

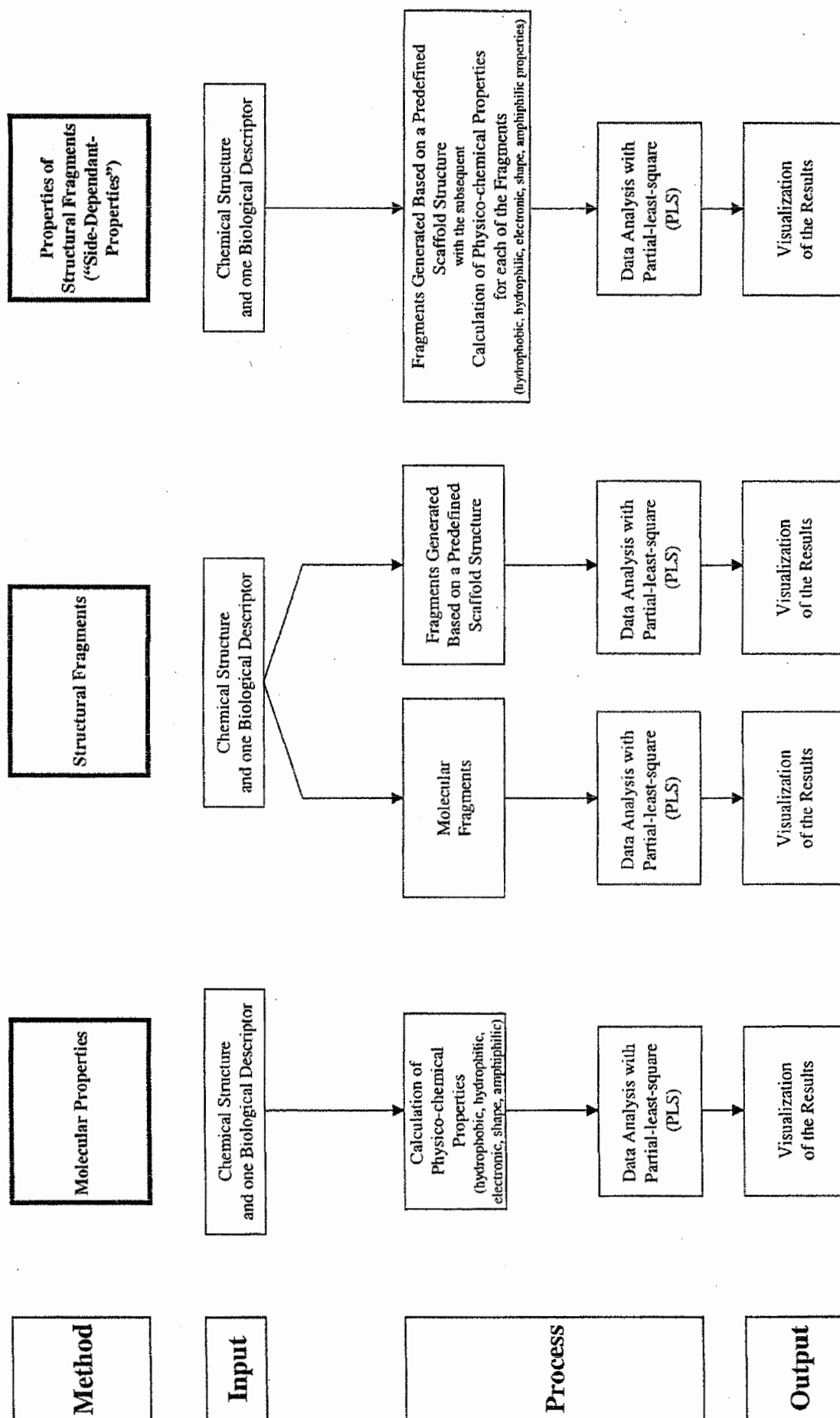
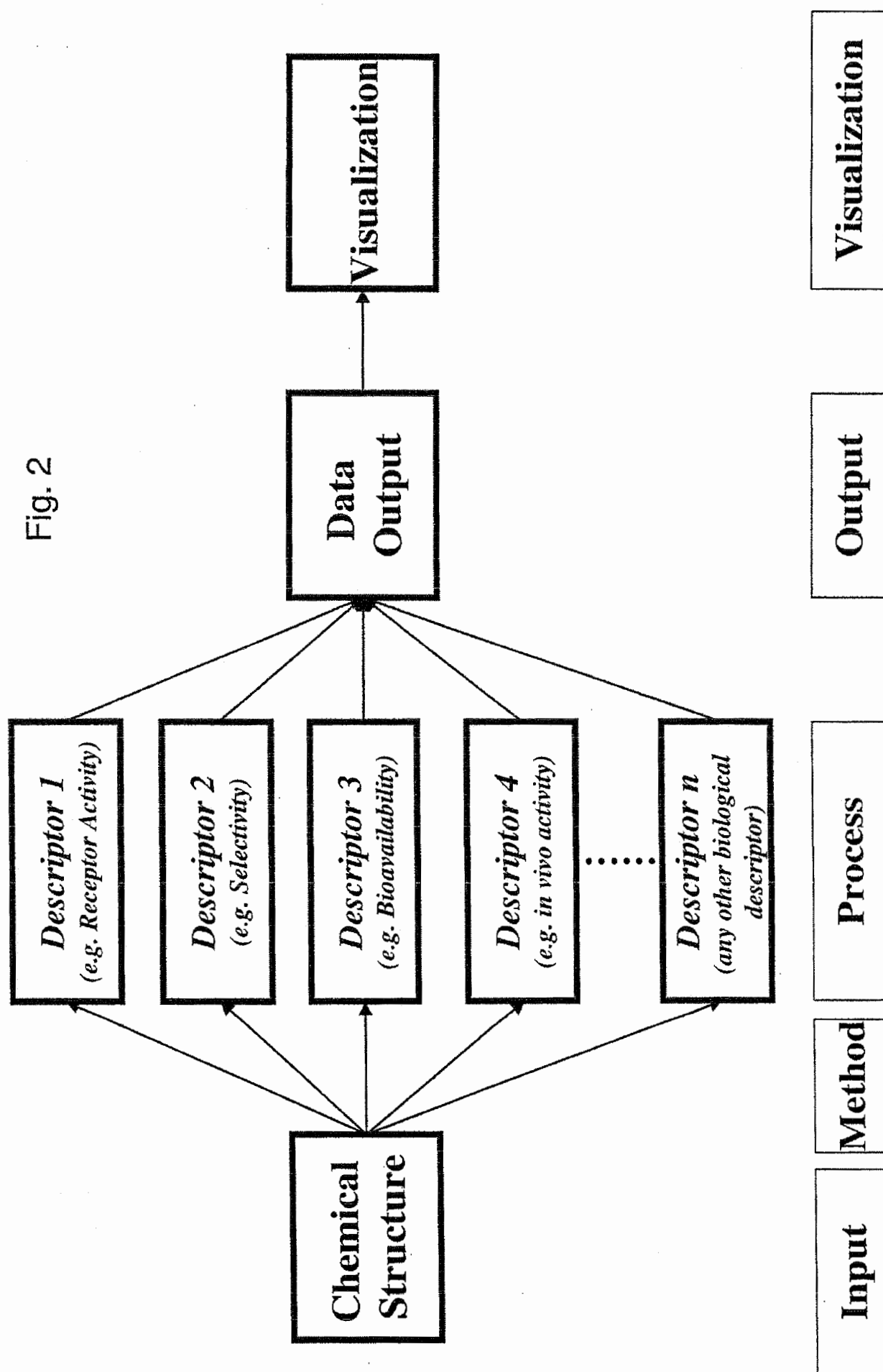


Fig. 1



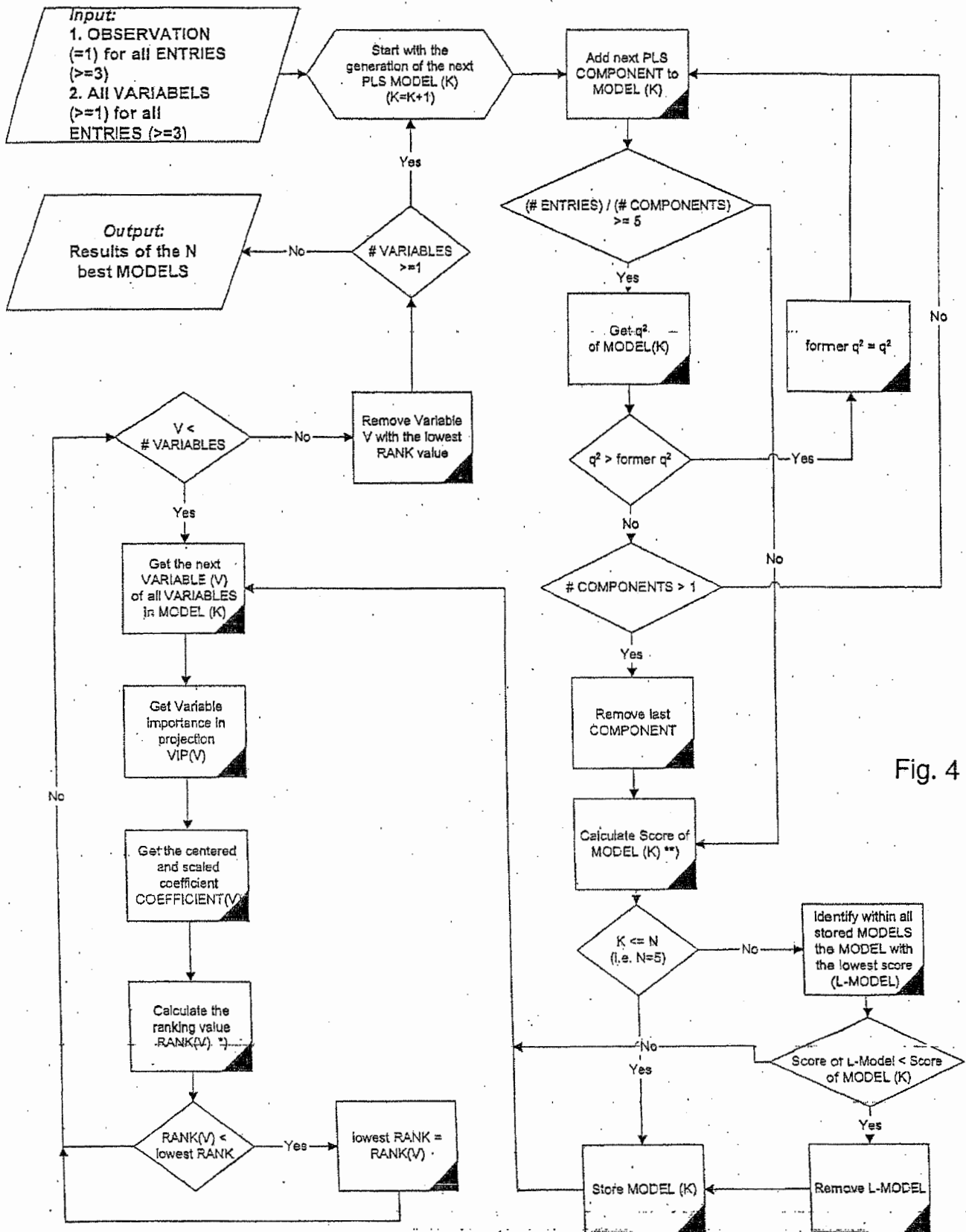


Fig. 4

*) $\text{Rank}(V) = \text{VIP}(V) \cdot |\text{Coefficient}(V)|$

**) $\text{Model Score} = \frac{r^2}{\sqrt{(r^2 - q^2) \cdot \sqrt{\#V}}}$ OR $\text{Model Score} = \frac{r^2}{\sqrt{(r^2 - q^2) \cdot \sqrt{0.05 \cdot (\#V - 1)^2 + 0.01 \cdot (\#V - 1) + 1}}}$
for $\#V > 1$

Rosara - Microsoft Internet Explorer provided by F.Hoffmann-La Roche Ltd

File Edit View Favorites Tools Help

Back Journals Physico-chemical properties Google Compendium_CH LEO New E-Journal Link PDR Roche Lexikon Medizin ROSARA

Address http://compchem.bas.roche.com:8080/cgi-bin/MP_ENTRY?ROSARA.html

Google

ROSARA

Roche SAR Analyser

Tries to find elementary correlations between your data (e.g. from PD, PK, Tox) and molecular properties

Data submission fields:

List with SRN numbers

List with observations

Calculate **Reset**

Example

Header required (SRN)

(Name of Observation)

List with SRN numbers

RO0635290-000
RO0638207-000
RO0635590-000
RO0674294-000
RO0678361-000
RO0638208-000
RO0678867-000
RO0631908-000
RO0256981-000
RO0161536-000
RO0628081-000

List with observations

phERG
7.04
5.85
5.4
5
4.51
5
4.59
6.16
5.89
5.8
4.54

Number of rows has to be identical (please delete empty rows)

For comments or additional information, please contact [Holger Fischer](#)

Done Local Intranet

Fig. 5

Rosara - Model Overview - Microsoft Internet Explorer provided by F.Hoffmann-La Roche Ltd

File Edit View Favorites Tools Help

Back
New E-Journal Link
PDR
Roche Lexikon Medizin
ROSARA

Address
http://rbaw01.bas.roche.com:8080/htbin/pc1_fisch_PLS.cgi?FIRST

Google



Model Overview

Model	Regression Coeff. - R2	Cross Validation - Q2	Number of Variables
15	0.544	0.466	5
16	0.727	0.586	4
17	0.674	0.558	3
18	0.635	0.595	2
19	0.638	0.609	1

General Remarks:

- The higher R2 and Q2 the "better" the model.
- The lower the Number of Variables the easier the interpretation of the model.

Additional calculations are performed. Please wait...

Model	Model Summary	Transfer Plots to Spotfire	Validate the Model	Keep the Model
15		☒ Regression ☐ Coefficients	Predict List Predict Single	Not yet available
16		☒ Regression ☐ Coefficients	Predict List Predict Single	Not yet available
17		☒ Regression ☐ Coefficients	Predict List Predict Single	Not yet available
18		☒ Regression ☐ Coefficients	Predict List Predict Single	Not yet available
19		☒ Regression ☐ Coefficients	Predict List Predict Single	Not yet available

See List with Abbreviations

Interpretation Coefficients

Local Intranet

Fig. 6

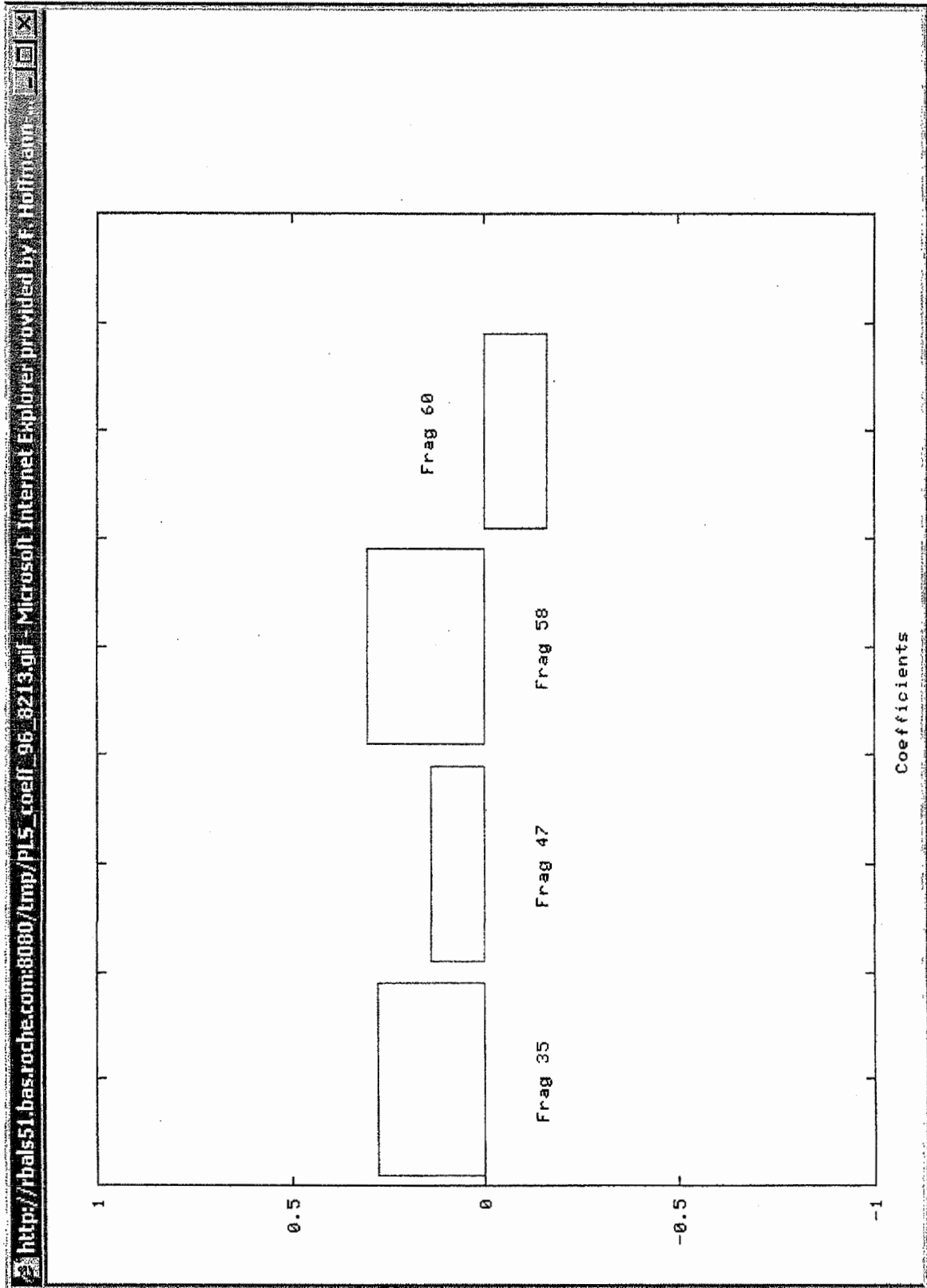


Fig. 7

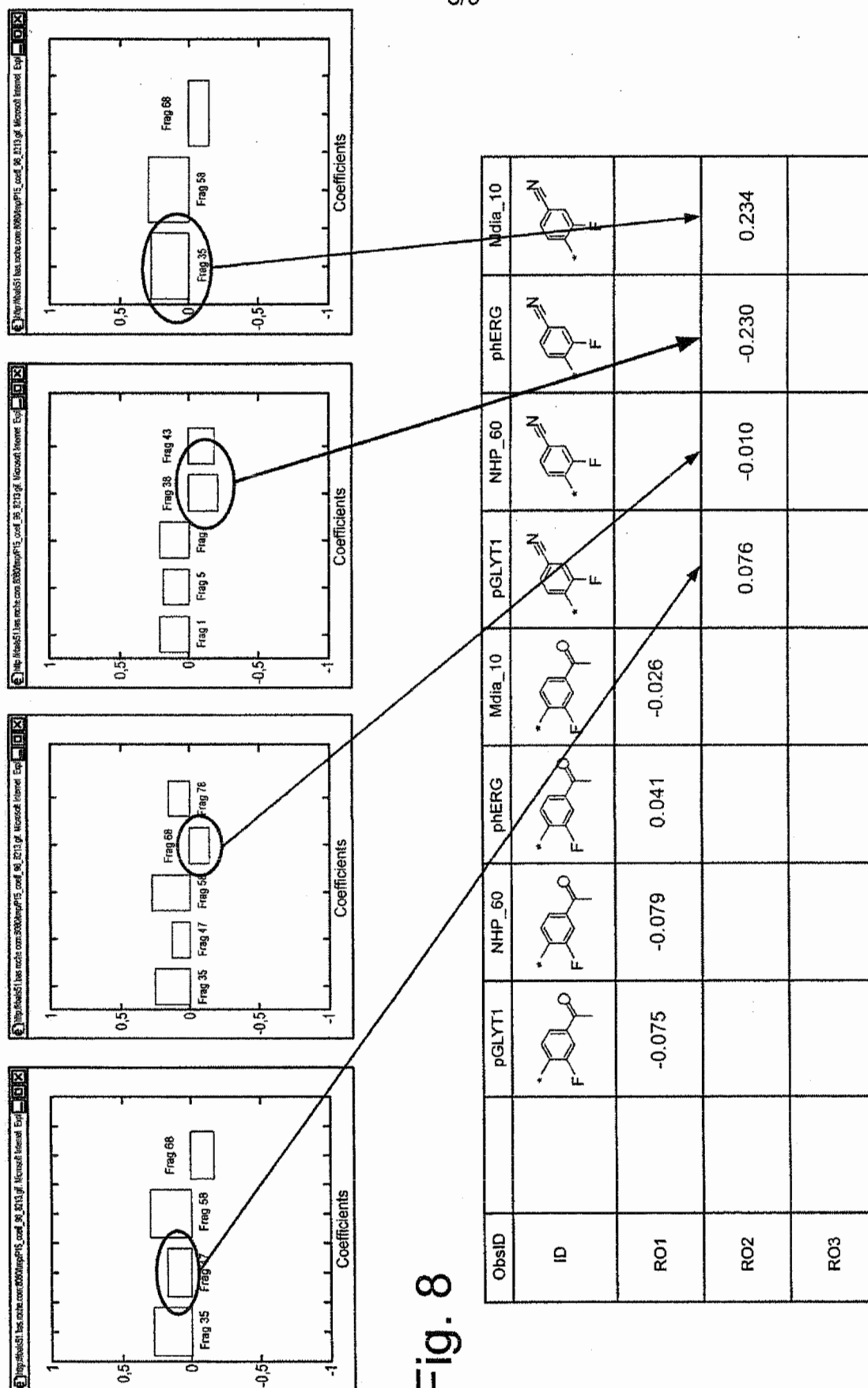


Fig. 8

Structure	pGLYT1	NHP_60	phERG	Mdia_10	Ranking Score
Chemistry 12	0.222	0.14	0.126	0.122	0.528
Chemistry 13	0.222	0.14	0.126	0.122	0.528
Chemistry 14	0.222	0.14	0.126	0.122	0.528
Chemistry 15	0.18	0.132	0.107	0.143	0.514
Chemistry 16	0.18	0.132	0.107	0.143	0.514
Chemistry 17	0.18	0.132	0.107	0.143	0.514
Chemistry 21	0.192	0.15	0.054	0.134	0.488
Chemistry 22	0.192	0.15	0.054	0.134	0.488
Chemistry 23	0.192	0.15	0.054	0.134	0.488
Chemistry 41	0.074	0.121	0.072	0.169	0.483
Chemistry 42	0.074	0.121	0.072	0.169	0.483
Chemistry 43	0.074	0.121	0.072	0.169	0.483
Chemistry 27	0.15	0.142	0.035	0.155	0.474
Chemistry 28	0.15	0.142	0.035	0.155	0.474
Chemistry 29	0.15	0.142	0.035	0.155	0.474
Chemistry 30	0.118	0.112	0.077	0.171	0.472
Chemistry 31	0.118	0.112	0.077	0.171	0.472
Chemistry 32	0.118	0.112	0.077	0.171	0.472
Chemistry 38	0.069	0.096	0.112	0.162	0.466
Chemistry 39	0.069	0.096	0.112	0.162	0.466
Chemistry 40	0.069	0.096	0.112	0.162	0.466

Fig. 9