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English - Or. English

**ENVIRONMENT DIRECTORATE**
**JOINT MEETING OF THE CHEMICALS COMMITTEE AND THE WORKING PARTY ON CHEMICALS, PESTICIDES AND BIOTECHNOLOGY**

# ADDENDUM TO THE SUMMARY DOCUMENT ON THE STATISTICAL PERFORMANCE OF METHODS IN OECD TEST GUIDELINE 431 FOR SUB-CATEGORISATION

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**or contact:**

**OECD Environment Directorate,**
**Environment, Health and Safety Division**
**2 rue André-Pascal**
**75775 Paris Cedex 16**
**France**

**Fax: (33-1) 44 30 61 80**

**E-mail: ehscont@oecd.org**

## FOREWORD

This document contains an addendum to the document reviewing the Statistical Performance of Methods in OECD Test Guideline 431 for Sub-categorisation among corrosives [ENV/JM/MONO(2013)14] approved and declassified in 2103.

The addendum summarises the statistical performance of the epiCS (previously known as EST-1000) method for the partial sub-categorisation among corrosives. It was presented at the 26th Meeting of the Working Group of the National Coordinators of the Test Guidelines Programme in April 2014 and endorsed in support of the update to TG 431. The Joint Meeting of the Chemicals Committee and the Working Party on Chemicals, Pesticides and Biotechnology agreed to its declassification on 7th July, 2014.

This document is published under the responsibility of the Joint Meeting of the Chemicals Committee and the Working Party on Chemicals, Pesticides and Biotechnology.

**Table 1.4 Results including accuracy values, correct classification, over-prediction and under-prediction rates for epiCS on entire set of chemicals (80 chemicals per run, two runs performed), when MTT reducers are included (substance #58 only one test due to limited substance amount)**

| epiCS with entire set of chemicals | | | | |
|---|---|---|---|---|
| | Test method: epiCS | | | |
| *In vivo* categories | Classified as Cat. 1A | Classified as Cat. 1BC | Classified as Cat. NC | Sum |
| *In vivo* Cat. 1A | 22 | 2 | 0 | 24 |
| *In vivo* Cat. 1BC | 28 | 29 | 4 | 61 |
| *In vivo* Cat. NC | 0 | 21 | 53 | 74 |
| *Sum* | 50 | 52 | 57 | 159 |

| | |
|---|---|
| **Within 1A Vs. 1BC** | |
| Sensitivity for 1A | 91.67% |
| Specificity = Sensitivity for 1BC | 50.88% |
| *Accuracy* | 62.96% |
| **Corr. Vs. Non Corr** | |
| Sensitivity for Corr | 95.29% |
| Sp for Coor = Se for Non Corr | 71.62% |
| *Accuracy* | 84.28% |

| Calculations over the 3 chemicals categories: | | | |
|---|---|---|---|
| | Checking the misclassifications over the 3 categories: | | |
| **Accuracy (Pred. C)** | **% OverClass 1BC as 1A** | **%OverClassNC as 1BC** | **% OverClass NC as 1A** |
| 65.41% | 45.90% | 28.38% | 0.00% |
| | **% UnderClass 1A as 1BC** | **% underClass 1A as NC** | **% UnderClass 1BC as NC** |
| | 8.33% | 0.00% | 6.56% |
| **Correctly Class** | | | |
| Cat.1A 91.67% | | | |
| Cat.1BC 47.54% | **% of OverClass** | **% of UnderClass** | |
| Cat. NC 71.62% | 30.82% | 3.77% | |

**Table 2.4 Results including accuracy values, correct classification, over-prediction and under-prediction rates for epiCS on entire set of chemicals, when MTT reducers are excluded (2 runs)**

| epiCS Without its MTT Reducers | | | | |
|---|---|---|---|---|
| | Test method: epiCS | | | |
| *In vivo* categories | Classified as Cat. 1A | Classified as Cat. 1BC | Classified as Cat. NC | Sum |
| *In vivo* Cat. 1A | 20 | 0 | 0 | 20 |
| *In vivo* Cat. 1BC | 17 | 18 | 4 | 39 |
| *In vivo* Cat. NC | 0 | 14 | 42 | 56 |
| *Sum* | 37 | 32 | 46 | 115 |

| Within 1A Vs. 1BC | |
|---|---|
| Sensitivity for 1A | 100.00% |
| Specificity = Sensitivity for 1BC | 51.43% |
| *Accuracy* | 69.09% |
| **Corr. Vs. Non Corr** | |
| Sensitivity for Corr | 93.22% |
| Sp for Coor = Se for Non Corr | 75.00% |
| *Accuracy* | 84.35% |

| Calculations over the 3 chemicals categories: | | | |
|---|---|---|---|
| | Checking the misclassifications over the 3 categories: | | |
| **Accuracy (Pred. C)** 69.57% | **% OverClass 1BC as 1A** 43.59% | **%OverClassNC as 1BC** 25.00% | **% OverClass NC as 1A** 0.00% |
| | **% UnderClass 1A as 1BC** 0.00% | **% underClass 1A as NC** 0.00% | **% UnderClass 1BC as NC** 10.26% |
| **Correctly Class** | | | |
| Cat.1A 100.00% | | | |
| Cat.1BC 46.15% | **% of OverClass** 26.96% | **% of UnderClass** 3.48% | |
| Cat. NC 75.00% | | | |

**Table 3.4 Results including accuracy values, correct classification, over-prediction and under-prediction rates for epiCS on MTT reducers only (2 runs)**

| epiCS Within MTT Reducers specific to epiCS only (i.e. non-MTT excluded) | | | | |
|---|---|---|---|---|
| | Test method: epiCS | | | |
| *In vivo* categories | Classified as Cat. 1A | Classified as Cat. 1BC | Classified as Cat. NC | Sum |
| *In vivo* Cat. 1A | 2 | 2 | 0 | 4 |
| *In vivo* Cat. 1BC | 11 | 11 | 0 | 22 |
| *In vivo* Cat. NC | 0 | 7 | 11 | 18 |
| *Sum* | 13 | 20 | 11 | 44 |

| | |
|---|---|
| **Within 1A Vs. 1BC** | |
| Sensitivity for 1A | 50.00% |
| Specificity = Sensitivity for 1BC | 50.00% |
| *Accuracy* | 50.00% |
| **Corr. Vs. Non Corr** | |
| Sensitivity for Corr | 100.00% |
| Sp for Coor = Se for Non Corr | 61.11% |
| *Accuracy* | 84.09% |

| Calculations over the 3 chemicals categories: | | | |
|---|---|---|---|
| | Checking the misclassifications over the 3 categories: | | |
| **Accuracy (Pred. C)** | **% OverClass 1BC as 1A** | **%OverClassNC as 1BC** | **% OverClass NC as 1A** |
| | 50.00% | 38.89% | 0.00% |
| 54.55% | **% UnderClass 1A as 1BC** | **% underClass 1A as NC** | **% UnderClass 1BC as NC** |
| | 50.00% | 0.00% | 0.00% |
| **Correctly Class** | | | |
| Cat.1A 50.00% | | | |
| Cat.1BC 50.00% | **% of OverClass** | **% of UnderClass** | |
| Cat. NC 61.11% | 40.91% | 4.55% | |

**Table 4.4 Results including accuracy values, correct classification, over-prediction and under-prediction rates for epiCS after organic base removal (2 runs)**

| epiCS Without Organic Bases (8 substances) | | | | |
|---|---|---|---|---|
| | Test method: epiCS | | | |
| *In vivo* categories | Classified as Cat. 1A | Classified as Cat. 1BC | Classified as Cat. NC | Sum |
| *In vivo* Cat. 1A | 20 | 0 | 0 | 20 |
| *In vivo* Cat. 1BC | 24 | 25 | 4 | 53 |
| *In vivo* Cat. NC | 0 | 20 | 50 | 70 |
| *Sum* | 44 | 45 | 54 | 143 |

| | |
|---|---|
| **Within 1A Vs. 1BC** | |
| Sensitivity for 1A | 100.00% |
| Specificity = Sensitivity for 1BC | 51.02% |
| *Accuracy* | 65.22% |
| **Corr. Vs. Non Corr** | |
| Sensitivity for Corr | 94.52% |
| Sp for Coor = Se for Non Corr | 71.43% |
| *Accuracy* | 83.22% |

| Calculations over the 3 chemicals categories: | | | |
|---|---|---|---|
| | Checking the misclassifications over the 3 categories: | | |
| **Accuracy (Pred. C)** | **% OverClass 1BC as 1A** | **%OverClassNC as 1BC** | **% OverClass NC as 1A** |
| 66.43% | 45.28% | 28.57% | 0.00% |
| | **% UnderClass 1A as 1BC** | **% underClass 1A as NC** | **% UnderClass 1BC as NC** |
| **Correctly Class** | 0.00% | 0.00% | 7.55% |
| Cat.1A 100.00% | | | |
| Cat.1BC 47.17% | **% of OverClass** | **% of UnderClass** | |
| Cat. NC 71.43% | 30.77% | 2.80% | |

**Table 5.4 Results including accuracy values, correct classification, over-prediction and under-prediction rates for epiCS on organic base only (2 runs)**

| WITHIN {MTT-Red. & Organic Bases} ONLY | | | | |
|---|---|---|---|---|
| epiCS entire set of chemicals | | | | |
| *In vivo* categories | Test method: epiCS | | | |
| | Classified as Cat. 1A | Classified as Cat. 1BC | Classified as Cat. NC | Sum |
| *In vivo* Cat. 1A | 2 | 2 | 0 | 4 |
| *In vivo* Cat. 1BC | 4 | 4 | 0 | 8 |
| *In vivo* Cat. NC | 0 | 1 | 1 | 2 |
| *Sum* | 6 | 7 | 1 | 14 |

| | |
|---|---|
| **Within 1A Vs. 1BC** | |
| Sensitivity for 1A | 50% |
| Specificity = Sensitivity for 1BC | 50% |
| *Accuracy* | 50% |
| **Corr. Vs. Non Corr** | |
| Sensitivity for Corr | 100% |
| Sp for Coor = Se for Non Corr | 50.00% |
| *Accuracy* | 92.86% |

| Calculations over the 3 chemicals categories: | | | |
|---|---|---|---|
| | Checking the misclassifications over the 3 categories: | | |
| **Accuracy (Pred. C)** | **% OverClass 1BC as 1A** | **%OverClassNC as 1BC** | **% OverClass NC as 1A** |
| 50.00% | 50.00% | 50.00% | 0.00% |
| | **% UnderClass 1A as 1BC** | **% underClass 1A as NC** | **% UnderClass 1BC as NC** |
| | 50.00% | 0.00% | 0.00% |
| **Correctly Class** | | | |
| Cat.1A 50% | | | |
| Cat.1BC 50% | **% of OverClass** | **% of UnderClass** | |
| Cat. NC 50% | 35.71% | 14.29% | |