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Synthetic organic pigments of the 20th and 21st century relevant to artist's paints: Raman spectra reference collection

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ABSTRACT

Some 170 organic pigments relevant to artist's paints have been collected from historic collections and modern manufacturers. The number includes multiples of the same pigment from different sources and comprises 118 different color indices (C.I.). All of them have been analysed with FTIR spectroscopy and 125 pigments (93 different C.I. No.s) of particular relevance to artist's paints have been characterised with Raman spectroscopy so far. The pigment collection encompasses the following pigment classes and subgroups: monoazo pigments represented by acetoacetic arylide yellow (hansa yellow), β-naphthol, BON, naphthol AS and benzimidazolone; disazo pigments with disazo condensation, diarylide, bisacetoacetarylide, pyrazolone; azo-azomethin metal complex pigments; non-azo, polycyclic pigments such as phthalocyanines, diketopyrrolo-pyrroles (DPP), perylenes and perinones, quinacridones, isoindolinones, polycarbocyclic anthraquinones and dioxanines. The selection of references was based on availability (historic collections) and current use in 16 acrylic, alkyd and oil-based artist's paints, and it covers pigment colors PY yellow (27 C.I. No.s), PR red (38), PO orange (9), PB blue (8), PV violet (6), PG green (3) and PBr brown (2). Besides peak tables and spectra patterns, flow charts based on color, pigment class, group and individual color index are presented to help identification of unknowns and mixed paint samples. While Raman could isolate all different C.I. numbers, multiple references of the same C.I. from different sources could not be distinguished.

1. Introduction

The use of synthetic organic pigments in artist's paint products has dramatically increased and is now well established [1,2]. This sets additional challenges to art technological research. There are clear advantages over inorganic pigments in the sense of optical properties and processability. The application of synthetic organic pigments in artist's paints has grown proportionally to their historic development. Their industrial manufacturing has always been a sideproduct of the dyestuff industry. The history of synthetic dyes begins with the discovery of mauve in 1856 [3–6]. Of particular relevance was the discovery of the diazo compounds in 1861 laying the foundation for the currently largest class of synthetic dyes [5,7]. In the early 20th century, there has been an enormous expansion of synthetic pigment developments. There are examples where new organic pigments in were found in artwork or prints shortly after their introduction to the market [8,9]. In the following years, more and more synthetic pigments were developed and marketed. While organic pigment usage in artist's paint products has been conservative for a long time, the range of pigment C.I.s and numbers of pigments mixed within the same product has dramatically increased. More recently, synthetic organic pigments have largely replaced particularly the yellow and red tones of the classical artist's pigment palette. Table 1 gives an overview on the pigments and mixtures thereof in 16 current acrylic, oil and alkyd artist's paint. There are no less than 71 synthetic organic pigments within those 16 products, making up almost 60% of the pigments used (120) to create a painter's palette. Furthermore, the combination of pigments to achieve a specific hue varies largely across the products. This, of course, generates new analytical challenges for forensic and art technological laboratories.

Pigment analysis is well established as a means to answer forensic and authentication questions regarding artwork. Spectroscopic techniques like FTIR and Raman spectroscopy form part of the available armory that can cope with minute samples or, in the case of Raman, even fully non-destructive in situ analysis [10–14]. The range of organic pigments and mixtures thereof both in current and historic artwork is very wide. Additionally, successful Raman instrument settings may vary considerably. It is

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Table 1
Summary of pigments contained in 16 current products of artist's paint.

Bold Spectrum in Tab. 3 / *organic pigments*	Acrylic, Oil and Alkyd Artist's paint	Schmincke Primacryl	Schmincke Akademie Acryl	Talens Rembrandt Acryl	Talens Van Gogh Acryl	Winsor & Newton Artist's Acrylic Colour	Winsor & Newton Galerie Acrylic Colour	Golden Acrylics	Schmincke Mussini Oil / Resin	Schmincke Norma Oil prof.	Talens Rembrandt Oil	Talens Van Gogh Oil	Talens Amsterdam Oil	Talens Van Gogh H_2O	Winsor & Newton Artist's Oil Colour	Winsor & Newton Oil Colour	Winsor & Newton Gryffin Alkyd
	1 pigment (single pigment colour)	55	24	38	18	62	34	79	59	34	58	32	17	16	82	21	35
	2 pigments	15	19	21	16	11	14	6	18	22	35	24	9	18	27	17	10
	3 pigments	14	14	15	6	1	10	2	17	13	30	10	9	5	9	7	5
	4 pigments		2	1						8	11						
	5 pigments		1							1	1						

Synthetic organic pigment
Bold Generic name: Synthetic organic pigment
Regular Generic name: Not synth. organic pigment
Italic Pigment only used in combination, not as a single pigment

Information from colour chart declarations 2008

Pigments in Artist's paint
total: 120 pigments
Synthetic organic pigments: 71 pigments
Inorganic pigments: 49 pigments

Colour		Colour Index Generic Name																Pigment combinations
PY 3	Monoazo, Acetoacetarylide	**PY 3**	***PY 3***	***PY 3***	**PY 3**	**PY 3**	**PY 3**	**PY 3**	**PY 3**	**PY 3**		***PY 3***	***PY 3***	***PY 3***	**PY 3**	**PY 3**	**PY3**	PW4,5,7, **PY53,74,150,154**, **PO67, PB15,15:3, PG7**,19,**36**
PY 53	Cadmium zinc sulfide	PY 35		PY 35		PY 35	PY 35	PY 35	PY 35	PY 35	PY 35	PY 35			PY 35		PY 35	PW6,21, PO20, **PB15:3,** PG18
PY 42	Synthetic iron oxide	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	PY 42	*PY 42*	PW4,6, **PY43,74,138,153,154,155**,184, **PO43**, PR101,**188**, PV19, PB15,15:6,27, PG7,17,36, PBr7,24, PBk6,7,10,11,19
PY 43	Natural iron oxide					*PY 43*		PY 43	PY 43	PY 43		PY 43	*PY 43*		PY 43	*PY 43*	PY 43	PY42, PR57:1,101, **PG7, PB15,15:4**, PBr 6,7, PBk11
PY 47	Lead titanate														*PY 47*			PW6, **PG7**
PY 53	Nickel antimony titanate, Rutile	PY 53	PY 53	*PY 53*	*PY 53*			PY 53	*PY 53*	*PY 53*					PY 53			PW4,6, **PY3,153,154,155**, PG19, PBr24
PY 65	Monoazo, Acetoacetarylide						**PY 65**								**PY 65**	**PY 65**		PW6, **PY74,138, PO73, PR9**, **PB**27,**60**, PBr24
PY 73	Monoazo, Acetoacetarylide						**PY 73**	**PY 73**										
PY 74	Monoazo, Acetoacetarylide	***PY 74***	**PY 74**	**PY 74**	***PY 74***	**PY 74**	**PY 74**	**PY 74**	***PY 74***		***PY 74***	***PY 74***	***PY 74***		**PY 74**	**PY 74**	**PY 74**	PW5,6,7, **PY3**,42,**65,154, PO43,62, PB15,15:1, PG7,36**
PY 83	Diazo, Diarylide		**PY 83**			**PY 83**	***PY 83***	**PY 83**		***PY 83***								**PY74,138, PB15**,27,**60**, PBr24
PY 100	Monoazo, Tartrazine lake															***PY 100***		**PG12**
PY 109	Isoindolinone, Azomethine-type										***PY 109***							PW4, PG36
PY 110	Isoindolinone, Azomethine-type			***PY 110***						***PY 110***	**PY 110**	**PY 110**		**PY 110**	***PY 110***			**PR177,264, PB15, PG7**, PBk6
PY 119	Zinc magnesium ferrite, Spinel	*PY 119*	*PY 119*															PW 6
PY 128	Disazo, Disazo condensation			**PY 128**	***PY 128***	**PY 128**					**PY 128**	***PY 128***			**PY 128**			PG 7
PY 129	Azomethine copper complex						**PY 129**		***PY 129***		**PY 129**			***PY 129***	**PY 129**		***PY 129***	PG7, PBk7
PY 138	Quinophthalone														***PY 138***			PW4,6, **PY42,83,153,154, PO62, PR188, PG7**, PB27
PY 139	Isoindoline, Methine-type														***PY 139***		**PY 139**	PR101
PY 150	Azo, Nickel complex	**PY 150**					**PY 150**	**PY 150**	**PY 150**	***PY 150***	**PY 150**				**PY 150**			**PY3, PO48, PB60, PG36**, PBr7
PY 153	Nickel Dioxine, Ni-complex	**PY 153**							**PY 153**	**PY 153**								PW6, **PY42**,53,**138,154**, PR101, **PG7**, BBr24
PY 154	Monoazo, Benzimidazolone	**PY 154**								***PY 154***	**PY 154**	***PY 154***	***PY 154***	***PY 154***				PW4,5,6, **PY3**,42,27,53,**74,138,153, PO43, PG7**, PBr24
PY 155	Disazo, Bisacetoacetarylide	**PY 155**							**PY 155**									PW4,6, PY42,53, PV15, PG17
PY 184	Bismuth vanadate	PY 184				PY 184			PY 184	*PY 184*	PY 184				PY 184			PW4, PY42, **PO67, PG7**,18,38,50
PO 5	Monoazo, β-Naphtol		PO 5															
PO 20	Cadmium sulfo-selenide	PO 20		PO 20		PO 20		PO 20	PO 20	PO 20	*PO 20*	PO 20			PO 20		PO 20	PW21, PY35, PR108, **PB15:3**
PO 34	Disazo, Bisacetoacetarylide				***PO 34***						***PO 34***	***PO 34***	***PO 34***	***PO 34***				**PR**57:1,**112**
PO 36	Monoazo, Benzimidazolone															***PO 36***	***PO 36***	**PR170**
PO 43	Polycyclic, Perinone		**PO 43**	***PO 43***	***PO 43***	**PO 43**		**PO 43**			***PO 43***	***PO 43***	***PO 43***	***PO 43***				PW6, PY42,**74,154, PR112**, PBr24
PO 48	Polycyclic, Quinacridone							***PO 48***										**PY150**
PO 49	Polycyclic, Quinacridone					**PO 49**												**PB15,60, PG36**
PO 62	Monoazo, Benzimidazolone					**PO 62**				***PO 62***					***PO 62***			PW6, **PY74,138, PR255**
PO 67	Monoazo, Pyrazoloquinazolone	**PO 67**							**PO 67**	***PO 67***		***PO 67***	***PO 67***					**PY3**,183, **PR255**
PO 71	Polycyclic, Diketopyrrolo-pyrrole	**PO 71**							**PO 71**									
PO 73	Polycyclic, Diketopyrrolo-pyrrole							**PO 73**			**PO 73**				**PO 73**	**PO 73**		**PY65, PR255**
PR 5	Monoazo, Naphthol AS							**PR 5**										
PR 9	Monoazo, Naphthol AS					**PR 9**												**PY65**
NR 9	Lake of natural madder														**NPR 9**			
PR 12	Monoazo, Naphthol AS				***PR 12***									***PR 12***				**PV19**
PR 23	Disazo, Disazo condensation			**PR 23**	**PR 23**									**PR 23**				
PR 57:1	Monoazo, BON											***PR 57:1***	***PR 57:1***					PO34, PR83
PR 83	Polycyclic, Antraquinone											**PR 83**			**PR 83**			PV19, PR57:1
PR 83:1	Polycyclic, Antraquinone (Al)								**PR 83:1**									
PR 88	Polycyclic, Thioindigo									***PR 88***								PW5, PV23
PR 101	Synthetic iron oxide	PR 101	PR 101	PR 101	PR 101	PR 101	PR 101	PR 101	PR 101	PR 101	PR101	PR 101	PR 101	PR 101	PR 101	PR 101	PR 101	PW4,6,15,20, **PY**42,43,**139,153**, PR101,**112,170,179,264,** PB15:1,29,60, PG7,18, PV19, PBk6,7,11,19
PR 108	Cadmium sulfo-selenide	PR 108		PR 108		PR 108	PR 108	PR 108	*PR 108*	PR 108	PR 108	PR 108			PR 108		PR 108	PW21, PO20
PR 112	Monoazo, Naphthol AS		**PR 112**	**PR 112**	**PR 112**		**PR 112**	**PR 112**						**PR 112**				**PO34,43, PR170**, PBr24
PR 122	Polycyclic, Quinacridone	**PR 122**	***PR 122***	***PR 122***	***PR 122***	**PR 122**	***PR 122***	**PR 122**	**PR 122**	**PR 122**		***PR 122***		***PR 122***	**PR 122**	***PR 122***	***PR 122***	PW4,6, **PR170, PV23, PB15, PB60**
PR 149	Polycyclic, Perylene					**PR 149**					**PR 149**				**PR 149**			
PR 170	Monoazo, Naphthol AS		**PR 170**			**PR 170**	**PR 170**									**PR 170**	***PR 170***	PW4, **PO36, PR**101,**112,122,188, PV23**, PBr24
PR 176	Monoazo, Benzimidazolone										**PR 176**							
PR 177	Polycyclic, Anthraquinone					***PR 177***				**PR 177**				**PR 177**	**PR 177**	**PR 177**	**PR 177**	PR110, **PV19,23**, PB29, PBr7
PR 179	Polycyclic, Perylene	**PR 179**	**PR 179**						**PR 179**	**PR 179**								PR101, BBk7

PR 187	Monoazo, Naphthol AS									***PR 187***								**PV19**
PR 188	Monoazo, Naphthol AS							***PR 202***							***PR 188***	**PR 188**	**PR 188**	PW 6, PY 42,138, **PR170**
PR 202	Polycyclic, Quinacridone										**PR 202**							**PR 206**
PR 206	Polycyclic, Quinacridone	**PR 206**				**PR 206**		**PR 206**	**PR 206**									**PR 202**
PR 207	Polycyclic, Quinacridone							**PR 207**			**PR 207**							
PR 209	Polycyclic, Quinacridone	**PR 209**		**PR 209**		**PR 209**			**PR 209**						**PR 209**	**PR 209**	**PR 209**	
PR 242	Disazo, Disazo condensation								**PR 242**									**PV 19**
PR 254	Polycyclic, Diketopyrrolo-pyrrole	***PR 254***	***PR 254***	**PR 254**		**PR 254**		**PR 254**			**PR 254**	**PR 254**			**PR 254**			PW6, **PR255,264, PV19,42**
PR 255	Polycyclic, Diketopyrrolo-pyrrole	**PR 255**	***PR 255***			**PR 255**		**PR 255**	**PR 255**	**PR 255**	**PR 255**				**PR 255**			PW6, **PO62,67,73**, **PR**101,**254**, PBr24
PR 264	Polycyclic, Diketopyrrolo-pyrrole			**PR 264**	**PR 264**						***PR 264***							PW4, **PY110**, **PR**101,**254, PV19**, PB29, **PG7**
PV 14	Cobalt phoshate								PV 14		PV 14				PV 14			
PV 15	Sodium aluminium sulfur silicate			PV 15				PV 15	*PV 15*		PV 15				PV 15			
PV 16	Manganese ammonium pyrophosphate										PV 16				PV 16	*PV 16*		PB 29
PV 19	Polycyclic, Quinacridone	**PV 19**		**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	**PV 19**	PW6, PY42, **PR12,83**,101,**177,187,242,254,264, PV23,42,** PB15:6,23,60, PBk7,10,11
PV 23	Polycyclic, Dioxazine	**PV 23**	**PV 23**	***PV 23***	***PV 23***	**PV 23**	**PV 23**	**PV 23**	**PV 23**	***PV 23***		***PV 23***	***PV 23***	***PV 23***	**PV 23**	***PV 23***	**PV 23**	PW5,6, **PR88,122,170, PV19, PB15,15:1,15:4,15:6**,29, **PBr25**
PV 42	Polycyclic, Quinacridone								**PV 42**									**PR254, PV19**
PB 15	Polycyclic, Phthalocyanine (Cu)				***PB 15***	***PB 15***	**PB 15**			**PB 15**		**PB 15**			**PB 15**	**PB 15**	**PB 15**	PW4, **PY3**,42,43,**74,83,110, PO49, PR122, PV19,23,** PB15,15:6,29, PG7, PBk7,9
PB 15:1	Polycyclic, Phthalocyanine (Cu,Cl), alpha	***PB 15:1***	***PB 15:1***			**PB 15:1**		**PB 15:1**										PW6, **PY74**, PR101, P**V23, PB15:1,60, PG7**, PBk7
PB 15:2	Polycyclic, Phthalocyanine (Cu)	***PB 15:2***																PB15:6
PB 15:3	Polycyclic, Phthalocyanine (Cu), beta	**PB 15:3**	**PB 15:3**			**PB 15:3**	**PB 15:3**		**Pb 15:3**	**PB 15:3**								PW4,6, **PY3, PB15:4,16**,29,**60, PG7**,19, PBk11
PB 15:4	Polycyclic, Phthalocyanine (Cu)			**PB 15:4**	**PB 15:4**			**PB 15:4**			**PB 15:4**		***PB 15:4***	**PB 15:4**				PW4, PW6, **PY3, PV23, PG7**, PBk11
PB 15:6	Polycyclic, Phthalocyanine (Cu)	***PB 15:6***		***PB 15:6***	***PB 15:6***				**PB 15:6**		**PB 15:6**			***PB 15:6***				PW4, PY42, **PV19, PV23, PB15:2**,29, PBk9,11
PB 16	Polycyclic, Phthalocyanine, gamma	**PB 16**				***PB 16***			***PB 16***									PW4,6, **PB15:3**,29
PB 17	Polycyclic, Phthalocyanine (Cu), trisulfonated	***PB 17***																PW6, PY42
PB 27	Ferriammonium ferrocyanide								PB 27	PB 27	PB 27	PB 27	PB 27	PB 27	PB 27	PB 27	PB 27	PY42,**83,154**,183
PB 28	Cobalt aluminate, Spinel	PB 28		PB 28	PB 28	PB 28	PB 28	PB 28	PB 28	PB 28	*PB 28*	PB 28			PB 28		PB 28	PW4,6, **PB60**
PB 29	Sodium aluminium-sulfosilicate	PB 29	PB 29	PB 29	PB 29	Pb 29	PB 29	PB 29	PB 29	PB 29	*PB 29*	PB 29	PB 29		PB 29	PB 29	PB 29	PW4,6, **PR**101,**177,264, PV16, PB15,15:1,15:3,15:6,16,60,** PV23, PBk7,9,11,19
PB 35	Cobalt stanate			PB 35		PB 35			PB 35	PB 35	PB 35	PB 35			PB 35			PB36
PB 36	Cobalt chromate					PB 36		PB 36	*PB 36*	*PB 36*	PB 36				PB 36			PW4,6, PY109, PB35
PB 36:1	Cobalt chromate							PB 36:1										
PB 60	Polycyclic, Indanthrene	**PB 60**	**PB 60**			**PB 60**		**PB 60**	**PB 60**	**PB 60**	***PB 60***				**PB 60**			PW4, **PY83,150, PO49**, **PR**101,**122, PB15:1**, PB28, **PV19**, PBk10,11
PB 66	Unsubstituted indigo								**PB 66**									
PB 73	Cobalt silicate					**PB 73**												
PB 74	Cobalt zinc silicate								**PB 74**	**PB 74**	**PB 74**				**PB 74**			
PG7	Polycyclic, Phthalocyanine (Cu) chlorinated	**PG 7**		**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	**PG 7**	PW4,6, **PY3**,42,43,47,53,**74,110,128,129,138,153,154**,184, PR101,264, PB15,15:3,15:4, PG18,23
PG 8	Azo metal complex, nitroso iron complex			**PG 8**	**PG 8**								**PG 8**					
PG 12	Monoazo, Ferrous nitroso β-Naphthol															***PG 12***		**PY100**
PG 17	Anhydrous chromium oxide	PG 17		PG 17	PG 17	PG 17		PG 17	PG 17	PG 17	PG 17	PG 17			PG 17	PG 17	PG 17	PW4,6, **PY42**,**155**, PR101, PBk11
PG 18	Hydrated chromium hydroxide	PG 18							PG 18	*PG 18*	PG 18				PG 18		PG 18	PW4, PY35,42,184, PR101, PG17, PBk11
PG 19	Copper stanate	PG 19							PG 19	*PG 19*								PW4, PY3, PY53, **PB15:3**
PG 23	Green earth, Celadonite									*PG 23*								PBr7
PG 24	Polysulfide of sodium alumino silicate										PG 24							
PG 26	Cobalt chromate	PG 26				PG 26		PG 26	PG 26		PG 26				PG 26			PG50
PG 36	Polycyclic, Phthalocyanine (Cu), bromated	**PG 36**	**PG 36**			**PG 36**		**PG 36**	**PG 36**		**PG 36**				**PG 36**		**PG 36**	PW4,6, PY42,**74,184, PO49, PB15:3**, PG35
PG 50	Cobalt titanate, Spinel (Co,Li, Ni,Zn,Ti)	PG 50				PG 50		PG 50	PG 50	PG 50	PG 50				PG 50			**PY184**, PG26
PBr 6	Synthetic iron oxide	PBr 6						PBr 6										
PBr 7	Calcined earth pigment, Natural iron oxide	PBr 7				PBr 7	PBr 7	PBr 7	PBr 7	PBr 7		PBr 7	PBr 7		PBr 7	PBr 7	PBr 7	PW6, **PY**42,43,**150**, **PR**101,**177, PB15,15:1**, PBk6
PBr 8	Bitumeous earth														*NBr 8*	*NBr 8*		PBr7
PBr 24	Chromium titanate, Rutile (Ti,Cr,Sb)	PBr 24	PBr 24	PBr 24	PBr 24	PBr 24			PBr 24	*PBr 24*	PBr 24	*PBr 24*		PBr 24	PBr 24			PW4,6, **PY**42,53,**74,83,153,154, PO43**, PR101, **PR255**
PBr 25	Monoazo, Benzimidazolone														**PBr 25**			PBr7
PBr 33	Zinc iron chromite	PBr 33																
PBk 6	Lamp black	*PBk 6*					PBk 6								PBk 6	PBk 6	PBk 6	PW6, **PY42**,**110**, PBr7
PBk 7	Carbon black, Vegetable carbon	PBk 7	PBk 7	PBk 7			*PBk 7*	*PBk 7*	PBk 7		Pbk 7				*PBk 7*	*PBk 7*	PBk 7	PW6, **PY**42,**129**, PR101, **PR179, PB15,29**, PG27, **PV19**, PBr6, PBk11,19
PBk 8	Ground charcoal														PBk 8			
PBk 9	Bone black, Carbonised bones	PBk 9		PBk 9		PBk 9	PBk 9	PBk 9	PBk 9	PBk 9	*PB 29*	PBk9	PBk 9	PBk 9	PBk 9	PBk 9	PBk 9	PBr7, **PB15:6**,29, PV19
PBk 10	Graphite	PBk 10				PBk 10		PBk 10	PBk 10									PW4,6, PY42, **PV19, PB60**, PBr24,
PBk 11	Synthetic iron oxide	PBk 11		PBk 11	PBk 11	PBk 11	PBk 11	*PBk 11*	PBk 11	PBk 11	*PBk 11*			*PBk 11*	*PBk 11*			PW4,6,15,20, PY42, PR101, **PV19, PB15:1,15:4,15:6**,29,**60**, PG17,18, PBk7
PBK 19	Slate powder, black chalk mineral					*PBk 19*									*PBk 19*	*PBk 19*	*PBk 19*	PB29, PY42, PR101, PBk6,7
PBK 29	Copper chromate, Spinel					*PBk 29*			PBk 28						*PBk 29*			
PBk 31	Polycyclic, Perylene	**PBK 31**							**PBk 31**						**PBk 31**			
PW 1	Basic lead carbonate														PW 1			PW 4
PW 4	Zinc oxide	PW 4		PW 4			PW 4	PW 4	PW 4	PW 4	PW 4	PW 4	PW4	PW 4	PW 4	PW 4		several
PW 5	Lithopone		*PW 5*							*PW 5*								several
PW 6	Titanum dioxide	PW 6	PW 6	*PW 6*	*PW 6*	PW 6	PW 6	PW 6		*PW 6*	*PW 6*	*PW 6*	*PW 6*	PW 6	*PW 6*	*PW 6*	PW 6	several
PW 7	Zinc sulfide		*PW 7*							*PW 7*								several
PW 15	Coated mica			*PW 15*							*PW 15*							PW6,20, PR101, PBk11
PW 20	Coated mica			*PW20*							*PW 20*							PW6,15, PR101, PBk11
PW 21	Barium sulfate								*PW 21*									PR108, PO20, **PB15:3,**

Not included are the metal oxide coated mica and the fluorescence pigments

Table 2
List of reference materials and analytical settings for Raman spectra acquired.

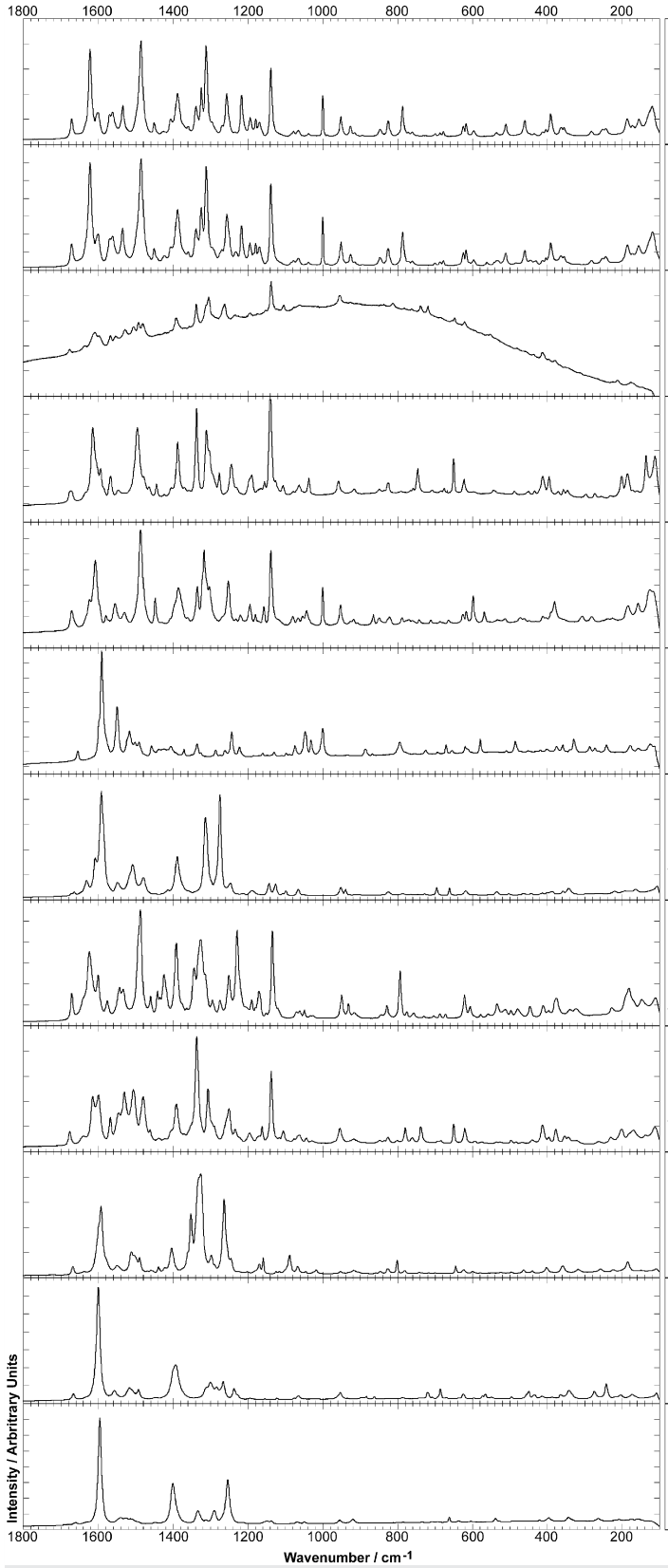
Pigment	C.I.	Laser (nm)	P sample (mW)	Time scan (s)	No. of scans	Product name	Manufacturer / supplier	Collection	Year prod.	Pigment class	Pigment group	# n=125
PB15	74160	785	0.0121	10	10	DY HG 502 Hostapermblau A 3R	Hoechst	Coll.: TU Dresden		Polycyclic	Phthalocyanine	1
PB15	74160	785	0.0121	10	10	Heliogenblau 23050	Kremer		≤ 2006	Polycyclic	Phthalocyanine	2
PB15:1	74160:1	785	0.0121	10	10	MONASTRAL Blue CSN	Heubach		≤ 2007	Polycyclic	Phthalocyanine	3
PB15:2	74160:2	785	0.121	10	10	MONASTRAL Blue FBN	Heubach		≤ 2007	Polycyclic	Phthalocyanine	4
PB15:3	74160:3	785	0.0000121	10	15	DY HB 502 Hostapermblau B3G	Hoechst	Coll.: TU Dresden		Polycyclic	Phthalocyanine	5
PB15:3	74160:3	785	0.0000121	10	15	Heliogenblau, königs-blau	Kremer		≤ 2006	Polycyclic	Phthalocyanine	6
PB15:4	74160:4	785	0.0121	10	15	HEUCO-Blau	Heubach		≤ 2007	Polycyclic	Phthalocyanine	7
PB15:6	74160:6	514	0.57	10	10	Heliogenblau, rotstichig	Kremer		≤ 2006	Polycyclic	Phthalocyanine	8
PB16	74100	514	5.7	10	15	Sample, Monstral Fast Blue GS, Powder	Imp. Chem. Indust.	Coll.: TU Dresden	1962	Polycyclic	Phthalocyanine	9
PB60	69800	514	1.14	30	10	Indanthrenblau	Kremer		≤ 2006	Polycyclic	Polycarbocyclic anthraquinone	10
PBr23	20060	785	0.0605	20	5	Gubbi Rot 23493	Kremer		≤ 2006	Disazo	Condensation	11
PBr25	12510	633	1.03	20	10	Hostaperm-Braun HFR 01	Clariant		≤ 2007	Monoazo	Benzimidazolone	12
PG7	74260	514	0.114	10	5	Heliogengrün 23000	Kremer		≤ 2006	Polycyclic	Phthalocyanine	13
PG9	49415	785	0.121	10	10	Hansagrün GS	Lucius & Brüning	Coll.: TU Dresden		Metal complex	Azo metal complex	14
PG36	74265	514	1.14	30	5	Heliogengrün 23010	Kremer		≤ 2006	Polycyclic	Phthalocyanine	15
PO5	12075	785	0.0121	10	10	Hansa-Rot GG	Clariant		≤ 2006	Monoazo	B-Naphthol	16
PO5	12075	633	0.0515	10	10	Hansaorange		Coll.: SIAR, Zurich		Monoazo	B-Naphthol	17
PO5	12075	785	0.0121	10	10	Permanentrot GG extra	Hoechst	Coll.: TU Dresden		Monoazo	B-Naphthol	18
PO13	21110	785	0.0121	10	10	Permanent-Orange G	Clariant		≤ 2007	Disazo	Pyrazolone	19
PO34	21115	785	0.0121	10	10	Permanent-Orange RL 70	Clariant		≤ 2007	Disazo	Pyrazolone	20
PO36	11780	785	1.21	10	5	HEUCO-Orange	Heubach		≤ 2007	Monoazo	Benzimidazolone	21
PO36	11780	785	1.21	20	5	Novoperm-Orange HL	Clariant		≤ 2007	Monoazo	Benzimidazolone	22
PO43	71105	785	0.121	10	10	Hostaperm-Orange GR	Clariant		≤ 2007	Polycyclic	Perinone	23
PO48	73900	785	0.121	10	10	Chinquasia rotgold	Kremer		≤1995	Polycyclic	Quinacridone	24
PO49	564800	633	1.03	20	10	Chinquasia braungold	Kremer		≤1995	Polycyclic	Quinacridone	25
PO62	11775	785	0.0605	10	10	HEUCO-Orange	Heubach		≤ 2007	Monoazo	Benzimidazolone	26
PO73	561170	785	0.121	10	12	Iragazin Orange DPP RTR 23168	Kremer		≤ 2006	Polycyclic	Diketopyrrolo-Pyrrole (DPP)	27
PO73	561170	785	0.121	10	10	Irgazin Orange DPP RA	Kremer		≤ 2006	Polycyclic	Diketopyrrolo-Pyrrole (DPP)	28
PR2	12310	785	0.0121	10	10			Coll.: SIAR, Zurich		Monoazo	Naphthol AS	29
PR3	12120	785	0.121	10	10	Hansa-Rot 3B	Clariant		≤ 2006	Monoazo	B-Naphthol	30
PR3	12120	785	0.121	10	10	Hansa-Rot B	Clariant		≤ 2006	Monoazo	B-Naphthol	31
PR4	12085	785	0.121	10	10	Permanentrot R, extra	Hoechst	Coll.: TU Dresden		Monoazo	B-Naphthol	32
PR5	12490	785	0.121	20	3	Monolite Red CB	Heubach		≤ 2007	Monoazo	Naphthol AS	33
PR5	12490	785	0.121	20	10	Permanentcarmin FB, extra	Hoechst	Coll.: TU Dresden		Monoazo	Naphthol AS	34
PR7	12420	785	0.0121	10	15	Permanentrot, Antiquität	Kremer			Monoazo	Naphthol AS	35
PR8	12335	785	0.0121	10	15	Permanentrot F4R	Schoenfeld & Co.	Coll.: SIAR, Zurich	1968	Monoazo	Naphthol AS	36
PR9	12460	785	0.121	20	5	Permanentrot FRLL	Kremer	Coll.: SIAR, Zurich		Monoazo	Naphthol AS	37
PR10	12440	785	0.00605	10	15	Permanentrot FRL		Coll.: SIAR, Zurich		Monoazo	Naphthol AS	38
PR11	12430	785	0.0121	10	15	Permanentrubin FBH, extra	Hoechst	Coll.: TU Dresden		Monoazo	Naphthol AS	39
PR12	12385	785	0.121	10	10	MONOLITE Rubine2R	Heubach		≤ 2007	Monoazo	Naphthol AS	40
PR12	12385	785	0.121	10	10	Permanent Bordeaux FRR	Schoenfeld & Co.	Coll.: SIAR, Zurich	1968	Monoazo	Naphthol AS	41
PR12	12385	785	0.121	10	10	Permanent Bordo FRR	Clariant		≤ 2007	Monoazo	Naphthol AS	42
PR12	12385	785	0.121	10	10	Sample, Monolite Fast Bordeaux 2RS Powder D	Imp. Chem. Indust.	Coll.: TU Dresden	1961	Monoazo	Naphthol AS	43
PR16	12500	785	0.0121	10	15	Permanentbordeaux F3R, extra	Hoechst	Coll.: TU Dresden		Monoazo	Naphthol AS	44
PR18	12350	785	0.0605	10	15	Sample, Monolite Maroon NS Powder	Imp. Chem. Indust.	Coll.: TU Dresden	1962	Monoazo	Naphthol AS	45
PR48:3	15865:3	785	0.121	10	5	HEUCO-Rot	Heubach		≤ 2007	Monoazo	BON lake	46
PR49	15630	785	0.121	10	10			Coll.: SIAR, Zurich		Monoazo	B-Naphthol	47
PR49:1	15630:1	785	0.121	10	10	Lackrot RB 8051, BaSO4 substrate		Coll.: TU Dresden		Monoazo	B-Naphthol lake	48
PR49:2	15630:2	785	0.121	10	10	Lackrot RC 8052, CaCO3 substrate		Coll.: TU Dresden		Monoazo	B-Naphthol lake	49
PR53	15585	785	0.0121	10	10			Coll.: SIAR, Zurich		Monoazo	B-Naphthol	50

Pigment	C.I.	Laser (nm)	P sample (mW)	Time scan (s)	No. of scans	Product name	Manufacturer / supplier	Collection	Year prod.	Pigment class	Pigment group	# n=125
PR53:1	15585:1	785	0.0605	10	10	Lackrot B 8056, BaSO4 substrate		Coll.: TU Dresden		Monoazo	B-Naphthol lake	51
PR57	15850	785	0.121	10	5			Coll.: SIAR, Zurich		Monoazo	BON lake	52
PR57:1	15858:1	785	0.121	10	10	Graphtol-Rubin 6BP	Clariant		≤ 2007	Monoazo	BON lake	53
PR68	15525	785	0.121	10	10	Permanentrottoner NCR	Hoechst	Coll.: TU Dresden		Monoazo	B-Naphthol	54
PR83:1	58000:1	633	0.103	30	15	Alizarin-Krapplack dunkel	Kremer		≤ 2006	Polycyclic	Polycarbocyclic Anthraquinone	55
PR112	12370	785	0.0121	10	10	HEUCO-Rot	Heubach		≤ 2007	Monoazo	Naphthol AS	56
PR122	73915	514	0.114	40	10	Quindo Rot R 6713	Kremer		≤ 2006	Polycyclic	Quinacridone	57
PR144	20735	785	0.0605	10	10	CPT Rot 23293	Kremer		≤ 2006	Disazo	Condensation	58
PR146	12485	785	0.121	10	10	Permanent Carmin FBB 02	Clariant		≤ 2007	Monoazo	Naphthol AS	59
PR149	71137	785	0.0000121	20	30	PV Fast Red B	Clariant		≤ 2007	Polycyclic	Perylene & Perinone	60
PR166	20730	785	0.00605	10	10	CPT Scharlach 23202	Kremer		≤ 2006	Disazo	Condensation	61
PR166	20730	785	0.00605	10	15	HEUCO-Rot 316600	Heubach		≤ 2007	Disazo	Condensation	62
PR170	12475	785	0.00605	10	15	HEUCO-Rot 317000	Heubach		≤ 2007	Monoazo	Naphthol AS	63
PR170	12475	785	0.121	10	10	Permanentrot	Kremer		≤ 2006	Monoazo	Naphthol AS	64
PR179	71130	785	0.00605	10	10	Paliogenmarron	Kremer		≤ 2006	Polycyclic	Perylene & Perinone	65
PR185	12516	785	0.121	10	5	Novoperm-Carmin HF4C	Clariant		≤ 2007	Monoazo	Benzimidazolone	66
PR187	12486	785	0.0605	10	10	Novoperm-Rot HF4B	Clariant		≤ 2007	Monoazo	Naphthol AS	67
PR188	12467	785	0.121	20	5	Novoperm-Rot HF3S	Clariant		≤ 2007	Monoazo	Naphthol AS	68
PR214	200660	785	0.0605	10	10	Novoperm Red BN 103502	Clariant		≤ 2007	Disazo	Condensation	69
PR242	20067	785	0.0605	10	10	Novoperm Scarlet 4RF 01	Clariant		≤ 2007	Disazo	Condensation	70
PR254	56110	785	0.0605	10	15	Hostaperm-Rot D3G 70 VP 2884	Clariant		≤ 2007	Polycyclic	Diketopyrrolo-Pyrrole (DPP)	71
PR254	56110	785	0.00605	10	10	Irgazin Rot DPP BO	Kremer		≤ 2006	Polycyclic	Diketopyrrolo-Pyrrole (DPP)	72
PR255	561050	785	0.121	10	10	Irgazin Scharlach DPP EK	Kremer		≤ 2006	Polycyclic	Diketopyrrolo-Pyrrole (DPP)	73
PR264	561300	785	0.00605	10	10	Iragzin Rubin DPP/TR	Kremer		≤ 2006	Polycyclic	Diketopyrrolo-Pyrrole (DPP)	74
PV5	58055	785	0.605	10	10	Alizarinviolett	Kremer		≤ 2006	Polycyclic	Polycarbocyclic Anthraquinone	75
PV19	73900	633	0.103	10	10	Hostaperm magenta	Kremer		≤ 2006	Polycyclic	Quinacridone	76
PV23	51319	514	0.114	20	10	MONOLITE Violet RN	Heubach		≤ 2007	Polycyclic	Dioxazine	77
PV32	12517	785	0.121	10	5	Novoperm Bordo HF3R	Clariant		≤ 2007	Monoazo	Benzimidazolone	78
PV36	73385	514	0.114	20	10	Indathrenrot Violett RH	Bayer	Coll.: TU Dresden		Polycyclic	Indigoide	79
PV37	51345	785	0.121	10	10	Dioxazinviolett	Kremer		≤ 2006	Polycyclic	Dioxazine	80
PY1	11680	785	1.21	20	1	Echtgelb rein RG	Rasquin, Köln	Coll.: SIAR, Zurich		Monoazo	Acetoacetic arylide	81
PY1	11680	785	1.21	30	1	Hansagelb G	Schoenfeld & Co.	Coll.: SIAR, Zurich	1968	Monoazo	Acetoacetic arylide	82
PY1	11680	785	1.21	20	1	Hansagelb G	Siegle & Co.	Coll.: Musee Suisse, Zurich		Monoazo	Acetoacetic arylide	83
PY1	11680	785	1.21	30	1	Hansagelb G 02	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	84
PY1	11680	785	6.05	30	1	Hansagelb G trans. Pulver	IG Farbenindustrie	Coll.: Musee Suisse, Zurich	1925-45	Monoazo	Acetoacetic arylide	85
PY1	11680	785	1.21	20	1	Hansagelb GSA, Pulver	IG Farbenindustrie	Coll.: Musee Suisse, Zurich	1925-45	Monoazo	Acetoacetic arylide	86
PY1	11680	785	1.21	30	1	HEUCO-Gelb	Heubach		≤ 2007	Monoazo	Acetoacetic arylide	87
PY1:1	11680:1	785	1.21	30	1	MONOLITE Yellow 2R	Heubach		≤ 2007	Monoazo	Acetoacetic arylide	88
PY2	11730	785	0.121	20	5	Hansagelb GR		Coll.: SIAR, Zurich		Monoazo	Acetoacetic arylide	89
PY3	11710	785	1.21	10	1	Echtgelb rein R	Rasquin, Köln	Coll.: SIAR, Zurich		Monoazo	Acetoacetic arylide	90
PY3	11710	785	0.121	10	10	Hansagelb		Coll.: Doerner Inst., Munich		Monoazo	Acetoacetic arylide	91
PY3	11710	785	1.21	30	1	Hansagelb 10G	Schoenfeld & Co.	Coll.: SIAR, Zurich	1968	Monoazo	Acetoacetic arylide	92
PY3	11710	785	1.21	30	1	Hansagelb 10G	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	93
PY3	11710	785	0.121	10	10	Hansagelb 10G		Coll.: SIAR, Zurich		Monoazo	Acetoacetic arylide	94
PY3	11710	785	1.21	30	1	Hansagelb 10G	Schmincke		≤ 2006	Monoazo	Acetoacetic arylide	95
PY3	11710	785	1.21	20	1	Hansagelb 10G 41	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	96
PY3	11710	785	1.21	30	1	Studiogelb	Kremer		≤ 2006	Monoazo	Acetoacetic arylide	97
PY5	11660	785	0.121	20	5	Hansagelb 5G		Coll.: SIAR, Zurich		Monoazo	Acetoacetic arylide	98
PY10	12710	785	0.121	10	10	Hansagelb R	Hoechst	Coll.: TU Dresden		Monoazo	Pyrazolone	99
PY16	20040	785	0.121	10	10	DHS DS 005 Permanent-Gelb NCG-O	Hoechst	Coll.: TU Dresden		Disazo	Bisacetoacetarylide	100

Table 2 (*Continued*)

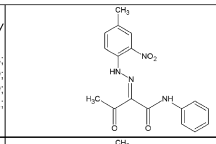
Pigment	C.I.	Laser (nm)	P sample (mW)	Time scan (s)	No. of scans	Product name	Manufacturer / supplier	Collection	Year prod.	Pigment class	Pigment group	# *n=125*
PY16	20040	785	0.121	10	10	Permanent-Gelb NCG	Clariant		≤ 2007	Disazo	Bisacetoacetarylide	101
PY65	11740	785	1.21	10	1	Pigmentmuster	Schmincke		≤ 2006	Monoazo	Acetoacetic arylide	102
PY73	11738	785	1.21	20	1	Hansa-Brillantgelb 4GX	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	103
PY74	11741	785	0.121	10	10	Hansa-Brillantgelb	Kremer		≤ 2006	Monoazo	Acetoacetic arylide	104
PY74	11741	785	0.121	10	10	Hansa-Brillantgelb 2GX 70	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	105
PY74	11741	785	0.121	10	1	Hansa-Brillantgelb 2GX 70-S	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	106
PY74	11741	785	0.121	20	1	Hansa-Brillantgelb 5GX	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	107
PY74	11741	785	0.121	10	10	Hansa-Brillantgelb 5GX 03	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	108
PY81	21127	785	0.121	10	5	Novoperm-Gelb H10G 01	Clariant		≤ 2007	Disazo	Diarylide	109
PY83	21108	785	0.0121	10	10	Novoperm-Gelb HR	Clariant		≤ 2007	Disazo	Diarylide	110
PY93	20710	785	0.0121	10	10	HEUCO-Gelb 109300	Heubach		≤ 2007	Disazo	Condensation	111
PY95	20034	785	0.121	20	10	HEUCO-Gelb 109500	Heubach		≤ 2007	Disazo	Condensation	112
PY97	11767	785	1.21	30	1	Novoperm-Gelb FGL	Clariant		≤ 2007	Monoazo	Acetoacetic arylide	113
PY109	56284	785	0.0121	10	10	Isoindolgelb 23340	Kremer		≤ 2006	Isoindolinone	Azomethine type	114
PY111	11745	785	0.121	20	5	Hansa-Brillantgelb 9GX	Clariant		≤ 2006	Monoazo	Acetoacetic arylide	115
PY120	11783	785	1.21	30	5	Novoperm-GelbH2G	Clariant		≤ 2007	Monoazo	Benzimidazolone	116
PY129	48042	785	0.0121	10	10	Irazingelb, grünstichig	Kremer		≤ 2006	Metal complex	Azomethine metal complex	117
PY139	56298	785	0.00605	10	10	Paliotolgelb-orange	Kremer		≤ 2006	Isoindoline	Methine type	118
PY150	12764	785	0.0121	10	10	Indischgelb, imitiert	Kremer		≤ 2006	Metal complex	Azo metal complex	119
PY151	13980	785	1.21	30	5	Permanentgelb hell	Kremer		≤ 2005	Monoazo	Benzimidazolone	120
PY154	11781	785	1.21	30	5	Permanentgelb mittel	Kremer		≤ 2005	Monoazo	Benzimidazolone	121
PY155	200310	785	1.21	10	10	Novoperm-Gelb 5GD71	Clariant		≤ 2007	Disazo	Bisacetoacetarylide	122
PY175	11784	785	0.121	30	10	Hostaperm-Gelb H6G	Clariant		≤ 2007	Monoazo	Benzimidazolone	123
PY181	11777	785	1.21	10	10	PV-Echtgelb H3R	Clariant		≤ 2007	Monoazo	Benzimidazolone	124
PY194	11785	785	1.21	10	10	Novoperm-Gelb F2G	Clariant		≤ 2007	Monoazo	Benzimidazolone	125

Table 3
Raman spectral library of 93 synthetic organic pigments, sorted by C.I. pigment name. Main signals are marked with vs = very strong, s = strong or m = medium in the peak tables. Bold band positions in the tables relate to discriminating features differentiating between pigment class, group and individual C.I. number (refer to flowcharts in Figs. 2–6). No baseline correction has been applied to any spectrum.



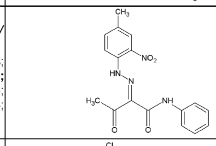
PY1 C.I. 11680, Monoazopigment, Acetoacetic arylide
Schoenfeld & Co.; Laser: 785nm 1.21mW

1671m; 1622vs; 1601m; 1565m; 1534m; **1485vs;** 1450; 1407; 1388s; 1359; 1339m; **1324s;** 1311vs; 1257s; **1217s;** 1194; 1179; 1169; **1138vs;** 1078; 1065; 1038; **1000s; 951m;** 926; 847; 825m; **786s;** 760; 699; 678; 617; 597; 536; **511m; 460m;** 391m; 362; 282; 244; 186; 172; 155; 120m



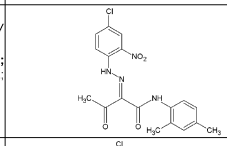
PY1:1 C.I. 11680:1, Monoazopigment, Acetoacetic arylide
Heubach; Laser: 785nm 1.21mW

1671m; 1622vs; 1600m; 1565m; 1535m; **1485vs;** 1450; 1424; 1388s; 1359; 1339; **1325s;** 1311vs; 1256s; 1232; **1217s;** 1194; 1169; **1138vs;** 1079; 1065; 1038; **1000s; 951m;** 925; 847; 825m; **786s;** 760; 700; 678; 617m; 596; 561; 534; **511m; 460m;** 444; 430; 391m; 363; 282; 244; 186m; 156; 119m



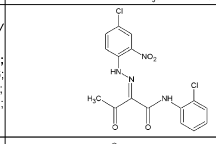
PY2 C.I. 11730, Monoazopigment, Acetoacetic arylide
Coll.: SIAR, Zurich; Laser: 785nm 0.121mW

1676m; 1609m; 1568; 1554; 1528; 1506; 1492; 1480m; 1391m; **1338s;** 1305m; 1263m; 1235; 1194; **1138s;** 1104; 1063; **954m;** 836; 812; **738m; 719m; 648m;** 620; 552; 436; 412; 379; 212; 176



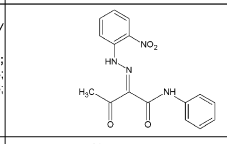
PY3 C.I. 11710, Monoazopigment, Acetoacetic arylide
Schoenfeld & Co.; Laser: 785nm 1.21mW

1673m; 1614vs; 1567m; 1546; 1495vs; 1444; 1424; 1387s; **1337vs;** 1310vs; 1276; 1244m; 1192m; **1140vs;** 1106; 1063; 1037; **958;** 916; 849; 825; 791; **746m;** 707; 676; **650s;** 622m; 542; 487; 450; 434; 412m; 395m; 371; 356; 345; 297; 272; 255; 231; 202m; 185m; 159; 136m; 111m



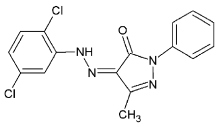
PY5 C.I. 11660, Monoazopigment, Acetoacetic arylide
Coll.: SIAR, Zurich; Laser: 785nm 0.121mW

1670m; 1608s; 1579; 1555m; 1529; **1486vs;** 1447m; 1385s; **1336s;** 1316vs; 1252s; 1220; 1194m; 1180; 1157; **1138vs;** 1080; 1066; 1043; **1000s; 952m;** 917; 865; 849; 822; 788; 770; 742; 711; 686; 663; 616; 598m; 568; 533; 513; 472; 412; 380m; 307; 281; 225; 185; 158; 125m



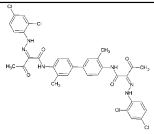
PY10 C.I. 12710, Monoazopigment, Pyrazolone
Hoechst; Laser: 785nm 0.121mW

1655m; 1590vs; 1549s; 1517m; 1490; 1457; 1437; 1405; 1371; 1336; 1286; 1261; 1243m; 1222; 1161; 1130; 1074; 1047; 1031; 1000m; 886; 794m; 725; 670; 654; 617; 578m; 485; 400; 375; 358; 328m; 287; 272; 242; 178; 156; 121



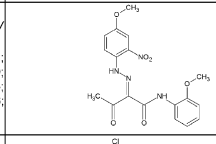
PY16 C.I. 20040, Disazopigment, Bisacetoacetarylide
Clariant; Laser: 785nm 0.121mW

1664; 1631; **1591vs;** 1548m; **1508s;** 1479; 1389s; **1313vs; 1274vs;** 1247; 1212; **1189;** 1143m; 1126; 1099; 1065; 1006; 951m; 939; 905; 886; 825; 786; 765; 746; 728; 695; 661m; 618; 592; 535; 503; 464; 443; 414; 388; 358; 342m; 290; 258; 220; 193; 164; 107



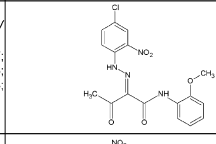
PY65 C.I. 11740, Monoazopigment, Acetoacetic arylide
Schmincke; Laser: 785nm 1.21mW

1670m; 1623s; 1600m; 1575; 1544m; 1532m; 1489vs; 1460; 1441; 1423m; 1391s; 1344m; **1326s;** 1294; 1274; 1251m; 1228s; 1189; 1170m; **1134s;** 1062; 1049; 1027; **950m;** 931; 915; 828; 793s; 775; 757; 730; 703; 687; 672; 621m; 606; 578; 558; 534; 512; 497; 479; 446; 411; 396; 376m; 340; 322; 227; 183m; 147; 111



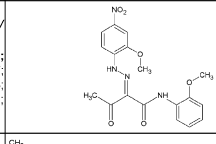
PY73 C.I. 11738, Monoazopigment, Acetoacetic arylide
Clariant; Laser: 785nm 1.21mW

1676m; 1642; **1615s; 1598s;** 1568; 1530s; 1505s; 1480s; 1437; 1391m; **1336vs;** 1306s; 1251m; 1233; 1195; 1162; **1137s;** 1105; 1063; 1044; **954s;** 917; 825; 801; **779m;** 761; **738m;** 685; **650m;** 620m; 593; 497; 440; 413m; 395; 377m; 353; 263; 230; 202; 171; 112



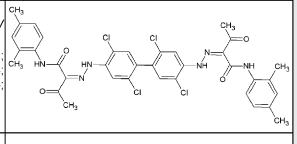
PY74 C.I. 11741, Monoazopigment, Acetoacetic arylide
Clariant; Laser: 785nm 0.121mW

1720; **1667m;** 1638; 1593s; 1549; 1507m; 1458; 1438; 1403m; **1352s; 1328vs;** 1297; 1263s; 1202; 1170; 1159m; 1125; 1116; 1088m; 1067; 1045; 1018; **952;** 916; 846; 826; 801m; 780; 741; 717; 699; 645m; 623; 600; 579; 547; 524; 496; 463; 440; 402; 359m; 317; 258; 223; 185m; 149; 109



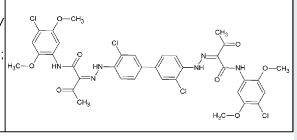
PY81 C.I. 21127, Disazopigment, Diarylide
Clariant; Laser: 785nm 0.121mW

1666; **1600vs;** 1557; 1516; 1492; 1447; **1394s;** 1301m; 1283; 1265m; 1237m; 1194; 1122; 1065; 953m; 883; 862; 786; 719m; 686m; 669; 624; 596; 565; 549; 495; 450; 434; 413; 364; 341m; 274; **242m;** 204; 173; 108



PY83 C.I. 21108, Disazopigment, Diarylide
Clariant; Laser: 785nm 0.0121mW

1660; **1596vs;** 1541; 1511; **1400s; 1334m;** 1290m; **1254s;** 1136; 1068; 1049; 955; 919; 662; 637; 538; 396; 343; **264m**



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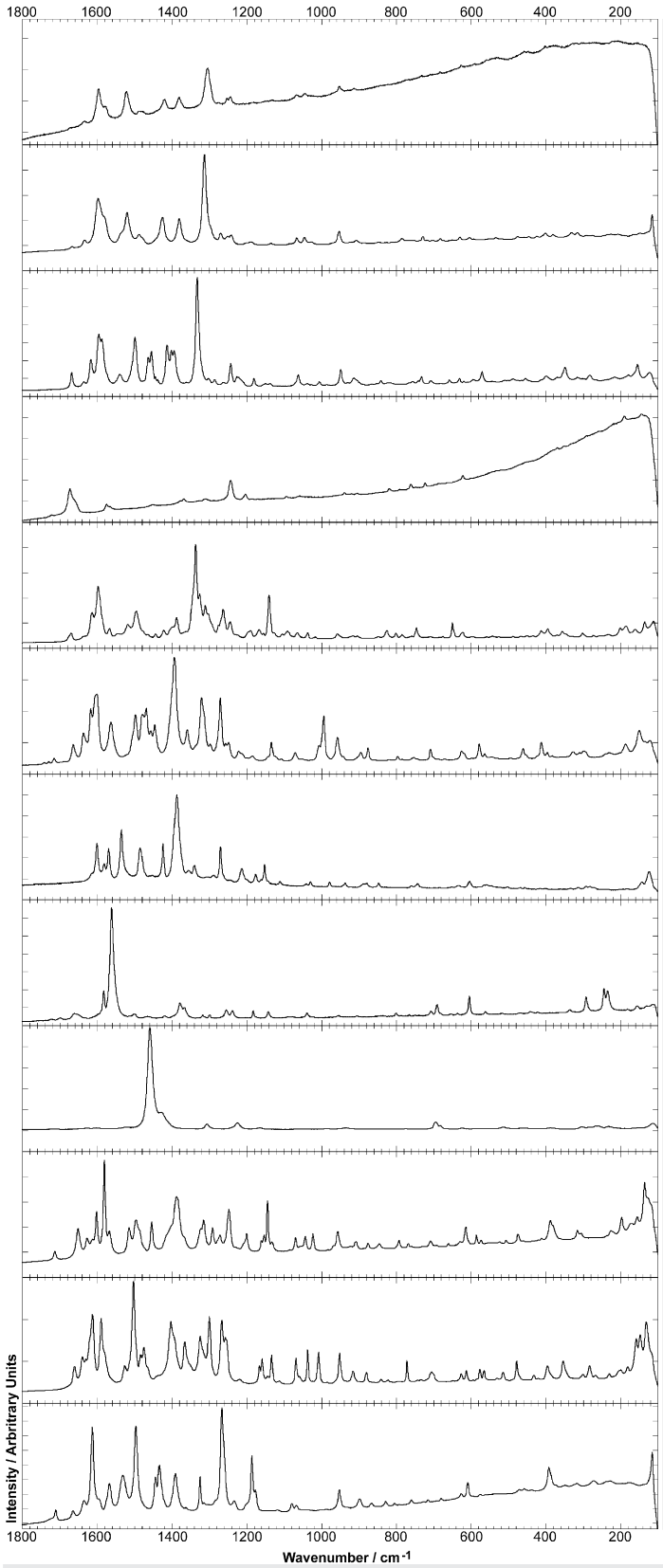
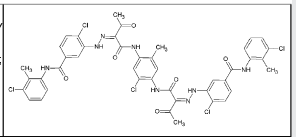


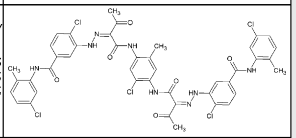
PY93 C.I. 20710, Disazopigment, Condensation
Heubach; Laser: 785nm 0.0121mW

1634; **1596s; 1521s;** 1484; 1420m; **1381m; 1305s;** 1244m; 1067w; 1045w; 952m



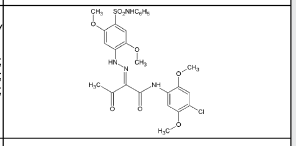
PY95 C.I. 20034, Disazopigment, Condensation
Heubach; Laser: 785nm 0.121mW

1667; 1634; **1596s; 1520s;** 1486m; 1426s; **1381s; 1313vs; 1269m;** 1241; 1189; 1135; 1066m; 1045; 1026; 953m; 907; 886; 848; 785; 754; 729; 702; 682; 650; 630; 604; 551; 533; 475; 459; 445; 424; 401; 381; 331; 315; 291; 274; 231; 206; 165; 149; 115m



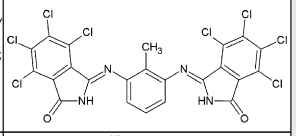
PY97 C.I. 11767, Monoazopigment, Acetoacetic arylide
Clariant; Laser: 785nm 1.21mW

1668m; 1636; 1617m; 1591s; 1539m; 1499s; 1455s; 1413s; 1394; **1332vs;** 1301; 1286; 1263; 1243m; 1222; 1180; 1137; 1062m; 1038; 1006; **949m;** 912; 841; 757; 733; 707; 658; 631; 595; 570m; 487; 454; 399; 349m; 315; 282; 216; 179; 155m; 121;



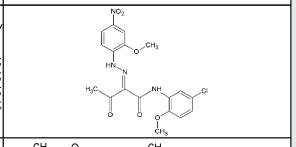
PY109 C.I. 56284, Isoindolinone, Azomethine type
Kremer; Laser: 785nm 0.0121mW

1721; **1672s;** 1575m; 1452; 1368; 1310; **1243s;** 1204m; 1094; 1060; 938; 904; 818; 791; 761; 723; 622; 370; 352; 190; 143



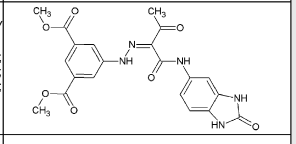
PY111 C.I. 11745, Monoazopigment, Acetoacetic arylide
Clariant; Laser: 785nm 0.121mW

1670m; 1614m; 1596s; 1567; 1546; 1519; 1495m; 1443; 1422; 1387m; **1337vs;** 1310m; 1263m; 1244; 1192; 1167; **1140s;** 1091; 1065; 1037; 1016; **957;** 917; 904; 849; 825; 801; 784; **746;** 708; 675; **649m;** 623; 596; 543; 487; 467; 449; 434; 412; 395m; 355; 301; 272; 234; 201; 185m; 161; 136m



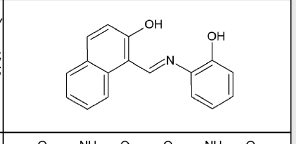
PY120 C.I. 11783, Monoazopigment, Benzimidazolone
Clariant; Laser: 785nm 1.21mW

2590; 1741; 1730; 1715; **1664m;** 1637m; 1603s; 1563s; 1498s; 1469s; 1445m; 1394vs; 1358m; 1319s; 1270s; 1248; 1220; 1184; 1134m; 1107; 1070; 994s; **957m;** 895; 876; 819; 796; 753; **708;** 671; 624; 578m; 563; 544; 494; 461; 412m; 396; 383; 327; 296; 231; 187; 150m



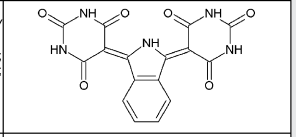
PY129 C.I. 48042, Metal complex, Azomethine metal complex
Kremer; Laser: 785nm 0.0121mW

1601s; 1581; 1569m; 1535s; 1484s; 1424s; **1387vs;** 1355; 1339; 1289; 1270s; 1213; 1176; 1152n; 1111; 1029; 978; 937; 878; 847; 742; 633; 604; 313; 293; 143; 123m



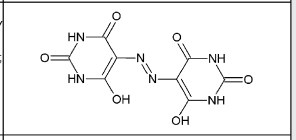
PY139 C.I. 56298, Isoindoline, Methine type
Kremer; Laser: 785nm 0.00605mW

1699; 1658; 1582m; **1561vs;** 1500; 1419; 1379m; 1366; 1317; 1299; 1255; 1238; 1182; 1142; 1039; 954; 801; 765; 707; 690; 654; 637; 604m; 561; 468; 441; 336; 292m; **245m; 234m;** 181; 156



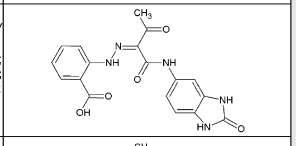
PY150 C.I. 12764, Metal complex, Azo metal complex
Kremer; Laser: 785nm 0.0121mW

1459vs; 1306m; 1224m; 1165w; 935w; **694m;** 624; 514w; 387; 305; 262; 230; 114m



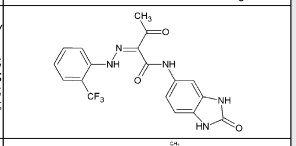
PY151 C.I. 13980, Monoazopigment, Benzimidazolone
Kremer; Laser: 785nm 1.21mW

2938; 1713; **1651m;** 1627; **1602m; 1581vs;** 1515m; 1495m; 1454m; 1387s; 1315m; 1291m; 1272; 1248s; 1200m; 1144s; 1070m; **1043m;** 1023m; **956m;** 923; 908; 875; 845; 792; 768; **708;** 660; 614m; 586; 573; 553; 524; 506; 474; 411; 387m; 315; 225; 197m; 174; 156; 130m



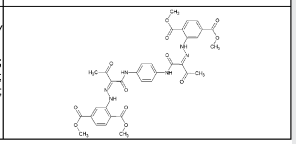
PY154 C.I. 11781, Monoazopigment, Benzimidazolone
Kremer; Laser: 785nm 1.21mW

1660m; 1640m; **1613s; 1589s;** 1527; 1503vs; 1475m; 1402s; 1365m; 1324m; 1300s; 1266s; 1219; 1159m; 1133m; 1113; 1068m; **1037m;** 1008m; 984; **951m;** 915; 880; 840; 822; 793; 771m; 734; **704;** 626; 612; 576; 565; 530; 514; 478m; 432; 395m; 353m; 301; 283; 266; 230; 202; 181; 159s; 147s; 130s



PY155 C.I. 200310, Disazopigment, Bisacetoacetarylide
Clariant; Laser: 785nm 1.21mW

1711; 1664; 1636; **1613vs;** 1567m; **1531m;** 1496vs; **1433s; 1391s;** 1325m; **1266vs;** 1233; **1186s;** 1139; 1118; 1079; 1067; 1037; 1002; 987; 952m; 898; 866; 828; 805; 792; 759; 727; 715; 680; 626; 609m; 575; 518; 472; 457; 437; **391m;** 349; 317; 272; 231; 173; 116m



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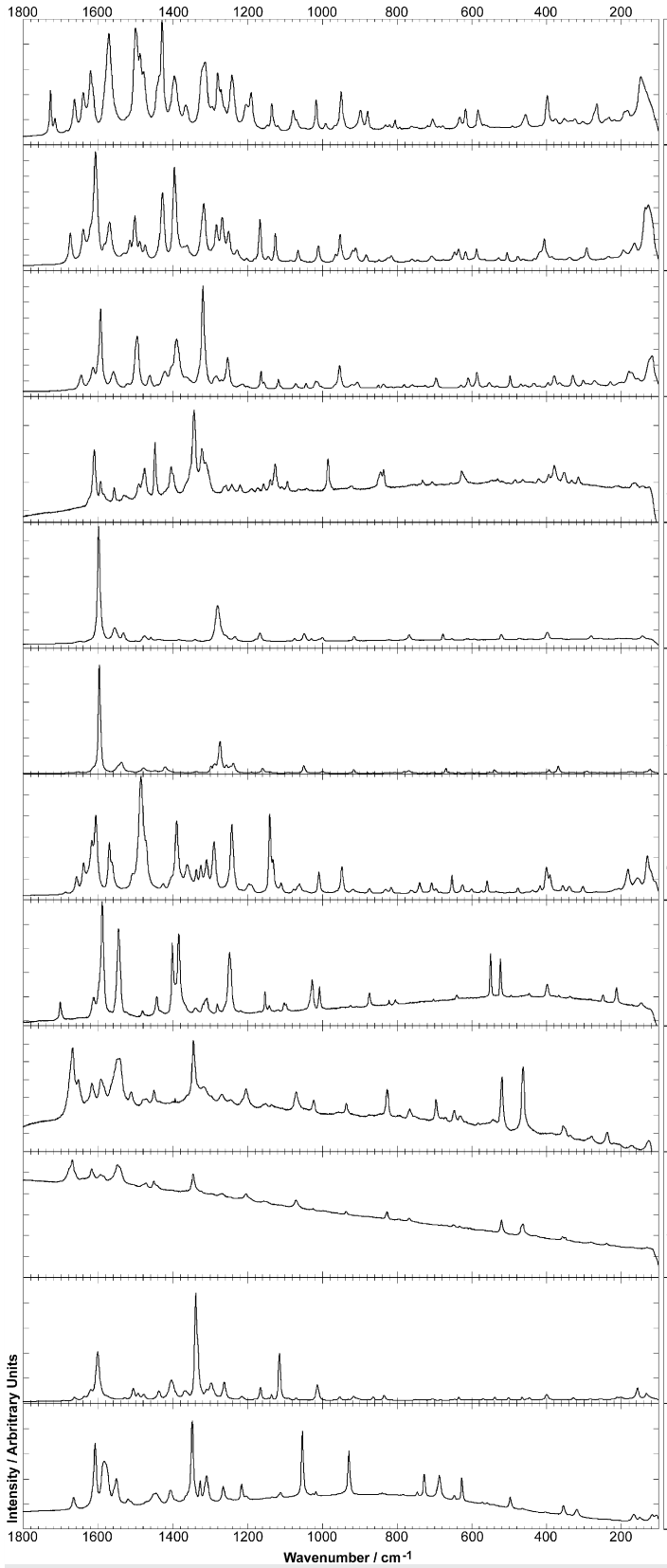
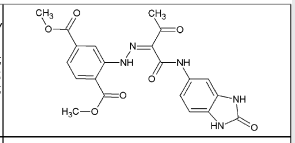


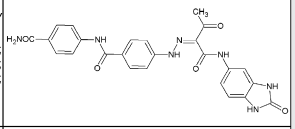
PY175 C.I. 11784, Monoazopigment, Benzimidazolone
Clariant; Laser: 785nm 0.121mW

1727s; 1715; **1663m;** 1640m; 1619s; 1571vs; 1498vs; **1429vs;** 1395m; 1364; 1317s; 1279m; 1241m; 1205; 1190m; 1135m; 1078m; 1016m; 991; **950m;** 898; 878; 831; 820; 805; 760; **705;** 677; 633; 616m; 583m; 456; 398m; 376; 352; 324; 303; 266m; 234; 188; 143s



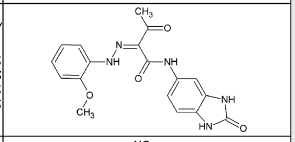
PY181 C.I. 11777, Monoazopigment, Benzimidazolone
Clariant; Laser: 785nm 1.21mW

1674m; 1640m; 1607vs; 1569m; 1502m; 1474; **1428s;** 1395vs; 1361; 1317s; 1284m; 1267m; 1250m; 1227; 1202; **1167m;** 1144; 1126m; 1065; 1010; **952m;** 911; 882; 848; 815; 760; 744; **707;** 676; 636; 616; 587; 528; 505; 477; 462; 406m; 338; 293m; 235; 194; 165; 129s



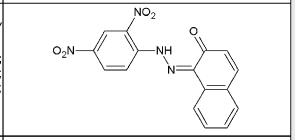
PY194 C.I. 11785, Monoazopigment, Benzimidazolone
Clariant; Laser: 785nm 1.21mW

1645m; 1614m; 1593vs; 1559; 1522; 1496s; 1462; 1422; 1389s; **1319vs;** 1285; 1253m; 1214; 1164m; 1118; 1071; **1043;** 1015; **954m;** 907; 874; 850; 836; 817; 800; 781; 760; 724; **695;** 629; 610; 586m; 553; 532; 497m; 469; 457; 434; 419; 396; 379; 364; 329m; 302; 271; 229; 176m; 154; 121m



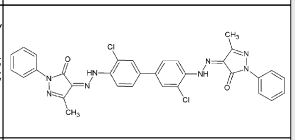
PO5 C.I. 12075, Monoazopigment, B-Naphthol
Clariant; Laser: 785nm 0.0121mW

1610s; 1593; 1557; 1530; 1476m; **1447s;** 1404m; **1343vs; 1321s;** 1260; 1242; 1220; 1190; 1173; 1157; 1126m; 1093; 1042; **985s;** 922; 836m; 732; 706; 626m; 531; 484; 463; 421; 395; 379m; 352; 332; 314; 209; 166



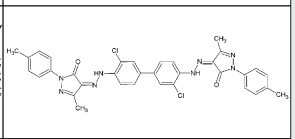
PO13 C.I. 21110, Disazopigment, Pyrazolone
Clariant; Laser: 785nm 0.0121mW

1598vs; 1555m; 1532; 1476; 1459; 1437; 1384; 1340; **1280s;** 1234; 1167m; 1074; 1048; 1029; 1000; 914; 767m; 677; 653; 612; **521;** 473; 398m; 281; 256; 141



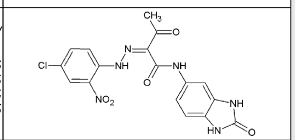
PO34 C.I. 21115, Disazopigment, Pyrazolone
Clariant; Laser: 785nm 0.0121mW

1653; **1597vs;** 1538m; 1478; 1446; 1420; 1374; 1337; 1298; 1289; **1273s;** 1257; 1238; 1189; 1160; 1138; 1091; 1049m; 1000; 916; 805; 781; 768; 706; 669; 636; 602; 587; 553; 539; 446; 429; 393; **369m;** 331; 292; 272; 253; 175; 123



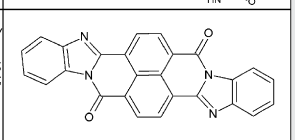
PO36 C.I. 11780, Monoazopigment, Benzimidazolone
Heubach; Laser: 785nm 1.21mW

1687; 1657; 1639m; **1617s;** 1606s; 1570s; 1485vs; 1426; **1390s;** 1361m; 1337; 1325; 1309m; 1290s; **1242s;** 1193; **1140s;** 1110; 1077; 1061; **1009m; 948m;** 917; 874; 830; 816; 762; 740; 707; 695; 683; 653m; 625; 600; 574; 559; 535; 476; 437; 418; 401m; 390; 356; 339; 302; 267; 207; 182m; 156; 129m



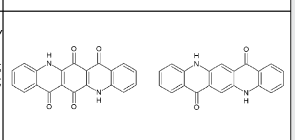
PO43 C.I. 71105, Polycyclic pigment, Perinone
Clariant; Laser: 785nm 0.121mW

1701m; 1612; 1588vs; **1545vs;** 1481; 1442m; **1401s; 1384vs;** 1339; 1310; 1281; **1248s;** 1153m; 1118; 1102; 1027m; 1007m; 924; 873; 822; 805; 702; 640; **550s;** 523s; 446; 398; 367; 338; 283; 249; **212m**



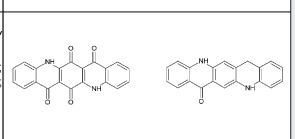
PO48 C.I. 73900, Polycyclic pigment, Quinacridone
Kremer; Laser: 785nm 0.121mW

1669vs; 1616m; 1592m; **1546s;** 1511; 1478; 1450; 1344vs; 1268; 1204m; 1151; **1070m;** 1023; 987; 936; **826m;** 789; 766; **695m;** 646; 589; 583; **519s; 463vs;** 387; 353; 280; **238m;** 172; 125



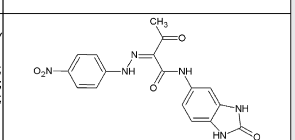
PO49 C.I. 564800, Polycyclic pigment, Quinacridone
Kremer; Laser: 633nm 1.03mW

1669s; 1617m; 1590; **1545s;** 1473; 1450; 1345s; 1294; 1268; 1204; 1153; **1070m;** 1025; 936; **827m;** 795; 767; 648; 632; **520m; 465m;** 356; 280; **239m**



PO62 C.I. 11775, Monoazopigment, Benzimidazolone
Heubach; Laser: 785nm 0.0605mW

1692; 1663; **1601s;** 1528; 1506; 1492; 1478; 1437; 1403m; 1367; **1338vs;** 1297; 1262m; 1215; 1166; 1136; 1115s; 1070; **1013m; 953;** 915; 864; 834; 750; 735; 705; 684; 635; 590; 569; 538; 501; 466; 446; 399; 328; 305; 283; 256; 211; 200; 157m; 132



PO73 C.I. 561170, Polycyclic p., Diketopyrrolo-Pyrrole (DPP)
Kremer; Laser: 785nm 0.121mW

1665m; 1608vs; 1582s; **1551m;** 1519; 1447; 1406; 1348vs; 1327; 1309m; 1265; 1216; 1134; 1112; **1053vs;** 1017; **929s;** 839; 783; 746; **727m; 687m;** 647; **626m;** 571; 559; 497; 463; 403; 354; 319; 241; 166; 150; 118

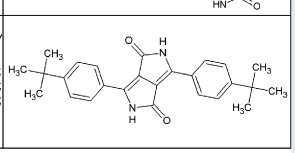
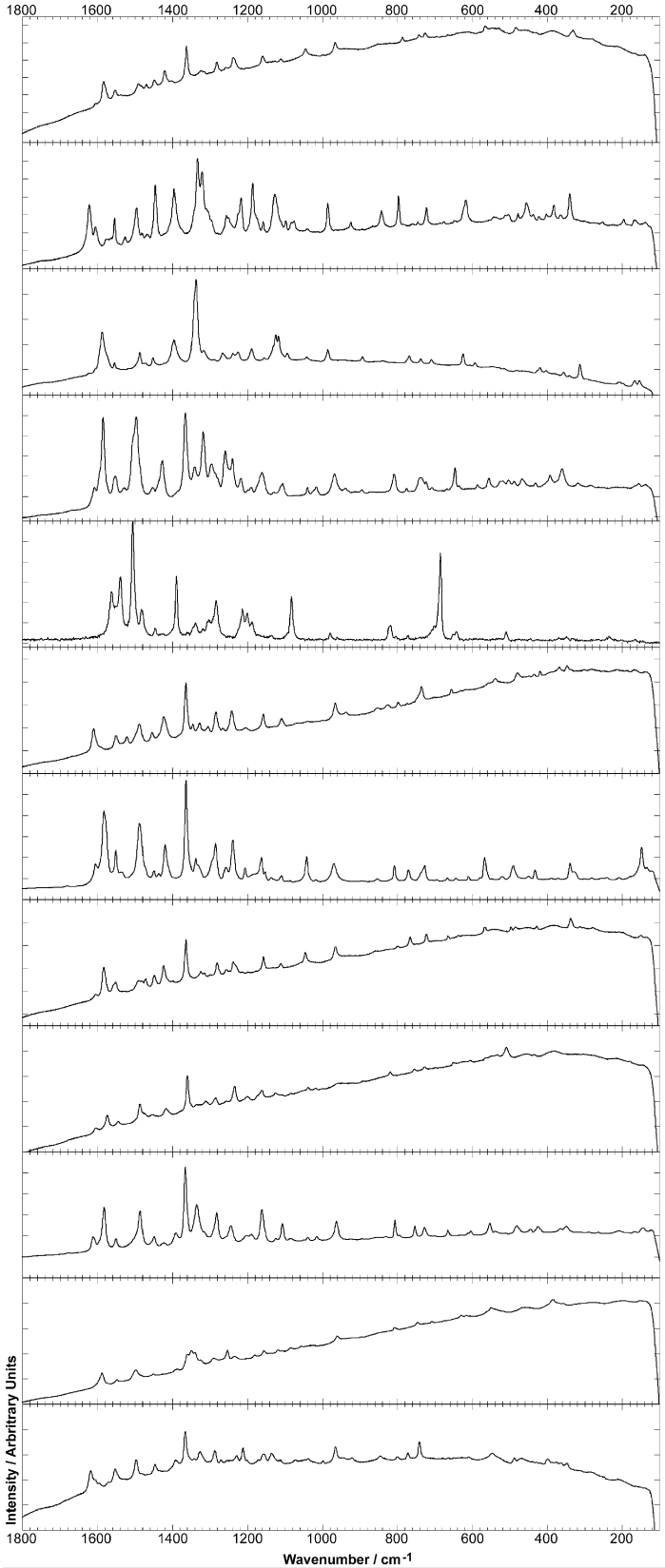
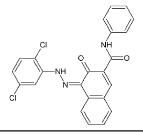


Table 3 (*Continued*)



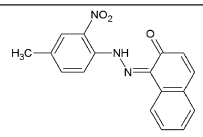
PR2 C.I. 12310, Monoazopigment, Naphthol AS
Coll.: SIAR, Zurich; Laser: 785nm 0.0121mW

1583s; **1553m; 1491m;** 1470; 1448; **1421m; 1362vs;** 1323; **1281m;** 1236m; **1159m;** 1111; 1045m; 966m; **786m;** 742; 725; 566; 484; 385; 332



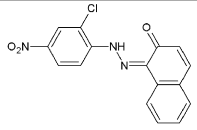
PR3 C.I. 12120, Monoazopigment, B-Naphthol
Clariant; Laser: 785nm 0.121mW

1621s; 1554m; 1526; 1496m; 1470; 1445vs; 1395s; **1333vs;** 1256; **1217s;** 1186s; 1127; 1076; 1057; 1040; 985s; 924; 842m; 797s; 759; 723m; 676; **617m;** 542; 504; 455m; 383m; 340s; 253; 225; 196; 166



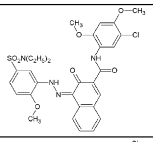
PR4 C.I. 12085, Monoazopigment, B-Naphthol
Hoechst; Laser: 785nm 0.121mW

1587s; 1554; 1487m; 1451; 1396m; **1338vs;** 1288; 1266; 1239; **1224;** 1189; 1156; 1124m; 1093; 1041; 986m; 942; 893; 838; 769; 737; 709; 654; **624m;** 593; 514; 466; 420; 403; 356; 340; 313m; 208; 167



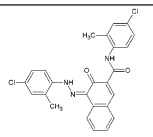
PR5 C.I. 12490, Monoazopigment, Naphthol AS
Heubach; Laser: 785nm 0.121mW

1585vs; **1553m;** 1530; **1498vs;** 1453; **1427m; 1365vs;** 1341m; Pigment Red **1295m;** 1259s; 1239m; 1217; 1190; **1161m;** 1107; 1040; 1016; 967m; 938; 894; 809m; 775; 737; 707; **646m;** 586; 556; 523; 503; 487; 467; 431; 393m; 360m; 318; 283; 215; 157



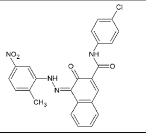
PR7 C.I. 12420, Monoazopigment, Naphthol AS
Kremer; Laser: 785nm 0.0121mW

1601m; 1574s; **1550m; 1481vs;** 1409; **1361vs;** 1329; 1310; **1278s;** 1239s; 1202; **1161s; 1122m;** 1089; 1039; 964m; 842; 760; 728m; 669; 604m; 554m; **497m;** 443; 407; 379; 302



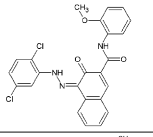
PR8 C.I. 12335, Monoazopigment, Naphthol AS
Schoenfeld & Co.; Laser: 785nm 0.0121mW

1610m; **1550m;** 1521; **1488m;** 1454; **1423m; 1364vs;** 1345; 1327; 1304; **1284m;** 1265; 1241m; 1205; **1158m;** 1109; 965m; 937; 854; 826; 798; 736m; 655; **539m;** 480; 435; 419; 368; 347; 283; 214; 166



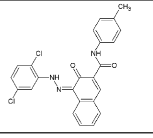
PR9 C.I. 12460, Monoazopigment, Naphthol AS
Kremer; Laser: 785nm 0.121mW

1681; 1605; 1580vs; **1551m;** 1533; **1487s;** 1449; 1437; **1419m; 1363vs;** 1337m; **1285m;** 1258; 1238m; 1206; **1163m;** 1136; 1109; 1086; **1042s;** 1017; 969m; 894; 854; 808m; 770m; 728m; 695; 666; 644; 610; **567s;** 520; 491m; 450; 433; 389; 372; 339m; 301; 282; 255; 240; 209; **148s**



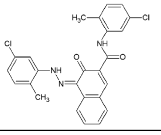
PR10 C.I. 12440, Monoazopigment, Naphthol AS
Coll.: SIAR, Zurich; Laser: 785nm 0.00605mW

1605; 1583s; **1553m; 1491m;** 1471; 1448m; **1423s; 1364vs;** 1325; 1314; **1280m;** 1257; 1236m; **1157m;** 1111; 1045m; 965m; 799; **766m; 722m;** 665; 567; 497; 485; 428; 338m; 278; 157



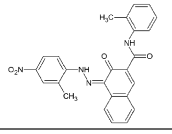
PR11 C.I. 12430, Monoazopigment, Naphthol AS
Hoechst; Laser: 785nm 0.0121mW

1605; 1573m; **1545m; 1486m;** 1453; 1417; **1359vs;** 1311; **1285m;** 1234m; 1200; **1162m;** 1125; 1038; 1018; 819; 754; 727; 650; 605; 533; **509m;** 435; 386



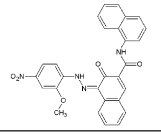
PR12 C.I. 12385, Monoazopigment, Naphthol AS
Schoenfeld & Co.; Laser: 785nm 0.121mW

1677; 1611; 1582s; **1550m; 1486s;** 1448; 1423; 1391; **1365vs; 1335s; 1282s;** 1244m; 1204; 1188; **1161s;** 1125; **1106m;** 1084; 1039; 1015; 962m; 923; 894; 856; 830; 806m; 753; 727; 700; 665; 604; 554m; 537; 512; **481m; 445**; 425; 365; 349; 317; 289; 264; 210; 167; 145



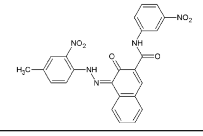
PR16 C.I. 12500, Monoazopigment, Naphthol AS
Hoechst; Laser: 785nm 0.0121mW

1588m; **1548m; 1498m;** 1451; 1389; **1359s; 1349vs; 1340s; 1290m;** 1253m; 1234; 1180; **1156m;** 1141; 1118; 1106; 1085; 1057; 1027; 960m; 807; 746; 707; 629; 615; 549m; 464; 385m; 356; 281



PR18 C.I. 12350, Monoazopigment, Naphthol AS
Imperial Chem. Indust. LDT. UK; Laser: 785nm 0.0605mW

1618m; 1553m; 1497m; 1446; 1391; **1365vs;** 1342; 1326; **1287m;** 1270; 1255; 1229; **1211m; 1157m;** 1134; 1112; 1073; 1038; 998; 965m; 943; 920; 846; 800; **772m;** 741m; 680; 664; 630; 609; 546; 488; 467; 429; 418; 399; 375; 363; 348; 280



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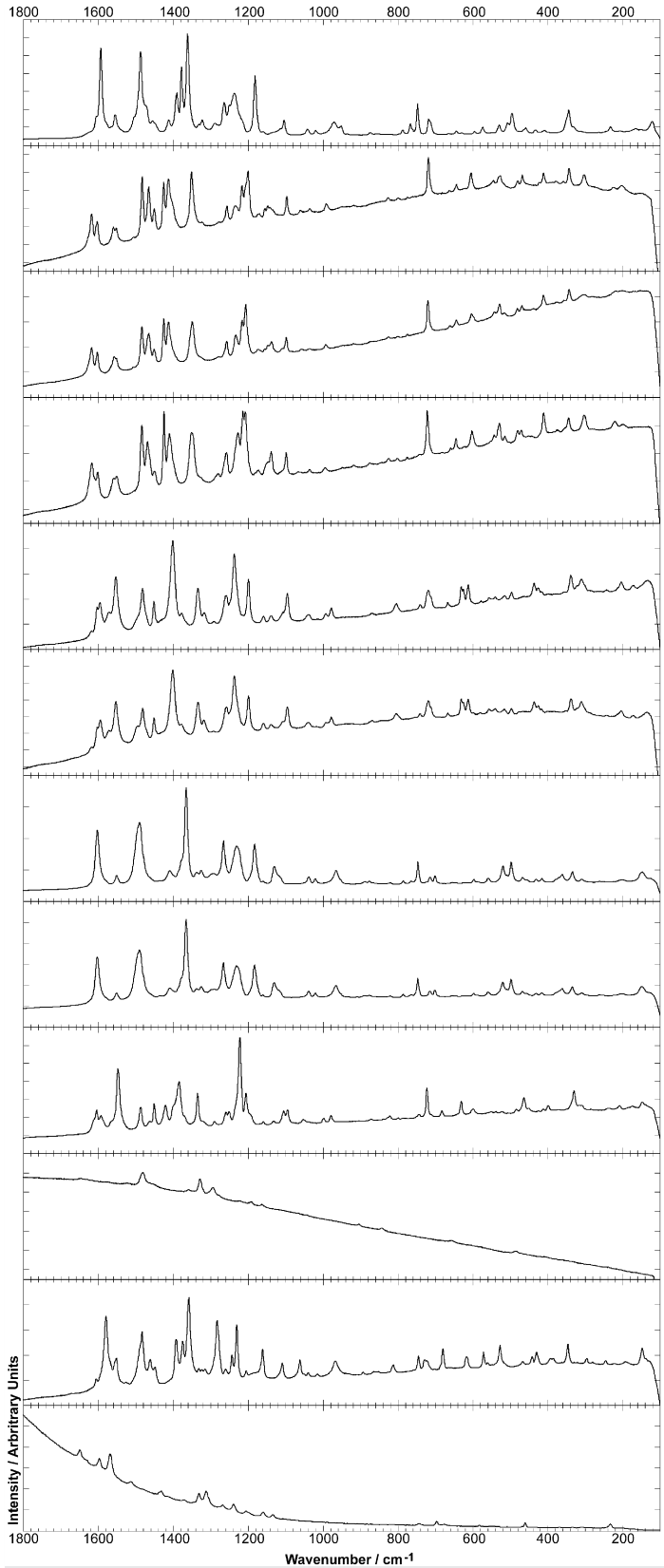


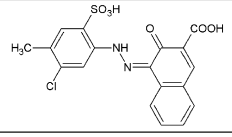
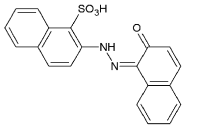
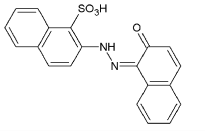
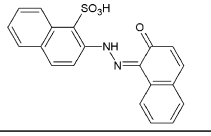
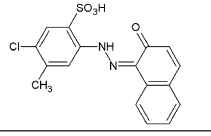
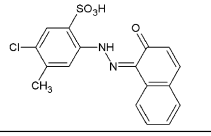
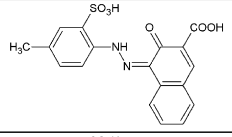
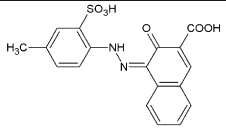
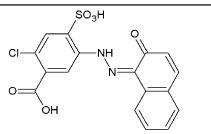
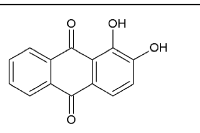
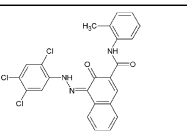
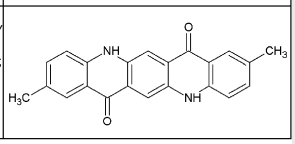
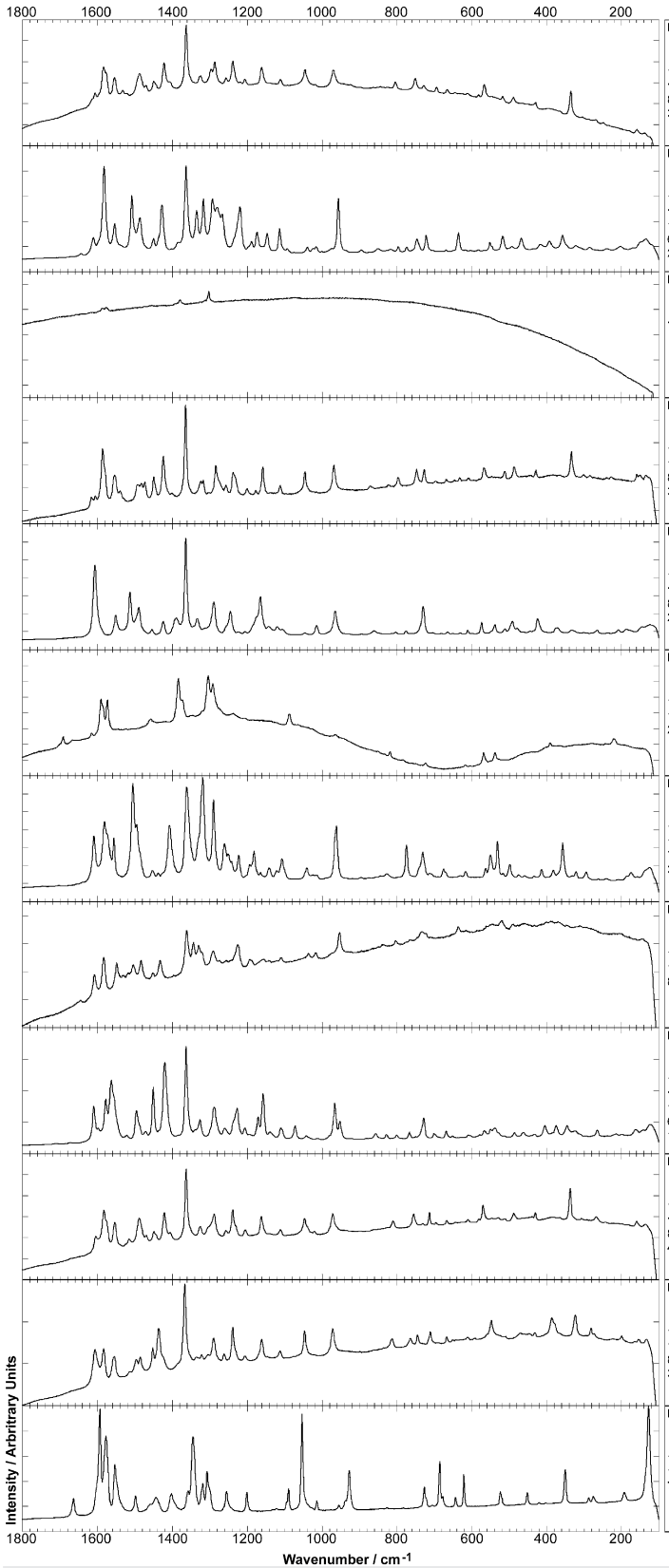
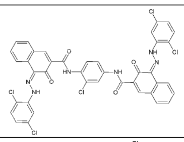
PR48:3 C.I. 15865:3, Monoazopigment, BON lake *Heubach; Laser: 785nm 0.121mW* 1593vs; 1555m; 1487vs; 1452; 1412; **1391s; 1378vs;** 1361vs; 1322; 1289; 1264m; 1236m; **1181s;** 1104m; 1041; 1019; 971m; 952; 873; 787; 767; **747m;** 716m; 664; 644; 629; 596; 573; 530; 495m; 459; 433; 409; 344m; 232; 206; 166; 121	
PR49 C.I. 15630, Monoazopigment, B-Naphthol *Coll.: SIAR, Zurich; Laser: 785nm 0.121mW* 1618s; 1603m; 1560m; 1551m; 1483vs; 1465vs; 1450m; 1426vs; 1412vs; **1351vs;** 1323; 1257m; 1235; 1216s; **1200vs;** 1172; 1156; 1148; 1097m; 1060; 1035; 991; 918; 826; 800; 775; 719s; 662; 644; **605m;** 545; 528; 480; 468; 411; 377; 359; 343m; **303m;** 225; 201	
PR49:1 C.I. 15630:1, Monoazopigment, B-Naphthol lake *Coll.: TU Dresden; Laser: 785nm 0.121mW* 1618m; 1603m; 1556m; 1483vs; 1466s; 1450m; 1425vs; 1412vs; **1349s;** 1258m; 1233m; 1216s; **1206vs;** 1173; 1136; 1098m; 1057; 1036; 992; 826; 775; 720s; 661; 644; **603m;** 529m; 515; 481; 469; 411m; 343m; **305**	
PR49:2 C.I. 15630:2, Monoazopigment, B-Naphthol lake *Coll.: TU Dresden; Laser: 785nm 0.121mW* 1617m; 1601m; 1560m; 1550m; 1484vs; 1468s; 1449; 1424vs; 1409s; **1350s;** 1281; 1258m; 1228s; 1215vs; **1207vs;** 1173; 1138m; 1098m; 1067; 1036; 994; 918; 875; 825; 801; 776; 722s; 659; 645; **602m;** 543; 529m; 515; 480; 470; 411m; 375; 344m; **302m;** 221; 198	
PR53 C.I. 15585, Monoazopigment, B-Naphthol *Coll.: SIAR, Zurich; Laser: 785nm 0.0121mW* 1604; 1594m; 1573; 1553vs; 1482s; 1451m; 1401vs; 1376; **1334s;** 1316; 1291; 1260; **1236vs;** 1199s; 1159; 1138; 1095m; 1039; 993; 977; 869; 805; 740; 719m; 667; 631m; **612m;** 578; 557; 540; 516; 497; 436m; 425; 338m; 310; 242; 203; 172; 134	
PR53:1 C.I. 15585:1, Monoazopigment, B-Naphthol lake *Coll.: TU Dresden; Laser: 785nm 0.0605mW* 1594m; 1573; 1553s; **1497m;** 1481s; 1451m; 1401vs; 1377; **1334s;** 1317; 1293; 1259; **1236vs;** 1199s; 1159; 1138; 1095m; 1040; 977; 869; 804; 740; 719m; 667; 631m; **612m;** 579; 557; 540; 516; 497; 436m; 425; 338m; 310m; 244; 204; 172; 135	
PR57 C.I. 15850, Monoazopigment, BON lake *Coll.: SIAR, Zurich; Laser: 785nm 0.121mW* 1603s; 1551; 1491s; 1410; 1365vs; 1338; 1324; 1295; 1265s; 1229s; **1182s;** 1129m; 1038; 1020; 965m; 889; 876; 820; 786; 765; **746m;** 714; 701; 654; 597; 559; 520m; 497m; 467; 431; 415; 362m; 334m; 308; 261; 202; 148m	
PR57:1 C.I. 15858:1, Monoazopigment, BON lake *Clariant; Laser: 785nm 0.121mW* 1603s; 1551; 1492s; 1436; 1409; 1365vs; 1339; 1324; 1296; 1266s; 1229s; **1182s;** 1130m 1039; 1020; 965m; 932; 890; 876; 821; 786; 765; **746m;** 714; 701; 654; 623; 598; 559; 520m; 498m; 467; 431; 416; 362m; 334m; 308; 261; 202; 148m	
PR68 C.I. 15525, Monoazopigment, B-Naphthol *Hoechst; Laser: 785nm 0.121mW* 1605m; 1592; 1547s; 1487m; 1450m; 1421m; 1385s; **1335m;** 1289; 1259; **1222vs**(tw); 1205m; 1159; 1132; 1105m; 1094m; 1052; 998; 979; 872; 822; 799; 744; 722m; 682; **631m;** 599; 553; 538; 522; 484; 463m; 412; 398; 330m; 308; 238; 208; 174; 147	
PR83:1 C.I. 58000:1, Polycarbocyclic Anthraquinone *Kremer; Laser: 633nm 0.103mW* 1646; 1522; **1481s;** 1358m; **1328vs; 1294s;** 1221m; 1191m; 1163m; **904m;** 843m; 655m; 484m	
PR112 C.I. 12370, Monoazopigment, Naphthol AS *Heubach; Laser: 785nm 0.0121mW* 1579vs; **1552m;** 1526; **1484s;** 1461m; 1448; **1392m; 1375m; 1358vs;** 1332; 1314; **1282s;** 1260; 1243; 1230s; 1205; **1161m;** 1109m; 1061m; 1039; 1015; 967m; 893; 865; 813; 745; 725; 680m; 616; 571; 527m; 467; 442; 429; 389; 346m; 296; 280; 245; 222; 191; 148m	
PR122 C.I. 73915, Polycyclic pigment, Quinacridone *Kremer; Laser: 514nm 0.114mW* **1649s; 1597s; 1568vs;** 1512; 1432; 1370; **1331m;** 1311s; 1267; 1238m; 1204; **1160m;** 1133; 818; 743; 696; 676; 582; 460m; 309; 233m	

Table 3 (*Continued*)



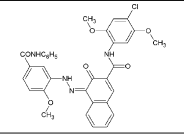
PR144 C.I. 20735, Disazopigment, Condensation
Kremer; Laser: 785nm 0.0605mW

1606; 1581s; **1554m;** 1532; **1487s;** 1448; **1421m; 1362vs;** 1325; **1286m;** 1257; 1238m; 1206; **1161m;** 1110; 1045m; 969m; 923; 844; 824; 804; 751m; 728; 694; 665; 644; 610; 582; 566m; 517; 489; 429; 386; **336s;** 304; 268; 248; 158



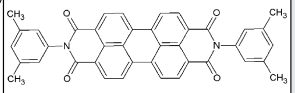
PR146 C.I. 12485, Monoazopigment, Naphthol AS
Clariant; Laser: 785nm 0.121mW

1877; 1643; 1611; 1582vs; **1554m; 1508s; 1486m;** 1450; **1427s; 1363vs;** 1335m; **1316s; 1293s;** 1265m; **1219m;** 1188; **1173m;** 1146m; 1113m; 1092; 1039; 1015; 956s; 895; 851; 817; 796; 774; 746; 722m; 668; 636m; 603; 582; 551; 517m; 493; 467; 417; 392; 357m; 321; 285; 239; 203; 134m



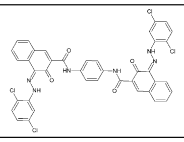
PR149 C.I. 71137, Polycyclic pigment, Perylene & Perinone
Clariant; Laser: 633nm 0.515mW

1585s; 1577s; 1379s; 1302vs



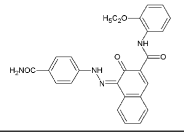
PR166 C.I. 20730, Disazopigment, Condensation
Heubach Laser: 785nm 0.00605mW

1605; 1585s; **1553m; 1492m; 1482m;1472m;** 1449m; 1423s; **1364vs;** 1317; 1283m; 1256; 1235m; 1200; 1177; **1158m;** 1111; 1045m; 968m; 871; 821; 796; 747m; 727m; 667; 632; 609; 567m; 512; 487; 429; 386; **334m;** 301; 226; 159 301; 226; 159



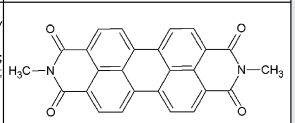
PR170 C.I. 12475, Monoazopigment, Naphthol AS
Kremer; Laser: 785nm 0.121mW

1606vs; **1551m; 1513s; 1489m;** 1453; 1424; 1390; **1363vs;** 1333; **1289s;** 1245m; 1206; **1165s;** 1141; 1119; 1046; 1014; 964m; 893; 861; 803; 775; 730m; 664; 631; 610; 573; 538; 492m; **423m;** 372; 332; 300; 265; 237; 208; 186; 121



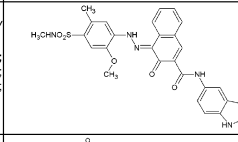
PR179 C.I. 71130, Polycyclic pigment, Perylene & Perinone
Kremer; Laser: 785nm 0.00605mW

1692; 1667; 1615; **1590s;** 1573s; 1458; **1384vs;** 1346; **1304vs; 1291s;** 1237; 1205; 1136; 1087m; 963; 818; 723; 617; **568m;** 538m; 457; 390; 279; 220



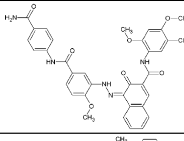
PR185 C.I. 12516, Monoazopigment, Benzimidazolone
Clariant; Laser: 785nm 0.121mW

1609s; 1580s; 1556m; 1505vs; 1452; 1406s; **1360vs; 1319vs; 1289vs;** 1260m; 1222; **1181m;** 1141; 1107m; 1040; 1014; **962s;** 896; 827; 774m; 731m; 675; 616; 550m; 531m; 498; 474; 458; 433; 413; 382; 357m; 322; 295; 239; 175; 125



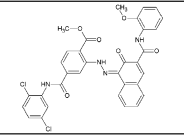
PR187 C.I. 12486, Monoazopigment, Naphthol AS
Clariant; Laser: 785nm 0.0605mW

1646; 1608m; 1583vs; **1548s; 1504m; 1483m;** 1451; 1432m; **1361vs;** 1343s; 1328s; **1291m; 1224s;** 1191; **1158m;** 1109; 1037; 1016; 953s; 837; 803; 733; 636; 546; 520; 491; 460; 366; 202



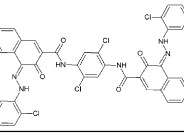
PR188 C.I. 12467, Monoazopigment, Naphthol AS
Clariant; Laser: 785nm 0.121mW

1711; 1672; 1609m; 1578s; **1562s;** 1521; **1495m;** 1471; 1450s; **1419vs; 1363vs;** 1326; **1288m;** 1259; 1227m; 1206; **1157s;** 1137; 1109; 1072; 1041; 1011; 965s; 857; 827; 800; 766; 729m; 700; 668; 606; 566; 538m; 486; 462; 432; 404m; 375m; 346; 323; 265; 216; 199; 162; 121



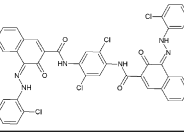
PR214 C.I. 200660, Disazopigment, Condensation
Clariant; Laser: 785nm 0.0605mW

1604; 1582s; **1553m;** 1515; **1487m;** 1448; **1421m; 1362vs;** 1325; **1288m;** 1257; 1238m; 1205; **1161m;** 1111; 1046m; 1020; 971m; 898; 863; 810; 755m; 731; **713m;** 695; 666; 644; 610; 569m; 546; 529; 511; 488; 430; 388; 364; **337s;** 306; 266; 243; 181; 159; 134



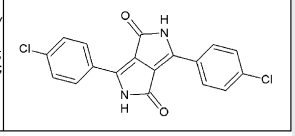
PR242 C.I. 20067, Disazopigment, Condensation
Clariant; Laser: 785nm 0.0605mW

1606m; 1583m; **1556m;** 1496; 1485; 1452; **1436s; 1366vs;** 1336; 1321; **1289m;** 1261; 1238s; 1205; **1160m;** 1111; 1046m; 971m; 898; 813; 764; 744; 711; 666; 651; 643; 610; 592; 547m; 509; 471; 446; 431; **385m; 324m;** 281; 224; 200; 153; 133



PR254 C.I. 56110, Polycyclic p., Diketopyrrolo-Pyrrole (DPP)
Kremer; Laser: 785nm 0.00605mW

1664m; 1593vs; 1576vs; 1553s; 1498m; 1443m; 1402m; 1344vs; 1319m; 1306s; 1255m; 1200m; 1089m; **1053vs;** 1013; 955; **927s; 727m;** 685s; 643; 621m; **523m;** 451; 420; **350s;** 288; 275; 192; 127vs



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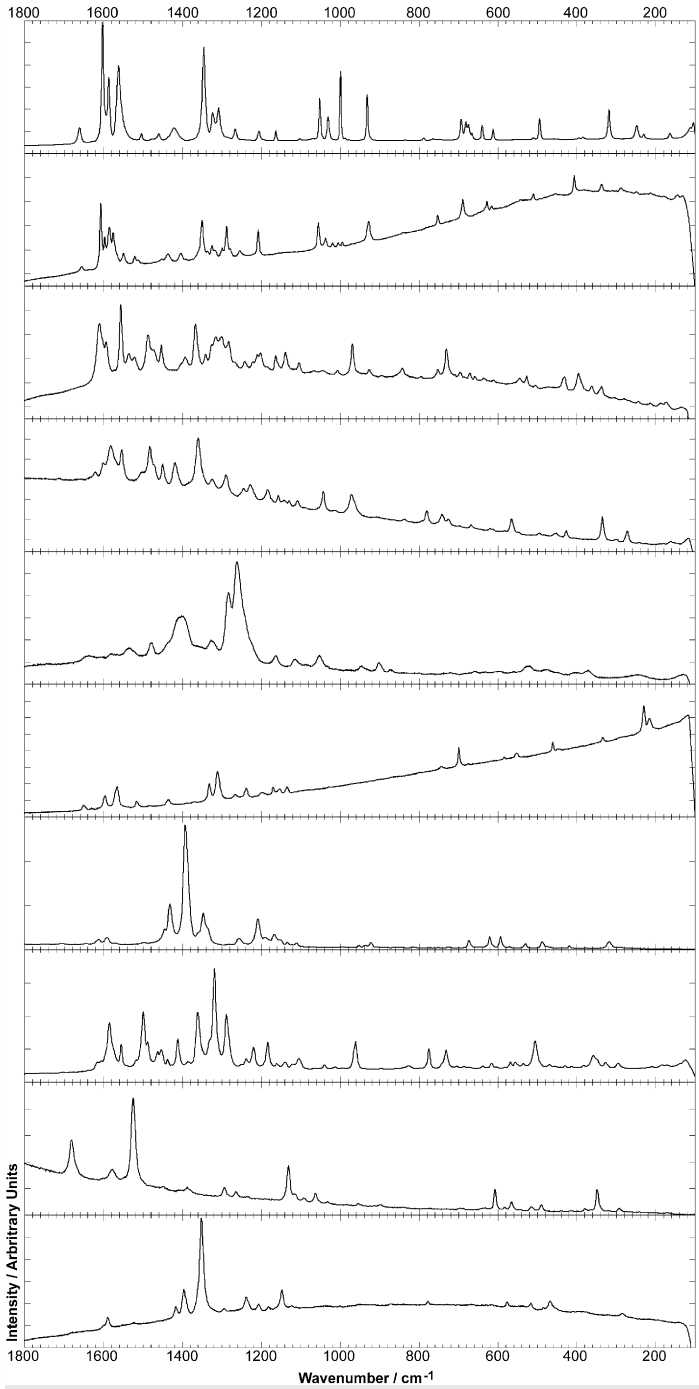
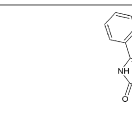


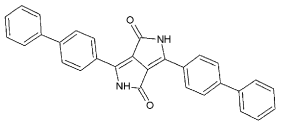
PR255 C.I. 561050, Polycyclic p., Diketopyrrolo-Pyrrole (DPP)
Kremer; Laser: 785nm 0.121mW

3060; 1660m; 1602vs; 1586s; 1562s; 1503; 1460; 1421m; 1346vs; 1323m; 1308m; 1265; 1206; 1163; 1102; **1051s;** 1030m; **999s; 931s;** 834; 788; 764; 693m; 681m; 640; 612; 494m; 457; 385; **318s;** 248; 230; 164; 107



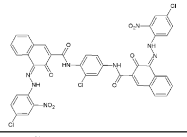
PR264 C.I. 561300, Polycyclic p., Diketopyrrolo-Pyrrole (DPP)
Kremer; Laser: 785nm 0.00605mW

1655; 1607vs; 1584vs; 1575s; 1549; 1521; 1437; 1404; 1350vs; 1325; **1288s;** 1255; 1208s; **1055s;** 1037; 1019; 1005; 994; 928s; 752m; 689s; 628m; 615; 510; 455; **406s;** 337m; 288; 249; 212; 145; 131



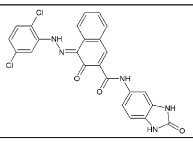
PBr23 C.I. 20060, Disazopigment, Condensation
Kremer; Laser: 785nm 0.0605mW

1610vs; 1556vs; 1536m; 1520m; **1487s;** 1453m; 1393; **1366s;** 1341; 1317s; 1300s; 1282m; 1242; 1205; 1163; 1138m; 1104; 1067; 1043; 1007; 969s; 926; 895; 842m; 795; 752; 730s; 696; 671; 635; 611; 545; 527; 504; 472; 432m; 395m; 362; 337; 302; 278; 244; 213; 188; 173



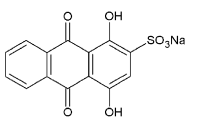
PBr25 C.I. 12510, Monoazopigment, Benzimidazolone
Clariant; Laser: 633nm 1.03mW

1621; **1582s; 1553s; 1482s;** 1449m; 1418m; **1359vs;** 1324; 1289m; 1245; 1226; 1183; 1157; 1129; 1108; 1043m; 970m; 837; 780m; 741; 725; 668; 619; 565m; 453; 426; 335m; 272; 162; 116



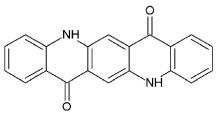
PV5 C.I. 58055, Polycyclic p., Polycarbocyclic Anthraquinone
Kremer; Laser: 785nm 0.605mW

1641; 1581; 1534; 1479m; **1403s;** 1325m; **1284s; 1260vs;** 1163; 1114; 1052m; 946; **901m;** 871; 721; 659; 597; 524m; 474; 406; 371; 243



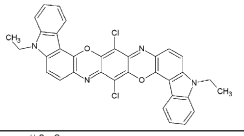
PV19 C.I. 73900, Polycyclic pigment, Quinacridone
Kremer; Laser: 633nm 0.103mW

1650; 1596m; **1566s;** 1516; 1483; 1435; 1369; 1332m; **1310s;** 1266; 1238m; 1198; 1170; 1153; 1134; 743; **699s;** 584; 553; **461m;** 334; **230s;** 215m



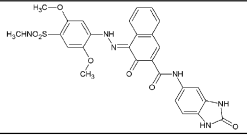
PV23 C.I. 51319, Polycyclic pigment, Dioxazine
Heubach; Laser: 514nm 0.114mW

2819; 2776m; 2733; 2641; 2598m; 2554; 1613; 1591; 1431m; **1391vs; 1347s;** 1256; 1208m; 1167; 922; 673; **621m; 593m;** 530; 487; 317



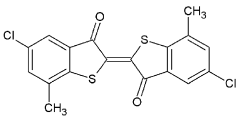
PV32 C.I. 12517, Monoazopigment, Benzimidazolone
Clariant; Laser: 785nm 0.121mW

1585s; 1555m; **1499s;** 1453; 1437; 1411m; 1386; 1361s; 1318vs; 1288s; 1238; 1219m; 1184m; 1161; 1139; 1104; 1040; 1013; 994; **961m;** 896; 826; **775m; 731m;** 703; 686; 638; 616; 568; 555; 535; **505m;** 469; 430; 413; 383; 357m; 327; 295; 209; 185; 170; 124



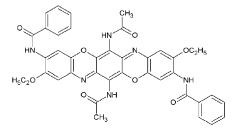
PV36 C.I. 73385, Polycyclic pigment, Indigoide
Bayer; Laser: 514nm 0.114mW

1680s; 1577m; **1524vs;** 1388; 1293; 1263; **1131s;** 1063; **607m;** 565; 515; 489; **348m;** 292



PV37 C.I. 51345, Polycyclic pigment, Dioxazine
Kremer; Laser: 785nm 0.121mW

1589m; 1416; **1396s; 1351vs;** 1294; 1237m; 1207; 1182; **1147m;** 777; 576; 517; 467m; 284



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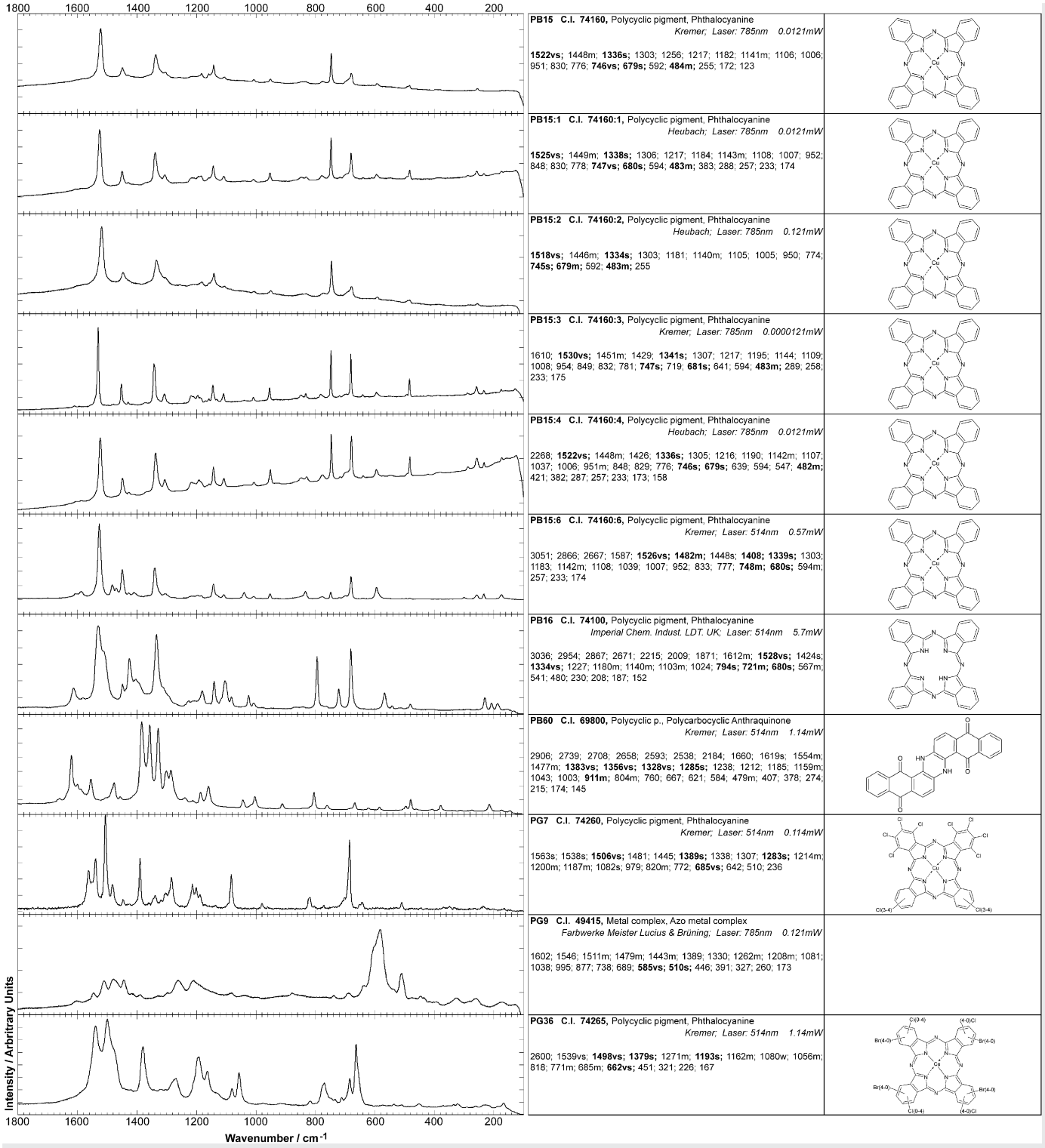


PB15 C.I. 74160, Polycyclic pigment, Phthalocyanine
Kremer; Laser: 785nm 0.0121mW
1522vs; 1448m; **1336s;** 1303; 1256; 1217; 1182; 1141m; 1106; 1006; 951; 830; 776; **746vs; 679s;** 592; **484m;** 255; 172; 123

PB15:1 C.I. 74160:1, Polycyclic pigment, Phthalocyanine
Heubach; Laser: 785nm 0.0121mW
1525vs; 1449m; **1338s;** 1306; 1217; 1184; 1143m; 1108; 1007; 952; 848; 830; 778; **747vs; 680s;** 594; **483m;** 383; 288; 257; 233; 174

PB15:2 C.I. 74160:2, Polycyclic pigment, Phthalocyanine
Heubach; Laser: 785nm 0.121mW
1518vs; 1446m; **1334s;** 1303; 1181; 1140m; 1105; 1005; 950; 774; **745s; 679m;** 592; **483m;** 255

PB15:3 C.I. 74160:3, Polycyclic pigment, Phthalocyanine
Kremer; Laser: 785nm 0.0000121mW
1610; **1530vs;** 1451m; 1429; **1341s;** 1307; 1217; 1195; 1144; 1109; 1008; 954; 849; 832; 781; **747s;** 719; **681s;** 641; 594; **483m;** 289; 258; 233; 175

PB15:4 C.I. 74160:4, Polycyclic pigment, Phthalocyanine
Heubach; Laser: 785nm 0.0121mW
2268; **1522vs;** 1448m; 1426; **1336s;** 1305; 1216; 1190; 1142m; 1107; 1037; 1006; 951m; 848; 829; 776; **746s; 679s;** 639; 594; 547; **482m;** 421; 382; 287; 257; 233; 173; 158

PB15:6 C.I. 74160:6, Polycyclic pigment, Phthalocyanine
Kremer; Laser: 514nm 0.57mW
3051; 2866; 2667; 1587; **1526vs; 1482m;** 1448s; **1408; 1339s;** 1303; 1183; 1142m; 1108; 1039; 1007; 952; 833; 777; **748m; 680s;** 594m; 257; 233; 174

PB16 C.I. 74100, Polycyclic pigment, Phthalocyanine
Imperial Chem. Indust. LDT. UK; Laser: 514nm 5.7mW
3036; 2954; 2867; 2671; 2215; 2009; 1871; 1612m; **1528vs;** 1424s; **1334vs;** 1227; 1180m; 1140m; 1103m; 1024; **794s; 721m; 680s;** 567m; 541; 480; 230; 208; 187; 152

PB60 C.I. 69800, Polycyclic p., Polycarbocyclic Anthraquinone
Kremer; Laser: 514nm 1.14mW
2906; 2739; 2708; 2658; 2593; 2538; 2184; 1660; 1619s; 1554m; 1477m; **1383vs; 1356vs; 1328vs; 1285s;** 1238; 1212; 1185; 1159m; 1043; 1003; **911m;** 804m; 760; 667; 621; 584; 479m; 407; 378; 274; 215; 174; 145

PG7 C.I. 74260, Polycyclic pigment, Phthalocyanine
Kremer; Laser: 514nm 0.114mW
1563s; 1538s; **1506vs;** 1481; 1445; **1389s;** 1338; 1307; **1283s;** 1214m; 1200m; 1187m; 1082s; 979; 820m; 772; **685vs;** 642; 510; 236

PG9 C.I. 49415, Metal complex, Azo metal complex
Farbwerke Meister Lucius & Brüning; Laser: 785nm 0.121mW
1602; 1546; 1511m; 1479m; 1443m; 1389; 1330; 1262m; 1208m; 1081; 1038; 995; 877; 738; 689; **585vs; 510s;** 446; 391; 327; 260; 173

PG36 C.I. 74265, Polycyclic pigment, Phthalocyanine
Kremer; Laser: 514nm 1.14mW
2600; 1539vs; **1498vs; 1379s;** 1271m; **1193s;** 1162m; 1080w; 1056m; 818; 771m; 685m; **662vs;** 451; 321; 226; 167

therefore of considerable interest to gain knowledge of successful analytical settings and approaches to systematic identification (flowcharts).

2. Experimental

Reference samples of synthetic organic pigment powders were supplied by several collections and pigment manufacturers, as listed in Table 2.

A Raman spectral database was compiled using the software SpectralID as part of the Grams/AI suite. Spectra are available on request in digital format from the corresponding author. Reference powder samples were loosely pressed on an aluminum plate for analysis. All Raman spectra were acquired on a Renishaw InVia dispersive Raman spectrometer (2007), equipped with a Leica DM microscope and 3 laser sources: 785 nm (diode-type), Renishaw HP NIR785 (300 mW); 633 nm (gas-type), Renishaw HeNe 633 (17 mW); 514 nm (gas-type), Spectra Physics Ar ion laser (24 mW).

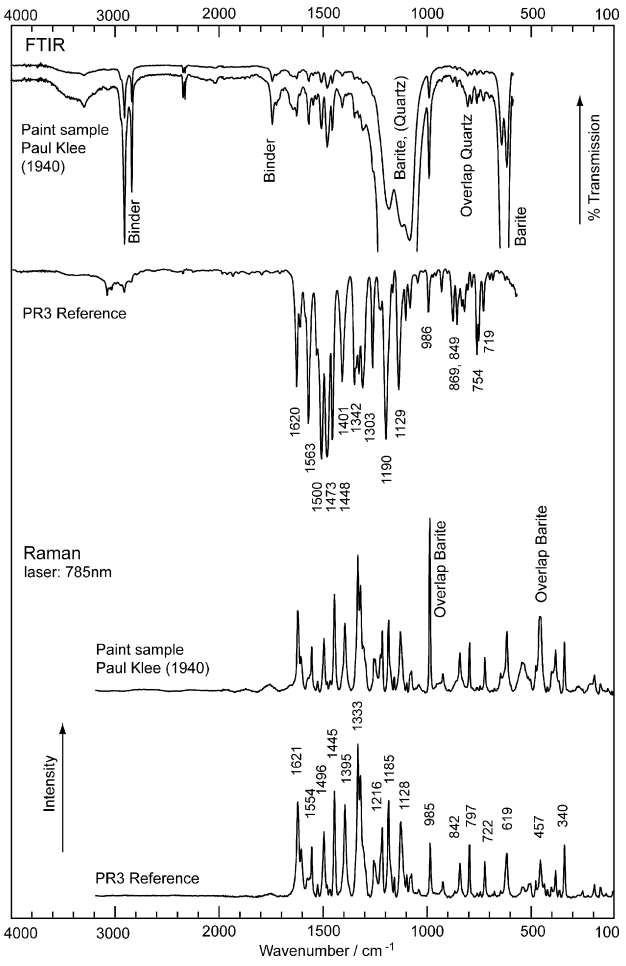


Fig. 1. Comparison of FTIR and Raman data of a red paint sample taken from the artwork "Glas-Fassade", 1940, by Paul Klee. This example demonstrates the different signal contributions of pigment, substrate and binding media and intensity ratios thereof. A baseline correction was applied to these spectra.

The general approach was to use the 785 nm laser (1200 l/mm grating), which did work successfully for about 90% of the pigments with different C.I. numbers, applying powers between 0.00001 and 1 mW (power on sample). The remaining pigments were analysed using the 514 nm laser (6%) with powers ranging between 0.1 and 5 mW, and the 633 nm laser (4%) with powers between 0.1 and 1 mW (both 1800 l/mm gratings). The spectral range covered for all spectra is 100–3200 wavenumbers (cm^{-1}) at a resolution of <2 cm^{-1}. Prior to each reference measurement, the instrument was calibrated on the internal Si-reference standard (520.6 ± 0.1 cm^{-1}). Integration times varied from 30 s to 200 s in total (Table 2). 5 random spots were analysed prior to the reference measurement to check the homogeneity of the pigment powder. All spectra are presented without baseline correction. According to other publications on organic pigments [15–19], the selected spectral range of 100–1800 cm^{-1} for presentation is the relevant range to identify such pigments. Signals above 1800 cm^{-1} are generally weak or absent, and for those observed in this upper range, the positions are listed in Table 3. Peak picking and peak table output was generated in WiRE 2.0, Renishaw's Raman software. To analyse the large dataset, a Filemaker Pro database was generated combining all information collected on a particular reference sample, spectra and peak tables in a single file to permit searching (peak range, class, group, etc.) and produce workable outputs in any wanted form.

Flowcharts were generated for colors where more than 5 different C.I. numbers were analysed (PB, PO, PR, PV, and PY). No flowcharts were produced for PG (3 pigments) and PBr (2), but the spectra have been included in Table 3. The flowchart hierarchy followed the path along color, pigment class, pigment group and individual C.I. constitution number. The discrimination criteria were the presence or absence of distinctive Raman bands of very strong to medium intensity, variations in relative intensities of two prominent signals, or specific features such as twin or triple peaks. Obviously, the comparison is restricted to the dataset available, which as such is limited, but nevertheless comprises about 3 times the number of different C.I. numbers presented in previous publications [15–17,19].

3. Results and discussion

Raman analysis is an excellent supplement to the standard analytical armory of forensic and art technological analysis, since both

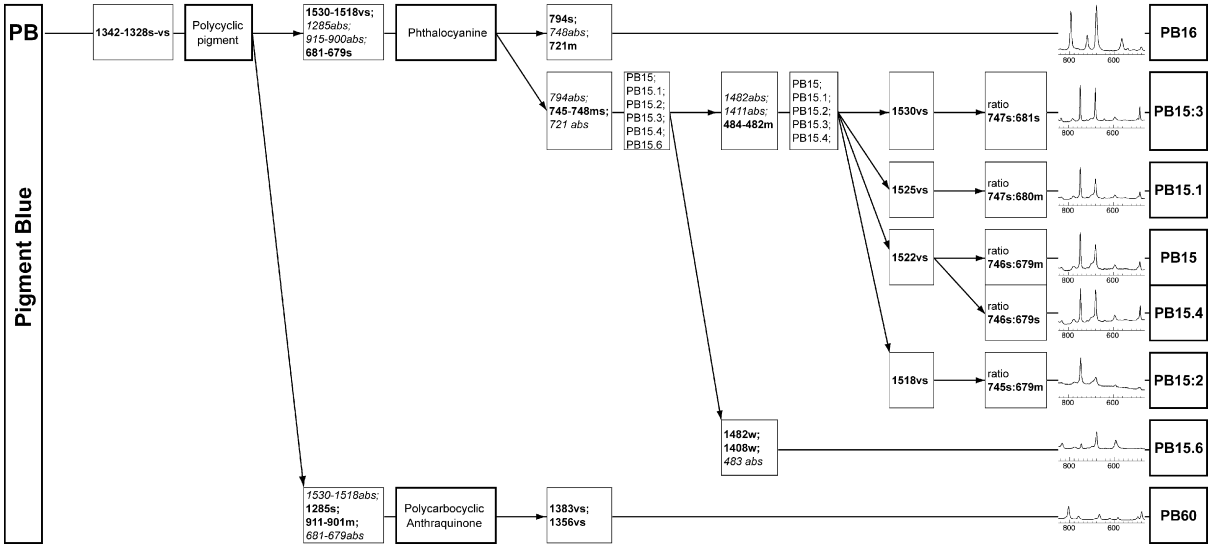


Fig. 2. Flowchart PB for the 8 blue pigments presented. Discriminating peak positions or ranges are given as Raman shift (cm^{-1}) and relative intensities are marked with: vs = very strong; s = strong; ms = medium to strong; m = medium, wm = weak to medium; w = weak; vw = very weak; abs = absent; br = broad; tw = twin peak. "Present" is given in bold, "absent" is marked with italic text. The distinct bands (or their absence) selected as discrimination criteria are also highlighted in the spectra table collection in Table 3.

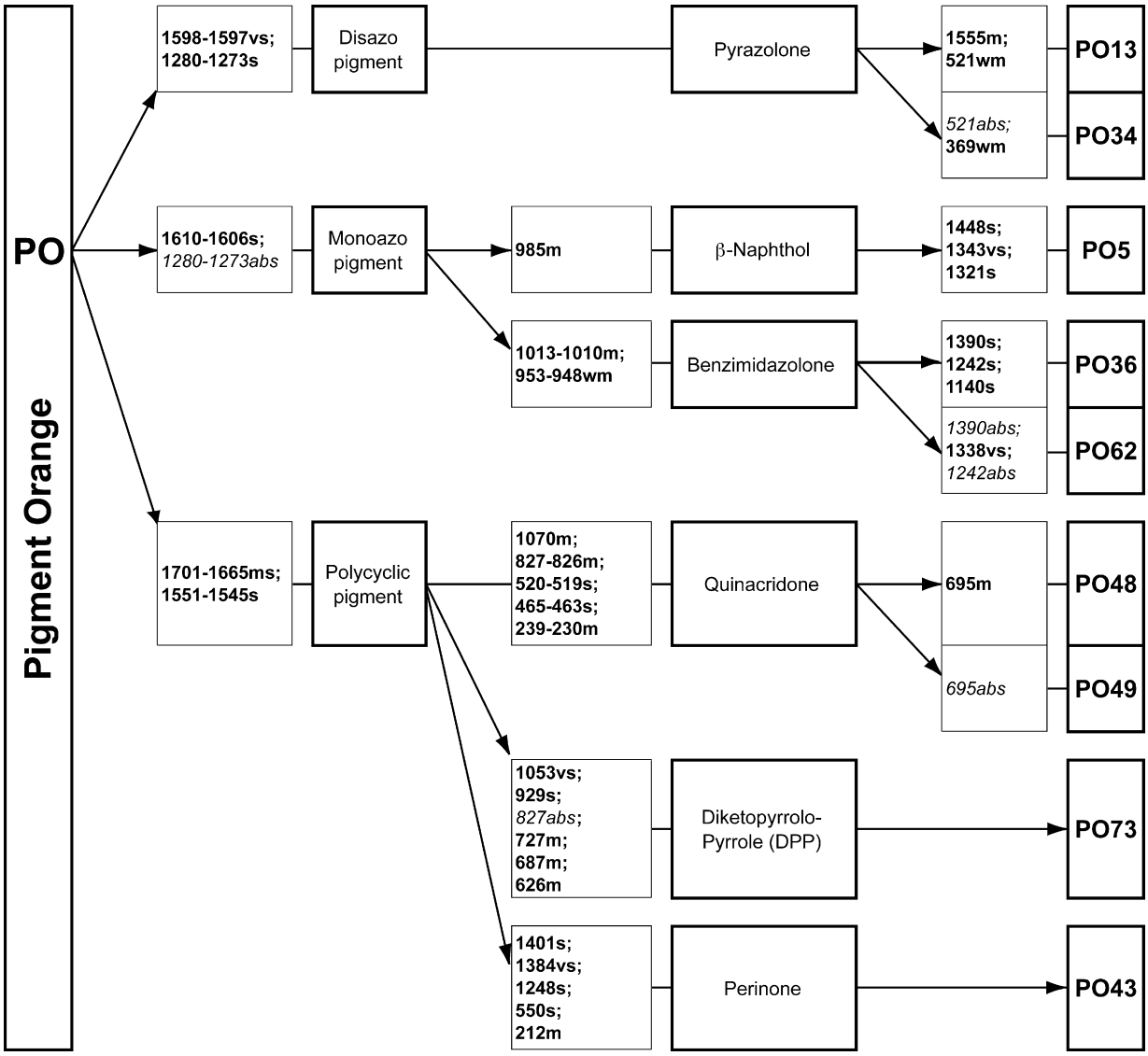


Fig. 3. Flowchart PO for the 9 orange pigments presented. Refer to Fig. 2 for the labeling convention.

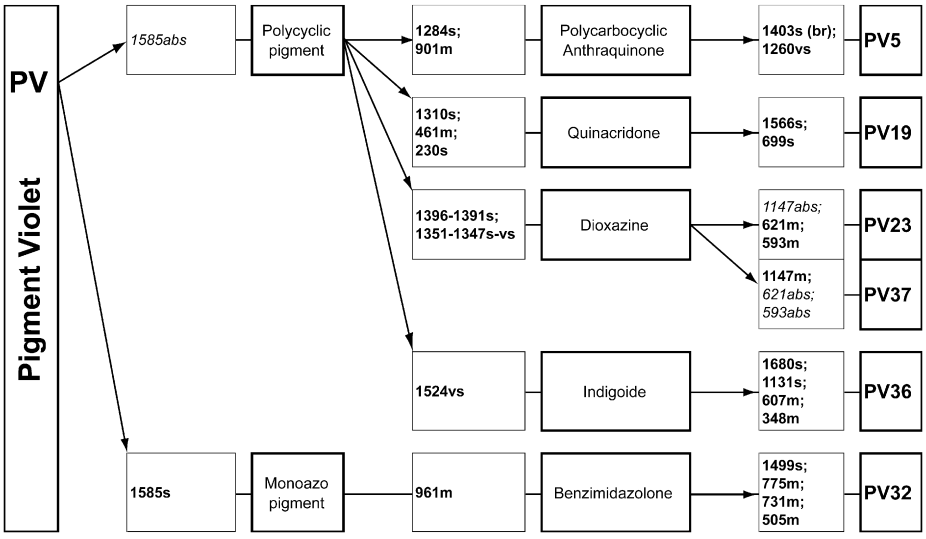


Fig. 4. Flowchart PV for the 6 violet pigments presented. Refer to Fig. 2 for the labeling convention.

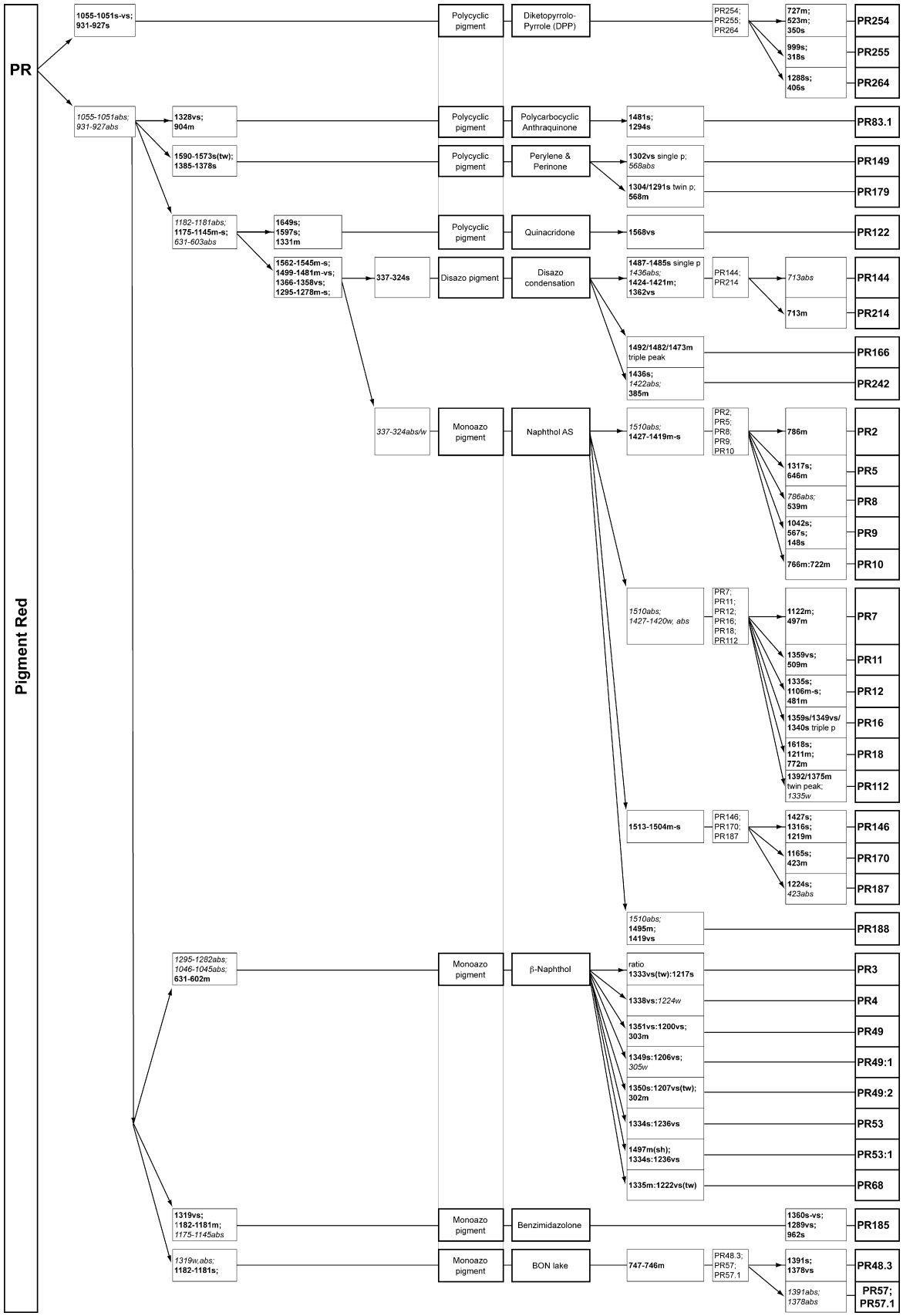


Fig. 5. Flowchart PR for the 38 red pigments presented. Refer to Fig. 2 for the labeling convention.

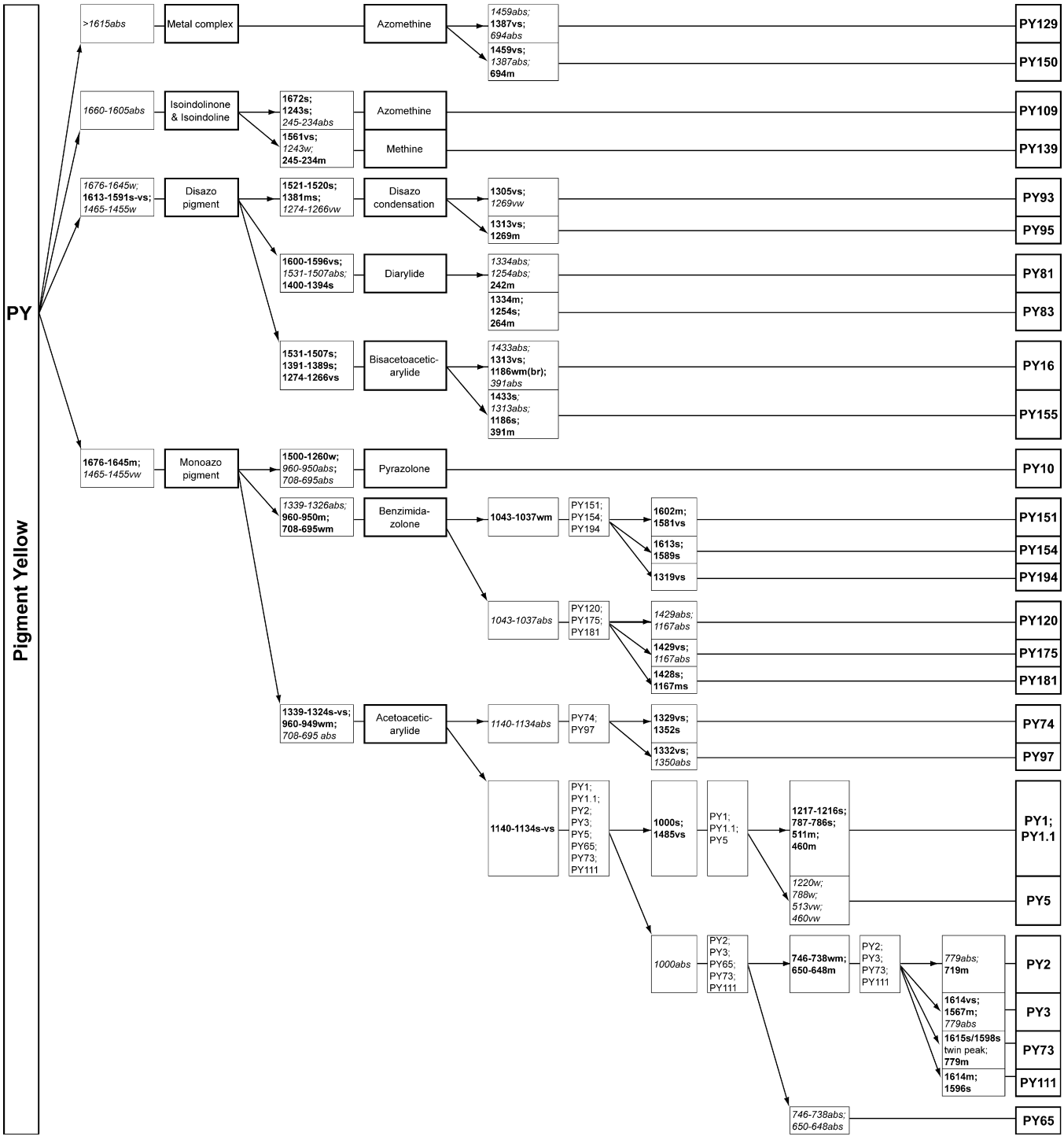


Fig. 6. Flowchart PY for the 27 yellow pigments presented. Refer to Fig. 2 for the labeling convention.

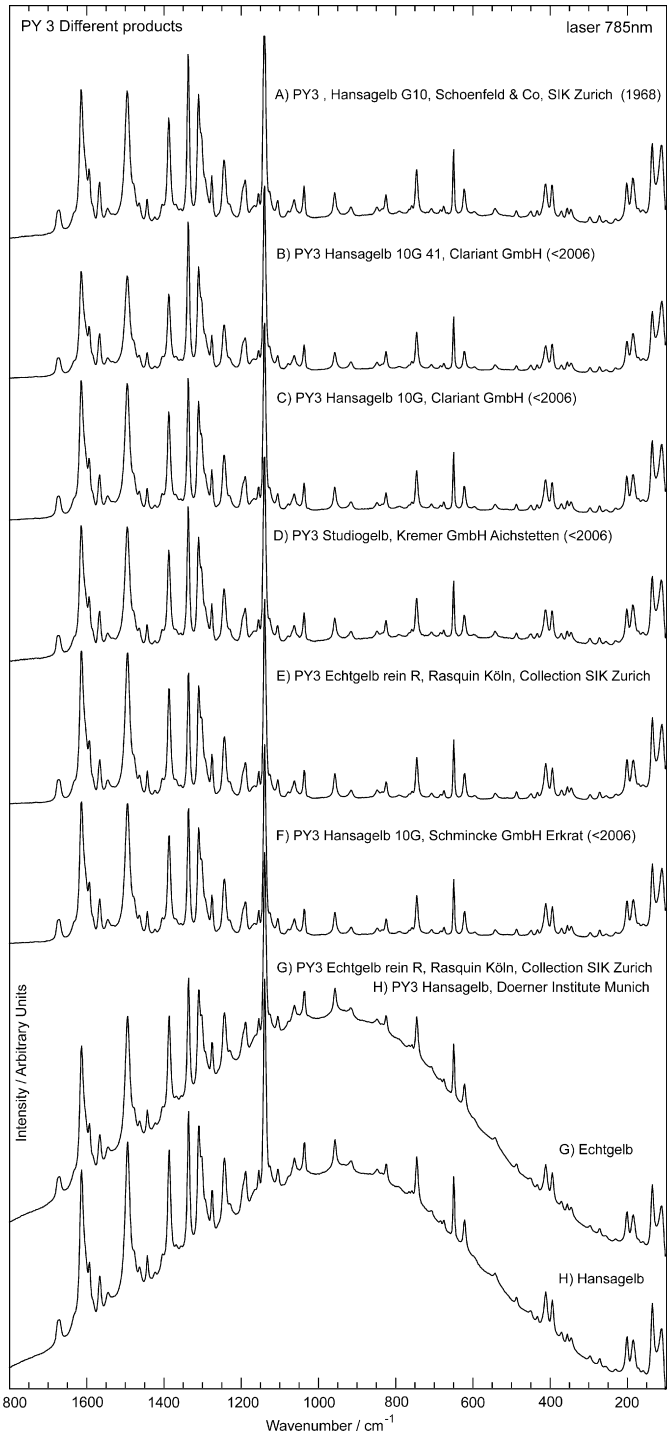
organic and inorganic pigments can be characterised reliably. XRF or SEM-EDS is powerful with inorganic pigments. In combination with FTIR, elemental analysis often leads to conclusive results. Organic pigments, whatsoever, require another combination of techniques. FTIR is very sensitive to organic compounds and often delivers information on pigments and substrates as well as binding media and fillers within the same analysis. This advantage of combined information may, however, be hampered by overlapping bands and relative signal intensities, making it difficult to separate the individual components of paint samples from artwork. Raman, on the other hand, while more complex in the choice of ideal analysis and instrument settings, appears to suffer far less from overlapping signals, since binding media such as oils or resins produce relatively weak Raman scattering compared to the pigments of interest [17,20–23]. Fig. 1 elucidates such a comparison of a sample taken from the painting “Glas-Fassade”, 1940, artwork 288(K8) of Paul Klee. Nevertheless, FTIR analysis provides a fast response on a routine basis, delivers in any case binding media and substrate information and hints at possible types of pigments. Raman complements excellently in pigment isolation and identification, or in case of requests for in situ and possibly mobile non-destructive analysis. The efficiency in information gain by the two spectroscopic methods may be expressed in terms of the difference in the number of reference measurements acquired within the same amount of time, where

FTIR has clear advantages for routine measurements and requires less experience of the operator. In order to compare the specificity of FTIR and Raman to pin down separate C.I. numbers, both spectra have been generated, with the priority given to the synthetic organic pigments most relevant to artist's paints of current products (Table 1), as well as historically important pigments from collection sources (Table 2). Published libraries of Raman spectra cover most of the inorganic pigments [10,24–33], whereas papers with Raman spectra of synthetic organic pigments cover a comparatively small palette [8,15–19,34–37]. Identification of inorganic pigments with few prominent signals is reasonably efficient using peak tables and spectra patterns. With the large number of signals generated from synthetic organic pigments, the use of peak tables and patterns only, seems inefficient and time consuming. Software solutions for automatic spectra matching such as SpectralID (Grams/AI) considerably ease the identification of unknowns in the presence of a reference database. The identification of multi-component paint samples suffering potentially from degradation phenomena may not always lead to a clear automatic match, however. A major goal was thus to generate flowcharts based on major peak discrimination, as has been presented by Vandenabeele et al. [19] for a selection of red and yellow azo pigments. While they set their flowchart criteria on structurally relevant bands across the colors, this paper separates first by color and empirically discriminates the same colors, based on the presence, absence or ratio of characteristic major signals within the individual patterns. This approach was chosen since major signal intensities may have different origins in relation to the structural elements. In most cases this will permit identification of the pigments contained in this reference collection, even with the lack of minor peaks expected for mixed or dilute samples. Based on the relatively large dataset available, the following points of interest were addressed on comparing reference spectra of synthetic organic pigments with

(a) different C.I. numbers,
(b) the same C.I. from different manufacturers (e.g. 8 products of PY3, Fig. 7),
(c) the same C.I. from the same manufacturer (e.g. 4 products of PY74, Table 2),
(d) the same C.I. root, but different modifications (e.g. PB15, PB15:1, PB15:2, PB15:3, PB15:4, PB15.6, Fig. 2)

to explore the possibility of pinpointing a particular C.I. number or even product of a unique manufacturer. The combination of automated spectra matching, use of flowcharts, tables and patterns should thus ease and speed up identification of synthetic organic pigments. A further step not addressed here will be the spectral separation of synthetic organic pigment mixtures in modern artist's paint products (compare Table 1).

Reference spectra and tables are summarised in Table 3, presenting one spectrum and peak table for each C.I. number. Within the adjacent peak tables, prominent signals are marked with very strong (vs), strong (s) or medium (m). Weak signals have not been labeled specifically. The main discriminating bands or spectral ranges guiding through the flowcharts (Figs. 2–6) have been marked with bold capitols in the peak tables. The flowcharts rely on relatively precise peak positions or bands, which have been derived from the dataset available and thus may be regarded with some tolerance for pigments of the same classes or groups not yet considered in this database. Nevertheless, for multiple products of the same C.I. number, current experience with the instrument used here is that the peak precision is within 1 wavenumber (a) for products from various sources and manufacturers, and (b) for spectra acquired on different days and up to 5 months apart. This is shown exemplarily for 8 pigment products of PY3 in Fig. 7. When comparing the associated peak tables (Fig. 7), the noted peak precision is



Peak table:

A) 1614vs; 1567m; 1495vs; 1387s; 1337vs; 1310vs; 1244m; 1192m; 1140vs; 746m; 650s; 622m; 412m; 395m; 202m; 185m
B) 1614vs; 1567m; 1495vs; 1387s; 1337vs; 1310vs; 1244m; 1192m; 1140vs; 746m; 650s; 622m; 412m; 395m; 202m; 185m
C) 1614vs; 1567m; 1495vs; 1387s; 1337vs; 1310vs; 1244m; 1192m; 1140vs; 746m; 650s; 622m; 412m; 395m; 201m; 185m
D) 1614vs; 1567m; 1495vs; 1387s; 1337vs; 1310vs; 1244m; 1192m; 1140vs; 746m; 650s; 622m; 412m; 395m; 201m; 185m
E) 1613vs; 1567m; 1495vs; 1387s; 1337vs; 1310vs; 1243m; 1191m; 1139vs; 745m; 649s; 621m; 411m; 394m; 201m; 184m
F) 1613vs; 1567m; 1495vs; 1387s; 1337vs; 1310vs; 1244m; 1191m; 1139vs; 745m; 649s; 622m; 411m; 394m; 201m; 184m
G) 1613vs; 1566m; 1494vs; 1387s; 1336vs; 1309vs; 1243m; 1190m; 1139vs; 745m; 649s; 621m; 411m; 394m; 201m; 184m
H) 1613vs; 1566m; 1494vs; 1386s; 1336vs; 1309vs; 1243m; 1190m; 1139vs; 745m; 649s; 621m; 411m; 394m; 201m; 184m

Fig. 7. Comparison of 8 Raman spectra of pigment yellow PY3 from different sources (Table 2) and analysed on different days. The peak precision is within one wavenumber for all peaks. The only conspicuous difference visible is the curved background of two samples from historic collections (G and H, refer to Table 2). The spectra have been normalised to the highest peak, but no baseline correction has been applied.

within 1 wavenumber for all peaks listed. The same applies to all other pigments in the collection, where multiple references were analysed (e.g. PY1/n = 7, PY74/8, PR12/4, PO5/3, PB15:3/2, PR5/2, PY16/2). It thus appears reasonable to view the positions given in the flowcharts with a tolerance of about ±1 wavenumber. Addressing the question regarding differences between older products from collections versus currently produced batches, e.g. due to process related changes, it is observed that in the cases of the 7 pigments PB15:3, PO5, PR5, PR12, PY1, PY3 (Fig. 7) and PY16, where old and new reference materials were available, older samples from collections may display a distinctly higher background, but otherwise are identical to within 1 wavenumber.

4. Conclusion

16 current products of acrylic, alkyd and oil-based artist's paints have been compared on the basis of pigment contents. The occurrence of more than 60% synthetic organic pigments within those states their relevance to contemporary artwork and the importance to build up analytical tools for the reconstruction of painter's color palettes, or to solve authenticity questions. A Raman spectral library of 93 synthetic organic pigments with separate C.I. numbers of particular reference to artist's paint products has been presented here. About 90% of those could readily be analysed using 785 nm excitation. The remaining pigments could be analysed applying the 514 and 633 nm lasers. The size of the reference collection also permitted comparison of products with the same C.I. from different sources, performed exemplarily in the case of PY3 (n = 8) and PY74 (n = 5). While it currently seems not possible to track down a particular product, this comparison elucidates the peak precision of spectra acquired up to 5 months apart to within 1 cm^{-1}. To help identification of unknowns, flowcharts have been generated for PY (comprising 27 C.I. numbers), PR (38), PO (9), PB (8) and PV (6). Raman spectroscopy has shown to be capable of distinguishing a large number of synthetic organic pigments, and under ideal conditions, may even differentiate between modifications of the same C.I. root number (PB15). A next step will be the spectral separation of multi-pigment samples.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.saa.2008.11.029.

References

[1] M. De Keijzer, ICOM, 12th Triennial Meeting, vol. 1, London Preprints, 29 August–3 September, 1999, pp. 369–374.
[2] S. Frowein, Synthetische organische Pigmente in zeitgenössischen Künstlerfarben Angebot, neue Entwicklungen und Nachweismöglichkeiten, s.n., München, 2004.
[3] K. Heumann, Die Anilinfarben und ihre Fabrikation, Fr. Vieweg, Braunschweig, 1888.
[4] K. Huebner, Chemie unserer Zeit 40 (2006) 274–275.
[5] H. Zollinger, Color chemistry syntheses properties and applications of organic dyes and pigments, second, revised ed., VCH, Weinheim [etc.], 1991.
[6] W. Herbst, K. Hunger, Industrielle organische Pigmente Herstellung, Eigenschaften, Anwendung, Zweite, vollständig überarb. Aufl. ed., VCH, Weinheim; Basel [etc.], 1995.
[7] W. Herbst, K. Hunger, Azo-Pigmente Eigenschaften - Anforderungen - Entwicklungstendenzen, 1978.
[8] S.A. Centeno, V.L. Buisan, P. Ropret, Journal of Raman Spectroscopy 37 (2006) 1111–1118.
[9] S. Zumbuehl, M. Gross, Reihe Bild und Wissenschaft, Forschungsbeiträge zu Leben und Werk Alexej von Jawlenskys 3 (2008).
[10] R.J.H. Clark, Comptes Rendus Chimie 5 (2002) 7–20.
[11] R.J.H. Clark, P.J. Gibbs, K.R. Seddon, N.M. Brovenko, Y.A. Petrosyan, Journal of Raman Spectroscopy 28 (1997) 91–94.
[12] P. Vandenabeele, K. Castro, M. Hargreaves, L. Moens, J.M. Madariaga, H.G.M. Edwards, Analytica Chimica Acta 588 (2007) 108–116.
[13] P. Vandenabeele, J. Tate, L. Moens, Analytical and Bioanalytical Chemistry 387 (2007) 813–819.
[14] P. Vandenabeele, F. Verpoort, L. Moens, Journal of Raman Spectroscopy 32 (2001) 263–269.
[15] J. De Gelder, P. Vandenabeele, F. Govaert, L. Moens, Journal of Raman Spectroscopy 36 (2005) 1059–1067.
[16] P. Ropret, S.A. Centeno, P. Bukovec, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 69 (2008) 486–497.
[17] F. Schulte, K.-W. Brzezinka, K. Lutzenberger, H. Stege, U. Panne, Journal of Raman Spectroscopy 9999 (2008), n/a.
[18] P. Vandenabeele, L. Moens, Analyst 128 (2003) 187–193.
[19] P. Vandenabeele, L. Moens, H.G.M. Edwards, R. Dams, Journal of Raman Spectroscopy 31 (2000) 509–517.
[20] H.G.M. Edwards, M.J. Falk, M.G. Sibley, J. Alvarez-Benedi, F. Rull, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 54 (1998) 903–920.
[21] P. Vandenabeele, D.M. Grimaldi, H.G.M. Edwards, L. Moens, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 59 (2003) 2221–2229.
[22] P. Vandenabeele, M. Ortega-Aviles, D.T. Castilleros, L. Moens, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 68 (2007) 1085–1088.
[23] P. Vandenabeele, B. Wehling, L. Moens, H. Edwards, M. De Reu, G. Van Hooydonk, Analytica Chimica Acta 407 (2000) 261–274.
[24] I.M. Bell, R.J.H. Clark, P.J. Gibbs, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 53 (1997) 2159–2179.
[25] M. Bouchard, D.C. Smith, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 59 (2003) 2247–2266.
[26] K. Castro, M. Perez, M.D. Rodriguez-Laso, J.M. Madariaga, Analytical Chemistry 75 (2003) 214A–221A.
[27] A. Zoppi, A. Perardi, E. Castellucci, Annali Di Chimica 91 (2001) 833–841.
[28] L. Burgio, R.J.H. Clark, Spectrochimica Acta Part a—Molecular and Biomolecular Spectroscopy 57 (2001) 1491–1521.
[29] K. Castro, M. Perez-Alonso, M.D. Rodriguez-Laso, L. Fernandez, J. Madariaga, Analytical and Bioanalytical Chemistry 382 (2005) 248–258.
[30] H.G.M. Edwards, Spectroscopy 17 (2002) 16–40.
[31] H.G.M. Edwards, E.M. Newton, J. Russ, Journal of Molecular Structure 550 (2000) 245–256.
[32] Q.L. Ma, A. Portmann, F. Wild, H. Berke, Studies in Conservation 51 (2006) 81–98.
[33] C. Sandalinas, S. Ruiz-Moreno, Studies in Conservation 49 (2004) 41–52.
[34] T.D. Chaplin, R.J.H. Clark, D.R. Beech, Journal of Raman Spectroscopy 33 (2002) 424–428.
[35] K. Chen, M. Leona, K.C. Vo-Dinh, F. Yan, M.B. Wabuyele, T. Vo-Dinh, Journal of Raman Spectroscopy 37 (2006) 520–527.
[36] K. Chen, K.C. Vo-Dinh, F. Yan, M.B. Wabuyele, T. Vo-Dinh, Analytica Chimica Acta 569 (2006) 234–237.
[37] G. Chiavari, D. Fabbri, S. Prati, A. Zoppi, Chromatographia 61 (2005) 403–408.