Advanced Reporting with ACD/Labs’ Manager Products

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European User’s Meeting

Advanced Chemistry Development, Inc. (ACD/Labs)
Advanced Reporting

- Two types of reporting
  - Default template
  - Custom template
    - Advanced reports from here

- Create custom templates in ChemSketch
Template Creation

Introduction

Using Templates

Template Options

Multi-Spec Templates

Macros with Reports

Context Sensitive Reports

Summary
Template Options
Template Creation

Introduction

Using Templates

Template Options

Multi-Spec Templates

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Context Sensitive Reports

Summary
Example Template

Introduction
Using Templates
Template Options
Multi-Spec Templates
Macros with Reports
Context Sensitive Reports
Summary
Report Multiple Spectra

- Report Multiple 1D and 2D NMR experiments in same report
- Increment ID#
- Order in window is important
Introduction

Using Templates

Template Options

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Context Sensitive Reports

Summary
Report Result

Introduction
Using Templates
Template Options
Multi-Spec Templates
Macros with Reports
Context Sensitive Reports
Summary
More Options

Combine ALL spectroscopic techniques in one report

- NMR, MS, Chrom, UV, IR, etc.
More Options
More Options

- Use dynamic date, time and page numbers
- Print report directly without stopping at ChemSketch
- Export report directly to PDF!
Flexibility

- Reported objects are still customizable
- Resizable and moveable
- Page numbers can be reordered easily
Special Examples

Context sensitive Reporting

- Use a decision macro
- Macro measures condition of a spectrum or spectra
- Chooses a specific report template based on the result
- Report indicates result of macro test and is a context sensitive report
Macros with Reports

Macro is used to identify if condition is satisfied
- Locate peak in particular region for example
- If found, use Report Template X
- If not found, use Report Template Y
Macros with Reports

Introduction

Using Templates

Template Options

Multi-Spec Templates

Macros with Reports

Context Sensitive Reports

Summary
Context Sensitive Report

Possible uses:

- Identify an impurity automatically
- Check spectrum referencing
- Ensure that all Multiplets have been defined
- If they haven’t, don’t waste space on a template for a multiplet report!
Assisted Verification Example

Screen a spectrum for a poor match factor

Level of match determines with report template to use
Context Sensitive Report Example

**Introduction**

Using Templates

Template Options

Multi-Spec Templates

Macros with Reports

Context Sensitive Reports

Summary
Context Sensitive Report Example

Introduction

Using Templates

Template Options

Multi-Spec Templates

Macros with Reports

Context Sensitive Reports

Summary
Context Sensitive Report

The Spectrum-Structure Match is Good.
Further manual evaluation is not required.
Context Sensitive Report

Introduction

Using Templates
Template Options
Multi-Spec Templates
Macros with Reports

Context Sensitive Reports

Summary
The Spectrum-Structure Match is Uncertain. Please consult the Spectroscopist for assistance.
The Spectrum-Structure Match is Poor.
Please re-evaluate the structure that has been proposed.
Summary

- **Standardize Reports**
  - For yourself
  - For your organization
- **Organize results quickly**
- **Maximize the value of your software!**