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Identification of Drugs and Other Toxic Compounds from Their Ultraviolet Spectra. Part III: Ultraviolet Absorption Properties of 22 Structural Groups

This paper concludes a series of three papers which present ultraviolet (UV) absorption data of drugs and toxic organic compounds systematically by grouping according to chemical structure. As in Parts I and II [*1,2*], structural groups are spectrophotometrically characterized by (1) an absorption profile which is a graph of wavelength versus absorbance from 200 to 340 nm, (2) the effect of pH change, (3) the effect of decreased solvent polarity relative to water, and (4) the intensity of the absorption bands. The purposes of this series are first, to aid in rapidly characterizing an unknown organic compound from UV data and second, to interpret UV spectra in terms of chemical structure. An analyst in a forensic situation should be able to defend an identification on the basis that a given molecular structure is specifically indicated by the tests conducted. Understanding the specificity of each test leads the analyst to more clear-cut decisions in establishing an identification with the degree of scientific certainty expected of him. Reviews and pertinent publications related to this presentation have been cited in Parts I and II [*1,2*].

Methods

Spectrophotometers used in this study, a Bausch & Lomb 200, a Beckman Acta IV, and a Perkin-Elmer 202, were calibrated according to the method of Haupt [*3*] with reagent grade potassium chromate, 0.0400 g/litre in 0.005*N* potassium hydroxide. Differences in spectra recorded on different spectrophotometers are slight if the instruments are calibrated and if comparable slit widths are used for absorption measurements. Absorption bands from 340 down to 200 nm were routinely examined except for compounds having bands above 340 nm. The different structural groups are given in Table 1. Considerable data in Tables 2 and 3 and the Appendix were abstracted from appropriate publications to present more complete information on each structural group.

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TABLE 1—*Compounds in the different structural groups.*

L1	Chlorpromazine
	Diethazine
	Fluphenazine
	Isothipendyl
	Mepazine
	Methdilazine
	Methotrimeprazine
	Methoxypromazine
	Perphenazine
	Pipamazine
	Prochlorperazine
	Promazine
	Promethazine
	Prothipendyl
	Pyrathiazine
	Thiethylperazine
	Thiopropazate
	Thioridazine
	Trifluoperazine
	Triflupromazine
	Trimeprazine
L2	Acetophenazine
	Acetylpromazine
	Carphenazine
	Dimethothiazine
	Dimethoxanate
	Mesoridazine
	Pericyazine
	Piperacetazine
	Propiomazine
	Thioproperazine
M	Acenocoumarol
	Coumarin
	Cyclocumarol
	Dicumarol®
	Warfarin
N1	Aminophylline
	Caffeine
	8-Chlorotheophylline
	Diphylline
	Etamiphylline
	Oxytriphylline
	Theobromine
	Theophylline
	Xanthine
N2	Adenine
	Adenosine monophosphate
	Guanine
	Idoxuridine
	Thymine
	Uracil
O1	Aramite®
	Benzethonium chloride
	Captodiamine
	4-Chloro-2-methylphenoxyacetic acid (MCP)
	Chlorphenesin
	Chlorphenesin carbamate
	Clofibrate
	Dextromethorphan
	2,4-Dichlorphenoxyacetic (2,4-D)
	2,4-Dichlorphenoxyacetic acid methyl ester
	Domiphen bromide
	Mephenesin
	Mephenesin carbamate
	Mephenoxalone
	Metaxalone
	Methantheline bromide
	Methixene
	Methocarbamol
	4-Methoxyamphetamine
	Methoxybenzene
	Methoxychlor
	Methoxyphenamine
	Methylbenzethonium chloride
	Phenoxybenzamine
	Phenoxymethyl penicillin
	Phenoxypropyl penicillin
	Phenyltoloxamine
	Pramoxine
	Propantheline bromide
	Sodium 2,4-dichlorphenoxyethyl sulfate (SES-T)
	Trithion®
O2	Benzquinamide
	Cotarnine
	Desmethylemetine
	Dimethoxyamphetamine
	2,4-Dimethoxy-4-methyl-amphetamine (STP)
	Dopamine
	Emetine
	Epinephrine
	Hexylresorcinol
	Isoproterenol
	Mescaline
	Methoxamine
	3,4-Methylenedioxy amphetamine (MDA)
	5-Methoxy-3,4-methylenedioxy amphetamine (MMDA)
	Nordefrin
	Norepinephrine
	Piperonyl butoxide
	Protokylol
	Ronnel®
	2,4,5-Trichlorphenoxy acetic acid (2,4,5-T)
	3,4,5-Trimethoxy amphetamine (TMA)
O3	Acetanilide
	Brucine
	Bupivacaine
	Diuron
	Fentanyl
	Isopropyl carbanilate (IPC)
	Isopropyl-N-3-chlorophenyl carbamate (CIPC)
	Lidocaine
	Mepivacaine
	Monuron
	Neburon
	Phenacetin
	Prilocaine
	Strychnine
P1	Amodiaquine
	Chiniofon
	Chloroquine
	Cinchonidine
	Cinchonine
	Cinchophen
	Dibucaine
	Dimethisoquin
	Hydroxychloroquine
	8-Hydroxyquinoline
	Papaverine
	Quinidine
	Quinine
	Quinoline
P2	Carbaryl
	Naphazoline
	α-Naphthalene acetic acid
	Propranolol
	Quinacrine
	Triamterene
Q1	Sulfacetamide
	Sulfachlorpyridazine
	Sulfadiazine
	Sulfadimethoxine
	Sulfaethidole
	Sulfaquanidine
	Sulfamerazine
	Sulfameter
	Sulfamethazine
	Sulfamethizole
	Sulfamethoxazole
	Sulfamethoxydiazine

TABLE 1—*Compounds in the different structural groups*—Continued.

	Sulfamethoxypyridazine		Flurazepam		Rotenone
	Sufanilamide		Nitrazepam		Salicylazosulfapyridine
	Sulfaphenazole		Oxazepam		Succinylsulfathiazole
	Sulfapyridine	T	Dihydroergotamine		Sulfinpyrazone
	Sulfathiazole		Ergonovine		Syrosingopine
	Sulfisomidine		Ergotamine		Tetracycline
	Sulfisoxazole		Lysergic acid		Thiamine
Q2	Bendroflumethiazide		Lysergic acid diethylamide (LSD)		Thiothixene
	Benzthiazide		Methylergonovine		Tolnaftate
	Chlorothiazide		Methylsergide		Trimethobenzamide
	Furosemide		Amolanone		Tubocurarine chloride
	Hydrochlorothiazide	U	Anisindione	X1	Acetone
	Hydroflumethiazide		Antipyrine		Amyl nitrite
	Methyclothiazide		Benzydamine		Camphor
	Polythiazide		Bephenium hydroxynaphthoate		Cantharidin
	Quinethazone		Berberine		Ethinamate
	Teclothiazide		Bisacodyl		Ethyl nitrate
	Trichlormethiazide		Bretylium tosylate		Methyprylon
R1	Acetorphine		Cephaloridine		MGK-264 (Octacide-264®)
	Apomorphine		Cetoxime		Nitroglycerin
	Cyprenorphine		Chlorbenside		Nitromethane
	Desomorphine [a]		Chlortetracycline		Pentaerythritol tetranitrate
	Diacetylmorphine		Chlorthalidone		Picrotoxin
	Dihydromorphinol [a]		Clemizole		Randox®
	Dihydromorphine [a]		Colchicine		δ-Valerolactam
	Dihydromorphinone		Crotamiton	X2	Aldrin
	Etorphine		Dequalinium chloride		Chlordane
	Methyldesorphine [a]		Deserpidine		Dieldrin
	Methyldihydromorphinone		Deslanoside		Ethchlorvynol
	Methyldihydromorphine [a]		Diaveridine		Heptachlor
	3-Monoacetylmorphine		Digitoxin		Thiodan®
	6-Monoacetylmorphine		Digoxin		Vapona®
	Morphine		Dimethindene	Y1	Furazolidone
	Morphine-*N*-oxide [b]		Diphenadione		Furfural
	Nalorphine		Dipyrone		Hydroxymethylfurfural
	Naloxone		Duraset®		Nitrofurantoin
	Nicomorphine [a]		Dyrene®		Nitrofurazone
	Normorphine		Haloperidol		Thiophene
	Oxymorphone		Hydrastine	Y2	Amitrole
R2	Acetyldihydrocodeine [a]		Indomethacin		Atrazine
	Benzylmorphine [a]		Methaqualone		Betazole
	Codeine		Methotrexate		Diazinon®
	Codeine-*N*-oxide [b]		Nalidixic acid		Histamine
	Dihydrocodeine		Narceine		Maleic hydrazide
	Dihydrocodeinone		Noscapine		Pilocarpine
	Ethylmorphine		Oxyphenbutazone		Pyrrole
	Myorphine [a]		Oxytetracycline		Simazine
	Neopine		Phenacaine		Sparteine
	Nicocodeine [a]		Phenolphthalein	Y3	Acetazolamide
	Oxycodone		Phenoxybenzamine		Acinitrazole
	Pholcodine		Phenylbutazone		Cycloserine
	Thebacon [a]		Phthalylsulfathiazole		Isocarboxazid
	Thebaine		Pyrolan®		Paramethadione
S	Chlordiazepoxide		Reserpine		Trimethadione
	Clorazepate				
	Diazepam				

[a] Obsolete narcotics whose manufacture is not authorized in the United States and which are not likely to be encountered as illegal drugs.

[b] May be encountered as metabolite or oxidation artifact.

TABLE 2—*Ultraviolet absorption data on a number of compounds in each of 17 structural groups.*

Compound and Molecular Weight [a]	Wavelength Max			Absorbance Data			
	Aqueous Acid	Aqueous Base	Other Solvent	Wavelength	Molar Absorptivity	Solvent [b]	Ref [c]
Group L1							
Chlorpromazine*—318.9	252,[d] 305, 0.1*N* HCl	255, 310, 0.1*N* NaOH	255, 305, ethanol	252	34 100	H_3O^+	5
				255	35 700	ethanol	5
				305	4 400	H_3O^+	5
Fluphenazine*—437.5	256, 306, 0.1*N* HCl	257, 306, 0.1*N* NaOH	259, 304, ethanol	256	33 300	H_3O^+	5,6
				306	4 100	H_3O^+	5
Isothipendyl—285.4	245, 315, 0.1*N* H_2SO_4	249, 315, 0.1*N* NaOH	249, 315, ethanol	245	27 200	H_3O^+	5,7
				315	5 100	H_3O^+	5
Mepazine—346.9	252, 302, 0.1*N* H_2SO_4	254, 304, 0.1*N* NaOH	254, 305, ethanol	252	32 200	H_3O^+	5
				302	4 200	H_3O^+	5
Methotrimeprazine—328	252, 302, 0.1*N* HCl	255, 310, 0.1*N* NaOH	255, 310, ethanol	252	32 400	H_3O^+	7
				302	5 800	H_3O^+	7
Perphenazine*—403.9	213s, 254, 305, 0.1*N* HCl	255, 310, 0.1*N* NaOH	257, 310, ethanol	255	33 200	H_3O^+	6,7
				306	3 700	H_3O^+	7
Prochlorperazine*—374	213s, 254, 305, 0.1*N* HCl	256, 308, 0.1*N* NaOH	257, 311, ethanol	see the Appendix			
Promazine*—284.4	251, 301, 0.1*N* H_2SO_4	253, 303, 0.1*N* NaOH	254, 306, ethanol	252	31 900	H_3O^+	7
				301	3 700	H_3O^+	7
Promethazine*—284.4	249, 299, 0.1*N* H_2SO_4	253, 304, 0.1*N* NaOH	252, 304, ethanol	249	31 200	H_3O^+	6,7
				299	3 800	H_3O^+	5
Pyrathiazine—296.4	248, 298, 0.1*N* H_2SO_4	252, 298, 0.1*N* NaOH	251, 300, methanol	248	27 600	H_3O^+	5
				298	4 200	H_3O^+	5
Thiopropazate—466	255, 306, 0.1*N* H_2SO_4	257, 310, 0.1*N* NaOH	257, 310, ethanol	255	33 700	H_3O^+	5,7
				305	4 400	H_3O^+	5,7
Thioridazine*—370.6	228, 262, 310, 0.1*N* HCl	273, 318, 0.1*N* NaOH	263, 314, ethanol	262	46 000	H_3O^+	5,7
				313	4 500	H_3O^+	5,7
Trifluoperazine*—480	235s, 255, 305, 0.1*N* HCl	257, 305, 0.1*N* NaOH	235s, 258, 308, ethanol	255	37 000	H_3O^+	authors
				305	4 300	H_3O^+	authors

Trifluprom azine—352.4	255, 306, 0.1*N* H_2SO_4	259, 311, 0.1*N* NaOH	258, 308, ethanol	256 305	38 700 4 200	H_3O^+ H_3O^+	5,7 5,7
Trimeprazine*—298.4	251, 299, 0.1*N* H_2SO_4	255, 306, 0.1*N* NaOH	228s, 255, 305, ethanol	251 299	26 100 3 900	H_3O^+ H_3O^+	5,7 5,7
Group L2							
Acetophenazine—411.6	243, 278, 374, 0.1*N* H_2SO_4	243, 280, 0.1*N* NaOH	243, 278, ethanol	243 278	19 300 13 600	H_3O^+ H_3O^+	7 7
Carphenazine—425.6	244, 277, 0.1*N* H_2SO_4	243, 280, 0.1*N* NaOH	243, 278, ethanol	243 277	25 300 18 800	H_3O^+ H_3O^+	7 7
Propiomazine*—340.5	204, 240, 274, 0.1*N* HCl	244, 280, 0.1*N* NaOH	244, 279, ethanolic HCl		see the Appendix		
Group M							
Acenocoumarol—353.3	284, 306, 0.1*N* HCl	243s, 292s, 303, 0.1*N* NaOH	...	284 306	24 400 21 900	H_3O^+ H_3O^+	5 5
Dicumarol®*—336.3	237, 281s, 295, 313, 329, 0.1*N* HCl	240s, 292s, 314, 0.1*N* NaOH	240s, 275, 303, 325s, ethanol	314 275	25 000 17 200	OH^- H_2O	authors authors
Warfarin*—308.3	215s, 232s, 270, 280, 302, 317s, 0.1*N* HCl	240s, 291s, 305, 0.1*N* NaOH	232s, 240, 259s, 269, 280, 303, 316, ethanol		see the Appendix		
Group N1							
Caffeine*—194.2	227s, 272, 0.01*N* HCl	227, 272 0.1*N* NaOH	273, ethanol	273	10 000	ethanol	7
8-Chlorotheophylline*—215	205, 230s, 276, 0.1*N* HCl	240s, 278, 0.1*N* NaOH	275, ethanol	276 205	11 500 28 300	H_3O^+ H_3O^+	authors authors
Diphylline*—254.2	206s, 232, 270, 0.1*N* H_2SO_4	232s, 273, 0.1*N* NaOH	232s, 273, ethanol	273 206	9 300 23 000	H_2O H_2O	authors authors
Oxytriphylline*—281.2	205s, 231, 268, 0.1*N* H_2SO_4	274, 0.1*N* NaOH	230s, 271, H_2O, pH 6.6	271 205	10 500 20 000	H_2O H_2O	authors authors
Theobromine*—180.2	231s, 271, 0.1*N* H_2SO_4	234, 274, 0.5*N* NaOH	205, 271, H_2O pH 7		see the Appendix		
Theophylline*—180.2	203, 229s, 271, 0.1*N* HCl	230s, 275, H_2O, pH 10	274, chloroform	274 272	10 400 10 500	OH^- H_2O	7 8
Xanthine—152.1	225, 266, H_2O, pH 5	242, 283, 0.1*N* NaOH	241, 276, H_2O, pH 10	266 241	10 700 8 900	H_3O^+ OH^-	8 8

TABLE 2—*Ultraviolet absorption data on a number of compounds in each of 17 structural groups*—Continued.

Compound and Molecular Weight [a]	Wavelength Max			Absorbance Data			
	Aqueous Acid	Aqueous Base	Other Solvent	Wavelength	Molar Absorptivity	Solvent [b]	Ref [c]
Group N2							
Adenosine monophosphate*—347.2	210s, 256, 0.1*N* HCl	259, 0.1*N* NaOH	209, 258, ethanol	256	14 200	H_3O^+	authors
				259	14 900	OH^-	authors
Guanine*—151.1	248, 270s, 0.1*N* HCl	273, 0.1*N* NaOH	245, 274, H_2O, pH 7	see the Appendix			
Idoxuridine*—354.1	215, 287, 0.1*N* HCl	279, 0.1*N* NaOH	216, 283, ethanol	279	6 000	OH^-	authors
				287	8 500	H_3O^+	authors
Thymine*—126.1	265, H_2O, pH 4	289, 270s, H_2O, pH 12	265, H_2O, pH 7	265	7 900	H_3O^+	authors
				289	5 400	OH^-	authors
Uracil*—112.1	260, 1*N* HCl	284, 262s, H_2O, pH 12	260, H_2O, pH 7	260	7 800	H_3O^+	authors
				284	6 200	OH^-	authors
Group O1							
Chlorphenesin carbamate*—245.7	226, 279, 285s, 0.1*N* HCl	281, 286s, 0.1*N* NaOH	227, 280, 288s, ethanol	280	1 600	ethanol	authors
				227	10 700	ethanol	authors
Clofibrate*—242	224, 270s, 276, 284, 0.1*N* HCl	224, 271s, 277, 285, 0.1*N* NaOH	226, 278, 287, 269s, ethanol	226	12 000	ethanol	authors
				279	1 200	ethanol	authors
Dextromethorphan*—271	218, 278, 283s, 0.1*N* HCl	278, 282, 0.1*N* NaOH	221, 280, 288s, ethanol	see the Appendix			
Domiphen bromide*—414	217, 268, 274 0.1*N* HCl	268, 274, 0.1*N* NaOH	...	217	6 500	H_3O^+	authors
				268	1 500	H_3O^+	authors
Mephenesin*—182.2	216, 270, 276, 0.1*N* HCl	270, 275, 0.1*N* NaOH	216, 271, 278, methanol	216	7 200	methanol	9
				271	1 680	methanol	9
Methocarbamol*—241.1	222, 272, 279s, 0.1*N* HCl	222, 272, 0.1*N* NaOH	224, 274, 280s, ethanol	224	7 600	ethanol	authors
				274	2 500	ethanol	authors
Phenoxymethyl penicillin—350.4	218s, 268, 262, 275, 0.1*N* HCl	268, 274, 262, 0.1*N* NaOH	263, 268, 275, methanol	268	1 360	methanol	7
				268	1 230	OH^-	6
Phenyltoloxamine*—255.4	218s, 269, 276, 0.1*N* HCl	270, 277, 0.1*N* NaOH	269, 276, ethanol	269	1 900	H_3O^+	authors
				276	1 600	H_3O^+	authors
Propantheline bromide*—448.4	243, 281, 0.1*N* H_2SO_4	246, 281, 286s, 0.1*N* NaOH	246, 281, 286s, methanol	243	4 600	H_3O^+	7
				281	2 300	H_3O^+	7

Group O2							
Cotarnine—237.3	205, 246, 320, 0.1*N* H_2SO_4	245, 275s, 320, 0.1*N* NaOH	248, 325, ethanol	246 320	12 600 8 000	H_3O^+ H_3O^+	12 12
2,4-Dimethoxy-4-methyl amphetamine*—209.3	225, 288, 0.1*N* HCl	222, 290, 0.1*N* NaOH	227, 290, ethanol	see the Appendix			
Emetine—470.7	227, 282, 285s, 0.1*N* H_2SO_4	281, 285s, 290s, 0.1*N* NaOH	230, 283, ethanol	230 283	17 000 7 400	ethanol ethanol	8 8
Epinephrine—183.2	222, 279, 0.1*N* H_2SO_4	245s, 280, 296s, 0.1*N* NaOH	230, 281, methanol	279 281	4 400 4 900	H_3O^+ methanol	5 9
Mescaline*—211.3	226s, 268, 276s, 0.1*N* HCl	267, 276s, 0.1*N* NaOH	225s, 269, ethanol	225 269	16 000 1 600	H_3O^+ H_3O^+	8 8
Methoxamine—211.3	225, 289, 0.1*N* H_2SO_4	289, 0.1*N* NaOH	227, 291 methanol	227 291	7 800 3 700	H_3O^+ methanol	9 9
3,4-Methylenedioxy amphetamine*—179.2	234, 284, 0.1*N* HCl	233, 285, 0.1*N* NaOH	235, 286, ethanol	234 284	3 500 3 500	H_3O^+ H_3O^+	authors authors
Norepinephrine*—169.2	220s, 279, 0.1*N* HCl	241, 293, 0.4% NH_4OH	225, 281, ethanol	279 241	4 400 8 100	H_3O^+ OH^-	authors authors
Group O3							
Acetanilide—135.2	239, 0.1*N* H_2SO_4	239, 0.1*N* NaOH	242, ethanol	242	15 300	ethanol	7
Brucine—466.5	265, 300, 0.1*N* H_2SO_4	265, 300, 0.1*N* NaOH	267, 301, ethanol	265 300	15 300 10 200	H_3O^+ H_3O^+	7 7
Isopropyl-N-(3-chlorophenyl) carbamate*—214	206, 237, 277, 284, 0.1*N* HCl	237, 277, 284, 0.1*N* NaOH	239, 278, 286, ethanol	237 277	15 100 10 000	H_3O^+ H_3O^+	authors authors
Lidocaine*—234.5	200, 262, 271, 0.1*N* HCl	262, 271, 0.1*N* NaOH	271, 262, ethanol	262 262	500 600	H_3O^+ H_3O^+	authors 5
Mepivacaine*—246.3	200, 262, 270, 0.1*N* HCl	262, 270, 0.1*N* NaOH	...	272 270	480 400	H_3O^+ H_3O^+	authors authors
Phenacetin*—179.2	243, 280s, 0.1*N* HCl	243, 280s, 0.1*N* NaOH	249, ethanol	249 243	16 300 16 000	ethanol H_3O^+	7 12
Strychnine*—334.4	206, 254, 261s, 286, 0.1*N* HCl	254, 263s, 279, 288, 0.1*N* NaOH	255, 280, 290, ethanol	see the Appendix			

TABLE 2—*Ultraviolet absorption data on a number of compounds in each of 17 structural groups*—Continued.

Compound and Molecular Weight [a]	Wavelength Max			Absorbance Data			
	Aqueous Acid	Aqueous Base	Other Solvent	Wavelength	Molar Absorptivity	Solvent [b]	Ref [c]
Group P1							
Amodiaquine—355.9	223, 237s, 247s, 343, 0.1*N* HCl	222, 253, 344, 0.1*N* NaOH	222, 253, 339, methanol	223 237	33 900 20 300	H_3O^+ H_3O^+	7,12 7,12
Cinchonidine—294.4	236, 316, 0.1*N* HCl	226, 283, 300, 313, H_2O, pH 7	225, 284, 300, 314, ethanol	236 316	32 200 6 200	H_3O^+ H_3O^+	12 12
Cinchophen*—249.3	242, 267, 344, 0.1*N* HCl	258, 322, 0.1*N* NaOH	222s, 260, 330, methanol	244 257	27 400 37 200	H_3O^+ OH^-	6 6
Dibucaine—343.5	225s, 247, 318, 328s, 0.1*N* H_2SO_4	225, 238, 274, 314, 326, 0.1*N* NaOH	270, 317, 327, ethanol	247 318	29 400 7 600	H_3O^+ H_3O^+	7 7
Hydroxychloroquine—336	220, 235, 256,324, 343, 0.1*N* HCl	219, 253, 325, 0.1*N* NaOH	...	221 342	29 400 19 500	H_3O^+ H_3O^+	7,12 6
Papaverine—339.4	251, 279s, 284, 309, 325s, 0.1*N* HCl	237, 277, 314, 326, 0.1*N* NaOH	239, 280, 314, 327, ethanol	see the Appendix			
Quinidine—378.5	208s, 250, 316, 345, 0.1*N* HCl	234, 273s, 279, 286, 322, 331, H_2O, pH 8	236, 278, 332, ethanol	250 279 331	36 300 4 100 5 600	H_3O^+ H_2O H_2O	12 8 8
Quinine*—378.5	208s, 250, 316, 345, 0.1*N* HCl	234, 273s, 280, 284, 320, 331, H_2O, pH 7.5	235, 281, 333, ethanol	250 280 331	38 000 4 800 6 300	H_3O^+ H_2O H_2O	12 8 8
Group P2							
Carbaryl*—201.2	220, 280, 269, 260s, 287s, 290s, 312, 0.1*N* HCl	245, 321s, 332, 0.1*N* NaOH[d]	222, 280, 270s, 260s, 291s, 313, 317, hexane	220 280 222	85 000 6 800 80 000	H_3O^+ H_3O^+ hexane	authors authors 4
Naphazoline—210.2	223, 281, 271, 288, 291, 312, 0.1*N* HCl	281, 271, 312, 0.1*N* NaOH	...	281 282	5 400 6 900	H_3O^+ H_3O^+	12 6
Propranolol*—259.4	215, 228s, 287, 292, 305, 318, 0.1*N* HCl	292, 305, 318, 0.1*N* NaOH	231, 291, 305, 319, ethanol	280 215	6 800 50 000	H_3O^+ H_3O^+	authors authors
Quinacrine*—402	279, 222, 344, 0.1*N* HCl	268, 229, 343, 0.1*N* NaOH	268, 228, 283s, 323s, 343, methanol	see the Appendix			

Group Q1							
Sulfacetamide*—214.3	215, 269, 0.1*N* HCl	256, 0.01*N* NaOH	272, ethanol	256	16 500	OH^-	authors
				272	19 600	ethanol	authors
Sulfachlorpyridazine*—284.7	215s, 256, 272s, 315, 0.1*N* HCl	258, 248s, 0.1*N* NaOH	274, ethanol		see the Appendix		
Sulfadiazine—250.3	242, 270s, 314, 0.1*N* HCl	238, 255, 0.1*N* NaOH	270, ethanol	270	21 100	ethanol	7
				242	14 600	H_3O^+	6
Sulfaethidole—284.4	214s, 275, 0.1*N* HCl	261, 280s, 0.1*N* NaOH	284, 250s, ethanol	261	18 100	OH^-	9
				275	15 700	H_3O^+	9
Sulfamerazine*—264.3	244, 305, 0.1*N* HCl	241, 255, 0.1*N* NaOH	270, ethanol	244	15 800	H_3O^+	authors
				255	21 400	OH^-	authors
Sulfamethazine—278.3	243, 300, 0.1*N* HCl	241, 258, 0.1*N* NaOH	242, 260, ethanol	243	14 900	H_3O^+	6,12
				262	16 900	OH^-	6
Sulfamethizole—270.3	214s, 275, 0.1*N* HCl	261, 0.1*N* NaOH	258s, 283, ethanol	261	18 600	OH^-	9
				275	15 300	H_3O^+	9
Sulfamethoxazole*—253.3	215s, 265, 271, 0.1*N* HCl	256, 0.1*N* NaOH	270, ethanol	256	16 800	OH^-	authors
				270	19 600	ethanol	authors
Sulfamethoxydiazine*—280.3	220s, 265, 0.1*N* HCl	245, 0.1*N* NaOH	240, 272, ethanol	245	24 100	OH^-	authors
				272	19 600	ethanol	authors
Sulfanilamide—172.2	258, 0.1*N* HCl	255, 0.1*N* NaOH	262, ethanol	258	18 900	H_3O^+	12
				255	24 000	OH^-	5
Sulfapyridine*—249.3	215s, 238, 310, 0.1*N* HCl	246, 310s, 0.1*N* NaOH	231s, 270, ethanol	246	19 400	OH^-	authors
				270	19 400	ethanol	authors
Sulfathiazole*—255.3	216s, 280, 0.1*N* HCl	256, 280s, 0.1*N* NaOH	260, 289, ethanol	256	15 400	OH^-	authors
				280	12 500	H_3O^+	authors
Sulfisoxazole*—267.3	214s, 225s, 264, 272s, 0.1*N* HCl	254, 269s, 0.1*N* NaOH	268, ethanol	254	21 200	OH^-	6
				264	10 900	H_3O^+	12
Group Q2							
Bendroflumethiazide—421.4	272, 319, 0.1*N* HCl	273, 328, 0.1*N* NaOH	272, 328, ethanol	273	17 400	OH^-	7
				329	3 400	OH^-	7
Benzthiazide*—431.9	224, 282, 304s, 0.1*N* HCl	296, 316s, 0.1*N* NaOH	283, 300s, 319, ethanol	282	10 100	H_3O^+	authors
				296	12 800	OH^-	authors
Chlorothiazide*—295.7	225, 278, 292, 300, 0.1*N* HCl	228, 292, 310, 0.1*N* NaOH	280, ethanol	228	20 700	OH^-	authors
				292	13 600	OH^-	authors

TABLE 2—*Ultraviolet absorption data on a number of compounds in each of 17 structural groups*—Continued.

Compound and Molecular Weight [a]	Wavelength Max			Absorbance Data			
	Aqueous Acid	Aqueous Base	Other Solvent	Wavelength	Molar Absorptivity	Solvent [b]	Ref [c]
Furosemide*—330.8	234, 273, 342, 0.1*N* HCl	228, 270, 333, 0.1*N* NaOH	228, 276, 328, ethanol	234	7 000	H_3O^+	authors
				270	4 000	OH^-	authors
Hydrochlorothiazide*—297.8	222s, 226, 271, 317, 0.1*N* HCl	273, 323, 0.1*N* NaOH	222, 226, 271, 318, ethanol	see the Appendix			
Hydroflumethiazide*—331.3	213, 272, 325, 0.1*N* HCl	273, 331, 0.1*N* NaOH	213, 273, 329, ethanol	273	14 500	OH^-	authors
				331	3 200	OH^-	authors
Methyclothiazide*—360.2	225, 270, 314, 0.1*N* HCl	264, 300s, 318, 0.1*N* NaOH	226, 267, 311, ethanol	264	16 200	OH^-	authors
				270	17 100	H_3O^+	authors
Polythiazide*—439.9	224, 270, 310, 0.1*N* HCl	265, 315, 0.1*N* NaOH	225, 270, 313, ethanol	265	20 800	OH^-	authors
				270	26 000	H_3O^+	authors
Quinethazone*—289.7	235, 280, 346, 0.1*N* HCl	233, 268, 345, 0.1*N* NaOH	234, 278, 346, ethanol	280	10 400	H_3O^+	authors
				234	44 000	H_3O^+	authors
Trichlormethiazide*—381	226, 267, 313, 0.1*N* HCl	224, 263, 310, 0.1*N* NaOH	267, 313, ethanol	267	19 000	ethanol	authors
				263	14 700	OH^-	authors
Group R1							
Apomorphine—267.3	211, 225s, 272, 287s, 301s, 0.1*N* HCl	295, 0.1*N* NaOH	274, 310, methanol	211	32 400	H_3O^+	10
				272	16 200	H_2O	8
Diacetylmorphine*—369.4	204, 235s, 278.5, 274s, 0.1*N* HCl	298, 251s, 0.1*N* NaOH [f]	240s, 281, ethanol	278	1 860	H_3O^+	7,10,12
				281	1 920	ethanol	12,15
Dihydromorphine—287.4	284, 0.1*N* HCl	297, 0.2*N* NaOH	210s, 235s, 285, ethanol	284	1 600	H_3O^+	11
				297	2 560	OH^-	11
Dihydromorphinone*—285.3	207s, 235s, 282, 0.1*N* HCl	235s, 290, 0.1*N* NaOH	236s, 284, ethanol	207	33 900	H_3O^+	9
				282	1 520	H_3O^+	7,11
Methyldihydromorphinone—299.4	208s, 230s, 281, 0.1*N* HCl	240s, 292, 0.1*N* NaOH	235s, 285, ethanol	281	1 200	H_3O^+	7,10
				292	1 980	OH^-	11
3-Monoacetylmorphine—327.4	205, 278, 274s, 0.1*N* HCl	251, 298, 0.1*N* NaOH [g]	240s, 282, ethanol	282	2 050	ethanol	15

6-Monoacetylmorphine—327.4	210, 240s, 285, 0.1*N* HCl	251, 297, 0.1*N* NaOH [h]	287, ethanol	285 287	1 420 1 460	H_3O^+ ethanol	11 15
Morphine*—285.4	210, 240s, 284, 280s, 0.1*N* HCl	251, 298, 0.1*N* NaOH	208s, 241s, 286, ethanol	see the Appendix			
Nalorphine*—311.4	210, 240s, 284, 280s, 0.1*N* HCl	251, 298, 0.1*N* NaOH	208s, 241s, 286, ethanol	284 298	1 470 2 440	H_3O^+ OH^-	11 11
Naloxone*—327.4	230s, 280, 0.1*N* HCl	239s, 292, 0.1*N* NaOH	. . .	280 292	1 800 3 000	H_3O^+ OH^-	authors authors
Oxymorphone—301.3	281, 0.1*N* HCl	240s, 292, 0.1*N* NaOH	206, 230s, 284, methanol	206 281	25 400 1 800	methanol H_3O^+	9 12
Group R2							
Benzylmorphine—375.5	213, 283, 0.1*N* HCl	. . .	215, 246s, 284, ethanol	213 284	31 600 1 840	H_3O^+ H_3O^+	10 7,10
Codeine*—299.4	211, 240s, 284, 278s, 0.1*N* HCl	238s, 284, 278s, 0.1*N* NaOH	211, 239s, 286, ethanol	see the Appendix			
Dihydrocodeine—301.4	230s, 284, 278s, 0.1*N* HCl	283, 277s, 0.1*N* NaOH	285, ethanol	230 284	6 800 1 720	H_3O^+ H_3O^+	12 10
Dihydrocodeinone—299.4	204, 228s, 280, 0.1*N* HCl	279, 0.1*N* NaOH	234s, 282 ethanol	208 280	34 500 1 300	methanol H_3O^+	9 7,10,11
Ethylmorphine*—313.4	211, 241s, 284, 279s, 0.1*N* HCl	284, 279s, 0.1*N* NaOH	211, 240s, 285, ethanol	211 284	25 500 1 700	H_3O^+ H_3O^+	authors authors
Oxycodone*—315.4	205, 227s, 280, 0.1*N* HCl	280, 0.1*N* NaOH	232s, 284, ethanol	280 280	1 380 1 200	H_3O^+ OH^-	12 6
Thebaine—311.4	228s, 284, 0.1*N* HCl	228s, 284, 0.1*N* NaOH	226s, 285, ethanol	226 285	15 100 7 400	ethanol ethanol	8 12
Group S							
Chlordiazepoxide*—299.8	204s, 244, 307, 0.1*N* HCl	244, 260, 307s, 0.1*N* NaOH	244, 264, 310, methanol	see the Appendix			
Clorazepate*—332.7	238, 283, 320, 0.1*N* HCl	235s, 256s, 362, 0.1*N* NaOH	. . .	238 283	28 600 13 100	H_3O^+ H_3O^+	18 18
Diazepam*—284.7	240, 284, 360, 0.1*N* H_2SO_4	228, 251s, 310, 0.1*N* NaOH	230, 254s, 313, ethanol	240 284	28 200 12 800	H_3O^+ H_3O^+	18 18

TABLE 2—*Ultraviolet absorption data on a number of compounds in each of 17 structural groups*—Continued.

Compound and Molecular Weight [a]	Absorbance Data			Wavelength Max			
	Aqueous Acid	Aqueous Base	Other Solvent	Wavelength	Molar Absorptivity	Solvent [b]	Ref [c]
Flurazepam*—388	236, 284, 356, 0.1*N* HCl	230s, 254s, 311, 0.05*N* NaOH	228, 255s, 316, ethanol	237	44 600	H_3O^+	18
				282	16 800	H_3O^+	18
Nitrazepam—281.3	278, 340s, 0.1*N* HCl	230s, 263, 375, 0.1*N* NaOH	218, 360, ethanol	278	42 200	H_3O^+	7
Oxazepam—286.7	236, 282, 0.2*N* H_2SO_4	235, 260s, 343, 0.1*N* NaOH	230, 315, ethanol	236	28 100	H_3O^+	18
				230	34 400	ethanol	7
Group T							
Dihydroergotamine—583.7	279, 0.1*N* HCl	279, 0.1*N* NaOH	...	279	6 200	H_3O^+	12
Ergonovine—325.4	222, 240s, 311, 0.1*N* HCl	235, 307, 0.1*N* NaOH	240, 311, ethanol	311	8 100	H_3O^+	7
Ergotamine—581.7	239s, 317, 0.1*N* HCl	235, 307, 0.1*N* NaOH	240, 320, methanol	239	21 100	H_3O^+	7,12
				317	6 600	H_3O^+	7
Lysergic acid diethylamide*—323.4	225s, 240s, 310, 0.1*N* HCl	238, 308, 0.05*N* NaOH	226s, 242s, 311, ethanol	see the Appendix			
Methylergonovine—339.4	226, 313, 0.1*N* H_2SO_4	226, 240s, 311, 0.1*N* NaOH	208, 240s, 311, methanol	226	23 700	H_3O^+	7
				313	8 600	H_3O^+	7
Group U							
Antipyrine*—188.2	231, 258s, 264s, 0.1*N* HCl	242, 258, 0.1*N* NaOH	235, 244, 270, ethanol	241	9 000	H_2O	6
				231	11 000	H_3O^+	7
Berberine—353.4	228, 264, 345, 0.1*N* H_2SO_4	228, 264, 0.5*N* NaOH	267, 347, ethanol	228	20 400	H_3O^+	7
				267	27 100	ethanol	7
Chlortetracycline—478.9	228, 265, 319, 337, 0.1*N* HCl	223, 253, 284, 346, 0.1*N* NaOH	231, 255, 320, 340, methanol	253	29 200	OH^-	7
				265	17 500	H_3O^+	7
Chlorthalidone*—333.8	207s, 227s, 275, 283, 0.1*N* HCl	273s, 281, 0.1*N* NaOH	274, 283, ethanol	275	20 300	ethanol	7
				284	15 300	ethanol	7
Clemizole—325.9	275, 282s, 0.1*N* H_2SO_4	254, 267, 274, 282, 0.1*N* NaOH	253, 268, 276, 283, ethanol	274	11 000	H_3O^+	5
				254	8 500	OH^-	5
Diphenadione*—340.4	238, 277, 288, 306, 314, 0.1*N* H_2SO_4	246, 275, 284, 312, 323, 0.1*N* NaOH	221, 238, 275s, 285, 313, 325, ethanol	238	61 200	H_3O^+	7
				246	17 000	OH^-	7

Dimethindene*—292.4	260, 290s, 225s, 0.1*N* HCl	262, 269s, 227s, 0.1*N* NaOH	258, 263s, 269s, ethanol	260	16 400	H_3O^+	authors
Haloperidol*—375.9	220, 225s, 248, 0.1*N* HCl	248, 0.1*N* NaOH	220, 225s, 247, ethanol	248	13 000	H_3O^+	7
Methaqualone*—250.4	234, 229s, 269, 275, 294, 0.1*N* HCl	226, 231s, 263, 294s, 305, 316, 0.1*N* NaOH	227, 266, 273s, 305, 317s, ethanol	see the Appendix			
Oxyphenbutazone*—342.4	235, 280, 0.1*N* HCl	253, 0.1*N* NaOH	242, 275s, ethanol	254	51 300	OH^-	7
Oxytetracycline—496.5	267, 0.1*N* HCl	245, 267, 0.1*N* NaOH	269, 339, ethanol	269	19 900	H_3O^+	7
Phenylbutazone*—308.4	236, 274s, 0.1*N* HCl	266, 0.1*N* NaOH	240, ethanol	264	20 600	OH^-	7,5
Reserpine—608.7	217, 268, 292, methanolic HCl	217, 267, 295, methanolic KOH	217, 267, 295, methanol	217	15 500	methanol	7,9
Rotenone*—394.4	234, 242s, 292, 0.1*N* HCl	240s, 294, 0.1*N* NaOH	234, 241s, 291, 315s, ethanol	235 292	18 900 21 700	H_3O^+ H_3O^+	7 7
Sulfinpyrazone*—404.5	237, 0.1*N* HCl	259, 0.1*N* NaOH	265, ethanol	259 265	24 000 28 300	OH^- ethanol	authors authors
Trimethobenzamide—424.9	213, 257, 0.1*N* HCl	212, 260, 0.1*N* NaOH	213, 261, methanol	257 261	17 500 12 400	H_3O^+ methanol	5 9

[a] Compounds are listed by group as in Table 1; not all substances in Table 1 are given in this table. Molecular weights are given so that molar absorptivity values can be converted to 1%, 1-cm cell absorptivities ($A^{1\%}_{1\,cm}$ or $E^{1\%}_{1\,cm}$). Starred (*) compounds were analyzed spectrophotometrically by the authors. The values given in Columns 2, 3, and 4 under "Wavelength Max" were chosen to reflect a consensus or average of all sources available, including the authors', and are not always in exact agreement with the values in Column 5, which were taken from specifically cited sources.

[b] Solvents are abbreviated as follows: H_3O^+ is 0.05 to 0.5*N* aqueous HCl or H_2SO_4; OH^- is 0.05 to 0.5*N* NaOH or KOH; ethanol is either absolute or 95% ethanol.

[c] Where more than one reference is given, absorptivities have been averaged.

[d] The strongest absorption max is underlined.

[e] Hydrolyzed to α-naphthol in alkaline solution.

[f] Diacetylmorphine (heroin) converts to 6-monoacetylmorphine and morphine within 1 to 2 min after being placed in 0.1*N* NaOH.

[g] UV scan similar to diacetylmorphine; hydrolyzed in 0.1*N* NaOH to morphine.

[h] UV scan similar to morphine.

TABLE 3—*Ultraviolet absorption data for a number of compounds containing isolated chromophores and for several heterocyclic compounds.*

Compound and Molecular Weight	Group Number	Chemical Class	Wavelength Max	Molar Absorptivity	Solvent	Ref
Acetone—58	X1	aliphatic ketone	279	15	*n*-hexane	19
Amyl nitrite—117.1	X1	nitro-alkane	358	27	0.1*N* H_2SO_4	12
Camphor—152.2	X1	aliphatic ketone	289	30	ethanol	7
Ethinamate—167.2	X1	carbamate ester	265	40	0.1*N* H_2SO_4	7
Methyprylon—183.3	X1	aliphatic ketone and amide	291	30	0.1*N* HCl	authors
Nitroglycerin—227.1	X1	aliphatic nitric acid ester	276	10	water	authors
Aldrin—364.9	X2	chlorinated hydrocarbon with ethylene groups	211	2 400	ethanol	authors
Dieldrin—380.9	X2	chlorinated hydrocarbon with ethylene groups	226	6 700	hexane	4
Ethchlorvynol—144.6	X2	acetylene and ethylene groups	253	40	water	authors
			200s	1 000	water	authors
Furfural—96	Y1	furan ring with conjugated carbonyl	276	16 300	water, pH 6	authors
			228	3 700	water, pH 6	authors
Furazolidone—225.2	Y1	furan ring with conjugated carbonyl and azo	261	12 400	methanol	9
			204	7 300	methanol	9
Nitrofurazone—198.1	Y1	furan ring with conjugated azo and nitro	260	11 500	0.1*N* NaOH	12
			375	. . .	0.1*N* NaOH	12
Amitrole—84.1	Y2	nitrogenous heterocycle with unsaturation	341	4 960	ethanol	6
			235	. . .	ethanol	12
Atrazine—216.1	Y2	nitrogenous heterocycle with unsaturation	221	21 000	0.1*N* HCl	authors
			272	4 500	0.1*N* HCl	authors
Pilocarpine—208.3	Y2	nitrogenous heterocycle with unsaturation	214	5 100	0.1*N* HCl	authors
Acetazolamide—222.2	Y3	nitrogen-sulfur heterocycle with a chromophore	240	3 600	0.1*N* NaOH	authors
			291	12 800	0.1*N* NaOH	authors
			265	10 300	0.1*N* HCl	authors
Isocarboxazid—231.3	Y3	nitrogen-oxygen heterocycle with a chromophore	272	7 400	0.1*N* NaOH	7,12

Each compound listed in Table 1 is known to have absorption characteristics of the group in which it is listed. Efforts were made by the authors to include in Table 1 current drugs, new drugs, and drugs sold illegally in the United States. A qualification of the structural features of each group is given in the Appendix. An example of at least one compound in each group is shown in Figs. 1–3.

Table 2 presents the absorption properties of groups L1 through U in terms of maximum wavelength (λ_{max}) and molar absorbancies. Spectra λ_{max} are given in aqueous acid, aqueous base, and a third solvent. Each compound was checked for agreement of spectral data from at least two sources, those being chiefly Ref *4–12*, and the authors' accumulated collections. Specific references are given for molar absorptivity (ϵ) values appearing in Table 2; where more than one source is given, the ϵ values are averages. Not all compounds listed in Table 1 are presented in Table 2, as space limitations required some selectivity in data presentation.

Properties of the Individual Groups

The more common phenothiazine derivatives, Group L1, typically have a very strong central absorption band near 255 nm in aqueous acid solution. A dilute aqueous base produces a λ_{max} shift of a few nanometres and a slight increase in absorptivity. An upper but weaker band near 300 nm is invariably present. Group L1 phenothiazines can be differentiated from other groups on the basis of UV absorption characteristics. Phenothiazines isolated from biological specimens contain sulfoxide metabolites which have four or five maxima between 230 and 350 nm [*13*]. Group L2 contains a smaller group of phenothiazine derivatives characterized by two strong central bands. Conjugation in Group L2 is extended by one more double bond than Group L1 by a ring chromophore substituent.

Some coumarin derivatives (Group M) are used in humans for medical purposes. Other coumarins find use as rodenticides (for example, warfarin). The strong, detailed absorption pattern above 275 nm, which is very pH dependent, gives Group M compounds a high level of UV specificity.

Group N1 compounds have spectra which differ perceptibly from the spectra of all other groups (those in Refs *1* and *2* and in this paper). The 272±5-nm band (aqueous solution) is the prominent feature; subtle absorption changes occur when the acidity is drastically changed. For example, λ_{max} shifts downward slightly in changing from 0.1*N* HCl to 2*N* HCl. Theobromine, 8-chlorotheophylline, and xanthine have acidic protons within a conjugated system and show moderate changes as the pH is raised. Purines and pyrimidines (Group N2) have amino and oxygen substituent groups and exhibit greater variation in spectra with pH change than do Group N1 substances. Other than adenosine monophosphate and idoxuridine, Group N2 compounds are not available to the public. Some of these compounds may occur in extracts of biological specimens [*14*].

The spectra of Group O1 compounds might be mistaken for some compounds in Groups C1, F2 [*1*], or O2. However, careful attention to the details of spectra will generally narrow down the number of "look alikes" to a few compounds within the groups mentioned. The position and kind of substituent on the benzene ring influences the position and intensity of λ_{max}, as Bailey et al [*16*] demonstrated with six isomeric dimethoxyamphetamines. Groups O1 and O2 are separated on the basis of the number of O-alkyl and alkyl groups present, Group O1 having up to three substituents, one of which may be O-alkyl, and Group O2 having two or more O-alkyl substituents in addition to one or more alkyl substituents. Di-O-alkyls with no alkyl substituent have been placed in Group O1 because of greater resemblance to Group O1 compounds, Group O2 compounds have absorption patterns like those of Group O1 except that in Group O2 the two major absorption bands are of approximately the same intensity. In

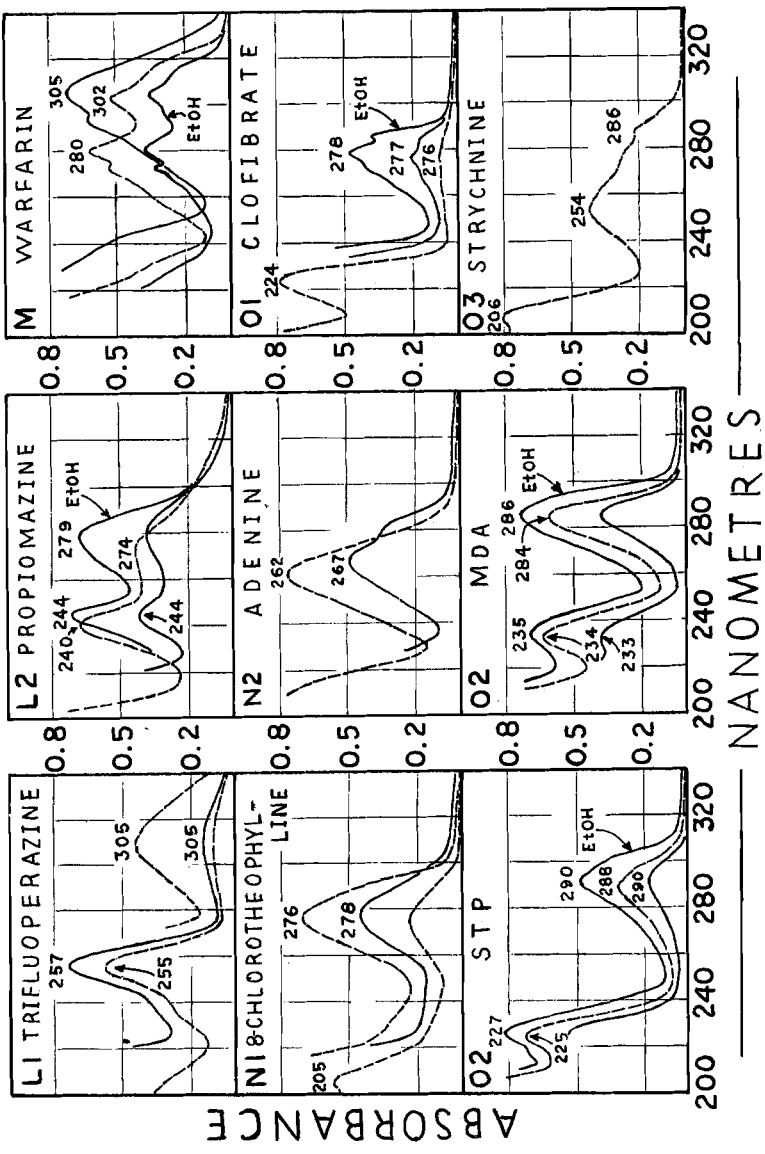

FIG. 1—*Ultraviolet spectra representing eight structural groups. The dashed line traces the absorbance scan in 0.1N HCl; a solid line traces the absorbance scan in 0.1N NaOH; solid lines marked "EtOH" trace scans made in 95% ethanol. STP is 2,4-dimethoxy-4-methylamphetamine and MDA is 3,4-methylenedioxy amphetamine.*

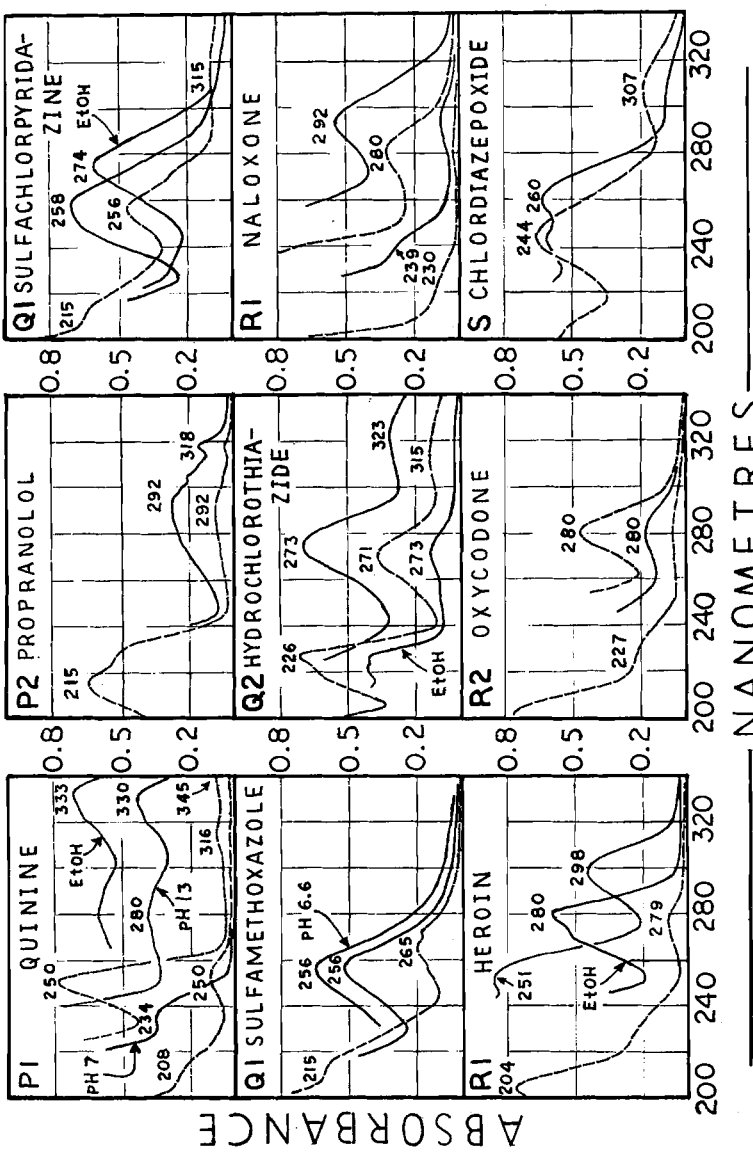

FIG. 2—*Ultraviolet spectra representing seven structural groups. Dashed and solid lines are used as in Fig. 1. The 0.1 N NaOH scan for heroin is indentical to the aqueous base scan for morphine, since heroin is converted to morphine and 6-monoacetylmorphine in aqueous base (see text). The spectrum of 3-monoacetylmorphine in 0.1 N HCl is practically identical to that of heroin* [15].

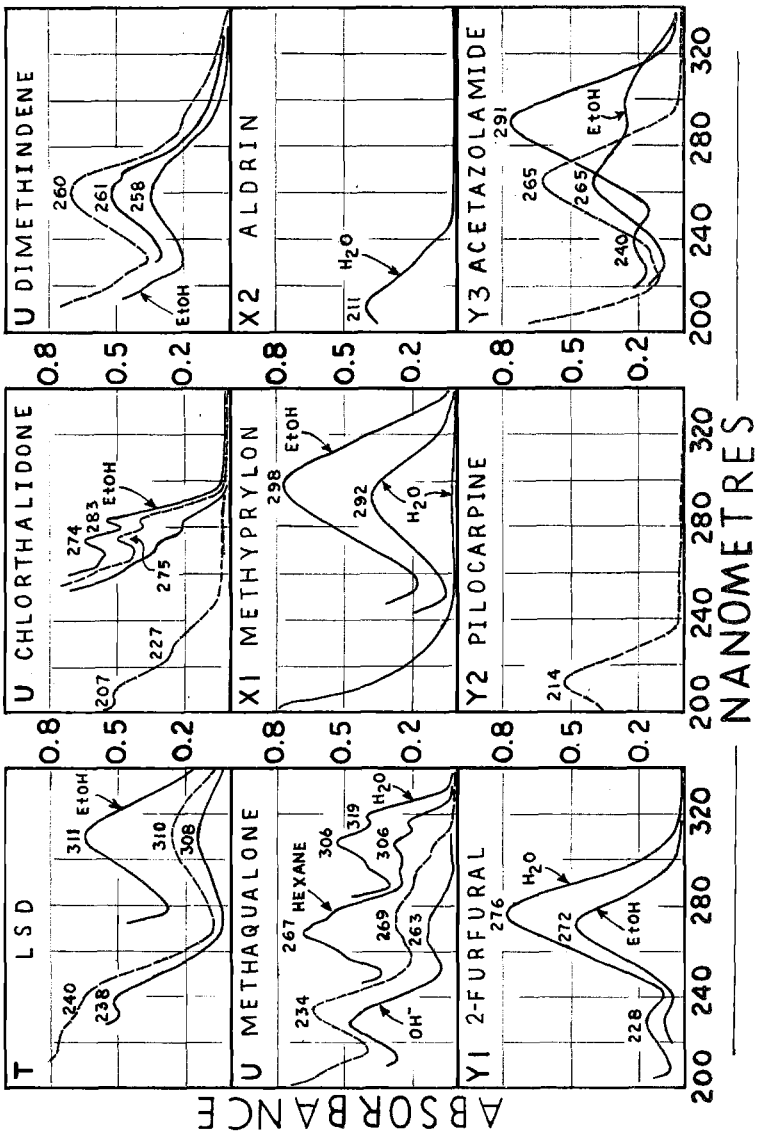

FIG. 3—*Ultraviolet scans representing seven structural groups. Dashed and solid lines are used as in Fig. 1. LSD designates lysergic acid diethylamide.*

Group O1, the lower band is usually at least three times as intense as the upper band. Group O3 compounds, all of which contain the acetanilide unit phenyl–NCO–C–, differ widely in absorption profiles depending on the substituents on the aromatic ring. The spectra of lidocaine and mepivacaine are identical, as both are *ortho*-dimethyl substituted acetanilides.

Several features characterize Group P1 compounds: (1) absorption bands above 300 nm which are pH dependent, (2) a strong central absorption area which changes appearance significantly as the pH is raised above 7, and (3) fluorescence in sulfuric acid solutions. Naphthalene derivatives of Group P2 may be recognized by the presence of a very strong band near 220 nm and a broad, finely structured band near 285 nm with minor maxima above 300 nm. Compounds of Group P2 with three aromatic rings exhibit complex absorption patterns, with some bands above 340 nm.

The various sulfonamide derivatives all have the same general absorption profile; however, with a few exceptions, each sulfonamide derivative in Group Q1 has a specific UV absorption. Solvent changes and pH changes in the 4 to 7 range will cause moderate λ_{max} shifts with these sulfonamides. Group Q1 and Q2 compounds have structural similarities. The differences are that in Q2 the central band is positioned at a slightly higher wavelength (270 nm), and a lower band near 225 nm and an upper band near 310 nm are present.

The UV absorption properties of morphine and codeine-type narcotics, Groups R1 and R2 respectively, have been studied by a number of authors [*10,11,15*]. The two groups each have three absorption bands: one near 208 nm; a broad, low-profile band in the 225 to 245 nm region; and a third band near 280 nm. Group R1 compounds all show a phenol shift as the pH is raised above 8; in Group R2, the phenol is alkylated to a neutral ether bond and very little change with pH is observed.

Morphine derivatives such as heroin (diacetylmorphine), 3-monoacetyl-morphine, and nicomorphine have been placed in Group R1 because in alkaline solution (pH 9 or greater) the phenolic ester group is rapidly cleaved by hydrolysis, yielding a free phenol, and therefore giving a typical Group R1 scan. Morphine, nalorphine, 6-monoacetylmorphine, morphine-*N*-oxide, and normorphine all have the same absorption profile and cannot be differentiated by ordinary UV analysis. On the other hand, if heroin free of other UV absorbing compounds is scanned first in water or dilute aqueous acid, then in aqueous base, and finally in dilute acid by re-acidifying the solution that was made basic, a highly specific absorption profile is obtained. Only 3-monoacetylmorphine would show the same absorption picture using the three scans described. A number of morphine and codeine-type narcotics in Table 1 are obsolete or used only in research studies. Acetorphine, cyprenorphine, and etorphine, opium derivatives listed in Schedule I(b) of Public Law 91—513,[4] have found use in veterinary medicine. Pholcodine, originally on Schedule I(b), is now being marketed as a cough suppressant.

Group S includes six benzodiazepines now being marketed in the United States or Europe. Specific analysis of lysergic acid diethylamide (LSD) by UV spectrophotometry does not appear to be attainable, as several other ergot alkaloids show very similar absorption patterns.

The major weakness of the classification system presented here and previously [*1,2*] lies in the fact that those compounds with isolated conjugated systems within the same molecule have absorption properties which preclude a practical systematic classification. However, the number of such drugs is not large, and these chemically complex drugs have been placed in Group U. Certain compounds in Group U have a relatively

[4] Public Law 91–513, the Controlled Substances Act of 1970 passed by the United States Congress, lists 22 opium derivatives under Schedule I(b). Most of these are virtually unobtainable, either legally or illegally.

simple absorption profile and could be mistaken for compounds in other groups. Most substances in Group U have highly specific absorption profiles.

The letters V, W, and Z were not used so that additional groups could be accommodated in the system, if needed. The X and Y groups do not have easily recognized absorption patterns, and many of the compounds in these groups absorb so weakly that they are not amenable to UV analysis. The UV absorption properties of the X and Y groups are summarized in Table 3. Group X1 includes compounds having an isolated chromophore, $-C=0$ or $-N=0$. Group X2 compounds include those with nonconjugated chlorinated double bonds. Many pesticides possess the structural requirements of Group X2, but are not presented in Table 3 as Gore et al [*4*] have published the spectra of 76 pesticides, including Group X2 compounds. The Y groups (Y1, Y2, and Y3) each contain a particular type of heterocyclic ring. The hetero-atom in Group Y1 is oxygen or sulfur, in Group Y2 nitrogen, and in Group Y3, nitrogen and oxygen or nitrogen and sulfur.

Conclusion

The classification system presented by the authors here and in two previous publications was developed by simply placing compounds with identical conjugated systems in the same group. Similarities in UV spectra are an aspect of structural similarities. Biological properties of drugs (as well as every physical and chemical property) are likewise a consequence of chemical structure. Therefore, Table 1 classifies not only by structural group but also by pharmacological action for many of the groups, which is advantageous in toxicology. A second advantage of Table 1 is that when an unknown is found to match the spectra of a certain known, one has a list of other compounds which may have identical or nearly identical UV spectra. In no case would the authors claim that an identification should or even can be made on the basis of UV spectra alone. The UV analysis more often than not will rapidly narrow the possibilities, sometimes to a single choice. Confirmation of a UV identification may be accomplished by the right selection of other analytical techniques. Those using this system should save analysis time and be forced to think of drugs, pesticides, and various toxic substances in terms of chemical structure. The identification of an unknown compound is accomplished by showing that a certain chemical structure is specifically indicated, not by merely showing that the unknown has X number of properties which match a certain known compound or by doing a specified number of tests.

Summary

The ultraviolet absorption spectra of 22 different chemical (structural) groups of drugs and toxic compounds were studied. This paper completes a three-part series in which more than 500 individual compounds have been grouped according to structure as it pertains to characteristics of the ultraviolet absorption scan. Each group has a typical absorption profile with respect to the number of bands between 200 and 340 nm, the intensity of the band(s), and the changes in absorption pattern with solvent and pH changes.

Phenothiazines, xanthines, coumarins, quinolines, naphthalene derivatives, O-alkyl benzene derivatives, opiates, ergot alkaloids, benzodiazepines, and various heterocyclic compounds are among the groups of compounds covered in this paper.

APPENDIX

Summary of the Ultraviolet Absorption Characteristics of Compounds in the Different Structural Groups

Group L1—Phenothiazines without a ring chromophore substituent.

1. Maxima (given in nm).
   a. 205–218 nm in H_2O/H_3O^+; shoulder apparent with higher molecular weight phenothiazines.
   b. 254±4 nm in H_3O^+ (a few phenothiazines are slightly outside these limits); 1–3-nm red shift in OH^-; shoulder on low wavelength side may be noted.
   c. 308±8 nm in H_3O^+; 2–5-nm red shift in OH^-.
2. Solvent polarity effects (water versus organic solvents)—Middle and upper bands show a moderate red shift (2–6 nm), and fine structure is more pronounced in less polar solvents.
3. Example (compound having spectra typical of this group)—Prochlorperazine.

Band Max [a]	Molar Absorptivity	Solvent	Ref
213s, 254, 305	—,42 400, 6 700	0.1*N* HCl	authors, 5
257, 312	46 000, 6 100	ethanol	7
256, 307	44 200, 7 200	0.1*N* NaOH	5

[a] Where more than one maxima is given, the strongest is underlined.

Group L2—Phenothiazines with a chromophone substituent.

1. Maxima.
   a. 239±5 nm in H_3O^+; shows a 1–3-nm red shift in OH^-.
   b. 270±10 nm in H_3O^+; connected to the 239-nm band by a shallow minimum; 2–10-nm shift in OH^-.
   c. Above 300 nm in H_2O; a broad, very weak R band.
2. Solvent polarity effects—Moderate changes in less polar solvents including ethanol.
3. Example—Propiomazine.

Band Max	Molar Absorptivity	Solvent	Ref
204, 240, 274	—,30 200, 21 000	0.1*N* HCl	authors
244, 280	23 100, 21 000	0.1*N* NaOH	authors
244, 270s, 279	. . .	ethanol	authors

Group M—Coumarin derivatives.

1. Maxima.
   a. 200–240 nm in H_2O/H_3O^+; several shoulders or inflections, or both, in this range following a minimum near 245 nm.
   b. 280±10 nm and 305±10 nm in H_2O; this band is very pH dependent, showing a large phenol shift in OH^-; pH 7 scan is unlike H_3O^+ or OH^- scan.
2. Solvent polarity effects—Very pronounced for all bands with increased fine structure in less polar solvents.
3. Example—Warfarin.

Band Max	Molar Absorptivity	Solvent	Ref
215s, 232s, 270, 280, 302, 317s	10 500 at 280 nm	0.1*N* HCl	authors
240s, 291s, 305	12 600 at 305 nm	0.1*N* NaOH	authors
232s, 240, 259s, 269, 280, 291, 304, 311s, 317	8 600 at 304 nm	95% ethanol	authors

Group N1—Alkylated and halogenated xanthines.

1. Maxima.
   a. 272±6 nm in H_2O; position of this max is pH dependent.
   b. 205±2 nm in H_2O; this band is slightly more intense than the 272 band, but it may appear only as a shoulder or inflection.
   c. 235±5 nm in H_2O; shoulder or slight inflection following a minimum near 240 nm; more pronounced in OH^- whenever the compound is acidic.
2. Solvent polarity effects—272 band shows a red shift of a few nanometres in less polar solvents.
3. Example—Theobromine (3,7-dimethyl xanthine).

Band Max	Molar Absorptivity	Solvent	Ref
205, 271	20 000, 10 400	H_2O, pH 7	authors
234s, 274	5 250, 10 500	H_2O, pH 10	8
234, 274	7 080, 10 300	H_2O, pH 13	6,7,8

Group N2—Purines and pyrimidines, biological bases associated with nucleic acids.

1. Maxima.
   a. 250–290 nm in H_2O; two bands or one band with an extended shoulder.
   b. Below 220 nm a strong band is present.
2. Solvent and pH effects—Bands are strongly pH dependent with respect to position and intensity; N2 compounds are poorly soluble in solvents less polar than ethanol.
3. Example—Guanine.

Band Max	Molar Absorptivity	Solvent	Ref
248, 270s	11 500, 7 240	H_2O, pH 0	8
245, 274	11 000, 8 300	H_2O, pH 6	8
243, 273	8 500, 10 000	H_2O, pH 11	8
273	9 500	H_2O, pH 14	8

Group O1—Alkyl and O-alkyl substituted benzene derivatives containing not more than three substituents and only one O-alkyl if three substituents are present.

1. Maxima.
   a. 226±6 nm in H_3O^+; an E_2 band transition.
   b. 273±7 nm in H_3O^+; a B band transition.
2. Solvent polarity and pH effects—B band shows a slight red shift and more fine structure in less polar solvents; pH effects are slight.
3. Example—Dextromethorphan.

Band Max	Molar Absorptivity	Solvent	Ref
218, 278	7 560, 2 000	dilute HCl	10,6

Group O2—Alkyl and O-alkyl substituted benzene derivatives containing three or more substituents at least two of which are O-alkyl; also compounds related to epinephrine (diphenols with one alkyl group).

1. Maxima.
   a. 230±9 nm in H_3O^+; an E_2 band transition.
   b. 280±10 nm in H_3O^+; a B band transition.
2. Solvent polarity and pH effects—Both bands show a moderate red shift in less

polar solvents, the B band showing more fine structure; pH effects are slight except for epinephrine-type compounds which show the phenol red shift.

3. Example—2,4-Dimethoxy-4-methylamphetamine (STP).

Band Max	Molar Absorptivity	Solvent	Ref
225, 288	7 100, 3 300	0.1*N* HCl	authors
222, 290	6 900, 3 100	0.1*N* NaOH	authors
227, 290	...	95% ethanol	authors

Group O3—Acetanilide derivatives with one or more ring substituents.

1. Maxima.
   a. 200±10 nm in H_2O; a strong band which may be below ordinary UV range.
   b. 248±17 nm in H_2O; most O3 compounds have a strong max in this range; di-*ortho* alkylated acetanilides such as lidocaine and mepivacaine have a weak band near 265 nm and a strong band near 200 nm.
2. Solvent polarity and pH effects—Moderate red shift in less polar solvents; pH effects are not significant.
3. Example—Strychnine.

Band Max	Molar Absorptivity	Solvent	Ref
206	25 000	0.1*N* HCl	authors
254±1	12 670±240 [a]	dilute HCl	7 sources
277, 286	4 400, 3 500	0.1*N* HCl	authors

[a] An average of the reference sources ±1 SD.

Group P1—Quinolines with one to three substituents.

1. Maxima.
   a. 203±10 nm; H_2O or non-acidic solution.
   b. 275±15 nm in H_2O with secondary max or shoulders.
   c. 310–360 nm in H_2O; usually a compounded max with two or more absorption peaks.
2. Solvent polarity and pH effects—Spectrum shows additional fine structure in nonpolar solvents; a red shift of 4–16 nm in H_3O^+ as the ring nitrogen becomes protonated near pH 5.
3. Example—Papaverine.

Band Max	Molar Absorptivity	Solvent	Ref
251, 284, 309	60 700, 6 400, 8 200	1*N* H_2SO_4	6
251, 309	57 500, 8 600	dilute HCl	7,12

Group P2—Polynuclear aromatics, two or more fused aromatic rings.

1. Maxima.
   a. Naphthalene derivatives: very strong band at 220±5 nm and a broad band centered near 285 in H_2O or ethanol; upper band has secondary max above 300.
   b. Three rings: very strong band near mid-UV with lesser bands above and below the central band.
2. Solvent polarity and pH effects—Additional fine structure in less polar solvents; changes occur with pH when an amine group is part of the aromatic system.
3. Example—Quinacrine.

Band Max	Molar Absorptivity	Solvent	Ref
222, 279, 344	11 900, 42 200, 7 900	0.1*N* HCl	authors
228, 268, 325, 343	38 700 at 268	0.1*N* NaOH	authors
228, 268, 325, 345	58 100 at 268	95% ethanol	authors

Group Q1—Sulfonamides.

1. Maxima.
   a. Sulfonamides with a second nitrogenous unsaturated heterocycle: strong band at 260±20 nm in H_3O^+ which forms a doublet or broadened max in OH^-; lower band or shoulder at 200–220 nm in H_3O^+
   b. Sulfonamides with one unsaturated aromatic ring: strong band in the 245–275-nm range which is pH dependent; lower band or shoulder below 220 nm.
2. Solvent polarity effects—Central band shifts to higher wavelength in ethanol.
3. Example—Sulfachlorpyridazine.

Band Max	Molar Absorptivity	Solvent	Ref
215s, 256	16 200, 12 900	0.1*N* HCl	authors
249s, 258	21 000, 22 000	0.1*N* NaOH	authors
212s, 274	. . .	95% ethanol	authors

Group Q2—Benzothiadiazines and related compounds.

1. Maxima.
   a. 224±10 nm in H_3O^+; this band may exhibit fine structure.
   b. 275±8 nm in H_3O^+; about ⅓ as intense as the lower band.
   c. 320±10 nm in H_3O^+; a broad weak band.
2. Solvent polarity and pH effects—Two lower bands show slight changes in less polar solvents and a slight ± shift in OH^-; upper band shows a 2–10-nm shift in OH^-.
3. Example—Hydrochlorothiazide.

Band Max	Molar Absorptivity	Solvent	Ref
226, 271, 317	45 000, 18 300, 3 000	0.1*N* HCl	authors
273, 323	15 200, 2 900	0.1*N* NaOH	authors
222, 226, 271, 318	17 900 at 271	95% ethanol	authors

Group R1—Morphine-type opiates (free phenol functional group).

1. Maxima.
   a. 210±5 nm in H_2O/H_3O^+; max or pronounced shoulder.
   b. 235±10 nm in H_2O/H_3O^+; a broad, smooth, low profile band showing a red shift of approximately 10–15 nm in OH^-.
   c. 284±4 nm in H_2O/H_3O^+; red shift of approximately 15 nm in OH^- above pH 8.
2. Solvent polarity effects—Upper band shows a slight to moderate red shift in ethanol.
3. Example—Morphine.

Band Max	Molar Absorptivity	Solvent	Ref
210±1	27 050±926	dilute HCl	4 sources
285±1	1 611±71	dilute HCl	7 sources
298±1, 251	2 662, 6 920	dilute NaOH	5 sources

Group R2—Codeine-type opiates (phenol group is alkylated).

1. Maxima.
   a. 210±5 nm in H_2O; max or pronounced shoulder.
   b. 235±10 nm in H_2O; a broad shoulder.
   c. 283±3 nm in H_2O; no shifting of max with pH change.
2. Solvent polarity and pH effects—Upper band shows a slight red shift in ethanol; pH effects are negligible.
3. Example—Codeine.

Band Max	Molar Absorptivity	Solvent	Ref
212±1	25 275±896	dilute HCl	4 sources
285	1 612±87	dilute HCl	9 sources
239s	4 680	95% ethanol	8

Group S—Benzodiazepines.

1. Maxima.
   a. 200±6 nm in H_2O; this band follows a minimum near 220; may be a shoulder.
   b. 240±5 nm in H_3O^+; this band changes its pattern in OH^-.
   c. 294±15 nm in H_3O^+; this band is pH dependent, shifting or broadening in OH^-
2. Solvent polarity effects—Slight to moderate changes in less polar solvents.
3. Example—Chlordiazepoxide.

Band Max	Molar Absorptivity	Solvent	Ref
204s, 245, 307	23 000, 31 000, 8 700	dilute HCl	5 sources
243, 260, 308	29 100, 30 600, 6 500	0.1*N* NaOH	4 sources

Group T—Ergot alkaloids including lysergic acid diethylamide and derivatives.

1. Maxima.
   a. One or more maxima below 230 nm in H_2O.
   b. 240±5 nm in H_2O/H_3O^+.
   c. 312±5 nm in H_2O; a relatively strong, broad band.
2. Solvent polarity and pH effects—Upper band shows slight changes in less polar solvents; all bands show some changes as pH is elevated.
3. Example—Lysergic acid diethylamide (LSD).

Band Max	Molar Absorptivity	Solvent	Ref
225s, 240s, 310	22 600, 20 000, 7 100	0.1*N* HCl	authors
226s, 242s, 311	23 300, 18 000, 8 300	95% ethanol	authors
238, 308	. . .	0.1*N* NaOH	authors

Group U—Compounds with two or more conjugated systems separated by saturated atoms.

1. Maxima—Spectra are complex and not easily predictable from considerations of chemical structure; three or more bands may occur, or a single central band between 230–280 nm with minor lower and upper bands.
2. Solvent polarity and pH effects—Solvent effects are pronounced for compounds with polar auxochrome and chromophore substituents adjacent to conjugated systems; pH effects are noted when acidic or basic functional groups are present.
3. Example—Methaqualone.

Band Max	Molar Absorptivity	Solvent	Ref
234, 269, 275, 294	33 600, 8 000, —, —	0.1*N* HCl	authors
226, 231s, 263, 305, 316	9 300 at 363	H_2O, pH 6.6	authors
227, 266, 273s, 305, 317s	33 400 at 227	ethanol	6, authors

Group X1—Unconjugated carbonyl, nitro- or nitroso-chromophores.

1. Maxima.
   a. 278–294 nm in ethanol for n→π^* transitions of >C=O (carbonyl) or −N=O (nitro); a very weak band.
   b. Below 210 nm in H_2O or ethanol for a polynitrated alcohol or alkane; absorbance increases gradually from about 230 nm and down.
2. Solvent polarity and pH effects—n→π^* transitions show a red shift as solvent polarity decreases; pH effects are not significant.

Group X2—Chlorinated alkenes and alkanes; includes many chloro-organic pesticides.

1. Maxima—Absorbance begins at approximately 250 nm with no sharp maxima before 200 nm; some compounds show very weak bands above 240 nm.
2. Solvent polarity and pH effects—Both effects are slight or negligible.

Group Y1—Saturated and unsaturated heterocycles containing oxygen.

1. Maxima—Two bands of moderate intensity are usually present in conjugated, unsaturated compounds.
2. Solvent polarity and pH effects—Moderately large solvent effects; pH effects are noted with acidic and basic substances.

Group Y2—Unsaturated heterocycles containing nitrogen.

1. Maxima—Moderately strong band near 215 nm; compounds with extensive unsaturation or chromophore substituents have an upper and lower band.
2. Solvent polarity and pH effects—Both effects are moderately pronounced.

Group Y3—Unsaturated heterocycles containing both nitrogen and oxygen or nitrogen and sulfur.

1. Maxima—Two or more bands are generally present.
2. Solvent polarity and pH effects—Both effects are generally pronounced.

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