# PDF-4/Organics
# Results

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The purpose of this tutorial is to demonstrate the results possible with the use of PDF-4+/Organics and high quality experimental data

We are grateful to Bruker-AXS, Rigaku, PANalytical, Oak Ridge National Laboratory, and the Argonne Synchrotron Light Source who generously donated instrument time and expertise for data collection

# Results

- All results were obtained using PDF-4/Organics and embedded software contained in this product. Similar results would be expected with most commercial search/match programs using this database
- Please note that most results required multiple data sources for phase identification, which demonstrates the power of using multi-source databases that spans a wide range of chemistry.
- Polymeric, inorganic and organic materials were all used in the identifications
- Each slide presents the commercial material being analyzed, the SIeve+ identification results and a comparison of the experimental data with a data simulation based on the identification results

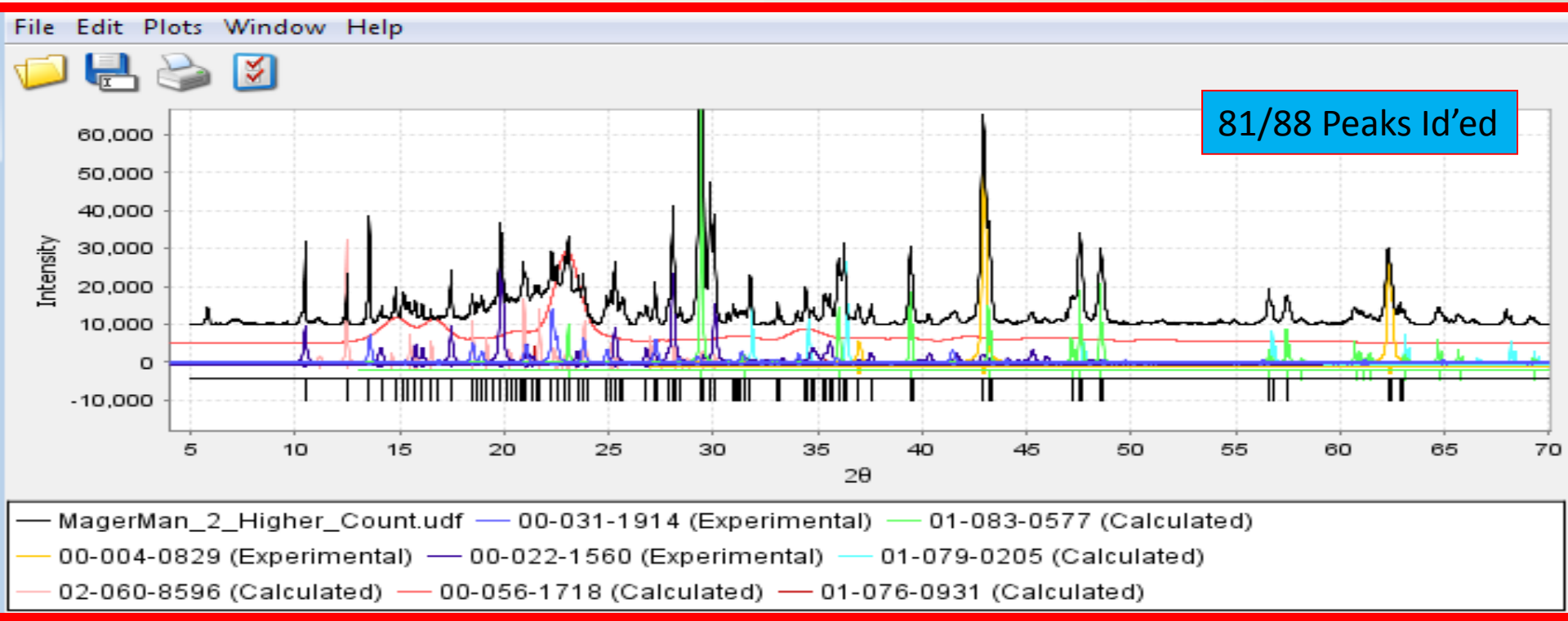
# Laboratory Data

In each data set all major phases were identified.

Many data sets contain minor phases (1-10 wt %) where identification was dependent on the data quality (signal to noise, resolution) and phase complexity (overlapping peaks).

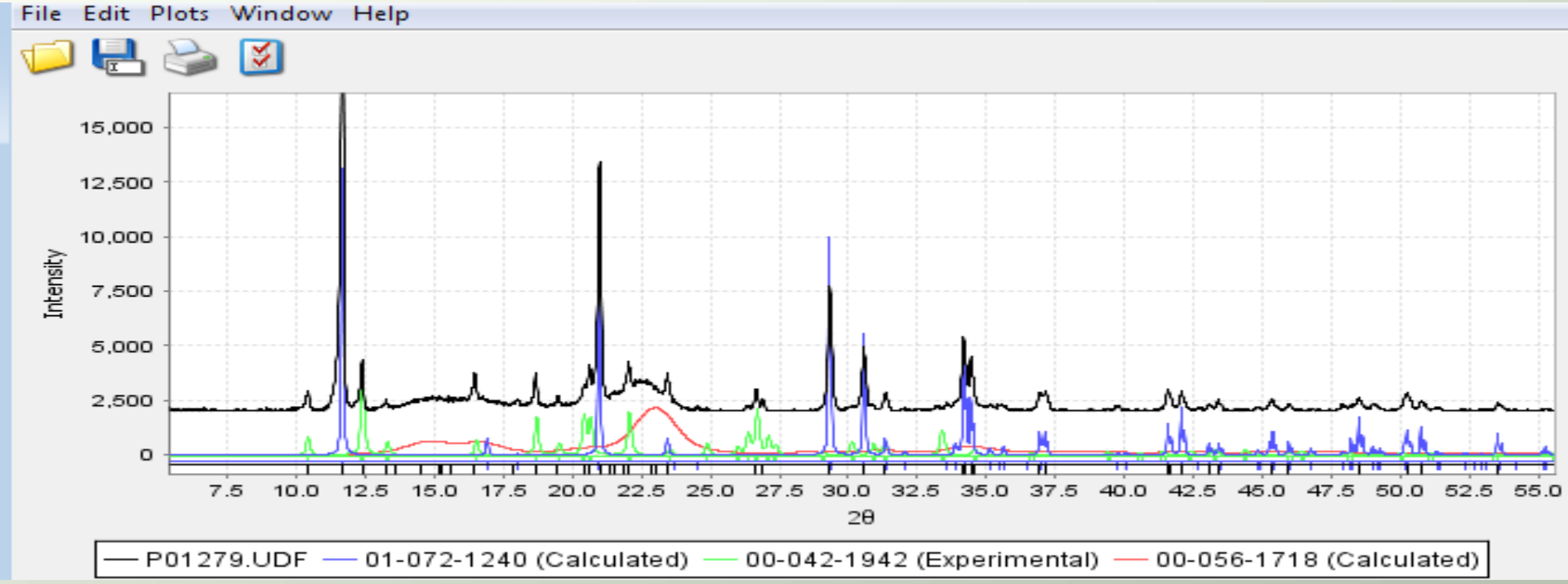
The experiments were not optimized to look for minor phases.

# Megaman Vitamin
# 8 Phases – 3 Database sources




| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-031-1914 | Taurine | 0.199 | 7 | | 15.7s |
| 2 | ☑ | 01-083-0577 | Calcium Carbonate | 0.806 | 27 | 3.21 | 5.2s |
| 3 | ☑ | 00-004-0829 | Magnesium Oxide | 0.228 | 8 | 2.1 | 4.6s |
| 4 | ☑ | 00-022-1560 | Ascorbic acid | 0.396 | 13 | | 12.8s |
| 5 | ☑ | 01-079-0205 | Zinc Oxide | 0.084 | 3 | 5.22 | 8.4s |
| 6 | ☑ | 02-060-8596 | Calcium ascorbate dihydrate | 0.489 | 16 | 0.55 | 7.8s |
| 7 | ☑ | 00-056-1718 | Cellulose Iβ | 0.679 | 22 | | 2s |
| 8 | ☑ | 01-076-0931 | Silicon Oxide | 0.061 | 2 | 5.59 | 1.1s |

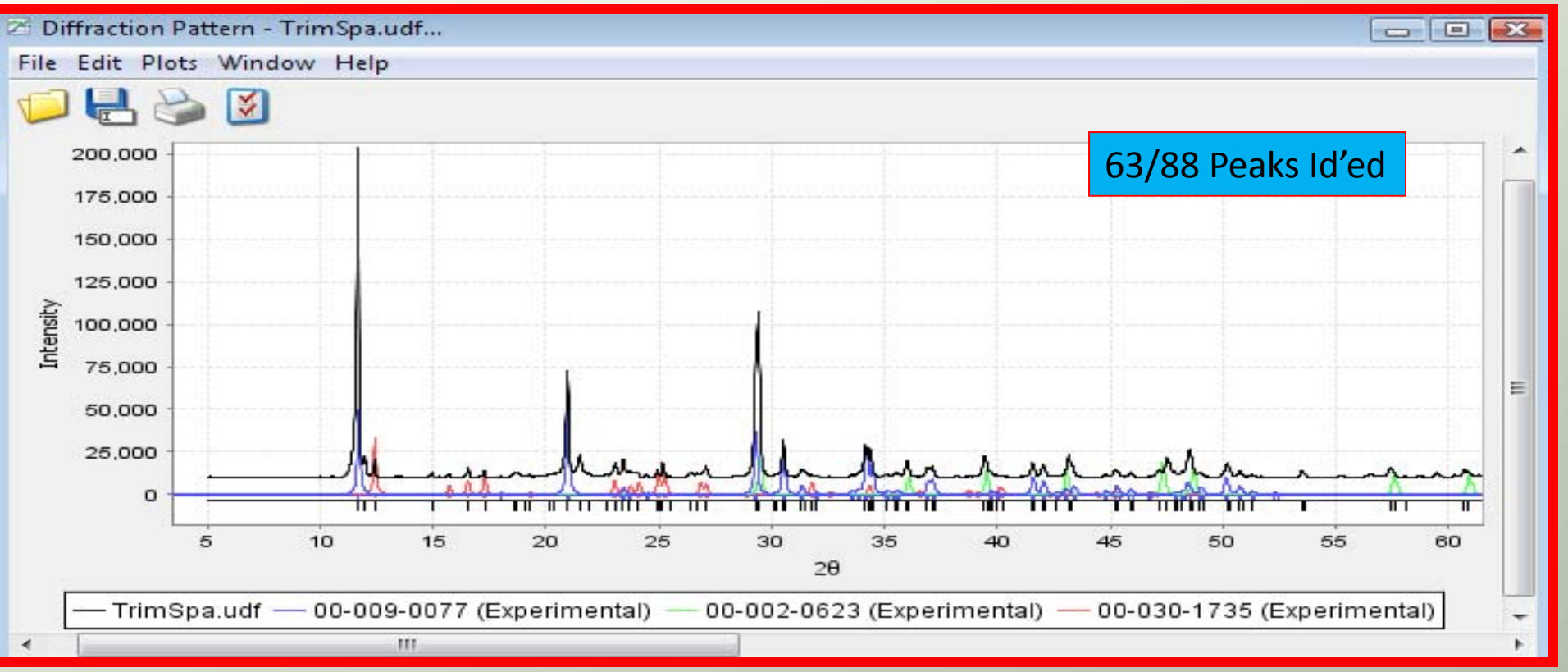
# Kroger Decongestant
# 3 phases – 2 sources




| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 01-072-1240 | Calcium Hydrogen Phosphate Hydrate | 0.586 | 61 | 1.39 | 2.3s |
| 2 | ☑ | 00-042-1942 | Diphenhydramine hydrochloride | 0.168 | 17 | | 6.3s |

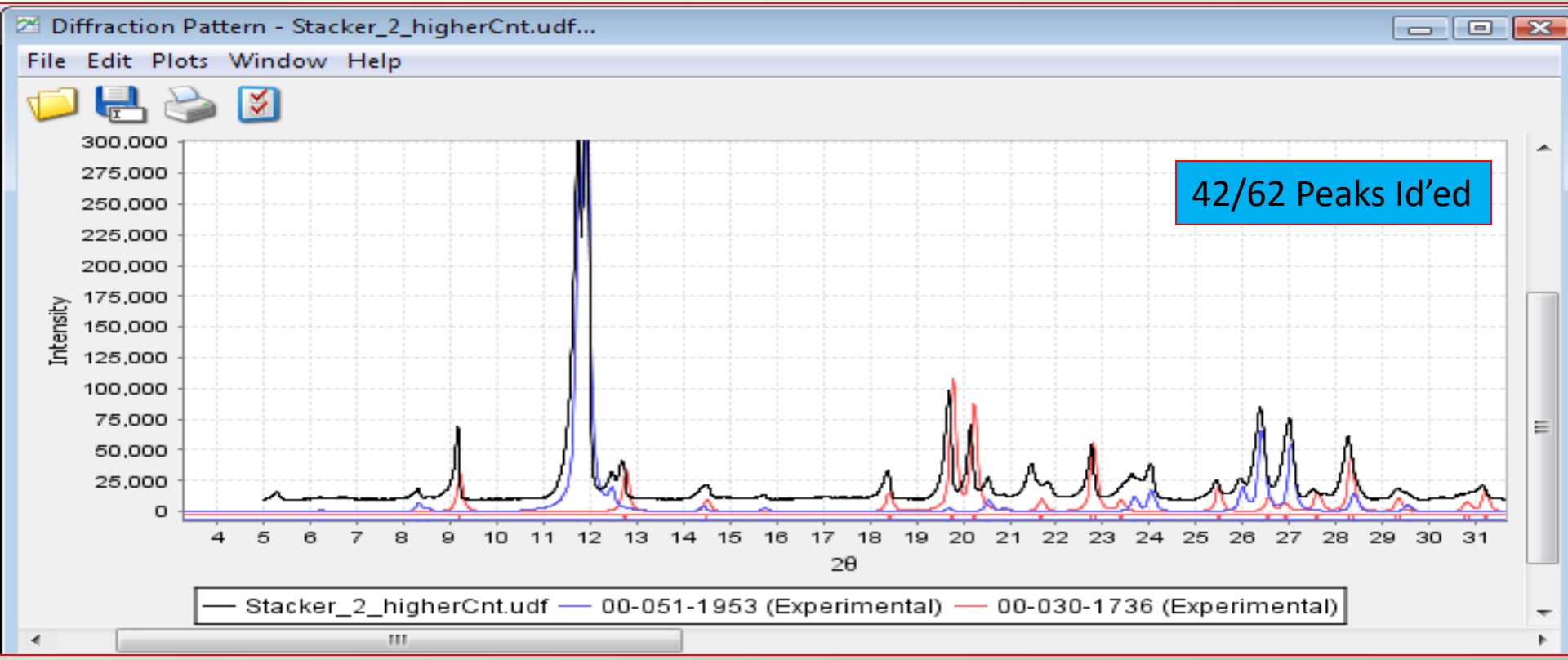
Note: Microcrystalline cellulose I beta (40A) was added to the simulation as shown in red fromm reference PDF 00-056-1718

# TrimSpa
# 3 Phases – 1 Data source



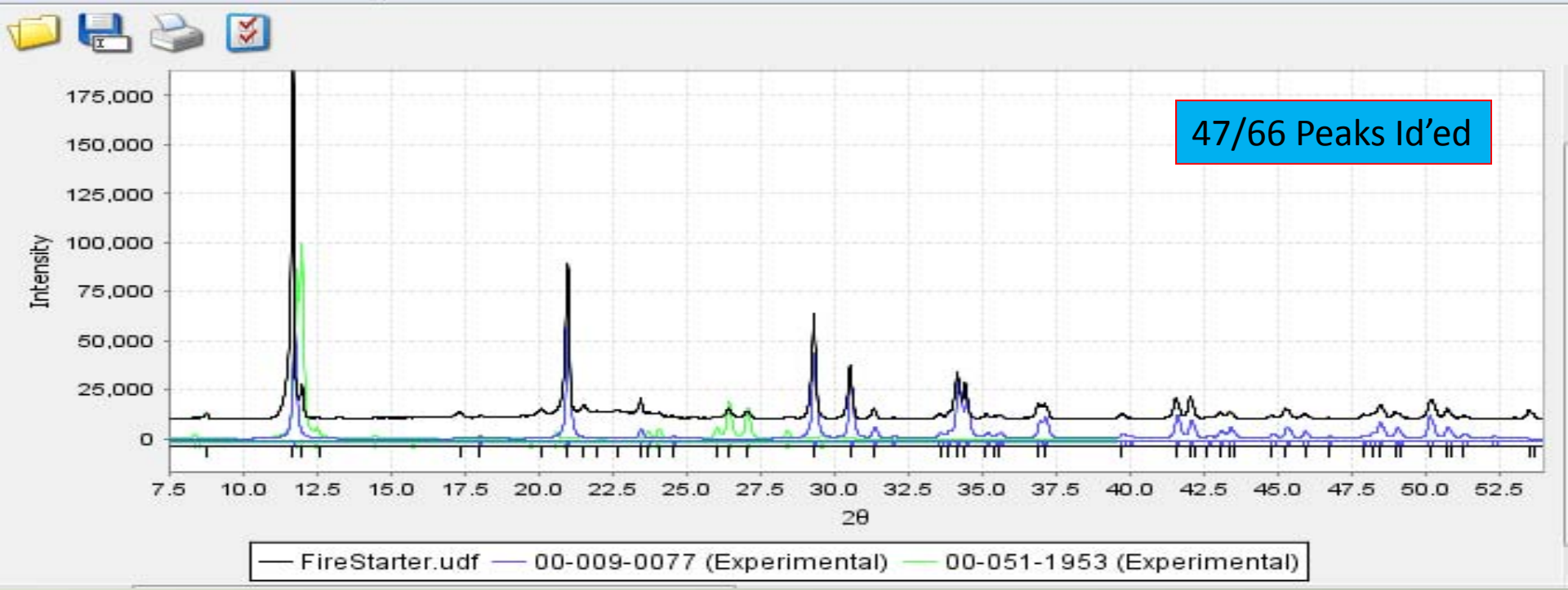

| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-009-0077 | Calcium Phosphate Hydroxide Hydrate | 0.413 | 27 | | 8.4s |
| 2 | ☑ | 00-002-0623 | Calcium Carbonate | 0.165 | 11 | | 6.8s |
| 3 | ☑ | 00-030-1735 | α-d-Glucosamine hydrochloride | 0.105 | 7 | 1.5 | 16.3s |

# Stacker
# 2 phases – 1 source



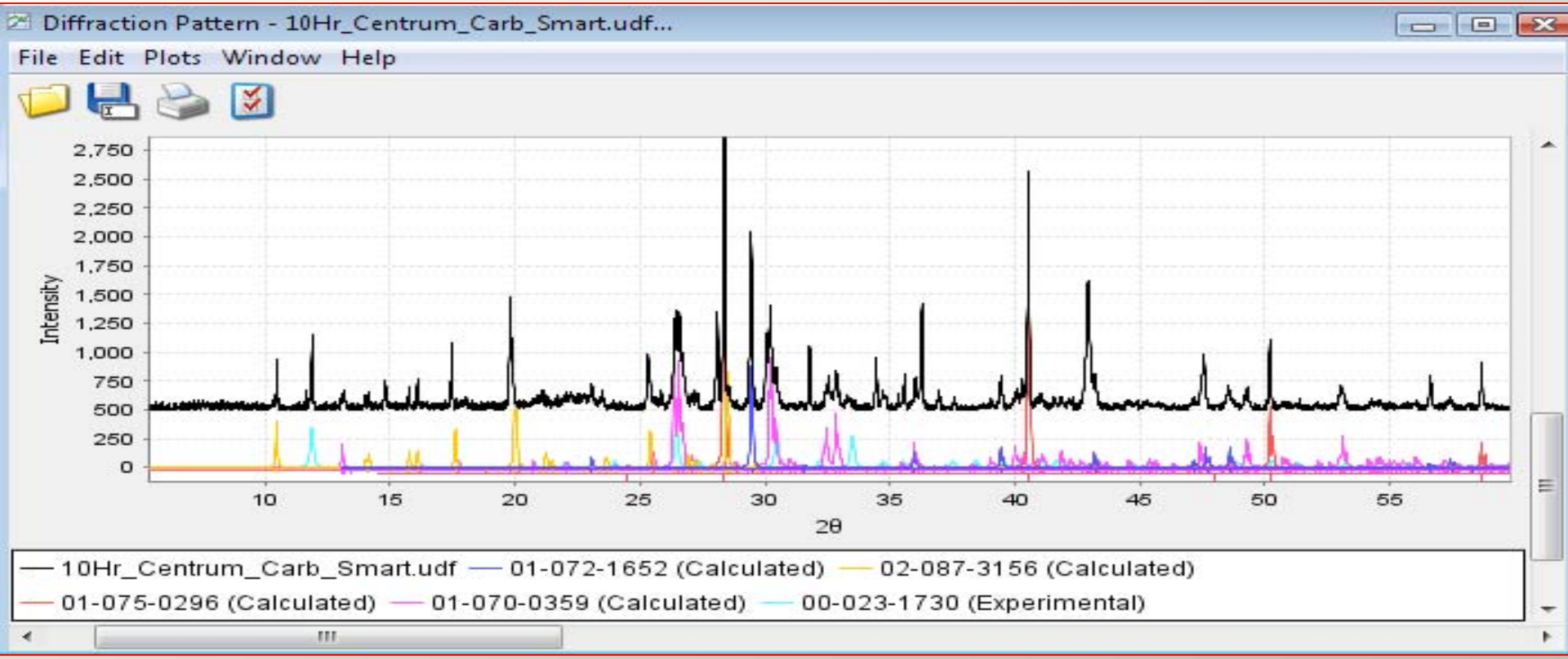

| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-051-1953 | Caffeine | 1.11 | 75 | | 7.1s |
| 2 | ☑ | 00-030-1736 | D-Glucose hydrate | 0.236 | 16 | 0.67 | 3.9s |

# Firestarter
# 2 phases – 1 source



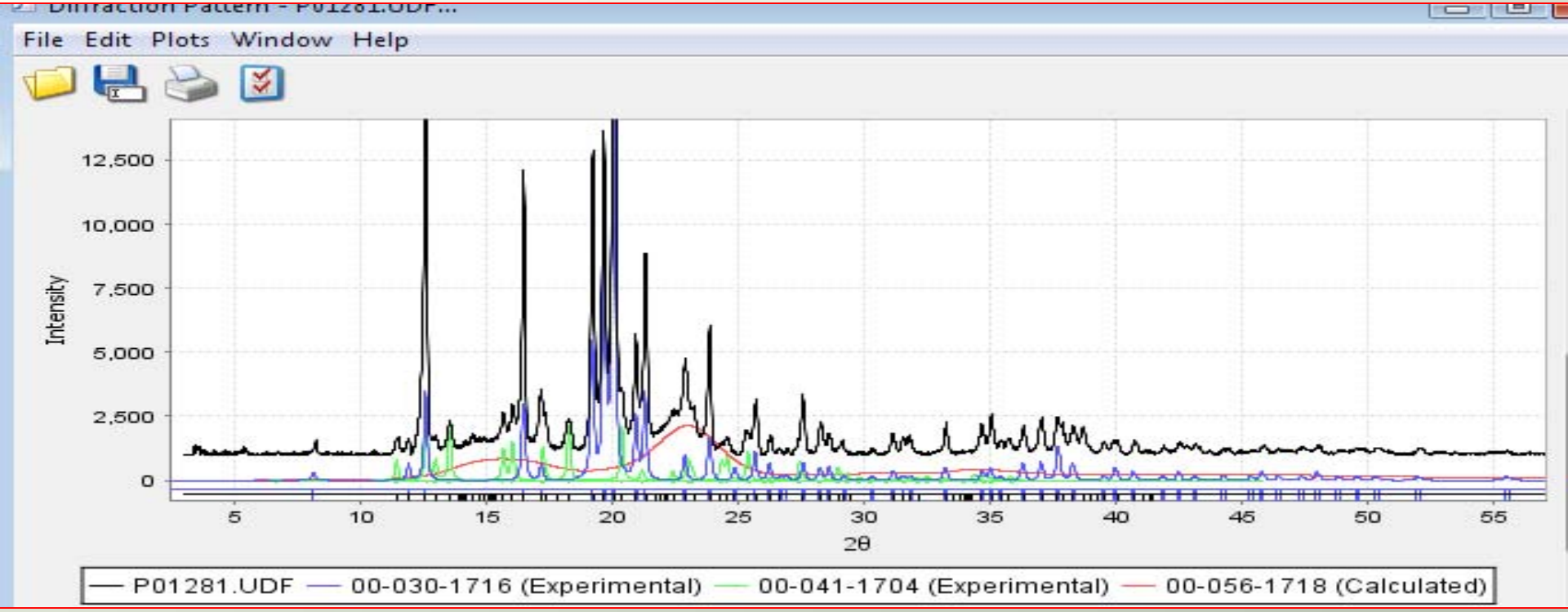

| # | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-009-0077 | Calcium Phosphate Hydroxide Hydrate | 0.417 | 32 | | 3s |
| 2 | ☑ | 00-051-1953 | Caffeine | 0.667 | 52 | | 1.8s |

# Centrum Carb Smart
# 5 phases – 3 data sources




| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 01-072-1652 | Calcium Carbonate | 0.233 | 13 | 3.24 | 1.5s |
| 2 | ☑ | 02-087-3156 | L-Ascorbic acid | 0.12 | 6 | 0.72 | 1.9s |
| 3 | ☑ | 01-075-0296 | Potassium Chloride | 0.768 | 41 | 6.07 | 0.6s |
| 4 | ☑ | 01-070-0359 | Calcium Hydrogen Phosphate | 0.253 | 14 | 0.71 | 2.3s |
| 5 | ☑ | 00-023-1730 | Iron fumarate | 0.091 | 5 | | 2.4s |

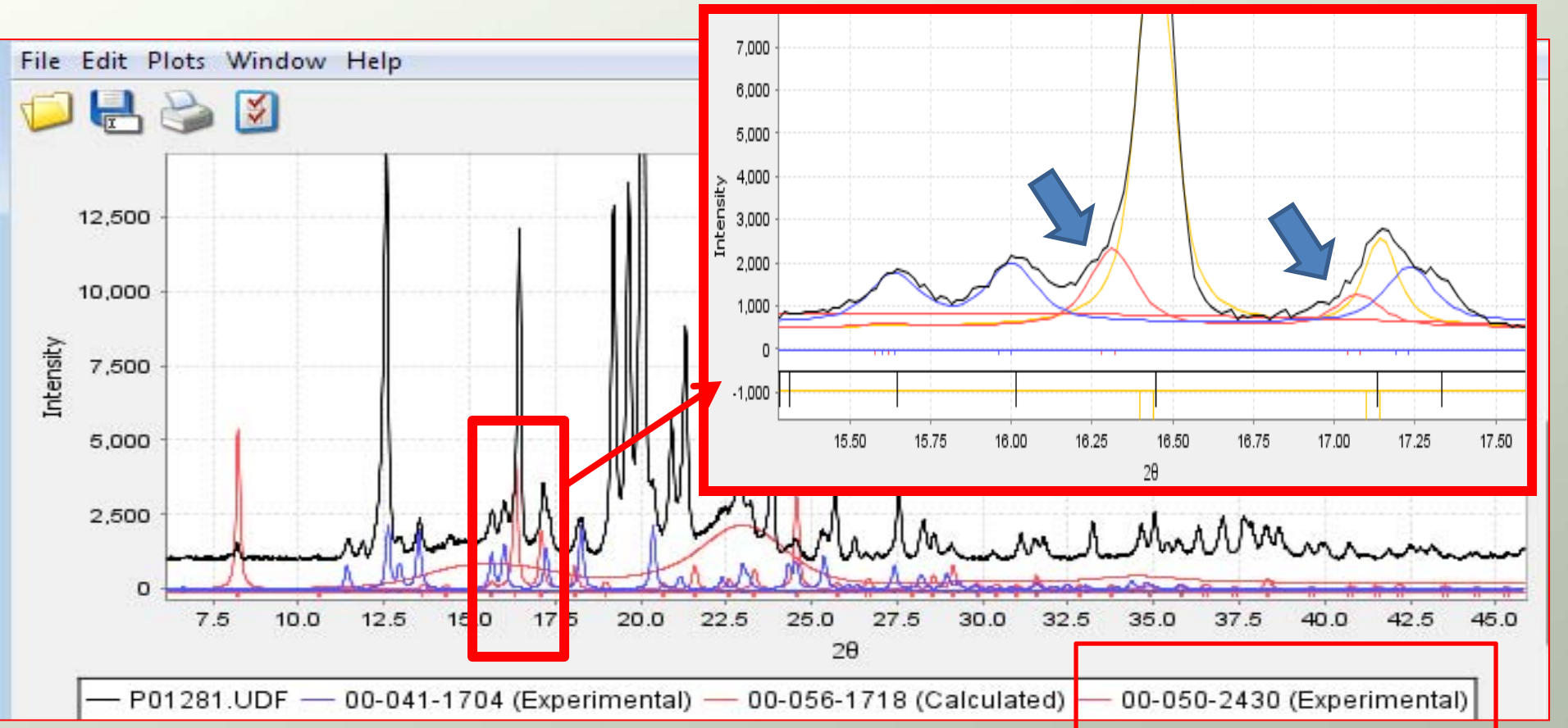
# Promethazine Formulation
# 3 phases – 1 source



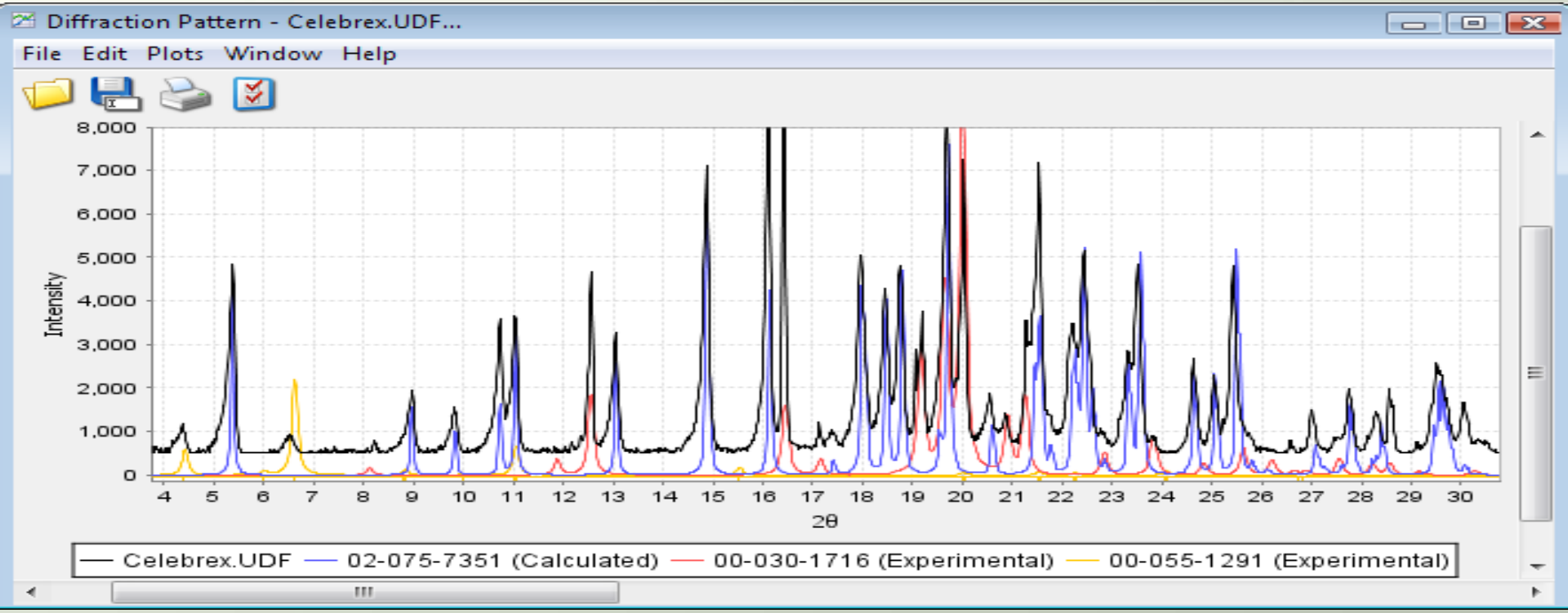

| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-030-1716 | Lactose hydrate | 1.264 | 61 | 1.55 | 2.8s |
| 2 | ☑ | 00-041-1704 | Promethazine hydrochloride | 0.158 | 8 | | 5.4s |
| 3 | ☑ | 00-056-1718 | Cellulose Iβ | 0.323 | 16 | | 1.9s |

Note: 25 A microcrystalline cellulose

# Promethazine – 2 polymorphs ?



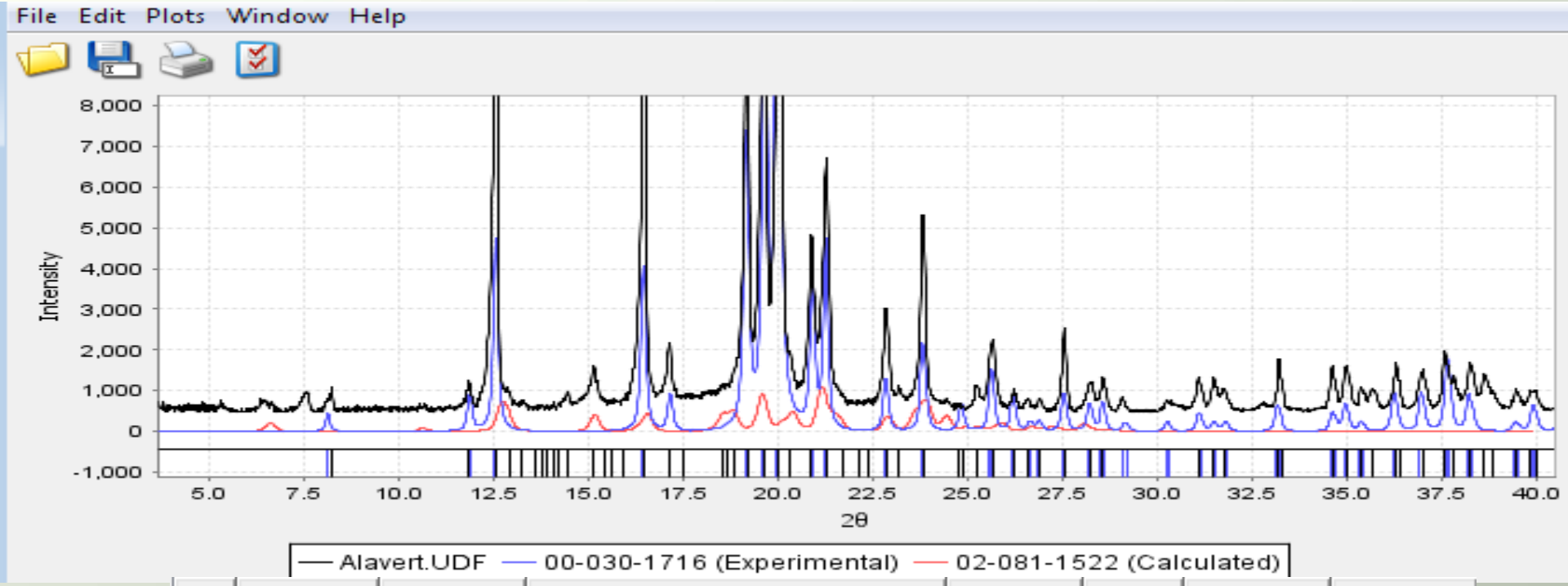
# Celebrex
# 3 phases – 2 sources




| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 02-075-7351 | 4-(5-(4-Methylphenyl)-3-(trifluorometh... | 0.831 | 13 | 0.36 | 15.9s |
| 2 | ☑ | 00-030-1716 | Lactose hydrate | 1.454 | 24 | 1.55 | 5.4s |
| 3 | ☑ | 00-055-1291 | Stearic acid | 3.303 | 54 | | 2.2s |

Celecoxib

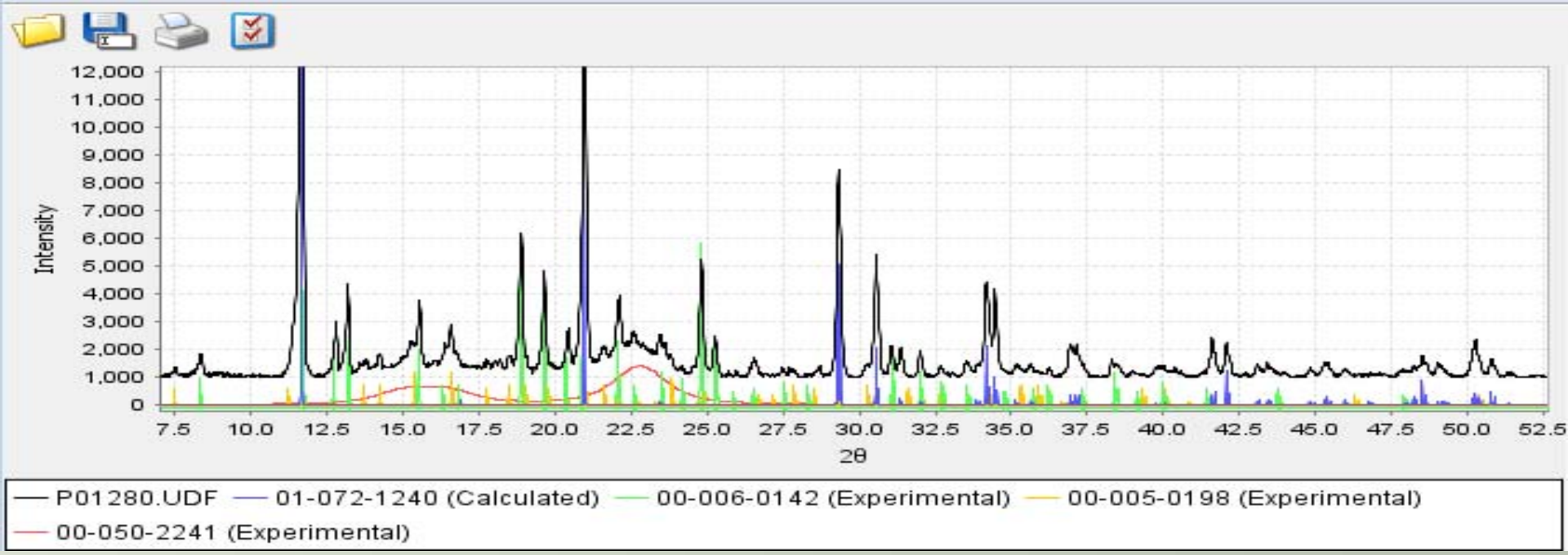
# Alavert
# 3 phases – 2 sources




| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-030-1716 | Lactose hydrate | 1.362 | 53 | 1.55 | 7.8s |
| 2 | ☑ | 02-081-1522 | 4-(8-Chloro-5,6-dihydro-11H-benzo(5,... | 0.523 | 20 | 0.45 | 1.4s |

Note: The third phase is Mg Stearate dihydrate (not shown) which accounts for the unidentified low angle peak at 7.5 degrees. The active ingredient is Loratadine, the chemical name is displayed. There are two polymorphs, only one was observed in this commercial specimen.

# Donnatal
# 4 phases – 2 sources




| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 01-072-1240 | Calcium Hydrogen Phosphate Hydrate | 0.748 | 51 | 1.39 | 13.4s |
| 2 | ☑ | 00-006-0142 | Sucrose | 0.428 | 29 | | 8.3s |
| 3 | ☑ | 00-005-0198 | Phenobarbital | 0.194 | 13 | | 11.9s |
| 4 | ☑ | 00-050-2241 | Cellulose | 0.108 | 7 | | 1.3s |

# Synchrotron Data

More peaks identified because of significant resolution and signal to noise improvements versus conventional data collection

# Vitapower – Yellow Tablet
# 6 phases – 2 sources

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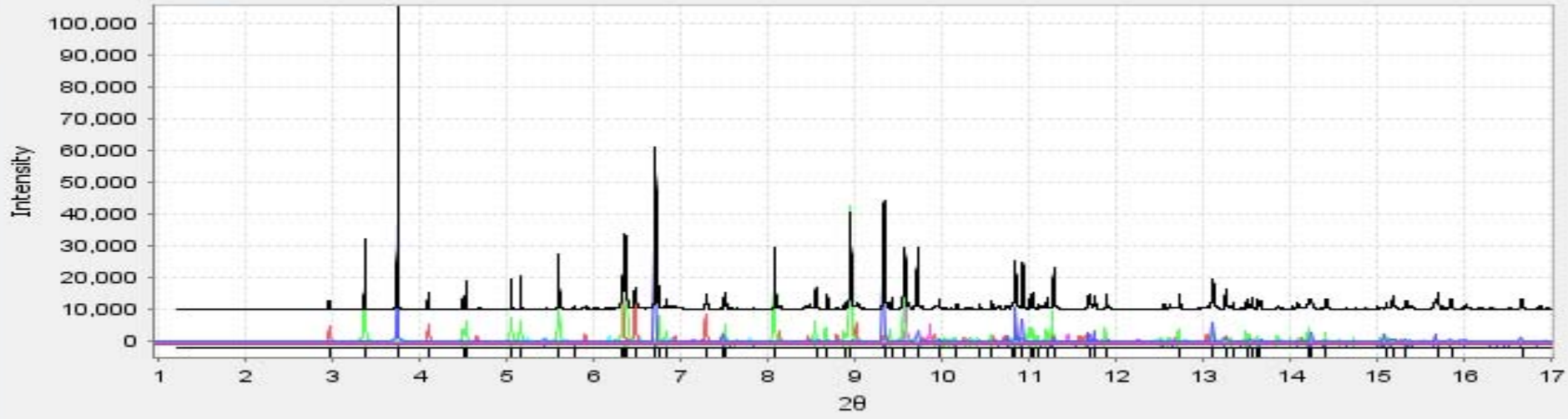


| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 01-072-1240 | Calcium Hydrogen Phosphate Hydrate | 0.7 | 31 | 1.39 | 21.4s |
| 2 | ☑ | 00-022-1560 | Ascorbic acid | 0.49 | 21 | | 10.8s |
| 3 | ☑ | 00-030-1736 | D-Glucose hydrate | 0.375 | 16 | 0.67 | 7.3s |
| 4 | ☑ | 01-075-1674 | Potassium Chloride | 0.115 | 5 | 8.32 | 0.2s |
| 5 | ☑ | 00-051-1524 | Calcium Carbonate | 0.315 | 14 | | 0.1s |
| 6 | ☑ | 00-017-1018 | β-D-Glucose | 0.288 | 13 | | 0s |

# Vitapower – Red Tablet
# 5 phases – 2 sources

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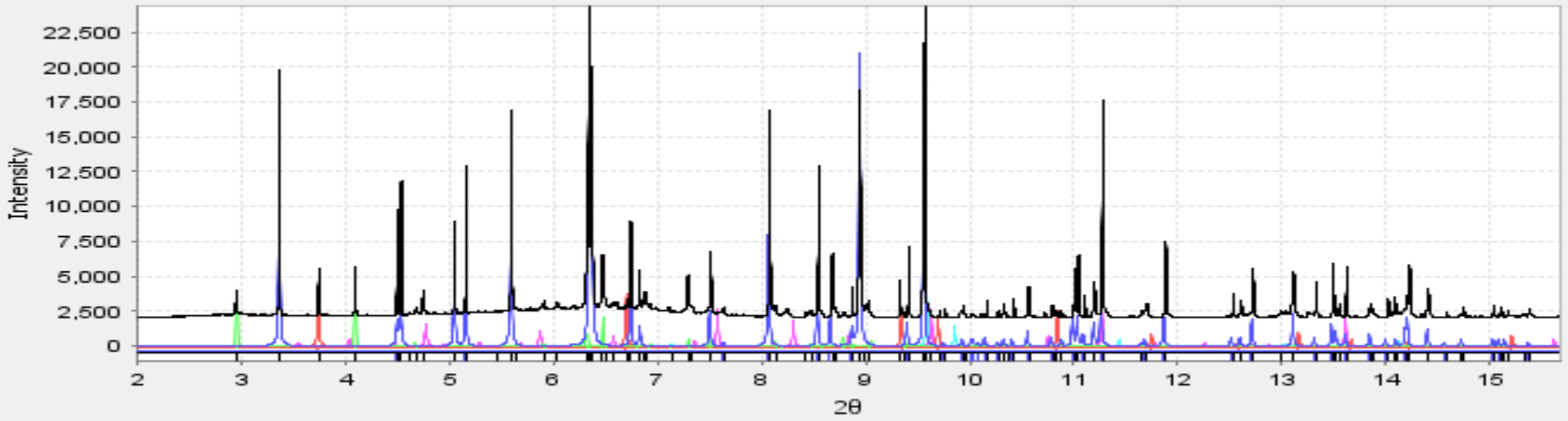


vitapower_red.gsas — 00-022-1560 (Experimental) — 02-063-0145 (Calculated) — 00-001-0395 (Experimental) — 00-015-0615 (Experimental) — 00-051-1524 (Experimental)

| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 00-022-1560 | Ascorbic acid | 1.406 | 38 | | 11.7s |
| 2 | ☑ | 02-063-0145 | alpha-D-Glucose monohydrate | 0.411 | 11 | 0.72 | 5.9s |
| 3 | ☑ | 00-001-0395 | Calcium Phosphate Hydrate | 0.153 | 4 | | 4.4s |
| 4 | ☑ | 00-015-0615 | Iron Oxide | 0.373 | 10 | | 2.8s |
| 5 | ☑ | 00-051-1524 | Calcium Carbonate | 0.828 | 23 | | 1s |

# Centrum Tablet
# 10 phases – 3 sources

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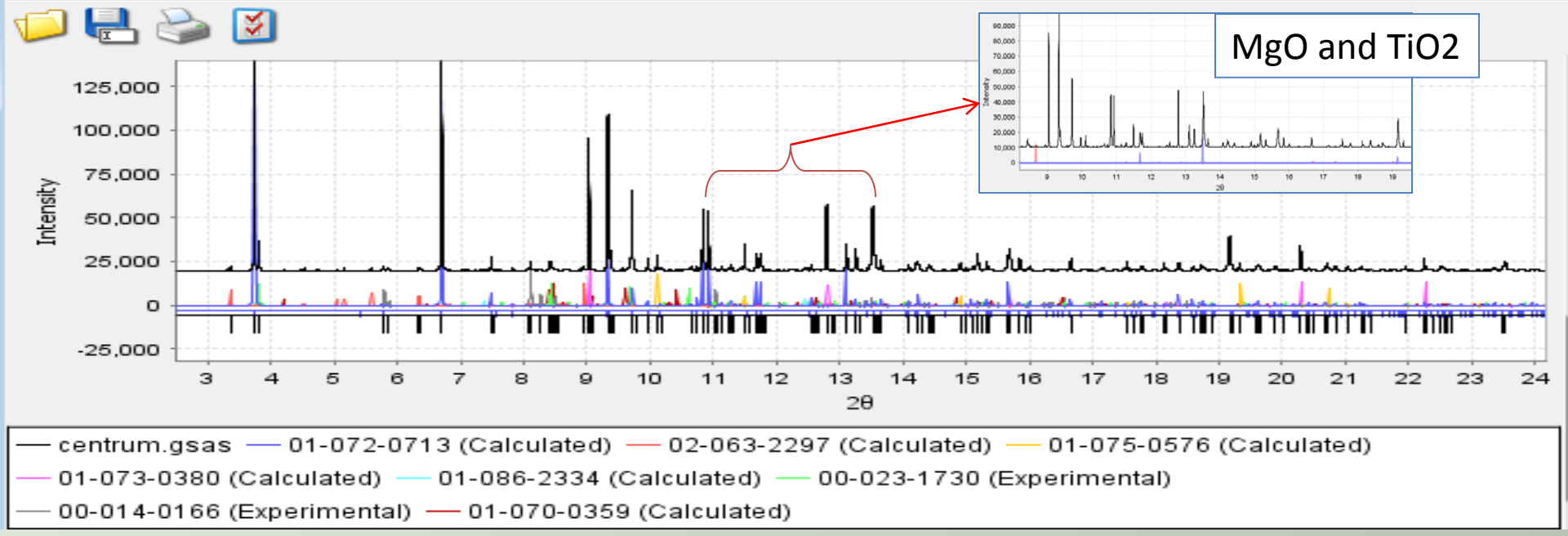


centrum.gsas — 01-072-0713 (Calculated) — 02-063-2297 (Calculated) — 01-075-0576 (Calculated)
01-073-0380 (Calculated) — 01-086-2334 (Calculated) — 00-023-1730 (Experimental)
00-014-0166 (Experimental) — 01-070-0359 (Calculated)

| # ▲ | Accepted | PDF # | Compound Name | Int. Ratio | Int. % | I/Ic | Time |
|---|---|---|---|---|---|---|---|
| 1 | ☑ | 01-072-0713 | Calcium Hydrogen Phosphate Hydrate | 0.485 | 29 | 1.42 | 51.1s |
| 2 | ☑ | 02-063-2297 | L-Ascorbic acid | 0.112 | 7 | 0.6 | 9.7s |
| 3 | ☑ | 01-075-0576 | Zinc Oxide | 0.079 | 5 | 5.53 | 24s |
| 4 | ☑ | 01-073-0380 | Potassium Chloride | 0.208 | 12 | 6.07 | 8.9s |
| 5 | ☑ | 01-086-2334 | Calcium Carbonate | 0.071 | 4 | 3.25 | 0.4s |
| 6 | ☑ | 00-023-1730 | Iron fumarate | 0.056 | 3 | | 0.3s |
| 7 | ☑ | 00-014-0166 | Manganese Sulfate Hydrate | 0.113 | 7 | | 1.2s |
| 8 | ☑ | 01-070-0359 | Calcium Hydrogen Phosphate | 0.264 | 16 | 0.71 | 1s |
| 9 | ☑ | 01-089-4248 | Magnesium Oxide | 0.122 | 7 | 3.04 | 0.1s |
| 10 | ☑ | 01-076-0323 | Titanium Oxide | 0.038 | 2 | 3.25 | 0s |

# Results

Complex multiphase materials can be identified using PDF-4/Organics when combined with high quality diffraction data from either laboratory diffractometers or synchrotron sources