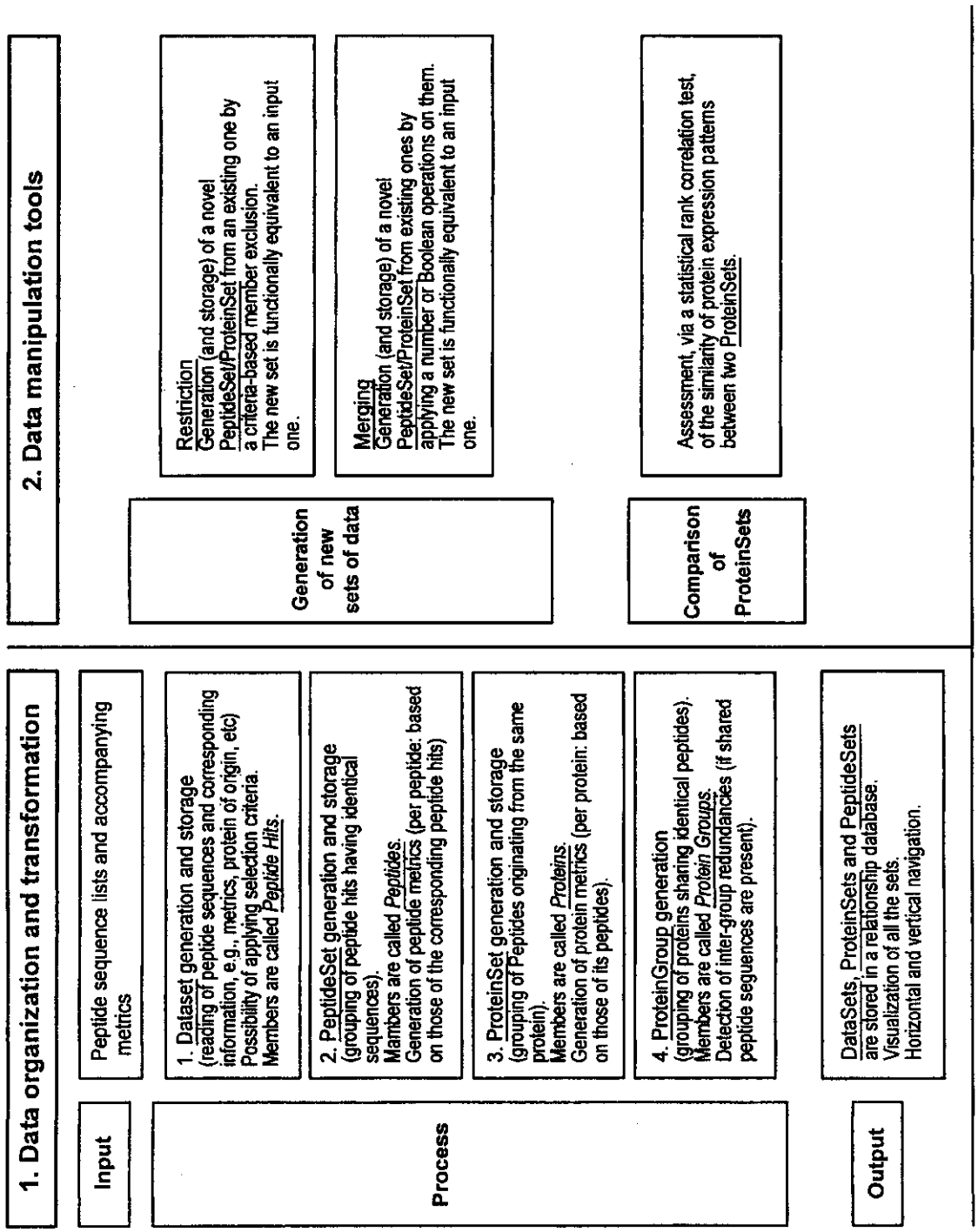

1. Data organization and transformation
2. Data manipulation tools
Input
Peptide sequence lists and accompanying metrics
Process
1. Dataset generation and storage
(reading of peptide sequences and corresponding information, e.g., metrics, protein of origin, etc)
Possibility of applying selection criteria.
Members are called Peptide Hits.
2. PeptideSet generation and storage
(grouping of peptide hits having identical sequences).
Members are called Peptides.
Generation of peptide metrics (per peptide: based on those of the corresponding peptide hits)
3. ProteinSet generation and storage
(grouping of Peptides originating from the same protein).
Members are called Proteins.
Generation of protein metrics (per protein: based on those of its peptides).
4. ProteinGroup generation
(grouping of proteins sharing identical peptides).
Members are called Protein Groups.
Detection of inter-group redundancies (if shared peptide sequences are present).
Output
DataSets, ProteinSets and PeptideSets are stored in a relationship database.
Visualization of all the sets.
Horizontal and vertical navigation.
Generation of new sets of data
Restriction
Generation (and storage) of a novel PeptideSet/ProteinSet from an existing one by a criteria-based member exclusion.
The new set is functionally equivalent to an input one.
Merging
Generation (and storage) of a novel PeptideSet/ProteinSet from existing ones by applying a number or Boolean operations on them.
The new set is functionally equivalent to an input one.
Comparison of ProteinSets
Assessment, via a statistical rank correlation test, of the similarity of protein expression patterns between two ProteinSets.

Fig. 1

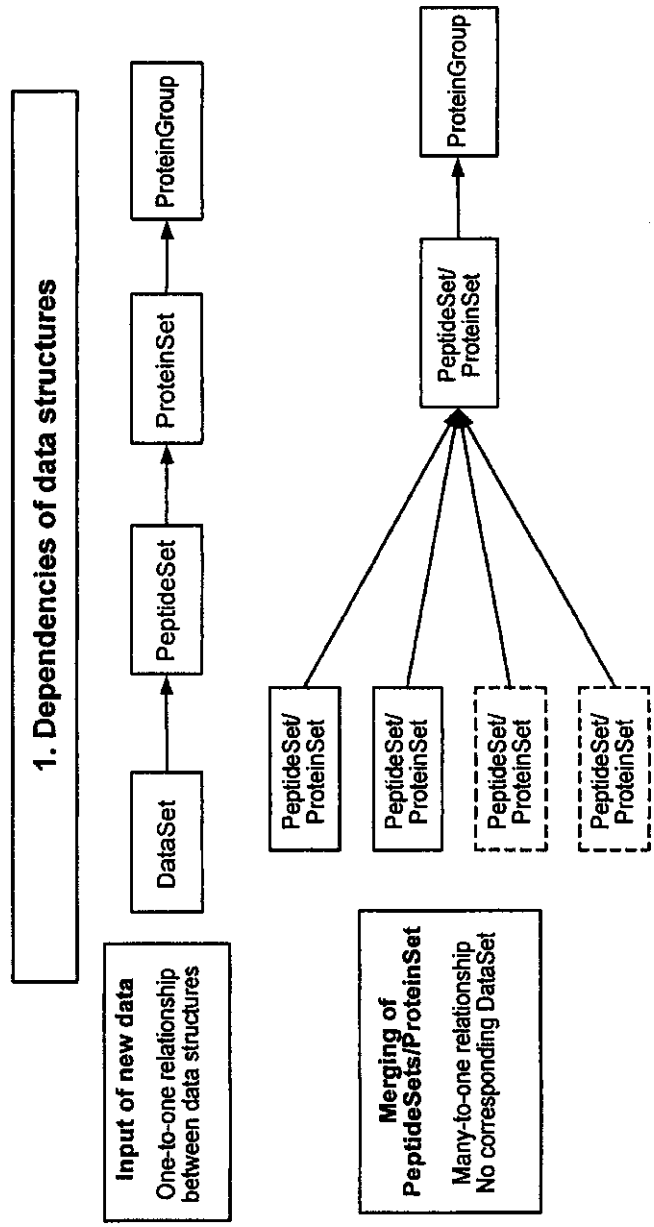
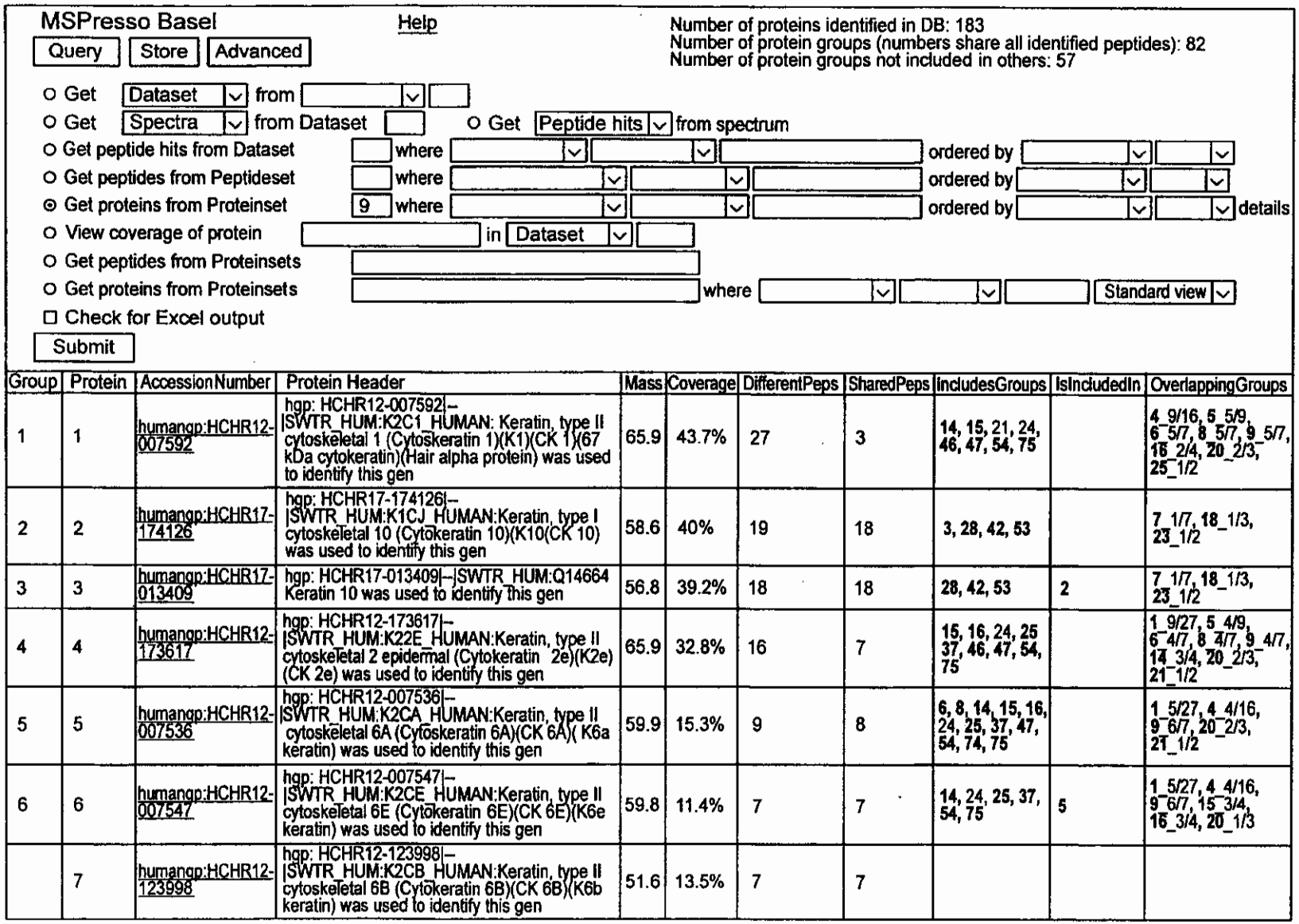

1. Dependencies of data structures
DataSet
PeptideSet
ProteinSet
ProteinGroup
Input of new data
One-to-one relationship
between data structures
PeptideSet/
ProteinSet
PeptideSet/
ProteinSet
PeptideSet/
ProteinSet
PeptideSet/
ProteinSet
PeptideSet/
ProteinSet
ProteinGroup
Merging of
PeptideSets/ProteinSet
Many-to-one relationship
No corresponding DataSet

Fig. 2

Sequence	MHplus	dM	Charge	RT	MaxCorr.	dCn	Rank	Duplicates	DuplicatesModified	Modifications
YVSAYIPDATWYDYETGEK	2271.013	-0.002	2	81.146	4.233	0.637	1	2	0	
YTGDYPSR	958.427	-0.001	2	16.282	2.02	0.477	1	1	0	
YPIEHGIITNWDDMEK	1976.906	-0.002	3	79.395	2.941	0.562	1	0	2	14 M
YNDEPVQIR	1133.559	0.002	2	37.426	2.462	0.426	1	3	0	
YLDGLTAER	1037.526	0	2	48.007	3.496	0.532	1	10	0	
YEVPVPLNIPSAPSSTNEGR	2127.072	-0.001	2	71.618	4.921	0.59	1	6	0	
YETELNLR	1037.526	0	2	45.054	2.131	0.244	1	1	0	
YENEVALR	993.5	0	2	34.583	2.864	0.31	1	5	0	
YEELQVTGR	1193.616	-0.001	2	53.142	3.291	0.634	1	11	0	
YEELQVTAGR	1165.585	-0.002	2	41.102	3.336	0.644	1	10	0	
YEELQQTAGR	1194.575	-0.002	2	28.098	3.45	0.548	1	5	0	
YEELQITAGR	1179.6	-0.001	2	90.315	3.673	0.603	1	67	0	
WTTQSFSDNEK	1342.591	-0.001	2	41.665	2.142	0.534	1	1	0	
WTLLQEQGTK	1203.637	-0.002	2	63.286	3.308	0.586	1	6	0	
WTLGGMVNR	1049.52	0	2	60.986	2.214	0.239	1	0	1	6 M

Fig. 3



Group	Protein	AccessionNumber	Protein Header	Mass	Coverage	DifferentPeps	SharedPeps	IncludesGroups	IsIncludedIn	OverlappingGroups
1	1	humangp:HCHR12-007592	hgp: HCHR12-007592|--|SWTR_HUM:K2C1_HUMAN: Keratin, type II cytoskeletal 1 (Cytoskeratin 1)(K1)(CK 1)(67 kDa cytokeratin)(Hair alpha protein) was used to identify this gen	65.9	43.7%	27	3	14, 15, 21, 24, 46, 47, 54, 75		4_9/16, 5_5/9, 6_5/7, 8_5/7, 9_5/7, 16_2/4, 20_2/3, 25_1/2
2	2	humangp:HCHR17-174126	hgp: HCHR17-174126|--|SWTR_HUM:K1CJ_HUMAN:Keratin, type I cytoskeletal 10 (Cytokeratin 10)(K10(CK 10) was used to identify this gen	58.6	40%	19	18	3, 28, 42, 53		7_1/7, 18_1/3, 23_1/2
3	3	humangp:HCHR17-013409	hgp: HCHR17-013409|--|SWTR_HUM:Q14664 Keratin 10 was used to identify this gen	56.8	39.2%	18	18	28, 42, 53	2	7_1/7, 18_1/3, 23_1/2
4	4	humangp:HCHR12-173617	hgp: HCHR12-173617|--|SWTR_HUM:K22E_HUMAN:Keratin, type II cytoskeletal 2 epidermal (Cytokeratin 2e)(K2e) (CK 2e) was used to identify this gen	65.9	32.8%	16	7	15, 16, 24, 25 37, 46, 47, 54, 75		1_9/27, 5_4/9, 6_4/7, 8_4/7, 9_4/7, 14_3/4, 20_2/3, 21_1/2
5	5	humangp:HCHR12-007536	hgp: HCHR12-007536|--|SWTR_HUM:K2CA_HUMAN:Keratin, type II cytoskeletal 6A (Cytoskeratin 6A)(CK 6A)(K6a keratin) was used to identify this gen	59.9	15.3%	9	8	6, 8, 14, 15, 16, 24, 25, 37, 47, 54, 74, 75		1_5/27, 4_4/16, 9_6/7, 20_2/3, 21_1/2
6	6	humangp:HCHR12-007547	hgp: HCHR12-007547|--|SWTR_HUM:K2CE_HUMAN:Keratin, type II cytoskeletal 6E (Cytokeratin 6E)(CK 6E)(K6e keratin) was used to identify this gen	59.8	11.4%	7	7	14, 24, 25, 37, 54, 75	5	1_5/27, 4_4/16, 9_6/7, 15_3/4, 16_3/4, 20_1/3
	7	humangp:HCHR12-123998	hgp: HCHR12-123998|--|SWTR_HUM:K2CB_HUMAN:Keratin, type II cytoskeletal 6B (Cytokeratin 6B)(CK 6B)(K6b keratin) was used to identify this gen	51.6	13.5%	7	7			

Fig. 4