

Supplemental Table 1 – Neat Standard Procurement and Storage Conditions

Vendor	Standard	CAS	Purity (%)	Physical State	Storage Condition
Acros Organics	Butanoic Acid	107-92-6	99+	Liquid	Chemical Shelf
Acros Organics	Isovanillin	621-59-0	98	Solid	Chemical Shelf
Acros Organics	L-Limonene	5989-54-8	96	Liquid	Chemical Shelf
Acros Organics	L-Menthol	2216-51-5	99.5	Solid	Chemical Shelf
Acros Organics	Maltol	118-71-8	99	Solid	Chemical Shelf
Acros Organics	Triacetin	102-76-1	99	Liquid	Chemical Shelf
Alfa Aesar	Benzyl Alcohol	100-51-6	99+	Liquid	Chemical Shelf
Alfa Aesar	D-Limonene	5989-27-5	97	Liquid	Chemical Shelf
Alfa Aesar	Ethyl Vanillin	121-32-4	98	Solid	Chemical Shelf
Alfa Aesar	Eucalyptol	470-82-6	99	Liquid	Chemical Shelf
Alfa Aesar	Vanillin	121-33-5	99	Solid	Chemical Shelf
Cambridge Isotopes	Acenaphthene-d10	15067-26-2	99	Solid	Chemical Shelf
Cambridge Isotopes	Benzene-d6	1076-43-3	99.5	Liquid	Chemical Shelf
Cambridge Isotopes	Chlorobenzene-d5	3114-55-4	99	Liquid	Chemical Shelf
Cambridge Isotopes	Pyridine-d5	7291-22-7	99.5	Liquid	Chemical Shelf
Santa Cruz Biotechnology	Acetoin	513-86-0	97	Solid	4-8°C
Santa Cruz Biotechnology	Naphthalene-d8	1146-65-2	NA	Solid	Chemical Shelf
Sigma Aldrich	Benzaldehyde	100-52-7	99.5	Liquid	Chemical Shelf, under argon
Sigma Aldrich	Eugenol	97-53-0	99	Liquid	Chemical Shelf
Sigma Aldrich	Furaneol	3658-77-3	99	Solid	4-8°C, under argon
Sigma Aldrich	Methyl Salicylate	119-36-8	99	Liquid	Chemical Shelf
TCI	(+)Pulegone	89-82-7	95	Liquid	Chemical Shelf
TCI	2,3,5-Trimethylpyrazine	14667-55-1	98	Liquid	Chemical Shelf
TCI	Ethyl Maltol	4940-11-8	99	Solid	Chemical Shelf
TCI	Ethyl Salicylate	118-61-6	99	Liquid	Chemical Shelf
TCI	trans-Cinnamaldehyde	14371-10-9	98	Liquid	Chemical Shelf

Supplemental Table 2 – Preparation Information for Calibration and Quality Control (QC) Standards

Standard ID	Volume of Neat Standard (µL)	Volume of 20mg/mL Working Solution ² (µL)	Volume of Previous Calibration Level (µL)	Volume of 50:50 PG:VG (5% H ₂ O) (µL)	Total Volume (µL)	Concentration (mg/mL)
Initial Calibration						
C10	100, each ¹	5000	NA	3700	10,000	10.0
C9	---	---	5000 (of C10)	5000	10,000	5.00
C8	---	---	5000 (of C9)	5000	10,000	2.50
C7	---	---	5000 (of C8)	5000	10,000	1.25
C6	---	---	5000 (of C7)	5000	10,000	0.63
C5	---	---	5000 (of C6)	5000	10,000	0.31
C4	---	---	5000 (of C5)	5000	10,000	0.16
C3	---	---	5000 (of C4)	5000	10,000	0.08
C2	---	---	5000 (of C3)	5000	10,000	0.04
C1	---	---	5000 (of C2)	5000	10,000	0.02
C0	---	---	---	5000	10,000	
Quality Control (QC)						
QC9	80, each ¹	4000	NA	4960	10,000	8.00
QC8	---	---	5000 (of QC9)	5000	10,000	4.00
QC7	---	---	5000 (of QC8)	5000	10,000	2.00
QC6	---	---	5000 (of QC7)	5000	10,000	1.00
QC5	---	---	5000 (of QC6)	5000	10,000	0.50
QC4	---	---	5000 (of QC5)	5000	10,000	0.25
QC3	---	---	5000 (of QC4)	5000	10,000	0.13
QC2	---	---	5000 (of QC3)	5000	10,000	0.06
QC1	---	---	5000 (of QC2)	5000	10,000	0.03

¹Refer to Supplemental Table 1 for each liquid neat standard to be added

²Prepared by weighting 2.0000 ± 0.0005mg of each neat solid standard (see Supplemental Table 1) into 100mL of methanol and hand-vortex 5 min, or until visible granules are dissolved.

Supplemental Table 3 – Initial Calibration Parameters of Twenty Flavoring Chemicals

	Instrument Linear Range ¹ (mg/mL)	Working Calibration Range ² (mg/mL)	Calibration Curve Fit	Average ³ Coefficient of Determination (r ²)	Average ³ RRF	Average ³ RRT	Average ³ RSE (%)	LLOQ (mg/mL)	S:N ⁴ at LLOQ
Acetoin	0.31-10.00	0.31-10.00	Quadratic, 1/x ²	0.995	0.03	1.24	6.9	0.31	715
Butanoic Acid	0.16-10.00	0.63-10.00	Quadratic, 1/x ²	0.995	0.34	1.13	7.2	0.63	59
Benzaldehyde	0.02-10.00	0.02-10.00	Quadratic, 1/x ²	0.996	0.56	1.12	6.7	0.02	45
2,3,5-Trimethylpyrazine	0.02-10.00	0.02-10.00	Quadratic, 1/x ²	0.995	0.70	1.24	7.9	0.02	846
DL-Limonene	0.08-10.00	0.08-10.00	Quadratic, 1/x ²	0.993	0.14	1.26	8.3	0.08	891
Eucalyptol	0.04-10.00	0.04-10.00	Quadratic, 1/x ²	0.995	0.09	1.29	7.0	0.04	438
Benzyl Alcohol	0.02-5.00	0.02-5.00	Quadratic, 1/x ²	0.995	0.54	1.35	7.1	0.02	164
Furaneol	0.02-5.00	0.02-5.00	Quadratic, 1/x ²	0.994	0.25	1.37	7.8	0.02	35
Maltol	0.16-10.00	0.63-10.00	Quadratic, 1/x ²	0.992	0.49	1.47	8.9	0.63	580
L-Menthol	0.08-10.00	0.08-10.00	Quadratic, 1/x ²	0.997	0.08	1.51	5.6	0.08	631
Methyl Salicylate	0.08-10.00	0.08-10.00	Quadratic, 1/x ²	0.993	0.36	1.00	8.5	0.08	2212
Ethyl Maltol	0.08-10.00	0.63-10.00	Quadratic, 1/x ²	0.992	0.24	1.02	8.4	0.63	492
(+)Pulegone	0.02-10.00	0.02-10.00	Quadratic, 1/x ²	0.995	0.19	1.04	6.5	0.02	1256
Ethyl Salicylate	0.02-10.00	0.02-10.00	Quadratic, 1/x ²	0.993	0.37	1.06	8.2	0.02	1986
trans-Cinnamaldehyde	0.02-5.00	0.16-5.00	Quadratic, 1/x ²	0.995	0.33	1.09	7.7	0.16	157
Triacetin	0.02-10.00	0.04-10.00	Quadratic, 1/x ²	0.997	0.18	1.12	5.7	0.04	10
Eugenol	0.04-10.00	0.04-10.00	Quadratic, 1/x ²	0.994	0.38	1.15	7.6	0.04	652
Vanillin	0.31-10.00	0.63-10.00	Quadratic, 1/x ²	0.994	0.24	1.26	7.9	0.63	159
Ethyl Vanillin	0.04-10.00	0.31-10.00	Quadratic, 1/x ²	0.995	0.14	1.32	7.3	0.31	1125
Isovanillin	0.04-10.00	0.31-10.00	Quadratic, 1/x ²	0.994	0.28	1.02	7.7	0.31	162

¹Determined from percent recovery values ($\pm 20\%$) of each calibrator

²Determined from method validation parameters, including LLOQ and carryover analysis and represents calibration range applicable to quantitation of e-cigarette liquids

³Average of 7 independent batches analyzed across 7 days

⁴S:N = Signal/Noise ratio. Value calculated and provided by automated instrument software during data analysis. Acceptable peak identification from baseline noise is considered 10:1.

Supplemental Table 4 – Average Recovery and Coefficient of Variation (CV) Across 7 Calibration Batches

Level	Initial Calibration										Quality Control									
	1	2	3	4	5	6	7	8	9	10	1	2	3	4	5	6	7	8	9	
	Expected Concentration (mg/mL)	0.02	0.04	0.08	0.16	0.31	0.63	1.25	2.5	5.0	10.0	0.03	0.06	0.13	0.25	0.5	1.0	2.0	4.0	8.0
Percent Recovery (%)¹																				
Acetoin	0	15	41	74	101	97	99	102	100	100	0	12	43	67	102	100	100	101	97	
Butanoic Acid	30	26	88	102	95	97	99	106	107	96	25	26	78	90	91	96	101	107	100	
Benzaldehyde	99	99	95	98	98	100	106	107	104	94	91	94	93	93	95	100	102	102	96	
2,3,5-Trimethylpyrazine	105	96	94	95	96	99	109	110	104	91	95	90	90	91	94	101	105	102	92	
DL-Limonene	55	90	97	99	99	98	99	98	108	97	58	81	102	100	105	103	102	111	105	
Eucalyptol	87	99	99	100	98	100	101	101	102	99	90	99	96	98	99	98	98	102	96	
Benzyl Alcohol	93	102	100	95	98	97	105	108	104	67	102	94	92	94	96	102	108	107	71	
Furaneol	102	88	100	97	102	102	106	104	96	13	104	105	95	101	103	106	104	105	14	
Maltol	45	55	86	93	94	96	104	111	108	93	43	56	79	90	94	100	107	109	98	
L-Menthol	73	82	100	100	101	98	102	101	101	99	61	87	99	99	98	100	99	101	100	
Methyl Salicylate	85	85	95	93	97	100	107	111	106	92	82	81	94	95	97	104	107	107	96	
Ethyl Maltol	45	71	100	91	95	96	104	109	110	94	42	65	95	92	94	103	109	113	100	
(+)Pulegone	98	99	103	95	100	97	101	104	106	96	104	94	103	98	98	101	103	104	99	
Ethyl Salicylate	99	95	94	97	97	100	107	112	107	92	98	93	95	93	98	105	109	110	97	
trans-Cinnamaldehyde	99	98	97	97	101	101	107	104	94	14	103	97	95	97	100	104	106	102	14	
Triacetin	100	98	98	99	98	100	101	104	104	97	93	94	95	93	96	96	99	102	97	
Eugenol	86	95	95	95	97	100	106	110	108	92	87	96	94	96	99	106	110	112	99	
Vanillin	71	70	70	81	96	101	101	105	108	95	67	65	66	80	94	98	104	109	100	
Ethyl Vanillin	91	95	97	96	96	100	103	106	108	95	86	99	95	94	95	102	104	110	99	
Isovanillin	90	98	97	95	96	100	104	106	107	94	92	95	92	95	99	101	104	108	97	
Benzene-d6	107	104	103	103	102	103	100	101	101	101	95	95	94	95	94	95	95	94	96	
Pyridine-d5	105	104	102	102	102	101	100	100	100	100	97	98	97	96	96	96	94	95	95	
Chlorobenzene-d5	107	105	101	102	103	103	100	101	101	102	97	98	97	98	97	97	97	97	97	
Naphthalene-d8	106	104	101	101	101	102	100	100	98	97	96	97	96	96	97	96	95	94	93	
Acenaphthene-d10	107	105	102	102	103	102	100	101	100	99	98	98	98	98	97	98	98	96	95	
Coefficient of Variation (CV) (%)¹																				
Acetoin	N/A	265	125	69	6	7	6	4	3	2	N/A	265	126	70	14	6	5	4	4	

Butanoic Acid	171	171	46	6	4	5	3	2	3	2	171	171	45	9	5	5	3	3	2
Benzaldehyde	6	8	5	3	3	4	3	2	2	3	10	7	7	4	4	3	4	2	4
2,3,5-Trimethylpyrazine	3	6	2	4	3	2	1	2	2	4	7	7	3	5	3	3	3	4	4
DL-Limonene	95	46	9	10	6	3	2	4	3	2	95	46	7	7	8	8	7	5	2
Eucalyptol	44	13	8	9	7	4	3	4	3	2	46	8	8	6	4	3	2	4	2
Benzyl Alcohol	8	6	4	6	3	3	1	3	5	68	11	11	6	5	6	5	4	4	68
Furaneol	5	7	8	3	4	2	4	5	7	265	8	8	9	6	3	2	2	3	265
Maltol	125	94	44	6	3	4	3	3	2	2	125	94	44	4	6	5	3	3	3
L-Menthol	68	45	7	6	6	6	4	3	3	2	70	47	9	5	3	5	2	3	4
Methyl Salicylate	46	44	6	3	3	3	4	2	2	3	44	45	6	4	2	2	4	2	4
Ethyl Maltol	125	69	5	5	4	5	2	2	2	1	125	68	6	5	4	5	1	3	1
(+)Pulegone	7	9	7	5	3	3	3	3	2	2	12	7	7	4	4	2	2	4	1
Ethyl Salicylate	7	5	7	3	2	3	2	1	3	2	4	4	5	3	2	3	1	3	3
trans-Cinnamaldehyde	10	8	4	3	4	3	4	2	6	265	11	6	5	3	3	2	2	5	265
Triacetin	6	8	4	6	4	4	2	2	2	1	15	11	5	2	4	3	2	3	1
Eugenol	44	6	6	1	4	2	4	2	2	3	45	3	4	2	3	4	2	3	2
Vanillin	70	68	69	44	2	4	6	4	3	3	69	69	68	44	6	6	5	4	3
Ethyl Vanillin	45	10	5	8	3	4	3	2	3	1	48	6	6	4	2	5	2	3	4
Isovanillin	45	8	7	5	4	3	3	2	4	3	45	7	6	5	4	8	4	3	2
Benzene-d6	4	6	4	3	3	4	0	2	2	3	4	6	2	4	3	4	4	3	3
Pyridine-d5	5	6	4	5	3	3	0	3	2	2	3	4	4	3	4	4	4	3	3
Chlorobenzene-d5	6	8	4	3	2	1	0	3	2	1	3	5	3	4	2	4	3	2	3
Naphthalene-d8	4	5	2	2	3	3	0	2	2	2	2	3	2	2	2	4	3	3	3
Acenaphthene-d10	7	7	3	3	3	3	0	3	2	3	3	2	2	3	2	4	3	2	2

¹Averaged from 7 independent batches analyzed across 7 days

Italicized and grey indicates values outside of the instrument linear range where recovery is estimated. Bold indicates values outside of 80-120% percent recovery or $\pm 20\%$ CV.

Supplemental Table 5 – Method Validation Parameters for Mid-Range and Low-Range Fortified Matrix Samples Across 7 Batches

Method Validation Measure ¹	Mid-Range Fortified Matrix Samples						LLOQ Fortified Matrix Samples					
	Expected Concentration (mg/mL)											
	0.04	0.10	0.88	1.75	3.5	7.0	0.01	0.04	0.07	0.10	0.27	
Acetoin												
Within Batch Precision (%)												
<i>Batch #</i>	1	8	19	4	7	4	2	---	21	29	7	5
	2	27	4	9	6	3	1	---	33	3	20	11
	3	9	8	3	4	3	4	---	8	4	9	10
	4	6	38	4	6	1	3	---	41	50	19	14
	5	---	5	6	2	6	7	---	---	---	20	15
	6	---	92	5	6	2	5	---	5	---	---	9
	7	---	---	7	4	9	2	---	---	5	29	4
Between Batch Precision (%)		68	33	6	6	6	5	---	50	53	29	12
Between Batch Bias (%)		37	17	2	1	1	1	---	48	0	9	5
Butanoic Acid												
Within Batch Precision (%)												
<i>Batch #</i>	1	8	7	5	5	3	1	19	5	6	9	3
	2	7	10	2	2	3	2	2	5	5	11	2
	3	10	5	0	2	3	2	7	14	7	8	6
	4	4	6	0	1	1	4	7	6	5	5	2
	5	6	3	1	2	2	2	20	8	0	2	5
	6	17	10	4	3	2	1	51	19	14	10	7
	7	11	7	3	3	3	3	---	29	9	3	7
Between Batch Precision (%)		32	14	4	3	3	5	43	30	17	14	8
Between Batch Bias (%)		39	-2	-8	-2	4	1	252	36	4	-4	-13
Benzaldehyde												
Within Batch Precision (%)												
<i>Batch #</i>	1	11	2	5	2	4	5	18	7	4	4	0
	2	6	4	1	3	2	4	15	3	4	1	5
	3	2	3	1	2	3	4	10	4	6	4	4
	4	4	7	3	5	1	1	18	2	3	5	6
	5	11	6	1	1	2	3	21	6	7	13	2
	6	13	4	2	1	3	1	28	1	8	4	5
	7	8	2	1	2	4	0	4	9	4	3	5
Between Batch Precision (%)		8	6	4	5	4	4	30	12	8	7	6

Between Batch Bias (%)	-5	-10	-5	-1	0	-2	-5	-5	-6	-5	-5
-------------------------------	----	-----	----	----	---	----	----	----	----	----	----

2,3,5-Trimethylpyrazine

Within Batch Precision (%)												
Batch #	1	3	2	1	1	1	4	2	7	7	6	2
	2	4	1	2	2	1	2	5	0	5	1	2
	3	7	4	2	2	2	2	7	9	2	4	3
	4	4	3	2	4	0	2	9	11	3	8	0
	5	1	4	2	2	0	2	5	6	3	2	1
	6	2	2	0	1	1	2	13	6	5	7	2
	7	5	5	3	2	3	2	4	5	6	7	2
Between Batch Precision (%)	6	5	2	3	3	3	8	18	9	7	6	3
Between Batch Bias (%)	2	-9	1	7	7	0		19	-4	-7	-6	-8

DL-Limonene

Within Batch Precision (%)												
Batch #	1	6	1	3	7	2	3	3	3	9	5	5
	2	12	9	0	1	1	2	5	9	9	7	7
	3	18	10	3	1	3	1	17	9	7	11	8
	4	12	12	5	5	1	1	89	19	5	8	10
	5	3	11	6	2	2	1	19	3	13	9	1
	6	14	8	5	2	2	1	---	33	17	9	10
	7	12	6	3	3	0	1	8	9	14	5	6
Between Batch Precision (%)	14	10	10	6	4	3	3	46	19	13	9	10
Between Batch Bias (%)	32	11	-2	-17	-5	12		66	11	1	1	-6

Eucalyptol

Within Batch Precision (%)												
Batch #	1	22	12	2	2	2	4	28	26	9	17	11
	2	10	7	4	1	1	2	19	12	11	2	7
	3	8	5	3	5	2	1	10	22	8	8	2
	4	13	4	1	1	1	2	36	1	3	12	10
	5	24	4	2	4	2	1	48	11	25	2	5
	6	25	15	3	3	2	0	76	18	16	14	3
	7	18	9	2	6	1	2	146	6	13	7	7
Between Batch Precision (%)	19	9	3	5	4	4	4	62	19	13	10	8
Between Batch Bias (%)	4	-1	-1	-2	0	-1		-32	-13	-7	-6	-8

Benzyl Alcohol

Within Batch Precision (%)												
Batch #	1	8	6	4	1	4	3	23	1	5	8	5
	2	11	6	4	7	1	1	5	9	10	3	1
	3	14	6	7	2	1	2	14	4	5	2	7

	4	4	4	1	2	1	2	11	11	2	6	3
	5	5	13	4	1	1	2	22	6	6	2	1
	6	4	4	5	3	1	2	13	9	6	2	3
	7	16	3	3	2	3	2	4	8	2	1	2
Between Batch Precision (%)	13	11	7	5	4	4	9	21	13	14	9	11
Between Batch Bias (%)	-1	-7	2	8	8	8	-2	12	1	2	0	0

Furaneol

Within Batch Precision (%)												
Batch #	1	11	8	4	3	4	5	22	15	10	10	5
	2	11	4	4	4	7	---	2	7	3	3	5
	3	9	5	2	4	7	24	7	9	4	6	1
	4	14	1	3	4	6	---	18	13	5	5	5
	5	10	9	6	6	10	---	18	14	9	2	7
	6	19	5	5	2	4	---	10	8	4	11	2
	7	4	3	4	4	13	---	35	9	3	8	2
Between Batch Precision (%)	13	5	4	4	7	7	17	21	12	9	9	5
Between Batch Bias (%)	6	-3	3	5	8	8	7	7	-4	-7	-7	-8

Maltol

Within Batch Precision (%)												
Batch #	1	5	5	0	0	4	3	1	1	4	5	3
	2	3	5	5	3	4	2	8	2	3	4	3
	3	4	2	3	2	2	3	2	3	3	0	3
	4	9	4	1	2	1	0	5	5	5	3	3
	5	5	1	3	1	2	1	4	4	7	2	5
	6	7	4	2	2	2	2	12	8	6	3	2
	7	9	8	3	4	3	2	9	2	3	5	5
Between Batch Precision (%)	37	16	4	3	3	3	5	67	38	23	16	5
Between Batch Bias (%)	42	-2	-3	5	9	9	3	217	34	2	-6	-14

L-Menthol

Within Batch Precision (%)												
Batch #	1	27	16	5	2	3	4	65	17	4	10	11
	2	13	9	1	1	4	3	39	16	7	6	3
	3	14	10	2	3	1	3	34	27	29	11	7
	4	6	13	6	4	1	1	53	33	7	13	9
	5	4	9	1	4	3	2	96	2	7	26	12
	6	10	8	2	2	2	1	88	4	16	8	7
	7	17	14	4	4	2	3	---	20	25	13	3
Between Batch Precision (%)	18	12	4	3	4	4	4	114	29	22	17	8
Between Batch Bias (%)	8	0	-2	-1	0	1	1	-29	6	0	-5	-8

Methyl Salicylate												
Within Batch Precision (%)												
Batch #	1	6	6	2	3	1	2	22	8	8	7	3
	2	2	4	0	1	1	1	14	10	3	1	3
	3	10	2	1	2	1	1	9	5	3	5	3
	4	4	5	3	3	1	1	4	2	5	3	6
	5	2	4	2	3	4	1	7	7	5	3	1
	6	2	2	2	1	2	2	14	6	3	4	8
	7	15	8	3	2	1	2	3	12	3	7	6
Between Batch Precision (%)		18	7	3	3	2	3	54	22	11	9	5
Between Batch Bias (%)		6	-4	0	4	7	0	35	-3	-7	-9	-11

Ethyl Maltol												
Within Batch Precision (%)												
Batch #	1	2	7	2	1	1	1	4	5	9	8	4
	2	1	10	3	2	4	0	9	3	3	9	3
	3	3	6	2	2	1	1	5	2	3	7	3
	4	7	6	1	4	2	1	4	2	11	6	2
	5	9	3	4	3	2	1	5	3	7	8	4
	6	1	6	2	3	2	1	13	5	5	5	4
	7	4	8	3	2	3	2	8	10	4	1	7
Between Batch Precision (%)		18	8	5	5	4	3	40	22	14	10	5
Between Batch Bias (%)		25	-6	-2	7	11	3	148	12	-9	-13	-18

(+)Pulegone												
Within Batch Precision (%)												
Batch #	1	6	11	1	3	1	3	26	13	13	9	5
	2	4	3	3	2	1	0	9	6	4	4	2
	3	5	5	2	2	0	1	13	5	4	4	3
	4	15	4	4	3	1	2	4	6	6	3	3
	5	12	3	2	3	6	1	9	13	6	9	6
	6	1	7	2	3	2	1	13	5	5	9	5
	7	12	13	1	1	2	3	17	4	10	7	0
Between Batch Precision (%)		9	7	3	3	3	3	17	9	9	7	5
Between Batch Bias (%)		1	-7	-4	-1	2	0	7	-4	-10	-7	-7

Ethyl Salicylate												
Within Batch Precision (%)												
Batch #	1	7	6	1	1	0	1	2	13	8	7	3
	2	10	4	0	2	1	1	5	1	6	4	3
	3	1	5	4	1	0	2	8	3	2	5	2
	4	4	4	1	1	2	1	7	8	8	1	4

	5	7	4	2	0	3	1	13	5	2	6	4
	6	10	3	1	3	3	2	6	3	10	4	3
	7	13	4	2	2	1	1	10	4	4	4	4
Between Batch Precision (%)	7	5	2	2	2	2	3	18	8	6	5	4
Between Batch Bias (%)	-2	-6	0	4	8	1		8	-9	-10	-11	-10

trans-Cinnamaldehyde

Within Batch Precision (%)												
Batch #	1	4	4	4	4	4	1	2	4	5	2	4
	2	3	7	2	5	5	---	23	10	2	7	4
	3	1	4	4	2	5	13	18	13	4	4	3
	4	9	5	2	1	8	13	8	11	11	3	4
	5	5	5	2	2	11	---	7	2	5	8	5
	6	9	8	5	6	7	---	6	11	3	5	3
	7	9	4	2	2	11	---	29	9	4	9	4
Between Batch Precision (%)	9	6	5	5	8	8	11	19	10	6	7	5
Between Batch Bias (%)	-3	-13	-5	-2	-1	-18		9	-6	-7	-9	-8

Triacetin

Within Batch Precision (%)												
Batch #	1	14	3	1	3	2	2	28	16	2	4	6
	2	3	4	4	1	2	1	40	4	3	5	5
	3	8	6	3	3	2	2	33	11	5	3	3
	4	16	8	5	4	1	3	36	9	7	9	0
	5	12	12	4	3	3	1	16	22	8	5	4
	6	20	8	6	1	3	1	40	12	7	9	9
	7	4	4	5	3	3	1	45	4	12	4	8
Between Batch Precision (%)	16	7	4	3	3	3	3	41	19	11	8	8
Between Batch Bias (%)	-6	-7	-4	-1	1	-2		-7	-8	-11	-8	-13

Eugenol

Within Batch Precision (%)												
Batch #	1	0	4	4	3	2	3	7	8	2	8	2
	2	1	6	1	2	1	3	3	7	3	4	3
	3	3	4	1	3	2	3	4	4	3	4	2
	4	4	5	2	3	3	2	13	4	7	8	7
	5	10	5	1	2	5	1	11	7	10	5	4
	6	5	4	3	1	1	2	5	8	6	4	4
	7	7	2	2	1	3	3	13	13	8	3	0
Between Batch Precision (%)	11	5	3	3	3	3	3	30	14	8	6	4
Between Batch Bias (%)	-1	-10	-1	5	9	0		13	-15	-20	-21	-22

Vanillin

Within Batch Precision (%)												
Batch #	1	4	2	1	1	4	3	4	5	3	5	4
	2	10	9	1	2	1	2	5	5	8	9	3
	3	4	4	3	3	1	3	41	14	7	5	7
	4	5	3	3	3	1	1	4	9	3	3	7
	5	18	3	4	3	3	1	21	17	2	5	2
	6	11	2	1	2	3	1	10	2	7	7	5
	7	16	3	3	1	4	2	10	6	3	2	5
Between Batch Precision (%)		35	13	6	7	5	6	86	41	21	14	9
Between Batch Bias (%)		31	-3	-5	1	7	2	97	17	-3	-11	-20

Ethyl Vanillin

Within Batch Precision (%)												
Batch #	1	2	7	1	3	2	3	21	10	7	21	2
	2	16	7	2	4	0	2	8	17	1	2	4
	3	9	4	2	3	1	1	35	9	9	4	5
	4	4	6	5	2	2	2	13	19	9	9	1
	5	16	7	4	2	4	1	75	6	8	9	4
	6	9	2	2	2	2	2	20	4	13	12	10
	7	13	4	2	3	3	2	9	8	7	5	5
Between Batch Precision (%)		13	6	3	3	3	4	47	15	9	11	10
Between Batch Bias (%)		5	-6	1	5	9	2	9	-7	-7	-16	-15

Isovanillin

Within Batch Precision (%)												
Batch #	1	14	2	3	3	2	4	5	8	3	4	8
	2	1	1	1	5	6	4	10	4	10	5	3
	3	2	7	4	5	7	2	57	4	8	6	4
	4	11	8	5	6	5	6	39	11	3	6	2
	5	9	8	1	5	2	6	14	5	11	3	3
	6	3	1	4	2	5	6	27	8	3	11	2
	7	11	3	6	1	6	3	23	16	7	5	1
Between Batch Precision (%)		12	5	5	4	5	5	49	10	9	7	6
Between Batch Bias (%)		1	-7	1	5	8	1	11	-6	-14	-12	-12

¹Averaged from 7 independent batches analyzed across 7 days

Italicized and grey indicates values outside of the instrument linear range where recovery is estimated. Bold indicates values outside of 80-120% percent recovery or $\pm 20\%$ CV.

Supplemental Table 6 – Carryover Assessment with 50:50 PG:VG and Methanol Matrix Blanks

<i>Matrix blank assessed</i>	<i>50:50 PG:VG</i>		<i>Methanol</i>	
	<i>8mg/mL</i>	<i>10mg/mL</i>	<i>8mg/mL</i>	<i>10mg/mL</i>
<i>Standard concentration injected prior to matrix blank</i>				
<i>Average Carryover (mg/mL)</i>				
Acetoin	0.00	0.00	0.00	0.00
Butanoic Acid	0.04	0.04	0.00	0.00
Benzaldehyde	0.00	0.00	0.00	0.00
2,3,5-Trimethylpyrazine	0.00	0.00	0.00	0.00
DL-Limonene	0.00	0.00	0.00	0.00
Eucalyptol	0.00	0.00	0.00	0.00
Benzyl Alcohol	0.00	0.00	0.00	0.00
Furaneol	0.00	0.00	0.00	0.00
Maltol	0.04	0.04	0.03	0.03
L-Menthol	0.00	0.00	0.00	0.00
Methyl Salicylate	0.00	0.00	0.00	0.00
Ethyl Maltol	0.03	0.03	0.02	0.01
(+)Pulegone	0.00	0.00	0.00	0.00
Ethyl Salicylate	0.00	0.00	0.00	0.00
trans-Cinnamaldehyde	0.00	0.00	0.01	0.01
Triacetin	0.00	0.00	0.00	0.00
Eugenol	0.00	0.00	0.00	0.00
Vanillin	0.05	0.00	0.04	0.00
Ethyl Vanillin	0.01	0.00	0.00	0.00
Isovanillin	0.00	0.01	0.02	0.01

Supplemental Table 7 – Dilution Precision and Bias Determined from Four Dilution Factors

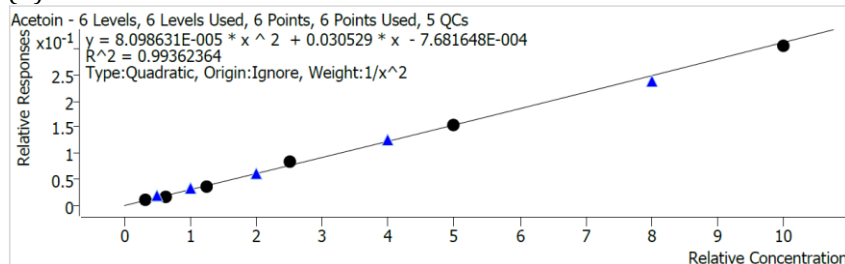
<i>Dilution Factor</i>	2X			5X			10X		50X	
<i>Fortified Matrix Sample Concentration (mg/mL)</i>	5	10	18.6	5	10	18.6	10	18.6	10	18.6
<i>Concentration after dilution (mg/mL)</i>	2.5	5	9.3	1	2	3.72	1	1.86	0.2	0.372
<i>Between Run Precision (CV%)</i>										
Acetoin	7	7	2	7	9	6	11	6	17	17
Butanoic Acid	14	16	19	15	13	4	20	5	16	14
Benzaldehyde	3	2	6	3	5	6	9	5	8	11
2,3,5-Trimethylpyrazine	5	6	10	7	6	5	7	4	9	16
DL-Limonene	10	7	16	13	13	14	19	8	11	7
Eucalyptol	4	3	10	4	5	4	9	7	7	8
Benzyl Alcohol	10	4	14	26	18	7	23	21	41	46
Furaneol	11	17	28	11	19	27	18	17	10	23
Maltol	4	6	5	3	6	3	6	6	9	10
L-Menthol	3	5	10	4	5	4	6	6	5	14
Methyl Salicylate	4	3	9	6	4	4	7	6	6	16
Ethyl Maltol	4	4	3	5	6	5	7	7	12	13
(+)Pulegone	5	2	9	6	6	4	5	5	8	17
Ethyl Salicylate	3	5	10	3	3	5	6	5	6	13
trans-Cinnamaldehyde	4	12	---	9	15	13	19	17	15	23
Triacetin	4	4	8	7	6	5	7	6	13	20
Eugenol	4	4	7	5	5	4	6	3	8	17
Vanillin	9	7	9	7	7	8	8	9	16	19
Ethyl Vanillin	5	6	3	8	4	6	5	7	14	17
Isovanillin	5	2	19	5	4	13	9	15	11	23
<i>Between Run Bias (CV%)</i>										
Acetoin	9	6	-2	7	1	-7	17	-10	19	-14
Butanoic Acid	-11	-5	-14	-17	-14	-3	-14	-4	-14	-33
Benzaldehyde	16	16	0	14	16	7	25	6	16	-10
2,3,5-Trimethylpyrazine	14	8	-5	10	10	3	21	5	13	-15
DL-Limonene	26	28	-9	11	42	8	41	1	45	4
Eucalyptol	5	7	-9	3	5	-9	14	-10	8	-23
Benzyl Alcohol	24	10	-12	33	25	6	47	20	54	19
Furaneol	-11	-21	-37	-18	-26	-42	-14	-38	-11	-39

Maltol	11	13	-3	0	9	5	14	1	-2	-26
L-Menthol	5	9	-4	5	7	-4	22	1	29	-6
Methyl Salicylate	13	12	-10	8	17	3	24	5	15	-13
Ethyl Maltol	13	13	-6	2	11	0	13	-4	-3	-28
(+)Pulegone	9	7	-9	6	6	-5	17	-2	18	-11
Ethyl Salicylate	20	14	-9	16	21	6	31	10	20	-9
trans-Cinnamaldehyde	15	9	-8	7	-4	-13	7	-14	19	-17
Triacetin	6	5	-8	4	6	-7	15	-5	16	-15
Eugenol	15	10	-8	9	12	1	19	3	12	-14
Vanillin	-1	-8	7	-5	-13	1	-7	2	<i>-8</i>	-15
Ethyl Vanillin	6	-5	11	1	-7	8	2	9	-1	-6
Isovanillin	-2	-18	53	-4	-26	20	-21	17	-19	1

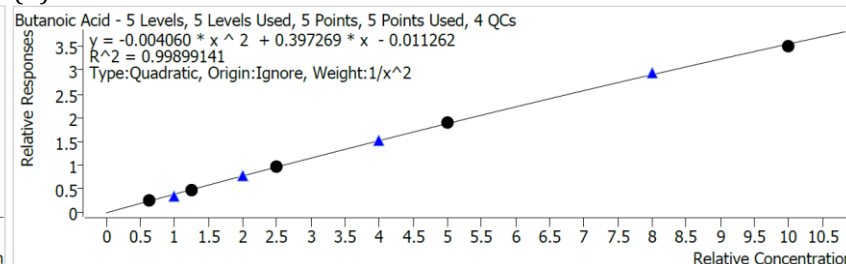
Italicized and grey indicates values outside of the instrument linear range where recovery is estimated. Bold indicates values outside of $\pm 20\%$ CV.

Supplemental Figure 1 – Calibration Curves for Twenty Flavoring Chemicals

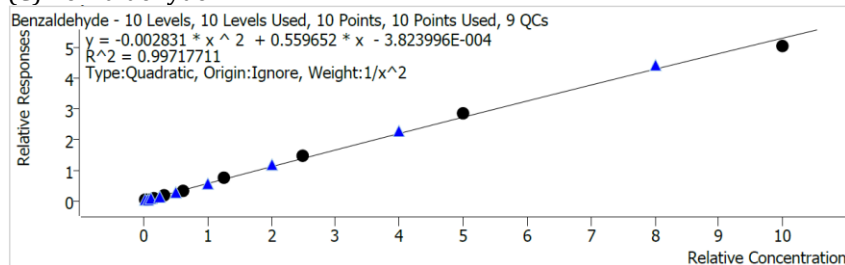
(A) Acetoin



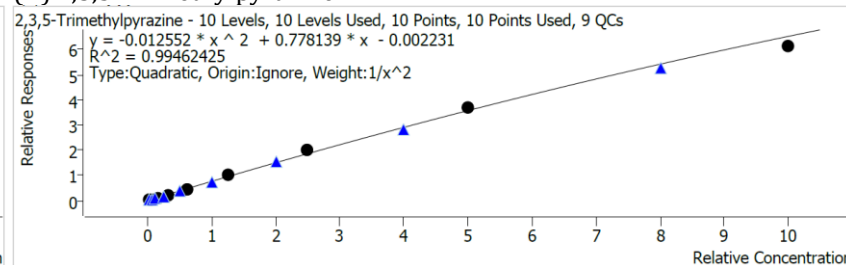
(B) Butanoic Acid



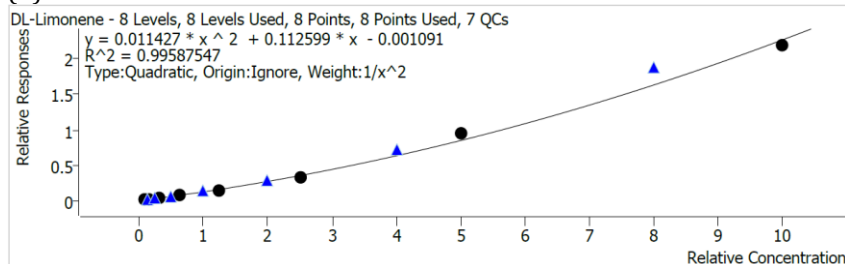
(C) Benzaldehyde



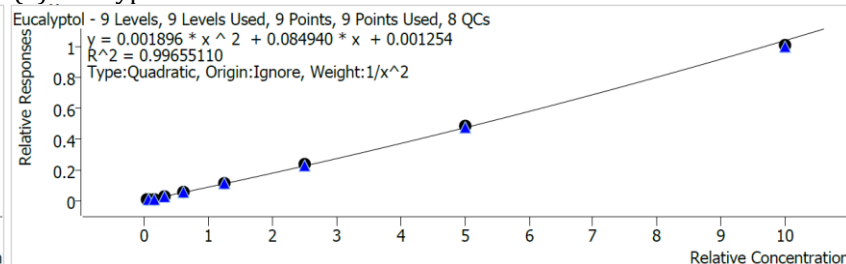
(D) 2,3,5-Trimethylpyrazine



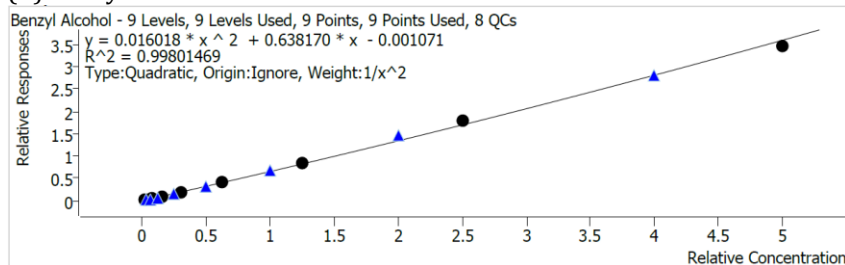
(E) DL-Limonene



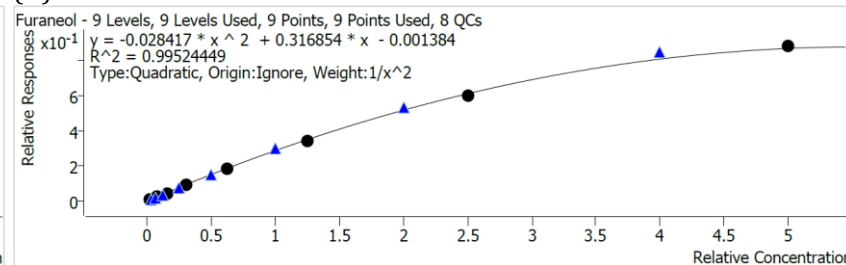
(F) Eucalyptol



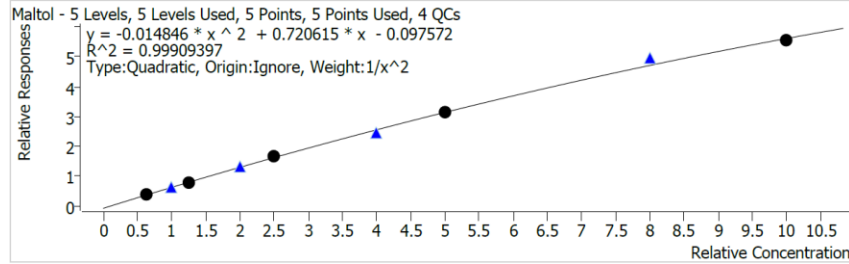
(G) Benzyl Alcohol



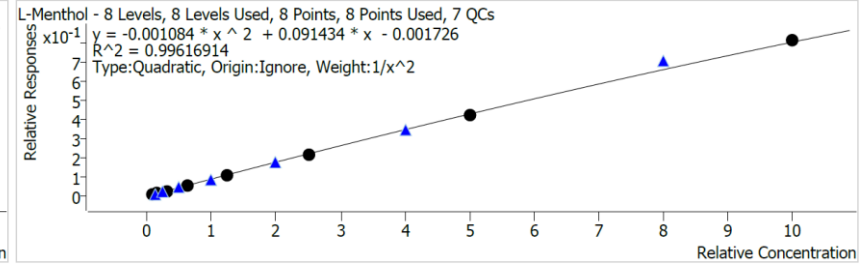
(H) Furaneol



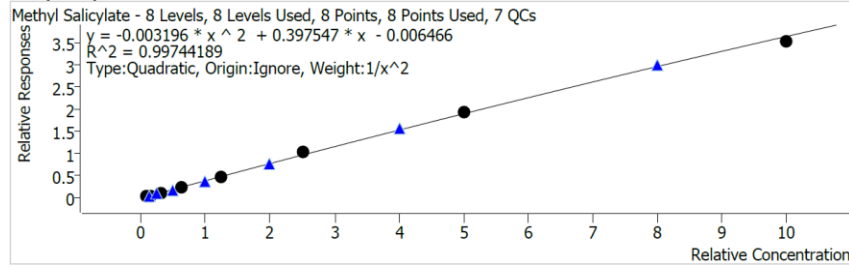
(I) Maltol



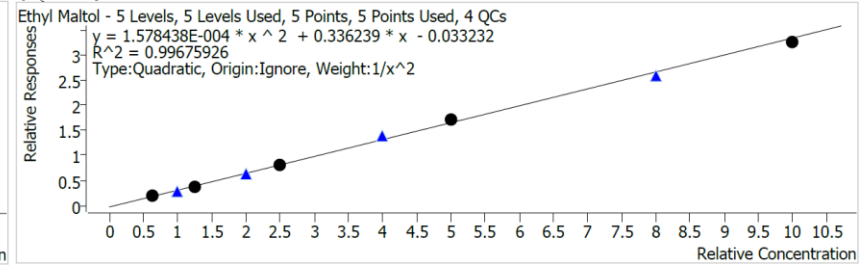
(J) L-Menthol



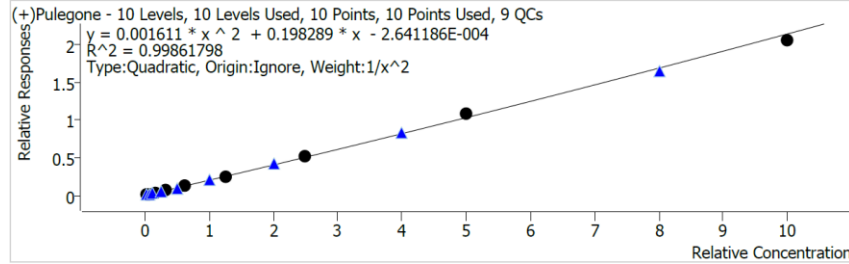
(K) Methyl Salicylate



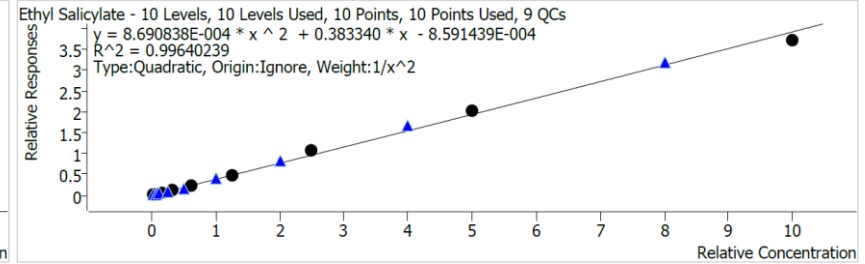
(L) Ethyl Maltol



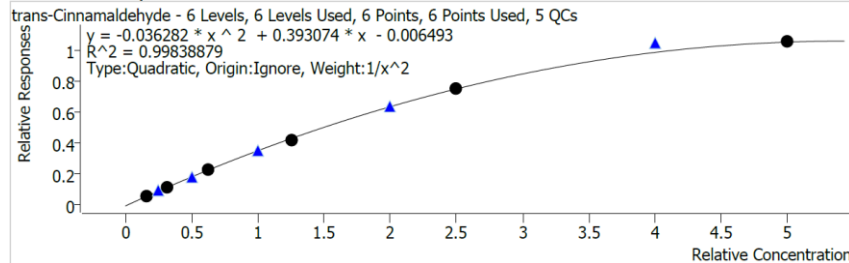
(M) (+)Pulegone



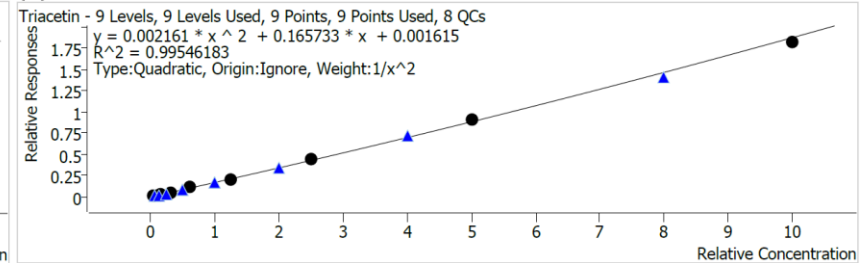
(N) Ethyl Salicylate



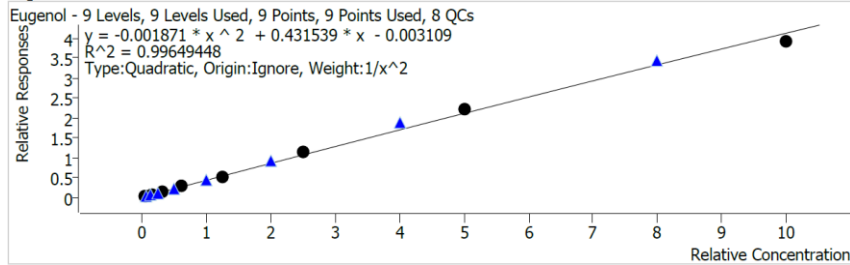
(O) trans-Cinnamaldehyde



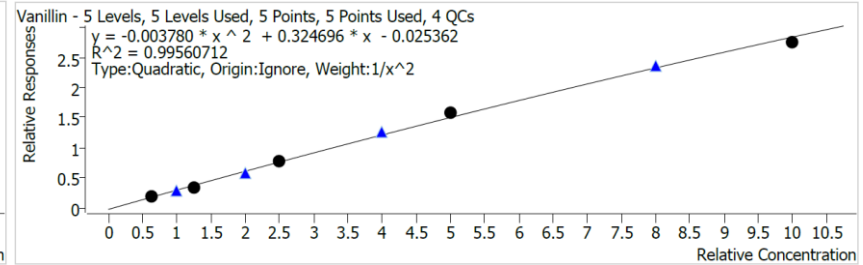
(P) Triacetin



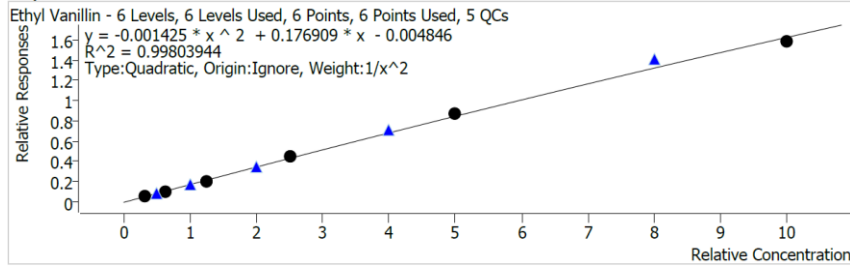
(Q) Eugenol



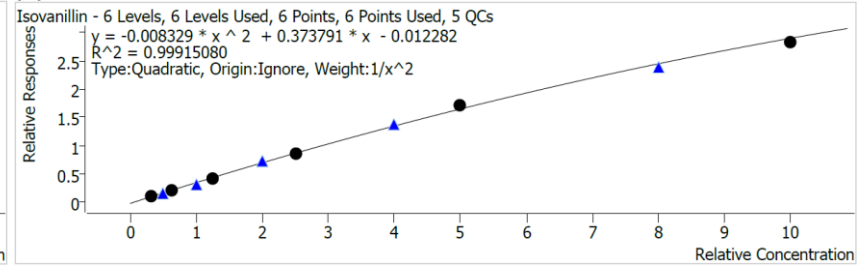
(R) Vanillin



(S) Ethyl Vanillin



(T) Isovanillin



Circles (black) indicate calibration standards within the working calibration range (Supplemental Table 3) and are included in the calculation of the curve and corresponding r² value.

Triangles (blue) indicate quality control standards within the working calibration range.