









Development of a Low-Cost Web-Based Information System for Managing a University Department Chemical Warehouse

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Supplementary Materials

| | | | | |
|--|--------------------------|---------------------------|---|-----------|
|  | ACID0012 | ortho-Phosphoric acid 85% | <div><div>-</div><div>1</div><div>+</div></div> | 52,400 € |
|  | ALCO0001 | 1-Butanol | <div><div>-</div><div>1</div><div>+</div></div> | 19,400 € |
|  | AMAC0002 | L-Alanine | <div><div>-</div><div>1</div><div>+</div></div> | 72,580 € |
|  | SAIN0034 | Calcium carbonate | <div><div>-</div><div>1</div><div>+</div></div> | 21,400 € |
|  | SAIN0049 | Magnesium sulfate dried | <div><div>-</div><div>1</div><div>+</div></div> | 30,000 € |
|  | SAIN0037 | Potassium bicarbonate | <div><div>-</div><div>2</div><div>+</div></div> | 27,480 € |
|  | SAIN0025 | Sodium acetate anhydrous | <div><div>-</div><div>1</div><div>+</div></div> | 13,500 € |
|  | CONS0005 | PARAFILM M - 10 cm x 33 m | <div><div>-</div><div>2</div><div>+</div></div> | 38,400 € |
| Total: | | | | 275,160 € |

Proceed with the order

Empty cart

Back to products catalog

Figure S1. Shopping cart page view.































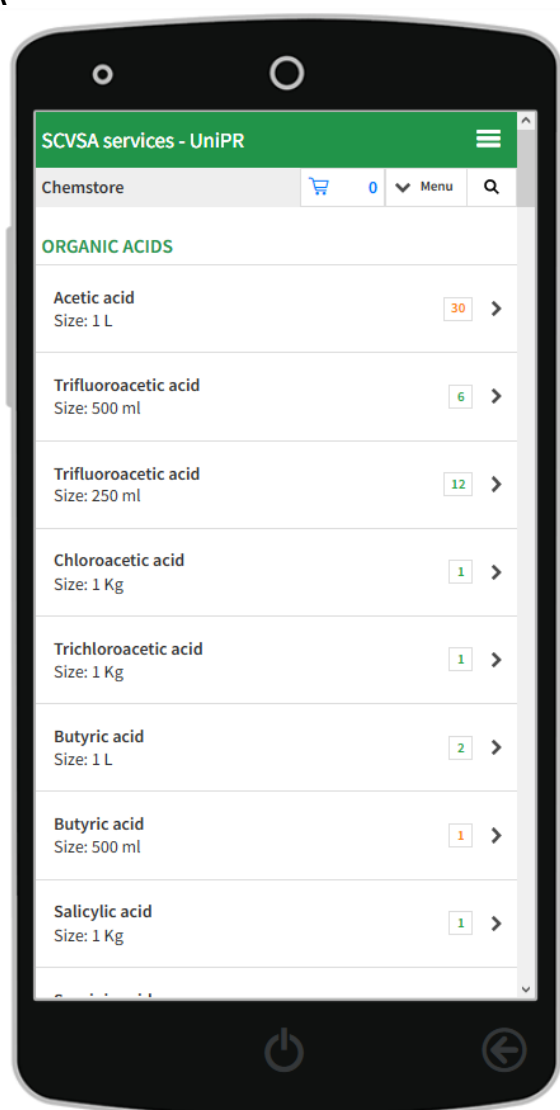
| Date | Product ID | Product name | Load/Unload | Reason | Destination | Destination PI |
|--|--------------------------|-----------------------------|-------------|---------------------------------|---------------------|----------------|
|  02/04/2024 09:09 | SOPU0005 | Chloroform | -1 | Order 0618/2024 | 13.01.S.075 | Name Lastname |
|  29/03/2024 12:04 | ALOD0026 | 1-Iodohehexane | -1 | Transfer | 13.01.S.049 | Name Lastname |
|  29/03/2024 11:59 | ALOD0024 | Iodotrimethylsilane | -2 | Transfer | 13.01.S.049 | Name Lastname |
|  29/03/2024 11:56 | ETER0003 | Chloromethyl octyl ether | -4 | Transfer | 13.01.S.049 | Name Lastname |
|  29/03/2024 09:19 | BASU0002 | Potassium hydroxide pellets | -1 | Order 0615/2024 | 13.01.S.049 | Name Lastname |
|  29/03/2024 09:19 | CONS0095 | NMR Tubes – 5mm OD | -1 | Order 0614/2024 | 13.01.0.021 | Name Lastname |
|  29/03/2024 09:19 | SAIN0022 | Sodium chloride | -1 | Order 0614/2024 | 13.01.0.021 | Name Lastname |
|  29/03/2024 09:19 | SOPU0017 | 2-Propanol | -1 | Order 0614/2024 | 13.01.0.021 | Name Lastname |
|  29/03/2024 09:19 | SOPU0022 | Ethyl alcohol denatured 90% | -2 | Order 0612/2024 | 13.01.S.049 | Name Lastname |
|  29/03/2024 09:19 | SOPU0023 | Ethyl alcohol 96% | -1 | Order 0614/2024 | 13.01.0.021 | Name Lastname |
|  28/03/2024 13:01 | ETEC0019 | Carbazole | -1 | Transfer | 13.01.0.021 | Name Lastname |
|  28/03/2024 11:08 | SODE0006 | Acetonitrile-d3 | -2 | Transfer | 13.01.1.056 | Name Lastname |
|  28/03/2024 09:40 | ACID0001 | Hydrochloric acid | -2 | Order 0603/2024 | 13.01.S.049 | Name Lastname |
|  28/03/2024 09:40 | CONS0005 | PARAFILM M - 10 cm x 33 m | -1 | Order 0605/2024 | 13.01.S.103 | Name Lastname |
|  28/03/2024 09:40 | SODE0001 | Chloroform-d | -1 | Order 0606/2024 | 13.01.0.021 | Name Lastname |
|  28/03/2024 09:40 | SOPU0002 | Hexane | -1 | Order 0604/2024 | 13.01.1.024 | Name Lastname |
|  28/03/2024 09:40 | SOPU0002 | Hexane | -1 | Order 0609/2024 | 13.01.1.026 | Name Lastname |
|  28/03/2024 09:40 | SOPU0003 | Ethyl acetate | -1 | Order 0604/2024 | 13.01.1.024 | Name Lastname |
|  27/03/2024 12:31 | SOPU0023 | Ethyl alcohol 96% | +48 | Purchase | 13.01.S.127 S10.R03 | Name Lastname |
|  27/03/2024 12:29 | HPLC0005 | Dichloromethane for HPLC | +2 | Purchase | 13.01.S.127 S11.R03 | Name Lastname |
|  27/03/2024 12:27 | AMAR0006 | Benzylamine | -1 | Transfer | 13.01.0.021 | Name Lastname |
|  27/03/2024 12:26 | SAIN0029 | Sodium acetate trihydrate | +2 | Purchase | 13.01.S.058 S02.R04 | Name Lastname |
|  27/03/2024 12:26 | SAIN0062 | Zinc sulfate heptahydrate | +2 | Purchase | 13.01.S.058 S01.R05 | Name Lastname |
|  27/03/2024 12:25 | SAIN0025 | Sodium acetate anhydrous | +16 | Purchase | 13.01.S.058 S02.R04 | Name Lastname |
|  27/03/2024 12:24 | SAIN0088 | Potassium sulfate | +6 | Purchase | 13.01.S.058 S01.R06 | Name Lastname |
|  27/03/2024 12:21 | SOPU0007 | Dimethyl sulfoxide | +6 | Purchase | 13.01.S.127 S07.R04 | Name Lastname |
|  27/03/2024 12:21 | SOPU0028 | 1,4-Dioxane | -1 | Transfer | 13.01.0.021 | Name Lastname |
|  27/03/2024 12:19 | SAIN0050 | Barium chloride dihydrate | +1 | Purchase | 13.01.S.058 S01.R05 | Name Lastname |
|  27/03/2024 12:19 | SOPU0025 | Methyl tert-butyl ether | +16 | Purchase | 13.01.S.127 S10.R05 | Name Lastname |
|  27/03/2024 12:17 | HPLC0006 | Chloroform for HPLC | +2 | Purchase | 13.01.S.127 S11.R03 | Name Lastname |
|  27/03/2024 12:16 | SOPU0010 | Pentane | +18 | Purchase | 13.01.S.127 S08.R02 | Name Lastname |

Figure S2. List view of the Inventory Transaction table. The "Destination PI" column indicates the name of the principal investigator of the destination laboratory for unloading movements, or the name of the warehouse manager for loading movements.

A



B

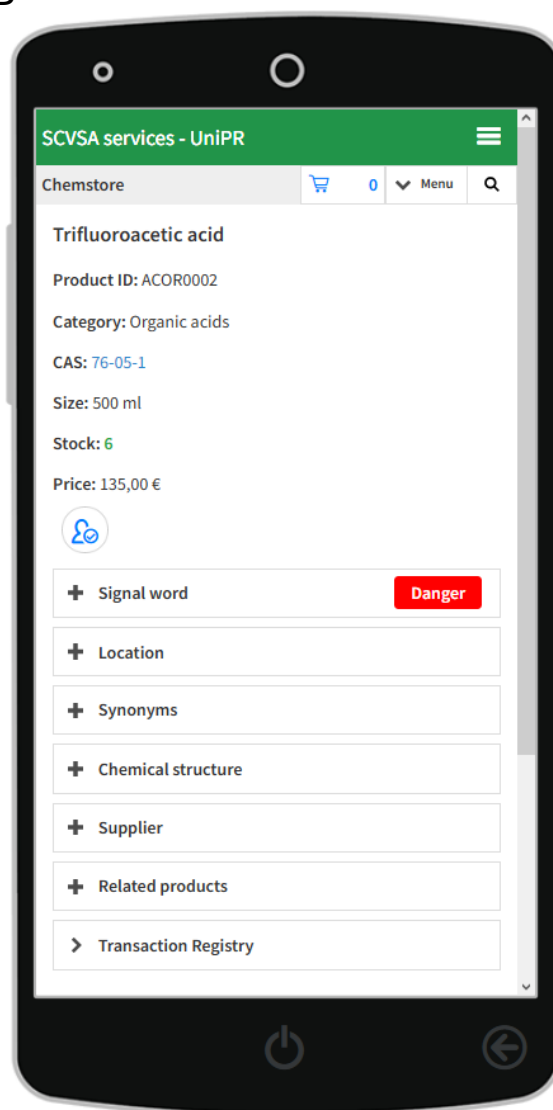


Figure S3. Mobile front-end of the Digital Warehouse application. Android app screenshots of A) products list view and B) product page view.

Table S1. Products table data fields

| Field | Data type | Chemical compound | Generic product | Source |
|------------------------------|-----------------|-------------------|-----------------|-----------------|
| Product ID | Primary key | Yes | Yes | Computed |
| Category | Multiple choice | Yes | Yes | User input |
| Subcategory | Multiple choice | No | Yes | User input |
| CAS number | Text | Yes | No | User input |
| Product name | Text | Yes | Yes | PubChem |
| IUPAC name | Text | Yes | No | PubChem |
| LANG name | Text | Yes | No | MyMemory |
| Synonyms | Text | Yes | No | PubChem |
| Formula | Text | Yes | No | PubChem |
| SMILES | Text | Yes | No | PubChem |
| M. weight | Text | Yes | No | PubChem |
| PubChem CID | Text | Yes | No | PubChem |
| Supplier ID | Multiple choice | Yes | Yes | Suppliers table |
| Supplier code | Text | Yes | Yes | User input |
| Barcode | Text | Yes | Yes | User input |
| Supplier size | Text | Yes | Yes | User input |
| Product size | Text | Yes | Yes | User input |
| Product price | Number | Yes | Yes | User input |
| Stock | Number | Yes | Yes | User input |
| Understock | Number | Yes | Yes | User input |
| Overstock | Number | Yes | Yes | User input |
| Last purchase | Date | Yes | Yes | Computed |
| Room location | Text | Yes | Yes | User input |
| Shelf location | Text | Yes | Yes | User input |
| Notes | Text | Yes | Yes | User input |
| Automatic reordering | Yes/No | Yes | Yes | User input |
| Product for teaching | Yes/No | Yes | Yes | User input |
| Product without stock | Yes/No | Yes | Yes | User input |
| Delivered to staff only | Yes/No | Yes | Yes | User input |
| Store at low temperature | Yes/No | Yes | Yes | User input |
| Description | Text | Yes | Yes | User input |
| Images | Drag & Drop | Yes | Yes | User input |
| SDS | File | Yes | No | User input |
| SDS date | Date | Yes | No | SDS scan |
| Signal Word | Yes/No | Yes | No | SDS scan |
| Not hazardous (EC) 1272/2008 | Multiple choice | Yes | No | SDS scan |
| Pictogram | Multiple choice | Yes | No | SDS scan |
| Hazard Statement | Multiple choice | Yes | No | SDS scan |
| Precautionary statement | Multiple choice | Yes | No | SDS scan |
| Attachments | Drag & Drop | Yes | Yes | User input |
| Epoch time last changes | Number | Yes | Yes | Computed |

Table S2. Sale Orders table data fields

| Field | Data type | Source |
|-------------------------|-----------------|-----------------------|
| Order ID | Primary key | Computed |
| Order number | Text | Computed |
| Date | Date | Computed |
| User ID | Text | Users table |
| Type of activity | Multiple choice | User input |
| Account ID | Text | Accounts table |
| Joint purchase ID | Text | Joint Purchases table |
| Destination | Text | User input |
| Notes | Text | User input |
| Attachments | Drag & Drop | User input |
| Order state | Multiple choice | Computed |
| Discount | Number | User input |
| VAT | Number | Computed |
| Product ID | Text | Products table |
| Product name | Text | Products table |
| Quantity | Number | Shopping cart |
| Unit price | Number | Products table |
| Product cost | Number | Computed |
| Total cost | Number | Computed |
| Epoch time last changes | Number | Computed |

Table S3. Inventory Transactions table data fields

| Field | Data type | Source |
|-------------------------|-----------------|-------------------|
| Transaction ID | Primary key | Computed |
| Date | Date | Computed |
| Product ID | Text | Products table |
| Product name | Text | Products table |
| Product category | Multiple choice | Products table |
| Quantity | Number | Sale Orders table |
| Transaction reason | Text | Computed |
| Destination | Text | Sale Orders table |
| Product size | Text | Products table |
| Product price | Number | Products table |
| User ID | Text | Users table |
| Grant Holder ID | Text | Accounts table |
| Epoch time last changes | Number | Computed |

Table S4. Accounts table data fields

| Field | Data type | Source |
|-------------------------|-----------------|-------------|
| Account ID | Primary key | Computed |
| Account name | Text | User input |
| Grant ID | Text | User input |
| Grant Holder ID | Text | Users table |
| Type of account | Multiple choice | User input |
| Start date | Date | User input |
| End date | Date | User input |
| Budget | Number | User input |
| Authorized users | Multiple choice | Users table |
| Epoch time last changes | Number | Computed |

Table S5. Suppliers table data fields

| Field | Data type | Source |
|-------------------------|-------------|------------|
| Supplier ID | Primary key | Computed |
| Supplier name | Text | User input |
| Supplier code | Text | User input |
| VAT number | Text | User input |
| Telephone number | Text | User input |
| Email address | Text | User input |
| Website url | Text | User input |
| Address | Text | User input |
| Notes | Text | User input |
| Attachments | Drag & Drop | User input |
| Local agent name | Text | User input |
| Local agent email | Text | User input |
| Local agent telephone | Text | User input |
| Epoch time last changes | Number | Computed |

Table S6. Joint Purchases table data fields

| Field | Data type | Source |
|-------------------------|-----------------|-----------------|
| Joint purchase ID | Primary key | Computed |
| Title | Text | User input |
| Description | Text | User input |
| Start date | Date | User input |
| End date | Date | User input |
| Suppliers ID | Multiple choice | Suppliers table |
| Products ID | Multiple choice | Products table |
| Attachments | Drag & Drop | User input |
| Epoch time last changes | Number | Computed |