

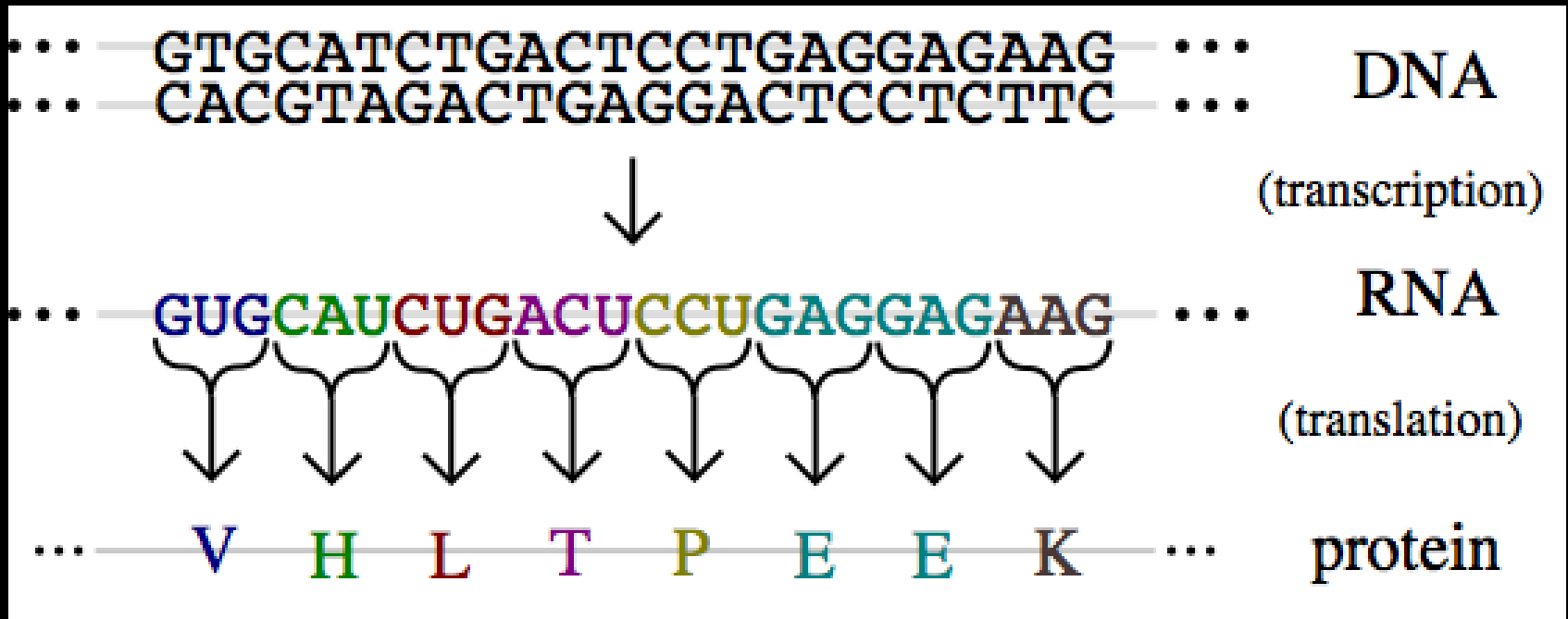


LEIDEN UNIVERSITY
MEDICAL CENTER

Use of ontologies for automated data
processing and their challenges:
a bioinformatics view

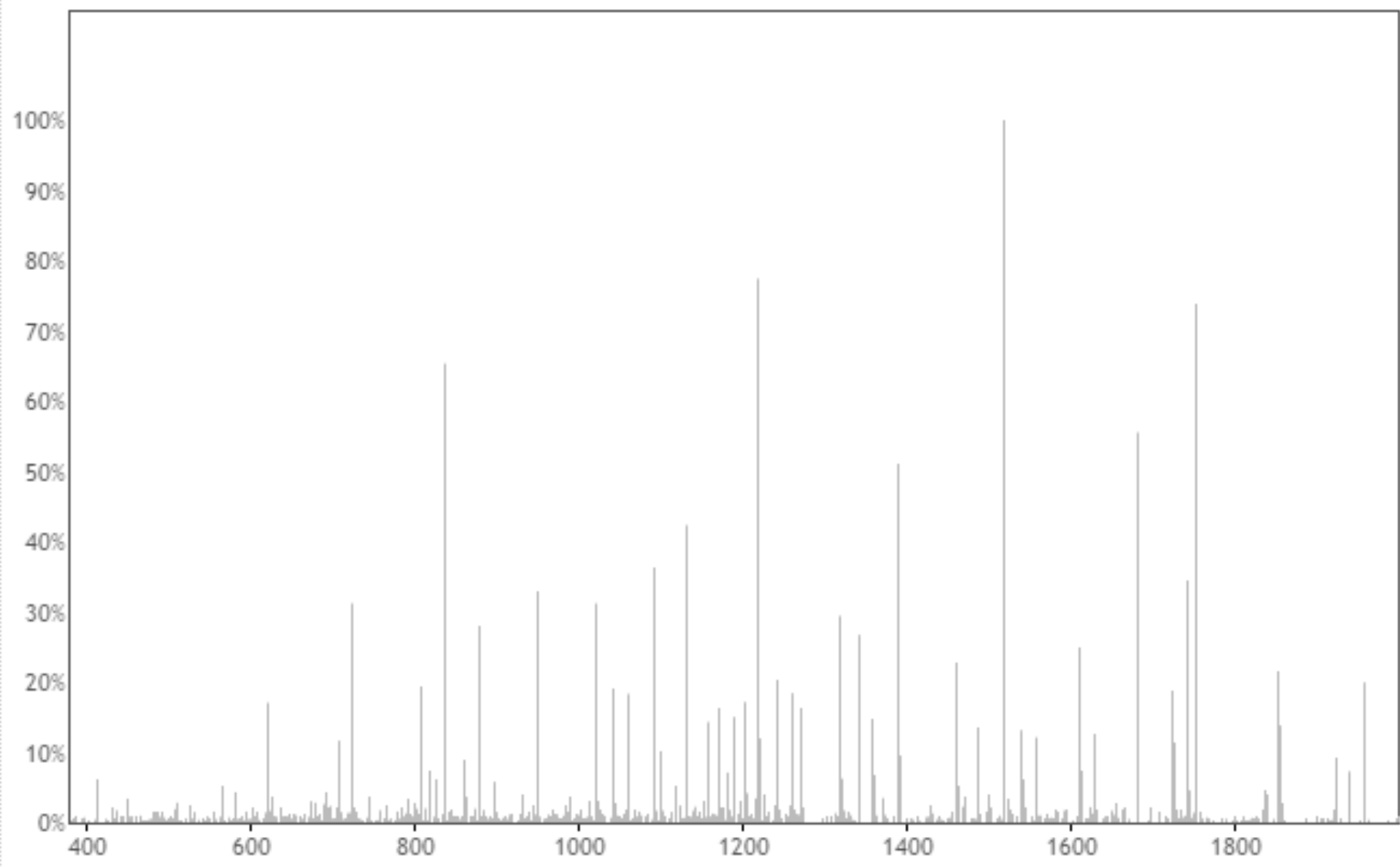
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**Image from Bruker
Daltonics**



- Identification
- Quantification

Identification

MS/MS

eg. **Ion trap**: low resolution > Relatively cheap per run

Quantification

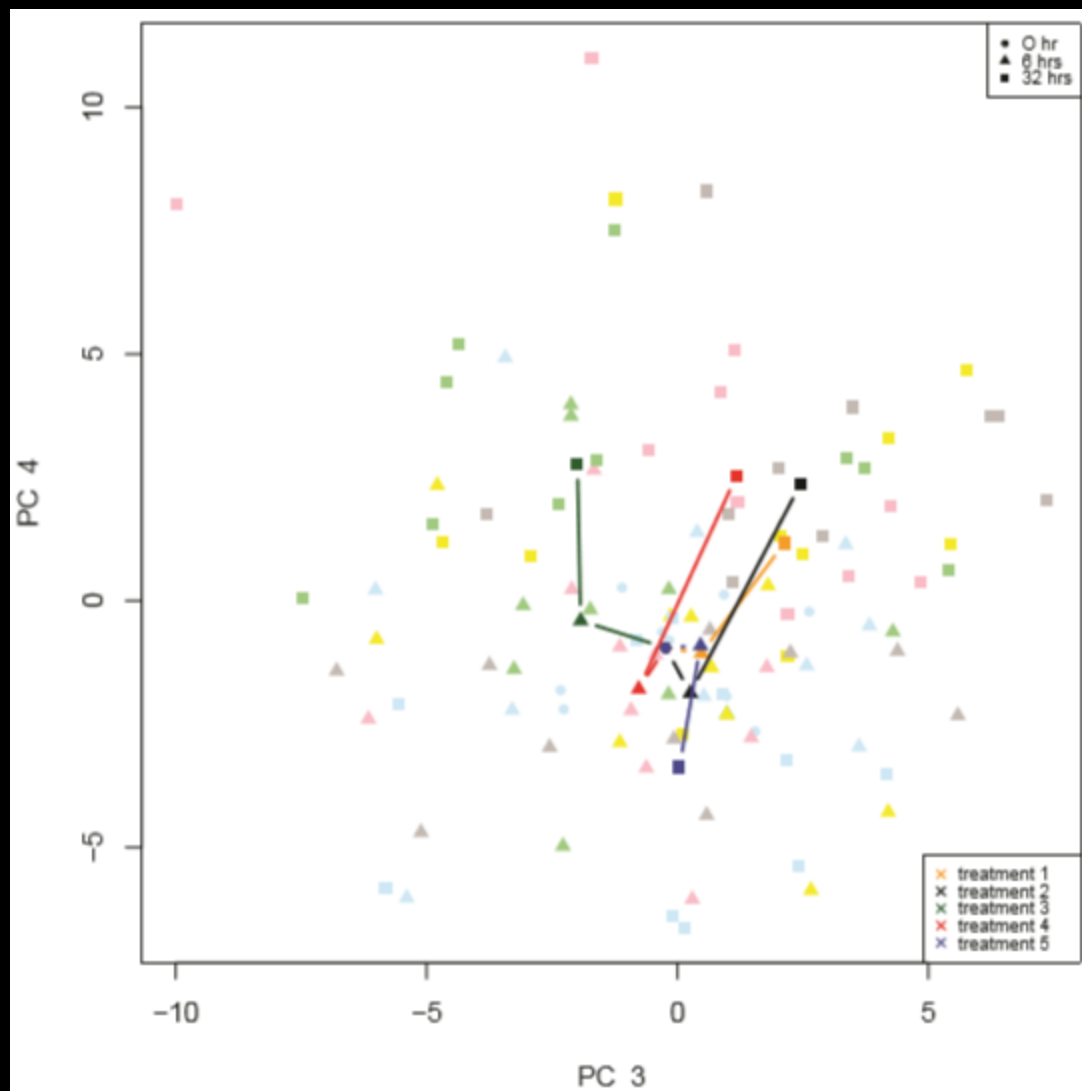
MS

eg. **FTICR**: high resolution > Expensive

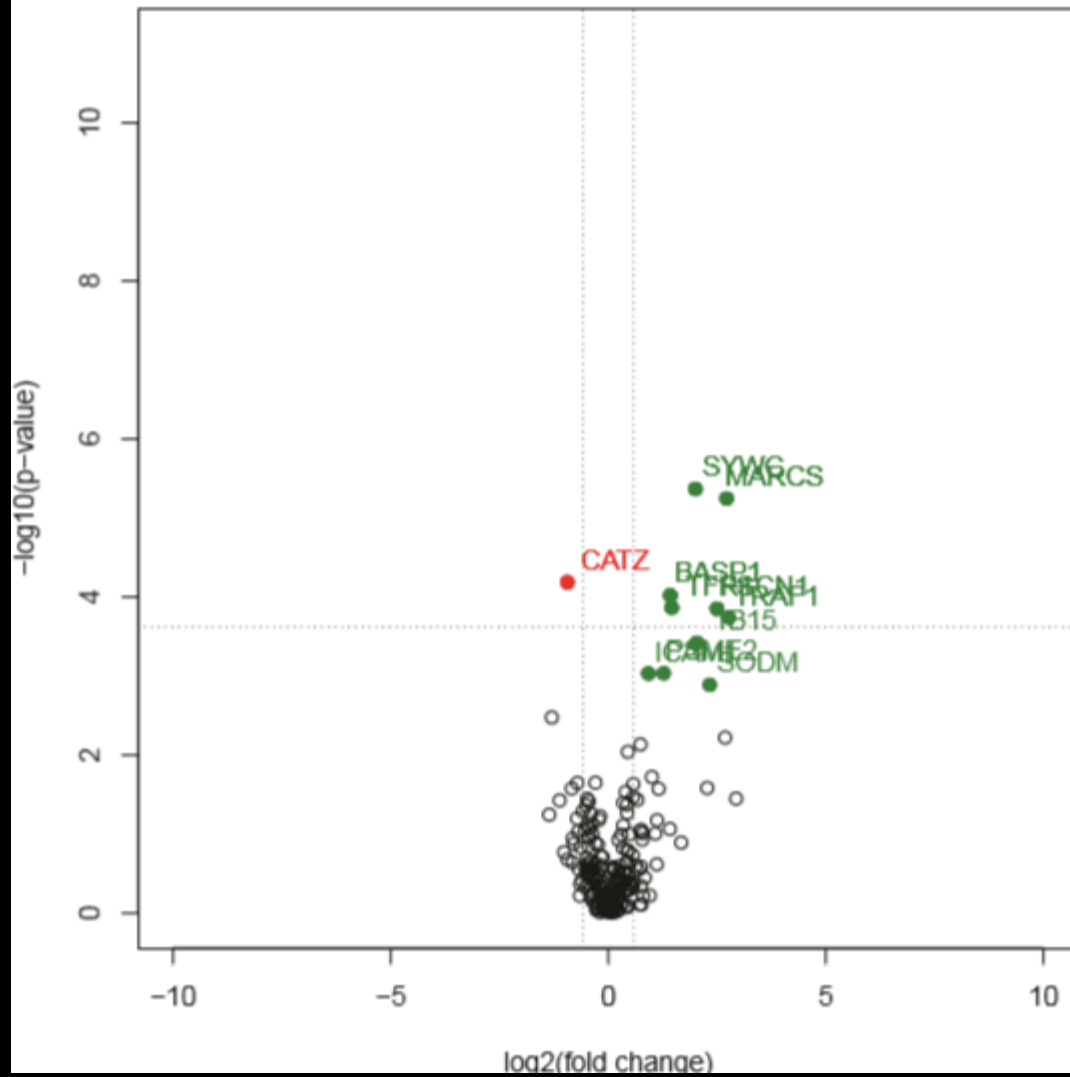
1. Peptide/protein identification
2. Alignment
3. Warping
4. Peptide assignment validation
5. Recalibration
6. Quantification

1	PEPTIDE	PROTEIN		
2			SEA	IFNy
3			32	6
4			591	594
5				
6	SYVTTSTR	sp P08670 VIME_HUMAN	399514816	855244864
7	DSYVGDEAQSKR	sp P60709 ACTB_HUMAN	1103222.625	2741537
8	FSDAASPR	sp P30464 1B15_HUMAN	8596512	12697854
9	VPVHDVTDASK	sp P21333 FLNA_HUMAN	3440370.25	13634095
10	DAVTYTEHAK	sp P62805 H4_HUMAN	36951160	216957504
11	QVDQLTNDK	sp P08670 VIME_HUMAN	369075392	825738432
12	DSYVGDEAQSK	sp P60709 ACTB_HUMAN	858582272	2200605696
13	ISAEGGEQVER	sp Q9BQE5 APOL2_HUMAN	1441425.125	2202019.25
14	VGEFSGANK	sp P10599 THIO_HUMAN	204935168	159583760
15	VLVQNAAGSQEK	sp Q9Y490 TLN1_HUMAN	2738871.75	12318588
16	VYSTSVTGSR	sp Q9H299 SH3L3_HUMAN	154226192	310132832
17	QDVNDASLAR	sp P08670 VIME_HUMAN	455627616	1012007808
18	LLEGEESR	sp P08670 VIME_HUMAN	299053056	655997120
19	VTDALNATR	sp P10809 CH60_HUMAN	13392219	50331816
20	VLANPGNSQVAR	sp Q14974 IMB1_HUMAN	2003451.125	5595640
21	LQDAEIAR	sp P06703 S10A6_HUMAN	271635744	458409952
22	TPGPGAQSALR	sp P62263 RS14_HUMAN	3307595	21660038
23	MATNAAAQNAIK	sp Q9Y490 TLN1_HUMAN	1118888.625	5458304
24	TIQVDNTDAEGR	sp P28838 AMPL_HUMAN	6126292	14676089
25	SGAQASSTPLSPTR	sp P02545 LMNA_HUMAN	1671472	8454731

1. Peptide/protein identification
2. Alignment
3. Warping
4. Peptide assignment validation
5. Recalibration
6. Quantification
7. Statistics
8. Plotting



treatment 1 32 vs 6 h



“...And Hera swiftly touched the horses with the lash, and self-bidden (αὐτ’ ὀματα) groaned upon their hinges the gates of heaven which the Hours had in their keeping...”

Illiad, Book V, 749

automatic (adj):

capable of operating without external control or intervention



>>Information processing analogy<<

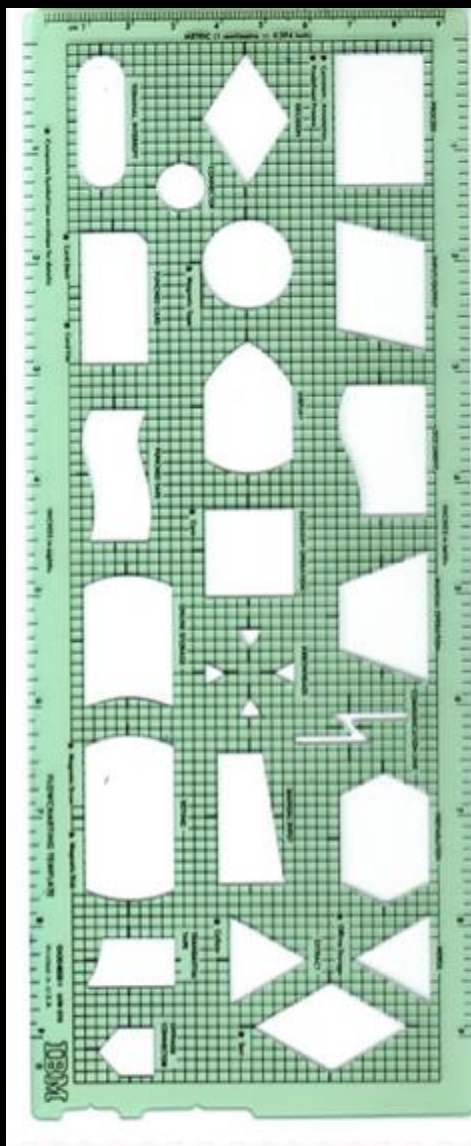
compute -> information processing

computer -> information processing machine

Konrad Zuse, Rechnender Raum



1. Peptide/protein identification
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IBM

FLOWCHARTING TEMPLATE

The symbols on this envelope and the enclosed template conform to the International Organization for Standardization (ISO) International Standard 1028 - "Information Processing-Flowchart Symbols", and American National Standard, Flowchart Symbols and Their Usage in Information Processing, ANSI X3.5-1970. IBM usages beyond the above standards are three symbols: off-page connector, transmittal tape, and keying, which are identified IBM.

* Composite Symbols (preceded by a star) are those drawn by adding to or combining shapes provided by cutouts in the template.

On this envelope, symbols are in three groups: (1) basic symbols; (2) processing and sequencing symbols related to programming; (3) input/output, communication link, and processing symbols related to systems.

BASIC Symbols

	Any processing function defined operation, including change in routing form, or location of information.	Additional descriptive classification, comment, or other data normally to symbols as operations.		Composite, Alternative
	General life function; information available for processing (input), or recording of processed information (output).			CONNECTOR: Exit to, or entry from, another part of chart.
				OFFPAGE CONNECTOR: for entry to or exit from a page.

ARROWHEADS and Flowlines: In linking symbols, these show operations sequence and direction. Arrowheads required if path on any linkage is not left-to-right or top-to-bottom.



Symbols related to PROGRAMMING

	A decision or switching-type operation that determines which of a number of alternative paths followed.	Iteration modification to change program set to include, modify an inner routine, terminate a routine.	
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	One or more named operations or program areas specified in a reference to another set of flowcharts.	A terminal gate in a flowchart; stop, skip, delay, or transfer may show exit from a closed subroutine.	
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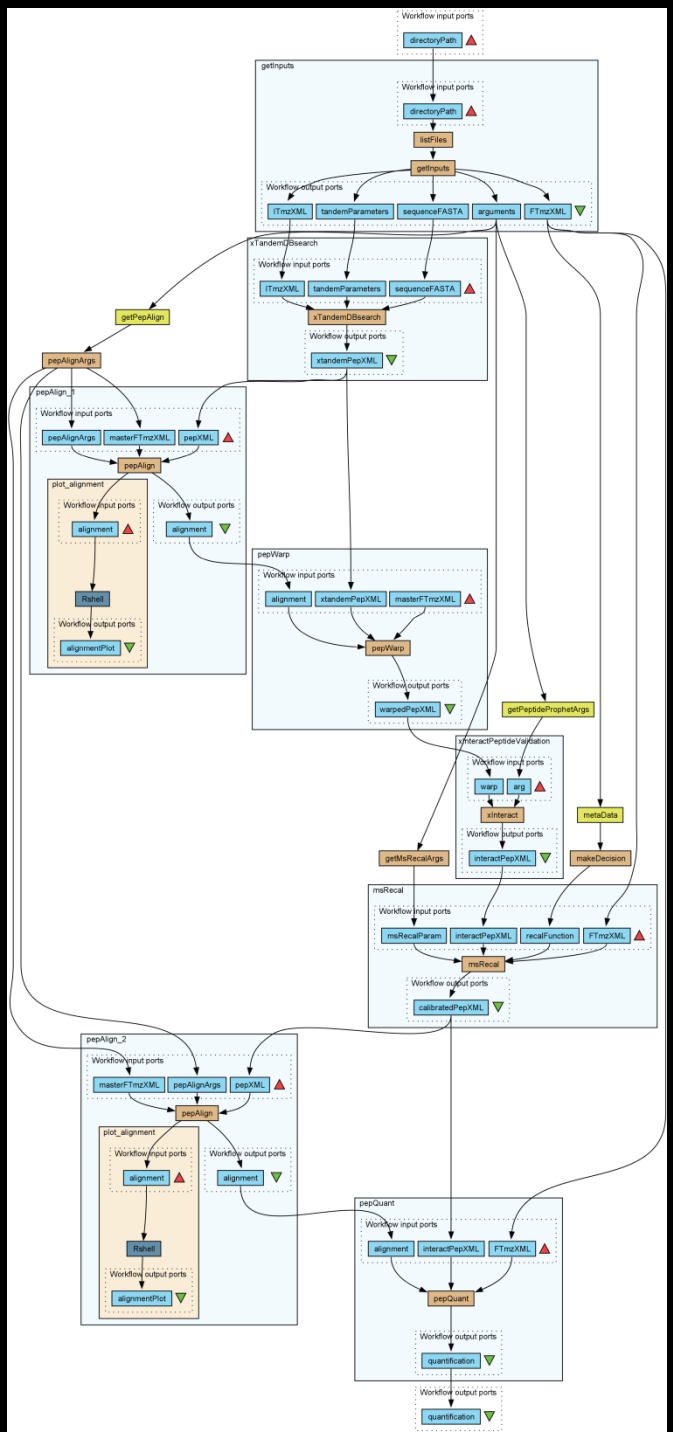


BASIC Symbols (shown at left) also are used in program flowcharting and in systems flowcharting (see other side of envelope).



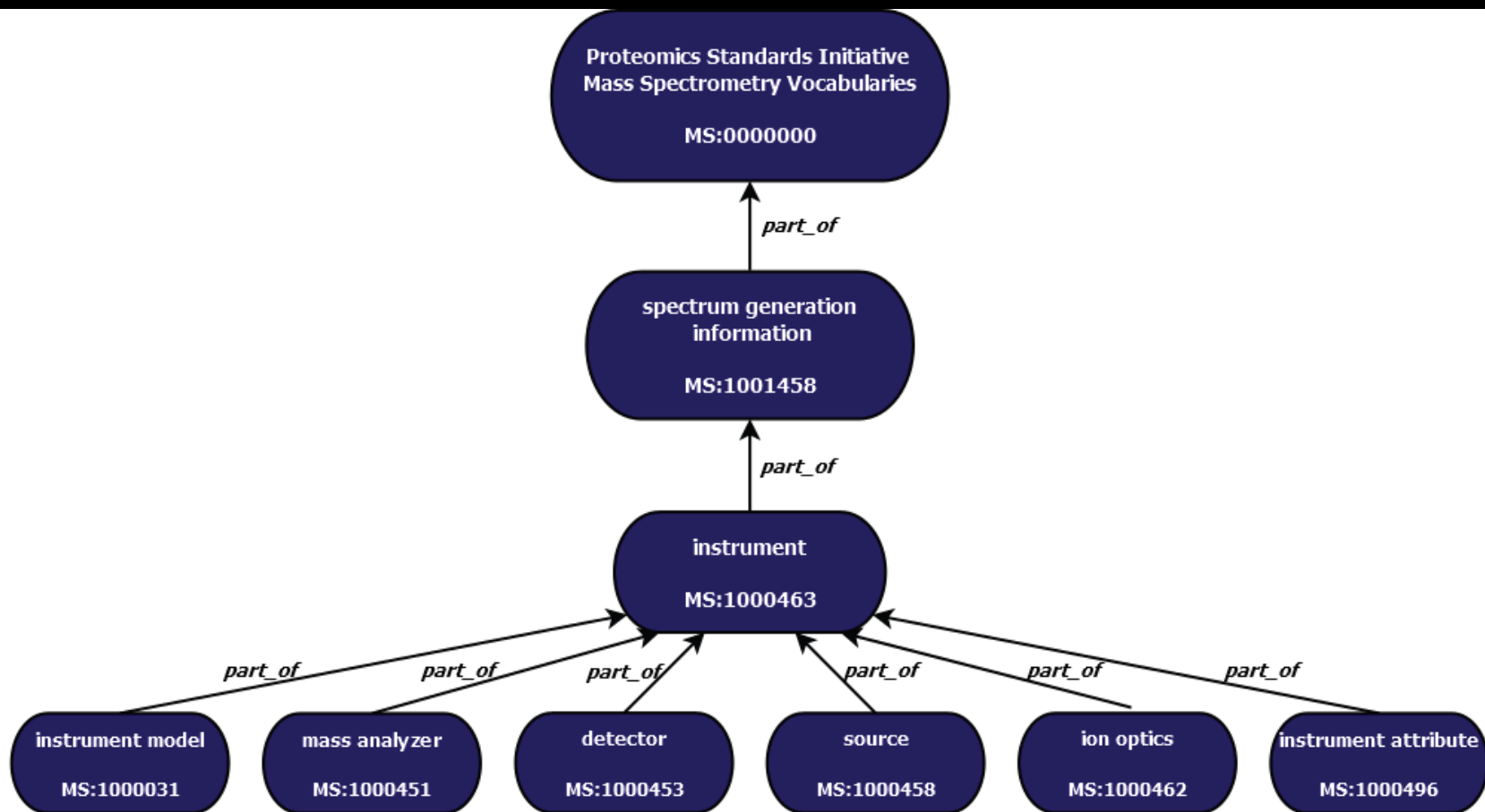
Ceci n'est pas une pipe.

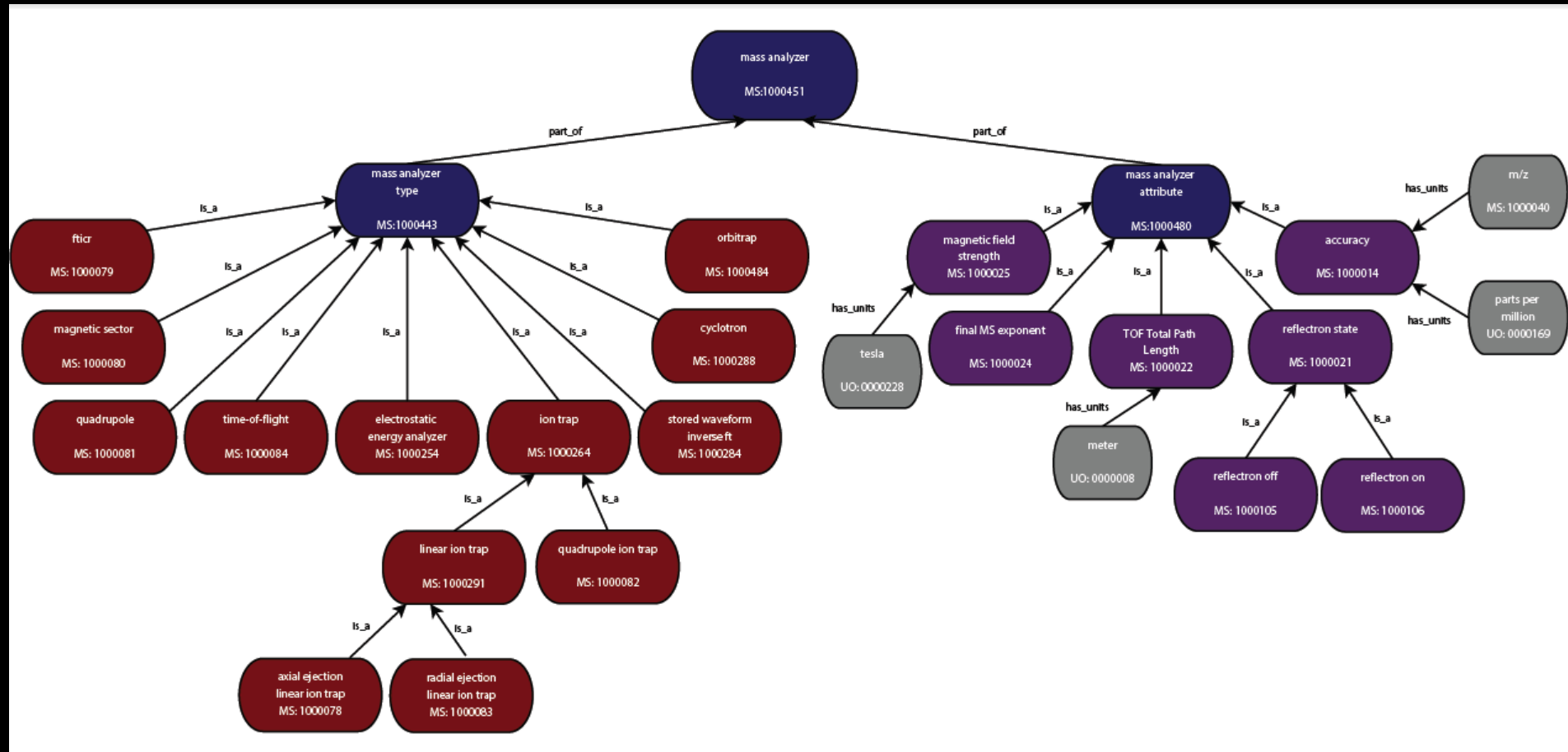
Magnific




Systems that think like humans	Systems that think rationally
Systems that act like humans	Systems that act rationally

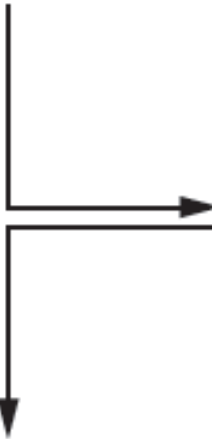
- *A scientific ontology* is a concise and unambiguous description of what principle entities are relevant to an application domain and the relationships between them.
- There are many existing subject-specific ontologies







MS:1000443	default_calibration_function
MS:1000082	$(m/z)_1 = A(m/z)_0 + B$
MS:1000084	$(m/z)_1 = At_0^2 + Bt_0 + C$
MS:1000079	$(m/z)_1 = A/(f_0 + B)$
MS:1000484	$(m/z)_1 = A/f_0^2$



MS:1000008	default_calibrants
MS:1000397	[]
MS:1000398	[593.157605, 667.176396, ...]
MS:1000075	[379.092463, 401.074407, ...]

+





- Intelligent workflows making automated decisions according to metadata, using ontologies.
- Recovery from errors caused by non-optimal parameters.
- The user can focus on the general information flow and the task in hand.

“One always looks at biology as a kind of guide, even though it never invents the wheel, and even though we don’t make flapping wings for airplanes because we thought of a better way.”

Richard Feynman

Infinitesimal Machinery, 1983