

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
 Data File : BM048296.D
 Acq On : 29 Oct 2024 20:41
 Operator : RC/JU
 Sample : P4493-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A4EC1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM048296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.169	28	31	38	rVB	46877	62595	1.17%	0.116%
2	3.587	99	102	116	rBV	232876	377044	7.03%	0.697%
3	3.810	136	140	149	rVB4	19804	30962	0.58%	0.057%
4	3.910	154	157	161	rVB4	12719	17559	0.33%	0.032%
5	4.198	204	206	209	rVB2	9459	9864	0.18%	0.018%
6	4.275	215	219	226	rVB6	17611	29328	0.55%	0.054%
7	5.057	346	352	358	rBV8	10286	18070	0.34%	0.033%
8	5.228	376	381	391	rVB3	20290	37704	0.70%	0.070%
9	5.769	468	473	476	rBV	44377	68190	1.27%	0.126%
10	5.804	476	479	489	rVB	127182	189539	3.53%	0.350%
11	6.369	568	575	584	rBV2	62770	103816	1.94%	0.192%
12	6.734	633	637	644	rBV6	12667	24940	0.47%	0.046%
13	6.892	655	664	675	rVB	166182	306516	5.72%	0.566%
14	7.051	685	691	702	rBV	664136	1065163	19.86%	1.968%
15	7.251	718	725	736	rBV	684301	1120967	20.91%	2.071%
16	7.339	736	740	747	rVB10	8471	14373	0.27%	0.027%
17	7.504	764	768	772	rBV3	11824	20753	0.39%	0.038%
18	7.716	797	804	810	rBV	563451	911201	16.99%	1.684%
19	7.781	810	815	828	rVB	124563	215775	4.02%	0.399%
20	7.875	828	831	837	rVB8	10561	17248	0.32%	0.032%
21	7.963	840	846	851	rBV2	56451	107946	2.01%	0.199%
22	8.334	906	909	913	rVB4	9408	13392	0.25%	0.025%
23	8.428	919	925	934	rBV	516606	882821	16.46%	1.631%
24	8.504	934	938	942	rVV	56911	98003	1.83%	0.181%
25	8.539	942	944	949	rVV3	26239	37128	0.69%	0.069%
26	8.581	949	951	956	rVB6	7522	10236	0.19%	0.019%
27	8.810	983	990	994	rBV2	75895	137159	2.56%	0.253%
28	8.869	994	1000	1010	rVV	734744	1258053	23.46%	2.324%
29	8.963	1010	1016	1020	rVV2	158688	263229	4.91%	0.486%
30	9.028	1020	1027	1040	rVB2	174872	457024	8.52%	0.844%
31	9.298	1067	1073	1081	rVB3	24674	51573	0.96%	0.095%
32	9.439	1091	1097	1105	rVB10	12827	28101	0.52%	0.052%
33	9.592	1115	1123	1140	rBV	617320	1113446	20.77%	2.057%
34	9.769	1146	1153	1163	rBV3	118939	246603	4.60%	0.456%
35	9.845	1163	1166	1173	rVB7	19011	38111	0.71%	0.070%
36	9.980	1184	1189	1202	rVB3	109784	247932	4.62%	0.458%

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Stop Thrs : 0

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
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37	10.133	1207	1215	1236	rBV	934639	1657226	30.91%	3.062%
38	10.292	1236	1242	1249	rBV7	33383	65913	1.23%	0.122%
39	10.369	1249	1255	1258	rVB6	11860	20650	0.39%	0.038%
40	10.416	1258	1263	1271	rVB9	15761	34384	0.64%	0.064%
41	10.504	1271	1278	1286	rBV	781777	1379603	25.73%	2.549%
42	10.645	1294	1302	1321	rBV	654776	1373192	25.61%	2.537%
43	10.798	1323	1328	1336	rVV4	74087	155642	2.90%	0.288%
44	10.904	1340	1346	1355	rVB2	35427	76263	1.42%	0.141%
45	11.051	1365	1371	1376	rBV3	18212	39097	0.73%	0.072%
46	11.110	1376	1381	1386	rVV3	16987	32462	0.61%	0.060%
47	11.157	1386	1389	1397	rVB2	18371	33590	0.63%	0.062%
48	11.316	1402	1416	1429	rBV2	26000	81399	1.52%	0.150%
49	11.527	1448	1452	1457	rVB6	7163	11391	0.21%	0.021%
50	11.674	1472	1477	1483	rBV8	6382	12297	0.23%	0.023%
51	11.792	1488	1497	1502	rBV	26072	44202	0.82%	0.082%
52	11.910	1513	1517	1519	rBV5	10287	16653	0.31%	0.031%
53	12.098	1543	1549	1557	rVB4	13816	26313	0.49%	0.049%
54	12.257	1573	1576	1585	rVB9	5413	10452	0.19%	0.019%
55	12.474	1610	1613	1617	rBV5	6390	9797	0.18%	0.018%
56	12.645	1636	1642	1648	rBV6	6519	12821	0.24%	0.024%
57	12.716	1648	1654	1668	rVV2	79425	166464	3.10%	0.308%
58	12.821	1668	1672	1678	rVB3	7317	13314	0.25%	0.025%
59	12.910	1683	1687	1692	rBV2	10815	15683	0.29%	0.029%
60	12.963	1692	1696	1705	rVB	115161	171592	3.20%	0.317%
61	13.204	1729	1737	1740	rBV7	9737	18532	0.35%	0.034%
62	13.292	1740	1752	1766	rVV3	83958	252788	4.71%	0.467%
63	13.486	1779	1785	1788	rBV7	9228	14794	0.28%	0.027%
64	13.598	1797	1804	1814	rVB4	38623	73452	1.37%	0.136%
65	13.768	1826	1833	1850	rBV	1800207	2522216	47.04%	4.660%
66	13.898	1850	1855	1860	rVB6	25307	37045	0.69%	0.068%
67	14.051	1869	1881	1892	rBV	1940047	2949137	55.00%	5.449%
68	14.233	1907	1912	1921	rVB4	21023	40472	0.75%	0.075%
69	14.357	1921	1933	1945	rBV3	1366808	2460443	45.89%	4.546%
70	14.445	1945	1948	1952	rVB4	10604	14449	0.27%	0.027%
71	14.598	1966	1974	1989	rBV3	61511	192240	3.59%	0.355%
72	14.798	2001	2008	2011	rBV9	7267	14038	0.26%	0.026%
73	15.051	2042	2051	2056	rBV4	17041	37445	0.70%	0.069%
74	15.104	2056	2060	2066	rVV	22920	35722	0.67%	0.066%
75	15.180	2066	2073	2080	rVV3	34481	66453	1.24%	0.123%
76	15.351	2094	2102	2116	rBV	2690625	3830368	71.44%	7.077%

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 Title : SVOA CALIBRATION

77	15.480	2118	2124	2140	rVV	821602	1251527	23.34%	2.312%
78	15.592	2140	2143	2148	rVB5	14309	21665	0.40%	0.040%
79	15.721	2157	2165	2171	rBV4	22486	38270	0.71%	0.071%
80	15.915	2194	2198	2204	rVB6	12994	22296	0.42%	0.041%
81	16.062	2217	2223	2229	rBV5	18116	35981	0.67%	0.066%
82	16.133	2229	2235	2258	rVV2	71292	205861	3.84%	0.380%
83	17.098	2392	2399	2406	rBV	1401312	1964062	36.63%	3.629%
84	17.198	2409	2416	2429	rVV2	2941391	4298796	80.17%	7.943%
85	17.327	2434	2438	2443	rVV	35854	52123	0.97%	0.096%
86	17.386	2444	2448	2454	rVB	14473	21209	0.40%	0.039%
87	17.774	2508	2514	2524	rVV	2474282	3034113	56.59%	5.606%
88	17.998	2548	2552	2561	rVV4	35439	58040	1.08%	0.107%
89	18.068	2561	2564	2565	rVV2	19043	20918	0.39%	0.039%
90	18.092	2565	2568	2576	rVB8	23479	38701	0.72%	0.072%
91	18.209	2584	2588	2591	rBV2	15639	22148	0.41%	0.041%
92	18.251	2591	2595	2598	rVV3	17595	24728	0.46%	0.046%
93	19.056	2728	2732	2735	rBV2	38836	51996	0.97%	0.096%
94	19.127	2740	2744	2748	rBV	37350	55010	1.03%	0.102%
95	19.280	2766	2770	2774	rBV3	35655	51703	0.96%	0.096%
96	19.421	2789	2794	2798	rBV6	29769	48255	0.90%	0.089%
97	19.492	2800	2806	2820	rVV	3746188	5258378	98.07%	9.716%
98	21.321	3112	3117	3130	rBV	1345062	2150895	40.11%	3.974%
99	24.068	3575	3584	3603	rVB	2144214	5362013	100.00%	9.907%
100	24.268	3610	3618	3636	rVB	926590	2381620	44.42%	4.400%

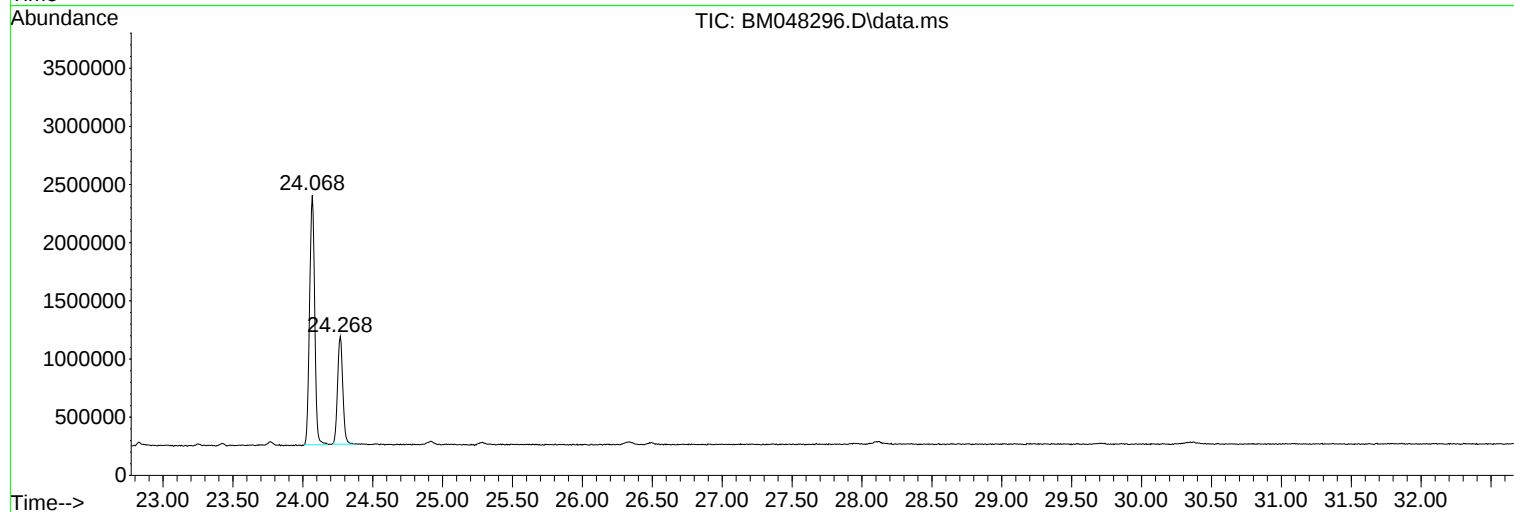
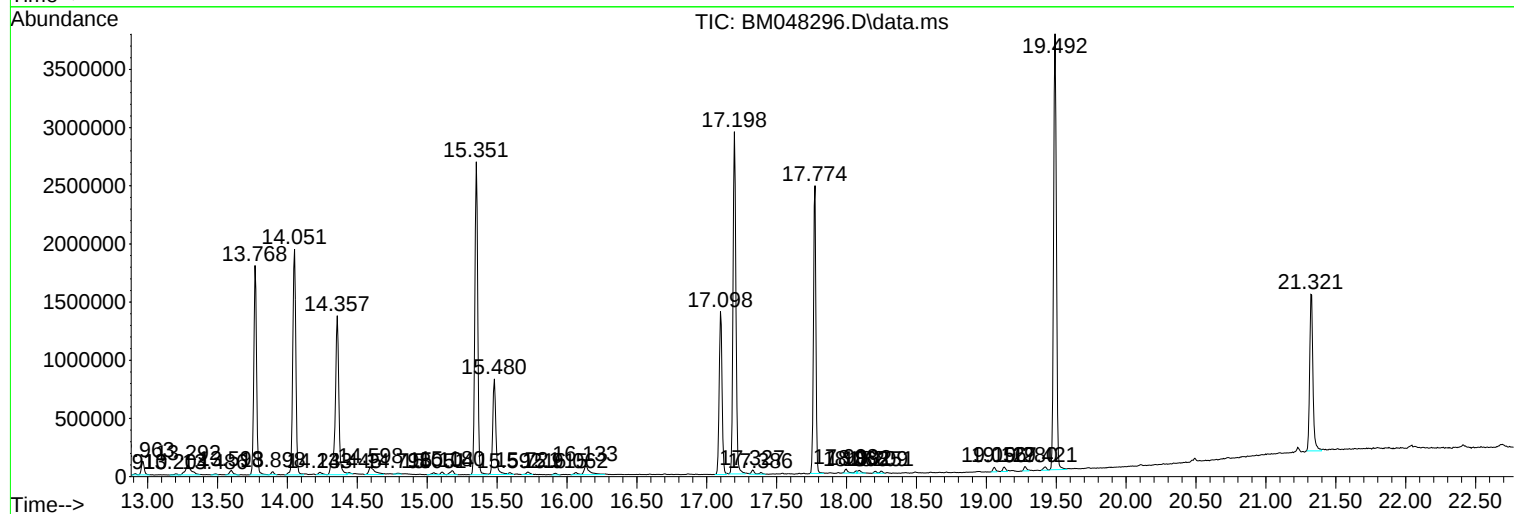
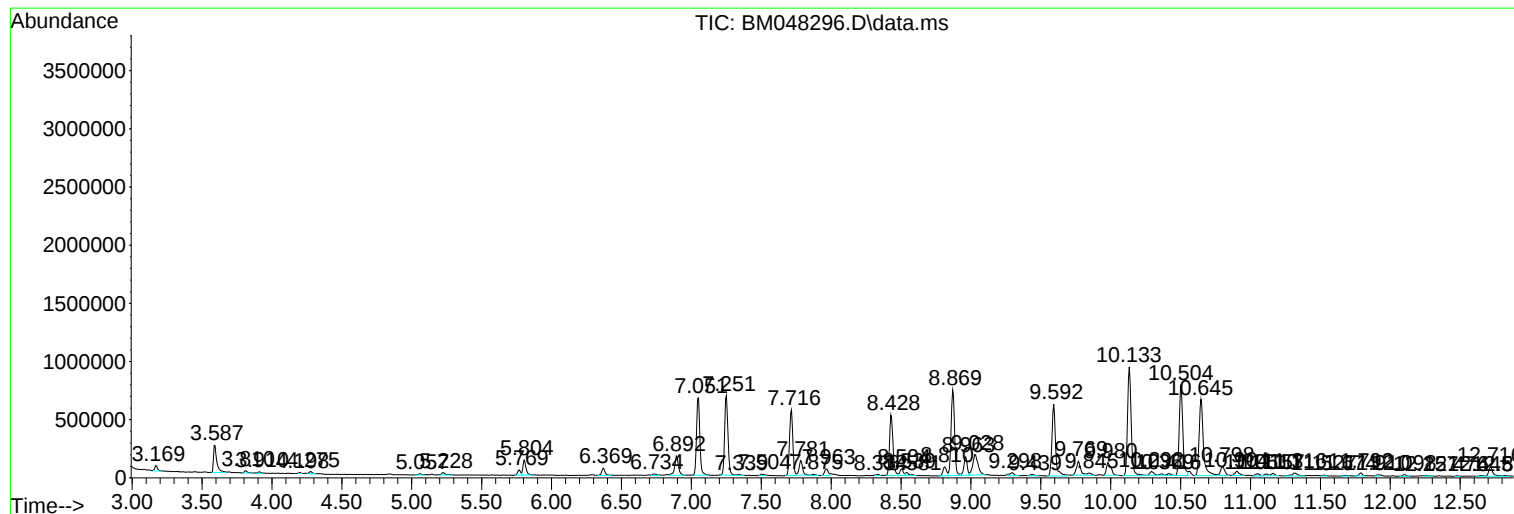
Sum of corrected areas: 54122666

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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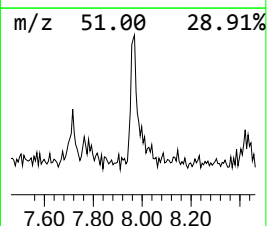
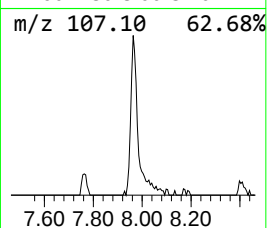
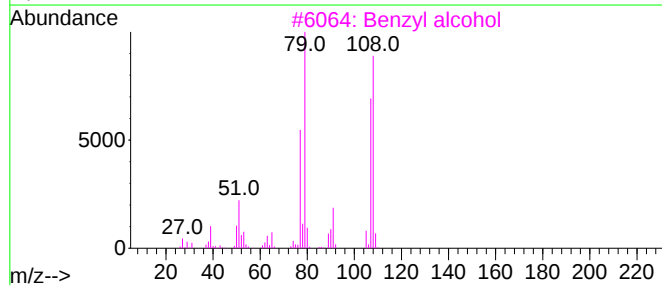
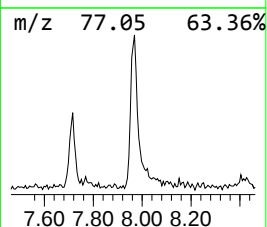
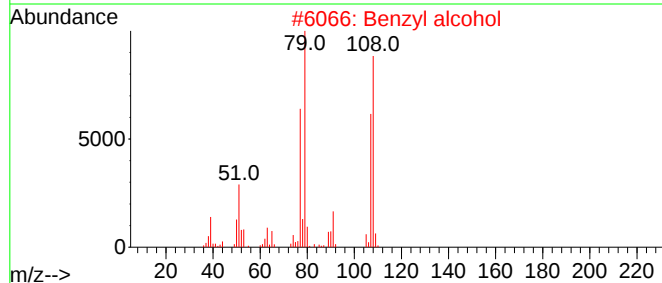
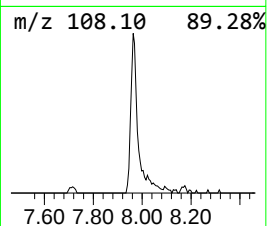
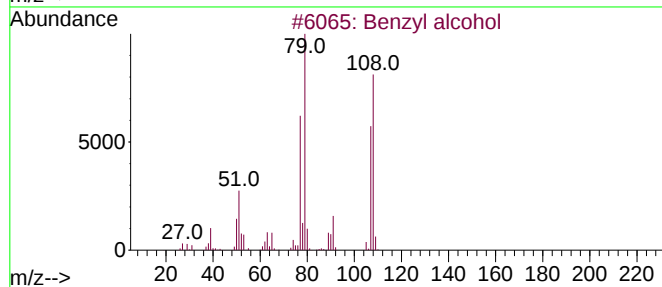
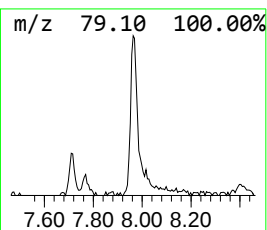
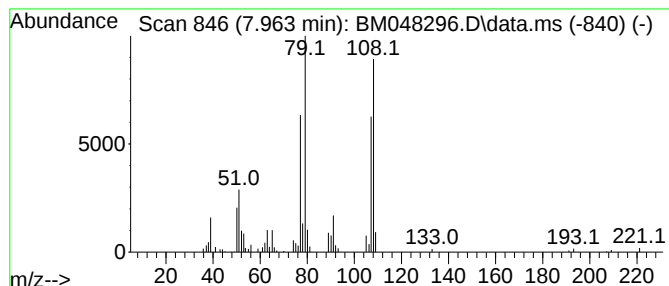
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzyl alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.963	2.37 ng/ul	107946	1,4-Dichlorobenzene-d4	7.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl alcohol	108	C7H8O	000100-51-6	95
2			Benzyl alcohol	108	C7H8O	000100-51-6	94
3			Benzyl alcohol	108	C7H8O	000100-51-6	94
4			Benzyl alcohol	108	C7H8O	000100-51-6	93
5			N-Cbz-glycylglycine p-nitropheny...	387	C18H17N3O7	013574-81-7	91



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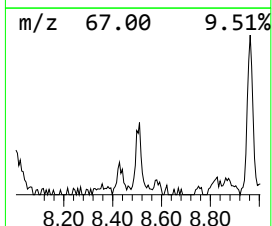
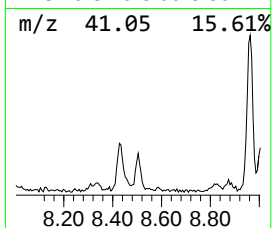
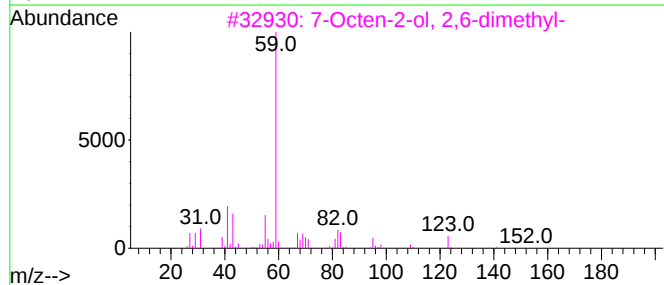
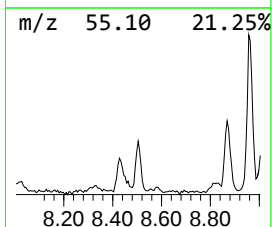
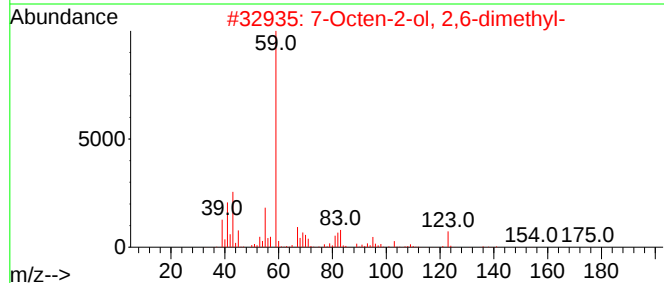
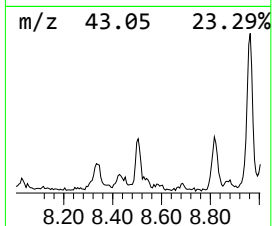
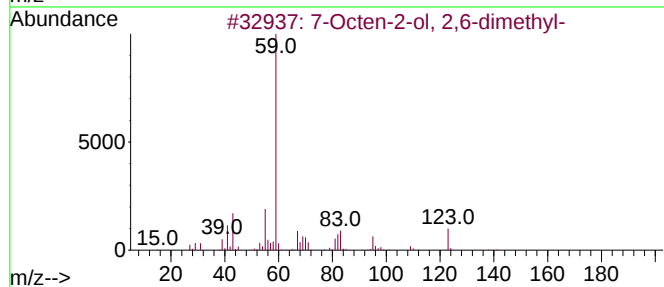
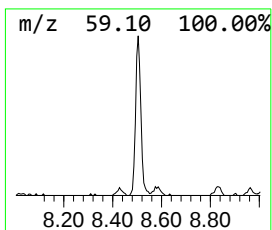
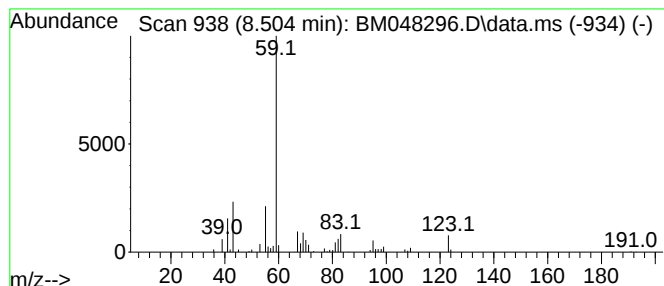
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.504	2.15 ng/ul	98003	1,4-Dichlorobenzene-d4	7.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	90
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	64
5			Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	64



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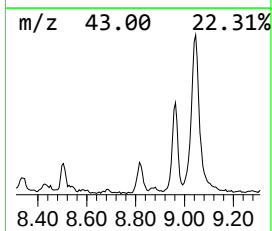
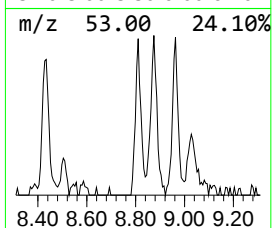
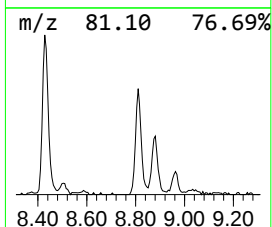
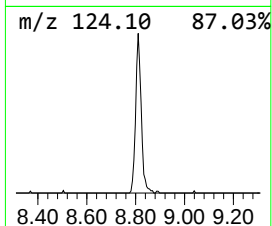
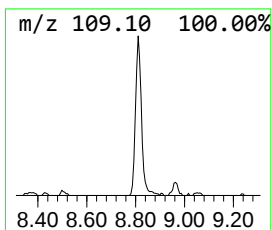
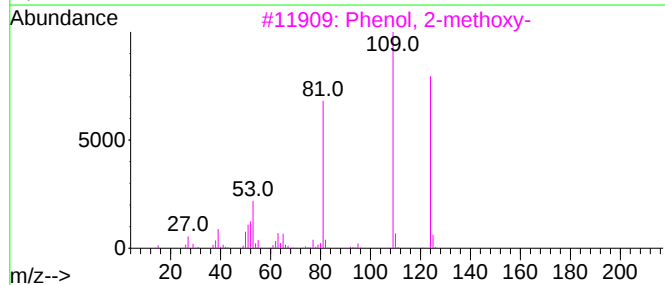
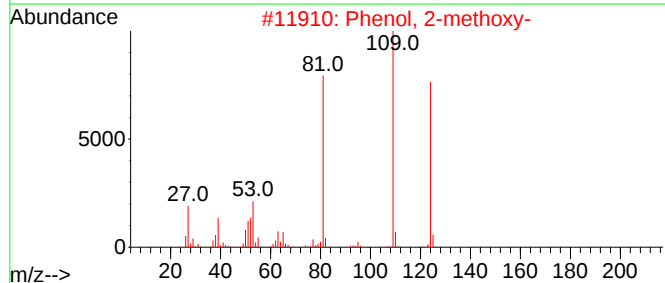
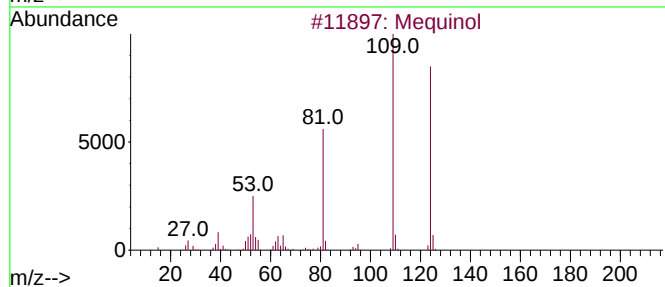
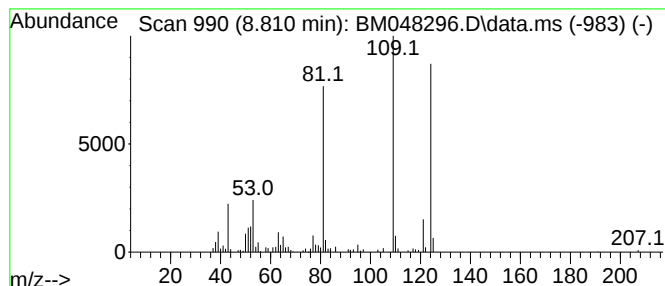
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Mequinol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.810	3.01 ng/ul	137159	1,4-Dichlorobenzene-d4	7.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mequinol	124	C7H8O2	000150-76-5	94
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	93
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	93
4			Mequinol	124	C7H8O2	000150-76-5	91
5			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048296.D
Acq On : 29 Oct 2024 20:41
Operator : RC/JU
Sample : P4493-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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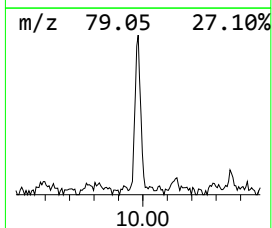
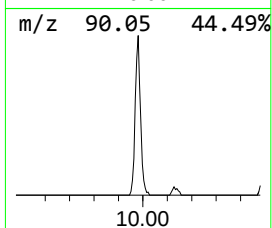
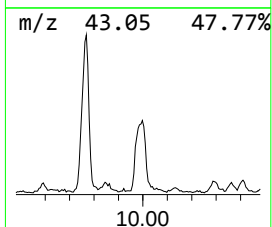
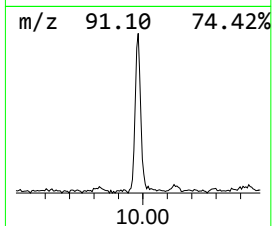
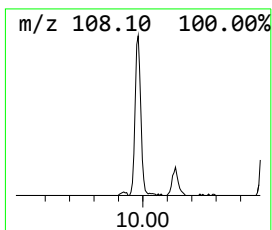
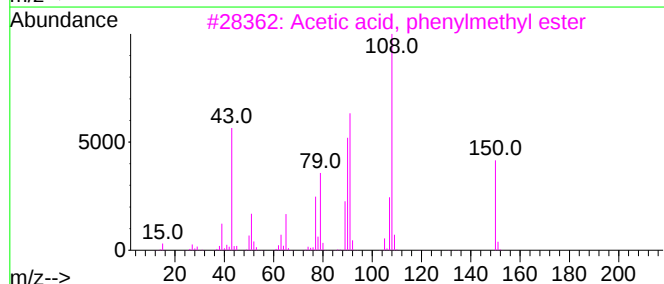
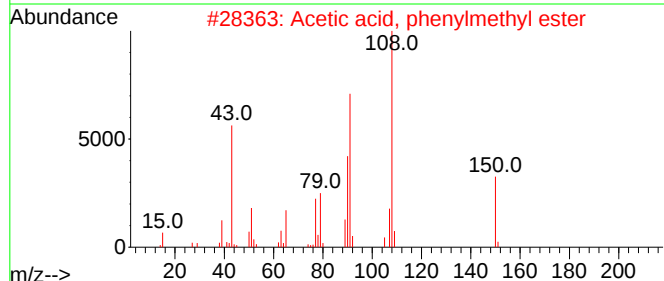
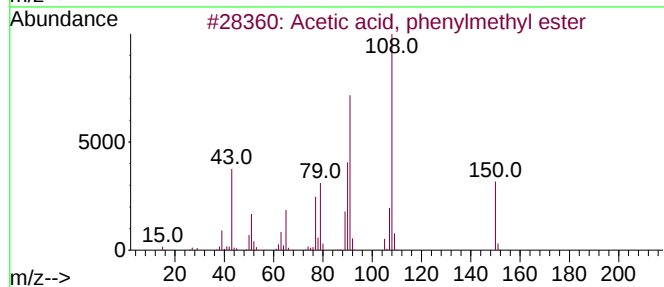
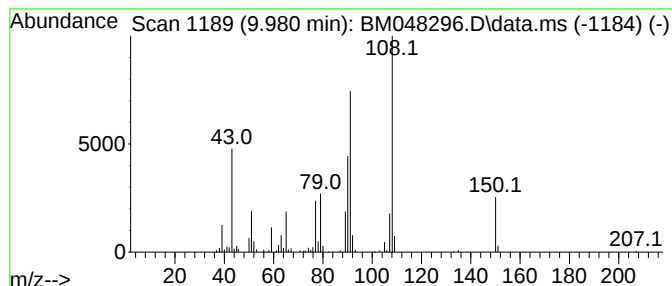
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Acetic acid, phenylmethyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	3.59 ng/ul	247932	Naphthalene-d8	10.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	98
2			Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	96
3			Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	90
4			Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	87
5			Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048296.D
Acq On : 29 Oct 2024 20:41
Operator : RC/JU
Sample : P4493-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4EC1

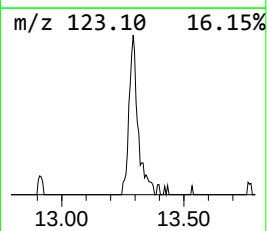
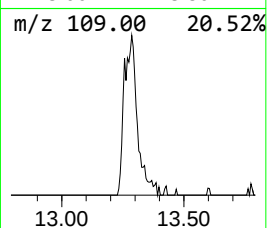
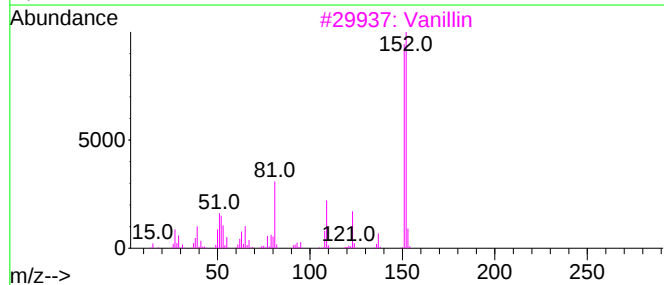
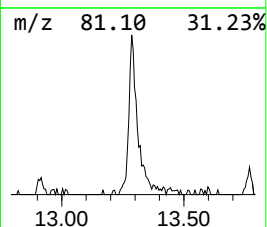
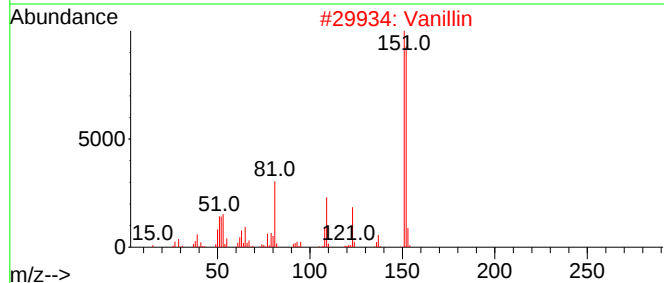
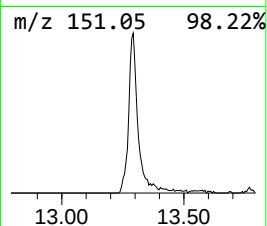
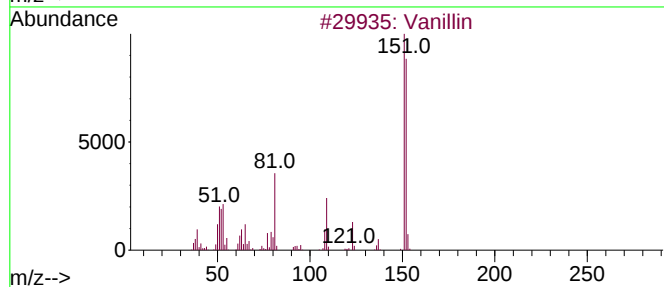
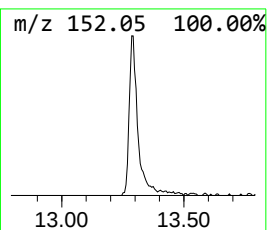
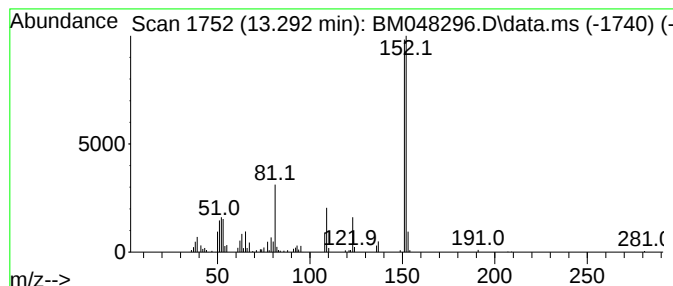
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Vanillin Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	2.05 ng/ul	252788	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	97
2			Vanillin	152	C8H8O3	000121-33-5	96
3			Vanillin	152	C8H8O3	000121-33-5	96
4			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
5			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048296.D
Acq On : 29 Oct 2024 20:41
Operator : RC/JU
Sample : P4493-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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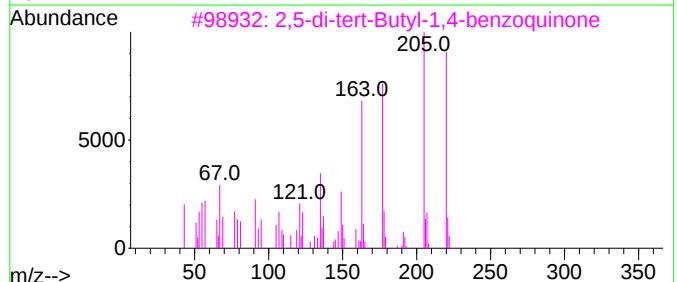
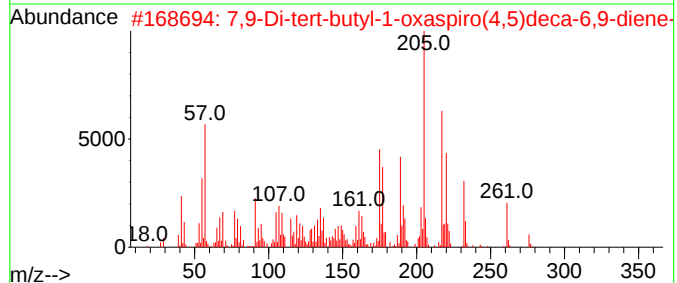
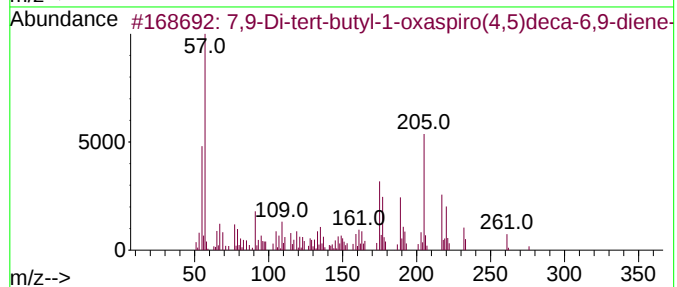
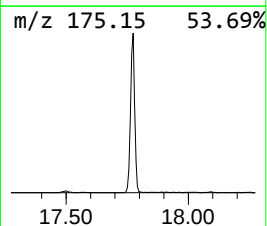
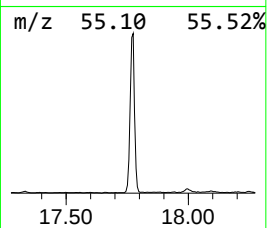
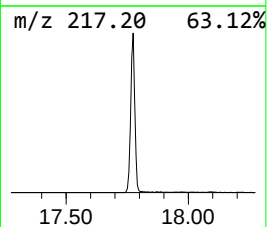
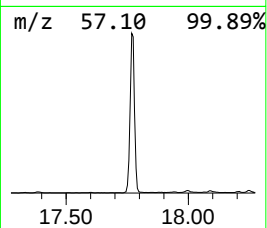
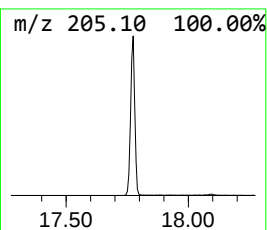
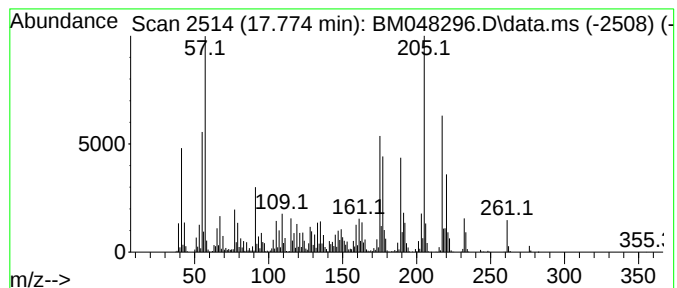
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.774	30.90 ng/ul	3034110	Phenanthrene-d10	17.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90		
3	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	70		
4	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	55		
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102824\
Data File : BM048296.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM102624.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzyl alcohol	7.963	2.4	ng/ul	107946	1	7.716	911201	20.0
7-Octen-2-ol, 2...	8.504	2.1	ng/ul	98003	1	7.716	911201	20.0
Mequinol	8.810	3.0	ng/ul	137159	1	7.716	911201	20.0
Acetic acid, ph...	9.980	3.6	ng/ul	247932	2	10.504	1379600	20.0
Vanillin	13.292	2.0	ng/ul	252788	3	14.357	2460440	20.0
7,9-Di-tert-but...	17.774	30.9	ng/ul	3034110	4	17.098	1964060	20.0