

Iron Traffics in Circulation Bound to Siderocalin-Catechol Complex

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Supplementary dataset 1: Urinary Compounds and Derivatives (at 10 μ M)

	Compounds IUPAC name	Compound	Purity (Company)	Paper Chromatography Fe Solubilization	%Retention of 55Fe complex by Scn-Ngal
1	benzene-1,2-diol	Catechol	99% (Fluka)	Yes	56
2	3-methylbenzene-1,2-diol	3-methylcatechol	98% (Aldrich)	Yes	56
3	4-methylbenzene-1,2-diol	4-methylcatechol	95% (Aldrich)	Yes	29
4	benzene-1,2,3-triol	Pyrogallol	99% (Aldrich)	Yes	73
5	2,3-dihydroxybenzoic acid	2,3-Dihydroxybenzoic acid	99% (Aldrich)	Yes	35
6	3,4-Dihydroxybenzoic Acid	3,4-Dihydroxybenzoic Acid	97% (Aldrich)	Yes	5
7	(E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid	Caffeic acid	99% (Sigma)	No	7
8	(1S,3R,4R,5R)-3-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy-1,4,5-trihydroxycyclohexane-1-carboxylic acid	Chlorogenic acid	98% (Aldrich)	Yes	6
9	[(2R,3R)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-chromen-3-yl]3,4,5-trihydroxybenzoate	(-) Epigallocatechin gallate	80% (Sigma)	Yes	45
10	Catechol cyclic sulfate	Catechol cyclic sulfonate	95%	No	6
11	Catechol sulfate sodium	Catechol sulfonate sodium	Salts	No	4
12	2-methoxyphenol	Guaiacol	98% (Aldrich)	No	4
13	1,2-Dimethoxybenzene	1,2Dimethoxy benzene	99% (Aldrich)	No	3
14	2-amino-3-(3,4-dihydroxyphenyl)propanoic acid	3,4-Dihydroxy-DL-phenylalanine	97% (Aldrich)	Yes	12

15	2-amino-3-(3,4-dihydroxy-phenyl)-propionic acid	Dihydroxyphenyl alanine (L-DOPA)	98% (Sigma)	Yes	10
16	4-(2-amino-1-hydroxy-ethyl)-2-methoxy-phenol	DL-Norepinephrine	97% (Aldrich)	No	5
17	(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	Ferulic acid	98% (Fluka)	No	3
18	phenethyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	Caffeic acid phenethyl ester	97% (Sigma)	No	8
19	(2R)-3-(3,4-dihydroxyphenyl)-2-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxypropanoic acid	Rosmarinic acid	97% (Aldrich)	Yes	50
20	5-(2-aminoethyl)benzene-1,2,3-triol	5-Hydroxydopamine	98% (Aldrich)	No	10
21	5-(2-aminoethyl)benzene-1,2,4-triol	6-Hydroxydopamine	95% (Aldrich)	No	4
22	3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)chromen-4-one	Myricetin	85% (Sigma)	No	28
23	2, 3-Dimethoxybenzoic acid	2,3-Dimethoxy benzoic acid	99% (Aldrich)	No	6
24	2-amino-3-hydroxybenzoic acid	3-Hydroxyanthranilic acid	97% (Aldrich)	No	10
25	2-hydroxybenzoic acid	Salicylic acid	99% (Sigma)	No	15
26	Ellagic acid	Ellagic acid	95% (Sigma)	Yes	24
27	2-(2,5-dihydroxyphenyl)acetic acid	Homogentisic acid	98% (Sigma)	No	7
28	2,5-dihydroxybenzoic acid	Gentistic Acid	99% (Sigma)	No	6
29	2-amino-4-(2-amino-3-hydroxyphenyl)-4-oxobutanoic acid	3-Hydroxy-DL-kynurenine	(Sigma)	Yes	3
30	2-amino-3-phenyl-propanoic acid	L-Phenylalanine	98% (Sigma)	No	8
31	3-acetamido-3-phenylpropanoic acid	N-Acetyl-DL-phenylalanine	97% (Sigma)	No	5
32	(2S)-2-amino-3-(1H-indol-3-yl)propanoic acid	L-Tryptophan	99% (Sigma)	No	5
33	2-amino-3-(5-hydroxy-1H-indol-3-yl)propanoic acid	5-Hydroxytryptophan	99% (Sigma)	No	4
34	5-Hydroxy-indoleacetic acid	5-Hydroxy-Indole acetic acid	98% (Sigma)	No	7
35	1H-pyrimidine-2,4-dione	Uracil	99% (Sigma)	No	7
36	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	Orotic acid	98% (Sigma)	No	13

37	2,6-dioxo-1,3-diazinane-4-carboxylic acid	DL-Dihydroorotic acid	98% (Sigma)	No	7
38	pyridine-3-carboxylic acid	Nicotinic acid	99.5% (Fluka)	No	3
39	2, 3-Pyridinedicarboxylic acid	2, 3-Pyridine-dicarboxylic acid	99% (Aldrich)	No	6
40	3-hydroxy-5-(hydroxymethyl)-2-methylpyridine-4-carbaldehyde	Pyridoxal	99% (Sigma)	No	1
41	3-hydroxy-5-(hydroxymethyl)-2-methyl-pyridine-4-carboxylic acid	4-Pyridoxic Acid	98% (Sigma)	No	12
42	2-(2-furylcarbonylamino)acetic acid	2-Furoylglycine	98% (Aldrich)	No	6
43	3-[5-(aminomethyl)-4-(carboxymethyl)-1H-pyrrol-3-yl]propanoic acid	Porphobilinogen	97% (Frontier)	No	3
44	1-(2-aminoacetyl)pyrrolidine-2-carboxylic acid	Glycyl-L-proline	99% (Aldrich)	No	4
45	5-ureidohydantoin (2,5-dioxoimidazolidin-4-yl)urea	Allantoin	98% (Sigma)	No	7
46	3-[2-[[3-(2-carboxyethyl)-5-[(Z)-(3-ethenyl-4-methyl-5-oxo-pyrrol-2-ylidene)methyl]-4-methyl-1H-pyrrol-2-yl]methyl]-5-[(Z)-(4-ethenyl-3-methyl-5-oxo-pyrrol-2-ylidene)methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid	Bilirubin	Salts (Frontier)	No	3
47	3-[2-[(E)-[(5E)-3-(2-carboxyethyl)-5-[(4-ethenyl-3-methyl-5-oxo-pyrrol-2-yl)methylidene]-4-methyl-pyrrol-2-ylidene]methyl]-5-[(E)-(3-ethenyl-4-methyl-5-oxo-pyrrol-2-ylidene)methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid. HCl	Biliverdin HCl	97% (Frontier)	No	9
48	3-[2-[[3-(2-carboxyethyl)-5-[(3-ethyl-4-methyl-5-oxo-1,2-dihydropyrrol-2-yl)methyl]-4-methyl-1H-pyrrol-2-yl]methylidene]-5-[(4-ethyl-3-methyl-5-oxo-1,2-dihydropyrrol-2-yl)methyl]-4-methyl-pyrrol-3-yl]propanoic acid.HCl	Urobilin HCl	Salts (Frontier)	No	3
49	7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-Porphine-2,18-dipropanoic acid	Protoporphyrin IX	97% (Frontier)	No	3
50	Riboflavin 5'-(trihydrogen diphosphate)	FAD	95% (Sigma)	Yes	6
51	[(2R,3R,4R,5R)-2-(6-aminopurin-9-yl)-5-[[[(2R,3S,4R,5R)-5-(5-carbamoylpyridin-1-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl]oxymethyl]-4-hydroxy-oxolan-3-yl]oxyphosphonic acid	NADP	97% (Sigma)	Yes	7
52	[(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-3-hydroxy-4-phosphonoxyoxolan-2-yl]methyl	NADPH	95% (Sigma)	Yes	3

	[[[(2R,3S,4R,5R)-5-(3-carbamoyl-4H-pyridin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-hydroxyphosphoryl] hydrogen phosphate				
53	[(2S,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-[[[(2S,3S,4R,5R)-5-(5-carbamoylpyridin-1-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-oxido-phosphoryl]oxy-phosphonic acid	NAD	99% (Sigma)	No	12
54	2-[4-[(2-amino-4-hydroxy-pteridin-6-yl)methylamino]benzoyl]amino]pentanedioic acid	Folic acid	98% (Sigma)	No	3
55	but-2-enedioic acid	Maleic acid	99% (Fluka)	No	4
56	2-hydroxypropane-1,2,3-tricarboxylic acid sodium	Citric acid sodium	(Sigma)	Yes	6
57	Succinic acid	Succinic acid	99% (Sigma)	No	11
58	5-amino-4-oxo-pentanoic acid	5-Aminolevulinic acid	98% (Sigma)	No	3
59	(1Z)-1-Propene-1,2,3-tricarboxylic acid	Cis-Aconitic acid	98% (Aldrich)	No	11
60	1-hydroxypropane-1,2,3-tricarboxylic acid	Isocitric acid	98% (Sigma)	Yes	6