

Supplementary Materials

A Data-Challenge Case Study of Analyte Detection and Identification with Comprehensive Two-Dimensional Gas Chromatography with Mass Spectrometry (GCxGC-MS)

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The supplementary materials comprise three tables:

Table S1: Analyte Identifications.

Table S2: Detected Ion-Peak Sets.

Table S3: MS Search Experiments.

For descriptions of these tables, refer to the case-study paper.

Table S1: Analyte identifications (compound name and CAS#), blob metadata (percent response, 1D and 2D retention times, computed retention index, base peak), library search results (direct match factor, reverse match factor, probability, retention index, base peak), and identification tests (direct match factor > 850, analyte base peak = library base peak, computed retention index – library retention index ≤ 15).

Analyte ID			Blob					Library					Tests		
ID	Compound Name	CAS#	%Rsp	1 _{tr}	2 _{tr}	I'	BsPk	DMF	RMF	Prob	I	BsPk	DMF	RI	BsPk
1	β-Myrcene	123-35-3	5.38	14.33	0.70	991	41	936	947	66	991	93	PASS	PASS	FAIL
2	D-Limonene	5989-27-5	5.59	16.17	0.70	1030	68	930	931	24		68	PASS		PASS
3	Linalool	78-70-6	4.99	19.21	0.92	1099	43	929	929	72	1099	71	PASS	PASS	FAIL
4	β-Pinene	127-91-3	5.41	13.92	0.75	979	93	944	945	42	979	93	PASS	PASS	PASS
5	Camphene	79-92-5	5.86	12.75	0.72	952	93	947	962	35	952	93	PASS	PASS	PASS
6	Isopulegol	89-79-2	4.39	21.42	1.13	1153	41	935	942	37	1146	41	PASS	PASS	PASS
7	Humulene	6753-98-6	4.95	33.63	0.84	1454	93	949	953	73	1454	93	PASS	PASS	PASS
8	3-Carene	13466-78-9	5.13	15.29	0.70	1010	93	905	924	7	1011	93	PASS	PASS	PASS
9	α-Pinene	80-56-8	5.30	12.00	0.70	937	93	945	952	28	937	93	PASS	PASS	PASS
10	Caryophyllene	87-44-5	4.52	32.33	0.84	1419	41	926	926	29	1419	93	PASS	PASS	FAIL
11	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	586-62-9	4.78	18.67	0.68	1088	93	916	923	11	1088	93	PASS	PASS	PASS
12	τ-Terpinene	99-85-4	5.43	17.46	0.69	1060	93	912	933	33	1060	93	PASS	PASS	PASS
13	trans-β-Ocimene	3779-61-1	4.31	16.88	0.73	1049	93	913	914	10	1049	93	PASS	PASS	PASS
14	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-	99-86-5	4.93	15.63	0.74	1017	93	907	916	16	1017	121	PASS	PASS	FAIL
15	α-Bisabolol	515-69-5	4.49	41.25	0.85	1684	43	929	944	76	1684	43	PASS	PASS	PASS
16	p-Cymene	99-87-6	5.02	15.96	0.79	1025	119	924	947	17	1025	119	PASS	PASS	PASS
17	Guaiol	489-86-1	4.10	38.42	0.94	1603	59	908	908	39	1596	161	PASS	PASS	FAIL
18	1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	3338-55-4	2.52	16.38	0.69	1036	93	904	905	9	1038	93	PASS	PASS	PASS
19	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	40716-66-3	2.43	37.04	0.82	1564	41	939	946	37	1564	41	PASS	PASS	PASS
20	Geraniol	106-24-1	3.19	25.54	0.99	1255	41	922	922	37	1255	69	PASS	PASS	FAIL
21	Nerolidol	142-50-7	1.46	36.00	0.82	1530	41	949	954	42	1544	41	PASS	PASS	PASS
22	β-Pinene	127-91-3	0.88	15.04	0.75	1005	93	902	903	18	979	93	PASS	FAIL	PASS
23	Eucalyptol	470-82-6	0.71	16.29	0.84	1034	43	913	913	69	1032	43	PASS	PASS	PASS
24	7-Oxabicyclo[2.2.1]heptane, 1-methyl-4-(1-methylethyl)-	470-67-7	0.28	15.50	0.82	1014	43	904	918	62	1016	43	PASS	PASS	PASS
30	α-Phellandrene	99-83-2	0.19	15.17	0.72	1008	93	926	931	63	1005	93	PASS	PASS	PASS
32	Fenchol, exo-	22627-95-8	0.13	20.17	0.99	1123	81	938	942	50	1116	81	PASS	PASS	PASS
33	cis-2,6-Dimethyl-2,6-octadiene	2492-22-0	0.03	14.17	0.65	986	41	880	915	32		69	PASS		FAIL
34	2-Furanmethanol, tetrahydro-α,α,5-trimethyl-5-(4-methyl-3-cyclohexen-1-yl)-, [2S-[2α,5β(R*)]]-	26184-88-3	0.14	40.33	0.98	1658	43	891	894	90	1655	143	PASS	PASS	FAIL
35	Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-	508-32-7	0.10	11.58	0.70		93	921	925	23	925	93	PASS		PASS
36	β-Ocimene	13877-91-3	0.05	14.96	0.71	1004	93	918	920	14	1037	93	PASS	FAIL	PASS
37	2,4,6-Octatriene, 2,6-dimethyl-, (E,Z)-	7216-56-0	0.12	20.46	0.78	1130	121	918	924	25	1131	121	PASS	PASS	PASS
38	(1R,3E,7E,11R)-1,5,5,8-Tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	19888-34-7	0.09	38.96	1.34	1619	43	891	892	63	1606	109	PASS	PASS	FAIL
39	Aromandendrene	489-39-4	0.09	33.79	0.77	1459	41	909	923	20	1440	41	PASS	FAIL	PASS
40	1R,3Z,9s-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene	0-00-0	0.10	33.33	0.79	1446	41	877	883	15	1505	41	PASS	FAIL	PASS

Analyte ID			Blob					Library					Tests		
ID	Compound Name	CAS#	%Rsp	¹ tr	² tr	I'	BsPk	DMF	RMF	Prob	I	BsPk	DMF	RI	BsPk
41	Santolina triene	2153-66-4	0.09	15.92	0.70	1024	93	813	849	9	908	93	FAIL	FAIL	PASS
42	o-Cymene	527-84-4	0.06	15.75	0.83	1020	119	942	959	40	1022	119	PASS	PASS	PASS
43	5,5,6-Trimethylhept-3-en-2-one	0-00-0	0.07	29.42	0.95	1349	43	737	761	18		43	FAIL		PASS
44	Limonene oxide, cis-	13837-75-7	0.11	20.71	1.23	1136	43	914	933	38	1134	43	PASS	PASS	PASS
46	Caryophyllene oxide	1139-30-6	0.01	38.04	1.35	1593	41	841	844	43	1581	43	FAIL	PASS	FAIL
49	1,2-Dihydrolinalool	18479-51-1	0.07	20.71	0.92	1136	41	883	907	75	1120	109	PASS	PASS	FAIL
53	trans-Ascaridol glycol	21473-37-0	0.07	29.13	1.01	1342	43	834	878	70	1272	109	FAIL	FAIL	FAIL
54	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	483-76-1	0.06	34.13	0.71	1470	105	853	875	26	1524	161	PASS	FAIL	FAIL
55	β-Myrcene	123-35-3	0.07	14.75	0.65	999	41	826	857	27	991	93	FAIL	PASS	FAIL
56	3-Oxabicyclo[4.3.0]non-8-en-2-one, cis-	0-00-0	0.06	21.17	1.21	1147	79	769	784	14		79	FAIL		PASS
57	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	110823-68-2	0.06	34.04	0.83	1467	41	851	855	11		81	PASS		FAIL
58	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	0.07	13.67	0.76	973	91	850	866	21	1131	91	PASS	FAIL	PASS
59	Limonene oxide, trans-	4959-35-7	0.05	20.92	1.23	1141	43	908	924	66	1138	43	PASS	PASS	PASS
60	2-Isopropylidene-3-methylhexa-3,5-dienal	0-00-0	0.02	18.92	0.84	1093	91	772	780	10	1164	91	FAIL	FAIL	PASS
61	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-	497-32-5	0.06	12.29	0.72	943	79	910	917	43	940	79	PASS	PASS	PASS
68	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, trans-	7212-40-0	0.05	20.29	1.02	1126	43	900	903	51	1123	109	PASS	PASS	FAIL
69	trans-Ascaridol glycol	21473-37-0	0.03	30.38	0.97	1372	109	802	829	36	1272	109	FAIL	FAIL	PASS
70	3-Oxatricyclo[4.1.1.0(2,4)]octane, 2,7,7-trimethyl-	1686-14-2	0.03	19.29	1.33	1101	67	869	876	38	1095	67	PASS	PASS	PASS
74	Carvone	99-49-0	0.03	25.46	1.55	1253	82	924	949	50	1242	82	PASS	PASS	PASS
75	α-Bisabolol	515-69-5	0.06	40.71	0.87	1669	43	851	876	30	1684	43	PASS	FAIL	PASS
77	α-Guaiene	3691-12-1	0.04	32.79	0.71	1431	41	888	901	14	1439	105	PASS	PASS	FAIL
79	cis-p-Mentha-2,8-dien-1-ol	3886-78-0	0.05	20.92	1.03	1141	43	853	863	28	1102	43	PASS	FAIL	PASS
81	(E)-Bisabol-11-ol	73416-20-3	0.03	40.63	0.87	1666	93	822	843	10	1670	93	FAIL	PASS	PASS
82	Cyclohexene, 3-methyl-6-(1-methylethyl)-	5256-65-5	0.02	14.88	0.74	1002	41	828	848	9	1004	95	FAIL	PASS	FAIL
83	Fenchone	1195-79-5	0.03	18.83	1.56	1091	81	916	924	64	1096	81	PASS	PASS	PASS
84	5-Azulenemethanol, 1,2,3,3a,4,5,6,7-octahydro-α,α,3,8-tetramethyl-, [3S-(3α,3aβ,5α)]-	22451-73-6	0.03	40.71	0.94	1669	59	875	881	48	1667	59	PASS	PASS	PASS
87	(1S,2R,4R,7R)-4-Isopropyl-7-methyl-3,8-dioxatricyclo[5.1.0.02,4]octane	1619-26-7	0.03	24.58	1.47	1231	43	879	900	77	1306	43	PASS	FAIL	PASS
88	cis-Calamenene	72937-55-4	0.02	35.88	0.78	1526	159	870	875	26	1531	159	PASS	PASS	PASS
89	10,10-Dimethyl-2,6-dimethylenebicyclo[7.2.0]undecane	357414-37-0	0.03	32.58	0.81	1426	41	850	852	15	1440	120	PASS	PASS	FAIL
90	1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hexahydro-1,4,9,9-tetramethyl-, (1α,3α,7α,8aβ)-	560-32-7	0.02	33.88	0.78	1462	93	850	858	11	1457	107	PASS	PASS	FAIL
91	cis-(-)-1,2-Epoxy-p-menth-8-ene	32543-51-4	0.02	20.75	1.35	1137	43	830	830	8	1136	43	FAIL	PASS	PASS
92	Guaiol	489-86-1	0.03	38.83	0.93	1615	59	854	855	13	1596	161	PASS	PASS	FAIL
94	Oxirane, 2-(hexyn-1-yl)-3-methoxymethylene-	0-00-0	0.02	18.08	0.91	1074	43	767	777	22		79	FAIL		FAIL
97	Benzenemethanol, α,α,4-trimethyl-	1197-01-9	0.06	23.17	1.02	1197	43	827	848	73	1183	43	FAIL	PASS	PASS
99	cis-Verbenol	1845-30-3	0.02	19.75	1.12	1112	43	802	807	20	1142	41	FAIL	FAIL	FAIL
101	Carvone	99-49-0	0.05	25.54	1.54	1255	41	833	864	55	1242	82	FAIL	PASS	FAIL
102	β-Bisabolene	495-61-4	0.02	35.33	0.66	1509	41	867	882	33	1509	69	PASS	PASS	FAIL

Analyte ID			Blob					Library					Tests		
ID	Compound Name	CAS#	%Rsp	¹ t _R	² t _R	I'	BsPk	DMF	RMF	Prob	I	BsPk	DMF	RI	BsPk
103	2,6,11,15-Tetramethyl-hexadeca-2,6,8,10,14-pentaene	38259-79-9	0.03	47.29	0.65		41	803	805	15		69	FAIL		FAIL
108	Humulene	6753-98-6	0.02	36.42	0.64	1544	93	878	886	26	1454	93	PASS	FAIL	PASS
111	(Z)-((3,7-dimethylocta-2,6-dien-1-yl)oxy)trimethylsilane	0-00-0	0.04	29.83	0.68	1359	41	815	830	35		73	FAIL		FAIL
112	2,4-Hexadiene, 2,5-dimethyl-	764-13-6	0.01	19.38	0.79	1103	95	729	771	9	861	95	FAIL	FAIL	PASS
118	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	0.04	19.88	0.79	1115	41	835	891	28	1131	91	FAIL	FAIL	FAIL
119	3,6-Heptadien-2-ol, 2,5,5-trimethyl-, (E)-	26127-98-0	0.02	18.29	0.90	1079	43	771	771	10	1000	43	FAIL	FAIL	PASS
120	(1R,2S,4R)-2,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol	3247-40-3	0.02	19.54	1.01	1107	43	836	836	18		43	FAIL		PASS
123	2,6-Octadienal, 3,7-dimethyl-, (E)-	141-27-5	0.04	26.38	1.67	1275	41	867	894	37	1270	69	PASS	PASS	FAIL
128	Longifolene	475-20-7	0.02	32.00	0.81	1411	41	877	881	10	1405	41	PASS	PASS	PASS
129	trans-2-Caren-4-ol	4017-82-7	0.01	19.42	1.08	1104	43	827	829	27	1178	109	FAIL	FAIL	FAIL
131	trans-Carveol	1197-07-5	0.03	24.50	0.97	1229	109	902	912	44	1217	109	PASS	PASS	PASS
139	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, cis-	1197-06-4	0.02	25.00	0.96	1242	41	894	898	41	1229	84	PASS	PASS	FAIL
140	(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	206115-88-0	0.06	22.67	0.98	1184	43	801	845	11		43	FAIL		PASS
151	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-	118-65-0	0.01	31.75	0.79	1405	41	867	876	16	1406	41	PASS	PASS	PASS
154	trans-2-Caren-4-ol	4017-82-7	0.02	25.21	0.99	1247	43	815	819	17	1178	109	FAIL	FAIL	FAIL
171	Ribitol, 1,3:2,4-di-O-benzylidene-	4148-60-1	0.01	8.79	0.71		149	709	709	57		179	FAIL		FAIL
174	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	0.02	20.88	0.82	1140	91	869	897	28	1131	91	PASS	PASS	PASS
184	α-Phellandrene	99-83-2	0.01	11.67	0.66		93	869	907	33	1005	93	PASS		PASS
188	2-Isopropenyl-5-methylhex-4-enal	75697-98-2	0.03	24.75	0.97	1236	41	801	874	36		41	FAIL		PASS
196	Caryophyllene oxide	1139-30-6	0.01	36.96	1.32	1561	43	783	809	23	1581	43	FAIL	FAIL	PASS
201	(1R,2S,4R)-2,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol	3247-40-3	0.01	20.21	1.11	1124	43	827	827	30		43	FAIL		PASS
208	1,5-Decadiyne	53963-03-4	0.00	20.83	1.28	1139	39	712	713	6		91	FAIL		FAIL
212	cis-α-Bisabolene	29837-07-8	0.02	40.00	0.90	1648	43	805	842	12	1504	93	FAIL	FAIL	FAIL
217	cis-β-Farnesene	28973-97-9	0.01	33.29	0.67	1445	41	862	903	35	1444	41	PASS	PASS	PASS
222	Germacrene D	23986-74-5	0.01	30.63	0.74	1378	105	864	871	19	1481	161	PASS	FAIL	FAIL
227	2,4,6-Octatriene, 2,6-dimethyl-, (E,E)-	3016-19-1	0.03	21.04	0.84	1144	91	829	892	12	1144	121	FAIL	PASS	FAIL
228	cis-β-Farnesene	28973-97-9	0.01	32.38	0.67	1420	41	825	885	49	1444	41	FAIL	FAIL	PASS
229	Santolina triene	2153-66-4	0.01	13.54	0.68	970	93	872	888	27	908	93	PASS	FAIL	PASS
236	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethenyl)-, [2R-(2α,4α,8aβ)]-	473-13-2	0.01	39.00	0.91	1620	43	727	775	5	1494	41	FAIL	FAIL	FAIL
245	cis-Verbenol	1845-30-3	0.01	20.50	0.99	1131	81	753	793	6	1142	41	FAIL	FAIL	FAIL
251	Cyclohexene, 4-methylene-1-(1-methylethyl)-	99-84-3	0.01	17.33	0.81	1058	93	844	910	10	1028	93	FAIL	FAIL	PASS
254	α-Terpineol	98-55-5	0.02	23.46	0.98	1204	43	695	803	8	1189	59	FAIL	PASS	FAIL
256	Humulene	6753-98-6	0.01	39.08	0.86	1622	93	783	840	13	1454	93	FAIL	FAIL	PASS
257	Santolina triene	2153-66-4	0.01	13.46	0.69	968	67	855	860	32	908	93	PASS	FAIL	FAIL
269	1,3,7-Octatriene, 3,7-dimethyl-	502-99-8	0.01	38.58	1.32	1608	93	791	852	20	1047	93	FAIL	FAIL	PASS
272	Nerolidol	142-50-7	0.01	36.46	0.77	1545	41	792	875	25	1544	41	FAIL	PASS	PASS
276	11-Tridecyn-1-ol	33925-75-6	0.01	39.67	1.21	1639	41	814	835	14		68	FAIL		FAIL

Analyte ID			Blob					Library					Tests		
ID	Compound Name	CAS#	%Rsp	¹ tr	² tr	I'	BsPk	DMF	RMF	Prob	I	BsPk	DMF	RI	BsPk
282	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, trans-	7212-40-0	0.01	23.63	1.15	1208	39	747	770	8	1123	43	FAIL	FAIL	FAIL
285	cis- α -Bisabolene	29837-07-8	0.01	35.04	0.64	1500	41	817	836	16	1504	93	FAIL	PASS	FAIL
286	β -Myrcene	123-35-3	0.01	11.08	0.72		41	845	899	59	991	93	FAIL		FAIL
290	2-Methyl-1-nonene-3-yne	70058-00-3	0.01	18.04	0.73	1074	79	822	905	17		79	FAIL		PASS
304	1,4-dihydroxy-p-menth-2-ene	0-00-0	0.01	26.75	1.27	1284	43	819	848	71		109	FAIL		FAIL
311	Cubenol	21284-22-0	0.01	40.21	0.93	1654	43	757	825	6	1642	119	FAIL	PASS	FAIL
317	Germacrene D	23986-74-5	0.01	34.67	0.69	1488	41	822	880	10	1481	161	FAIL	PASS	FAIL
321	1,1,3,3-Tetramethyl-3-(1-methylpropoxy)disiloxan-1-ol	0-00-0	0.00	11.88	0.73		165	784	788	92		163	FAIL		FAIL
333	1,3-Cyclopentadiene, 5,5-dimethyl-2-propyl-	0-00-0	0.01	17.92	0.82	1071	91	806	826	13		107	FAIL		FAIL
342	Butylated Hydroxytoluene	128-37-0	0.01	35.08	0.81	1501	41	752	816	75	1513	205	FAIL	PASS	FAIL
345	(-)-trans-Isopiperitenol	74410-00-7	0.01	23.75	1.07	1211	84	745	843	63	1210	84	FAIL	PASS	PASS
355	(+)-cis-Verbenol, acetate	29135-27-1	0.00	23.83	1.12	1213	91	744	773	14	1279	119	FAIL	FAIL	FAIL
362	Benzenemethanol, 4-(methoxymethyl)- α -methyl-	66190-31-6	0.01	18.50	0.90	1084	151	611	777	30		151	FAIL		PASS
367	2,4-Cycloheptadien-1-one, 2,6,6-trimethyl-	503-93-5	0.01	24.50	1.57	1229	107	806	828	37	1243	107	FAIL	FAIL	PASS
371	3-Oxabicyclo[3.2.1]octane-2,4-dione, 1-bromo-5,8,8-trimethyl-	13441-28-6	0.00	20.63	1.27	1134	41	628	661	19		69	FAIL		FAIL
373	2-Furanmethanol, 5-ethenyltetrahydro- $\alpha,\alpha,5$ -trimethyl-, cis-	5989-33-3	0.01	18.00	1.10	1073	43	818	831	38	1074	59	FAIL	PASS	FAIL
375	1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	3479-89-8	0.01	33.13	0.72	1440	119	729	782	7	971	119	FAIL	FAIL	PASS
379	1,3,7-Octatriene, 3,7-dimethyl-	502-99-8	0.01	23.46	1.14	1204	79	749	817	9	1047	93	FAIL	FAIL	FAIL
383	2-Methyl-1-nonene-3-yne	70058-00-3	0.01	18.46	0.80	1083	93	709	861	7		79	FAIL		FAIL
386	trans- α -Bergamotene	13474-59-4	0.01	34.38	0.69	1478	41	708	823	8	1435	93	FAIL	FAIL	FAIL
389	α -Bisabolol	515-69-5	0.00	40.50	1.06	1663	43	737	771	13	1684	43	FAIL	FAIL	PASS
395	trans-Ascaridol glycol	21473-37-0	0.00	30.58	0.97	1377	43	693	702	40	1272	109	FAIL	FAIL	FAIL
396	Formic acid, 3,7,11-trimethyl-1,6,10-dodecatrien-3-yl ester	0-00-0	0.01	42.21	0.90		43	686	690	10	1752	43	FAIL		PASS
399	4-Hydroxy-4-(2-methylcyclohex-3-enyl)butan-2-one	0-00-0	0.00	34.46	0.93	1481	43	515	612	36		43	FAIL		PASS
400	trans-Ascaridol glycol	21473-37-0	0.00	27.58	1.29	1304	43	559	639	30	1272	109	FAIL	FAIL	FAIL
402	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	26560-14-5	0.00	35.13	0.68	1502	41	785	867	28	1491	41	FAIL	PASS	PASS
406	Hydroxylamine, O-decyl-	29812-79-1	0.01	27.54	0.61	1303	43	736	835	12	1100	43	FAIL	FAIL	PASS
409	Oxalic acid, allyl nonyl ester	0-00-0	0.00	34.96	0.59	1497	43	777	843	4		41	FAIL		FAIL
413	Cyclohexane, 1,5-diethenyl-3-methyl-2-methylene-, (1 α ,3 α ,5 α)-	74742-35-1	0.00	32.17	0.82	1415	41	720	725	13		79	FAIL		FAIL
414	1,3,7-Octatriene, 3,7-dimethyl-	502-99-8	0.03	19.25	0.61	1100	41	766	844	7	1047	93	FAIL	FAIL	FAIL
416	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, (1R)-	5794-03-6	0.15	14.17	0.72	986	93	883	893	11	951	93	PASS	FAIL	PASS
417	Caryophyllene oxide	1139-30-6	0.06	38.04	1.39	1593	41	877	878	45	1581	43	PASS	PASS	FAIL
418	(1,3-Dimethyl-2-methylene-cyclopentyl)-methanol	0-00-0	0.02	15.00	0.66	1004	41	797	814	22		109	FAIL		FAIL
419	α -Pinene	80-56-8	0.03	16.42	0.79	1037	91	785	843	7	937	93	FAIL	FAIL	FAIL
421	2-Furanmethanol, 5-ethenyltetrahydro- $\alpha,\alpha,5$ -trimethyl-, cis-	5989-33-3	0.01	18.71	1.11	1089	59	794	810	47	1074	59	FAIL	PASS	PASS
422	Benzene, 1-methyl-4-(1-methylethenyl)-	1195-32-0	0.06	18.92	0.88	1093	117	944	952	33	1090	117	PASS	PASS	PASS

Table S2: Detected ion-peak sets.

ID	%Rsp	¹ t _R	² t _R	RI	BsPk	Ion Peaks
38	0.0154	14.38	0.64	992	69	69, 70, 82, 95, 96, 123, 138
50	0.0061	16.25	0.78	1030	93	51, 62, 63, 64, 65, 77, 78, 80, 89, 91, 93, 136
60	0.0027	20.75	1.23	1137	43	40, 43, 55, 67, 68, 71, 81, 82
351	0.0009	9.21	1.95		39	39, 41, 43
374	0.0010	12.88	0.74	955	91	91, 92
382	0.0004	12.58	0.67	949	93	93, 108
474	0.0017	20.71	1.20	1136	137	94, 137
501	0.0019	14.96	0.75	1004	119	119, 134
526	0.0001	8.83	2.10		31	31
529	0.0004	14.00	0.65	981	41	41, 69
564	0.0030	14.54	0.70	995	55	55
583	0.0030	14.38	0.80	992	81	81
700	0.0004	22.79	0.94	1187	69	69
748	0.0001	10.63	0.99		43	43
813	0.0003	35.46	0.67	1513	41	41
819	0.0005	22.67	0.99	1184	91	39, 41, 91
895	0.0003	22.58	0.98	1182	109	109
907	0.0002	23.50	0.61	1205	43	41, 43
928	0.0002	18.63	1.75	1087	69	69
938	0.0040	13.96	0.68	980	97	97

Table S3: Mass spectral search experimental settings (source spectrum, blob spectrum integration threshold, spectrum subtraction, intensity threshold, presearch) and resulting performance for all blobs and top blobs (direct match factor, reverse match factor, probability, average match factor, coefficient of determination). Groups of experiments are shown with alternate shading. Results for All analytes are colorized by column to indicate performance (red for low, green for high).

Row	Experimental Settings					Results All					Results Top				
	Src	Intgr.	Subtr.	Thr.	Search	DMF	RMF	Prob.	AMF	R ²	DMR	RMF	Prob.	AMF	R ²
1	Apex	0	None	0	None	775	818	21%	797	0.80	923	928	39%	926	0.99
2	Apex	0	None	0	Quick	772	820	25%	796	0.75	923	928	40%	926	0.99
3	Apex	0	None	0	Norm	774	818	25%	796	0.78	923	928	40%	926	0.99
4	Blob	0	None	0	None	785	835	18%	810	0.72	914	922	38%	918	0.99
5	Blob	0	None	0	Quick	783	834	23%	809	0.68	914	922	39%	918	0.99
6	Blob	0	None	0	Norm	784	835	23%	809	0.72	914	922	40%	918	0.99
7	Apex	0	None	5	Norm	777	822	25%	800	0.83	923	928	40%	926	0.99
8	Apex	0	None	10	Norm	779	826	25%	803	0.84	923	928	40%	926	0.99
9	Apex	0	None	15	Norm	782	831	26%	806	0.86	923	928	40%	926	0.99
10	Apex	0	None	16	Norm	782	831	26%	807	0.87	923	928	40%	926	0.99
11	Apex	0	None	17	Norm	783	832	26%	808	0.87	923	928	40%	926	0.99
12	Apex	0	None	18	Norm	784	831	26%	808	0.87	923	928	40%	926	0.99
13	Apex	0	None	19	Norm	786	834	26%	810	0.90	923	928	40%	926	0.99
14	Apex	0	None	20	Norm	786	834	27%	810	0.90	923	928	40%	926	0.99
15	Apex	0	None	21	Norm	787	834	27%	810	0.86	923	928	40%	926	0.99
16	Apex	0	None	22	Norm	787	833	27%	810	0.89	923	928	40%	926	0.99
17	Apex	0	None	23	Norm	788	832	27%	810	0.89	923	928	40%	926	0.99
18	Apex	0	None	24	Norm	789	832	27%	811	0.85	923	928	40%	926	0.99
19	Apex	0	None	25	Norm	790	832	27%	811	0.85	923	928	40%	926	0.99
20	Apex	0	None	26	Norm	790	831	27%	811	0.85	923	928	40%	926	0.99
21	Apex	0	None	27	Norm	791	831	27%	811	0.92	923	928	40%	926	0.99
22	Apex	0	None	28	Norm	791	829	27%	810	0.92	923	928	40%	926	0.99
23	Apex	0	None	29	Norm	791	829	27%	810	0.87	923	928	40%	926	0.99
24	Apex	0	None	30	Norm	791	828	27%	809	0.85	923	928	40%	926	0.99
25	Apex	0	None	32	Norm	791	828	27%	809	0.83	923	928	40%	926	0.99
26	Apex	0	None	35	Norm	791	826	28%	809	0.80	923	928	40%	926	0.99
27	Apex	0	None	50	Norm	791	825	28%	808	0.73	923	928	40%	926	0.99
28	Blob	0	None	50	Norm	785	836	23%	811	0.69	914	922	40%	918	0.99
29	Blob	0	None	150	Norm	787	836	23%	811	0.88	914	922	40%	918	0.99
30	Blob	0	None	200	Norm	789	838	23%	813	0.81	914	922	40%	918	0.99
31	Blob	0	None	250	Norm	790	838	23%	814	0.82	914	922	40%	918	0.99
32	Blob	0	None	300	Norm	792	839	24%	815	0.82	914	922	40%	918	0.99
33	Blob	0	None	350	Norm	795	839	24%	817	0.88	914	922	40%	918	0.99
34	Blob	0	None	400	Norm	798	840	25%	819	0.83	914	922	40%	918	0.99
35	Blob	0	None	450	Norm	801	842	25%	822	0.90	914	922	40%	918	0.99
36	Blob	0	None	500	Norm	803	842	25%	822	0.89	914	922	40%	918	0.99
37	Blob	0	None	550	Norm	805	840	26%	823	0.89	914	922	40%	918	0.99
38	Blob	0	None	575	Norm	805	839	26%	822	0.88	914	922	40%	918	0.99
39	Blob	0	None	600	Norm	806	839	26%	822	0.87	914	922	40%	918	0.99
40	Blob	0	None	625	Norm	807	840	27%	823	0.88	914	922	40%	918	0.99
41	Blob	0	None	650	Norm	807	839	26%	823	0.88	914	922	40%	918	0.99
42	Blob	0	None	675	Norm	807	839	26%	823	0.85	914	922	40%	918	0.99
43	Blob	0	None	700	Norm	808	840	26%	824	0.86	914	922	40%	918	0.99
44	Blob	0	None	725	Norm	808	838	26%	823	0.86	914	922	40%	918	0.99
45	Blob	0	None	750	Norm	809	839	27%	824	0.83	914	922	40%	918	0.99
46	Blob	0	None	775	Norm	809	837	26%	823	0.81	914	922	40%	918	0.99
47	Blob	0	None	800	Norm	809	836	27%	823	0.82	914	922	40%	918	0.99
48	Blob	0	None	900	Norm	810	835	27%	822	0.86	914	922	39%	918	0.99
49	Blob	0	None	1000	Norm	811	833	28%	822	0.80	914	922	39%	918	0.99
50	Blob	0	None	1200	Norm	807	826	28%	817	0.76	914	922	39%	918	0.99
51	Apex	0	Start	0	Norm	759	803	25%	781	0.69	924	928	41%	926	0.99
52	Apex	0	Start	5	Norm	762	807	25%	784	0.88	924	928	41%	926	0.99
53	Apex	0	Start	10	Norm	763	808	26%	785	0.90	924	928	41%	926	0.99
54	Apex	0	Start	15	Norm	764	811	26%	787	0.88	924	928	41%	926	0.99
55	Apex	0	Start	20	Norm	768	813	27%	791	0.89	924	928	41%	926	0.99
56	Apex	0	Start	25	Norm	771	815	27%	793	0.85	924	928	41%	926	0.99
57	Apex	0	Start	30	Norm	771	810	27%	791	0.86	924	928	41%	926	0.99
58	Apex	0	Start	35	Norm	772	811	28%	792	0.66	924	928	41%	926	0.99
59	Apex	0	Start	40	Norm	775	812	29%	794	0.78	924	928	41%	926	0.99

60	Apex	0	Start	50	Norm	775	807	30%	791	0.78	924	928	41%	926	0.99
61	Blob	0	Start	0	Norm	753	795	24%	774	0.66	913	920	39%	917	0.99
62	Blob	0	Start	50	Norm	755	798	24%	776	0.65	913	920	39%	917	0.99
63	Blob	0	Start	100	Norm	755	798	24%	777	0.84	913	920	39%	917	0.99
64	Blob	0	Start	200	Norm	756	803	24%	779	0.93	913	920	39%	917	0.99
65	Blob	0	Start	300	Norm	761	813	25%	787	0.85	913	920	39%	917	0.99
66	Blob	0	Start	400	Norm	767	813	26%	790	0.79	913	920	39%	917	0.99
67	Blob	0	Start	500	Norm	773	811	28%	792	0.76	913	920	39%	917	0.99
68	Blob	0	Start	600	Norm	781	814	28%	797	0.67	913	920	39%	917	0.99
69	Blob	0	Start	700	Norm	787	813	28%	800	0.69	913	920	39%	917	0.99
70	Blob	0	Start	800	Norm	785	806	28%	796	0.55	913	920	39%	917	0.99
71	Blob	0	Start	900	Norm	767	785	28%	776	0.68	913	920	39%	917	0.99
72	Apex	0	S&E	0	Norm	761	801	25%	781	0.57	923	929	40%	926	0.99
73	Apex	0	S&E	5	Norm	764	807	25%	786	0.66	923	929	40%	926	0.99
74	Apex	0	S&E	10	Norm	766	812	25%	789	0.84	923	929	40%	926	0.99
75	Apex	0	S&E	15	Norm	769	818	25%	793	0.85	923	929	40%	926	0.99
76	Apex	0	S&E	20	Norm	774	818	26%	796	0.83	923	929	40%	926	0.99
77	Apex	0	S&E	25	Norm	776	820	27%	798	0.81	923	929	40%	926	0.99
78	Apex	0	S&E	30	Norm	777	819	27%	798	0.77	923	929	40%	926	0.99
79	Apex	0	S&E	35	Norm	778	815	27%	796	0.73	923	929	40%	926	0.99
80	Apex	0	S&E	40	Norm	780	815	28%	797	0.75	923	929	40%	926	0.99
81	Apex	0	S&E	50	Norm	779	814	29%	796	0.57	923	929	40%	926	0.99
82	Blob	0	S&E	0	Norm	763	811	24%	787	0.65	915	921	39%	918	0.99
83	Blob	0	S&E	50	Norm	765	814	24%	789	0.70	915	921	39%	918	0.99
84	Blob	0	S&E	100	Norm	766	815	24%	790	0.76	915	921	39%	918	0.99
85	Blob	0	S&E	200	Norm	768	819	24%	793	0.83	915	921	39%	918	0.99
86	Blob	0	S&E	300	Norm	773	821	25%	797	0.86	915	921	39%	918	0.99
87	Blob	0	S&E	400	Norm	781	825	26%	803	0.88	915	921	39%	918	0.99
88	Blob	0	S&E	500	Norm	787	823	27%	805	0.89	915	921	39%	918	0.99
89	Blob	0	S&E	600	Norm	793	821	27%	807	0.75	915	921	39%	918	0.99
90	Blob	0	S&E	700	Norm	787	813	28%	800	0.82	915	921	39%	918	0.99
91	Blob	0	S&E	800	Norm	789	813	28%	801	0.77	915	921	39%	918	0.99
92	Blob	0	S&E	900	Norm	789	811	29%	800	0.75	915	921	39%	918	0.99
93	Blob	5	None	700	Norm	812	839	27%	825	0.85	918	924	40%	921	0.99
94	Blob	10	None	700	Norm	818	841	28%	830	0.86	919	925	41%	922	0.98
95	Blob	15	None	700	Norm	819	839	28%	829	0.87	919	925	40%	922	0.99
96	Blob	20	None	700	Norm	822	841	29%	831	0.81	919	925	40%	922	0.99
97	Blob	25	None	700	Norm	822	839	29%	831	0.81	920	925	41%	922	0.99
98	Blob	30	None	700	Norm	822	836	30%	829	0.80	920	926	40%	923	0.99
99	Blob	35	None	700	Norm	820	833	30%	827	0.76	920	926	40%	923	0.99
100	Blob	5	None	600	Norm	811	842	27%	826	0.82	918	924	40%	921	0.99
101	Blob	10	None	600	Norm	816	843	28%	829	0.88	919	925	41%	922	0.98
102	Blob	15	None	600	Norm	820	843	28%	831	0.89	919	925	40%	922	0.99
103	Blob	20	None	600	Norm	821	843	28%	832	0.92	919	925	40%	922	0.99
104	Blob	25	None	600	Norm	823	842	29%	832	0.82	920	925	41%	922	0.99
105	Blob	30	None	600	Norm	824	840	29%	832	0.74	920	926	40%	923	0.99
106	Blob	35	None	600	Norm	823	837	30%	830	0.77	920	926	40%	923	0.99
107	Blob	5	None	500	Norm	808	842	26%	825	0.90	918	924	40%	921	0.99
108	Blob	10	None	500	Norm	813	844	27%	828	0.94	919	925	41%	922	0.98
109	Blob	15	None	500	Norm	817	842	27%	830	0.94	919	925	40%	922	0.99
110	Blob	20	None	500	Norm	820	845	28%	832	0.87	919	925	40%	922	0.99
111	Blob	25	None	500	Norm	822	844	28%	833	0.87	920	925	41%	922	0.99
112	Blob	30	None	500	Norm	824	845	29%	834	0.79	920	926	40%	923	0.99
113	Blob	35	None	500	Norm	825	843	29%	834	0.75	920	926	40%	923	0.99
114	Blob	40	None	500	Norm	825	841	30%	833	0.83	920	926	40%	923	0.99
115	Blob	5	None	400	Norm	803	841	25%	822	0.84	918	924	40%	921	0.99
116	Blob	10	None	400	Norm	809	843	27%	826	0.76	919	925	41%	922	0.98
117	Blob	15	None	400	Norm	814	845	27%	830	0.86	919	925	40%	922	0.99
118	Blob	20	None	400	Norm	818	846	28%	832	0.92	919	925	40%	922	0.99
119	Blob	25	None	400	Norm	820	844	28%	832	0.84	920	925	41%	922	0.99
120	Blob	30	None	400	Norm	823	846	29%	835	0.89	920	926	40%	923	0.99
121	Blob	35	None	400	Norm	825	846	29%	836	0.83	920	926	40%	923	0.99
122	Blob	40	None	400	Norm	827	846	30%	836	0.88	920	926	40%	923	0.99
123	Blob	45	None	400	Norm	827	843	30%	835	0.86	920	926	40%	923	0.99
124	Blob	50	None	400	Norm	825	838	30%	831	0.81	920	926	40%	923	0.99
125	Blob	5	None	350	Norm	799	842	25%	821	0.83	918	924	40%	921	0.99
126	Blob	10	None	350	Norm	806	844	26%	825	0.88	919	925	41%	922	0.98

127	Blob	15	None	350	Norm	811	844	27%	827	0.91	919	925	40%	922	0.99
128	Blob	20	None	350	Norm	815	845	27%	830	0.92	919	925	40%	922	0.99
129	Blob	25	None	350	Norm	818	845	28%	831	0.92	920	925	41%	922	0.99
130	Blob	30	None	350	Norm	822	847	28%	834	0.88	920	926	40%	923	0.99
131	Blob	35	None	350	Norm	825	847	29%	836	0.91	920	926	40%	923	0.99
132	Blob	40	None	350	Norm	827	847	30%	837	0.85	920	926	40%	923	0.99
133	Blob	45	None	350	Norm	827	844	30%	836	0.83	920	926	40%	923	0.99
134	Blob	50	None	350	Norm	825	841	29%	833	0.76	920	926	40%	923	0.99
135	Blob	5	None	300	Norm	796	841	24%	819	0.83	918	924	40%	921	0.99
136	Blob	10	None	300	Norm	803	844	26%	823	0.77	919	925	41%	922	0.98
137	Blob	15	None	300	Norm	808	846	26%	827	0.89	919	925	40%	922	0.99
138	Blob	20	None	300	Norm	813	847	27%	830	0.91	919	925	40%	922	0.99
139	Blob	25	None	300	Norm	815	845	27%	830	0.91	920	925	41%	922	0.99
140	Blob	30	None	300	Norm	819	847	28%	833	0.87	920	926	40%	923	0.99
141	Blob	35	None	300	Norm	822	849	29%	835	0.91	920	926	40%	923	0.99
142	Blob	40	None	300	Norm	825	848	29%	836	0.89	920	926	40%	923	0.99
143	Blob	45	None	300	Norm	827	848	30%	837	0.91	920	926	40%	923	0.99
144	Blob	50	None	300	Norm	828	845	30%	836	0.89	920	926	40%	923	0.99
145	Blob	55	None	300	Norm	826	842	30%	834	0.86	920	926	40%	923	0.99
146	Blob	5	None	250	Norm	794	840	24%	817	0.83	918	924	40%	921	0.99
147	Blob	10	None	250	Norm	800	844	25%	822	0.74	919	925	41%	922	0.98
148	Blob	15	None	250	Norm	805	847	26%	826	0.92	919	925	40%	922	0.99
149	Blob	20	None	250	Norm	810	849	26%	830	0.89	919	925	40%	922	0.99
150	Blob	25	None	250	Norm	812	848	27%	830	0.90	920	925	41%	922	0.99
151	Blob	30	None	250	Norm	815	846	27%	831	0.93	920	926	40%	923	0.99
152	Blob	35	None	250	Norm	819	848	28%	833	0.95	920	926	40%	923	0.99
153	Blob	40	None	250	Norm	822	849	29%	836	0.94	920	926	40%	923	0.99
154	Blob	45	None	250	Norm	826	851	30%	838	0.95	920	926	40%	923	0.99
155	Blob	50	None	250	Norm	826	846	29%	836	0.92	920	926	40%	923	0.99
156	Blob	55	None	250	Norm	825	845	29%	835	0.85	920	926	40%	923	0.99
157	Blob	5	None	200	Norm	792	839	23%	816	0.85	918	924	40%	921	0.99
158	Blob	10	None	200	Norm	798	843	25%	820	0.75	919	925	41%	922	0.98
159	Blob	15	None	200	Norm	802	845	25%	824	0.88	919	925	40%	922	0.99
160	Blob	20	None	200	Norm	806	847	26%	826	0.80	919	925	40%	922	0.99
161	Blob	25	None	200	Norm	809	846	26%	827	0.91	920	925	41%	922	0.99
162	Blob	30	None	200	Norm	812	848	27%	830	0.90	920	926	40%	923	0.99
163	Blob	35	None	200	Norm	815	847	27%	831	0.92	920	926	40%	923	0.99
164	Blob	40	None	200	Norm	819	851	28%	835	0.91	920	926	40%	923	0.99
165	Blob	45	None	200	Norm	821	849	28%	835	0.91	920	926	40%	923	0.99
166	Blob	50	None	200	Norm	821	848	29%	835	0.94	920	926	40%	923	0.99
167	Blob	55	None	200	Norm	822	847	29%	835	0.95	920	926	40%	923	0.99
168	Blob	60	None	200	Norm	822	845	29%	834	0.91	920	926	40%	923	0.99
169	Blob	65	None	200	Norm	822	845	30%	834	0.91	920	926	40%	923	0.99
170	Blob	70	None	200	Norm	821	842	30%	832	0.83	921	926	40%	923	0.99
171	Blob	5	None	150	Norm	790	838	23%	814	0.77	918	924	40%	921	0.99
172	Blob	10	None	150	Norm	795	843	24%	819	0.76	919	925	41%	922	0.99
173	Blob	15	None	150	Norm	800	843	25%	822	0.79	919	925	40%	922	0.99
174	Blob	20	None	150	Norm	804	846	25%	825	0.84	919	925	40%	922	0.99
175	Blob	25	None	150	Norm	807	846	25%	826	0.92	920	925	41%	922	0.99
176	Blob	30	None	150	Norm	809	847	26%	828	0.90	920	926	40%	923	0.99
177	Blob	35	None	150	Norm	811	845	26%	828	0.81	920	926	40%	923	0.99
178	Blob	40	None	150	Norm	814	852	27%	833	0.90	920	926	40%	923	0.99
179	Blob	45	None	150	Norm	816	849	28%	833	0.85	920	926	40%	923	0.99
180	Blob	50	None	150	Norm	816	850	28%	833	0.94	920	926	40%	923	0.99
181	Blob	55	None	150	Norm	817	848	28%	832	0.95	920	926	40%	923	0.99
182	Blob	60	None	150	Norm	817	848	28%	833	0.93	920	926	40%	923	0.99
183	Blob	65	None	150	Norm	818	847	29%	833	0.89	920	926	40%	923	0.99
184	Blob	70	None	150	Norm	815	845	29%	830	0.89	921	926	40%	923	0.99