SUPPORTING INFORMATION

Presence of *N, N'*-Substituted *p*-Phenylenediamine-Derived Quinones in Human Urine

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Table S1. List of Target PPDQs in the Present Study and Their Abbreviations and Full Names.

Abbreviation	Full name
IPPDQ	2-(isopropylamino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione
DPPDQ	2,5-bis(phenylamino)cyclohexa-2,5-diene-1,4-dione
CPPDQ	2-(cyclohexylamino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione
6PPDQ	2-((4-methylpentan-2-yl)amino)-5-(phenylamino)cyclohexa-2,5-diene-1,4-dione
77PDQ	2,5-bis((5-methylhexan-2-yl)amino)cyclohexa-2,5-diene-1,4-dione
DTPDQ	2,5-bis(o-tolylamino)cyclohexa-2,5-diene-1,4-dione

Table S2. Demographic Characteristics of Participants (*n* = 149) Recruited in This Study.

	n (%) or mean ± SD [a]
Gender	
Males	67 (45%)
Females	82 (55%)
Age	
Males	46 ± 11
Females	47 ± 14
Age group	
24−30 years	15 (10%)
31−40 years	42 (28%)
41−50 years	45 (30%)
51−62 years	47 (32%)
BMI (kg/m^2)	
Males	28 ± 6.1
Females	24 ± 5.5
Education level	
College	20 (14%)
High school	69 (46%)
Below high school	60 (40%)
Annual household income (CNY)	
< 80, 000	51 (34%)
80, 000−150, 000	82 (55%)
> 150, 000	16 (11%)

[a] % means the percentage to the total participants, and ± means the +/−.

Table S3. MRM Transition Parameters for PPDQs and Internal Standard.

	MRM transition		Cone voltage	Collision energy	SRM ratio
	Parent ion	Daughter ion	(eV)	(eV)	(average)
6PPDQ	299	215	38	15	4.5
		187	38	27	
IPPDQ	257	187	33	28	9.8
		215	33	22	
DPPDQ	291	263	38	12	2.2
		170	38	30	
DTPDQ	319	301	40	14	2.8
		212	40	22	
CPPDQ	297	187	35	28	2.5
		98	35	35	
77PDQ	335	237	40	15	4.1
		139	40	28	
6PPDQ-d_5	304	192	38	27	

Table S4. LODs and Extraction Recoveries of PPDQs in Human Urine.

	LOD (ng/mL)	Extraction Recovery (%) Spiked at 0.5 ng/mL			Spiked at 5.0 ng/mL			Spiked at 50 ng/mL			Equation	R^2
		mean	SD	Range	mean	SD	Range	mean	SD	Range		
IPPDQ	0.095	82	9.0	71-92	87	10	75-98	87	8.0	80-96	y = 0.36 x -0.022	0.9956
DPPDQ	0.017	107	5.2	102-114	105	5.4	98-113	102	7.4	95-110	y = 2.1 x + 0.81	0.9991
CPPDQ	0.052	105	10	92-116	92	6.6	86-99	98	10	85-110	y = 1.4 x + 0.66	0.9989
6PPDQ	0.033	92	8.6	98-101	86	5.9	83-96	96	5.8	90-105	y = 2.9 x -0.53	0.9978
77PDQ	0.081	92	6.3	86-100	87	5.1	81-95	88	5.9	82-94	y = 0.44 x + 0.25	0.9990
DTPDQ	0.097	99	8.1	90-107	89	7.3	81-97	99	6.2	92-106	y = 1.9 x + 0.69	0.9979

Table S5. Correlations among Concentrations of Various PPDQs in Human Urine.

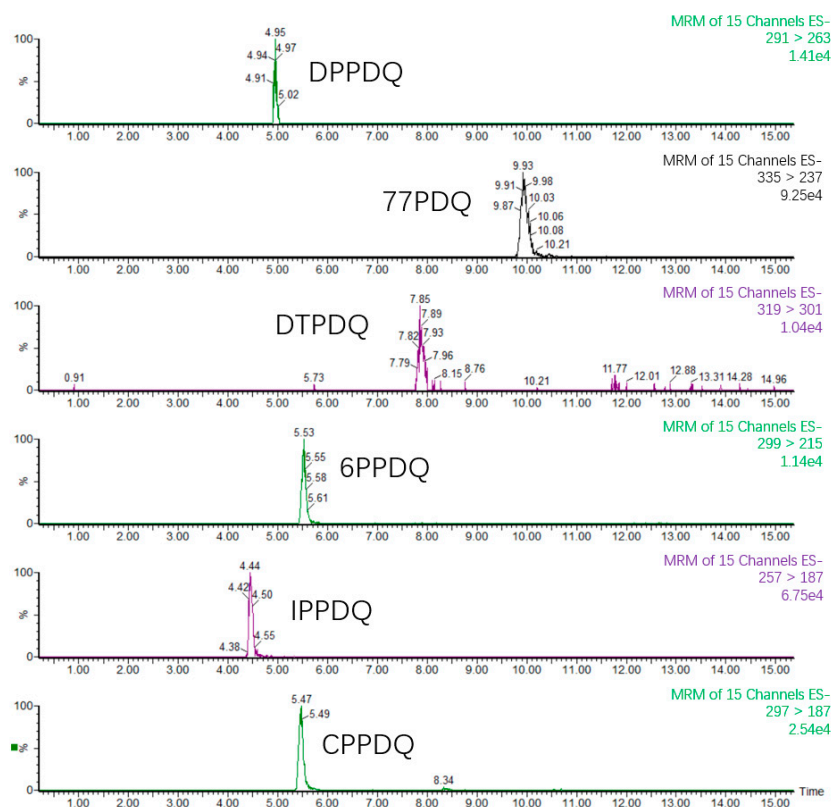|		DPPDQ	CPPDQ	77PDQ	6PPDQ	DTPDQ
IPPDQ	r_s	.134	.139	.003	.208	.296
	p	.265	.239	.982	.066	.130
DPPDQ	r_s	1	.278	.123	.288	.592**
	p		.164	.221	.202	.000
CPPDQ	r_s		1	.232	.733**	.267
	p			.115	.000	.117
77PDQ	r_s			1	.129	.048
	p				.244	.676
6PPDQ	r_s				1	.290
	p					.206

Figure S1. Representative chromatograms of target analytes in the human urine sample.