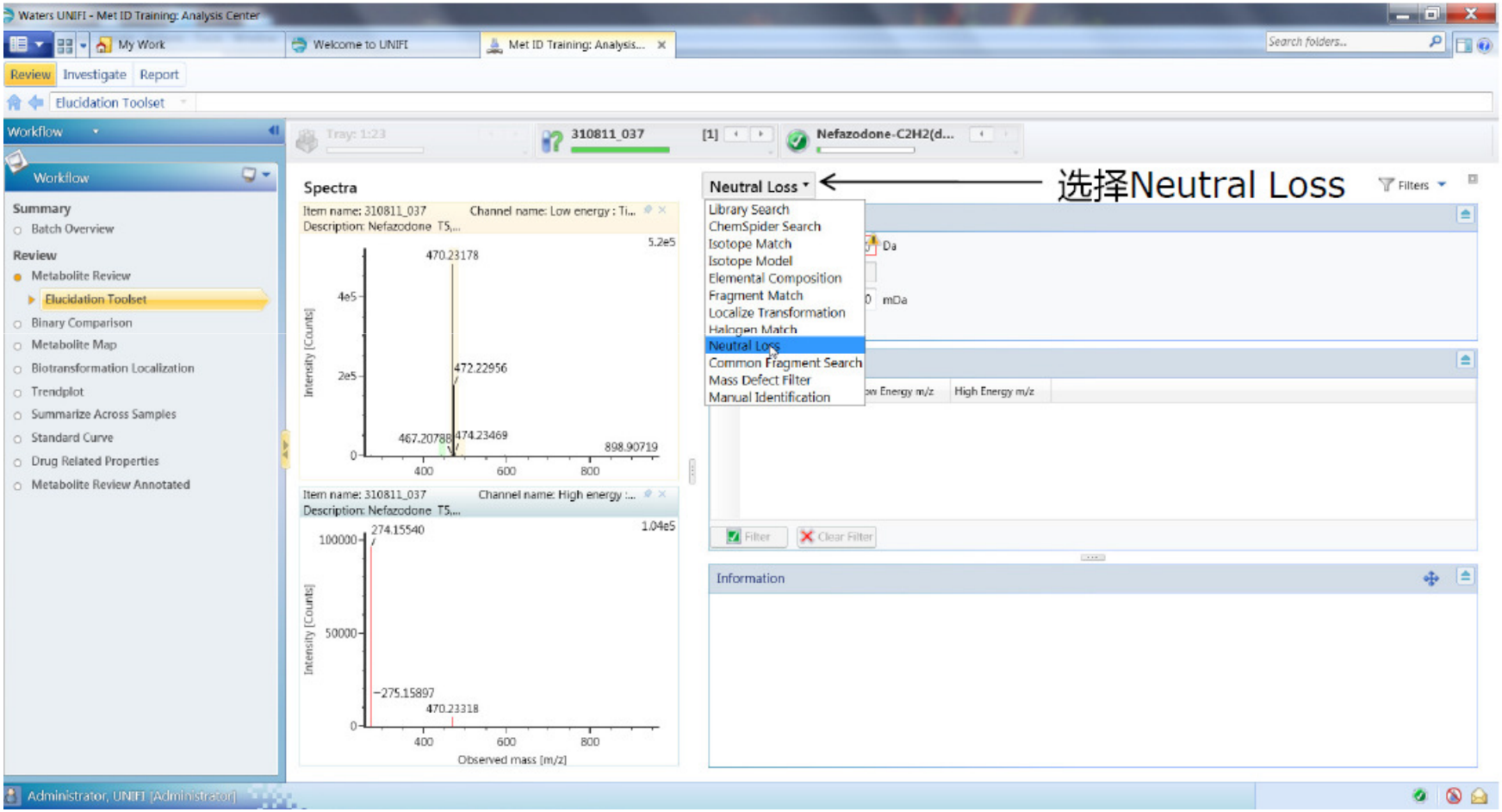


中性丢失扫描，寻找具有相同中性丢失的化合物

Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

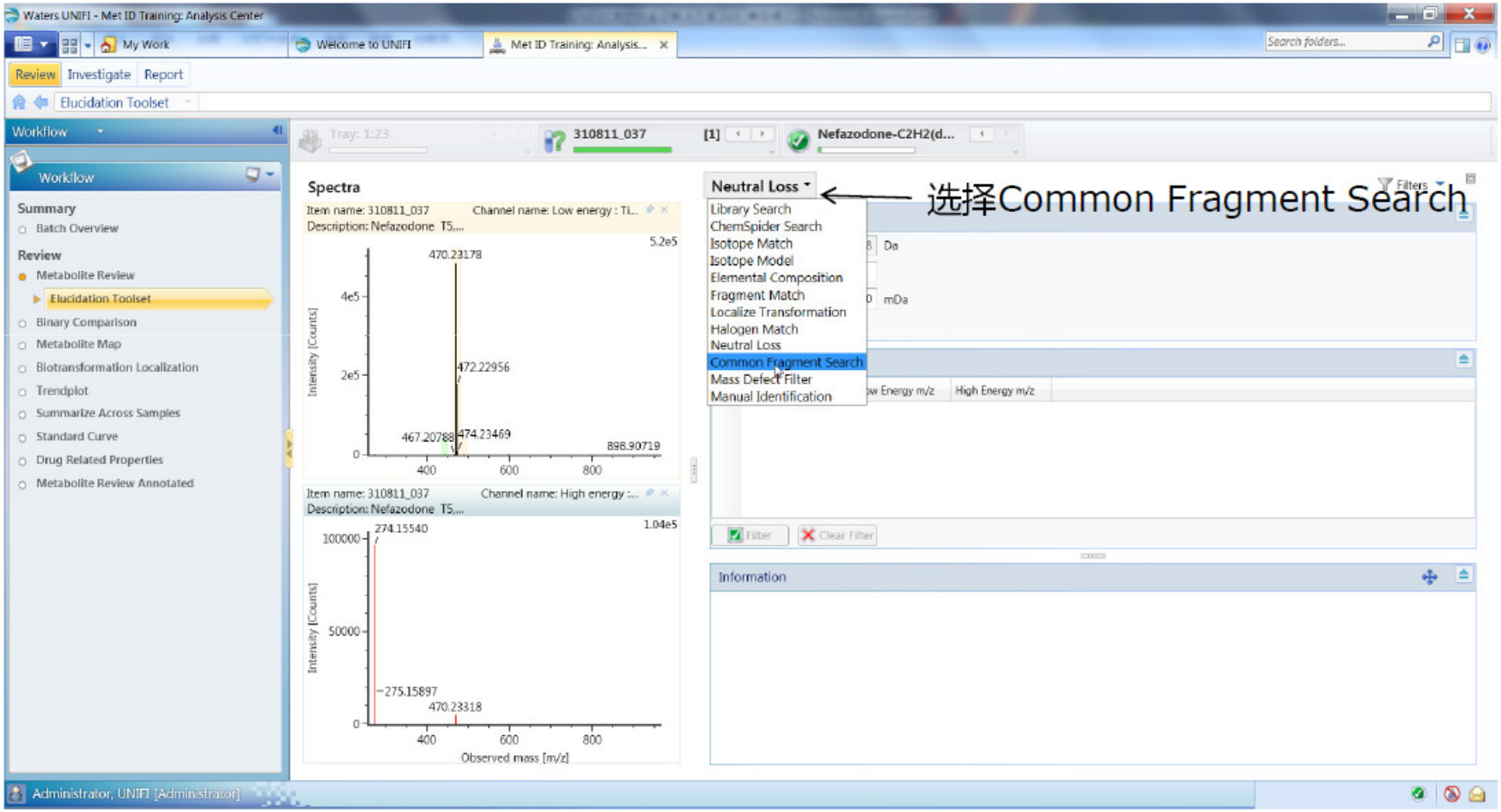


中性丢失扫描，寻找具有相同中性丢失的化合物



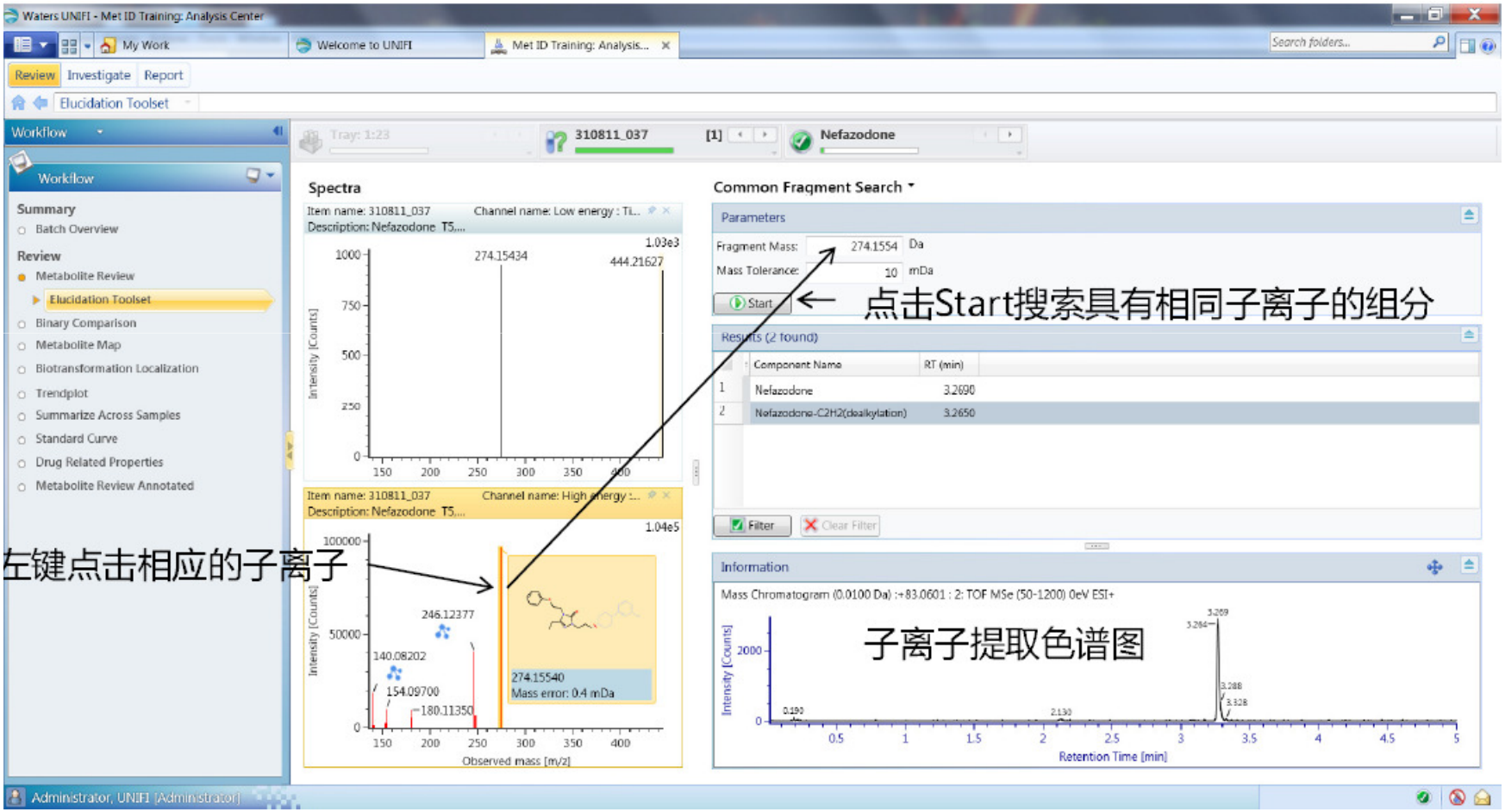
子离子扫描，寻找具有相同子离子的化合物

Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

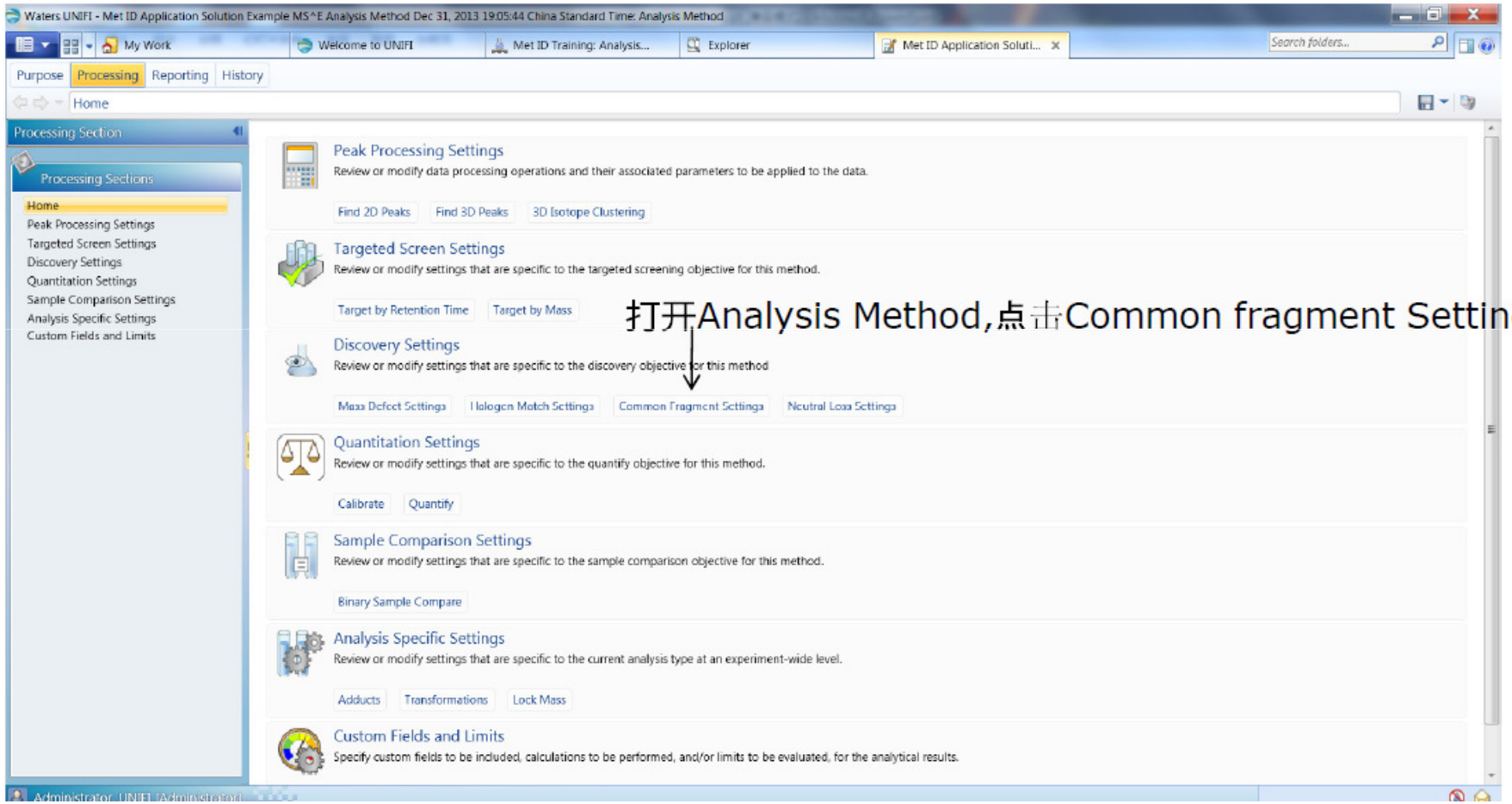


子离子扫描，寻找具有相同子离子的化合物

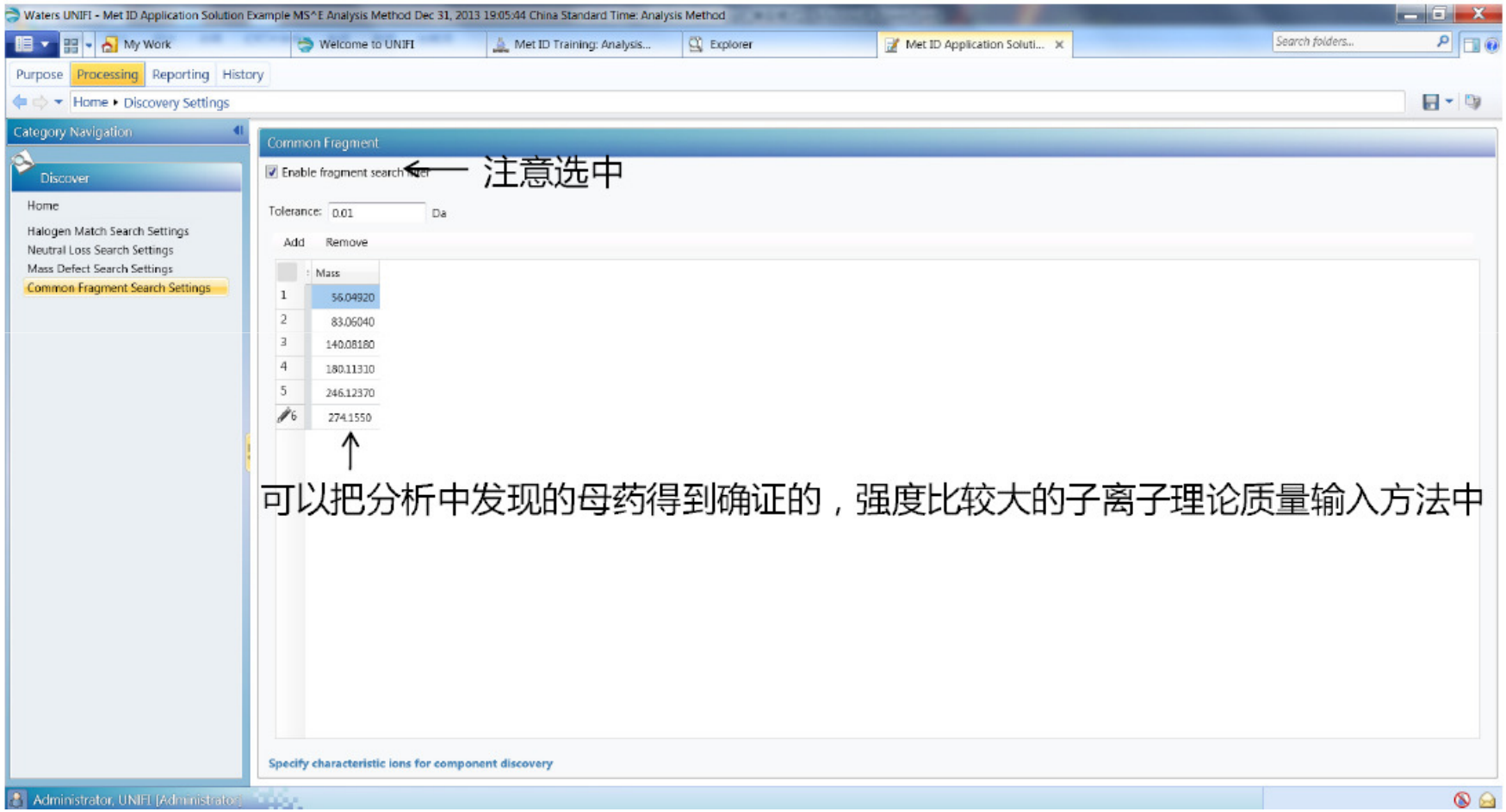
Waters
THE SCIENCE OF WHAT'S POSSIBLE.®



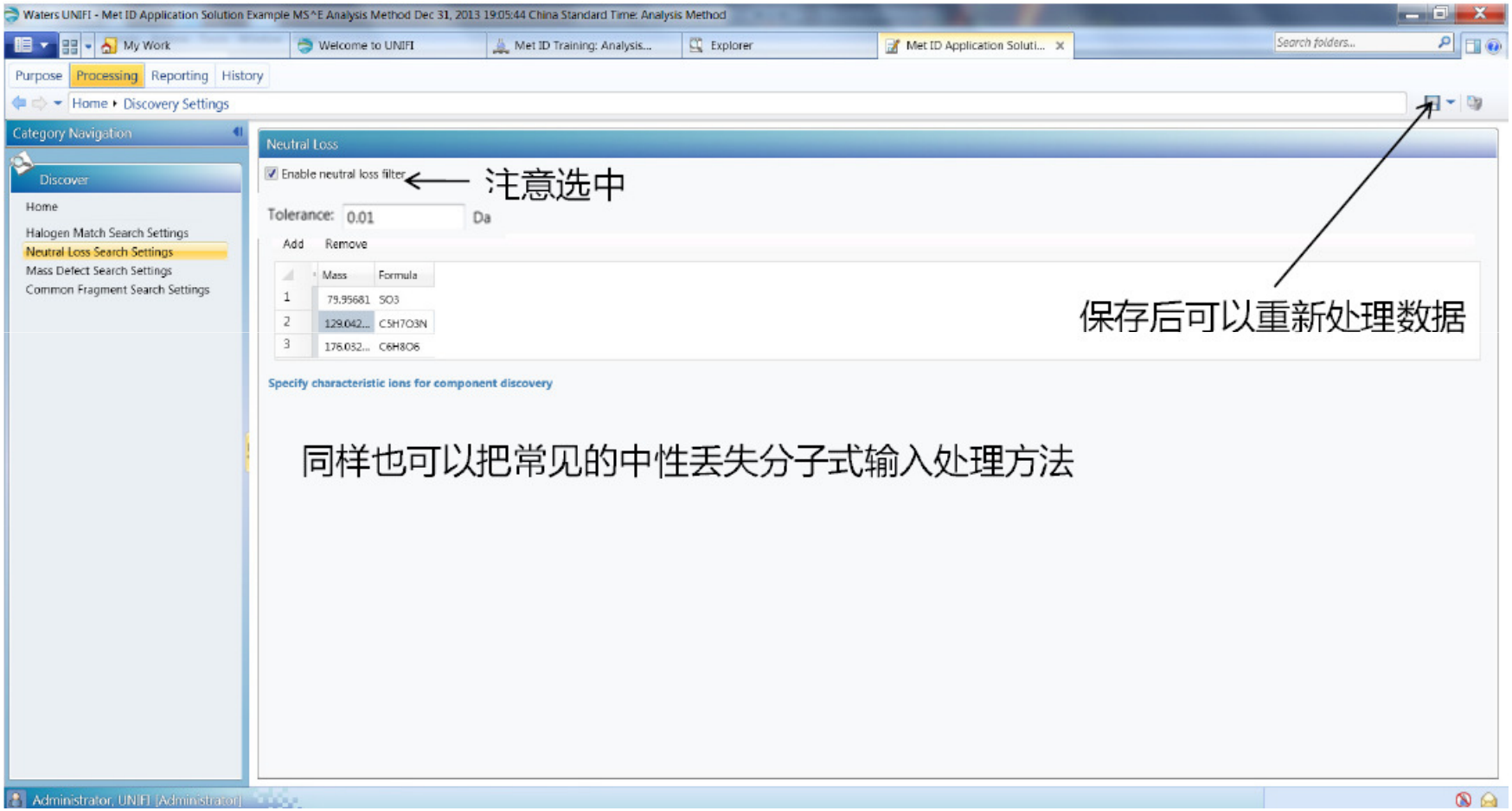
可以将得到的母离子碎片信息添加到方法中



设置子离子丢失

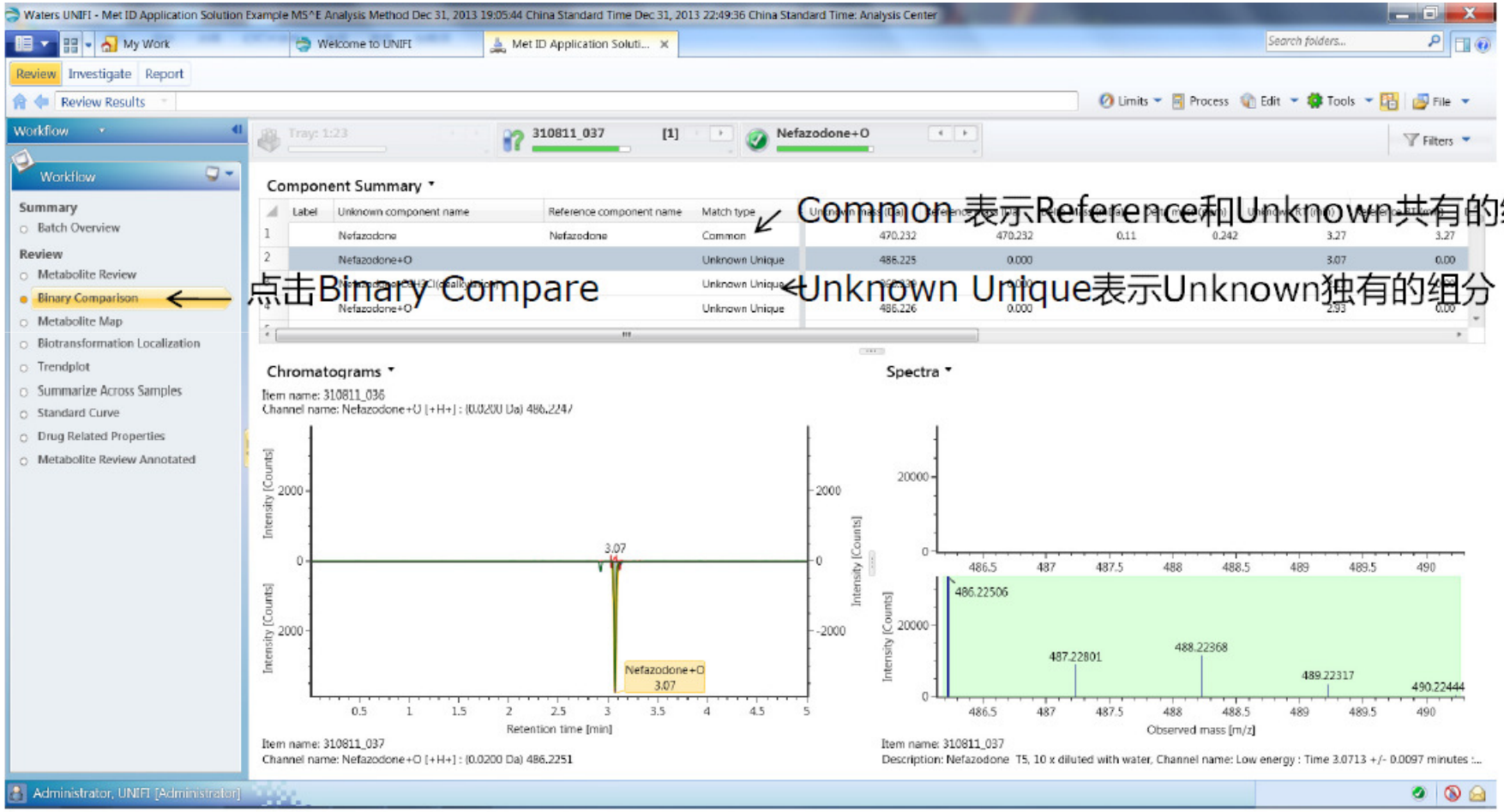


设置中性丢失

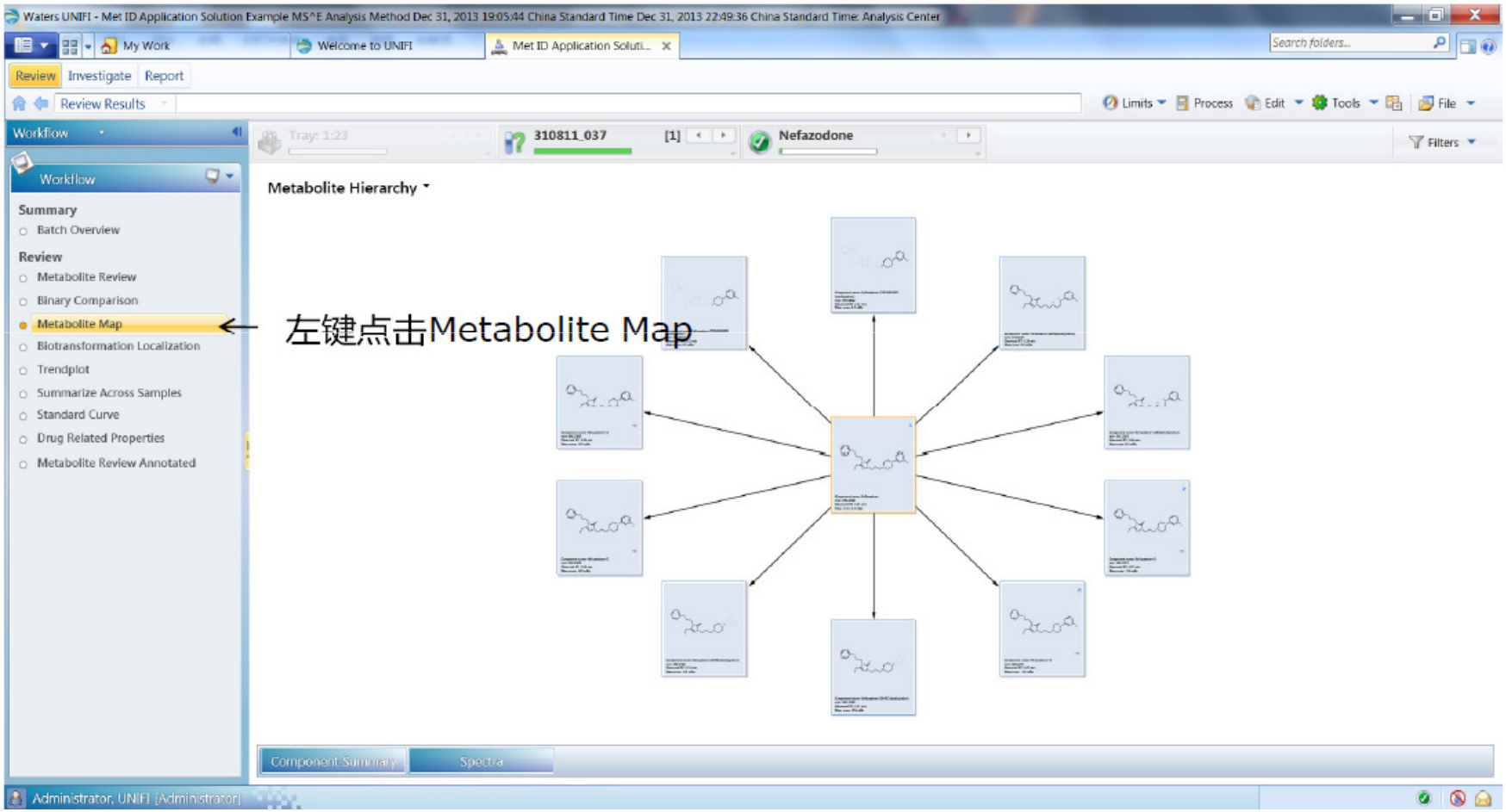


浏览二元比较结果

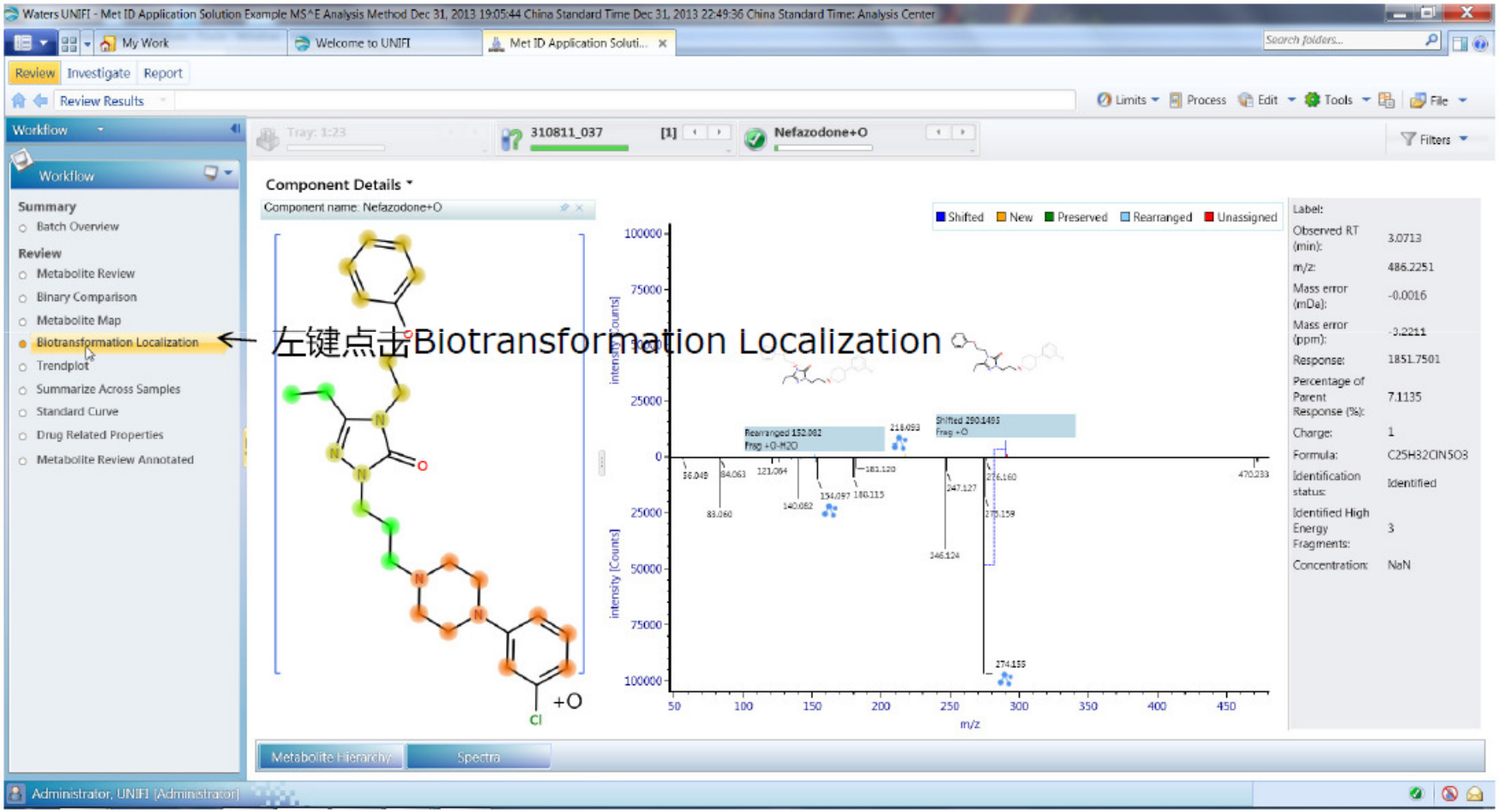
Waters
THE SCIENCE OF WHAT'S POSSIBLE.®



Metabolite map

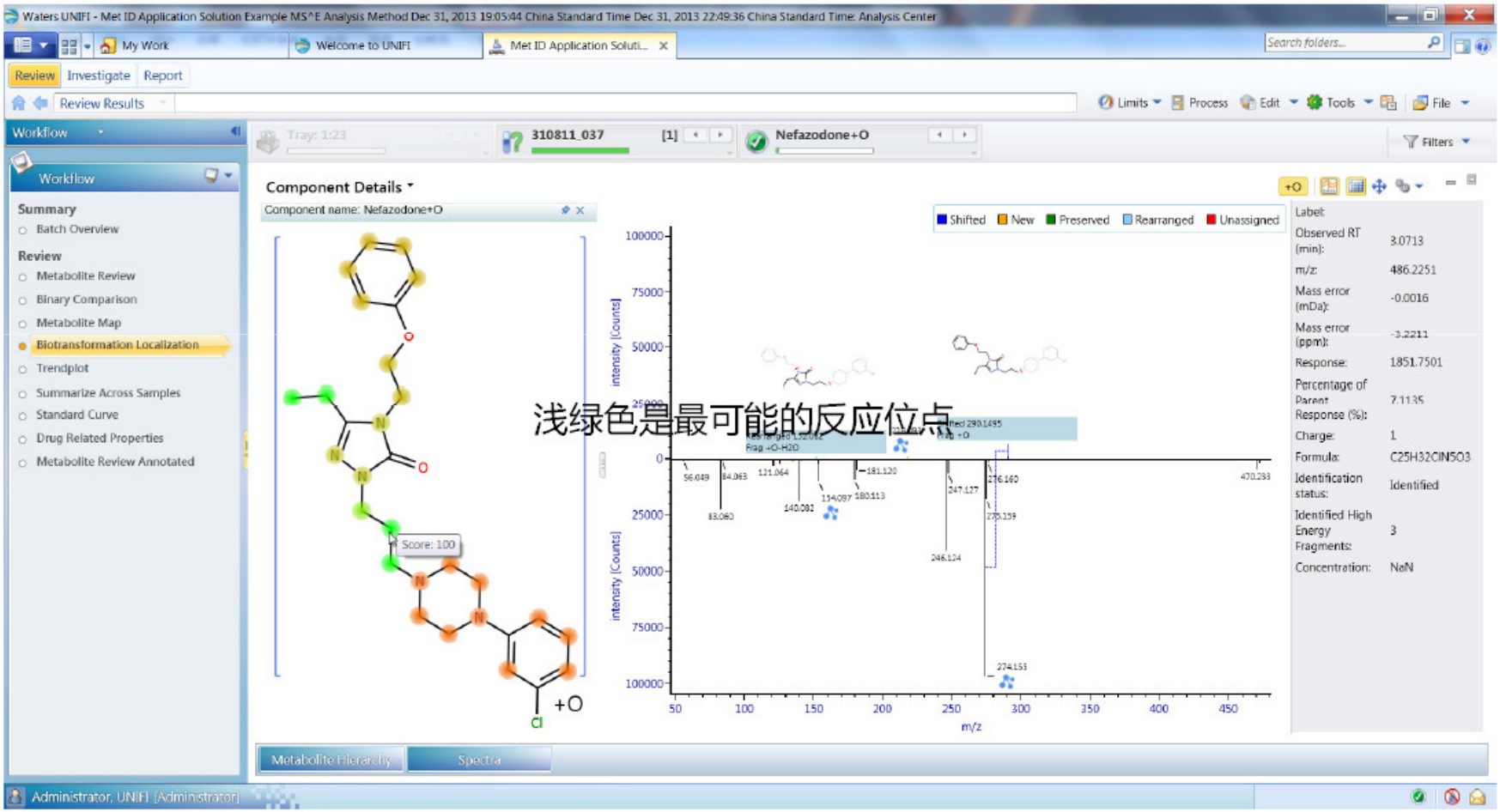


代谢位点

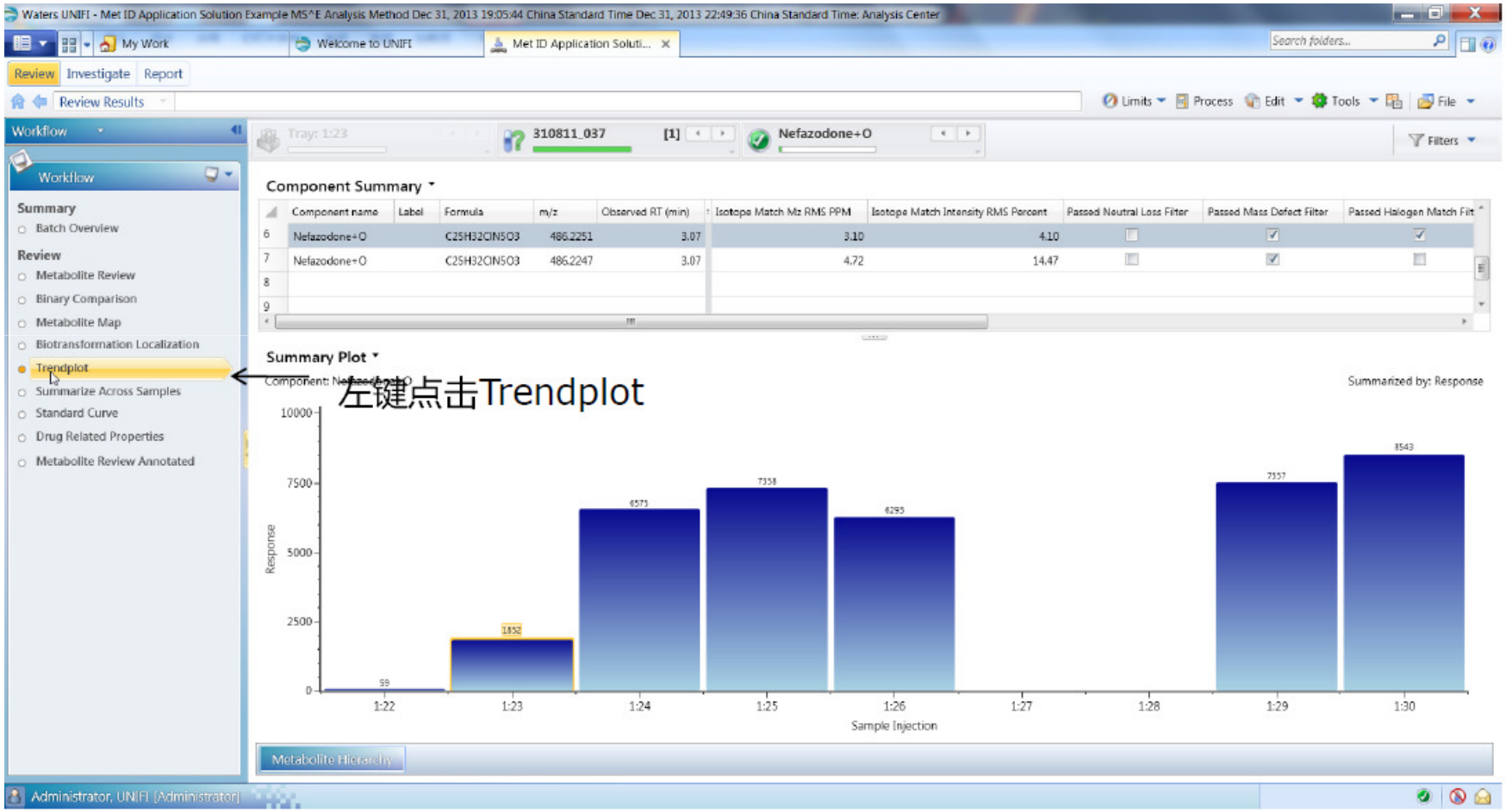


代谢位点

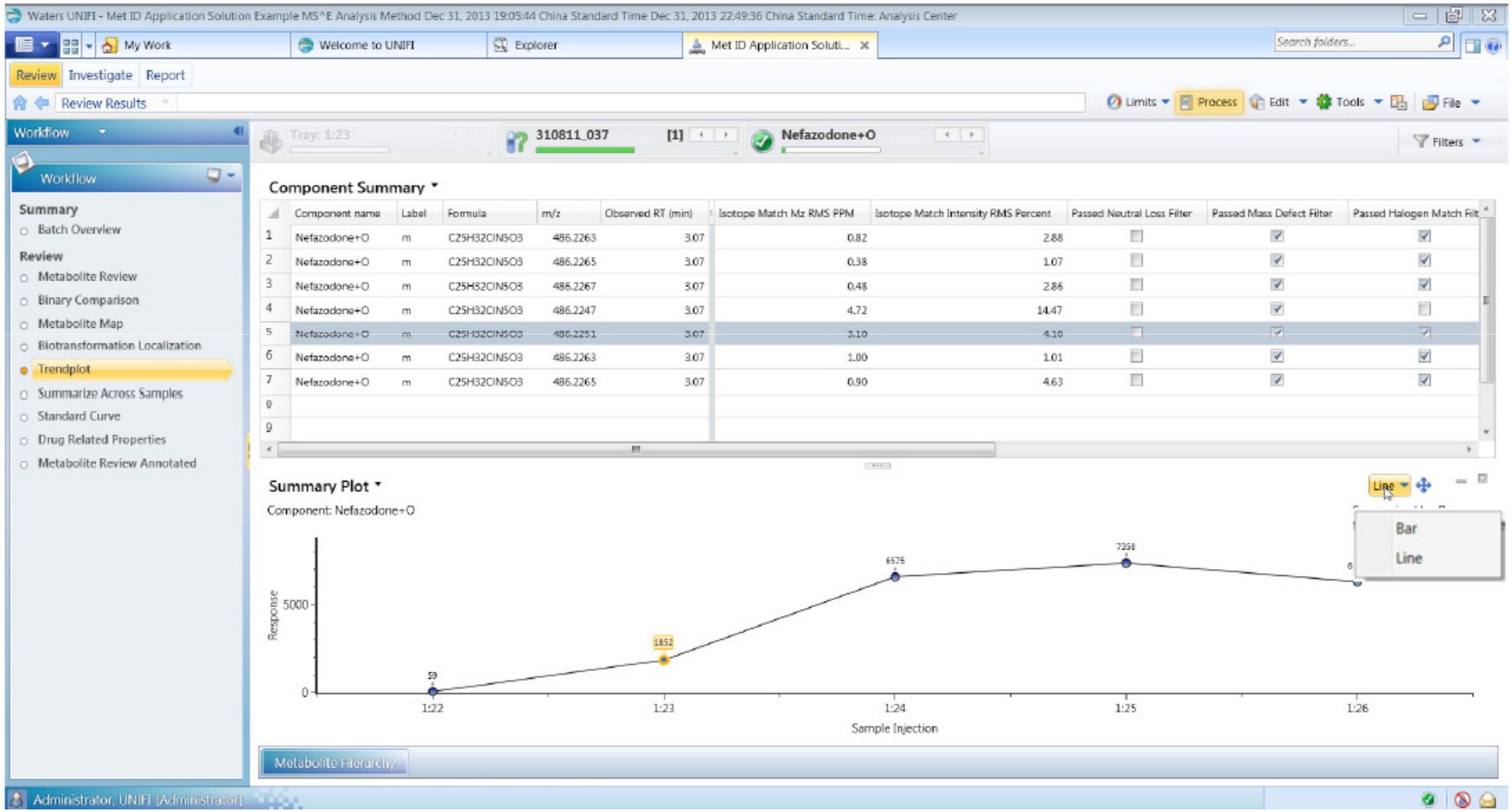
Waters
THE SCIENCE OF WHAT'S POSSIBLE.®



强度趋势图

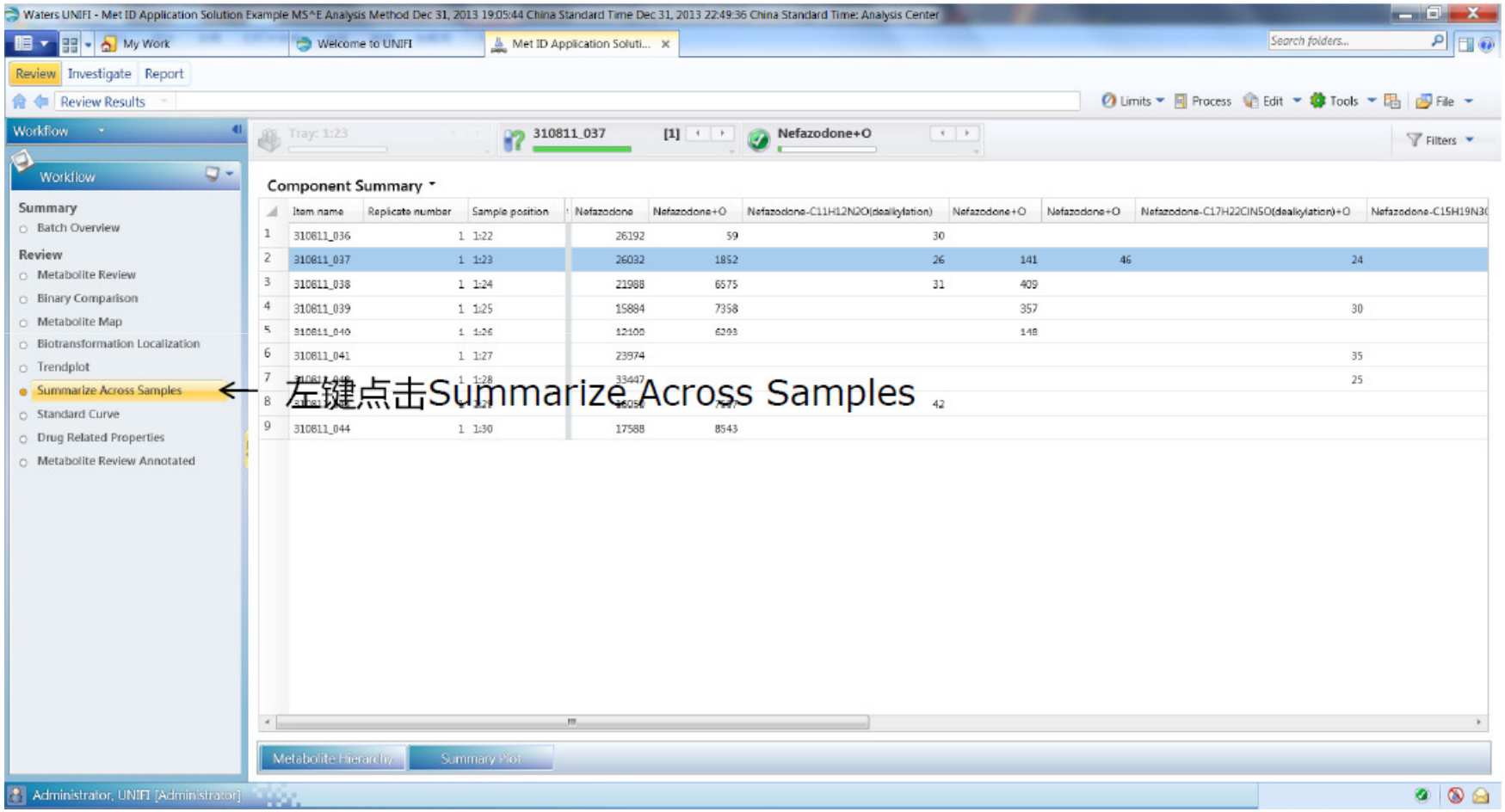


强度趋势图

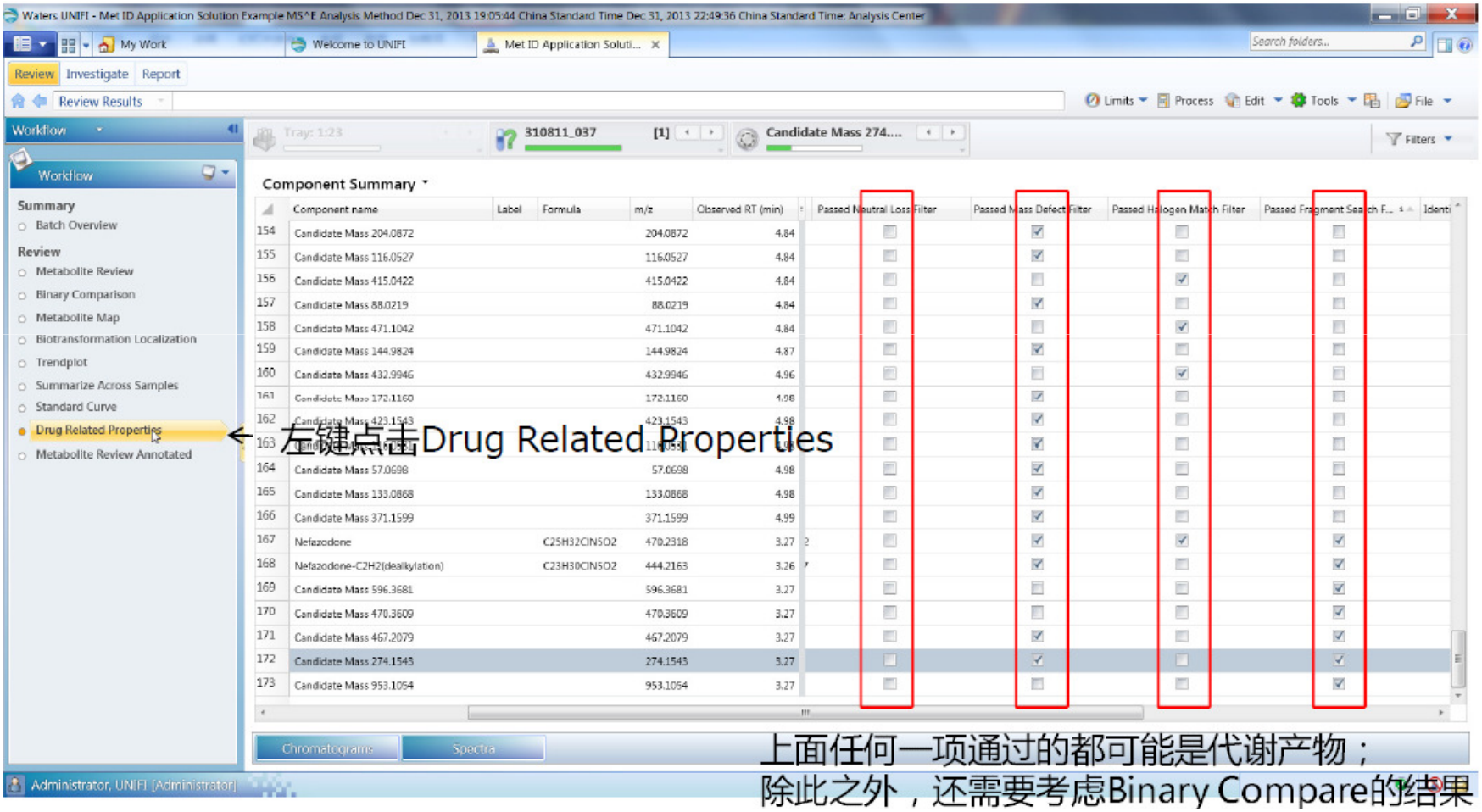


考察某一代谢物在所有样品中的情况

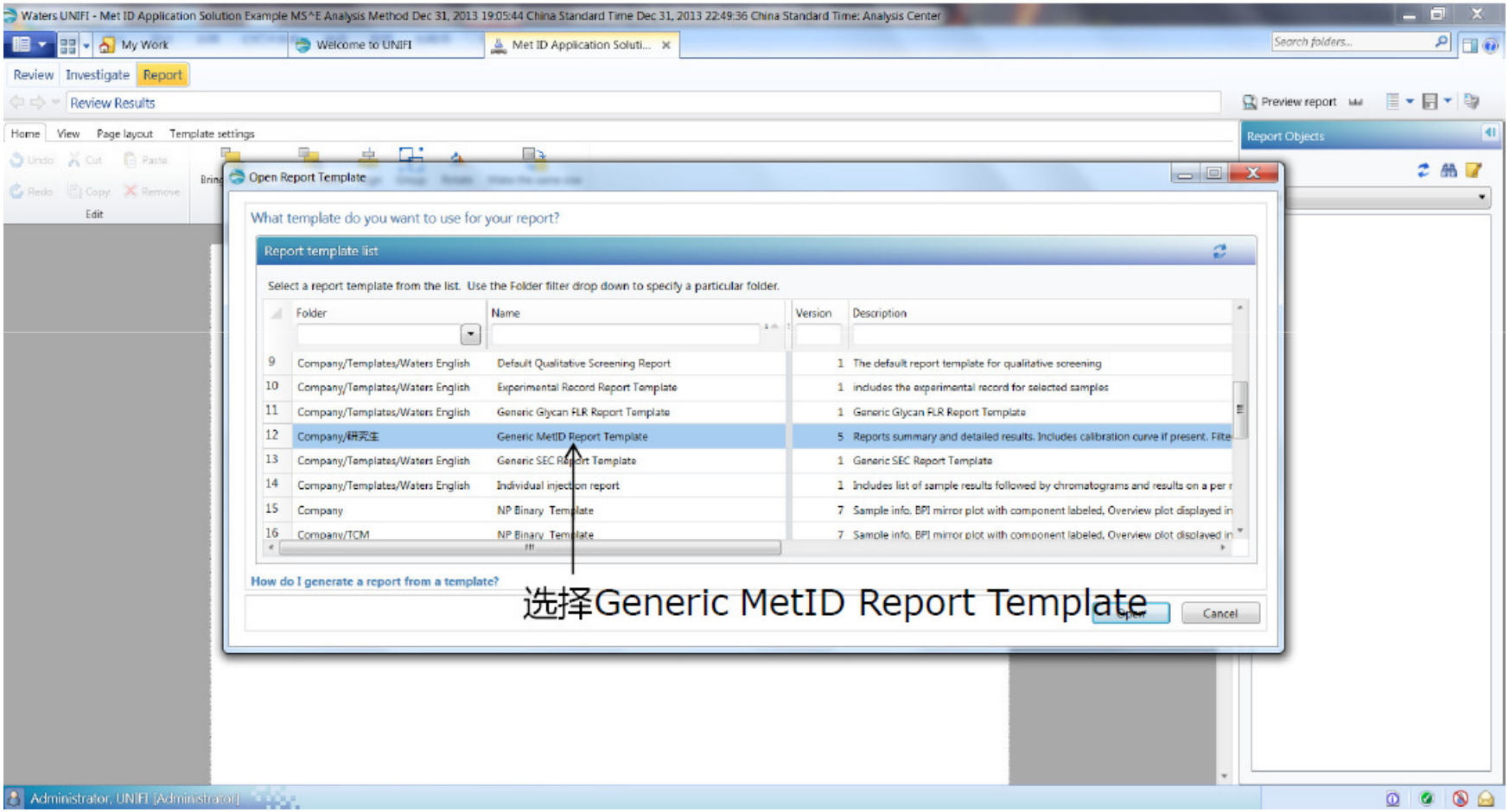
Waters
THE SCIENCE OF WHAT'S POSSIBLE.®



代谢产物与原药的相关性

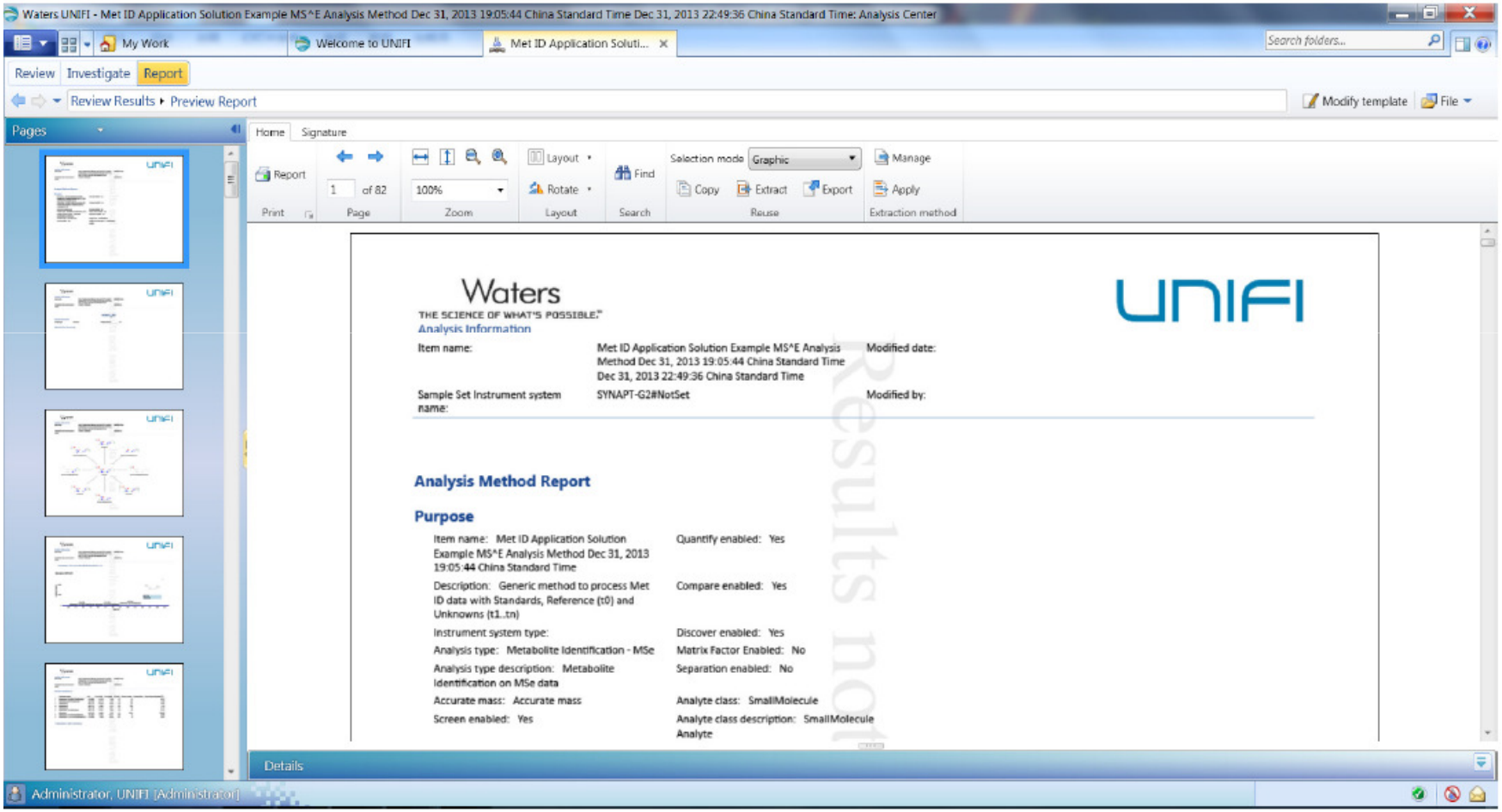


选择报告模板



预览报告

预览报告



储存报告为PDF格式