SimSite3D search_sitemaps reference sheet

Purpose: search_sitemaps may be used to query a database of sitemaps for sitemaps similar to the query sitemap or may be used to compare two sitemaps

Note: `<text>` : denotes a required argument supplied by a user
`[text]` : denotes an optional argument supplied by a user

Getting help on screen

- Short help:
  `search_sitemaps [--usage]`
- Longer help:
  `search_sitemaps --help`
- Getting the version of search_sitemaps:
  `search_sitemaps --version`

Comparing sitemaps with search_sitemaps – Note: either one or two sitemaps are required. If one sitemap is present on the command line, that sitemap will be used as the query versus the database of sitemaps. If two sitemaps are present on the command line, the second sitemap will be compared to the first sitemap.

- Querying the default database:
  `search_sitemaps <query_s>.csv`
- Querying a specific database:
  `search_sitemaps --dbase_sites <path/to/dbase/sitemaps> --dbase_ligs <path/to/dbase/ligands> <query_s>.csv`
- Comparing two sitemaps:
  `search_sitemaps <query_s>.csv <sitemap_2_s>.csv`
- Specifying a specific results (output) file:
  `search_sitemaps -o <path/to/output/file> <query_s>.csv [<sitemap_2_s>.csv]`
- Specifying a directory other than the **`$SIMSITE3D_PROJ_OUTPUT`** directory to save the sitemap
  `gen_points --proj_output <saved/sitemap/directory>`

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Advanced search_sitemaps options – options that should only be used if you are familiar with the way SimSite3D compares sitemaps. These options have been extensively tested, but could have unintended results

- Keep more than the top scoring orientation for each pair of sitemaps. By default, search_sitemaps keeps the top scoring orientation for each pair of sitemaps if the score met the score threshold, otherwise no score is saved for that pair.

  search_sitemaps --keep_n_scores <N> <query_s>.csv [<sitemap_2_s>.csv]

- Specifying a score threshold; please recall that more negative scores are more favorable. Typically, scores better than -2.0 are highly significant and scores above 0.0 are likely to be irrelevant.

  search_sitemaps --score_threshold <real number> <query_s>.csv [<sitemap_2_s>.csv]

- Have search_sitemaps use an external protein-ligand scoring function to score ligand fragments. At the present, DrugScore is the only supported scoring function; please consult the SimSite3D Quick Guide for a discussion on using protein-ligand scoring functions.

  search_sitemaps --prot_lig_score <SF_name> <query_s>.csv [<sitemap_2_s>.csv]

- Specifying the minimum number of heavy atoms for a ligand fragment to be kept

  search_sitemaps --lig_frag_size N <query_s>.csv [<sitemap_2_s>.csv]

Expert search_sitemaps options – options that should only be used if you have a clear understanding of their implications and requirements.

- Specifying a directory for SimSite3D temporary files. We recommend only using this option if the temporary directory specified by your systems administrator cannot be used.

  search_sitemaps --scratch_dir <path/to/temp/dir> <query_s>.csv [<sitemap_2_s>.csv]

- Omitting the writing of database ligands and ligand fragments corresponding to the saved hits:

  search_sitemaps --DO_NOT_WRITE_LIGANDS <query_s>.csv [<sitemap_2_s>.csv]

- Computing SimSite3D score of sitemaps without aligning; of course this option implies both that the database sitemaps are all aligned to the query sitemap and the database proteins and ligands are in the same reference frame as the database sitemaps

  search_sitemaps --SCORE_ONLY <query_s>.csv [<sitemap_2_s>.csv]