LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101723\
Data File : BM042335.D
Acq On : 17 Oct 2023 23:53
Operator : MA/JU
Sample : 04885-04 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0M28

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-BM101223.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM042335.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	8	11	16	rVB	37792	45460	0.79%	0.083%
2	3.369	27	31	32	rBV	35306	37482	0.65%	0.068%
3	3.399	32	36	48	rVV	378665	491888	8.58%	0.894%
4	3.499	50	53	59	rVB3	6333	9361	0.16%	0.017%
5	3.716	86	90	97	rVB	33166	44352	0.77%	0.081%
6	3.810	101	106	125	rBV2	297333	597903	10.43%	1.086%
7	4.005	133	139	146	rVB	42928	69154	1.21%	0.126%
8	4.099	150	155	166	rVB2	60027	100019	1.75%	0.182%
9	4.228	174	177	181	rVV3	4355	5762	0.10%	0.010%
10	4.275	181	185	190	rVB	17413	23716	0.41%	0.043%
11	4.375	198	202	209	rVV	120954	173624	3.03%	0.315%
12	4.457	212	216	221	rVV4	12504	19718	0.34%	0.036%
13	4.504	221	224	229	rVB4	7209	11303	0.20%	0.021%
14	4.569	231	235	242	rVB	124376	162472	2.84%	0.295%
15	4.640	242	247	252	rBV	60540	82384	1.44%	0.150%
16	5.028	306	313	322	rBV	242209	349975	6.11%	0.636%
17	5.546	397	401	405	rVB3	6170	8849	0.15%	0.016%
18	5.910	458	463	470	rVB	13565	20437	0.36%	0.037%
19	6.963	638	642	646	rBV7	4192	8229	0.14%	0.015%
20	7.157	669	675	686	rVB	247087	383791	6.70%	0.697%
21	7.351	701	708	718	rVB	939763	1439029	25.11%	2.615%
22	7.528	731	738	750	rBV	825962	1297216	22.64%	2.357%
23	7.622	750	754	764	rVB2	8023	16548	0.29%	0.030%
24	8.010	813	820	830	rBV	635709	1016168	17.73%	1.846%
25	8.716	933	940	953	rBV	670334	1043163	18.20%	1.895%
26	8.857	957	964	974	rVB2	34258	56078	0.98%	0.102%
27	9.210	1015	1024	1039	rBV	1091444	1768470	30.86%	3.213%
28	9.322	1039	1043	1047	rVV5	3782	6342	0.11%	0.012%
29	9.369	1047	1051	1056	rVV	5376	8180	0.14%	0.015%
30	9.439	1056	1063	1071	rVB2	8531	19322	0.34%	0.035%
31	9.634	1091	1096	1100	rBV6	4300	8192	0.14%	0.015%
32	9.922	1135	1145	1153	rBV	866424	1370837	23.92%	2.491%
33	10.045	1159	1166	1171	rBV6	5133	12241	0.21%	0.022%
34	10.092	1171	1174	1180	rVB7	4095	8004	0.14%	0.015%
35	10.275	1201	1205	1211	rBV7	2852	5872	0.10%	0.011%
36	10.445	1226	1234	1248	rBV	1113467	1853866	32.35%	3.369%

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ClientSampleId :
C0M28

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101223.MA.M
Title : SVOA CALIBRATION

37	10.833	1293	1300	1307	rBV	935177	1528004	26.67%	2.776%
38	10.992	1319	1327	1346	rBV	1015729	1662374	29.01%	3.021%
39	11.322	1377	1383	1388	rBV	89310	135096	2.36%	0.245%
40	11.381	1388	1393	1405	rVB	122453	201321	3.51%	0.366%
41	11.581	1421	1427	1431	rBV8	7895	15093	0.26%	0.027%
42	11.657	1435	1440	1444	rVV4	6400	12395	0.22%	0.023%
43	12.410	1563	1568	1574	rBV2	18746	31807	0.56%	0.058%
44	12.528	1584	1588	1597	rBV6	5427	12020	0.21%	0.022%
45	12.663	1606	1611	1617	rVB6	4861	8447	0.15%	0.015%
46	12.980	1660	1665	1669	rBV5	4150	6585	0.11%	0.012%
47	13.498	1747	1753	1760	rBV	36313	58868	1.03%	0.107%
48	13.722	1788	1791	1795	rBV6	4469	6656	0.12%	0.012%
49	14.069	1843	1850	1857	rBV	2257042	3062196	53.44%	5.564%
50	14.351	1891	1898	1906	rBV2	2475090	3572962	62.35%	6.492%
51	14.651	1942	1949	1957	rVB	1422996	2026340	35.36%	3.682%
52	14.786	1966	1972	1976	rBV7	2866	5803	0.10%	0.011%
53	14.863	1979	1985	2003	rVV	190037	318094	5.55%	0.578%
54	15.021	2008	2012	2014	rBV5	5622	7443	0.13%	0.014%
55	15.439	2078	2083	2092	rVB4	16495	33010	0.58%	0.060%
56	15.645	2111	2118	2124	rBV	3184933	4470343	78.01%	8.123%
57	15.768	2132	2139	2153	rBV	1241256	1581178	27.59%	2.873%
58	15.880	2154	2158	2162	rVB	15451	20503	0.36%	0.037%
59	16.286	2222	2227	2235	rVB8	4945	10322	0.18%	0.019%
60	17.186	2376	2380	2386	rVB6	4608	7314	0.13%	0.013%
61	17.404	2410	2417	2424	rBV	1689653	2380735	41.55%	4.326%
62	17.504	2427	2434	2446	rBV	3594331	4977319	86.86%	9.044%
63	17.798	2480	2484	2487	rBV4	4159	6849	0.12%	0.012%
64	17.827	2487	2489	2494	rVV5	4907	6968	0.12%	0.013%
65	17.898	2498	2501	2505	rVB6	6170	7717	0.13%	0.014%
66	18.021	2518	2522	2528	rVB2	14165	22126	0.39%	0.040%
67	18.198	2546	2552	2555	rBV8	3856	6093	0.11%	0.011%
68	18.245	2555	2560	2569	rVV	97519	130208	2.27%	0.237%
69	18.339	2573	2576	2580	rVB	11246	14948	0.26%	0.027%
70	18.521	2604	2607	2610	rVB4	5991	7151	0.12%	0.013%
71	19.351	2744	2748	2753	rBV2	33247	45103	0.79%	0.082%
72	19.421	2754	2760	2765	rVB2	43580	78948	1.38%	0.143%
73	19.521	2773	2777	2783	rBV	46895	63177	1.10%	0.115%
74	19.662	2798	2801	2805	rBV5	12694	14595	0.25%	0.027%
75	19.792	2817	2823	2834	rBV	4623362	5730167	100.00%	10.412%
76	20.709	2977	2979	2981	rBV2	12154	8578	0.15%	0.016%

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Instrument :
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ClientSampleId :
C0M28

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Title : SVOA CALIBRATION

77	21.239	3065	3069	3076	rBV3	69716	124108	2.17%	0.226%
78	21.580	3122	3127	3133	rBV	1972863	2381804	41.57%	4.328%
79	23.891	3512	3520	3535	rVB2	2714706	5302329	92.53%	9.634%
80	24.050	3540	3547	3556	rVB	1172309	2356754	41.13%	4.282%

Sum of corrected areas: 55035258

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Instrument :
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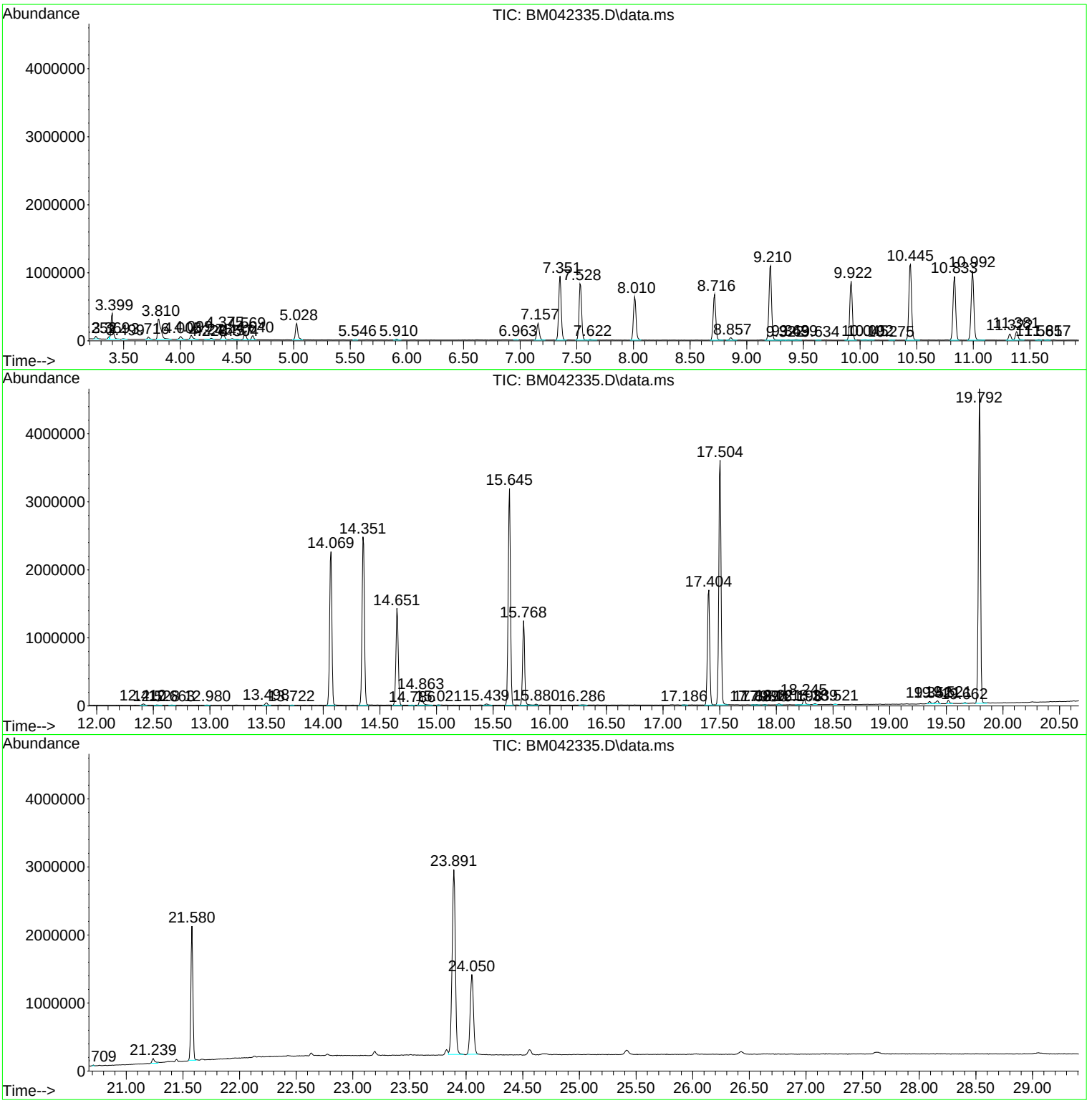
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101223.MA.M
Quant Title : SVOA CALIBRATION

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



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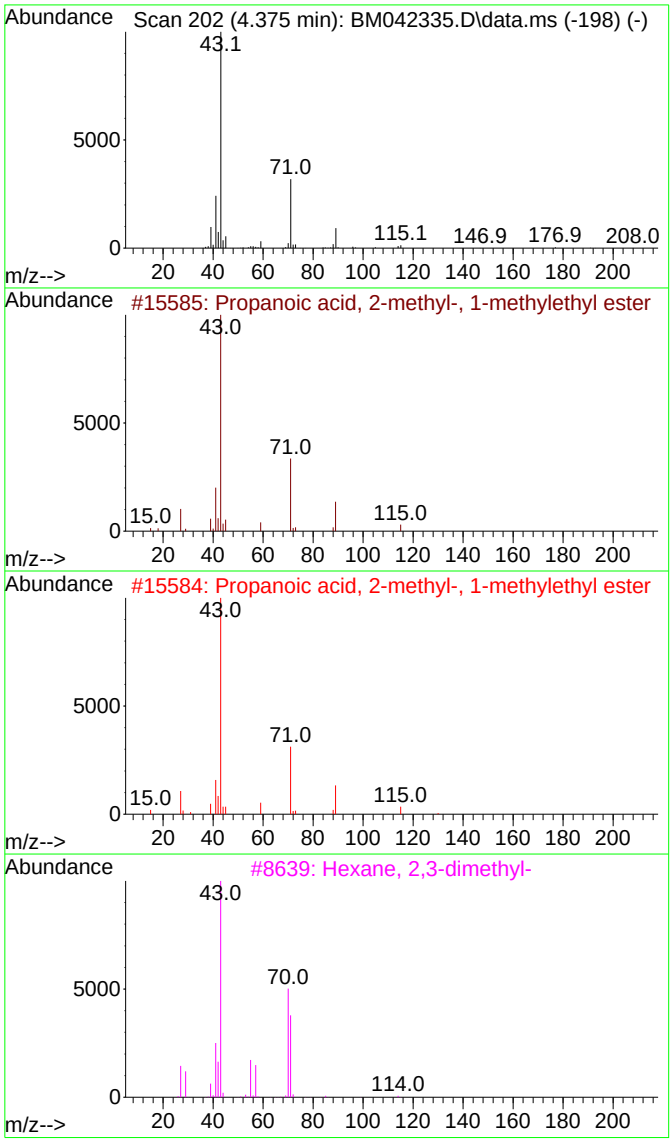
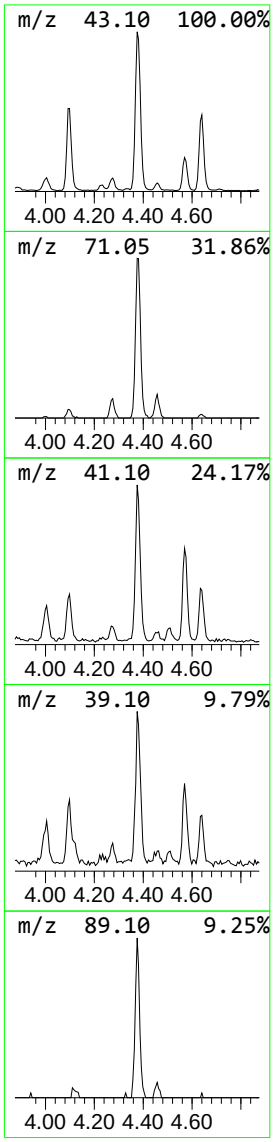
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2-methyl-, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.375	3.42 ng/ul	173624	1,4-Dichlorobenzene-d4	8.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
3	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	50
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	50
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	50





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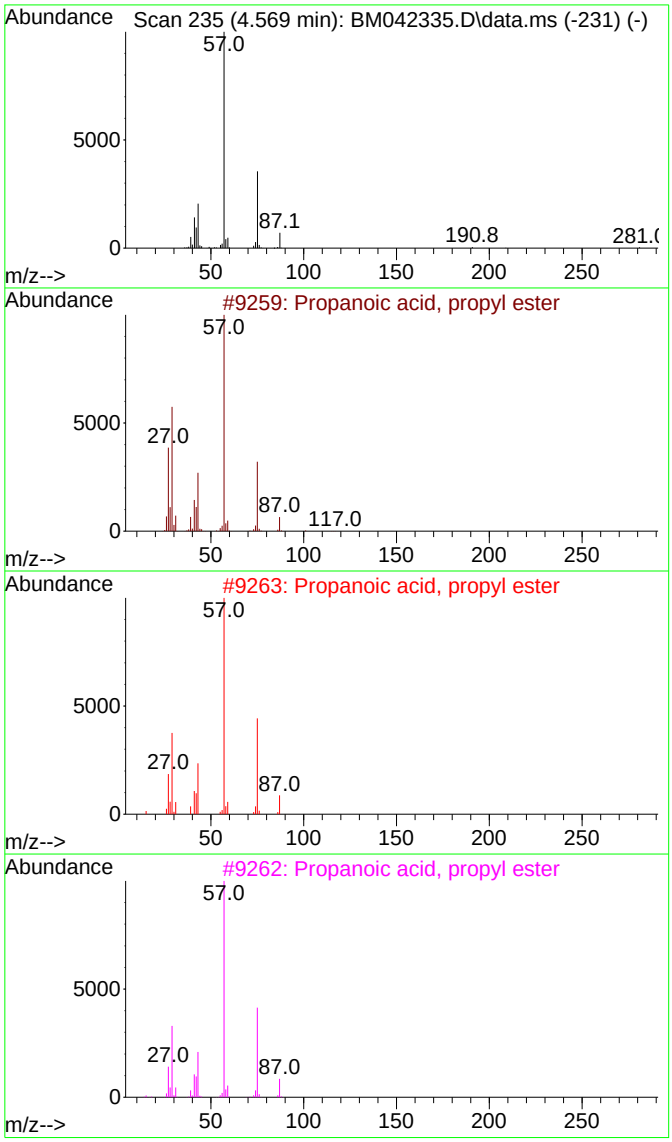
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101223.MA.M
Quant Title : SVOA CALIBRATION

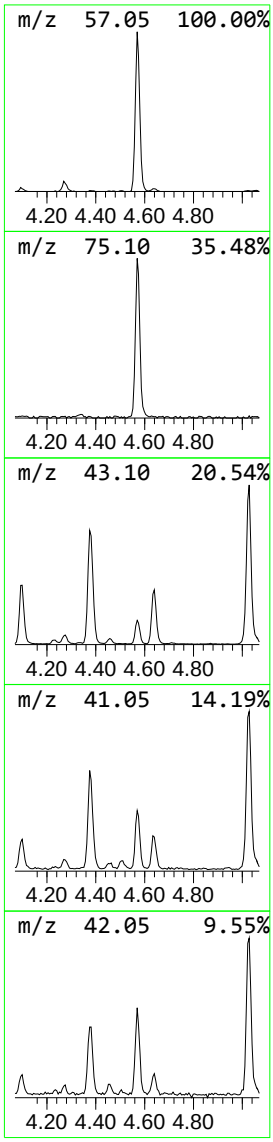
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.20 ng/ul	162472	1,4-Dichlorobenzene-d4	8.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM101223.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
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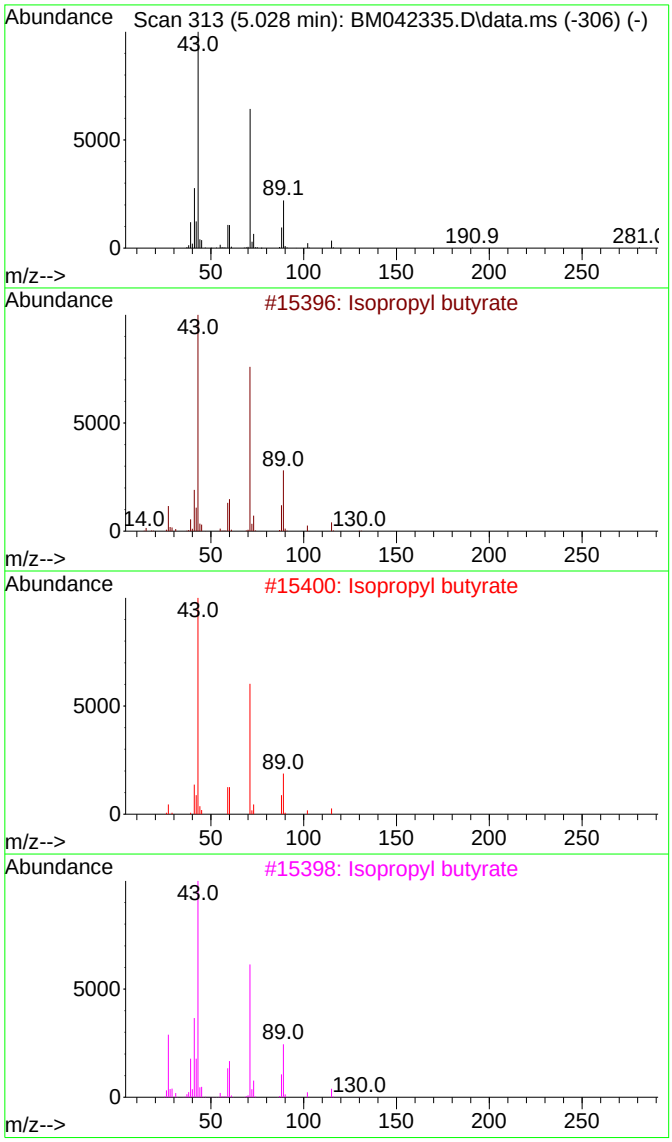
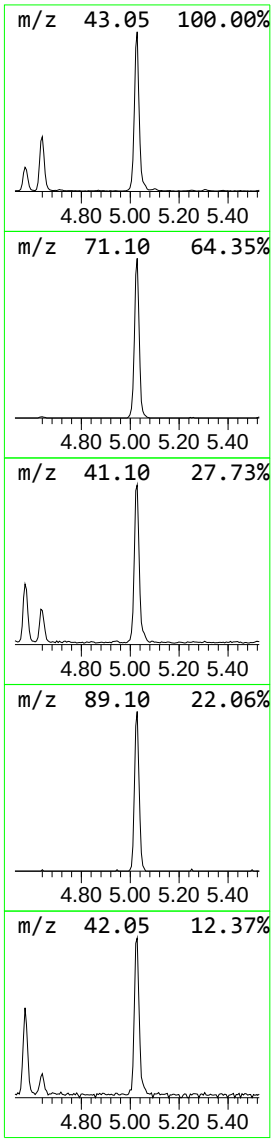
****
Peak Number 3 Isopropyl butyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	6.89 ng/ul	349975	1,4-Dichlorobenzene-d4	8.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





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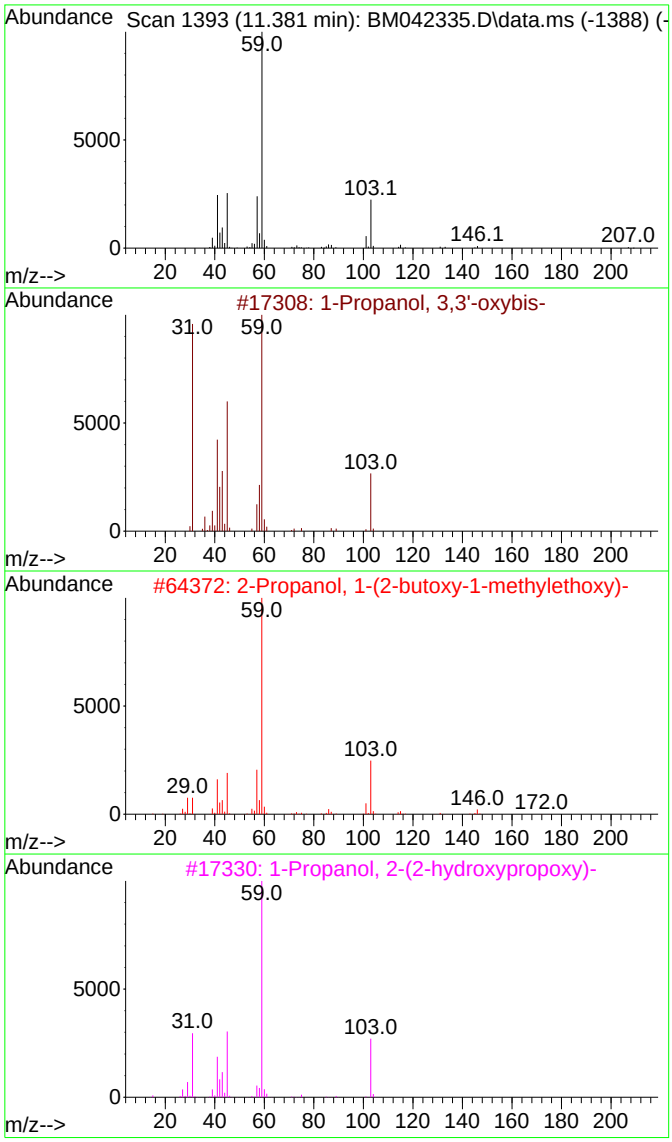
Quant Title : SVOA CALIBRATION

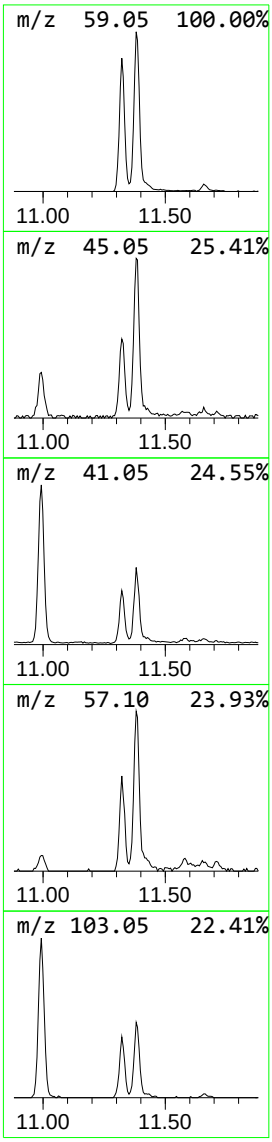
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol, 3,3'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.381	2.64 ng/ul	201321	Naphthalene-d8	10.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	78
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72





Tentatively Identified Compound (LSC) summary

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Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid,...	4.375	3.4	ng/ul	173624	1	8.010	1016170	20.0
Propanoic acid,...	4.569	3.2	ng/ul	162472	1	8.010	1016170	20.0
Isopropyl butyrate	5.028	6.9	ng/ul	349975	1	8.010	1016170	20.0
1-Propanol, 3,3...	11.381	2.6	ng/ul	201321	2	10.834	1528000	20.0