

Supporting Information:

Peak	Solvent	Retention Time	Principal ion (m/z)	Qualifying ion (m/z)
1	Chloromethane	3.272	50	52
2	Methanol	3.422	31	29
3	Ethanol	4.075	31	45
4	Acetone	4.524	43	58
5	Isopentane	4.526	41	57
6	2-propanol	4.751	45	59
7	Pentane	5.018	43	51
8	Ethyl Ether	5.073	59	74
9	Methyl propyl ether	5.498	45	74
10	1-Chloropropane	5.951	42	41
11	1-propanol	6.434	31	59
12	Cyclopentane	6.902	42	55
13	2-methylpentane	7.146	43	42/41
14	Methyl Ethyl Ketone (MEK)	7.566	43	72
15	3-methylpentane	7.792	57	41
16	Hexane	8.698	57	41/86
17	Chloroform	8.767	83	47
18	Ethyl Acetate	9.101	43	70
19	Isobutanol	9.979	43	41/39
20	Benzene	11.524	78	77/50/51
21	Isopropyl Acetate	11.709	43	61
22	Cyclohexane	11.878	84	56
23	2,3-dimethylpentane	12.294	56	41
24	Heptane	12.537	43	71
25	n-propyl Acetate	13.304	43	61/73/42

26	Methyl Isobutyl Ketone (MIBK)	13.900	43	58
27	Toluene	14.662	91	65
28	Isobutyl Acetate	14.770	43	56
29	Mesityl Oxide	15.168	83	55
30	o-xylene	16.349	91	106
31	m-xylene	16.459	91	106
32	p-xylene	16.752	91	106
33	Mesitylene	17.546	105	120

Table S1. List of the residual solvents HS–GC-MS method sorted by retention time.

Class	1	2	3	4	5	6	7	8	9
1	100	43.3	0.13	59.4	13.1	0.01	0.02	0.02	22.6
2	-	100	0.08	0.12	38.67	1.16	0.05	0.21	60.7
3	-	-	100	0.001	0.02	0.02	0.0007	0.002	0.02
4	-	-	-	100	0.07	0.03	0.01	0.004	0.09
5	-	-	-	-	100	70.0	1.02	6.57	94.3
6	-	-	-	-	-	100	1.37	8.94	48.1
7	-	-	-	-	-	-	100	94.6	0.69
8	-	-	-	-	-	-	-	100	4.60
9	-	-	-	-	-	-	-	-	100

Table S2. Correlation ρ values among the means that characterize the nine classes of the simulated dataset.

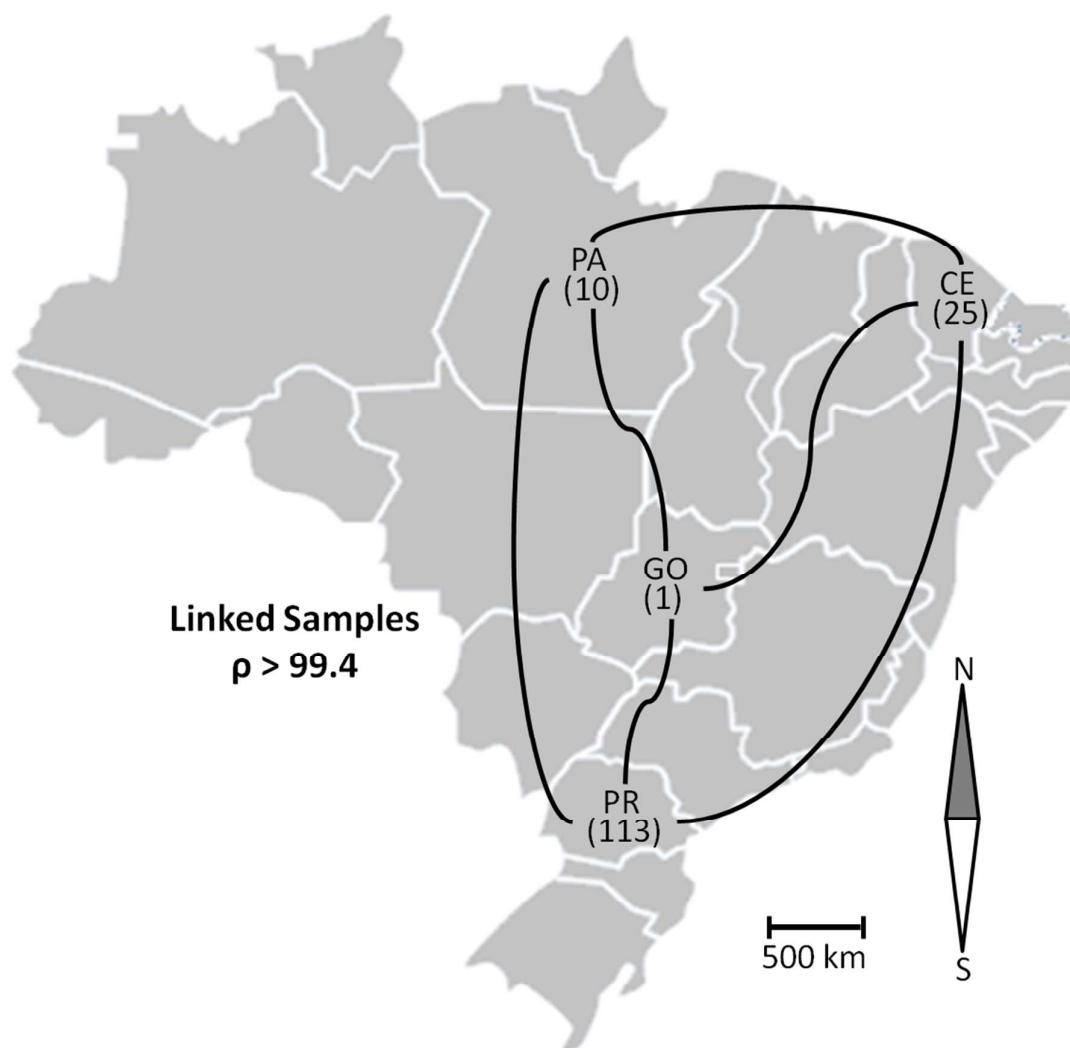


Figure S1. Correlated seizures of cocaine hydrochloride made by the Federal Police, (number of samples seized in each state).