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[**added missing figures from old computer to repo**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/51dcad880a641db7b2d46e0bcbdf2e996f869a42)

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* [](mailto:dbandyo3@its.jnj.com)

[**TCAMS cluster data added, exported as data table from Spotfire file for planned analysis**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/fd7ec65aec0122f1ea5f9ff81185b217b1f2177e)

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* [](mailto:rajarshi_guha@vrtx.com)

[**Fixed bib style issue**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/f0fb513e4f80abf5188d602bc13b4982f8b438e8)

[Rajarshi Guha](mailto:rajarshi_guha@vrtx.com) committed 2 months ago

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* [](mailto:rajarshi_guha@vrtx.com)

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* [](mailto:dbandyo3@its.jnj.com)

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* [](mailto:dbandyo3@its.jnj.com)

[**Little endian data files in Stats zip fixed (dos2unix)**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/1e0ec625a278b3197fd992c6d44d4fa7569f2415)

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* [](mailto:dbandyo3@its.jnj.com)

[**just some small changes after merging Raj version**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/f428ab16cad4def7688a4fd6c0743dc717707d54)

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* [](mailto:dbandyo3@its.jnj.com)

[**Removing qualitative comparison section - since some conclusions in it need to r…**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/d752bc9314f00a120af9cdc5ac5bf91676d76d93) ...

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* [](mailto:dbandyo3@its.jnj.com)

[**changes made to paper morning of May 10... may still get few more in by mtg time**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/2490d0f489e72fe0fc28fa858c23f5e87d367df8)

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* [](mailto:dbandyo3@its.jnj.com)

[**changes made to paper afternoon of May 10**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/8caae4ff742575d7f6cf6996d94a6c7b2be4416c)

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* [](mailto:dbandyo3@its.jnj.com)

[**Figure ?? removed**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/47580f610bb8d752d5afe773eef570baf6e7f8bf)

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* [](mailto:dbandyo3@its.jnj.com)

[**updates to the stats code to compare clustering**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/872318c99836d395a7fdf1454552e1fb9e9a6765)

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* [](mailto:dbandyo3@its.jnj.com)

[**stats changes to include clustering - no interpretation yet**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/eebd66e289b5a79a5ac597c6fe857721848f0fe8)

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* [](mailto:dbandyo3@its.jnj.com)

[**more stats changes to include clustering**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/f7abe04e6d58f3f7fed4d261b9242389ee4e8c2f)

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* [](mailto:dbandyo3@its.jnj.com)

[**changes made over weekend June 7-9**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/4758b2582b17df02ba1e1bd8c511b40b9870700f)

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* [](mailto:dbandyo3@its.jnj.com)

[**moving some stuff off old computer that wasn't in git**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/11314d6786f5f4b606b6ca0c6c7203586daa63ba)

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* [](mailto:dbandyo3@its.jnj.com)

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* [](mailto:dbandyo3@its.jnj.com)

[**added Fig 2 structures as SMILES for others to render**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/a0b34526b40d37321017a95a93aa6d0a59a71fae)

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* [](mailto:dbandyo3@its.jnj.com)

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* [](mailto:dbandyo3@its.jnj.com)

[**changes to structures and figs weekend of June 14**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/f447a514ef4769a064087f44c4c34f4b2d7f42b4)

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* [](mailto:dbandyo3@its.jnj.com)

[**renaming a couple of figures**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/4e4ce578c862e6034b2530c35f3f5558d30ac92c)

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* [](mailto:dbandyo3@its.jnj.com)

[**quick add few more SMILES in a break**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/532d54a194c670fc01fd490edb94655b68b9f176)

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* [](mailto:dbandyo3@its.jnj.com)

[**more progress on SMILES & structure figs, till 4**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/a40676eebd4b6336024ab6d02bc881a877002c0c)

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* [](mailto:dbandyo3@its.jnj.com)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fig 7 structures SMILES added**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/333f6b26436e521ae53f82276161d6e1d8dc85b8)

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* [](mailto:dbandyo3@its.jnj.com)

[**weekend of 6/23 changes Sunday AM - structures done**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/70b682c4b25bce5a25bb2007a387ee238322e5f0)

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* [](mailto:dbandyo3@its.jnj.com)

[**added TOC image**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/db383476454b89a131bd3f31c7e6035c05f38d4a)

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* [](mailto:dbandyo3@its.jnj.com)

[**added TOC image new version**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/08f3191b18af818d6231954d7ce0f6a4aed9ebc1)

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* [](mailto:dbandyo3@its.jnj.com)

[**small updates to PDF & PPT**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/e591d27f32bf69faf811151583cd235905656416)

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* [](mailto:dbandyo3@its.jnj.com)

[**some figures refreshed based on CK input, more to do**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/e2db80c9db14ee5f1c64bac1f4e3bb1a12a10ae6)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fig 4 refreshed**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/a202942c0ba62e603794906afa213a8c81da26e6)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fig 5 refreshed**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/b02404f01c5f36c04e0449cfa654cd99a18ad5d2)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fig 7 refreshed**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/f004ebff4e6d77caa060ceb672cc002ac1e14127)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fig 8 refreshed - two takes**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/2c9f2919bc4d8738f2b71b2d37b2e129e0476a3b)

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* [](mailto:dbandyo3@its.jnj.com)

[**All figs in main paper upgraded**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/3b8a92dd0df4f7fb5ab96178f9b0b3a82fb6b786)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fig 10/11 sizes adjusted**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/060733efa16d0f72674d0993cd3b5b1714d4ba45)

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* [](mailto:dbandyo3@its.jnj.com)

[**Fixing up SI sections order and exporting figure SMILES for rendering**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/bce1935747e4297d02922c8b787343767491a9c8)

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* [](mailto:dbandyo3@its.jnj.com)

[**Refresh SI figures where structures are available**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/42339e793247bcf133575fd84b0d39b63f9f93bd)

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* [](mailto:dbandyo3@its.jnj.com)

[**stats code generalized and updated, display env changed to listing from verbatim to reduce font size**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/dca66742376822ff23137ff500aae6aa2ae52ecf)

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* [](mailto:dbandyo3@its.jnj.com)

[**last three (first three) figure changes in SI**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/e2fd1ad2f51502cae8fc87d034966872c49f636b)

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* [](mailto:dbandyo3@its.jnj.com)

[**changes made while preparing eLNB figure changes**](https://spotlite.nih.gov/ncats/scaffoldanalytics/commit/5164c3886656ccfe8cde15e2d4b514559ddb59a0)

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|  |  | title = {Ligand-Based Virtual Screening Using Graph Edit Distance as Molecular Similarity Measure}, |
|  |  | journal = {Journal of Chemical Information and Modeling}, |
|  |  | volume = {59}, |
|  |  | number = {4}, |
|  |  | pages = {1410-1421}, |
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|  |  | abstract = { Extended reduced graphs provide summary representations of chemical structures using pharmacophore-type node descriptions to encode the relevant molecular properties. Commonly used similarity measures using reduced graphs convert these graphs into 2D vectors like fingerprints, before chemical comparisons are made. This study investigates the effectiveness of a graph-only driven molecular comparison by using extended reduced graphs along with graph edit distance methods for molecular similarity calculation as a tool for ligand-based virtual screening applications, which estimate the bioactivity of a chemical on the basis of the bioactivity of similar compounds. The results proved to be very stable and the graph editing distance method performed better than other methods previously used on reduced graphs. This is exemplified with six publicly available data sets: DUD-E, MUV, GLL\&GDD, CAPST, NRLiSt BDB, and ULS-UDS. The screening and statistical tools available on the ligand-based virtual screening benchmarking platform and the RDKit were also used. In the experiments, our method performed better than other molecular similarity methods which use array representations in most cases. Overall, it is shown that extended reduced graphs along with graph edit distance is a combination of methods that has numerous applications and can identify bioactivity similarities in a structurally diverse group of molecules. } |
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|  |  | @Unpublished{SmallWorld, |
|  |  | title={SmallWorld: Efficient maximum common subgraph searching of large databases}, |
|  |  | abstract = {We report a novel chemical database search method-based upon explicit representation of chemical space. A pre-computed index allows the exact size of the maximum common edge subgraph (MCES) between a query molecule and molecules in the index to be calculated rapidly. In practice, this allows the 100 nearest neighbors having the largest MCES to a query molecule to be determined in a few seconds even for target databases containing millions of molecules. This work builds upon the previous efforts of Wipke and Rogers in the late 1980s and of Messmer and Bunke in the 1990s, but takes advantage of the rapid advances in parallel processing power and storage technology now available to researchers. Data will be presented on the size of the index/chemical universe as a function heavy atom count and number of represented molecules. |
|  |  | }, |
|  |  | author = {Roger Sayle and Jose Batista and Andrew Grant}, |
|  |  | affiliation = {NextMove Software LLC}, |
|  |  | details = {https://tpa.acs.org/session/244tNM/COMP/drug-discovery}, |
|  |  | location = {Philadelphia, Pennsylvania, USA}, |
|  |  | note = {244th American Chemistry Society National Meeting, Philadelphia, PA, August 19-23, 2012}, |
|  |  | year = {2012} |
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|  |  | Author="Hassan, M. and Brown, R. D. and Varma-O'brien, S. and Rogers, D. ", |
|  |  | Title="{{C}heminformatics analysis and learning in a data pipelining environment}", |
| ... | ... | @@ -56,7 +86,7 @@ title={{D}ynamic {SA}/reports: Analyzing current project and {HTS} data by inter |
|  |  | abstract = {Diverse compound sets, such as high-throughput screening (HTS) hit sets containing an unknown number of chemotypes, have traditionally been analyzed by clustering, nearest neighbors, or other scaffold-agnostic methods rather than by rigorous R-group analysis. Here we describe how MOE SA/Report has been applied to analyze 2-4k compound subsets of the GSK screening collection having measured activity (percent inhibition or pIC50) against one or more screened targets. Since the default scaffold auto-detection within SA/Report is tuned for datasets with many exemplars of a few scaffolds as opposed to more diverse HTS hit sets, we use an interactive scaffold selection approach. The user is allowed to pick a scaffold from the highest ranked (most frequent and largest) fragments found in the data, and frequent fragments are then found in the remaining unmapped compounds. Both these steps continue iteratively until scaffold selection is complete. We also describe how MOE SA/Report has been integrated into project data delivery mechanisms at GSK, with reports being run automatically for several projects on their current set of compounds via custom KNIME workflows.}, |
|  |  | author = {Deepak Bandyopadhyay}, |
|  |  | affiliation = {GlaxoSmithKline}, |
|  |  | details = {http://acselb-529643017.us-west-2.elb.amazonaws.com/chem/244nm/program/view.php}, |
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|  |  | year = {2012} |
| ... | ... | @@ -67,7 +97,17 @@ title={On the compound annotation and cleaning the {GSK} screening collection in |
|  |  | abstract = {High throughput screening (HTS) constitutes a critical tool for the identification of lead molecules from primary screening assays for novel targets. GlaxoSmithKline (GSK) has continuously invested in the development and curation of its HTS collection to maximize the number of quality starting points for drug discovery and reduce the number of false positives from primary screens. An Inhibition Frequency Index (IFI) has been defined as a measure of promiscuity of individual compounds in HTS primary assays based upon activities tabulated over time in GSK's exhaustive screening assay tables. In this talk, we will present our analysis of the IFI profile across the GSK HTS collection. We will characterize the IFI profile with respect to desired physical properties, will discuss obvious substructures that may be less attractive as starting points, and will describe new classes of nuisance compounds revealed by our IFI analysis. In addition, we will examine the IFI of promiscuity filters described in the literature. There are many reasons why any particular molecule might display promiscuity: physical properties of the compound, properties of the target or target class, details of the assay and the assay technology and methodology. All of these factors must be considered when deciding whether to remove or retain a compound in a curated HTS collection.}, |
|  |  | author = {Subhas J Chakravorty and James A Chan and Juan Luengo and Nicole M Greenwood and Ioana Popa-Burke and Ricardo Macarron}, |
|  |  | affiliation = {GlaxoSmithKline}, |
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|  |  | details = {https://tpa.acs.org/session/245tNM/CINF/advances-in-visualizing-and-analyzing-biomolecular-screening-data}, |
|  |  | location = {New Orleans, Louisiana, USA}, |
|  |  | note = {245th American Chemistry Society National Meeting, New Orleans, LA, April 7-11, 2013}, |
|  |  | year = {2013} |
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|  |  | @Unpublished{RGTool, |
|  |  | title={From hits to leads: Data visualization of chemical scaffolds beyond traditional {SAR} exploration}, |
|  |  | author = {Tyler Peryea and John Braisted and Ajit Jadhav and Rajarshi Guha and Noel Southall and Dac-Trung Nguyen}, |
|  |  | affiliation = {NCATS}, |
|  |  | details = {https://tpa.acs.org/session/245tNM/CINF/advances-in-visualizing-and-analyzing-biomolecular-screening-data}, |
|  |  | location = {New Orleans, Louisiana, USA}, |
|  |  | note = {245th American Chemistry Society National Meeting, New Orleans, LA, April 7-11, 2013}, |
|  |  | year = {2013} |
| ... | ... | @@ -190,6 +230,17 @@ CONCLUSIONS: Currently used lead libraries make little use of the metabolites an |
|  |  | Year = {2013}, |
|  |  | Bdsk-Url-1 = {http://dx.doi.org/10.1007/s10822-013-9641-y}} |
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|  |  | @Article{Mulrooney2013JCAMD, |
|  |  | Author="Mulrooney, C. A. and Lahr, D. L. and Quintin, M. J. and Youngsaye, W. and Moccia, D. and Asiedu, J. K. and Mulligan, E. L. and Akella, L. B. and Marcaurelle, L. A. and Montgomery, P. and Bittker, J. A. and Clemons, P. A. and Brudz, S. and Dandapani, S. and Duvall, J. R. and Tolliday, N. J. and De Souza, A. ", |
|  |  | Title="{{A}n informatic pipeline for managing high-throughput screening experiments and analyzing data from stereochemically diverse libraries}", |
|  |  | Journal="J. Comput. Aided Mol. Des.", |
|  |  | Year="2013", |
|  |  | Volume="27", |
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|  |  | Pages="455--468", |
|  |  | Month="May" |
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|  |  | @article{Torres2009, |
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|  |  | Journal = {Int J Electr Comput Syst Eng}, |
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|  |  |  |
|  |  |  |
|  |  | **\subsection**{Qualitative Comparison of Scaffold-Generation Methods and Clustering} |
|  |  | {**\bf** Complete-Linkage Clustering}: As shown in **\fref**{clusterlanes}, the defining feature of a partitioning clustering is that every molecule maps to one and only one cluster. Thus if a chemotype is broken up among two or more clusters, using the cluster ID to map Related Molecules can retrieve only neighbors from the same cluster, ignoring the other cluster. This is not ideal for purposes of the visualization and navigation method presented here, as arbitrary neighbors would be excluded depending on how the clustering is defined. Thus we do not advocate the use of clustering, unless it is a fuzzy clustering where all meaningful class memberships a molecule might have are considered. |
|  |  |  |
|  |  | \begin{figure} |
|  |  | **\includegraphics**[width=6in]{fig/clusterlanes.png} |
|  |  | **\caption**{Illustrating one problem with clustering: bifurcation of related molecules. When two molecules of the same chemotype differing by a halogen are split across Complete Linkage Clusters, searches of cluster neighbors for one molecule do not find its analogs in the other cluster, **\ie** the two related clusters are not linked.} |
|  |  | **\label**{fig:clusterlanes} |
|  |  | \end{figure} |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  | {**\bf** NCATS R-group tool}: As opposed to the clustering method, |
|  |  | if any two molecules share a common substructure that meets the standards required of a scaffold by the NCATS method (**\eg** being bordered by rings on each end), then those molecules will be found to contain that shared substructure as a scaffold and their activities will be used to compute aggregate properties for it. |
|  |  |  |
|  |  | {**\bf** Other Scaffold Generation Methods}: As shown earlier, even though another scaffold generation method (represented here by the **\citet**{Harper2004DDclus} implementation of Frameworks) differed in its implementation details and produced different numbers of scaffolds for the same molecule, it was roughly equivalent in a qualitative sense with regard to the insights obtained. Due to substantial overlap between sets of scaffolds, ring systems responsible for activity of a molecule were generally revealed by either method. For example, the insights mentioned in **\sref**{scafwalk} were more or less consistent across the methods. However, there were cases where the Frameworks revealed negative information about a fragment being not important for activity that is also useful for a drug discovery scientist. For example, in **\fref**{frameswalk} a substructure is highlighted that is on the aggregate inactive and could be removed or substituted. This insight is not available from SSSR-based scaffolding methods such as the NCATS R-group tool since they don't define or find that fragment as a scaffold. |
|  |  |  |
|  |  | \begin{figure} |
|  |  | **\includegraphics**[width=5in]{fig/mol1\_frames\_scafpie.png} |
|  |  | **\caption**{Using Frameworks with the Scaffold Pies visualization. One framework is highlighted that has no equivalent in the NCATS scaffolds, but is shown to reduce activity as related molecules containing it are less active than the parent molecule. The star symbol shows the location of the parent molecule in this Related Molecules plot, and the compass device at the origin shows the direction of favorable properties (+X and +Y axes).} |
|  |  | **\label**{fig:frameswalk} |
|  |  | \end{figure} |
|  |  |  |
|  |  |  |
|  |  | To summarize, both multiple-scaffold decomposition methods considered in this study, **\ie** NCATS R-group Tool and Frameworks give comparable insights when exploring the TCAMS dataset, with some differences stemming from individual substructures that are considered shared scaffolds or not by the individual methods. We now explore these overlaps, similarities and differences in the aggregate using the statistical methods described earlier in **\sref**{statmethod}. |
|  |  |  |
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[**datasets/chemblntd\_gsk\_clusters.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#e9ca89200ea14a2053e7b991770d161c74081ecd) 0 → 100644

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25.2 KB

[**fig/CP\_TCAMS\_CLink\_RGT\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#eb8c86d47b889bde6a113ac352eba52dc90e6748) 0 → 100644

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29.3 KB

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54.5 KB

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40 KB

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214 KB

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32.4 KB

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423 KB

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56.2 KB

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|  |  |  |
| --- | --- | --- |
|  |  | SCAFFOLD\_ID ID STRUCTURE pIC50\_3D7 mw SCAFFOLD R1 R2 R3 R4 R5 |
|  |  | 4719 531021 CC1(C)N=C(N)N=C(N)N1OCCSCCON2C(N)=NC(N)=NC2(C)C 7.29597 400.5 "[$([#1,\*])]C1([$([#1,\*])])N=C([$([#1,\*])])N=C([$([#1,\*])])N1[$([#1,\*])] |$\_R1;;\_R2;;;\_R5;;;\_R4;;\_R3$,t:3,6|" C\* C\* "CC1(C)N=C(N)N=C(N)N1OCCSCCO\* |t:3,6|" N\* N\* |
|  |  | 4719 526851 CC1(C)N=C(N)N=C(N)N1C2=CC3=C(C=CC=C3)C=C2 7.26898 267.33 "[$([#1,\*])]C1([$([#1,\*])])N=C([$([#1,\*])])N=C([$([#1,\*])])N1[$([#1,\*])] |$\_R1;;\_R2;;;\_R5;;;\_R4;;\_R3$,t:3,6|" C\* C\* "\*C1=CC2=C(C=CC=C2)C=C1 |c:5,7,10,t:1,3|" N\* N\* |
|  |  | 4719 535903 CC1=CC=C(C=C1)N2C(N=C(N)N=C2N)C3=CC=CC=C3 7.2471099 279.34 "[$([#1,\*])]C1([$([#1,\*])])N=C([$([#1,\*])])N=C([$([#1,\*])])N1[$([#1,\*])] |$\_R1;;\_R2;;;\_R5;;;\_R4;;\_R3$,t:3,6|" "\*C1=CC=CC=C1 |c:3,5,t:1|" "CC1=CC=C(\*)C=C1 |c:6,t:1,3|" N\* N\* |

[**fig/Fig4c\_scafaggr\_struc.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#09f978dee9a6712560b2abda5f8c3fcfffc8d23c) 0 → 100644

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217 KB

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159 KB

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31.4 KB

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105 KB

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231 KB

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116 KB

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333 KB

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420 KB

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193 KB

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228 KB

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244 KB

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123 KB

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328 KB

[**fig/mol3\_RGtool\_scafpie\_iter\_struc\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#934b51f68ed9d891b3d11a64f595e1b1efa16b30) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/mol3_RGtool_scafpie_iter_struc_v2.png)

88.9 KB

[**fig/mol4\_541531.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#ab90ef0cea642ca52db7d7ab5e3571d19cde2dc4) 0 → 100644

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14.7 KB

[**fig/statcompare\_CLink\_RGtool\_transparent\_density.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#7ba74a6540c8ebcf10e43128de11dd66fa242012) 0 → 100644

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163 KB

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[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/statcompare_CLink_RGtool_transparent_density_v2.png)

350 KB

[**fig/statcompare\_frames\_RGtool\_transparent\_density\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#ec8a3b5b3c051f58d13537261e13f121f445c6b7) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/statcompare_frames_RGtool_transparent_density_v2.png)

396 KB

[**fig/statcompare\_frames\_RGtool\_transparent\_density\_v3.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#b8e38bf279fc0b9e5a4f362f3ae4be2eb8a00a4d) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/statcompare_frames_RGtool_transparent_density_v3.png)

914 KB

[**fig/structure\_group\_C\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#4b821e1fd241fd7a4b1e649de6322c615ceddd6a) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/structure_group_C_v2.png)

103 KB

[**fig/structures.smi**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#b68742967311302a905d82bc8eed4dad6969b13e) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/structures.smi)

|  |  |  |
| --- | --- | --- |
|  |  | CC1(N=C(N=C(N1OCc2ccc3ccccc3c2)N)NC(=O)c4ccc(cc4)N(=O)=O)C 536182\_mol1\_Fig2a\_scafDD |
|  |  | CC1(C)NC(N)=NC(=N)N1OCc1cccs1 Fig4a\_mol\_541127 |
|  |  | [$([#1,\*])]C1([$([#1,\*])])N=C([$([#1,\*])])N=C([$([#1,\*])])N1[$([#1,\*])] |$\_R1;;\_R2;;;\_R5;;;\_R4;;\_R3$,t:3,6| Fig4a\_scaf\_4719 |
|  |  | [$([#1,\*])]C1=C([$([#1,\*])])SC([$([#1,\*])])=C1[$([#1,\*])] |$\_R1;;;\_R4;;;\_R3;;\_R2$,c:1,6| Fig4a\_scaf\_89 |
|  |  | [\*]C1=C([\*])SC([\*])=C1[\*] Fig4b\_scaf\_89 |
|  |  | [\*]C1([\*])N=C([\*])N=C([\*])N1[\*] Fig4b\_scaf\_4719 |
|  |  | Cc1ccccc1Cn2ccc3c2ccc4c3c(nc(n4)N)N Fig5a\_mol\_541564 |
|  |  | c1ncccc1-c2ccc3nc([\*:1])n([\*:2])c3c2 Fig7\_central |
|  |  | c1([\*])n([\*])c([\*])c([\*])c([\*])c1-c2c([\*])c([\*])c([\*])c([\*])c2 Fig7\_left |
|  |  | c1([\*])n([\*])c2c([\*])c([\*])c([\*])cc2n1([\*]) Fig7\_right |
|  |  | CC1(C)N=C(NC(=O)C2=CC=C(C=C2)[N+]([O-])=O)N=C(N)N1OCC3=CC4=C(C=CC=C4)C=C3 Fig8\_mol\_536182\_top\_ScafWalk |
|  |  | CC1(NC(=NC(=N)N1OCc2ccc(cc2)c3ccccc3)N)C Fig8\_mol\_540655\_bluepink\_scaf\_2467 |
|  |  | [$([#1,\*])]C(ON1C([$([#1,\*])])=NC([$([#1,\*])])=NC1([$([#1,\*])])[$([#1,\*])])C2=C([$([#1,\*])])C([$([#1,\*])])=C([$([#1,\*])])C([$([#1,\*])])=C2[$([#1,\*])] |$\_R1;;;;;\_R5;;;\_R4;;;\_R2;\_R3;;;\_R10;;\_R9;;\_R8;;\_R7;;\_R6$,c:5,8,14,22,t:18| Fig8\_scaf\_2467\_pink |
|  |  | [$([#1,\*])]C1([$([#1,\*])])N=C([$([#1,\*])])N=C([$([#1,\*])])N1[$([#1,\*])] |$\_R1;;\_R2;;;\_R5;;;\_R4;;\_R3$,t:3,6| Fig8\_scaf\_4719\_blue |
|  |  | CC1(C)N=C(N)N=C(N)N1C2=CC(Cl)=C(Cl)C(Cl)=C2 Fig8\_mol\_525631\_blue\_scaf\_4719 |
|  |  | [$([#1,\*])]C1=C([$([#1,\*])])C2=C(C([$([#1,\*])])=C1[$([#1,\*])])C([$([#1,\*])])=C([$([#1,\*])])C=C2[$([#1,\*])] |$\_R1;;;\_R7;;;;\_R3;;\_R2;;\_R4;;\_R5;;;\_R6$,c:1,4,7,15,t:12| Fig8\_scaf\_978\_yellow |
|  |  | OCCN1CCN(CC1)C2=CC=C(NC3=C4C=C5C=CC=CC5=CC4=NC=C3)C=C2 Fig8\_mol\_529200\_yellow\_scaf\_978 |
|  |  | NC(=N)c1ccc(cc1)-c1cc(on1)-c1cccc(c1)C(N)=N Fig10a\_542503\_grey\_CP0.99 |
|  |  | CN(C)CCn1c2ccccc2n(CC(O)c2ccc(Cl)c(Cl)c2)c1=N Fig10a\_525973\_orange\_PIUB\_RG\_high |
|  |  | C(SC1=NNC(S1)c1ccccn1)c1ccccc1 Fig10a\_541131\_purple\_PIUA\_FW\_high |
|  |  | CC(=O)OCCn1c(=O)c2ccc3c4c(ccc(c24)c1=O)c(=O)n(CCOC(C)=O)c3=O Fig10b\_535874\_orange\_PIUB\_RG\_high |
|  |  | C[C@H](Cc1ccc(OCCCCCCCOc2ccc(C[C@@H](C)NC[C@H](O)c3cccc(Cl)c3)cc2)cc1)NC[C@H](O)c1cccc(Cl)c1 Fig10b\_539523\_purple\_PIUD\_CL\_high |
|  |  | CC1(NC(=NC(=N)N1OCCCc2ccc(cc2Cl)Cl)N)C Fig11c\_524739 |
|  |  | CCN(CC)CCN(Cc1ccc(cc1)c2ccc(cc2)C#N)C(=O)Cn3c4ccccc4c(=O)nc3CCc5cccc(c5F)F Fig11d\_541941 |
|  |  | CN(C)CCCNCc1ccc(cc1)c2ccc(cc2)CNCCOc3ccccc3 Fig11e\_531249 |

[**fig/tcam1\_FW\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#24388407c5f93bcbe85ca744a76214e351fda21e) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/tcam1_FW_v2.png)

183 KB

[**fig/tcam1\_RGscaf\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#4c51c075a73e75e4e601fb41748899206ca6df80) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/tcam1_RGscaf_v2.png)

108 KB

[**fig/tcam1\_mol\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#ab00f861d0b1a7657e88262c0a3f641b891f4ffa) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/tcam1_mol_v2.png)

73.8 KB

[**fig/tcam2\_541564\_6scaf\_col.PNG**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#033562acb519de89d8498ec3fdb439c837ad7e22) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/fig/tcam2_541564_6scaf_col.PNG)

51.6 KB

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92.5 KB

[**fig/tcam2\_541564\_6scaf\_row\_v2.PNG**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#8018e3ffeafc68c4f85867a6c6945f5dffa02880) 0 → 100644

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55.4 KB

[**fig/tcam2\_mol\_541564\_v2.png**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#51dc70375ba8f78168beac8311252fa8d975afba) 0 → 100644

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22.8 KB

[**pres/DBandyopadhyay\_FigChanges\_eLNB\_revision\_2019.pptx**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#f155d3bb2b45f5e70f8e19fc08218f7128f8efb9) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/pres/DBandyopadhyay_FigChanges_eLNB_revision_2019.pptx)

No preview for this file type

[**pres/Scaffold analytics figures to modify with chemical structures.pptx**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#d02adb280dfd351e9b52afa451e141b302d40f96) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/pres/Scaffold%20analytics%20figures%20to%20modify%20with%20chemical%20structures.pptx)

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[**pres/Scaffold-Based Analytics ACS figures scratch.pptx**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#0dbeefa9b9d18b2822b1b219a1d0c84b0ec09dde) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/pres/Scaffold-Based%20Analytics%20ACS%20figures%20scratch.pptx)

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[**scaffoldAnalyticsJCIM.pdf**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#49274ce5aa17b2cfa8d5b0dee94a0f2986b8fa6b)

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/scaffoldAnalyticsJCIM.pdf)

No preview for this file type

[**scaffoldAnalyticsJCIM.tex**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#57eacaa2478e9f8de477650df3c4a120b229c96b)

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/scaffoldAnalyticsJCIM.tex)

This diff is collapsed. Click to expand it.

[**spotfire/chemblntd\_gsk\_TCAMS\_RG\_frames\_eLNB\_v2.dxp**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#f8057306b05a75dba9362252ad2a5c4447beb283) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/spotfire/chemblntd_gsk_TCAMS_RG_frames_eLNB_v2.dxp)

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[**spotfire/chemblntd\_gsk\_TCAMS\_Stats\_PropByCompd\_DD\_RG\_CLink\_eLNB.dxp**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#850a4428c0299c99ed4e0ad50435cc68aa92ccbb) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/spotfire/chemblntd_gsk_TCAMS_Stats_PropByCompd_DD_RG_CLink_eLNB.dxp)

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[**spotfire/chemblntd\_gsk\_cpd\_search\_hier\_SNG\_v4.dxp**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#0684513fbd641d02f314276d54af4134c6fa7af6) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/spotfire/chemblntd_gsk_cpd_search_hier_SNG_v4.dxp)

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[**stats/A\_DDclus.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#b2c1a681d7fb0de202111951ae71c03be28f994f) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/A_DDclus.txt)

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[**stats/B\_RGD.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#6ba331f8b32ffbe3418ac895a2e3cc3296919400) 0 → 100644

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[**stats/CLinkClusters.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#90d7657b3613cff35af292808a1f0cb5fade3919) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/CLinkClusters.txt)

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[**stats/DDframes.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#dea6571bc7418f78c829ce607b556fee74b08a71) 0 → 100644

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[**stats/D\_CLinkClusters.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#ef7e6ebce17269fa1cf52ce86105b7a52459d5ec) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/D_CLinkClusters.txt)

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[**stats/PropByCompound\_Cluster\_RGD.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#d8c4758d3f07d3aa51bec6160a184af2cb9716ae) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/PropByCompound_Cluster_RGD.txt)

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[**stats/PropByCompound\_FW\_RGD.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#e7892c357eafd47b3bb18ae2511fd0f61d952719) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/PropByCompound_FW_RGD.txt)

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[**stats/PropByCompound\_RGD\_Cluster.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#8bea63e4ecaf1e0c73d3fdd56db3531eb1659985) 0 → 100644

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This diff could not be displayed because it is too large.

[**stats/ProportionScoresClusters\_5212019.R**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#407f2b8db7e7ed017f50a64b5c0319ddfc18e12c) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/ProportionScoresClusters_5212019.R)

|  |  |  |
| --- | --- | --- |
|  |  | *#Note: To do the calculations comparing 2 fragmentation methods* |
|  |  | *#took about 10 minutes of computer time.* |
|  |  |  |
|  |  | *#Set working directory to location of the data files* |
|  |  |  |
|  |  | *#setwd("C:\\Work\\Consulting\\MDR\\Other MDR Issues\\CSC\\FragmentOntologies")* |
|  |  | setwd("C:/Work/git/NIH/scaffoldanalytics/stats") |
|  |  | *#####################* |
|  |  | rm(list **=** ls()) *#Erase anything in R's working memory* |
|  |  |  |
|  |  | DDData **<-** read.table("DDframes.txt", header **=** T, sep **=** "\t") |
|  |  | RGData **<-** read.table("RGD.txt", header **=** T, sep **=** "\t") |
|  |  | CLData **<-** read.table("CLinkClusters.txt", header **=** T, sep **=** "\t") |
|  |  |  |
|  |  | *#Create a list of compounds shared between two datasets.* |
|  |  | *#Scores will not make sense if we include non-common compounds* |
|  |  |  |
|  |  | DDCompounds **<-** unique(DDData**$**COMPOUND\_ID) |
|  |  | RGCompounds **<-** unique(RGData**$**COMPOUND\_ID) |
|  |  | CLCompounds **<-** unique(CLData**$**COMPOUND\_ID) |
|  |  |  |
|  |  | *# Compounds <- intersect(DDCompounds, RGCompounds)* |
|  |  | Compounds **<-** intersect(intersect(RGCompounds, DDCompounds), CLCompounds) |
|  |  |  |
|  |  | *# Compounds <- as.numeric(as.character(intersect(DDCompounds, RGCompounds)))* |
|  |  | N **<-** **length**(Compounds) |
|  |  |  |
|  |  | *#Calculate PI's and common proportions for each compound* |
|  |  |  |
|  |  | *#Proportions by compound* |
|  |  |  |
|  |  | PropByCompound **<-** data.frame(CompoundID **=** **rep**(**NA**, N), |
|  |  | FragA **=** **rep**(**NA**, N), |
|  |  | FragB **=** **rep**(**NA**, N), |
|  |  | Ca **=** **rep**(**NA**, N), |
|  |  | Cb **=** **rep**(**NA**, N), |
|  |  | IntAB **=** **rep**(**NA**, N), |
|  |  | UnionAB **=** **rep**(**NA**, N), |
|  |  | CommonProp **=** **rep**(**NA**, N), |
|  |  | PIa **=** **rep**(**NA**, N), |
|  |  | PIb **=** **rep**(**NA**, N), |
|  |  | PIaU **=** **rep**(**NA**, N), |
|  |  | PIbU **=** **rep**(**NA**, N), |
|  |  | FragEffA **=** **rep**(**NA**, N), |
|  |  | FragEffB **=** **rep**(**NA**, N)) |
|  |  |  |
|  |  | **for** (index **in** 1**:**N){ |
|  |  |  |
|  |  | PropByCompound**$**CompoundID[index] **<-** Compounds[index] |
|  |  |  |
|  |  | *# MethodABelongsTo <- DDData[DDData$COMPOUND\_ID == Compounds[index],* |
|  |  | *# "StrucUniqueID"]* |
|  |  | MethodABelongsTo **<-** CLData[CLData**$**COMPOUND\_ID **==** Compounds[index], |
|  |  | "CLink"] |
|  |  |  |
|  |  | MethodBBelongsTo **<-** RGData[RGData**$**COMPOUND\_ID **==** Compounds[index], |
|  |  | "SCAFFOLD\_ID"] |
|  |  |  |
|  |  | PropByCompound**$**FragA[index] **<-** **length**(unique(MethodABelongsTo)) |
|  |  | PropByCompound**$**FragB[index] **<-** **length**(unique(MethodBBelongsTo)) |
|  |  |  |
|  |  | *# MethodACompoundCluster <- unique(DDData[DDData$StrucUniqueID %in% MethodABelongsTo,* |
|  |  | *# "COMPOUND\_ID"])* |
|  |  | MethodACompoundCluster **<-** unique(CLData[CLData**$**CLink **%in%** MethodABelongsTo, |
|  |  | "COMPOUND\_ID"]) |
|  |  |  |
|  |  | MethodBCompoundCluster **<-** unique(RGData[RGData**$**SCAFFOLD\_ID **%in%** MethodBBelongsTo, |
|  |  | "COMPOUND\_ID"]) |
|  |  |  |
|  |  | PropByCompound**$**Ca[index] **<-** **length**(MethodACompoundCluster) |
|  |  | PropByCompound**$**Cb[index] **<-** **length**(MethodBCompoundCluster) |
|  |  | PropByCompound**$**IntAB[index] **<-** **length**(intersect(MethodACompoundCluster, |
|  |  | MethodBCompoundCluster)) |
|  |  | PropByCompound**$**UnionAB[index] **<-** **length**(union(MethodACompoundCluster, |
|  |  | MethodBCompoundCluster)) |
|  |  | PropByCompound**$**CommonProp[index] **<-** PropByCompound**$**IntAB[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIa[index] **<-** PropByCompound**$**Ca[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIb[index] **<-** PropByCompound**$**Cb[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIaU[index] **<-** 1 **-** PropByCompound**$**Cb[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIbU[index] **<-** 1 **-** PropByCompound**$**Ca[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**FragEffA[index] **<-** PropByCompound**$**Ca[index]**/**PropByCompound**$**FragA[index] |
|  |  | PropByCompound**$**FragEffB[index] **<-** PropByCompound**$**Cb[index]**/**PropByCompound**$**FragB[index] |
|  |  |  |
|  |  | } |
|  |  |  |
|  |  | *#Create output -- averages, quantiles, and histograms* |
|  |  |  |
|  |  | ACP **<-** mean(PropByCompound**$**CommonProp, na.rm **=** T) |
|  |  | APIa **<-** mean(PropByCompound**$**PIa, na.rm **=** T) |
|  |  | APIb **<-** mean(PropByCompound**$**PIb, na.rm **=** T) |
|  |  | APIaU **<-** mean(PropByCompound**$**PIaU, na.rm **=** T) |
|  |  | APIbU **<-** mean(PropByCompound**$**PIbU, na.rm **=** T) |
|  |  | AFragA **<-** mean(PropByCompound**$**FragA, na.rm **=** T) |
|  |  | AFragB **<-** mean(PropByCompound**$**FragB, na.rm **=** T) |
|  |  | AFragEffA **<-** mean(PropByCompound**$**FragEffA, na.rm **=** T) |
|  |  | AFragEffB **<-** mean(PropByCompound**$**FragEffB, na.rm **=** T) |
|  |  | ACa **<-** mean(PropByCompound**$**Ca, na.rm **=** T) |
|  |  | ACb **<-** mean(PropByCompound**$**Cb, na.rm **=** T) |
|  |  |  |
|  |  | CP90 **<-** quantile(PropByCompound**$**CommonProp, **c**(0.1,0.5,0.9)) |
|  |  | PIa90 **<-** quantile(PropByCompound**$**PIa, na.rm **=** T , **c**(0.1,0.5,0.9)) |
|  |  | PIb90 **<-** quantile(PropByCompound**$**PIb, na.rm **=** T , **c**(0.1,0.5,0.9)) |
|  |  | PIaU90 **<-** quantile(PropByCompound**$**PIaU, na.rm **=** T , **c**(0.1,0.5,0.9)) |
|  |  | PIbU90 **<-** quantile(PropByCompound**$**PIbU, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragA90 **<-** quantile(PropByCompound**$**FragA, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragB90 **<-** quantile(PropByCompound**$**FragB, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragEffA90 **<-** quantile(PropByCompound**$**FragEffA, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragEffB90 **<-** quantile(PropByCompound**$**FragEffB, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | Ca90 **<-** quantile(PropByCompound**$**Ca, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | Cb90 **<-** quantile(PropByCompound**$**Cb, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  |  |
|  |  | ACP |
|  |  | APIa |
|  |  | APIb |
|  |  | APIaU |
|  |  | APIbU |
|  |  | AFragA |
|  |  | AFragB |
|  |  | AFragEffA |
|  |  | AFragEffB |
|  |  | ACa |
|  |  | ACb |
|  |  |  |
|  |  | CP90 |
|  |  | PIa90 |
|  |  | PIb90 |
|  |  | PIaU90 |
|  |  | PIbU90 |
|  |  | FragA90 |
|  |  | FragB90 |
|  |  | FragEffA90 |
|  |  | FragEffB90 |
|  |  | Ca90 |
|  |  | Cb90 |
|  |  |  |
|  |  | write.table(PropByCompound,"PropByCompound\_RGD\_Cluster.txt",sep**=**"\t",row.name**=**F,col.name**=**T) |
|  |  | *#########################################################################################* |
|  |  |  |
|  |  | *################# Plot #####################* |
|  |  | attach(PropByCompound) |
|  |  |  |
|  |  | hist(FragA,main**=**"FragA") |
|  |  | hist(FragB,main**=**"FragB") |
|  |  | hist(CommonProp,main**=**"CommonProp") |
|  |  |  |
|  |  | plot(CommonProp**~**UnionAB) |
|  |  | plot(CommonProp**~**IntAB) |
|  |  | plot(Ca**~**Cb) |
|  |  |  |
|  |  | plot(UnionAB, IntAB) |
|  |  | plot(FragA **+** FragB, CommonProp) |
|  |  |  |
|  |  | detach(PropByCompound) |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

[**stats/ProportionScoresNewEdits7302015.R**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#fbf5b80d0c322cca693301e45f8b5b343146d830)

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/ProportionScoresNewEdits7302015.R)

|  |  |  |
| --- | --- | --- |
| ... | ... | @@ -2,7 +2,8 @@ |
|  |  | *#took about 10 minutes of computer time.* |
|  |  |  |
|  |  | *#Set working directory to location of the data files* |
|  |  | setwd("C:\\Work\\Consulting\\MDR\\Other MDR Issues\\CSC\\FragmentOntologies") |
|  |  | *#setwd("C:\\Work\\Consulting\\MDR\\Other MDR Issues\\CSC\\FragmentOntologies")* |
|  |  | setwd("C:/Work/git/NIH/scaffoldanalytics/stats") |
|  |  | *#####################* |
|  |  | rm(list **=** ls()) *#Erase anything in R's working memory* |
|  |  |  |
| ... | ... |  |

[**stats/ProportionScores\_Clus\_or\_FW\_vs\_RG\_07012019.R**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#aa359a212d1498d6d337190ef0dac7087a914ad1) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/ProportionScores_Clus_or_FW_vs_RG_07012019.R)

|  |  |  |
| --- | --- | --- |
|  |  | *#Note: To do the calculations comparing 2 fragmentation methods* |
|  |  | *#took about 10 minutes of computer time.* |
|  |  |  |
|  |  | *#Set working directory to location of the data files* |
|  |  |  |
|  |  | *#setwd("C:\\Work\\Consulting\\MDR\\Other MDR Issues\\CSC\\FragmentOntologies")* |
|  |  | setwd("C:/Work/git/NIH/scaffoldanalytics/stats") *# Deepak's folder* |
|  |  | *#####################* |
|  |  | rm(list **=** ls()) *#Erase anything in R's working memory* |
|  |  |  |
|  |  | DDData **<-** read.table("DDframes.txt", header **=** T, sep **=** "\t") |
|  |  | RGData **<-** read.table("RGD.txt", header **=** T, sep **=** "\t") |
|  |  | CLData **<-** read.table("CLinkClusters.txt", header **=** T, sep **=** "\t") |
|  |  |  |
|  |  | *#Create a list of compounds shared between two datasets.* |
|  |  | *#Scores will not make sense if we include non-common compounds* |
|  |  |  |
|  |  | DDCompounds **<-** unique(DDData**$**COMPOUND\_ID) |
|  |  | RGCompounds **<-** unique(RGData**$**COMPOUND\_ID) |
|  |  | CLCompounds **<-** unique(CLData**$**COMPOUND\_ID) |
|  |  |  |
|  |  | *# Compounds <- intersect(DDCompounds, RGCompounds)* |
|  |  | *# if comparing 3 methods pairwise, make sure we use the same set of compounds* |
|  |  | Compounds **<-** intersect(intersect(RGCompounds, DDCompounds), CLCompounds) |
|  |  |  |
|  |  | *# Compounds <- as.numeric(as.character(intersect(DDCompounds, RGCompounds)))* |
|  |  | N **<-** **length**(Compounds) |
|  |  |  |
|  |  | *#Calculate PI's and common proportions for each compound* |
|  |  |  |
|  |  | *#Proportions by compound* |
|  |  | statcompare **<-** **function**(ScafSetA, ScafSetB, |
|  |  | ScafColA**=**"StrucUniqueID", ScafColB**=**"SCAFFOLD\_ID", CompoundSet) { |
|  |  | N **<-** **length**(CompoundSet) |
|  |  | PropByCompound **<-** data.frame(CompoundID **=** **rep**(**NA**, N), |
|  |  | FragA **=** **rep**(**NA**, N), FragB **=** **rep**(**NA**, N), |
|  |  | Ca **=** **rep**(**NA**, N), Cb **=** **rep**(**NA**, N), |
|  |  | IntAB **=** **rep**(**NA**, N), UnionAB **=** **rep**(**NA**, N), |
|  |  | CommonProp **=** **rep**(**NA**, N), |
|  |  | PIa **=** **rep**(**NA**, N), PIb **=** **rep**(**NA**, N), |
|  |  | PIaU **=** **rep**(**NA**, N), PIbU **=** **rep**(**NA**, N), |
|  |  | FragEffA **=** **rep**(**NA**, N), FragEffB **=** **rep**(**NA**, N)) |
|  |  |  |
|  |  | **for** (index **in** 1**:**N){ |
|  |  |  |
|  |  | PropByCompound**$**CompoundID[index] **<-** CompoundSet[index] |
|  |  |  |
|  |  | MethodABelongsTo **<-** ScafSetA[ScafSetA**$**COMPOUND\_ID **==** Compounds[index], |
|  |  | ScafColA] *# StrucUniqueID or CLink* |
|  |  |  |
|  |  | MethodBBelongsTo **<-** ScafSetB[ScafSetB**$**COMPOUND\_ID **==** Compounds[index], |
|  |  | ScafColB] *# SCAFFOLD\_ID* |
|  |  |  |
|  |  | PropByCompound**$**FragA[index] **<-** **length**(unique(MethodABelongsTo)) |
|  |  | PropByCompound**$**FragB[index] **<-** **length**(unique(MethodBBelongsTo)) |
|  |  |  |
|  |  | MethodACompoundCluster **<-** unique(ScafSetA[ScafSetA[,ScafColA] **%in%** MethodABelongsTo, |
|  |  | "COMPOUND\_ID"]) |
|  |  |  |
|  |  | MethodBCompoundCluster **<-** unique(ScafSetB[ScafSetB[,ScafColB] **%in%** MethodBBelongsTo, |
|  |  | "COMPOUND\_ID"]) |
|  |  |  |
|  |  | PropByCompound**$**Ca[index] **<-** **length**(MethodACompoundCluster) |
|  |  | PropByCompound**$**Cb[index] **<-** **length**(MethodBCompoundCluster) |
|  |  | PropByCompound**$**IntAB[index] **<-** **length**(intersect(MethodACompoundCluster, |
|  |  | MethodBCompoundCluster)) |
|  |  | PropByCompound**$**UnionAB[index] **<-** **length**(union(MethodACompoundCluster, |
|  |  | MethodBCompoundCluster)) |
|  |  | PropByCompound**$**CommonProp[index] **<-** PropByCompound**$**IntAB[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIa[index] **<-** PropByCompound**$**Ca[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIb[index] **<-** PropByCompound**$**Cb[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIaU[index] **<-** 1 **-** PropByCompound**$**Cb[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**PIbU[index] **<-** 1 **-** PropByCompound**$**Ca[index]**/**PropByCompound**$**UnionAB[index] |
|  |  | PropByCompound**$**FragEffA[index] **<-** PropByCompound**$**Ca[index]**/**PropByCompound**$**FragA[index] |
|  |  | PropByCompound**$**FragEffB[index] **<-** PropByCompound**$**Cb[index]**/**PropByCompound**$**FragB[index] |
|  |  | } *# for index* |
|  |  | **return**(PropByCompound) |
|  |  | } *# function* |
|  |  |  |
|  |  | *# call function - A is FW, B is RGT, D is CLink* |
|  |  | PropByCompound\_AB **<-** statcompare(ScafSetA **=** DDData , ScafSetB **=** RGData, |
|  |  | ScafColA**=**"StrucUniqueID", ScafColB**=**"SCAFFOLD\_ID", |
|  |  | CompoundSet **=** Compounds) |
|  |  | PropByCompound\_DB **<-** statcompare(ScafSetA **=** CLData , ScafSetB **=** RGData, |
|  |  | ScafColA**=**"CLink", ScafColB**=**"SCAFFOLD\_ID", |
|  |  | CompoundSet **=** Compounds) |
|  |  |  |
|  |  | *#Create output -- averages, quantiles, and histograms* |
|  |  | summarize\_prop **<-** **function**(PropByCompound) { |
|  |  | ACP **<-** mean(PropByCompound**$**CommonProp, na.rm **=** T) |
|  |  | APIa **<-** mean(PropByCompound**$**PIa, na.rm **=** T) |
|  |  | APIb **<-** mean(PropByCompound**$**PIb, na.rm **=** T) |
|  |  | APIaU **<-** mean(PropByCompound**$**PIaU, na.rm **=** T) |
|  |  | APIbU **<-** mean(PropByCompound**$**PIbU, na.rm **=** T) |
|  |  | AFragA **<-** mean(PropByCompound**$**FragA, na.rm **=** T) |
|  |  | AFragB **<-** mean(PropByCompound**$**FragB, na.rm **=** T) |
|  |  | AFragEffA **<-** mean(PropByCompound**$**FragEffA, na.rm **=** T) |
|  |  | AFragEffB **<-** mean(PropByCompound**$**FragEffB, na.rm **=** T) |
|  |  | ACa **<-** mean(PropByCompound**$**Ca, na.rm **=** T) |
|  |  | ACb **<-** mean(PropByCompound**$**Cb, na.rm **=** T) |
|  |  |  |
|  |  | CP90 **<-** quantile(PropByCompound**$**CommonProp, **c**(0.1,0.5,0.9)) |
|  |  | PIa90 **<-** quantile(PropByCompound**$**PIa, na.rm **=** T , **c**(0.1,0.5,0.9)) |
|  |  | PIb90 **<-** quantile(PropByCompound**$**PIb, na.rm **=** T , **c**(0.1,0.5,0.9)) |
|  |  | PIaU90 **<-** quantile(PropByCompound**$**PIaU, na.rm **=** T , **c**(0.1,0.5,0.9)) |
|  |  | PIbU90 **<-** quantile(PropByCompound**$**PIbU, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragA90 **<-** quantile(PropByCompound**$**FragA, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragB90 **<-** quantile(PropByCompound**$**FragB, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragEffA90 **<-** quantile(PropByCompound**$**FragEffA, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | FragEffB90 **<-** quantile(PropByCompound**$**FragEffB, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | Ca90 **<-** quantile(PropByCompound**$**Ca, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  | Cb90 **<-** quantile(PropByCompound**$**Cb, na.rm **=** T, **c**(0.1,0.5,0.9)) |
|  |  |  |
|  |  | ret **<-** **list**(ACP**=**ACP, CP90**=**CP90, |
|  |  | APIa**=**APIa, PIa90**=**PIa90, APIb**=**APIb, PIb90**=**PIb90, |
|  |  | APIaU**=**APIaU, PIaU90**=**PIaU90, APIbU**=**APIbU, PIbU90**=**PIbU90, |
|  |  | AFragA**=**AFragA, FragA90**=**FragA90, AFragB**=**AFragB, FragB90**=**FragB90, |
|  |  | AFragEffA**=**AFragEffA, FragEffA90**=**FragEffA90, AFragEffB**=**AFragEffB, FragEffB90**=**FragEffB90, |
|  |  | ACa**=**ACa, Ca90**=**Ca90, ACb**=**ACb, Cb90**=**Cb90) |
|  |  |  |
|  |  | **return**(ret) |
|  |  | } |
|  |  |  |
|  |  | *######### create summaries #######* |
|  |  | SumProp\_AB **<-** summarize\_prop(PropByCompound\_AB) |
|  |  | SumProp\_DB **<-** summarize\_prop(PropByCompound\_DB) |
|  |  |  |
|  |  | *# write output to CSV* |
|  |  | write.table(PropByCompound\_AB,"PropByCompound\_FW\_RGD.txt",sep**=**"\t",row.name**=**F,col.name**=**T) |
|  |  | write.table(PropByCompound\_DB,"PropByCompound\_Cluster\_RGD.txt",sep**=**"\t",row.name**=**F,col.name**=**T) |
|  |  | *#########################################################################################* |
|  |  |  |
|  |  | *################# Plot #####################* |
|  |  | createPlots **<-** **function**(PropByCompound) { |
|  |  | attach(PropByCompound) |
|  |  |  |
|  |  | hist(FragA,main**=**"FragA") |
|  |  | hist(FragB,main**=**"FragB") |
|  |  | hist(CommonProp,main**=**"CommonProp") |
|  |  |  |
|  |  | plot(CommonProp**~**UnionAB) |
|  |  | plot(CommonProp**~**IntAB) |
|  |  | plot(Ca**~**Cb) |
|  |  |  |
|  |  | plot(UnionAB, IntAB) |
|  |  | plot(FragA **+** FragB, CommonProp) |
|  |  |  |
|  |  | detach(PropByCompound) |
|  |  | } |
|  |  |  |
|  |  | createPlots(PropByCompound\_AB) |
|  |  | createPlots(PropByCompound\_DB) |
|  |  | \ No newline at end of file |

[**stats/RGD.txt**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#5a9f1024cdb87c3d49d79c1da6e7f4a49b3b7bd0) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/RGD.txt)

This diff could not be displayed because it is too large.

[**stats/stats.Rproj**](https://spotlite.nih.gov/ncats/scaffoldanalytics/compare/28575ec708dd8bb0f33062c15d36b8d3781e911b...5164c3886656ccfe8cde15e2d4b514559ddb59a0#c67d83a7b73e62e709c7ba75876b171786be58b8) 0 → 100644

[View file @5164c38](https://spotlite.nih.gov/ncats/scaffoldanalytics/blob/5164c3886656ccfe8cde15e2d4b514559ddb59a0/stats/stats.Rproj)

|  |  |  |
| --- | --- | --- |
|  |  | Version: 1.0 |
|  |  |  |
|  |  | RestoreWorkspace: Default |
|  |  | SaveWorkspace: Default |
|  |  | AlwaysSaveHistory: Default |
|  |  |  |
|  |  | EnableCodeIndexing: Yes |
|  |  | UseSpacesForTab: Yes |
|  |  | NumSpacesForTab: 2 |
|  |  | Encoding: UTF-8 |
|  |  |  |
|  |  | RnwWeave: Sweave |
|  |  | LaTeX: pdfLaTeX |