

1	R	945	945R	54.7P	Cocaine
2	R	935	936R	54.7P	Cocaine
3	R	932	933R	54.7P	Cocaine
4	R	931	940R	34.3P	Allopseudococaine
5	R	931	934R	54.7P	Cocaine
6	M	926	935R	54.7P	Cocaine
7	R	916	916R	54.7P	Cocaine
8	M	902	903R	9.71P	Pseudococaine
9	R	881	884R	9.71P	Pseudococaine
10	M	859	928R	34.3P	Allopseudococaine
11	M	823	895R	1.10P	Allococaine
12	M	703	772R	0.05P	m-Hydroxycocaine
13	M	689	885R	0.03P	Isobutyroylecgonine methyl ester
14	M	674	750R	0.02P	trans-Cinnamoylcocaine
15	M	666	853R	0.01P	Propionylecgonine methyl ester
16	M	662	734R	0.01P	Cinnamoylcocaine
17	M	654	820R	0.01P	Acetoxyecgonine methyl ester
18	M	648	772R	0.00P	Phenylacetoxyecgonine methyl ester
19	M	636	840R	0.00P	Valeroylecgonine methyl ester
20	M	602	675R	0.00P	o-Chlorococaine
21	M	568	675R	0.00P	Acetic acid, 2-(3-hydroxy-8-azabicyclo[3.2.1]oct-8-yl)-1,1-diphenylethyl ester
22	R	554	650R	0.00P	Ecgonine methyl ester
23	M	544	665R	0.00P	Benzenepropanol, $\alpha$ -phenyl- $\gamma$ -(phenylamino)-
24	M	534	620R	0.00P	Ecgonine methyl ester
25	M	526	696R	0.00P	8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, ethyl ester
26	M	524	558R	0.00P	Benzoylecgonine isopropyl ester
27	M	512	723R	0.00P	cis-Cinnamoylcocaine
28	ni	500	558R	0.00P	Clidinium Bromide
29	M	500	547R	0.00P	Propylbenzoylecgonine
30	M	499	586R	0.00P	N-(8-Methyl-8-azabicyclo[3.2.1]oct-3-yl)-2-((4-methylphenyl)sulfanyl)acetamide
31	M	496	565R	0.00P	Propanedioic acid, 2-(3-dimethylaminopropenyldiene)-, dimethyl ester
32	M	493	587R	0.00P	5-(Benzoyloxy)-6-[dimethyl(thexyl)silyloxymethyl]-5,6-dihydro-2(1H)-pyridinone
33	M	490	563R	0.00P	Cyclohexanone, 3,3,5-trimethyl-, semicarbazone
34	M	486	498R	0.00P	(3-Benzoyl-2-t-butyl-4-isopropyl-1-methyl-5-oxo-imidazolidin-4-yl)-acetic acid
35	M	475	530R	0.00P	1-(4-Amino-furazan-3-yl)-piperidine-4-carboxylic acid
36	R	469	641R	0.00P	Ecgonine methyl ester
37	M	466	676R	0.00P	2,5-Dimethyl-7,7-diphenyl-3-aza-4,6-dioxabicyclo[3.2.0]hept-2-ene
38	M	461	644R	0.00P	Pseudoecgonine methyl ester
39	R	461	583R	0.00P	Scopolamine
40	R	460	621R	0.00P	Benzoylecgonine
41	M	459	650R	0.00P	Tropacocaine
42	M	459	488R	0.00P	Benzoylecgonine-TMS
43	M	455	478R	0.00P	L-Isoleucine, N-trifluoroacetyl-, 2,2,3,3,3-pentafluoropropyl ester
44	M	452	651R	0.00P	1-Isobutoxycarbonyl-4(5)-methylimidazole
45	R	450	638R	0.00P	Tropacocaine
46	M	450	610R	0.00P	Benzoylecgonine, 2,2,3,3,3-pentafluoropropyl ester
47	M	449	537R	0.00P	N-(8-Methyl-8-azabicyclo[3.2.1]oct-3-yl)-2-(phenylsulfanyl)acetamide
48	M	448	640R	0.00P	Benzoylecgonine
49	M	448	552R	0.00P	Scopolamine
50	M	447	611R	0.00P	(4-Aminophenyl)phenylmethanol
51	M	447	565R	0.00P	3,9-Diazabicyclo[4.2.1]nonan-4-one, 3-ethyl-9-methyl-
52	R	446	672R	0.00P	Ecgonine
53	R	446	641R	0.00P	Tropacocaine
54	M	444	455R	0.00P	Lycorenan,7-desoxy-12,4-dihydro-9,10-dimethoxy-1-methyl-
55	M	440	488R	0.00P	2-(p-(Phenylazo)phenyl)hydrazinesulfonic acid
56	M	439	520R	0.00P	Acetamide, 2-phenoxy-N-(4-biphenyl)-
57	M	436	608R	0.00P	1,2,4-Trioxolane, 3,3,5-triphenyl-
58	R	435	537R	0.00P	Benzoylecgonine
59	M	435	457R	0.00P	Thiophene-2-carboxylic acid, 3-benzoylamino-4,5-dimethyl-, ethyl ester
60	R	433	624R	0.00P	Tropacocaine
61	R	432	537R	0.00P	Scopolamine
62	M	432	457R	0.00P	Benzoylecgonine, tert-butyl dimethylsilyl ester
63	R	430	647R	0.00P	Ecgonine
64	M	430	613R	0.00P	Ecgonine

65	M	430	482R	0.00P	Tropine, trimethylsilyl ether
66	M	428	527R	0.00P	2-((4-Fluorophenyl)sulfanyl)-N-(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)acetamide
67	M	427	510R	0.00P	Nicotinamide, 2-benzylamino-N-phenyl-
68	M	425	498R	0.00P	Ethyl 2-benzamido-3,3,3-trifluoro-2-(4-fluorophenethylamino)propionate
69	M	425	488R	0.00P	Benzamide, N-(2-methoxyphenyl)-4-phenyl-
70	M	424	511R	0.00P	1,3-Dioxolane, 2-(1-imidazolylmethyl)-2-phenyl-4-[2-(methylthiopyrimidinyl-5-o
71	R	421	583R	0.00P	Benzophenone dimethyl ketal
72	R	421	576R	0.00P	Phenol, 4-methyl-2,6-dinitro-
73	M	420	506R	0.00P	2-((2,4-Difluorophenyl)sulfanyl)-N-(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)acetan
74	M	420	502R	0.00P	2-((4-tert-Butylphenyl)sulfanyl)-N-(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)acetam
75	R	420	486R	0.00P	Benzeneacetic acid, $\alpha$ -hydroxy- $\alpha$ -phenyl-, 1-methyl-3-piperidinyl ester
76	M	418	628R	0.00P	Histamine-2-carboxylic acid
77	M	416	556R	0.00P	Uracil, 5-acetyl-6-amino-1,3-dimethyl
78	M	416	501R	0.00P	2-((4-Chlorophenyl)sulfanyl)-N-(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)acetamide
79	R	412	589R	0.00P	Benzoylcegonine
80	M	409	434R	0.00P	Phenol, 2-[3-[2-(1H-indol-3-yl)ethenyl]-1,2,4-oxadiazol-5-yl]-
81	M	408	457R	0.00P	Ethyl 2-benzamido-3,3,3-trifluoro-2-(2-fluorophenethylamino)propionate
82	M	407	623R	0.00P	Ecgonine, o-pentafluoropropionyl-, pentafluoropropyl ester
83	M	407	564R	0.00P	Glycopyrrolate
84	M	407	451R	0.00P	1,2-Benzisothiazole-2-acetamide, 6-fluoro-2,3-dihydro-3-oxo-N-phenyl-
85	M	406	481R	0.00P	5,7-Dimethyl-2H,5H-pyrimido[4,5-E][1,2,4]triazine-3,6,8-trione
86	M	405	556R	0.00P	Propenoic acid, 2-phenyl-, 8-methyl-8-azabicyclo[3.2.1]octan-3-yl ester
87	M	404	501R	0.00P	Bis(trimethylsilyl)histidine
88	M	404	469R	0.00P	Methanesulfonamide, N-(1,2-dihydro-5-acenaphthylenyl)-N-(2-oxopropyl)-
89	M	402	627R	0.00P	3-Hexen-1-ol benzoate
90	M	401	607R	0.00P	2,5-Methanopyrano[3,2-b]pyrrole, 8-chlorohexahydro-1-methyl-, (2 $\alpha$ ,3 $\alpha$ $\beta$ ,5 $\alpha$ ,7 $\epsilon$
91	M	401	538R	0.00P	Ethyl 2-benzamido-4,5-dimethyl-3-thiophenecarboxylate
92	M	401	462R	0.00P	13a,3a-(Epoxyethano)-1H-indolizino[8,1-cd]carbazol-7-ol, 6-acetyl-2,3,4,5,5a,(
93	M	400	401R	0.00P	Albomaculine
94	M	399	581R	0.00P	4-(2-Fluorobenzoylamino)piperidine-1-carboxylic acid, (2-fluorophenyl)amide
95	M	398	532R	0.00P	trans-1-Benzoyloxy-cis-3-hydroxy-trans-4,trans-5-isopropylidenedioxycyclohex
96	M	397	456R	0.00P	Ethyl 2-benzamido-3,3,3-trifluoro-2-(phenethylamino)propionate
97	M	396	447R	0.00P	N1-(8-Methyl-8-azabicyclo[3.2.1]oct-3-yl)-2-(2-fluorophenyl)acetamide
98	M	395	584R	0.00P	3-Tropanyl 2-[2,6-dichlorophenyl]acrylate
99	M	394	447R	0.00P	Spiro[cyclohexanone-3,6'-hexahydropyridin-2-one]
100	M	394	407R	0.00P	Benzoic acid, [1-amino-2-(2,4-dichlorophenoxy)ethylidenamino] ester