

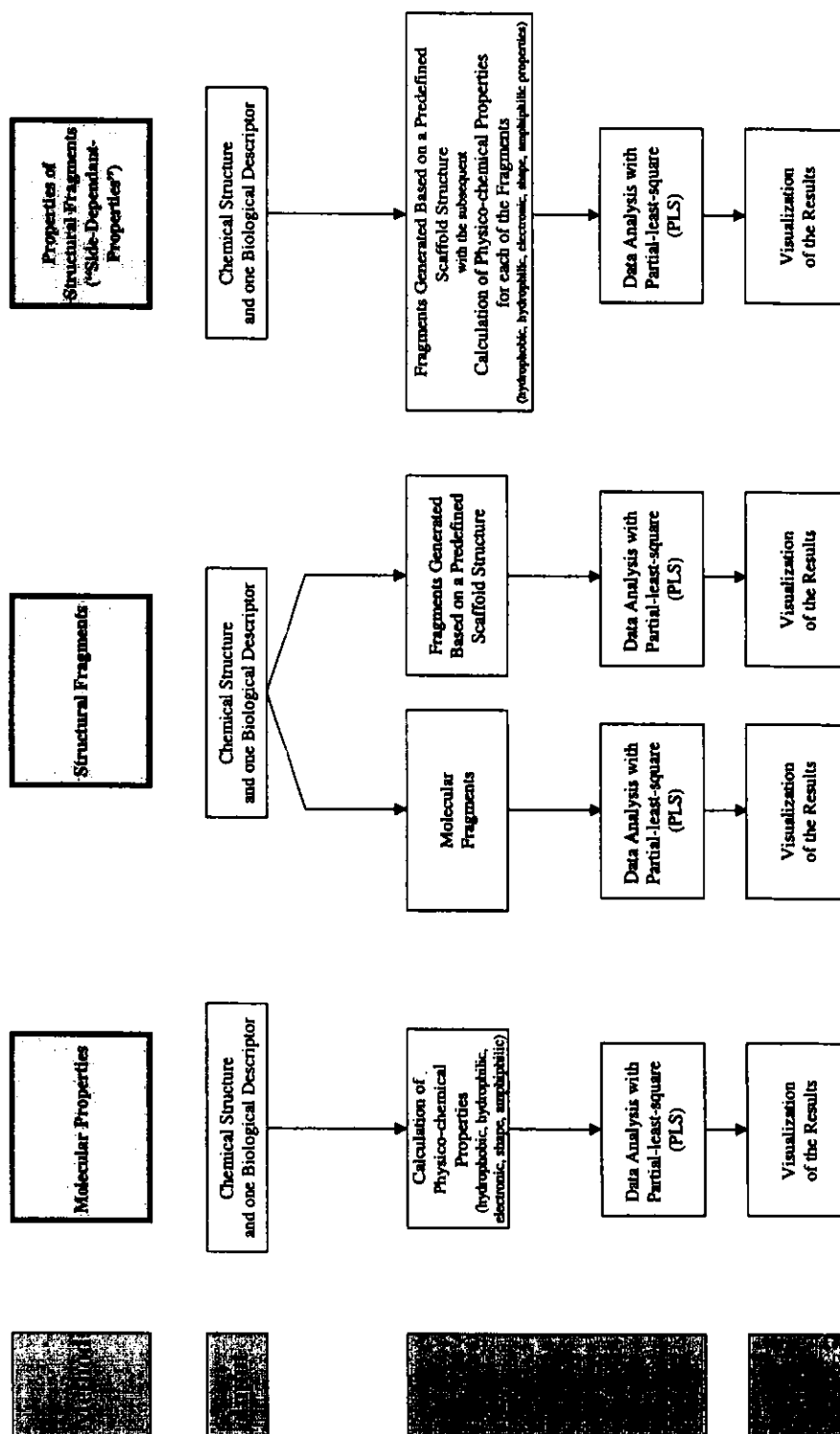
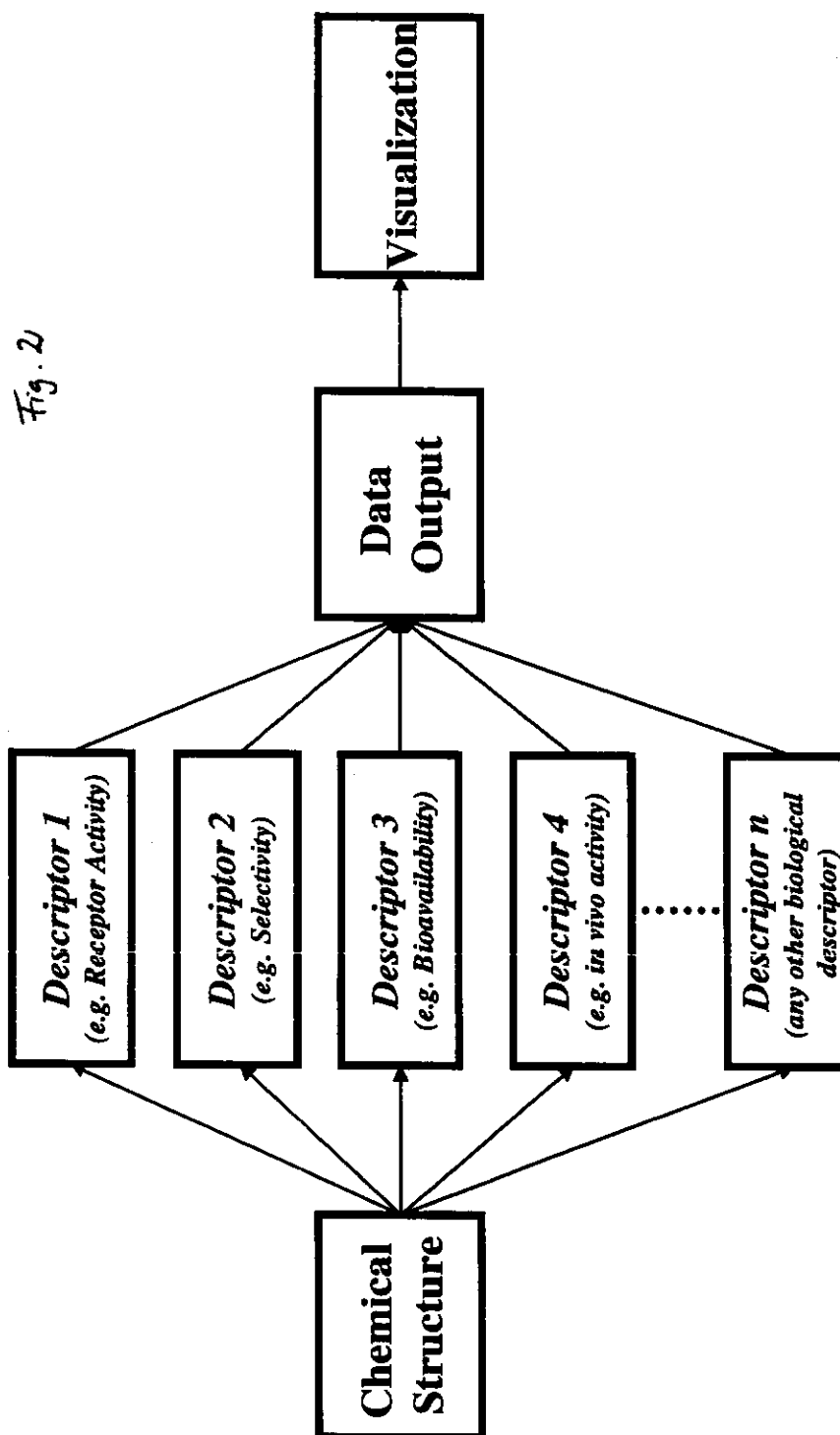


Fig. 1



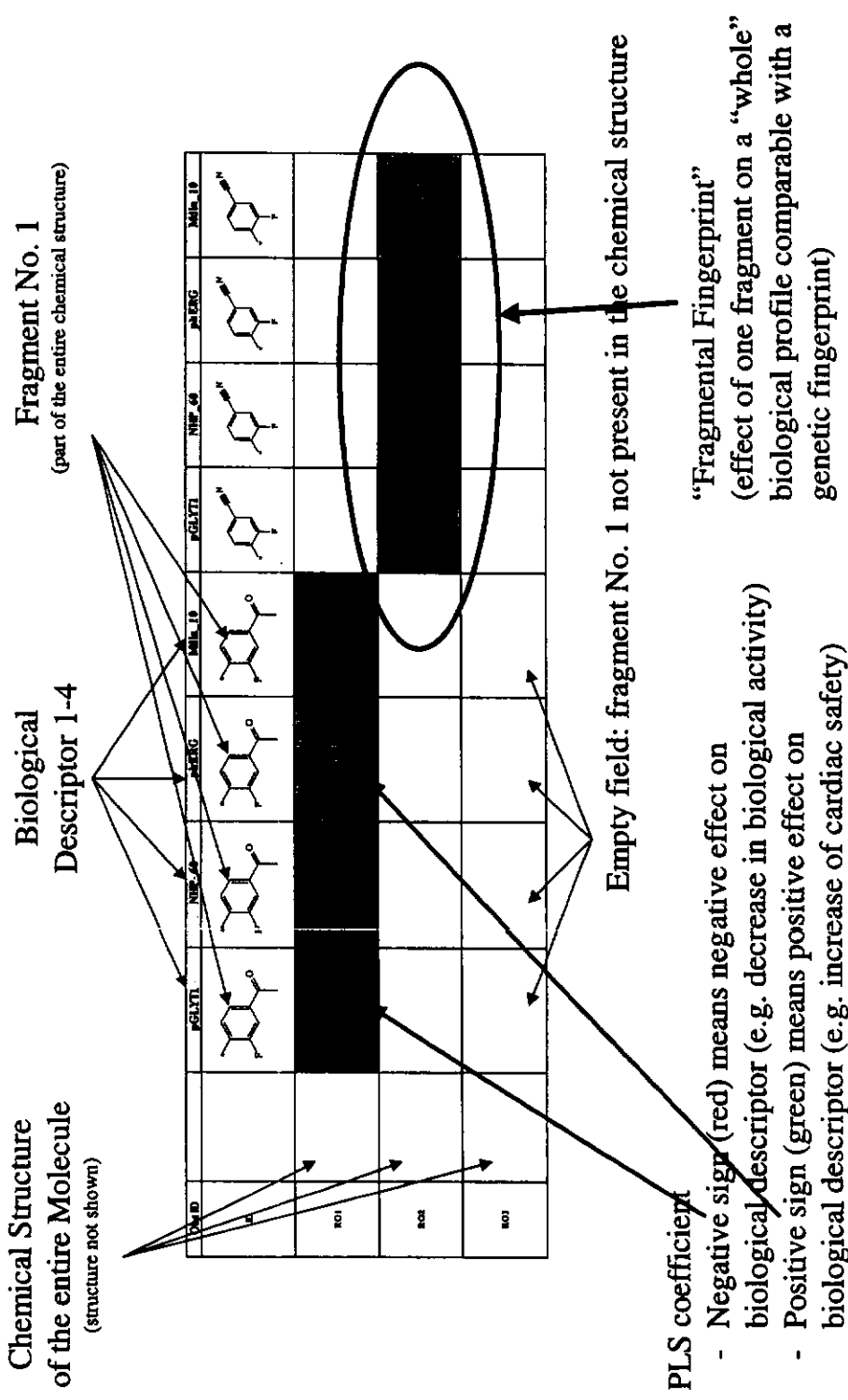


Fig. 3

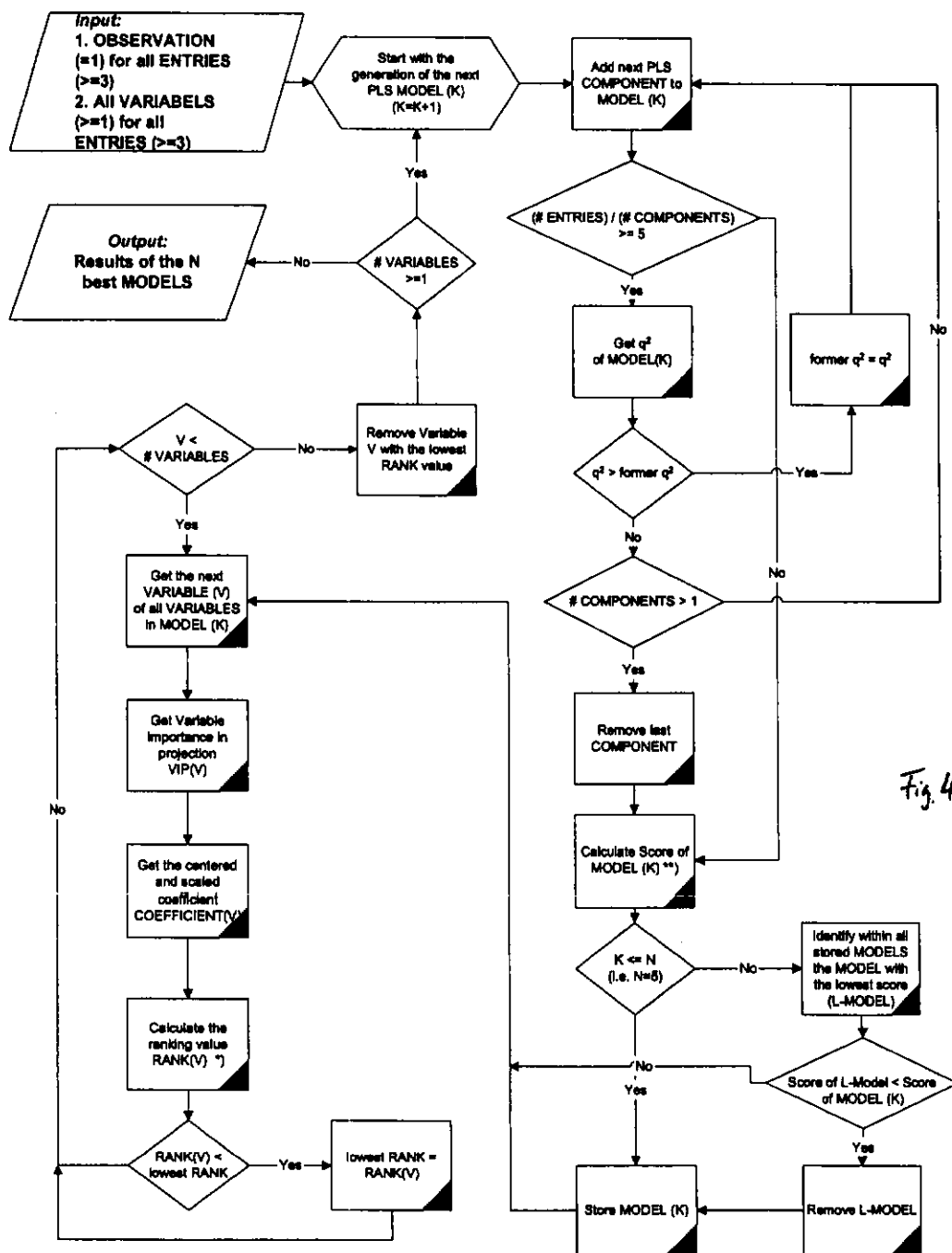


Fig. 4

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

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

for #V > 1

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Fig 5

ROCHE

ROSAARA

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

Example

List with SRN numbers

List with observations

Header required (SRN)

Name of Observation

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

Example

RO0635290-000	PKERG
RO0635290-000	7.04
RO0635290-000	5.85
RO0635290-000	5.4
RO0635290-000	5
RO0635290-000	4.51
RO0635290-000	5
RO0635290-000	4.56
RO0635290-000	5.16
RO0635290-000	5.89
RO0635290-000	5.8
RO0635290-000	4.54

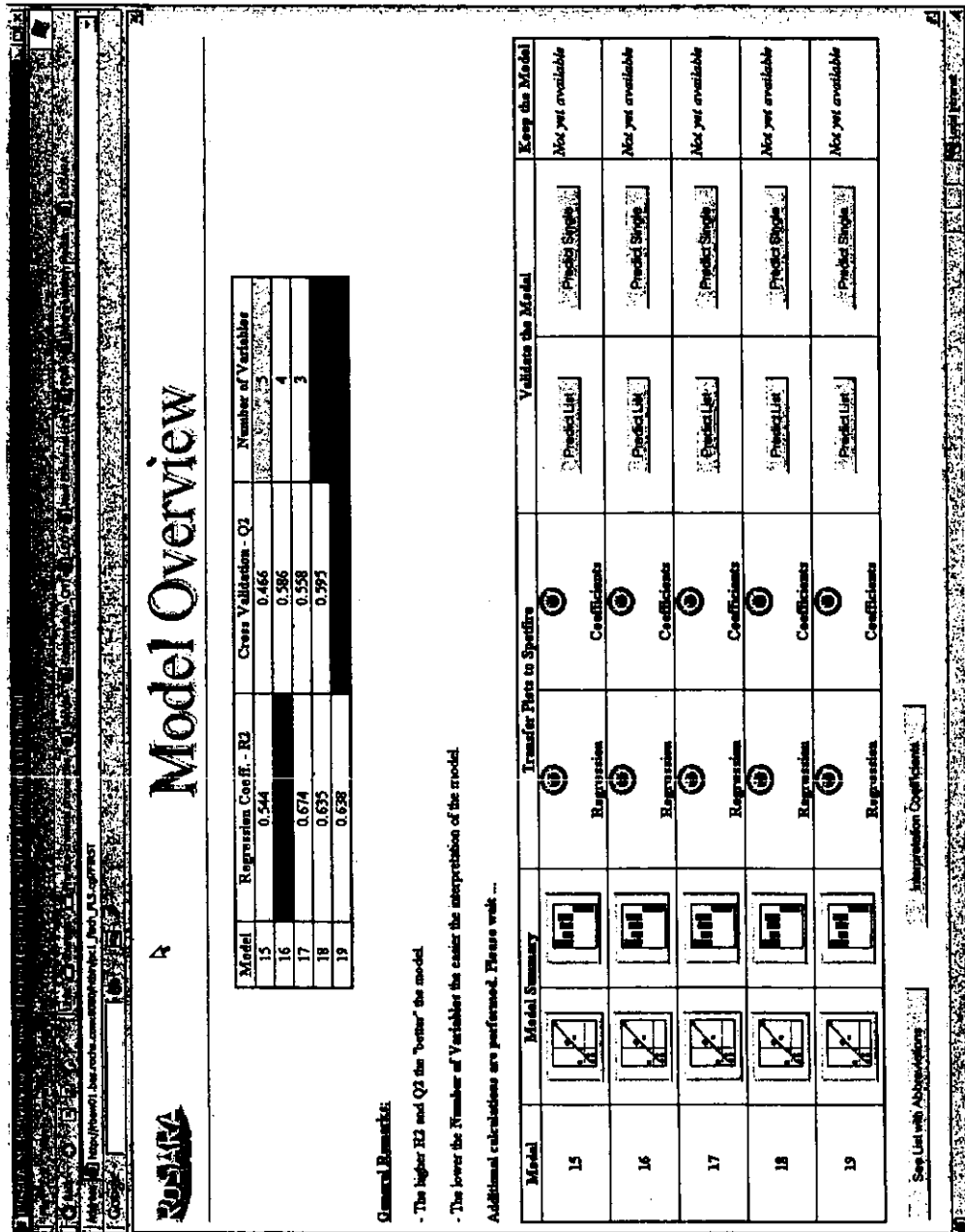
Calculate **Sheet**

Done

For comments or additional information, please contact holger.fischer@roche.com

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Fig 6



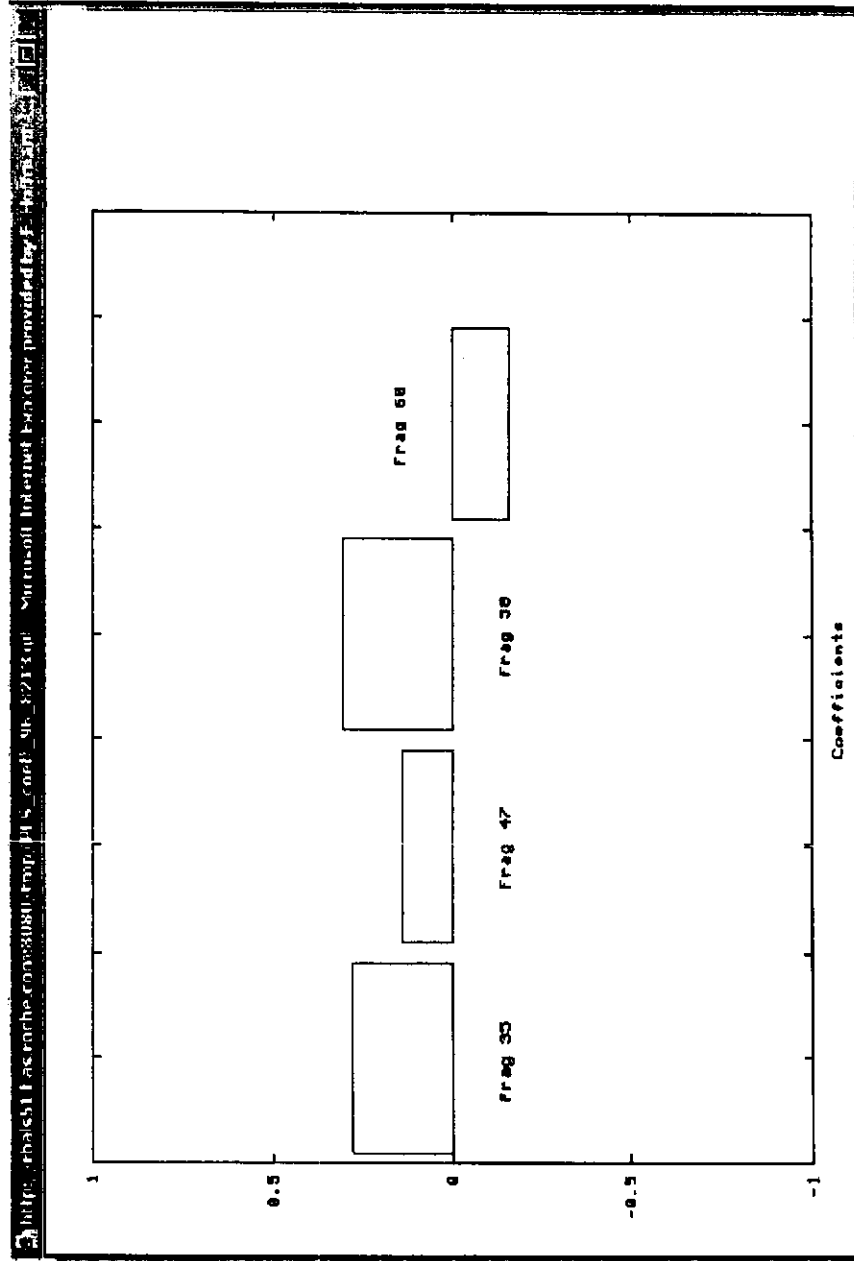


Fig. 7

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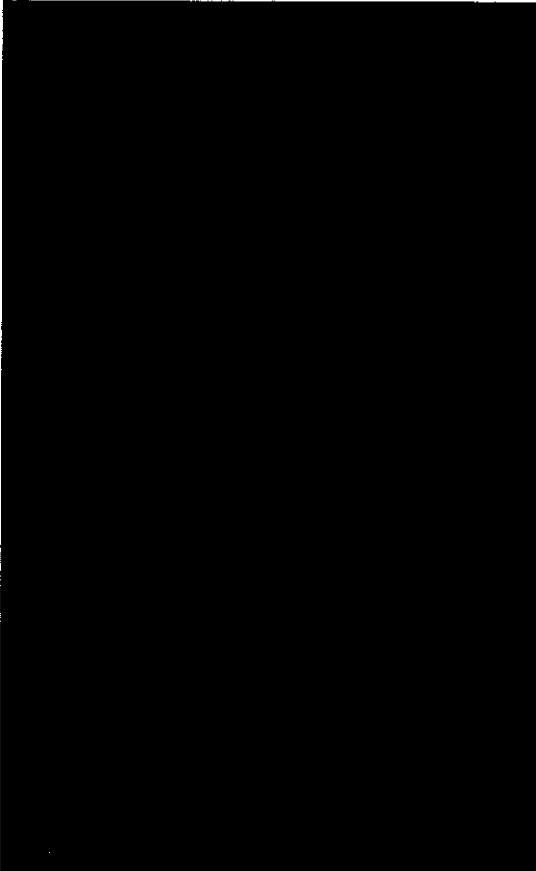
Structure	pGLYT1	NHP_60	phERG	Mdla_10
Chemistry 12				
Chemistry 13				
Chemistry 14				
Chemistry 15				
Chemistry 16				
Chemistry 17				
Chemistry 21				
Chemistry 22				
Chemistry 23				
Chemistry 41				
Chemistry 42				
Chemistry 43				
Chemistry 27				
Chemistry 28				
Chemistry 29				
Chemistry 30				
Chemistry 31				
Chemistry 32				
Chemistry 38				
Chemistry 39				
Chemistry 40				

Fig. 9