

Appendix B: External Standard Compounds and Data

Example

RT1	RT2	Description	Column_T	Retention_d_alkane_	Contributor	Num Peak: MS
57.46	0.69	cis-Vaccenic Acid, TMS	SemiStdNF	2259	2260 Emily Barn	221 40 7; 41 207; 42 38; 43 144; 44
29.32	0.53	citronellol	SemiStdNF	1338	1339 Emily Barn	113 40 10; 41 213; 42 15; 43 44; 44
30.04	0.65	cycloisolongifolene	SemiStdNF	1355	1355 Emily Barn	136 40 11; 41 143; 42 8; 43 67; 44
78.9	0.97	deoxycholic Acid (maybe)	SemiStdNF	3347	3347 Emily Barn	308 40 2; 41 31; 42 4; 43 28; 44 10;
77.79	1.52	dibenz(ah)anthracene	SemiStdNF	3280	3280 Emily Barn	107 50 1; 51 1; 62 1; 63 3; 74 3;
34	0.9	dimethyl Glutaric Acid, TMS	SemiStdNF	1456	1457 Emily Barn	155 40 2; 41 17; 42 8; 43 36; 44 17;
48.66	0.62	dodecyl benzene	SemiStdNF	1920	1921 Emily Barn	69 40 2; 41 56; 42 7; 43 64; 44 2;
60.54	0.55	eicosanol, TMS	SemiStdNF	2390	2390 Emily Barn	114 40 2; 41 83; 42 13; 43 123; 44
78.06	0.84	ergosterol	SemiStdNF	3296	3297 Emily Barn	307 40 6; 41 179; 42 15; 43 179; 44
46.15	0.55	farnesol	SemiStdNF	1832	1832 Emily Barn	157 40 12; 41 297; 42 24; 43 139;
41.62	0.84	galactosan	SemiStdNF	1684	1684 Emily Barn	130 40 2; 41 4; 42 2; 43 15; 44 9;
42.42	1.9	gamma dodecalactone	SemiStdNF	1709	1710 Emily Barn	86 40 4; 41 83; 42 21; 43 60; 44 4;
42.61	1.97	beta-caryophyllene aldehyde	SemiStdNF	1715	1716 Emily Barn	138 40 14; 41 231; 42 22; 43 999;
36.82	0.54	SESQ7	SemiStdNF	1537	1538 Emily Barn	115 40 15; 41 539; 42 28; 43 36; 44
37.93	0.5	SESQ8	SemiStdNF	1569	1569 Emily Barn	111 40 11; 41 117; 42 9; 43 44; 44
52.47	0.93	beta-caryophyllinic acid, TMS	SemiStdNF	2060	2061 Emily Barn	209 40 1; 41 36; 42 4; 43 26; 44 8;
48.97	1.33	beta-caryophyllonic acid, TMS	SemiStdNF	1931	1932 Emily Barn	200 40 6; 41 93; 42 11; 43 384; 44
54.18	1.25	beta-nocaryophyllinic acid, TMS	SemiStdNF	2127	2127 Emily Barn	236 40 2; 41 46; 42 5; 43 34; 44 13;
43.9	0.27	beta-nocaryophyllone aldehyde	SemiStdNF	1757	1757 Emily Barn	146 40 15; 41 200; 42 21; 43 999;
50.49	1.73	beta-nocaryophyllonic acid, TMS	SemiStdNF	1985	1985 Emily Barn	213 40 8; 41 134; 42 15; 43 795; 44
79.89	0.87	beta-sitosterol	SemiStdNF	3406	3407 Emily Barn	286 40 6; 41 124; 42 15; 43 286; 44
44.32	0.56	bisabolol	SemiStdNF	1770	1771 Emily Barn	146 40 7; 41 168; 42 9; 43 39; 44 8;
25.78	0.62	borneol	SemiStdNF	1254	1254 Emily Barn	115 40 3; 41 79; 42 6; 43 42; 44 9;
76.61	0.84	cholesterol	SemiStdNF	3209	3209 Emily Barn	265 40 3; 41 136; 42 11; 43 183; 44
63.63	1.3	chrysene	SemiStdNF	2531	2532 Emily Barn	65 50 2; 51 1; 61 1; 62 3; 63 4;
27.34	0.72	C8 acid	SemiStdNF	1293	1293 Emily Barn	119 40 4; 41 59; 42 15; 43 51; 44
45.88	0.95	C9 Diacid (azelaic acid)	SemiStdNF	1822	1823 Emily Barn	172 40 1; 41 32; 42 10; 43 70; 44
31.22	0.69	C9 acid	SemiStdNF	1381	1382 Emily Barn	115 40 6; 41 75; 42 18; 43 70; 44
38.99	1.79	DEET	SemiStdNF	1600	1600 Emily Barn	55 40 1; 41 4; 42 8; 44 6; 50 3;
49.69	0.73	FAME16 (Methyl Palmitate)	SemiStdNF	1957	1957 Emily Barn	94 40 4; 41 134; 42 25; 43 181; 44
55.06	0.72	FAME18 (Methyl Stearate)	SemiStdNF	2161	2161 Emily Barn	105 40 4; 41 139; 42 25; 43 206; 44
44.51	0.98	MBTCA	SemiStdNF	1776	1777 Emily Barn	157 40 1; 41 24; 42 7; 43 31; 44 13;
39.72	0.83	Me-OH-glutatric acid (?)	SemiStdNF	1623	1623 Emily Barn	142 41 2; 42 2; 43 31; 44 12; 45 81;
81.14	1.06	a-Amyrin	SemiStdNF	3479	3479 Emily Barn	210 41 75; 42 4; 43 38; 44 3; 45 19;

62.26	0.84 abietic acid	SemiStdNF	2468	2468 Emily Barn	177 40 1; 41 35; 42 2; 43 31; 44 3;
51.37	1.45 anthraquinone	SemiStdNF	2017	2018 Emily Barn	88 49 5; 50 70; 51 17; 52 4; 53 5;
41.01	1.18 benzophenone	SemiStdNF	1664	1665 Emily Barn	44 49 3; 50 35; 51 121; 52 6; 53 1;
48.7	0.94 C10 diacid (sebacic acid)	SemiStdNF	1922	1922 Emily Barn	183 40 1; 41 40; 42 10; 43 83; 44
53.99	0.91 C12 diacid	SemiStdNF	2120	2120 Emily Barn	203 40 1; 41 44; 42 10; 43 56; 44
44.51	0.69 C13 acid	SemiStdNF	1776	1777 Emily Barn	127 40 2; 41 84; 42 16; 43 85; 44 8;
58.83	0.89 C14 Diacid	SemiStdNF	2317	2318 Emily Barn	229 40 2; 41 47; 42 9; 43 56; 44 12;
52.93	0.69 C16 Acid	SemiStdNF	2078	2079 Emily Barn	132 40 2; 41 98; 42 18; 43 122; 44
55.48	0.67 C17 acid	SemiStdNF	2177	2178 Emily Barn	157 40 2; 41 96; 42 18; 43 124; 44
57.95	0.7 C18 Acid	SemiStdNF	2280	2281 Emily Barn	135 40 2; 41 105; 42 19; 43 143; 44
66.83	0.69 C22 acid	SemiStdNF	2684	2685 Emily Barn	169 40 2; 41 104; 42 20; 43 174; 44
70.79	0.7 C24 acid	SemiStdNF	2886	2887 Emily Barn	171 40 2; 41 103; 42 18; 43 184; 44
74.48	0.72 C26 acid	SemiStdNF	3088	3088 Emily Barn	178 40 3; 41 111; 42 21; 43 218; 44
77.98	0.74 C28 acid	SemiStdNF	3291	3292 Emily Barn	185 40 2; 41 111; 42 20; 43 223; 44
23.15	0.77 C7 acid	User	0	Emily Barn	110 40 4; 41 45; 42 10; 43 57; 44
33.74	1.63 SESQ2	SemiStdNF	1449	1449 Emily Barn	85 42 4; 43 45; 44 4; 45 9; 47 9;
61.72	0.55 C24	SemiStdNF	2443	2444 Emily Barn	104 40 5; 41 199; 42 40; 43 440; 44
63.93	0.56 C25	SemiStdNF	2545	2546 Emily Barn	105 40 5; 41 187; 42 37; 43 449; 44
66.1	0.57 C26	SemiStdNF	2649	2649 Emily Barn	109 40 5; 41 186; 42 36; 43 439; 44
68.16	0.57 C27	SemiStdNF	2750	2751 Emily Barn	101 40 4; 41 179; 42 35; 43 442; 44
70.14	0.58 C28	SemiStdNF	2852	2853 Emily Barn	101 40 4; 41 170; 42 34; 43 429; 44
72.08	0.59 C29	SemiStdNF	2955	2956 Emily Barn	101 40 5; 41 167; 42 32; 43 430; 44
73.95	0.6 C30	SemiStdNF	3058	3058 Emily Barn	101 40 4; 41 160; 42 31; 43 427; 44
75.74	0.62 C31	SemiStdNF	3159	3159 Emily Barn	98 40 4; 41 156; 42 30; 43 427; 44
77.45	0.63 C32	SemiStdNF	3259	3260 Emily Barn	97 40 4; 41 147; 42 29; 43 420; 44
79.16	0.64 C33	SemiStdNF	3363	3363 Emily Barn	104 40 4; 41 144; 42 29; 43 412; 44
82.63	0.72 C35	SemiStdNF	3564	3565 Emily Barn	109 40 4; 41 133; 42 27; 43 386; 44
34.8	0.69 C10 carboxylic acid	SemiStdNF	1479	1480 Emily Barn	128 40 3; 41 89; 42 22; 43 81; 44
44.28	1.57 4-nitrocatechol	SemiStdNF	1769	1770 Emily Barn	85 42 1; 43 13; 44 7; 45 79; 46 5;
23.88	0.78 4-terpineol (?)	SemiStdNF	1206	1207 Emily Barn	92 40 16; 41 141; 42 20; 43 282;
44.55	1.39 9H-Florenone	SemiStdNF	1778	1778 Emily Barn	55 49 2; 50 13; 51 9; 52 2; 53 1;
32.82	0.47 C14	SemiStdNF	1422	1423 Emily Barn	69 40 9; 41 251; 42 57; 43 549; 44
39.83	0.49 C16	SemiStdNF	1626	1627 Emily Barn	73 40 7; 41 238; 42 51; 43 512; 44
43.07	0.49 C17	SemiStdNF	1730	1730 Emily Barn	78 40 7; 41 232; 42 48; 43 493; 44
46.11	0.5 C18	SemiStdNF	1830	1831 Emily Barn	82 40 7; 41 230; 42 47; 43 471; 44

49.04	0.51 C19	SemiStdNF	1934	1934 Emily Barn	86 40 7; 41 224; 42 46; 43 474; 44
51.79	0.52 C20	SemiStdNF	2034	2034 Emily Barn	89 40 7; 41 225; 42 46; 43 467; 44
54.45	0.52 C21	SemiStdNF	2137	2138 Emily Barn	93 40 7; 41 220; 42 44; 43 463; 44
56.96	0.54 C22	SemiStdNF	2238	2239 Emily Barn	97 40 7; 41 210; 42 42; 43 452; 44
59.4	0.55 C23	SemiStdNF	2341	2342 Emily Barn	104 40 5; 41 203; 42 39; 43 440; 44
62.29	0.7 12-OH C18 Acid, TMS	SemiStdNF	2470	2470 Emily Barn	180 41 38; 42 5; 43 39; 44 8; 45 51;
61.42	0.69 16-OH C16 Acid, TMS	SemiStdNF	2429	2430 Emily Barn	229 40 2; 41 73; 42 12; 43 82; 44
39.91	0.8 2-Ketoglutaric acid, tri-TMS	SemiStdNF	1629	1629 Emily Barn	136 42 1; 43 16; 44 16; 45 115; 46
36.4	0.88 3-5-dimethoxyphenol	SemiStdNF	1525	1526 Emily Barn	124 41 2; 42 1; 43 13; 44 4; 45 31;
58.26	1.45 4, 4 dimethoxy-benzophenone	SemiStdNF	2293	2294 Emily Barn	81 50 10; 51 8; 52 1; 53 3; 61 2;
40.59	0.89 4-hydroxybenzoic acid	SemiStdNF	1651	1651 Emily Barn	129 42 1; 43 15; 44 5; 45 61; 46 4;
29.93	0.69 glyceric acid (?)	SemiStdNF	1352	1353 Emily Barn	96 40 1; 41 2; 42 3; 43 24; 44 9;
56.36	1.23 hexadecanamide	SemiStdNF	2212	2213 Emily Barn	78 40 4; 41 103; 42 20; 43 132; 44
50.61	0.53 hexadecanol, TMS	SemiStdNF	1989	1989 Emily Barn	98 40 1; 41 55; 42 9; 43 69; 44 5;
52.32	0.93 homosalate, TMS	SemiStdNF	2054	2055 Emily Barn	93 41 27; 42 1; 43 13; 44 1; 45 9;
32.75	0.73 hydroquinone	SemiStdNF	1420	1421 Emily Barn	129 42 1; 43 18; 44 5; 45 67; 46 3;
33.74	1.34 ionone	SemiStdNF	1449	1449 Emily Barn	106 40 10; 41 69; 42 6; 43 243; 44
33.51	0.64 SESQ3	SemiStdNF	1442	1443 Emily Barn	109 40 13; 41 523; 42 1; 43 193; 45
33.81	0.66 SESQ4	SemiStdNF	1451	1451 Emily Barn	122 40 74; 41 541; 42 27; 43 77; 44
38.69	0.78 isoeugenol	SemiStdNF	1591	1591 Emily Barn	125 40 1; 41 2; 42 1; 43 8; 44 4;
60.43	0.87 isopimaric acid	SemiStdNF	2385	2385 Emily Barn	190 40 2; 41 63; 42 4; 43 20; 44 5;
36.56	1.33 ketopinic acid	SemiStdNF	1530	1530 Emily Barn	176 40 7; 41 96; 42 12; 43 70; 44
42.95	0.85 levoglucosan	SemiStdNF	1726	1727 Emily Barn	149 41 4; 42 1; 43 17; 44 10; 45 88;
57.12	0.7 linoleic Acid, TMS	SemiStdNF	2245	2245 Emily Barn	213 40 5; 41 205; 42 18; 43 85; 44
81.22	1.04 lupeol	SemiStdNF	3483	3484 Emily Barn	281 40 6; 41 207; 42 12; 43 114; 44
28.33	1.1 maltol	SemiStdNF	1316	1316 Emily Barn	88 40 2; 41 1; 42 6; 43 23; 44 4;
42.3	0.86 mannosan	SemiStdNF	1706	1706 Emily Barn	148 41 4; 42 1; 43 14; 44 10; 45 89;
65.68	0.75 monopalmitin	SemiStdNF	2628	2628 Emily Barn	183 40 2; 41 104; 42 20; 43 183; 44
68.92	0.71 monostearin TMS	SemiStdNF	2788	2789 Emily Barn	194 40 2; 41 119; 42 21; 43 212; 44
28.41	0.51 nonanol	SemiStdNF	1318	1318 Emily Barn	88 40 2; 41 35; 42 6; 43 31; 44 7;
52.36	0.87 octadecanal (?)	SemiStdNF	2056	2056 Emily Barn	180 40 15; 41 519; 42 87; 43 606;
55.82	0.55 octadecanol	SemiStdNF	2191	2191 Emily Barn	103 40 1; 41 65; 42 10; 43 89; 44 5;
51.71	0.85 octadecanone	SemiStdNF	2031	2031 Emily Barn	97 40 5; 41 167; 42 33; 43 297; 44
57.27	0.7 oleic Acid, TMS	SemiStdNF	2251	2252 Emily Barn	205 40 5; 41 196; 42 30; 43 146; 44
37.05	0.97 p-anisic acid (4-methoxybenzoic ac	SemiStdNF	1544	1544 Emily Barn	95 42 1; 43 10; 44 3; 45 27; 46 2;

52.36	0.71 palmitoleic Acid	SemiStdNF	2056	2056 Emily Barn	192 40 6; 41 182; 42 32; 43 122; 44
42.95	0.95 pentadecanone	SemiStdNF	1726	1727 Emily Barn	115 40 6; 41 153; 42 33; 43 548; 44
72.31	1.46 perylene	SemiStdNF	2967	2968 Emily Barn	63 50 1; 51 1; 62 2; 63 1; 74 4;
42.57	1.11 phthalic acid	SemiStdNF	1714	1715 Emily Barn	94 43 8; 44 5; 45 49; 46 3; 47 4;
38.76	1.14 phthalimide	SemiStdNF	1593	1593 Emily Barn	70 42 1; 43 7; 44 2; 45 10; 47 1;
41.89	0.97 pinic acid 1	SemiStdNF	1692	1693 Emily Barn	146 40 1; 41 22; 42 3; 43 19; 44 9;
42.04	0.98 pinic acid 2	SemiStdNF	1697	1698 Emily Barn	149 40 1; 41 20; 42 3; 43 17; 44 9;
37.28	1.47 pinonic acid	SemiStdNF	1550	1551 Emily Barn	132 40 3; 41 39; 42 6; 43 123; 44
55.33	1.22 pyrene	SemiStdNF	2171	2172 Emily Barn	48 50 2; 51 1; 61 2; 62 3; 63 3;
29.36	0.68 pyrocatechol	SemiStdNF	1339	1340 Emily Barn	70 42 1; 43 11; 44 5; 45 73; 46 3;
26.73	1.1 quinoline	SemiStdNF	1278	1278 Emily Barn	35 49 5; 50 43; 51 62; 52 16; 53 1;
31.99	0.73 resorcinol	SemiStdNF	1399	1399 Emily Barn	145 42 1; 43 18; 44 4; 45 65; 46 4;
32.18	0.57 SESQ1	SemiStdNF	1404	1404 Emily Barn	112 40 26; 41 148; 42 18; 43 68; 44
57.65	1.05 retene	SemiStdNF	2267	2268 Emily Barn	104 41 1; 50 2; 51 2; 62 3; 63 6;
51.75	1.54 sinapinaldehyde	SemiStdNF	2032	2033 Emily Barn	192 41 1; 42 2; 43 18; 44 6; 45 68;
70.44	0.6 squalene	SemiStdNF	2868	2869 Emily Barn	99 40 5; 41 176; 42 9; 43 13; 44 1;
78.86	0.86 stigmasterol	SemiStdNF	3344	3345 Emily Barn	248 40 2; 41 97; 42 5; 43 84; 44 5;
42.95	1.33 syringaldehyde	SemiStdNF	1726	1727 Emily Barn	115 41 1; 42 1; 43 11; 44 3; 45 31;
48.78	0.88 syringic acid	SemiStdNF	1924	1925 Emily Barn	187 42 1; 43 17; 44 7; 45 70; 46 3;
32.67	0.82 syringol	SemiStdNF	1418	1419 Emily Barn	104 42 1; 43 10; 44 3; 45 29; 46 1;
36.25	0.53 threitol	SemiStdNF	1521	1521 Emily Barn	124 41 4; 42 1; 43 10; 44 8; 45 67;
36.52	0.54 erythreitol	SemiStdNF	1528	1529 Emily Barn	133 41 5; 42 1; 43 11; 44 8; 45 68;
30.39	2.11 triacetin	SemiStdNF	1362	1363 Emily Barn	31 40 1; 41 2; 42 16; 43 999; 44
36.82	0.93 tridecanal (?)	SemiStdNF	1537	1538 Emily Barn	96 40 22; 41 629; 42 132; 43 670;
44.89	0.88 vanillic acid	SemiStdNF	1789	1789 Emily Barn	155 42 1; 43 16; 44 6; 45 64; 46 3;
37.55	1.34 vanillin	SemiStdNF	1558	1558 Emily Barn	103 41 1; 42 1; 43 14; 44 5; 45 40;
25.09	2.07 verbenone (-)	SemiStdNF	1237	1237 Emily Barn	93 40 38; 41 169; 42 33; 43 45; 44
48.24	1.38 xanthone	SemiStdNF	1906	1906 Emily Barn	64 49 2; 50 23; 51 7; 52 1; 53 5;
39.33	1.07 SESQ9	SemiStdNF	1610	1611 Emily Barn	124 41 8; 42 2; 43 31; 44 13; 45
35.3	0.62 SESQ6	SemiStdNF	1493	1494 Emily Barn	118 40 35; 41 450; 42 39; 43 89; 44
34.5	0.62 SESQ5	SemiStdNF	1471	1471 Emily Barn	122 40 28; 41 484; 42 65; 43 140;