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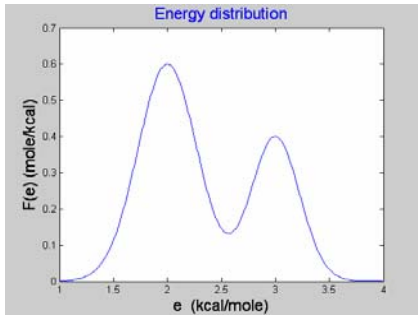.[-]

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: ( ) $1\frac{Kcal}{mol} < e < 4\frac{Kcal}{mol}$

$f(e) = 1.125 \exp(-(e - 2.5)^2 / 0.25)$
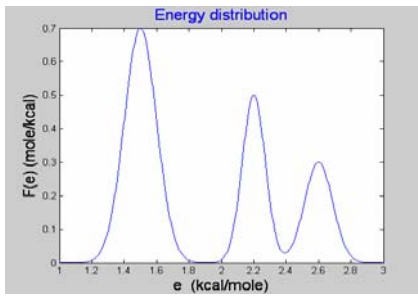
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Email:ahaghighi@semnan.ac.ir   -   :   ,   -   :   :   *

Energy distribution

F(e) (mole/kcal)

e (kcal/mole)

: .(Overlapped)

f(e) =1.125*exp(-(e-2.5)²/.25)

f(e) mole/Kcale

e (Kcal/mole)

: .(Single peak)

Non overlapped triple Peak -

-

:

$$f(e) = 0.7\exp(-(e-1.5)^2/0.02) + 0.5\exp(-(e-2.2)^2/0.01)$$
$$+ 0.3\exp(-(e-2.6)^2/0.015)$$

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Non overlapped double Peak -

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$$f(e) = 0.7\exp(-(e-1.7)^2/0.05) +$$
$$0.4\exp(-(e-3.1)^2/0.09)$$

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Energy distribution

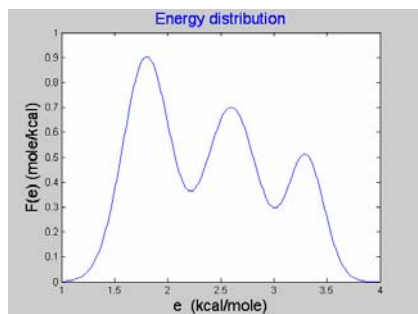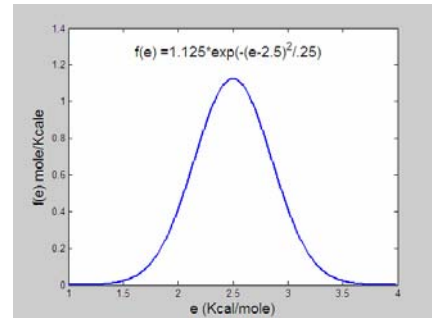F(e) (mole/kcal)

e (kcal/mole)

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.(Non overlapped)

Overlapped triple Peak -

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$$f(e) = 0.9\exp(-(e-1.8)^2/0.1) + 0.7\exp(-(e-2.6)^2/0.12)$$
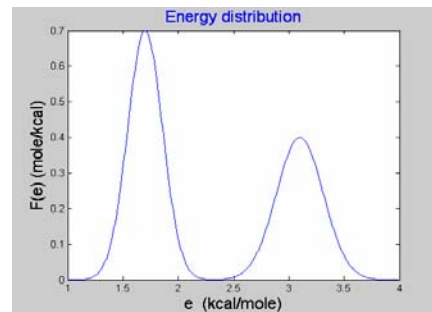$$+ 0.5\exp(-(e-3.3)^2/0.06)$$

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Energy distribution

F(e) (mole/kcal)

e (kcal/mole)

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.(Non overlapped)

Overlapped double Peak -

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$$f(e) = 0.6\exp(-(e-2.0)^2/0.15) +$$
$$0.4\exp(-(e-3.0)^2/0.1)$$

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Energy distribution

F(e) (mole/kcal)

e (kcal/mole)

: .(Overlapped)

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$$F(e) = 1.125 \exp\left[-\frac{(e-0.25)^2}{0.25}\right]$$

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$$g(p_i) = \int_{e_{\min}}^{e_{\max}} k(p_i, e) f(e) de$$

( )

77.5   f(e)

$1\,mbar < P_i < 1000\,mbar$ k(p,e)

( )

$1\frac{Kcal}{mol} < e < 4\frac{Kcal}{mol}$.

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:

$$\theta(P_i, T) = \int_{e_{\min}}^{e_{\max}} \frac{k_0 \exp\left[\dfrac{e}{RT}\right] P_i}{1 + k_0 \exp(\dfrac{e}{RT}) P_i} . F(e) de$$

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$F(e)$

:

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$$k(e, P_i, T) = \frac{K_0 \exp\left[\dfrac{e}{RT}\right] P_i}{1 + K_0 \exp(\dfrac{e}{RT}) P_i}$$

$\theta(P_i, T)$ k_0

.   T P_i ( )

K_0

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$$f = \left\{A^T A + \gamma I\right\}^{-1} A^T g.$$

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:g   :I   :A

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λ :

(GCV)

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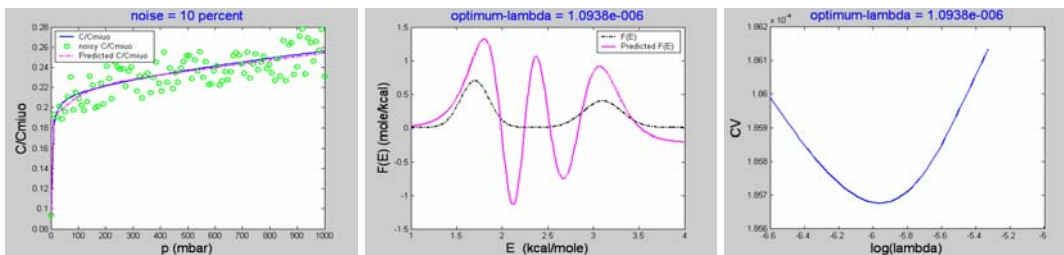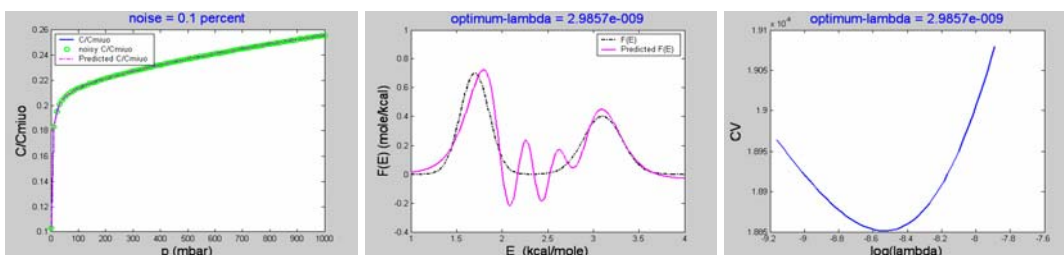:   -

λ : (a)   -

(GCV)

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-                               : (b)

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: (c)   .   ( )   ( ) ( )

(   ) (k_o)

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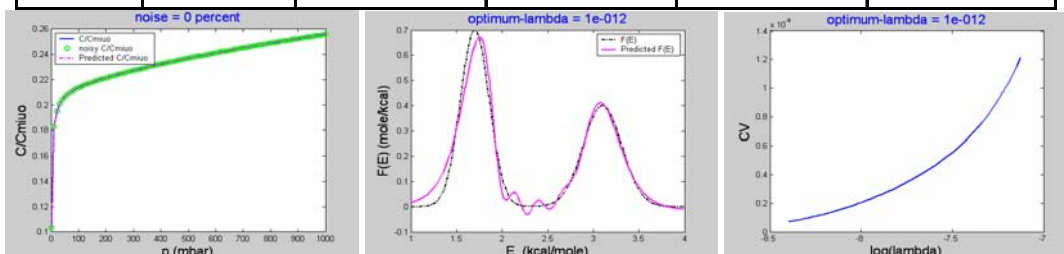**Non overlapped double peak**   -

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(k0)				
Type	Double peak		Triple peak	
	Non overlaped	Overlaped	Non overlaped	Overlaped
equi space	3.136E-09	4.306E-09	1.752E-08	1.874E-09
Non equi space	1.120E-08	2.343E-09	7.107E-09	2.856E-09

.«   »   :

(equi space)					
Noise		Double		Triple	
		Non overlapped	Overlapped	Non overlapped	Overlapped
0.10%	2.000E-03	2.986E-09	8.652E-08	4.863E-09	5.362E-09
0.50%	1.000E-02	1.011E-08	3.076E-07	1.002E-07	5.856E-08
1%	2.000E-02	1.906E-08	6.395E-07	1.554E-07	1.409E-07
3%	6.000E-02	3.392E-07	1.681E-05	3.739E-07	7.051E-07
5%	1.000E-01	6.091E-07	4.460E-05	6.715E-07	1.836E-04
10%	2.000E-01	1.094E-06	2.125E-04	1.127E-04	5.921E-04
20%	4.000E-01	.....	1.013E-03	.....	.....

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| (Non equi space)					
Noise		Double		Triple	
		Non overlapped	Overlapped	Non overlapped	Overlapped
0.10%	2.000E-03	3.775E-08	1.217E-07	2.683E-08	4.588E-08
1%	2.000E-02	8.162E-07	1.964E-06	1.539E-06	1.329E-06
3%	6.000E-02	1.871E-06	4.288E-06	3.889E-06	3.047E-06
5%	1.000E-01	2.632E-06	6.034E-06	5.473E-06	4.288E-06
10%	2.000E-01	3.704E-06	8.914E-06	7.700E-06	6.335E-06
20%	4.000E-01	.....	.....	1.084E-05	.....
30%	6.000E-01	.....	.....	1.317E-05	.....
50%	1.000E+00	.....	.....	1.681E-05	.....

(c)   (b)   (a)

.   **Non Overlapped double peak**   **cv**   :
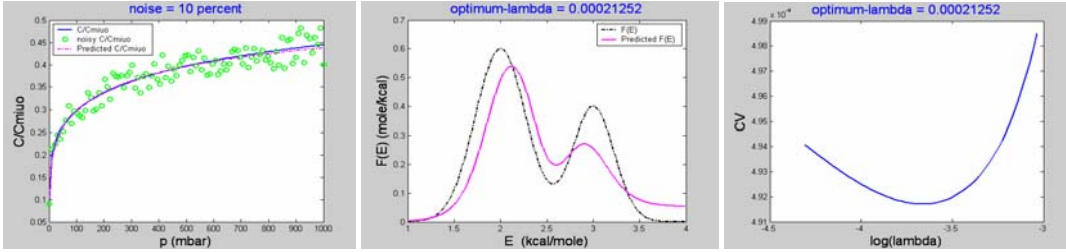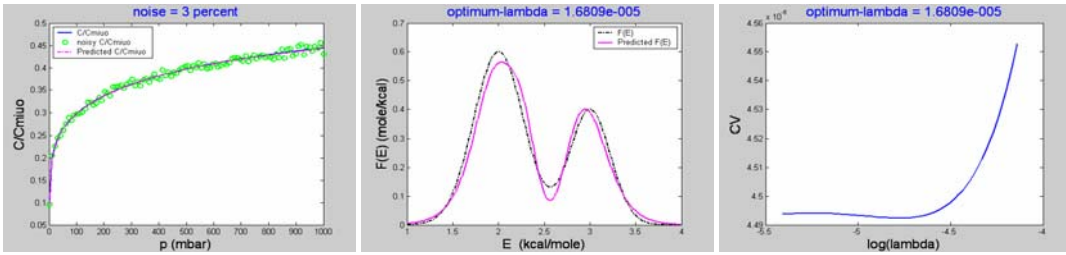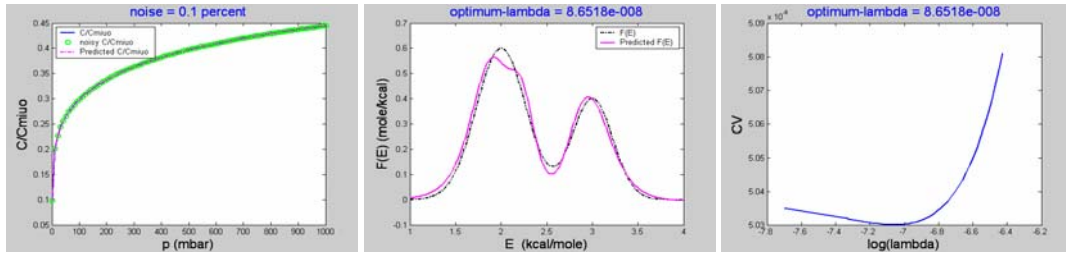
. **Overlapped double peak** cv :
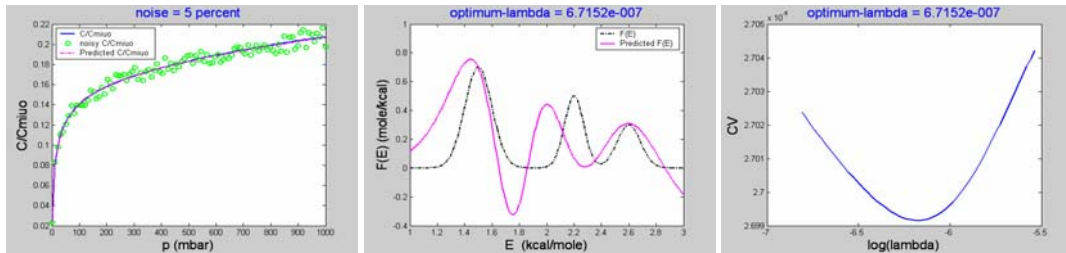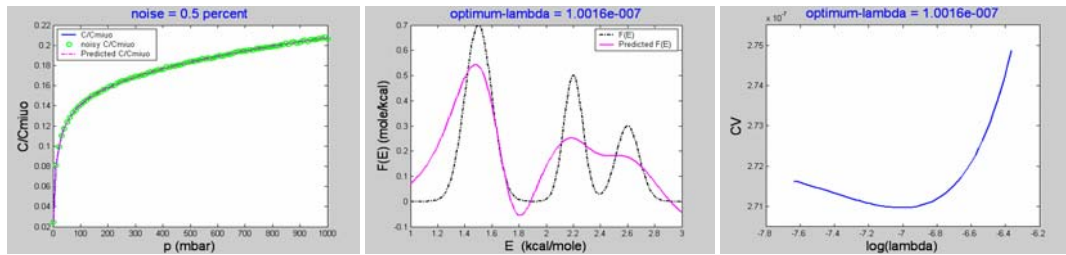

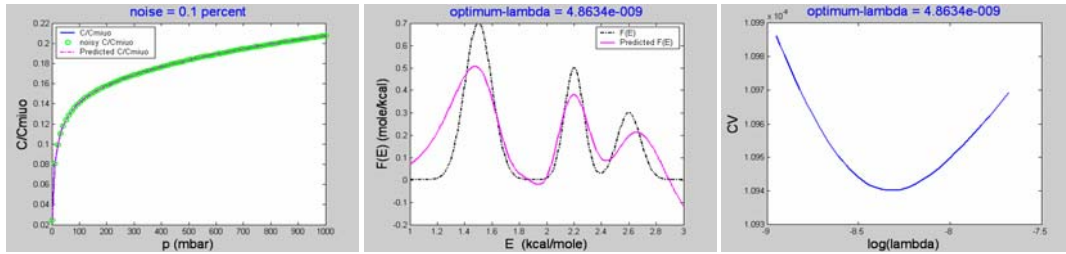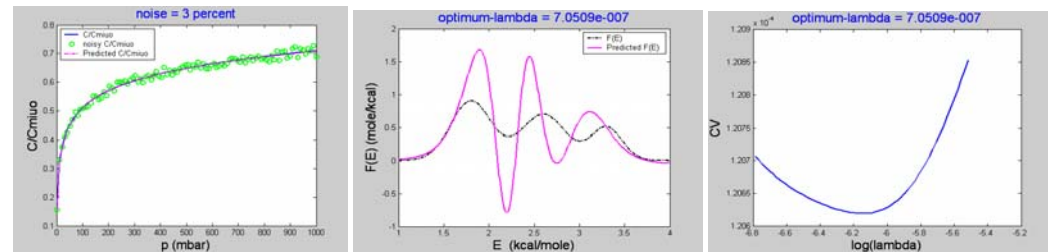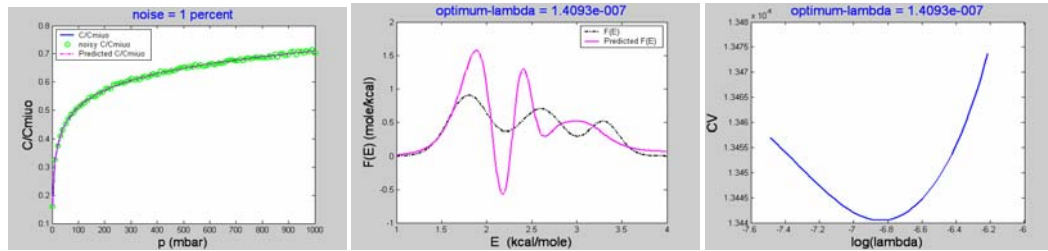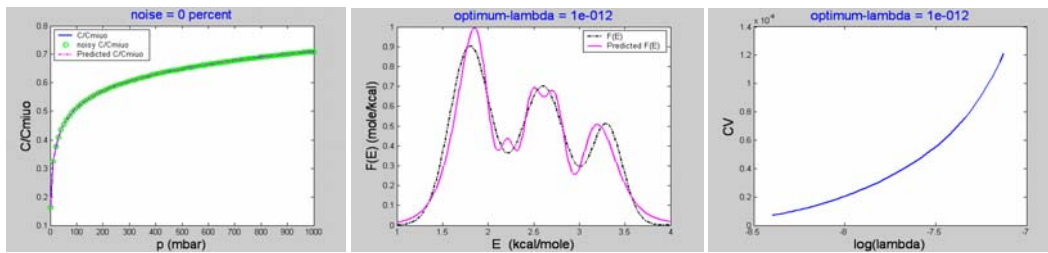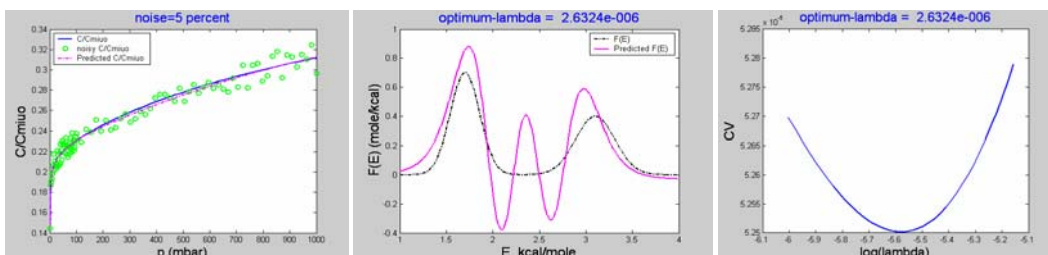
. **Non overlapped triple peak** :

. **Overlapped triple peak** cv :

. **Non overlapped double peak** cv :

. **Overlapped double peak** cv :

. **Non overlapped triple peak** :

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-   **Overlapped double peak**

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Overlapped double peak   -
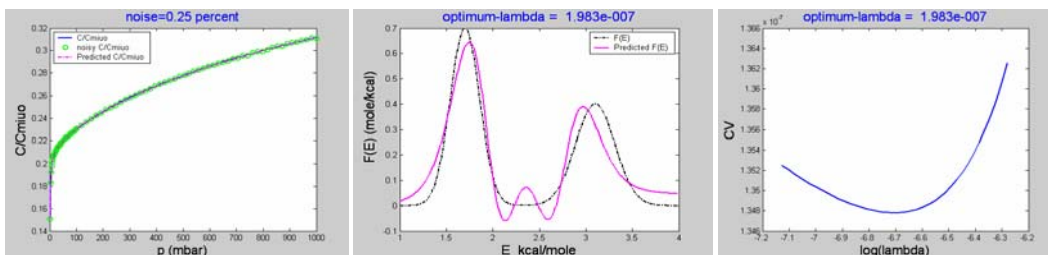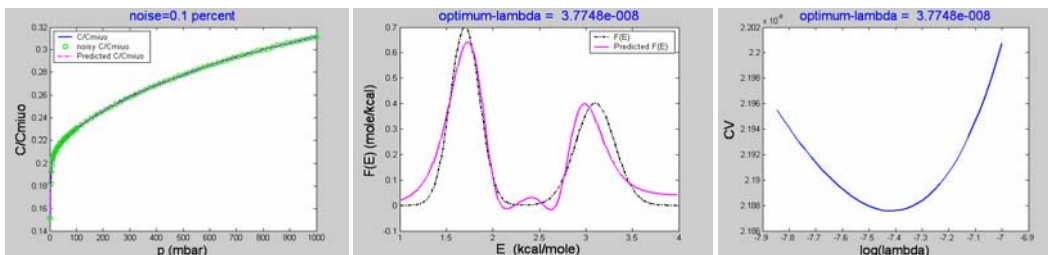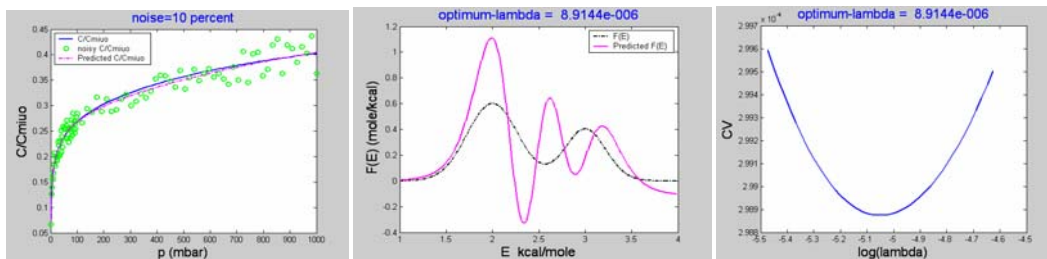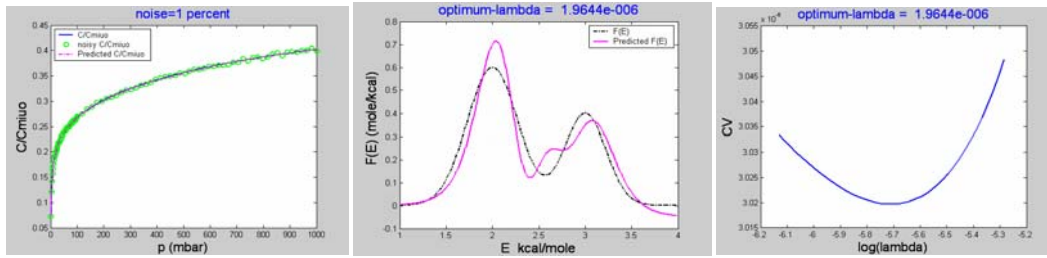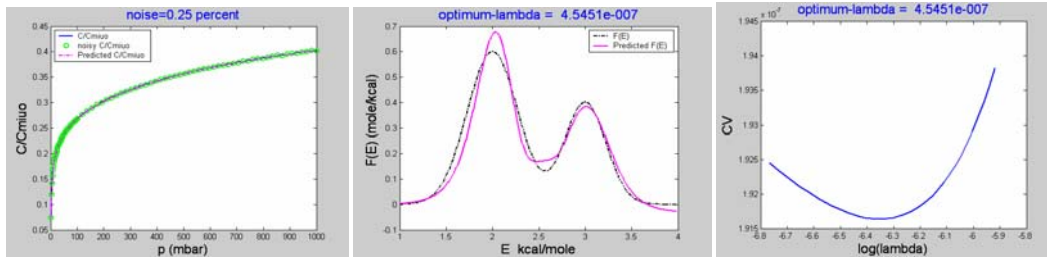
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(( )   )   **Non overlapped triple peak**   -

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Non overlapped triple peak   -

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Overlapped triple peak   -

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Overlapped triple peak   -

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Non overlapped double peak   -

Triple

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.   **Overlapped triple peak**   **cv**   :

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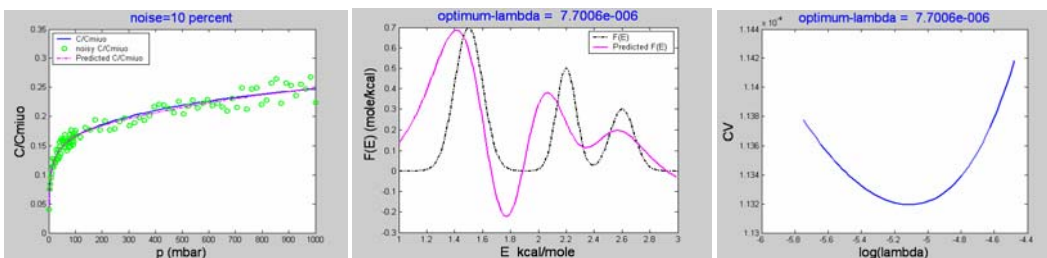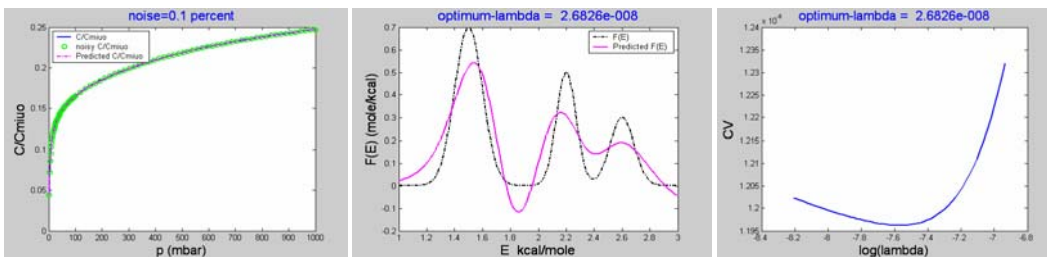
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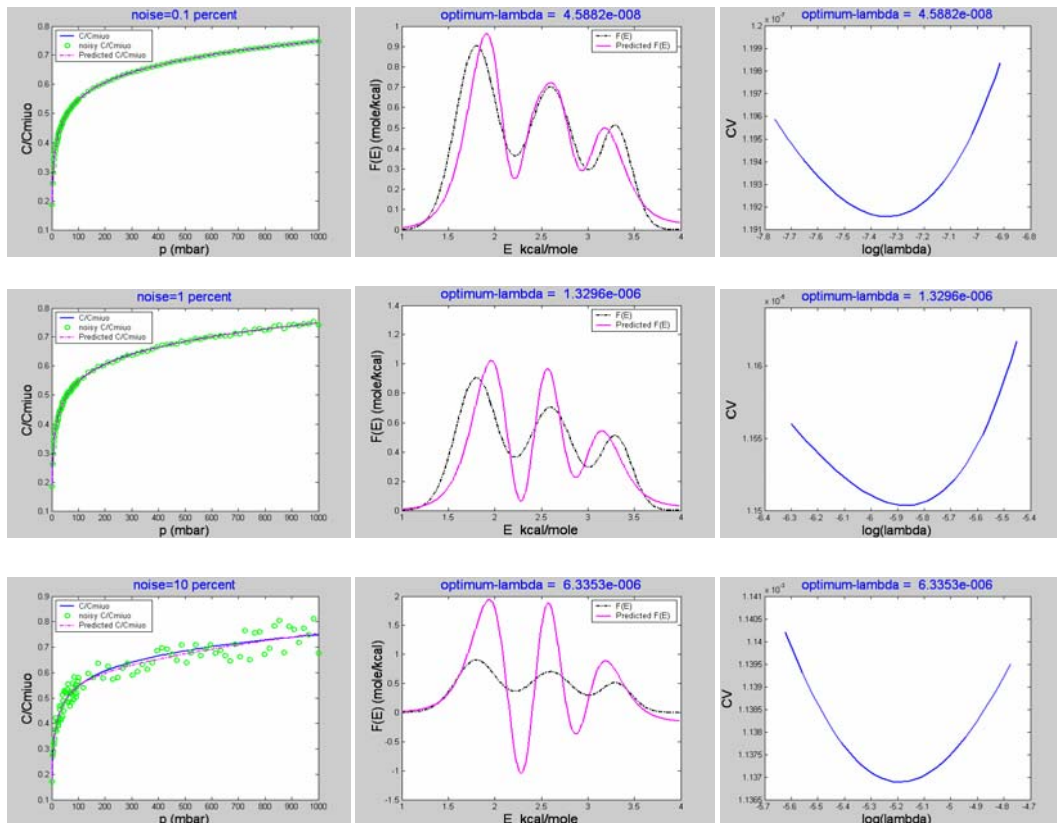
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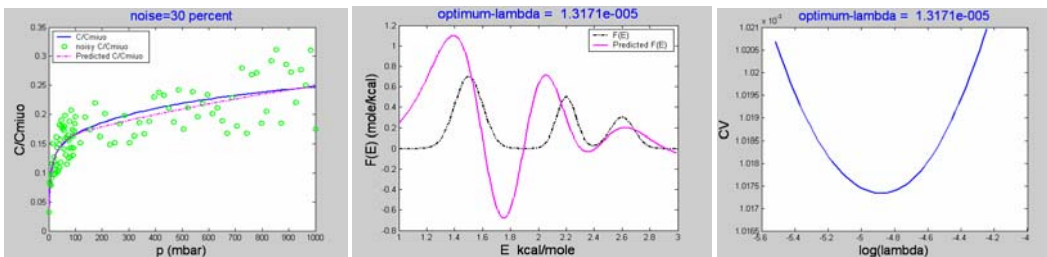
1 - Russell, B. P. and Levan, M. D. (1994). "Pour size distribution of BPL activated carbon determined by different methods." *Carbon, ELSEVIER,* Vol. 32, No. 5, PP. 845-855.

2 - William, H. Press, Brian P. Flannery, Saul A. Teukolsky, William T. Vetterling, (1992). *Numerical Recipes (The art of scientific computing*), 2nd Ed.

3 - Szombathely, M. V., Brauer, P. and Jaroniec, M. (1992). "The solution of adsorption integral equations by means of the regularization ,ethod." *Journal of Computational Chemistry*, Vol. 13, No. 1, PP. 17-32.

4 - Glob and Loan. (1996). *Matrix computation*,Third edition.

5 - Venkatesh, P. K. (2000). "On tikhonov regularization." *Physica A*, Elsevier, Vol. 284, PP. 448-460.

6 - Merz, P. H. (1980). "Determination of adsorption energy distribution by regularization and a characterization of certain adsorption isotherms." *Journal of Computational Physics,* Vol. 38, PP. 64-85.

7 - Hansen, O[1]., Fischer, S[2]. and Ramlau, R[3]. (2003). *Regularization of mellin–type inverse problems with an application to oil engineering.* 1- Johannes Gutenberg–University Mainz and 2- University of Bremen.

8 - Lamm, P. K. (2000). *Variable-Smoothing Regularization Methods for Inverse Problems*, Michigan State University, East Lansing, MI 48824-1027, USA.

9 - Doung, D. Do. (1998). *Adsorption Analysis: Equilibria and Kinetics*, Imperical college press, Singapore.

10 - Ahmadian, H., Mottershead, J. E. and Friswell, M. I. (1998). "Regularization methods for finite element model updating." *Mechanical systems and Signal Processing, AP*, Vol. 12, No. 1, PP. 47-64.

11 - Yagola, A. and Titarenko, V. (2000). *Numerical methods and regularization techniques for the solution of ill-posed problems*, Department of Mathematics, Faculty of Physics, Moscow State University Moscow 119899 Russia.

12 - Yeun, Y. S., Lee, K. H., Han, S. M. and Yang, Y. S. (2001). "Smooth fitting with a method for determining the regularization parameter under the genetic programming algorithm." *Information Sciences*, Elsevier, Vol. 133, PP. 175-194.

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1 - Gaussian Distribution   2 - Local adsorption isotherm   3 - Generalized cross validation