

# Product data sheet



MedKoo Cat#: 525618 Name: Methylenebis(chloroaniline) CAS: 101-14-4 Chemical Formula: C <sub>13</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> Exact Mass: 266.0378 Molecular Weight: 267.153	
Product supplied as: Powder	
Purity (by HPLC): ≥ 98%	
Shipping conditions: Ambient temperature	
Storage conditions: Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

## 1. Product description:

Aromatic diamine used in the plastics industry as curing agent for epoxy resins and urethane rubbers. It is a curing agent in polyurethane production. It causes bladder, liver, lung, and other neoplasms.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
TBD	TBD	TBD

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.74 mL	18.72 mL	37.43 mL
5 mM	0.75 mL	3.74 mL	7.49 mL
10 mM	0.37 mL	1.87 mL	3.74 mL
50 mM	0.08 mL	0.37 mL	0.75 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

1. DeBord DG, Cheever KL, Booth-Jones AD, Swearingin TF, Savage RE Jr. Alterations of histone phosphorylation in rat spleen cells after treatment with the aromatic amine, 4,4'-methylene-bis(2-chloroaniline). *J Biochem Toxicol.* 1995 Feb;10(1):19-23. PMID: 7595928.
2. Segerbäck D, Kadlubar FF. Characterization of 4,4'-methylenebis(2-chloroaniline)--DNA adducts formed in vivo and in vitro. *Carcinogenesis.* 1992 Sep;13(9):1587-92. doi: 10.1093/carcin/13.9.1587. PMID: 1394844.

### In vivo study

1. Swaminathan S, Frederickson SM, Hatcher JF, Reznikoff CA, Butler MA, Cheever KL, Savage RE Jr. Neoplastic transformation and DNA-binding of 4,4'-methylenebis(2-chloroaniline) in SV40-immortalized human uroepithelial cell lines. *Carcinogenesis.* 1996 Apr;17(4):857-64. doi: 10.1093/carcin/17.4.857. PMID: 8625501.
2. DeBord DG, Cheever KL, Werren DM, Reid TM, Swearingin TF, Savage RE Jr. Determination of 4,4'-methylene-bis(2-chloroaniline)-DNA adduct formation in rat liver and human uroepithelial cells by the 32P postlabeling assay. *Fundam Appl Toxicol.* 1996 Mar;30(1):138-44. doi: 10.1006/faat.1996.0050. PMID: 8812257.

## 7. Bioactivity

### Biological target:

Aromatic diamine used in the plastics industry as curing agent for epoxy resins and urethane rubbers.

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## In vitro activity

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Alterations of the phosphorylation pattern of histones by the carcinogen, 4,4'-methylene-bis(2-chloroaniline) (MOCA) were investigated using rodent spleen cells. Spleen cells were isolated from Sprague-Dawley rats and treated with either 5, 10, 25, or 50 microM MOCA or acetone vehicle controls for 1, 2, 4, or 8 hours. Marked stimulation of histone phosphorylation was observed with the 10 microM MOCA treatment.

Reference: J Biochem Toxicol. 1995 Feb;10(1):19-23. <https://pubmed.ncbi.nlm.nih.gov/7595928/>

## In vivo activity

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Male Sprague-Dawley rats were treated with different dosing regimens of MOCA, and DNA was isolated from the liver. Five MOCA adducts were detected in rat liver DNA. Adduct A, which corresponded to N-(deoxyadenosin-8-yl)-4-amino-3-chlorobenzyl alcohol, was the major adduct in rat liver DNA appearing in all treatment groups. Levels of adduct A were higher when MOCA was administered by ip injection versus oral gavage.

Reference: Fundam Appl Toxicol. 1996 Mar;30(1):138-44. <https://pubmed.ncbi.nlm.nih.gov/8812257/>

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*