

Supplemental Materials

Table A1: Averaged peaks retention times and abundances for viral infected cell lines at 24 hours exposure. R.T.: retention time (min.), A.: abundance (a.u.), D.P.: discriminating peaks (p<0.05). Any two cell lines that have a same letter in their D.P. column are mutually distinguishable. ‘--’: either no peak or not detected by the peak criteria. (*): standard deviation].

Peak No.	Cntrl			MOI 1 H1N1			MOI 10 H1N1			MOI 10 H6N2			MOI 10 H9N2			Tentative Chemical ID (alternative structure(s))
	R.T.	A.	D.P.	R.T.	A.	D.P.	R.T.	A.	D.P.	R.T.	A.	D.P.	R.T.	A.	D.P.	
1	1.43 (0.04)	146783 (134582)		1.44 (0.03)	187363 (103803)	g.	1.46 (0.00)	182485 (101271)		1.46 (0.00)	226571 (154656)	j.	1.46 (0.01)	112734 (62588)	g, j.	Carbon dioxide
2- C1	1.92 (0.12)	10047 (3800)	a, b, c, d.	2.05 (0.04)	18975 (5286)	a, e, f, g.	2.07 (0.01)	34638 (7187)	b, e, h, i.	2.06 (0.01)	53071 (6207)	c, f, h, j.	2.07 (0.00)	27768 (4821)	d, g, i, j.	2-methoxy-ethanol
3	2.50 (0.05)	9148 (1859)	d.	2.51 (0.04)	9882 (1794)		--	--		2.51 (0.07)	11372 (4022)		2.55 (0.06)	11777 (3259)	d.	Isopropanol
4- C2	3.87 (0.04)	25721 (14735)		3.86 (0.03)	33571 (13207)	g.	3.90 (0.01)	35777 (19539)		3.90 (0.01)	31622 (11886)		3.90 (0.01)	23009 (9401)	g.	Thiirane
5- C3	--	--		5.96 (0.09)	109624 (136496)	e, f, g.	6.09 (0.07)	15356 (13469)	e.	6.11 (0.09)	15183 (8325)	f.	6.06 (0.09)	14263 (4506)	g.	Propanoic acid, ethyl ester
6- C4	12.62 (0.08)	8601 (2233)	a, b, c, d.	12.62 (0.03)	18629 (7844)	a, f.	12.71 (0.03)	17975 (4401)	b, h.	12.69 (0.03)	30312 (12957)	c, f, h, j.	12.71 (0.03)	15104 (5906)	d, j.	Butanoic acid, 2-methyl-, methyl ester
7- C5	19.71 (0.07)	10925 (2735)	c, d.	19.75 (0.05)	11214 (1939)	f, g.	19.79 (0.09)	8924 (3672)		19.85 (0.07)	8271 (3269)	c, f.	19.87 (0.04)	7127 (1269)	d, g.	Butanoic acid, 2-methyl-, ethyl ester
8	22.25 (0.07)	10726 (3997)	d.	22.27 (0.07)	11983 (4571)	g.	--	--		22.42 (0.08)	8181 (5616)		22.43 (0.08)	5748 (1357)	d, g.	Octane (Nonane)
9	23.56 (0.05)	8462 (1779)	b.	--	--		23.64 (0.03)	7310 (509)	b.	23.63 (0.04)	8170 (1540)		23.63 (0.04)	7857 (1097)		4-Ethylbenzoic acid, 2-butyl ester (4-formylbenzoic acid, ethyl ester)
10- C6	30.13 (0.04)	10292 (3091)	a, b, c.	30.11 (0.06)	18579 (7496)	a, g.	30.26 (0.04)	13955 (3882)	b, h, i.	30.25 (0.04)	23767 (13960)	c, h, j.	30.26 (0.04)	10047 (2748)	g, i, j.	3-Hexanone, 5-methyl-
11	--	--		31.59 (0.06)	7670 (1371)	e, g.	31.72 (0.04)	5233 (865)	e.	31.71 (0.05)	6102 (3247)		31.71 (0.03)	5124 (652)	g.	o-Xylene (p-Xylene)
12- C7	--	--		35.43 (0.06)	9945 (1756)	e, f, g.	35.59 (0.03)	6493 (772)	e.	35.59 (0.04)	7526 (2329)	f.	35.58 (0.04)	6829 (1452)	g.	3-Heptanone
13- C8	--	--		36.06 (0.11)	7882 (842)	e, f, g.	36.25 (0.05)	6463 (778)	e.	36.27 (0.05)	6569 (1613)	f.	36.24 (0.05)	5955 (528)	g.	2-Octanone
14	46.14 (0.04)	10404 (2318)	c, d.	46.10 (0.07)	9922 (1506)	f, g.	46.30 (0.06)	8301 (3177)		46.31 (0.04)	8228 (1789)	c, f.	46.30 (0.04)	7760 (1206)	d, g.	Benzaldehyde
15- C9	48.10 (0.08)	10895 (5148)		48.10 (0.09)	9703 (2285)	e, f, g.	48.16 (0.05)	13743 (6077)	e.	48.17 (0.07)	13705 (4113)	f.	48.15 (0.04)	13617 (3724)	g.	Not identified
16	49.10 (0.05)	8023 (1342)	d.	49.09 (0.07)	7883 (1102)		49.30 (0.07)	7074 (1950)		--	--		49.30 (0.06)	6822 (1440)	d.	1-Heptanol
17	--	--		53.07 (0.07)	7533 (822)	e, f, g.	53.24 (0.04)	6350 (650)	e.	53.25 (0.05)	6454 (1573)	f.	53.24 (0.04)	6179 (974)	g.	Not identified
18	--	--		57.23 (0.07)	7272 (973)	f, g.	57.41 (0.04)	6267 (1843)		57.40 (0.05)	6073 (1417)	f.	57.39 (0.05)	6072 (1194)	g.	Not identified
19- C10	67.17 (0.05)	22904 (3975)	b, c, d.	67.20 (0.06)	22780 (3323)	e, f, g.	67.34 (0.04)	14834 (4705)	b, e.	67.35 (0.04)	14875 (3667)	c, f.	67.33 (0.04)	13788 (2653)	d, g.	1-Phenyl-1-butene (1-ethenyl-4-ethyl-Benzene, 1-ethenyl-3-ethyl-Benzene, 1-methyl-4-(2-propenyl)-Benzene)
20-	68.59	18440	b, c.	68.59	17319	e, f.	68.76	11818	b, e.	68.77	11820	c, f.	68.76	11314	d, g.	1-Phenyl-1-butene (1-ethenyl-4-

C11	(0.06)	(4064)	d,	(0.06)	(3374)	g,	(0.04)	(3835)		(0.05)	(2142)		(0.03)	(2118)		ethyl-Benzene, 1-ethenyl-3-ethyl-Benzene, 1-methyl-4-(2-propenyl)-Benzene)
21	--	--		--	--		69.25 (0.05)	9487 (2036)	i,	69.24 (0.04)	10765 (4045)	j,	69.24 (0.04)	7184 (1790)	i, j,	Benzoic acid, methyl ester
22- C12	70.92 (0.06)	9138 (2726)	b,	70.92 (0.07)	8959 (1387)	e,	71.11 (0.03)	7200 (1726)	b, e,	71.12 (0.04)	7978 (1823)		71.11 (0.05)	7729 (1855)		3,7-dimethyl-3-Octanol
23	74.71 (0.06)	19220 (31982)		74.71 (0.07)	9778 (3313)	f,	74.90 (0.04)	47013 (141880)		74.89 (0.04)	6391 (1383)	f,	74.89 (0.04)	7673 (3784)		Not identified
24- C13	79.81 (0.06)	15112 (4098)	c, d,	79.82 (0.07)	13800 (2201)	f, g,	80.02 (0.04)	11344 (8837)		80.02 (0.03)	9559 (1669)	c, f,	80.00 (0.03)	9119 (1420)	d, g,	4-ethyl-Benzaldehyde
25- C14	88.63 (0.07)	15356 (23190)		88.61 (0.04)	7988 (2512)	e, f, g,	88.78 (0.14)	28348 (15442)	e,	88.82 (0.10)	23635 (13835)	f,	88.87 (0.04)	18743 (6348)	g,	Decanal (isomers, homologs)

Table A2: Averaged peaks retention times and abundances for viral infected cell lines at 48 hours exposure. R.T.: retention time (min.). A.: abundance (a.u.), D.P.: discriminating peaks (p<0.05). Any two cell lines that have a same letter in their D.P. column are mutually distinguishable. ‘--’: either no peak or not detected by the peak criteria. (*): standard deviation].

Peak No.	Cntrl			MOI 1 H1N1			MOI 10 H1N1			MOI 10 H6N2			MOI 10 H9N2			Tentative Chemical ID (alternative structure(s))
	R.T.	A.	D.P.	R.T.	A.	D.P.	R.T.	A.	D.P.	R.T.	A.	D.P.	R.T.	A.	D.P.	
1-C1	1.94 (0.12)	25529 (51445)		2.06 (0.03)	18854 (5856)	e, f, g.	2.06 (0.01)	33738 (5590)	e, h, i.	2.04 (0.06)	53547 (18986)	f, h, j.	2.07 (0.01)	25269 (7255)	g, i, j.	2-methoxy-ethanol
2-C2	3.86 (0.03)	40346 (20248)	d.	3.87 (0.03)	46689 (21178)	g.	3.95 (0.09)	34018 (34063)		3.94 (0.09)	29199 (40753)		3.94 (0.09)	18437 (8217)	d, g.	Thiirane
3-C3	5.97 (0.10)	102677 (139578)	b, c.	5.97 (0.09)	89269 (126787)	f.	6.14 (0.13)	15467 (13608)	b.	6.13 (0.07)	12979 (3486)	c, f.	--	--		Propanoic acid, ethyl ester
4-C4	12.61 (0.09)	24798 (55836)		12.63 (0.04)	19591 (5864)	g.	12.69 (0.04)	16392 (8453)		12.69 (0.04)	26769 (18189)	j.	12.71 (0.04)	13415 (6804)	g, j.	Butanoic acid, 2-methyl-, methyl ester
5	14.72 (0.06)	179950 (154023)	c, d.	14.72 (0.04)	113587 (94050)	f, g.	--	--		14.82 (0.05)	26444 (23106)	c, f.	14.81 (0.04)	15569 (13826)	d, g.	Dimethyldisulfide
6-C5	19.72 (0.09)	9553 (2108)	b, d.	--	--		19.84 (0.08)	7130 (1356)	b.	19.82 (0.08)	8032 (2811)		19.83 (0.08)	6812 (943)	d.	Butanoic acid, 2-methyl-, ethyl ester
7-C6	30.14 (0.06)	22483 (45752)		30.13 (0.06)	16363 (5726)	e, g.	30.25 (0.03)	11215 (5801)	e.	30.24 (0.03)	13882 (8658)		30.24 (0.02)	9213 (3919)	g.	3-Hexanone, 5-methyl-
8-C7	35.41 (0.08)	9775 (2076)	b, c, d.	--	--		35.57 (0.03)	7075 (1161)	b.	35.57 (0.03)	7462 (2059)	c.	35.56 (0.02)	7940 (2096)	d.	3-Heptanone
9-C8	36.08 (0.09)	8018 (1601)	b.	--	--		36.23 (0.09)	6586 (1313)	b.	36.21 (0.10)	6805 (2256)		36.24 (0.02)	6810 (2098)		2-Octanone
10-C9	48.09 (0.06)	9725 (2024)	b, d.	48.11 (0.05)	10410 (2421)	e, g.	48.17 (0.08)	14765 (4105)	b, e.	48.17 (0.08)	30011 (55623)		48.16 (0.07)	14344 (3465)	d, g.	Not identified
11	54.14 (0.11)	10403 (2693)	b, d.	--	--		54.18 (0.04)	13995 (2952)	b.	54.17 (0.04)	14774 (7340)		54.15 (0.04)	14641 (3457)	d.	6-Nonenoic acid, methyl ester (Octanal)
12	59.29 (0.09)	111010 (222322)	d.	59.30 (0.06)	84668 (153458)	f, g.	59.36 (0.04)	168103 (201143)		59.35 (0.04)	302273 (255840)	f.	59.35 (0.03)	323340 (238440)	d, g.	2-ethyl-1-Hexanol
13	64.02 (0.07)	9273 (1674)	b, c, d.	64.02 (0.07)	9604 (1234)	e, f, g.	64.17 (0.04)	11473 (1753)	b, e.	64.18 (0.04)	12581 (3356)	c, f.	64.17 (0.03)	11034 (1462)	d, g.	2-Hexenyl benzoate
14-C10	67.18 (0.06)	19993 (3883)	b, c, d.	67.18 (0.06)	20658 (3291)	e, f, g.	67.31 (0.03)	12935 (1536)	b, e.	67.31 (0.04)	14845 (2888)	c, f.	67.30 (0.02)	14429 (2331)	d, g.	1-Phenyl-1-butene (1-ethenyl-4-ethyl-Benzene, 1-ethenyl-3-ethyl-Benzene, 1-methyl-4-(2-propenyl)-Benzene)
15-C11	68.59 (0.07)	15346 (4069)	b, d.	68.60 (0.06)	16455 (2832)	e, f, g.	68.73 (0.05)	11029 (1260)	b, e, h.	68.73 (0.03)	12784 (2488)	f, h.	68.73 (0.02)	12172 (1807)	d, g.	1-Phenyl-1-butene (1-ethenyl-4-ethyl-Benzene, 1-ethenyl-3-ethyl-Benzene, 1-methyl-4-(2-propenyl)-Benzene)
16-C12	70.89 (0.09)	8421 (1189)		70.91 (0.07)	8850 (1185)	e.	71.08 (0.04)	7600 (1047)	e.	71.08 (0.03)	31796 (75434)		71.08 (0.03)	62545 (127604)		3,7-dimethyl-3-Octanol
17	71.91 (0.11)	11507 (4414)	b, c, d.	--	--		72.02 (0.03)	19162 (7885)	b.	72.02 (0.04)	25760 (16566)	c.	72.01 (0.02)	23731 (10620)	d.	2-Nonen-1-ol (Nonanal)
18-C13	79.81 (0.07)	12586 (2391)	b, d.	79.82 (0.07)	13369 (2263)	e, g.	79.99 (0.04)	9402 (1136)	b, e.	79.99 (0.03)	11363 (3899)		79.97 (0.02)	10182 (1530)	d, g.	4-ethyl-Benzaldehyde
19	82.45 (0.08)	9234 (1691)	b, d.	82.44 (0.08)	9489 (1650)	e, g.	82.65 (0.04)	6864 (811)	b, e.	82.63 (0.04)	8171 (2632)		82.62 (0.03)	7477 (1220)	d, g.	3,4-dimethyl-Benzaldehyde
20	87.42 (0.10)	9159 (2849)	b.	87.42 (0.10)	10775 (2610)	e.	87.22 (0.04)	5061 (776)	b, e.	--	--		--	--		2-Methyl-4-tetradecene (isomers)
21-	88.65	7924	d.	88.64	9122	g.	88.82	36445		88.82	38360		88.83	13851	d, g.	Decanal (isomers,

C14	(0.09)	(3340)		(0.09)	(4012)		(0.07)	(52712)		(0.08)	(73221)		(0.02)	(2398)		homologs)
22	103.62 (0.10)	8448 (1468)	b, d,	103.64 (0.09)	8617 (1278)	e, g,	103.82 (0.03)	6849 (949)	b, e,	103.82 (0.03)	8540 (3389)		103.81 (0.03)	7038 (1340)	d, g,	3-ethyl-5-(2-ethylbutyl)- Octadecane (isomers)
23	160.54 (0.08)	8393 (2970)	b, c, d,	160.56 (0.08)	8994 (3189)	f, g,	160.44 (0.04)	11476 (3815)	b,	160.43 (0.04)	15905 (6750)	c, f,	160.43 (0.03)	13941 (4602)	d, g,	2,6- Diisopropylnaphthalene
24	--	--		--	--		173.27 (0.03)	24008 (5060)	h,	173.24 (0.08)	30585 (9475)	h,	173.28 (0.04)	27760 (5113)		Not identified