CAPE-OPEN Update in PRO/II v10.1

CAPE-OPEN Property Package in compound Databank Search Order List

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CAPE-OPEN 2017 Annual Meeting

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Agenda

PRO/II v10.1 was released in June 2017

- **CAPE-OPEN Property Package Limitations with PRO/II v9.4 & v10.0**
- **CAPE-OPEN Property Package behavior in PRO/II v10.1**
- **Demo of PRO/II v10.1 - Property Package in compound Databank Search Order**
- **Q&A**

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CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Limitations with PRO/II v9.4 and v10.0 :

  - The CO PP compounds are added as non-library compounds in PRO/II irrespective of whether the PP compounds are having CAS number or not.
  - Constant pure compound properties for the non-library compounds are taken from the CO PP.
  - This approach is having a limitation that user can’t use PRO/II native thermo as the required temperature dependent properties are not filled for the non-library compounds.
  - The results of CO PP can’t be compared with PRO/II native thermo in the same flowsheet.

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CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Behavior in PRO/II v10.1 :

  - Both CO PP and PRO/II native thermo can co-exist in the same flowsheet and be used in parallel by unit operations within the flowsheet.
  - If PP compounds are having CAS numbers and matching CAS number is found in the SIMSCI or PROCESS libraries.
    - CO PP compounds are added as library compounds in PRO/II.
    - CO PP is made available in the compound databank search order list and will be first in the list with the “cascade” option checked by default.
    - Constant pure compound properties are taken from the CO PP, if it is first in the databank search order list.

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CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Behavior in PRO/II v10.1 :

  - The constant pure compound properties are disabled in PRO/II and user is not allowed to modify the properties, if they are taken from CO PP.
  - The temperature dependent properties (such as vapor pressure, thermal conductivity, viscosity, Ideal Gas Enthalpy, Surface Tension etc.) are not taken from the PP and they are always filled from SIMSCI or PROCESS libraries.
  - User is allowed to change the global databank search order list or for each individual compound.

- Multiple CO PP in a flowsheet are allowed. Each newly added PP will have its corresponding databank inserted at the top of the search order.

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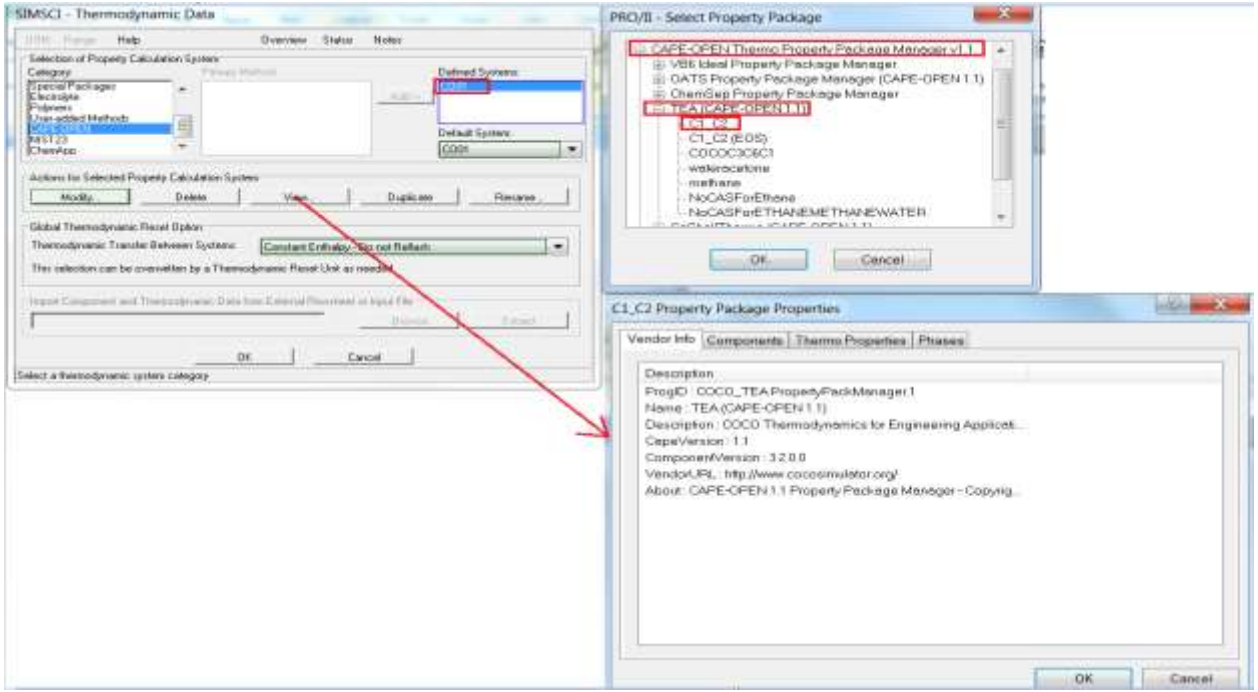
CO PP in compound Databank Search Order List in PRO/II v10.1

Selecting CO PP in PRO/II



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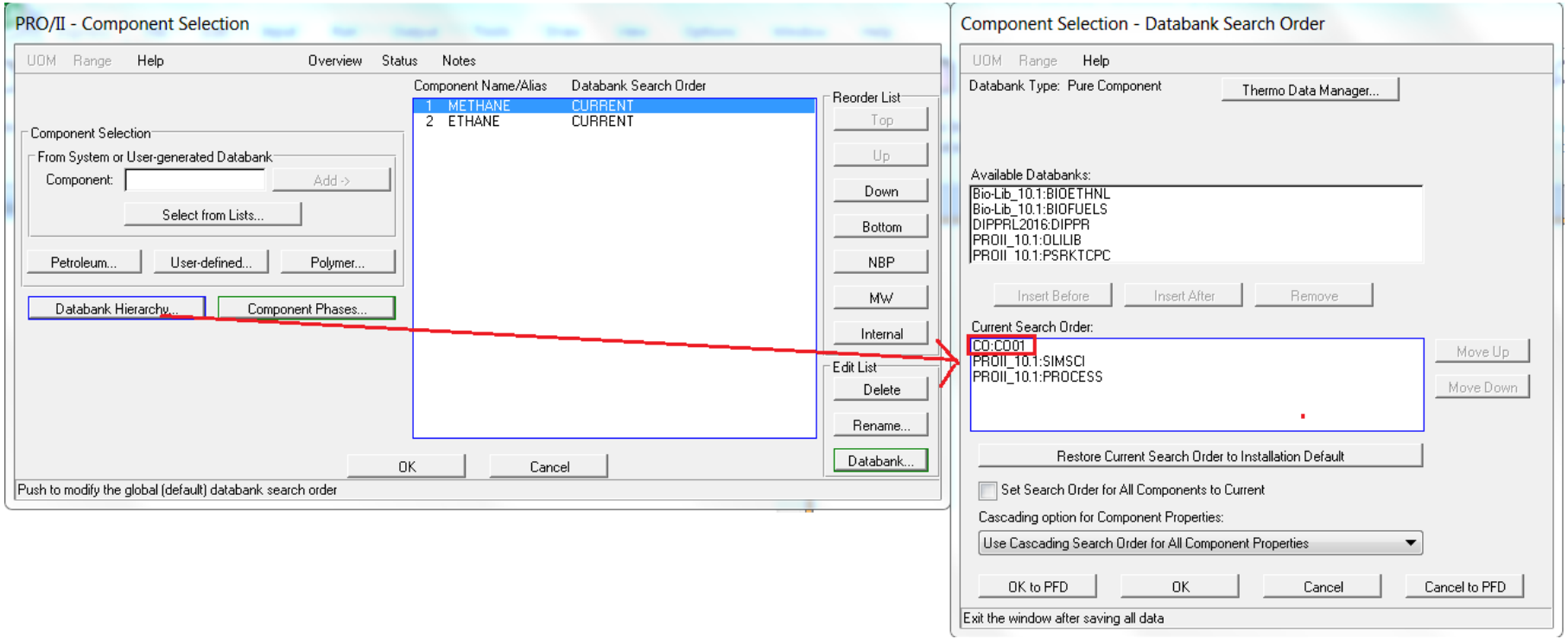
CO PP in compound Databank Search Order List in PRO/II v10.1



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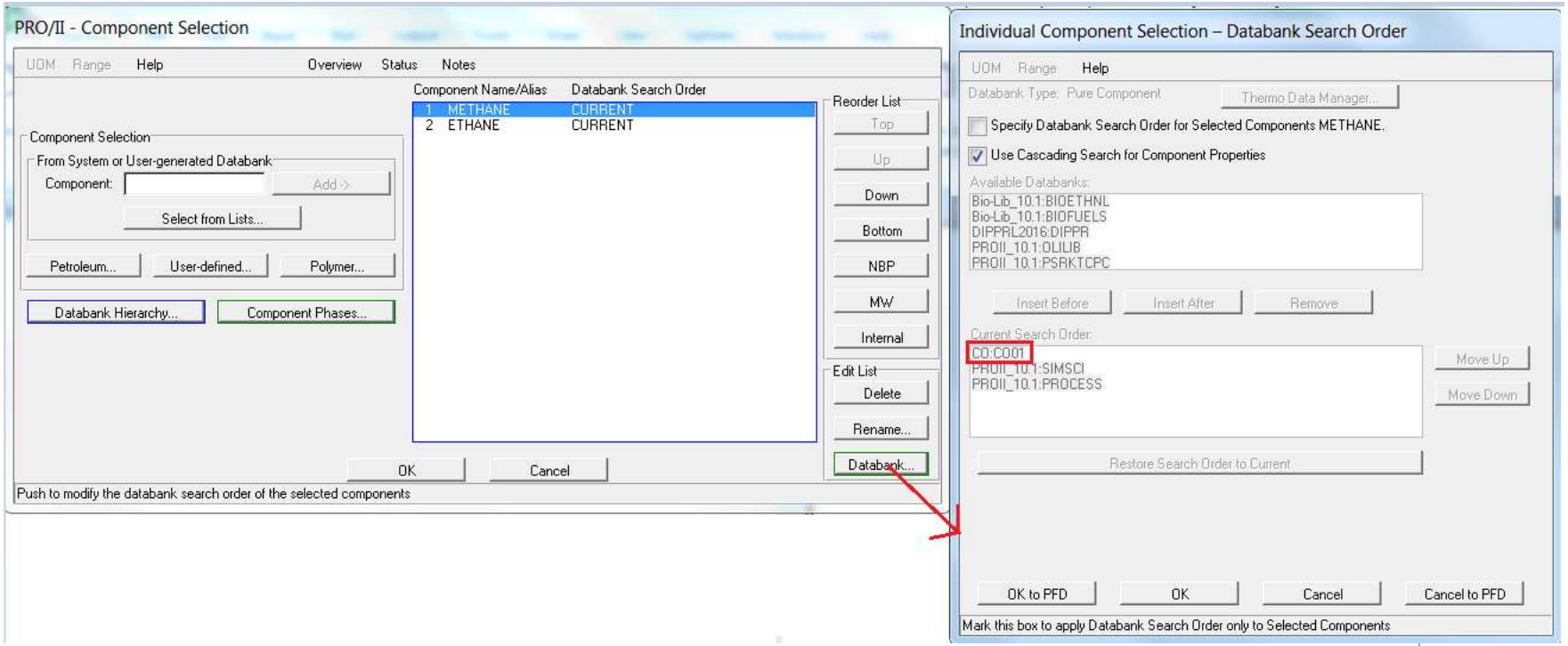
CO PP in compound Databank Search Order List in PRO/II v10.1



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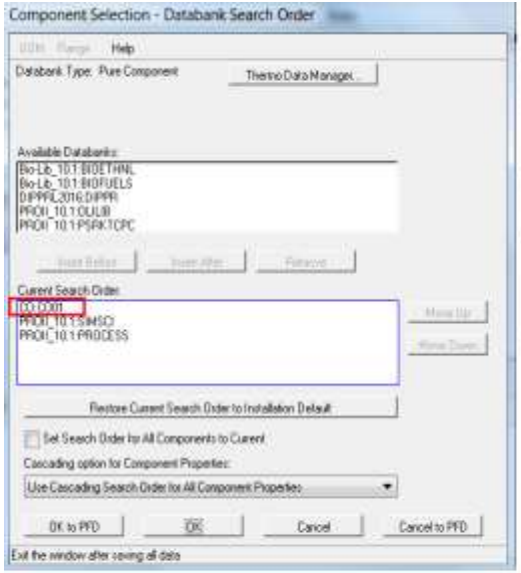
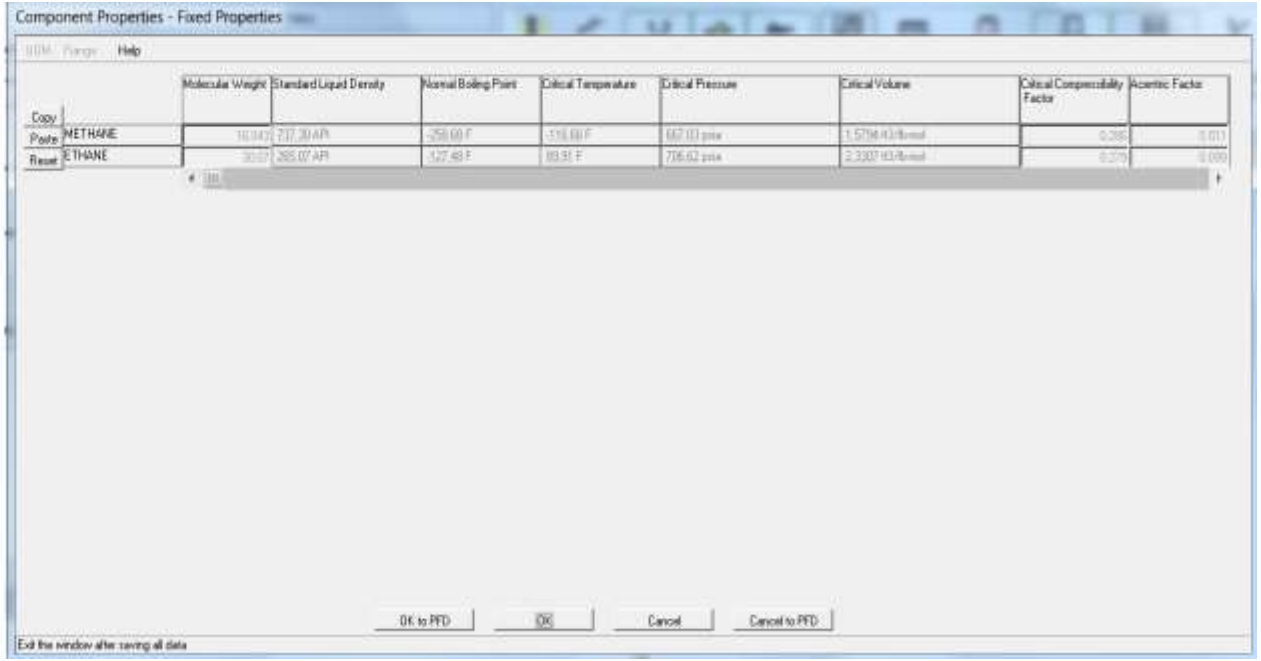
CO PP in compound Databank Search Order List in PRO/II v10.1





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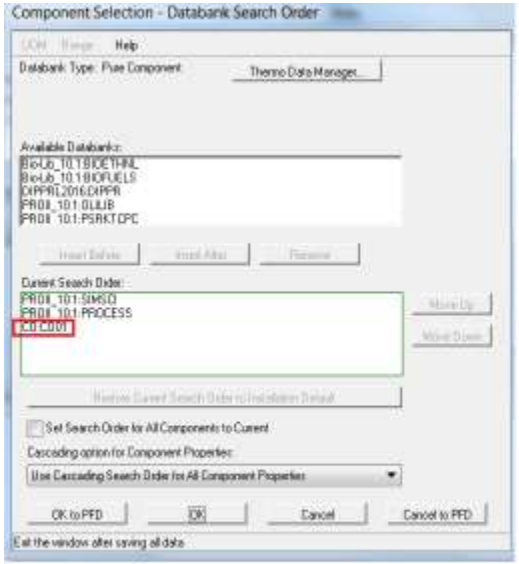

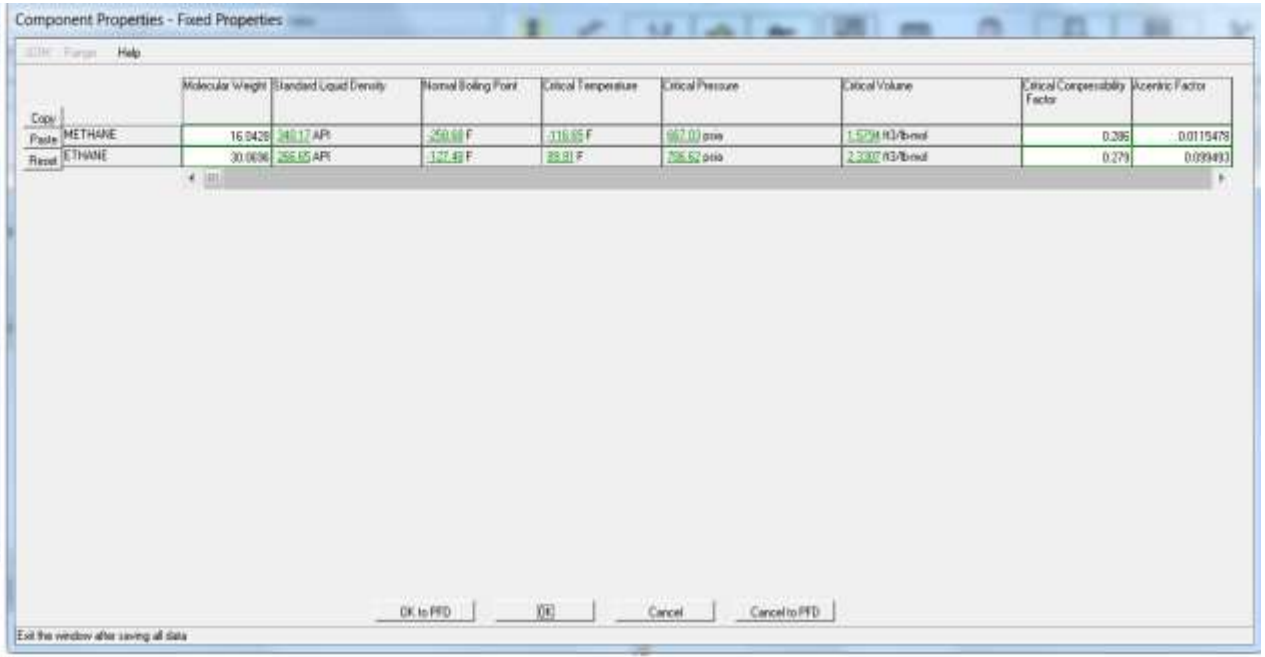

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CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Behavior in PRO/II v10.1

  - If PP compounds are not having CAS numbers or matching CAS number is not found in the SIMSCI or PROCESS libraries
    - CO PP compounds are added as non-library compounds in PRO/II.
    - The constant pure compound properties are taken from the CO PP.
    - The temperature dependent properties are not filled from the CO PP.
    - Compound Databank Search Order is not available for non-library compounds

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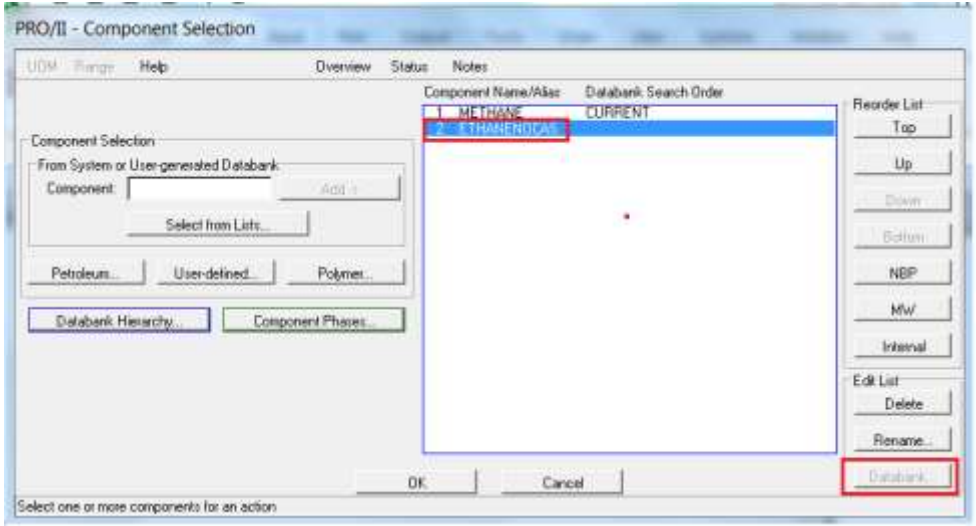
CO PP in compound Databank Search Order List in PRO/II v10.1



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- If user deletes CO PP in PRO/II, the corresponding CO thermoset is deleted from the databank search order. The compounds associated with that PP are either deleted or retained in the PRO/II compound slate based on conditions.

- If user renames CO thermoset, the databank search order list having the CO thermoset should be renamed accordingly.
- If CO PP supports persistence and user modifies the constant pure compound properties by editing the CO PP, the updates values are reflected in PRO/II.

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CO PP in compound Databank Search Order List in PRO/II v10.1

Demo of CO PP in compound Databank Search Order in PRO/II v10.1

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CO PP in compound Databank Search Order List in PRO/II v10.1

Q&A

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