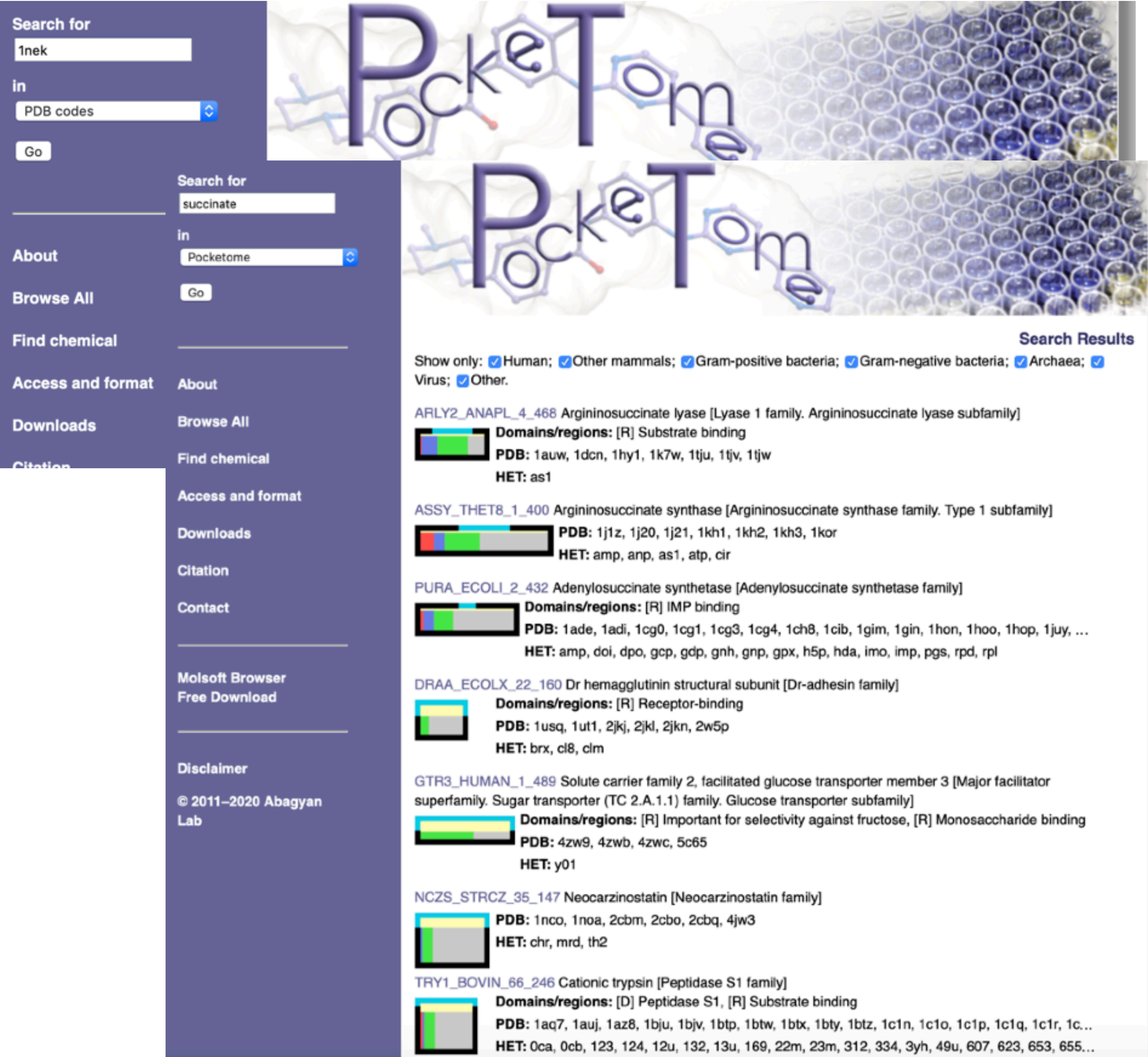


- Also take a look at “Structural information”
- There is no crystal structures and the homology models from Modbase are not high quality. The homology model could be a guide, but I would not base an SBDD campaign against a *T. brucei* homology model.

Structural information									
Modbase 3D models:									
There are 3 models calculated for this protein. More info on these models, including the models themselves is available at: Modbase									
Target Beg	Target End	Template	Template Beg	Template End	Identity	Evalue	Model Score	MPQS	zDope
32	156	1zoy (B)	16	151	46.00	0	1	0.950829	0.33
32	156	4ysx (B)	40	175	46.00	0	0.99	0.956829	0.26
168	229	5i9f (A)	348	409	23.00	0.53	0.98	0.708498	-1.37
+ Help me make sense of these data.									
Target Beg: first modeled residue Target End: last modeled residue Template: template structure used for modelling (PDB accession and chain) Template Beg: first template residue in target-template alignment Template End: last template residue in target-template alignment Identity: sequence identity Evalue: E value for target-template hit Model Score: GA341 score (>0.7 for reliable model) MPQS: ModPipe Quality Score (>1.1 for reliable model)									

- The structure we have used as a basis for modeling studies has been 1NEK. I tried this in the PockeTome (<http://ablab.ucsd.edu/POCKETOME/>). There was no record for it.
- Try a search for “succinate”. Did you find SDH?



The screenshot displays the PockeTome web application interface. On the left, there is a navigation menu with links: About, Browse All, Find chemical, Access and format, Downloads, and Citation. The main search area has two input fields: 'Search for' (containing '1nek') and 'in' (set to 'PDB codes'). A 'Go' button is present. Below this, a second search area shows 'Search for' (containing 'succinate') and 'in' (set to 'Pocketome'), also with a 'Go' button.

The right side of the interface shows 'Search Results' for 'succinate'. It includes a filter section with checkboxes for 'Human', 'Other mammals', 'Gram-positive bacteria', 'Gram-negative bacteria', 'Archaea', 'Virus', and 'Other'. The results list several proteins with their domain regions, PDB codes, and HET codes:

- ARLY2_ANAPL_4_468** Argininosuccinate lyase [Lyase 1 family. Argininosuccinate lyase subfamily]
Domains/regions: [R] Substrate binding
PDB: 1auw, 1dcn, 1hy1, 1k7w, 1tju, 1tjv, 1tjw
HET: as1
- ASSY_THET8_1_400** Argininosuccinate synthase [Argininosuccinate synthase family. Type 1 subfamily]
PDB: 1j1z, 1j20, 1j21, 1kh1, 1kh2, 1kh3, 1kor
HET: amp, anp, as1, atp, cir
- PURA_ECOLI_2_432** Adenylosuccinate synthetase [Adenylosuccinate synthetase family]
Domains/regions: [R] IMP binding
PDB: 1ade, 1adi, 1cg0, 1cg1, 1cg3, 1cg4, 1ch8, 1cib, 1gim, 1gin, 1hon, 1hoo, 1hop, 1juy, ...
HET: amp, doi, dpo, gcp, gdp, gnh, gnp, gpx, h5p, hda, imo, imp, pgs, rpd, rpl
- DRAA_ECOLX_22_160** Dr hemagglutinin structural subunit [Dr-adhesin family]
Domains/regions: [R] Receptor-binding
PDB: 1usq, 1ut1, 2jkl, 2jkn, 2w5p
HET: brx, cl8, clm
- GTR3_HUMAN_1_489** Solute carrier family 2, facilitated glucose transporter member 3 [Major facilitator superfamily. Sugar transporter (TC 2.A.1.1) family. Glucose transporter subfamily]
Domains/regions: [R] Important for selectivity against fructose, [R] Monosaccharide binding
PDB: 4zw9, 4zwb, 4zwc, 5c65
HET: y01
- NCZS_STRCZ_35_147** Neocarzinostatin [Neocarzinostatin family]
PDB: 1nco, 1noa, 2cbm, 2cbo, 2cbq, 4jw3
HET: chr, mrd, th2
- TRY1_BOVIN_66_246** Cationic trypsin [Peptidase S1 family]
Domains/regions: [D] Peptidase S1, [R] Substrate binding
PDB: 1aq7, 1auj, 1az8, 1bjv, 1btv, 1btw, 1btv, 1btv, 1btz, 1c1n, 1c1o, 1c1p, 1c1q, 1c1r, 1c...
HET: Oca, Ocb, 123, 124, 12u, 132, 13u, 169, 22m, 23m, 312, 334, 3yh, 49u, 607, 623, 653, 655...

At the bottom, there is a 'Molsoft Browser Free Download' link and a 'Disclaimer' section stating '© 2011–2020 Abagyan Lab'.