

Parent level amendment

In a parent level amendment (PLA) structural changes, converting structures to multi-component compounds, adding CSTs or additional data can be performed, but changes involving isotopes, charges or salts/solvates (since these are not stored on a parent level) are not stored.

When amending a parent the Id (PCN) will be always kept.

- Amending single structure compounds
- Amendment of single compounds used in multi-component compounds
- Amendment of multi-component compounds

Amending single structure compounds

No match

In the case when the amendment was initiated from a parent structure and there are no parent matches to the modified structure an empty Suggestion list will appear where the new structure is displayed as a "New compound" (Figure D1). By clicking the **[Register as selected]** button, the structural change will be saved and the Ids will be kept.

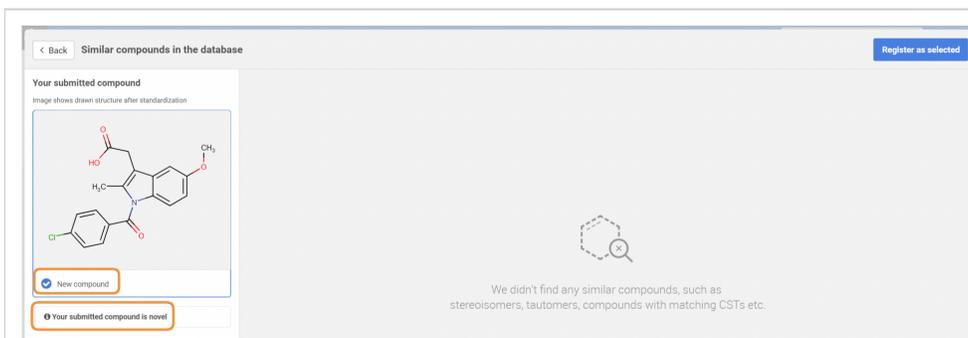


Figure D1. Empty Suggestion list in case of no match

Exact match (no other matches)

Independently from which level of the tree was the amendment initiated (parent, version or lot level), if there is an exact parent match and non-exact (e.g. stereoisomer, tautomer) matches are not found, an empty Suggestion list will appear (Figure D2). The modified structure will be a new lot (or new version) of an existing parent after clicking the **[Register as selected]** button.

Figure D2. Empty Suggestion list in case of exact match

Stereoisomer, tautomer and stereoisomer & tautomer match

Stereoisomer, tautomer or tautomer&stereoisomer matches, if available, are displayed on the right side of the Suggestion list.

When amending a compound, e.g. CXN14: 5-methylpiperidin-3-one on parent level to (5S)-5-methyl-1,2,5,6-tetrahydropyridin-3-ol, having CXN13: (5R)-5-methylpiperidin-3-one as a stereoisomer & tautomer match, the Suggestion list (Figure D3) will display the matching CXN13A version and also its own parent version (CXN14A).

The Ids will be kept, if "New compound" is chosen before clicking the **[Register as selected]** button. Otherwise, if a suggested structure is chosen, all the lots that belong to the modified parent structure will be moved under the chosen version structure and will receive new Ids.

Figure D3. Suggestion list with stereoisomer & tautomer matches

Amendment of single compounds used in multi-component compounds

Currently, editing compounds on parent level that are part as components of multi-component compounds is not allowed.

Amendment of multi-component compounds

Currently, editing multi-component compounds on parent level is not allowed.