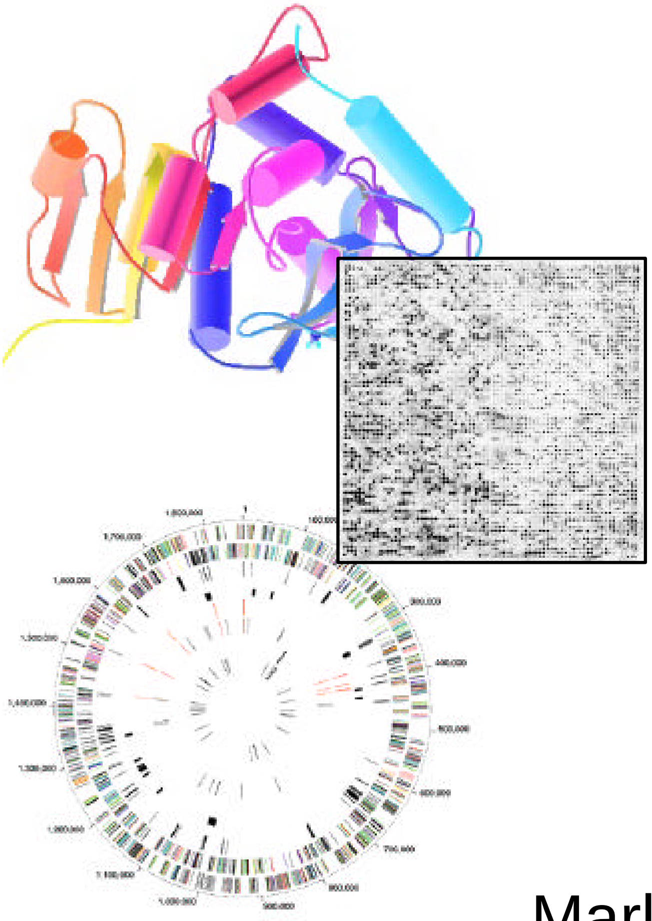
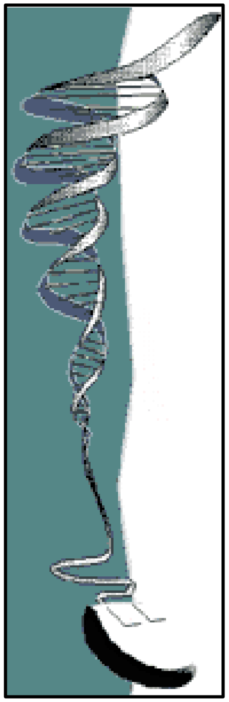
BIOINFORMATICS
Databases





Mark Gerstein, Yale University

bioinfo.mbb.yale.edu/mbb452a

Contents: Databases

- Structuring Information in Tables
- Keys and Joins
- Normalization
- Complex RDB encoding
- Indexes and Optimization
- Forms and Reports

Unstructured Data

This type of “membership” analysis has been performed previously in terms of the occurrence of sequence motifs, families, functions, and biochemical pathways. Starting from the most basic units, genomes have been compared in terms of the relative frequencies of short oligonucleotide and oligopeptide “words” (Blaisdell et al., 1996; Karlin & Burge, 1995; Karlin et al., 1992; Karlin et al., 1996). The degree of gene duplication in a number of genomes has been ascertained (Brenner et al., 1995; Koonin et al., 1996b; Riley & Labedan, 1997; Wolfe & Shields, 1997; Gerstein, 1997; Tamames et al., 1997). Other analyses have looked at how many highly conserved sequence families in one organism are present in another (Green et al., 1993; Koonin et al., 1995; Tatusov et al., 1997; Ouzounis et al., 1995a,b; Clayton et al., 1997). Finally, if sequences can be related to specific functions and pathways, one can see whether homologous sequences in two organisms truly have the same role (ortholog vs. paralog) and whether particular pathways are present or absent in different organisms (Karp et al., 1996a; Karp et al., 1996b; Koonin et al., 1996a; Mushegian & Koonin, 1996; Tatusov et al., 1996, 1997). This work has yielded many interesting conclusions in terms of pathways that are modified or absent in certain organisms. For instance, the essential citric acid cycle is found to be highly modified in H. influenzae (Fleischmann et al.,

Semi-Structured Data

```
REMARK   8 HET GROUP TRIVIAL NAME: FLAVIN ADENINE DINUCLEOTIDE (FAD)     1FNB  79
REMARK   8 CAS REGISTRY NUMBER: 146-14-5                                1FNB  80
REMARK   8 SEQUENCE NUMBER: 315                                         1FNB  81
REMARK   8 NUMBER OF ATOMS IN GROUP: 53                                 1FNB  82
REMARK   8                                                              1FNB  83
REMARK   8 HET GROUP TRIVIAL NAME: PHOSPHATE                            1FNB  84
REMARK   8 SEQUENCE NUMBER: 316                                         1FNB  85
REMARK   8 NUMBER OF ATOMS IN GROUP: 5                                  1FNB  86
REMARK   8                                                              1FNB  87
REMARK   8 HET GROUP TRIVIAL NAME: SULFATE                              1FNB  88
REMARK   8 SEQUENCE NUMBER: 317                                         1FNB  89
REMARK   8 NUMBER OF ATOMS IN GROUP: 5                                  1FNB  90
REMARK   8                                                              1FNB  91
REMARK   8 HET GROUP TRIVIAL NAME: K2 PT(CN)4                           1FNB  92
REMARK   8 CHARGE: 2- ( PT(CN)4 -- )                                    1FNB  93
REMARK   8 SEQUENCE NUMBER: PT1 - PT7                                   1FNB  94
REMARK   8 NUMBER OF ATOMS IN GROUP: 9                                  1FNB  95
REMARK   8 ADDITIONAL COMMENTS: BINDING SITES USED IN MIR PHASING       1FNB  96
REMARK   8                                                              1FNB  97
REMARK   8 HEAVY ATOM PARAMETERS ARE AS FOLLOWS:                        1FNB  98
REMARK   8  PT    PT     1      11.832  -8.309  27.027  0.68 33.00      1FNB  99
REMARK   8  PT    PT     2      13.996  -2.135  13.212  0.42 40.00      1FNB 100
REMARK   8  PT    PT     3      33.293  18.752  27.229  0.32 42.00      1FNB 101
REMARK   8  PT    PT     4      19.961 -15.348 -10.328  0.23 28.00      1FNB 102
REMARK   8  PT    PT     5       8.312  14.713  35.679  0.26 31.00      1FNB 103
REMARK   8  PT    PT     6      27.594  -7.790  23.540  0.14 35.00      1FNB 104
REMARK   8  PT    PT     7      15.917  -9.001  12.608  0.30 50.00      1FNB 105
REMARK   8                                                              1FNB 106
REMARK   8 HET GROUP TRIVIAL NAME: URANYL NITRATE (UO2--)               1FNB 107
REMARK   8 EMPIRICAL FORMULA: UO2 (NO3)2                                1FNB 108
REMARK   8 CHARGE: 2-                                                   1FNB 109
REMARK   8 SEQUENCE NUMBER: UR1 - UR13                                  1FNB 110
REMARK   8 NUMBER OF ATOMS IN GROUP: 3                                  1FNB 111
REMARK   8 ADDITIONAL COMMENTS: BINDING SITES USED IN MIR PHASING       1FNB 112
REMARK   8                                                              1FNB 113
REMARK   8 HEAVY ATOM PARAMETERS ARE AS FOLLOWS:                        1FNB 114
REMARK   8   U    UR     1       8.513  16.214  36.081  0.49 27.00      1FNB 115
```

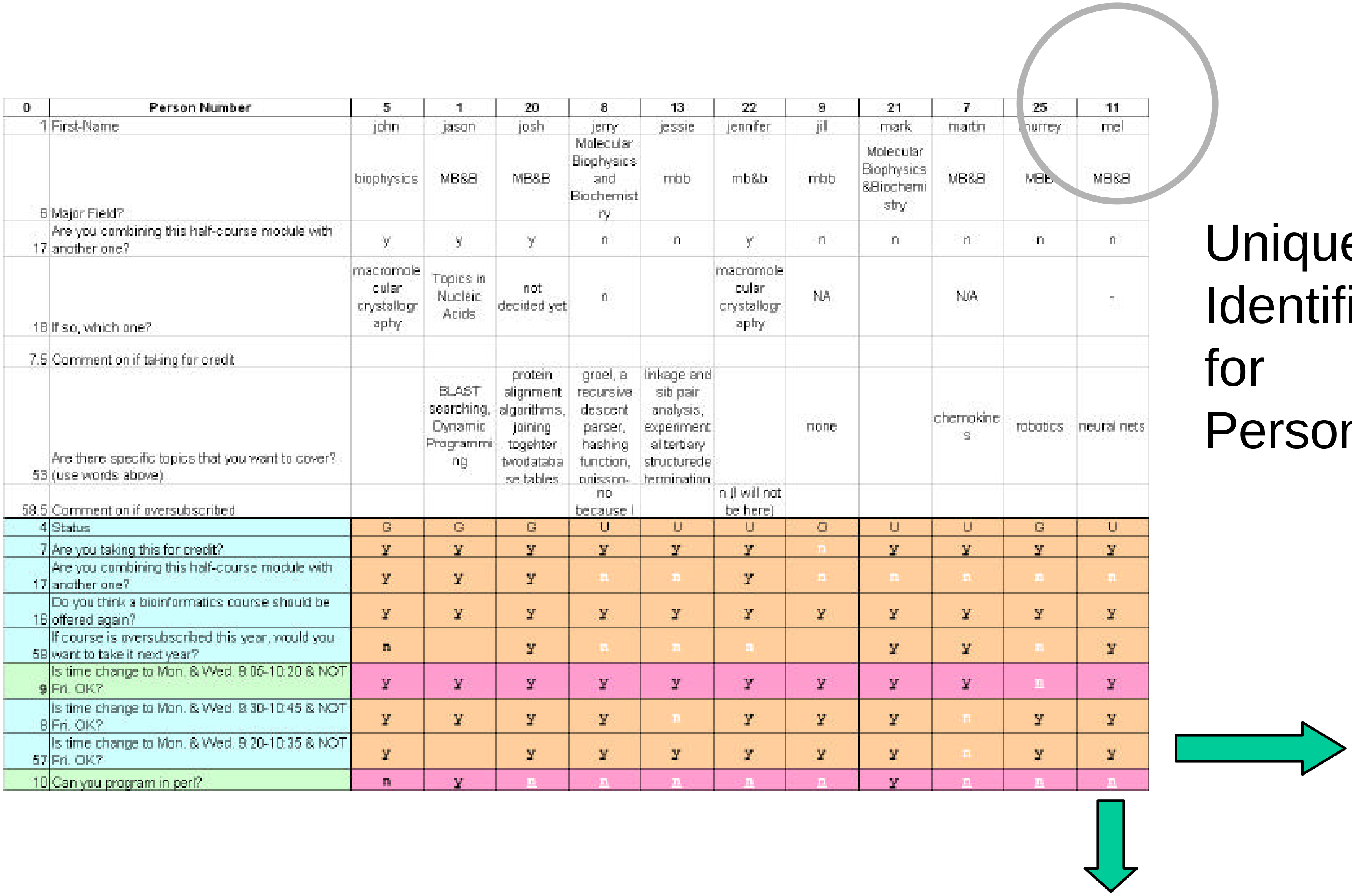
Structured Data

did_	fids
d2rs51_	1.002.007
d1imr__	1.010.002
d1pyib1	1.007.030
d1dxtd_	1.001.001
d181l__	1.004.002
d1vmoa_	1.002.044
d2gsq_1	1.001.031
d1etb2_	1.002.003
d1guha1	1.001.031
d1hrc__	1.001.003
d150lc_	1.004.002
d1dmf__	1.007.035
d1l19__	1.004.002
d1yrnc_	1.010.002
d1apld_	1.001.004
d1ndab2	1.003.004
d2rmai_	1.002.036

gid_	TrgStrt	TrgStop	did
HI0299	119	135	d193l__
HI0572	180	240	d1aba__
HI0989	56	125	d1aco_1
HI0988	106	458	d1aco_2
HI0154	2	76	d1acp__
HI1633	2	432	d1adea_
HI0349	1	183	d1aky__
HI1309	35	52	d1alo_3
HI0589	8	25	d1alo_3
HI1358	239	444	d1amg_2
HI1358	218	410	d1amy_2
HI0460	20	24	d1ans__
HI1386	139	147	d1ans__
HI0421	11	14	d1ans__
HI0361	285	295	d1ans__
HI0835	100	106	d1ans__

fid_	bestrep	N_minsp	N_scop	objname
1.001.001	d1flp__	8	340	Globin-like
1.001.002	d1hdj__	4	33	Long alpha-hairpin
1.001.003	d1ctj__	9	78	Cytochrome c
1.001.004	d1enh__	18	76	DNA-binding 3-helical bundle
1.001.005	d1dtr_2	1	3	Diphtheria toxin repressor (DtxR) dimeriz
1.001.006	d1tns__	1	2	Mu transposase, DNA-binding domain
1.001.007	d2spca_	1	2	Spectrin repeat unit
1.001.008	d1bdd__	1	4	Immunoglobulin-binding protein A modules
1.001.009	d1bal__	1	5	Peripheral subunit-binding domain of 2-ox
1.001.010	d2erl__	3	5	Protozoan pheromone proteins

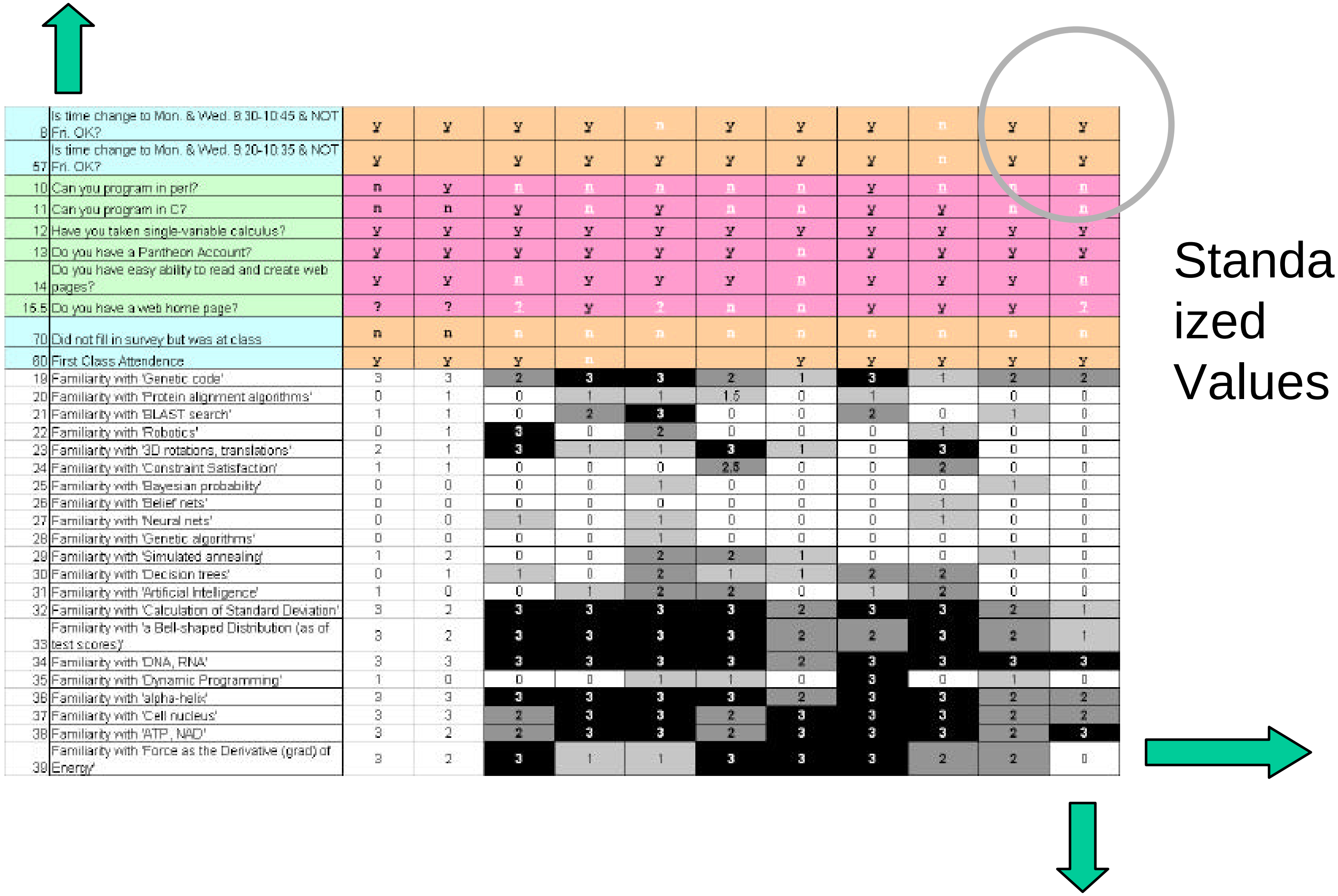
Turn the Survey into a Table (I)



0	Person Number	5	1	20	8	13	22	9	21	7	25	11
1	First-Name	john	jason	josh	jerry	jessie	jennifer	jill	mark	martin	murrey	mel
6	Major Field?	biophysics	MB&B	MB&B	Molecular Biophysics and Biochemistry	mbb	mb&b	mbb	Molecular Biophysics &Biochemistry	MB&B	MBB	MB&B
17	Are you combining this half-course module with another one?	y	y	y	n	n	y	n	n	n	n	n
18	If so, which one?	macromolecular crystallography	Topics in Nucleic Acids	not decided yet	n		macromolecular crystallography	NA		N/A		-
7.5	Comment on if taking for credit											
53	Are there specific topics that you want to cover? (use words above)		BLAST searching, Dynamic Programming	protein alignment algorithms, joining togehter twodatabase tables	groel, a recursive descent parser, hashing function, poisson-	linkage and sib pair analysis, experimental tertiary structuredetermination		none		chemokines	robotics	neural nets
58.5	Comment on if oversubscribed				no because I		n (I will not be here)					
4	Status	G	G	G	U	U	U	O	U	U	G	U
7	Are you taking this for credit?	y	y	y	y	y	y	n	y	y	y	y
17	Are you combining this half-course module with another one?	y	y	y	n	n	y	n	n	n	n	n
16	Do you think a bioinformatics course should be offered again?	y	y	y	y	y	y	y	y	y	y	y
58	If course is oversubscribed this year, would you want to take it next year?	n		y	n	n	n		y	y	n	y
9	Is time change to Mon. & Wed. 9:05-10:20 & NOT Fri. OK?	y	y	y	y	y	y	y	y	y	n	y
8	Is time change to Mon. & Wed. 8:30-10:45 & NOT Fri. OK?	y	y	y	y	n	y	y	y	n	y	y
57	Is time change to Mon. & Wed. 9:20-10:35 & NOT Fri. OK?	y		y	y	y	y	y	y	n	y	y
10	Can you program in perl?	n	y	n	n	n	n	n	y	n	n	n

Unique Identifier for Person?

Turn the Survey into a Table (II)

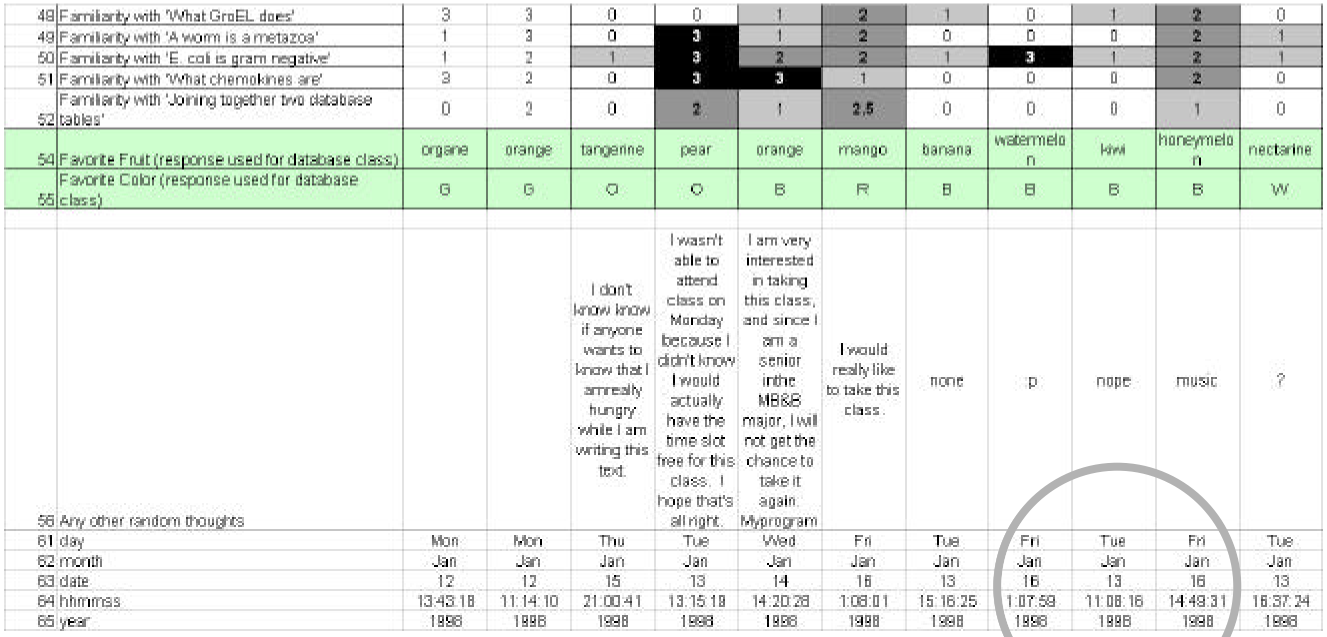


8	Is time change to Mon. & Wed. 8:30-10:45 & NOT Fri. OK?	y	y	y	y	n	y	y	y	n	y	y
57	Is time change to Mon. & Wed. 8:20-10:35 & NOT Fri. OK?	y		y	y	y	y	y	y	n	y	y
10	Can you program in perl?	n	y	n	n	n	n	n	y	n	n	n
11	Can you program in C?	n	n	y	n	y	n	n	y	y	n	n
12	Have you taken single-variable calculus?	y	y	y	y	y	y	y	y	y	y	y
13	Do you have a Pantheon Account?	y	y	y	y	y	y	n	y	y	y	y
14	Do you have easy ability to read and create web pages?	y	y	n	y	y	y	n	y	y	y	n
15.5	Do you have a web home page?	?	?	?	y	?	n	n	y	y	y	?
70	Did not fill in survey but was at class	n	n	n	n	n	n	n	n	n	n	n
80	First Class Attendence	y	y	y	n			y	y	y	y	y
19	Familiarity with 'Genetic code'	3	3	2	3	3	2	1	3	1	2	2
20	Familiarity with 'Protein alignment algorithms'	0	1	0	1	1	1.5	0	1		0	0
21	Familiarity with 'BLAST search'	1	1	0	2	3	0	0	2	0	1	0
22	Familiarity with 'Robotics'	0	1	3	0	2	0	0	0	1	0	0
23	Familiarity with '3D rotations, translations'	2	1	3	1	1	3	1	0	3	0	0
24	Familiarity with 'Constraint Satisfaction'	1	1	0	0	0	2.5	0	0	2	0	0
25	Familiarity with 'Bayesian probability'	0	0	0	0	1	0	0	0	0	1	0
26	Familiarity with 'Belief nets'	0	0	0	0	0	0	0	0	1	0	0
27	Familiarity with 'Neural nets'	0	0	1	0	1	0	0	0	1	0	0
28	Familiarity with 'Genetic algorithms'	0	0	0	0	1	0	0	0	0	0	0
29	Familiarity with 'Simulated annealing'	1	2	0	0	2	2	1	0	0	1	0
30	Familiarity with 'Decision trees'	0	1	1	0	2	1	1	2	2	0	0
31	Familiarity with 'Artificial Intelligence'	1	0	0	1	2	2	0	1	2	0	0
32	Familiarity with 'Calculation of Standard Deviation'	3	2	3	3	3	3	2	3	3	2	1
33	Familiarity with 'a Bell-shaped Distribution (as of test scores)'	3	2	3	3	3	3	2	2	3	2	1
34	Familiarity with 'DNA, RNA'	3	3	3	3	3	3	2	3	3	3	3
35	Familiarity with 'Dynamic Programming'	1	0	0	0	1	1	0	3	0	1	0
36	Familiarity with 'alpha-helix'	3	3	3	3	3	3	2	3	3	2	2
37	Familiarity with 'Cell nucleus'	3	3	2	3	3	2	3	3	3	2	2
38	Familiarity with 'ATP, NAD'	3	2	2	3	3	2	3	3	3	2	3
39	Familiarity with 'Force as the Derivative (grad) of Energy'	3	2	3	1	1	3	3	3	2	2	0

Standard-ized Values

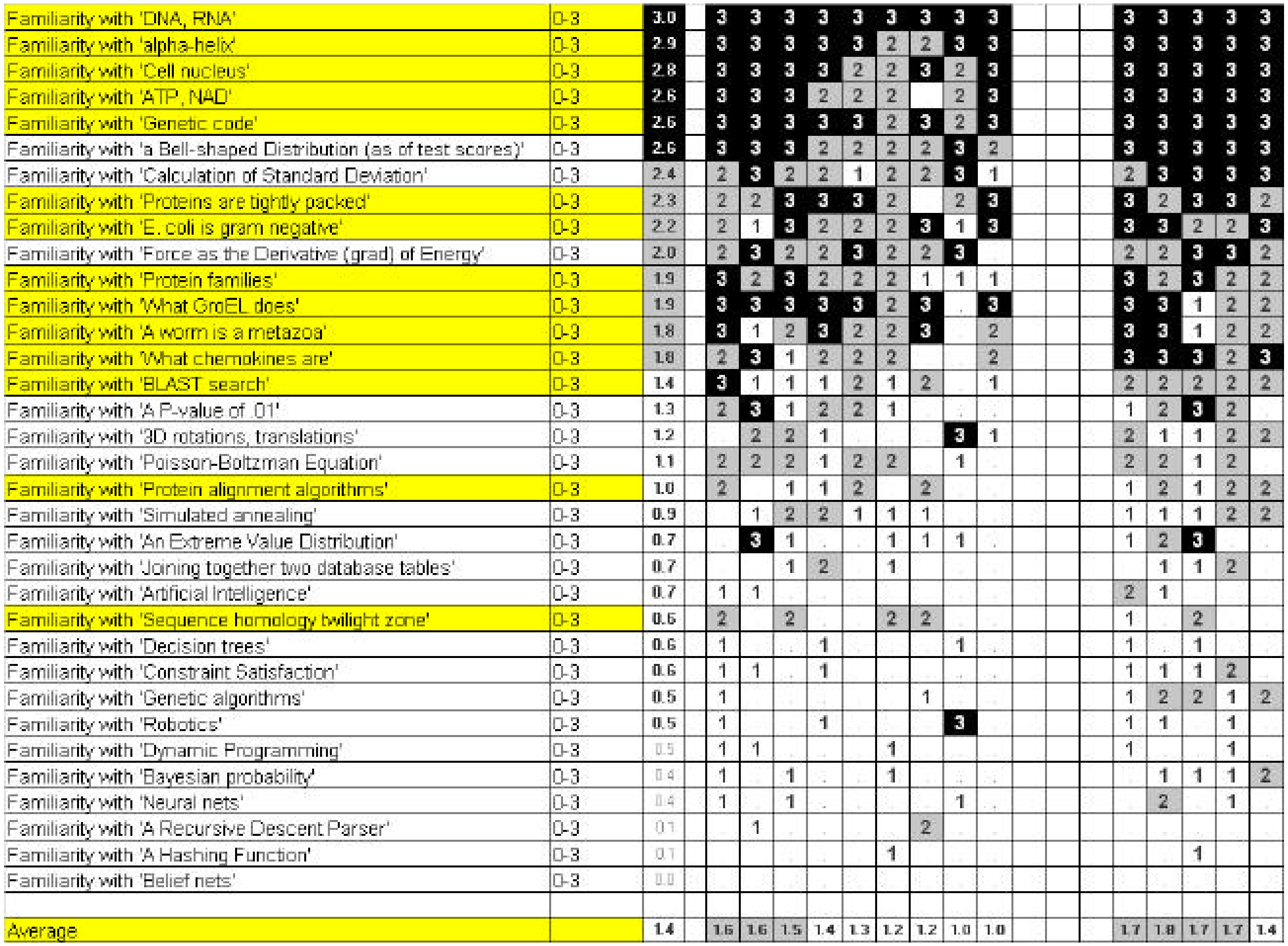
Turn the Survey into a Table (III)

- Dependencies between Values (dates)
- Unstructured Text



48	Familiarity with 'What GroEL does'	3	3	0	0	1	2	1	0	1	2	0
49	Familiarity with 'A worm is a metazoa'	1	3	0	3	1	2	0	0	0	2	1
50	Familiarity with 'E. coli is gram negative'	1	2	1	3	2	2	1	3	1	2	1
51	Familiarity with 'What chemokines are'	3	2	0	3	3	1	0	0	0	2	0
52	Familiarity with 'Joining together two database tables'	0	2	0	2	1	2.5	0	0	0	1	0
54	Favorite Fruit (response used for database class)	organe	orange	tangerine	pear	orange	mango	banana	watermelon	kiwi	honeymelon	nectarine
55	Favorite Color (response used for database class)	G	G	O	O	B	R	B	B	B	B	W
56	Any other random thoughts			I don't know know if anyone wants to know that I amreally hungry while I am writing this text.	I wasn't able to attend class on Monday because I didn't know I would actually have the time slot free for this class. I hope that's all right.	I am very interested in taking this class, and since I am a senior inthe MB&B major, I will not get the chance to take it again. Myprogram	I would really like to take this class.	none	:p	nope	music	?
61	day	Mon	Mon	Thu	Tue	Wed	Fri	Tue	Fri	Tue	Fri	Tue
62	month	Jan	Jan	Jan	Jan	Jan	Jan	Jan	Jan	Jan	Jan	Jan
63	date	12	12	15	13	14	16	13	16	13	16	13
64	hhmmss	13:43:18	11:14:10	21:00:41	13:15:18	14:20:28	1:08:01	15:16:25	1:07:59	11:08:16	14:49:31	16:37:24
65	year	1998	1998	1998	1998	1998	1998	1998	1998	1998	1998	1998

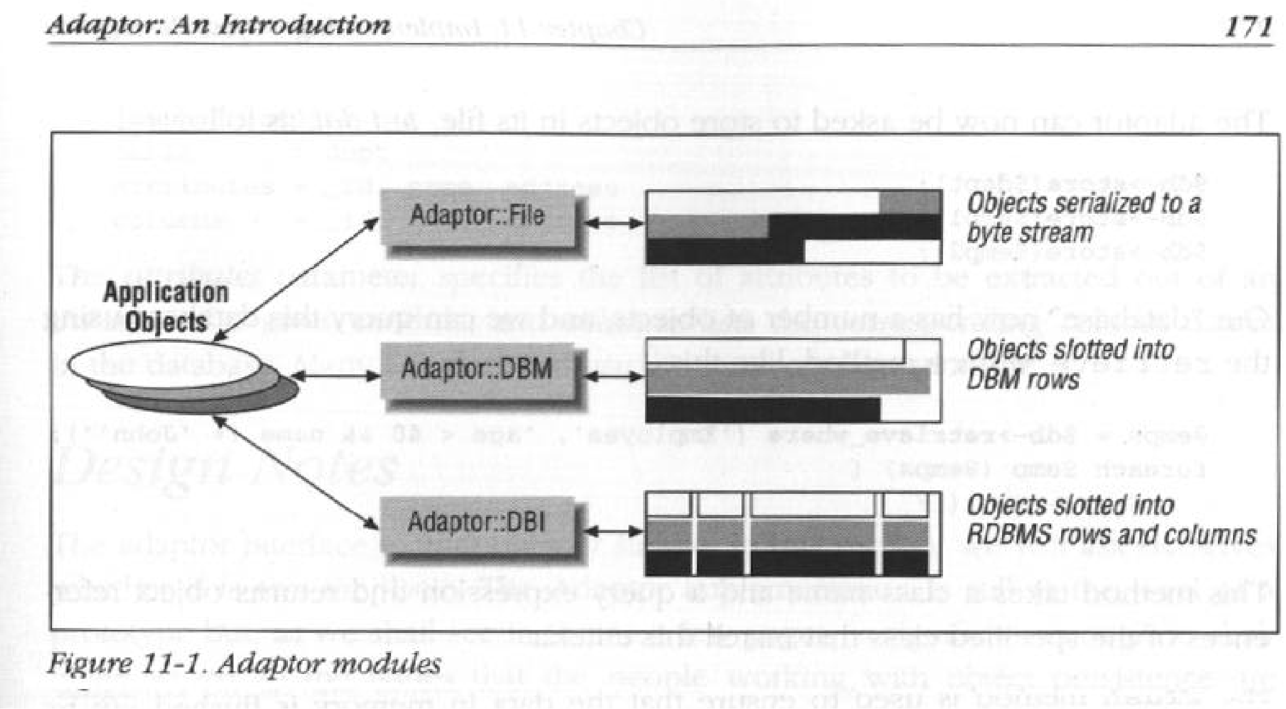
Statistics are only Possible on Standarized Values



Familiarity with 'DNA, RNA'	0-3	3.0		3	3	3	3	3	3	3	3	3				3	3	3	3	3
Familiarity with 'alpha-helix'	0-3	2.9		3	3	3	3	3	2	2	3	3				3	3	3	3	3
Familiarity with 'Cell nucleus'	0-3	2.8		3	3	3	3	2	2	3	2	3				3	3	3	3	3
Familiarity with 'ATP, NAD'	0-3	2.6		3	3	3	2	2	2		2	3				3	3	3	3	3
Familiarity with 'Genetic code'	0-3	2.6		3	3	3	3	3	2	3	2	3				3	3	3	3	3
Familiarity with 'a Bell-shaped Distribution (as of test scores)'	0-3	2.6		3	3	3	2	2	2	2	3	2				3	3	3	3	3
Familiarity with 'Calculation of Standard Deviation'	0-3	2.4		2	3	2	2	1	2	2	3	1				2	3	3	3	3
Familiarity with 'Proteins are tightly packed'	0-3	2.3		2	2	3	3	3	2		2	3				3	2	3	3	2
Familiarity with 'E. coli is gram negative'	0-3	2.2		2	1	3	2	2	2	3	1	3				3	3	2	2	3
Familiarity with 'Force as the Derivative (grad) of Energy'	0-3	2.0		2	3	2	2	3	2	2	3					2	2	3	3	2
Familiarity with 'Protein families'	0-3	1.9		3	2	3	2	2	2	1	1	1				3	2	3	2	2
Familiarity with 'What GroEL does'	0-3	1.9		3	3	3	3	3	2	3		3				3	3	1	2	2
Familiarity with 'A worm is a metazoa'	0-3	1.8		3	1	2	3	2	2	3		2				3	3	1	2	2
Familiarity with 'What chemokines are'	0-3	1.8		2	3	1	2	2	2			2				3	3	3	2	3
Familiarity with 'BLAST search'	0-3	1.4		3	1	1	1	2	1	2		1				2	2	2	2	2
Familiarity with 'A P-value of .01'	0-3	1.3		2	3	1	2	2	1							1	2	3	2	
Familiarity with '3D rotations, translations'	0-3	1.2			2	2	1				3	1				2	1	1	2	2
Familiarity with 'Poisson-Boltzman Equation'	0-3	1.1		2	2	2	1	2	2		1					2	2	1	2	
Familiarity with 'Protein alignment algorithms'	0-3	1.0		2		1	1	2		2						1	2	1	2	2
Familiarity with 'Simulated annealing'	0-3	0.9			1	2	2	1	1	1						1	1	1	2	2
Familiarity with 'An Extreme Value Distribution'	0-3	0.7			3	1			1	1	1					1	2	3		
Familiarity with 'Joining together two database tables'	0-3	0.7				1	2		1								1	1	2	
Familiarity with 'Artificial Intelligence'	0-3	0.7		1	1											2	1			
Familiarity with 'Sequence homology twilight zone'	0-3	0.6		2		2			2	2						1		2		
Familiarity with 'Decision trees'	0-3	0.6		1			1				1					1		1		
Familiarity with 'Constraint Satisfaction'	0-3	0.6		1	1		1									1	1	1	2	
Familiarity with 'Genetic algorithms'	0-3	0.5		1						1						1	2	2	1	2
Familiarity with 'Robotics'	0-3	0.5		1			1				3					1	1		1	
Familiarity with 'Dynamic Programming'	0-3	0.5		1	1				1							1			1	
Familiarity with 'Bayesian probability'	0-3	0.4		1		1			1								1	1	1	2
Familiarity with 'Neural nets'	0-3	0.4		1		1					1						2		1	
Familiarity with 'A Recursive Descent Parser'	0-3	0.1			1					2										
Familiarity with 'A Hashing Function'	0-3	0.1							1									1		
Familiarity with 'Belief nets'	0-3	0.0																		
Average		1.4		1.6	1.6	1.5	1.4	1.3	1.2	1.2	1.0	1.0				1.7	1.8	1.7	1.7	1.4

Relational Databases

- Databases make program data **persistent**
- RDB’s turn formless data in a number of structured tables
  - ◊ Ways of joining together tables to give various views of the data



Adaptor: An Introduction **171**

Adaptor::File
Objects serialized to a byte stream
Application Objects
Adaptor::DBM
Objects slotted into DBM rows
Adaptor::DBI
Objects slotted into RDBMS rows and columns

Figure 11-1. Adaptor modules

SQL

- SIMPLE Language for Building and Querying Tables
- CREATE a table
- INSERT values into it
- SELECT various entries from it (tuples, rows)
- UPDATE the values

- Example: How Many Globin Folds
  are there in E. coli versus Yeast?

matches table

gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0988	106	458	d1aco_2	4.4e-14
HI0154	2	76	d1acp__	1.2e-23
HI1633	2	432	d1adea_	0
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	**239**	**444**	**d1amg_2**	**0.002**
HI1358	**218**	**410**	**d1amy_2**	**0.00037**
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	11	14	d1ans__	6.4
HI0361	285	295	d1ans__	8.2
HI0835	100	106	d1ans__	9.7

```
create table
matches(
  gid char255,
      # Genome_ID
 TrgStrt int,
      # Start of
      # Match in Gene
  TrgStop int,
      # End of Match
      # in Gene
  did char255,
      # ID Matching
      # Structure
  score real
      # e-value
      # of Match
)
```

matches table 2

gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0988	106	458	d1aco_2	4.4e-14
HI0154	2	76	d1acp__	1.2e-23
HI1633	2	432	d1adea_	0
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	239	444	d1amg_2	0.002
HI1358	218	410	d1amy_2	0.00037
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	11	14	d1ans__	6.4
HI0361	285	295	d1ans__	8.2
HI0835	100	106	d1ans__	9.7

```
insert into
matches
(gid, TrgStrt,
  TrgStop, did,
  score)
values
(HI0299, 119,
 135, d193l__,
 3.1)
```

structures table

did_	fid
d2rs51_	1.002.007
d1imr__	**1.010.002**
d1pyib1	1.007.030
d1dxtd_	1.001.001
d181l__	**1.004.002**
d1vmoa_	1.002.044
d2gsq_1	1.001.031
d1etb2_	1.002.003
d1guha1	1.001.031
d1hrc__	1.001.003
d150lc_	**1.004.002**
d1dmf__	1.007.035
d1l19__	1.004.002
d1yrnc_	**1.010.002**
d1apld_	1.001.004
d1ndab2	1.003.004
d2rmai_	1.002.036

```
create table
structures(
  did char255,
      # ID Matching
      # Structure
  fid char255,
      # ID of fold that
      # structure has
)
```

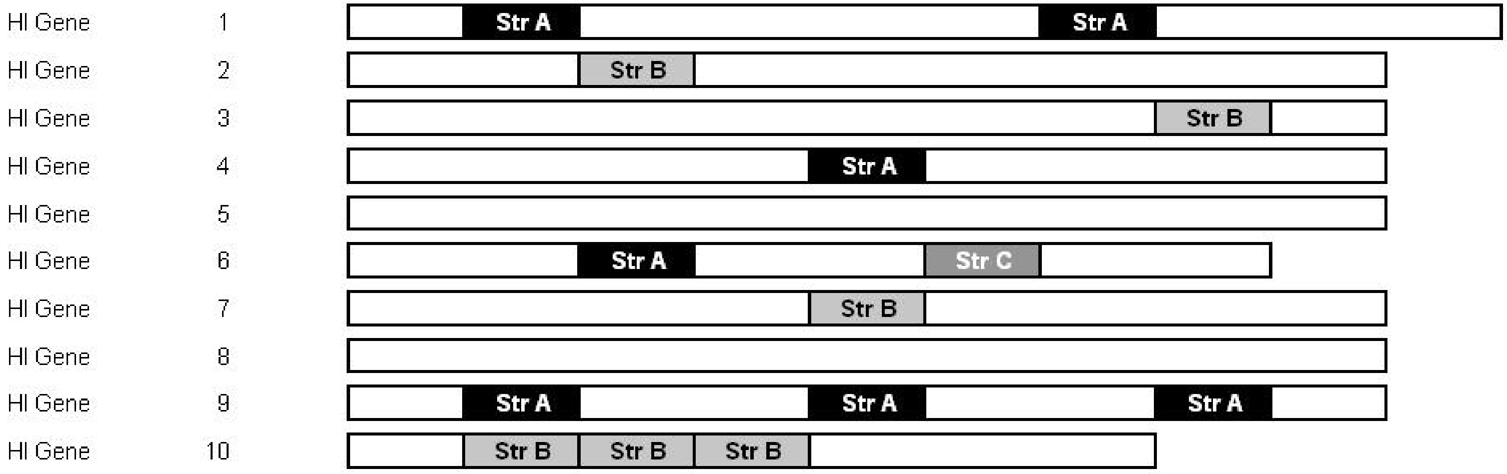
10 K domain structure IDs (did) vs. 300 fold IDs (fid)

folds table

```
create table
folds(
 fid char255,
    # fold ID
 bestrep char255,
 N_hlx  int,
 N_beta int,
    # number of helices & sheets
 name char255
    # name of fold
)
```

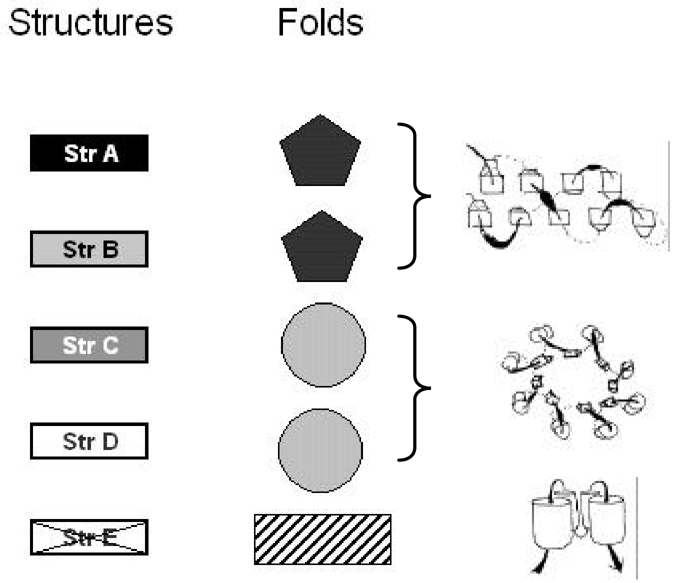
```
fid_            bestrep N_hlx  N_beta  name
1.001.001       d1flp__ 8       0       Globin-like
1.001.002       d1hdj__ 4       0       Long alpha-hairpin
1.001.003       d1ctj__ 9       0       Cytochrome c
1.001.004       d1enh__ 2       0       DNA-binding 3-helical bundle
1.001.005       d1dtr_2 1       3       Diphtheria toxin repressor (DtxR) dimeriz
1.001.006       d1tns__ 1       2       Mu transposase, DNA-binding domain
1.001.007       d2spca_ 0       2       Spectrin repeat unit
1.001.008       d1bdd__ 0       4       Immunoglobulin-binding protein A modules
1.001.009       d1bal__ 0       5       Peripheral subunit-binding domain of 2-ox
1.001.010       d2erl__ 3       5       Protozoan pheromone proteins
```

Table Interpretation



Match Table: Ways Structures A, B, and C can match HI Genome

Structures have a limited number of folds, which have various characteristics



Structure of a Table

- Row
  - Entity, Tuple, Instance
- Column
  - Field
  - Attribute of an Entity
  - dimension
- Key
  - Certain Attributes (or combination of attributes) can uniquely identify an object, these are keys
- NULL
  - Variant Records

	key	**key**				
Table	**attr-a**	**attr-b**	**attr-c**	**attr-d**	**attr-e**	**attr-f**
tuple-1	**a1**	**b1**	c1	d1	e1	f1
tuple-2	**a2**	**b2**	c2	d2	e2	f2
tuple-3	**a3**	**b3**	c3	d3	e3	f3
tuple-4	**a4**	**b4**	c4	d4	e4	f4
tuple-5	**a5**	**b5**	c5	d5	e5	f5
tuple-6	**a6**	**b6**	c6	d6		
tuple-7	**a7**	**b7**	c7	d7		f7
tuple-8	**a8**	**b8**	c8	d8	e8	f8
tuple-9	**a9**	**b9**	c9	d9	e9	f9
tuple-10	**a10**	**b10**	c10	d10		f10
tuple-11	**a11**	**b11**	c11	d11	e11	f11
tuple-12	**a12**	**b12**	c12	d12	e12	f12
tuple-13	**a13**	**b13**	c13	d13	e13	f13
tuple-14	**a14**	**b14**	c14	d14	e14	f14

What is a Key?

```
table matches(gid, TrgStrt, TrgStop, did, score)
table structures(did, fid)
table folds(fid, bestrep, N_hlx, N_beta, name)
```

gid -> many matches

gid,TrgStrt -> unique match (one tuple)

thus, primary key gid,TrgStrt

gid,TrgStop -> unique match as well

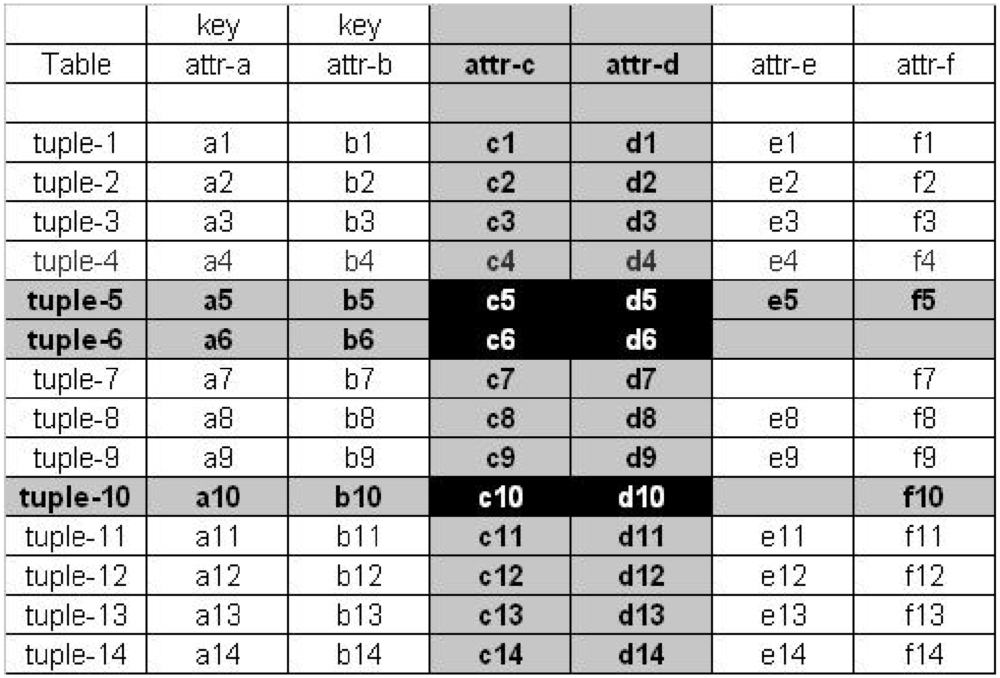
fid -> many did's, but did -> one fid

thus, primary key did

one-to-one between fid and name

1<->1
1->many
many->1

SQL Select on a Single Table



	key	key				
Table	attr-a	attr-b	**attr-c**	**attr-d**	attr-e	attr-f
tuple-1	a1	b1	**c1**	**d1**	e1	f1
tuple-2	a2	b2	**c2**	**d2**	e2	f2
tuple-3	a3	b3	**c3**	**d3**	e3	f3
tuple-4	a4	b4	**c4**	**d4**	e4	f4
tuple-5	**a5**	**b5**	**c5**	**d5**	**e5**	**f5**
tuple-6	**a6**	**b6**	**c6**	**d6**		
tuple-7	a7	b7	**c7**	**d7**		f7
tuple-8	a8	b8	**c8**	**d8**	e8	f8
tuple-9	a9	b9	**c9**	**d9**	e9	f9
tuple-10	**a10**	**b10**	**c10**	**d10**		**f10**
tuple-11	a11	b11	**c11**	**d11**	e11	f11
tuple-12	a12	b12	**c12**	**d12**	e12	f12
tuple-13	a13	b13	**c13**	**d13**	e13	f13
tuple-14	a14	b14	**c14**	**d14**	e14	f14

- Select {columns} from {a table} where {row-selection is true}
- projection of a selection
- Sort result on a attribute

SQL Select on a Single Table, Example

gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	239	444	d1amg_2	0.002
HI0016	1	173	d1dar_2	2e-07
HI0016	179	274	d1dar_1	8.5e-06
HI0016	399	476	d1dar_4	0.00031
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	11	14	d1ans__	6.4
HI0361	285	295	d1ans__	8.2
HI0835	100	106	d1ans__	9.7

- Select * from matches where gid= HI0016

```
HI0016  1       173     d1dar_2    2e-07
HI0016  179     274     d1dar_1   8.5e-06
HI0016  399     476     d1dar_4   0.00031
```

- Select * from matches where gid= HI0016 and TrgStrt=179

```
HI0016  179     274     d1dar_1   8.5e-06
```

SQL Select on a Single Table, Example 2

```
gid_    TrgStrt TrgStop did        score
HI0299  119     135     d193l__      3.1
HI0572  180     240     d1aba__   0.0032
HI0989  56      125     d1aco_1   0.0049
HI0349  1       183     d1aky__   7.6e-36
HI1309  35      52      d1alo_3      1.1
HI0589  8       25      d1alo_3      1.8
HI1358  239     444     d1amg_2    0.002
HI0016  1       173     d1dar_2   2e-07
HI0016  179     274     d1dar_1  8.5e-06
HI0016  399     476     d1dar_4  0.00031
HI0460  20      24      d1ans__      1.8
HI1386  139     147     d1ans__      3.3
HI0421  11      14      d1ans__      6.4
HI0361  285     295     d1ans__      8.2
HI0835  100     106     d1ans__      9.7
```

- Select did from matches where score < 0.0001

d1aky__, d1dar_2, d1dar_1

```
HI0349  1       183     d1aky__    7.6e-36
I0016  1       173      d1dar_2    2e-07
HI0016  179     274     d1dar_1   8.5e-06
```

Joins

Foreign Key

Matches

gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0988	106	458	d1aco_2	4.4e-14
HI0154	2	76	d1acp__	1.2e-23
HI1633	2	432	d1adea_	0
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	239	444	d1amg_2	0.002
HI1358	218	410	d1amy_2	0.00037
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	**11**	**14**	**d1ans__**	**6.4**
HI0361	**285**	**295**	**d1ans__**	**8.2**
HI0835	**100**	**106**	**d1ans__**	**9.7**

Structures

did_	fid
d2rs51_	1.002.007
d1imr__	1.010.002
d1pyib1	1.007.030
d1dxtd_	1.001.001
d181l__	1.004.002
d1vmoa_	1.002.044
d2gsq_1	1.001.031
d1etb2_	1.002.003
d1guha1	1.001.031
d1hrc__	1.001.003
d150lc_	1.004.002
d1dmf__	1.007.035
d1l19__	1.004.002
d1yrnc_	1.010.002
d1ans__	**1.007.008**
d2rmai_	1.002.036

Folds

fid_	bestrep	N_hlx	N_beta	name
1.001.001	d1flp__	8	0	Globin-like
1.001.002	d1hdj__	4	0	Long alpha-hairpin
1.001.003	d1ctj__	9	0	Cytochrome c
1.001.004	d1enh__	2	0	DNA-binding 3-helical bundle
1.001.005	d1dtr_2	1	3	Diphtheria toxin repressor (DtxR) dimeriz
1.001.006	d1tns__	1	2	Mu transposase, DNA-binding domain
1.001.007	d2spca_	0	2	Spectrin repeat unit
1.001.008	d1bdd__	0	4	Immunoglobulin-binding protein A modules
1.007.008	**d1qkt__**	**4**	**3**	**Neurotoxin III (ATX III)**
1.001.010	d2erl__	3	5	Protozoan pheromone proteins

SQL Select on Multiple Tables

- Select *
  from matches, structures, folds
  where
  matches.gid = HI0361
  and matches.did=structures.did
  and structures.fid = folds.fid
- Returns

```
matches |  structures | folds
HI0361,285,295,d1ans__ ,8.2  | d1ans__,1.007.008 | 1.007.008,d1qkt__,4, 3,Neurotoxin III ...
```

- Select score,name from matches, structures, folds
  where gid = HI0361and matches.did=structures.did
  and structures.fid = folds.fid

```
8.2, Neurotoxin III ...
```

Foreign Key

matches

gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0988	106	458	d1aco_2	4.4e-14
HI0154	2	76	d1acp__	1.2e-23
HI1633	2	432	d1adea_	0
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	239	444	d1amg_2	0.002
HI1358	218	410	d1amy_2	0.00037
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	**11**	**14**	**d1ans__**	**6.4**
HI0361	**285**	**295**	**d1ans__**	**8.2**
HI0835	**100**	**106**	**d1ans__**	**9.7**

structures

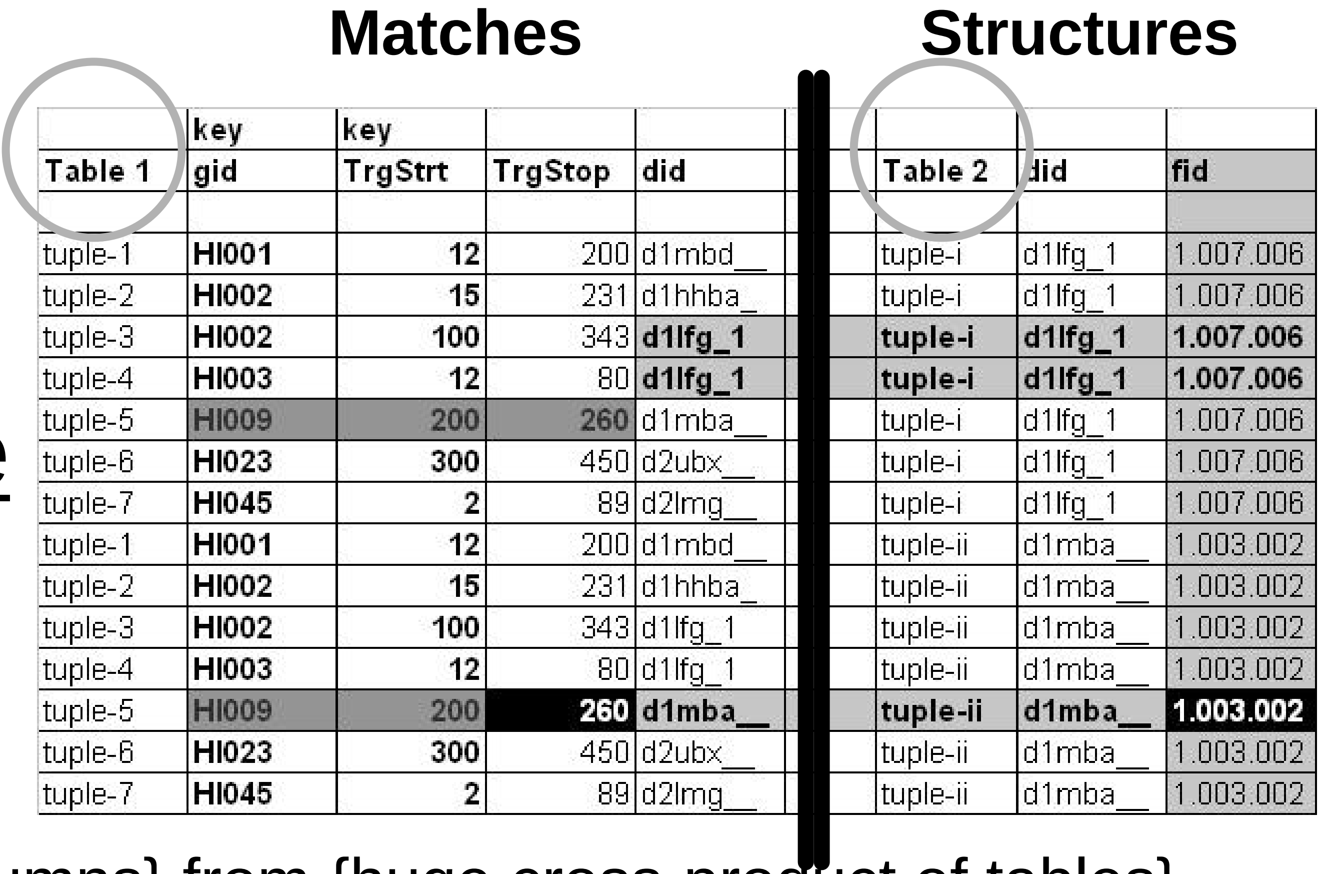
did_	fid
d2rs51_	1.002.007
d1imr__	1.010.002
d1pyib1	1.007.030
d1dxtd_	1.001.001
d181l__	1.004.002
d1vmoa_	1.002.044
d2gsq_1	1.001.031
d1etb2_	1.002.003
d1guha1	1.001.031
d1hrc__	1.001.003
d150lc_	1.004.002
d1dmf__	1.007.035
d1l19__	1.004.002
d1yrnc_	1.010.002
d1ans__	**1.007.008**
d2rmai_	1.002.036

matches.did is a (foreign) key in the structures table -- i.e. looks up exactly one structure.

Selection as Array Lookup

- Same for a fold identifier from a structure id
  - ◊ $fid=$structure{$did}
  - ◊ (perl pseudo-code)
- Same for matches and folds tables, but this time arrays return multiple values and have multiple field keys
  - ◊ ($bestrep, $N_hlx, $N_beta, $name) = $folds{$fid}
  - ◊ ($TrgStop,$did,$score)=$match{$gid,$TrgStrt}
- Joining as a double-lookup
  - ◊ $did = 1mbd__
    ($bestrep, $N_hlx, $N_beta, $name) = $folds{ $structures{$did} }
  - ◊ Select bestrep,N_hlx,N_beta,name from structures, folds where structures.fid = folds.fid and structures.did = 1mbd__

SQL Select on Multiple Tables



Matches **Structures**

	key	key						
Table 1	gid	TrgStrt	TrgStop	did		Table 2	did	fid
tuple-1	HI001	12	200	d1mbd__		tuple-i	d1lfg_1	1.007.006
tuple-2	HI002	15	231	d1hhba_		tuple-i	d1lfg_1	1.007.006
tuple-3	HI002	100	343	**d1lfg_1**		**tuple-i**	**d1lfg_1**	**1.007.006**
tuple-4	HI003	12	80	**d1lfg_1**		**tuple-i**	**d1lfg_1**	**1.007.006**
tuple-5	HI009	200	260	d1mba__		tuple-i	d1lfg_1	1.007.006
tuple-6	HI023	300	450	d2ubx__		tuple-i	d1lfg_1	1.007.006
tuple-7	HI045	2	89	d2lmg__		tuple-i	d1lfg_1	1.007.006
tuple-1	HI001	12	200	d1mbd__		tuple-ii	d1mba__	1.003.002
tuple-2	HI002	15	231	d1hhba_		tuple-ii	d1mba__	1.003.002
tuple-3	HI002	100	343	d1lfg_1		tuple-ii	d1mba__	1.003.002
tuple-4	HI003	12	80	d1lfg_1		tuple-ii	d1mba__	1.003.002
tuple-5	HI009	200	**260**	**d1mba__**		**tuple-ii**	**d1mba__**	**1.003.002**
tuple-6	HI023	300	450	d2ubx__		tuple-ii	d1mba__	1.003.002
tuple-7	HI045	2	89	d2lmg__		tuple-ii	d1mba__	1.003.002

- Select {columns} from {huge cross-product of tables} where {row-selection is true}
  - ◊ cross-product T(1) x T(2) builds a huge virtual table where every row of T(1) is paired with every row of T(2). Then perform selection on this.
- Select fid from matches,structures where gid=HI009 and matches.did = structures.did

Cross Product A x B

A(1) = Row 1 of Table A
A(2) = Row 2 of Table A
A(i) = Row i of Table A

A has N rows
and C columns

B(1) = Row 1 of Table B
B(2) = Row 2 of Table B
B(i) = Row i of Table B

B has M rows
and K columns

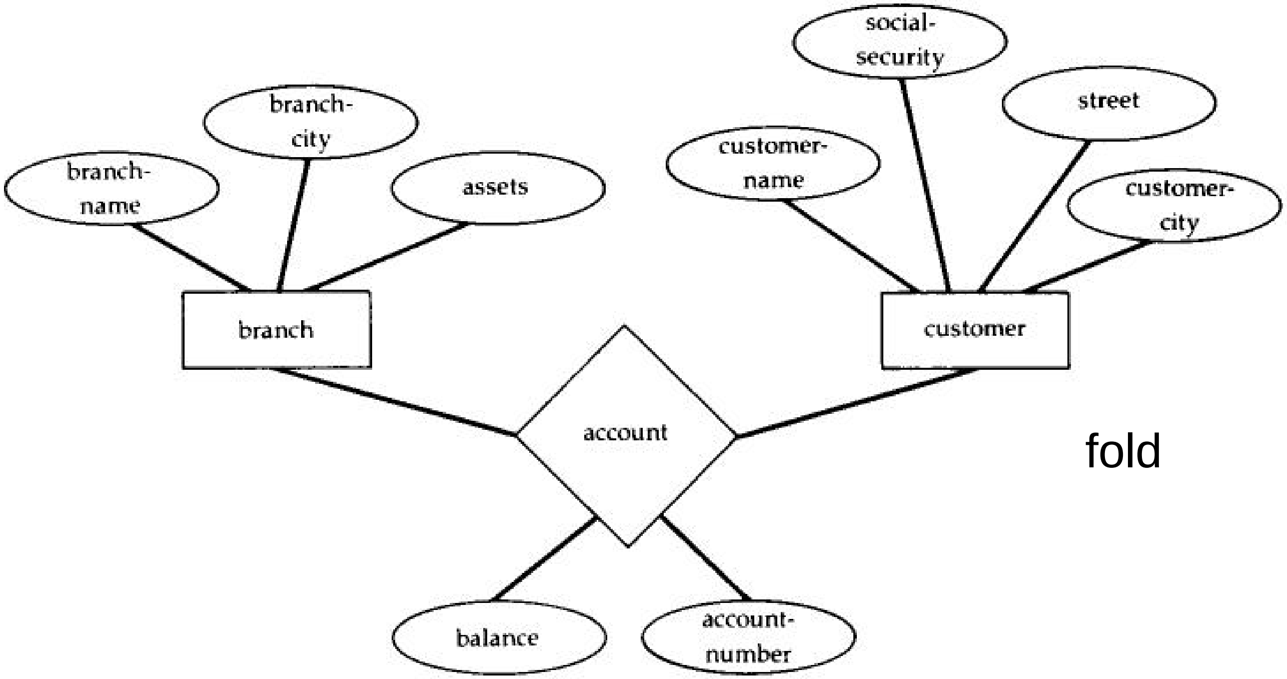
A x B =

A x B has
N x M rows
and
C+K columns

A(1)B(1)
A(1)B(2)
A(1)B(3)
...
A(1)B(M)
A(2)B(1)
A(2)B(2)
A(2)B(3)
...
A(2)B(M)
A(N)B(1)
A(N)B(2)
A(N)B(3)
...
A(N)B(M)

ER-diagrams

Start gid structure



fold

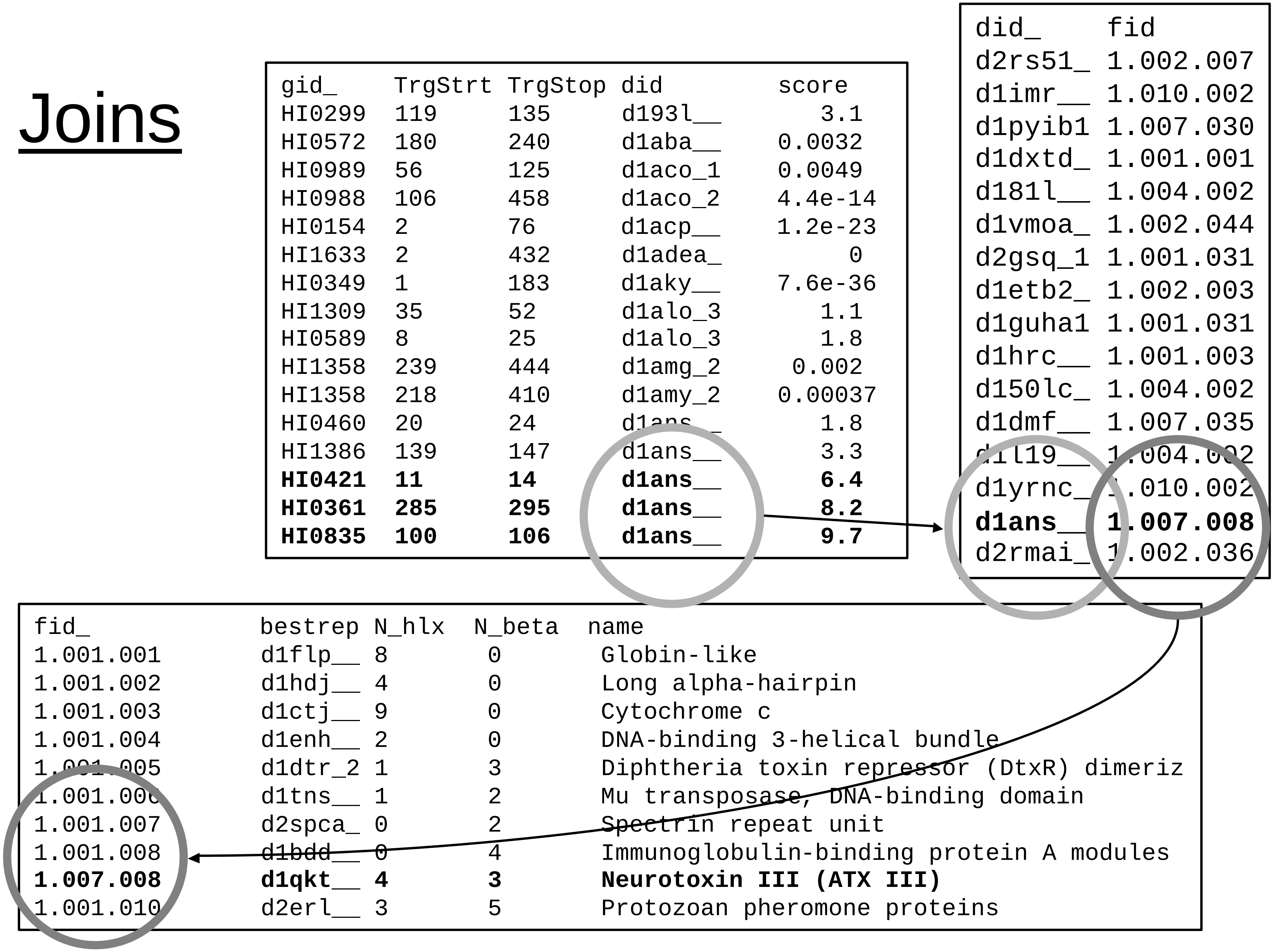
Figure 2.23 E-R diagram with *account* as a relationship set.

- Korth & Silberschatz
  - ◊ branch <=> matches (gid-start +++ did)
  - ◊ customer <=> folds (fid +++)
  - ◊ linked by
    account <=> structures (did fid)

Aggregate Functions--Statistics on Attributes

- Query Statistics
  - ◊ select gid, count (distinct did) from matches
  - ◊ select max(N_hlx) from folds where N_beta = 0
- How many matches to globins in the E. coli genome
- Complex Query by nesting selections
  - ◊ F <= select fid from folds where name contains “globin”
  - ◊ D <= select did from structures where fid in F
  - ◊ N <= select count(distinct gid,TrgStrt) from matches where did in D and score < .01

Joins



gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0988	106	458	d1aco_2	4.4e-14
HI0154	2	76	d1acp__	1.2e-23
HI1633	2	432	d1adea_	0
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	239	444	d1amg_2	0.002
HI1358	218	410	d1amy_2	0.00037
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	**11**	**14**	**d1ans__**	**6.4**
HI0361	**285**	**295**	**d1ans__**	**8.2**
HI0835	**100**	**106**	**d1ans__**	**9.7**

did_	fid
d2rs51_	1.002.007
d1imr__	1.010.002
d1pyib1	1.007.030
d1dxtd_	1.001.001
d181l__	1.004.002
d1vmoa_	1.002.044
d2gsq_1	1.001.031
d1etb2_	1.002.003
d1guha1	1.001.031
d1hrc__	1.001.003
d150lc_	1.004.002
d1dmf__	1.007.035
d1l19__	1.004.002
d1yrnc_	1.010.002
d1ans__	**1.007.008**
d2rmai_	1.002.036

fid_	bestrep	N_hlx	N_beta	name
1.001.001	d1flp__	8	0	Globin-like
1.001.002	d1hdj__	4	0	Long alpha-hairpin
1.001.003	d1ctj__	9	0	Cytochrome c
1.001.004	d1enh__	2	0	DNA-binding 3-helical bundle
1.001.005	d1dtr_2	1	3	Diphtheria toxin repressor (DtxR) dimeriz
1.001.006	d1tns__	1	2	Mu transposase, DNA-binding domain
1.001.007	d2spca_	0	2	Spectrin repeat unit
1.001.008	d1bdd__	0	4	Immunoglobulin-binding protein A modules
1.007.008	**d1qkt__**	**4**	**3**	**Neurotoxin III (ATX III)**
1.001.010	d2erl__	3	5	Protozoan pheromone proteins

Join Gives Unnormalized Table

Joining Two or More Tables with a Select Query Gives a New, “Bigger” Table

```
gid_  TrgStrt TrgStop did     score   fid      N_hlx N_beta name

HI0299 119     135    d193l__    3.1  1.010.002 0      2    Spectrin repeat unit
HI0572 180     240    d1aba__ 0.0032  1.002.045 1      2    Mu transposase, DNA-binding domain
HI0989 56      125    d1aco_1 0.0049  1.001.031 8      0    Globin-like
HI0988 106     458    d1aco_2 4.4e-14 1.001.031 8      0    Globin-like
HI0154 2       76     d1acp__ 1.2e-23 1.001.031 8      0    Globin-like
HI1633 2       432    d1adea_      0  1.010.002 0      2    Spectrin repeat unit
HI0349 1       183    d1aky__ 7.6e-36 1.001.031 8      0    Globin-like
HI1309 35      52     d1alo_3    1.1  1.007.008 4      3    Neurotoxin III (ATX III)
HI0589 8       25     d1alo_3    1.8  1.002.045 1      2    Mu transposase, DNA-binding domain
HI1358 239     444    d1amg_2  0.002  1.004.002 1      3    Diphtheria toxin repressor (DtxR)
HI1358 218     410    d1amy_2 0.00037 1.002.044 0      4    Immunoglobulin-binding protein A
HI0460 20      24     d1ans__    1.8  1.007.008 4      3    Neurotoxin III (ATX III)
HI1386 139     147    d1ans__    3.3  1.007.008 4      3    Neurotoxin III (ATX III)
HI0421 11      14     d1ans__    6.4  1.007.008 4      3    Neurotoxin III (ATX III)
HI0361 285     295    d1ans__    8.2  1.007.008 4      3    Neurotoxin III (ATX III)
HI0835 100     106    d1ans__    9.7  1.007.008 4      3    Neurotoxin III (ATX III)
```

Normalization

- What if Want to update Fold 1.007.008 to be “Neurotoxin IV”?
  - Many Updates
- So Good if Previously Normalized into Separate Tables
  - Eliminate Redundancy
  - Allow Consistent Updating

```
gid_  TrgStrt TrgStop did     score   fid      N_hlx N_beta name

HI0299 119     135    d193l__    3.1  1.010.002 0      2    Spectrin repeat unit
HI0572 180     240    d1aba__ 0.0032  1.002.045 1      2    Mu transposase, DNA-binding domain
HI0989 56      125    d1aco_1 0.0049  1.001.031 8      0    Globin-like
HI0988 106     458    d1aco_2 4.4e-14 1.001.031 8      0    Globin-like
HI0154 2       76     d1acp__ 1.2e-23 1.001.031 8      0    Globin-like
HI1633 2       432    d1adea_       0 1.010.002 0      2    Spectrin repeat unit
HI0349 1       183    d1aky__ 7.6e-36 1.001.031 8      0    Globin-like
HI1309 35      52     d1alo_3    1.1  1.007.008 4      3    Neurotoxin III (ATX III)
HI0589 8       25     d1alo_3    1.8  1.002.045 1      2    Mu transposase, DNA-binding domain
HI1358 239     444    d1amg_2  0.002  1.004.002 1      3    Diphtheria toxin repressor (DtxR)
HI1358 218     410    d1amy_2 0.00037 1.002.044 0      4    Immunoglobulin-binding protein A
HI0460 20      24     d1ans__    1.8  1.007.008 4      3    Neurotoxin III (ATX III)
HI1386 139     147    d1ans__    3.3  1.007.008 4      3    Neurotoxin III (ATX III)
HI0421 11      14     d1ans__    6.4  1.007.008 4      3    Neurotoxin III (ATX III)
HI0361 285     295    d1ans__    8.2  1.007.008 4      3    Neurotoxin III (ATX III)
HI0835 100     106    d1ans__    9.7  1.007.008 4      3    Neurotoxin III (ATX III)
```

Normalization Example

Un-normalized

Name	City	Area-Code	Phone-Number
Charles	NY	212	345-6789
Mark	SF	415	236-8982
Jane	NY	212	567-2345
Jeff	SF	415	435-3535
Jack	Boston	617	234-9988

→

Normalized

Name	City	Phone-Number
Charles	NY	345-6789
Mark	SF	236-8982
Jane	NY	567-2345
Jeff	SF	435-3535
Jack	Boston	234-9988

City	Area-Code
NY	212
SF	415
Boston	617

Normalized Tables

Theory of Normalization

gid_	TrgStrt	TrgStop	did	score
HI0299	119	135	d193l__	3.1
HI0572	180	240	d1aba__	0.0032
HI0989	56	125	d1aco_1	0.0049
HI0988	106	458	d1aco_2	4.4e-14
HI0154	2	76	d1acp__	1.2e-23
HI1633	2	432	d1adea_	0
HI0349	1	183	d1aky__	7.6e-36
HI1309	35	52	d1alo_3	1.1
HI0589	8	25	d1alo_3	1.8
HI1358	239	444	d1amg_2	0.002
HI1358	218	410	d1amy_2	0.00037
HI0460	20	24	d1ans__	1.8
HI1386	139	147	d1ans__	3.3
HI0421	**11**	**14**	**d1ans__**	**6.4**
HI0361	**285**	**295**	**d1ans__**	**8.2**
HI0835	**100**	**106**	**d1ans__**	**9.7**

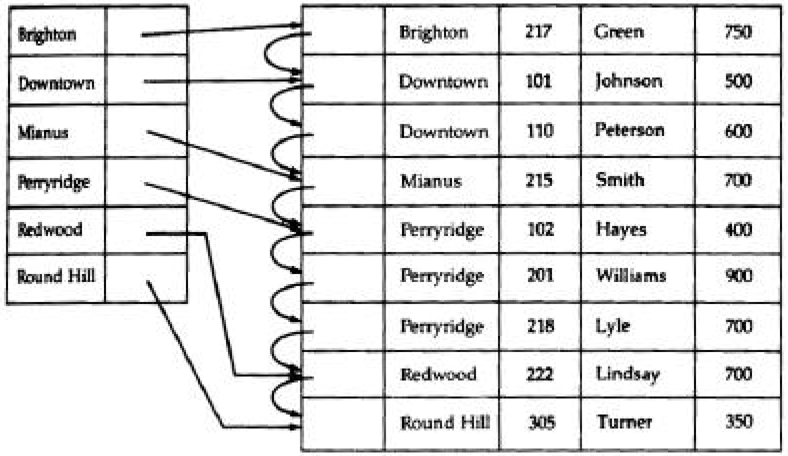
did_	fid
d2rs51_	1.002.007
d1imr__	1.010.002
d1pyib1	1.007.030
d1dxtd_	1.001.001
d181l__	1.004.002
d1vmoa_	1.002.044
d2gsq_1	1.001.031
d1etb2_	1.002.003
d1guha1	1.001.031
d1hrc__	1.001.003
d150lc_	1.004.002
d1dmf__	1.007.035
d1l19__	1.004.002
d1yrnc_	1.010.002
d1ans__	**1.007.008**
d2rmai_	1.002.036

fid_	bestrep	N_hlx	N_beta	name
1.001.001	d1flp__	8	0	Globin-like
1.001.002	d1hdj__	4	0	Long alpha-hairpin
1.001.003	d1ctj__	9	0	Cytochrome c
1.001.004	d1enh__	2	0	DNA-binding 3-helical bundle
1.001.005	d1dtr_2	1	3	Diphtheria toxin repressor (DtxR) dimeriz
1.001.006	d1tns__	1	2	Mu transposase, DNA-binding domain
1.001.007	d2spca_	0	2	Spectrin repeat unit
1.001.008	d1bdd__	0	4	Immunoglobulin-binding protein A modules
1.007.008	**d1qkt__**	**4**	**3**	**Neurotoxin III (ATX III)**
1.001.010	d2erl__	3	5	Protozoan pheromone proteins

Query Optimization

- Get at the Data Quickly!!
- Indexes
- Hash Function Reproduce the Effect of Indexes
  - ◊ Rapidly Associate a Bucket with Each Key
- Joining 10 tables, which to do first?
  - ◊ Joining is slow so store some tables in unnormalized form
    - o Speed vs Memory

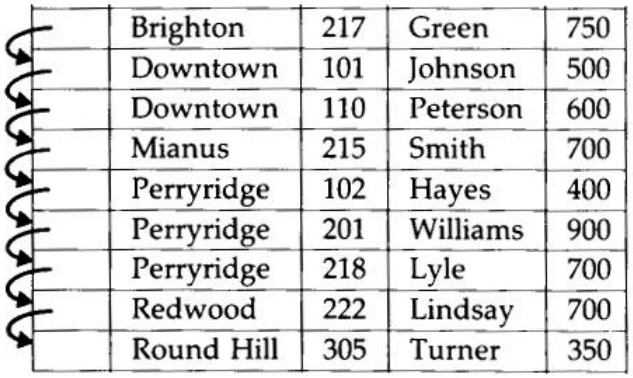
Indexes Speed Access



Brighton	
Downtown	
Mianus	
Perryridge	
Redwood	
Round Hill	

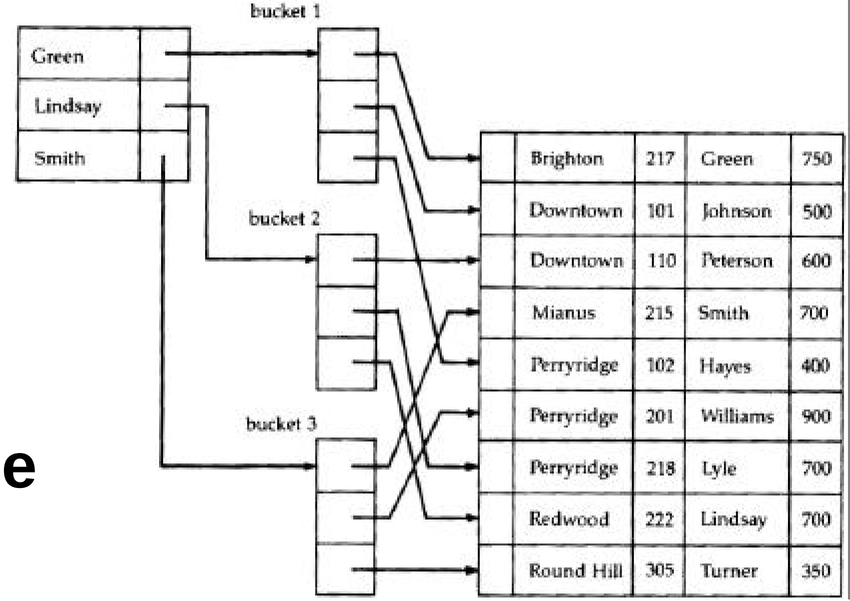
	Brighton	217	Green	750
	Downtown	101	Johnson	500
	Downtown	110	Peterson	600
	Mianus	215	Smith	700
	Perryridge	102	Hayes	400
	Perryridge	201	Williams	900
	Perryridge	218	Lyle	700
	Redwood	222	Lindsay	700
	Round Hill	305	Turner	350

One Index



	Brighton	217	Green	750
	Downtown	101	Johnson	500
	Downtown	110	Peterson	600
	Mianus	215	Smith	700
	Perryridge	102	Hayes	400
	Perryridge	201	Williams	900
	Perryridge	218	Lyle	700
	Redwood	222	Lindsay	700
	Round Hill	305	Turner	350

No Index

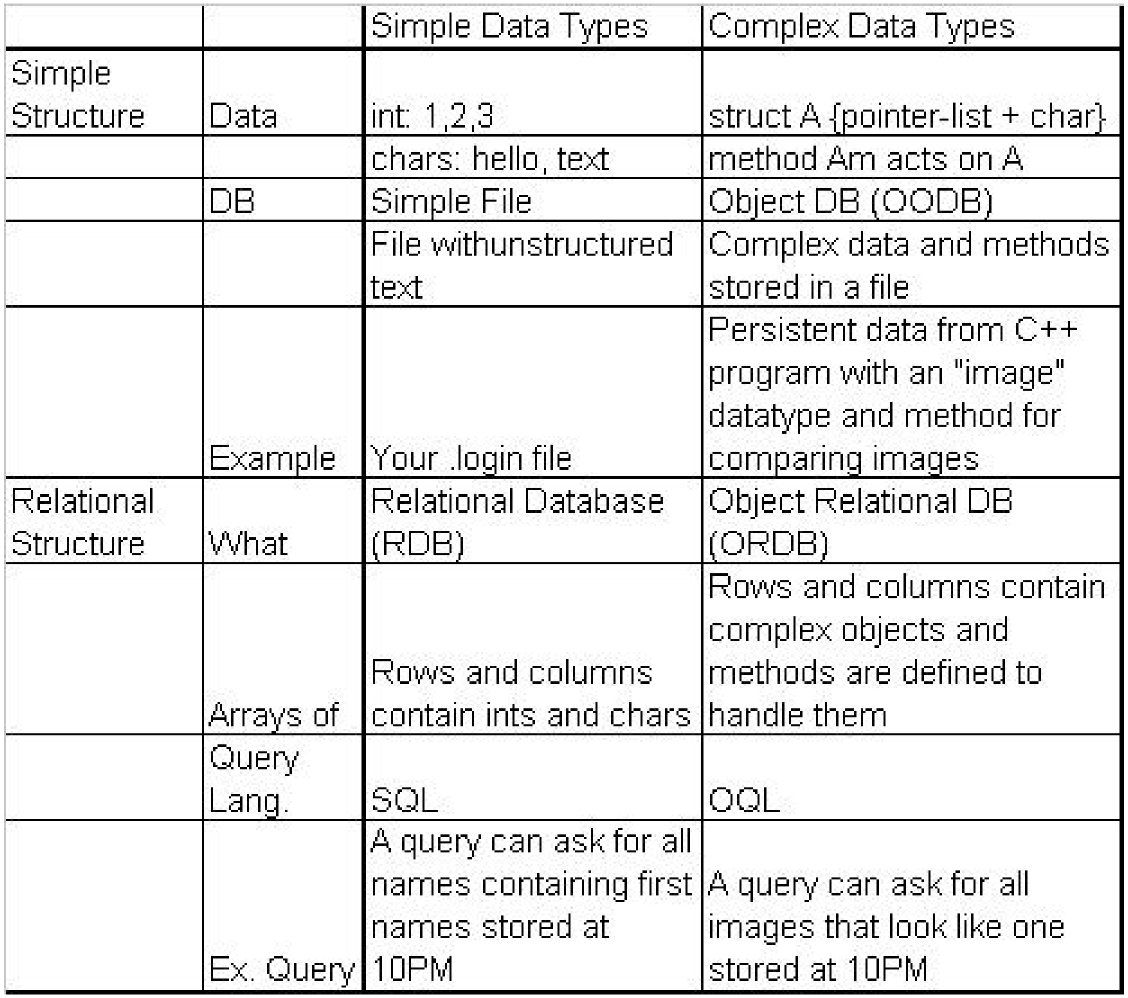


Green	
Lindsay	
Smith	

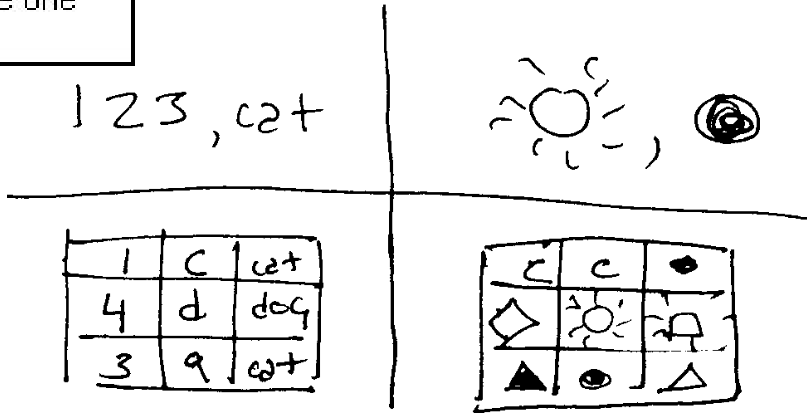
	Brighton	217	Green	750
	Downtown	101	Johnson	500
	Downtown	110	Peterson	600
	Mianus	215	Smith	700
	Perryridge	102	Hayes	400
	Perryridge	201	Williams	900
	Perryridge	218	Lyle	700
	Redwood	222	Lindsay	700
	Round Hill	305	Turner	350

Double Index

Object Databases



		Simple Data Types	Complex Data Types
Simple Structure	Data	int: 1,2,3	struct A {pointer-list + char}
		chars: hello, text	method Am acts on A
	DB	Simple File	Object DB (OODB)
		File withunstructured text	Complex data and methods stored in a file
	Example	Your .login file	Persistent data from C++ program with an "image" datatype and method for comparing images
Relational Structure	What	Relational Database (RDB)	Object Relational DB (ORDB)
	Arrays of	Rows and columns contain ints and chars	Rows and columns contain complex objects and methods are defined to handle them
	Query Lang.	SQL	OQL
	Ex. Query	A query can ask for all names containing first names stored at 10PM	A query can ask for all images that look like one stored at 10PM



C, fortran vs. C++

Forms & reports [user views]

- Reports are the result of running a succession of selects queries on a database, joining together a number of tables, and then pasting the results together
- Forms are the same but they are editable
- Forms and Reports represent particular views of the data
    - ◊ For instance, one can be keyed on gene id listing all the structures matching a gene and the other could be keyed on structure id listing all the gene matching a given structure

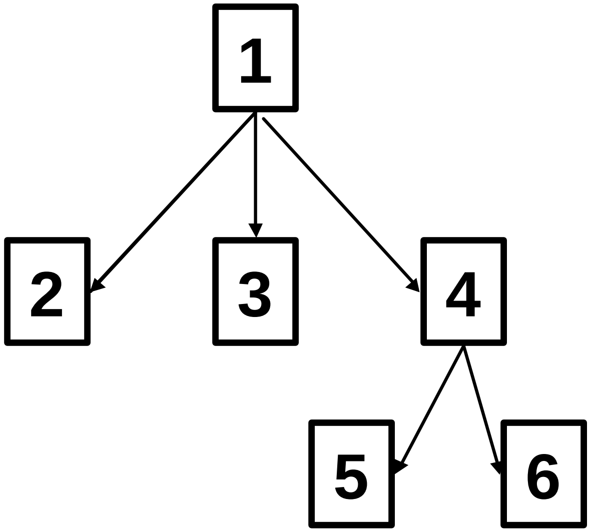
Aspects of Forms: Transactions and Security

- Transactions
  - ◊ Genome Centers and United Airlines!
  - ◊ Log each entry and enable **UNDO**
- Security
  - ◊ Only certain users can modify certain fields

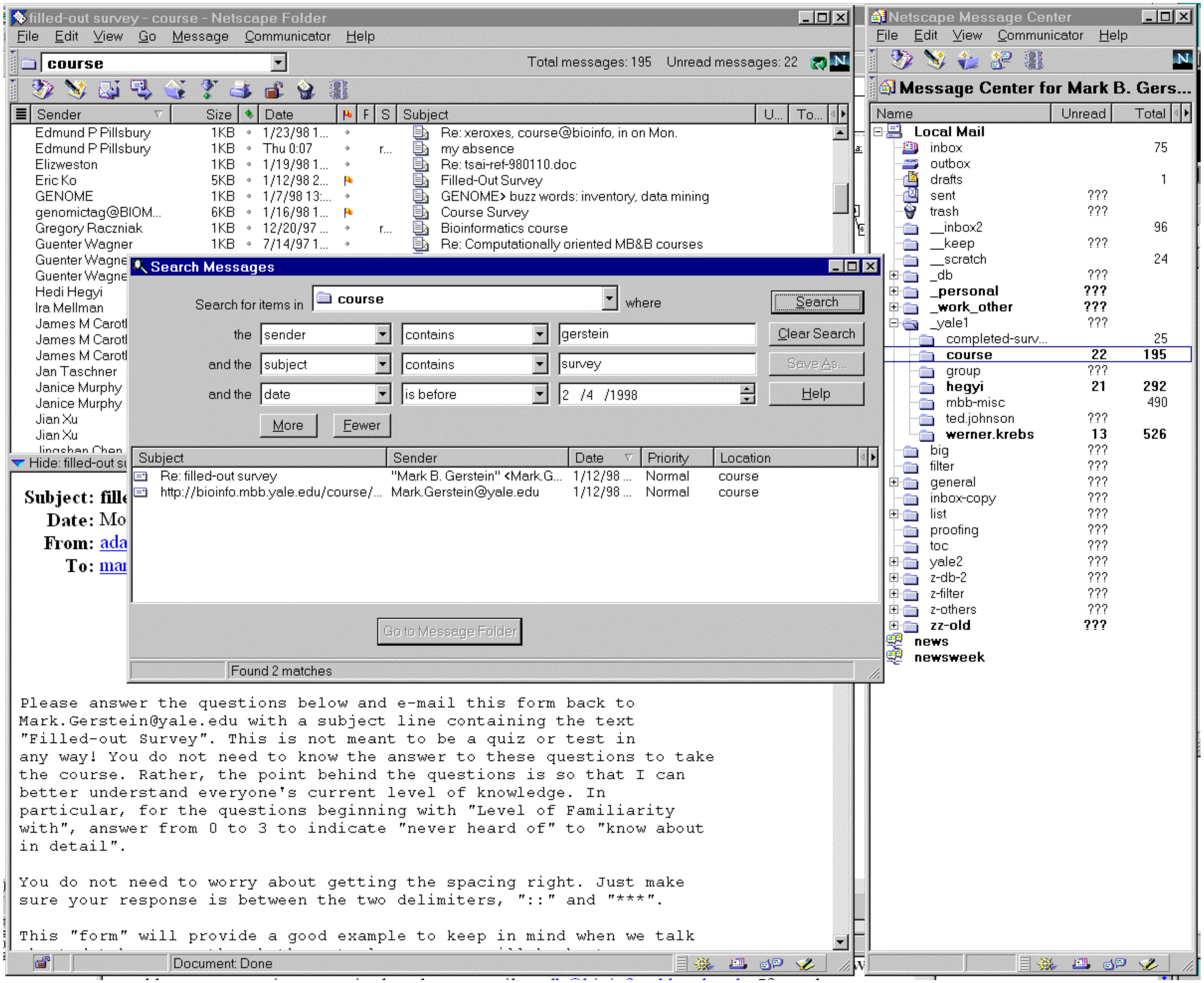
Complex Data Example: Encoding Trees in RDBs

Node	Parent
1	0
2	1
3	1
4	1
5	4
6	4

Node	Name
1	Organism
2	Bacteria
3	Archea
4	Eukarya
5	Metazoa
6	Plants



RDBs Everywhere: Internet Mail


filled-out survey - course - Netscape Folder
File Edit View Go Message Communicator Help
Netscape Message Center
File Edit View Communicator Help
Message Center for Mark B. Gers...
Search Messages
Search
Clear Search
Save As...
Help
More
Fewer
Go to Message Folder
Hide: filled-out su
Document: Done

course — Total messages: 195 Unread messages: 22

Sender	Size	Date	F	S	Subject
Edmund P Pillsbury	1KB	1/23/98 1...			Re: xeroxes, course@bioinfo, in on Mon.
Edmund P Pillsbury	1KB	Thu 0:07		r...	my absence
Elizweston	1KB	1/19/98 1...			Re: tsai-ref-980110.doc
Eric Ko	5KB	1/12/98 2...			Filled-Out Survey
GENOME	1KB	1/7/98 13:...			GENOME> buzz words: inventory, data mining
genomictag@BIOM...	6KB	1/16/98 1...			Course Survey
Gregory Raczniak	1KB	12/20/97 ...		r...	Bioinformatics course
Guenter Wagner	1KB	7/14/97 1...			Re: Computationally oriented MB&B courses
Guenter Wagne					
Guenter Wagne					
Hedi Hegyi					
Ira Mellman					
James M Carotl					
James M Carotl					
James M Carotl					
Jan Taschner					
Janice Murphy					
Janice Murphy					
Jian Xu					
Jian Xu					
Jingshan Chen					

Search for items in course where

the sender contains gerstein

and the subject contains survey

and the date is before 2 /4 /1998

Subject	Sender	Date	Priority	Location
Re: filled-out survey	"Mark B. Gerstein" <Mark.G...	1/12/98 ...	Normal	course
http://bioinfo.mbb.yale.edu/course/...	Mark.Gerstein@yale.edu	1/12/98 ...	Normal	course

Found 2 matches

Subject: fille
Date: Mo
From: ada
To: mai

Please answer the questions below and e-mail this form back to Mark.Gerstein@yale.edu with a subject line containing the text "Filled-out Survey". This is not meant to be a quiz or test in any way! You do not need to know the answer to these questions to take the course. Rather, the point behind the questions is so that I can better understand everyone's current level of knowledge. In particular, for the questions beginning with "Level of Familiarity with", answer from 0 to 3 to indicate "never heard of" to "know about in detail".

You do not need to worry about getting the spacing right. Just make sure your response is between the two delimiters, "::" and "***".

This "form" will provide a good example to keep in mind when we talk

Name	Unread	Total
Local Mail		
inbox		75
outbox		
drafts		1
sent	???	
trash	???	
__inbox2		96
__keep	???	
__scratch		24
_db	???	
_personal	???	
_work_other	???	
_yale1	???	
completed-surv...		25
course	22	195
group	???	
hegyi	21	292
mbb-misc		490
ted.johnson	???	
werner.krebs	13	526
big	???	
filter	???	
general	???	
inbox-copy	???	
list	???	
proofing	???	
toc	???	
yale2	???	
z-db-2	???	
z-filter	???	
z-others	???	
zz-old	???	
news		
newsweek		

RDBs Everywhere: File System

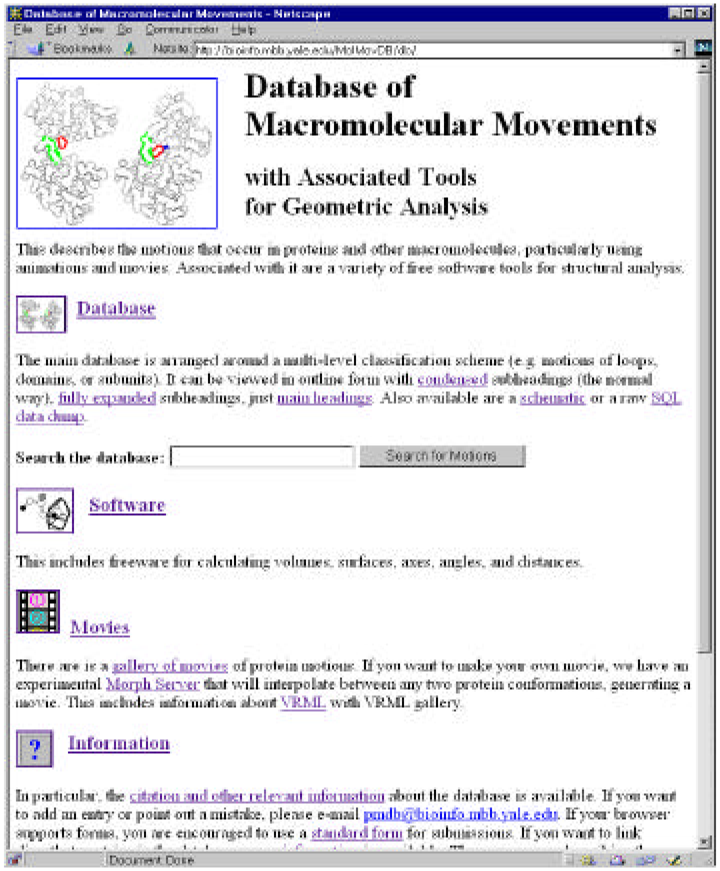
```
INODE   SIZE PERMISSION    USER     GROUP       BYTES MMM-DD--YEAR NAME

120462    1 drwxr-xr-x  10 mbg      gerstein     1024 Feb 12  1997 .
120463    1 drwxr-xr-x   2 mbg      gerstein     1024 Jan 30  1997 ./hi-tbl
120464  514 -rw-r--r--   1 mbg      gerstein   525335 Nov 10  1996 ./hi-tbl/id_gorss.tbl
120465   19 -rw-r--r--   1 mbg      gerstein    18469 Nov 10  1996 ./hi-tbl/id_kytedool.tbl
120466  514 -rw-r--r--   1 mbg      gerstein   525372 Nov 10  1996 ./hi-tbl/id_seq.tbl
108224  507 -rw-r--r--   1 mbg      gerstein   518822 Nov 10  1996 ./mj-tbl/id_gorss.tbl
108227   54 -rw-r--r--   1 mbg      gerstein    54775 Jan 30  1997 ./mj-tbl/id_abcode.tbl
108228   19 -rw-r--r--   1 mbg      gerstein    19131 Nov 11  1996 ./mj-tbl/id_kytedool.tbl
108229  106 -rw-r--r--   1 mbg      gerstein   108345 Nov 16  1996 ./mj-tbl/word_stats.tbl.bak
108230  106 -rw-r--r--   1 mbg      gerstein   108354 Jan 28  1997 ./mj-tbl/word_stats.tbl
108231    7 -rw-r--r--   1 mbg      gerstein     6962 Jan 30  1997 ./mj-tbl/hist_seqlen.tbl
108232    7 -rw-r--r--   1 mbg      gerstein     6967 Jan 30  1997 ./mj-tbl/hist_num_H_res.tbl
 91903    1 drwxr-xr-x   2 mbg      gerstein     1024 Nov 19  1996 ./po-tbl
```

```
USER:PASSWD:UID:GID:COMMENT:DIR:SHELL

ftp:*:14:50:FTP User:/home/ftp:
nobody:*:99:99:Nobody:/:
mlml:cw5ZrAmNBAxvU:106:100:Michael Levitt (linux):/u1/mlml:/bin/tcsh
dabushne:ErR3hu4q0tO7Y:108:100:Dave:/u1/dabushne:/bin/tcsh
mbg:V9CPWXAG.mo3E:5514:165:Mark Gerstein,432A, BASS,2-6105,:/u0/mbg:/bin/tcsh
mbgmbg:V9CPWXAG.mo3E:5515:165:logs into mbg,,,,:/u0/mbg:/bin/tcsh
mbg10:V9CPWXAG.mo3E:5516:165:alternate account for mbg:/home/mbg10:/bin/tcsh
local::502:20:Local Installed Packages:/u1/local:/bin/tcsh
login::503:20:Hyper Login:/u0/login:/u0/login/hyper-login.pl
```

find -ls

/etc/passwd

Example Report: Motions Database



Database of Macromolecular Movements - Netscape
File Edit View Go Communicator Help
Bookmarks Netsite: http://bioinfo.mbb.yale.edu/MolMovDB/db/
Search for Motions
Document: Done

Database of Macromolecular Movements

with Associated Tools for Geometric Analysis

This describes the motions that occur in proteins and other macromolecules, particularly using animations and movies. Associated with it are a variety of free software tools for structural analysis.

Database

The main database is arranged around a multi-level classification scheme (e.g. motions of loops, domains, or subunits). It can be viewed in outline form with condensed subheadings (the normal way), fully expanded subheadings, just main headings. Also available are a schematic or a raw SQL data dump.

Search the database:

Software

This includes freeware for calculating volumes, surfaces, axes, angles, and distances.

Movies

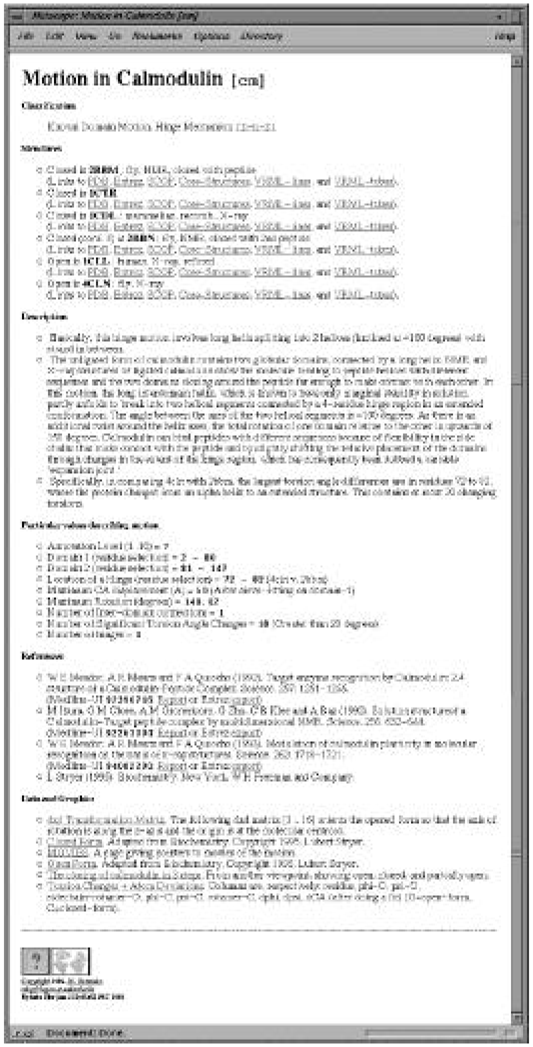
There are is a gallery of movies of protein motions. If you want to make your own movie, we have an experimental Morph Server that will interpolate between any two protein conformations, generating a movie. This includes information about VRML with VRML gallery.

Information

In particular, the citation and other relevant information about the database is available. If you want to add an entry or point out a mistake, please e-mail pmdb@bioinfo.mbb.yale.edu. If your browser supports forms, you are encouraged to use a standard form for submissions. If you want to link

Report on Calmodulin

→



Netscape: Motion in Calmodulin [cm]
File Edit View Go Bookmarks Options Directory Help
Document: Done

Motion in Calmodulin [cm]

Classification

Known Domain Motion, Hinge Mechanism [illegible]

Structures

- Closed is **2BBM**, fly, NMR, closed with peptide
  (Links to PDB, Entrez, SCOP, Cose-Structures, VRML - lines, and VRML - tubes).
- Closed is **1CTR**
  (Links to PDB, Entrez, SCOP, Cose-Structures, VRML - lines, and VRML - tubes).
- Closed is **1CDL**, mammalian, recomb., X-ray
  (Links to PDB, Entrez, SCOP, Cose-Structures, VRML - lines, and VRML - tubes).
- Closed (cont. ?) is **2BBN**, fly, NMR, closed with 2nd peptide
  (Links to PDB, Entrez, SCOP, Cose-Structures, VRML - lines, and VRML - tubes).
- Open is **1CLL**, human, X-ray, refined
  (Links to PDB, Entrez, SCOP, Cose-Structures, VRML - lines, and VRML - tubes).
- Open is **4CLN**, fly, X-ray
  (Links to PDB, Entrez, SCOP, Cose-Structures, VRML - lines, and VRML - tubes).

Description

- Basically, this hinge motion involves long helix splitting into 2 helices (kinked at ~100 degrees) with strand in between.
- The unligated form of calmodulin contains two globular domains, connected by a long helix. NMR and X-ray structures of ligated calmodulin show the molecule bending to [illegible] peptide [illegible] sequence and the two domains closing around the peptide far enough to make contact with each other. In this motion, the long intervening helix, which is known to have only marginal stability in solution, partly unfolds to break into two helical segments connected by a 4-residue hinge region in an extended conformation. The angle between the axes of the two helical segments is ~100 degrees. As there is an additional twist around the helix axis, the total rotation of one domain relative to the other is upwards of 150 degrees. Calmodulin can bind peptides with different sequences because of flexibility in the side chains that make contact with the peptide and by slightly shifting the relative placement of the domains through changes in torsion of the hinge region, which has consequently been dubbed a variable 'expansion joint.'
- Specifically, in comparing 4cln with 2bbm, the largest torsion angle differences are in residues 72 to 81, where the protein changes from an alpha helix to an extended structure. This contains at most 20 changing torsions.

Particular values describing motion

- Annotation Level (1..10) = 7
- Domain 1 (residue selection) = 2 - 80
- Domain 2 (residue selection) = 81 - 147
- Location of a Hinge (residue selection) = 72 - 80 (4cln v. 2bbm)
- Maximum CA Displacement (A) = [illegible] (After Gerstein fitting on domain-1)
- Maximum Rotation (degrees) = 148.42
- Number of Inter-domain connections = 1
- Number of Significant Torsion Angle Changes = 18 (Greater than 20 degrees)
- Number of hinges = 1

References

- W.E. Meador, A.R. Means and F.A. Quiocho (1992). Target enzyme recognition by Calmodulin: 2.4 Å structure of a Calmodulin-Peptide Complex. Science. 257: 1251-1255. (Medline-UI 92386795 Report or Entrez-report)
- M. Ikura, G.M. Clore, A.M. Gronenborn, G. Zhu, C.B. Klee and A. Bax (1992). Solution structure of a Calmodulin-Target peptide complex by multidimensional NMR. Science. 256: 632-638. (Medline-UI 92261393 Report or Entrez-report)
- W.E. Meador, A.R. Means and F.A. Quiocho (1993). Modulation of calmodulin plasticity in molecular recognition on the basis of x-ray structures. Science. 262: 1718-1721. (Medline-UI 94082292 Report or Entrez-report)
- L. Stryer (1995). Biochemistry. New York, W.H. Freeman and Company.

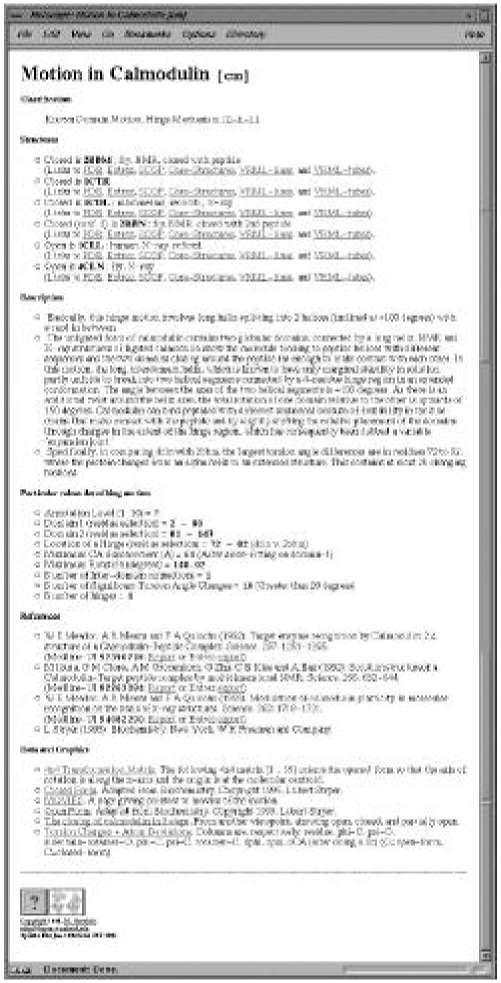
Data and Graphics

- 4x4 Transformation Matrix. The following 4x4 matrix (1 .. 16) orients the opened form so that the axis of rotation is along the z-axis and the origin is at the molecular centroid.
- Closed Form. Adapted from Biochemistry. Copyright 1995. Lubert Stryer.
- MOVIES. A page giving pointers to movies of the motion.
- Open Form. Adapted from Biochemistry. Copyright 1995. Lubert Stryer.
- The closing of calmodulin in 3 steps. From another viewpoint, showing open, closed, and partially open.
- Torsion Changes + Alpha Deviations. Columns are, respectively: residue, phi-O, psi-O, [illegible] phi-C, psi-C, [illegible] Closed-form.

Copyright 1996, M. Gerstein
[illegible]

Example Report: Motions Database

Report shows information, merging together many tables with variable amounts of information. Form same but allows entry.



Motion in Calmodulin [cm]

Classification

Known Domain Motion, Hinge Mechanism [illegible]

Structures

- Closed in 2BBM: fly, NMR, closed with peptide (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines and VRML-tubes).
- Closed in 1CTR (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines and VRML-tubes).
- Closed in 1CTR, [illegible], X-ray (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines and VRML-tubes).
- Closed (conf. 1) in 2BBN: fly, NMR, closed with 2nd peptide (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines and VRML-tubes).
- Open in 1CLL: human, X-ray refined (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines and VRML-tubes).
- Open in 4CLN: fly, X-ray (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines and VRML-tubes).

Description

- Basically, this hinge motion involves long helix splitting into 2 helices (inclined at ~100 degrees) with strand in between.
- The unligated form of calmodulin contains two globular domains, connected by a long helix. NMR and X-ray structures [illegible]
- Specifically, in comparing 4cln with 2bbm, the largest torsion angle differences are in residues 72 to 82, where the protein changes from an alpha helix to an extended structure. [illegible]

Particular values describing motion

- Annotation Level (1 - 10) = ?
- Domain1 (residue selection) = 2 - 80
- Domain2 (residue selection) = 81 - 147
- Location of a Hinge (residue selection) = 72 - 82 (4cln v. 2bbm)
- Maximum CA displacement (A) = [illegible]
- Maximum Rotation (degrees) = 148.[illegible]
- Number of Inter-domain connections = 1
- Number of Significant Torsion Angle Changes = 18 (Greater than 20 degrees)
- Number of Hinges = 1

References

- W. E. Meador, A. R. Means and F. A. Quiocho (1992). Target enzyme recognition by Calmodulin: 2.4 structure of a Calmodulin-Peptide Complex. Science 257: 1251-1255. (Medline UI 92396788: Report or Entrez-report)
- M. Ikura, G. M. Clore, A. M. Gronenborn, G. Zhu, C. B. Klee and A. Bax (1992). Solution structure of a Calmodulin-Target peptide complex by multidimensional NMR. Science 256: 632-638. (Medline UI 92263394: Report or Entrez-report)
- W. E. Meador, A. R. Means and F. A. Quiocho (1993). Modulation of calmodulin plasticity in molecular recognition on the basis of X-ray structures. Science 262: 1718-1721. (Medline UI 94082290: Report or Entrez-report)
- L. Stryer (1995). Biochemistry. New York: W.H. Freeman and Company.

Movies and Graphics

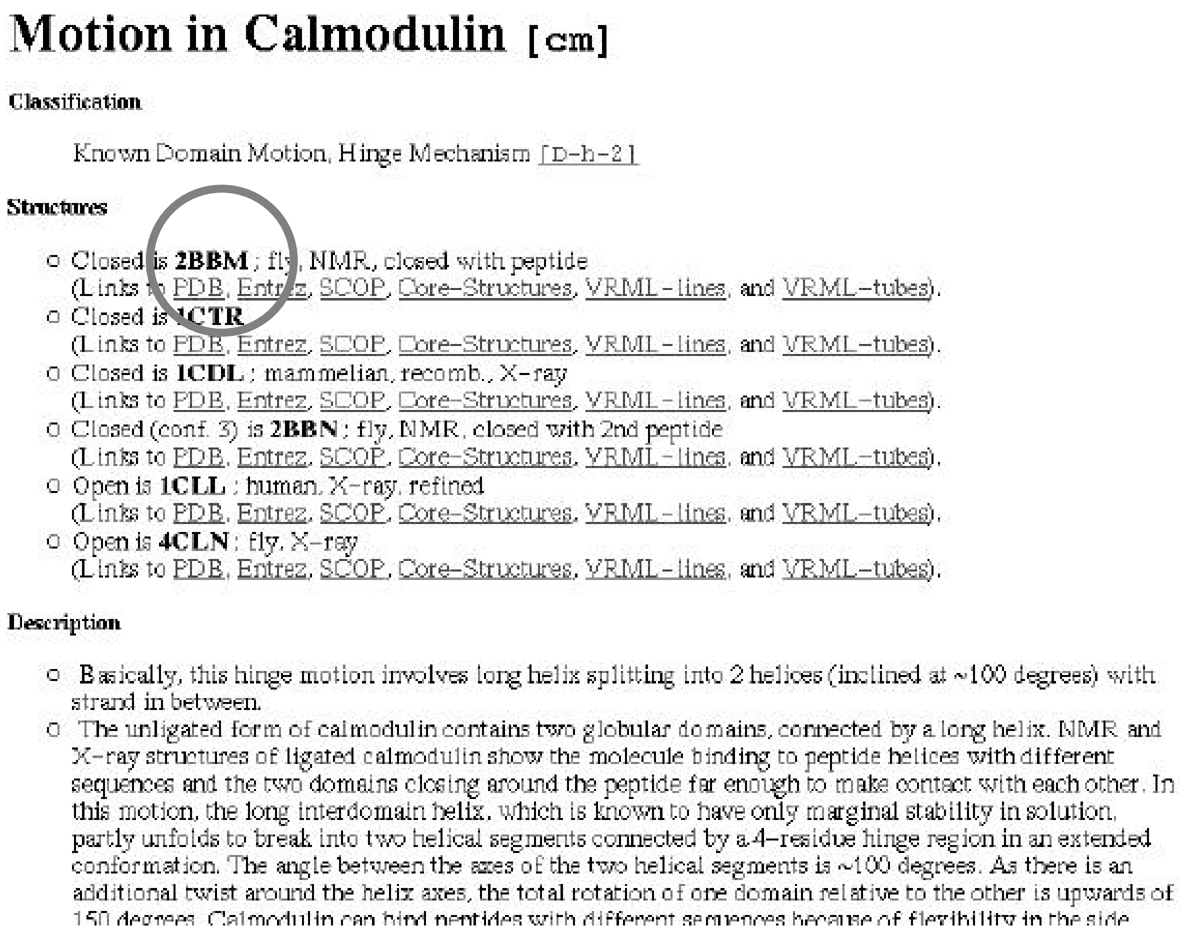
- [illegible]
- [illegible] Adapted from Biochemistry. Copyright 1995, Lubert Stryer.
- [illegible]
- [illegible] Copyright 1995, Lubert Stryer.
- The closing of calmodulin in [illegible]
- Torsion Changes + [illegible]

Schema

```
CREATE TABLE relations (
 id_ CHAR(15),
  id_to_ CHAR(15),
  type CHAR(30),
  comment CHAR(512)
)
CREATE TABLE single_vals (
 id_ CHAR(10),
  name_ CHAR(30),
  val CHAR(30),
  comment CHAR(500)
)
CREATE TABLE structures (
 id_ CHAR(10),
  pdb_id_ CHAR(8),
  name_short CHAR(50),
  chain CHAR(1),
  name_long CHAR(100)
)
CREATE TABLE value_names (
  abbrev_ CHAR(15),
  name CHAR(50)
)
CREATE TABLE endnote_refs (
  num_I INT,
  name CHAR(512)
)
```

```
CREATE TABLE classes (
  class_num_ CHAR(10),
  new CHAR(10),
  class_name CHAR(80)
)
CREATE TABLE classifications (
  id_ CHAR(10),
  class_num CHAR(10)
)
CREATE TABLE links (
  id_ CHAR(10),
  url_ CHAR(150),
  hilit_text CHAR(100),
  other_text CHAR(500),
  flag CHAR(5)
)
CREATE TABLE names (
 id_ CHAR(10),
  seq_num_n INT,
  name CHAR(255)
)
CREATE TABLE refs (
 id_ CHAR(10),
  medline_I INT,
  endnote_I INT,
  flag_n INT
)
CREATE TABLE descriptions (
 id_ CHAR(10),
  num_I INT,
  prose CHAR(5000)
)
```

Example Report: Motions Database



Motion in Calmodulin [cm]

Classification

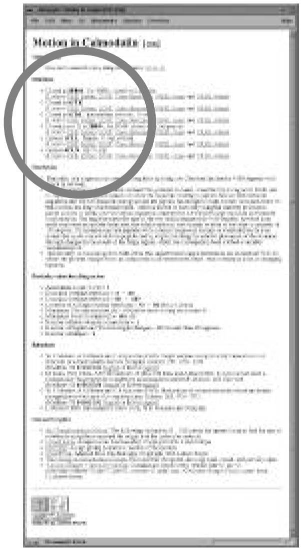
Known Domain Motion, Hinge Mechanism [D-h-2]

Structures

- Closed is **2BBM** ; fly, NMR, closed with peptide
  (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines, and VRML-tubes).
- Closed is **1CTR**
  (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines, and VRML-tubes).
- Closed is **1CDL** ; mammelian, recomb., X-ray
  (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines, and VRML-tubes).
- Closed (conf. 3) is **2BBN** ; fly, NMR, closed with 2nd peptide
  (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines, and VRML-tubes).
- Open is **1CLL** ; human, X-ray, refined
  (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines, and VRML-tubes).
- Open is **4CLN** ; fly, X-ray
  (Links to PDB, Entrez, SCOP, Core-Structures, VRML-lines, and VRML-tubes).

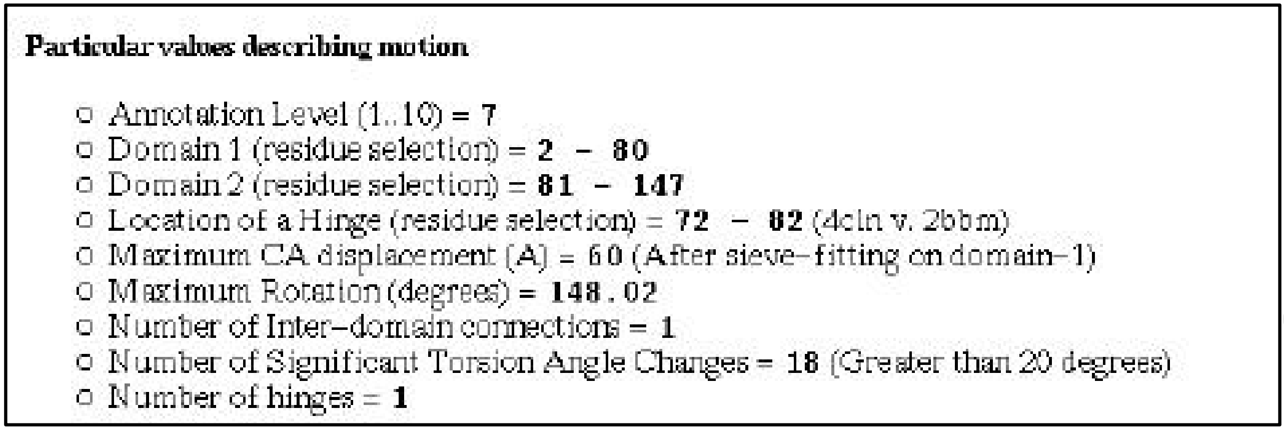
Description

- Basically, this hinge motion involves long helix splitting into 2 helices (inclined at ~100 degrees) with strand in between.
- The unligated form of calmodulin contains two globular domains, connected by a long helix. NMR and X-ray structures of ligated calmodulin show the molecule binding to peptide helices with different sequences and the two domains closing around the peptide far enough to make contact with each other. In this motion, the long interdomain helix, which is known to have only marginal stability in solution, partly unfolds to break into two helical segments connected by a 4-residue hinge region in an extended conformation. The angle between the axes of the two helical segments is ~100 degrees. As there is an additional twist around the helix axes, the total rotation of one domain relative to the other is upwards of 150 degrees. Calmodulin can bind peptides with different sequences because of flexibility in the side



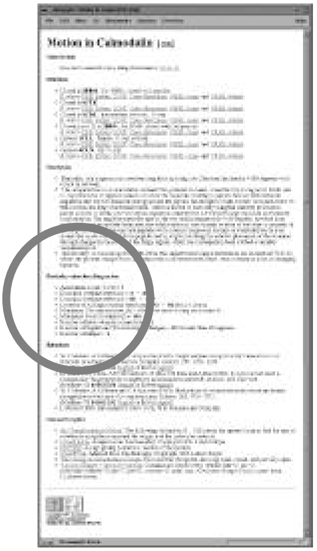
Structures: Variable Number Per ID (Var. Num. of Phone Num. per Person), Foreign Key into PDB

Example Report: Motions Database



Particular values describing motion

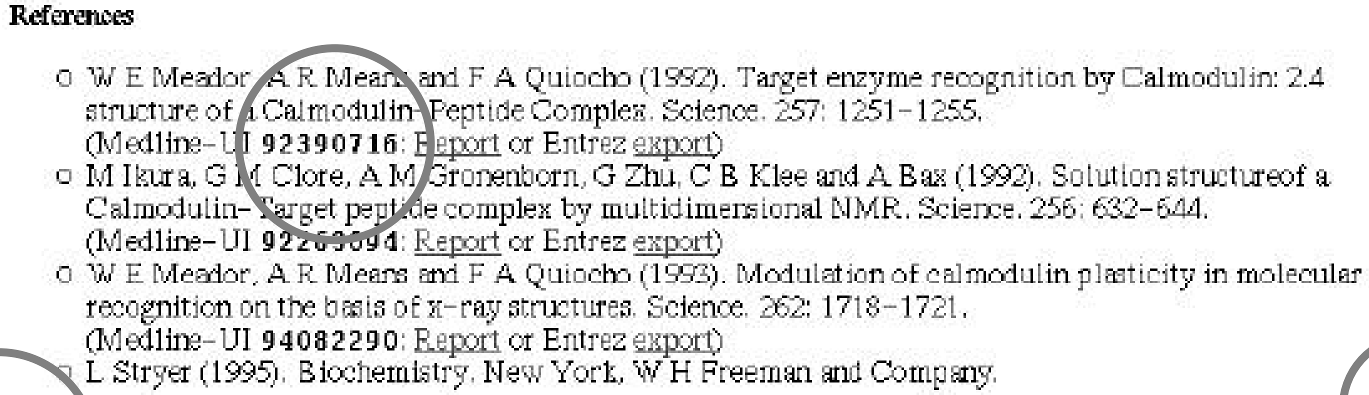
- ○ Annotation Level (1..10) = **7**
- ○ Domain 1 (residue selection) = **2 - 80**
- ○ Domain 2 (residue selection) = **81 - 147**
- ○ Location of a Hinge (residue selection) = **72 - 82** (4cln v. 2bbm)
- ○ Maximum CA displacement (A) = **60** (After sieve-fitting on domain-1)
- ○ Maximum Rotation (degrees) = **148.02**
- ○ Number of Inter-domain connections = **1**
- ○ Number of Significant Torsion Angle Changes = **18** (Greater than 20 degrees)
- ○ Number of hinges = **1**



```
$sth = $dbh->query("SELECT value_names.name,
                     single_vals.val,single_vals.comment ".
                "FROM value_names,single_vals ".
                "WHERE single_vals.id_ = '$id' AND
                single_vals.name_ = value_names.abbrev_ ".
                "ORDER BY value_names.name");

 $rows = $sth->numrows;

 if ($rows > 0) {
   &PrintHead("Particular values describing motion");
   for ($i=0; $i<$rows; $i++) {
     @values = $sth->fetchrow;
     PrintSingleVals(@values);
   }
 }
```

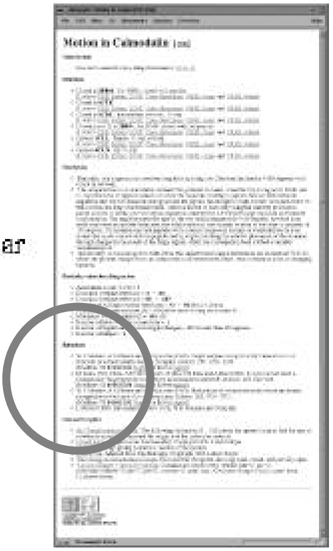
Single Values: Joining Two Tables and Iterating in Perl

Example Report: Motions Database



References

- W E Meador, A R Means and F A Quiocho (1992). Target enzyme recognition by Calmodulin: 2.4 structure of a Calmodulin-Peptide Complex. Science. 257: 1251-1255. (Medline-UI **92390716**: Report or Entrez export)
- M Ikura, G M Clore, A M Gronenborn, G Zhu, C B Klee and A Bax (1992). Solution structureof a Calmodulin-Target peptide complex by multidimensional NMR. Science. 256: 632-644. (Medline-UI **92263094**: Report or Entrez export)
- W E Meador, A R Means and F A Quiocho (1993). Modulation of calmodulin plasticity in molecular recognition on the basis of x-ray structures. Science. 262: 1718-1721. (Medline-UI **94082290**: Report or Entrez export)
- L Stryer (1995). Biochemistry. New York, W H Freeman and Company.

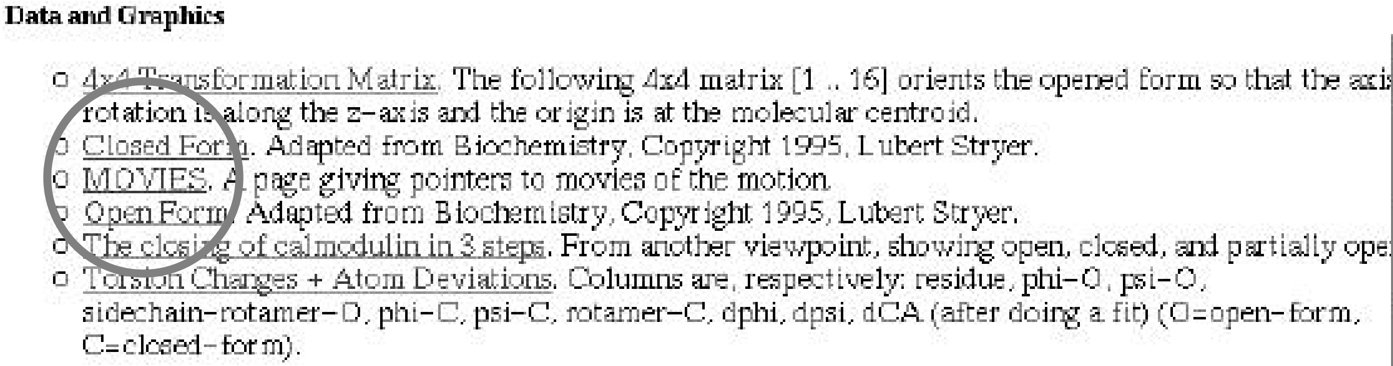


```
NAMES
id_     seq_num_n  name
aat       7        Aspartate Amino Transferase (AAT)
acetyl  1005       Acetylcholinesterase
br        97       Bacteriorhodopsin (bR)
cm        23       Calmodulin

REFS
id_           medline_I      endnote_I
acetyl        0              1007
br            90294303       893
br            93154310       313
cm            92263094       648
cm            92390716       647
cm            94082290       673

ENDNOTE_REFS
num_I         name
313           S Subramaniam, M Gerstein, D Oesterhelt and R H Hender
893           R Henderson, J M Baldwin, T A Ceska, F Zemlin, E Beckm
1007          M K Gilson, T P Straatsma, JA A McCammon, D R Ripoll,
647           W E Meador, A R Means and F A Quiocho (1992). Target e
648           M Ikura, G M Clore, A M Gronenborn, G Zhu, C B Klee an
649           B-H Oh, J Pandit, C-H Kang, K Nikaido, S Gokcen, G F-L
```

References:
Join Two Lists (Protein Names and References) with a Table Containing Key for each List (a Relation: protein has reference.)

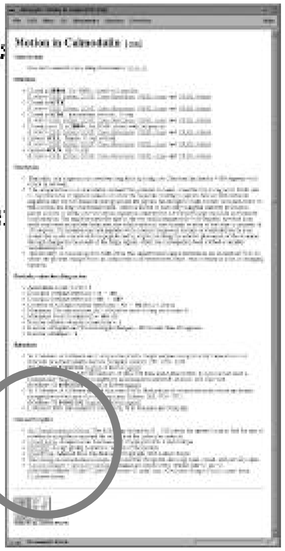
SELECT endnote_refs.name, refs.medline_I FROM endnote_refs,refs WHERE refs.id_ = ’cm' AND refs.endnote_I = endnote_refs.num_I

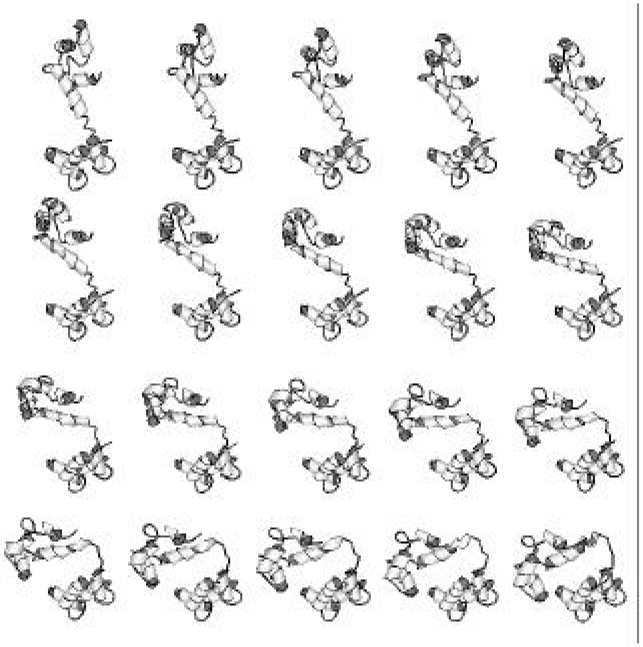
Example Report: Motions Database



Data and Graphics

- 4x4 Transformation Matrix. The following 4x4 matrix [1 .. 16] orients the opened form so that the axi rotation is along the z-axis and the origin is at the molecular centroid.
- Closed Form. Adapted from Biochemistry, Copyright 1995, Lubert Stryer.
- MOVIES. A page giving pointers to movies of the motion.
- Open Form. Adapted from Biochemistry, Copyright 1995, Lubert Stryer.
- The closing of calmodulin in 3 steps. From another viewpoint, showing open, closed, and partially ope
- Torsion Changes + Atom Deviations. Columns are, respectively: residue, phi-O, psi-O, sidechain-rotamer-O, phi-C, psi-C, rotamer-C, dphi, dpsi, dCA (after doing a fit) (O=open-form, C=closed-form).





Graphics:
How to Store Complex Data?
(File Pointers, BLOBS, OODB)