Contents

[Phthalates 12](#_Toc124056640)

[Benzyl butyl phthalate 12](#_Toc124056641)

[Biological location 12](#_Toc124056642)

[General References 13](#_Toc124056643)

[Material Safety Data Sheet (MSDS) 13](#_Toc124056644)

[Bis(2-ethylhexyl) phthalate 13](#_Toc124056645)

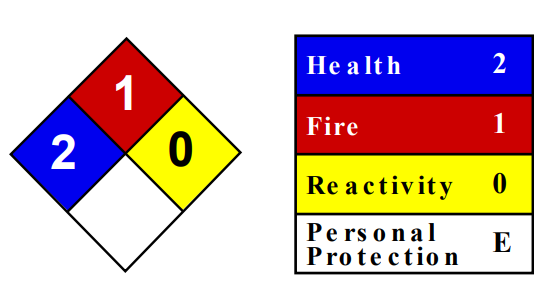
[General References 14](#_Toc124056646)

[Bis(2-ethylhexyl) terephthalate 14](#_Toc124056647)

[Material Safety Data Sheet (MSDS) 14](#_Toc124056648)

[General References 14](#_Toc124056649)

[Deoxycholic acid 15](#_Toc124056650)

[ 15](#_Toc124056651)

[Biological location 16](#_Toc124056652)

[Disease References 16](#_Toc124056653)

[General References 17](#_Toc124056654)

[Dibutyl phthalate 18](#_Toc124056655)

[Biological location 18](#_Toc124056656)

[General References 19](#_Toc124056657)

[Diisobutyl phthalate 20](#_Toc124056658)

[Biological Role(s): 20](#_Toc124056659)

[Application(s): 21](#_Toc124056660)

[Citations 21](#_Toc124056661)

[Diisooctyl phthalate 22](#_Toc124056662)

[Biological location 23](#_Toc124056663)

[Ageratriol (nasty chemotherapy) 24](#_Toc124056664)

[Genetic research 24](#_Toc124056665)

[Isophthalic acid 26](#_Toc124056666)

[Applications 26](#_Toc124056667)

[Health Hazard 27](#_Toc124056668)

[Mono(2-ethylhexyl) phthalate 27](#_Toc124056669)

[Biological location 27](#_Toc124056670)

[Monobutyl phthalate 28](#_Toc124056671)

[Health Hazard 28](#_Toc124056672)

[Cellular Locations 29](#_Toc124056673)

[Material Safety Data Sheet (MSDS) 29](#_Toc124056674)

[General References 29](#_Toc124056675)

[Phthalic acid 29](#_Toc124056676)

[Biospecimen Locations 30](#_Toc124056677)

[Tissue Locations 30](#_Toc124056678)

[Disease References 30](#_Toc124056679)

[General References 30](#_Toc124056680)

[Terephthalic acid 31](#_Toc124056681)

[Biospecimen Locations 31](#_Toc124056682)

[Tissue Locations 31](#_Toc124056683)

[General References 31](#_Toc124056684)

[Benzoic 32](#_Toc124056685)

[Benzoic acid 32](#_Toc124056686)

[(1R,9S)-11-Benzoyl-5-[(E)-2-(4-chlorophenyl)vinyl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4- 32](#_Toc124056687)

[dien-6-one 32](#_Toc124056688)

[1,2,4-Benzenetricarboxylic acid 33](#_Toc124056689)

[2,4-Dihydroxybenzoic acid 33](#_Toc124056690)

[3,5-Dihydroxybenzoic acid 33](#_Toc124056691)

[3,5-Di-tert-butyl-4-hydroxybenzaldehyde 33](#_Toc124056692)

[4-Ethoxy ethylbenzoate 33](#_Toc124056693)

[4-Hydroxybenzaldehyde 33](#_Toc124056694)

[Benzoguanamine 33](#_Toc124056695)

[Hydro 34](#_Toc124056696)

[(3S,4R)-3-(1-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one 34](#_Toc124056697)

[5-Hydroxymethyl-2-furancarboxaldehyde 34](#_Toc124056698)

[16-Hydroxyhexadecanoic acid 35](#_Toc124056699)

[2-Hydroxynicotinic acid 35](#_Toc124056700)

[3-Hydroxypicolinic acid 35](#_Toc124056701)

[3-Methoxysalicylic acid 35](#_Toc124056702)

[4-Hydroxy-6-methyl-2-pyrone 35](#_Toc124056703)

[4-Hydroxycoumarin 35](#_Toc124056704)

[4-Hydroxymandelic acid 35](#_Toc124056705)

[5-(1-Hydroxyethyl)-3-(2-hydroxypropyl)-2(5H)-furanone 35](#_Toc124056706)

[5-Hydroxynicotinic acid 35](#_Toc124056707)

[6-Hydroxynicotinic acid 35](#_Toc124056708)

[DL-4-Hydroxyphenyllactic acid 35](#_Toc124056709)

[Methyl 4-hydroxyphenylacetate 35](#_Toc124056710)

[3-Hydroxypicolinic acid 35](#_Toc124056711)

[4-Hydroxycoumarin 35](#_Toc124056712)

[4-Hydroxymandelic acid 35](#_Toc124056713)

[5-(1-Hydroxyethyl)-3-(2-hydroxypropyl)-2(5H)-furanone 35](#_Toc124056714)

[5-Hydroxymethyl-2-furaldehyde 35](#_Toc124056715)

[5-Hydroxynicotinic acid 35](#_Toc124056716)

[6-Hydroxynicotinic acid 36](#_Toc124056717)

[6-Hydroxypicolinic acid 36](#_Toc124056718)

[7-Hydroxycoumarine 36](#_Toc124056719)

[2-Hydroxynicotinic acid 36](#_Toc124056720)

[Critic acid cycle 36](#_Toc124056721)

[Citric acid 36](#_Toc124056722)

[Isocitric acid 36](#_Toc124056723)

[Methox 37](#_Toc124056724)

[2-(4-Methoxyphenoxy)ethanamine 37](#_Toc124056725)

[2-(4-Methoxyphenoxy)ethanamine 37](#_Toc124056726)

[2-Methoxyresorcinol 37](#_Toc124056727)

[2-Methyl-5-propionylfuran 37](#_Toc124056728)

[3,4-Dimethoxymethcathinone 37](#_Toc124056729)

[3-Methoxyphenylacetic acid 37](#_Toc124056730)

[3-Methoxysalicylic acid 37](#_Toc124056731)

[3-Methoxytyramine 37](#_Toc124056732)

[4-Methoxysalicylic acid 37](#_Toc124056733)

[5-Methoxysalicylic acid 37](#_Toc124056734)

[6-Methoxysalicylic acid 37](#_Toc124056735)

[DL-α-Methoxyphenylacetic acid 37](#_Toc124056736)

[PEG's 37](#_Toc124056737)

[Xxx PEG n6 37](#_Toc124056738)

[Physico-chemical properties and general characteristics 38](#_Toc124056739)

[Other applications of PEG-6 38](#_Toc124056740)

[PEG n11 39](#_Toc124056741)

[PEG n12 39](#_Toc124056742)

[PEG n5 39](#_Toc124056743)

[PEG n6 39](#_Toc124056744)

[PEG n7 39](#_Toc124056745)

[PEG-7 GLYCERYL COCOATE 39](#_Toc124056746)

[What is PEG-7 GLYCERYL COCOATE used for? 39](#_Toc124056747)

[Origin 40](#_Toc124056748)

[Xxx PEG n8 40](#_Toc124056749)

[Sugar 40](#_Toc124056750)

[D-(-)-Fructose 40](#_Toc124056751)

[D-(+)-Galactose 40](#_Toc124056752)

[D-(+)-Glucose 40](#_Toc124056753)

[Description 40](#_Toc124056754)

[Cellular Locations 42](#_Toc124056755)

[Biospecimen Locations 42](#_Toc124056756)

[Tissue Locations 42](#_Toc124056757)

[Disease References 43](#_Toc124056758)

[Growth hormone deficiency 43](#_Toc124056759)

[Acute myelogenous leukemia 43](#_Toc124056760)

[Hyperlipoproteinemia 43](#_Toc124056761)

[3-Methyl-crotonyl-glycinuria 43](#_Toc124056762)

[Addison's Disease 43](#_Toc124056763)

[Early preeclampsia 43](#_Toc124056764)

[Pregnancy 43](#_Toc124056765)

[Late-onset preeclampsia 44](#_Toc124056766)

[Glucagon deficiency 44](#_Toc124056767)

[Primary hypomagnesemia 44](#_Toc124056768)

[3-Hydroxy-3-methylglutaryl-CoA lyase deficiency 44](#_Toc124056769)

[3-Hydroxy-3-Methylglutaryl-CoA Synthase Deficiency 44](#_Toc124056770)

[21-Hydroxylase deficiency 45](#_Toc124056771)

[3-Hydroxyacyl-CoA dehydrogenase deficiency 45](#_Toc124056772)

[Short-chain L-3-hydroxyacyl-CoA dehydrogenase deficiency 45](#_Toc124056773)

[2-Methyl-3-hydroxybutyryl-CoA dehydrogenase deficiency 46](#_Toc124056774)

[Lipodystrophy 46](#_Toc124056775)

[Long-chain Fatty Acids, Defect in Transport of 46](#_Toc124056776)

[Partial lipodystrophy 47](#_Toc124056777)

[Phosphoenolpyruvate Carboxykinase Deficiency 1, Cytosolic 47](#_Toc124056778)

[Fructose-1,6-diphosphatase deficiency 47](#_Toc124056779)

[Hypoglycemia, familial neonatal 47](#_Toc124056780)

[Leigh's syndrome, subacute necrotizing encephalopathy, SNE 47](#_Toc124056781)

[Donohue Syndrome 48](#_Toc124056782)

[Leptin Deficiency or Dysfunction 48](#_Toc124056783)

[Mitochondrial trifunctional protein deficiency 49](#_Toc124056784)

[Carnitine palmitoyltransferase I deficiency 49](#_Toc124056785)

[Carnitine transporter defect; primary systemic carnitine deficiency 49](#_Toc124056786)

[Diabetes and Deafness, Maternally Inherited 49](#_Toc124056787)

[Beckwith-Wiedemann Syndrome 49](#_Toc124056788)

[Familial partial lipodystrophy 49](#_Toc124056789)

[Fanconi Bickel syndrome 49](#_Toc124056790)

[Sepsis 50](#_Toc124056791)

[Alzheimer's disease 50](#_Toc124056792)

[Glucose transporter type 1 deficiency syndrome 50](#_Toc124056793)

[Ulcerative colitis 50](#_Toc124056794)

[Colorectal cancer 51](#_Toc124056795)

[Diverticular disease 51](#_Toc124056796)

[Gout 51](#_Toc124056797)

[Rheumatoid arthritis 51](#_Toc124056798)

[Diabetes mellitus type 2 51](#_Toc124056799)

[Eosinophilic esophagitis 52](#_Toc124056800)

[General References 52](#_Toc124056801)

[Known gene associations 55](#_Toc124056802)

[D-(+)-Mannose 56](#_Toc124056803)

[Maltol 56](#_Toc124056804)

[Biological location 57](#_Toc124056805)

[Cellular Locations 57](#_Toc124056806)

[Disease References 58](#_Toc124056807)

[α-Lactose 58](#_Toc124056808)

[Tetramor's 58](#_Toc124056809)

[Tetranor-12(S)-HETE 58](#_Toc124056810)

[Tetranor-12R-HETE 58](#_Toc124056811)

[Amino acid and or derivative 58](#_Toc124056812)

[Alpha-Lactose 58](#_Toc124056813)

[Disease References 59](#_Toc124056814)

[Genes associated with Lactose 59](#_Toc124056815)

[cis-4-Hydroxy-D-proline 60](#_Toc124056816)

[3-Hydroxy-L-proline 60](#_Toc124056817)

[4-Oxoproline 60](#_Toc124056818)

[Isovanillic acid 60](#_Toc124056819)

[L-Pyroglutamic acid 60](#_Toc124056820)

[N-Acetyl-D-alloisoleucine 60](#_Toc124056821)

[N-Acetyl-DL-norvaline 60](#_Toc124056822)

[N-Acetyl-L-leucine 60](#_Toc124056823)

[N-Acetylvaline 60](#_Toc124056824)

[N-Isovalerylglycine 60](#_Toc124056825)

[trans-4-Hydroxy-L-proline 60](#_Toc124056826)

[Valine 60](#_Toc124056827)

[Hex 61](#_Toc124056828)

[Hexanoylglycine 61](#_Toc124056829)

[Bis(2-ethylhexyl) isophthalate 61](#_Toc124056830)

[Bis(2-ethylhexyl) sebacate 61](#_Toc124056831)

[Bis(2-ethylhexyl) adipate (nasty) 61](#_Toc124056832)

[Safety Profile 61](#_Toc124056833)

[Cyclohexylamine 61](#_Toc124056834)

[Hexadecanedioic acid 61](#_Toc124056835)

[Acids 63](#_Toc124056836)

[(-)-Camphanic acid 63](#_Toc124056837)

[(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid 63](#_Toc124056838)

[(5ξ,9ξ,16ξ)-17-Hydroxykauran-19-oic acid 63](#_Toc124056839)

[(R)-3-Hydroxy myristic acid 63](#_Toc124056840)

[1-(Carboxymethyl)cyclohexanecarboxylic acid 63](#_Toc124056841)

[11(Z)-Eicosenoic acid 63](#_Toc124056842)

[16-Hydroxyhexadecanoic acid 63](#_Toc124056843)

[2-(6-Hydroxyhexyl)-3-methylenesuccinic acid 63](#_Toc124056844)

[2-[(2S,4aR,8aS)-2-Hydroxy-4a-methyl-8-methylenedecahydro-2-naphthalenyl]acrylic acid 63](#_Toc124056845)

[2-Furoic acid 63](#_Toc124056846)

[2-Phenoxypropanoic acid 63](#_Toc124056847)

[3-(4-Hydroxyphenyl)propionic acid 63](#_Toc124056848)

[3-Methyladipic acid 63](#_Toc124056849)

[3-tert-Butyladipic acid 63](#_Toc124056850)

[5-Aminolevulinic acid 63](#_Toc124056851)

[5-Aminovaleric acid 63](#_Toc124056852)

[9-Oxo-10(E),12(E)-octadecadienoic acid 64](#_Toc124056853)

[Adipic acid 64](#_Toc124056854)

[Health effect 64](#_Toc124056855)

[Biological location 64](#_Toc124056856)

[Disease References 65](#_Toc124056857)

[General References 67](#_Toc124056858)

[Azelaic acid 68](#_Toc124056859)

[cis,cis-Muconic acid 68](#_Toc124056860)

[Dehydroacetic acid 68](#_Toc124056861)

[DL-4-Hydroxyphenyllactic acid 68](#_Toc124056862)

[Gabapentin 68](#_Toc124056863)

[Gentisic acid 68](#_Toc124056864)

[Kojic acid 68](#_Toc124056865)

[Myristic acid 68](#_Toc124056866)

[Oleic acid 68](#_Toc124056867)

[Palmitic acid 68](#_Toc124056868)

[Penicillic acid 68](#_Toc124056869)

[Pimelic acid 68](#_Toc124056870)

[Protocatechuic acid 68](#_Toc124056871)

[Sebacic acid 68](#_Toc124056872)

[Stearic acid 69](#_Toc124056873)

[Suberic acid 69](#_Toc124056874)

[Tetradecanedioic acid 69](#_Toc124056875)

[Tranexamic acid 69](#_Toc124056876)

[trans-10-Heptadecenoic acid 69](#_Toc124056877)

[trans-Petroselinic acid 69](#_Toc124056878)

[Drugs 69](#_Toc124056879)

[Caffeic acid 69](#_Toc124056880)

[Paracetamol 69](#_Toc124056881)

[DEET 69](#_Toc124056882)

[Methyl 70](#_Toc124056883)

[(3S)-3-Methyl-5-[(1S,8aR)-2,5,5,8a-tetramethyl-4-oxo-1,4,4a,5,6,7,8,8a-octahydro-1- 70](#_Toc124056884)

[naphthalenyl]pentanoic acid 70](#_Toc124056885)

[(3S)-5-[(4aR,8aS)-2,5,5,8a-Tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3- 70](#_Toc124056886)

[methylpentanoic acid 70](#_Toc124056887)

[1,2,3,4-Tetramethyl-1,3-cyclopentadiene 70](#_Toc124056888)

[2,2,6,6-Tetramethyl-4-piperidinol 70](#_Toc124056889)

[3,3,5,5-Tetramethylpyrroline-N-oxide 70](#_Toc124056890)

[Dimethyl Sebacate 70](#_Toc124056891)

[Major applications 70](#_Toc124056892)

[Hydro's 71](#_Toc124056893)

[(4E)-3-Hydroxy-2,4-dimethyl-4-heptenamide 71](#_Toc124056894)

[2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid 71](#_Toc124056895)

[2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid 71](#_Toc124056896)

[2,2-Dimethylglutaric acid 71](#_Toc124056897)

[2,6-Dimethyl-γ-pyrone 71](#_Toc124056898)

[3,3-Dimethylglutaric acid 71](#_Toc124056899)

[3-Acetyl-2,5-dimethylfuran 71](#_Toc124056900)

[Dimethyl cyclohexane-1,4-dicarboxylate 71](#_Toc124056901)

[Dimethyl sebacate 71](#_Toc124056902)

[N,N-Dimethylaniline (nasty) 71](#_Toc124056903)

[Tissue Locations 71](#_Toc124056904)

[Potential Acute Health Effects: 72](#_Toc124056905)

[Potential Chronic Health Effects: 72](#_Toc124056906)

[General References 72](#_Toc124056907)

[Dioctyl sebacate 72](#_Toc124056908)

[Decan's 73](#_Toc124056909)

[12-Aminododecanoic acid 73](#_Toc124056910)

[Dodecanedioic acid 73](#_Toc124056911)

[Dodecyl sulfate 73](#_Toc124056912)

[Dodecyltrimethylammonium 73](#_Toc124056913)

[Ethyl's 73](#_Toc124056914)

[Ethyl myristate 73](#_Toc124056915)

[Ethyl oleate 73](#_Toc124056916)

[N-Ethylpentylone 73](#_Toc124056917)

[Single compounds 73](#_Toc124056918)

[trans,trans-2,4-Heptadienal (nasty / antibiotic) 73](#_Toc124056919)

[Hazard Statements 74](#_Toc124056920)

[Chemical-Disease Co-Occurrences in Literature 74](#_Toc124056921)

[Health Hazards 75](#_Toc124056922)

[Antibiotic 75](#_Toc124056923)

[(-)-Caryophyllene oxide 80](#_Toc124056924)

[(+/-)12(13)-DiHOME 80](#_Toc124056925)

[(+/-)-C75 80](#_Toc124056926)

[(3S,4R)-3-(1-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one 80](#_Toc124056927)

[1,6-Hexanediol diglycidyl ether 80](#_Toc124056928)

[10-HDA 80](#_Toc124056929)

[13(S)-HOTrE 80](#_Toc124056930)

[13,14-Dihydro-15-keto-tetranor prostaglandin F1α 80](#_Toc124056931)

[18-HETE 80](#_Toc124056932)

[1-Adamantanamine 80](#_Toc124056933)

[1-Linoleoyl glycerol 80](#_Toc124056934)

[1-Tetradecylamine 80](#_Toc124056935)

[2,4-Xylidine 80](#_Toc124056936)

[2,5-Bis(5-tert-butyl-benzoxazol-2-yl)thiophene 80](#_Toc124056937)

[2,5-di-tert-Butylhydroquinone 80](#_Toc124056938)

[2,6-Xylidine 80](#_Toc124056939)

[4-Hydroxy-6-methyl-2-pyrone 80](#_Toc124056940)

[4-Nitrophenol 80](#_Toc124056941)

[9-Oxo-ODE 81](#_Toc124056942)

[Ageratriol 81](#_Toc124056943)

[Betaine 81](#_Toc124056944)

[Description 81](#_Toc124056945)

[Physiological effect 81](#_Toc124056946)

[Cellular Locations 82](#_Toc124056947)

[Tissue Locations 82](#_Toc124056948)

[Disease References 83](#_Toc124056949)

[Chronic renal failure 83](#_Toc124056950)

[Continuous ambulatory peritoneal dialysis 83](#_Toc124056951)

[Hemodialysis 83](#_Toc124056952)

[Colorectal cancer 83](#_Toc124056953)

[Schizophrenia 83](#_Toc124056954)

[Early preeclampsia 83](#_Toc124056955)

[Pregnancy 83](#_Toc124056956)

[Late-onset preeclampsia 84](#_Toc124056957)

[Hypermethioninemia 84](#_Toc124056958)

[Crohn's disease 84](#_Toc124056959)

[Ulcerative colitis 84](#_Toc124056960)

[Perillyl alcohol administration for cancer treatment 85](#_Toc124056961)

[Pancreatic cancer 85](#_Toc124056962)

[Periodontal disease 85](#_Toc124056963)

[Alzheimer's disease 85](#_Toc124056964)

[Frontotemporal dementia 85](#_Toc124056965)

[Lewy body disease 85](#_Toc124056966)

[Lung Cancer 85](#_Toc124056967)

[Argininosuccinic aciduria 86](#_Toc124056968)

[Propionic acidemia 86](#_Toc124056969)

[Phenylketonuria 86](#_Toc124056970)

[Eosinophilic esophagitis 86](#_Toc124056971)

[Known gene relationship 86](#_Toc124056972)

[Caprolactam 87](#_Toc124056973)

[Capryloylglycine 87](#_Toc124056974)

[Decanamide 87](#_Toc124056975)

[D-Raffinose 87](#_Toc124056976)

[Disease References 87](#_Toc124056977)

[Colorectal cancer 87](#_Toc124056978)

[Sepsis 87](#_Toc124056979)

[Erucamide 88](#_Toc124056980)

[Eucalyptol 89](#_Toc124056981)

[Methyl 4-hydroxyphenylacetate 89](#_Toc124056982)

[Pestalotin 89](#_Toc124056983)

[Phloroglucinol 89](#_Toc124056984)

[WARNING 90](#_Toc124056985)

[IBS RESEARCH PAPER 90](#_Toc124056986)

[Polygodial 91](#_Toc124056987)

[Pregabalin 91](#_Toc124056988)

[Pyrogallol 91](#_Toc124056989)

[Stearamide 91](#_Toc124056990)

[trans,trans-2,4-Heptadienal 91](#_Toc124056991)

[Tributylphosphine oxide 91](#_Toc124056992)

[Triethanolamine 91](#_Toc124056993)

[Triisopropanolamine 91](#_Toc124056994)

[Trinexapac 91](#_Toc124056995)

[Valpromide 91](#_Toc124056996)

[Vanillin 91](#_Toc124056997)

[Veratrole 91](#_Toc124056998)

[Pyrogallol (nasty stuff) 91](#_Toc124056999)

[Mechanism of Action 91](#_Toc124057000)

[Hazards Summary 92](#_Toc124057001)

# Phthalates

## Benzyl butyl phthalate

A red and black sign

Description automatically generated with medium confidence

Description - Benzyl butyl phthalate belongs to the class of organic compounds known as benzoic acid esters. These are ester derivatives of benzoic acid. Based on a literature review a significant number of articles have been published on Benzyl butyl phthalate. This compound has been identified in human blood as reported by (PMID: 31557052). Benzyl butyl phthalate is not a naturally occurring metabolite and is only found in those individuals exposed to this compound or its derivatives. Technically Benzyl butyl phthalate is part of the human exposome. The exposome can be defined as the collection of all the exposures of an individual in a lifetime and how those exposures relate to health. An individual's exposure begins before birth and includes insults from environmental and occupational sources.

### Biological location

Non-excretory biofluid

Biofluid or Excreta

Blood (PMID:31557052)

Cellular substructure

Membrane (HMDB:HMDB0249068)

### General References

Barupal DK, Fiehn O: Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach. Environ Health Perspect. 2019 Sep;127(9):97008. doi: 10.1289/EHP4713. Epub 2019 Sep 26. [PubMed:31557052]

### Material Safety Data Sheet (MSDS)

Not Available

## Bis(2-ethylhexyl) phthalate

A red and black sign

Description automatically generated with medium confidence

Description - Di(2-ethylhexyl)phthalate, also known as DEHP or di-iso-octyl phthalate, belongs to the class of organic compounds known as benzoic acid esters. These are ester derivatives of benzoic acid. Di(2-ethylhexyl)phthalate is a primary metabolite. Primary metabolites are metabolically or physiologically essential metabolites. They are directly involved in an organism’s growth, development or reproduction. Di(2-ethylhexyl)phthalate is formally rated as a possible carcinogen (by IARC 2B) and is also a potentially toxic compound.

Based on a literature review a significant number of articles have been published on Di(2-ethylhexyl)phthalate. This compound has been identified in human blood as reported by (PMID: 31557052). Bis(2-ethylhexyl) phthalate is not a naturally occurring metabolite and is only found in those individuals exposed to this compound or its derivatives. Technically Bis(2-ethylhexyl) phthalate is part of the human exposome. The exposome can be defined as the collection of all the exposures of an individual in a lifetime and how those exposures relate to health. An individual's exposure begins before birth and includes insults from environmental and occupational sources.

General References

Barupal DK, Fiehn O: Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach. Environ Health Perspect. 2019 Sep;127(9):97008. doi: 10.1289/EHP4713. Epub 2019 Sep 26. [PubMed:31557052]

## Bis(2-ethylhexyl) terephthalate

A red and black sign

Description automatically generated with medium confidence

Description - Eastman DOTP Plasticizer, also known as 1,4-deht, belongs to the class of organic compounds known as p-phthalate esters. These are ester derivatives of p-phthalic acids, which are based on a benzene 1,4-dicarboxylic acid skeleton. Based on a literature review a significant number of articles have been published on Eastman DOTP Plasticizer. This compound has been identified in human blood as reported by (PMID: 31557052 ). Bis(2-ethylhexyl) terephthalate is not a naturally occurring metabolite and is only found in those individuals exposed to this compound or its derivatives. Technically Bis(2-ethylhexyl) terephthalate is part of the human exposome. The exposome can be defined as the collection of all the exposures of an individual in a lifetime and how those exposures relate to health. An individual's exposure begins before birth and includes insults from environmental and occupational sources.

### Material Safety Data Sheet (MSDS)

Not Available

### General References

Barupal DK, Fiehn O: Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach. Environ Health Perspect. 2019 Sep;127(9):97008. doi: 10.1289/EHP4713. Epub 2019 Sep 26. [PubMed:31557052]

Decyl hexyl phthalate

## Deoxycholic acid

## 

Deoxycholic acid

Description - Deoxycholic acid is a secondary bile acid produced in the liver and is usually conjugated with glycine or taurine. It facilitates fat absorption and cholesterol excretion. Bile acids are steroid acids found predominantly in the bile of mammals. The distinction between different bile acids is minute, and depends only on the presence or absence of hydroxyl groups on positions 3, 7, and 12. Bile acids are physiological detergents that facilitate excretion, absorption, and transport of fats and sterols in the intestine and liver. Bile acids are also steroidal amphipathic molecules derived from the catabolism of cholesterol. They modulate bile flow and lipid secretion, are essential for the absorption of dietary fats and vitamins and have been implicated in the regulation of all the key enzymes involved in cholesterol homeostasis. Bile acids recirculate through the liver, bile ducts, small intestine, and portal vein to form an enterohepatic circuit. They exist as anions at physiological pH, and consequently require a carrier for transport across the membranes of the enterohepatic tissues. The unique detergent properties of bile acids are essential for the digestion and intestinal absorption of hydrophobic nutrients. Bile acids have potent toxic properties (e.g. membrane disruption) and there are a plethora of mechanisms to limit their accumulation in blood and tissues (PMID: 11316487, 16037564, 12576301, 11907135). When present in sufficiently high levels, deoxycholic acid can act as a hepatotoxin, a metabotoxin, and an oncometabolite. A hepatotoxin causes damage to the liver or liver cells. A metabotoxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. An oncometabolite is a compound, when present at chronically high levels, that promotes tumour growth and survival. Among the primary bile acids, cholic acid is considered to be the least hepatotoxic while deoxycholic acid is the most hepatoxic (PMID: 1641875). The liver toxicity of bile acids appears to be due to their ability to peroxidate lipids and to lyse liver cells. High bile acid levels lead to the generation of reactive oxygen species and reactive nitrogen species, disruption of the cell membrane and mitochondria, induction of DNA damage, mutation and apoptosis, and the development of reduced apoptosis capability upon chronic exposure (PMID: 24884764). Chronically high levels of deoxycholic acid are associated with familial hypercholanemia. In hypercholanemia, bile acids, including deoxycholic acid, are elevated in the blood. This disease causes liver damage, extensive itching, poor fat absorption, and can lead to rickets due to lack of calcium in bones. The deficiency of normal bile acids in the intestines results in a deficiency of vitamin K, which also adversely affects clotting of the blood. The bile acid ursodiol (ursodeoxycholic acid) can improve symptoms associated with familial hypercholanemia. Chronically high levels of deoxycholic acid are also associated with several forms of cancer including colon cancer, pancreatic cancer, esophageal cancer, and many other GI cancers.

### Biological location

Cell

Erythrocyte (HMDB:HMDB0000626)

Fibroblasts (HMDB:HMDB0000626)

Organ

Intestine (HMDB:HMDB0000626)

Biofluid or Excreta

Non-excretory biofluid

Bile (PMID:16548228)

Blood (PMID:15185309)

Excreta

Urine (PMID:2621422)

Feces (PMID:22664055)

Cellular substructure

Extracellular (HMDB:HMDB0000626)

Intestine (HMDB:HMDB0000626)

### Disease References

1. Cystic fibrosis

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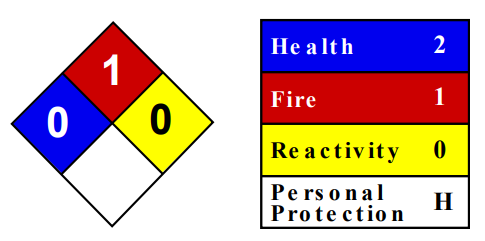
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Batta AK, Arora R, Salen G, Tint GS, Eskreis D, Katz S: Characterization of serum and urinary bile acids in patients with primary biliary cirrhosis by gas-liquid chromatography-mass spectrometry: effect of ursodeoxycholic acid treatment. J Lipid Res. 1989 Dec;30(12):1953-62. [PubMed:2621422]

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## Dibutyl phthalate



Dibutyl phthalate

Description - Dibutyl phthalate is found in cloves. DBP was added to the California Proposition 65 (1986) list of suspected teratogens in November 2006. It is a suspected endocrine disruptor. It was used in some nail polishes; all major producers began eliminating this chemical from nail polishes in the Fall of 2006. Dibutyl phthalate (DBP) is a commonly used plasticizer. It is also used as an additive to adhesives or printing inks. It is soluble in various organic solvents, e.g. in alcohol, ether and benzene. DBP is also used as an ectoparasiticide. Belongs to the class of organic compounds known as benzoic acid esters. These are ester derivatives of benzoic acid.

### Biological location

Cellular substructure

Membrane (HMDB:HMDB0244288)

Biofluid or Excreta

Non-excretory biofluid

Blood (PMID:31557052)

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## Diisobutyl phthalate

A red and black sign

Description automatically generated with low confidence

Diisobutyl phthalate (DIBP) is prepared by esterification process of isobutanol and phthalic anhydride. Its structural formula is C6H4(COOCH2CH(CH3)2)2. DIBP is an odorless plasticizer and has excellent heat and light stability. It is the lowest cost plasticizer for cellulose nitrate. DIBP has lower density and freezing point than the related compound dibutyl phthalate (DBP). Otherwise, it has similar properties DBP and can often be used as a substitute for it. Its refractive index is 1.488–1.492 (at 20 °C, D).

### Biological Role(s):

1. teratogenic agent

2. A role played by a chemical compound in biological systems with adverse consequences in embryo developments, leading to birth defects, embryo death or altered development, growth retardation and functional defect.

3. PPAR modulator

### Application(s):

1. plasticiser - Any compound that is used as an additive to increase the plasticity or fluidity of a substance, particularly but not exclusively to synthetic polymers.

2. endocrine disruptor - Any compound that can disrupt the functions of the endocrine (hormone) system

(via phthalate ester)

Citations

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## Diisooctyl phthalate

A red and black sign

Description automatically generated with medium confidence

Description - Diisooctyl phthalate belongs to the class of organic compounds known as benzoic acid esters. These are ester derivatives of benzoic acid. Phthalate esters are endocrine disruptors. Diisooctyl phthalate is an extremely weak basic (essentially neutral) compound (based on its pKa). The terminal or next-to-last carbon atom in the monoester can also be oxidized to an alcohol, which can be excreted as is or first oxidized to an aldehyde, ketone, or carboxylic acid. Diisooctyl phthalate is a potentially toxic compound. Phthalate esters are first hydrolyzed to their monoester derivative. Phthalate esters are esters of phthalic acid and are mainly used as plasticizers, primarily used to soften polyvinyl chloride. They decrease foetal testis testosterone production and reduce the expression of steroidogenic genes by decreasing mRNA expression. Phthalates are hazardous due to their ability to act as endocrine disruptors. The combination of effects associated with phthalates is called 'phthalate syndrome’. This compound has been identified in human blood as reported by (PMID: 31557052). Diisooctyl phthalate is not a naturally occurring metabolite and is only found in those individuals exposed to this compound or its derivatives. Technically Diisooctyl phthalate is part of the human exposome. The exposome can be defined as the collection of all the exposures of an individual in a lifetime and how those exposures relate to health. An individual's exposure begins before birth and includes insults from environmental and occupational sources.

Biological location

Non-excretory biofluid

Biofluid or Excreta

Blood (PMID: 31557052)

Cellular substructure - Membrane (HMDB: HMDB0251353)

Health Hazard - Danger - GHS Hazard Statements H360FD: May damage fertility; May damage the unborn child [Danger Reproductive toxicity]

## Ageratriol (nasty chemotherapy)

A red and black sign

Description automatically generated with medium confidence

Terpenoids and also known as a SESQUITERPENOIDS

Asolute configuration of ageratriol germacranic sesquiterpene from Achillea ageratum

Grandi R, Marchesini A, Pagnoni UM, Trave R, Garanti L, 1974. A L. Tetrahedron, 30, 3821-3826.

### Genetic research

|  |  |  |  |
| --- | --- | --- | --- |
| Target Name | BioAssay Name (Chemotherapeutic ) | BioAssay AID | Substance SID |
| [Chain A, Calcium and integrin-binding protein 1 (human)](https://pubchem.ncbi.nlm.nih.gov/protein/2LM5_A) | Calcium Integrin Binding Protein 1 (CIB1) Competitor | [1508620](https://pubchem.ncbi.nlm.nih.gov/bioassay/1508620) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [CIB1 - calcium and integrin binding 1 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/10519) | Calcium Integrin Binding Protein 1 (CIB1) Competitor | [1508620](https://pubchem.ncbi.nlm.nih.gov/bioassay/1508620) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [FH - fumarate hydratase (human)](https://pubchem.ncbi.nlm.nih.gov/gene/2271) | human fumarate hydratase | [1347055](https://pubchem.ncbi.nlm.nih.gov/bioassay/1347055) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [FH - fumarate hydratase (human)](https://pubchem.ncbi.nlm.nih.gov/gene/2271) | Calcium Integrin Binding Protein 1 (CIB1) Competitor | [1347055](https://pubchem.ncbi.nlm.nih.gov/bioassay/1347055) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [GPT2 - glutamic--pyruvic transaminase 2 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/84706) | Glutamate pyruvate transaminase 2 (GPT2) | [1671188](https://pubchem.ncbi.nlm.nih.gov/bioassay/1671188) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [GPT2 - glutamic--pyruvic transaminase 2 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/84706) | Glutamate pyruvate transaminase 2 (GPT2) | [1671188](https://pubchem.ncbi.nlm.nih.gov/bioassay/1671188) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [IP6K1 - inositol hexakisphosphate kinase 1 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/9807) | inhibitors of Inositol hexaphosphate kinase 1 (IP6K1) | [1645851](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645851) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [IP6K1 - inositol hexakisphosphate kinase 1 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/9807) | inhibitors of Inositol hexaphosphate kinase 1 (IP6K1) | [1645851](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645851) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [NSD2 - nuclear receptor binding SET domain protein 2 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/7468) | nuclear receptor binding SET domain protein 2 (NSD2) | [1645876](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645876) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [NSD2 - nuclear receptor binding SET domain protein 2 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/7468) | nuclear receptor binding SET domain protein 2 (NSD2) | [1645876](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645876) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [NSD2 - nuclear receptor binding SET domain protein 2 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/7468) | nuclear receptor binding SET domain protein 2 (NSD2) | [1645877](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645877) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [NSD2 - nuclear receptor binding SET domain protein 2 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/7468) | nuclear receptor binding SET domain protein 2 (NSD2) | [1645877](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645877) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [NTMT1 - N-terminal Xaa-Pro-Lys N-methyltransferase 1 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/28989) | N-terminal methyltransferase 1 (NTMT1) | [1645870](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645870) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |
| [NTMT1 - N-terminal Xaa-Pro-Lys N-methyltransferase 1 (human)](https://pubchem.ncbi.nlm.nih.gov/gene/28989) | N-terminal methyltransferase 1 (NTMT1) | [1645870](https://pubchem.ncbi.nlm.nih.gov/bioassay/1645870) | [363679670](https://pubchem.ncbi.nlm.nih.gov/substance/363679670) |

|  |  |  |
| --- | --- | --- |
| The cytotoxic and antitumor activities of GE. |  |  |
| Cancer type | Suppressive effect | Cellular processes |
| Colon cancer | Anti-proliferation | Apoptosis, DNA damage, and cell cycle arrest |
| Endometrial carcinoma | Anti-migration | Antiangiogenesis |
| Liver cancer | Anti-proliferation | Apoptosis |
| Lung cancer | Anti-proliferation | Apoptosis |
| Pancreatic cancer | Anti-proliferation | Apoptosis |
| Prostate cancer | Anti-proliferation | Cell cycle arrest |
| Skin cancer | Anti-proliferation | Apoptosis |

## Isophthalic acid

A red and black sign

Description automatically generated with medium confidence

Isophthalic acid (PIA) is a non-toxic organic compound with the formula C6H4(CO2H)2. This colorless solid is an isomer of phthalic acid and terephthalic acid. These aromatic dicarboxylic acids are used as precursors (in the form of acylchlorides) to commercially important polymers. The high-performance polymer polybenzimidazole is produced from isophthalic acid.

### Applications

Isophthalic acid (PIA) has three major uses:

1. PET (PolyEthylene Terephthalate) copolymer, which is used in bottle resins and to a much lesser extent, for fibers. PIA (Purified Isophthalic Acid) reduces the crystallinity of PET, which serves to improve clarity and increase the productivity of bottle-making.
2. Unsaturated polyester resins, where the addition of PIA improves thermal resistance and mechanical performance, as well as resistance to chemicals and water.
3. Polyester/alkyd surface coating resins, where PIA increases resistance to water, overall durability and weatherability.Health Hazards

Isophthalic acid is a colorless crystalline solid. It is used as an intermediate primarily for unsaturated polyester resins and alkyd and polyester coating resins; other applications include use in aramid fibers, as a component of copolyester resins and in high-temperature polymers. Nearly pure isophthalic acid has a purity of >99.8%. This material is called purified isophthalic acid or PIA.

IPA has excellent performance characteristics including exceptional hardness, corrosion and stain resistance, hydrolytic stability of coatings and gel coats, outstanding thermal stability and low resin color in coatings industry.

Isophthalic acid is a key ingredient in FRP (Fiberglass Reinforced Plastics) markets for such products as marine, automotive, and corrosion resistant pipes and tanks. Polyesters containing isophthalic acid are also used extensively in industrial coatings applications for home appliances, automobiles, aluminum siding, and metal office furniture. It used as an intermediate for polyesters, polyurethane resins, plasticizers.

### Health Hazard

May cause slight to moderate irritation of eyes, skin, and mucous membranes on prolonged contact. Ingestion may cause gastrointestinal irritation. (USCG, 1999)

## Mono(2-ethylhexyl) phthalate

A red and black sign

Description automatically generated with medium confidence

Mono-(2-ethyl-5-hydroxyhexyl) phthalate

Description - Mono-(2-ethyl-5-hydroxyhexyl) phthalate, also known as 40321-99-1 or phthalic acid mono(2-ethyl-5-hydroxyhexyl) ester, is classified as a member of the benzoic acid esters. Benzoic acid esters are ester derivatives of benzoic acid. 40321-99-1 is considered to be practically insoluble (in water) and acidic. (ChemoSummarizer) Mono-(2-ethyl-5-hydroxyhexyl) phthalate is a metabolite of mono(2-ethylhexyl) phthalate (MEHP) and a secondary metabolite of di(2-ethylhexyl) phthalate (DEHP) [Exposome-Explorer]. Di(2-ethylhexyl) phthalate (DEHP) is added to polyvinyl chloride (PVC) plastics used widely in medical devices and toys to impart flexibility and durability (Pubmed:16332407).

### Biological location

Excreta

Biofluid or Excreta

Urine (HMDB: HMDB0094679)

Cellular substructure

Membrane (HMDB: HMDB0094679)

Peroxisome (HMDB: HMDB0094679)

Metabolic pathway

Fatty Acid Metabolism (HMDB:HMDB0094679)

General References

1. Hauser R, Gaskins AJ, Souter I, Smith KW, Dodge LE, Ehrlich S, Meeker JD, Calafat AM, Williams PL: Urinary Phthalate Metabolite Concentrations and Reproductive Outcomes among Women Undergoing in Vitro Fertilization: Results from the EARTH Study. Environ Health Perspect. 2016 Jun;124(6):831-9. doi: 10.1289/ehp.1509760. Epub 2015 Nov 6. [PubMed:26545148]
2. Wang YX, Zeng Q, Sun Y, Yang P, Wang P, Li J, Huang Z, You L, Huang YH, Wang C, Li YF, Lu WQ: Semen phthalate metabolites, semen quality parameters and serum reproductive hormones: A cross-sectional study in China. Environ Pollut. 2016 Apr;211:173-82. doi: 10.1016/j.envpol.2015.12.052. Epub 2016 Jan 14. [PubMed:26766535]
3. Alves A, Vanermen G, Covaci A, Voorspoels S: Ultrasound assisted extraction combined with dispersive liquid-liquid microextraction (US-DLLME)-a fast new approach to measure phthalate metabolites in nails. Anal Bioanal Chem. 2016 Sep;408(22):6169-80. doi: 10.1007/s00216-016-9727-1. Epub 2016 Jul 2. [PubMed:27372718]
4. Yao HY, Han Y, Gao H, Huang K, Ge X, Xu YY, Xu YQ, Jin ZX, Sheng J, Yan SQ, Zhu P, Hao JH, Tao FB: Maternal phthalate exposure during the first trimester and serum thyroid hormones in pregnant women and their newborns. Chemosphere. 2016 Aug;157:42-8. doi: 10.1016/j.chemosphere.2016.05.023. Epub 2016 May 18. [PubMed:27208644]

## Monobutyl phthalate



Monobuty lphthalate

Description - Monobutylphthalate belongs to the class of organic compounds known as benzoic acid esters. These are ester derivatives of benzoic acid. Monobutylphthalate has been detected, but not quantified in, breakfast cereal and cereals and cereal products. This could make monobutylphthalate a potential biomarker for the consumption of these foods. Based on a literature review very few articles have been published on Monobutylphthalate.

### Health Hazard

Hu Y, Dong C, Chen M, Chen Y, Gu A, Xia Y, Sun H, Li Z, Wang Y (2015). "Effects of monobutyl phthalate on steroidogenesis through steroidogenic acute regulatory protein regulated by transcription factors in mouse Leydig tumor cells". Journal of Endocrinological Investigation. 38 (8): 875–884. doi:10.1007/s40618-015-0279-6. PMID 25903692. S2CID 21965989.

### Cellular Locations

Membrane

Blood

Urine

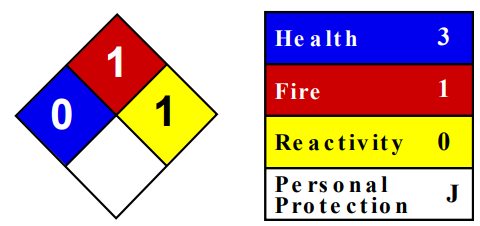
### Material Safety Data Sheet (MSDS)

Not Available

### General References

Blount BC, Silva MJ, Caudill SP, Needham LL, Pirkle JL, Sampson EJ, Lucier GW, Jackson RJ, Brock JW: Levels of seven urinary phthalate metabolites in a human reference population. Environ Health Perspect. 2000 Oct;108(10):979-82. [PubMed:11049818]

## Phthalic acid



Description - Phthalic acid is an aromatic dicarboxylic acid, with formula C6H4(COOH)2. Phthalic acid is used mainly in the form of the anhydride to produce other chemicals such as dyes, perfumes, saccharin, phthalates and many other useful products. Phthalic acid, when found in tissues or biofluids arises from exposure to these phthalate products. Phthalate is an environmental chemical of heightened public concern because reports of its potential risk to male reproductive health (PMID 16804814 ), being significantly associated with reduced sperm concentration to pesticide concentration in men's urine (PMID 16804812 ). Within the reproductive tract, the male is exquisitely vulnerable to the effects of anti-androgens during development due the reliance on the synthesis and action of androgens for the masculinization of the male reproductive tract. The ability of phthalates to suppress androgen synthesis during development and to induce testicular dysgenesis together with cryptorchidism and hypospadias has raised considerable concern. (PMID 15016950). Belongs to the class of organic compounds known as benzoic acids. These are organic Compounds containing a benzene ring which bears at least one carboxyl group.

### Biospecimen Locations

Blood

Feces

Saliva

Urine

### Tissue Locations

Liver

### Disease References

1. Hemodialysis

Pollack GM, Buchanan JF, Slaughter RL, Kohli RK, Shen DD: Circulating concentrations of di(2-ethylhexyl) phthalate and its de-esterified phthalic acid products following plasticizer exposure in patients receiving hemodialysis. Toxicol Appl Pharmacol. 1985 Jun 30;79(2):257-67. [PubMed:4002227 ]

1. Colorectal cancer

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. Carcinogenesis. 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. [PubMed:25037050 ]

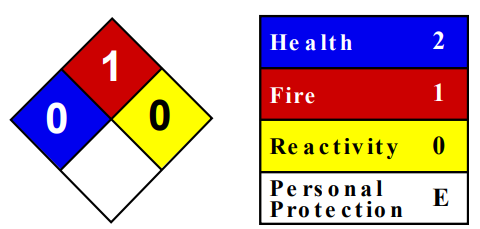
1. Eosinophilic esophagitis

Slae, M., Huynh, H., Wishart, D.S. (2014). Analysis of 30 normal pediatric urine samples via NMR spectroscopy (unpublished work). NA.

# General References

1. Silva MJ, Reidy JA, Samandar E, Herbert AR, Needham LL, Calafat AM: Detection of phthalate metabolites in human saliva. Arch Toxicol. 2005 Nov;79(11):647-52. Epub 2005 Jul 2. [PubMed:15995852]
2. Lapinskas PJ, Brown S, Leesnitzer LM, Blanchard S, Swanson C, Cattley RC, Corton JC: Role of PPARalpha in mediating the effects of phthalates and metabolites in the liver. Toxicology. 2005 Feb 1;207(1):149-63. [PubMed:15590130]
3. Hurst CH, Waxman DJ: Activation of PPARalpha and PPARgamma by environmental phthalate monoesters. Toxicol Sci. 2003 Aug;74(2):297-308. Epub 2003 Jun 12. [PubMed:12805656]
4. Hauser R: The environment and male fertility: recent research on emerging chemicals and semen quality. Semin Reprod Med. 2006 Jul;24(3):156-67. [PubMed:16804814]
5. Swan SH: Does our environment affect our fertility? Some examples to help reframe the question. Semin Reprod Med. 2006 Jul;24(3):142-6. [PubMed:16804812]
6. Fisher JS: Environmental anti-androgens and male reproductive health: focus on phthalates and testicular dysgenesis syndrome. Reproduction. 2004 Mar;127(3):305-15. [PubMed:15016950]

## Terephthalic acid



Terephthalic acid

Description - Terephthalic acid is a benzenedicarboxylic acid carrying carboxy groups at positions 1 and 4. One of three possible isomers of benzenedicarboxylic acid, the others being phthalic and isophthalic acids. It is a conjugate acid of a terephthalate(1-). Terephthalic acid is one isomer of the three phthalic acids. It finds important use as a commodity chemical, principally as a starting compound for the manufacture of polyester (specifically PET), used in clothing and to make plastic bottles. It is also known as 1,4-benzenedicarboxylic acid, and it has the chemical formula C6H4(COOH)2. Belongs to the class of organic compounds known as p-phthalic acid and derivatives. P-phthalic acid and derivatives are compounds containing a benzene ring bearing a carboxylic acid group at ring carbon atoms 1 and 4.

### Biospecimen Locations

Blood

Saliva

Urine

### Tissue Locations

Fibroblasts

Platelet

### General References

1. Guneral F, Bachmann C: Age-related reference values for urinary organic acids in a healthy Turkish pediatric population. Clin Chem. 1994 Jun;40(6):862-6. [PubMed:8087979]
2. Iwasaki Y, Yamasaki A, Ishihara K: Platelet compatible blood filtration fabrics using a phosphorylcholine polymer having high surface mobility. Biomaterials. 2003 Sep;24(20):3599-604. [PubMed:12809789]
3. Bot I, von der Thusen JH, Donners MM, Lucas A, Fekkes ML, de Jager SC, Kuiper J, Daemen MJ, van Berkel TJ, Heeneman S, Biessen EA: Serine protease inhibitor Serp-1 strongly impairs atherosclerotic lesion formation and induces a stable plaque phenotype in ApoE-/-mice. Circ Res. 2003 Sep 5;93(5):464-71. Epub 2003 Aug 14. [PubMed:12919945]
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5. Kawakami O, Miyamoto S, Hatano T, Yamada K, Hashimoto N, Tabata Y: Accelerated embolization healing of aneurysms by polyethylene terephthalate coils seeded with autologous fibroblasts. Neurosurgery. 2005 May;56(5):1075-81; discussion 1075-81. [PubMed:15854257]
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7. Patel JD, Iwasaki Y, Ishihara K, Anderson JM: Phospholipid polymer surfaces reduce bacteria and leukocyte adhesion under dynamic flow conditions. J Biomed Mater Res A. 2005 Jun 1;73(3):359-66. [PubMed:15800952]
8. Tremaine LM, Quebbemann AJ: The renal handling of terephthalic acid. Toxicol Appl Pharmacol. 1985 Jan;77(1):165-74. [PubMed:3966238]
9. Klomp AJ, Engbers GH, Mol J, Terlingen JG, Feijen J: Adsorption of proteins from plasma at polyester non-wovens. Biomaterials. 1999 Jul;20(13):1203-11. [PubMed:10395389]
10. Roald HE, Barstad RM, Bakken IJ, Roald B, Lyberg T, Sakariassen KS: Initial interactions of platelets and plasma proteins in flowing non-anticoagulated human blood with the artificial surfaces Dacron and PTFE. Blood Coagul Fibrinolysis. 1994 Jun;5(3):355-63. [PubMed:8075307]
11. Gappa-Fahlenkamp H, Lewis RS: Improved hemocompatibility of poly(ethylene terephthalate) modified with various thiol-containing groups. Biomaterials. 2005 Jun;26(17):3479-85. [PubMed:15621237]

# Benzoic

## Benzoic acid

## (1R,9S)-11-Benzoyl-5-[(E)-2-(4-chlorophenyl)vinyl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-

## dien-6-one

No data is viewable in any web site.

## 1,2,4-Benzenetricarboxylic acid

## 2,4-Dihydroxybenzoic acid

## 3,5-Dihydroxybenzoic acid

## 3,5-Di-tert-butyl-4-hydroxybenzaldehyde

Description - 3,5-Di-tert-butyl-4-hydroxybenzaldehyde, also known as BHT-CHO or 4-formyl-2,6-di-tert-butylphenol, belongs to the class of organic compounds known as hydroxybenzaldehydes. These are organic aromatic compounds containing a benzene ring carrying an aldehyde group and a hydroxyl group. BHT-CHO is a metabolite of 2,6-di-tert-butyl-4-methylphenol (BHA), a synthetic phenolic antioxidant (SPA). SPAs are a family of chemicals used widely in foods, polymers, and cosmetics as radical trapping agents to slow down degradation due to oxidation. Given their widespread use, human exposure is unavoidable and there is public concern regarding environmental contamination by these chemicals. BHT-CHO was detected in human urine (PMID: 31265952).

General References

Liu R, Mabury SA: Unexpectedly high concentrations of 2,4-di-tert-butylphenol in human urine. Environ Pollut. 2019 Sep;252(Pt B):1423-1428. doi: 10.1016/j.envpol.2019.06.077. Epub 2019 Jun 21. [PubMed:31265952]

## 4-Ethoxy ethylbenzoate

## 4-Hydroxybenzaldehyde

## Benzoguanamine

# Hydro

## (3S,4R)-3-(1-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one

## 5-Hydroxymethyl-2-furancarboxaldehyde

Description - 5-Hydroxymethyl-2-furancarboxaldehyde belongs to the family of Furans. These are compounds containing a furan ring, which is a five-member aromatic ring with one oxygen atom, four carbon atoms. 5-Hydroxymethyl-2-furancarboxaldehyde is found in garden onion. Obtainable from various carbohydrates. 5-Hydroxymethyl-2-furancarboxaldehyde is present in tomatoes, tobacco oil etc. 5-Hydroxymethyl-2-furancarboxaldehyde is a constituent of numerous plant species. 5-Hydroxymethyl-2-furancarboxaldehyde is used as an index of heat treatment and deterioration in food such as tomato paste, honey and fruit juices. Also an indicator of adulteration with acid-converted invert sugars. 5-Hydroxymethylfurfural is a biomarker for the consumption of beer.

## 16-Hydroxyhexadecanoic acid

## 2-Hydroxynicotinic acid

## 3-Hydroxypicolinic acid

## 3-Methoxysalicylic acid

## 4-Hydroxy-6-methyl-2-pyrone

## 4-Hydroxycoumarin

## 4-Hydroxymandelic acid

## 5-(1-Hydroxyethyl)-3-(2-hydroxypropyl)-2(5H)-furanone

## 5-Hydroxynicotinic acid

## 6-Hydroxynicotinic acid

## DL-4-Hydroxyphenyllactic acid

## Methyl 4-hydroxyphenylacetate

## 3-Hydroxypicolinic acid

## 4-Hydroxycoumarin

## 4-Hydroxymandelic acid

## 5-(1-Hydroxyethyl)-3-(2-hydroxypropyl)-2(5H)-furanone

## 5-Hydroxymethyl-2-furaldehyde

## 5-Hydroxynicotinic acid

## 6-Hydroxynicotinic acid

## 6-Hydroxypicolinic acid

## 7-Hydroxycoumarine

## 2-Hydroxynicotinic acid

# Critic acid cycle

## Citric acid

## Isocitric acid

# Methox

## 2-(4-Methoxyphenoxy)ethanamine

## 2-(4-Methoxyphenoxy)ethanamine

## 2-Methoxyresorcinol

## 2-Methyl-5-propionylfuran

## 3,4-Dimethoxymethcathinone

## 3-Methoxyphenylacetic acid

## 3-Methoxysalicylic acid

## 3-Methoxytyramine

## 4-Methoxysalicylic acid

## 5-Methoxysalicylic acid

## 6-Methoxysalicylic acid

## DL-α-Methoxyphenylacetic acid

# PEG's

## Xxx PEG n6

SYNONYMS - 3,6,9,12,15-PENTAOXAHEPTADECANE-1,17-DIOL, HEXAETHYLENE GLYCOL, PEG-6, and POLYETHYLENE GLYCOL 300

A clear viscous polymer (a molecule from repeated subunits) liquid that works as a solvent and humectant. According to manufacturer info, it's recommended for all kinds of washing products (like hand dishwashing detergents or fine-fabric washing powders) and is ideal as a viscosity regulator, detergent booster, and solubilizer.

Physico-chemical properties and general characteristics

The chemical compound named PEG-6 in the INCI taxonomy is a derivative resulting from the ethoxylation of polyethylene glycol with six moles of ethylene oxide. Chemically, it is a synthetic substance that is a product of ethylene oxide polymerization. The chemical name of PEG-6 is polyoxyethylene glycol. The CAS number of this compound, thanks to which it can be easily found, for example in the catalogues of chemical wholesalers, is 25322-68-3.

PEG-6 is a non-ionic surfactant. At room temperature, it is a liquid with a faint smell. The colour in the Hazen scale, i.e. a scale based on the assessment and comparison of the colours of liquid platinum-cobalt standards with the analysed compounds, for PEG-6 reaches a maximum value of 30. The pH of a 10% aqueous solution is in the range from 4.6 to 7.4. In a commercial product, such as POLIkol 300, offered by the PCC Group, the content of the main ingredient, i.e. PEG-6, exceeds 99%. The amount of water as an impurity is not higher than 0.5%, and the molar mass is about 300 g/mol. The density of PEG-6 at 20ᵒC is about 1.13 g/ml. Its solidification occurs when the temperature drops below 0ᵒC, while the substance ignites above 137ᵒC. PEG-6 dissolves very well in water, and due to its chemical nature and molecular structure, it forms proper solutions together with low aliphatic alcohols, diethyl ether or chloroform. PEG-6 is also characterized by good alkali resistance and strong hygroscopic properties. As a result of its hygroscopicity, PEG-6 not only dissolves very well in water, but also absorbs moisture from the air.

Other applications of PEG-6

The anti-electrostatic properties of PEG-6 are not only used in hair care products, but also in industrial cleaning and metalworking processes.

PEG-6 is one of the ingredients of preparations used in the agrochemical industry. It has the unique ability to bind to water molecules, which is why it is said to be highly hygroscopic. Thanks to this, it is suitable for the production of, for example, plant fertilizers.

In the chemical industry, PEG-6 is one of the raw materials for the production of esters.

The American Food and Drug Agency (FDA) has approved PEG-6 for indirect food contact based on CFR 21 lists: 175.105, 175.210, 176.180, 176.200.

## PEG n11

Cannot any data

Aka NEOPRENE PRIMER N11

Most usages are it the cement industry

## PEG n12

## PEG n5

## PEG n6

## PEG n7

PEG-7 GLYCERYL COCOATE

PEG-7 Glyceryl Cocoate is a water-soluble ingredient that has many benefits in the cosmetic industry. It conditions the skin and hair while also thickening the formulations. It is basically an oil that is light yellow in color and has a distinctive odor. Categorizing broadly, it is an emulsifier, emollient, and surfactant. PEG-7 Glyceryl Cocoate can be found in products like cleansers, moisturizers, hair conditioners, etc.

What is PEG-7 GLYCERYL COCOATE used for?

PEG-7 Glyceryl Cocoate is a multi-functional ingredient that can be found in a range of products such as cleansers, hair conditioners, and shampoos. It has benefits for both skin and hair.

Hair care: It effortlessly combines oil and water together - thus proving beneficial in cleaning the dirt and oil out of the hair. It treats rough and dry hair to leave them feeling healthy

Skin care: It helps in restoring the skin’s natural barrier and locks in moisture to give smoothness and flawlessness. It is lightweight and non-greasy, so it does not weigh the skin down

Cosmetic products: It improves the look and feel of cosmetic products by adding desired thickness and texture to them. It mixes oil and water components together and thus stabilizes the formulations

Origin

PEG-7 Glyceryl Cocoate is a synthetic polymer that is made by the reaction of polyethylene glycol (PEG) and the fatty acids derived from coconut or palm kernel oil. It is a mild compound that helps to combine oil-based and water-based ingredients together.

What does PEG-7 GLYCERYL COCOATE do in a formulation?

Emollient - Emulsifying -

Surfactant

Safety Profile of PEG-7 GLYCERYL COCOATE

A red and white sign

Description automatically generated with low confidence

PEG-7 Glyceryl Cocoate is safe for use in rinse-off products such as cleansers and shampoos. It can also be used in leave-on products up to a concentration of 10%. However, there are still some concerns regarding this ingredient because of the presence of ethylene oxide. The process of ethoxylation has the risk of contamination with 1,4-dioxane which is a potential carcinogen. But its presence can be avoided through purification steps taken before adding PEG-7 Glyceryl Cocoate to the formulations.

## Xxx PEG n8

# Sugar

## D-(-)-Fructose

## D-(+)-Galactose

## D-(+)-Glucose

Description

Glucose is a monosaccharide containing six carbon atoms and an aldehyde group. It is referred to as an aldohexose. The glucose molecule can exist in an open-chain (acyclic) and ring (cyclic) form, the latter being the result of an intramolecular reaction between the aldehyde C atom and the C-5 hydroxyl group to form an intramolecular hemiacetal. In aqueous solution, both forms are in equilibrium and at pH 7 the cyclic one is predominant. Glucose is a primary source of energy for all living organisms. It is a fundamental metabolite found in all organisms, ranging from bacteria to plants to humans. Most of the glucose generated on the Earth is made by plants and algae during photosynthesis from water and carbon dioxide, where it is used to make cellulose (and other polymeric forms of glucose called polysaccharides) that stabilize plant cell walls. Glucose is also found in fruits and other parts of plants in its free state. In animals, glucose can be generated from the breakdown of glycogen in a process known as glycogenolysis. Glucose can also be synthesized de novo in animals. In particular, it can be synthesized in the liver and kidneys from non-carbohydrate intermediates, such as pyruvate and glycerol (and gluconeogenic amino acids such as glycine, serine and alanine), by a process known as gluconeogenesis. Humans also consume large amounts of glucose as part of their regular diet. Ingested glucose initially binds to the receptor for sweet taste on the tongue in humans. This complex of the proteins T1R2 and T1R3 makes it possible to identify glucose-containing food sources. Glucose in the body mainly comes from food - about 300 g per day for the average adult. In humans, the breakdown of glucose-containing polysaccharides happens partly during chewing by means of the enzyme known as amylase, which is contained in saliva, as well as by other enzymes such as maltase, lactase and sucrase on the brush border of the small intestine. The blood sugar content of a healthy person in the short-time fasting state, e.g. after overnight fasting, is about 70 to 100 mg/dL of blood (4 to 5.5 mM). In blood plasma, the measured values are about 10-15% higher. Dysregulated metabolism of glucose can lead to a number of diseases including diabetes. Diabetes is a metabolic disorder where the body is unable to regulate levels of glucose in the blood either because of a lack of insulin in the body or the failure, by cells in the body, to respond properly to insulin. Each of these situations can be caused by persistently high elevations of blood glucose levels (called hyperglycemia), through pancreatic burnout and insulin resistance. Persistently elevated levels of glucose (>6 mM or >120 mg/dL) can lead to the formation of covalent adducts of glucose with plasma proteins through a non-enzymatic process known as glycation. This glycation reaction leads to advanced glycation end products or AGEs (PMID: 24634591 ). AGEs are thought to be the major causes of different diabetic complications. High glucose levels may induce glycation of various structural and functional proteins including plasma proteins and collagen. The non-enzymatic modification of plasma proteins such as albumin, fibrinogen, hemoglobin and globulins may produce various deleterious effects including alteration in drug binding in the plasma, platelet activation, generation of oxygen free radicals, impaired fibrinolysis and impairment in immune system regulation (PMID: 24634591 ). Transiently elevated glucose (up to 7.3 mM or 133 mg/dL) is often seen shortly after the consumption of a meal or a food item that is rich in carbohydrates -- even among very healthy people (PMID: 19885137 ). Glucose is also elevated when an individual is fighting viral or bacterial infections or suffering from traumatic injuries (burns, wounds). In fact, glucose can be significantly elevated (>11 mM or 200 mg/dL) when individuals are experiencing sepsis or septic shock (PMID: 16006275 ). On the other hand, low blood glucose levels (hypoglycemia) where blood glucose is <3.9 mM (70 mg/dL) are common among people with type 1 diabetes and people with type 2 diabetes who take certain diabetic medicines. Certain conditions, such as liver disease, may also cause low levels of blood glucose. Hypoglycemia can lead to fatigue, sleepiness, short temper or feeling faint.

Cellular Locations

Cytoplasm

Extracellular

Lysosome

Endoplasmic reticulum

Golgi apparatus

Biospecimen Locations

Blood

Breast Milk

Cerebrospinal Fluid (CSF)

Feces

Saliva

Sweat

Urine

Tissue Locations

Adipose Tissue

Adrenal Cortex

Adrenal Gland

Adrenal Medulla

Bladder

Brain

Epidermis

Eye Lens

Fibroblasts

Intestine

Kidney

Liver

Lung

Neuron

Ovary

Pancreas

Placenta

Prostate

Skeletal Muscle

Testis

Disease References

Growth hormone deficiency

Darzy KH, Murray RD, Gleeson HK, Pezzoli SS, Thorner MO, Shalet SM: The impact of short-term fasting on the dynamics of 24-hour growth hormone (GH) secretion in patients with severe radiation-induced GH deficiency. J Clin Endocrinol Metab. 2006 Mar;91(3):987-94. Epub 2005 Dec 29. [PubMed:16384844]

Acute myelogenous leukemia

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### Known gene associations

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| [HMDBP ID](https://hmdb.ca/metabolites/HMDB0000122/metabolite_protein_links?c=hmdbp_id&d=down) | [Name](https://hmdb.ca/metabolites/HMDB0000122/metabolite_protein_links?c=name&d=down) | [Gene Name](https://hmdb.ca/metabolites/HMDB0000122/metabolite_protein_links?c=gene_name&d=down) | [Type](https://hmdb.ca/metabolites/HMDB0000122/metabolite_protein_links?c=protein_type&d=down) | References |
| [HMDBP00088](https://hmdb.ca/proteins/HMDBP00088) | Aldose reductase | AKR1B1 | Unknown | N/a |
| [HMDBP00119](https://hmdb.ca/proteins/HMDBP00119) | Ectonucleotide pyrophosphatase/phosphodiesterase family member 1 | ENPP1 | Unknown | N/a |
| [HMDBP00210](https://hmdb.ca/proteins/HMDBP00210) | Glucokinase | GCK | Enzyme | N/a |
| [HMDBP00212](https://hmdb.ca/proteins/HMDBP00212) | Hexokinase-3 | HK3 | Enzyme | N/a |
| [HMDBP00213](https://hmdb.ca/proteins/HMDBP00213) | Hexokinase-2 | HK2 | Enzyme | N/a |
| [HMDBP00215](https://hmdb.ca/proteins/HMDBP00215) | Hexokinase-1 | HK1 | Enzyme | N/a |
| [HMDBP00290](https://hmdb.ca/proteins/HMDBP00290) | Sucrase-isomaltase, intestinal | SI | Enzyme | N/a |
| [HMDBP00329](https://hmdb.ca/proteins/HMDBP00329) | GDH/6PGL endoplasmic bifunctional protein | H6PD | Unknown | N/a |
| [HMDBP00365](https://hmdb.ca/proteins/HMDBP00365) | Lactase-phlorizin hydrolase | LCT | Enzyme | N/a |
| [HMDBP00366](https://hmdb.ca/proteins/HMDBP00366) | Neutral alpha-glucosidase AB | GANAB | Enzyme | N/a |
| [HMDBP00367](https://hmdb.ca/proteins/HMDBP00367) | Glycogen debranching enzyme | AGL | Enzyme | N/a |
| [HMDBP00369](https://hmdb.ca/proteins/HMDBP00369) | ADP-dependent glucokinase | ADPGK | Unknown | N/a |
| [HMDBP00371](https://hmdb.ca/proteins/HMDBP00371) | Beta-1,4-galactosyltransferase 2 | B4GALT2 | Unknown | N/a |
| [HMDBP00372](https://hmdb.ca/proteins/HMDBP00372) | Alpha-lactalbumin | LALBA | Enzyme | N/a |
| [HMDBP00374](https://hmdb.ca/proteins/HMDBP00374) | Trehalase | TREH | Enzyme | N/a |
| [HMDBP00376](https://hmdb.ca/proteins/HMDBP00376) | Glucose-6-phosphatase | G6PC | Enzyme | N/a |
| [HMDBP00377](https://hmdb.ca/proteins/HMDBP00377) | Beta-1,4-galactosyltransferase 1 | B4GALT1 | Unknown | N/a |
| [HMDBP00483](https://hmdb.ca/proteins/HMDBP00483) | UDP-glucuronosyltransferase 1-1 | UGT1A1 | Enzyme | N/a |
| [HMDBP00723](https://hmdb.ca/proteins/HMDBP00723) | Alpha-galactosidase A | GLA | Enzyme | N/a |
| [HMDBP00806](https://hmdb.ca/proteins/HMDBP00806) | Glucose-6-phosphate isomerase | GPI | Enzyme | N/a |
| [HMDBP00843](https://hmdb.ca/proteins/HMDBP00843) | Beta-galactosidase | GLB1 | Enzyme | N/a |
| [HMDBP01107](https://hmdb.ca/proteins/HMDBP01107) | Phosphoglucomutase-1 | PGM1 | Unknown | N/a |
| [HMDBP01795](https://hmdb.ca/proteins/HMDBP01795) | Glucosylceramidase | GBA | Enzyme | N/a |
| [HMDBP01817](https://hmdb.ca/proteins/HMDBP01817) | Lysosomal alpha-glucosidase | GAA | Enzyme | N/a |
| [HMDBP02083](https://hmdb.ca/proteins/HMDBP02083) | Alpha-amylase 1 | AMY1A | Unknown | N/a |
| [HMDBP02114](https://hmdb.ca/proteins/HMDBP02114) | Solute carrier family 2, facilitated glucose transporter member 1 | SLC2A1 | Enzyme | N/a |
| [HMDBP02909](https://hmdb.ca/proteins/HMDBP02909) | Glucokinase regulatory protein | GCKR | Enzyme | N/a |
| [HMDBP03061](https://hmdb.ca/proteins/HMDBP03061) | Cytosolic beta-glucosidase | GBA3 | Unknown | N/a |
| [HMDBP03069](https://hmdb.ca/proteins/HMDBP03069) | Maltase-glucoamylase, intestinal | MGAM | Enzyme | N/a |
| [HMDBP05099](https://hmdb.ca/proteins/HMDBP05099) | Glucose-6-phosphatase 3 | G6PC3 | Enzyme | N/a |
| [HMDBP05100](https://hmdb.ca/proteins/HMDBP05100) | Glucose-6-phosphatase 2 | G6PC2 | Enzyme | N/a |
| [HMDBP05979](https://hmdb.ca/proteins/HMDBP05979) | Neutral alpha-glucosidase C | GANC | Enzyme | N/a |
| [HMDBP07277](https://hmdb.ca/proteins/HMDBP07277) | Aldose 1-epimerase | GALM | Enzyme | N/a |
| [HMDBP09169](https://hmdb.ca/proteins/HMDBP09169) | Non-lysosomal glucosylceramidase | GBA2 | Enzyme | N/a |
| [HMDBP11606](https://hmdb.ca/proteins/HMDBP11606) | Aldo-keto reductase family 1 member B10 | AKR1B10 | Unknown | N/a |
| [HMDBP11783](https://hmdb.ca/proteins/HMDBP11783) | Putative hexokinase HKDC1 | HKDC1 | Unknown | N/a |
| [HMDBP11831](https://hmdb.ca/proteins/HMDBP11831) | Mannosyl-oligosaccharide glucosidase | MOGS | Unknown | N/a |

## D-(+)-Mannose

## Maltol

Description - Maltol, also known as E636 or fema 2656, belongs to the class of organic compounds known as pyranones and derivatives. Pyranones and derivatives are compounds containing a pyran ring which bears a ketone. Some synthetic derivatives of maltol, developed at the University of Urbino, showed limited in vitro antiproliferative activity towards cancer cells lines, perhaps inducing apoptosis in these cells. Maltol is a sweet, baked, and bread tasting compound. Maltol has been detected, but not quantified, in several different foods, such as milk and milk products, nuts, soybeans, pepper (c. annuum), and coffee and coffee products. Maltol's sweetness adds to the odor of freshly baked bread and is used as a flavor enhancer (INS Number 636) in breads and cakes. Related to this property, maltol has been reported to greatly increase aluminum uptake in the body and to increase the oral bioavailability of gallium and iron. Maltol is a naturally occurring organic compound that is used primarily as a flavor enhancer. It is a white crystalline powder that is soluble in hot water, chloroform, and other polar solvents. Maltol is registered as a flavor component in the EU. Maltol, like related 3-hydroxy-4-pyrones such as kojic acid, binds to hard metal centers such as Fe3+, Ga3+, Al3+, and VO2+. It is known in the European E number food additive series as E636. Because it has the odor of cotton candy and caramel, maltol is used to impart a sweet aroma to fragrances.

### Biological location

Excreta

Biofluid or Excreta

Feces (PMID: 25037050)

Cellular substructure

Extracellular (HMDB: HMDB0030776)

Cytoplasm (HMDB: HMDB0030776)

Route of exposure

Enteral

Ingestion (HMDB: HMDB0030776)

### Cellular Locations

Cytoplasm

Extracellular

### Disease References

Colorectal cancer - Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. Carcinogenesis. 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. [PubMed:25037050]

## α-Lactose

# Tetramor's

## Tetranor-12(S)-HETE

## Tetranor-12R-HETE

# Amino acid and or derivative

## Alpha-Lactose

Description - alpha-Lactose is the major sugar present in milk and the main source of energy supplied to the newborn mammalian in its mother's milk. Lactose is also an important osmotic regulator of lactation. It is digested by the intestinal lactase (EC 3.2.1.108), an enzyme expressed in newborns. Its activity declines following weaning. As a result, adult mammals are normally lactose-intolerant and more than 75% of the human adult population suffers from lactase deficiency. Lactase deficiency is present in up to 80 percent of blacks and Latinos, and up to 100 percent of American Indians and Asians. Persons with lactose intolerance are unable to digest significant amounts of lactose. Common symptoms include abdominal pain and bloating, excessive flatus, and watery stool following the ingestion of foods containing lactose. A sizable number of adults believe they are lactose intolerant but do not actually have impaired lactose digestion, and some persons with lactase deficiency can tolerate moderate amounts of ingested lactose. A diagnosis of lactose intolerance can usually be made with a careful history supported by dietary manipulation. If necessary, diagnosis can be confirmed by using a breath hydrogen or lactose tolerance test. These mostly uncomfortable symptoms of lactose maldigestion are blamed for a variably dairy consumption. There is, however, emerging evidence that certain lactic acid-producing bacteria, which selectively consume prebiotics, may be beneficial against some lower intestinal diseases. Lactose maldigestion and lactose should perhaps be re-evaluated as a potential provider of such a prebiotic. Treatment consists primarily of avoiding lactose-containing foods. Lactase enzyme supplements may be helpful. The degree of lactose malabsorption varies greatly among patients with lactose intolerance, but most of them can ingest up to 350 mL of milk daily without symptoms. Lactose-intolerant patients must ensure adequate calcium intake. (PMID: 13130292, 12216958, 12197838, 12018807). Lactose in the urine is a biomarker for the consumption of milk.

Disease References

Eosinophilic esophagitis

Slae, M., Huynh, H., Wishart, D.S. (2014). Analysis of 30 normal pediatric urine samples via NMR spectroscopy (unpublished work). NA.

Lactose Intolerance

Hoskova A, Sabacky J, Mrskos A, Pospisil R: Severe lactose intolerance with lactosuria and vomiting. Arch Dis Child. 1980 Apr;55(4):304-5. [PubMed:7416780]

1. Overington JP, Al-Lazikani B, Hopkins AL: How many drug targets are there? Nat Rev Drug Discov. 2006 Dec;5(12):993-6. [PubMed:17139284]

2. Imming P, Sinning C, Meyer A: Drugs, their targets and the nature and number of drug targets. Nat Rev Drug Discov. 2006 Oct;5(10):821-34. [PubMed:17016423]

Genes associated with Lactose

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| [HMDBP ID](https://hmdb.ca/metabolites/HMDB0000186/metabolite_protein_links?c=hmdbp_id&d=down) | [Name](https://hmdb.ca/metabolites/HMDB0000186/metabolite_protein_links?c=name&d=down) | [Gene Name](https://hmdb.ca/metabolites/HMDB0000186/metabolite_protein_links?c=gene_name&d=down) | [Locus](https://hmdb.ca/metabolites/HMDB0000186/metabolite_protein_links?c=locus&d=down) | [Type](https://hmdb.ca/metabolites/HMDB0000186/metabolite_protein_links?c=protein_type&d=down) | References |
| [HMDBP00365](https://hmdb.ca/proteins/HMDBP00365) | Lactase-phlorizin hydrolase | LCT | 2q21 | Enzyme | N/a |
| [HMDBP00371](https://hmdb.ca/proteins/HMDBP00371) | Beta-1,4-galactosyltransferase 2 | B4GALT2 | 1p34-p33 | Unknown | N/a |
| [HMDBP00372](https://hmdb.ca/proteins/HMDBP00372) | Alpha-lactalbumin | LALBA |  | Enzyme | N/a |
| [HMDBP00377](https://hmdb.ca/proteins/HMDBP00377) | Beta-1,4-galactosyltransferase 1 | B4GALT1 | 9p13 | Unknown | N/a |
| [HMDBP00843](https://hmdb.ca/proteins/HMDBP00843) | Beta-galactosidase | GLB1 |  | Enzyme | N/a |
| [HMDBP11449](https://hmdb.ca/proteins/HMDBP11449) | Glycolipid transfer protein | GLTP | 12q24.11 | Unknown | 1,2 |

## cis-4-Hydroxy-D-proline

## 3-Hydroxy-L-proline

## 4-Oxoproline

## Isovanillic acid

## L-Pyroglutamic acid

## N-Acetyl-D-alloisoleucine

## N-Acetyl-DL-norvaline

## N-Acetyl-L-leucine

## N-Acetylvaline

## N-Isovalerylglycine

## trans-4-Hydroxy-L-proline

## Valine

# Hex

## Hexanoylglycine

## Bis(2-ethylhexyl) isophthalate

## Bis(2-ethylhexyl) sebacate

Bis(2-ethylhexyl) adipate (nasty)

Definition - ChEBI: A diester resulting from the formal condensation of the carboxy groups of adipic acid with 2-ethylhexan-1-ol. It is used as a plasticiser in the preparation of various polymers.

Uses - Bis(2-ethylhexyl) adipate also known as dioctyl adipate (DOA) can be used as a plasticizer for improving the impact properties of polymers. DOA is also used to produce clear films for food packaging applications and in synthetic rubber industries due to its compatibility with nitrocellulose and ethylcellulose. Plasticizer in polyvinyl chloride films, sheeting, extrusions, and plastisols; solvent and

Health Hazard - Liquid may cause mild eye irritation. Repeated or prolonged skin contact may cause irritation.

Safety Profile

A red and black sign

Description automatically generated with low confidence

Moderately toxic by intravenous route. Mildly toxic by ingestion. Experimental reproductive effects. Mutation data reported. An eye and skin irritant. Questionable carcinogen with experimental carcinogenic data. See also ESTERS. When heated to decomposition it emits acrid smoke and irritating fumes.

## Cyclohexylamine

## Hexadecanedioic acid

# Acids

## (-)-Camphanic acid

## (15Z)-9,12,13-Trihydroxy-15-octadecenoic acid

## (5ξ,9ξ,16ξ)-17-Hydroxykauran-19-oic acid

## (R)-3-Hydroxy myristic acid

## 1-(Carboxymethyl)cyclohexanecarboxylic acid

## 11(Z)-Eicosenoic acid

## 16-Hydroxyhexadecanoic acid

## 2-(6-Hydroxyhexyl)-3-methylenesuccinic acid

## 2-[(2S,4aR,8aS)-2-Hydroxy-4a-methyl-8-methylenedecahydro-2-naphthalenyl]acrylic acid

## 2-Furoic acid

## 2-Phenoxypropanoic acid

## 3-(4-Hydroxyphenyl)propionic acid

## 3-Methyladipic acid

## 3-tert-Butyladipic acid

## 5-Aminolevulinic acid

## 5-Aminovaleric acid

## 9-Oxo-10(E),12(E)-octadecadienoic acid

## Adipic acid

Description - Adipic acid is an important inudstrial dicarboxylic acid with about 2.5 billion kilograms produced per year. It is used mainly in the production of nylon. It occurs relatively rarely in nature. It has a tart taste and is also used as an additive and gelling agent in jello or gelatins. It is also used in some calcium carbonate antacids to make them tart. Adipic acid has also been incorporated into controlled-release formulation matrix tablets to obtain pH-independent release for both weakly basic and weakly acidic drugs. Adipic acid in the urine and in the blood is typically exogenous in origin and is a good biomarker of jello consumption. In fact, a condition known as adipic aciduria is actually an artifact of jello consumption (PMID: 1779643 ). However, certain disorders (such as diabetes and glutaric aciduria type I.) can lead to elevated levels of adipic acid snd other dicarboxcylic acids (such as suberic acid) in urine (PMID: 17520433 ; PMID: 6778884 ). Moreover, adipic acid is also found to be associated with 3-hydroxy-3-methylglutaryl-CoA lyase deficiency, carnitine-acylcarnitine translocase deficiency, malonyl-Coa decarboxylase deficiency, and medium Chain acyl-CoA dehydrogenase deficiency, which are inborn errors of metabolism. Adipic acid is also microbial metabolite found in Escherichia.

Health effect

Cancer

1. Lung cancer (HMDB:HMDB0000448)
2. Anorexia nervosa (HMDB:HMDB0000448)
3. Glutaric aciduria type 2 (HMDB:HMDB0000448)

Biological location

1. Cellular substructure
2. Cytoplasm (HMDB: HMDB0000448)
3. extracellular (HMDB: HMDB0000448)
4. Cell membrane (HMDB: HMDB0000448)
5. Adiposome (HMDB: HMDB0000448)
6. Biofluid or Excreta
7. Cerebrospinal fluid (HMDB: HMDB0000448)
8. Excreta
9. Urine (PMID: 8087979)
10. Feces (PMID: 20669995)
11. Non-excretory biofluid
12. Blood (PMID: 32966057)
13. Cerebrospinal Fluid (CSF) (PMID: 9439441)
14. Saliva (HMDB: HMDB0000448)
15. Organ
16. Liver (HMDB: HMDB0000448)
17. Kidney (HMDB: HMDB0000448)

Disease References

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## Azelaic acid

## cis,cis-Muconic acid

## Dehydroacetic acid

## DL-4-Hydroxyphenyllactic acid

## Gabapentin

## Gentisic acid

## Kojic acid

## Myristic acid

## Oleic acid

## Palmitic acid

## Penicillic acid

## Pimelic acid

## Protocatechuic acid

## Sebacic acid

Description - Sebacic acid is a saturated, straight-chain naturally occurring dicarboxylic acid with 10 carbon atoms. Sebacic acid is a normal urinary acid. In patients with multiple acyl-CoA-dehydrogenase deficiency (MADD), also known as glutaric aciduria type II (GAII), a group of metabolic disorders due to deficiency of either electron transfer flavoprotein or electron transfer flavoprotein ubiquinone oxidoreductase, biochemical data shows an increase in urine sebacic acid excretion. Sebacic acid is found to be associated with carnitine-acylcarnitine translocase deficiency and medium chain acyl-CoA dehydrogenase deficiency, which are inborn errors of metabolism. Sebacic acid is a white flake or powdered crystal slightly soluble in water that has been proposed as an alternative energy substrate in total parenteral nutrition. Sebacic Acid was named from the Latin sebaceus (tallow candle) or sebum (tallow) in reference to its use in the manufacture of candles. Sebacic acid and its derivatives such as azelaic acid have a variety of industrial uses as plasticizers, lubricants, hydraulic fluids, cosmetics, candles, etc. It is used in the synthesis of polyamide and alkyd resins. It is also used as an intermediate for aromatics, antiseptics and painting materials (PMID: 10556649, 1738216, 8442769, 12706375).

## Stearic acid

## Suberic acid

## Tetradecanedioic acid

## Tranexamic acid

## trans-10-Heptadecenoic acid

## trans-Petroselinic acid

# Drugs

## Caffeic acid

## Paracetamol

## DEET

# Methyl

## (3S)-3-Methyl-5-[(1S,8aR)-2,5,5,8a-tetramethyl-4-oxo-1,4,4a,5,6,7,8,8a-octahydro-1-

## naphthalenyl]pentanoic acid

## (3S)-5-[(4aR,8aS)-2,5,5,8a-Tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-

## methylpentanoic acid

## 1,2,3,4-Tetramethyl-1,3-cyclopentadiene

## 2,2,6,6-Tetramethyl-4-piperidinol

## 3,3,5,5-Tetramethylpyrroline-N-oxide

Dimethyl Sebacate

Dimethyl Sebacate (DMS) is a dimethyl ester of sebacic acid. DMS has a vegetal origin since it is processed from castor oil.

## Major applications

Oleris® Dimethyl Sebacate can be used as an intermediate to produce light stabilizers. It can also be employed as a plasticizer, softening agent and solvent for cellulosic resins, synthetic resins and rubbers.

# Hydro's

## (4E)-3-Hydroxy-2,4-dimethyl-4-heptenamide

## 2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid

## 2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid

## 2,2-Dimethylglutaric acid

## 2,6-Dimethyl-γ-pyrone

## 3,3-Dimethylglutaric acid

## 3-Acetyl-2,5-dimethylfuran

## Dimethyl cyclohexane-1,4-dicarboxylate

## Dimethyl sebacate

N,N-Dimethylaniline (nasty)

Description - N,N-Dimethylaniline, also known as dimethylaminobenzene or dimethylphenylamine, belongs to the class of organic compounds known as dialkylarylamines. These are aliphatic aromatic amines in which the amino group is linked to two aliphatic chains and one aromatic group. N,N-dimethylaniline is a tertiary amine that is aniline in which the amino hydrogens are replaced by two methyl groups. It is a tertiary amine and a dimethylaniline. N,N-dimethylaniline appears as a yellow to brown colored oily liquid with a fishlike odor. It is less dense than water and insoluble in water. Its flash point is 150 °F, and is toxic by ingestion, inhalation, and skin absorption. N,N-Dimethylaniline was used to make dyes and as a solvent.

Tissue Locations

Intestine

Potential Acute Health Effects:

Very hazardous in case of ingestion. Hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of inhalation.

Potential Chronic Health Effects:

Hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of inhalation. The substance is toxic to blood, kidneys, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

A red and white sign

Description automatically generated with low confidence

General References

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Dioctyl sebacate

Dioctyl sebacate (also di(2-ethylhexyl) sebacate, commonly abbreviated as DOS, DEHS, and BEHS) is an organic compound which is the diester of sebacic acid and 2-ethylhexanol. It is an oily colorless liquid and is used as a plasticizer, including in the explosive C4.[3] It has also found use in Dot 5 brake fluid, in ester based engine oils and additives, as seed particle for Particle Image Velocimetry (PIV) and as a model compound that forms stable aerosols.

# Decan's

## 12-Aminododecanoic acid

## Dodecanedioic acid

## Dodecyl sulfate

## Dodecyltrimethylammonium

# Ethyl's

## Ethyl myristate

## Ethyl oleate

## N-Ethylpentylone

# Single compounds

trans,trans-2,4-Heptadienal (nasty / antibiotic)

Icon

Description automatically generated

Description - 2,4-Heptadienal or (E,E)-2,4-heptadienal belongs to the class of organic compounds known as medium-chain aldehydes. These are an aldehyde with a chain length containing between 6 and 12 carbon atoms. Thus, 2,4-heptadienal is considered to be a fatty aldehyde. 2,4-heptadienal is also known as polyunsaturated aldehyde. These compounds are classified by an aldehyde group covalently bound to long carbon chains containing two or more carbon-carbon double bonds. 2,4-heptadienal is a very hydrophobic molecule, practically insoluble in water, and relatively neutral. 2,4-heptadienal is an aldehydic, cake, and cinnamon tasting compound. 2,4-heptadienal has been detected, but not quantified in, several different foods, such as evergreen blackberries, cabbages, broccoli, corns, and tortilla chips. This could make 2,4-heptadienal a potential biomarker for the consumption of these foods. 2,4-heptadienal is also used as a flavoring additive in cigarettes.

Hazard Statements

1. H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral]
2. H311 (100%): Toxic in contact with skin [Danger Acute toxicity, dermal]
3. H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation]
4. H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

Chemical-Disease Co-Occurrences in Literature

1. Persistent Mullerian Duct Syndrome

Studies on the aroma of maté (Ilex paraguariensis St. Hil.) using headspace solid-phase microextraction PMID 17624890; DOI 10.1002/pca.1002; Phytochemical analysis : PCA 2007 Nov; 18(6):469-74 Name matches: pmds (e,e)-2,4-heptadienal

1. Taste Disorders

ron-lactoferrin complex reduces iron-catalyzed off-flavor formation in powdered milk with added fish oil PMID 22860577; DOI 10.1111/j.1750-3841.2012.02809.x; Journal of food science 2012 Aug; 77(8):C853-8 Name matches: metallic taste 2,4-heptadienal

1. Kidney Tubular Necrosis, Acute

Induction of a wide range of C(2-12) aldehydes and C(7-12) acyloins in the kidney of Wistar rats after treatment with a renal carcinogen, ferric nitrilotriacetate PMID 9034241; DOI 10.1016/s0891-5849(96)00489-3; Free radical biology & medicine 1997; 22(6):1019-27 Name matches: tubular necrosis trans,trans-2,4-heptadienal

Health Hazards

1. Harmful if swallowed [Warning Acute toxicity, oral]
2. Toxic in contact with skin [Danger Acute toxicity, dermal]
3. Causes skin irritation [Warning Skin corrosion/irritation]
4. Causes serious eye irritation [Warning Serious eye damage/eye irritation]
5. Acute toxicity, dermal
6. Acute toxicity, oral
7. Serious eye damage/eye irritation
8. Skin corrosion/irritation

Antibiotic

|  |  |  |  |
| --- | --- | --- | --- |
| Target Name | BioAssay Name | BioAssay AID | Substance SID |
| [Escherichia coli O157:H7](https://pubchem.ncbi.nlm.nih.gov/taxonomy/83334) | Antimicrobial activity against Escherichia coli O157:H7 ATCC 43894 assessed as growth inhibition rate at 0.34 mg/l after 72 hr by spectrophotometry | [1102651](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102651) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Vibrio parahaemolyticus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/670) | Antimicrobial activity against Vibrio parahaemolyticus ATCC 33844 assessed as growth inhibition rate at 0.068 mg/l after 72 hr by spectrophotometry | [1102721](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102721) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Staphylococcus aureus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1280) | Antimicrobial activity against Staphylococcus aureus ATCC 25923 assessed as growth inhibition rate at 6.8 mg/l after 72 hr by spectrophotometry | [1102682](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102682) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Salmonella enterica subsp. enterica serovar Typhimurium](https://pubchem.ncbi.nlm.nih.gov/taxonomy/90371) | Antimicrobial activity against Salmonella enterica subsp. enterica serovar Typhimurium ATCC 14028 assessed as growth inhibition rate at 0.017 mg/l after 72 hr by spectrophotometry | [1102745](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102745) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Bacillus cereus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1396) | Antimicrobial activity against Bacillus cereus ATCC 11778 assessed as growth inhibition rate at 0.68 mg/l after 72 hr by spectrophotometry | [1102775](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102775) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Salmonella enterica subsp. enterica serovar Typhimurium](https://pubchem.ncbi.nlm.nih.gov/taxonomy/90371) | Antimicrobial activity against Salmonella enterica subsp. enterica serovar Typhimurium ATCC 14028 assessed as growth inhibition rate at 6.8 mg/l after 72 hr by spectrophotometry | [1102751](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102751) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Bacillus cereus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1396) | Antimicrobial activity against Bacillus cereus ATCC 11778 assessed as growth inhibition rate at 0.068 mg/l after 72 hr by spectrophotometry | [1102767](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102767) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Escherichia coli O157:H7](https://pubchem.ncbi.nlm.nih.gov/taxonomy/83334) | Antimicrobial activity against Escherichia coli O157:H7 ATCC 43894 assessed as growth inhibition rate at 3.4 mg/l after 72 hr by spectrophotometry | [1102796](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102796) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Escherichia coli O157:H7](https://pubchem.ncbi.nlm.nih.gov/taxonomy/83334) | Antimicrobial activity against Escherichia coli O157:H7 ATCC 43894 assessed as growth inhibition rate at 6.8 mg/l after 72 hr by spectrophotometry | [1102659](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102659) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Listeria monocytogenes](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1639) | Antimicrobial activity against Listeria monocytogenes ATCC 19111 assessed as growth inhibition rate at 6.8 mg/l after 72 hr by spectrophotometry | [1102705](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102705) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Salmonella enterica subsp. enterica serovar Typhimurium](https://pubchem.ncbi.nlm.nih.gov/taxonomy/90371) | Antimicrobial activity against Salmonella enterica subsp. enterica serovar Typhimurium ATCC 14028 assessed as growth inhibition rate at 0.68 mg/l after 72 hr by spectrophotometry | [1102752](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102752) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Vibrio parahaemolyticus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/670) | Antimicrobial activity against Vibrio parahaemolyticus ATCC 33844 assessed as growth inhibition rate at 3.4 mg/l after 72 hr by spectrophotometry | [1102889](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102889) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Escherichia coli O157:H7](https://pubchem.ncbi.nlm.nih.gov/taxonomy/83334) | Antimicrobial activity against Escherichia coli O157:H7 ATCC 43894 assessed as growth inhibition rate at 0.068 mg/l after 72 hr by spectrophotometry | [1102652](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102652) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Escherichia coli O157:H7](https://pubchem.ncbi.nlm.nih.gov/taxonomy/83334) | Antimicrobial activity against Escherichia coli O157:H7 ATCC 43894 assessed as growth inhibition rate at 0.017 mg/l after 72 hr by spectrophotometry | [1102653](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102653) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Listeria monocytogenes](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1639) | Antimicrobial activity against Listeria monocytogenes ATCC 19111 assessed as growth inhibition rate at 0.068 mg/l after 72 hr by spectrophotometry | [1102698](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102698) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Escherichia coli O157:H7](https://pubchem.ncbi.nlm.nih.gov/taxonomy/83334) | Antimicrobial activity against Escherichia coli O157:H7 ATCC 43894 assessed as growth inhibition rate at 0.68 mg/l after 72 hr by spectrophotometry | [1102660](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102660) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Listeria monocytogenes](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1639) | Antimicrobial activity against Listeria monocytogenes ATCC 19111 assessed as growth inhibition rate at 0.34 mg/l after 72 hr by spectrophotometry | [1102697](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102697) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Vibrio parahaemolyticus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/670) | Antimicrobial activity against Vibrio parahaemolyticus ATCC 33844 assessed as growth inhibition rate at 6.8 mg/l after 72 hr by spectrophotometry | [1102728](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102728) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Vibrio parahaemolyticus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/670) | Antimicrobial activity against Vibrio parahaemolyticus ATCC 33844 assessed as growth inhibition rate at 0.68 mg/l after 72 hr by spectrophotometry | [1102729](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102729) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Staphylococcus aureus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1280) | Antimicrobial activity against Staphylococcus aureus ATCC 25923 assessed as growth inhibition rate at 0.068 mg/l after 72 hr by spectrophotometry | [1102675](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102675) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Bacillus cereus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1396) | Antimicrobial activity against Bacillus cereus ATCC 11778 assessed as growth inhibition rate at 0.017 mg/l after 72 hr by spectrophotometry | [1102768](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102768) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Staphylococcus aureus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1280) | Antimicrobial activity against Staphylococcus aureus ATCC 25923 assessed as growth inhibition rate at 0.34 mg/l after 72 hr by spectrophotometry | [1102674](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102674) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Staphylococcus aureus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1280) | Antimicrobial activity against Staphylococcus aureus ATCC 25923 assessed as growth inhibition rate at 0.68 mg/l after 72 hr by spectrophotometry | [1102683](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102683) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Listeria monocytogenes](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1639) | Antimicrobial activity against Listeria monocytogenes ATCC 19111 assessed as growth inhibition rate at 0.017 mg/l after 72 hr by spectrophotometry | [1102699](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102699) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Salmonella enterica subsp. enterica serovar Typhimurium](https://pubchem.ncbi.nlm.nih.gov/taxonomy/90371) | Antimicrobial activity against Salmonella enterica subsp. enterica serovar Typhimurium ATCC 14028 assessed as growth inhibition rate at 0.068 mg/l after 72 hr by spectrophotometry | [1102744](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102744) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Staphylococcus aureus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1280) | Antimicrobial activity against Staphylococcus aureus ATCC 25923 assessed as growth inhibition rate at 3.4 mg/l after 72 hr by spectrophotometry | [1102827](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102827) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Listeria monocytogenes](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1639) | Antimicrobial activity against Listeria monocytogenes ATCC 19111 assessed as growth inhibition rate at 0.68 mg/l after 72 hr by spectrophotometry | [1102706](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102706) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Bacillus cereus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1396) | Antimicrobial activity against Bacillus cereus ATCC 11778 assessed as growth inhibition rate at 3.4 mg/l after 72 hr by spectrophotometry | [1102951](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102951) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Staphylococcus aureus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1280) | Antimicrobial activity against Staphylococcus aureus ATCC 25923 assessed as growth inhibition rate at 0.017 mg/l after 72 hr by spectrophotometry | [1102676](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102676) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Bacillus cereus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1396) | Antimicrobial activity against Bacillus cereus ATCC 11778 assessed as growth inhibition rate at 6.8 mg/l after 72 hr by spectrophotometry | [1102774](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102774) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Vibrio parahaemolyticus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/670) | Antimicrobial activity against Vibrio parahaemolyticus ATCC 33844 assessed as growth inhibition rate at 0.34 mg/l after 72 hr by spectrophotometry | [1102720](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102720) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Vibrio parahaemolyticus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/670) | Antimicrobial activity against Vibrio parahaemolyticus ATCC 33844 assessed as growth inhibition rate at 0.017 mg/l after 72 hr by spectrophotometry | [1102722](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102722) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Salmonella enterica subsp. enterica serovar Typhimurium](https://pubchem.ncbi.nlm.nih.gov/taxonomy/90371) | Antimicrobial activity against Salmonella enterica subsp. enterica serovar Typhimurium ATCC 14028 assessed as growth inhibition rate at 3.4 mg/l after 72 hr by spectrophotometry | [1102920](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102920) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Salmonella enterica subsp. enterica serovar Typhimurium](https://pubchem.ncbi.nlm.nih.gov/taxonomy/90371) | Antimicrobial activity against Salmonella enterica subsp. enterica serovar Typhimurium ATCC 14028 assessed as growth inhibition rate at 0.34 mg/l after 72 hr by spectrophotometry | [1102743](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102743) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Bacillus cereus](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1396) | Antimicrobial activity against Bacillus cereus ATCC 11778 assessed as growth inhibition rate at 0.34 mg/l after 72 hr by spectrophotometry | [1102766](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102766) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
| [Listeria monocytogenes](https://pubchem.ncbi.nlm.nih.gov/taxonomy/1639) | Antimicrobial activity against Listeria monocytogenes ATCC 19111 assessed as growth inhibition rate at 3.4 mg/l after 72 hr by spectrophotometry | [1102857](https://pubchem.ncbi.nlm.nih.gov/bioassay/1102857) | [194177446](https://pubchem.ncbi.nlm.nih.gov/substance/194177446) |
|  |  |  |  |

## (-)-Caryophyllene oxide

## (+/-)12(13)-DiHOME

## (+/-)-C75

## (3S,4R)-3-(1-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one

## 1,6-Hexanediol diglycidyl ether

## 10-HDA

## 13(S)-HOTrE

## 13,14-Dihydro-15-keto-tetranor prostaglandin F1α

## 18-HETE

## 1-Adamantanamine

## 1-Linoleoyl glycerol

## 1-Tetradecylamine

## 2,4-Xylidine

## 2,5-Bis(5-tert-butyl-benzoxazol-2-yl)thiophene

## 2,5-di-tert-Butylhydroquinone

## 2,6-Xylidine

## 4-Hydroxy-6-methyl-2-pyrone

## 4-Nitrophenol

## 9-Oxo-ODE

## Ageratriol

## Betaine

Description

Betaine (CAS: 107-43-7), also known as N,N,N-trimethylglycine, was named after its discovery in sugar beet (Beta vulgaris) in the 19th century. It is a small N-trimethylated amino acid, existing in zwitterionic form at neutral pH. It is now often called glycine betaine to distinguish it from other betaines that are widely distributed in microorganisms, plants, and animals. Many naturally occurring betaines serve as organic osmolytes, substances synthesized or taken up from the environment by cells for protection against osmotic stress, drought, high salinity, or high temperature. Intracellular accumulation of betaines permits water retention in cells, thus protecting from the effects of dehydration (Wikipedia). Betaine functions as a methyl donor in that it carries and donates methyl functional groups to facilitate necessary chemical processes. In particular, it methylates homocysteine to methionine, also producing N,N-dimethylglycine. The donation of methyl groups is important to proper liver function, cellular replication, and detoxification reactions. Betaine also plays a role in the manufacture of carnitine and serves to protect the kidneys from damage. Betaine comes from either the diet or by the oxidation of choline. Betaine insufficiency is associated with metabolic syndrome, lipid disorders, and diabetes, and may have a role in vascular and other diseases (PMID: 20346934 ). Betaine is important in development, from the pre-implantation embryo to infancy. Betaine is also widely regarded as an anti-oxidant. Betaine has been shown to have an inhibitory effect on NO release in activated microglial cells and may be an effective therapeutic component to control neurological disorders (PMID: 22801281 ). As a drug, betaine hydrochloride has been used as a source of hydrochloric acid in the treatment of hypochlorhydria. Betaine has also been used in the treatment of liver disorders, for hyperkalemia, for homocystinuria, and for gastrointestinal disturbances (Martindale, The Extra Pharmacopoeia, 30th Ed, p1341).

Physiological effect

Health effect

Liver damage (PMID: 31434538)

Nerve damage (PMID: 31434538)

Hemodialysis (HMDB: HMDB0000043)

Schizophrenia (HMDB: HMDB0000043)

Continuous ambulatory peritoneal dialysis (HMDB: HMDB0000043)

Cancer

Lung cancer (HMDB: HMDB0000043)

Renal system and urinary system

Renal disorder

Chronic renal failure (HMDB: HMDB0000043)

Cellular Locations

Cytoplasm

Extracellular

Mitochondria

Biospecimen Locations

Blood

Breast Milk

Feces

Saliva

Urine

Tissue Locations

Adipose Tissue

Adrenal Cortex

Adrenal Gland

Bladder

Epidermis

Fibroblasts

Intestine

Kidney

Liver

Ovary

Pancreas

Placenta

Platelet

Prostate

Skeletal Muscle

Spleen

Testis

Disease References

Chronic renal failure

McGregor DO, Dellow WJ, Lever M, George PM, Robson RA, Chambers ST: Dimethylglycine accumulates in uremia and predicts elevated plasma homocysteine concentrations. Kidney Int. 2001 Jun;59(6):2267-72. [PubMed:11380830 ]

Continuous ambulatory peritoneal dialysis

McGregor DO, Dellow WJ, Lever M, George PM, Robson RA, Chambers ST: Dimethylglycine accumulates in uremia and predicts elevated plasma homocysteine concentrations. Kidney Int. 2001 Jun;59(6):2267-72. [PubMed:11380830 ]

Hemodialysis

McGregor DO, Dellow WJ, Lever M, George PM, Robson RA, Chambers ST: Dimethylglycine accumulates in uremia and predicts elevated plasma homocysteine concentrations. Kidney Int. 2001 Jun;59(6):2267-72. [PubMed:11380830 ]

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Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. J Proteome Res. 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. [PubMed:25105552 ]

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Koike S, Bundo M, Iwamoto K, Suga M, Kuwabara H, Ohashi Y, Shinoda K, Takano Y, Iwashiro N, Satomura Y, Nagai T, Natsubori T, Tada M, Yamasue H, Kasai K: A snapshot of plasma metabolites in first-episode schizophrenia: a capillary electrophoresis time-of-flight mass spectrometry study. Transl Psychiatry. 2014 Apr 8;4:e379. doi: 10.1038/tp.2014.19. [PubMed:24713860 ]

Early preeclampsia

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Pregnancy

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. [PubMed:22494326 ]

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Kolho KL, Pessia A, Jaakkola T, de Vos WM, Velagapudi V: Faecal and Serum Metabolomics in Paediatric Inflammatory Bowel Disease. J Crohns Colitis. 2017 Mar 1;11(3):321-334. doi: 10.1093/ecco-jcc/jjw158. [PubMed:27609529 ]

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Sugimoto M, Wong DT, Hirayama A, Soga T, Tomita M: Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. Metabolomics. 2010 Mar;6(1):78-95. Epub 2009 Sep 10. [PubMed:20300169 ]

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Wishart DS, Knox C, Guo AC, Eisner R, Young N, Gautam B, Hau DD, Psychogios N, Dong E, Bouatra S, Mandal R, Sinelnikov I, Xia J, Jia L, Cruz JA, Lim E, Sobsey CA, Shrivastava S, Huang P, Liu P, Fang L, Peng J, Fradette R, Cheng D, Tzur D, Clements M, Lewis A, De Souza A, Zuniga A, Dawe M, Xiong Y, Clive D, Greiner R, Nazyrova A, Shaykhutdinov R, Li L, Vogel HJ, Forsythe I: HMDB: a knowledgebase for the human metabolome. Nucleic Acids Res. 2009 Jan;37(Database issue):D603-10. doi: 10.1093/nar/gkn810. Epub 2008 Oct 25. [PubMed:18953024 ]

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Propionic acidemia

Gronwald W, Klein MS, Kaspar H, Fagerer SR, Nurnberger N, Dettmer K, Bertsch T, Oefner PJ: Urinary metabolite quantification employing 2D NMR spectroscopy. Anal Chem. 2008 Dec 1;80(23):9288-97. doi: 10.1021/ac801627c. [PubMed:19551947 ]

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Gronwald W, Klein MS, Kaspar H, Fagerer SR, Nurnberger N, Dettmer K, Bertsch T, Oefner PJ: Urinary metabolite quantification employing 2D NMR spectroscopy. Anal Chem. 2008 Dec 1;80(23):9288-97. doi: 10.1021/ac801627c. [PubMed:19551947 ]

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Gronwald W, Klein MS, Kaspar H, Fagerer SR, Nurnberger N, Dettmer K, Bertsch T, Oefner PJ: Urinary metabolite quantification employing 2D NMR spectroscopy. Anal Chem. 2008 Dec 1;80(23):9288-97. doi: 10.1021/ac801627c. [PubMed:19551947 ]

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Slae, M., Huynh, H., Wishart, D.S. (2014). Analysis of 30 normal pediatric urine samples via NMR spectroscopy (unpublished work). NA.

Dimethylglycine Dehydrogenase Deficiency

Moolenaar SH, Poggi-Bach J, Engelke UF, Corstiaensen JM, Heerschap A, de Jong JG, Binzak BA, Vockley J, Wevers RA: Defect in dimethylglycine dehydrogenase, a new inborn error of metabolism: NMR spectroscopy study. Clin Chem. 1999 Apr;45(4):459-64. [PubMed:10102904 ]

### Known gene relationship

|  |  |  |  |
| --- | --- | --- | --- |
| [HMDBP ID](https://hmdb.ca/metabolites/HMDB0000043/metabolite_protein_links?c=hmdbp_id&d=down) | [Name](https://hmdb.ca/metabolites/HMDB0000043/metabolite_protein_links?c=name&d=down) | [Gene Name](https://hmdb.ca/metabolites/HMDB0000043/metabolite_protein_links?c=gene_name&d=down) | References |
| [HMDBP00201](https://hmdb.ca/proteins/HMDBP00201) | Choline dehydrogenase, mitochondrial | CHDH | N/a |
| [HMDBP00293](https://hmdb.ca/proteins/HMDBP00293) | Alpha-aminoadipic semialdehyde dehydrogenase | ALDH7A1 | N/a |
| [HMDBP00559](https://hmdb.ca/proteins/HMDBP00559) | Betaine--homocysteine S-methyltransferase 1 | BHMT | N/a |
| [HMDBP02695](https://hmdb.ca/proteins/HMDBP02695) | Sodium- and chloride-dependent betaine transporter | SLC6A12 | [1](http://www.ncbi.nlm.nih.gov/pubmed/11380820) |
| [HMDBP04296](https://hmdb.ca/proteins/HMDBP04296) | S-methylmethionine--homocysteine S-methyltransferase BHMT2 | BHMT2 | N/a |

1. Basham JC, Chabrerie A, Kempson SA: Hypertonic activation of the renal betaine/GABA transporter is microtubule dependent. Kidney Int. 2001 Jun;59(6):2182-91. [PubMed:11380820 ]

## Caprolactam

## Capryloylglycine

## Decanamide

## D-Raffinose

Description -Belongs to the class of organic compounds known as oligosaccharides. These are carbohydrates made up of 3 to 10 monosaccharide units linked to each other through glycosidic bonds.

Disease References

A red and black sign

Description automatically generated with low confidence

Colorectal cancer

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. Cancer Metab. 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. [PubMed:27275383 ]

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Stewart CJ, Embleton ND, Marrs ECL, Smith DP, Fofanova T, Nelson A, Skeath T, Perry JD, Petrosino JF, Berrington JE, Cummings SP: Longitudinal development of the gut microbiome and metabolome in preterm neonates with late onset sepsis and healthy controls. Microbiome. 2017 Jul 12;5(1):75. doi: 10.1186/s40168-017-0295-1. [PubMed:28701177 ]

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Lobley RW, Burrows PC, Warwick R, Dawson DJ, Holmes R: Simultaneous assessment of intestinal permeability and lactose tolerance with orally administered raffinose, lactose and L-arabinose. Clin Sci (Lond). 1990 Aug;79(2):175-83. [PubMed:2167807 ]

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Toussaint M, Latger-Cannard V, Caron A, Lecompte T, Vigneron C, Menu P: Hemoglobin-based oxygen carriers do not alter platelet functions: study of three chemically modified hemoglobin solutions. Intensive Care Med. 2003 Jan;29(1):62-8. Epub 2002 Nov 30. [PubMed:12528024 ]

Xue S, Paterson W, Valdez D, Miller D, Christoff B, Wong LT, Diamant NE: Effect of an o-raffinose cross-linked haemoglobin product on oesophageal and lower oesophageal sphincter motor function. Neurogastroenterol Motil. 1999 Dec;11(6):421-30. [PubMed:10583849 ]

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Lieberthal W, Fuhro R, Alam H, Rhee P, Szebeni J, Hechtman HB, Favuzza J, Veech RL, Valeri CR: Comparison of the effects of a 50% exchange-transfusion with albumin, hetastarch, and modified hemoglobin solutions. Shock. 2002 Jan;17(1):61-9. [PubMed:11795671 ]

Gundermann KJ, Lie TS: Problems of competition in charcoal hemoperfusion for the treatment of intoxications. Artif Organs. 1979 Nov;3(4):346-9. [PubMed:533425 ]

## Erucamide

Description - 13-docosenamide, also known as erucamide, belongs to the class of organic compounds known as fatty amides. These are carboxylic acid amide derivatives of fatty acids, that are formed from a fatty acid and an amine. Based on a literature review very few articles have been published on 13-docosenamide. This compound has been identified in human blood as reported by (PMID: 31557052 ). 13-docosenamide is not a naturally occurring metabolite and is only found in those individuals exposed to this compound or its derivatives. Technically 13-Docosenamide is part of the human exposome. The exposome can be defined as the collection of all the exposures of an individual in a lifetime and how those exposures relate to health. An individual's exposure begins before birth and includes insults from environmental and occupational sources.

Barupal DK, Fiehn O: Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach. Environ Health Perspect. 2019 Sep;127(9):97008. doi: 10.1289/EHP4713. Epub 2019 Sep 26. [PubMed:31557052]

## Eucalyptol

## Methyl 4-hydroxyphenylacetate

## Pestalotin

## Phloroglucinol

Abstract

Substantial concentrations of phloroglucinol were synthesized by Pseudomonas fluorescens Pf-5 expressing the plasmid-localized phlACBDE gene cluster responsible for biosynthesis of 2,4-diacetylphloroglucinol. Expression in Escherichia coli of a single gene in this cluster, P. fluorescens Pf-5 phlD, led to extracellular accumulation of phloroglucinol. Purification of PhlD to homogeneity afforded an enzyme that catalyzed the conversion of malonyl-CoA into phloroglucinol with Km = 5.6 μM and kcat = 10 min-1. Acetylase and deacetylase activities were observed with the catalyzed interconversions of phloroglucinol, 2-acetylphloroglucinol, and 2,4-diacetylphloroglucinol when phlACB was expressed in E. coli. Beyond the mechanistic implications attendant with the identification of an enzyme that catalyzes the conversion of malonyl-CoA into phloroglucinol, PhlD provides the basis for environmentally benign syntheses of phloroglucinol and resorcinol from glucose.

WARNING

A red and white sign

Description automatically generated with low confidence

Irritates lungs, eyes, skin Alfa Aesar B25502

Harmful/Irritant/Mutagenic/Teratogenic/Light Sensitive/Hygroscopic SynQuest 2605-1-X0, 57138

SUPPLEMENT ABSTRACTS SUBMITTED FOR THE 70TH ANNUAL SCIENTIFIC MEETING OF THE AMERICAN COLLEGE OF GASTROENTEROLOGY: FUNCTIONAL BOWEL DISORDERS

Phloroglucinol (Spasfon) in Irritable Bowel Syndrome

Jafri, Wasim FRCP; Yakoob, Javed Ph.D.; Hussain, Sajjad M.B.B.S.; Jafri, Nadim M.B.B.S.; Islam, Muhammad M.S.C

IBS RESEARCH PAPER

American Journal of Gastroenterology 100():p S333, September 2005.

Purpose: To determine the efficacy and tolerability of phloroglucinol (Spasfon), an antispasmodic agent in the treatment of Irritable Bowel Syndrome (IBS).

Methods: An open label (quasi interventional) study. One hundred patients coming to the gastroenterology clinics of Aga Khan University Hospital with IBS as defined by the Rome II criteria were enrolled between February 2004 and September 2004 to participate in the trial and were treated as outpatients. Spasfon 50 mg orally three times daily was given for two months. Symptoms were assessed before and during treatment using a questionnaire.

Results: One hundred patients were enrolled in the study. Of them 61% (61/100) were males and 39% (39/100) were females. Their mean age was 41 ± 14 years. Sixty-eight patients completed the study and 32 dropped out. On Spasfon treatment there was an overall statistically significant improvement in abdominal pain p<0.001, frequency of stool per day p < 0.001, urgency p < 0.001, passage of mucus per rectum p < 0.001, sense of incomplete defecation p = 0.001 and bloating p = 0.001. However, no response was seen in the feature of straining in both genders p = 0.676. The difference in response to treatment according to gender separately showed statistically significant improvement in the sense of incomplete defecation in females alone with p = 0.003.

Conclusions: Spasfon in a dose of 50 mg three times daily is effective and well tolerated by the IBS patients. It relieves most of the symptoms of IBS.

## Polygodial

## Pregabalin

## Pyrogallol

## Stearamide

## trans,trans-2,4-Heptadienal

## Tributylphosphine oxide

## Triethanolamine

## Triisopropanolamine

## Trinexapac

## Valpromide

## Vanillin

## Veratrole

Pyrogallol (nasty stuff)

Mechanism of Action

Pyrogallol (PG) as a polyphenol induces apoptosis in cells. The effects of PG on the growth and death of endothelial cells (ECs) /were examined/. PG dose-dependently inhibited the growth of calf pulmonary artery endothelial cells (CPAEC) and human umbilical vein endothelial cells (HUVEC). PG also induced apoptosis in both cells accompanied by the loss of mitochondrial membrane potential (DeltaPsi(m)). CPAEC were more sensitive to PG than HUVEC concerning cell growth and death. Caspase inhibitors (pan-caspase, caspase-3, -8 or -9 inhibitor) did not affect the growth inhibition of CPAEC by PG. However, pan-caspase inhibitor (Z-VAD) significantly reduced apoptosis and the loss of DeltaPsi(m) in PG-treated CPAEC. PG reduced ROS level and increased GSH depleted cell numbers in CPAEC. While Z-VAD increased ROS levels in PG-treated CPAEC, it decreased GSH depleted cell numbers. In conclusion, PG inhibited the growth of ECs, especially CPAEC via caspase-dependent apoptosis and GSH depletion.

PMID:19913593

Han YH et al; Food Chem Toxicol 48 (2): 558-63 (2010)

Hazardous Substances Data Bank (HSDB)

Pyrogallol (PG) as a polyphenol compound induces apoptosis in several types of cells. Here, we evaluated the effects of PG on endothelial cells (ECs), especially calf pulmonary artery endothelial cells (CPAEC) in relation to the cell growth, ROS and glutathione (GSH) levels. PG dose-dependently inhibited the growth of CPAEC and human umbilical vein endothelial cells (HUVEC) at 24 h. PG also induced apoptosis in CPAEC, which was accompanied by the loss of mitochondrial membrane potential (MMP; DeltaPsim). PG decreased ROS level including O2\*- and PG dose-dependently increased GSH depleted cell number in both EC types. N-acetyl-cysteine (NAC; a well-known antioxidant) increased ROS levels in PG-treated CPAEC with the prevention of cell death and GSH depletion. In conclusion, PG inhibited the growth of ECs, especially CPAEC via apoptosis. PG-induced EC death was related to GSH depletion rather than ROS level changes.

Hazards Summary

A red and black sign

Description automatically generated with low confidence

Reported human toxicity after ingestion includes methemoglobinemia, hemolysis of red blood cells, and damage to the liver and kidneys; [HSDB] An eye, respiratory tract, and mild skin irritant; May cause skin sensitization; [ICSC] Allergic contact dermatitis reported in hairdressers; [Kanerva, p. 1832] Toxic by ingestion with adverse effects including convulsions; [CAMEO]

Kanerva - Rustemeyer L, Elsner P, John SM, Maibach HI (eds). Kanerva's Occupational Dermatology, 2nd Ed. Berlin: Springer-Verlag, 2012., p. 1832

Skin, Eye, and Respiratory Irritations HelpNew Window

The substance is irritating to the eyes and the respiratory tract and is mildly irritating to the skin.

International Program on Chemical Safety/Commission of the European Communities; International Chemical Safety Card on Pyrogallic acid (April 2006). Available from, as of May 20, 2010: https://www.inchem.org/pages/icsc.html

Hazardous Substances Data Bank (HSDB)

DUST /IS/ IRRITATING TO EYES, NOSE & THROAT. IF INHALED WILL CAUSE COUGHING & DIFFICULT BREATHING. SOLID /IS/ IRRITATING TO SKIN & EYES.

U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Manual Two. Washington, DC: U.S. Government Printing Office, Oct., 1978.

Hazardous Substances Data Bank (HSDB)

First Aid

EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop. SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment. INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Measurement** | **System** | **Route/Organism** | **Dose** | **Reference for effect** |
| Mutation Data | sister chromatid exchange | lung/hamster | 㔲딠潭⽬⁌ |  |
| Mutation Data | sex chromosome loss and nondisjunction | oral/Drosophila melanogaster | 125 mmol/L |  |
| Mutation Data | mutation in microorganisms | /Salmonella typhimurium | ‱涵汯瀯慬整⠠⼫攭穮浹瑡捩愠瑣癩瑡潩⁮瑳灥 |  |
| Mutation Data | mutation in microorganisms | /Escherichia coli | 㠷딠⽧汰瑡⁥⴨湥祺慭楴⁣捡楴慶楴湯猠整⥰ |  |
| Mutation Data | micronucleus test | intraperitoneal/mouse | 252 mg/kg |  |
| Mutation Data | micronucleus test | oral/mouse | 504 mg/kg |  |
| Mutation Data | micronucleus test | lung/hamster | 〵딠潭⽬⁌ |  |
| Mutation Data | gene conversion and mitotic recombination | /Saccharomyes cerevisiae | 300 mg/L |  |
| Mutation Data | DNA repair | /Bacillus subtilis | 50 mg/L |  |
| Mutation Data | DNA Damage | intraperitoneal/rat | 100 mg/kg |  |
| Mutation Data | DNA adduct | /Escherichia coli | 〳딠潭⽬⁌ |  |
| Mutation Data | DNA Damage | other cell types/human | 7.5 mg/L/18H |  |
| Mutation Data | Cytogenetic Analysis | intraperitoneal/mouse | 〱‰涵汯欯⁧ |  |
| Mutation Data | Cytogenetic Analysis | ovary/hamster | 100 mg/L |  |
| Mutation Data | Cytogenetic Analysis | lung/hamster | 〶딠潭⽬⽌䠲 |  |
| Skin and Eye Irritation |  | eye /rabbit | 20 mg/24H | 1 |
| Skin and Eye Irritation |  | skin /mouse | 0.13% |  |
| Skin and Eye Irritation |  | skin /rabbit | 2 mg/24H | 2 |
| Reproductive Effects |  | oral/rat | 3 gm/kg (6-15D pregnant) | 3 |
| Reproductive Effects |  | subcutaneous/rat | 5 mg/kg (1D prior to copulation) | 4 |
| Tumorigenic Data |  | subcutaneous/rat | lowest published toxic dose: 3950 mg/kg/58W- intermittent | 5 |
| Acute Toxicity Data |  | In Vitro/Rat, endocrine tumor | 湉楨楢潴⁲潃据湥牴瑡潩⁮潌㩷ㄠ㌮‴涵汯䰯 | 6 |
| Acute Toxicity Data |  | In Vitro/Rat, endocrine tumor | 湉楨楢潴⁲潃据湥牴瑡潩⁮潌㩷〠〮㠴딠潭⽬⁌ | 7 |
| Acute Toxicity Data |  | intraperitoneal/mouse | lethal dose (50 percent kill): 400 mg/kg | 8 |
| Acute Toxicity Data |  | intraperitoneal/mouse | lethal dose (50 percent kill): 400 mg/kg |  |
| Acute Toxicity Data |  | intravenous/Dog | lowest published lethal dose: 80 mg/kg | 9 |
| Acute Toxicity Data |  | intravenous/Dog | lowest published lethal dose: 80 mg/kg | 10 |
| Acute Toxicity Data |  | oral/Dog | lowest published lethal dose: 250 mg/kg |  |
| Acute Toxicity Data |  | oral/Dog | lowest published lethal dose: 25 mg/kg | 11 |
| Acute Toxicity Data |  | oral/human | lowest published lethal dose: 28 mg/kg |  |
| Acute Toxicity Data |  | oral/mouse | lethal dose (50 percent kill): 300 mg/kg | 12 |
| Acute Toxicity Data |  | oral/mouse | lethal dose (50 percent kill): 570 mg/kg | 13 |
| Acute Toxicity Data |  | oral/rabbit | lethal dose (50 percent kill): 1600 mg/kg | 14 |
| Acute Toxicity Data |  | oral/rabbit | lethal dose (50 percent kill): 1600 mg/kg | 15 |
| Acute Toxicity Data |  | oral/rat | lethal dose (50 percent kill): 790 mg/kg | 16 |
| Acute Toxicity Data |  | oral/wild bird | lethal dose (50 percent kill): 75 mg/kg |  |
| Acute Toxicity Data |  | subcutaneous/Dog | lowest published lethal dose: 300 mg/kg |  |
| Acute Toxicity Data |  | subcutaneous/Dog | lowest published lethal dose: 300 mg/kg | 17 |
| Acute Toxicity Data |  | subcutaneous/frog | lowest published lethal dose: 200 mg/kg | 18 |
| Acute Toxicity Data |  | subcutaneous/guinea pig | lowest published lethal dose: 800 mg/kg | 19 |
| Acute Toxicity Data |  | subcutaneous/man | lowest published lethal dose: 120 mg/kg | 20 |
| Acute Toxicity Data |  | subcutaneous/mouse | lethal dose (50 percent kill): 566 mg/kg |  |
| Acute Toxicity Data |  | subcutaneous/rabbit | lowest published lethal dose: 1 gm/kg |  |
| Acute Toxicity Data |  | subcutaneous/rabbit | lowest published lethal dose: 1000 mg/kg | 21 |
| Acute Toxicity Data |  | subcutaneous/rat | lowest published lethal dose: 650 mg/kg |  |
| Other Multiple Dose Data |  | intraperitoneal/mouse | lowest published toxic dose: 1120 mg/kg/4W- intermittent | 22 |
| Other Multiple Dose Data |  | intraperitoneal/rat | lowest published toxic dose: 175 mg/kg/7D- intermittent | 23 |
| Other Multiple Dose Data |  | intraperitoneal/rat | lowest published toxic dose: 350 mg/kg/7D- intermittent | 24 |
| Other Multiple Dose Data |  | oral/chicken | lowest published toxic dose: 98 gm/kg/4W- intermittent | 25 |
| Other Multiple Dose Data |  | oral/rat | lowest published toxic dose: 1200 mg/kg/60D- intermittent | 26 |
| Other Multiple Dose Data |  | oral/rat | lowest published toxic dose: 15200 mg/kg/152D- intermittent | 27 |
| Other Multiple Dose Data |  | skin/mouse | lowest published toxic dose: 18.75 mg/kg/3D- intermittent | 28 |
| Other Multiple Dose Data |  | skin/mouse | lowest published toxic dose: 3.12 mg/kg/4D- intermittent | 29 |

1. moderate

2. severe

3. Reproductive: Effects on fertility: Post- implantation mortality (e.g., dead and/or resorbed implants per total number of implants); Reproductive: Effects on embryo or fetus: Fetotoxicity (except death, e.g., stunted fetus)

4. Reproductive: Maternal effects: Ovaries, fallopian tubes

5. Tumorigenic: Equivocal tumorigenic agent by RTECS criteria; Tumorigenic: Tumors at site of application

6. Nutritional and Gross Metabolic: Changes in: Ca

7. Biochemical: Neurotransmitters or modulators (putative): Dopamine at other sites

8. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

10. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

11. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

12. Behavioral: Convulsions or effect on seizure threshold; Lung, Thorax, or Respiration: Dyspnea; Gastrointestinal: Other changes

13. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

14. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

15. Gastrointestinal: Gastritis; Lung, Thorax, or Respiration: Chronic pulmonary edema or congestion

16. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

17. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

18. Eye: Miosis (pupilliary constriction); Behavioral: Muscle weakness; Behavioral: Ataxia

19. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

20. Behavioral: Convulsions or effect on seizure threshold; Behavioral: Excitement; Gastrointestinal: Changes in structure or function of salivary glands

21. Behavioral: Tetany; Vascular: BP lowering not characterized in autonomic section; Blood: Other hemolysis with or without anemia

22. Liver: Other changes

23. Immunological Including Allergic: Decrease in humoral immune response

24. Immunological Including Allergic: Decrease in cellular immune response; Immunological Including Allergic: Decrease in humoral immune response; Biochemi

25. Related to Chronic Data: Death in the 'MULTIPLE DOSE' data type field

26. Blood: Changes in cell count (unspecified); Biochemical: Enzyme inhibition, induction, or change in blood or tissue levels: True cholinesterase

27. Biochemical: Enzyme inhibition, induction, or change in blood or tissue levels: Catalases; Biochemical: Enzyme inhibition, induction, or change in blood or tissue levels: Other oxidoreductases

28. Skin: After topical application: Cutaneous sensitization (experimental)

29. Skin: After topical application: Primary irritation