

The relationship between the molecular structure of linear aliphatic amines and biodegradation

The National Institute of Technology and Evaluation (NITE) classifies biodegradability test data of existing chemical substances under the Chemical Substance Control Law (CSCL), and analyzes the relationship between the molecular structure and biodegradation or bioconcentration. We obtained biodegradability test data on 1,565 chemical substances opened to the public as of July, 2014, and analyzed these data with a focus on 72 linear aliphatic amines (including an overlap of 12 chemical substances that have several functional groups). We have released the findings of the relationship between the molecular structure of 72 linear aliphatic amines and biodegradation here. Please use this information as reference of new chemical notification under CSCL.

The following are the breakdown of the functional groups (i.e., primary amines, secondary amines, and tertiary amines) of 72 chemical substances (Please read the attachment 1-6 for the details of biodegradation data of each chemical)

	Total	Readily biodegradable	Not readily biodegradable
Primary amines	30	15	15
Secondary amines	19	9	10
Tertiary amines	23	5	18

We found the following trends for biodegradation category:

	Amino group	Substituted group	Biodegradable*1	Number of	
				Existing chemical	New chemical
I	Primary amines	only straight chain alkyls group	RB	6	-
II	Primary amines	amino group at both terminals	RB	2	3
III	Primary amines	hydrazino groups	NB	3	-
IV	Primary amines	Chart 1	NB	4	-
V	Secondary amines	only straight chain alkyls group	RB	4	1

VI	Tertiary amines	Chart 2	RB	4	1
VII	Tertiary amines	Chart 3	NB	9	1
VIII	All	isopropyl group or tertiary butyl group at the alpha-position	NB	3	5

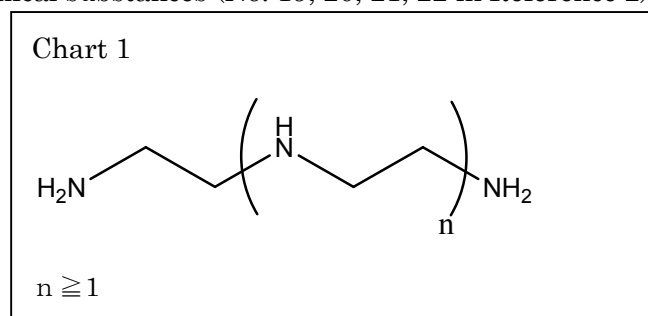
*1RB: Ready biodegradable, NB:Not

- I. Linear aliphatic primary amines that have only straight chain alkyls group in the side chain are all “Readily biodegradable” without exception: 6 existing chemical substances (No. 1, 2, 3, 4, 5, 6 in Reference 1)

- II. Linear aliphatic primary amines that have an amino group at both terminals are all “Readily biodegradable” without exception: 2 existing chemical substances (No. 7, 8 in Reference 1, and 3 new chemical substances*2)

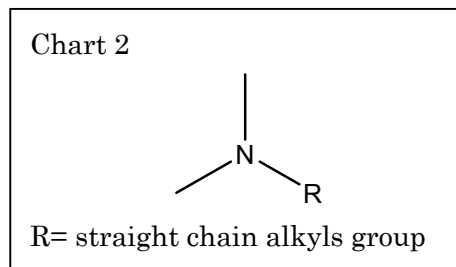
- III. Linear aliphatic primary amines that have hydrazino groups are all “Not readily biodegradable and no degradation products” without exception: 3 existing chemical substances (No. 16, 17, 18 in Reference 2)

- IV. Linear aliphatic primary amines that have the following molecular structure are all “Not readily biodegradable and no degradation products” without exception: 4 existing chemical substances (No. 19, 20, 21, 22 in Reference 2)

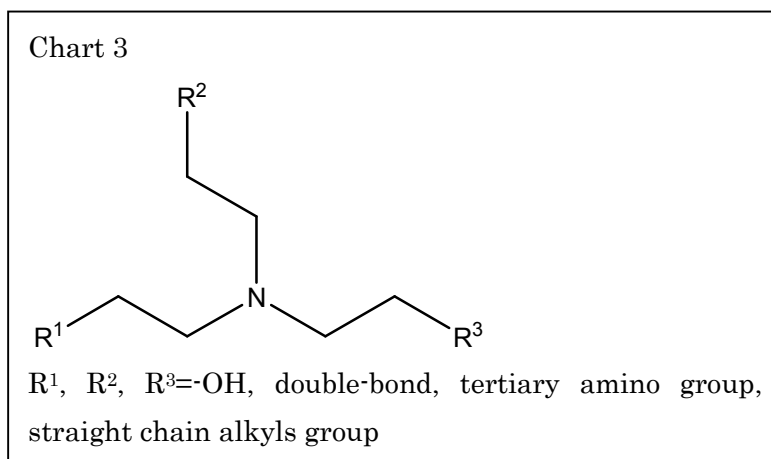


- V. Linear aliphatic secondary amines that have only straight chain alkyl groups in the side chain are all “Readily biodegradable” without exception: 4 existing chemical substances (No. 31, 32, 33, 34 in Reference 3, and 1 new chemical substance*2)

- VI. Linear aliphatic tertiary amines that have the following molecular structure are all “Readily biodegradable” without exception: 4 existing chemical substances (No. 50, 51, 52, 53 in Reference 5, and 1 new chemical substance*2)



VII. Linear aliphatic tertiary amines that have the following molecular structure are all “Not readily biodegradable and no degradation products” without exception: 9 existing chemical substances (No. 56, 57, 58, 59, 60, 61, 62, 63, 64 in Reference 6, and 1 new chemical substance*2)



VIII. Linear aliphatic amines that have an isopropyl group or tertiary butyl group at the alpha-position are all “Not readily biodegradable and no degradation products” without exception: 3 existing chemical substances (No. 24, 40, 41 in Reference 2 and 4, and 5 new chemical substance*2)

*2 biodegradability test data of 2,549 new chemical substances (not including polymers) notified from 1975 to March 2013 under CSCL (undisclosed data)