LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AH0

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-BM112322.M
Title : SVOA CALIBRATION

Signal : TIC: BM037734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.799	59	70	73	rBV	858046	1787514	3.60%	0.481%
2	3.887	81	85	86	rBV	638274	967922	1.95%	0.260%
3	4.028	105	109	119	rVB	197307	283336	0.57%	0.076%
4	4.216	119	141	145	rBV	759401	2942339	5.93%	0.792%
5	5.263	255	319	321	rVV	2830158	29153423	58.78%	7.843%
6	5.422	321	346	348	rVB	2068183	11199674	22.58%	3.013%
7	5.728	377	398	401	rBV	830019	2831912	5.71%	0.762%
8	5.916	426	430	435	rVV2	251248	402398	0.81%	0.108%
9	6.522	525	533	539	rVB	213475	422289	0.85%	0.114%
10	6.675	549	559	564	rVV	469833	1150215	2.32%	0.309%
11	6.951	597	606	622	rVB5	116458	352846	0.71%	0.095%
12	7.228	624	653	655	rBV	1132306	4915973	9.91%	1.323%
13	7.298	655	665	676	rVB	9813401	17220088	34.72%	4.633%
14	7.434	682	688	693	rBV	1554623	2347574	4.73%	0.632%
15	7.634	718	722	730	rVB	903474	1418506	2.86%	0.382%
16	8.110	798	803	808	rVB	1048478	1572857	3.17%	0.423%
17	8.175	808	814	825	rVB	1178858	1982479	4.00%	0.533%
18	8.269	825	830	835	rVB	281010	426603	0.86%	0.115%
19	8.345	835	843	849	rBV2	384946	795434	1.60%	0.214%
20	8.551	869	878	883	rBV	215174	365548	0.74%	0.098%
21	8.740	894	910	915	rBV3	552066	1485832	3.00%	0.400%
22	8.816	916	923	928	rBV	852799	1397581	2.82%	0.376%
23	8.881	928	934	940	rBV	5842693	9278350	18.71%	2.496%
24	8.998	949	954	965	rBV5	271346	631819	1.27%	0.170%
25	9.234	983	994	997	rBV5	166416	389271	0.78%	0.105%
26	9.281	997	1002	1008	rBV	1816036	2797251	5.64%	0.753%
27	9.363	1010	1016	1022	rVB	1522812	2469063	4.98%	0.664%
28	9.463	1022	1033	1044	rBV4	353044	1526227	3.08%	0.411%
29	9.616	1044	1059	1061	rBV3	888856	2598509	5.24%	0.699%
30	9.663	1063	1067	1079	rVB4	1268140	2796418	5.64%	0.752%
31	9.769	1079	1085	1086	rBV3	306254	490911	0.99%	0.132%
32	9.857	1096	1100	1114	rVB6	129898	342281	0.69%	0.092%
33	10.010	1118	1126	1131	rBV	1216145	2062958	4.16%	0.555%
34	10.269	1151	1170	1171	rBV3	952019	3624303	7.31%	0.975%
35	10.351	1176	1184	1187	rBV4	1492305	3848873	7.76%	1.035%
36	10.422	1194	1196	1203	rVB2	4292659	4250962	8.57%	1.144%

LSC Area Percent Report

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Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

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-BM112322.M
Title : SVOA CALIBRATION

37	10.545	1212	1217	1223	rVV	1591988	2632699	5.31%	0.708%
38	10.616	1226	1229	1240	rVB5	236108	456505	0.92%	0.123%
39	10.710	1240	1245	1253	rBV7	138578	350239	0.71%	0.094%
40	10.792	1253	1259	1265	rBV5	212472	427747	0.86%	0.115%
41	10.934	1271	1283	1288	rBV	1887514	3790834	7.64%	1.020%
42	10.986	1288	1292	1298	rVB2	678037	1158214	2.34%	0.312%
43	11.063	1298	1305	1311	rBV4	678830	1763589	3.56%	0.474%
44	11.134	1312	1317	1326	rBV7	273958	829013	1.67%	0.223%
45	11.398	1352	1362	1371	rVB7	186715	627512	1.27%	0.169%
46	11.704	1375	1414	1418	rBV	7368138	49596094	100.00%	13.343%
47	11.833	1431	1436	1443	rBV2	769646	1336498	2.69%	0.360%
48	11.963	1453	1458	1466	rVB4	208444	507342	1.02%	0.136%
49	12.257	1504	1508	1513	rVB	448130	663726	1.34%	0.179%
50	12.333	1514	1521	1524	rBV4	175096	408882	0.82%	0.110%
51	12.416	1529	1535	1543	rVB	3164328	5442548	10.97%	1.464%
52	12.551	1554	1558	1564	rVB3	300409	500724	1.01%	0.135%
53	12.886	1588	1615	1623	rBV	8736339	43824084	88.36%	11.790%
54	13.092	1644	1650	1656	rBV3	1497488	2567414	5.18%	0.691%
55	13.328	1682	1690	1691	rBV3	344260	619926	1.25%	0.167%
56	13.533	1721	1725	1731	rVV3	415228	702123	1.42%	0.189%
57	13.680	1742	1750	1759	rBV	10175116	16925881	34.13%	4.554%
58	13.839	1773	1777	1785	rBV4	345460	795312	1.60%	0.214%
59	13.916	1786	1790	1799	rVB4	400627	888312	1.79%	0.239%
60	14.033	1801	1810	1821	rVV2	1945582	4728958	9.53%	1.272%
61	14.145	1822	1829	1840	rVB	4182188	6565509	13.24%	1.766%
62	14.398	1866	1872	1874	rBV3	634762	1217422	2.45%	0.328%
63	14.433	1874	1878	1884	rVV	4670164	6776015	13.66%	1.823%
64	14.504	1887	1890	1894	rVV3	296481	493396	0.99%	0.133%
65	14.598	1897	1906	1912	rVB	4398236	7547371	15.22%	2.030%
66	14.739	1924	1930	1935	rBV	2633024	4085635	8.24%	1.099%
67	14.880	1950	1954	1958	rBV	761118	1042883	2.10%	0.281%
68	14.927	1958	1962	1971	rVB3	499949	1145874	2.31%	0.308%
69	15.145	1995	1999	2004	rVB	921368	1329583	2.68%	0.358%
70	15.227	2010	2013	2017	rVB3	425115	606741	1.22%	0.163%
71	15.310	2024	2027	2032	rVB3	178631	281080	0.57%	0.076%
72	15.727	2090	2098	2102	rBV	5709429	8427377	16.99%	2.267%
73	15.769	2102	2105	2110	rVB3	708491	942550	1.90%	0.254%
74	15.833	2111	2116	2127	rBV	1681634	2702736	5.45%	0.727%
75	15.986	2136	2142	2149	rBV	3001149	4998772	10.08%	1.345%
76	16.098	2158	2161	2169	rVB8	360756	686818	1.38%	0.185%

LSC Area Percent Report

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Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

77	16.180	2169	2175	2179	rBV7	246276	609505	1.23%	0.164%
78	16.416	2211	2215	2219	rBV4	242692	520646	1.05%	0.140%
79	16.574	2239	2242	2249	rVB	353089	537959	1.08%	0.145%
80	16.763	2271	2274	2279	rVB2	272643	343679	0.69%	0.092%
81	16.868	2289	2292	2299	rVB4	251095	413054	0.83%	0.111%
82	16.992	2308	2313	2319	rVB3	495491	963569	1.94%	0.259%
83	17.068	2322	2326	2331	rVB2	404333	597324	1.20%	0.161%
84	17.474	2390	2395	2405	rBV	3733568	6076634	12.25%	1.635%
85	17.574	2405	2412	2420	rVB	6205981	9212921	18.58%	2.479%
86	17.839	2454	2457	2462	rVB3	316585	407098	0.82%	0.110%
87	18.357	2542	2545	2551	rVB2	554289	752244	1.52%	0.202%
88	18.439	2555	2559	2563	rVV	549952	836485	1.69%	0.225%
89	18.486	2563	2567	2570	rVV	638615	919010	1.85%	0.247%
90	18.527	2570	2574	2580	rVB	1833211	2513843	5.07%	0.676%
91	19.621	2756	2760	2766	rBV	477468	598772	1.21%	0.161%
92	19.857	2794	2800	2803	rBV	6855491	9087189	18.32%	2.445%
93	19.892	2803	2806	2814	rVB	1811804	2220537	4.48%	0.597%
94	19.968	2815	2819	2824	rVB	2768228	3245119	6.54%	0.873%
95	20.856	2968	2970	2976	rVB	504095	640354	1.29%	0.172%
96	21.074	3004	3007	3017	rVB	470539	715330	1.44%	0.192%
97	21.180	3020	3025	3035	rBV2	1546838	2800659	5.65%	0.753%
98	21.639	3098	3103	3110	rBV	3128863	3987627	8.04%	1.073%
99	23.968	3492	3499	3513	rVB2	3512757	7513081	15.15%	2.021%
100	24.133	3520	3527	3536	rVB2	1596924	3264337	6.58%	0.878%

Sum of corrected areas: 371700453

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
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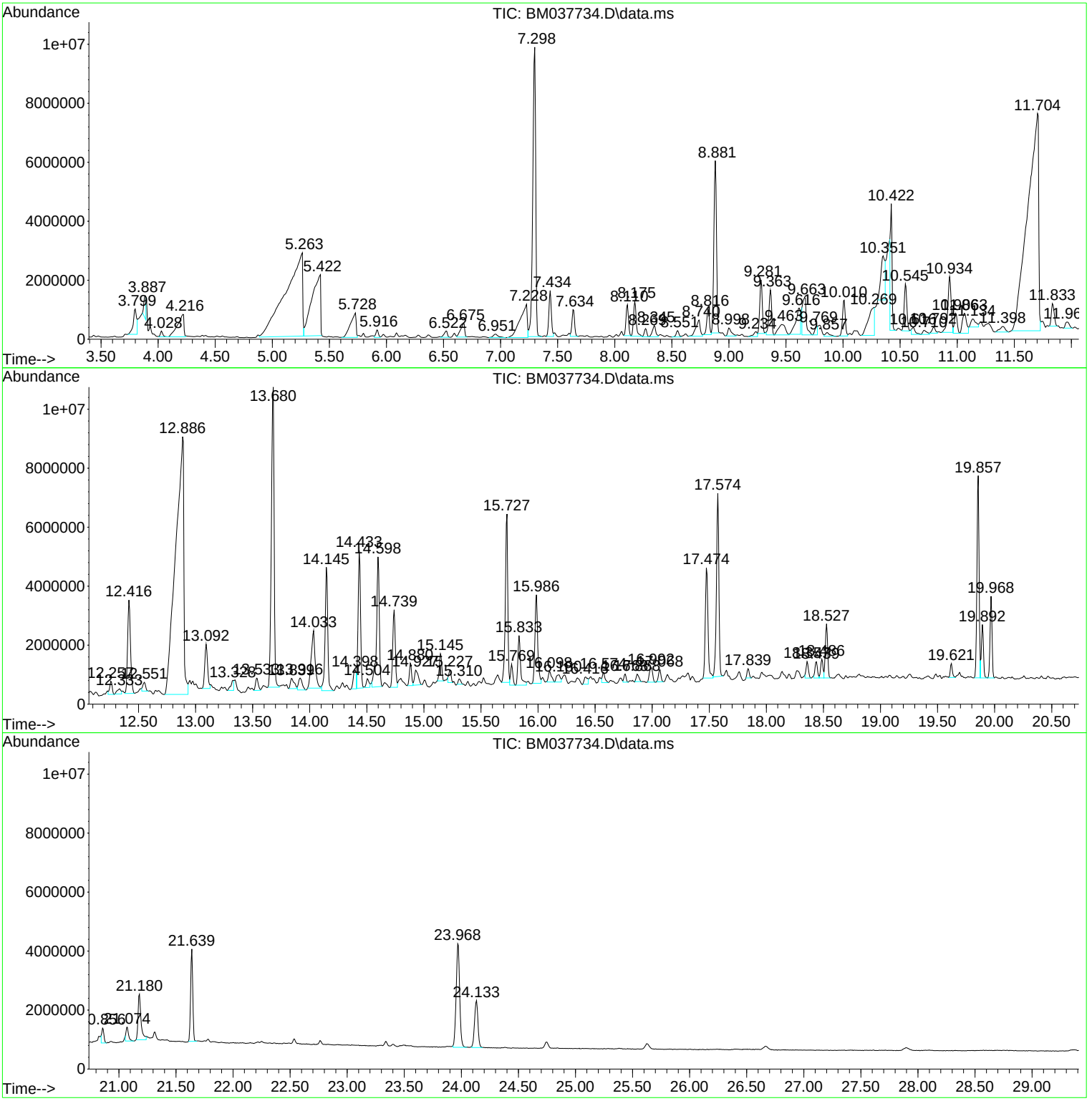
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
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ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

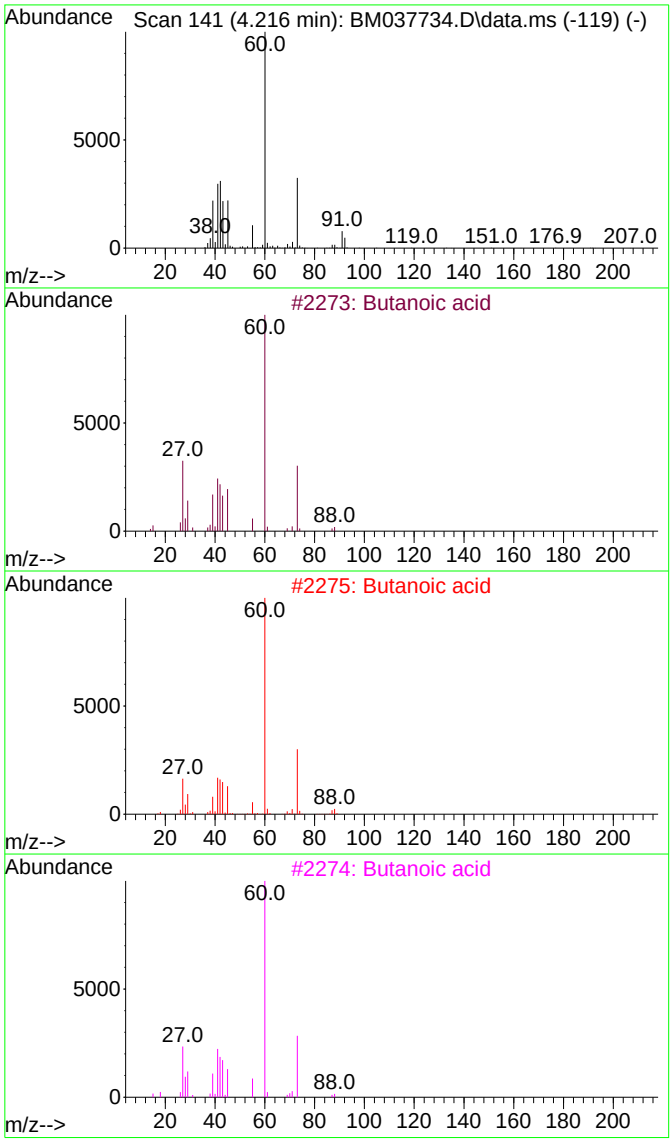
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

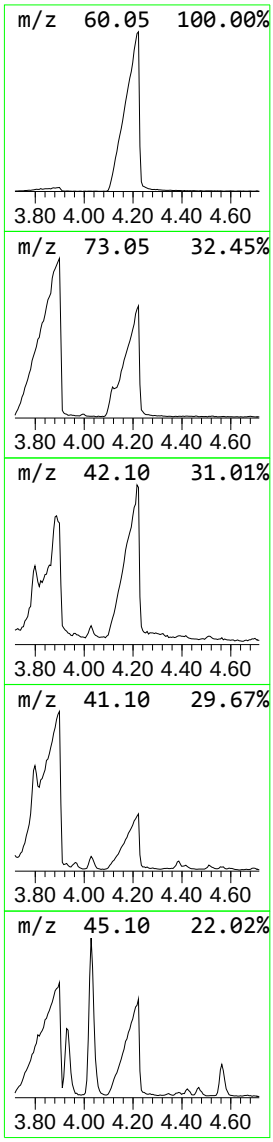
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.216	37.41 ng/ul	2942340	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	80
2	Butanoic acid	88	C4H8O2	000107-92-6	72
3	Butanoic acid	88	C4H8O2	000107-92-6	72
4	Butanoic acid	88	C4H8O2	000107-92-6	59
5	dl-Serine	105	C3H7NO3	000302-84-1	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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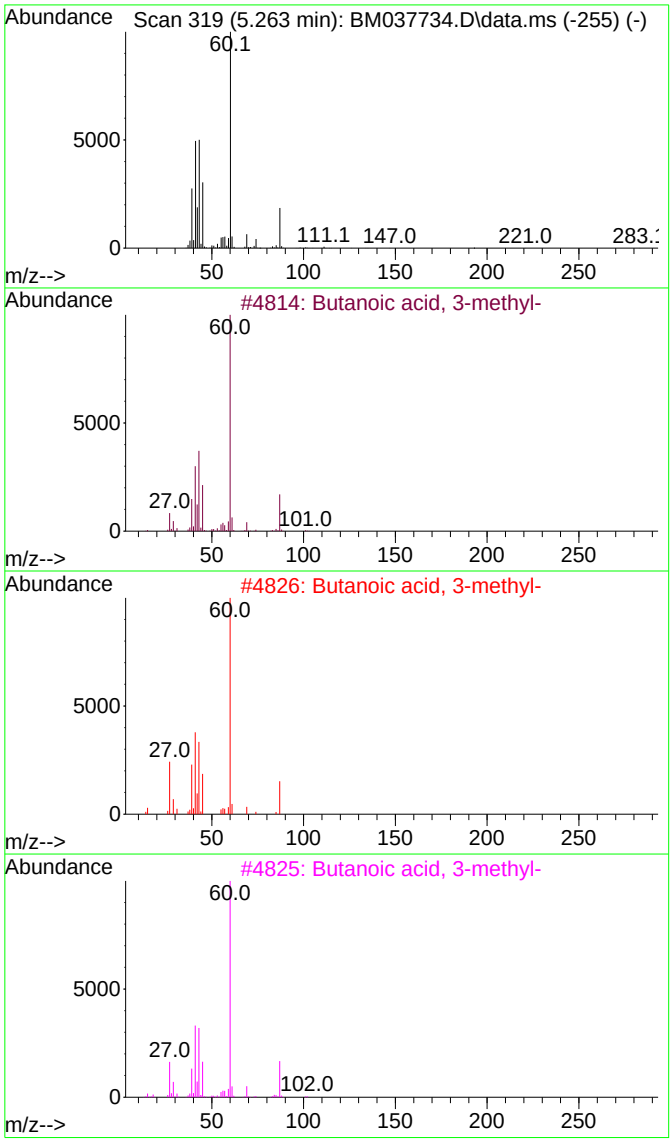
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

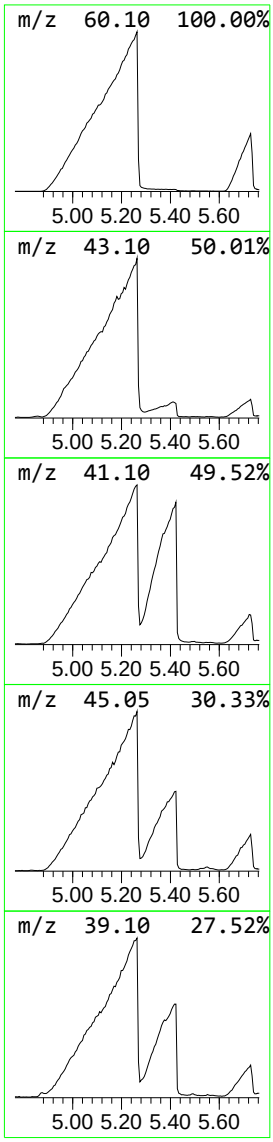
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.263	370.71 ng/ul	29153400	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
4	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	56
5	Formic acid hydrazide	60	CH4N2O	000624-84-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
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ALS Vial : 46 Sample Multiplier: 1

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BNA_M
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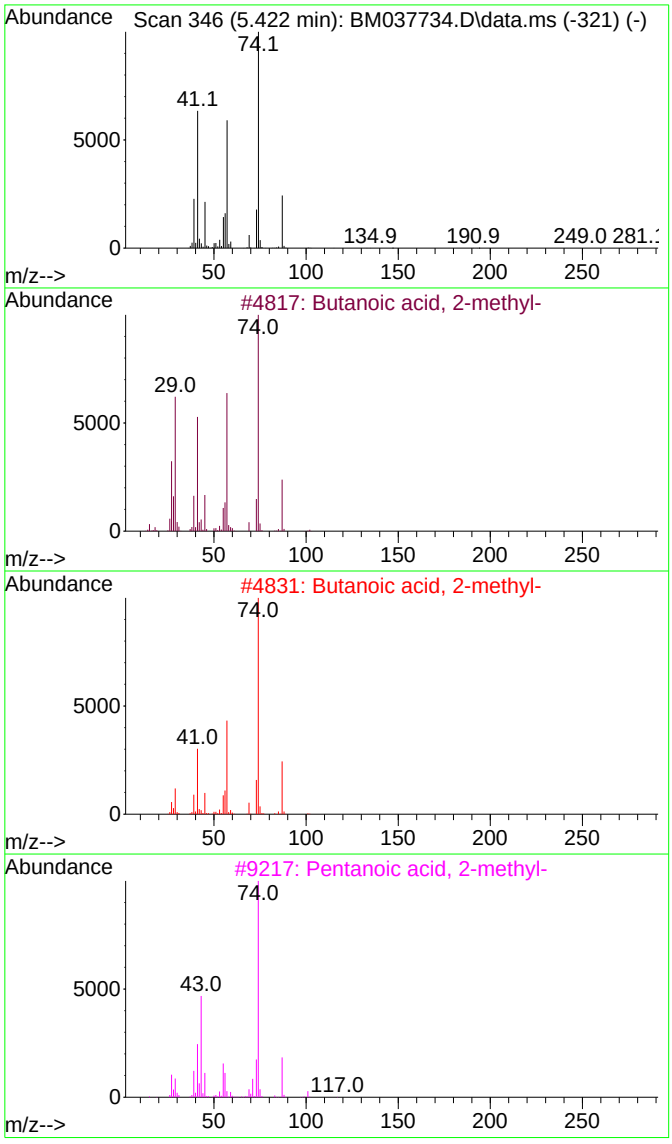
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

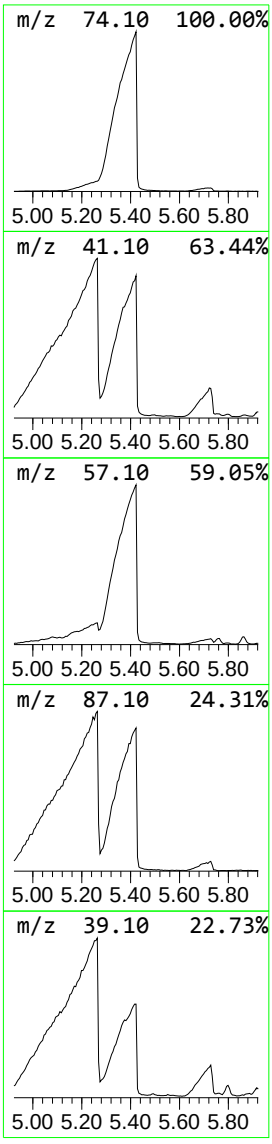
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.422	142.41 ng/ul	11199700	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
3	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
4	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
5	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	50





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Data File : BM037734.D
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Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

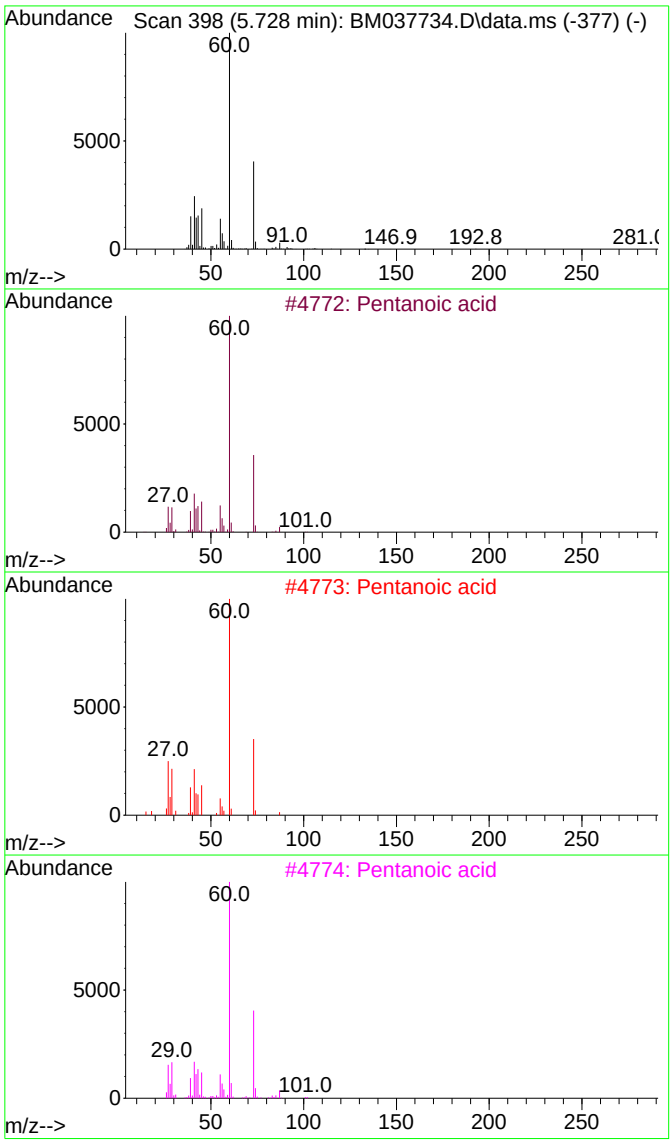
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

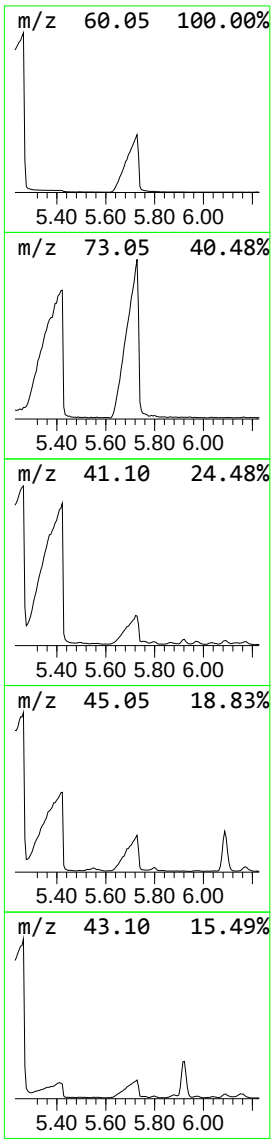
****

Peak Number 6 Pentanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.728	36.01 ng/ul	2831910	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	90
2	Pentanoic acid	102	C5H10O2	000109-52-4	83
3	Pentanoic acid	102	C5H10O2	000109-52-4	78
4	Butanoic acid	88	C4H8O2	000107-92-6	64
5	Butanoic acid	88	C4H8O2	000107-92-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

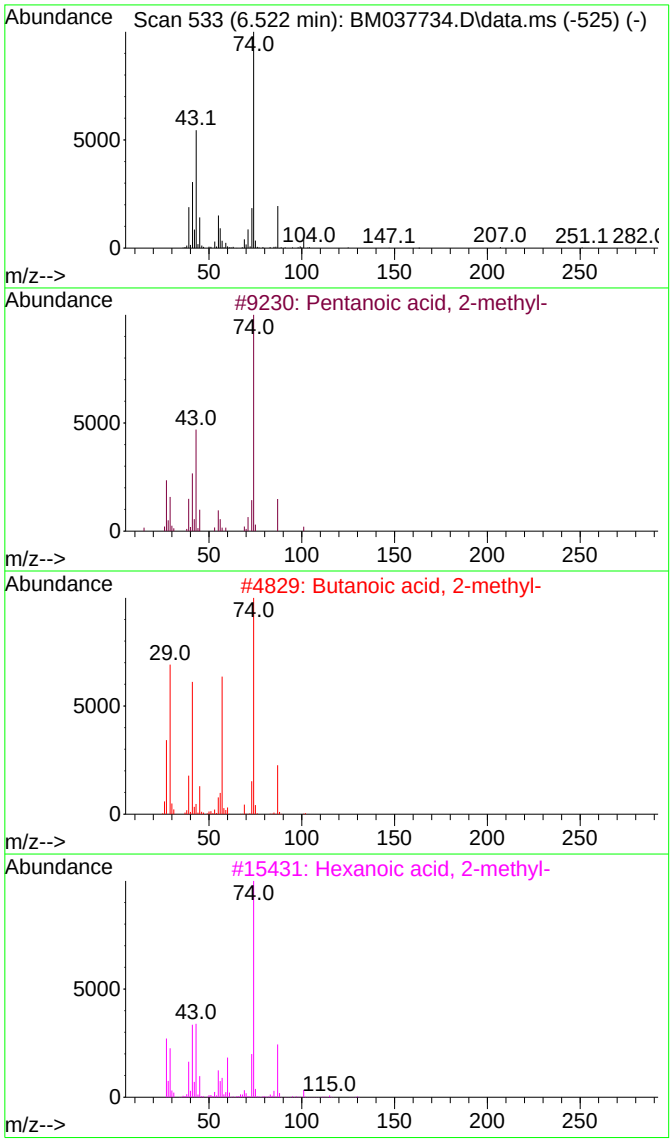
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

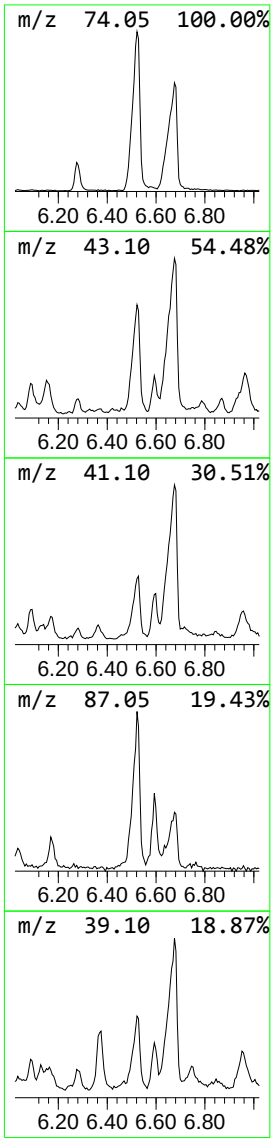
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentanoic acid, 2-methyl- Concentration Rank 32

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.522	5.37 ng/ul	422289	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	90
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
3	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
4	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72





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Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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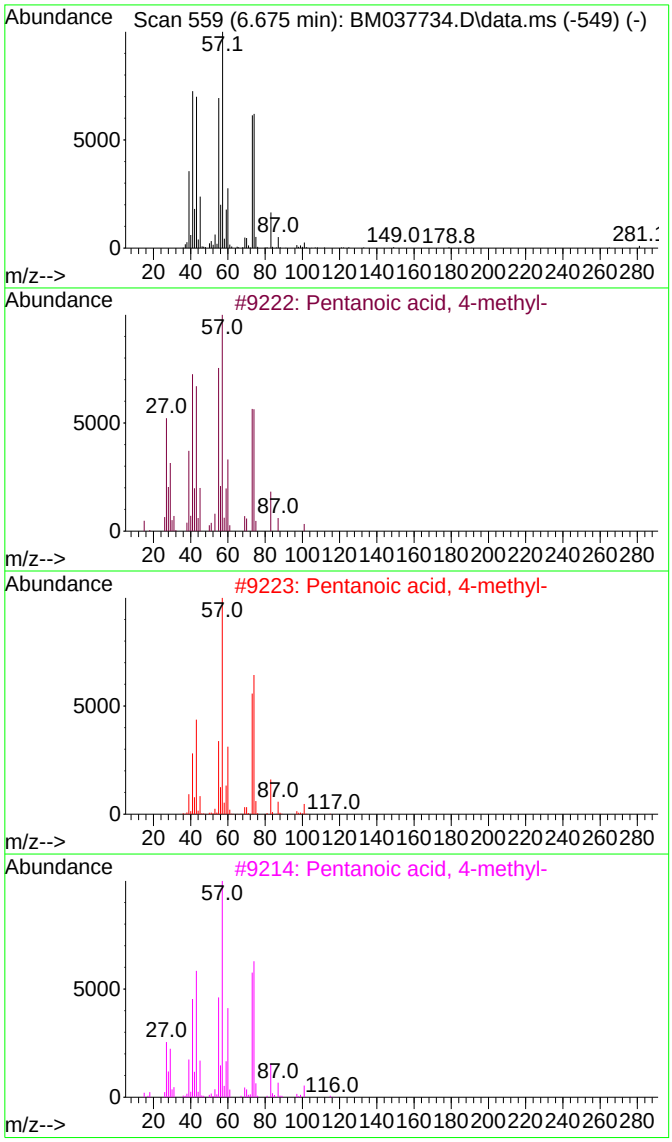
Quant Title : SVOA CALIBRATION

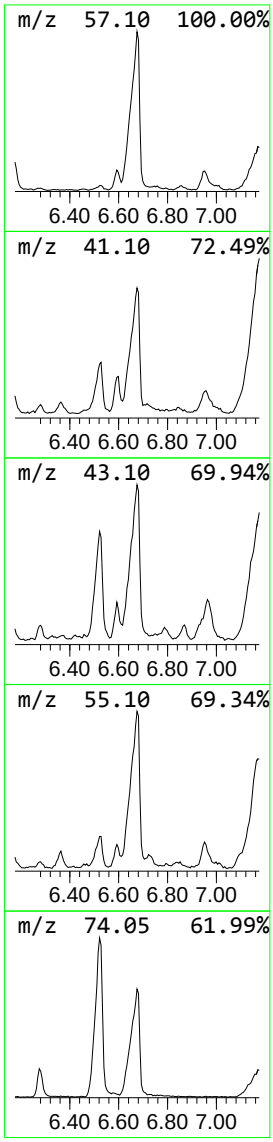
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentanoic acid, 4-methyl- Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	14.63 ng/ul	1150220	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	86
2	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	64
3	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	56
4	Butanoic acid, 3,3-dimethyl-, me...	130	C7H14O2	010250-48-3	37
5	Butanoic acid, 3,3-dimethyl-, me...	130	C7H14O2	010250-48-3	37





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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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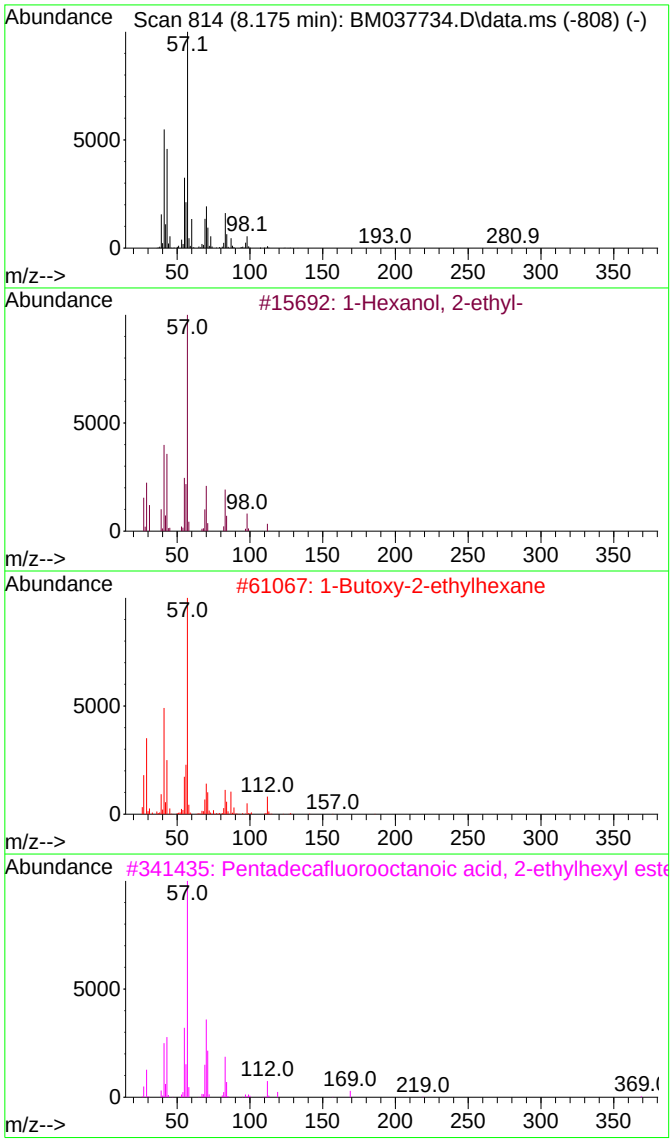
Quant Title : SVOA CALIBRATION

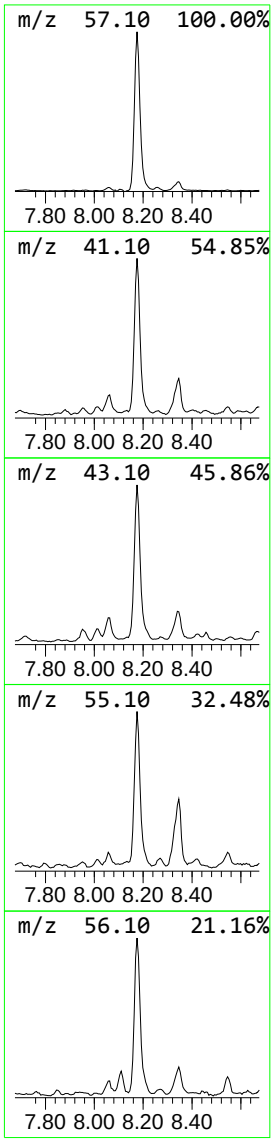
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1-Hexanol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	25.21 ng/ul	1982480	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
2	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	50
3	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	47





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Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

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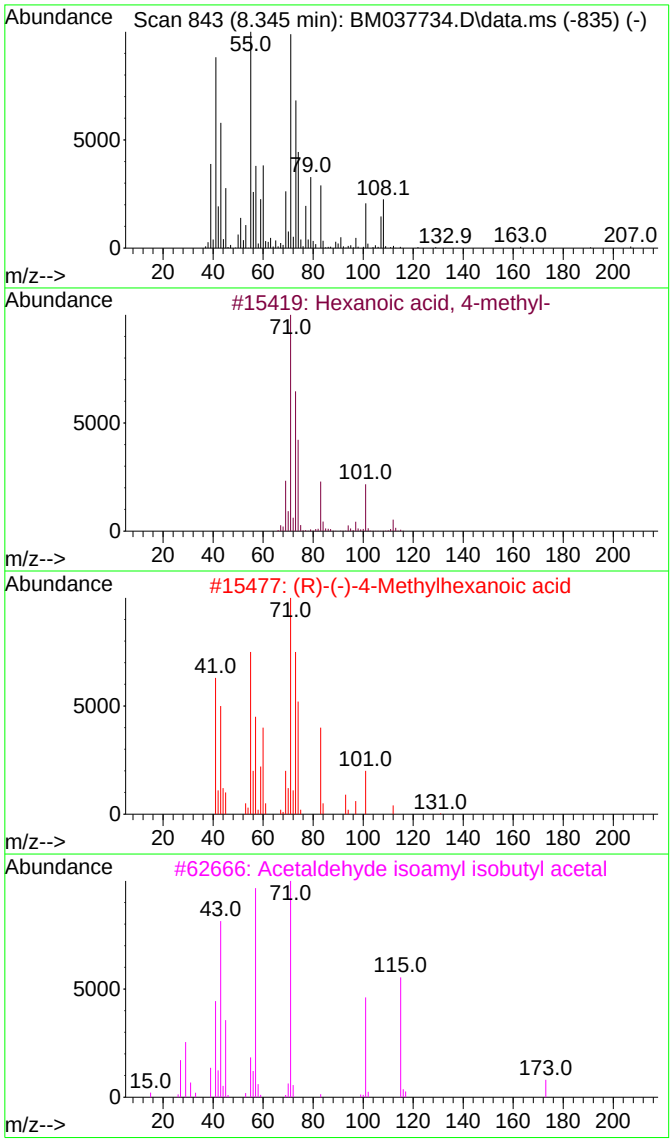
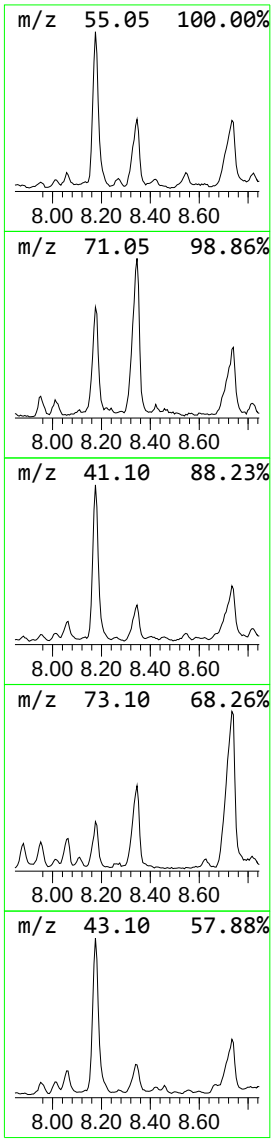
Peak Number 13 unknown-01 Concentration Rank 26

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.345	10.11 ng/ul	795434	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-methyl-	130	C7H14O2	001561-11-1	40
2	(R)-(-)-4-Methylhexanoic acid	130	C7H14O2	052745-93-4	38
3	Acetaldehyde isoamyl isobutyl ac...	188	C11H24O2	1000430-99-3	22
4	Phenylmethanediol dibutanoate	264	C15H20O4	002929-77-3	22
5	Oxalic acid, octyl propyl ester	244	C13H24O4	1010309-26-1	10





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Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

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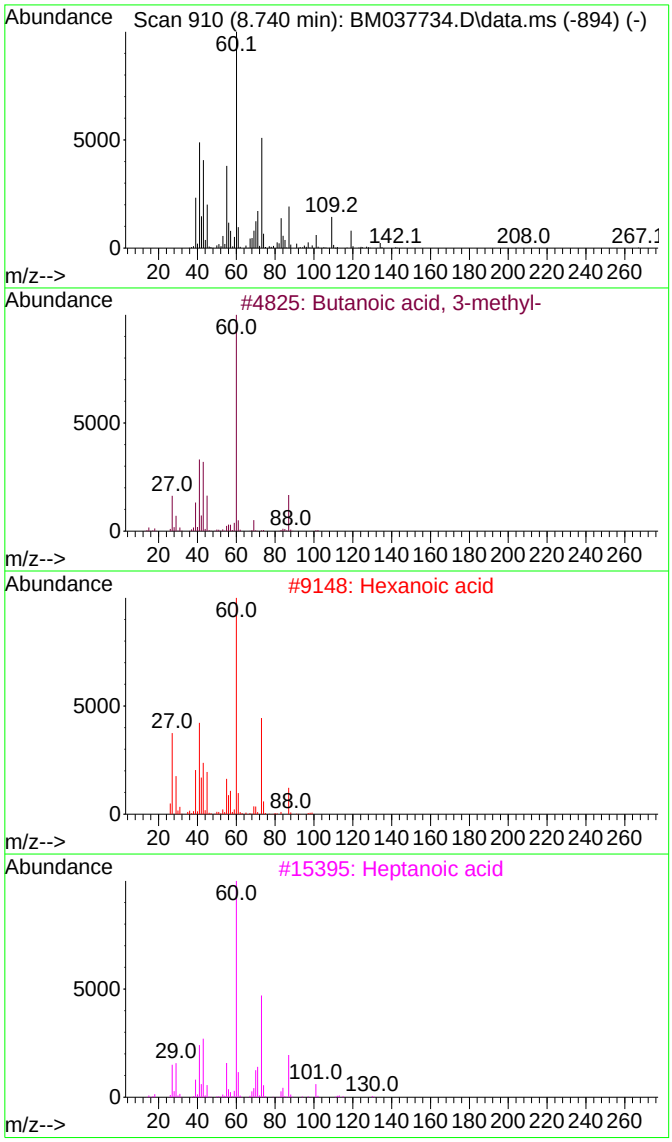
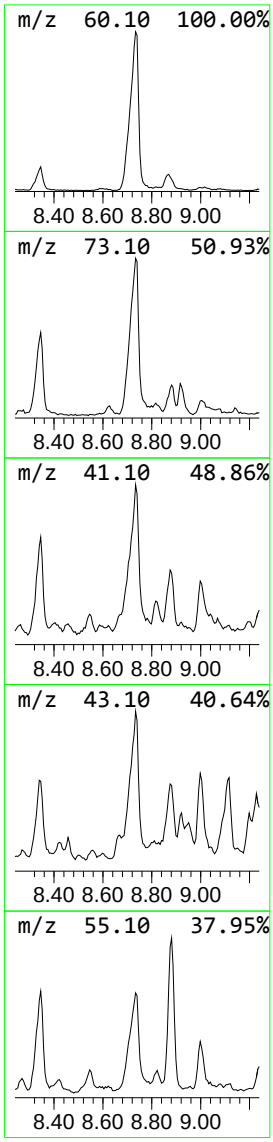
Peak Number 14 Hexanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.740	18.89 ng/ul	1485830	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	68
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Heptanoic acid	130	C7H14O2	000111-14-8	64
4	Heptanoic acid	130	C7H14O2	000111-14-8	64
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64





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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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

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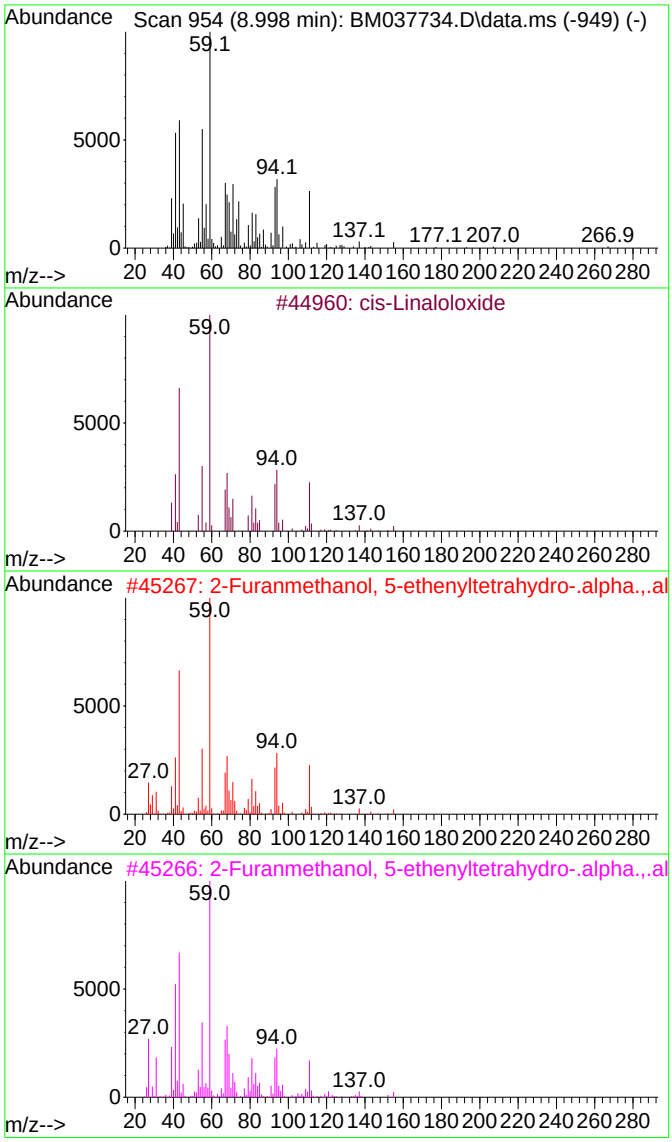
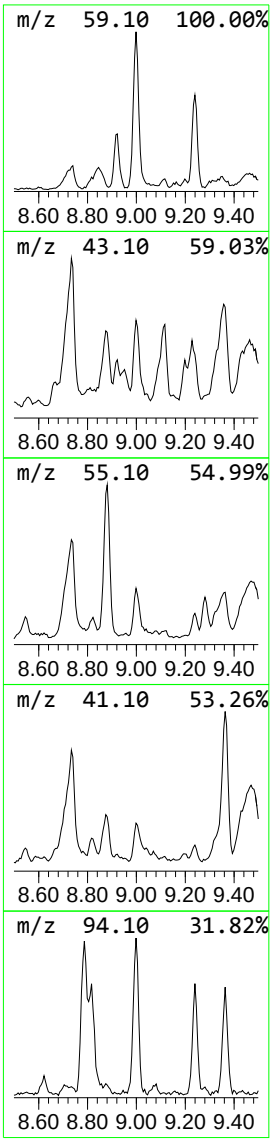
Peak Number 15 cis-Linaloloxide Concentration Rank 28

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.998	8.03 ng/ul	631819	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Linaloloxide	170	C10H18O2	1000121-97-4	50
2	2-Furanmethanol, 5-ethenyltetrah...	170	C10H18O2	005989-33-3	50
3	2-Furanmethanol, 5-ethenyltetrah...	170	C10H18O2	005989-33-3	47
4	Ethyl 2-(5-methyl-5-vinyltetrahy...	242	C13H22O4	1000373-80-3	47
5	2-Furanmethanol, 5-ethenyltetrah...	170	C10H18O2	005989-33-3	42





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Quant Title : SVOA CALIBRATION

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

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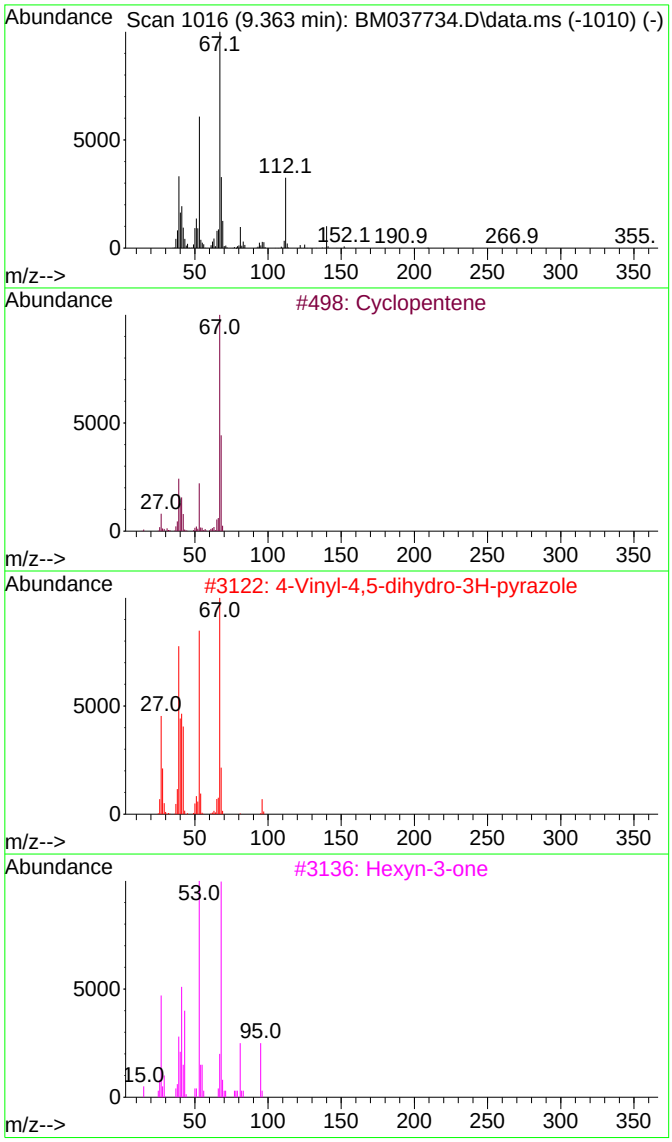
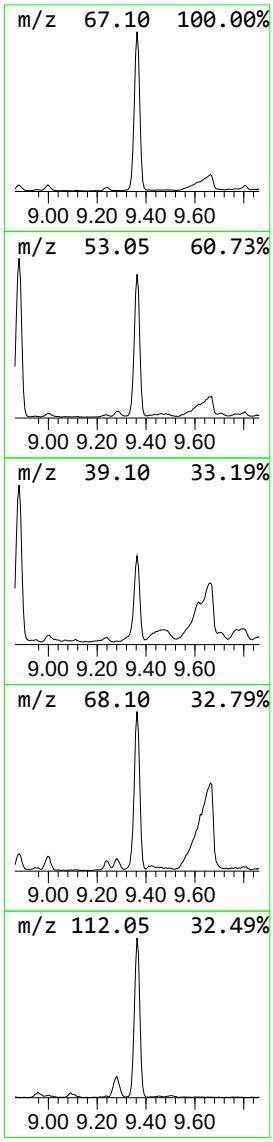
Peak Number 16 Cyclopentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.363	31.40 ng/ul	2469060	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	72
2	4-Vinyl-4,5-dihydro-3H-pyrazole	96	C5H8N2	063438-33-5	64
3	Hexyn-3-one	96	C6H8O	000689-00-9	38
4	Cyclopentene	68	C5H8	000142-29-0	30
5	Cyclopentene	68	C5H8	000142-29-0	30





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Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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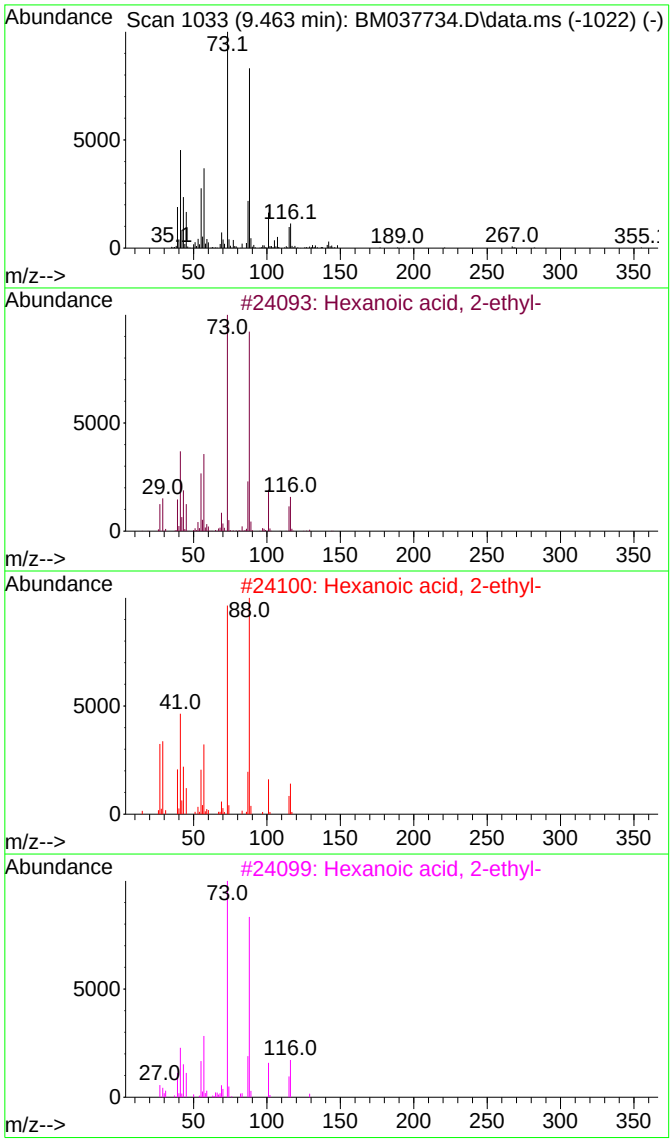
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

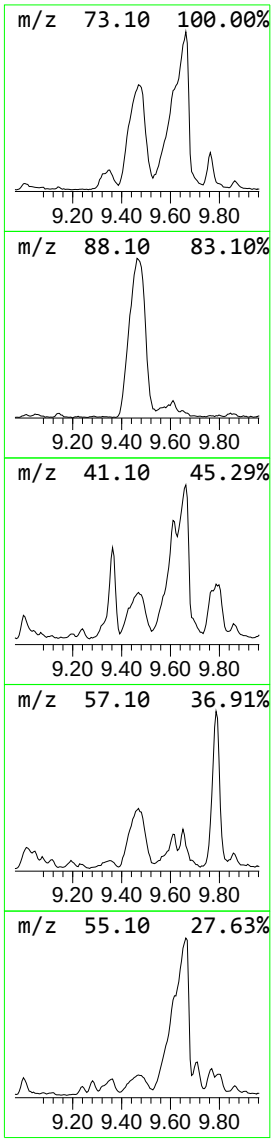
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Hexanoic acid, 2-ethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.463	19.41 ng/ul	1526230	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78





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ClientSampleId :
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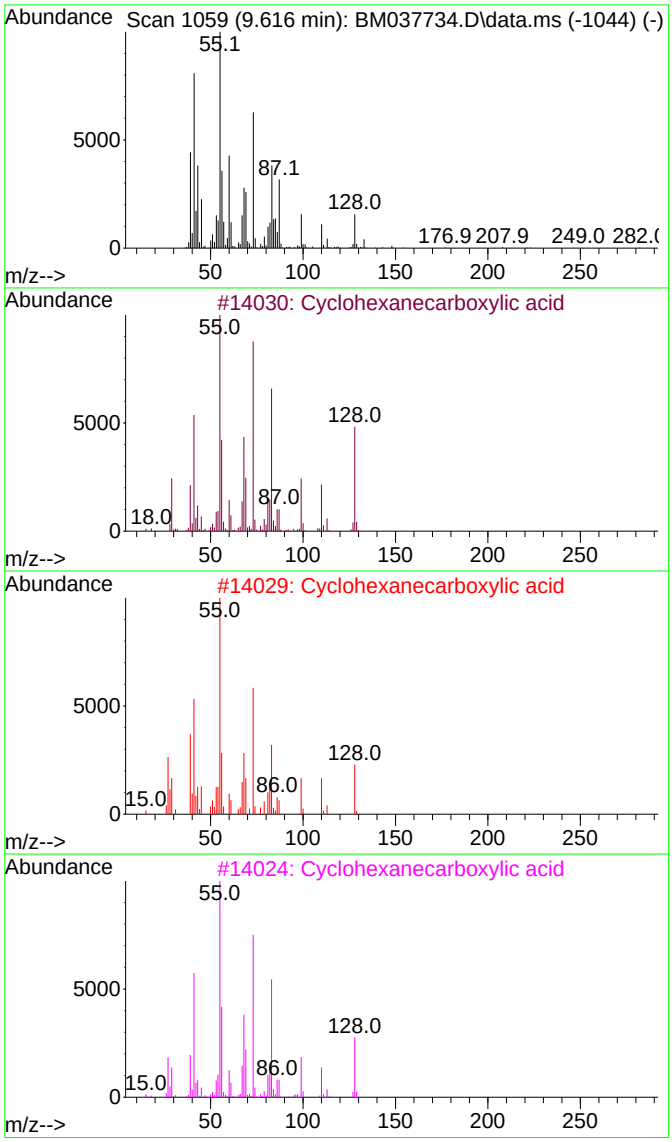
Quant Title : SVOA CALIBRATION

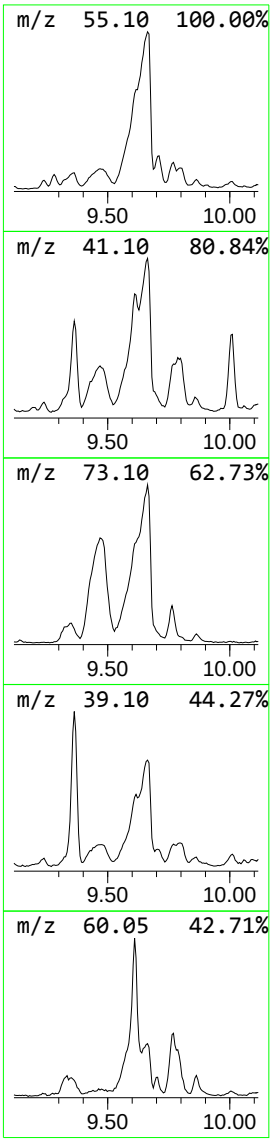
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Cyclohexanecarboxylic acid Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	13.71 ng/ul	2598510	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	78
2	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	60
3	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	60
4	Cyclopentaneundecanoic acid	254	C16H30O2	006053-49-2	50
5	9-Oxononanoic acid	172	C9H16O3	002553-17-5	38





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Quant Title : SVOA CALIBRATION

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

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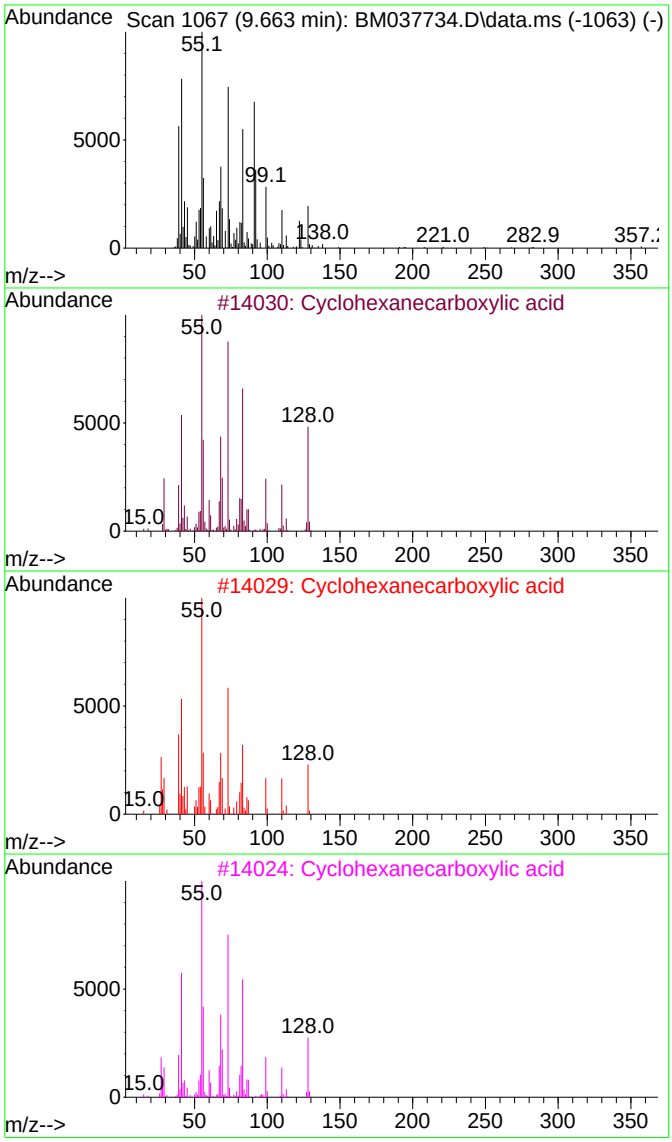
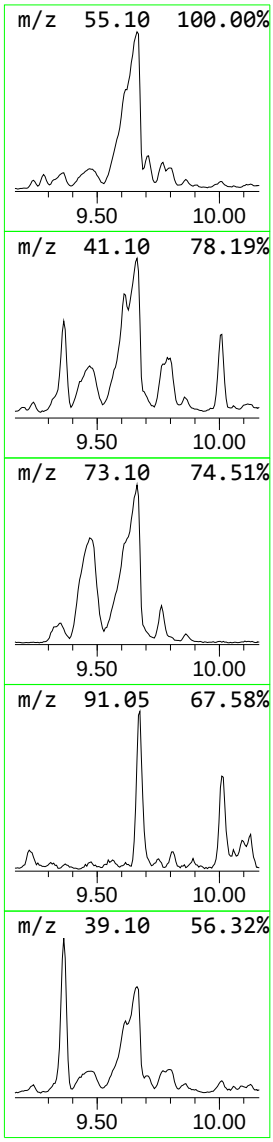
Peak Number 19 unknown-02 Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.663	14.75 ng/ul	2796420	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	60
2	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	52
3	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	38
4	2-Butenoic acid, 3-methyl-, ethy...	128	C7H12O2	000638-10-8	14
5	2-Hexenoic acid, (E)-	114	C6H10O2	013419-69-7	14





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Quant Title : SVOA CALIBRATION

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

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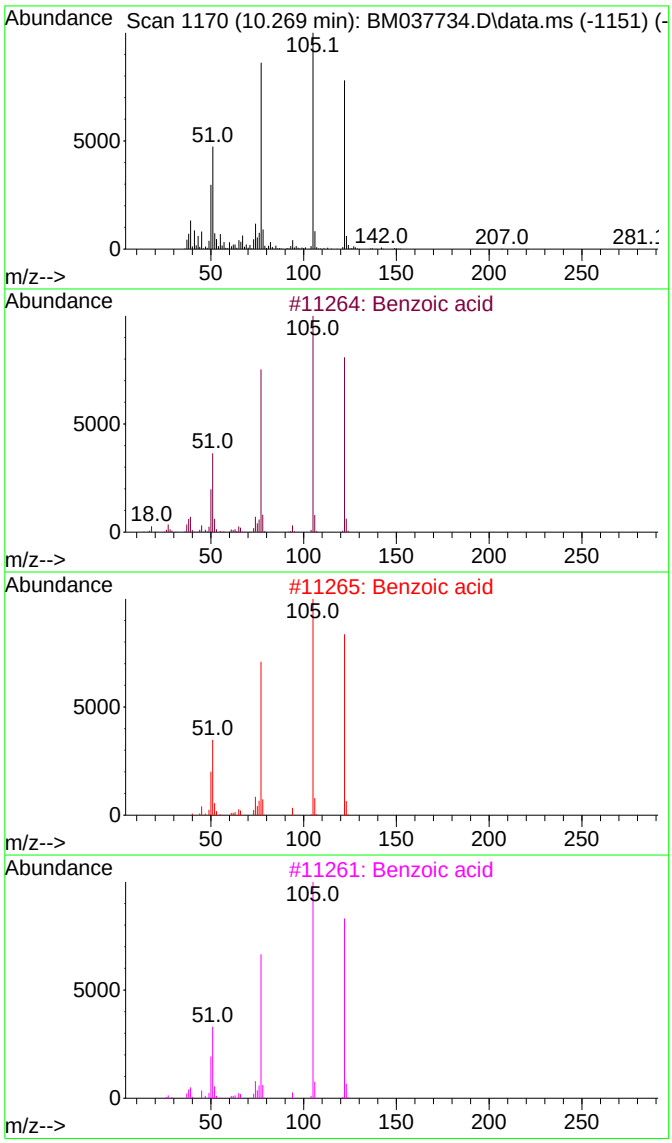
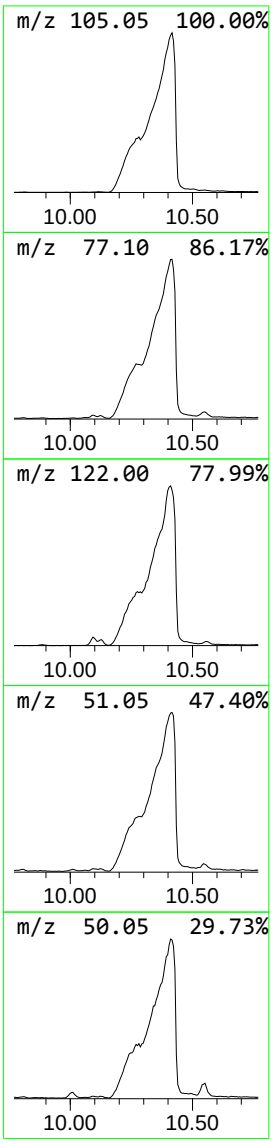
Peak Number 21 Benzoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.269	19.12 ng/ul	3624300	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid	122	C7H6O2	000065-85-0	97
2	Benzoic acid	122	C7H6O2	000065-85-0	95
3	Benzoic acid	122	C7H6O2	000065-85-0	95
4	Benzoic acid	122	C7H6O2	000065-85-0	91
5	Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	91





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Quant Title : SVOA CALIBRATION

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

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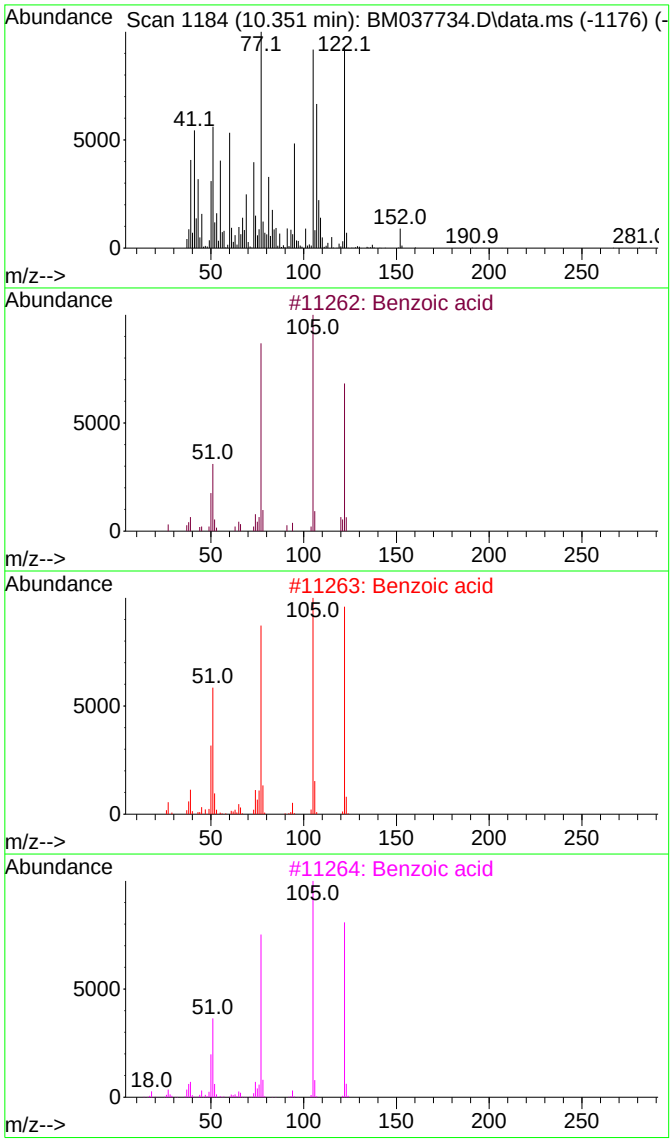
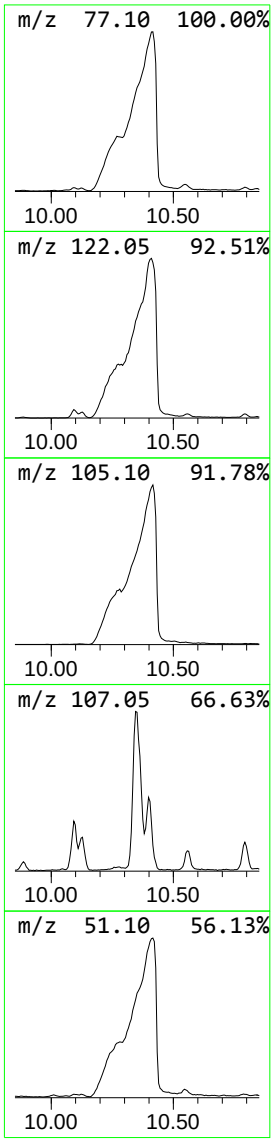
Peak Number 22 unknown-03 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.351	20.31 ng/ul	3848870	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid	122	C7H6O2	000065-85-0	70
2	Benzoic acid	122	C7H6O2	000065-85-0	70
3	Benzoic acid	122	C7H6O2	000065-85-0	64
4	Benzoic acid	122	C7H6O2	000065-85-0	55
5	Benzoic acid	122	C7H6O2	000065-85-0	55





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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

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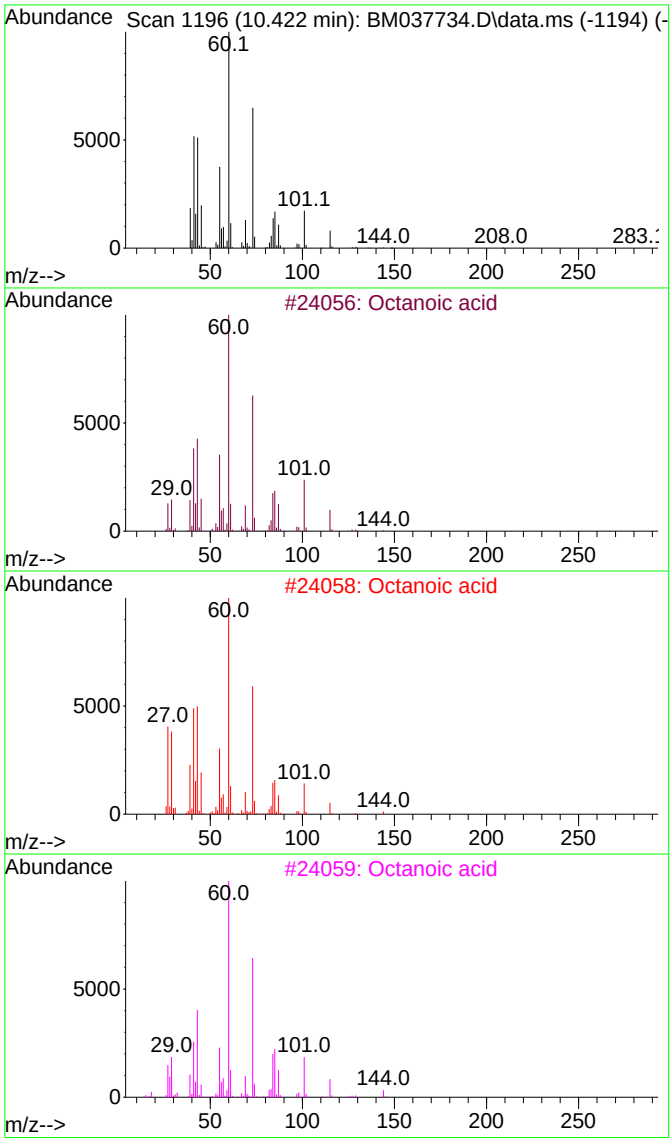
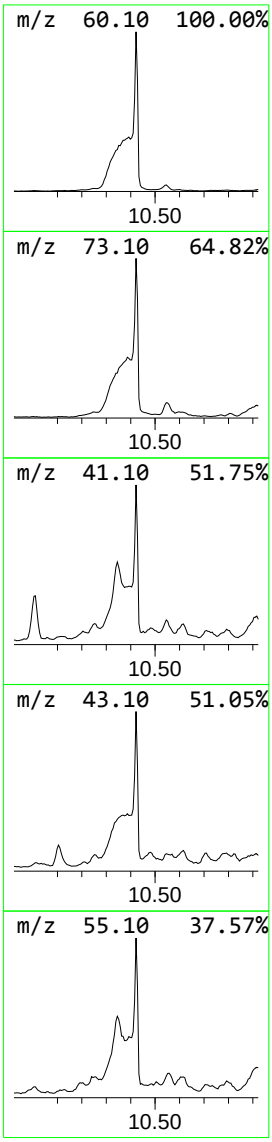
Peak Number 23 Octanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.422	22.43 ng/ul	4250960	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	97
2	Octanoic acid	144	C8H16O2	000124-07-2	90
3	Octanoic acid	144	C8H16O2	000124-07-2	80
4	Octanoic acid	144	C8H16O2	000124-07-2	78
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64





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Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

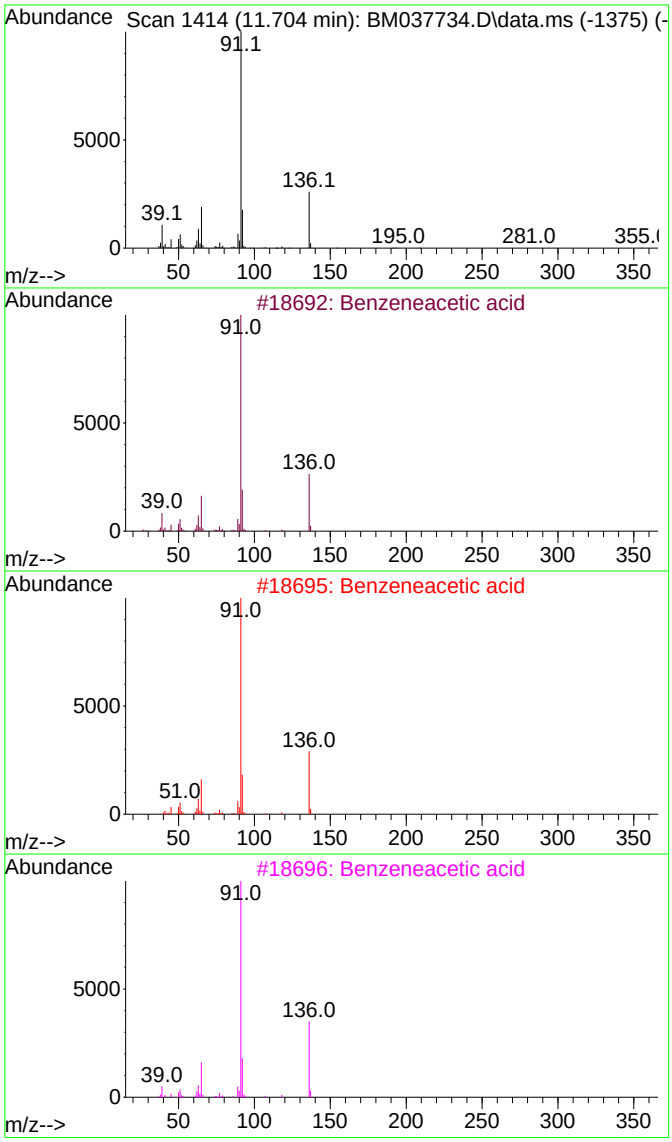
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

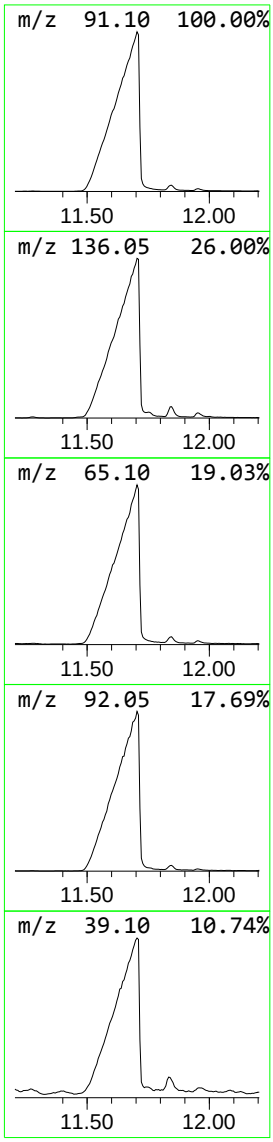
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 28 Benzeneacetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	261.66 ng/ul	49596100	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2	Benzeneacetic acid	136	C8H8O2	000103-82-2	94
3	Benzeneacetic acid	136	C8H8O2	000103-82-2	91
4	Benzeneacetic acid	136	C8H8O2	000103-82-2	91
5	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	64





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Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

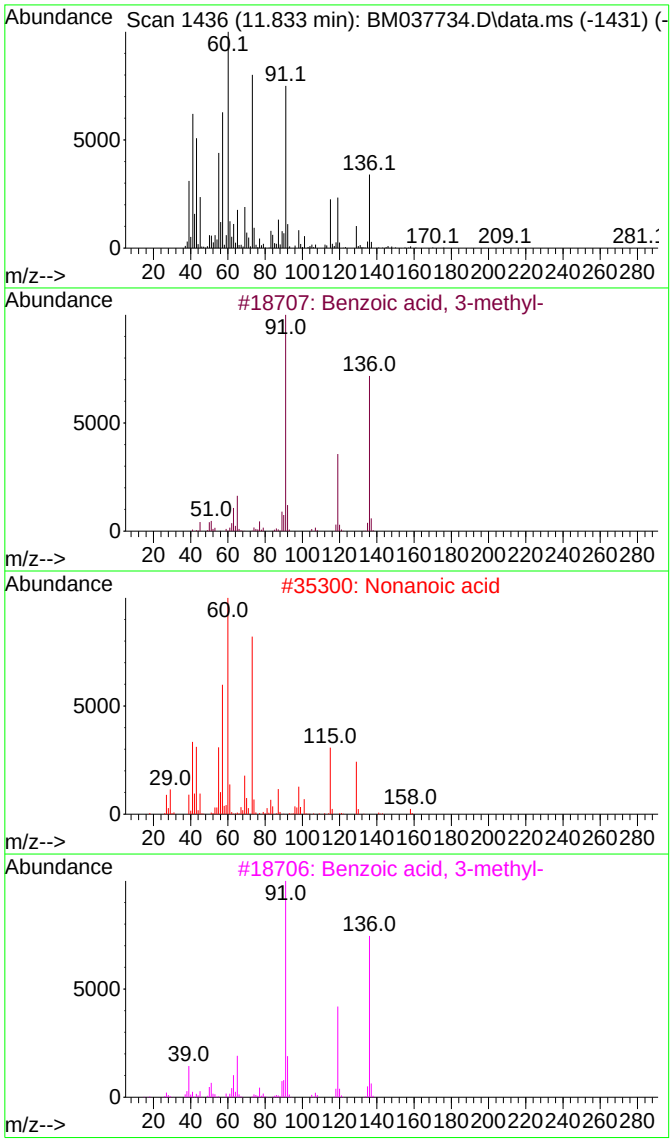
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

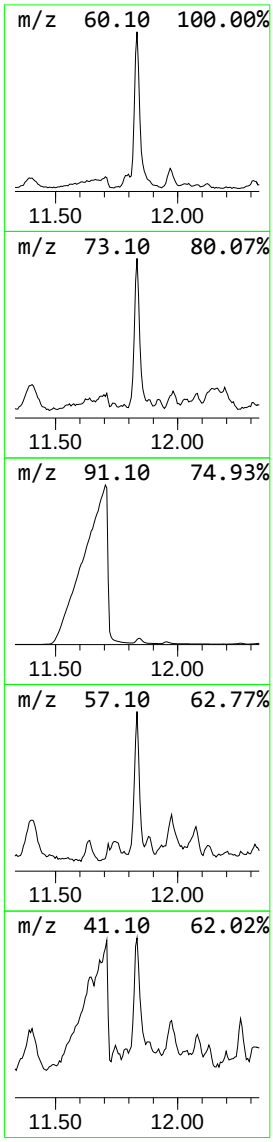
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 29 Benzoic acid, 3-methyl- Concentration Rank 29

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.834	7.05 ng/ul	1336500	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	66
2	Nonanoic acid	158	C9H18O2	000112-05-0	64
3	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	62
4	Nonanoic acid	158	C9H18O2	000112-05-0	47
5	Pentanoic acid	102	C5H10O2	000109-52-4	43





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ClientSampleId :
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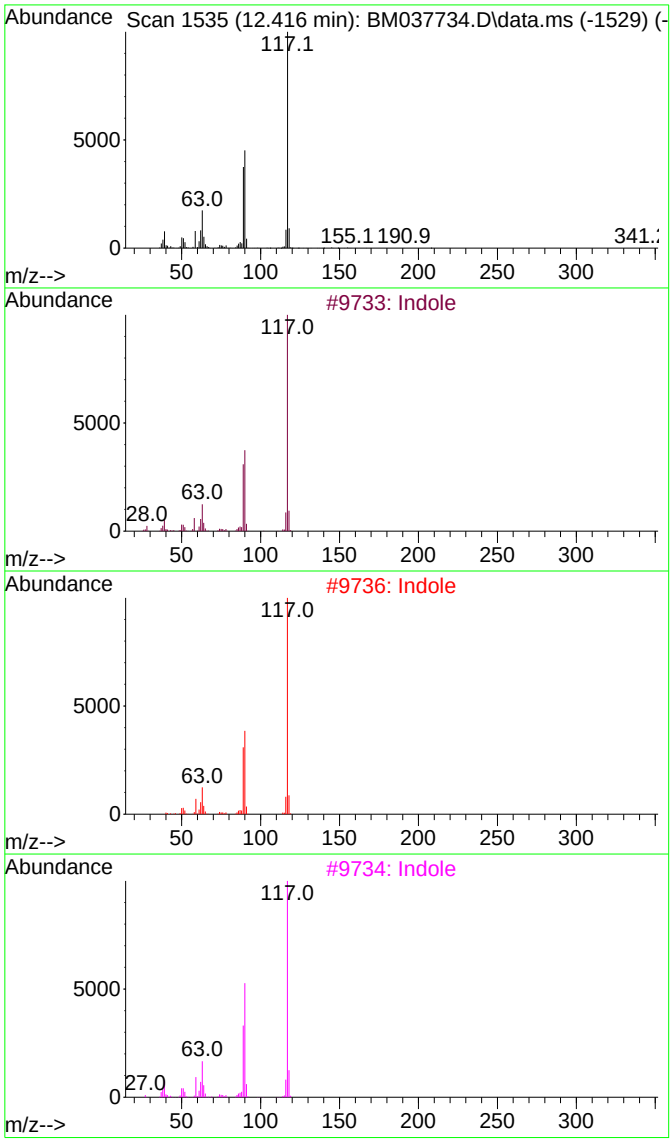
Quant Title : SVOA CALIBRATION

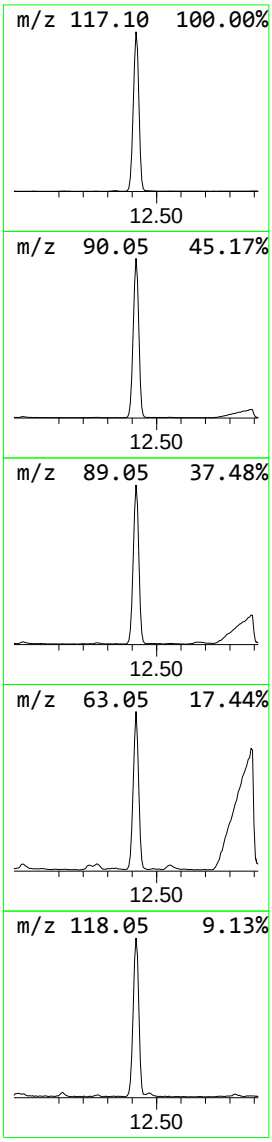
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 33 Indole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	28.71 ng/ul	5442550	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	97
2	Indole	117	C8H7N	000120-72-9	94
3	Indole	117	C8H7N	000120-72-9	94
4	Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	91
5	Indolizine	117	C8H7N	000274-40-8	91





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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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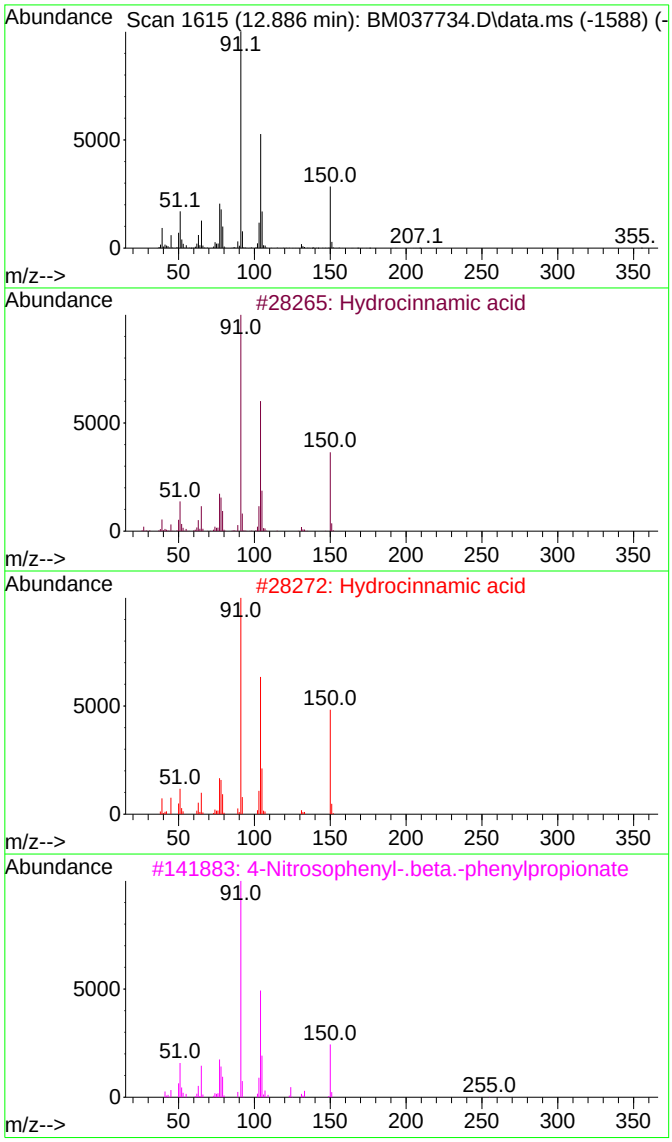
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

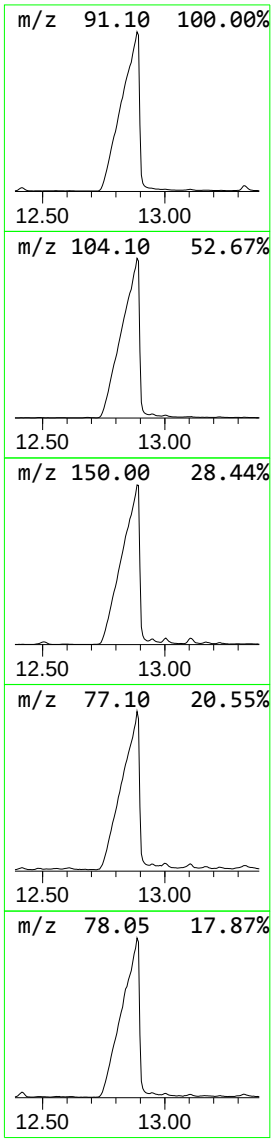
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 35 Hydrocinnamic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	214.53 ng/ul	43824100	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	95
2	Hydrocinnamic acid	150	C9H10O2	000501-52-0	95
3	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	91
4	Hydrocinnamic acid	150	C9H10O2	000501-52-0	87
5	Hydrocinnamic acid	150	C9H10O2	000501-52-0	87





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ALS Vial : 46 Sample Multiplier: 1

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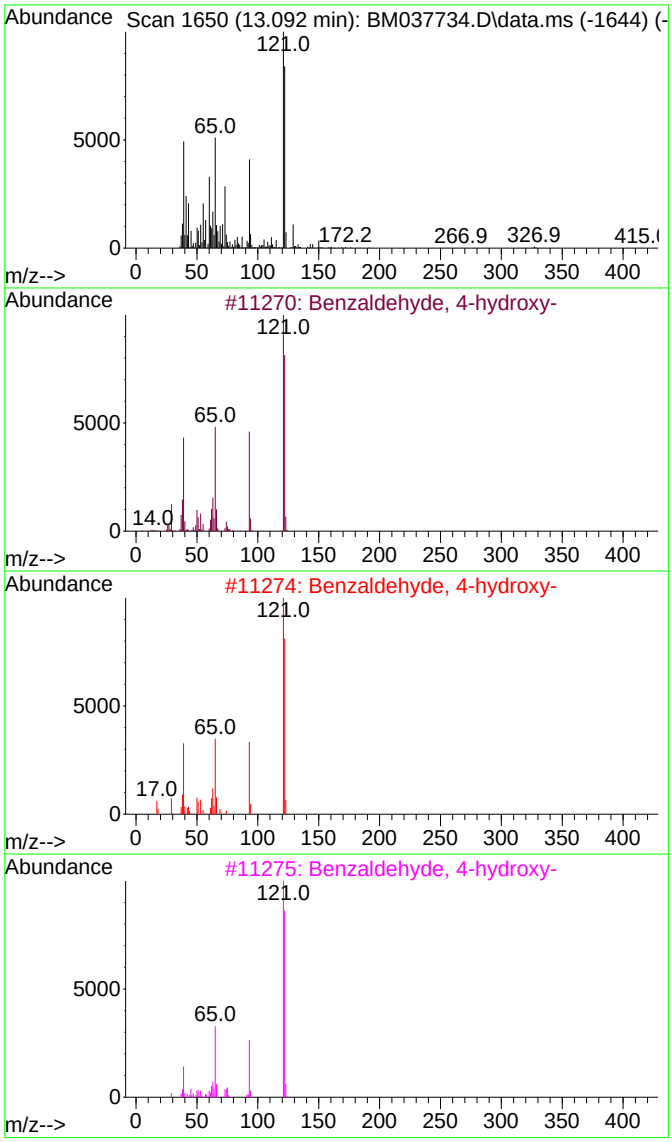
Quant Title : SVOA CALIBRATION

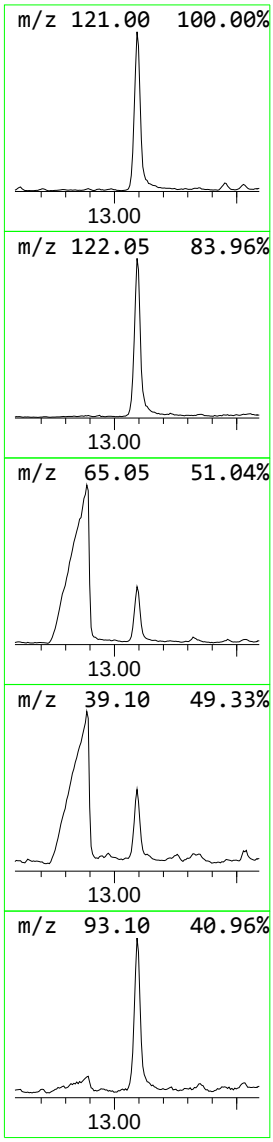
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 36 Benzaldehyde, 4-hydroxy- Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.092	12.57 ng/ul	2567410	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	97
2	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	96
3	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	87
4	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	81
5	Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	81





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Misc :
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Quant Title : SVOA CALIBRATION

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

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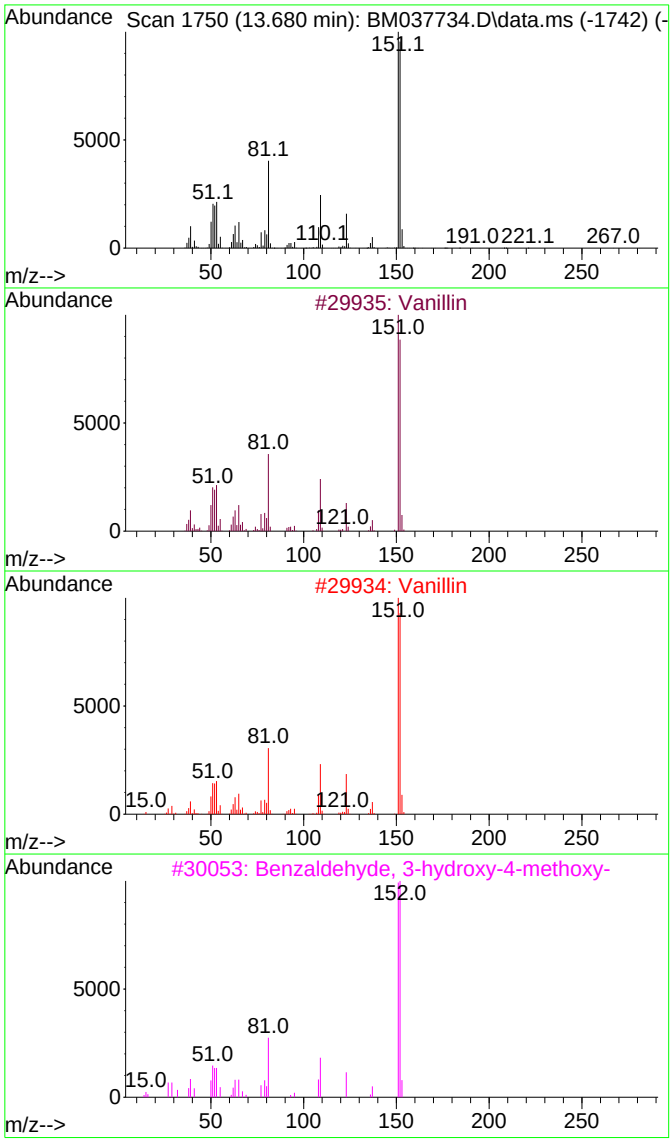
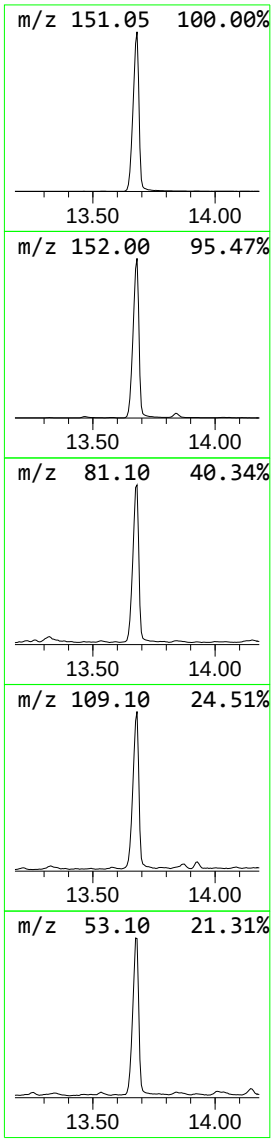
Peak Number 39 Vanillin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	82.86 ng/ul	16925900	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	98
2	Vanillin	152	C8H8O3	000121-33-5	97
3	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
4	Vanillin	152	C8H8O3	000121-33-5	97
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97





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Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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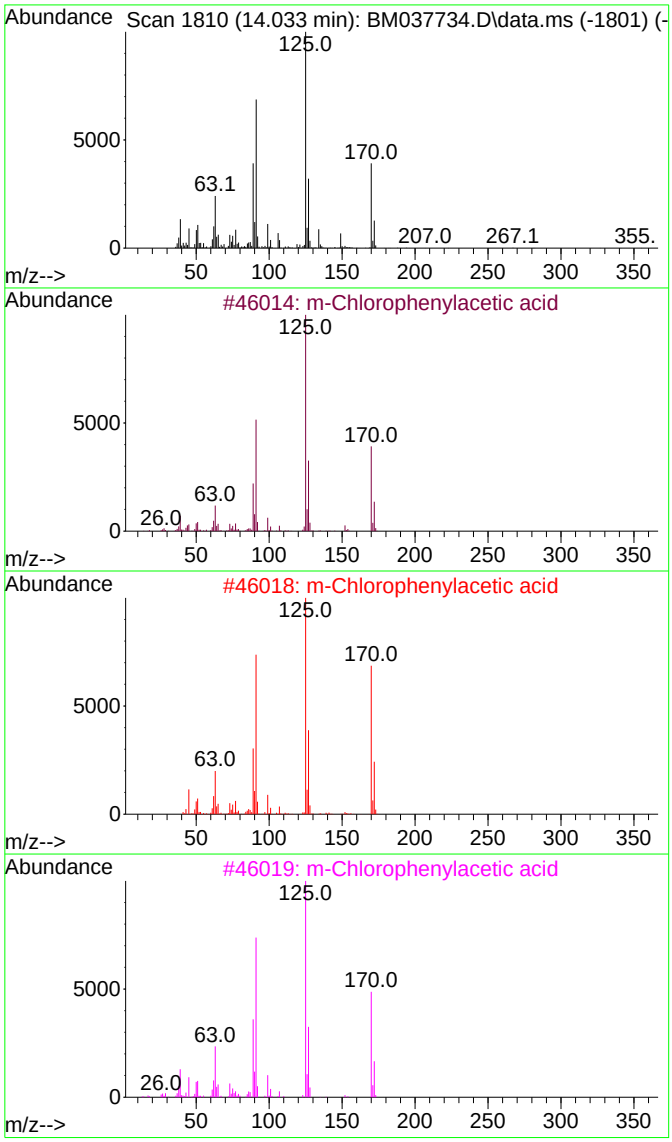
Quant Title : SVOA CALIBRATION

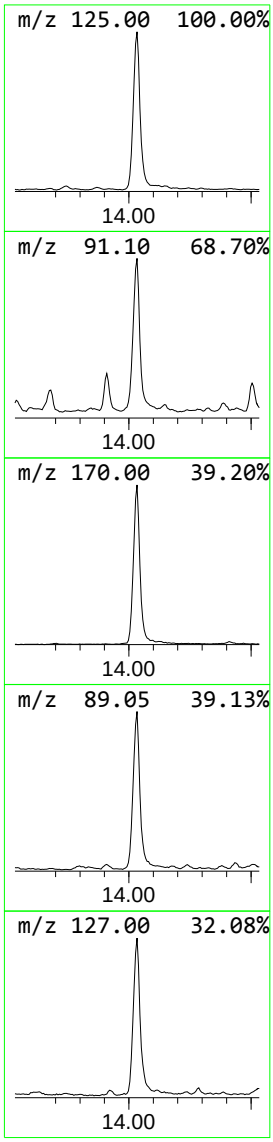
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 42 m-Chlorophenylacetic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	23.15 ng/ul	4728960	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	96
2	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	96
3	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	96
4	Benzeneacetic acid, 4-chloro-	170	C8H7ClO2	001878-66-6	95
5	Benzeneacetic acid, 2-chloro-	170	C8H7ClO2	002444-36-2	94





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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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Quant Title : SVOA CALIBRATION

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

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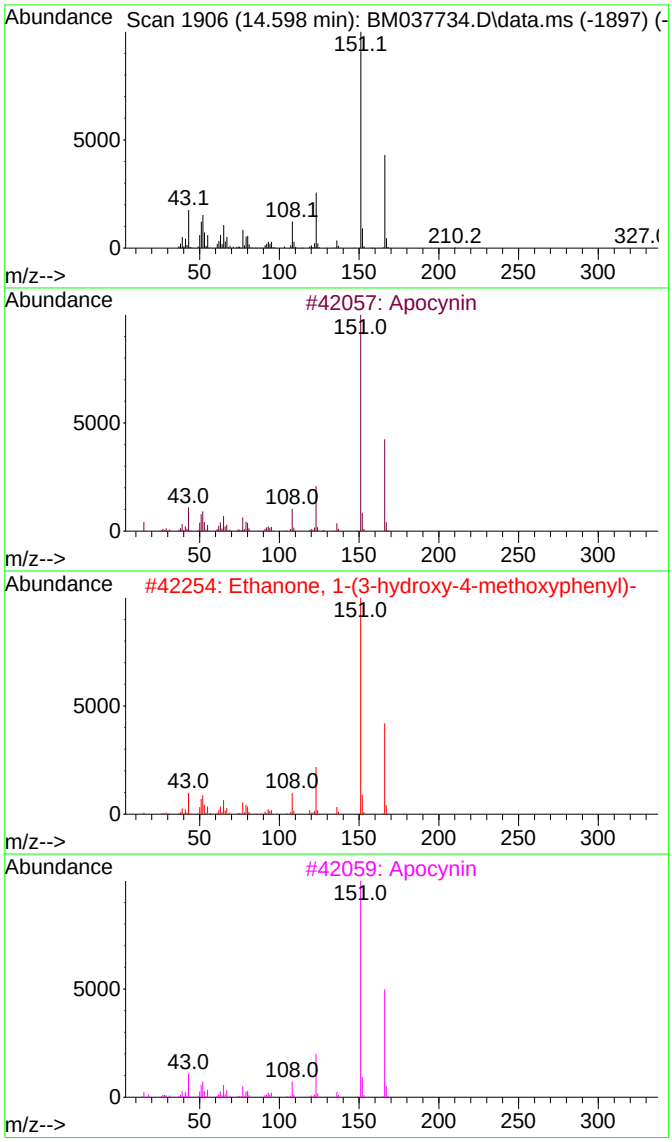
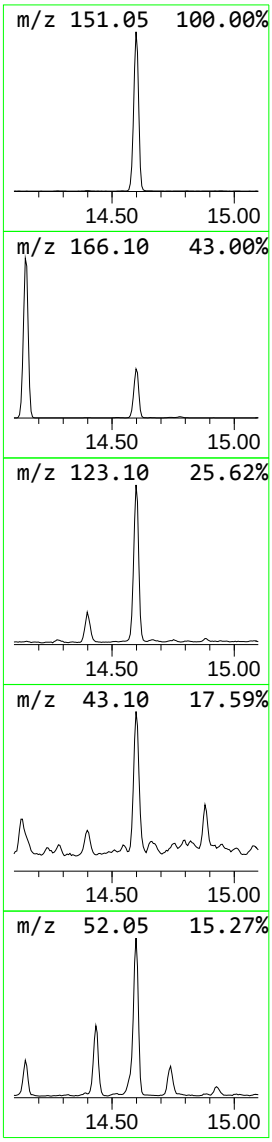
Peak Number 44 Apocynin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	36.95 ng/ul	7547370	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	96
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	94
3	Apocynin	166	C9H10O3	000498-02-2	93
4	Apocynin	166	C9H10O3	000498-02-2	91
5	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	90





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Quant Title : SVOA CALIBRATION

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

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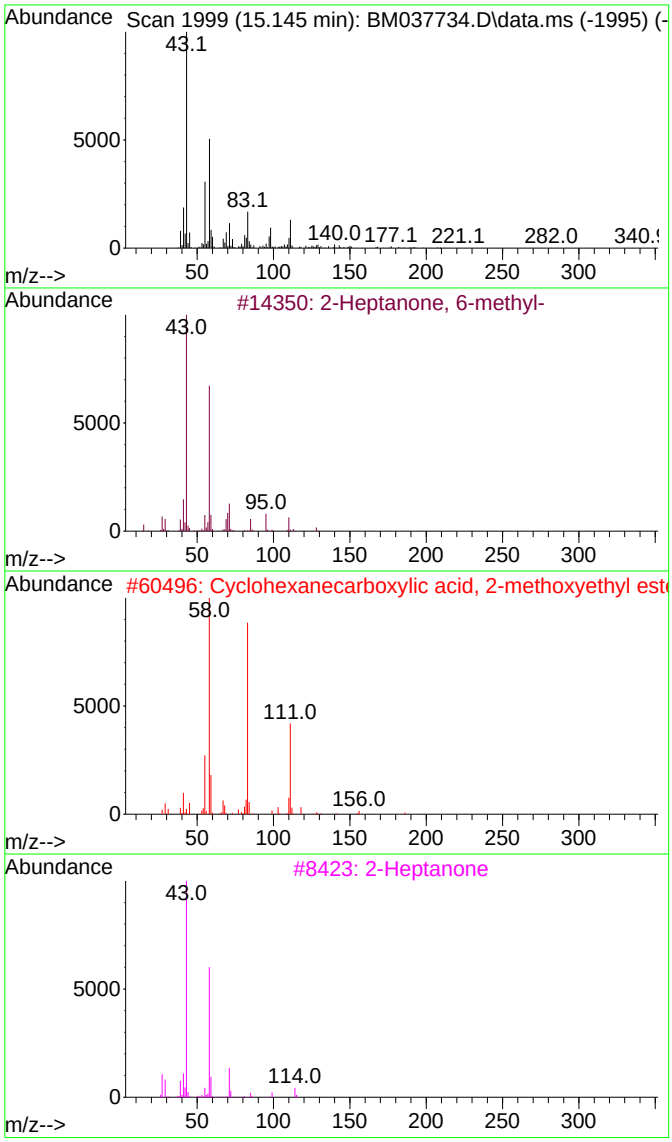
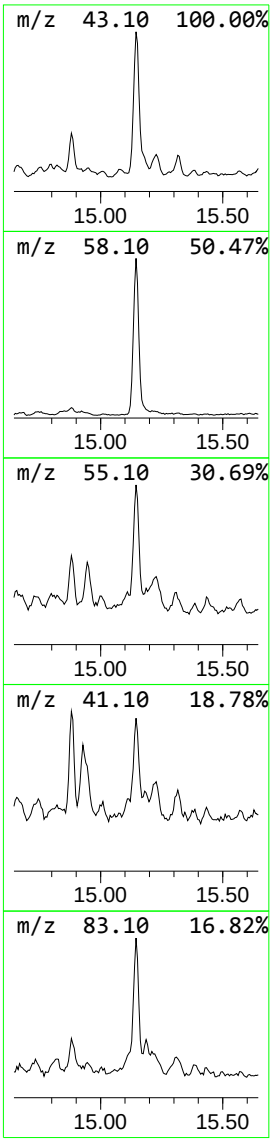
Peak Number 45 unknown-04 Concentration Rank 30

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	6.51 ng/ul	1329580	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	46
2	Cyclohexanecarboxylic acid, 2-me...	186	C10H18O3	1000330-87-5	40
3	2-Heptanone	114	C7H14O	000110-43-0	38
4	Acetic acid, 2-(dimethylamino)et...	131	C6H13NO2	001421-89-2	38
5	2-Heptanone	114	C7H14O	000110-43-0	38





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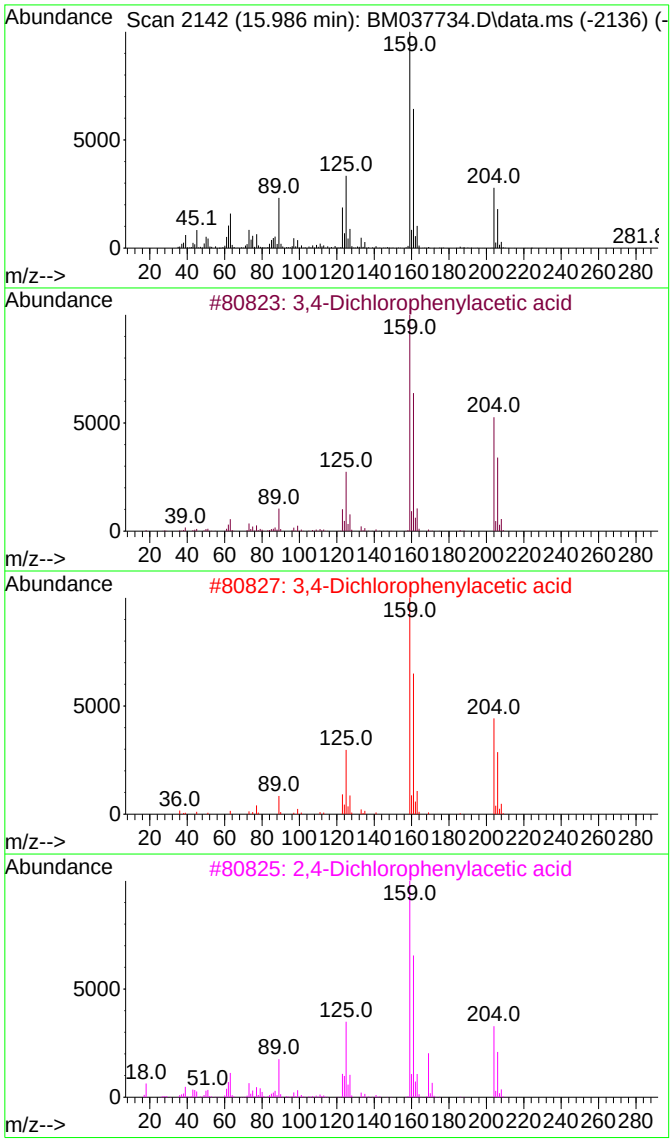
Quant Title : SVOA CALIBRATION

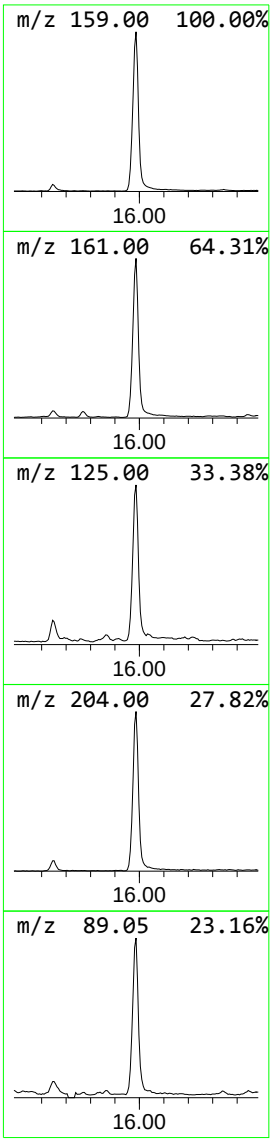
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 47 3,4-Dichlorophenylacetic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	24.47 ng/ul	4998770	Acenaphthene-d10	14.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	005807-30-7	97
2	3,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	005807-30-7	97
3	2,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	019719-28-9	96
4	3,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	005807-30-7	94
5	2,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	019719-28-9	94





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ALS Vial : 46 Sample Multiplier: 1

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ClientSampleId :
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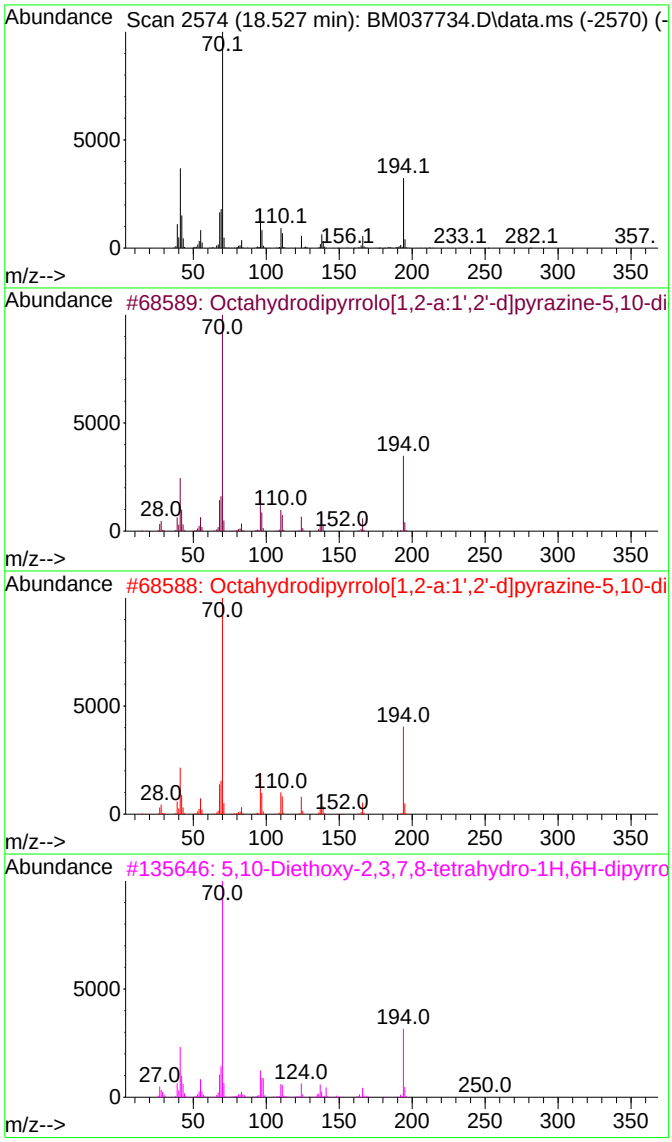
Quant Title : SVOA CALIBRATION

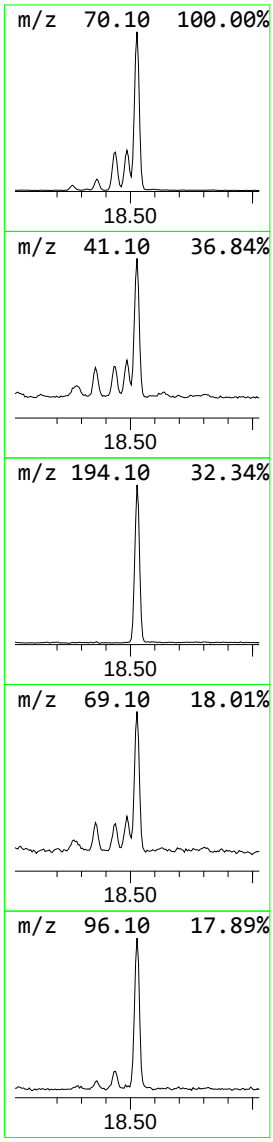
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 54 Octahydrodipyrrolo[1,2-a:1'... Concentration Rank 27

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.527	8.27 ng/ul	2513840	Phenanthrene-d10	17.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octahydrodipyrrolo[1,2-a:1',2'-d...	194	C10H14N2O2	1000497-90-3	97
2	Octahydrodipyrrolo[1,2-a:1',2'-d...	194	C10H14N2O2	1000497-90-2	96
3	5,10-Diethoxy-2,3,7,8-tetrahydro...	250	C14H22N2O2	1000190-75-5	91
4	6,6-Dimethyl-cyclohex-2-en-1-ol	126	C8H14O	038313-10-9	43
5	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

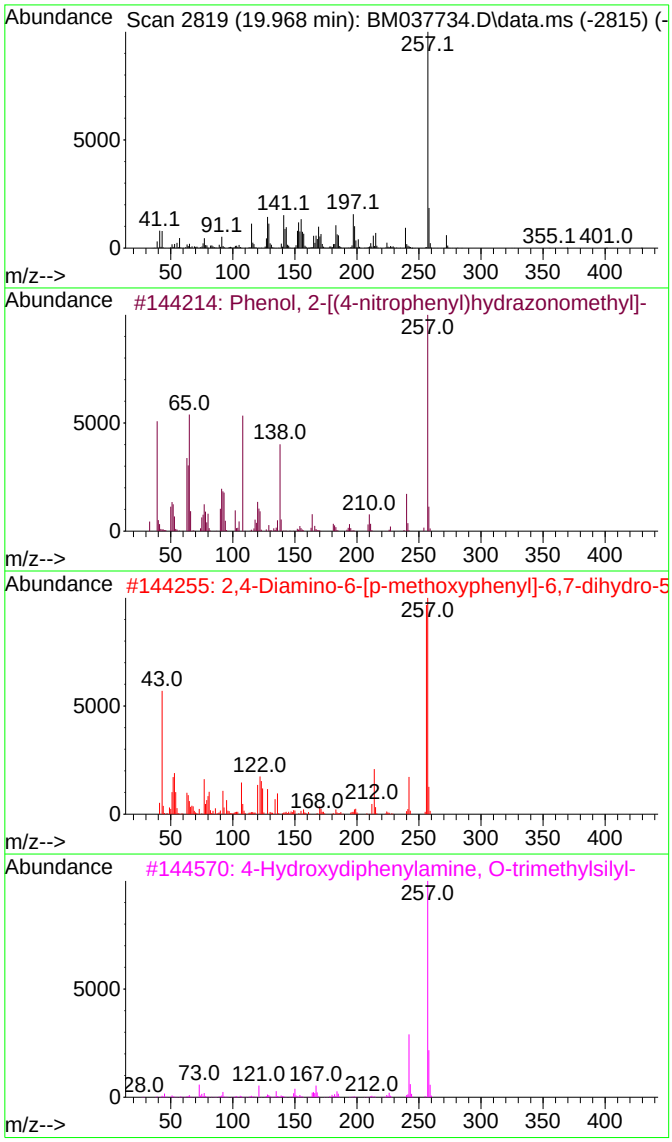
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

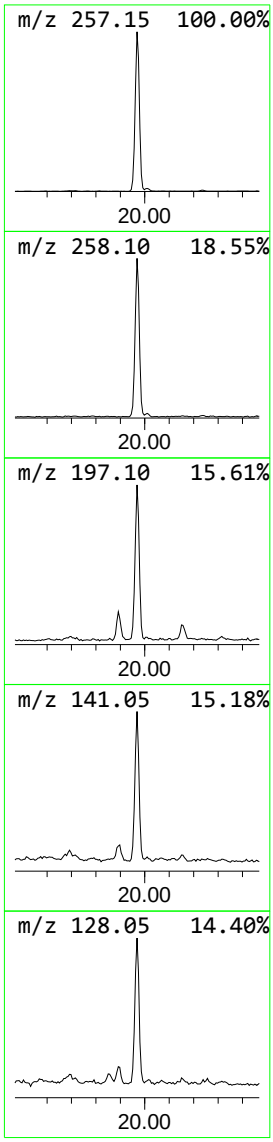
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 56 Phenol, 2-[(4-nitrophenyl)h... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.968	16.28 ng/ul	3245120	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-[(4-nitrophenyl)hydraz...	257	C13H11N3O3	003155-24-6	55
2	2,4-Diamino-6-[p-methoxyphenyl]-...	257	C13H15N5O	1000251-46-9	49
3	4-Hydroxydiphenylamine, O-trimet...	257	C15H19NOSi	1000417-42-0	47
4	9-Amino-7-nitro-3,4-dihydro-1(2H...	257	C13H11N3O3	104675-31-2	47
5	N-allylnormetazocine	257	C17H23NO	014198-28-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

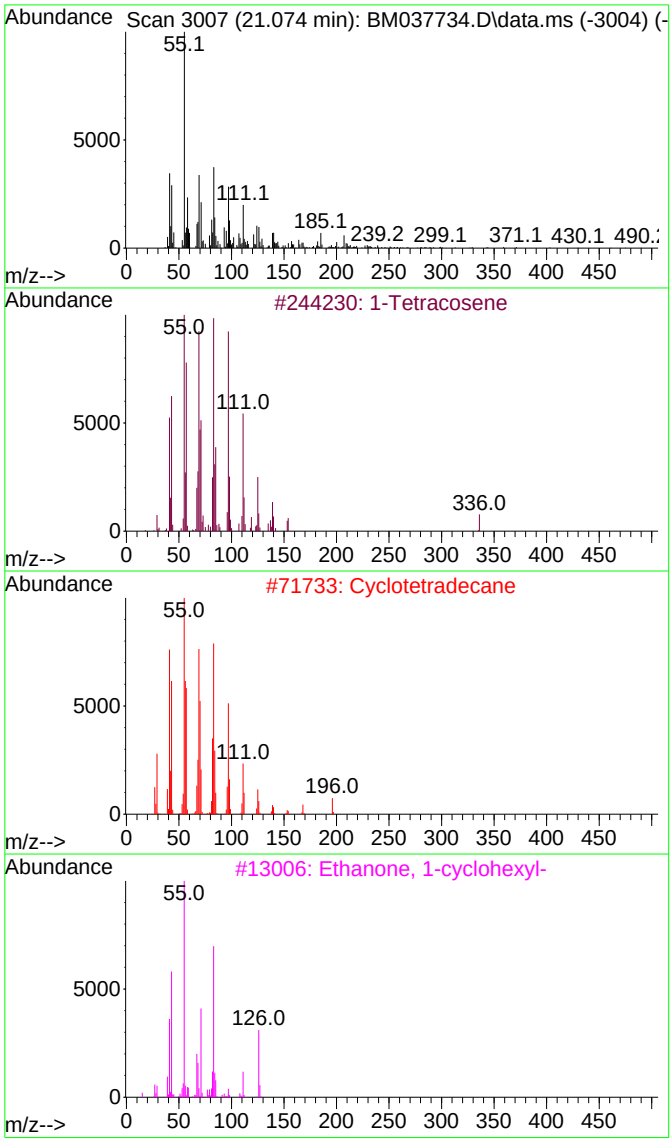
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

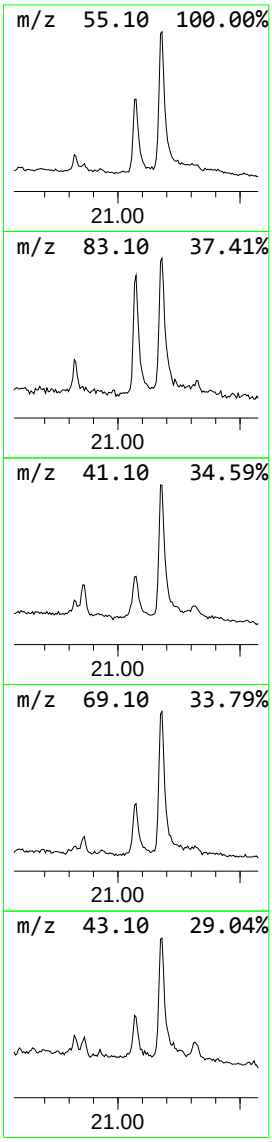
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 58 (DEL) Alkane: Straight-Chai... Concentration Rank 39

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	3.59 ng/ul	715330	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	47
2	Cyclotetradecane	196	C14H28	000295-17-0	38
3	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	38
4	5-Tetradecene, (Z)-	196	C14H28	041446-62-2	27
5	4,4-Dimethyl-cyclohex-2-en-1-ol	126	C8H14O	1010143-72-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

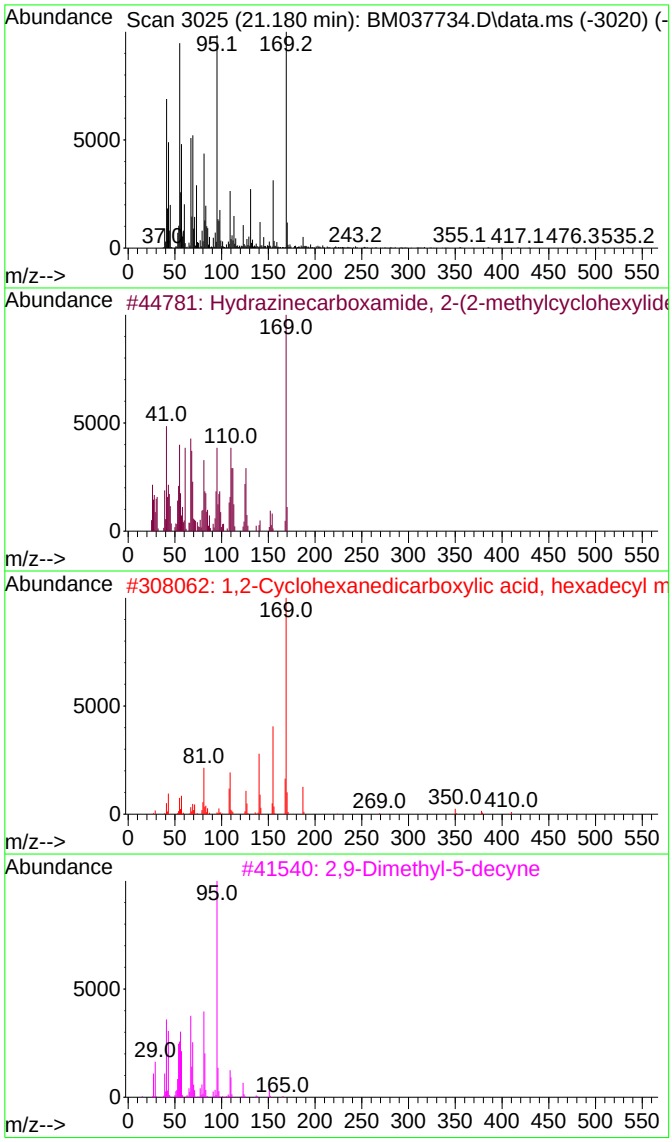
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

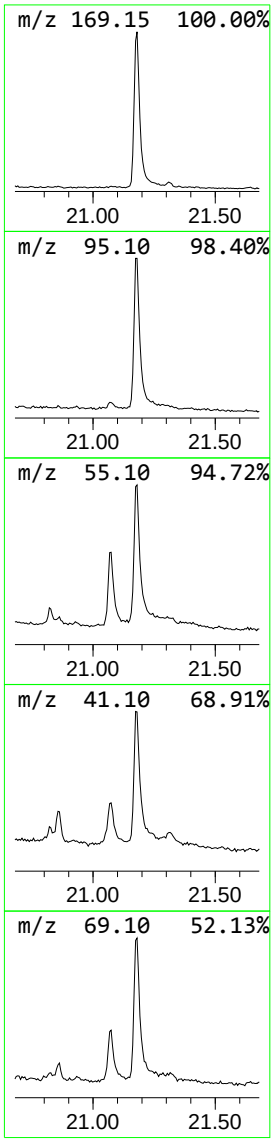
****

Peak Number 59 unknown-05 Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	14.05 ng/ul	2800660	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazinecarboxamide, 2-(2-methy...	169	C8H15N3O	004549-20-6	38
2	1,2-Cyclohexanedicarboxylic acid...	410	C25H46O4	1000339-66-2	27
3	2,9-Dimethyl-5-decyne	166	C12H22	019550-56-2	27
4	Cyclopropane, (2,2-dimethylpropy...	110	C8H14	039647-71-7	25
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037734.D
Acq On : 26 Nov 2022 15:38
Operator : CG/JU
Sample : N5602-18
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
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
Butanoic acid	4.216	37.4	ng/ul	2942340	1	8.110	1572860	20.0
Butanoic acid, ...	5.263	370.7	ng/ul	29153400	1	8.110	1572860	20.0
Butanoic acid, ...	5.422	142.4	ng/ul	11199700	1	8.110	1572860	20.0
Pentanoic acid	5.728	36.0	ng/ul	2831910	1	8.110	1572860	20.0
Pentanoic acid,...	6.522	5.4	ng/ul	422289	1	8.110	1572860	20.0
Pentanoic acid,...	6.675	14.6	ng/ul	1150220	1	8.110	1572860	20.0
1-Hexanol, 2-et...	8.175	25.2	ng/ul	1982480	1	8.110	1572860	20.0
unknown-01	8.345	10.1	ng/ul	795434	1	8.110	1572860	20.0
Hexanoic acid	8.740	18.9	ng/ul	1485830	1	8.110	1572860	20.0
cis-Linaloloxide	8.998	8.0	ng/ul	631819	1	8.110	1572860	20.0
Cyclopentene	9.363	31.4	ng/ul	2469060	1	8.110	1572860	20.0
Hexanoic acid, ...	9.463	19.4	ng/ul	1526230	1	8.110	1572860	20.0
Cyclohexanecarb...	9.616	13.7	ng/ul	2598510	2	10.934	3790830	20.0
unknown-02	9.663	14.8	ng/ul	2796420	2	10.934	3790830	20.0
Benzoic acid	10.269	19.1	ng/ul	3624300	2	10.934	3790830	20.0
unknown-03	10.351	20.3	ng/ul	3848870	2	10.934	3790830	20.0
Octanoic acid	10.422	22.4	ng/ul	4250960	2	10.934	3790830	20.0
Benzeneacetic acid	11.704	261.7	ng/ul	49596100	2	10.934	3790830	20.0
Benzoic acid, 3...	11.834	7.0	ng/ul	1336500	2	10.934	3790830	20.0
Indole	12.416	28.7	ng/ul	5442550	2	10.934	3790830	20.0
Hydrocinnamic acid	12.886	214.5	ng/ul	43824100	3	14.739	4085640	20.0
Benzaldehyde, 4...	13.092	12.6	ng/ul	2567410	3	14.739	4085640	20.0
Vanillin	13.680	82.9	ng/ul	16925900	3	14.739	4085640	20.0
m-Chlorophenyla...	14.033	23.1	ng/ul	4728960	3	14.739	4085640	20.0
Apocynin	14.598	37.0	ng/ul	7547370	3	14.739	4085640	20.0
unknown-04	15.145	6.5	ng/ul	1329580	3	14.739	4085640	20.0
3,4-Dichlorophe...	15.986	24.5	ng/ul	4998770	3	14.739	4085640	20.0
Octahydrodipyrr...	18.527	8.3	ng/ul	2513840	4	17.474	6076630	20.0
Phenol, 2-[(4-n...	19.968	16.3	ng/ul	3245120	5	21.639	3987630	20.0
(DEL) Alkane: S...	21.074	3.6	ng/ul	715330	5	21.639	3987630	20.0
unknown-05	21.180	14.1	ng/ul	2800660	5	21.639	3987630	20.0