

Sigma Dyes, Stains, and Natural Pigments FT-IR Spectral Library

Introduction

The Sigma Dyes, Stains, and Natural Pigments Library consists of 628 FT-IR spectra of interest to those in the biochemical field. The spectra were originally acquired at 2 cm⁻¹ spectral resolution, and then mathematically deresolved when converted to Nicolet library format.

The spectra are listed in this document in alphabetical order by compound name. The index number of each spectrum appears to the left of the name. If you are using Nicolet's OMNIC spectroscopy software, the molecular formula, CAS (Chemical Abstracts Services) registry number, when known, and the location number of the printed spectrum in *The Sigma Library of FT-IR Spectra* are available on-line. The Sigma location number is in the form:

<volume number> - <page number> <spectrum letter>

For example, the spectrum with the location number 1-234B refers to the second (B) spectrum on page 234 of Volume 1.

Abbreviations Used in Compound Names

Since the compound names associated with the spectra are often long, in many cases it has become necessary to abbreviate the full name of the substance. The table below defines the abbreviations used in the name field. The sequential index in this manual or the associated data may be consulted for the full name.

<i>Abbreviation</i>	<i>Name</i>
T-BOC	t-Butoxycarbonyl
:BSA	Bovine Serum Albumin conjugate
CBZ	Carbobenzyloxy
CHA	Cyclohexylammonium
CLPH	Chlorophenyl
CNET	Cyanoethyl
DANSYL	5-Dimethylamino-1-naphthalenesulfonyl
DCHA	Dicyclohexylammonium
DDZ	3,5-Dimethoxy- α,α -dimethylbenzyloxycarbonyl
DMT	4,4'-Dimethoxytrityl
2,4-DNP	2,4-Dinitrophenyl
DNPYR	3,5-Dinitro-2-pyridyl
FMOc	9-Fluorenylmethoxycarbonyl
IPREN	Isopropylidene

MESYL	Methanesulfonyl
MSOC	2-(Methanesulfonyl)ethoxycarbonyl
MTH	Methylthiohydantoin
PTH	Phenylthiohydantoin
TFA	Trifluoroacet(ate/yl)
TOSYL	p-Toluenesulfonyl

In addition to the above abbreviations, occasionally atomic symbols are used in place of element names: e.g. CL = chloro- or chloride. Also, Greek letters (alpha, beta, gamma,...,omega) are given as their lower-case Roman equivalents (a, b, g,...,w), and the standard abbreviations are used for amino acids in polypeptide names.

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Sigma Dyes, Stains, and Natural Pigments FT-IR Spectral Library

Index of Compounds

<u>No.</u>	<u>Compound Description</u>	<u>No.</u>	<u>Compound Description</u>
320	1-(2-Hydroxy-1-naphthylazo)-2-naphthol-4-sulfonic acid	230	1,1-Diphenyl-2-picrylhydrazyl
519	1-(2-Pyridylazo)-2-naphthol	227	2,3-Dimethylquinizarin
596	1-(2-Thiazolylazo)-2-naphthol	215	2,6-Dichlorophenol-indophenol, Na salt
211	1-Diazo-2-naphthol-4-sulfonic acid	205	3,3-Diaminobenzidine
324	1-Hydroxy-4-(p-toluidino)anthraquinone	327	5,5'-7-Indigotrisulfonic acid, K salt
131	2-(2'-Benzothiazolyl)-5-styryl-3-(4'-phthalhydrazidyl)tetrazolium cl	483	1,10-Phenanthroline .H2O
317	2-(4'-Hydroxyazobenzene)benzoic acid	614	1,3,5-Triphenyl-formazan
579	2-(p-Sulfophenylazo)-1,8-dihydroxy-3,6-naphthalenedisulfonic acid	442	a-Naphthyl red
597	2-(2-Thiazolylazo)-p-cresol	53	Acid black 48
154	2-(5-Bromo-2-pyridylazo)-5-(diethylamino)phenol	54	Acid blue 25
213	2-7-Dichlorofluorescein	55	Acid blue 29
172	2-Chloro-4-benzamido-5-methylbenzene diazonium chloride	56	Acid blue 45
318	2-Hydroxy-1-(2-hydroxy-4-sulfo-1-naphthylazo)-3-naphthoic acid	57	Acid blue 161
459	2-Nitro-4-(2,4-dinitrophenylazo)phenol	58	Acid fuchsin certified
458	2-Nitro-4-carboxyphenyl N,N-diphenylcarbamate	59	Acid orange 8
461	2-Nitroso-1-naphthol	60	Acid orange 51
217	2,2'-Dihydroxy-1,1'-azonaphthalene-3,3',6,6'-tetrasulfonic acid	61	Acid orange 63
174	3-Chloro-1-2-propanediol	62	Acid orange 74
334	3-Indoxyl phosphate di-p-toluidine	63	Acid red 1
333	3-Indoxyl phosphate, disodium salt	64	Acid red 4
335	3-Indoxyl sulfate, K salt	65	Acid red 88
372	3-O-Methylfluorescein	66	Acid red 106
373	3-O-Methylfluorescein phosphate, CHA salt	67	Acid red 114
588	3,3',5,5'-Tetramethylbenzidine	68	Acid red 150
589	3,3',5,5'-Tetramethylbenzidine .2HCl	69	Acid red 151
206	3,3'-Diaminobenzidine tetra .HCl	70	Acid red 183
520	4-(2-Pyridylazo)resorcinol	71	Acid violet 5
521	4-(2-Pyridylazo)resorcinol, disodium salt	72	Acid violet 7
522	4-(2-Pyridylazo)resorcinol, Na salt	73	Acid violet 17
460	4-(4-Nitrophenylazo)resorcinol	74	Acid yellow 17
212	4-5-Dibromofluorescein	75	Acid yellow 25
222	4-5-Dimethyl-o-phenylenediamine	76	Acid yellow 29
103	4-Amino-1,1'-azobenzene-3,4-disulfonic acid	77	Acid yellow 34
105	4-Amino-4'-dimethylamino-azobenzene	78	Acid yellow 38
102	4-Aminoantipyrine	79	Acid yellow 40
106	4-Aminodiphenylamine diazonium sulfate	80	Acid yellow 65
218	4-Dimethylaminoazobenzene-4'-isothiocyanate	81	Acid yellow 99
381	4-Methylumbelliferone	82	Acridine orange
382	4-Methylumbelliferone methyleneiminodiacetic acid	83	Acridine orange base
216	5-(4,6-Dichlorotriazin-2-yl)aminofluorescein .HCl	84	Acridine yellow
214	5-7-Dichloro-8-hydroxy-quinoline	85	Acriflavin .HCl
153	5-Bromo-4-chloro-3-indolyl phosphate, p-toluidine salt	86	Acriflavin neutral
338	5-Isatinsulfonic acid, Na salt	87	Adrenochrome
104	6-Aminochrysene	88	Adrenochrome semicarbazone sulfonate, Na salt
107	7-Amino-4-methylcoumarin	89	Alcian blue 8GX
220	8-Dimethylamino-2,3-benzophenoxazine, hemi(ZnCl2) salt	90	Alcian blue 8GX
321	8-Hydroxyquinoline	91	Alcian yellow
322	8-Hydroxyquinoline hemisulfate	92	Alizarin
323	8-Hydroxyquinoline-5-sulfonic acid	93	Alizarin blue black B
		94	Alizarin complexone
		96	Alizarin red S certified
		97	Alizarin violet R

<u>No.</u>	<u>Compound Description</u>	<u>No.</u>	<u>Compound Description</u>
98	Alizarin yellow R	162	Bromthymol blue sulfone
95	Alizarin-lanthanum complex buffered powder	163	Bromthymol blue, Na salt
99	Alkali blue 6B	52	C-Phycocyanin
100	Alphazurine A	164	Calcein
101	Amaranth	165	Calcion
108	Aniline blue	166	Calmagite
109	Aniline blue water soluble certified	167	Carbol fuchsin
110	Antipyrine	168	Carboxyarsenazo
111	Apigenin	169	Carminic acid
112	Arsenazo I, Na salt	170	Celestine blue
113	Arsenazo III	171	Chicago sky blue 6B
114	Arsenazo III, Na salt	173	Chlorophenol red
115	Auramine O, certified	4	Chlorophyllin, Na salt-copper
116	Aurintricarboxylic acid	175	Chrome azurol S
117	Aurintricarboxylic acid, ammonium salt	176	Chromotrope 2B
118	Azido fluorescein diacetate	177	Chromotrope 2R
119	Azocarmine B	178	Chrysin
120	Azure A eosinate	179	Chrysophanic acid
121	Azure B chloride	180	Chrysopenine
122	Azure B eosinate	5	Cobaltic protoporphyrin IX chloride
123	Azure II	181	Congo red
124	Azure II eosinate	182	Congo red certified
1	Bacteriochlorophyll A from rhodospseudomonas sphaeroides	183	Copper phthalocyanine
41	Bacteriorhodopsin from halobacterium halobium	6	Coproporphyrin I .2HCl
125	Basic blue 3	7	Coproporphyrin I ethyl ester type I
126	Basic blue 24 zinc chloride double	8	Coproporphyrin I ethyl ester type II
127	Basic yellow 11	9	Coproporphyrin I isopropyl ester
128	Benzidine .2HCl	10	Coproporphyrin I N-propyl ester
129	Benzidine .2HCl	11	Coproporphyrin I tetramethyl ester
130	Benzopurpurin 4B	12	Coproporphyrin I tetramethyl ester
132	Benzoxanthene yellow	13	Coproporphyrin III tetramethyl ester type III-H
133	Benzyl viologen dichloride	184	Coumarin
134	Biebrich scarlet	185	Coumarin 35
2	Bilirubin from bovine gall stones	186	Coumarin 138
3	Biliverdin .2HCl	187	Coumarin 152
135	Bisbenzimidazole Hoechst no 33258 .3HCl	188	Coumarin 153
136	Bismarck brown R	189	Coumarin 311
137	Bismarck brown Y	193	Cresol red
138	Bismarck brown Y certified	194	Cresol red, Na salt
139	Bordeaux red	195	Cresyl violet acetate
140	Brilliant black BN	196	Cresyl violet acetate certified
141	Brilliant blue G	197	Crocein orange G
142	Brilliant blue G	198	Crocein scarlet 7B
143	Brilliant blue R	199	Crystal ponceau 6R
144	Brilliant cresyl blue certified	200	Crystal violet
145	Brilliant green certified	201	Cupferron
146	Brilliant yellow, Na salt	202	Curcumin from curcuma longa
147	Bromchlorophenol blue alcohol soluble	203	Cymerin
148	Bromchlorophenol blue, Na salt	204	Delamar yellow
149	Bromcresol green	15	Deuteroporphyrin IX 2,4-disulfonic acid
150	Bromcresol green, Na salt	14	Deuteroporphyrin IX dimethyl ester from bovine blood
151	Bromcresol purple	221	Dimethylglyoxime
152	Bromcresol purple, Na salt	228	Diphenylamine-4-sulfonic acid, Ba salt
155	Bromo pyrogallol red	231	Direct orange 31
161	Bromophenol red, Na salt	232	Direct red 81
156	Bromosulfonazo III	233	Direct yellow 8
157	Bromoxylenol blue	234	Direct yellow 27
158	Bromphenol blue sulfone form	235	Direct yellow 29
159	Bromphenol blue, Na salt	236	Direct yellow 50
160	Bromphenol red sulfone form	237	Direct yellow 62

<u>No.</u>	<u>Compound Description</u>	<u>No.</u>	<u>Compound Description</u>
238	Disperse blue 1	42	Ferredoxin type V from clostridium pasteurianum
239	Disperse blue 14	43	Ferredoxin type VI from red marine algae
240	Disperse orange 1	298	Flavazin L
241	Disperse orange 3	299	Fluorescamine
242	Disperse orange 11	300	Fluorescein
243	Disperse red 1	304	Fluorescein diacetate
244	Disperse red 13	305	Fluorescein dilaurate
245	Disperse red 19	306	Fluorescein isothiocyanate isomer I
246	Disperse yellow 3	301	Fluorescein, Na salt
247	Disperse yellow 7	302	Fluoresceinamine isomer I
248	Disperse yellow 9	303	Fluoresceinamine isomer II
249	Disperse yellow 42	307	Fluorescent brightener 28
250	Drimarene brilliant blue K-BL	308	Fuchsin acid
251	Eosin B spirit soluble	309	Gallein
252	Eosin B, disodium salt	310	Gallocyanine
253	Eosin Y	311	Giemsa stain
254	Eosin Y certified	312	Giemsa stain, certified
255	Eriochrome blue black B	44	Gossypol
256	Eriochrome cyanine RC	45	Gossypol-acetic acid
257	Erioglaucine	313	Granular blue
258	Erythrosin B	46	Hematein from logwood
259	Erythrosin B, Na salt	16	Hematin from bovine blood
260	Ethidium bromide	17	Hematoporphyrin
261	Ethyl eosin	18	Hematoporphyrin .2HCl
262	Ethyl orange	315	Hematoxylin certified
263	Ethyl red	314	Hematoxylin; 7,11b-Dihydrobenz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol
264	Ethyl violet	19	Hemin type I bovine
265	Evans blue	20	Hemin type III equine
266	Fast black K salt	316	Hydrindantin anhydrous
267	Fast blue BB base	319	Hydroxynaphthol blue, Na salt
268	Fast blue BB salt	325	Indigo
269	Fast blue BB salt	326	Indigo carmine
270	Fast blue RR base	328	Indocyanine green
271	Fast blue RR salt	329	Indophenol blue
272	Fast corinth v	331	Indoxyl 1,3-diacetate
273	Fast dark blue R salt	330	Indoxyl acetate
274	Fast garnet GBC base	332	Indoxyl b-D-glucoside
276	Fast garnet GBC salt	336	Iodonitrotetrazolium formazan
275	Fast garnet GBC salt purified	337	Isatin
277	Fast green FCF	339	Janus green B
278	Fast green FCF certified	340	Janus green B certified
279	Fast red AL salt	341	Juglone
280	Fast red B salt	342	Kojic acid
281	Fast red ITR base	343	Lacmoid
282	Fast red ITR salt	344	Leishman's stain
283	Fast red KL salt	345	Leucocrystal violet
284	Fast red PDC	346	Leucomalachite green
285	Fast red RC salt diazotized	347	Light green SF yellowish
286	Fast red TR salt	348	Lissamine green B
287	Fast red violet LB salt	349	Litmus
288	Fast red violet LB salt	350	Lucifer yellow CH dilithium
289	Fast sulphon black F	351	Lucifer yellow VS dilithium
290	Fast violet B base	352	Lumazine
291	Fast violet B salt	353	Lumichrome
292	Fast violet B salt	191	m-Cresol purple
293	Fast violet B salt	192	m-Cresol purple, Na salt
294	Fast yellow GC salt	463	m-Nitrotetrazolium blue
295	Fat brown B	496	m-Phenylenediamine
296	Fat brown RR	354	Magon
297	Fat red 7B		

<u>No.</u>	<u>Compound Description</u>	<u>No.</u>	<u>Compound Description</u>
355	Malachite green .HCl	224	N,N-Dimethyl-p-phenylenediamine .2HCl
358	Malachite green base	225	N,N-Dimethyl-p-phenylenediamine .HCl
356	Malachite green oxalate	226	N,N-Dimethyl-p-phenylenediamine sulfate
357	Malachite green oxalate, certified	367	N-Methyl-9-(p-chlorophenoxy-carbonyl)-acridinium iodide
359	Martius yellow	375	N-Methylindoxyl acetate
360	May-Grunwald stain	501	N-Phenyl-1-naphthylamine
47	Melanin	402	Naphthol AS
361	Mercurochrome	403	Naphthol AS acetate
362	Mercury orange	412	Naphthol AS b-chloropropionate
363	Merocyanine 540	404	Naphthol AS benzoate
36	Meso-tetra(4-pyridyl)-porphine	430	Naphthol AS g-phenylbutyrate
34	Meso-tetra-(4-N-methyl-pyridyl) porphine tetratosyl	428	Naphthol AS nonanoate
35	Meso-tetraphenylporphine	429	Naphthol AS phenylacetate
21	Mesoporphyrin IX .2HCl	431	Naphthol AS phenylpropionate
22	Mesoporphyrin-IX dimethyl ester	432	Naphthol AS phosphate
48	Metallothionein from rabbit liver	433	Naphthol AS phosphate, Na salt
49	Metallothionein I	434	Naphthol AS propionate
50	Metallothionein II	405	Naphthol AS-BI
364	Metanil yellow	407	Naphthol AS-BI b-D-galactopyranoside
23	Methemoglobin bovine	408	Naphthol AS-BI b-D-glucuronic acid
24	Methemoglobin cat	406	Naphthol AS-BI N-acetyl-b-D-glucosaminide
25	Methemoglobin human	409	Naphthol AS-BI phosphate
365	Methyl calcein	410	Naphthol AS-BI phosphate, Na salt
366	Methyl calcein blue	411	Naphthol AS-BI sulfate, K salt
371	Methyl eosin	415	Naphthol AS-D acetate
374	Methyl green	416	Naphthol AS-D chloroacetate
376	Methyl orange	413	Naphthol AS-D type II practical
378	Methyl red .HCl; 2-[4-(Dimethylamino)phenylazo]benzoic acid .HCl	414	Naphthol AS-D type III
379	Methyl red, Na salt; 2-[4-(Dimethylamino)phenylazo]benzoic acid, Na salt	417	Naphthol AS-G
377	Methyl red; 2-[4-(Dimethylamino)phenylazo]benzoic acid	418	Naphthol AS-GR
383	Methyl violet 2B	419	Naphthol AS-GR phosphate
384	Methyl viologen	420	Naphthol AS-GR phosphate, Na salt
368	Methylene blue, certified	421	Naphthol AS-IRG
369	Methylene green	425	Naphthol AS-L3G
370	Methylene violet-bernthsen	422	Naphthol AS-LC
380	Methylthymol blue	423	Naphthol AS-LC acetate
28	Microperoxidase (MP-11), Na salt	424	Naphthol AS-LG
26	Microperoxidase (MP-8), Na salt	427	Naphthol AS-MX phosphate, Na salt
27	Microperoxidase (MP-9), ammonium salt	426	Naphthol AS-MX type III
385	Mordant blue 1	435	Naphthol AS-SG
386	Mordant blue 9	436	Naphthol AS-TR
387	Mordant brown 1	437	Naphthol AS-TR phosphate
388	Mordant brown 4	438	Naphthol AS-TR phosphate, Na salt
389	Mordant brown 6	439	Naphthol blue black
390	Mordant brown 24	440	Naphthol blue black
391	Mordant brown 33	441	Naphthol green B
392	Mordant brown 48	443	Neocuproine
393	Mordant orange 10	444	Neocuproine .HCl
394	Mordant red 19	445	Neotetrazolium chloride practical
395	Mordant yellow 7	448	Neutral red practical
396	Mordant yellow 10	446	Neutral red purified
397	Mordant yellow 12	447	Neutral red, certified
398	Morin	449	New coccine
399	MTT	450	Nigericin
400	MTT formazan	451	Nigrosin
401	Murexide	453	Nile blue sulfate
229	N,N'-Diphenylbenzidine	452	Nile blue, .HCl
223	N,N-Dimethyl-m-phenylenediamine .2HCl	454	Ninhydrin
		455	Nitrazine yellow
		456	Nitro blue diformazan

<u>No.</u>	<u>Compound Description</u>	<u>No.</u>	<u>Compound Description</u>
457	Nitro blue tetrazolium	511	Polymeric dye poly T-128
462	Nitrosulfonazo III	512	Ponceau 2R
464	Nuclear fast red	513	Ponceau S
190	o-Cresolphthalein	31	Porphin
207	o-Dianisidine	514	Primulin
208	o-Dianisidine .2HCl	515	Proflavine .HCl
209	o-Dianisidine, tetrazotized	33	Protoporphyrin IX dimethyl ester from ox hemin
497	o-Phenylenediamine	32	Protoporphyrin IX, disodium salt
498	o-Phenylenediamine	516	Purpald
499	o-Phenylenediamine .2HCl	517	Purpurin
607	o-Tolidine	518	Pyridine-2-azo-(p-dimethylaniline)
608	o-Tolidine .2HCl	523	Pyrocatechol violet
610	o-Toluidine	524	Pyrogallolsulfonphthalein
609	o-Toluidine practical	525	Pyronin B
29	Octaethylporphine	527	Pyronin Y
465	Oil blue N	526	Pyronin Y certified
466	Oil red EGN	531	Quin 2
467	Oil red O	532	Quin 2, tripotassium salt
470	Orange G, certified	533	Quin 2-AM
469	Orange G, Na salt	528	Quinaldic acid
468	Orange IV, Na salt	529	Quinaldine red
471	Orcein natural	530	Quinalizarin
472	Orcein synthetic	534	Quinizarin
210	p-Diazo-N,N-diethyl-m-toluidine zinc chloride	535	Quinizarinsulfonic acid
219	p-Dimethylaminobenzaldehyde	536	Quinoline yellow
494	p-Phenylazoaniline	537	Quinolinic acid
495	p-Phenylazoaniline .HCl	538	Reactive blue 2
500	p-Phenylenediamine	539	Reactive blue 4
611	p-Toluidine	540	Reactive blue 5
473	Palatine fast black WAN	541	Reactive brown 10
474	Palatine fast yellow BLN	542	Reactive green 19
475	Pararosaniline	543	Reactive orange 14
477	Pararosaniline .HCl	544	Reactive red 4
478	Pararosaniline .HCl, certified	545	Reactive red 120
476	Pararosaniline acetate	546	Reactive yellow 2
480	Patent blue violet	547	Reactive yellow 86
482	Patent blue violet	548	Remazol brilliant blue R
479	Patent blue violet purified	549	Resazurin, Na salt
481	Patent blue violet, Ca salt	553	Rhodamine 6G
30	Pentacarboxylporphyrin I permethyl ester	550	Rhodamine B
51	Perphenazine	551	Rhodamine B base
484	Phenazine ethosulfate	552	Rhodamine B isothiocyanate
485	Phenazine methosulfate	554	Rhodanile blue
491	Phenol red	555	Rhodanine
492	Phenol red, Na salt	556	Rhodizonic acid .2H2O
486	Phenolphthalein	557	Rhodizonic acid, Ba salt
487	Phenolphthalein dibutyrate	558	Rhodizonic acid, K salt
488	Phenolphthalein diphosphate, Na salt	559	Rhodizonic acid, Na salt
490	Phenolphthalin	560	Rose bengal
489	Phenolphthalein disulfate, tripotassium salt	561	Rosolic acid
493	Phenosafrafrin	562	Ruthenium red
502	Phloretin	563	Safranin O
503	Phloxine B	564	Safranin O, certified
504	Phloxine B certified	565	Solvent blue 37
505	Phthalein purple	566	Solvent blue 38
506	Pigment red 1	567	Solvent green 3
507	Pinacryptol yellow	568	Solvent yellow 7
508	Plasmocorinth B, disodium salt	574	Sudan black B
509	Polymeric dye poly R-478	569	Sudan I
510	Polymeric dye poly S-119	570	Sudan II

<u>No.</u>	<u>Compound Description</u>	<u>No.</u>	<u>Compound Description</u>
571	Sudan III	578	Sulfonazo III, Na salt
572	Sudan III certified	581	Sulforhodamine 101
573	Sudan IV certified	582	Sulforhodamine 101 acid chloride
575	Sudan orange G	580	Sulforhodamine B
576	Sulfobromophthalein, Na salt	583	Tartrazine
577	Sulfochlorophenol S, Na salt	584	Tetrabromophenol blue