

Supplementary materials

Preparation of thermodesorption tube standards: comparison of usual methods using accuracy profile evaluation

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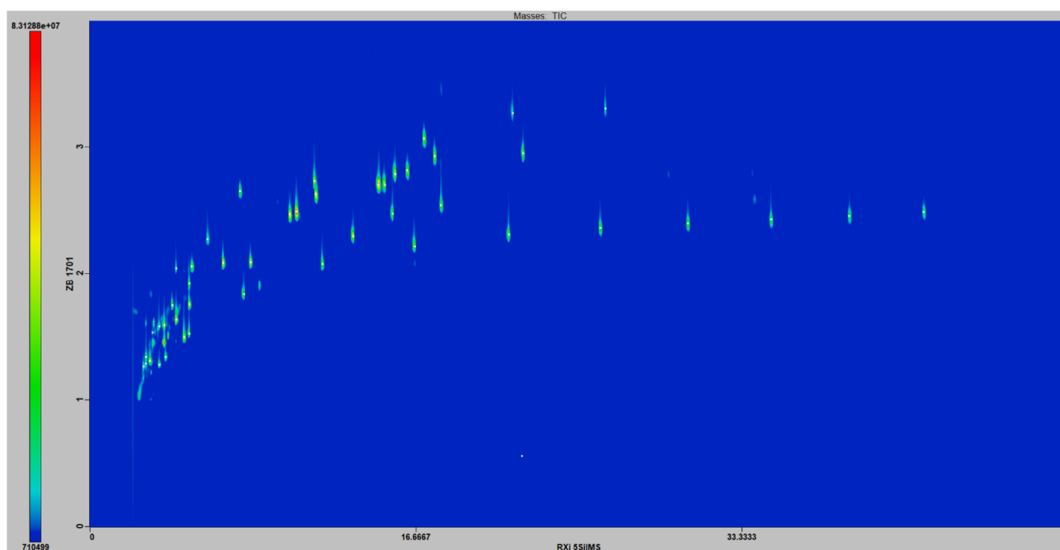


Figure S1. Chromatogram of reference solution loaded using GSAD (method described in materials and methods section).

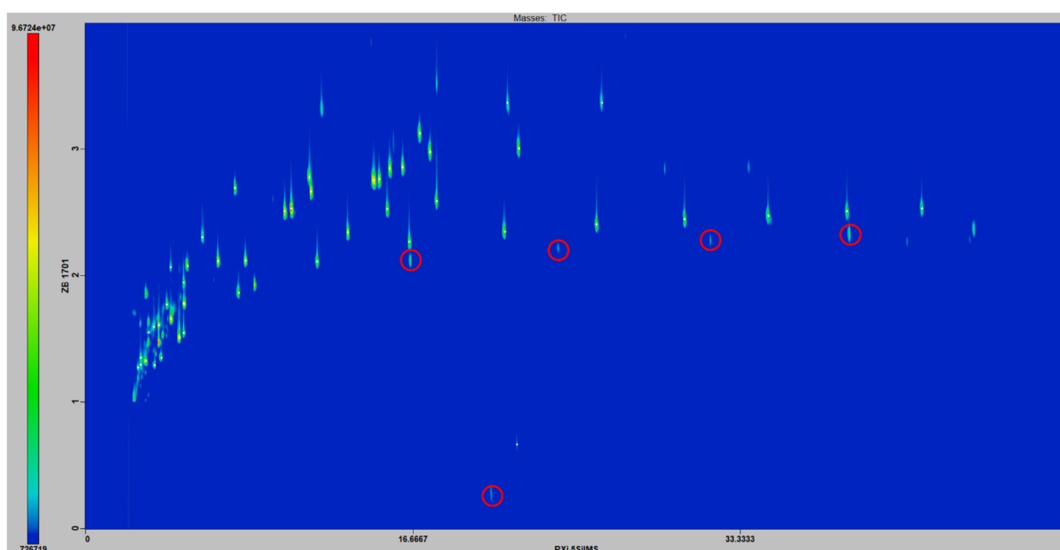


Figure S2. Chromatogram of reference solution loaded using VGSD (method described in materials and methods section) with a slight pollution (red circles around pollution peaks).

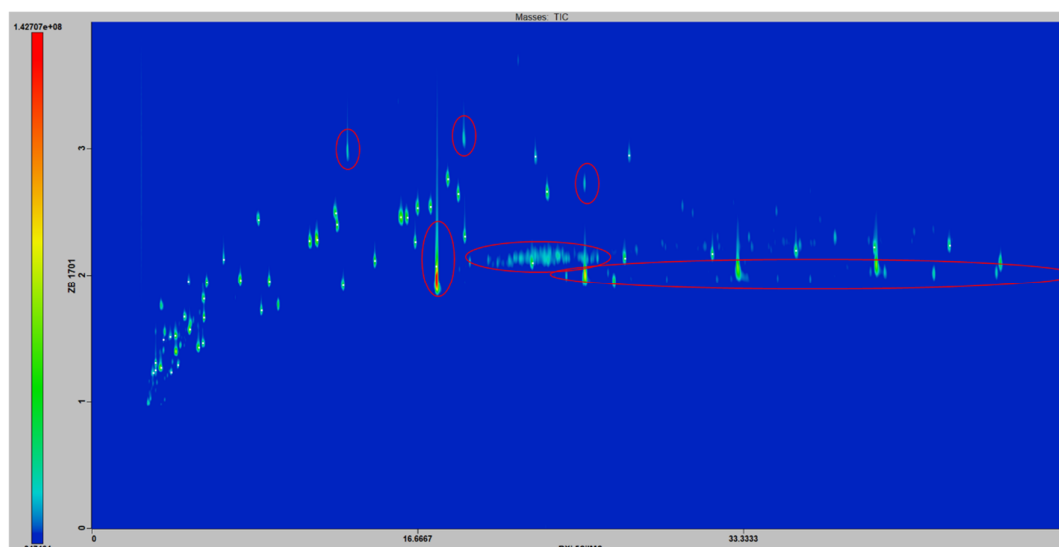
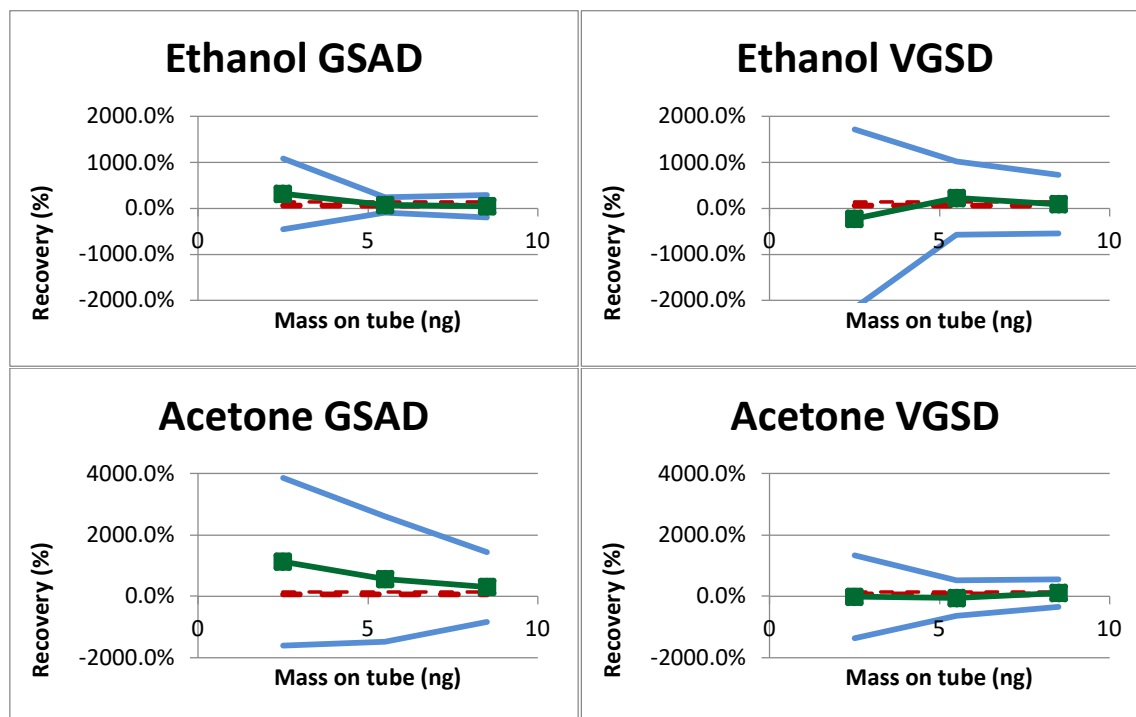


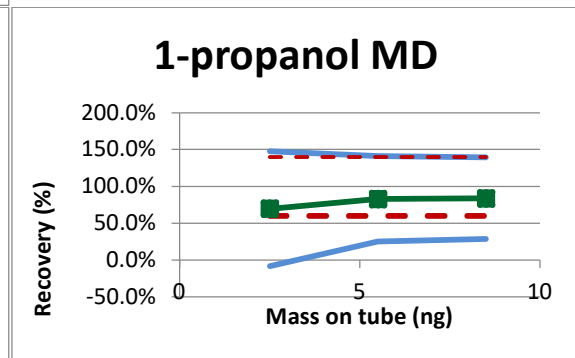
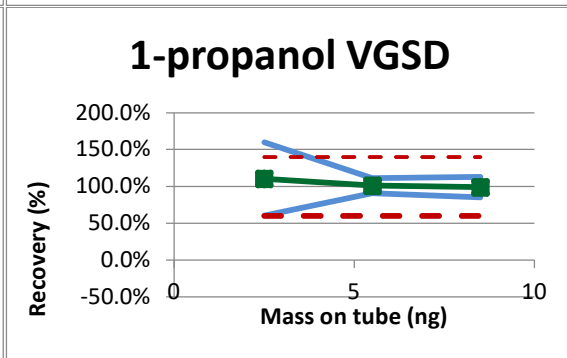
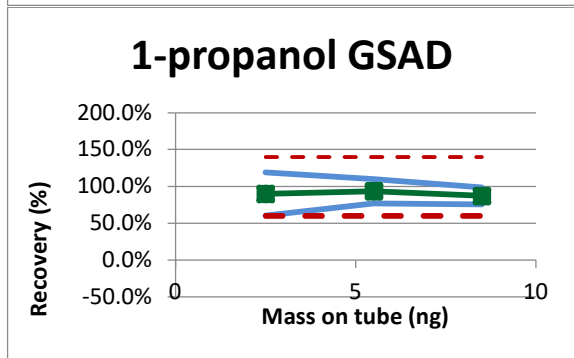
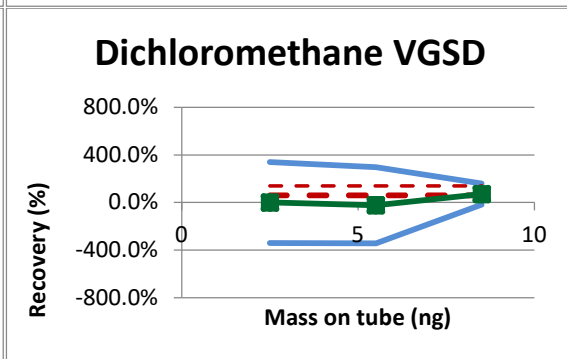
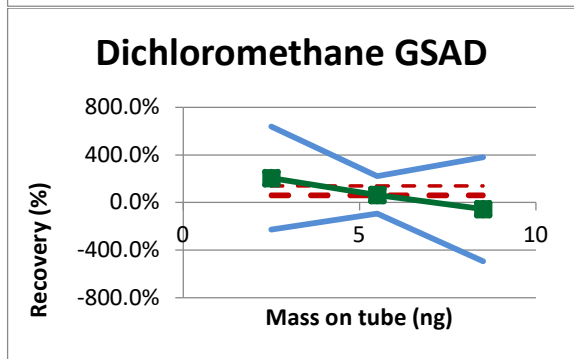
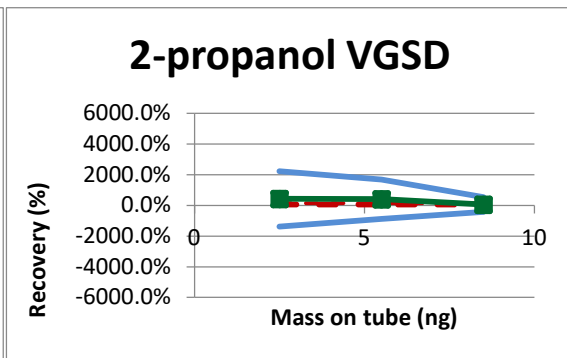
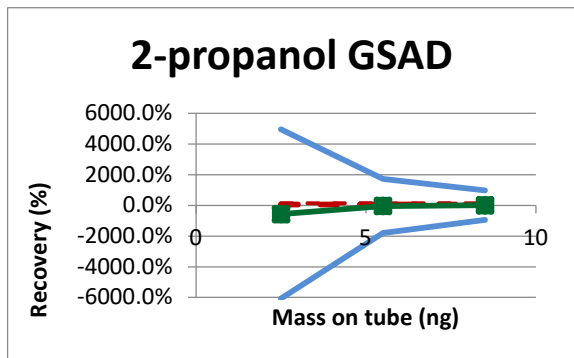
Figure S3. Chromatogram of reference solution loaded using GSAD (method described in materials and methods section) with an important pollution (red circles around pollution peaks).

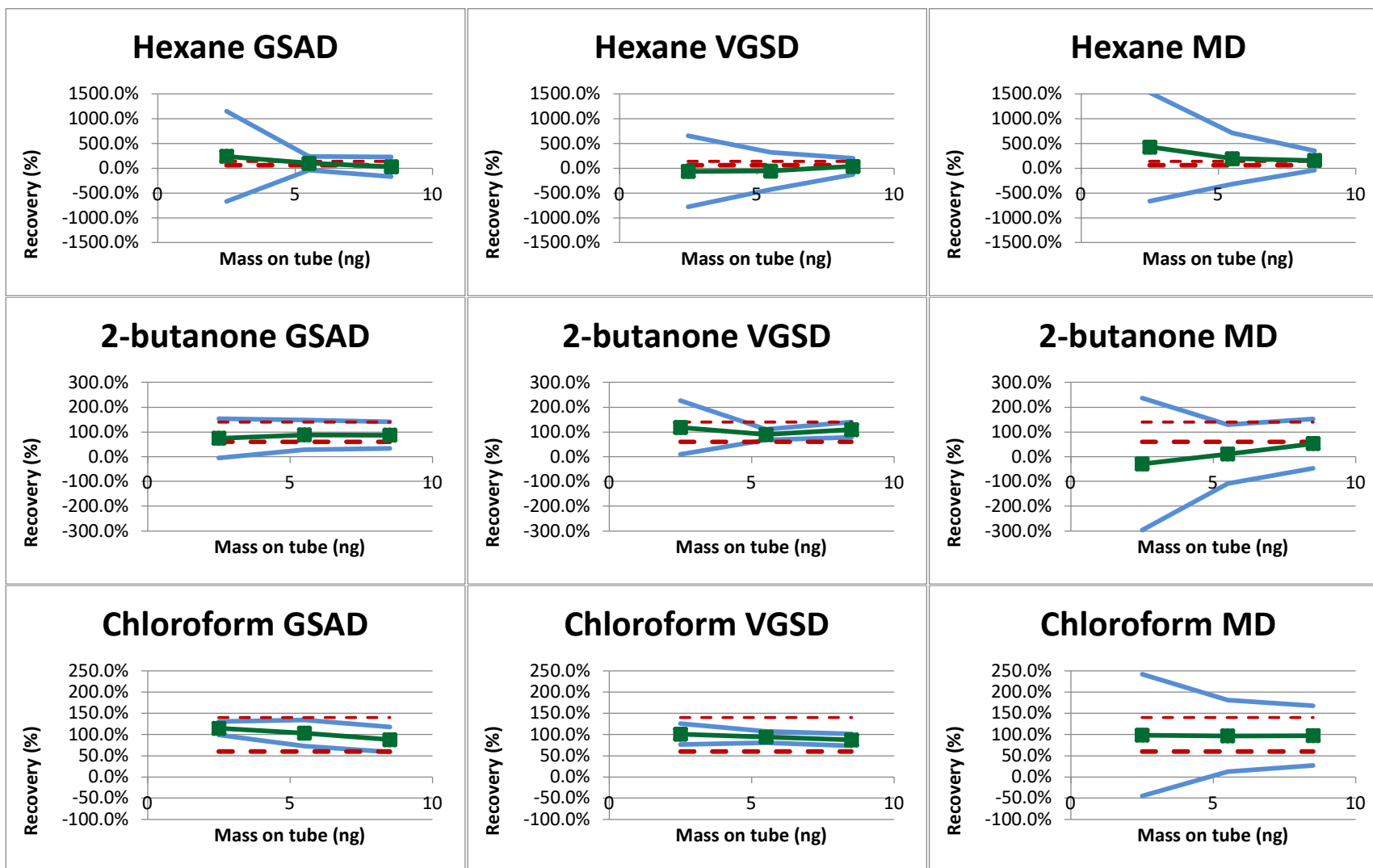
Table S1. Validation Range of each compound with each technique.

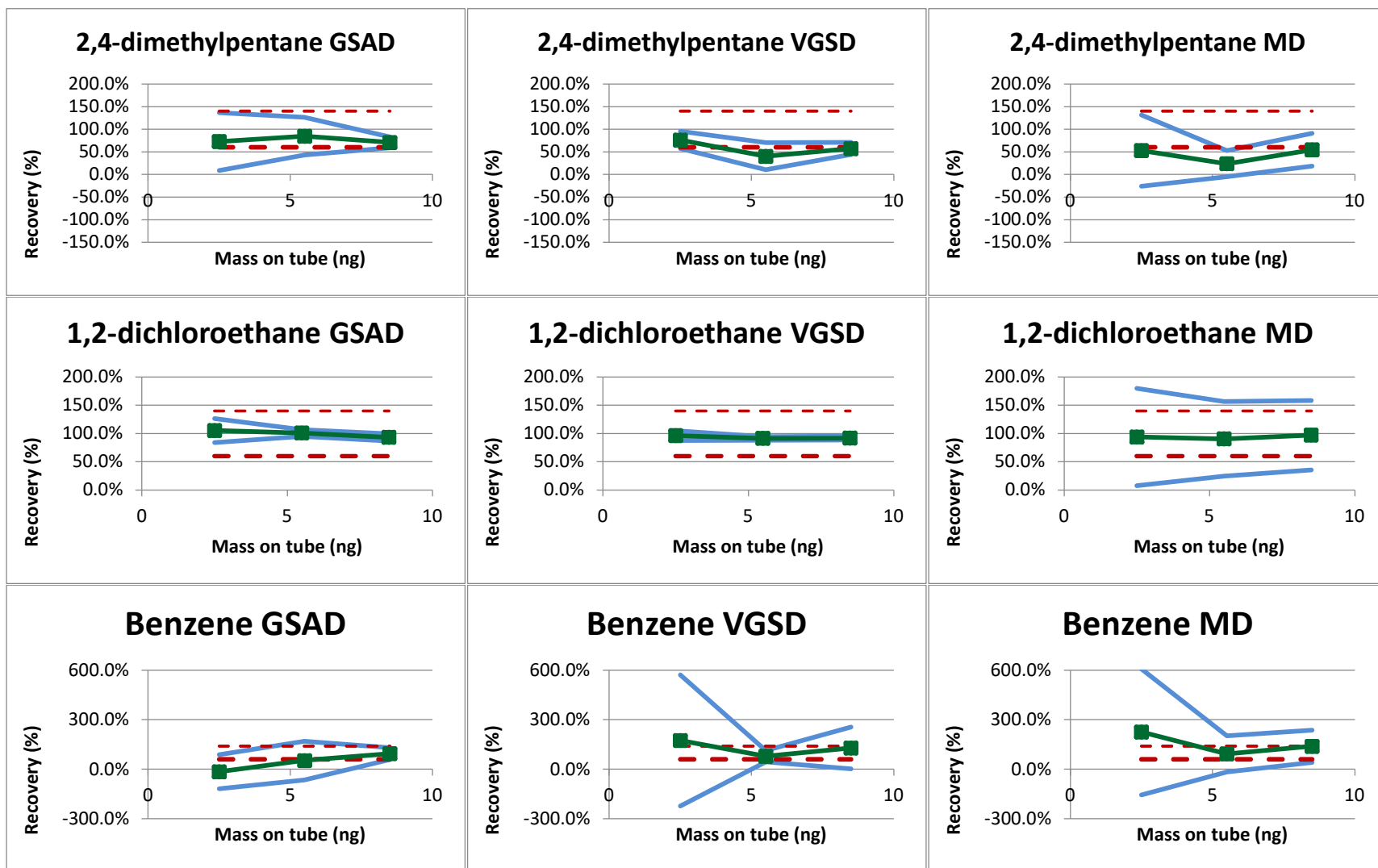
Compound Name	Family	Boiling Temperature (°C)	Score GSAD	Score VGSD	Score MD
Ethanol	Alcohol	78	0	0	N/A
Acetone	Ketone	56	0	0	N/A
2-Propanol	Alcohol	82.5	0	0	N/A
Methane dichloro-	Halogenate d	39.6	0	0	N/A
1-Propanol	Alcohol	97	100	79.5	0
Hexane	Alkane	68.7	0	0	0
2-Butanone	Ketone	79.6	0	57.2	0
Chloroform	Halogenate d	61.2	94.6	100	0
Pentane 2 4-dimethyl-	Alkane	80.5	0	0	0
Ethane 1 2-dichloro-	Halogenate d	83.5	100	100	0
Benzene	Aromatic	80.1	0	0	0
1-Butanol	Alcohol	117.7	39.8	98.3	0
Isooctane	Alkane	99	0	0	0
Heptane	Alkane	98.4	0	0	0
Propane 1 2-dichloro-	Halogenate d	96	80.8	100	0
Ethene trichloro-	Halogenate d	87.2	100	100	0
Methane bromodichloro-	Halogenate d	90	100	100	0
2-Pentanone 4-methyl-	Ketone	116	83.7	100	0
Toluene	Aromatic	110.6	0	78.6	0

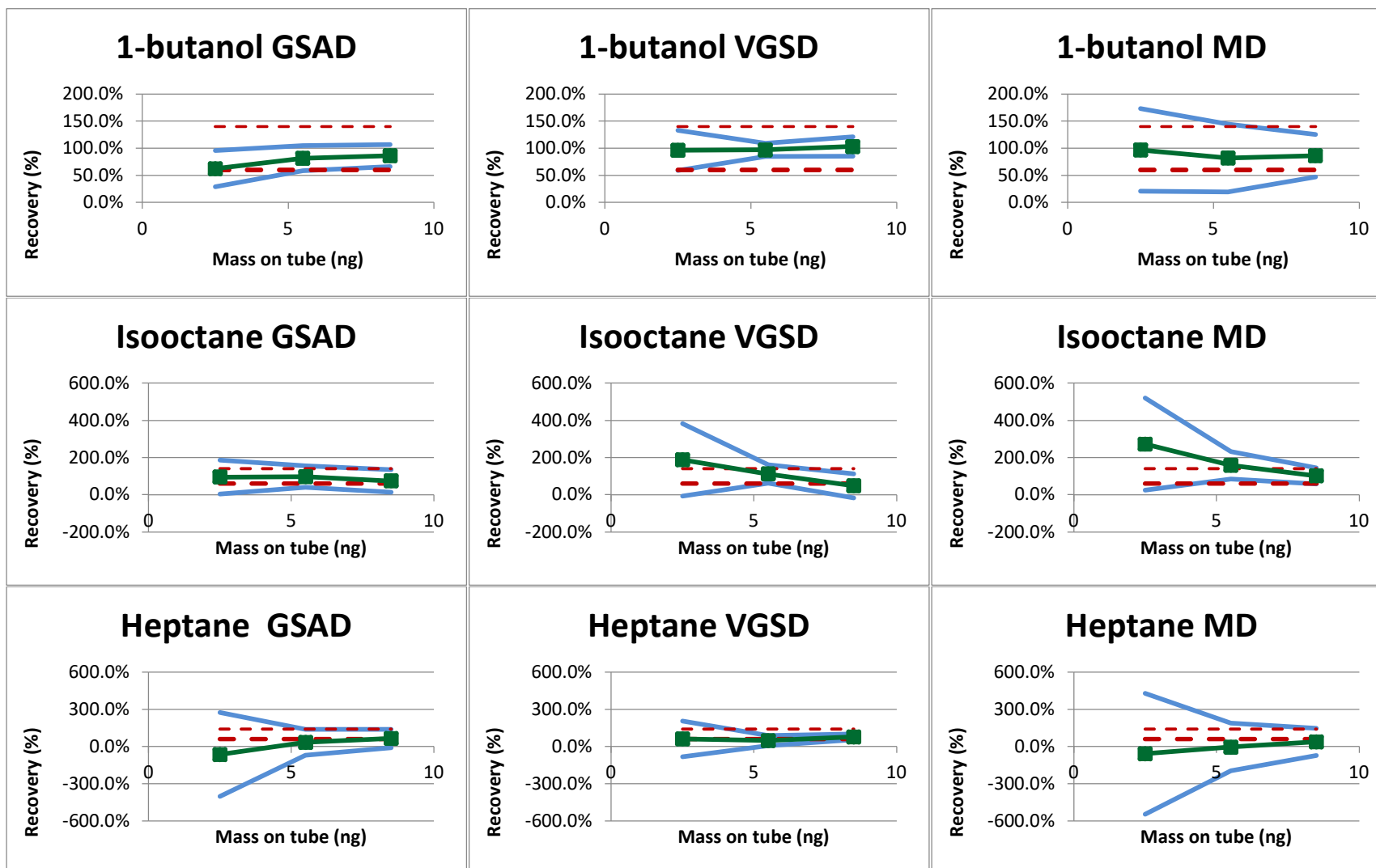
Methane dibromochloro-	Halogenate d	120	100	100	0
Octane	Alkane	125.6	0	100	0.2
Tetrachloroethylene	Halogenate d	121.1	100	100	0
Ethylbenzene	Aromatic	136	58.3	92	0
p-Xylene	Aromatic	138.4	99.4	73	0
Styrene	Aromatic	145	98.7	100	0
o-Xylene	Aromatic	144	85.6	100	0
Nonane	Alkane	151	55.1	100	1.2
α -Pinene	Terpene	156	75.9	100	0
Benzene 1-ethyl-4-methyl-	Aromatic	152	100	100	0
Mesitylene	Aromatic	164.7	71.9	100	0
β -Pinene	Terpene	166	76.7	100	0
Benzene 1-ethyl-2-methyl-	Aromatic	162	87.9	100	0
Benzene 1 2 4-trimethyl-	Aromatic	169.3	75.2	100	0
Decane	Alkane	174.1	0	100	0
Benzene 1 4-dichloro-	Aromatic	174	100	100	0
Benzene 1 2 3-trimethyl-	Aromatic	176	75.2	100	0
D-Limonene	Terpene	176	51.9	100	0
Undecane	Alkane	195.9	0	0	21.3
Nonanal	Aldehyde	195	0	59.3	0.5
Benzene 1 2 4 5-tetramethyl-	Aromatic	192	76.3	100	0
Dodecane	Alkane	216.2	55.4	20.1	38.2
Decanal	Aldehyde	207	0	53.1	2.4
Tridecane	Alkane	234	57.6	46.3	51.5
Tetradecane	Alkane	253.6	68.6	100	70.7
Pentadecane	Alkane	270.7	81.6	56.6	0
Hexadecane	Alkane	286.9	91.3	100	44.5
Mean score			53	70	5

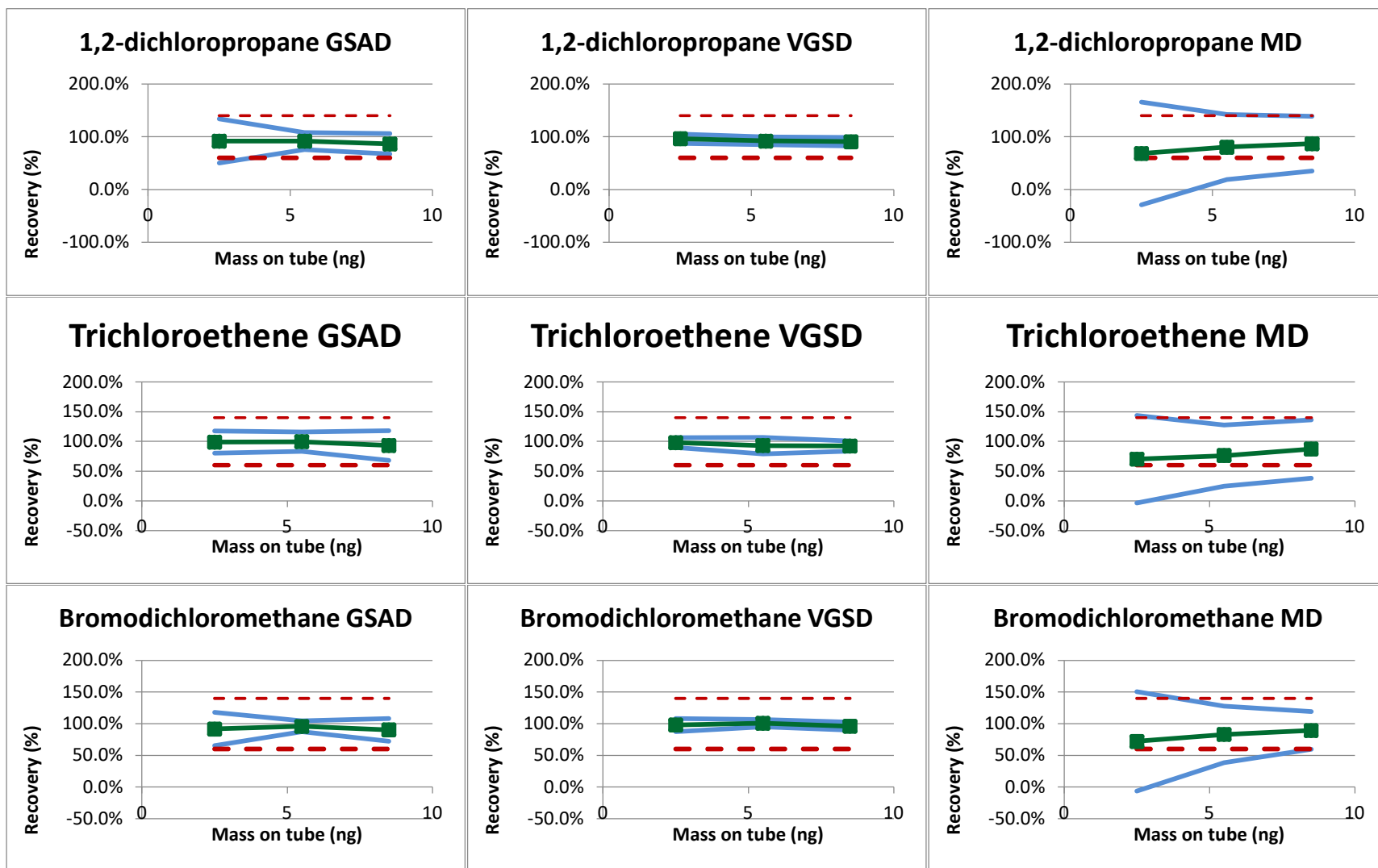


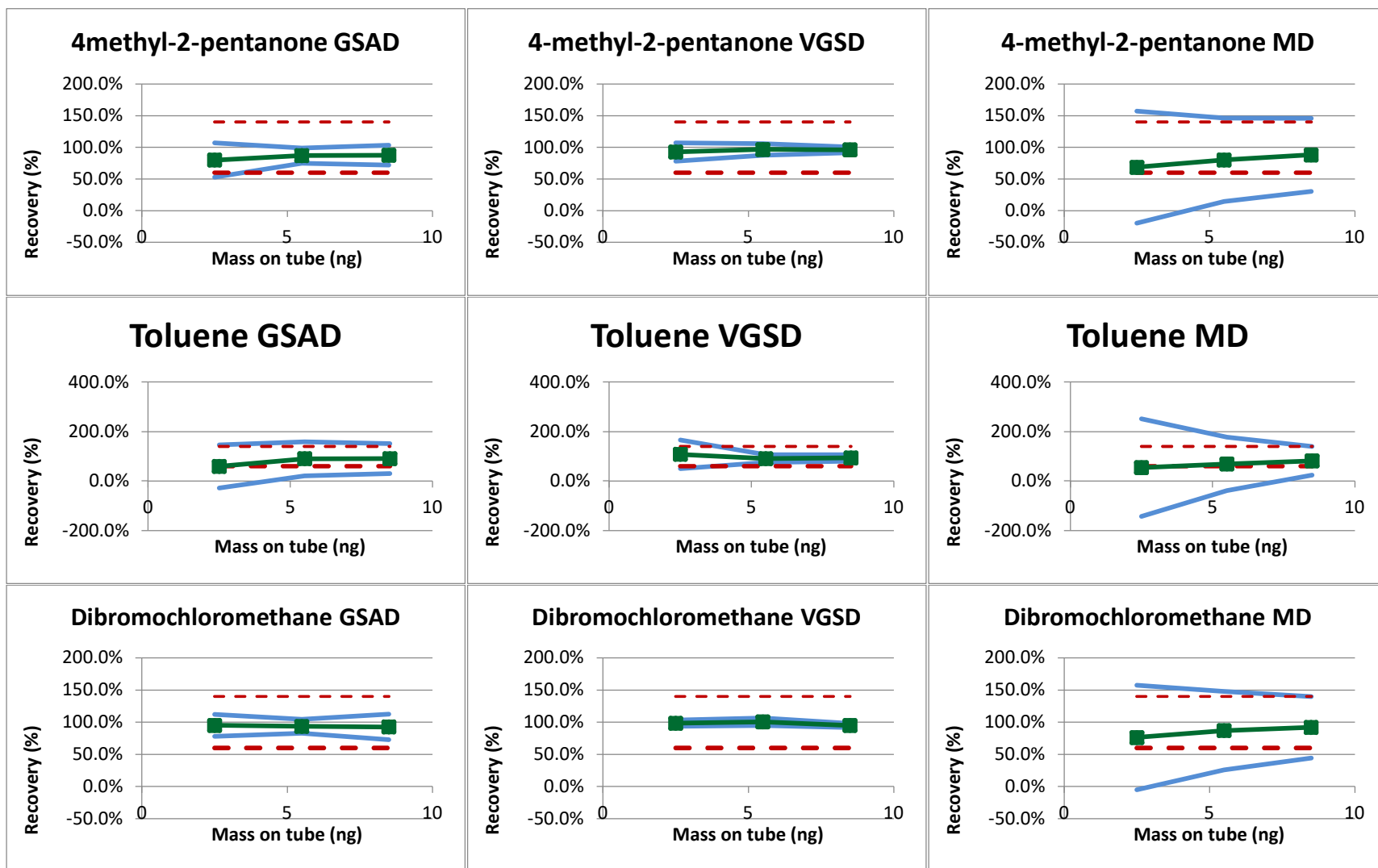


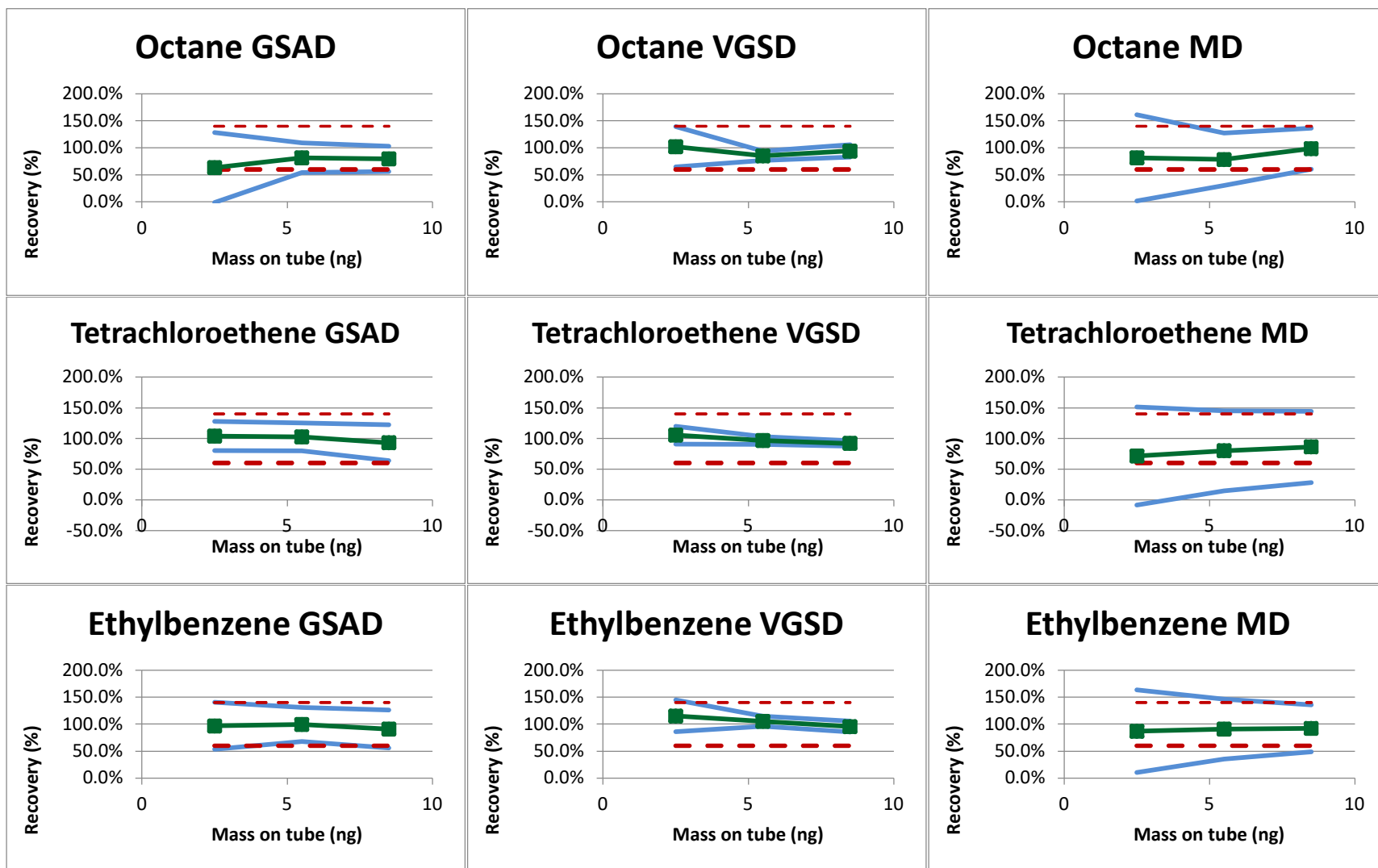


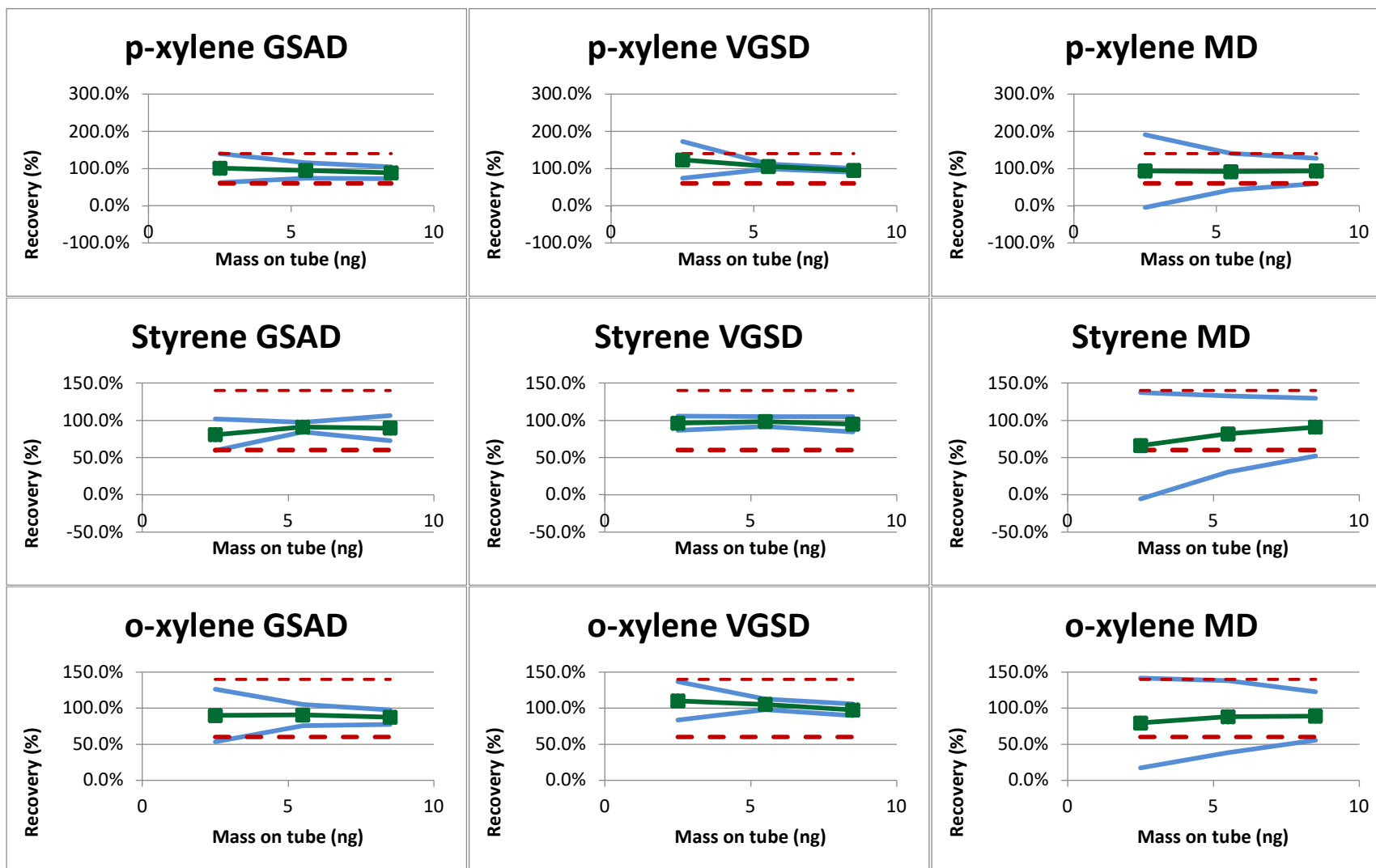


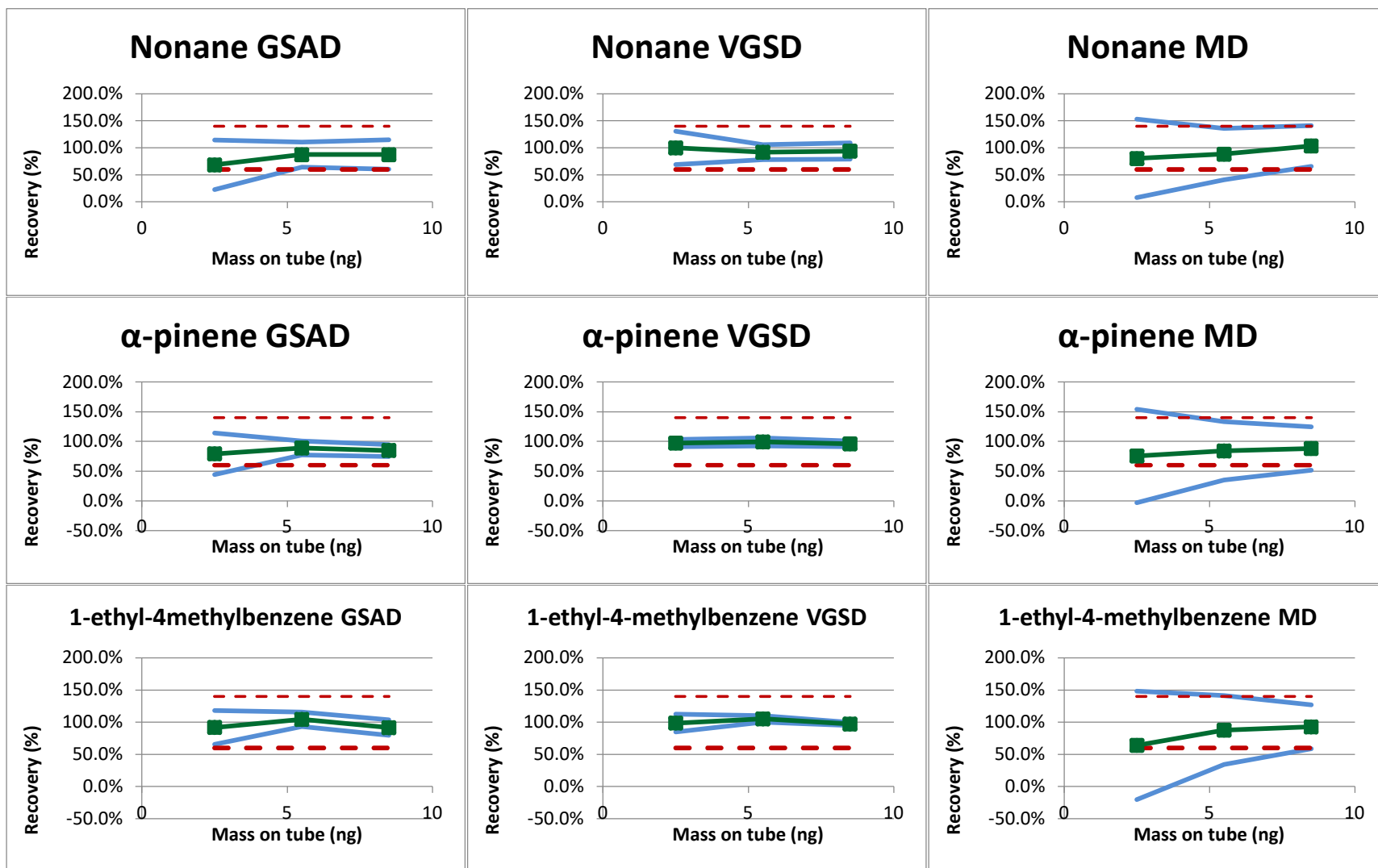


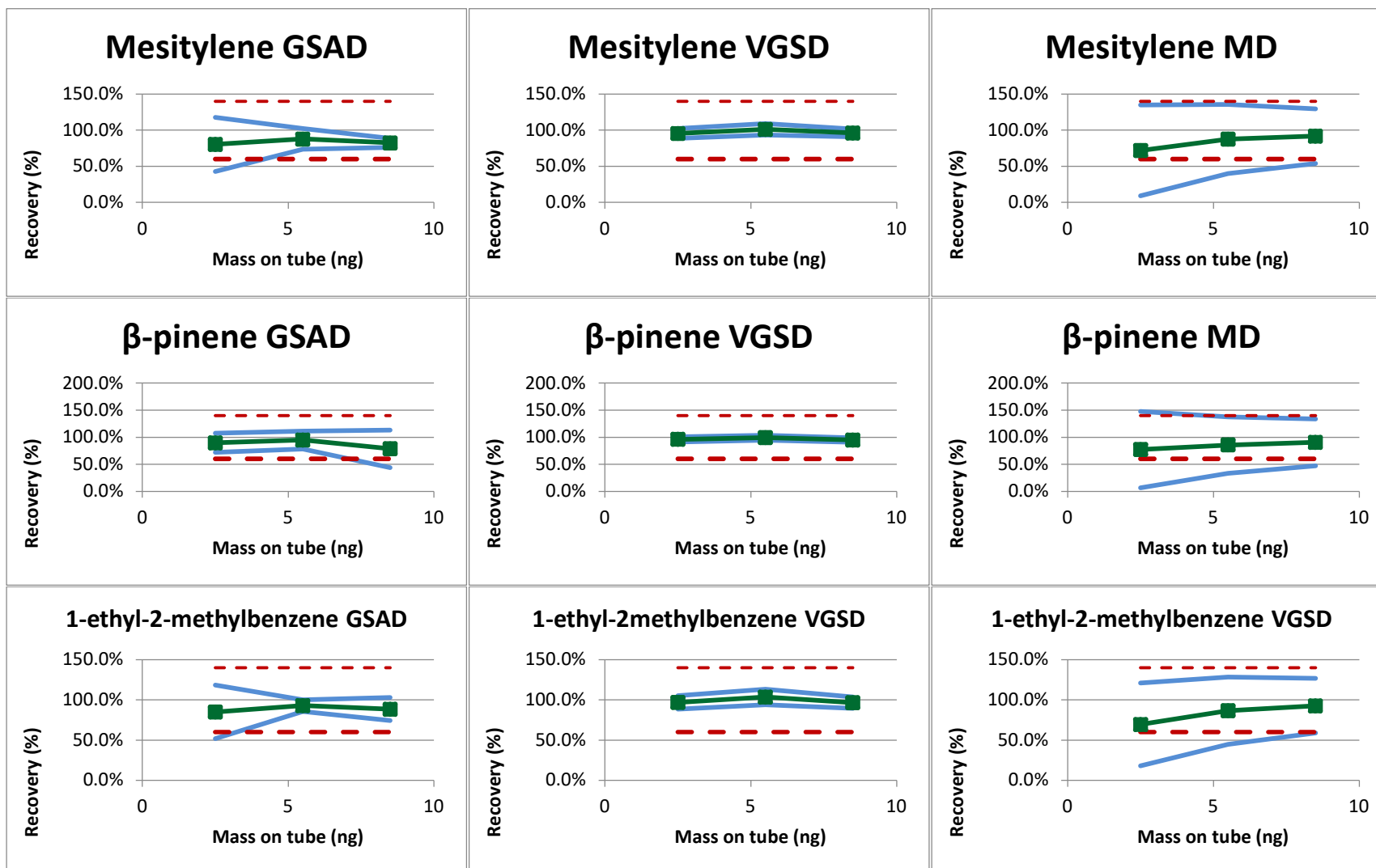


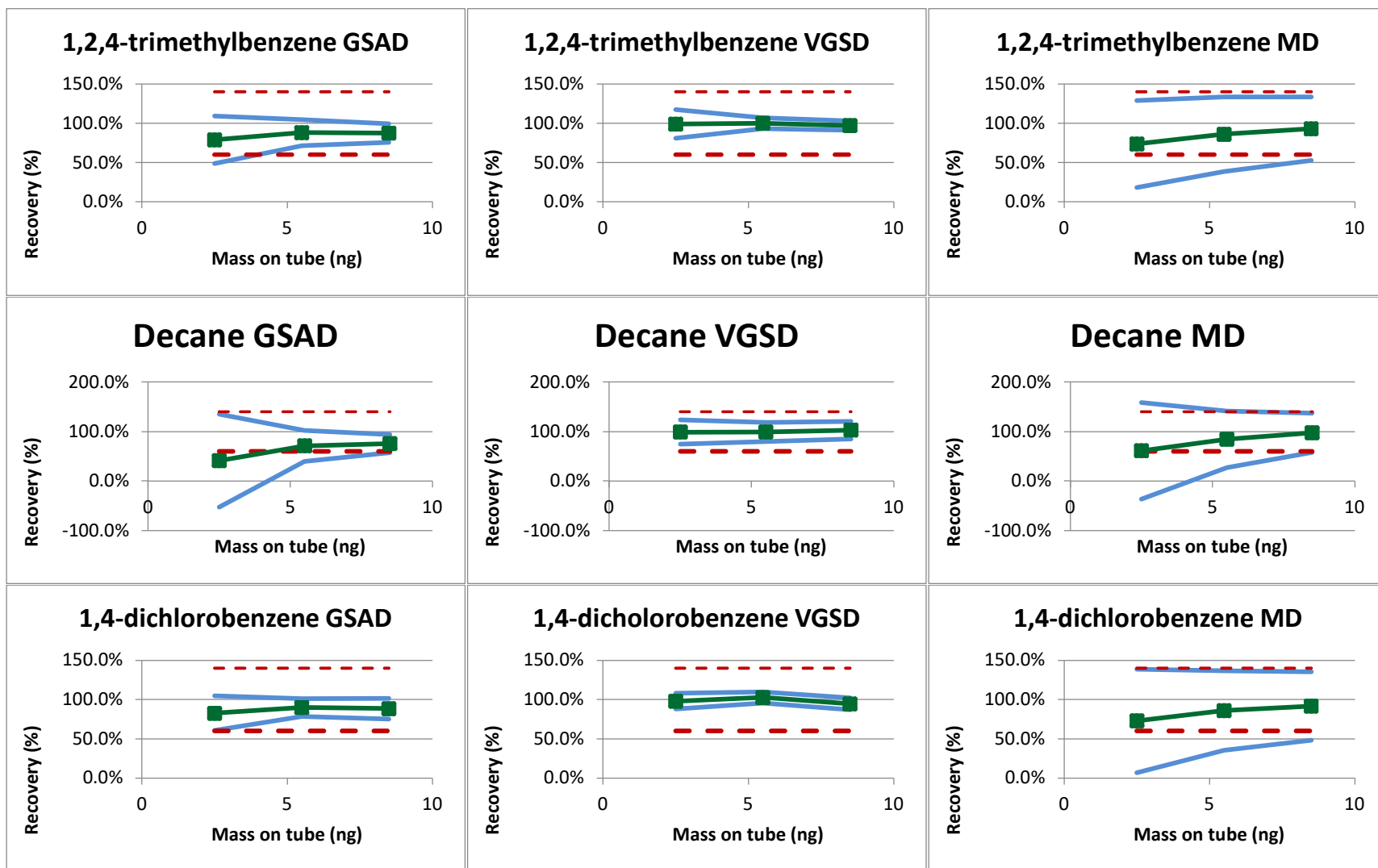


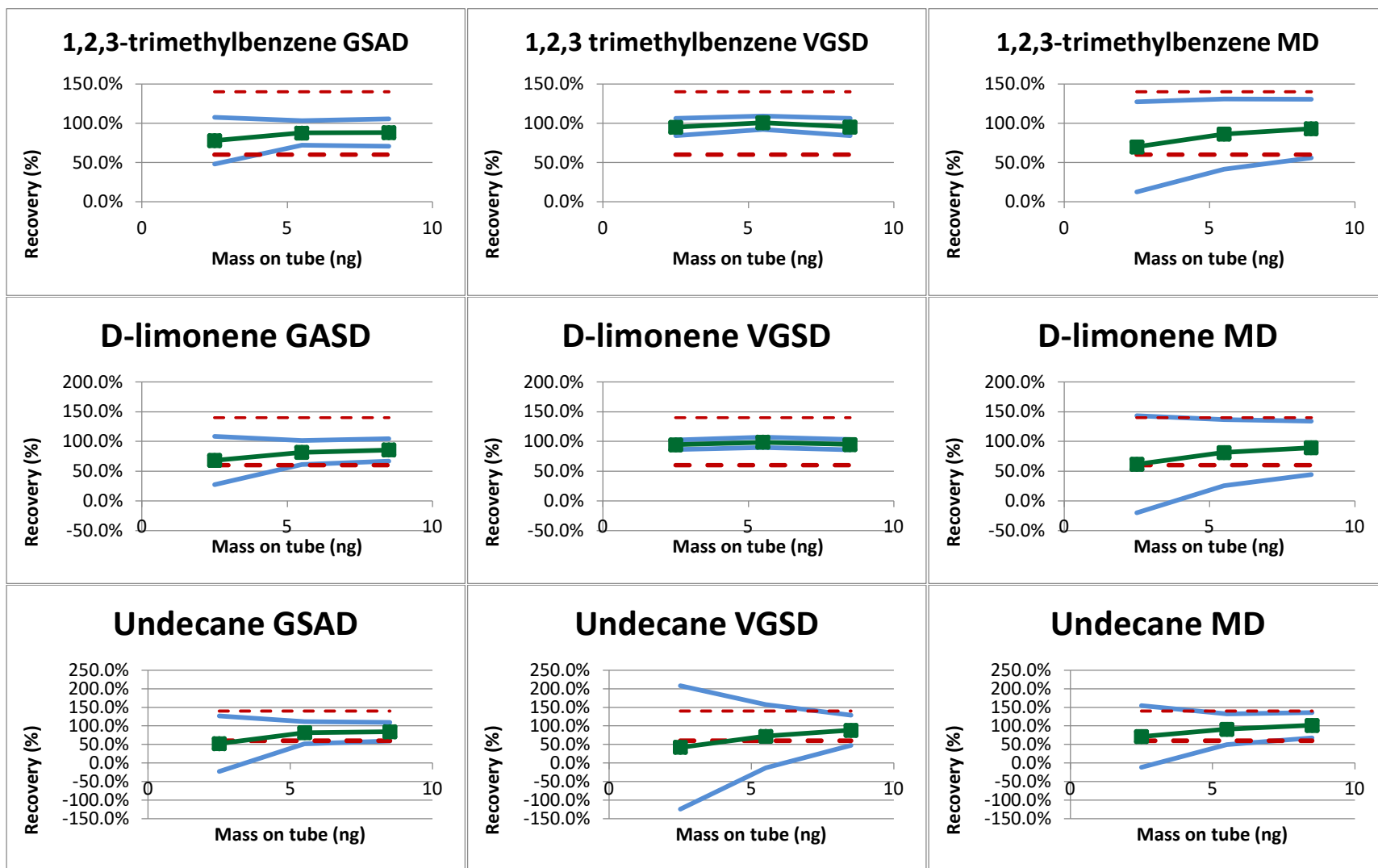


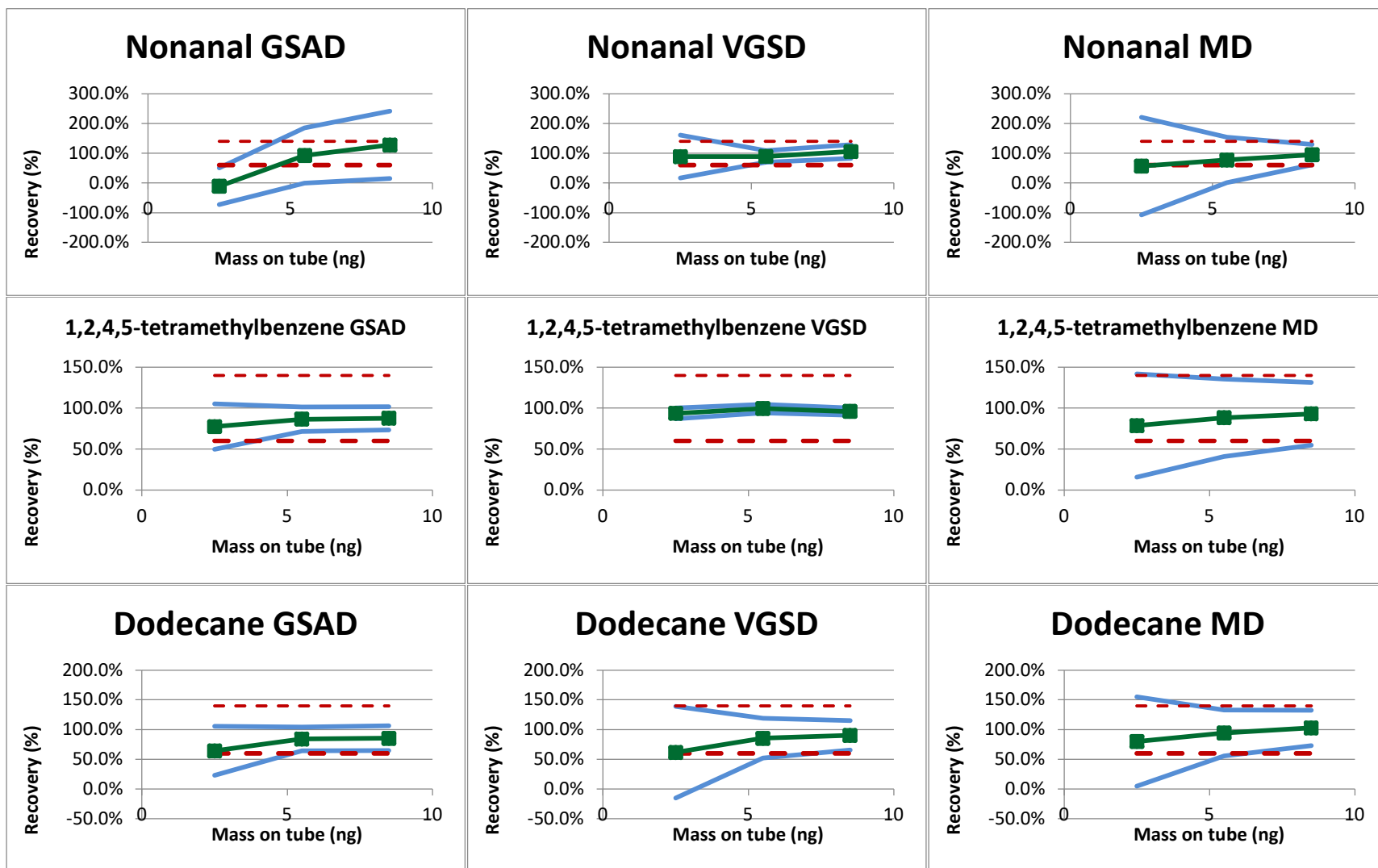


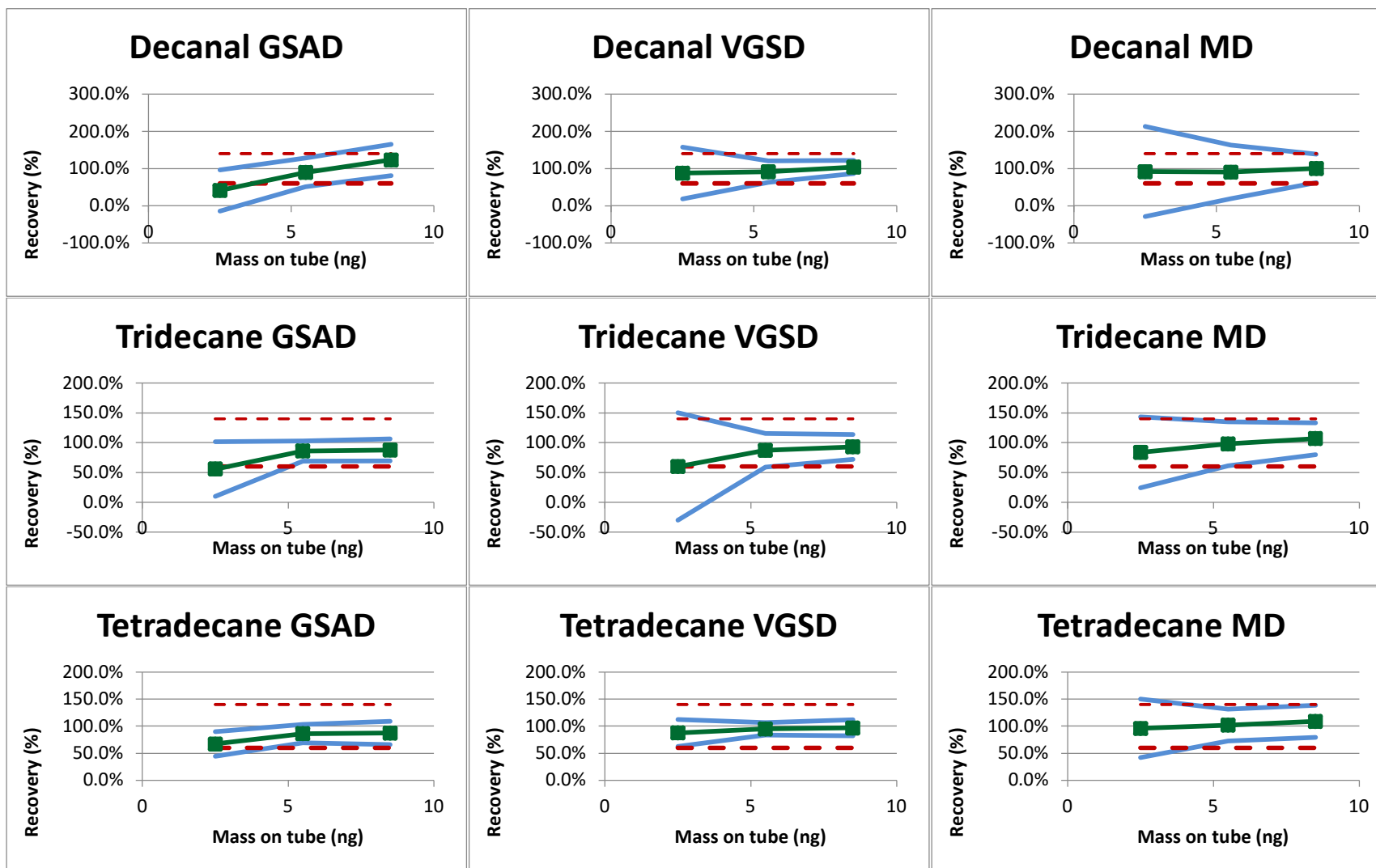


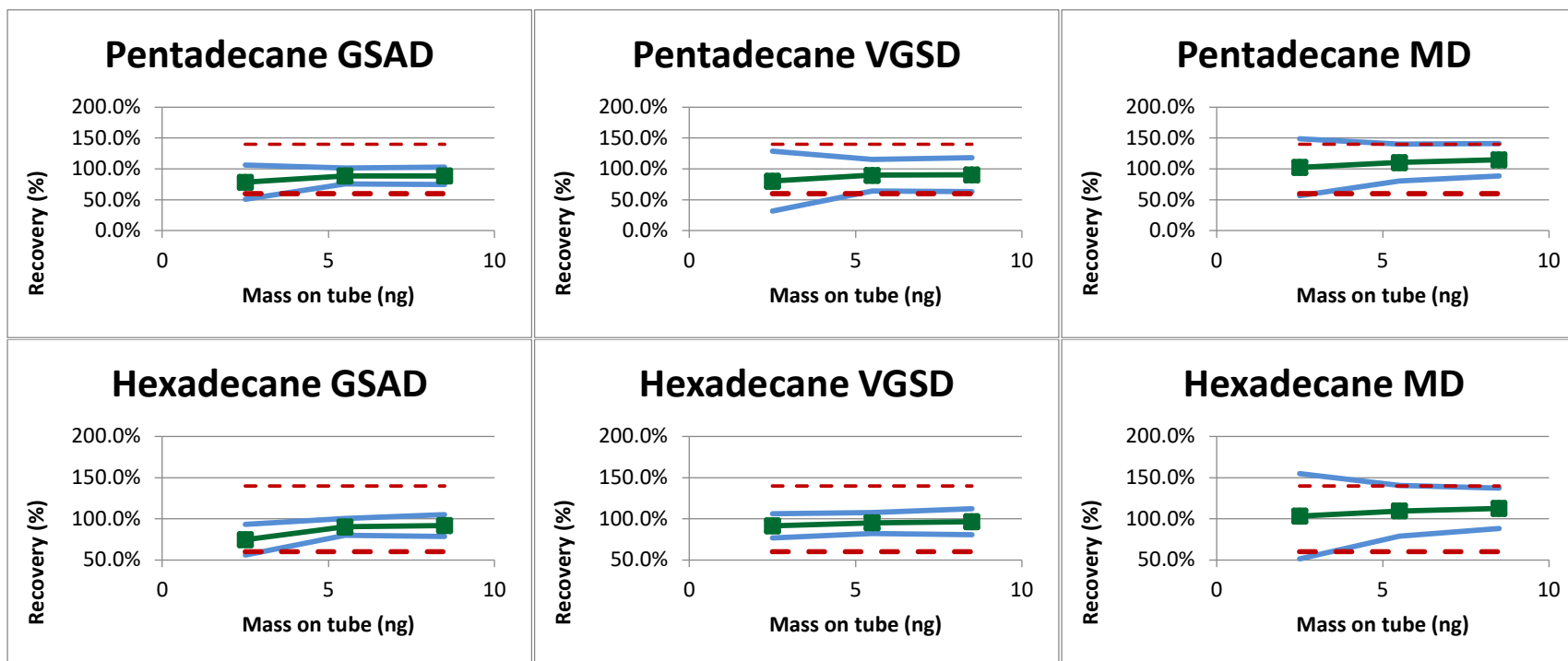












— Acceptance limits (%) — Tolerance limits (%) — Mean of experimental results (%)

Figure S4. Accuracy profile of all compounds.