

Table S1. Total NNN and total NNAL in the Persistence of Biomarkers (POB) Study

Subject	Total NNN, pmol/24h ^a								Total NNAL, pmol/24h							
	Baseline ^b	days since smoking cessation							baseline	days since smoking cessation						
		3	7	14	21	28	42	56		3	7	14	21	28	42	56
<i>Nicotine patch users</i>																
P1	253	3.51	2.49	13.9	IC ^c	0.535	79.8	1.81	2070	671	622	299	IC	143	92.4	103
P2	11.2	2.69	3.33	2.78	0.110	IC	0.200	3.61	2680	1120	666	555	289	IC	195	137
P3	19.9	0.136	2.43	0.174	0.104	0.150	0.113	0.092	5840	1270	1000	696	590	398	352	191
P4	30.3	0.100	0.190	2.03	0.180	0.173	1.75	0.134	8420	2030	1680	1340	743	668	443	224
P5	89.2	4.13	1.14	0.088	28.9	0.066	0.063	0.085	1990	1520	1210	368	578	384	389	175
P6	9.81	2.22	0.220	0.233	0.548	0.275	0.260	0.275	884	317	110	58.1	58.3	68.8	65.0	68.8
P7	4.28	0.330	0.310	0.335	1.80	17.9	0.345	0.295	2190	916	558	410	61.9	66.0	86.3	73.8
P8	145	0.275	0.552	3.19	0.545	1.04	0.260	0.205	2710	1170	614	378	309	254	65.0	51.3
P9	5.16	1.86	0.198	1.55	0.793	1.91	IC	1.01	1130	234	514	158	226	181	IC	23.8
<i>Oral NRT users</i>																
O1	67.4	219	IC	256	622	578	253	130	1330	641	IC	287	215	178	20.0	131
O2	81.5	87.7	59400	1250	11.3	558	6.83	118	237	291	30.6	28.5	19.8	22.5	39.8	40.6
O3	15.1	3.94	0.300	0.213	0.255	473	0.303	0.240	1710	508	600	256	261	136	159	60.0
O4	6.46	3.17	2.69	0.195	0.303	0.273	2.92	0.280	2080	880	540	527	650	429	535	476
O5	329	14.0	359	32.3	16.2	14.2	17.6	3.67	2930	752	507	217	171	228	71.3	89.4
O6	665	17900	103	18200	3310	23900	4080	8.65	197	744	93.1	569	68.8	665	74.4	47.5
O7	8.76	64.0	1.40	0.523	0.075	0.064	0.148	0.160	3050	1310	1020	473	356	206	310	40.0
O8	4.37	0.135	0.113	0.105	0.063	0.140	0.100	0.168	3870	1330	1740	900	520	480	263	223

^a The amount of NNN in some samples was verified by gas chromatography equipped with a thermal energy analyzer. All the values presented in this Table are from original analysis by liquid chromatography-electrospray ionization-tandem mass spectrometry.

^b Two baseline urine samples were collected and analyzed; each value represents mean of the two analyses

^c IC, incomplete collection

Table S2. Total NNN and total NNAL in the Quit Nicotine (QuitNic) Study ^a.

Subject	Total NNN, pmol/mg creatinine			Total NNAL, pmol/mg creatinine		
	study week			study week		
	baseline ^b	2	6	baseline	2	6
1	0.191	0.016	0.042	2.47	0.46	0.28
2	0.880	0.437	0.971	0.60	0.16	0.07
3	0.125	0.489	0.346	1.47	0.30	0.11
4	0.525	0.426	0.293	0.64	0.11	0.06
5	0.207	0.084	0.070	0.63	0.30	0.13
6	0.147	0.071	LOD ^c	1.51	0.64	0.15
7	0.059	0.025	0.019	3.26	0.32	0.18
8	0.063	0.025	0.019	0.73	0.15	0.01
9	0.037	0.033	LOD	0.90	0.08	0.05
10	0.057	0.001	S ^d	1.85	0.55	S
11	0.035	0.159	0.005	0.61	0.10	0.16
12	0.008	0.011	S	0.20	0.05	S
13	0.058	LOD	0.007	1.86	0.57	0.13
14	0.012	0.002	0.004	1.80	0.08	0.44
15	0.116	LOD	LOD	0.72	0.30	0.05
16	0.037	LOD	0.004	0.81	0.28	0.17
17	0.109	0.028	0.007	1.39	0.15	0.22
18	0.065	0.070	0.035	1.25	0.27	0.21
19	0.029	0.011	0.011	0.82	0.29	0.24
20	0.077	0.011	0.007	1.10	0.14	0.03
21	0.412	0.048	0.014	1.20	0.25	0.25
22	0.098	0.016	0.024	1.53	0.27	0.03
23	0.019	0.006	0.011	0.19	0.01	0.02
24	0.016	0.005	0.008	0.88	0.30	0.15
25	0.034	0.022	0.014	1.57	0.29	0.40
26	0.213	0.078	0.106	1.22	0.47	0.13

^a In this study, single-void urine samples were collected; therefore, the results are expressed per mg creatinine.

^b Two baseline urine samples were collected and analyzed; each value represents mean of the two analyses

^c LOD, below the limit of detection (0.001 pmol/ml urine)

^d S, the subject was smoking at this time point

Table S3. Anatabine, nitrate, and nitrite in selected samples from the POB study ^a.

Subject ^b	Baseline	days since smoking cessation						
		3	7	14	21	28	42	56
Anatabine, ng/ml urine								
<i>Nicotine patch user</i>								
7	1.5	na ^c	na	na	ND ^d	ND	ND	na
<i>Oral NRT users</i>								
1	na	ND	ND	ND	ND	ND	ND	ND
2	1.8	ND	0.3	ND	ND	ND	ND	ND
3	4.1	na	na	na	ND	ND	ND	na
5	5.9	0.2	0.2	0.1	na	na	na	na
6	1.2	0.2	ND	ND	ND	ND	ND	ND
7	9.5	ND	ND	na	na	na	na	na
Nitrate-N, µg/ml urine								
<i>Nicotine patch user</i>								
7	11.1	na	na	na	7.36	20.9	11.5	na
<i>Oral NRT users</i>								
1	na	8.62	6.09	12.5	12.9	9.53	11.1	16.4
2	7.43	11.9	5.83	2.13	11.8	5.96	10.9	1.59
3	5.61	na	na	na	3.46	1.74	5.51	na
5	7.35	9.22	0.77	9.75	na	na	na	na
6	11.4	6.86	30.1	4.64	7.01	3.09	0.82	36.3
7	7.29	0.29	23.0	na	na	na	na	na
Nitrite-N, µg/ml urine								
<i>Nicotine patch user</i>								
7	0.20	na	na	na	0.51	0.05	0.05	na
<i>Oral NRT users</i>								
1	na	4.04	1.91	2.25	1.86	3.04	NQ ^e	NQ
2	0.38	0.17	0.03	0.2	0.53	0.44	0.48	0.34
3	0.61	na	na	na	0.29	2.9	0.5	na
5	0.19	0.12	4.53	0.05	na	na	na	na
6	1.35	1.74	0.05	0.91	7.40	0.78	2.27	0.26
7	5.45	0.05	0.28	na	na	na	na	na

^a Time points were selected to include both high- and low-total NNN samples from different subjects.

^b Subject numbers correspond to those in Table S1 of Supplemental Information.

^c na, not analyzed.

^d ND, not detected.

^e NQ, not quantified due to interfering peaks.