Appendix2　SIRC-CVS:TEA の予測性一覧

表 1．Overall analysis by the judgment based on IC_{50} value of Triethanolamine (TEA) in UN GHS classification system in a bottom-up approach in the validation study

Regulatory System	Analysis
Accuracy	55.2% (64/116)
Sensitivity	60.0% (42/70)
Specificity	47.8% (22/46)
False Negative Rate	40.0% (28/70)
False Positive Rate	52.2% (24/46)

表 2. Analysis after cut Molecular weight <180 for alcohol, ester, ether , ketone heterocyclic compound and carboxylic acid , and purity ≧80% (GHS, Bottom-up, TEA) in the validation study.

Regulatory System	Analysis in applicability domain
Accuracy	64.9% (37/57)
Sensitivity	92.3% (24/26)
Specificity	41.9% (13/31)
False Negative Rate	7.6% (2/26)
False Positive Rate	58.1% (18/31)

表 3．Analysis after cut LogP (-1.5<log D<2) and pKa 4 or less (GHS, Bottom-up, TEA) in the validation study(see appendix 15).

Regulatory System	Analysis in applicability domain
Accuracy	57.7% (30/52)
Sensitivity	93.8% (15/16)
Specificity	41.7% (15/36)
False Negative Rate	6.3% (1/16)
False Positive Rate	58.3% (21/36)

表 4. Overall analysis by the judgment based on IC_{50} value of Triethanolamine (TEA) in UN GHS classification system in a bottom-up approach in the Shiseido in house 46 data (see appendix 16) and validated data

Regulatory System	Analysis
Accuracy	57.4% (93/162)
Sensitivity	64.8% (59/91)
Specificity	47.9% (34/71)
False Negative Rate	35.2% (32/91)
False Positive Rate	52.1% (37/71)

表 5. Analysis after cut Molecular weight <180 for alcohol, ester, ether , ketone heterocyclic compound and carboxylic acid , and purity ≧80% (GHS, Bottom-up, TEA) in the Shiseido in house 22 data (see appendix 11) and validated data

Regulatory System	Analysis in applicability domain
Accuracy	64.6% (51/79)
Sensitivity	94.6% (35/37)
Specificity	38.1% (16/42)
False Negative Rate	5.4% (2/37)
False Positive Rate	61.9% (26/42)

表 6. Analysis after cut LogP (-1.5<log D<2) and pKa 4 or less (GHS, Bottom-up, TEA) in the validation study(see appendix 15) (GHS, Bottom-up, TEA) in the Shiseido in house 31 data (see appendix 16) and validated data

Regulatory System	Analysis in applicability domain
Accuracy	65.1% (41/63)
Sensitivity	96.3% (26/27)
Specificity	42.9% (24/56)
False Negative Rate	3.7% (1/27)
False Positive Rate	57.1% (32/56)

表 7. Overall analysis by the judgment based on IC_{50} value of Triethanolamine (TEA) in UN GHS classification system in a bottom-up approach in the validated data based on Barroso' data (see appendix 14)

Regulatory System	Analysis
Accuracy	50.0% (49/98)
Sensitivity	52.9% (27/51)
Specificity	46.8% (22/47)
False Negative Rate	47.1% (24/51)
False Positive Rate	53.2% (25/47)

表 8. Analysis after cut Molecular weight <180 for alcohol, ester, ether , ketone heterocyclic compound and carboxylic acid , and purity ≧80% (GHS, Bottom-up, TEA) in the validated data based on Barroso' data (see appendix 14)

Regulatory System	Analysis in applicability domain
Accuracy	56.5% (26/46)
Sensitivity	87.5% (14/16)
Specificity	40.0% (12/30)
False Negative Rate	12.5% (2/16)
False Positive Rate	60.0% (18/30)