

A practical method for rapid screening and quantitative analysis of 130 pesticide residues in herbal medicines based on Kovats retention index principle: An exemplary study using *Panacis quinquefolii radix*

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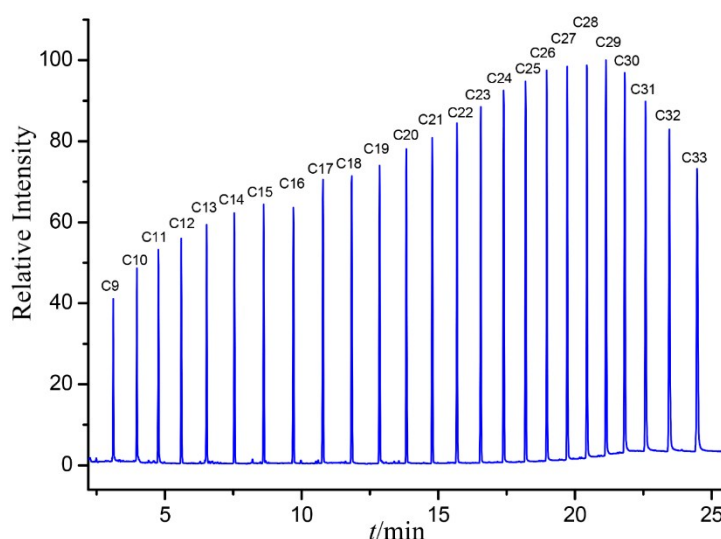


Fig. S1 Typical TIC chromatograms of n-alkanes C9~C33 mixed standard solution

Tab. S1 Monitoring ion pairs and collision energy of 130 pesticides

Number	Pesticide name	m/z 1	Collision energy (V)	m/z 2	Collision energy (V)	CAS Number
1	Dichlorvos	109.0>79.0	8	185.0>93.0	14	62-73-7
2	Dichlobenil	170.9>136.0	14	170.9>100.0	24	1194-65-6
3	Mevinphos-1	127.0>109.0	12	192.0>127.0	12	7786-34-7
3	Mevinphos-2	127.0>109.0	12	192.0>127.0	12	7786-34-7
4	Butylate	156.1>57.0	10	174.1>146.1	6	2008-41-5
5	Molinate	126.1>55.0	14	187.1>126.1	6	2212-67-1
6	Tecnazene	260.9>202.9	14	202.9>142.9	22	117-18-0
7	Omethoate	156.0>110.0	8	110.0>79.0	10	1113-02-6
8	Propachlor	120.0>77.0	20	176.1>57.0	8	1918-16-7
9	Chlorethoxyfos	153.0>97.0	12	153.0>125.0	4	54593-83-8
10	Diphenylamine	169.1>66.0	24	167.1>139.1	28	122-39-4
11	Ethoprophos	200.0>158.0	6	158.0>97.0	18	13194-48-4
12	Chlorpropham	127.1>65.0	22	213.1>171.1	6	101-21-3
13	Trifluralin	306.1>264.1	8	264.1>160.1	18	1582-09-8

14	Dicrotophos	127.1>109.0	12	127.1>95.0	18	141-66-2
15	Monocrotophos	127.1>109.0	12	127.1>95.0	16	6923-22-4
16	Flumethrin	187.0>159.0	10	216.0>187.0	10	69770-45-2
17	Phorate	260.0>75.0	8	231.0>129.0	24	298-02-2
18	Hexachlorobenzene	283.8>248.8	24	283.8>213.8	28	118-74-1
19	Desmedipham	181.0>109.0	10	122.0>94.0	10	13684-56-5
20	Simazine	201.1>173.1	6	201.1>186.1	6	122-34-9
21	Quintozene	264.8>236.8	10	294.8>236.8	16	82-68-8
22	Propazine	125.0>89.0	18	125.0>99.0	18	139-40-2
23	Lindane	180.9>144.9	16	218.9>182.9	8	58-89-9
24	Terbufos	231.0>128.9	26	231.0>174.9	14	13071-79-9
25	Fonofos	137.1>109.1	8	246.0>137.1	6	944-22-9
26	Diazinon	304.1>179.1	10	179.1>137.1	18	333-41-5
27	Phosphamidon-1	127.1>109.1	12	127.1>95.1	18	13171-21-6
27	Phosphamidon-2	127.1>109.1	12	127.1>95.1	18	13171-21-6
28	Pyrimethanil	198.1>183.1	14	198.1>118.1	28	53112-28-0
29	Chlorothalonil	263.9>168.0	24	263.9>228.8	18	1897-45-6
30	Tefluthrin	177.0>127.1	16	177.0>137.1	16	79538-32-2
31	Propanil	217.0>161.0	10	160.9>99.0	24	709-98-8
32	Chlorpyrifos-methyl	285.9>93.0	22	287.9>93.0	22	5598-13-0
33	Metribuzin	198.1>82.0	14	198.1>110.1	10	21087-64-9
34	Vinclozolin	212.0>172.0	16	285.0>212.0	12	50471-44-8
35	Parathion-methyl	263.0>109.0	14	125.0>47.0	12	298-00-0
36	Tolclofos-methyl	264.9>249.9	14	264.9>93.0	24	57018-04-9
37	Alachlor	188.1>160.1	10	188.1>132.1	18	15972-60-8
38	Heptachlor	271.8>236.9	20	273.8>238.9	16	76-44-8
39	Propisochlor	162.1>120.1	14	162.1>147.1	14	86763-47-5
40	Ametryn	227.1>185.1	6	227.1>58.0	14	834-12-8
41	Metalaxyl	249.2>190.1	8	206.1>132.1	20	57837-19-1
42	Prometryn	226.1>184.1	10	241.2>184.1	12	7287-19-6
43	Pirimiphos-methyl	290.1>125.0	22	290.1>233.1	12	29232-93-7
44	Fenitrothion	277.0>260.0	6	277.0>109.1	14	122-14-5
45	Bromacil	206.9>189.9	16	204.9>187.9	14	314-40-9
46	Malathion	173.1>99.0	14	173.1>127.0	6	121-75-5
47	Chlorpyrifos	196.9>168.9	14	313.9>257.9	14	2921-88-2
48	Aldrin	262.9>191.0	34	262.9>193.0	28	309-00-2
	Fenthion- <i>d</i> 6	284.0>115.0	20	284.0>169.0	15	1189662-83-6
49	Fenthion	278.0>109.0	20	278.0>169.0	14	55-38-9
50	Chlorthal-dimethyl	298.9>220.9	24	300.9>222.9	26	1861-32-1
51	Triadimefon	208.1>181.0	10	208.1>111.0	22	43121-43-3
52	Dicofol	139.0>111.0	16	139.0>75.0	28	0-00-0
53	Phthalide	272.0>242.9	14	243.0>214.9	9	27355-22-2
54	Isofenphos-methyl	199.0>121.0	14	241.1>121.1	22	99675-03-3
55	Pendimethalin	252.1>162.1	10	252.1>191.1	8	40487-42-1

56	Fipronil	366.9>212.9	30	368.9>214.9	30	120068-37-3
57	Penconazole	248.1>157.1	26	159.1>123.1	22	66246-88-6
58	Tolyfluanid	238.0>137.1	14	181.1>138.1	10	731-27-1
59	Phenthoate	273.9>125.0	20	273.9>246.0	6	2597-03-7
60	Quinalphos	146.1>118.0	10	146.1>91.0	24	13593-03-8
61	Captan	149.1>79.1	14	149.1>105.1	4	133-06-2
62	Procymidone	283.0>96.0	10	285.0>96.0	10	32809-16-8
63	Triadimenol-1	168.1>70.0	10	128.1>65.0	22	55219-65-3
63	Triadimenol-2	168.1>70.0	10	128.1>65.0	22	55219-65-3
64	Folpet	259.9>130.0	14	261.9>130.0	18	133-07-3
65	Methoprene	111.1>55.0	18	111.1>83.0	12	40596-69-8
66	Methidathion	145.0>85.0	8	145.0>58.0	14	950-37-8
67	Trans-Chlordane	374.8>265.9	26	372.8>263.9	28	5103-74-2
68	Paclobutrazol	236.1>125.0	14	236.1>167.0	10	76738-62-0
69	Butachlor	176.1>147.1	14	188.1>160.1	12	23184-66-9
70	Alpha-Endosulfan	194.9>160.0	8	194.9>125.0	24	959-98-8
71	Flutriafol	219.1>123.1	14	219.1>95.0	28	76674-21-0
72	Fenamiphos	303.1>195.1	8	288.1>260.1	6	22224-92-6
73	Napropamide	128.1>72.0	6	100.0>72.0	8	15299-99-7
74	Prothiophos	266.9>238.9	10	309.0>238.9	14	34643-46-4
75	Isoprothiolane	231.1>189.0	10	290.1>118.0	14	50512-35-1
76	Pretilachlor	262.1>202.1	10	238.1>162.1	10	51218-49-6
77	Profenofos	338.9>268.9	18	336.9>266.9	14	41198-08-7
78	Oxadiazon	258.0>175.0	8	302.0>175.0	14	19666-30-9
79	Tribufos	202.0>147.0	6	202.0>113.0	20	78-48-8
80	Myclobutanil	179.1>125.0	14	179.1>152.0	8	88671-89-0
81	Flusilazole	233.1>165.1	14	206.1>151.1	16	85509-19-9
82	Oxyfluorfen	252.0>196.0	22	361.0>300.0	14	42874-03-3
83	Chlorfenapyr	247.1>227.0	16	139.0>102.0	12	122453-73-0
84	Fluazifop-P-butyl	383.0>282.0	15	282.0>91.0	20	79241-46-6
85	Endrin	262.9>191.0	30	262.9>193.0	28	72-20-8
86	Flufenpyr-ethyl	408.0>345.0	16	408.0>321.0	14	188489-07-8
87	Beta-Endosulfan	194.9>160.0	8	194.9>125.0	24	33213-65-9
88	Diniconazole	268.0>232.0	12	270.0>234.0	10	83657-24-3
89	Ethion	153.0>97.0	14	230.9>129.0	24	563-12-2
90	Mepronil	119.1>91.0	12	119.1>65.0	24	55814-41-0
91	Triazophos	161.0>134.0	8	161.0>106.0	14	24017-47-8
92	Benalaxyl	148.1>105.1	16	148.1>79.1	24	71626-11-4
93	Trifloxystrobin	222.1>190.1	4	222.1>130.1	12	141517-21-7
94	Edifenphos	173.0>109.0	10	310.0>173.0	14	17109-49-8
95	Norflurazon	145.0>95.0	18	303.0>145.0	22	27314-13-2
96	Propiconazole-1	173.0>145.0	16	173.0>109.0	28	60207-90-1
96	Propiconazole-2	173.0>145.0	16	173.0>109.0	28	60207-90-1
97	Quinoxifen	237.1>208.1	28	307.1>237.1	22	124495-18-7

98	4,4'-DDT	235.0>165.0	24	237.0>165.0	28	50-29-3
99	Tebuconazole	250.1>125.1	22	125.1>89.0	18	107534-96-3
100	Diclofop-ethyl	340.0>253.0	14	253.0>162.0	22	51338-27-3
101	Piperonyl-butoxide	176.1>131.1	12	176.1>117.1	20	51-03-6
102	Zoxamide	187.0>159.0	16	187.0>123.0	24	156052-68-5
103	Iprodione	314.0>245.0	12	314.0>56.0	22	36734-19-7
104	Acetamiprid	152.0>116.0	18	152.0>89.0	26	135410-20-7
105	Phosmet	160.0>77.0	24	160.0>133.0	14	732-11-6
106	Bifenthrin	181.1>166.1	12	181.1>179.1	12	82657-04-3
107	Bromopropylate	340.9>182.9	18	340.9>184.9	20	18181-80-1
108	Etoxazole	359.1>187.1	14	330.1>300.1	26	153233-91-1
109	Fenpropathrin	181.1>152.1	22	265.1>210.1	12	39515-41-8
110	Phosalone	182.0>111.0	14	182.0>138.0	8	2310-17-0
111	Ipconazole	125.0>89.1	18	125.0>99.0	18	125225-28-7
112	Metrafenone	393.0>363.0	20	379.0>364.0	10	220899-03-6
113	Fenoxaprop-ethyl	361.1>288.1	12	288.1>119.1	12	66441-23-4
114	Oryzalin	275.0>258.0	6	317.0>258.0	14	19044-88-3
115	Permethrin-1	183.1>153.1	14	183.1>168.1	14	52645-53-1
115	Permethrin-2	183.1>153.1	14	183.1>168.1	14	52645-53-1
116	Coumaphos	362.0>109.0	16	362.0>226.0	14	56-72-4
117	Pyridaben	147.1>117.1	22	147.1>132.1	14	96489-71-3
118	Fenbuconazole	198.1>129.1	10	129.1>102.1	18	114369-43-6
119	Cyfluthrin-1	163.1>127.1	6	163.1>91.0	14	68359-37-5
119	Cyfluthrin-2	163.1>127.1	6	163.1>91.0	14	68359-37-5
119	Cyfluthrin-3	163.1>127.1	6	163.1>91.0	14	68359-37-5
119	Cyfluthrin-4	163.1>127.1	6	163.1>91.0	14	68359-37-5
120	Cypermethrin-1	163.1>127.1	6	163.1>91.0	14	52315-07-8
120	Cypermethrin-2	163.1>127.1	6	163.1>91.0	14	52315-07-8
120	Cypermethrin-3	163.1>127.1	6	163.1>91.0	14	52315-07-8
120	Cypermethrin-4	163.1>127.1	6	163.1>91.0	14	52315-07-8
121	Flucythrinate-1	199.1>157.1	10	157.1>107.1	12	70124-77-5
121	Flucythrinate-2	199.1>157.1	10	157.1>107.1	12	70124-77-5
122	Pyridalyl	204.1>148.1	20	204.1>176.1	12	179101-81-6
123	Flumioxazin	287.1>259.1	12	354.1>326.1	8	103361-09-7
124	Fenvalerate-1	225.1>119.1	20	225.1>147.1	10	51630-58-1
124	Fenvalerate-2	225.1>119.1	20	225.1>147.1	10	51630-58-1
125	Fluvalinate-1	250.1>55.0	20	250.1>200.0	20	69409-94-5
125	Fluvalinate-2	250.1>55.0	20	250.1>200.0	20	69409-94-5
126	Difenoconazole-1	323.0>265.0	14	265.0>202.0	20	119446-68-3
126	Difenoconazole-2	323.0>265.0	14	265.0>202.0	20	119446-68-3
127	Deltamethrin-1	180.9>151.9	22	252.9>93.0	20	52918-63-5
127	Deltamethrin-2	180.9>151.9	22	252.9>93.0	20	52918-63-5
128	Azoxystrobin	344.1>329.1	16	388.1>345.1	18	131860-33-8
129	Famoxadone	224.1>196.1	10	330.1>224.1	10	131807-57-3

130	Fluthiacet-methyl	403.0>56.0	24	403.0>84.0	14	117337-16-6
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Notes: (1) Compound Fenthion-*d*6 is internal standard compound.

(2) Some pesticides have multiple retention time because of isomers.

Tab. S2 Results of predicted retention time and actual measured retention time

Number	Pesticide name	Retention index from the database	Predicted retention time (min)	Actual measured retention index	Actual measured retention time (min)	Time deviation value (min)
1	Dichlorvos	1248	6.029	1245	6.013	-0.016
2	Dichlobenil	1348	6.997	1349	7.009	0.012
3	Mevinphos-1	1420	7.739	1427	7.759	0.020
3	Mevinphos-2	1423	7.771	1427	7.796	0.025
4	Butylate	1431	7.856	1432	7.862	0.006
5	Molinate	1548	9.116	1549	9.126	0.010
6	Tecnazene	1595	9.627	1598	9.649	0.022
7	Omethoate	1602	9.703	1598	9.682	-0.021
8	Propachlor	1611	9.800	1612	9.810	0.010
9	Chlorethoxyfos	1618	9.875	1620	9.895	0.020
10	Diphenylamine	1631	10.016	1633	10.035	0.019
11	Ethoprophos	1638	10.091	1639	10.098	0.007
12	Chlorpropham	1661	10.339	1661	10.339	0.000
13	Trifluralin	1666	10.393	1666	10.392	-0.001
14	Dicrotophos	1668	10.414	1667	10.398	-0.016
15	Monocrotophos	1686	10.609	1685	10.594	-0.015
16	Flumethrin	1689	10.641	1691	10.666	0.025
17	Phorate	1695	10.706	1697	10.723	0.017
18	Hexachlorobenzene	1710	10.865	1716	10.871	0.006
19	Desmedipham	1725	11.023	1729	11.039	0.016
20	Simazine	1746	11.244	1744	11.227	-0.017
21	Quintozene	1759	11.381	1764	11.401	0.020
22	Propazine	1760	11.391	1772	11.406	0.015
23	Lindane	1769	11.486	1772	11.502	0.016
24	Terbufos	1778	11.581	1779	11.586	0.005
25	Fonofos	1785	11.654	1787	11.675	0.021
26	Diazinon	1791	11.718	1791	11.713	-0.005
27	Phosphamidon-1	1798	11.791	1792	11.801	0.010
27	Phosphamidon-2	1868	12.506	1867	12.493	-0.013
28	Pyrimethanil	1799	11.802	1801	11.819	0.017
29	Chlorothalonil	1803	11.843	1806	11.870	0.027
30	Tefluthrin	1819	12.006	1818	11.994	-0.012
31	Propanil	1877	12.598	1880	12.622	0.024
32	Chlorpyrifos-methyl	1882	12.649	1884	12.671	0.022
33	Metribuzin	1884	12.669	1886	12.686	0.017
34	Vinclozolin	1891	12.741	1891	12.745	0.004

35	Parathion-methyl	1896	12.792	1896	12.791	-0.001
36	Tolclofos-methyl	1897	12.802	1898	12.813	0.011
37	Alachlor	1898	12.812	1899	12.819	0.007
38	Heptachlor	1909	12.921	1915	12.942	0.021
39	Propisochlor	1912	12.950	1912	12.951	0.001
40	Ametryn	1913	12.960	1913	12.961	0.001
41	Metalaxyl	1913	12.960	1912	12.953	-0.007
42	Prometryn	1919	13.019	1919	13.015	-0.004
43	Pirimiphos-methyl	1940	13.225	1940	13.229	0.004
44	Fenitrothion	1946	13.284	1946	13.286	0.002
45	Bromacil	1957	13.391	1954	13.398	0.007
46	Malathion	1964	13.460	1963	13.452	-0.008
47	Chlorpyrifos	1977	13.587	1978	13.598	0.011
48	Aldrin	1981	13.627	1988	13.632	0.005
	Fenthion- <i>d</i> 6	1982	13.637	1982	13.633	-0.004
49	Fenthion	1986	13.676	1986	13.677	0.001
50	Chlorthal-dimethyl	1986	13.676	1989	13.703	0.027
51	Triadimefon	1999	13.803	2000	13.811	0.008
52	Dicofol	2008	13.888	2010	13.908	0.020
53	Phthalide	2014	13.945	2018	13.971	0.026
54	Isofenphos-methyl	2031	14.105	2034	14.133	0.028
55	Pendimethalin	2044	14.228	2046	14.248	0.020
56	Fipronil	2055	14.332	2057	14.348	0.016
57	Penconazole	2058	14.360	2059	14.373	0.013
58	Tolyfluanid	2063	14.407	2065	14.425	0.018
59	Phenthoate	2077	14.539	2077	14.538	-0.001
60	Quinalphos	2079	14.558	2080	14.564	0.006
61	Captan	2082	14.586	2084	14.608	0.022
62	Procymidone	2086	14.624	2087	14.637	0.013
63	Triadimenol-1	2087	14.634	2087	14.638	0.004
63	Triadimenol-2	2103	14.783	2104	14.792	0.009
64	Folpet	2095	14.709	2097	14.725	0.016
65	Methoprene	2097	14.728	2097	14.727	-0.001
66	Methidathion	2108	14.828	2109	14.839	0.011
67	Trans-Chlordane	2110	14.847	2116	14.868	0.021
68	Paclobutrazol	2125	14.982	2127	15.003	0.021
69	Butachlor	2128	15.009	2129	15.020	0.011
70	Alpha-Endosulfan	2139	15.109	2145	15.116	0.007
71	Flutriafol	2150	15.208	2151	15.218	0.010
72	Fenamiphos	2154	15.245	2154	15.246	0.001
73	Napropamide	2156	15.263	2158	15.281	0.018
74	Prothiophos	2167	15.362	2170	15.389	0.027
75	Isoprothiolane	2172	15.407	2171	15.396	-0.011
76	Pretilachlor	2172	15.407	2173	15.417	0.010

77	Profenofos	2177	15.453	2179	15.470	0.017
78	Oxadiazon	2187	15.543	2187	15.544	0.001
79	Tribufos	2191	15.579	2192	15.588	0.009
80	Myclobutanil	2196	15.625	2197	15.630	0.005
81	Flusilazole	2199	15.652	2201	15.667	0.015
82	Oxyfluorfen	2200	15.661	2199	15.652	-0.009
83	Chlorfenapyr	2222	15.852	2223	15.858	0.006
84	Fluazifop-P-butyl	2236	15.974	2239	15.996	0.022
85	Endrin	2240	16.008	2248	16.017	0.009
86	Flufenpyr-ethyl	2254	16.130	2253	16.125	-0.005
87	Beta-Endosulfan	2266	16.234	2271	16.248	0.014
88	Diniconazole	2267	16.243	2271	16.265	0.022
89	Ethion	2276	16.321	2277	16.331	0.010
90	Mepronil	2308	16.597	2310	16.613	0.016
91	Triazophos	2310	16.613	2311	16.624	0.011
92	Benalaxyl	2328	16.764	2331	16.786	0.022
93	Trifloxystrobin	2339	16.856	2338	16.843	-0.013
94	Edifenphos	2341	16.873	2345	16.889	0.016
95	Norflurazon	2341	16.873	2346	16.893	0.020
96	Propiconazole-1	2344	16.898	2346	16.916	0.018
96	Propiconazole-2	2357	17.007	2360	17.031	0.024
97	Quinoxifen	2347	16.923	2351	16.955	0.032
98	4,4'-DDT	2359	17.023	2364	17.056	0.033
99	Tebuconazole	2391	17.291	2396	17.329	0.038
100	Diclofop-ethyl	2393	17.308	2395	17.325	0.017
101	Piperonyl-butoxide	2408	17.431	2409	17.440	0.009
102	Zoxamide	2425	17.567	2430	17.589	0.022
103	Iprodione	2451	17.776	2453	17.792	0.016
104	Acetamiprid	2457	17.825	2458	17.835	0.010
105	Phosmet	2466	17.897	2470	17.922	0.025
106	Bifenthrin	2469	17.921	2470	17.928	0.007
107	Bromopropylate	2475	17.969	2478	17.996	0.027
108	Etoazole	2488	18.074	2490	18.089	0.015
109	Fenpropathrin	2493	18.114	2493	18.117	0.003
110	Phosalone	2551	18.565	2555	18.579	0.014
111	Ipconazole	2611	19.026	2616	19.047	0.021
112	Metrafenone	2640	19.243	2642	19.259	0.016
113	Fenoxaprop-ethyl	2667	19.445	2670	19.467	0.022
114	Oryzalin	2674	19.497	2675	19.501	0.004
115	Permethrin-2	2702	19.706	2704	19.720	0.014
115	Permethrin-3	2720	19.835	2722	19.843	0.008
116	Coumaphos	2718	19.821	2726	19.845	0.024
117	Pyridaben	2724	19.864	2728	19.884	0.020
118	Fenbuconazole	2775	20.231	2782	20.248	0.017

119	Cyfluthrin-1	2777	20.246	2779	20.258	0.012
119	Cyfluthrin-2	2791	20.346	2792	20.355	0.009
119	Cyfluthrin-3	2799	20.404	2801	20.411	0.007
119	Cyfluthrin-4	2806	20.453	2807	20.458	0.005
120	Cypermethrin-1	2823	20.572	2825	20.583	0.011
120	Cypermethrin-2	2838	20.676	2839	20.686	0.010
120	Cypermethrin-3	2845	20.725	2848	20.745	0.020
120	Cypermethrin-4	2852	20.774	2854	20.786	0.012
121	Flucythrinate-1	2847	20.739	2848	20.749	0.010
121	Flucythrinate-2	2875	20.934	2876	20.945	0.011
122	Pyridalyl	2871	20.907	2876	20.933	0.026
123	Flumioxazin	2950	21.452	2952	21.466	0.014
124	Fenvalerate-1	2951	21.458	2954	21.482	0.024
124	Fenvalerate-2	2981	21.664	2985	21.689	0.025
125	Fluvalinate-1	2968	21.575	2971	21.593	0.018
125	Fluvalinate-2	2978	21.643	2980	21.657	0.014
126	Difenoconazole-1	3017	21.923	3022	21.934	0.011
126	Difenoconazole-2	3025	21.983	3032	22.003	0.020
127	Deltamethrin-1	3031	22.029	3035	22.060	0.031
127	Deltamethrin-2	3060	22.248	3064	22.278	0.030
128	Azoxystrobin	3086	22.444	3090	22.472	0.028
129	Famoxadone	3114	22.671	3122	22.702	0.031
130	Fluthiacet-methyl	3240	23.820	3247	23.847	0.027

Tab. S3 The limit of detection of 130 test pesticides for rapid pre-screening application

Number	Pesticide	LOD (ug/L)	Number	Pesticide	LOD (ug/L)
1	Dichlorvos	2.02	71	Flutriafol	1.60
2	Dichlobenil	0.57	72	Fenamiphos	0.02
3	Mevinphos-1	0.73	73	Napropamide	2.06
3	Mevinphos-2	0.73	74	Prothiophos	0.02
4	Butylate	1.73	75	Isoprothiolane	0.09
5	Molinate	1.92	76	Pretilachlor	0.01
6	Tecnazene	0.03	77	Profenofos	0.04
7	Omethoate	3.01	78	Oxadiazon	0.01
8	Propachlor	3.45	79	Tribufos	0.01
9	Chlorethoxyfos	1.75	80	Myclobutanil	0.01
10	Diphenylamine	0.47	81	Flusilazole	0.02
11	Ethoprophos	0.33	82	Oxyfluorfen	0.07
12	Chlorpropham	0.29	83	Chlorfenapyr	0.07
13	Trifluralin	0.03	84	Fluazifop-P-butyl	0.01
14	Diclotophos	1.10	85	Endrin	0.14
15	Monocrotophos	2.47	86	Flufenpyr-ethyl	0.02

16	Flumethrin	2.55	87	Beta-Endosulfan	0.13
17	Phorate	0.03	88	Diniconazole	0.01
18	Hexachlorobenzene	0.07	89	Ethion	1.21
19	Desmedipham	13.98	90	Mepronil	1.05
20	Simazine	0.58	91	Triazophos	0.08
21	Quintozone	0.01	92	Benalaxyl	0.59
22	Propazine	5.00	93	Trifloxystrobin	0.01
23	Lindane	0.07	94	Edifenphos	0.01
24	Terbufos	0.16	95	Norflurazon	0.02
25	Fonofos	0.41	96	Propiconazole-1	0.86
26	Diazinon	0.01	96	Propiconazole-2	0.83
27	Phosphamidon-1	4.36	97	Quinoxifen	0.00
27	Phosphamidon-2	0.56	98	4,4'-DDT	0.17
28	Pyrimethanil	1.09	99	Tebuconazole	0.01
29	Chlorothalonil	0.86	100	Diclofop-ethyl	0.01
30	Tefluthrin	0.02	101	Piperonyl-butoxide	0.03
31	Propanil	1.74	102	Zoxamide	2.58
32	Chlorpyrifos-methyl	0.01	103	Iprodione	0.08
33	Metribuzin	0.77	104	Acetamiprid	13.27
34	Vinclozolin	0.02	105	Phosmet	2.53
35	Parathion-methyl	0.44	106	Bifenthrin	0.13
36	Tolclofos-methyl	0.02	107	Bromopropylate	0.01
37	Alachlor	0.43	108	Etoxazole	0.02
38	Heptachlor	0.10	109	Fenpropathrin	1.02
39	Propisochlor	7.08	110	Phosalone	1.05
40	Ametryn	0.19	111	Ipconazole	0.82
41	Metalaxyl	0.01	112	Metrafenone	0.04
42	Prometryn	0.16	113	Fenoxaprop-ethyl	0.01
43	Pirimiphos-methyl	0.07	114	Oryzalin	2.68
44	Fenitrothion	0.03	115	Permethrin-1	2.07
45	Bromacil	0.96	115	Permethrin-2	0.51
46	Malathion	0.01	116	Coumaphos	0.57
47	Chlorpyrifos	0.23	117	Pyridaben	0.21
48	Aldrin	0.08	118	Fenbuconazole	0.01
49	Fenthion	0.19	119	Cyfluthrin-1	7.57
50	Chlorthal-dimethyl	0.02	119	Cyfluthrin-2	4.41
51	Triadimefon	0.06	119	Cyfluthrin-3	10.01
52	Dicofol	0.06	119	Cyfluthrin-4	2.85
53	Phthalide	0.31	120	Cypermethrin-1	4.05
54	Isofenphos-methyl	0.03	120	Cypermethrin-2	2.98
55	Pendimethalin	0.02	120	Cypermethrin-3	5.42
56	Fipronil	0.10	120	Cypermethrin-4	3.27
57	Penconazole	0.01	121	Flucythrinate-1	0.79
58	Tolyfluanid	0.01	121	Flucythrinate-2	1.09

59	Phenthoate	0.01	122	Pyridalyl	0.46
60	Quinalphos	0.50	123	Flumioxazin	0.78
61	Captan	13.45	124	Fenvalerate-1	0.30
62	Procymidone	0.01	124	Fenvalerate-2	0.28
63	Triadimenol-1	1.27	125	Fluvalinate-1	1.64
63	Triadimenol-2	2.12	125	Fluvalinate-2	1.94
64	Folpet	0.05	126	Difenoconazole-1	0.18
65	Methoprene	11.49	126	Difenoconazole-2	0.06
66	Methidathion	0.01	127	Deltamethrin-1	27.32
67	Trans-Chlordane	0.12	127	Deltamethrin-2	18.20
68	Paclobutrazol	0.01	128	Azoxystrobin	3.99
69	Butachlor	0.99	129	Famoxadone	4.81
70	Alpha-Endosulfan	0.18	130	Fluthiacet-methyl	1.02

Tab. S4 The accuracy and reproducibility of eight target pesticides in sample PQR19

Spiked level	10.0 (µg/L).		100.0 (µg/L)		200.0 (µg/L)		Reproducibility (µg/kg)	RSD% N = 6
	Recovery (%)	RSD% N = 6	Recovery (%)	RSD% N = 6	Recovery (%)	RSD% N = 6		
Tecnazene	84.57	6.34	86.17	5.89	86.18	5.04	324.71	3.81
Diphenylamine	80.77	5.03	84.93	6.12	84.77	4.85	14.25	5.49
Hexachlorobenzene	85.87	4.88	86.03	4.13	85.89	3.07	149.31	4.77
Quintozene	83.64	5.25	84.71	4.63	86.22	4.17	291.94	3.65
Lindane	80.14	6.68	81.93	6.84	82.36	5.37	35.89	5.71
Chlorpyrifos	84.79	4.01	85.26	3.87	85.94	4.02	110.11	4.03
Procymidone	80.28	5.63	85.25	4.15	86.09	3.79	38.88	5.16
4,4'-DDT	83.62	6.89	84.34	6.36	86.11	5.34	ND	ND

ND*--represents not detected.