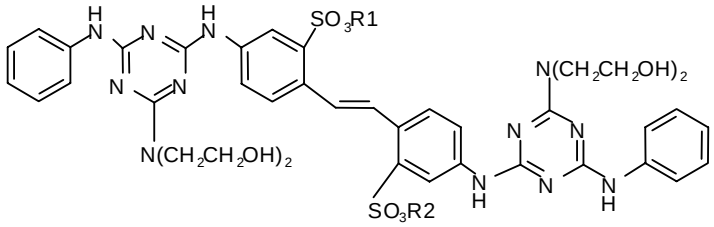
SIDS INITIAL ASSESSMENT PROFILE

CAS Nos. and Chemical Names	70942-01-7 Potassium sodium 4,4'-bis[6-anilino-4-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl] amino]stilbene-2,2'-disulphonate (C.I. Fluorescent Brightener 28/113) 71230-67-6 Dipotassium salt 4,4'-bis[6-anilino-4-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl] amino]stilbene-2,2'-disulphonate 4193-55-9 Disodium salt 4,4'-bis[6-anilino-4-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl] amino]stilbene-2,2'-disulphonate 4404-43-7 Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-[bis(2-hydroxyethyl)amino]-6-(phenylamino)-1,3,5-triazin-2-yl]amino]-
Structural Formulas	 70942-01-7: R1 = K; R2 = Na 71230-67-6: R1 = R2 = K 4193-55-9: R1 = R2 = Na 4404-43-7: R1 = R2 = H

SUMMARY CONCLUSIONS OF THE SIAR

Analogue Rational

C.I. Fluorescent Brightener 28/113 is a technical product which is manufactured as the potassium/sodium salt (CAS No. 70942-01-7), dipotassium salt (CAS No 71230-67-6), disodium salt (CAS No. 4193-55-9), and free acid (CAS No. 4404-43-7). All these types of C.I. Fluorescent Brightener 28/113 are based on the identical organic disulfonates which determines the ecological and the toxicological properties. Additionally there are a number of very similar fluorescent whitening agents with only minor differences of the structure and very similar physical and chemical properties. Data from these substances have been used to bridge possible data gaps in the section “Human health”: (C.I. Fluorescent Brighteners 24, 220, 225, and the Fluorescent Brightener 4,4´-bis[4-anilino -6-[(2-hydroxyethyl)methyl-amino]-s-triazin-2-yl)amino]2,2´-stilbenedisulphonate = CAS No. 12224-02-1, 16470-24-9, 24019-80-5, and 13863-31-5, respectively).

Human Health

The results of absorption/elimination/metabolism studies indicate virtually no absorption from the gut of the Fluorescent Brightener with CAS 13863-31-5 (chemical name see above) a chemically similar compound to C.I. Fluorescent Brightener 28/113. For this compound the faeces were the main elimination route. It is not metabolized in the gut. The excretion rate is solely dependent on the passage time through the gut.

The oral LD_{50} of C.I. Fluorescent Brightener 28/113 for rats is > 15 000 mg/kg bw. The acute inhalation toxicity study showed a reversible and sporadic reduction of general health after 4 hours exposure to > 1225 mg/m³ of rats. No pathological changes were seen in these animals. The 4h-LC_{50} value was > 1895 mg/m³ air.

No indication for skin irritation was seen in several rabbit studies (24-hour semi-occlusive or occlusive applications of 500 mg) or in the available human data. Slight signs of eye irritation were recorded in one of three studies.

The C.I. Fluorescent Brightener 28/113 is considered not to be a skin sensitizer in a guinea pig maximization assay according to Directive 84/449/EEC, B.6. Acute toxicity (skin sensitization).

Dermal application (90 weeks) on male mice (3 times/week, 50 µl, 7.8 %) revealed no toxicity. Two 2 years oral feeding studies in rats with the C.I. Fluorescent Brightener 28/113 were performed. The NOEL for male rats was 54.1 mg/kg bw and day in one study (only slight reduction of body weight), the NOAEL for female rats was ≥ 779 mg/kg bw and day, the NOAEL for male rats was ≥ 542.80 mg/kg bw/day. In the second study the NOAEL for female rats was ≥ 10 000 ppm (app. 500 - 1000 mg/kg bw /day). The NOEL for male rats was < 100 ppm because of an increased relative liver weight (up to 35 % at 10 000 ppm) in male rats considered as adaptive effect. The NOAEL for male rats is considered to be ≥ 10 000 ppm, however, this is a borderline case.

C.I. Fluorescent Brightener 28/113 is considered to be non-mutagenic as determined in vivo in a dominant lethal test with mice or in vitro up to 5000 µg/plate in *Salmonella typhimurium* strains TA1535, TA1537, TA98, TA100, and the *Escherichia coli* strain WP2 uvrA according to OECD TG 471. An in vitro cytogenetic study (chromosomal aberrations and sister chromatid exchanges) in Chinese hamster cells with a structurally very similar Fluorescent Brighteners (C.I. Fluorescent brighteners 24, and 225 = CAS No. 12224-02-1, and 24019-80-5) showed that these substances did not exhibit a potential to induce chromosomal aberrations nor sister chromatid exchanges. Another report describing the results of several tests in structurally very similar Fluorescent Brighteners (C.I. Fluorescent Brighteners 24, and 225 were tested) without giving experimental details (Ames Test in TA 100 TA 98; rec assay in *Bacillus subtilis*; Chromosomal aberrations in hamster lung fibroblasts and human embryo fibroblast; SCE in hamster lung fibroblasts and human embryo fibroblasts; chromosomal aberrations in rat bone marrow in vivo) confirmed the findings. Additionally no indication of mutagenic potential was found in the carcinogenicity studies conducted with these substances.

No indication for a carcinogenic potential of the C.I. Fluorescent Brightener 28/113 was seen, neither after dermal administration (3 times/week, up to 50 µl, 7.8 %) to mice on irradiated skin, nor after chronic oral administration (up to 10 000 ppm) to rats respectively.

A study available as secondary citation only described C.I. Fluorescent Brightener 28/113 as having no effect on reproduction and teratogenicity. In addition, well documented lack of effects on reproduction in rats and rabbits were reported for the chemically related optical brightener C.I. Fluorescent Brightener 220 (CAS 16470-24-9). These reports support the notion for C.I. Fluorescent Brightener 28/113 to have no effects on fertility, developmental and teratogenic properties.

Environment

C.I. Fluorescent Brightener 28/113 (K/Na- and Na_2-salts) is a yellowish solid without odour, with a melting point of 322 °C (K/Na-salt), 260 °C (Na_2-salt), and 290 °C (free acid). According to the structure of the substance and to decomposition starting at 351 °C, boiling point and vapor pressure are not measurable. The substance is soluble in

water with 27.1 g/l (K/Na-salt, at 20 °C [OECD TG 105]), 50 g/l (Na_2-salt, at 20 °C), and 80 g/l (free acid, at 25 °C). The bulk density of the Na_2-salt is 340 kg/m³. A log K_{OW} of 3.23 is estimated for the undissociated form of the free acid and a log K_{OW} of limited value of 0.65 for the salts of C.I. Fluorescent Brightener 28/113.

The calculated half-life of the C.I. Fluorescent Brightener 28/113 in air due to indirect photodegradation is $t_{1/2}$ = 1.2 hours.

C.I. Fluorescent Brightener 28/113 is not expected to undergo hydrolysis in the environment due to the lack of hydrolysable functional groups.

The calculation of the distribution of C.I. Fluorescent Brightener 28/113 between the environmental compartments according to the Mackay fugacity model level 1 and of the Henry's Law Constant are not practicable with the EPIWIN estimation program. From the physico-chemical properties it can be concluded that the sole target compartment for C.I. Fluorescent Brightener 28/113 is water. However, as a high adsorption to soil was calculated, it has to be assumed that the substance will strongly adsorb also to the sediment and soil compartments.

For C.I. Fluorescent Brightener 28/113 (free acid) biodegradation < 10 % during 28 days was determined in a Closed Bottle test [method similar to OECD TG 301D]. However, the elimination of the substances from waste water was shown by a Zahn-Wellens test according to OECD TG 302B. The elimination by adsorption was 83.6 % after 24 hours. In an OECD Confirmatory test (later modified to OECD TG 303A) two compounds containing C.I. Fluorescent Brightener 28/113 (Na_2-salt) showed a mean degradation rate of 11 % during 28 days and 56 % during 31 days, respectively. Based on these results, C.I. Fluorescent Brightener 28/113 can be classified as not readily biodegradable but elimination by adsorption is significant.

The calculated bioconcentration factor of 3 indicates no significant bioaccumulation potential in aquatic organisms via the water phase. Bioaccumulation from the sediment in benthic organisms due to the high adsorption potential of C.I. Fluorescent Brightener 28/113 cannot be excluded.

No experimental data on geoaccumulation is available. The calculated K_{OC} value of 8.1 x 10^9 for the salts and of 1.4 x 10^9 for the free acid of C.I. Fluorescent Brightener 28/113 indicates a very high sorption potential of the test substance onto the organic phase of soil or sediment.

Concerning the acute toxicity towards aquatic species valid studies for the three trophic levels are available. The lowest valid results for each aquatic trophic level are the following (n = nominal):

Danio rerio (fish):	96 h-LC_{50} = 5382 mg/l (n)	[OECD TG 203]
Daphnia magna (aq. invertebrate):	48 h-EC_{50} > 100 mg/l (n)	[Directive 92/69/EEC, C.2]
Selenastrum capricornutum) (algae):	72 h-E_rC_{50} > 22 mg/l (n)	[Directive 92/69/EEC, C.3]
Selenastrum capricornutum) (algae):	72 h-E_bC_{50} > 22 mg/l (n)	[Directive 92/69/EEC, C.3)
Activated sludge (bacteria):	3h-EC_{50} > 10 000 mg/l (n)	[OECD TG 209)]

No tests are available on chronic toxicity and on toxicity of C.I. Fluorescent Brightener 28/113 on sediment organisms.

For terrestrial organisms reliable experimental data are available with earthworms. A 14 d-LC_{50} of > 5000 mg/kg soil dry weight (n) was determined with the OECD TG 207.

Based on the acute aquatic toxicity data on three trophic levels (fish, *Daphnia*, algae), a Predicted No Effect Concentration ($PNEC_{aqua}$) can be calculated with an assessment factor of 1000 (EU Technical Guidance Document) applied to the lowest concentration tested of 22 mg/l towards algae, as no EC_{50} value could be determined at this level and the LC_{50} for *Daphnia* and fish was found at higher concentrations. This leads to a **$PNEC_{aqua}$ of > 22 µg/l.**

Exposure

In Germany there is only one manufacturer, which produces 1000 - 5000 tonnes/a of C.I. Fluorescent Brightener 28/113. In Western Europe there are about 5 producers, and presumably one in each of the following countries: USA, Japan, Russia, Poland, India, China, and Indonesia. Worldwide, 10 - 20 producers manufacture about 5000 - 10 000 tonnes/a of the active ingredient of C.I. Fluorescent Brightener 28/113.

C.I. Fluorescent Brightener 28/113 is exclusively used as a whitening agent in the paper and textile industry. It can also be used for brightening of polyamides.

C.I. Fluorescent Brightener 28/113 is confidentially listed in the Swedish Product Register as an industrial product in 2004. C.I. Fluorescent Brightener 28/113 and its salts are also listed in preparations in Sweden, Denmark, and Norway, but they are not reported to occur in consumer preparations in the Nordic countries in 2003 and in the Swiss Product Register in 2006. They are not listed in the Finnish Product Register Disodium salt 4,4'-bis[6-anilino-4-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl]amino]- stilbene-2,2'-disulphonate is listed with 4 industrial products in the Swiss Product Register.
From the manufacturing site of the Sponsor country virtually no C.I. Fluorescent Brightener 28/113 was emitted into the environment in 2000. Workplace air sampling shows that there is no exposure of workers at this site.

Releases into the hydrosphere may occur during processing of textiles and paper as well as during paper recycling and washing of treated textiles during cleaning processes. C.I. Fluorescent Brightener 28/113 is effectively eliminated predominantly by adsorption onto sludge from wastewater streams during secondary and tertiary wastewater treatment.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

The chemical is currently of low priority for further work, because of its low hazard profile.