

## Appendix

### Limit of detection (LOD) calculation [56]

The detection limit was calculated from the linear regression line of the calibration curve. It was determined as follows:

$$Y = a + bX \quad (1)$$

where

- Y = instrument signals
- X = normally are concentrations
- a = intercept
- b = slope of the straight line

$$Y_L = Y_B + kS_B \quad (2)$$

where  $Y_L$  = lowest detectable instrument signals

$Y_B \cong$  intercept, a

k = constant depend on definition such as k = 1.5, 3 or 10

according to IUPAC, in calculation of LOD, k = 3 was normally used and was also used in this work.

$S_B$  = blank signal standard deviation

$\cong S_{y/x}$

$S_{y/x}$  can be calculated from the equation

$$S_{y/x} = \{\sum(Y_i - \hat{Y}_i)^2 / (n-2)\}^{1/2} \quad (3)$$

where  $Y_i$  = response value from the instrument corresponding to the individual x - values

$\hat{Y}_i$  = value of y on the calculated regression line corresponding to the individual x – values

n = number of points on the calibration line

From equation (1) and (2)

$$Y_L = a + 3S_{y/x} \quad (4)$$

Thus, the concentration at detection limit ( $C_L$ ) can be calculated by using the equation

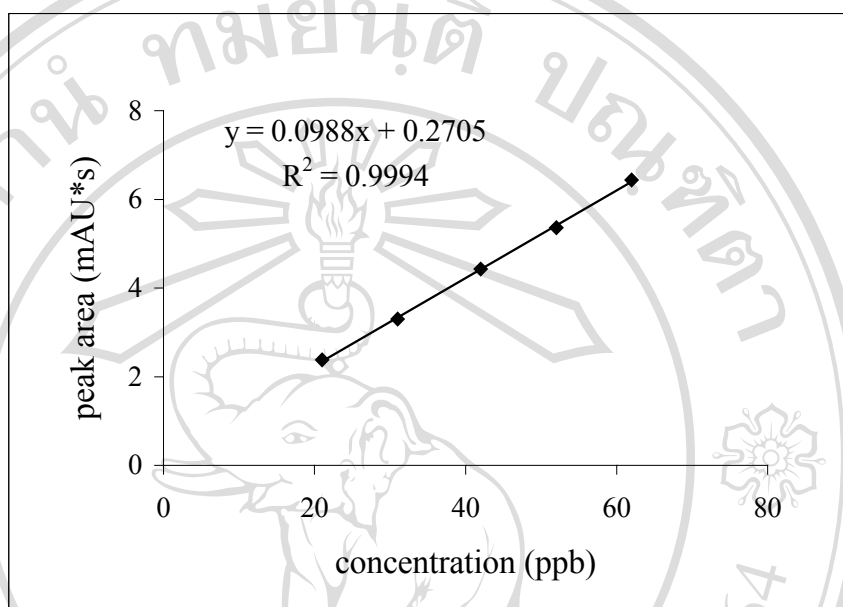
(6)

$$Y_L = a + bC_L \quad (5)$$

Thus,  $a + 3S_{y/x} = a + bC_L$

$$C_L = 3S_{y/x} / b \quad (6)$$

Example from the data of the calibration curve of C<sub>10</sub> LAS with the concentration range 21-62 ppb.



**Fig. A-1** Calibration curve of C<sub>10</sub> LAS used for calculating the detection limit.

**Table A-1** Calculation data of concentration on the linear regression line

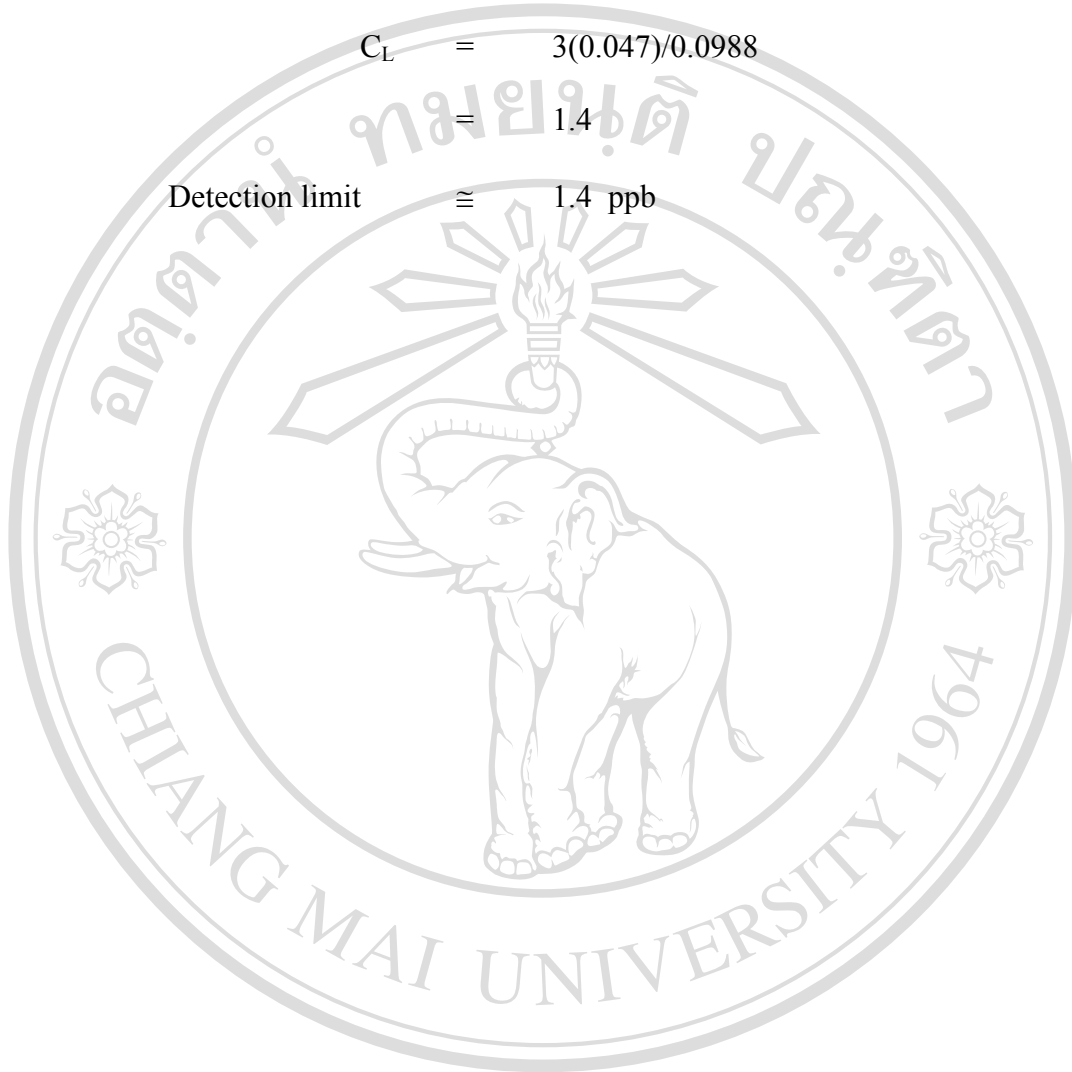
Concentration (ppb)	$Y_i$	$\hat{Y}_i$	$ Y_i - \hat{Y}_i $	$ Y_i - \hat{Y}_i ^2$
21	2.38	2.34	0.04	$1.6 \times 10^{-3}$
31	3.30	3.33	0.03	$9.0 \times 10^{-4}$
42	4.43	4.42	0.01	$1.0 \times 10^{-4}$
52	5.36	5.41	0.05	$2.5 \times 10^{-3}$
62	6.44	6.40	0.04	$1.6 \times 10^{-3}$
$\sum  Y_i - \hat{Y}_i ^2$				$6.7 \times 10^{-3}$

$$S_{y/x} = [6.7 \times 10^{-3}/(5-2)]^{1/2} = 0.047$$

$$C_L = 3(0.047)/0.0988$$

$$= 1.4$$

$$\text{Detection limit} \cong 1.4 \text{ ppb}$$




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