Reproducibility and Imputation of Air Toxics Data

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SUPPLEMENTAL MATERIALS – FIGURES AND TABLES

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Supplement 1. Statistics of concentrations at Dearborn, Michigan for VOCs and carbonyls analyzed by Eastern Research Group (ERG) laboratory. DF=detection frequency; MDL=method detection limit.

Compound	ERG laboratory-Sample 1						ERG laboratory-Sample 2						
	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	MDL (ppbv)
Carbonyls													
2,5-Dimethylbenzaldehyde	266	31	0.003	0.009	0.020	0.280	54	31	0.003	0.010	0.022	0.147	0.005
Acetaldehyde	266	100	0.007	1.203	0.998	4.406	54	100	0.024	0.972	0.604	3.056	0.014
Acetone	266	100	0.017	1.474	1.247	5.770	54	100	0.025	1.198	0.875	4.611	0.008
Benzaldehyde	266	98	0.002	0.050	0.043	0.422	54	98	0.002	0.048	0.035	0.152	0.004
Crotonaldehyde	266	79	0.003	0.027	0.051	0.309	54	80	0.003	0.021	0.044	0.307	0.006
Formaldehyde	266	100	0.008	2.406	1.972	20.980	54	100	0.019	2.373	1.512	7.061	0.016
Hexaldehyde	266	100	0.002	0.123	0.167	0.722	54	96	0.002	0.091	0.123	0.583	0.004
iso-Butyraldehyde	266	99	0.003	0.206	0.175	0.801	54	98	0.003	0.158	0.099	0.601	0.005
iso-Valeraldehyde	266	22	0.002	0.020	0.058	0.377	54	17	0.002	0.024	0.076	0.380	0.004
Propionaldehyde	266	89	0.004	0.147	0.153	1.440	54	93	0.004	0.124	0.082	0.377	0.007
Tolualdehydes	266	92	0.004	0.045	0.051	0.591	54	96	0.004	0.045	0.038	0.193	0.008
Valeraldehyde	266	90	0.002	0.061	0.067	0.377	54	94	0.002	0.040	0.034	0.213	0.003
VOCs													
1,1,1-Trichloroethane	282	5	0.030	0.033	0.014	0.167	52	4	0.030	0.032	0.008	0.072	0.060
1,1,2,2-Tetrachloroethane	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
1,1,2-Trichloroethane	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
1,1-Dichloroethane	282	0	0.040	0.040	0.000	0.040	52	0	0.040	0.040	0.000	0.040	0.080
1,1-Dichloroethene	282	0	0.050	0.050	0.000	0.050	52	0	0.050	0.050	0.000	0.050	0.100
1,2,4-Trichlorobenzene	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
1,2,4-Trimethylbenzene	282	91	0.035	0.212	0.138	1.029	52	85	0.035	0.195	0.146	0.854	0.070
1,2-Dibromoethane	282	0	0.040	0.040	0.000	0.040	52	0	0.040	0.040	0.000	0.040	0.080
1,2-Dichlorobenzene	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
1,2-Dichloroethane	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
1,2-Dichloropropane	282	0	0.035	0.035	0.000	0.035	52	0	0.035	0.035	0.000	0.035	0.070
1,3,5-Trimethylbenzene	282	39	0.035	0.065	0.046	0.312	52	38	0.035	0.081	0.125	0.900	0.070
1,3-Butadiene	282	26	0.035	0.057	0.045	0.292	52	27	0.035	0.060	0.045	0.209	0.070
1,3-Dichlorobenzene	282	0	0.025	0.025	0.000	0.025	52	0	0.025	0.025	0.000	0.025	0.050
1,4-Dichlorobenzene	282	1	0.045	0.046	0.008	0.142	52	6	0.045	0.049	0.016	0.130	0.090
2-Chloro-1,3-Butadiene	282	0	0.050	0.050	0.000	0.050	52	0	0.050	0.050	0.000	0.050	0.100
Acetonitrile	282	35	0.125	1.790	6.893	102.600	52	38	0.125	2.093	3.671	14.080	0.250
Acetylene	282	99	0.065	1.675	0.781	6.480	52	100	0.690	1.767	0.892	4.460	0.130
Acrylonitrile	282	0	0.105	0.105	0.000	0.105	52	0	0.105	0.105	0.000	0.105	0.210
Benzene	282	100	0.231	0.615	0.316	2.173	52	100	0.240	0.600	0.306	1.713	0.040
Benzyl chloride	282	0	0.035	0.035	0.000	0.035	52	0	0.035	0.035	0.000	0.035	0.070
Bromochloromethane	282	0	0.060	0.060	0.000	0.060	52	0	0.060	0.060	0.000	0.060	0.120
Bromodichloromethane	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
Bromoform	282	0	0.040	0.040	0.000	0.040	52	2	0.040	0.054	0.101	0.770	0.080
Bromomethane	282	0	0.045	0.045	0.000	0.045	52	0	0.045	0.045	0.000	0.045	0.090
Carbon tetrachloride	282	91	0.040	0.100	0.024	0.170	52	88	0.040	0.096	0.024	0.140	0.080
Chlorobenzene	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
Chloroethane	282	1	0.040	0.044	0.041	0.626	52	6	0.040	0.044	0.017	0.120	0.080

Supplement 1. (Cont.)

Compound	ERG laboratory-Sample 1						ERG laboratory-Sample 2						MDL
	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	(ppbv)
Chloroform	282	2	0.025	0.026	0.004	0.065	52	0	0.025	0.025	0.000	0.025	0.050
Chloromethane	282	100	0.408	0.608	0.082	0.988	52	100	0.480	0.600	0.098	1.190	0.060
2-Chloro-1,3-Butadiene	282	0	0.050	0.050	0.000	0.050	52	0	0.050	0.050	0.000	0.050	0.100
cis-1,2-Dichloroethylene	282	0	0.050	0.051	0.019	0.370	52	0	0.050	0.050	0.000	0.050	0.100
cis-1,3-Dichloroprene	282	0	0.050	0.050	0.000	0.050	52	0	0.050	0.050	0.000	0.050	0.100
Dibromochloromethane	282	0	0.040	0.040	0.000	0.040	52	0	0.040	0.040	0.000	0.040	0.080
Dichlorodifluoromethane	282	100	0.460	0.634	0.079	1.079	52	100	0.520	0.619	0.043	0.712	0.040
Dichlorotetrafluoroethane	282	0	0.025	0.025	0.000	0.025	52	0	0.025	0.025	0.000	0.025	0.050
Ethyl acrylate	282	0	0.080	0.080	0.000	0.080	52	0	0.080	0.080	0.000	0.080	0.160
Ethylbenzene	282	98	0.020	0.192	0.157	1.894	52	90	0.020	0.168	0.122	0.647	0.040
Ethyl-tert-butyl-ether	282	0	0.075	0.075	0.000	0.075	52	0	0.075	0.075	0.000	0.075	0.150
Hexachloro-1,3-Butadiene	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060
m,p-Xylene	282	100	0.100	0.551	0.482	6.082	52	98	0.025	0.489	0.375	1.893	0.050
Methyl ethyl ketone	282	72	0.075	0.604	0.510	2.920	52	73	0.075	0.601	0.446	1.761	0.150
Methyl isobutyl ketone	282	9	0.075	0.102	0.098	0.736	52	12	0.075	0.102	0.086	0.585	0.150
Methyl methacrylate	282	0	0.090	0.090	0.000	0.090	52	0	0.090	0.090	0.000	0.090	0.180
Methylene chloride	282	96	0.030	3.720	11.711	147.770	52	98	0.030	1.488	3.006	16.990	0.060
Methyl-tert-butyl-ether	282	6	0.090	0.102	0.056	0.585	52	8	0.090	0.109	0.073	0.484	0.180
n-Octane	282	32	0.030	0.055	0.058	0.750	52	46	0.030	0.072	0.064	0.310	0.060
o-Xylene	282	98	0.025	0.220	0.188	2.502	52	90	0.025	0.204	0.166	0.899	0.050
Propylene	282	100	0.110	1.210	1.474	14.137	52	100	0.180	1.248	1.842	11.490	0.050
Styrene	282	7	0.035	0.039	0.017	0.173	52	4	0.035	0.037	0.011	0.093	0.070
Tert-amyl-methyl-ether	282	0	0.060	0.060	0.000	0.060	52	0	0.060	0.060	0.000	0.060	0.120
Tertrachloroethylene	282	34	0.030	0.064	0.080	0.670	52	35	0.030	0.053	0.037	0.160	0.060
Toluene	282	100	0.250	1.112	1.099	13.428	52	100	0.210	1.057	0.929	6.431	0.060
trans-1,2-Dichloroethylene	282	0	0.030	0.030	0.004	0.090	52	0	0.030	0.030	0.000	0.030	0.060
trans-1,3-Dichloropropene	282	0	0.055	0.055	0.000	0.055	52	0	0.055	0.055	0.000	0.055	0.110
Trichloroethylene	282	1	0.035	0.043	0.085	1.268	52	4	0.035	0.329	2.099	15.172	0.070
Trichlorofluoromethane	282	100	0.020	0.321	0.120	1.540	52	100	0.190	0.299	0.052	0.497	0.040
Trichlorotrifluroethane	282	100	0.035	0.111	0.024	0.194	52	100	0.080	0.108	0.021	0.150	0.070
Vinyl chloride	282	0	0.030	0.030	0.000	0.030	52	0	0.030	0.030	0.000	0.030	0.060

Supplement 2. Statistics of concentrations at Dearborn, Michigan for VOCs and carbonyls analyzed by Michigan Department of Environmental Quality (MDEQ) laboratory.

TFE=trifluoroethane; TTFE=tetrafluoroethane; DF=detection frequency; MDL=method detection limit.

Compound	MDEQ laboratory-Sample 1						MDEQ laboratory-Sample 2						MDL
	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	(ppbv)
Carbonyls													
2,5-Dimethylbenzaldehyde	54	2	0.002	0.005	0.028	0.210	59	2	0.002	0.005	0.028	0.210	0.003
Acetaldehyde	54	89	0.005	1.005	1.207	6.721	59	98	0.005	1.005	1.207	6.721	0.009
Acetone	54	94	0.005	1.150	1.164	5.204	59	98	0.005	1.150	1.164	5.204	0.011
Benzaldehyde	54	72	0.002	0.042	0.085	0.509	59	56	0.002	0.042	0.085	0.509	0.004
Crotonaldehyde	54	24	0.004	0.016	0.030	0.139	59	14	0.004	0.016	0.030	0.139	0.008
Formaldehyde	54	91	0.004	2.046	1.689	8.735	59	97	0.004	2.046	1.689	8.735	0.008
Hexaldehyde	54	69	0.003	0.098	0.205	1.191	59	71	0.003	0.098	0.205	1.191	0.005
iso-Valeraldehyde	54	46	0.006	0.064	0.105	0.525	59	61	0.006	0.064	0.105	0.525	0.012
m,p-Tolualdehyde	54	31	0.001	0.017	0.033	0.161	59	29	0.001	0.017	0.033	0.161	0.002
n-Butyraldehyde	54	81	0.003	0.127	0.228	1.274	59	88	0.003	0.127	0.228	1.274	0.007
o-Tolualdehyde	54	4	0.001	0.002	0.003	0.020	59	0	0.001	0.002	0.003	0.020	0.002
Propionaldehyde	54	63	0.041	0.207	0.246	1.056	59	75	0.041	0.207	0.246	1.056	0.083
Valeraldehyde	54	31	0.011	0.053	0.096	0.519	59	34	0.011	0.053	0.096	0.519	0.022
VOCs													
1,1,1-Trichloroethane	57	5	0.024	0.026	0.007	0.057	58	2	0.024	0.026	0.007	0.057	0.048
1,1,2,2-Tetrachloroethane	57	0	0.041	0.041	0.000	0.041	58	0	0.041	0.041	0.000	0.041	0.081
1,1,2-Trichloro-1,2,2-TFE	57	95	0.017	0.083	0.023	0.178	58	95	0.017	0.083	0.023	0.178	0.034
1,1,2-Trichloroethane	57	0	0.024	0.024	0.000	0.024	58	0	0.024	0.024	0.000	0.024	0.048
1,1-Dichloroethane	57	0	0.045	0.045	0.000	0.045	58	0	0.045	0.045	0.000	0.045	0.089
1,1-Dichloroethene	57	0	0.023	0.023	0.000	0.023	58	2	0.023	0.023	0.000	0.023	0.046
1,2,4-Trichlorobenzene	57	2	0.041	0.042	0.009	0.110	58	0	0.041	0.042	0.009	0.110	0.081
1,2,4-Trimethylbenzene	57	86	0.031	0.174	0.122	0.589	58	83	0.031	0.174	0.122	0.589	0.062
1,2-Dibromoethane	57	0	0.027	0.027	0.000	0.027	58	0	0.027	0.027	0.000	0.027	0.054
1,2-Dichloro-1,1,2,2-TTFE	57	0	0.021	0.021	0.000	0.021	58	0	0.021	0.021	0.000	0.021	0.042
1,2-Dichlorobenzene	57	2	0.033	0.034	0.007	0.085	58	0	0.033	0.034	0.007	0.085	0.066
1,2-Dichloroethane	57	0	0.043	0.043	0.000	0.043	58	0	0.043	0.043	0.000	0.043	0.086
1,2-Dichloropropane	57	0	0.030	0.030	0.000	0.030	58	0	0.030	0.030	0.000	0.030	0.059
1,3,5-Trimethylbenzene	57	30	0.029	0.047	0.034	0.161	58	28	0.029	0.047	0.034	0.161	0.057
1,3-Butadiene	57	0	0.020	0.020	0.000	0.020	58	2	0.020	0.020	0.000	0.020	0.040
1,3-Dichlorobenzene	57	2	0.027	0.027	0.007	0.079	58	0	0.027	0.027	0.007	0.079	0.053
1,4-Dichlorobenzene	57	7	0.027	0.030	0.015	0.106	58	7	0.027	0.030	0.015	0.106	0.053
2,2,4-Trimethylpentane	57	96	0.009	0.118	0.085	0.523	58	98	0.009	0.118	0.085	0.523	0.017
2-Chloro-1,3-Butadiene	57	0	0.015	0.015	0.000	0.015	58	0	0.015	0.015	0.000	0.015	0.030
Acetonitrile	57	70	0.260	1.563	2.773	15.530	58	74	0.260	1.563	2.773	15.530	0.520
Acrylonitrile	57	0	0.195	0.195	0.000	0.195	58	0	0.195	0.195	0.000	0.195	0.390
Benzene	57	96	0.035	0.546	0.397	2.494	58	100	0.035	0.546	0.397	2.494	0.070
Benzyl chloride	57	0	0.038	0.038	0.000	0.038	58	0	0.038	0.038	0.000	0.038	0.076
Bromodichloromethane	57	0	0.037	0.037	0.000	0.037	58	0	0.037	0.037	0.000	0.037	0.073
Bromoform	57	0	0.030	0.030	0.000	0.030	58	0	0.030	0.030	0.000	0.030	0.059
Bromomethane	57	4	0.020	0.022	0.010	0.092	58	0	0.020	0.022	0.010	0.092	0.040

Supplement 2. (Cont.)

Compound	MDEQ laboratory-Sample 1						MDEQ laboratory-Sample 2						
	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	N	DF (%)	Min (ppbv)	Mean (ppbv)	SD (ppbv)	Max (ppbv)	MDL (ppbv)
Carbon tetrachloride	57	95	0.019	0.090	0.020	0.125	58	95	0.019	0.090	0.020	0.125	0.038
Chlorobenzene	57	2	0.020	0.021	0.004	0.049	58	2	0.020	0.021	0.004	0.049	0.040
Chloroethane	57	0	0.020	0.020	0.000	0.020	58	17	0.020	0.020	0.000	0.020	0.040
Chloroform	57	0	0.034	0.034	0.000	0.034	58	0	0.034	0.034	0.000	0.034	0.068
Chloromethane	57	98	0.031	0.568	0.169	1.426	58	100	0.031	0.568	0.169	1.426	0.062
2-Chloro-1,3-Butadiene	57	0	0.015	0.015	0.000	0.015	58	0	0.015	0.015	0.000	0.015	0.030
cis-1,2-Dichloroethylene	57	0	0.029	0.029	0.000	0.029	58	0	0.029	0.029	0.000	0.029	0.057
cis-1,3-Dichloroprene	57	0	0.027	0.027	0.000	0.027	58	0	0.027	0.027	0.000	0.027	0.054
Dibromochloromethane	57	0	0.030	0.030	0.000	0.030	58	0	0.030	0.030	0.000	0.030	0.059
Dichlorodifluoromethane	57	98	0.024	0.554	0.129	0.846	58	100	0.024	0.554	0.129	0.846	0.048
Ethylbenzene	57	68	0.042	0.118	0.086	0.413	58	48	0.042	0.118	0.086	0.413	0.083
Hexachloro-1,3-Butadiene	57	0	0.032	0.032	0.000	0.032	58	0	0.032	0.032	0.000	0.032	0.063
Hexane	57	21	0.250	0.427	0.482	3.318	58	22	0.250	0.427	0.482	3.318	0.500
m,p-Xylene	57	70	0.100	0.319	0.244	1.198	58	53	0.100	0.319	0.244	1.198	0.200
Methyl ethyl ketone	57	0	0.850	0.850	0.000	0.850	58	0	0.850	0.850	0.000	0.850	1.700
Methyl isobutyl ketone	57	0	0.420	0.420	0.000	0.420	58	0	0.420	0.420	0.000	0.420	0.840
Methylene chloride	57	82	0.115	1.621	3.545	22.196	58	81	0.115	1.621	3.545	22.196	0.230
Methyl-tert-butyl-ether	57	5	0.031	0.040	0.044	0.292	58	3	0.031	0.040	0.044	0.292	0.061
o-Xylene	57	89	0.022	0.139	0.098	0.487	58	88	0.022	0.139	0.098	0.487	0.043
Styrene	57	7	0.027	0.031	0.016	0.132	58	5	0.027	0.031	0.016	0.132	0.054
Tertrachloroethylene	57	33	0.036	0.064	0.053	0.343	58	22	0.036	0.064	0.053	0.343	0.071
Toluene	57	98	0.035	0.932	0.685	3.473	58	100	0.035	0.932	0.685	3.473	0.070
trans-1,2-Dichloroethylene	57	0	0.043	0.043	0.000	0.043	58	0	0.043	0.043	0.000	0.043	0.087
trans-1,3-Dichloropropene	57	0	0.031	0.031	0.000	0.031	58	0	0.031	0.031	0.000	0.031	0.062
Trichloroethylene	57	7	0.019	0.022	0.012	0.084	58	3	0.019	0.022	0.012	0.084	0.038
Trichlorofluoromethane	57	96	0.024	0.273	0.073	0.500	58	100	0.024	0.273	0.073	0.500	0.048
Vinyl chloride	57	0	0.022	0.022	0.000	0.022	58	0	0.022	0.022	0.000	0.022	0.044

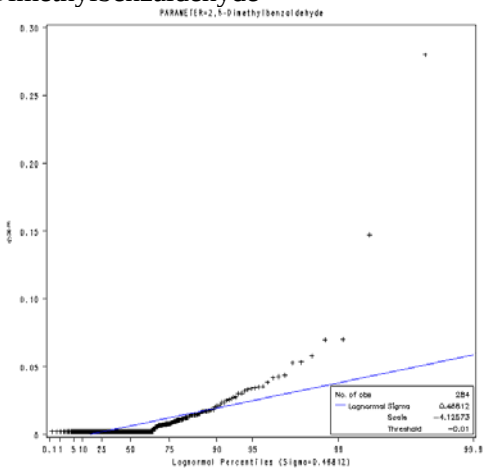
Supplement 3. Outlier analysis using Gumbel distribution (type I). ERG= Eastern Research Group; MDEQ= Michigan Department of Environmental Quality.

Compound	Date	Concentration (ppbv)	Laboratory	Sample
Carbonyls				
Formaldehyde	4/12/2002	20.98	ERG	1
Hexaldehyde	8/5/2001	1.19	MDEQ	1
Tolualdehyde	7/29/2001	0.59	ERG	1
VOCs				
Propylene	10/10/2001	14.14	ERG	1
	10/31/2001	11.49	ERG	1
n-Octane	3/11/2002	0.75	ERG	1
Methylene chloride	7/2/2001	61.71	ERG	1
	7/13/2001	61.41	ERG	1
	7/18/2001	199.27	MDEQ	2
	2/25/2002	51.19	ERG	1
	3/3/2002	147.77	ERG	1
m,p-Xylene	9/17/2001	6.08	ERG	1
	3/11/2002	3.49	ERG	1
Ethylbenzene	9/17/2001	1.89	ERG	1
	3/11/2002	1.26	ERG	1
o-Xylene	9/17/2001	2.50	ERG	1
1,3,5-Trimethylbenzene	8/20/2001	0.90	ERG	2
Toluene	5/20/2001	13.43	ERG	1
	9/17/2001	8.70	ERG	1

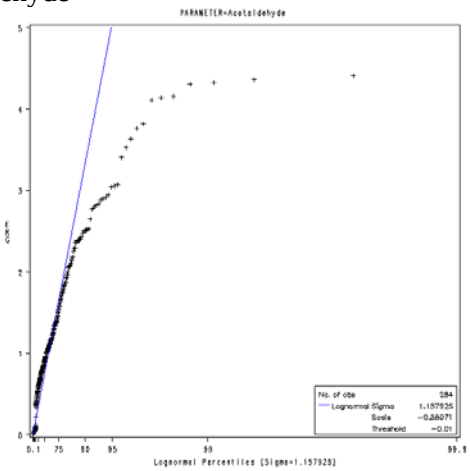
Supplement 4. Log-normal distribution plots for carbonyls and VOCs concentrations with detection frequencies above 20% from Eastern Research Group laboratory. Duplicates were averaged; Outliers were excluded.

a. ***Carbonyls***

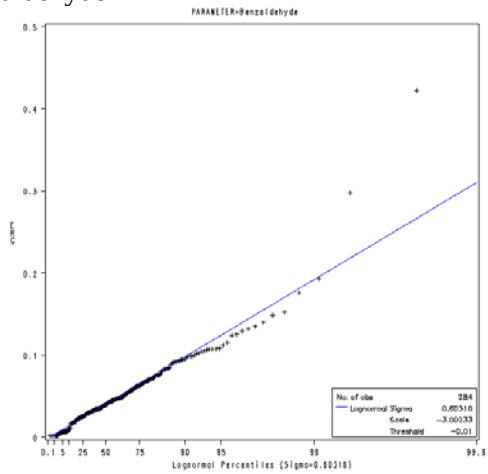
2,5-Dimethylbenzaldehyde



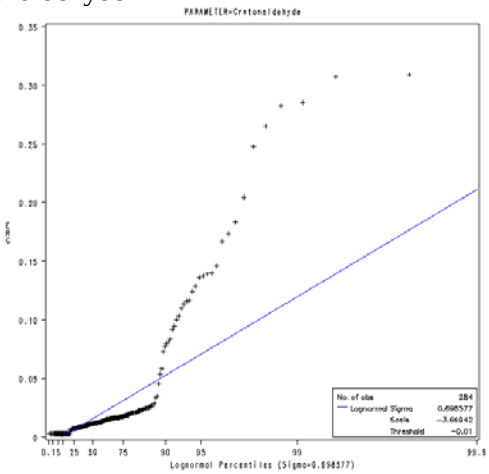
Acetaldehyde



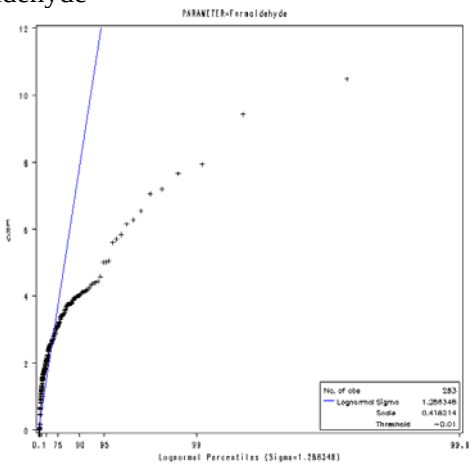
Benzaldehyde



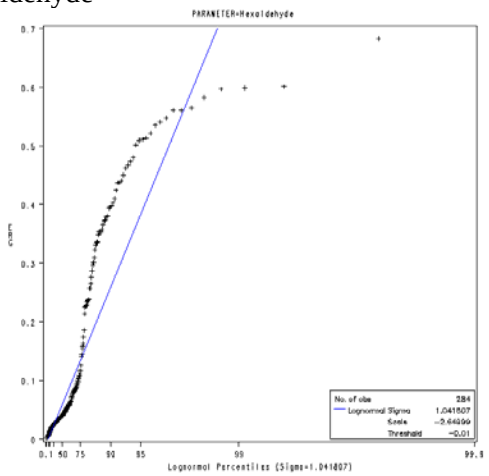
Crotonaldehyde



Formaldehyde

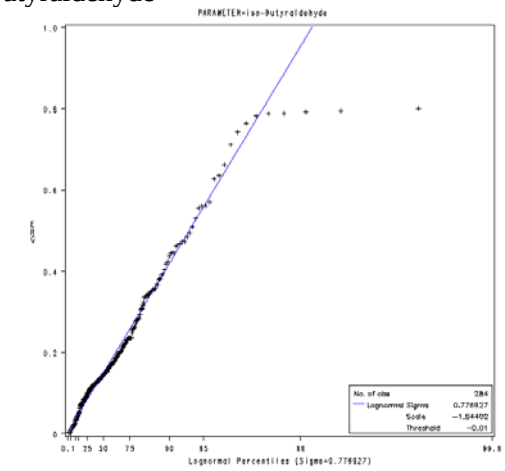


Hexaldehyde

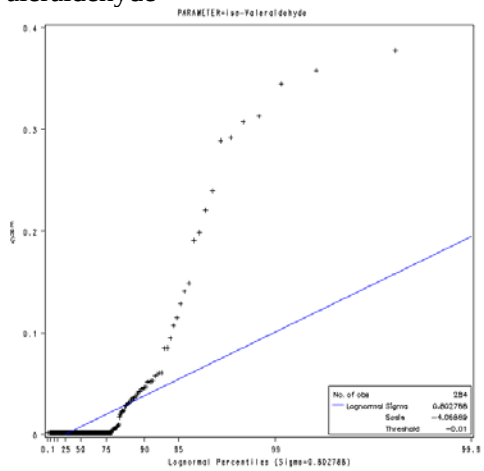


Carbonyls (Cont.)

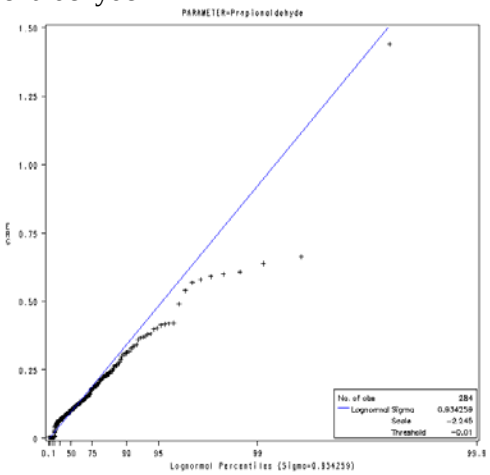
iso-Butyraldehyde



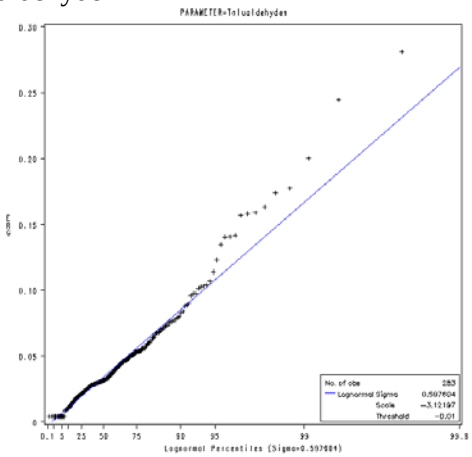
iso-Valeraldehyde



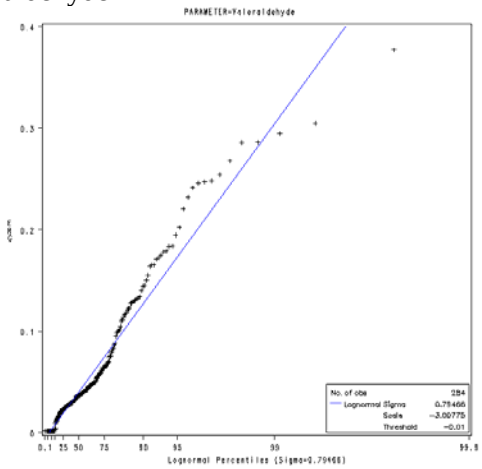
Propionaldehyde



Tolualdehyde

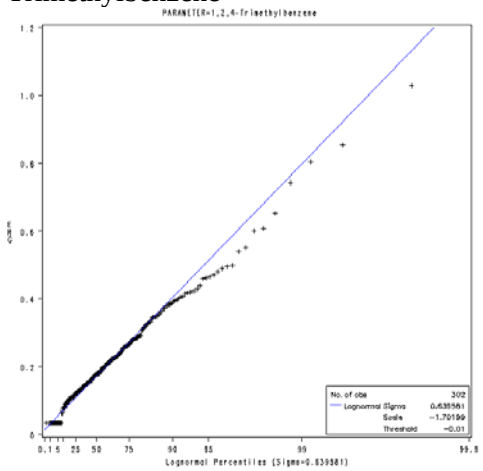


Valeraldehyde

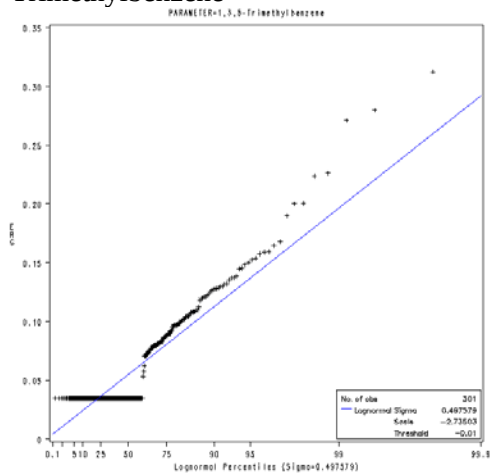


b. ***VOCs***

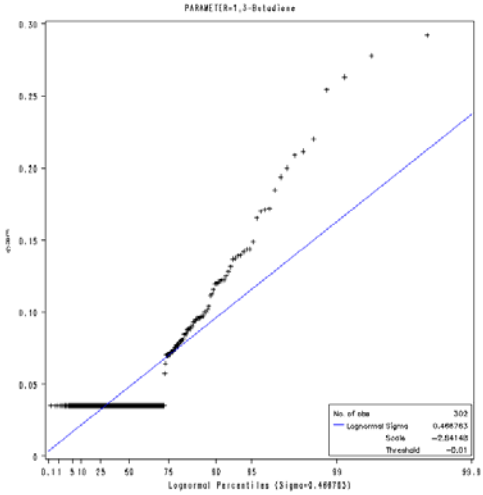
1,2,4-Trimethylbenzene



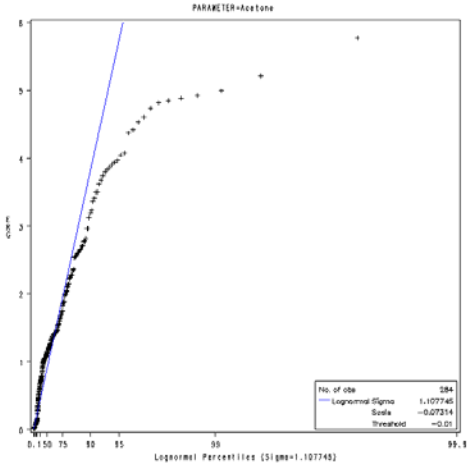
1,3,5-Trimethylbenzene



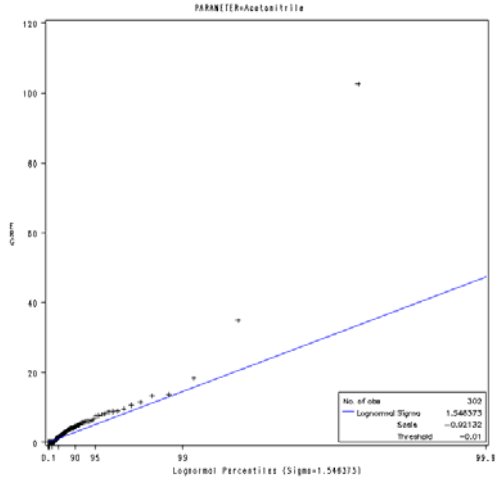
1,3-Butadiene



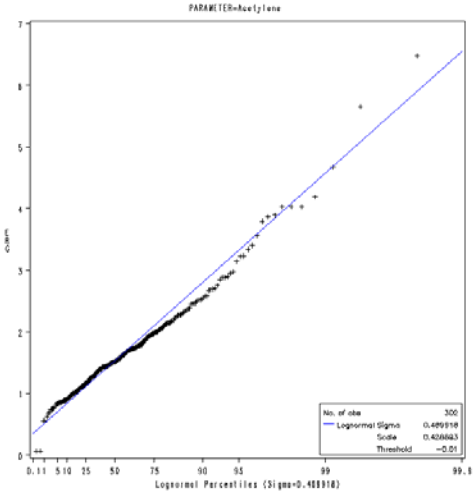
Acetone



Acetonitrile

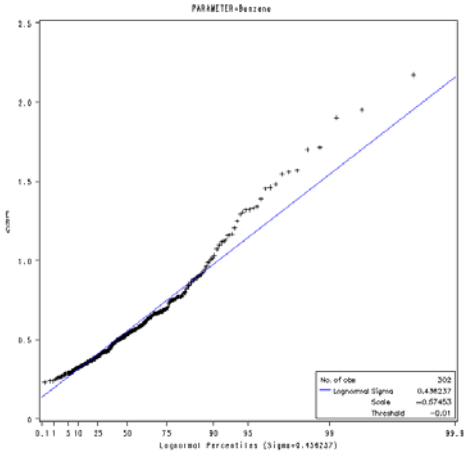


Acetylene

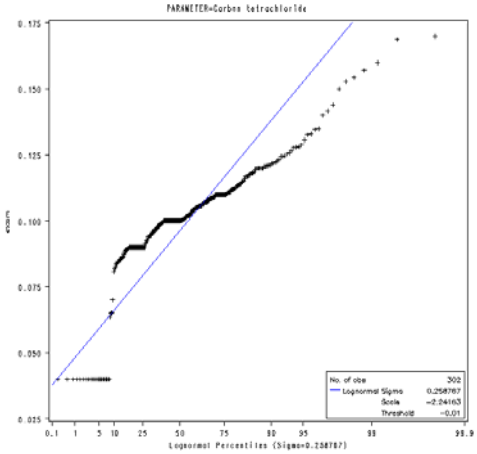


VOCs (Cont.)

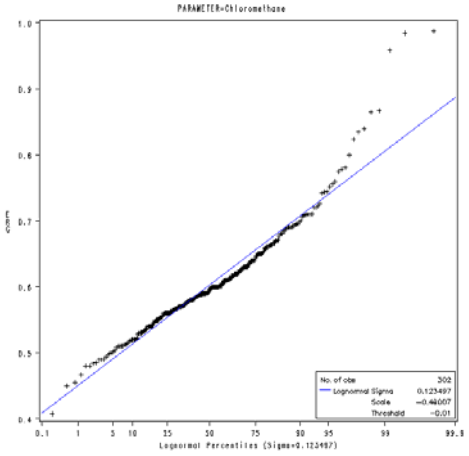
Benzene



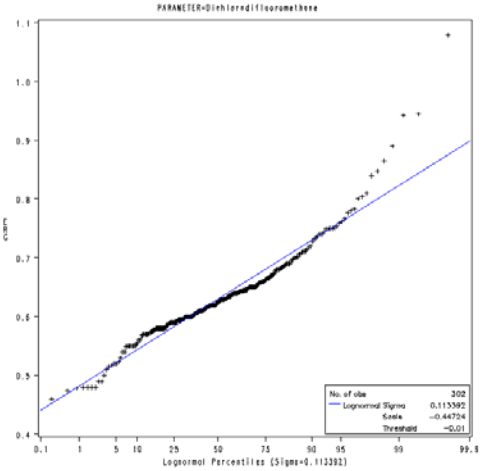
Carbon tetrachloride



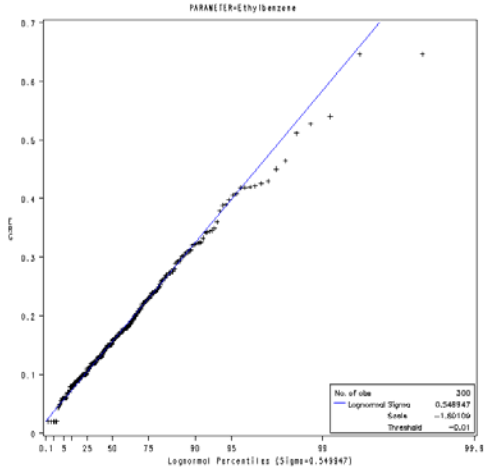
Chloromethane



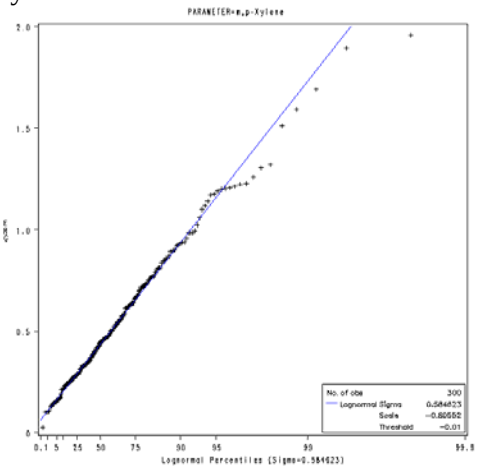
Dichlorodifluoromethane



Ethylbenzene

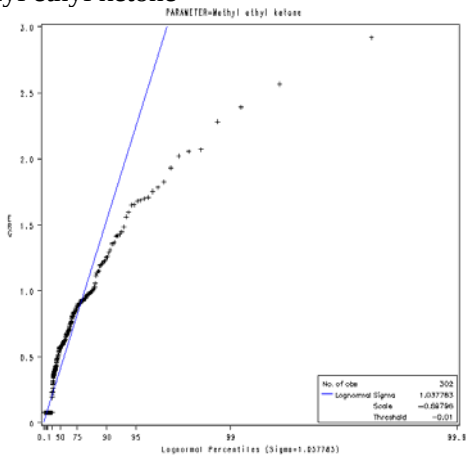


m,p-Xylene

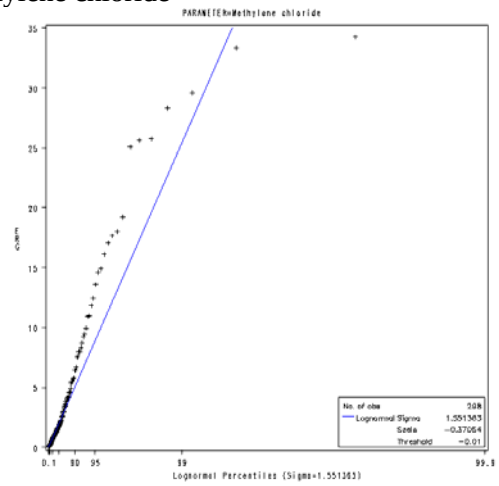


VOCs (Cont.)

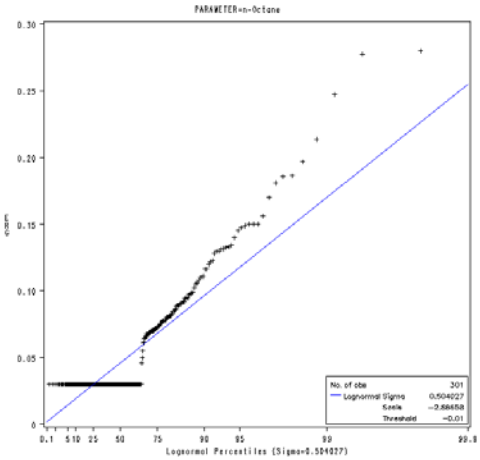
Methyl ethyl ketone



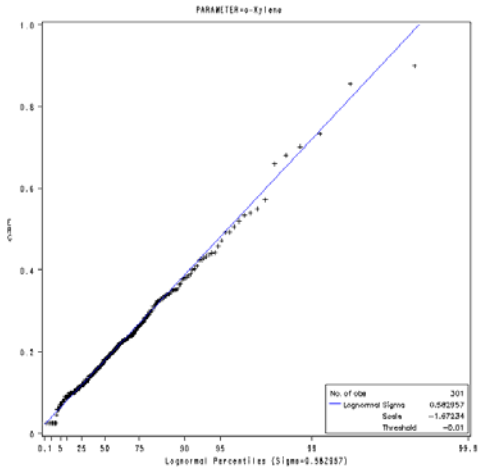
Methylene chloride



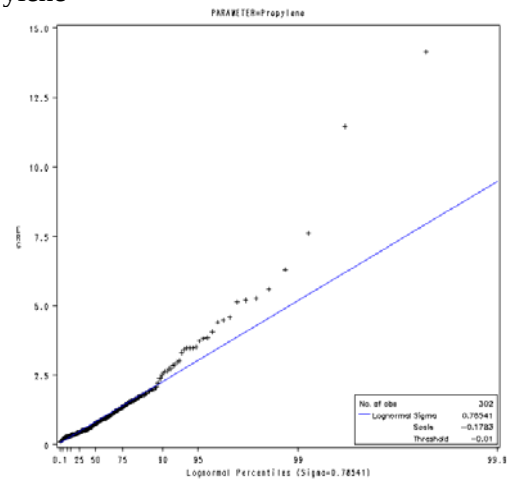
n-Octane



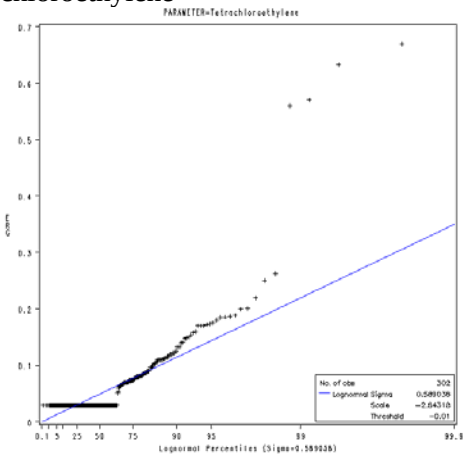
o-Xylene



Propylene

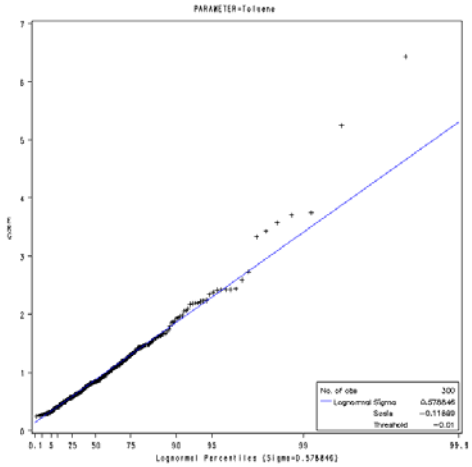


Tetrachloroethylene

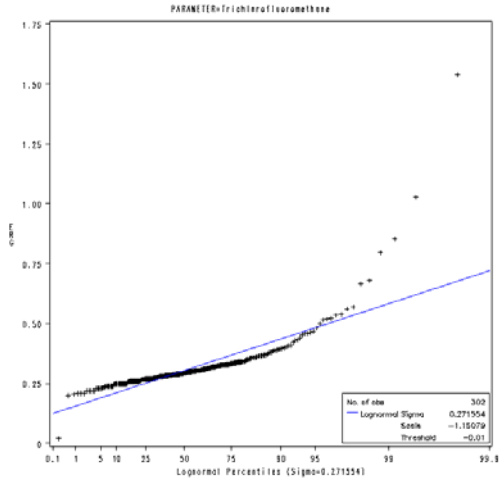


VOCs (Cont.)

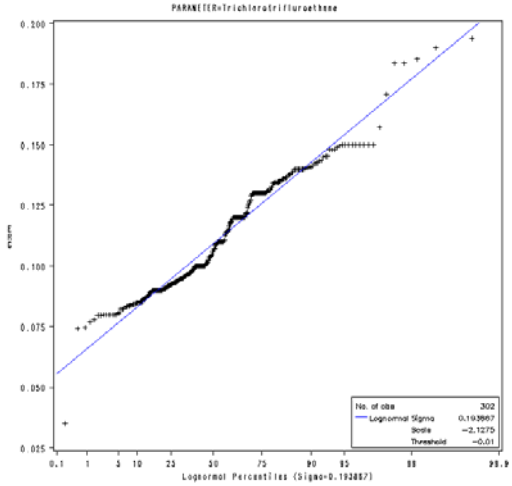
Toluene



Trichlorofluoromethane



Trichlorotrifluroethene

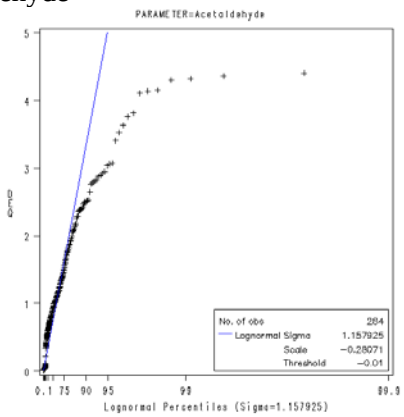


Supplement 5. Log-normal distribution plots for carbonyls and VOCs concentrations with detection frequencies above 20% from Michigan Department of Environmental Quality laboratory.

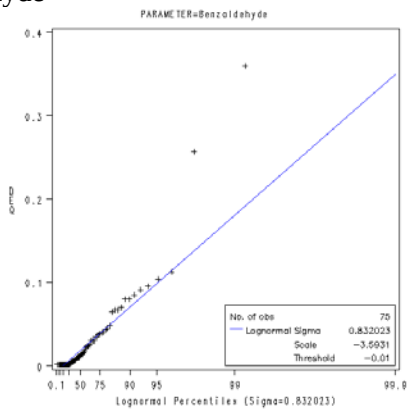
Duplicates were averaged; Outliers were excluded.

a. ***Carbonyls***

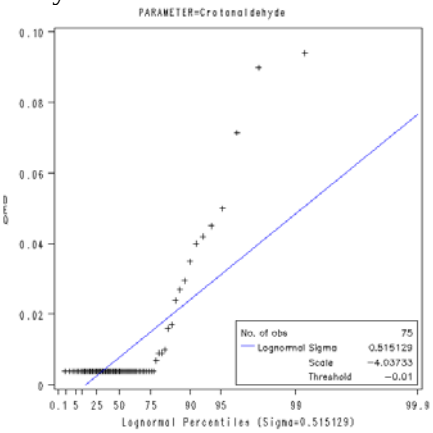
Acetaldehyde



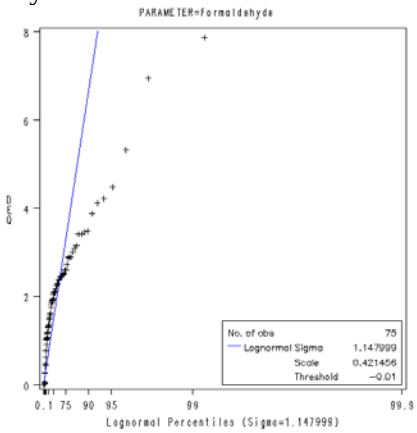
Benzaldehyde



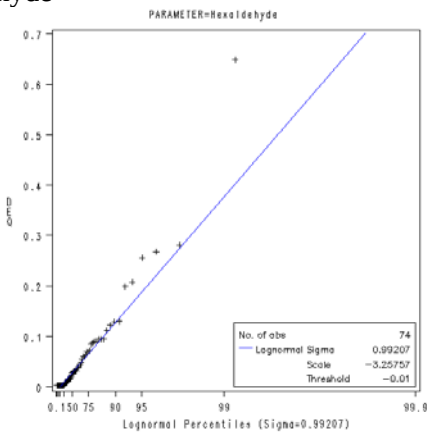
Crotonaldehyde



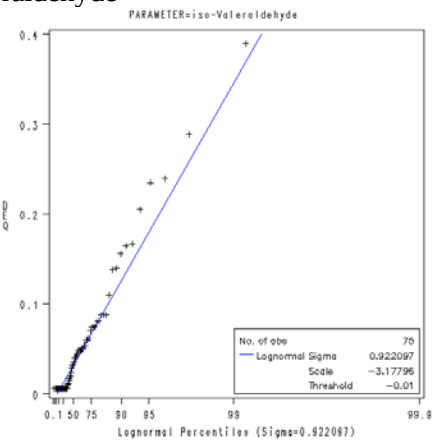
Formaldehyde



Hexaldehyde

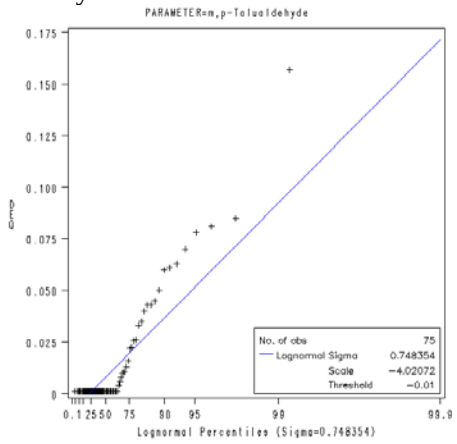


iso-Valeraldehyde

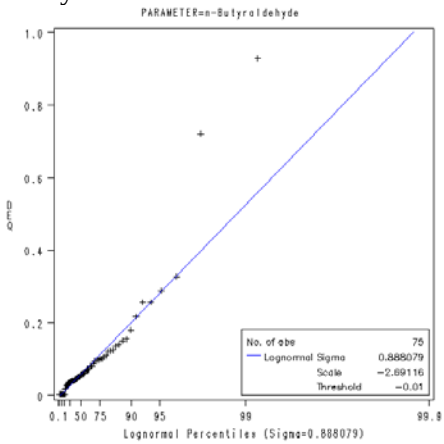


Carbonyls (Cont.)

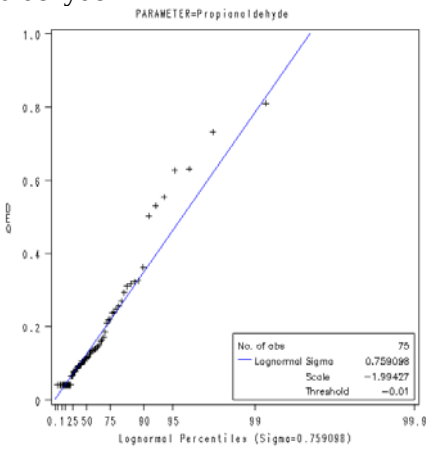
m,p-Tolualdehyde



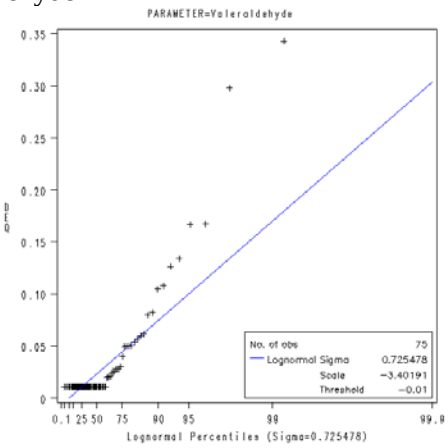
n-Butyraldehyde



Propionaldehyde

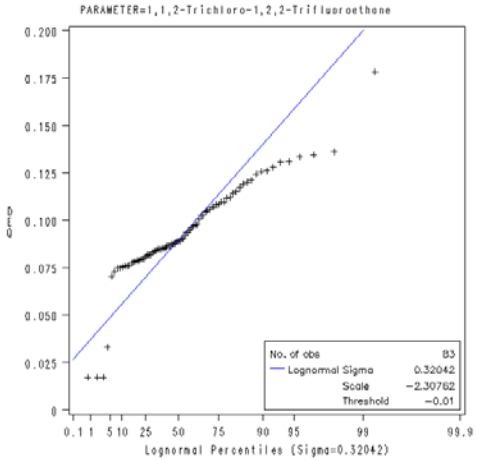


Valeraldehyde

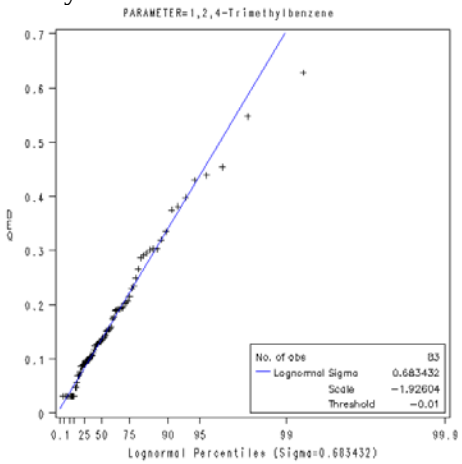


b. ***VOCs***

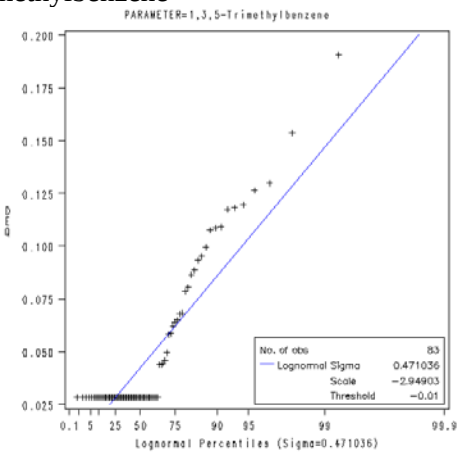
1,1,2-Trichloro-1,2,2-trifluoroethane



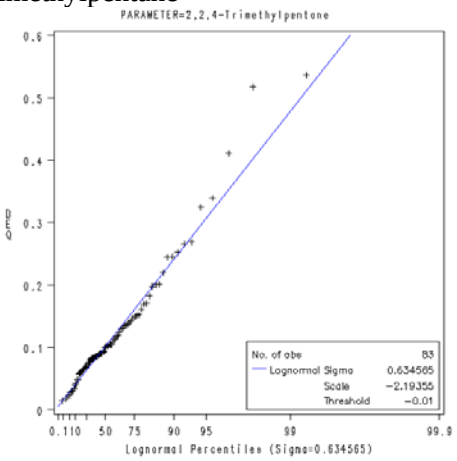
1,2,4-Trimethylbenzene



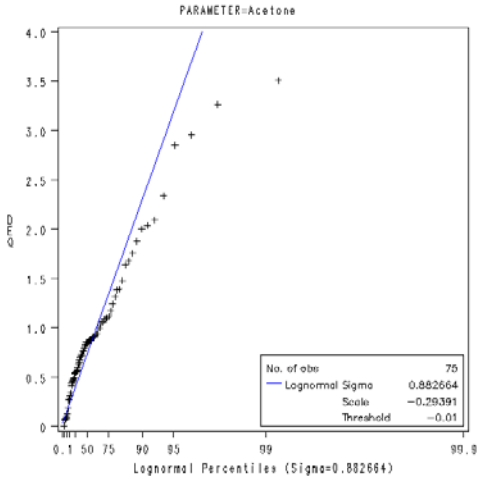
1,3,5-Trimethylbenzene



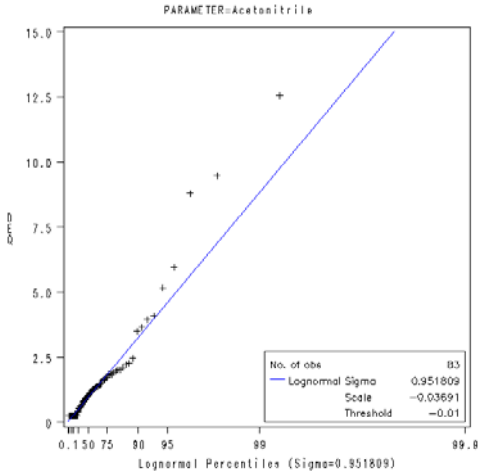
2,2,4-Trimethylpentane



Acetone

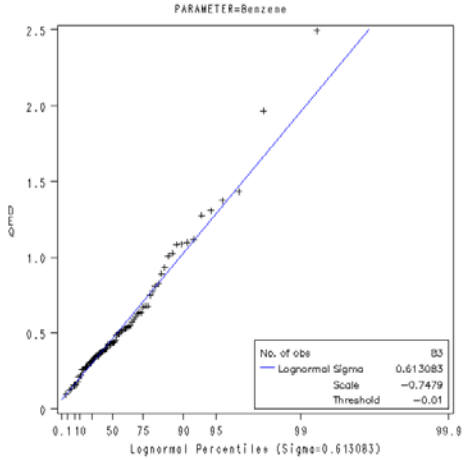


Acetonitrile

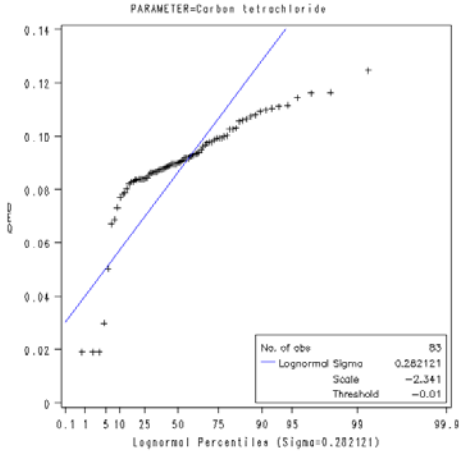


VOCs (Cont.)

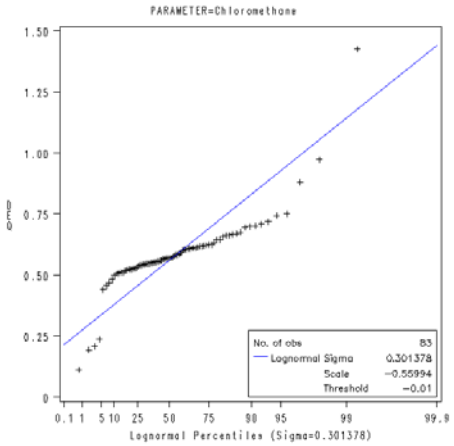
Benzene



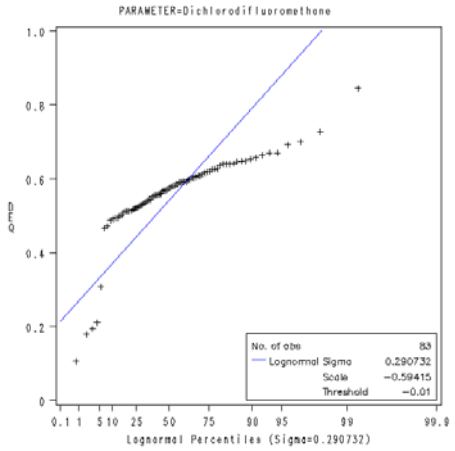
Carbon tetrachloride



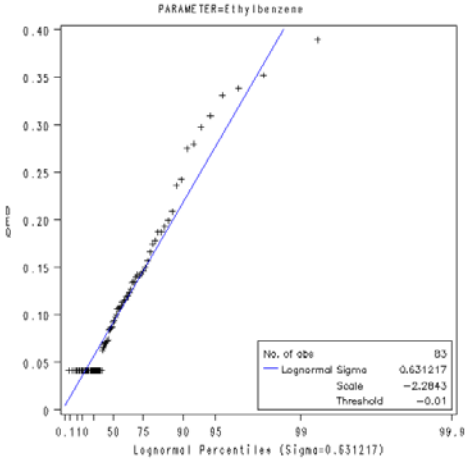
Chloromethane



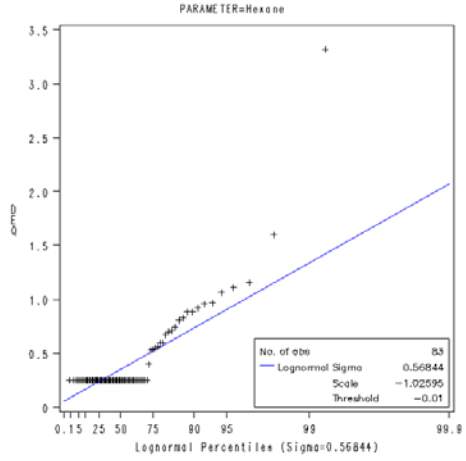
Dichlorodifluoromethane



Ethylbenzene

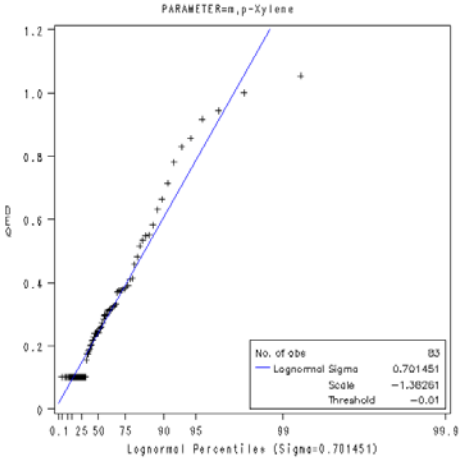


Hexane

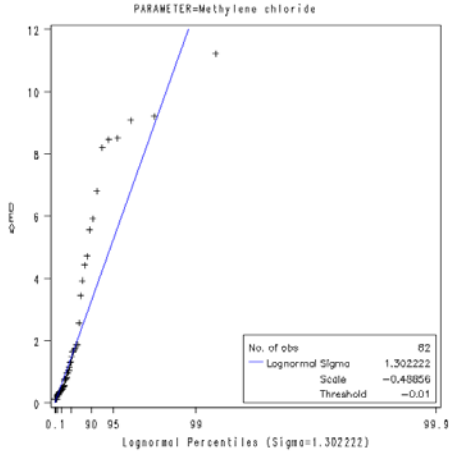


VOCs (Cont.)

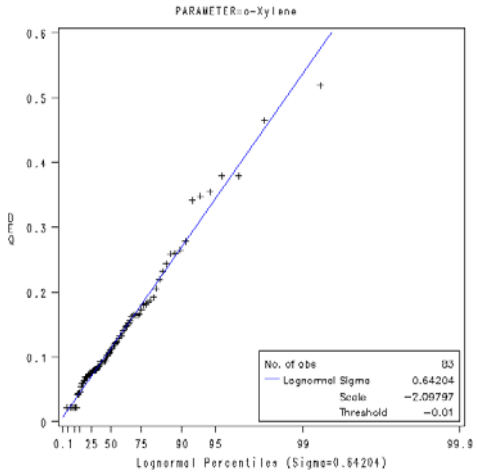
m,p-Xylene



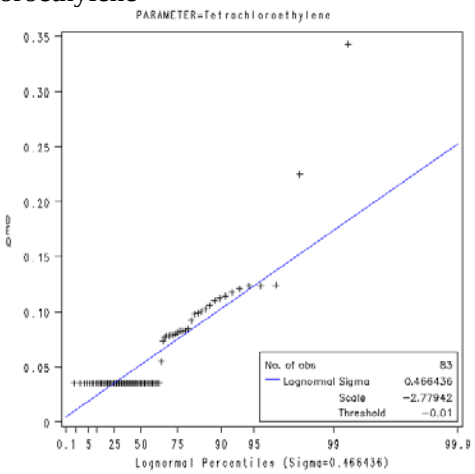
Methylene chloride



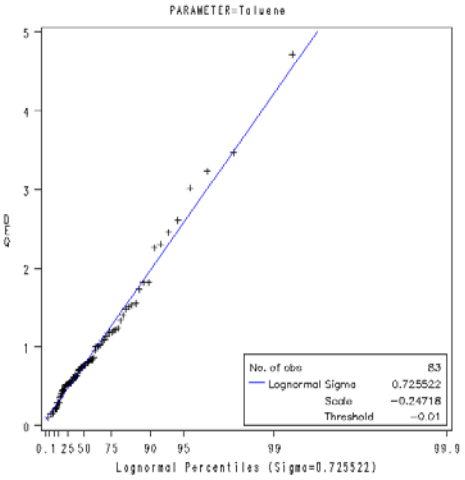
o-Xylene



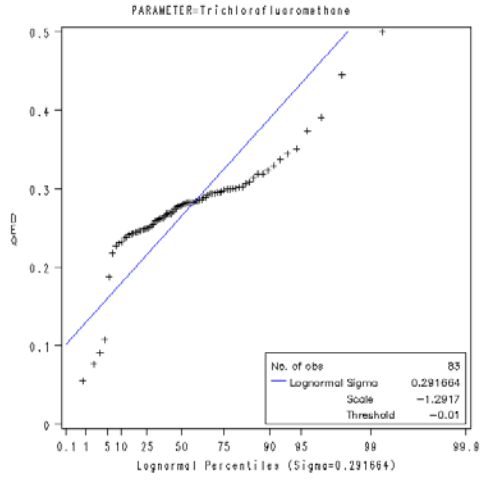
Tetrachloroethylene



Toluene



Trichlorofluoromethane



Supplement 6. Spearman rank correlation coefficients between air toxics and criteria pollutants and meteorological variables.

Variable dictionary is shown in Supplement 8.

VARIABLES	ACETALD	BNZALD	FORMALD	HEXALD	IBUTYRAL	PROPIONALD	TOLUALD	ACETYL	BNZ	BUTADNE	DCDFM	EBNZ	MEK	MPX	NOCTANE	OXY	PROPYL	TCEL	TCFM	TCTFE	TMBNZ_124	TMBNZ_135	TOLUENE
Criteria pollutants																							
APCO_24HR	0.30	0.25	0.30	0.11	0.21	0.26	0.12	0.60	0.57	0.43	0.15	0.49	0.18	0.48	0.21	0.50	0.48	0.20	0.12	-0.01	0.49	0.46	0.53
AP_PM25	0.41	0.43	0.39	0.40	0.31	0.38	0.34	0.25	0.45	0.12	0.17	0.39	0.56	0.39	0.22	0.41	0.38	0.16	0.28	-0.05	0.41	0.36	0.47
DB_pm10	0.19	0.22	0.15	0.06	0.09	0.18	0.15	0.09	0.10	-0.03	0.02	0.07	0.26	0.06	0.09	0.05	0.20	-0.09	-0.02	-0.06	0.03	0.08	0.05
E7MNO2_24HR	0.19	0.14	0.19	-0.03	0.15	0.17	-0.01	0.54	0.38	0.29	0.08	0.30	0.10	0.28	0.16	0.28	0.52	0.05	-0.02	0.10	0.27	0.20	0.28
E7MSO2_24HR	0.21	0.18	0.14	0.17	0.13	0.22	0.11	0.23	0.31	0.06	0.05	0.06	0.28	0.05	0.09	0.11	0.38	0.07	-0.02	-0.02	0.10	0.08	0.21
LWCO_24HR	0.30	0.30	0.31	0.09	0.21	0.27	0.16	0.54	0.49	0.38	0.09	0.47	0.22	0.46	0.21	0.47	0.58	0.13	0.11	0.04	0.42	0.39	0.47
LWNO2_24HR	0.27	0.30	0.30	0.15	0.23	0.24	0.18	0.47	0.48	0.19	0.03	0.35	0.20	0.33	0.16	0.35	0.48	0.09	-0.07	0.03	0.31	0.24	0.36
LWSO2_24HR	0.17	0.17	0.14	0.12	0.08	0.16	0.11	0.33	0.38	0.09	-0.05	0.15	0.21	0.15	0.15	0.20	0.47	0.09	-0.01	-0.02	0.18	0.13	0.26
LW_PM25	0.23	0.21	0.18	0.14	0.09	0.21	0.15	0.27	0.37	-0.03	0.00	0.19	0.33	0.17	0.11	0.19	0.35	0.06	0.03	-0.05	0.18	0.13	0.27
Meteorology																							
DPTP_DTW	0.54	0.61	0.51	0.70	0.45	0.53	0.54	-0.10	0.24	0.05	0.36	0.36	0.71	0.39	0.18	0.40	0.21	0.16	0.43	-0.11	0.39	0.31	0.45
MIX_HT	0.12	0.25	0.16	0.31	0.09	0.17	0.24	-0.30	-0.20	-0.18	0.14	-0.09	0.16	-0.08	-0.02	-0.09	-0.19	-0.06	0.00	-0.11	-0.09	-0.09	-0.10
MNRH_DTW	-0.12	-0.17	-0.12	-0.18	-0.14	-0.15	-0.14	0.05	0.03	0.00	-0.12	-0.01	-0.11	-0.01	-0.05	-0.01	0.14	0.05	0.03	0.13	-0.04	-0.01	-0.06
MNTP_DTW	0.54	0.62	0.51	0.71	0.46	0.54	0.54	-0.12	0.20	0.02	0.37	0.34	0.72	0.37	0.18	0.38	0.16	0.13	0.41	-0.16	0.38	0.29	0.44
MXRH_DTW	0.19	0.13	0.17	0.17	0.15	0.13	0.12	0.10	0.19	0.16	0.04	0.23	0.17	0.23	0.06	0.22	0.25	0.13	0.18	0.09	0.21	0.16	0.21
PRCP_DTW	-0.08	-0.10	-0.07	-0.01	-0.07	-0.10	-0.11	-0.14	-0.07	-0.14	-0.12	-0.08	-0.04	-0.08	-0.14	-0.09	0.04	-0.04	-0.09	0.05	-0.08	-0.13	-0.11
PRES_DTW	0.03	0.04	0.05	0.00	0.10	0.02	-0.03	0.23	0.21	0.24	0.05	0.18	0.01	0.17	0.10	0.21	0.05	0.04	0.06	-0.01	0.21	0.15	0.24
RWND_DTW	-0.37	-0.44	-0.36	-0.43	-0.32	-0.34	-0.29	-0.38	-0.59	-0.41	-0.26	-0.52	-0.44	-0.53	-0.24	-0.57	-0.25	-0.36	-0.28	0.17	-0.60	-0.54	-0.65
SLVP_DTW	0.00	0.00	0.01	-0.05	0.07	-0.01	-0.07	0.24	0.19	0.24	0.03	0.15	-0.04	0.14	0.09	0.18	0.04	0.02	0.04	0.01	0.18	0.13	0.20
WDIR_S1	0.14	0.16	0.16	0.23	0.16	0.15	0.11	0.18	0.22	0.25	0.24	0.26	0.15	0.28	0.14	0.32	-0.03	0.09	0.27	-0.06	0.36	0.31	0.37
WDIR_S2	0.12	0.09	0.15	0.17	0.15	0.08	0.08	0.13	0.28	0.11	0.08	0.15	0.13	0.15	0.09	0.19	0.02	0.14	0.08	-0.09	0.21	0.13	0.27
WDIR_S3	0.13	0.13	0.11	0.20	0.12	0.09	0.08	0.09	0.42	0.12	0.10	0.14	0.27	0.13	0.09	0.17	0.07	0.21	0.09	-0.09	0.20	0.14	0.27
WDIR_S4	0.23	0.21	0.17	0.20	0.18	0.19	0.09	0.13	0.36	0.07	0.09	0.11	0.32	0.10	0.17	0.15	0.42	0.06	0.11	0.03	0.11	0.08	0.21
WDIR_S5	0.07	-0.02	-0.02	-0.12	-0.01	0.05	-0.08	0.03	-0.08	-0.10	-0.16	-0.12	-0.03	-0.13	0.03	-0.14	0.30	-0.30	-0.11	0.11	-0.18	-0.15	-0.15
WDIR_S6	-0.16	-0.12	-0.12	-0.21	-0.16	-0.14	-0.10	-0.19	-0.35	-0.20	-0.16	-0.13	-0.21	-0.13	-0.18	-0.22	-0.26	-0.19	-0.16	-0.04	-0.23	-0.14	-0.33
WDIR_S7	-0.15	-0.06	-0.07	-0.07	-0.09	-0.11	0.03	-0.14	-0.24	-0.01	0.03	0.09	-0.14	0.10	-0.13	0.03	-0.23	0.14	-0.04	-0.15	0.05	0.07	-0.08
WDIR_S8	-0.01	0.03	0.00	0.11	0.10	0.01	0.08	-0.02	-0.05	0.16	0.10	0.07	-0.03	0.08	0.01	0.11	-0.19	0.16	0.06	-0.08	0.15	0.13	0.14

Supplement 7. Spearman rank correlation coefficients between selected carbonyls and VOCs.

Variable dictionary is shown in Supplement 8.

VARIABLES	ACETALD	BNZALD	FORMALD	HEXALD	IBUTYRAL	PROPIONALD	TOLUALD	ACETYL	BNZ	BUTADNE	DCDFM	EBNZ	MEK	MPX	NOCTANE	OXY	PROPYL	TCEL	TCFM	TCTFE	TMBNZ_124	TMBNZ_135	TOLUENE
Carbonyls																							
ACETALD	1.00																						
BNZALD	0.80	1.00																					
FORMALD	0.90	0.79	1.00																				
HEXALD	0.77	0.87	0.75	1.00																			
IBUTYRAL	0.85	0.69	0.80	0.72	1.00																		
PROPIONALD	0.95	0.80	0.87	0.79	0.80	1.00																	
TOLUALD	0.66	0.71	0.63	0.76	0.57	0.69	1.00																
VOCs																							
ACETYL	0.30	0.24	0.30	0.11	0.20	0.28	0.14	1.00															
BNZ	0.41	0.41	0.38	0.31	0.29	0.37	0.27	0.69	1.00														
BUTADNE	0.40	0.36	0.41	0.24	0.35	0.36	0.21	0.54	0.52	1.00													
DCDFM	0.38	0.33	0.36	0.40	0.39	0.39	0.31	0.22	0.24	0.26	1.00												
EBNZ	0.44	0.44	0.45	0.34	0.37	0.38	0.32	0.51	0.67	0.55	0.37	1.00											
MEK	0.51	0.59	0.48	0.58	0.47	0.50	0.42	0.16	0.45	0.25	0.40	0.47	1.00										
MPX	0.45	0.46	0.47	0.38	0.39	0.40	0.36	0.49	0.66	0.55	0.39	0.99	0.48	1.00									
NOCTANE	0.36	0.30	0.31	0.26	0.27	0.34	0.26	0.32	0.44	0.52	0.24	0.44	0.32	0.43	1.00								
OXY	0.49	0.50	0.49	0.42	0.40	0.44	0.38	0.53	0.72	0.57	0.40	0.97	0.51	0.97	0.47	1.00							
PROPYL	0.47	0.34	0.42	0.24	0.35	0.42	0.25	0.58	0.57	0.47	0.24	0.47	0.27	0.47	0.39	0.50	1.00						
TCEL	0.10	0.19	0.15	0.15	0.05	0.08	0.12	0.33	0.43	0.35	0.11	0.40	0.27	0.40	0.30	0.43	0.17	1.00					
TCFM	0.42	0.34	0.39	0.42	0.37	0.41	0.35	0.16	0.24	0.28	0.69	0.39	0.35	0.42	0.28	0.43	0.31	0.06	1.00				
TCTFE	0.12	-0.12	0.08	-0.04	0.15	0.07	-0.04	0.05	0.01	0.17	0.09	0.02	-0.01	0.00	0.16	-0.02	0.17	-0.11	0.06	1.00			
TMBNZ_124	0.46	0.47	0.47	0.40	0.38	0.40	0.35	0.53	0.70	0.59	0.40	0.94	0.52	0.94	0.45	0.94	0.44	0.44	0.41	-0.03	1.00		
TMBNZ_135	0.40	0.45	0.40	0.35	0.31	0.36	0.36	0.52	0.63	0.60	0.35	0.81	0.43	0.81	0.45	0.82	0.40	0.45	0.38	-0.04	0.86	1.00	
TOLUENE	0.52	0.55	0.52	0.48	0.43	0.47	0.36	0.57	0.80	0.55	0.37	0.84	0.56	0.84	0.43	0.88	0.51	0.45	0.42	-0.06	0.86	0.75	1.00

Supplement 8. Variable dictionary

Variables	Descriptions
Carbonyls	
ACETALD	Acetaldehyde
BNZALD	Benzaldehyde
FORMALD	Formaldehyde
HEXALD	Hexaldehyde
IBUTYRAL	iso-Butyraldehyde
PROPIONALD	Propionaldehyde
TOLUALD	Tolualdehyde
VOCs	
ACETYL	Acetylene
BNZ	Benzene
BUTADNE	1,3-Butadiene
CHLOMET	Chloromethane
DCDFM	Dichlorodifluoromethane
EBNZ	Ethylbenzene
MEK	Methyl ethyl ketone
MPX	m,p-Xylene
NOCTANE	n-Octane
OXY	o-Xylene
PROPYL	Propylene
TCEL	Tetrachloroethylene
TCFM	Trichlorofluoromethane
TCTFE	Trichlorotrifluoroethane
TMBNZ_124	1,2,4-Trimethylbenzene
TMBNZ_135	1,3,5-Trimethylbenzene
TOLUENE	Toluene
Criteria pollutants	
APCO_24HR	Allen Park-24H CO
AP_PM25	Allen Park-PM2.5
DB_pm10	PM10 at Dearborn
E7MNO2_24HR	East Seven Mile-24H NO2
E7MSO2_24HR	East Seven Mile-24H SO2
LWCO_24HR	Linwood-24H CO
LWNO2_24HR	Linwood-24H NO2
LWSO2_24HR	Linwood-24H SO2
LW_PM25	Linwood-PM2.5
Meteorology	
AWND_DTW	Detroit metro airport avg wind speed
DPTP_DTW	Detroit metro airport dewpoint
MIX_HT	Mixing height
MNRH_DTW	Detroit metro airport min relative humidity
MNTP_DTW	Detroit metro airport temperature
MXRH_DTW	Detroit metro airport max relative humidity
PRCP_DTW	Detroit metro airport precipitation
PRES_DTW	Detroit metro airport pressure
RDIR_DTW	Detroit metro airport resultant wind direction
RWND_DTW	Detroit metro airport resultant wind speed
SLVP_DTW	Detroit metro airport sea level pressure

Supplement 9. Performance indicators for MI and OLE estimates for carbonyls.

Bold values show highest performing model in group. Abbreviations: lag0=current day observation; lag1=current and previous day observations; lead1=current and next day observations; LL1=current, previous and next day observations; SD=standard deviation; d_2=Willmot's index of agreement; R^2=coefficient of determination; MAE=mean absolute error.

Performance indicators		Multiple imputation				Optimal estimation			
		lag0(SD)	lag1(SD)	lead1(SD)	LL1(SD)	lag0	lag1	lead1	LL1
Acetaldehyde									
Random	d_2	**0.95 (0.01)**	0.95 (0.01)	0.95 (0.01)	0.95 (0.00)	0.86	**0.89**	0.74	0.88
	R^2	**0.83 (0.02)**	0.80 (0.02)	0.83 (0.02)	0.83 (0.01)	0.69	**0.72**	0.51	0.70
	MAE	**0.29 (0.03)**	0.30 (0.03)	0.30 (0.02)	0.30 (0.01)	0.30	**0.26**	0.46	0.28
Block 5	d_2	**0.95 (0.01)**	0.95 (0.01)	0.95 (0.01)	0.94 (0.00)	0.79	0.81	0.71	**0.86**
	R^2	**0.84 (0.03)**	0.83 (0.02)	0.84 (0.03)	0.82 (0.01)	0.73	0.73	0.69	**0.79**
	MAE	**0.30 (0.03)**	0.31 (0.01)	0.30 (0.04)	0.31 (0.01)	0.43	0.42	0.57	**0.32**
Row-wise	d_2	0.58 (0.05)	**0.67 (0.04)**	0.51 (0.05)	0.63 (0.06)	**0.67**	0.63	0.47	0.46
	R^2	0.11 (0.05)	**0.20 (0.06)**	0.04 (0.02)	0.14 (0.08)	**0.32**	0.26	0.09	0.11
	MAE	0.87 (0.08)	**0.85 (0.12)**	0.91 (0.04)	0.87 (0.06)	**0.62**	0.66	0.83	0.79
Benzaldehyde									
Random	d_2	0.80 (0.03)	**0.83 (0.02)**	0.76 (0.05)	0.76 (0.01)	**0.88**	0.82	0.77	0.83
	R^2	0.46 (0.07)	**0.55 (0.03)**	0.38 (0.10)	0.38 (0.03)	**0.62**	0.48	0.44	0.51
	MAE	0.02 (0.00)	**0.02 (0.00)**	0.03 (0.00)	0.03 (0.00)	**0.00**	0.00	0.00	0.00
Block 5	d_2	**0.77 (0.03)**	0.72 (0.01)	0.63 (0.07)	0.73 (0.03)	**0.55**	0.50	0.36	0.51
	R^2	**0.49 (0.06)**	0.43 (0.06)	0.29 (0.11)	0.46 (0.07)	**0.41**	0.30	0.09	0.32
	MAE	**0.02 (0.00)**	0.03 (0.00)	0.03 (0.00)	0.03 (0.00)	**0.00**	0.00	0.00	0.00
Row-wise	d_2	0.48 (0.06)	**0.54 (0.03)**	0.35 (0.05)	0.38 (0.05)	0.50	**0.57**	0.25	0.31
	R^2	0.05 (0.05)	**0.09 (0.02)**	0.01 (0.01)	0.00 (0.01)	0.07	**0.13**	0.02	0.00
	MAE	0.04 (0.00)	**0.04 (0.00)**	0.05 (0.00)	0.05 (0.00)	0.00	**0.00**	0.00	0.00
Formaldehyde									
Random	d_2	0.84 (0.02)	0.80 (0.04)	**0.85 (0.01)**	0.81 (0.04)	**0.86**	0.82	0.84	0.83
	R^2	0.53 (0.05)	0.44 (0.07)	**0.54 (0.03)**	0.45 (0.09)	**0.63**	0.62	0.69	0.63
	MAE	0.80 (0.03)	0.90 (0.10)	**0.81 (0.03)**	0.86 (0.05)	**0.72**	0.78	0.69	0.77
Block 5	d_2	**0.88 (0.03)**	0.85 (0.03)	0.86 (0.01)	0.87 (0.04)	0.78	0.79	0.79	**0.80**
	R^2	**0.63 (0.09)**	0.56 (0.08)	0.58 (0.04)	0.60 (0.10)	0.55	0.65	0.66	**0.66**
	MAE	**0.84 (0.11)**	0.84 (0.11)	0.87 (0.04)	0.83 (0.12)	1.12	0.99	1.00	**0.97**
Row-wise	d_2	0.51 (0.06)	**0.53 (0.03)**	0.40 (0.06)	0.40 (0.06)	0.52	**0.54**	0.33	0.33
	R^2	0.05 (0.04)	**0.06 (0.03)**	0.01 (0.01)	0.01 (0.01)	0.09	**0.11**	0.00	0.00
	MAE	1.49 (0.14)	**1.58 (0.12)**	1.79 (0.14)	1.79 (0.14)	2.37	**2.31**	2.65	2.65

Supplement 9. (Cont.)

Performance indicators		Multiple imputation lag0(SD)	Multiple imputation lag1(SD)	Multiple imputation lead1(SD)	Multiple imputation LL1(SD)	Optimal estimation lag0	Optimal estimation lag1	Optimal estimation lead1	Optimal estimation LL1
Hexaldehyde									
Random	d_2	0.70 (0.04)	0.82 (0.03)	0.83 (0.02)	**0.85 (0.04)**	0.69	0.69	0.52	**0.81**
	R^2	0.26 (0.05)	0.46 (0.07)	0.50 (0.04)	**0.55 (0.09)**	0.29	0.41	0.13	**0.54**
	MAE	0.12 (0.01)	0.09 (0.00)	0.10 (0.01)	**0.07 (0.00)**	0.02	0.01	0.02	**0.01**
Block 5	d_2	0.71 (0.04)	0.68 (0.03)	0.70 (0.03)	**0.76 (0.03)**	0.62	0.54	0.56	**0.66**
	R^2	0.32 (0.07)	0.23 (0.07)	0.29 (0.05)	**0.37 (0.05)**	0.39	0.22	0.24	**0.44**
	MAE	0.12 (0.01)	0.13 (0.01)	0.12 (0.01)	**0.12 (0.01)**	0.02	0.03	0.03	**0.02**
Row-wise	d_2	0.64 (0.03)	**0.76 (0.05)**	0.64 (0.04)	0.75 (0.03)	0.71	0.74	0.73	**0.73**
	R^2	0.18 (0.04)	**0.34 (0.09)**	0.17 (0.05)	0.33 (0.06)	0.39	0.45	0.43	**0.42**
	MAE	0.14 (0.01)	**0.12 (0.01)**	0.14 (0.00)	0.12 (0.01)	0.02	0.02	0.02	**0.02**
iso-Butyraldehyde									
Random	d_2	**0.90 (0.01)**	0.90 (0.01)	0.90 (0.01)	0.89 (0.03)	**0.79**	0.79	0.79	0.79
	R^2	**0.68 (0.03)**	0.68 (0.03)	0.68 (0.03)	0.65 (0.09)	**0.74**	0.74	0.74	0.67
	MAE	**0.08 (0.00)**	0.08 (0.00)	0.08 (0.00)	0.09 (0.01)	**0.02**	0.02	0.02	0.02
Block 5	d_2	0.83 (0.02)	0.83 (0.02)	0.83 (0.02)	**0.85 (0.02)**	0.74	0.74	0.74	**0.81**
	R^2	0.52 (0.03)	0.52 (0.03)	0.52 (0.03)	**0.58 (0.05)**	0.47	0.47	0.47	**0.53**
	MAE	0.10 (0.01)	0.10 (0.01)	0.10 (0.01)	**0.09 (0.01)**	0.02	0.02	0.02	**0.01**
Row-wise	d_2	0.56 (0.10)	0.56 (0.03)	0.37 (0.05)	**0.58 (0.08)**	**0.64**	0.44	0.27	0.40
	R^2	0.12 (0.08)	0.09 (0.04)	0.01 (0.01)	**0.11 (0.05)**	**0.24**	0.06	0.01	0.05
	MAE	0.15 (0.02)	0.17 (0.01)	0.18 (0.00)	**0.15 (0.01)**	**0.02**	0.02	0.02	0.02
Propionaldehyde									
Random	d_2	**0.93 (0.01)**	0.93 (0.01)	0.93 (0.00)	0.93 (0.01)	0.84	0.86	0.86	**0.87**
	R^2	**0.77 (0.04)**	0.78 (0.02)	0.75 (0.02)	0.77 (0.04)	0.72	0.75	0.75	**0.76**
	MAE	**0.05 (0.00)**	0.05 (0.00)	0.05 (0.00)	0.05 (0.01)	0.01	0.01	0.01	**0.01**
Block 5	d_2	**0.93 (0.01)**	0.93 (0.01)	0.92 (0.01)	0.93 (0.01)	0.75	0.79	0.77	**0.83**
	R^2	**0.78 (0.03)**	0.76 (0.02)	0.74 (0.04)	0.76 (0.02)	0.65	0.71	0.67	**0.76**
	MAE	**0.05 (0.00)**	0.05 (0.00)	0.05 (0.00)	0.05 (0.00)	0.01	0.01	0.01	**0.01**
Row-wise	d_2	- -	0.62 (0.04)	0.56 (0.16)	**0.68 (0.02)**	**0.59**	0.41	0.27	0.32
	R^2	- -	0.16 (0.06)	0.13 (0.14)	**0.22 (0.04)**	**0.22**	0.06	0.00	0.01
	MAE	- -	0.11 (0.01)	0.05 (0.01)	**0.11 (0.01)**	**0.01**	0.02	0.02	0.02
Tolualdehyde									
Random	d_2	**0.72 (0.04)**	0.60 (0.07)	0.54 (0.09)	0.54 (0.09)	**0.58**	0.54	0.36	0.36
	R^2	**0.30 (0.07)**	0.15 (0.08)	0.10 (0.05)	0.10 (0.05)	**0.25**	0.23	0.05	0.05
	MAE	**0.03 (0.00)**	0.03 (0.00)	0.03 (0.00)	0.03 (0.00)	**0.00**	0.00	0.00	0.00
Block 5	d_2	**0.66 (0.05)**	0.59 (0.06)	0.50 (0.03)	0.50 (0.03)	**0.55**	0.50	0.39	0.39
	R^2	**0.22 (0.06)**	0.13 (0.06)	0.06 (0.03)	0.06 (0.03)	**0.20**	0.15	0.05	0.05
	MAE	**0.03 (0.00)**	0.03 (0.00)	0.03 (0.00)	0.03 (0.00)	**0.00**	0.00	0.00	0.00
Row-wise	d_2	**0.56 (0.08)**	0.51 (0.11)	0.46 (0.13)	0.53 (0.09)	**0.64**	0.52	0.45	0.52
	R^2	**0.10 (0.07)**	0.06 (0.05)	0.05 (0.09)	0.08 (0.07)	**0.26**	0.12	0.07	0.12
	MAE	**0.04 (0.00)**	0.04 (0.00)	0.04 (0.01)	0.03 (0.00)	**0.00**	0.00	0.00	0.00

Supplement 10. Performance indicators for MI and OLE estimates for VOCs. Otherwise as Supplement 9.

Performance indicators		Multiple imputation								Optimal estimation			
		lag0(SD)		lag1(SD)		lead1(SD)		LL1(SD)		lag0	lag1	lead1	LL1
Acetylene													
Random	d_2	**0.84**	**(0.04)**	0.72	(0.02)	0.76	(0.04)	0.66	(0.03)	**0.73**	0.65	0.59	0.46
	R^2	**0.52**	**(0.08)**	0.30	(0.04)	0.37	(0.08)	0.19	(0.04)	**0.57**	0.44	0.39	0.23
	MAE	**0.51**	**(0.05)**	0.66	(0.04)	0.60	(0.06)	0.71	(0.02)	**0.46**	0.55	0.60	0.68
Block 5	d_2	**0.86**	**(0.02)**	0.76	(0.03)	0.81	(0.04)	0.70	(0.03)	**0.69**	0.60	0.58	0.52
	R^2	**0.57**	**(0.05)**	0.37	(0.04)	0.44	(0.08)	0.28	(0.04)	**0.46**	0.36	0.35	0.21
	MAE	**0.46**	**(0.02)**	0.57	(0.03)	0.59	(0.02)	0.62	(0.03)	**0.47**	0.55	0.56	0.66
Row-wise	d_2	**0.65**	**(0.06)**	0.65	(0.03)	0.63	(0.07)	0.62	(0.05)	0.45	0.38	**0.46**	0.37
	R^2	**0.19**	**(0.08)**	0.18	(0.04)	0.16	(0.08)	0.15	(0.05)	0.09	0.06	**0.11**	0.04
	MAE	**0.63**	**(0.05)**	0.67	(0.06)	0.69	(0.06)	0.72	(0.05)	0.60	0.61	**0.58**	0.63
Benzene													
Random	d_2	**0.87**	**(0.03)**	0.84	(0.01)	0.87	(0.02)	0.84	(0.02)	**0.89**	0.85	0.84	0.79
	R^2	**0.61**	**(0.08)**	0.52	(0.03)	0.59	(0.06)	0.52	(0.05)	**0.71**	0.63	0.63	0.52
	MAE	**0.17**	**(0.02)**	0.18	(0.01)	0.17	(0.01)	0.18	(0.01)	**0.03**	0.04	0.04	0.04
Block 5	d_2	0.85	(0.02)	**0.85**	**(0.04)**	0.84	(0.04)	0.83	(0.02)	**0.88**	0.85	0.84	0.88
	R^2	0.55	(0.05)	**0.56**	**(0.09)**	0.54	(0.10)	0.49	(0.03)	**0.68**	0.62	0.60	0.65
	MAE	0.19	(0.02)	**0.19**	**(0.02)**	0.19	(0.02)	0.20	(0.02)	**0.03**	0.04	0.04	0.04
Row-wise	d_2	**0.64**	**(0.04)**	0.63	(0.03)	0.58	(0.06)	0.57	(0.06)	0.63	**0.65**	0.64	0.53
	R^2	**0.20**	**(0.05)**	0.18	(0.03)	0.13	(0.05)	0.12	(0.05)	0.22	**0.25**	0.24	0.17
	MAE	**0.26**	**(0.02)**	0.28	(0.02)	0.28	(0.03)	0.27	(0.01)	0.07	**0.07**	0.07	0.08
1,3-Butadiene													
Random	d_2	**0.89**	**(0.02)**	0.89	(0.01)	0.87	(0.01)	0.87	(0.02)	**0.78**	0.74	0.62	0.63
	R^2	**0.65**	**(0.06)**	0.65	(0.03)	0.58	(0.03)	0.58	(0.04)	**0.68**	0.67	0.52	0.52
	MAE	**0.03**	**(0.00)**	0.03	(0.00)	0.03	(0.00)	0.03	(0.00)	**0.00**	0.00	0.00	0.00
Block 5	d_2	0.88	(0.02)	0.86	(0.03)	0.88	(0.02)	**0.88**	**(0.01)**	0.76	0.75	0.77	**0.78**
	R^2	0.61	(0.06)	0.56	(0.08)	0.59	(0.05)	**0.61**	**(0.04)**	0.50	0.49	0.53	**0.56**
	MAE	0.03	(0.00)	0.03	(0.00)	0.03	(0.00)	**0.03**	**(0.00)**	0.00	0.00	0.00	**0.00**
Row-wise	d_2	**0.58**	**(0.04)**	0.50	(0.03)	0.52	(0.08)	0.46	(0.05)	**0.49**	0.43	0.41	0.30
	R^2	**0.09**	**(0.03)**	0.05	(0.03)	0.07	(0.05)	0.03	(0.03)	**0.13**	0.08	0.07	0.03
	MAE	**0.04**	**(0.00)**	0.04	(0.00)	0.05	(0.00)	0.04	(0.00)	**0.00**	0.00	0.00	0.00
Dichlorodifluoromethane													
Random	d_2	0.62	(0.06)	0.58	(0.07)	0.63	(0.05)	**0.64**	**(0.04)**	**0.52**	0.33	0.41	**0.52**
	R^2	0.15	(0.06)	0.12	(0.07)	0.17	(0.04)	**0.18**	**(0.06)**	**0.12**	0.04	0.12	**0.25**
	MAE	0.06	(0.01)	0.06	(0.01)	0.06	(0.00)	**0.06**	**(0.01)**	**0.01**	0.01	0.00	**0.00**
Block 5	d_2	0.59	(0.03)	0.57	(0.06)	**0.59**	**(0.02)**	0.58	(0.07)	0.35	0.34	0.37	**0.44**
	R^2	0.16	(0.02)	0.14	(0.07)	**0.17**	**(0.03)**	0.15	(0.07)	0.09	0.03	0.11	**0.18**
	MAE	0.06	(0.00)	0.07	(0.00)	**0.07**	**(0.01)**	0.07	(0.01)	0.01	0.01	0.01	**0.01**
Row-wise	d_2	0.44	(0.12)	0.44	(0.07)	**0.45**	**(0.05)**	0.38	(0.09)	0.29	**0.46**	0.22	0.29
	R^2	0.04	(0.05)	0.03	(0.04)	**0.03**	**(0.03)**	0.02	(0.02)	0.03	**0.16**	0.00	0.03
	MAE	0.08	(0.01)	0.08	(0.00)	**0.09**	**(0.01)**	0.09	(0.01)	0.01	**0.01**	0.01	0.01

Supplement 10. (Cont.)

Performance indicators		Multiple imputation lag0(SD)	Multiple imputation lag1(SD)	Multiple imputation lead1(SD)	Multiple imputation LL1(SD)	Optimal estimation lag0	Optimal estimation lag1	Optimal estimation lead1	Optimal estimation LL1
Ethylbenzene									
Random	d_2	0.99 (0.00)	**0.99 (0.00)**	0.99 (0.00)	0.99 (0.00)	0.88	**0.89**	0.88	0.87
	R^2	0.96 (0.01)	**0.96 (0.00)**	0.95 (0.01)	0.96 (0.01)	0.76	**0.76**	0.75	0.74
	MAE	0.02 (0.00)	**0.01 (0.00)**	0.02 (0.00)	0.02 (0.00)	0.00	**0.00**	0.00	0.00
Block 5	d_2	0.99 (0.00)	0.99 (0.00)	**0.99 (0.00)**	0.99 (0.00)	**0.90**	0.89	0.85	0.79
	R^2	0.97 (0.00)	0.97 (0.00)	**0.97 (0.00)**	0.97 (0.00)	**0.90**	0.87	0.86	0.71
	MAE	0.02 (0.00)	0.02 (0.00)	**0.01 (0.00)**	0.02 (0.00)	**0.00**	0.00	0.00	0.01
Row-wise	d_2	0.58 (0.09)	0.58 (0.05)	0.54 (0.10)	**0.60 (0.08)**	0.51	**0.62**	0.51	0.61
	R^2	0.12 (0.07)	0.10 (0.05)	0.08 (0.07)	**0.13 (0.08)**	0.06	**0.18**	0.07	0.15
	MAE	0.10 (0.01)	0.10 (0.01)	0.10 (0.01)	**0.10 (0.01)**	0.01	**0.01**	0.01	0.01
Methyl ethyl ketone									
Random	d_2	0.74 (0.04)	0.75 (0.05)	0.71 (0.02)	0.75 (0.05)	0.70	0.70	0.57	**0.70**
	R^2	0.32 (0.06)	0.34 (0.08)	0.25 (0.04)	0.33 (0.08)	0.36	0.38	0.18	**0.40**
	MAE	0.38 (0.04)	0.38 (0.02)	0.40 (0.02)	0.39 (0.02)	0.18	0.18	0.23	**0.17**
Block 5	d_2	**0.65 (0.05)**	0.64 (0.06)	0.63 (0.05)	0.62 (0.07)	0.74	**0.75**	0.73	0.73
	R^2	**0.20 (0.06)**	0.18 (0.07)	0.19 (0.06)	0.16 (0.07)	0.36	**0.38**	0.34	0.35
	MAE	**0.40 (0.03)**	0.40 (0.03)	0.45 (0.05)	0.41 (0.03)	0.12	**0.12**	0.14	0.12
Row-wise	d_2	**0.71 (0.02)**	0.69 (0.06)	0.65 (0.03)	0.68 (0.07)	**0.82**	0.80	0.81	0.80
	R^2	**0.28 (0.03)**	0.25 (0.10)	0.18 (0.05)	0.25 (0.10)	**0.49**	0.46	0.48	0.45
	MAE	**0.37 (0.02)**	0.38 (0.03)	0.38 (0.04)	0.39 (0.03)	**0.10**	0.10	0.10	0.11
m,p-Xylene									
Random	d_2	0.99 (0.00)	0.99 (0.00)	**0.99 (0.00)**	0.99 (0.00)	0.88	**0.88**	0.88	0.88
	R^2	0.97 (0.01)	0.97 (0.00)	**0.97 (0.00)**	0.97 (0.00)	0.77	**0.78**	0.78	0.78
	MAE	0.04 (0.01)	0.04 (0.01)	**0.04 (0.00)**	0.04 (0.01)	0.03	**0.03**	0.03	0.03
Block 5	d_2	0.99 (0.00)	**0.99 (0.00)**	0.99 (0.00)	0.99 (0.00)	0.87	0.87	0.86	**0.87**
	R^2	0.97 (0.01)	**0.97 (0.00)**	0.97 (0.00)	0.97 (0.01)	0.74	0.74	0.74	**0.75**
	MAE	0.04 (0.01)	**0.04 (0.00)**	0.04 (0.00)	0.04 (0.00)	0.03	0.03	0.03	**0.03**
Row-wise	d_2	0.50 (0.05)	0.56 (0.05)	0.52 (0.05)	**0.60 (0.04)**	0.50	**0.55**	0.52	0.45
	R^2	0.05 (0.03)	0.08 (0.03)	0.06 (0.03)	**0.13 (0.04)**	0.06	**0.12**	0.08	0.06
	MAE	0.31 (0.02)	0.32 (0.03)	0.31 (0.02)	**0.28 (0.02)**	0.11	**0.10**	0.10	0.10
n-Octane									
Random	d_2	**0.52 (0.04)**	0.52 (0.04)	0.53 (0.09)	0.47 (0.06)	0.32	0.32	0.42	**0.48**
	R^2	**0.06 (0.03)**	0.06 (0.03)	0.07 (0.07)	0.04 (0.05)	0.01	0.01	0.01	**0.04**
	MAE	**0.04 (0.00)**	0.04 (0.00)	0.04 (0.01)	0.04 (0.00)	0.00	0.00	0.00	**0.00**
Block 5	d_2	0.53 (0.05)	0.53 (0.05)	**0.57 (0.05)**	0.44 (0.06)	0.34	0.34	0.38	**0.39**
	R^2	0.06 (0.05)	0.06 (0.05)	**0.10 (0.05)**	0.02 (0.01)	0.01	0.01	0.02	**0.01**
	MAE	0.04 (0.00)	0.04 (0.00)	**0.04 (0.00)**	0.05 (0.00)	0.00	0.00	0.00	**0.00**
Row-wise	d_2	0.40 (0.06)	**0.38 (0.08)**	0.35 (0.10)	0.37 (0.12)	0.26	**0.31**	0.26	0.26
	R^2	0.01 (0.01)	**0.01 (0.02)**	0.01 (0.01)	0.03 (0.03)	0.01	**0.00**	0.01	0.01
	MAE	0.05 (0.00)	**0.05 (0.00)**	0.02 (0.00)	0.04 (0.00)	0.00	**0.00**	0.00	0.00

Supplement 10. (Cont.)

Performance indicators		Multiple imputation lag0(SD)	Multiple imputation lag1(SD)	Multiple imputation lead1(SD)	Multiple imputation LL1(SD)	Optimal estimation lag0	Optimal estimation lag1	Optimal estimation lead1	Optimal estimation LL1
o-Xylene									
Random	d_2	**0.98 (0.00)**	0.98 (0.00)	0.98 (0.00)	0.98 (0.00)	0.86	0.86	0.83	**0.94**
	R^2	**0.94 (0.01)**	0.94 (0.01)	0.92 (0.01)	0.93 (0.01)	0.89	0.89	0.85	**0.92**
	MAE	**0.03 (0.00)**	0.03 (0.00)	0.03 (0.00)	0.03 (0.00)	0.01	0.01	0.01	**0.00**
Block 5	d_2	**0.98 (0.00)**	0.98 (0.00)	0.98 (0.00)	0.98 (0.00)	0.87	0.88	0.84	**0.93**
	R^2	**0.94 (0.02)**	0.93 (0.01)	0.93 (0.01)	0.92 (0.01)	0.90	0.90	0.87	**0.89**
	MAE	**0.03 (0.00)**	0.03 (0.00)	0.03 (0.00)	0.03 (0.00)	0.01	0.01	0.01	**0.00**
Row-wise	d_2	0.60 (0.08)	**0.63 (0.05)**	0.59 (0.06)	0.63 (0.08)	0.60	0.63	0.55	**0.64**
	R^2	0.15 (0.08)	**0.17 (0.06)**	0.12 (0.06)	0.17 (0.09)	0.22	0.21	0.13	**0.24**
	MAE	0.13 (0.01)	**0.12 (0.01)**	0.12 (0.01)	0.12 (0.01)	0.02	0.02	0.02	**0.02**
Propylene									
Random	d_2	0.45 (0.04)	0.41 (0.11)	0.42 (0.06)	**0.45 (0.06)**	**0.66**	0.56	0.61	0.65
	R^2	0.07 (0.03)	0.06 (0.08)	0.04 (0.04)	**0.07 (0.05)**	**0.23**	0.10	0.15	0.19
	MAE	1.28 (0.15)	1.30 (0.10)	1.30 (0.15)	**1.24 (0.16)**	**0.76**	0.86	0.65	0.59
Block 5	d_2	**0.47 (0.11)**	0.44 (0.11)	0.29 (0.05)	0.32 (0.04)	**0.49**	0.36	0.28	0.27
	R^2	**0.09 (0.06)**	0.07 (0.05)	0.01 (0.01)	0.01 (0.01)	**0.24**	0.12	0.05	0.04
	MAE	**1.14 (0.07)**	1.21 (0.05)	1.33 (0.10)	1.27 (0.11)	**2.48**	2.79	3.04	3.09
Row-wise	d_2	**0.58 (0.05)**	0.51 (0.02)	0.54 (0.05)	0.44 (0.06)	0.65	0.53	**0.66**	0.57
	R^2	**0.14 (0.05)**	0.07 (0.02)	0.10 (0.04)	0.02 (0.02)	0.25	0.14	**0.27**	0.19
	MAE	**1.26 (0.15)**	1.30 (0.11)	1.23 (0.13)	1.30 (0.05)	1.08	1.25	**1.04**	1.15
Tetrachloroethylene									
Random	d_2	0.30 (0.07)	0.27 (0.03)	0.31 (0.06)	**0.33 (0.06)**	0.22	**0.27**	0.26	0.23
	R^2	0.02 (0.02)	0.01 (0.01)	0.01 (0.01)	**0.01 (0.02)**	0.01	**0.03**	0.03	0.00
	MAE	0.08 (0.01)	0.08 (0.00)	0.08 (0.00)	**0.07 (0.00)**	0.01	**0.01**	0.01	0.01
Block 5	d_2	0.39 (0.04)	**0.41 (0.12)**	0.34 (0.04)	0.32 (0.09)	0.27	0.33	**0.39**	0.26
	R^2	0.01 (0.02)	**0.04 (0.06)**	0.01 (0.00)	0.02 (0.02)	0.02	0.05	**0.11**	0.05
	MAE	0.07 (0.01)	**0.08 (0.01)**	0.07 (0.01)	0.08 (0.00)	0.01	0.01	**0.01**	0.01
Row-wise	d_2	**0.41 (0.11)**	0.38 (0.10)	- -	0.32 (0.06)	**0.37**	0.30	-	0.27
	R^2	**0.03 (0.02)**	0.02 (0.01)	- -	0.01 (0.00)	**0.15**	0.09	-	0.08
	MAE	**0.07 (0.01)**	0.08 (0.01)	- -	0.07 (0.01)	**0.01**	0.01	-	0.01
Trichlorofluoromethane									
Random	d_2	0.61 (0.08)	**0.62 (0.08)**	0.61 (0.08)	0.57 (0.05)	0.23	0.31	0.23	**0.51**
	R^2	0.17 (0.10)	**0.17 (0.09)**	0.17 (0.10)	0.12 (0.05)	0.02	0.01	0.02	**0.17**
	MAE	0.10 (0.01)	**0.10 (0.01)**	0.10 (0.01)	0.11 (0.01)	0.01	0.01	0.01	**0.01**
Block 5	d_2	0.47 (0.11)	**0.51 (0.05)**	0.47 (0.11)	0.29 (0.09)	0.39	**0.47**	0.39	0.43
	R^2	0.10 (0.07)	**0.10 (0.04)**	0.10 (0.07)	0.03 (0.04)	0.04	**0.10**	0.04	0.08
	MAE	0.10 (0.02)	**0.09 (0.01)**	0.10 (0.02)	0.12 (0.02)	0.00	**0.00**	0.00	0.00
Row-wise	d_2	- -	0.30 (0.08)	- -	**0.34 (0.10)**	-	0.34	-	**0.38**
	R^2	- -	0.01 (0.01)	- -	**0.03 (0.04)**	-	0.00	-	**0.01**
	MAE	- -	0.12 (0.02)	- -	**0.12 (0.01)**	-	0.01	-	**0.01**

Supplement 10. (Cont.)

Performance indicators		Multiple imputation								Optimal estimation			
		lag0(SD)		lag1(SD)		lead1(SD)		LL1(SD)		lag0	lag1	lead1	LL1
Trichlorotrifluoromethane													
Random	d_2	0.42	(0.09)	0.58	(0.02)	0.49	(0.06)	**0.67**	**(0.04)**	0.19	**0.20**	0.18	0.18
	R^2	0.02	(0.04)	0.09	(0.02)	0.03	(0.04)	**0.19**	**(0.07)**	0.01	**0.01**	0.02	0.01
	MAE	0.03	(0.00)	0.02	(0.00)	0.02	(0.00)	**0.02**	**(0.00)**	0.00	**0.00**	0.00	0.00
Block 5	d_2	0.44	(0.05)	0.39	(0.04)	0.39	(0.06)	**0.45**	**(0.04)**	0.21	0.18	0.20	**0.20**
	R^2	0.01	(0.02)	0.00	(0.01)	0.01	(0.01)	**0.01**	**(0.01)**	0.01	0.03	0.01	**0.01**
	MAE	0.03	(0.00)	0.03	(0.00)	0.03	(0.00)	**0.03**	**(0.00)**	0.00	0.00	0.00	**0.00**
Row-wise	d_2	0.42	(0.07)	0.56	(0.03)	0.49	(0.03)	**0.59**	**(0.03)**	0.18	0.18	**0.20**	0.19
	R^2	0.01	(0.01)	0.07	(0.02)	0.02	(0.01)	**0.10**	**(0.03)**	0.07	0.06	**0.03**	0.04
	MAE	0.03	(0.00)	0.02	(0.00)	0.03	(0.00)	**0.02**	**(0.00)**	0.00	0.00	**0.00**	0.00
1,2,4-Trimethylbenzene													
Random	d_2	**0.98**	**(0.00)**	0.98	(0.00)	0.98	(0.00)	0.98	(0.00)	0.65	**0.86**	0.60	0.63
	R^2	**0.92**	**(0.01)**	0.92	(0.02)	0.91	(0.02)	0.91	(0.02)	0.52	**0.69**	0.44	0.47
	MAE	**0.04**	**(0.00)**	0.04	(0.00)	0.04	(0.00)	0.04	(0.00)	0.02	**0.01**	0.02	0.02
Block 5	d_2	0.98	(0.00)	**0.98**	**(0.00)**	0.98	(0.00)	0.98	(0.00)	0.63	**0.88**	0.72	0.62
	R^2	0.92	(0.01)	**0.93**	**(0.01)**	0.93	(0.01)	0.92	(0.01)	0.42	**0.79**	0.54	0.41
	MAE	0.04	(0.00)	**0.04**	**(0.00)**	0.04	(0.00)	0.04	(0.00)	0.02	**0.01**	0.02	0.02
Row-wise	d_2	0.66	(0.07)	0.66	(0.03)	0.54	(0.04)	**0.69**	**(0.04)**	0.63	**0.70**	0.58	0.67
	R^2	0.21	(0.07)	0.20	(0.03)	0.07	(0.03)	**0.25**	**(0.06)**	0.24	**0.33**	0.17	0.26
	MAE	0.12	(0.01)	0.12	(0.01)	0.14	(0.01)	**0.12**	**(0.01)**	0.02	**0.02**	0.02	0.02
1,3,5-Trimethylbenzene													
Random	d_2	0.90	(0.01)	**0.91**	**(0.01)**	0.90	(0.02)	0.90	(0.01)	0.81	0.81	0.80	**0.85**
	R^2	0.66	(0.03)	**0.68**	**(0.03)**	0.68	(0.06)	0.65	(0.03)	0.51	0.51	0.48	**0.55**
	MAE	0.02	(0.00)	**0.02**	**(0.00)**	0.02	(0.00)	0.02	(0.00)	0.00	0.00	0.00	**0.00**
Block 5	d_2	0.90	(0.01)	**0.92**	**(0.01)**	0.91	(0.01)	0.92	(0.01)	0.85	0.84	0.84	**0.88**
	R^2	0.67	(0.02)	**0.73**	**(0.03)**	0.70	(0.04)	0.72	(0.02)	0.65	0.63	0.63	**0.61**
	MAE	0.02	(0.00)	**0.02**	**(0.00)**	0.02	(0.00)	0.02	(0.00)	0.00	0.00	0.00	**0.00**
Row-wise	d_2	0.58	(0.08)	0.57	(0.07)	**0.59**	**(0.12)**	0.56	(0.03)	0.46	0.48	**0.65**	0.58
	R^2	0.10	(0.06)	0.10	(0.07)	**0.14**	**(0.12)**	0.09	(0.03)	0.07	0.09	**0.24**	0.17
	MAE	0.04	(0.00)	0.04	(0.00)	**0.04**	**(0.00)**	0.04	(0.00)	0.00	0.00	**0.00**	0.00
Toluene													
Random	d_2	0.90	(0.02)	0.88	(0.02)	0.89	(0.02)	**0.91**	**(0.01)**	0.84	0.75	0.90	**0.95**
	R^2	0.68	(0.06)	0.64	(0.05)	0.67	(0.05)	**0.72**	**(0.04)**	0.61	0.44	0.74	**0.83**
	MAE	0.35	(0.04)	0.38	(0.04)	0.38	(0.04)	**0.36**	**(0.03)**	0.19	0.26	0.13	**0.08**
Block 5	d_2	**0.91**	**(0.01)**	0.87	(0.01)	0.90	(0.02)	0.89	(0.03)	0.60	0.51	**0.81**	0.81
	R^2	**0.70**	**(0.03)**	0.60	(0.04)	0.67	(0.05)	0.66	(0.07)	0.38	0.19	**0.63**	0.59
	MAE	**0.38**	**(0.02)**	0.40	(0.03)	0.36	(0.01)	0.36	(0.05)	0.56	0.69	**0.35**	0.36
Row-wise	d_2	**0.56**	**(0.05)**	0.52	(0.11)	0.55	(0.10)	0.51	(0.06)	0.50	0.46	0.50	**0.50**
	R^2	**0.11**	**(0.04)**	0.08	(0.09)	0.10	(0.09)	0.08	(0.04)	0.09	0.07	0.12	**0.12**
	MAE	**0.61**	**(0.04)**	0.69	(0.09)	0.68	(0.07)	0.67	(0.04)	0.68	0.69	0.64	**0.64**

Supplement 11. Performance indicators for OLE using both un-transformed and log-transformed data. Otherwise as Supplement 9.

Performance indicators		Untransformed				Log-transformed			
		lag0	**lag1**	**lead1**	**LL1**	**lag0**	**lag1**	**lead1**	**LL1**
Acetaldehyde									
Random	d2	0.86	**0.89**	0.74	0.88	0.78	0.80	0.78	**0.83**
	R2	0.69	**0.72**	0.51	0.70	0.62	0.66	0.62	**0.69**
	MAE	0.30	**0.26**	0.46	0.28	0.01	0.00	0.00	**0.00**
Row-wise	d2	**0.67**	0.63	0.47	0.46	**0.42**	0.35	0.35	0.36
	R2	**0.32**	0.26	0.09	0.11	**0.06**	0.02	0.01	0.03
	MAE	**0.62**	0.66	0.83	0.79	**0.00**	0.00	0.00	0.00
Benzaldehyde									
Random	d2	**0.88**	0.82	0.77	0.83	**0.65**	0.55	0.76	0.59
	R2	**0.62**	0.48	0.44	0.51	**0.34**	0.19	0.42	0.35
	MAE	**0.00**	0.00	0.00	0.00	**0.00**	0.00	0.00	0.00
Row-wise	d2	0.50	**0.57**	0.25	0.31	**0.55**	0.53	0.29	0.32
	R2	0.07	**0.13**	0.02	0.00	**0.14**	0.12	0.00	0.00
	MAE	0.00	**0.00**	0.00	0.00	**0.00**	0.00	0.00	0.00
Formaldehyde									
Random	d2	**0.86**	0.82	0.84	0.83	0.69	0.57	0.65	**0.70**
	R2	**0.63**	0.62	0.69	0.63	0.48	0.30	0.45	**0.37**
	MAE	**0.72**	0.78	0.69	0.77	0.00	0.00	0.00	**0.00**
Row-wise	d2	0.52	**0.54**	0.33	0.33	**0.41**	0.36	0.19	0.19
	R2	0.09	**0.11**	0.00	0.00	**0.09**	0.02	0.02	0.02
	MAE	2.37	**2.31**	2.65	2.65	**0.58**	0.00	0.00	0.00
Benzene									
Random	d2	**0.89**	0.85	0.84	0.79	**0.61**	0.43	0.45	0.41
	R2	**0.71**	0.63	0.63	0.52	**0.22**	0.08	0.10	0.07
	MAE	**0.03**	0.04	0.04	0.04	**0.00**	0.00	0.00	0.00
Row-wise	d2	0.63	**0.65**	0.64	0.53	0.70	**0.71**	0.70	0.69
	R2	0.22	**0.25**	0.24	0.17	0.30	**0.32**	0.30	0.29
	MAE	0.07	**0.07**	0.07	0.08	0.00	**0.00**	0.00	0.00
1,3-Butadiene									
Random	d2	**0.78**	0.74	0.62	0.63	**0.53**	0.30	0.29	0.29
	R2	**0.68**	0.67	0.52	0.52	**0.16**	0.03	0.02	0.02
	MAE	**0.00**	0.00	0.00	0.00	**0.00**	0.00	0.00	0.00
Row-wise	d2	**0.49**	0.43	0.41	0.30	**0.56**	0.49	0.48	0.45
	R2	**0.13**	0.08	0.07	0.03	**0.16**	0.13	0.09	0.06
	MAE	**0.00**	0.00	0.00	0.00	**0.00**	0.00	0.00	0.00
Tetrachloroethylene									
Random	d2	0.22	**0.27**	0.26	0.23	0.32	0.38	**0.55**	0.34
	R2	0.01	**0.03**	0.03	0.00	0.04	0.17	**0.30**	0.09
	MAE	0.01	**0.01**	0.01	0.01	0.00	0.00	**0.00**	0.00
Row-wise	d2	**0.37**	0.30	-	0.27	**0.48**	0.37	-	0.37
	R2	**0.15**	0.09	-	0.08	**0.17**	0.07	-	0.08
	MAE	**0.01**	0.01	-	0.01	**0.00**	0.00	-	0.00

Supplement 12. Performance indicators for MI using both untransformed and log-transformed data.

Otherwise as Supplement 9.

Performance indicators		Un-transformed								Log-transformed							
		lag0(SD)		lag1(SD)		lead1(SD)		LL1(SD)		lag0(SD)		lag1(SD)		lead1(SD)		LL1(SD)	
Acetaldehyde																	
Random	d_2	0.95	(0.01)	0.95	(0.01)	0.95	(0.01)	**0.95**	**(0.00)**	**0.93**	**(0.01)**	0.92	(0.02)	0.92	(0.03)	0.93	(0.01)
	R^2	0.83	(0.02)	0.80	(0.02)	0.83	(0.02)	**0.83**	**(0.01)**	**0.79**	**(0.04)**	0.75	(0.06)	0.76	(0.07)	0.77	(0.03)
	MAE	0.29	(0.03)	0.30	(0.03)	0.30	(0.02)	**0.30**	**(0.01)**	**0.31**	**(0.03)**	0.31	(0.04)	0.32	(0.05)	0.30	(0.02)
Row-wise	d_2	0.58	(0.05)	**0.67**	**(0.04)**	0.51	(0.05)	0.63	(0.06)	0.29	(0.19)	**0.31**	**(0.17)**	0.33	(0.13)	0.34	(0.09)
	R^2	0.11	(0.05)	**0.20**	**(0.06)**	0.04	(0.02)	0.14	(0.08)	0.04	(0.06)	**0.10**	**(0.08)**	0.02	(0.03)	0.04	(0.03)
	MAE	0.87	(0.08)	**0.85**	**(0.12)**	0.91	(0.04)	0.87	(0.06)	1.56	(0.48)	**1.53**	**(0.51)**	1.32	(0.25)	1.34	(0.15)
Benzaldehyde																	
Random	d_2	0.80	(0.03)	**0.83**	**(0.02)**	0.76	(0.05)	0.76	(0.01)	**0.85**	**(0.05)**	0.78	(0.04)	0.67	(0.08)	0.69	(0.12)
	R^2	0.46	(0.07)	**0.55**	**(0.03)**	0.38	(0.10)	0.38	(0.03)	**0.57**	**(0.10)**	0.41	(0.07)	0.27	(0.08)	0.28	(0.11)
	MAE	0.02	(0.00)	**0.02**	**(0.00)**	0.03	(0.00)	0.03	(0.00)	**0.02**	**(0.00)**	0.02	(0.00)	0.02	(0.00)	0.02	(0.00)
Row-wise	d_2	0.48	(0.06)	**0.54**	**(0.03)**	0.35	(0.05)	0.38	(0.05)	0.41	(0.09)	**0.43**	**(0.12)**	0.26	(0.06)	0.33	(0.06)
	R^2	0.05	(0.05)	**0.09**	**(0.02)**	0.01	(0.01)	0.00	(0.01)	0.04	(0.05)	**0.08**	**(0.04)**	0.01	(0.01)	0.00	(0.00)
	MAE	0.04	(0.00)	**0.04**	**(0.00)**	0.05	(0.00)	0.05	(0.00)	0.04	(0.00)	**0.04**	**(0.02)**	0.05	(0.00)	0.04	(0.01)
Formaldehyde																	
Random	d_2	0.84	(0.02)	0.80	(0.04)	**0.85**	**(0.01)**	0.81	(0.04)	0.74	(0.05)	0.66	(0.08)	**0.76**	**(0.03)**	0.75	(0.04)
	R^2	0.53	(0.05)	0.44	(0.07)	**0.54**	**(0.03)**	0.45	(0.09)	0.48	(0.05)	0.39	(0.08)	**0.52**	**(0.08)**	0.45	(0.09)
	MAE	0.80	(0.03)	0.90	(0.10)	**0.81**	**(0.03)**	0.86	(0.05)	1.13	(0.10)	1.27	(0.22)	**1.05**	**(0.04)**	1.09	(0.11)
Row-wise	d_2	0.51	(0.06)	**0.53**	**(0.03)**	0.40	(0.06)	0.40	(0.06)	0.16	(0.12)	**0.23**	**(0.14)**	0.16	(0.10)	0.16	(0.10)
	R^2	0.05	(0.04)	**0.06**	**(0.03)**	0.01	(0.01)	0.01	(0.01)	0.02	(0.02)	**0.03**	**(0.02)**	0.02	(0.02)	0.02	(0.02)
	MAE	1.49	(0.14)	**1.58**	**(0.12)**	1.79	(0.14)	1.79	(0.14)	3.92	(1.37)	**3.98**	**(1.84)**	3.79	(0.95)	3.79	(0.95)
Benzene																	
Random	d_2	**0.87**	**(0.03)**	0.84	(0.01)	0.87	(0.02)	0.84	(0.02)	**0.88**	**(0.04)**	0.78	(0.03)	0.83	(0.05)	0.81	(0.02)
	R^2	**0.61**	**(0.08)**	0.52	(0.03)	0.59	(0.06)	0.52	(0.05)	**0.62**	**(0.11)**	0.41	(0.06)	0.51	(0.11)	0.46	(0.05)
	MAE	**0.17**	**(0.02)**	0.18	(0.01)	0.17	(0.01)	0.18	(0.01)	**0.14**	**(0.02)**	0.17	(0.02)	0.17	(0.01)	0.17	(0.01)
Row-wise	d_2	**0.64**	**(0.04)**	0.63	(0.03)	0.58	(0.06)	0.57	(0.06)	**0.64**	**(0.07)**	0.63	(0.04)	0.59	(0.07)	0.58	(0.07)
	R^2	**0.20**	**(0.05)**	0.18	(0.03)	0.13	(0.05)	0.12	(0.05)	**0.20**	**(0.07)**	0.18	(0.04)	0.14	(0.08)	0.13	(0.06)
	MAE	**0.26**	**(0.02)**	0.28	(0.02)	0.28	(0.03)	0.27	(0.01)	**0.21**	**(0.02)**	0.22	(0.02)	0.22	(0.02)	0.23	(0.01)
1,3-Butadiene																	
Random	d_2	0.89	(0.02)	**0.89**	**(0.01)**	0.87	(0.01)	0.87	(0.02)	**0.81**	**(0.07)**	0.79	(0.04)	0.78	(0.05)	0.76	(0.07)
	R^2	0.65	(0.06)	**0.65**	**(0.03)**	0.58	(0.03)	0.58	(0.04)	**0.54**	**(0.11)**	0.52	(0.05)	0.44	(0.09)	0.42	(0.13)
	MAE	0.03	(0.00)	**0.03**	**(0.00)**	0.03	(0.00)	0.03	(0.00)	**0.03**	**(0.00)**	0.03	(0.00)	0.03	(0.00)	0.03	(0.00)
Row-wise	d_2	**0.58**	**(0.04)**	0.50	(0.03)	0.52	(0.08)	0.46	(0.05)	**0.57**	**(0.07)**	0.48	(0.04)	0.51	(0.10)	0.42	(0.03)
	R^2	**0.09**	**(0.03)**	0.05	(0.03)	0.07	(0.05)	0.03	(0.03)	**0.14**	**(0.07)**	0.05	(0.03)	0.10	(0.07)	0.02	(0.01)
	MAE	**0.04**	**(0.00)**	0.04	(0.00)	0.05	(0.00)	0.04	(0.00)	**0.03**	**(0.00)**	0.03	(0.00)	0.03	(0.00)	0.03	(0.00)
Tetrachloroethylene																	
Random	d_2	0.30	(0.07)	0.27	(0.03)	0.31	(0.06)	**0.33**	**(0.06)**	**0.29**	**(0.06)**	0.21	(0.04)	0.28	(0.04)	0.27	(0.04)
	R^2	0.02	(0.02)	0.01	(0.01)	0.01	(0.01)	**0.01**	**(0.02)**	**0.02**	**(0.02)**	0.00	(0.00)	0.01	(0.01)	0.02	(0.03)
	MAE	0.08	(0.01)	0.08	(0.00)	0.08	(0.00)	**0.07**	**(0.00)**	**0.06**	**(0.00)**	0.06	(0.00)	0.06	(0.00)	0.06	(0.00)
Row-wise	d_2	**0.41**	**(0.11)**	0.38	(0.10)	-	-	0.32	(0.06)	**0.40**	**(0.14)**	0.33	(0.11)	0.31	(0.12)	0.25	(0.05)
	R^2	**0.03**	**(0.02)**	0.02	(0.01)	-	-	0.01	(0.00)	**0.07**	**(0.07)**	0.03	(0.04)	0.02	(0.04)	0.01	(0.01)
	MAE	**0.07**	**(0.01)**	0.08	(0.01)	-	-	0.07	(0.01)	**0.05**	**(0.00)**	0.05	(0.00)	0.05	(0.00)	0.05	(0.01)