Welcome to iProtein – the proteome in the sky!

iProtein provides access to Eidogen-Sertanty's Target Informatics Platform (TIP) - the world's first protein structure informatics system and knowledgebase enabling structural interrogation of the druggable genome.

TIP amplifies the rapidly expanding body of experimental protein structural information found in the Protein Data Bank (PDB) by generating high accuracy protein structural models across sequences found in Swiss-Prot, RefSeq, Ensembl, IPI, etc. TIP leverages protein structural information across family members and corresponding crystal structure templates using an algorithm that has been validated in several top pharmaceutical companies and academic research sites. As such, TIP contains the world's largest repository of protein structures and models.

The TIP Database

The Target Informatics Platform's content includes high resolution protein structures with reliably annotated small molecule binding sites, including >200,000 chains and comparative models of human proteins, covering every major drug target family including proteases, kinases, phosphatases, phosphodiesterases, nuclear receptors, and GPCRs.

In addition to TIP's high quality structural annotation, it is the only database of its kind that stores all similarity relationships between every sequence, structure, and binding site, making it an incredibly powerful system for structural and comparative proteomics.

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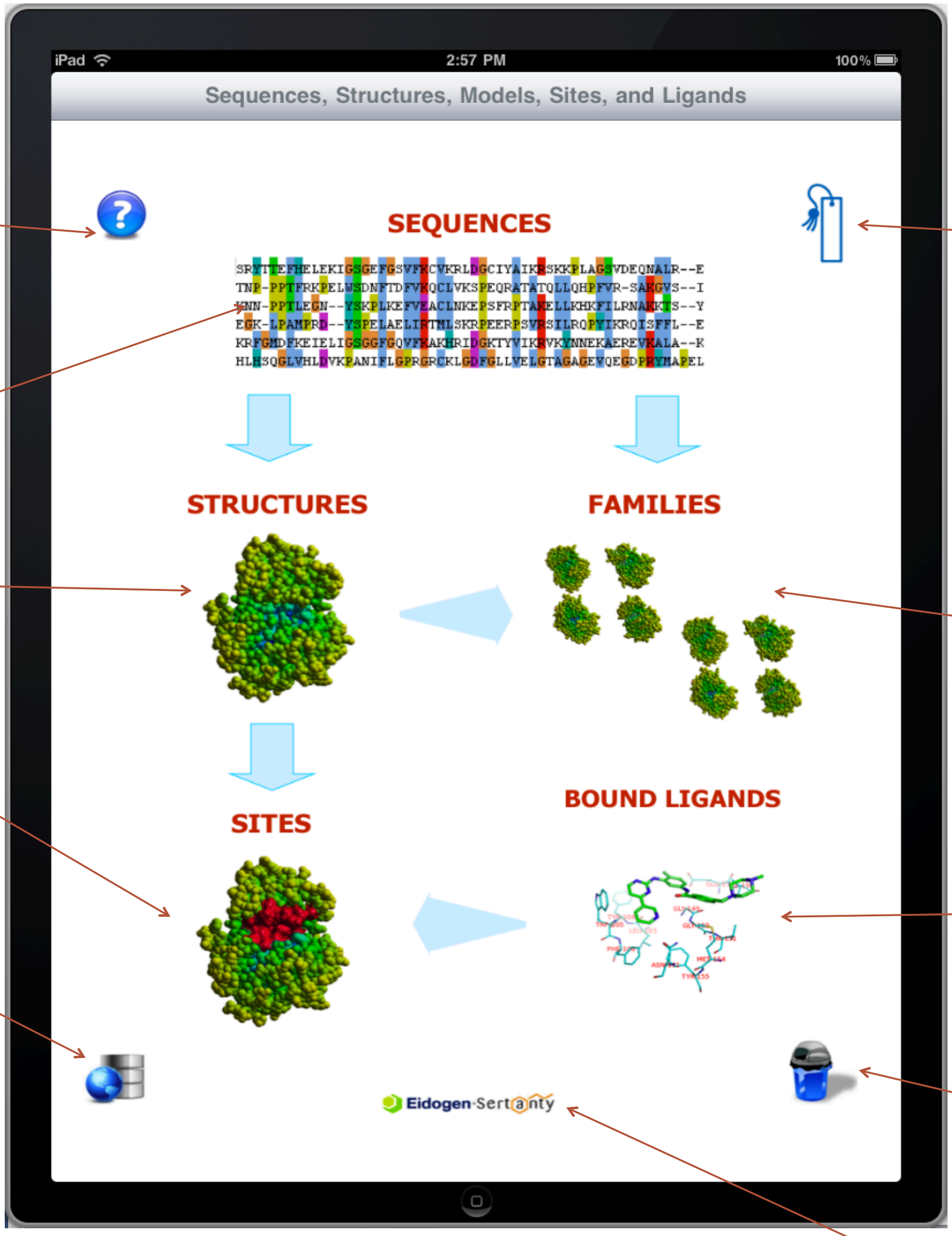
Accessing TIP content through iProtein

Through iProtein, the TIP database can be surveyed by Sequence, Structure/Model, Site, head-nodes (i.e. protein family), and by bound ligand structure searches. Simply click on any image in the main page to initiate a search. Future versions of iProtein may enable more complex searching – e.g. protein structure search, site-search, etc. So stay tuned….



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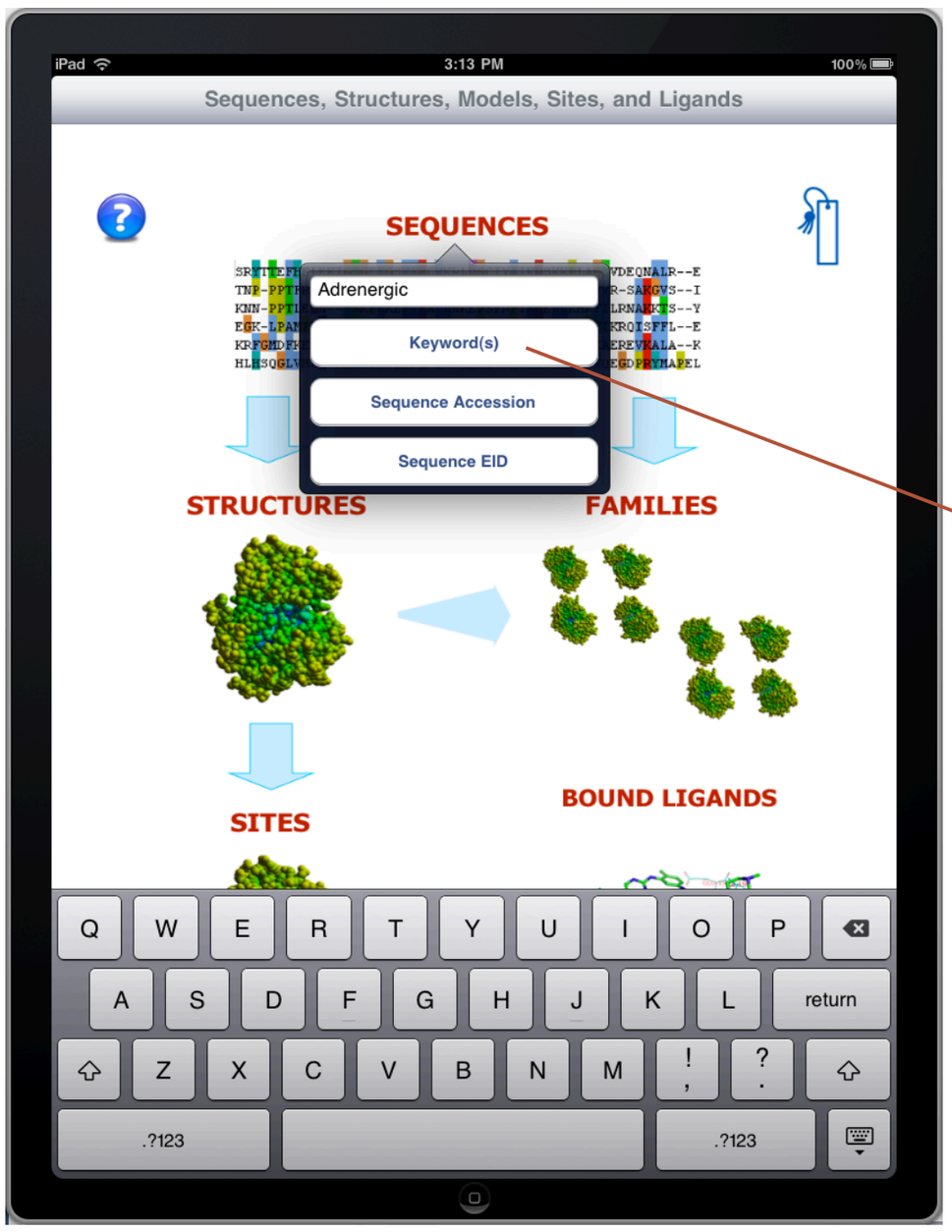
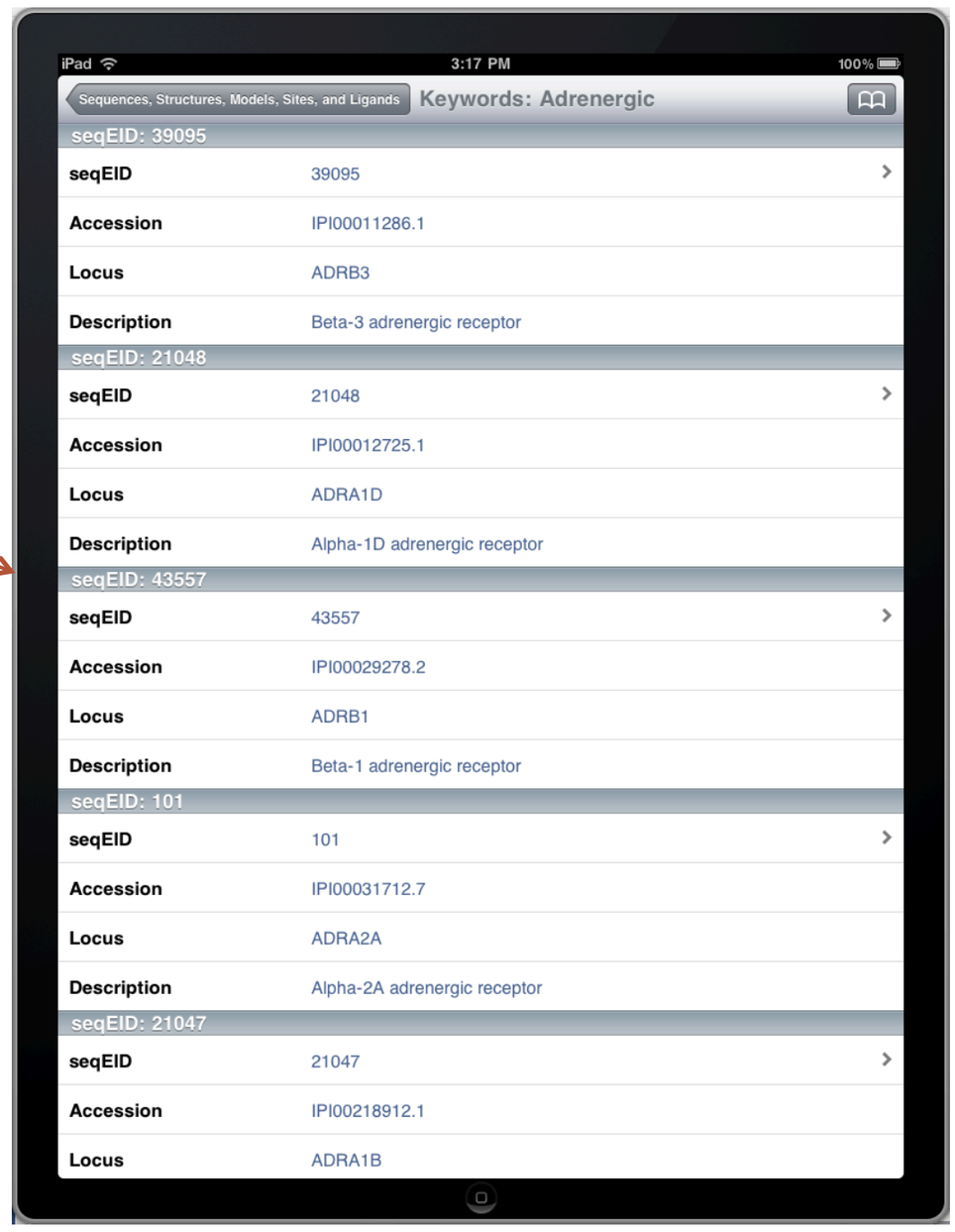
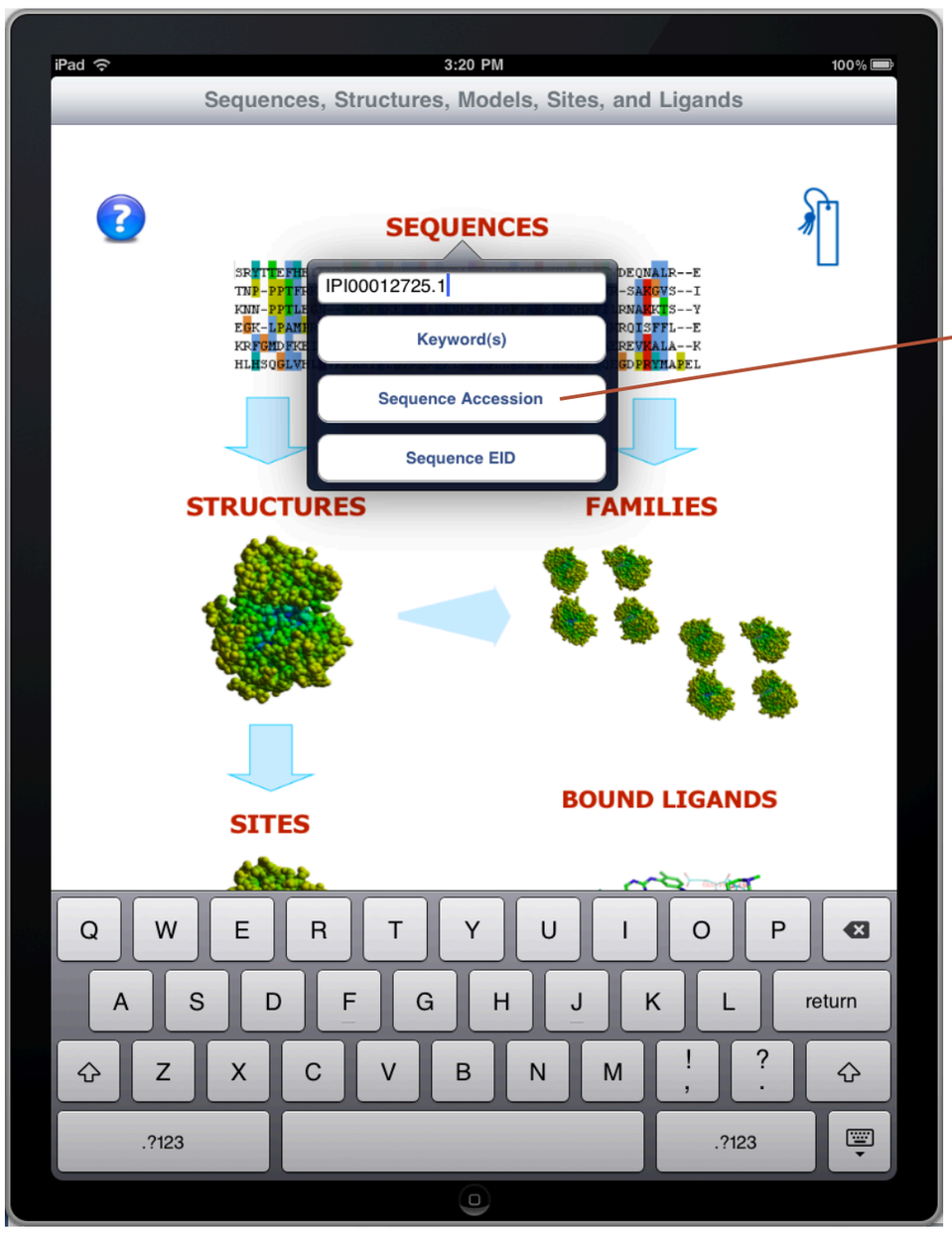
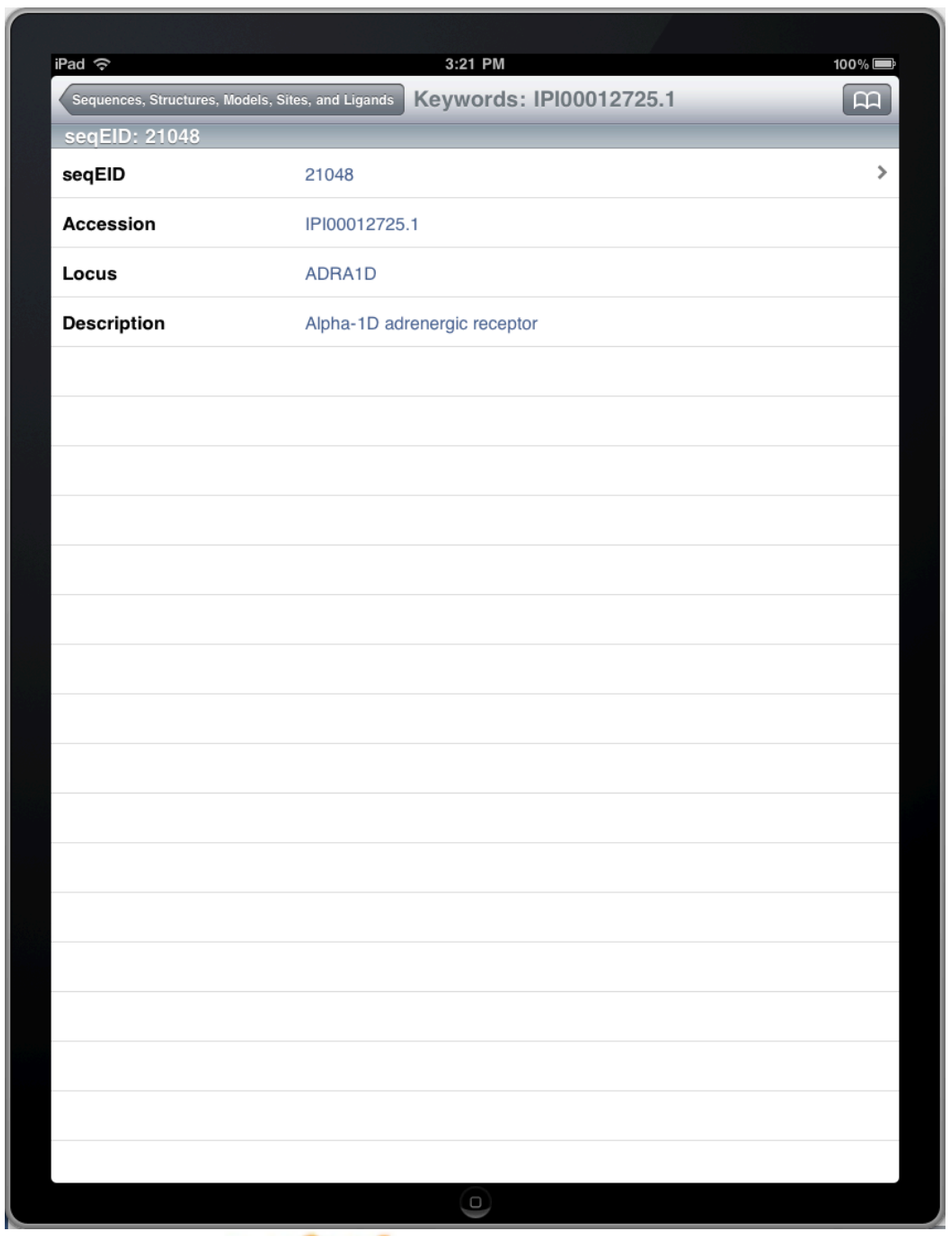
Sequence Searches

Within iProtein you can locate sequences by Keywords, Sequence Accessions (e.g. Swiss-Prot, RefSeq, Ensembl, IPI, etc.), and by Eidogen Identifiers (EID). Below are example queries:









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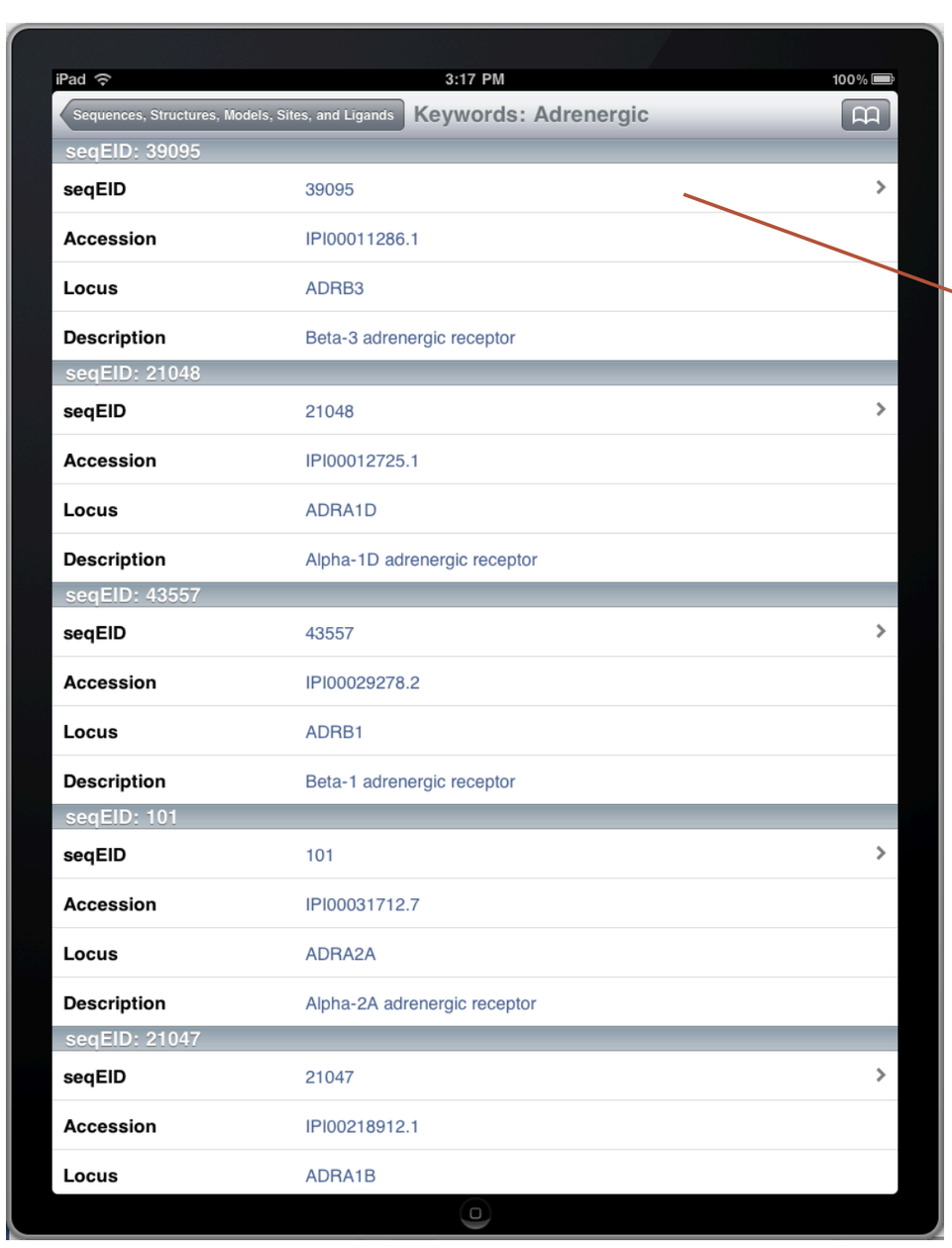
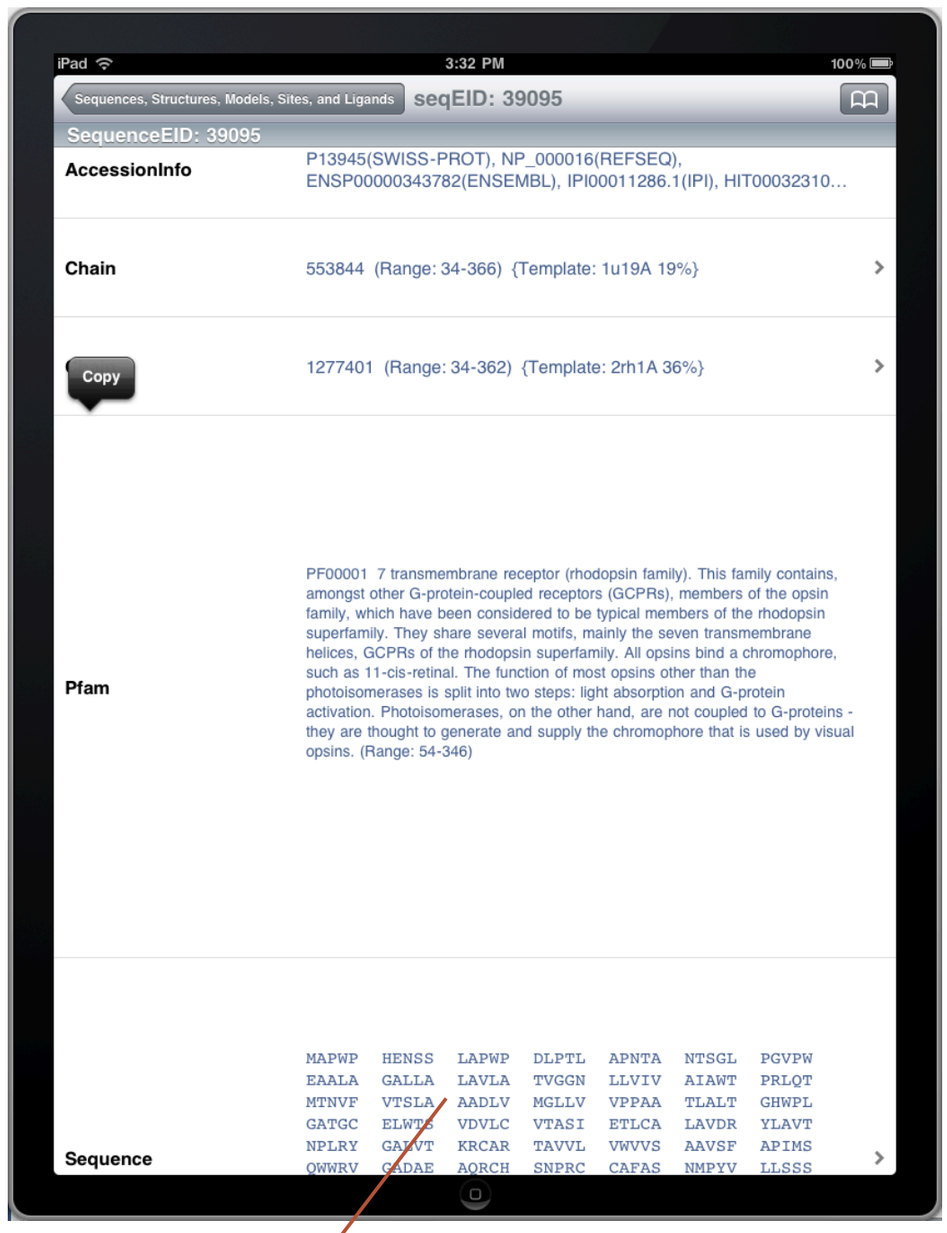
Sequence Searches (cont.)

Click on the arrow (when present) to see more data. You can double-tap on any row without an arrow (“>”) to initiate a copy-to-clipboard action or follow the arrow to see more detail. By clicking on the full sequence, a sequence search will be issued (homology >= 80%). Please note, sequence searches may take a several minutes, so please be patient…





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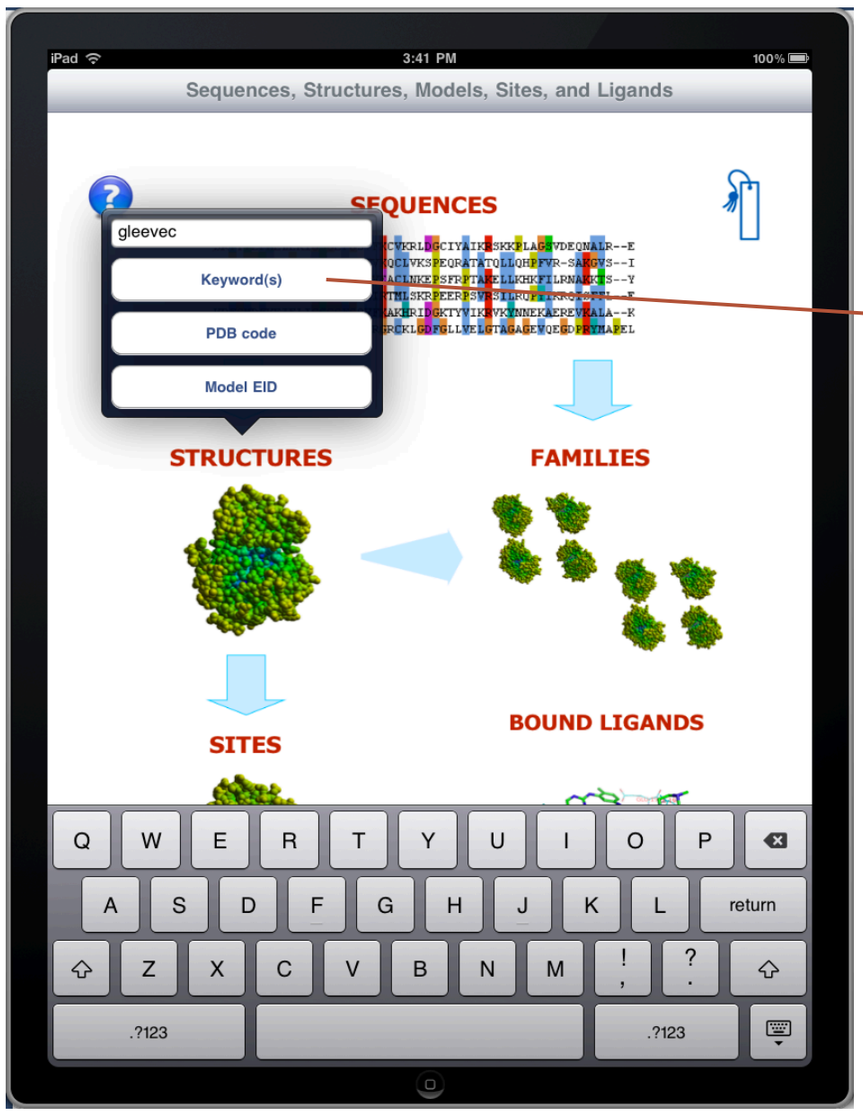
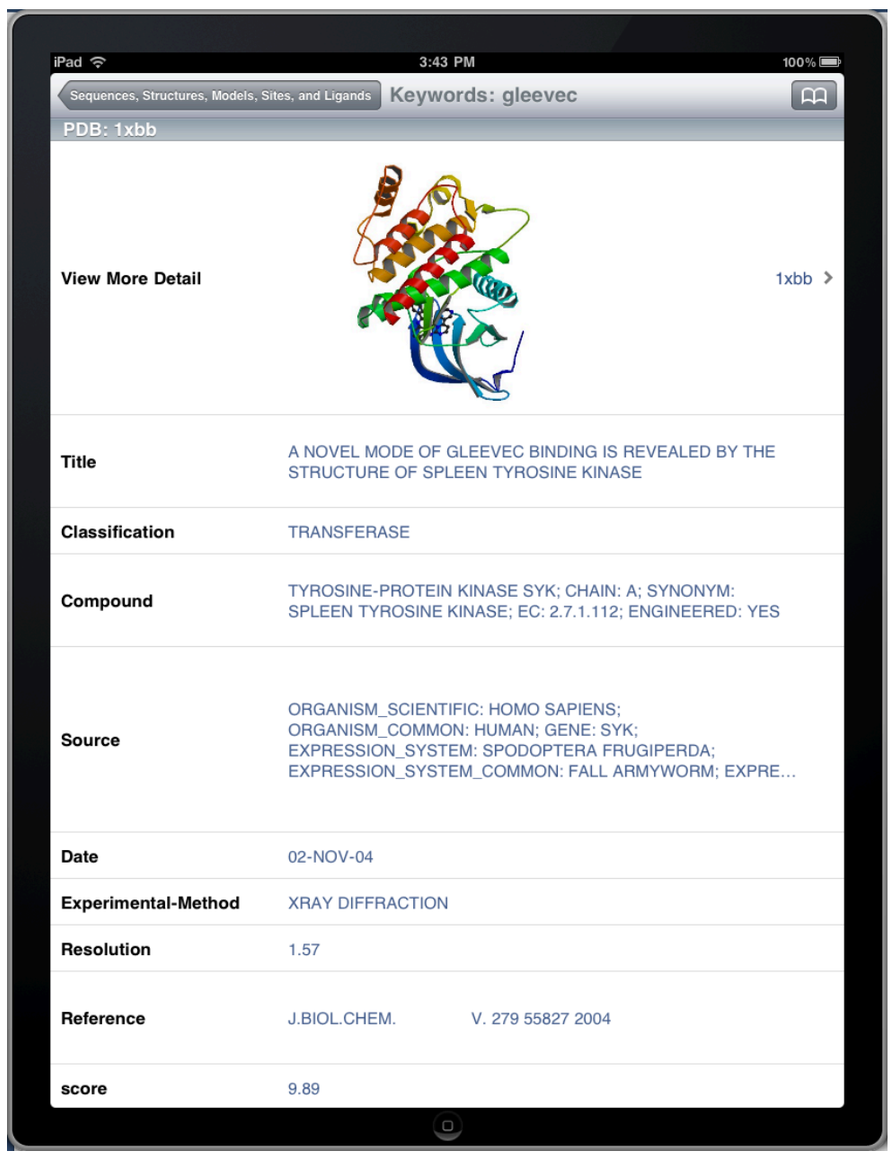
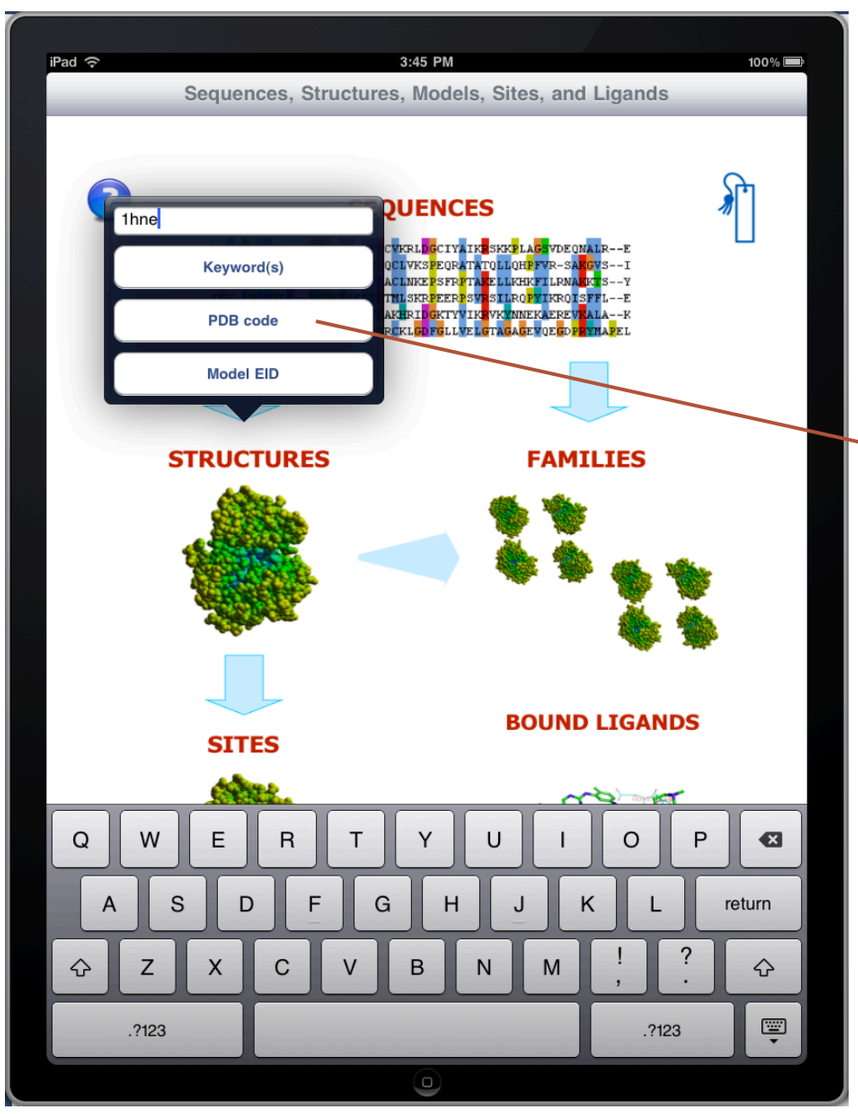
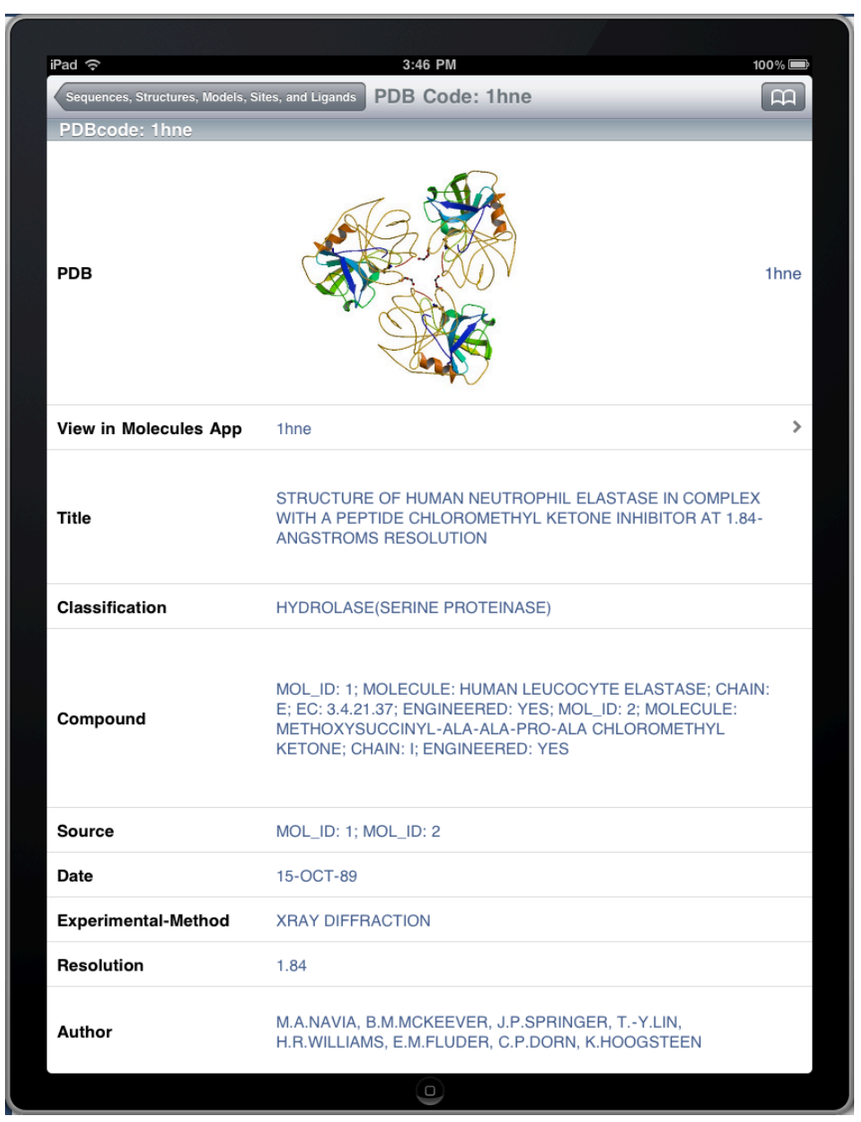
Structure/Model Searches

Within iProtein you can locate structures by Keywords, PDB codes, and by Eidogen Identifiers (EIDs). Below are a couple example queries:









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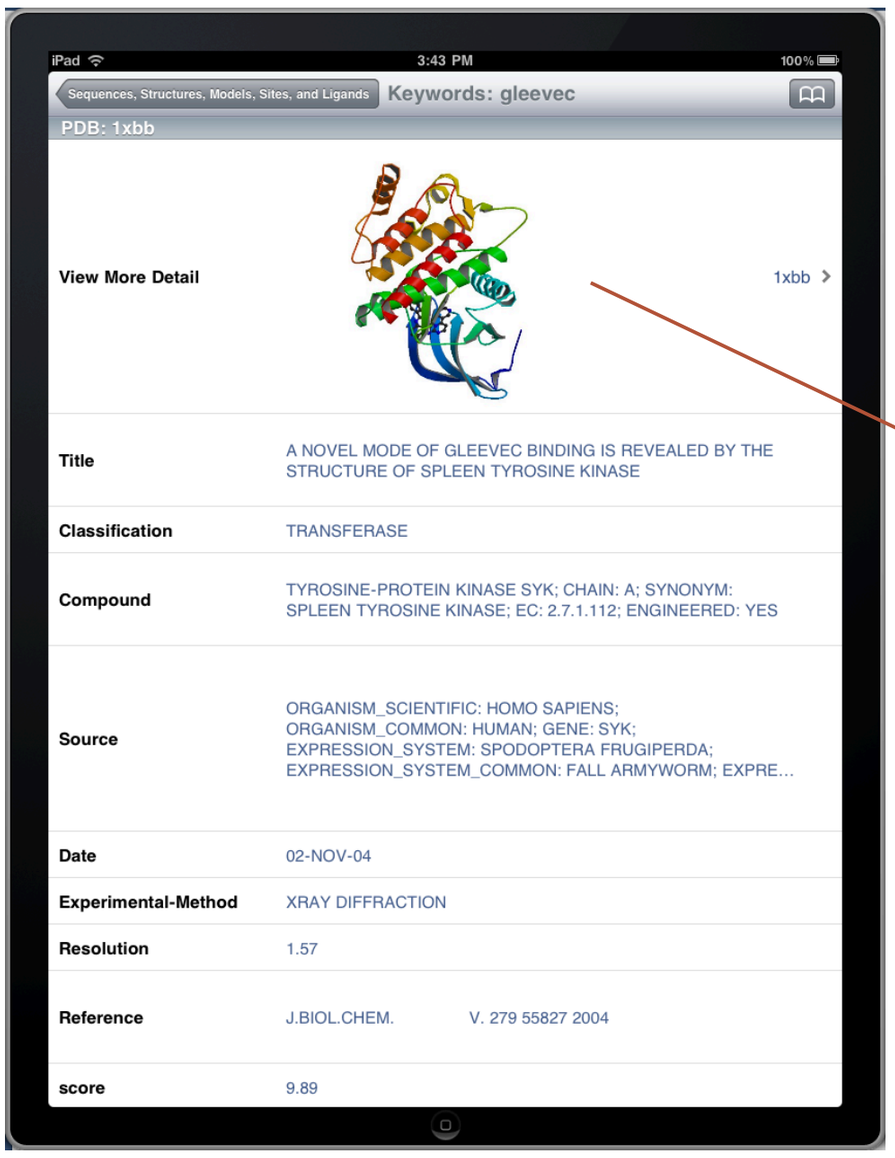
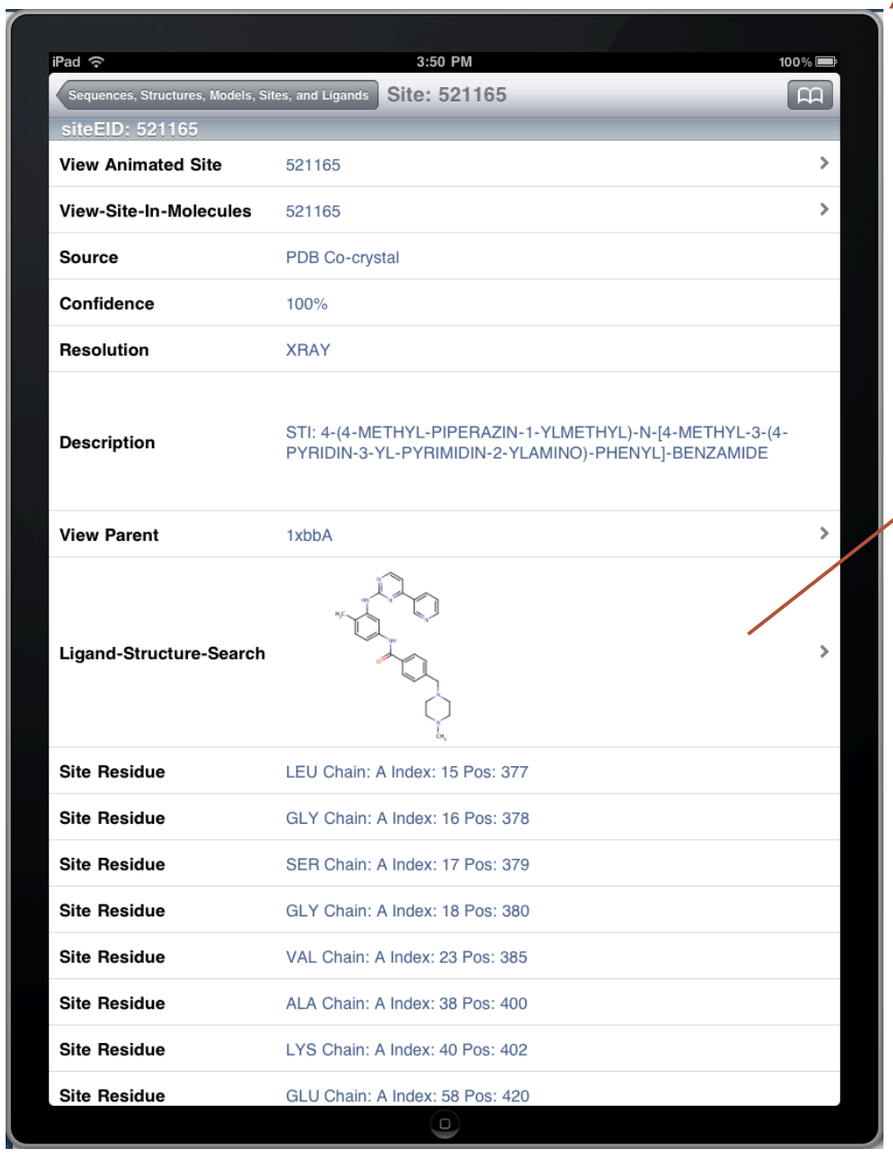
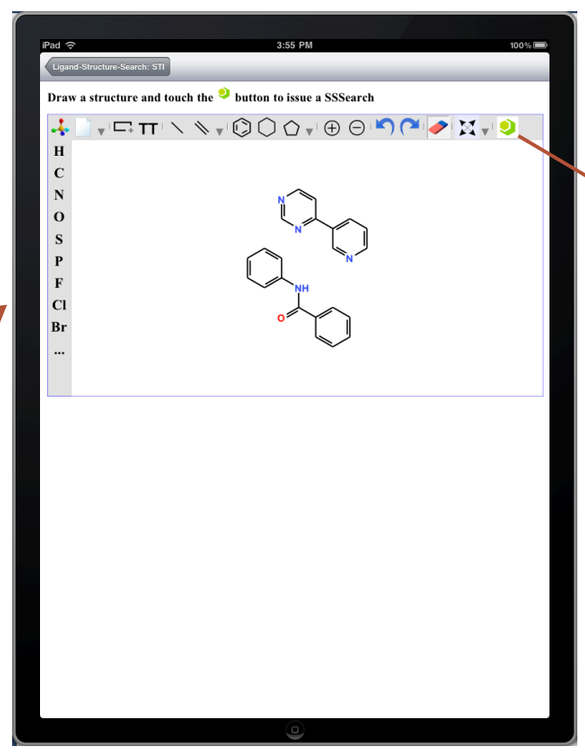
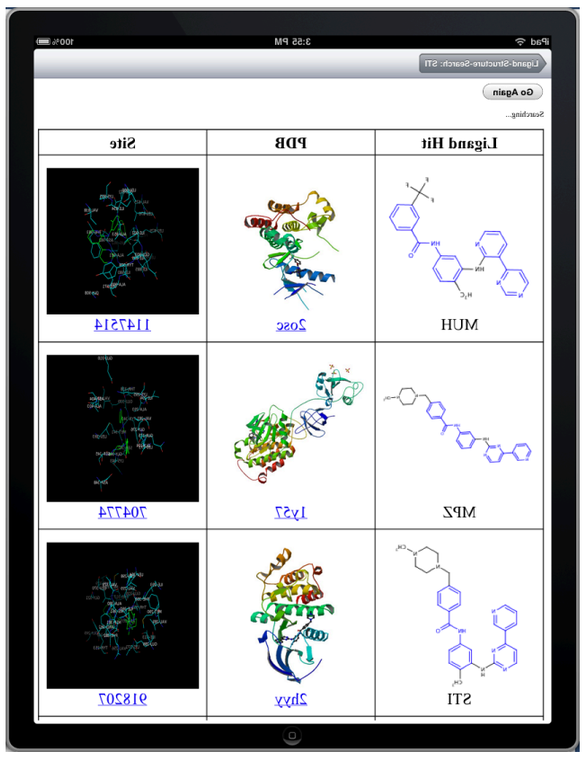
Structure/Model Searches (cont)

Click on the arrow (when present) to see more data. You can click the arrow (“>”) to see more detail. If there is a bound ligand, you can initiate ligand-based searches.









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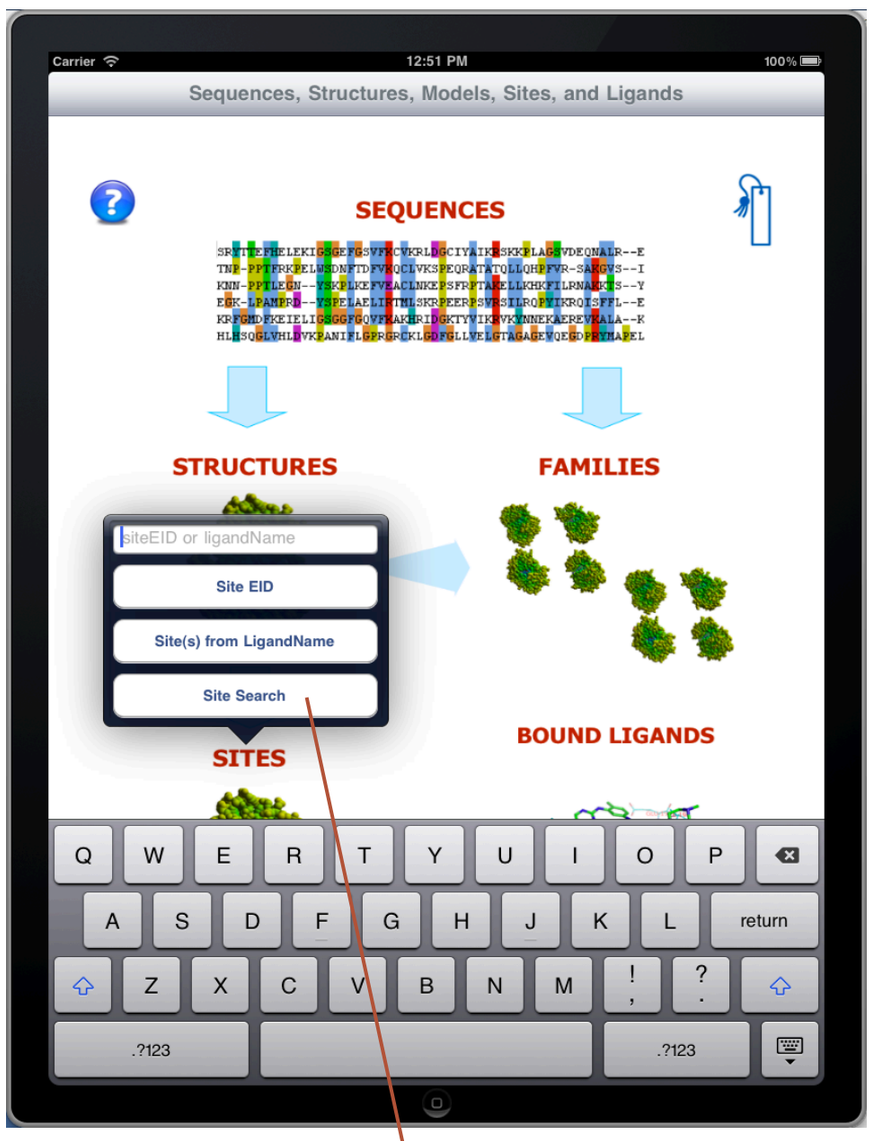
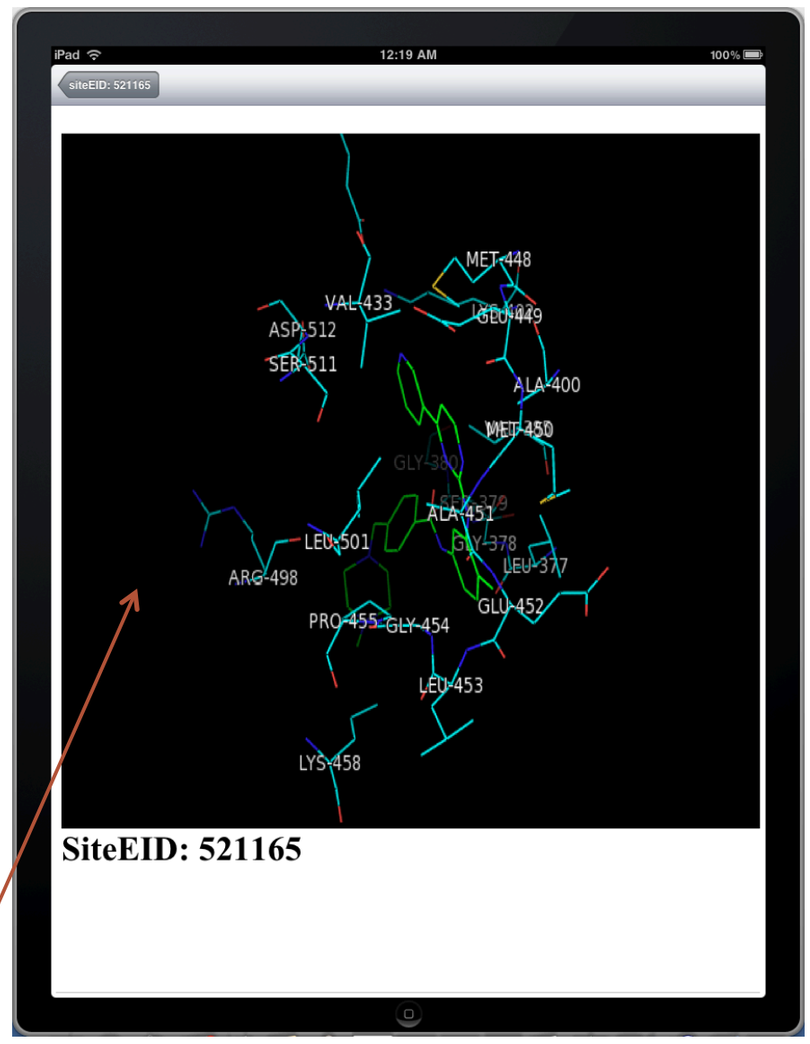
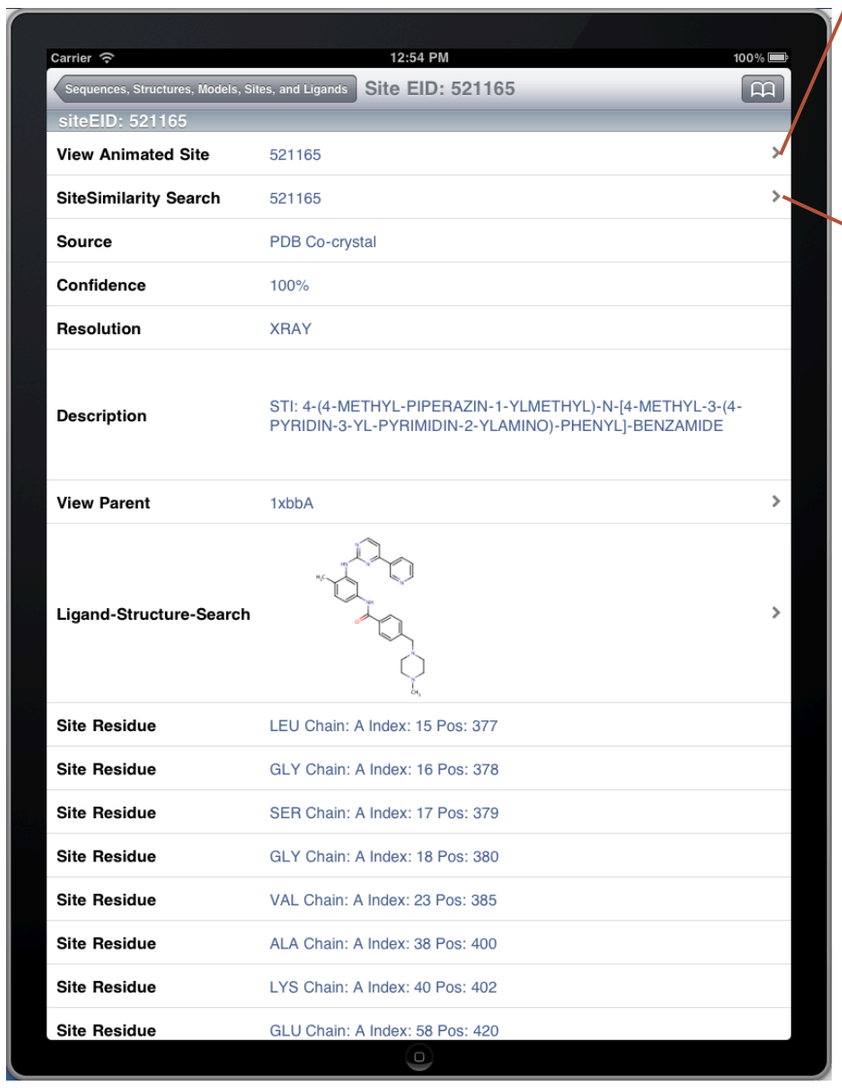
Site Searches

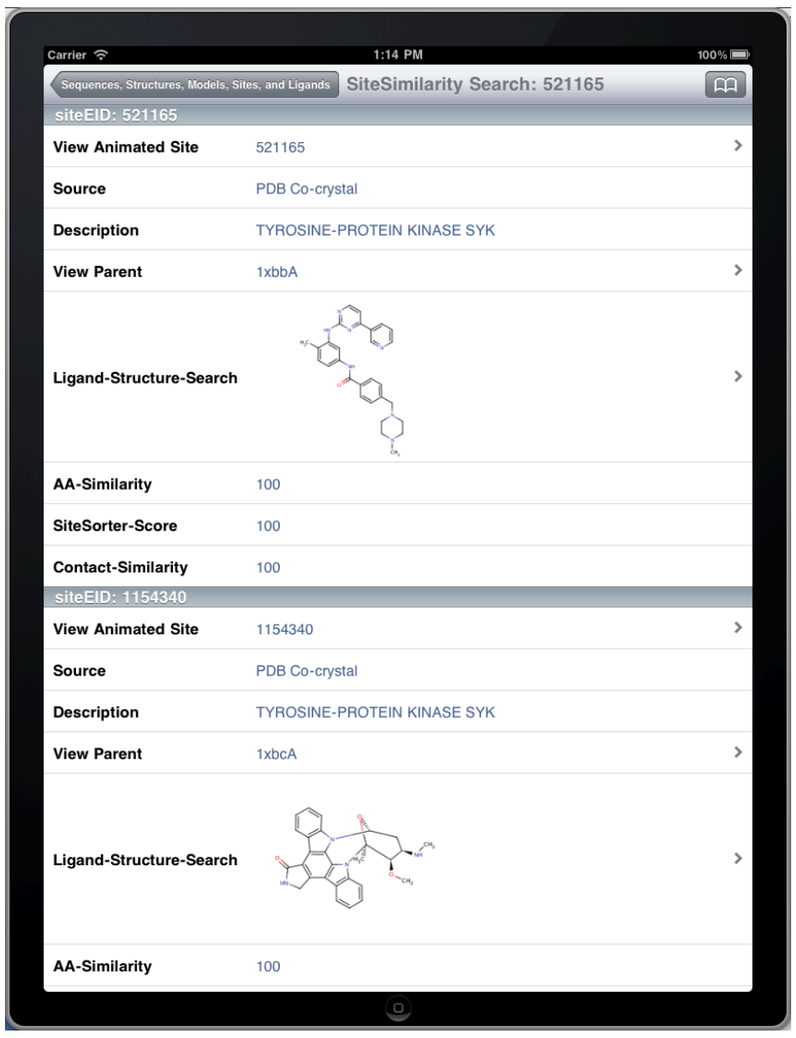
Within iProtein you can locate sites by Eidogen Identifiers (EIDs), PDB assigned ligand name and/or site ligand common name. Sites are annotated in both PDB structures and models. Ligand structures are shown if present in PDB co-complexes or inferred in models, given the template used in the modeling. Predicted sites within PDBs and models are also annotated. With version 2 of iProtein, Eidogen's powerful Site-Similarity searching capability is now accessible:





View Animated Site





SiteSimilarity Search
(Note: These can take several minutes)

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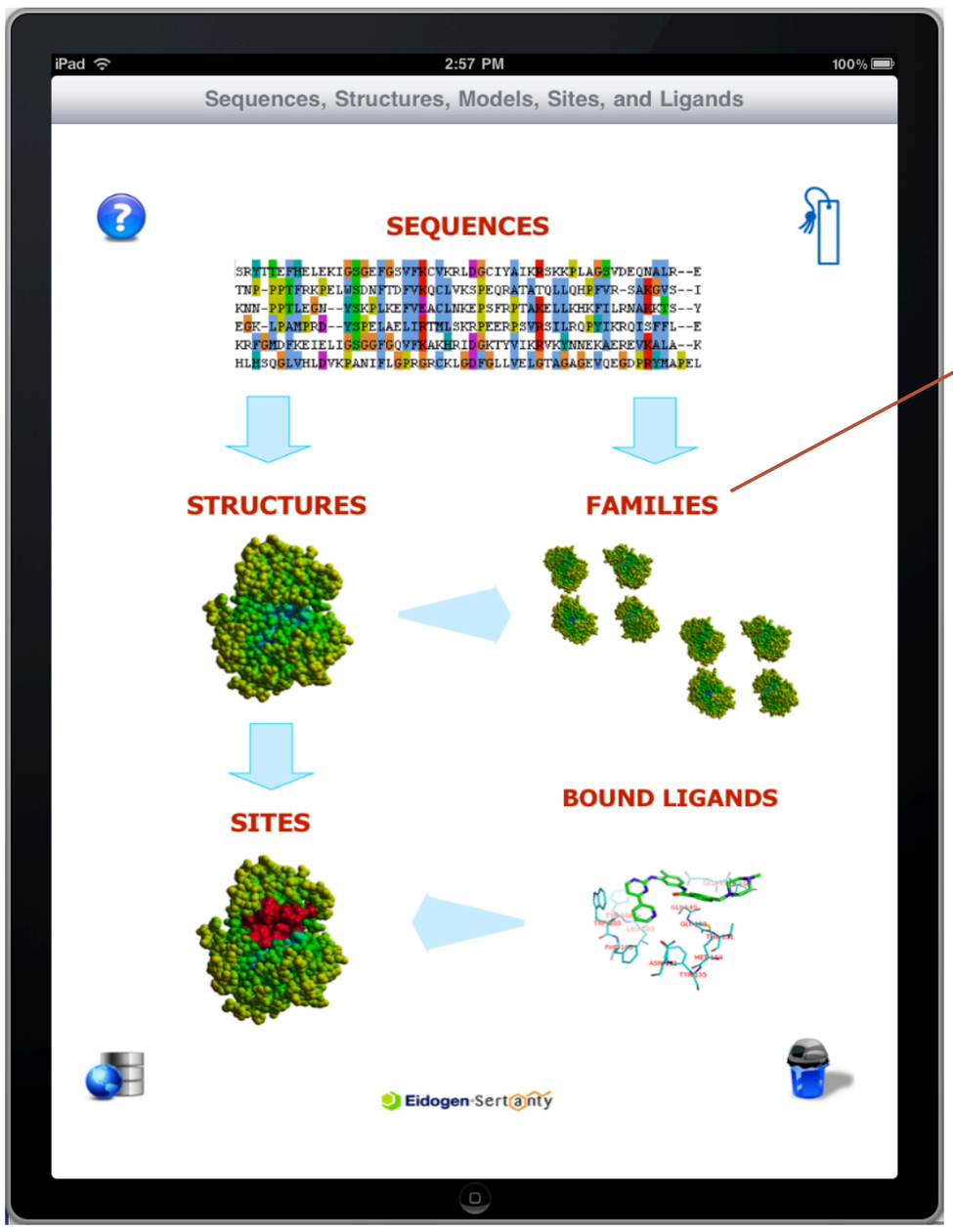
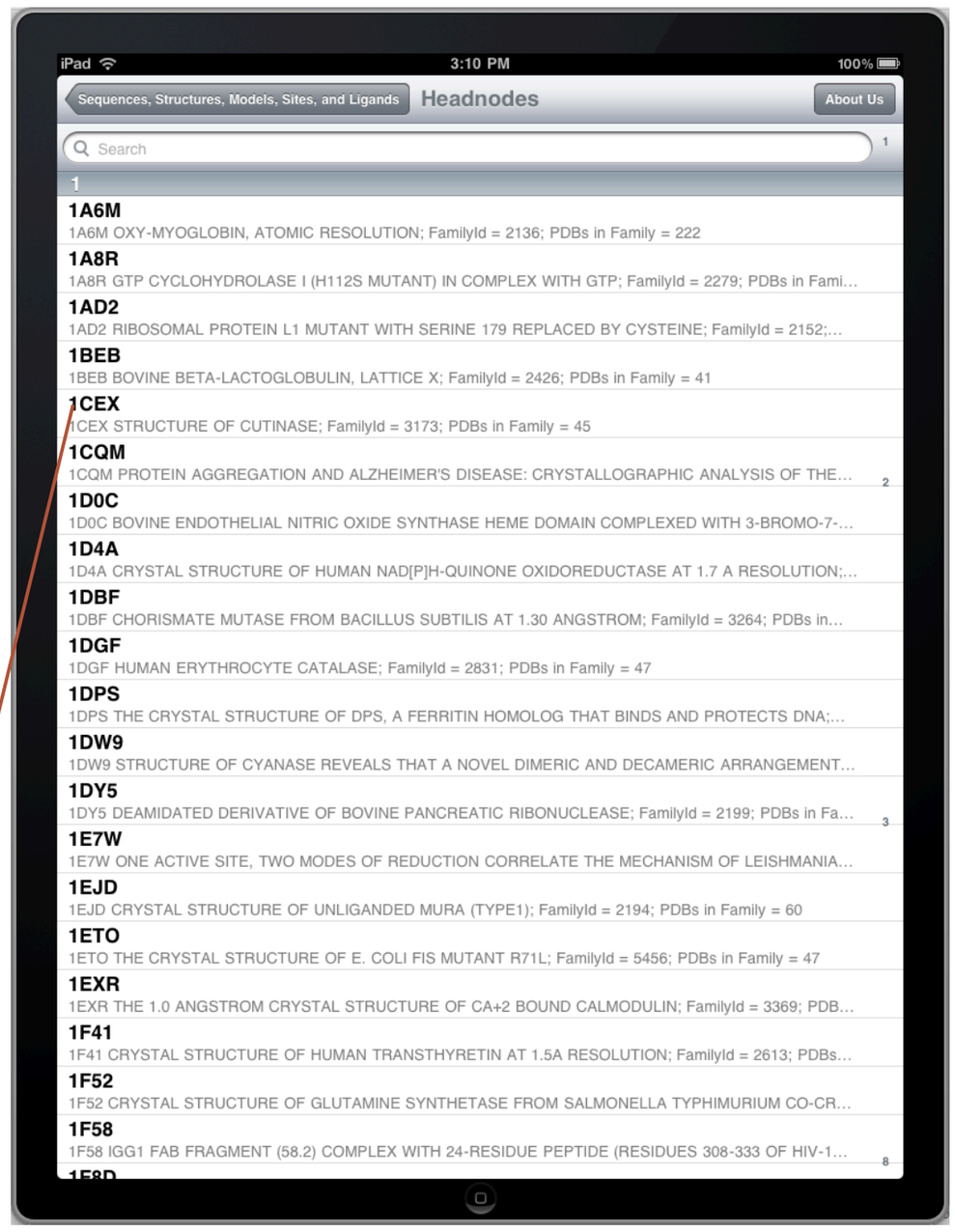
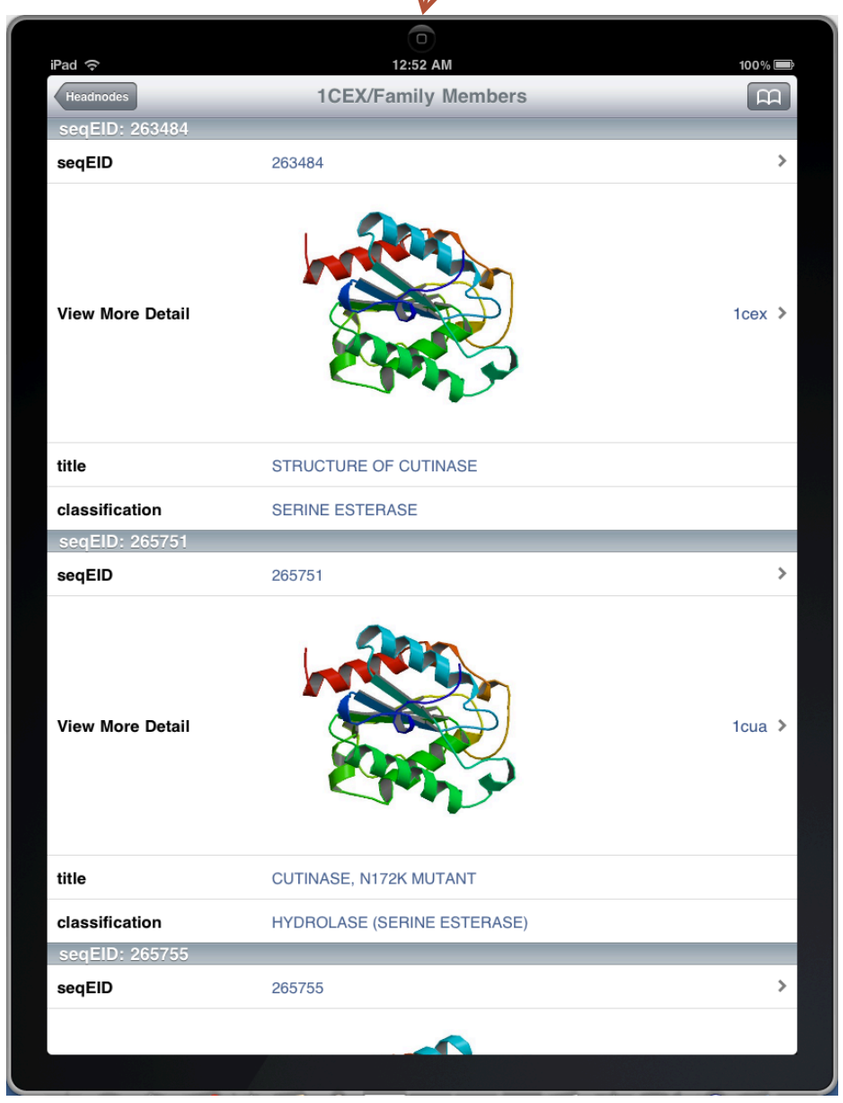
Family Searches

The TIP system clusters structurally similar protein structures. Representative members of each cluster are termed “headnodes.” Headnodes and corresponding family members are used in the sequence-to-structure modeling process. By touching “Families,” the current list of headnodes is downloaded. You can show representative family members by touching respective headnodes:







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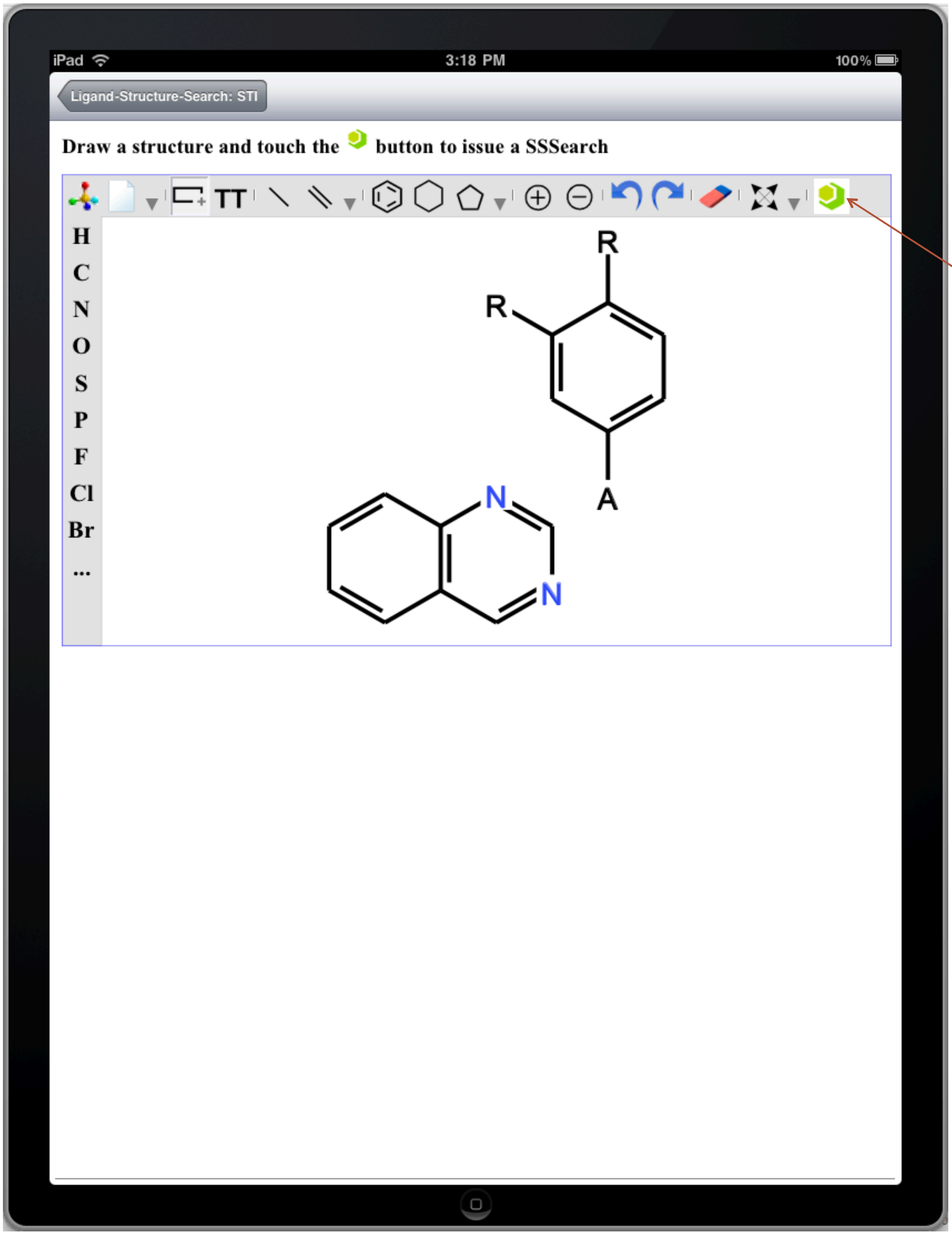
Ligand Searches

iProtein provides a chemical drawing interface that enables chemical structure drawing with your finger(s). After structures are drawn (or edited), you can issue substructure searches by tapping the iProtein icon.



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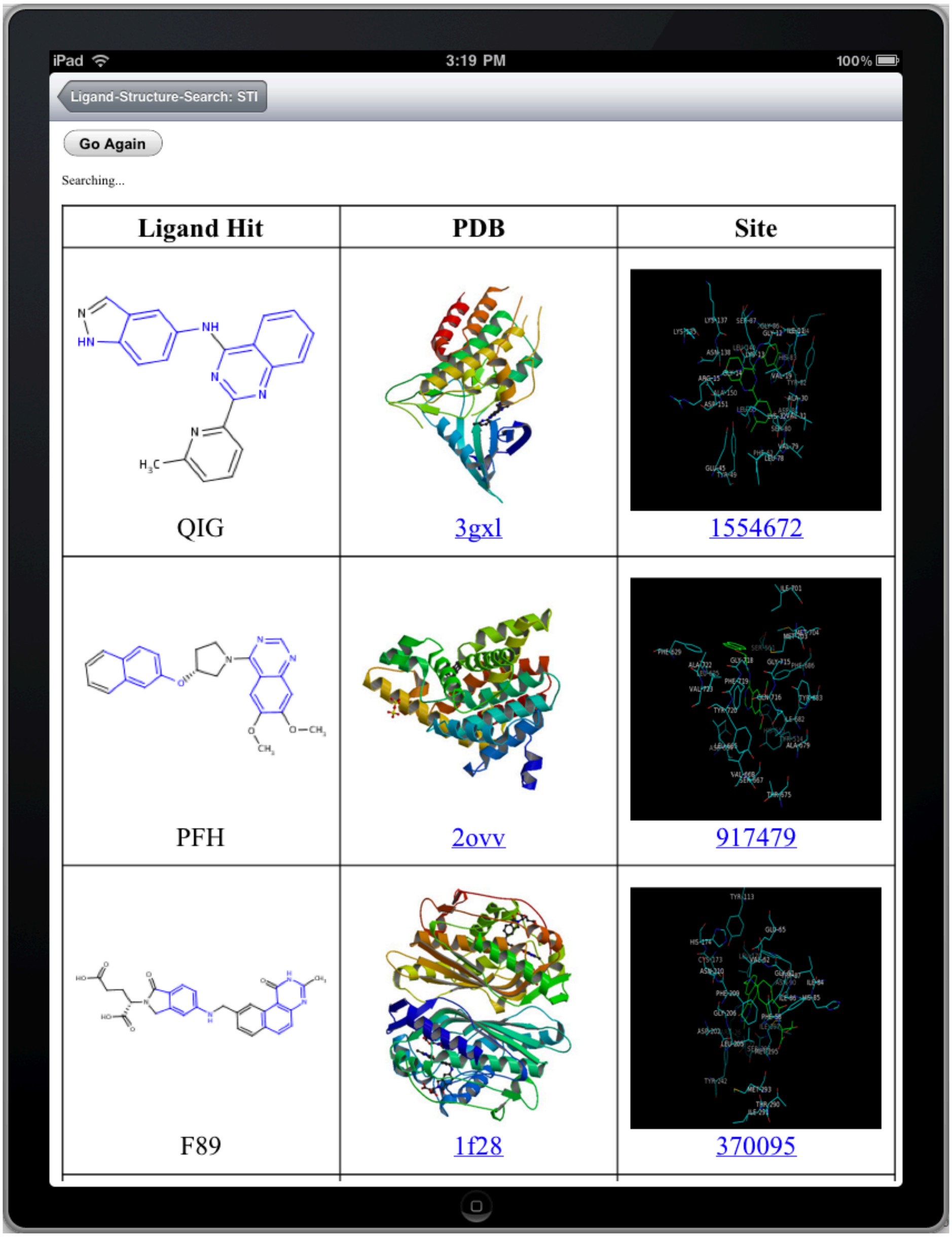
Ligand Searches (cont)

Ligand search results will tabulate the substructure hit(s), a ribbon diagram of the parent protein complex, and present an animated rendering of the co-complexed ligand within the receptor site. Site residues are annotated. You can click on the PDB code or the site EID to drill into more detail:



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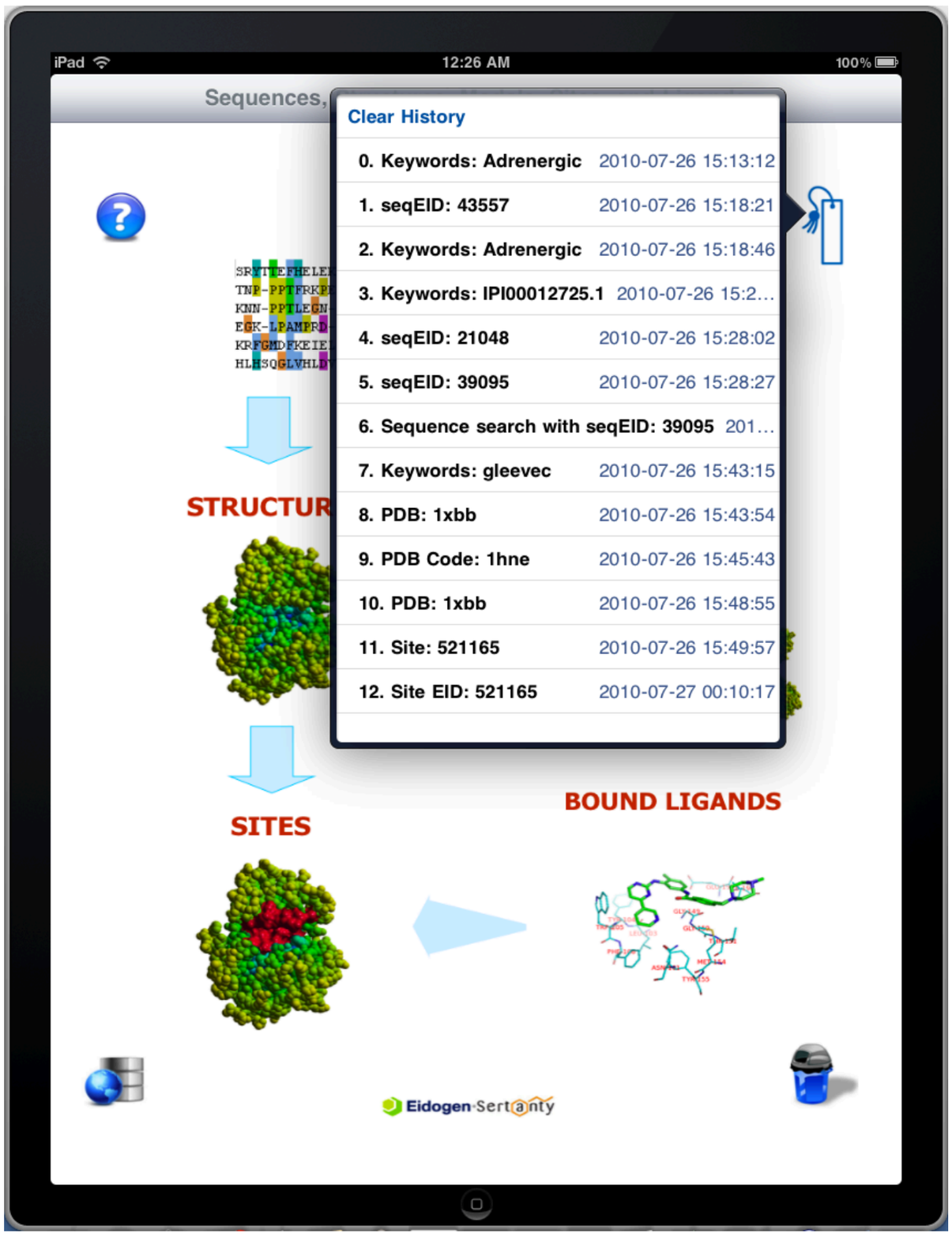
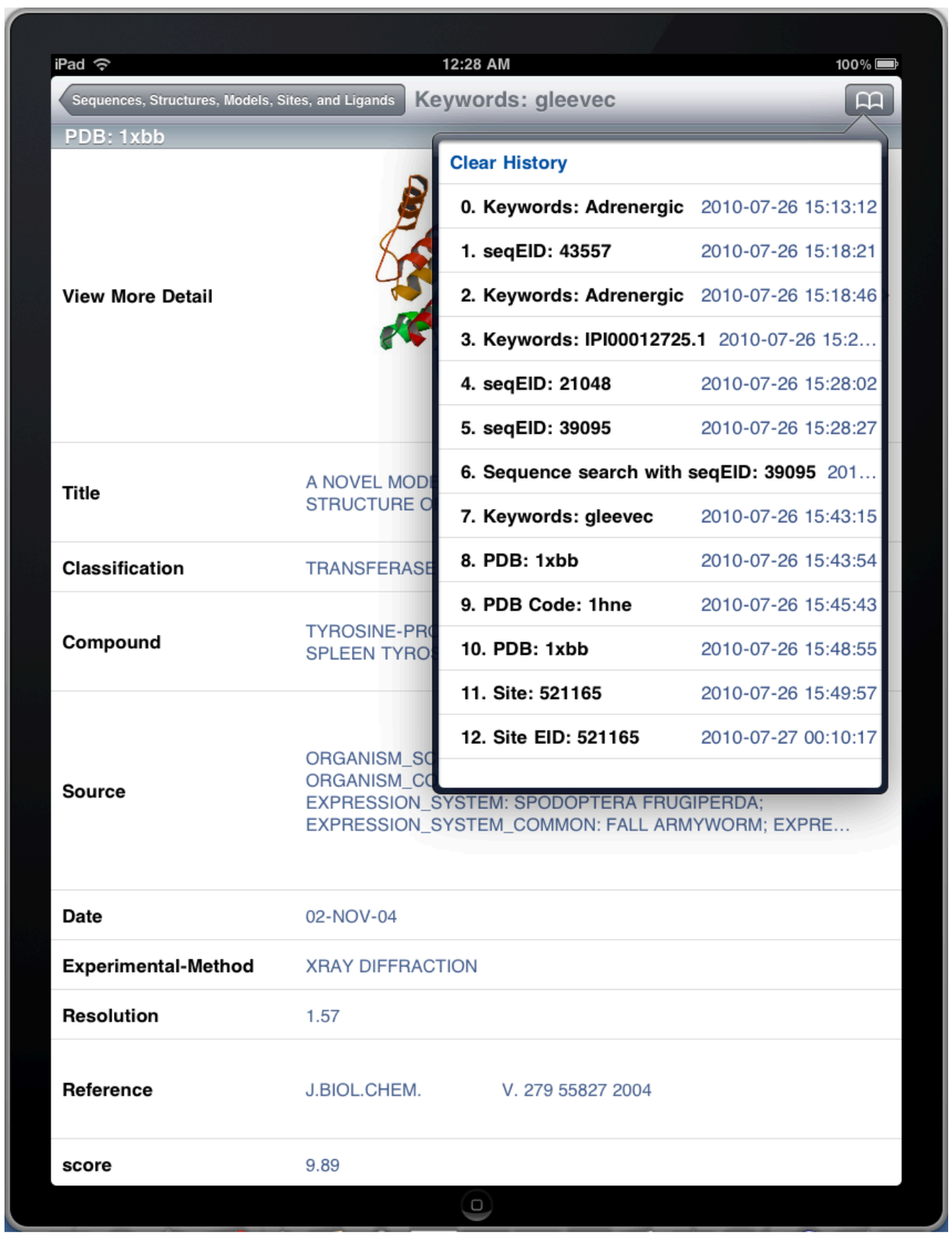
History

As you survey the proteome with iProtein, the results of your searches are stored locally on your device and accessible through the bookmark icons. You can use this history to quickly step backwards through past searches as you continue to survey the proteome:





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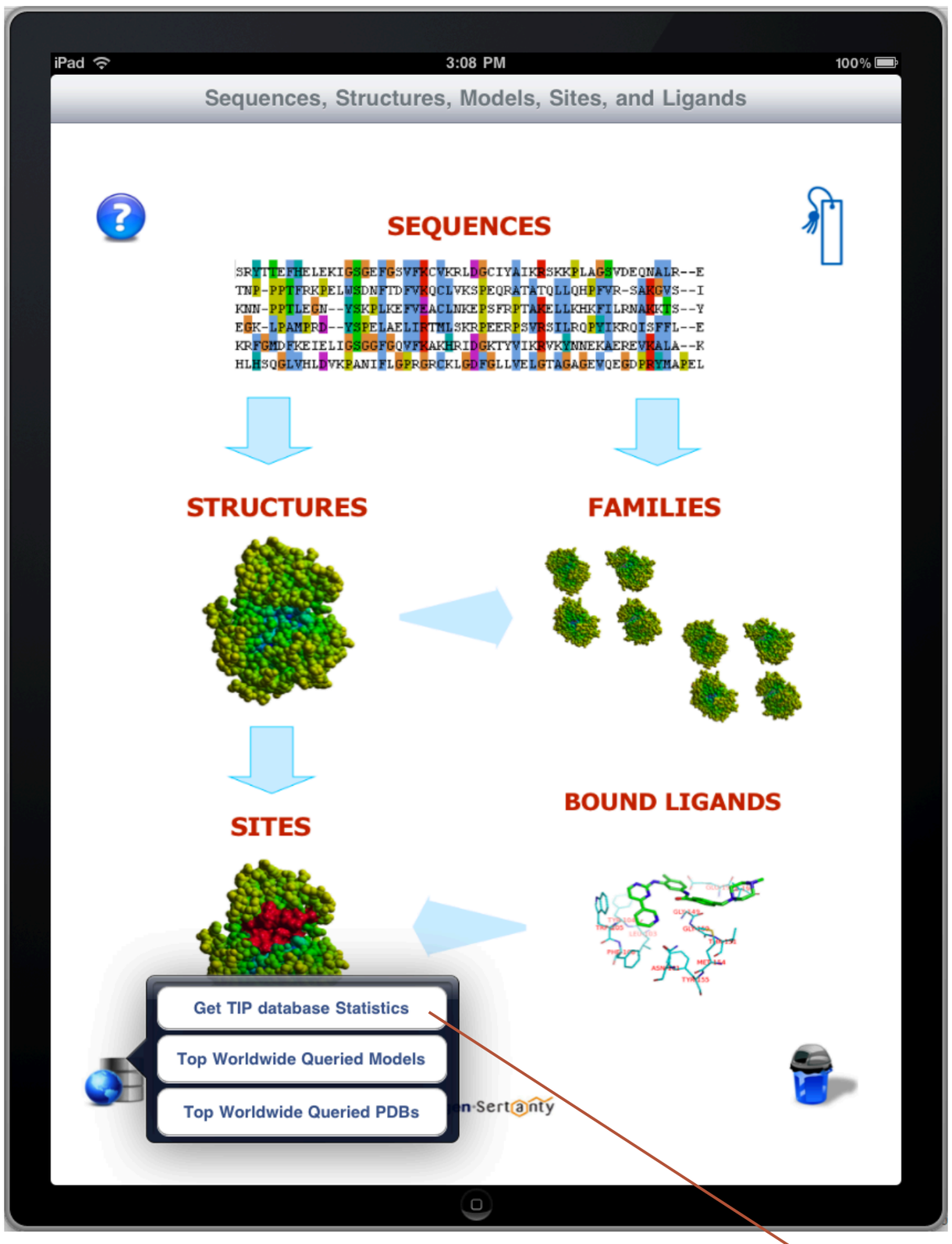
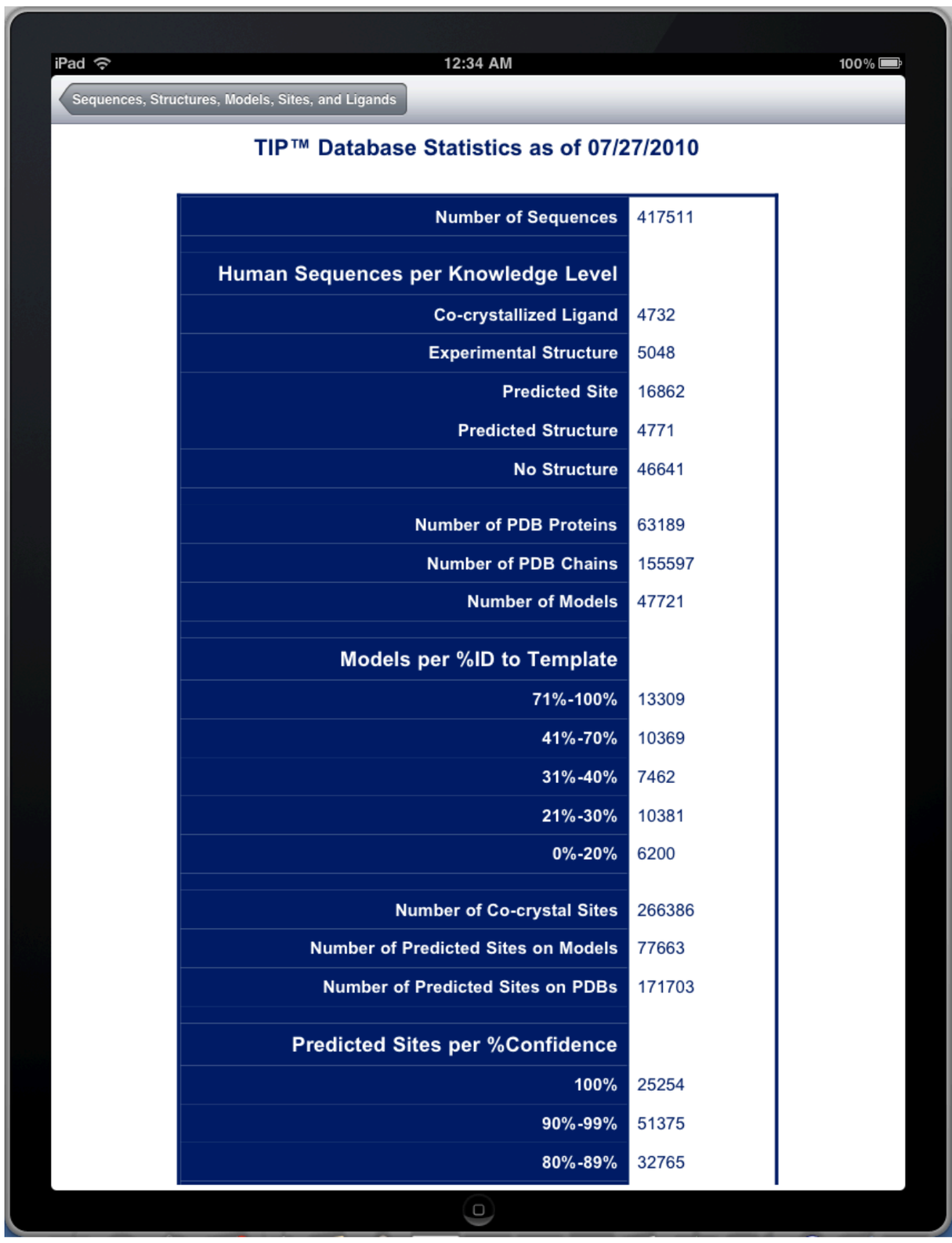
Database Statistics

The current TIP statistics can be retrieved from the mainpage, along with the top worldwide queried models and PDBs. These data will change weekly!





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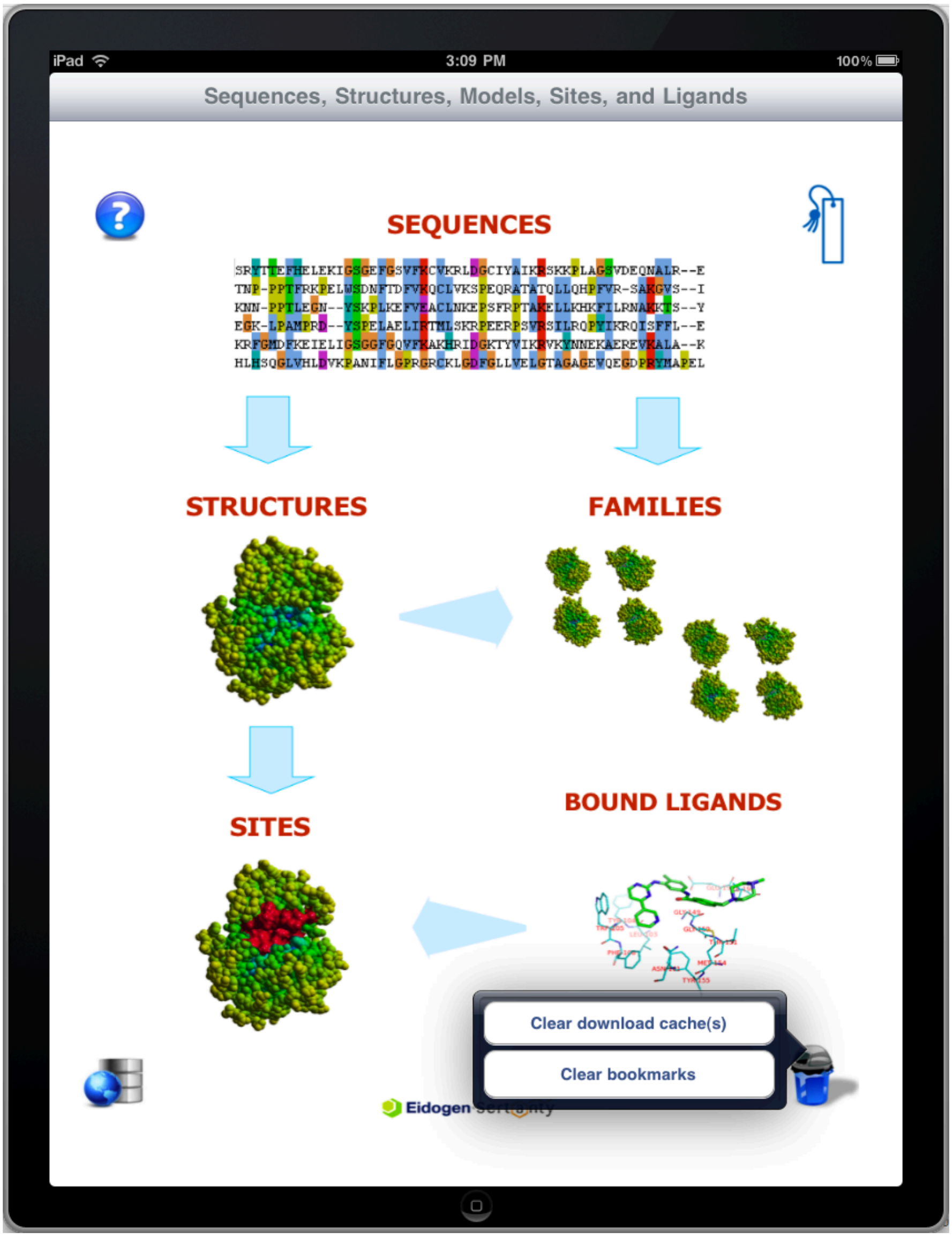
Clean-Up

All images, PDB structures, Models, Sites, and historical results (i.e. bookmarks) can be cleared from your device by touching the garbage can in the lower right:



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