LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112822\
Data File : BM037760.D
Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

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: BM037760.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.793	53	69	77	rVB	409379	1091874	11.90%	1.282%
2	3.893	83	86	90	rBV	54218	95795	1.04%	0.112%
3	3.928	90	92	104	rVB3	68707	131098	1.43%	0.154%
4	4.028	106	109	114	rVB	34753	45222	0.49%	0.053%
5	4.122	114	125	133	rBV	201162	464694	5.06%	0.546%
6	5.052	248	283	286	rBV	877641	4924880	53.66%	5.782%
7	5.199	290	308	311	rVV	612597	2095325	22.83%	2.460%
8	5.575	361	372	377	rBV	206379	447324	4.87%	0.525%
9	5.916	426	430	435	rVV	36813	50945	0.56%	0.060%
10	6.087	454	459	463	rBV2	24957	38756	0.42%	0.045%
11	6.463	518	523	531	rVB2	50215	83524	0.91%	0.098%
12	6.599	540	546	555	rVB	117143	208378	2.27%	0.245%
13	6.940	596	604	613	rBV	24419	68323	0.74%	0.080%
14	7.128	620	636	648	rBV	306075	823455	8.97%	0.967%
15	7.287	648	663	673	rVV	1968441	3148838	34.31%	3.697%
16	7.428	681	687	692	rBV	275492	415547	4.53%	0.488%
17	7.634	717	722	731	rVB	162707	267615	2.92%	0.314%
18	8.022	784	788	792	rVB	35277	53901	0.59%	0.063%
19	8.110	792	803	809	rBV	975825	1623007	17.68%	1.905%
20	8.169	809	813	819	rVB	139154	211287	2.30%	0.248%
21	8.269	825	830	832	rBV	51139	75302	0.82%	0.088%
22	8.298	832	835	841	rVV	61245	90183	0.98%	0.106%
23	8.545	871	877	882	rBV4	37879	69357	0.76%	0.081%
24	8.687	893	901	906	rVV	112649	215395	2.35%	0.253%
25	8.740	906	910	913	rVV5	23698	40503	0.44%	0.048%
26	8.810	917	922	927	rVV	167484	285019	3.11%	0.335%
27	8.869	927	932	941	rVV	1061750	1732873	18.88%	2.034%
28	8.981	947	951	960	rVB6	47088	105412	1.15%	0.124%
29	9.228	984	993	996	rBV7	29988	59745	0.65%	0.070%
30	9.275	996	1001	1010	rVV	334013	605334	6.60%	0.711%
31	9.357	1010	1015	1020	rVV	268543	427250	4.66%	0.502%
32	9.422	1020	1026	1034	rVV2	95351	225899	2.46%	0.265%
33	9.569	1039	1051	1060	rVB3	308281	924234	10.07%	1.085%
34	10.004	1118	1125	1131	rBV	213343	362002	3.94%	0.425%
35	10.245	1145	1166	1169	rVV	706320	2981686	32.49%	3.500%
36	10.287	1169	1173	1178	rVV	545183	932303	10.16%	1.095%

LSC Area Percent Report

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Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AH0DL

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	10.339	1178	1182	1188	rVV3	132531	252166	2.75%	0.296%
38	10.398	1188	1192	1196	rVB4	30988	49582	0.54%	0.058%
39	10.545	1211	1217	1224	rVB	298589	520588	5.67%	0.611%
40	10.704	1239	1244	1253	rBV8	30990	76696	0.84%	0.090%
41	10.822	1255	1264	1276	rBV5	123035	518614	5.65%	0.609%
42	10.928	1276	1282	1288	rVV	1454328	2394598	26.09%	2.811%
43	10.986	1288	1292	1298	rVB3	121587	203829	2.22%	0.239%
44	11.063	1298	1305	1314	rBV	222185	504975	5.50%	0.593%
45	11.204	1324	1329	1330	rBV3	33720	45194	0.49%	0.053%
46	11.351	1347	1354	1362	rVB7	50408	127978	1.39%	0.150%
47	11.557	1367	1389	1406	rBV	2443992	9177378	100.00%	10.774%
48	11.739	1415	1420	1427	rBV3	164642	300729	3.28%	0.353%
49	12.175	1490	1494	1499	rVB6	28048	45605	0.50%	0.054%
50	12.251	1501	1507	1512	rBV	92102	162640	1.77%	0.191%
51	12.328	1512	1520	1524	rVV8	46491	111250	1.21%	0.131%
52	12.410	1526	1534	1540	rVV	592891	1003897	10.94%	1.179%
53	12.486	1540	1547	1552	rVV6	43331	104852	1.14%	0.123%
54	12.545	1554	1557	1564	rVB4	44804	79660	0.87%	0.094%
55	12.775	1580	1596	1608	rBV	2743913	7868035	85.73%	9.237%
56	13.028	1634	1639	1641	rBV3	117515	180021	1.96%	0.211%
57	13.063	1641	1645	1654	rVB	255224	446636	4.87%	0.524%
58	13.269	1672	1680	1683	rBV6	43187	100479	1.09%	0.118%
59	13.486	1713	1717	1722	rVB4	66240	93664	1.02%	0.110%
60	13.657	1738	1746	1755	rBV	2480409	3617261	39.41%	4.247%
61	13.780	1764	1767	1773	rVB3	79757	126401	1.38%	0.148%
62	13.851	1774	1779	1780	rBV4	45931	64087	0.70%	0.075%
63	13.992	1798	1803	1812	rVV	357823	639153	6.96%	0.750%
64	14.139	1823	1828	1834	rVB	793092	1094319	11.92%	1.285%
65	14.275	1847	1851	1859	rBV8	37574	84907	0.93%	0.100%
66	14.392	1867	1871	1873	rBV3	77867	115938	1.26%	0.136%
67	14.427	1873	1877	1882	rVB	849648	1206321	13.14%	1.416%
68	14.533	1890	1895	1899	rBV3	115063	204508	2.23%	0.240%
69	14.586	1899	1904	1909	rVB	851132	1146282	12.49%	1.346%
70	14.733	1922	1929	1939	rBV	2423924	3538171	38.55%	4.154%
71	14.874	1948	1953	1956	rBV2	146856	214653	2.34%	0.252%
72	14.916	1956	1960	1967	rVB3	96125	156615	1.71%	0.184%
73	15.116	1990	1994	2001	rVV	132338	233713	2.55%	0.274%
74	15.627	2075	2081	2084	rBV8	41139	89014	0.97%	0.105%
75	15.716	2091	2096	2101	rBV	1047279	1530010	16.67%	1.796%
76	15.827	2110	2115	2123	rBV2	268828	413444	4.51%	0.485%

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Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

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

77	15.957	2132	2137	2146	rBV	489033	828659	9.03%	0.973%
78	16.092	2157	2160	2167	rVB5	65103	113794	1.24%	0.134%
79	16.157	2168	2171	2173	rBV3	54653	72624	0.79%	0.085%
80	16.398	2209	2212	2215	rBV4	37749	56873	0.62%	0.067%
81	16.545	2232	2237	2241	rBV4	56613	115714	1.26%	0.136%
82	16.851	2287	2289	2297	rVB7	46803	80455	0.88%	0.094%
83	16.980	2306	2311	2317	rVB3	103256	192572	2.10%	0.226%
84	17.057	2321	2324	2329	rVB2	97243	128925	1.40%	0.151%
85	17.116	2331	2334	2339	rVV6	38368	59906	0.65%	0.070%
86	17.468	2388	2394	2400	rBV	3055547	4308957	46.95%	5.059%
87	17.568	2406	2411	2418	rVB	1193955	1715933	18.70%	2.014%
88	18.127	2503	2506	2513	rVB7	52755	80695	0.88%	0.095%
89	18.345	2539	2543	2549	rVB3	106607	142816	1.56%	0.168%
90	18.404	2550	2553	2558	rVV	122120	165503	1.80%	0.194%
91	18.457	2558	2562	2566	rVV	128923	168657	1.84%	0.198%
92	18.510	2567	2571	2580	rVB	368509	509031	5.55%	0.598%
93	19.615	2755	2759	2764	rBV3	96265	127380	1.39%	0.150%
94	19.851	2794	2799	2802	rBV	1306371	1805027	19.67%	2.119%
95	19.886	2802	2805	2811	rVB	363193	442326	4.82%	0.519%
96	19.962	2814	2818	2823	rVV	541564	641155	6.99%	0.753%
97	21.168	3020	3023	3031	rBV4	135124	254472	2.77%	0.299%
98	21.633	3097	3102	3109	rBV	3109527	3976266	43.33%	4.668%
99	23.962	3493	3498	3508	rVB3	725969	1638993	17.86%	1.924%
100	24.127	3519	3526	3535	rVB2	1595278	3287532	35.82%	3.859%

Sum of corrected areas: 85180413

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112822\
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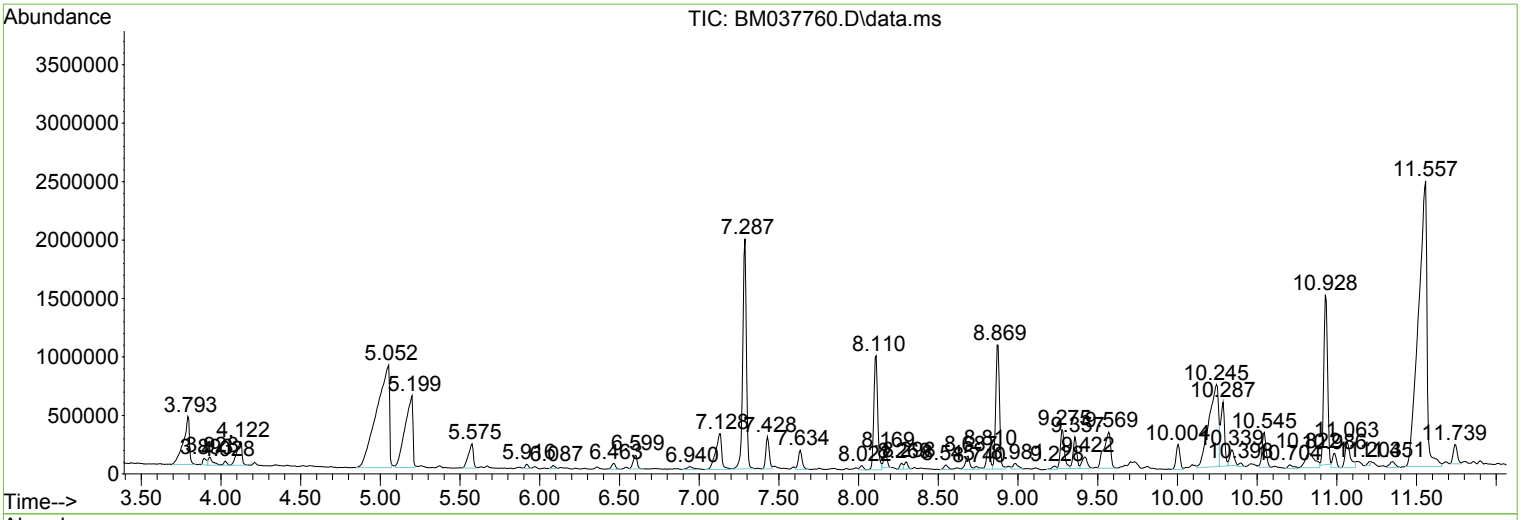
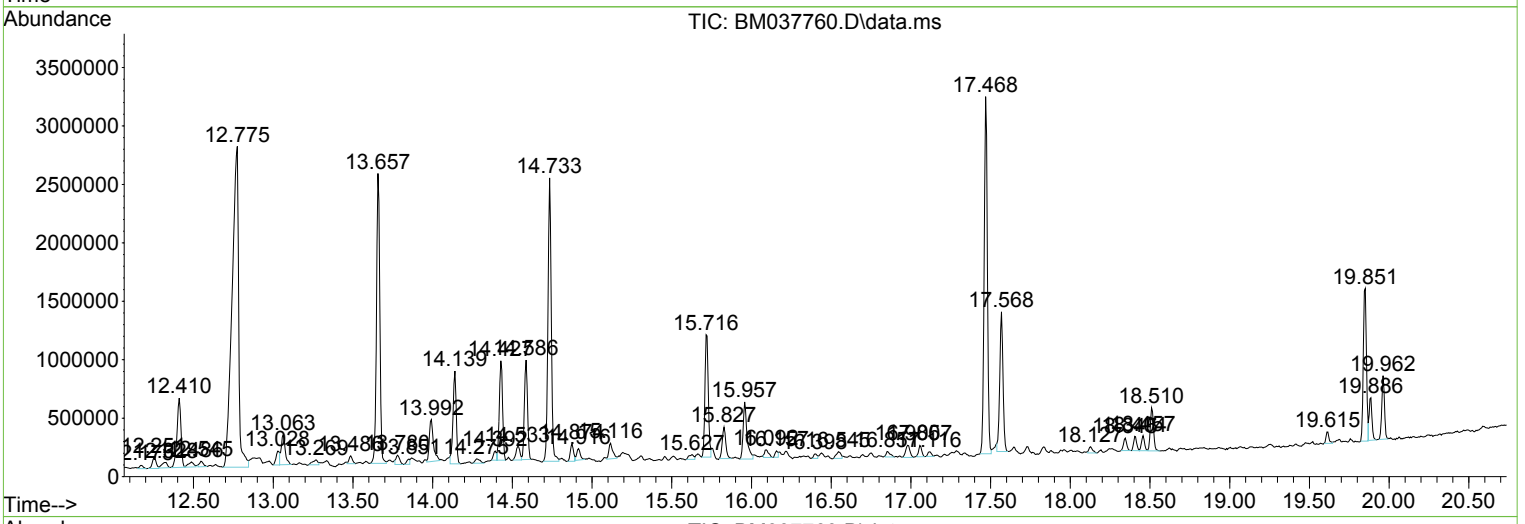
Misc :
ALS Vial : 10 Sample Multiplier: 1

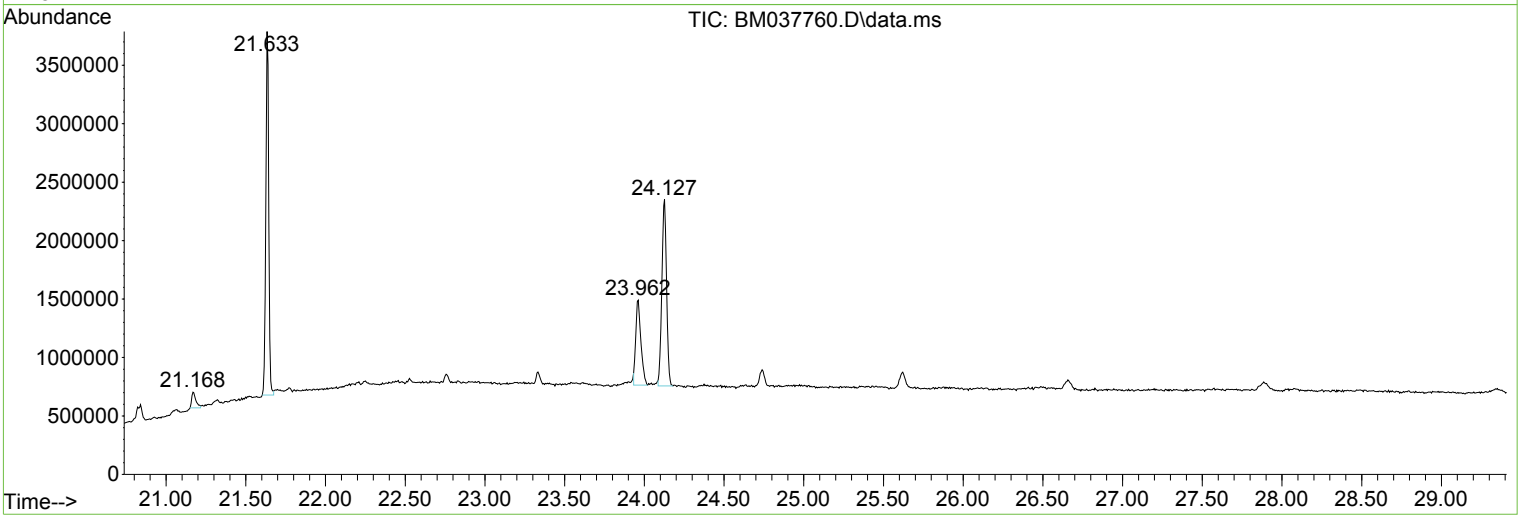
Instrument :
BNA_M
ClientSampleId :
C0AH0DL

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\BM112822\
Data File : BM037760.D
Acq On : 28 Nov 2022 15:24
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Sample : N5602-18DL 5X
Misc :
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Instrument :
BNA_M
ClientSampleId :
C0AH0DL

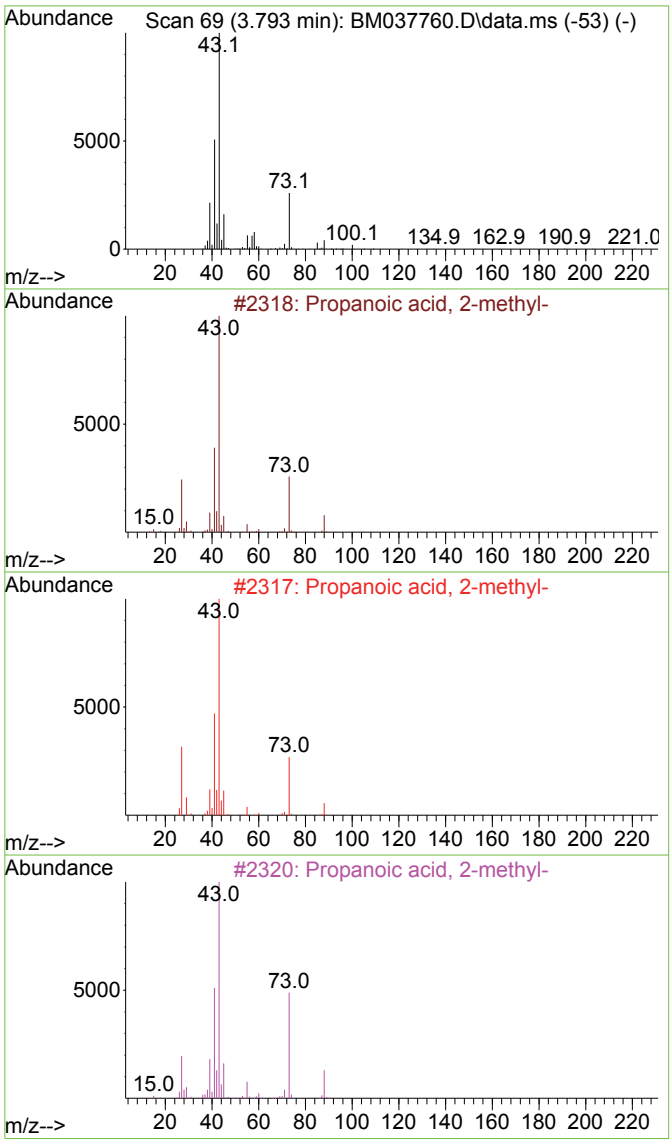
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

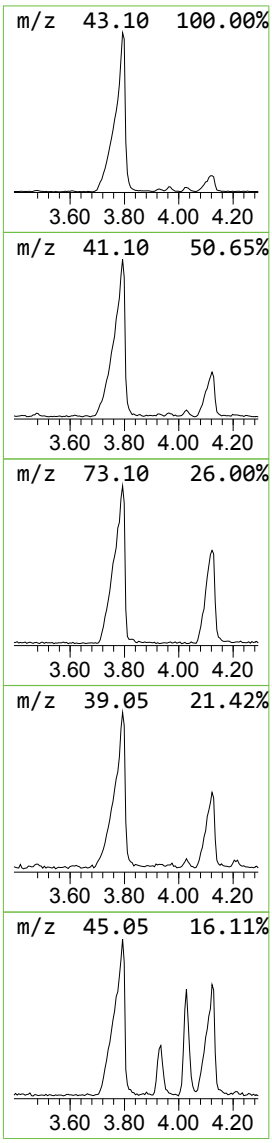
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.793	13.46 ng/ul	1091870	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	59
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	45
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	45
4	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	45
5	Glycine, N-acetyl-	117	C4H7NO3	000543-24-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112822\
Data File : BM037760.D
Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

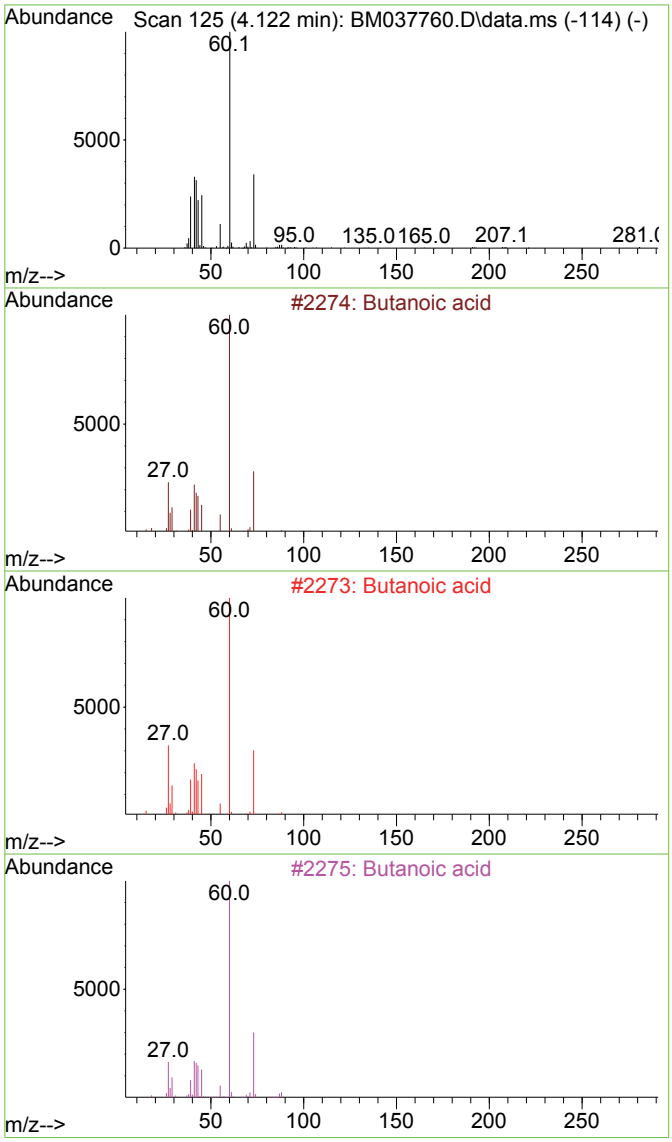
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

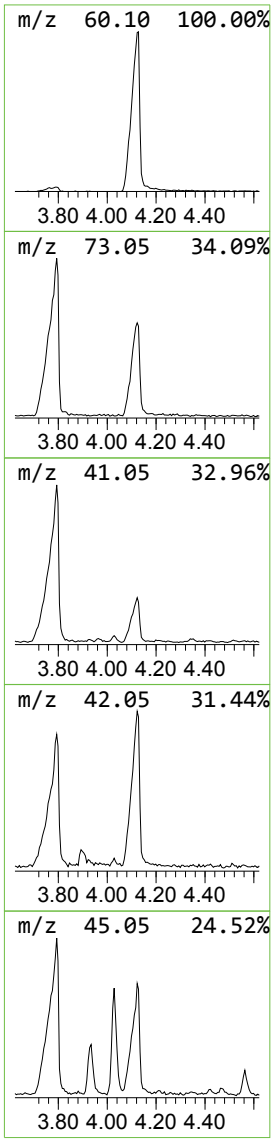
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.122	5.73 ng/ul	464694	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	72
2	Butanoic acid	88	C4H8O2	000107-92-6	72
3	Butanoic acid	88	C4H8O2	000107-92-6	64
4	Butanoic acid	88	C4H8O2	000107-92-6	64
5	Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	019467-01-7	40





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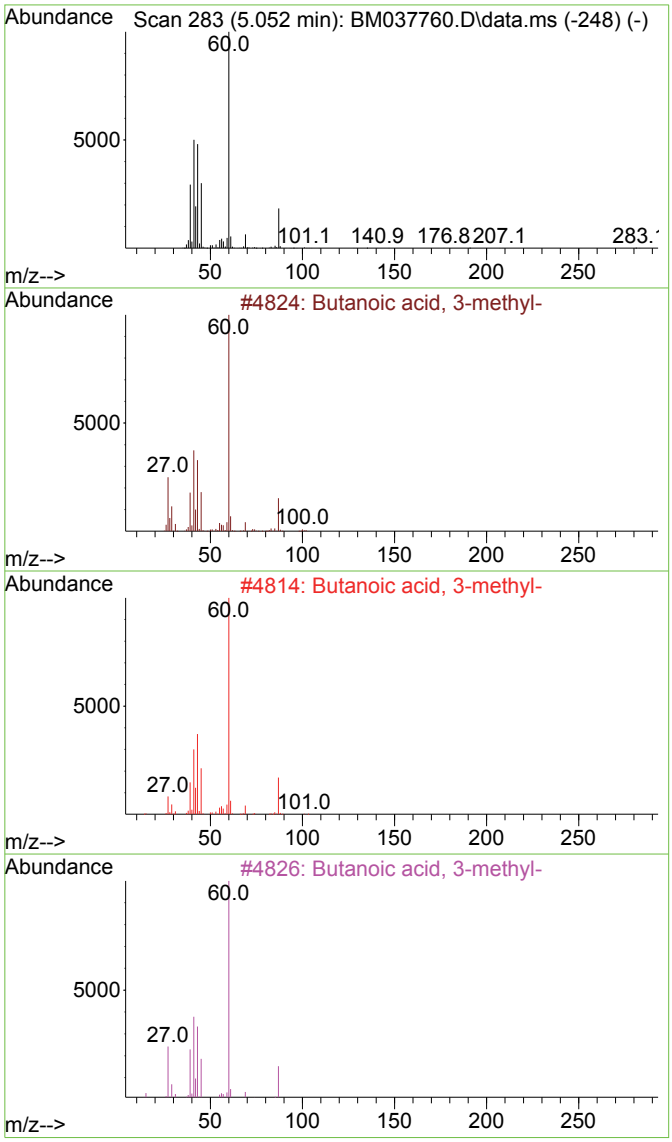
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

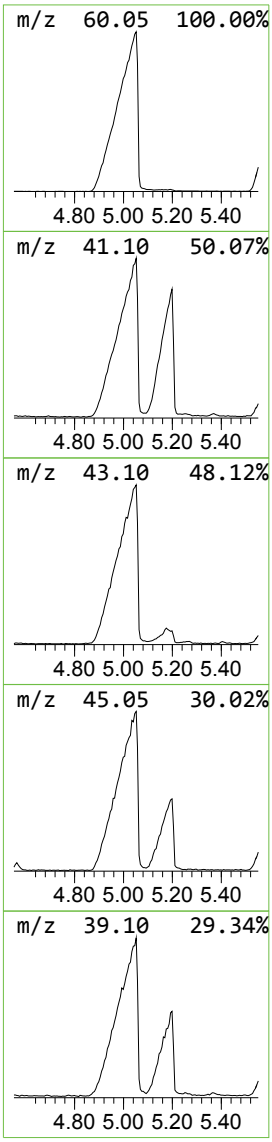
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	60.69 ng/ul	4924880	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	72
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
5	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112822\
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Acq On : 28 Nov 2022 15:24
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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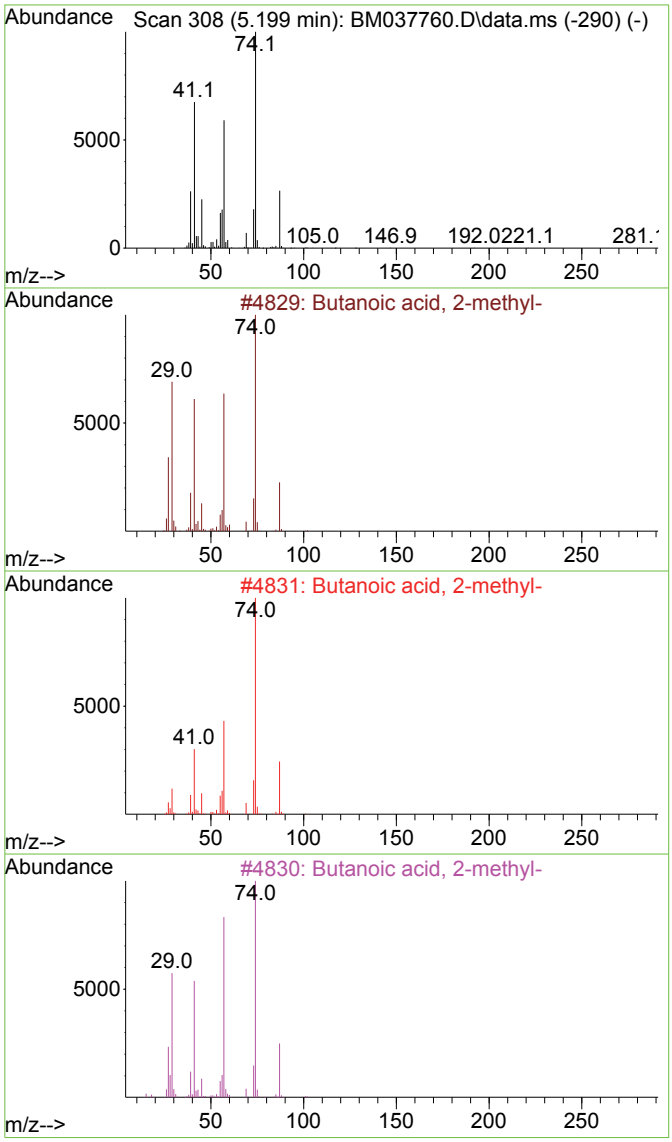
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

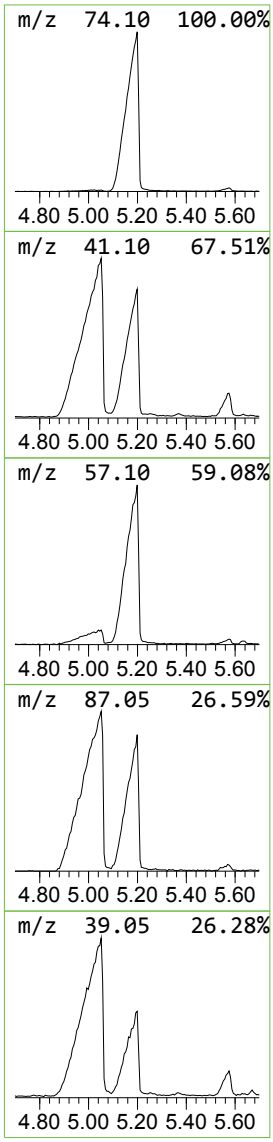
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	25.82 ng/ul	2095330	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	78
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
4	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
5	Thiirane, methyl-	74	C3H6S	001072-43-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112822\
Data File : BM037760.D
Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

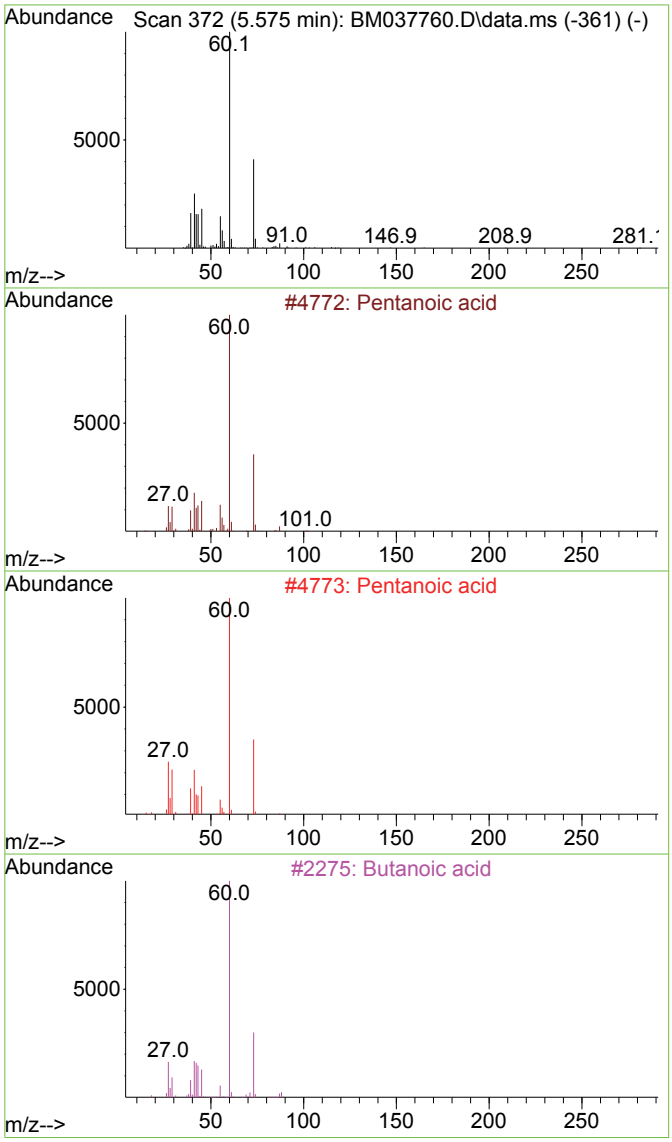
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

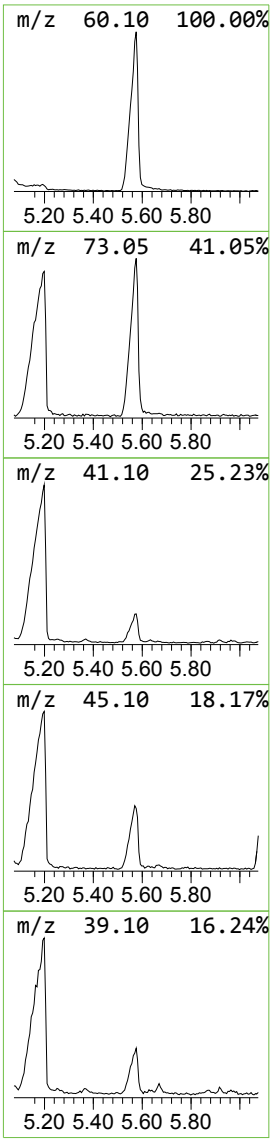
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.575	5.51 ng/ul	447324	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	83
2	Pentanoic acid	102	C5H10O2	000109-52-4	83
3	Butanoic acid	88	C4H8O2	000107-92-6	78
4	Butanoic acid	88	C4H8O2	000107-92-6	78
5	Pentanoic acid	102	C5H10O2	000109-52-4	74





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Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

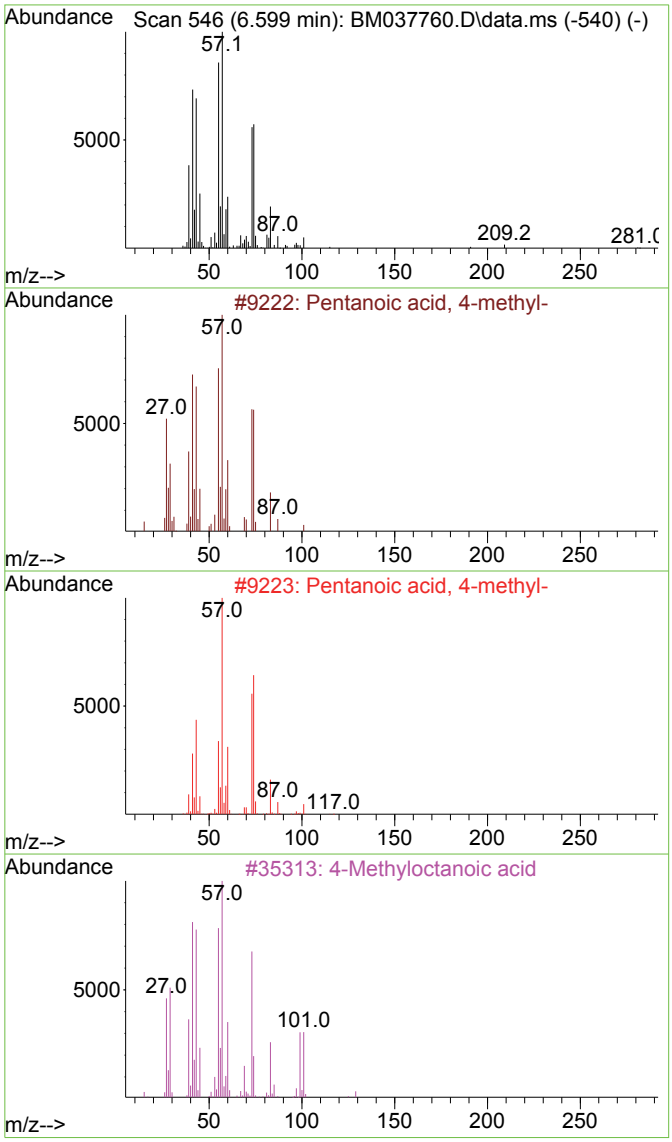
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

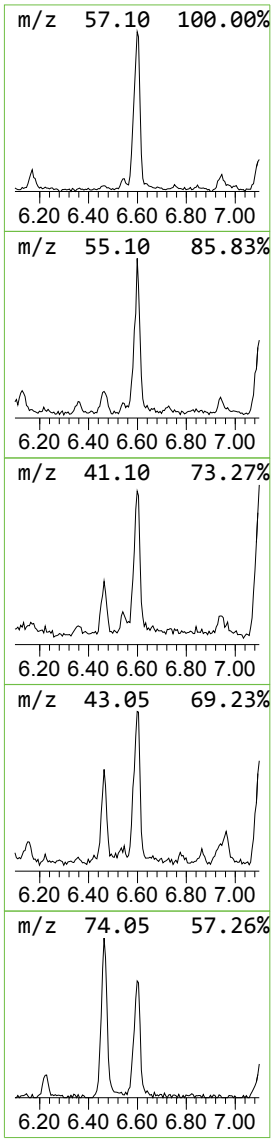
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentanoic acid, 4-methyl- Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.599	2.57 ng/ul	208378	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	58
2	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	53
3	4-Methyloctanoic acid	158	C9H18O2	054947-74-9	43
4	Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-30-8	32
5	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	28





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

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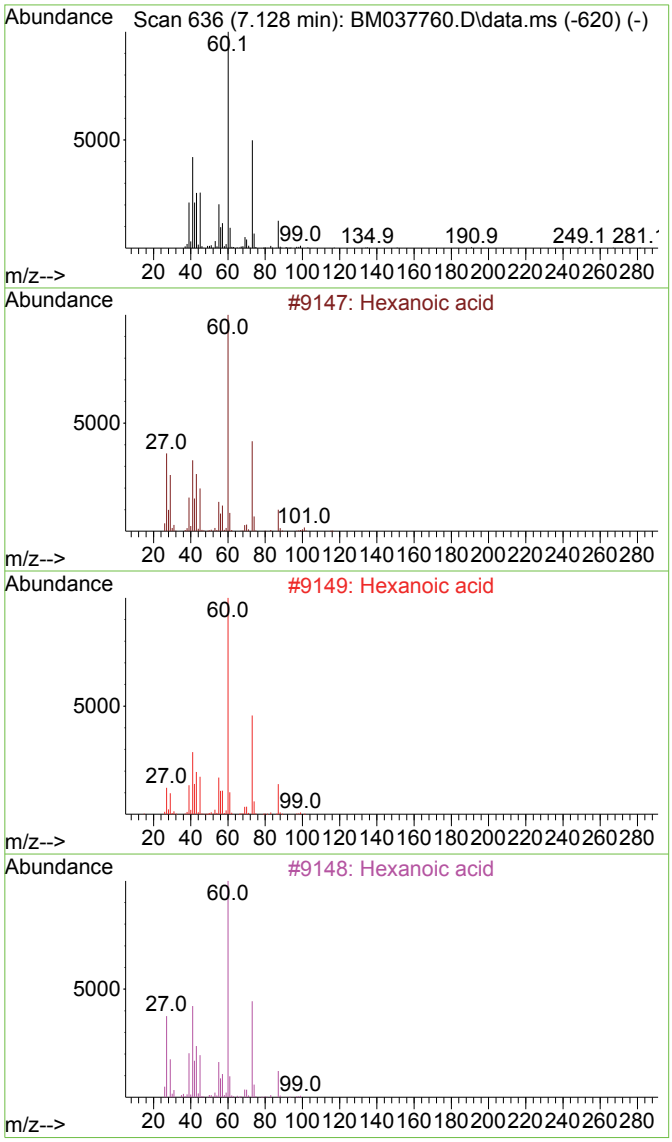
Quant Title : SVOA CALIBRATION

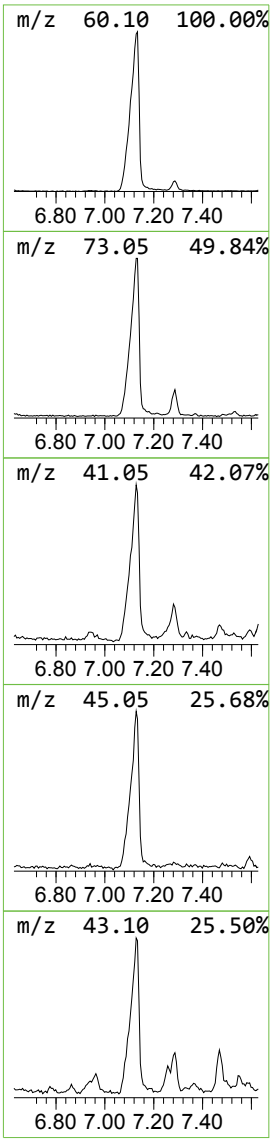
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.128	10.15 ng/ul	823455	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	83
2	Hexanoic acid	116	C6H12O2	000142-62-1	80
3	Hexanoic acid	116	C6H12O2	000142-62-1	72
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	64
5	Hexanoic acid	116	C6H12O2	000142-62-1	64





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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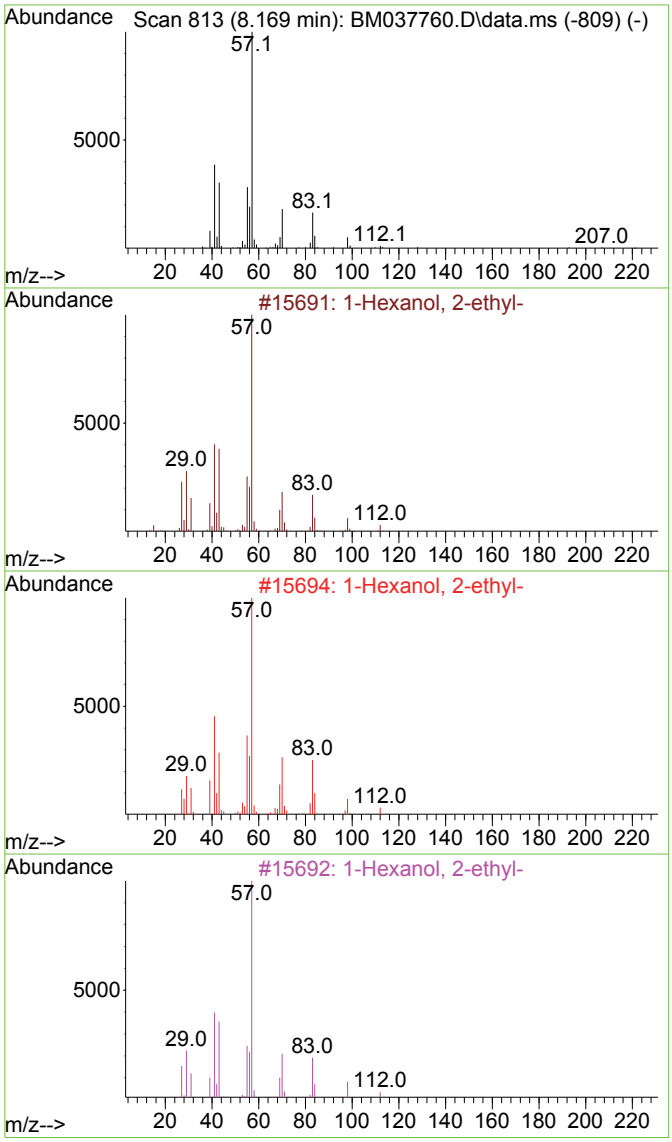
Quant Title : SVOA CALIBRATION

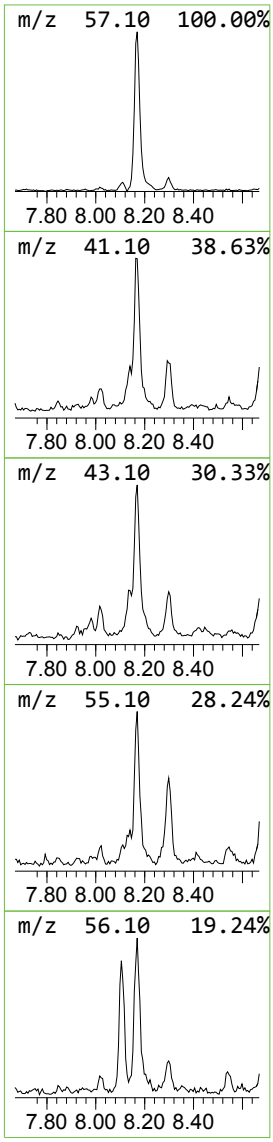
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.169	2.60 ng/ul	211287	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	83
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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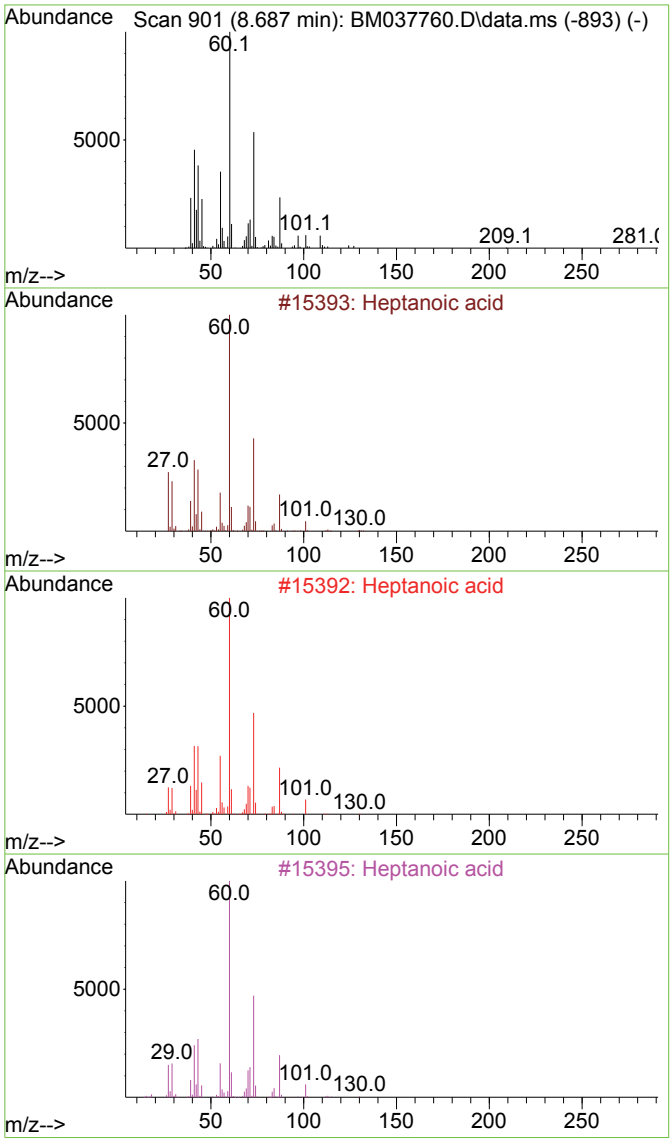
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

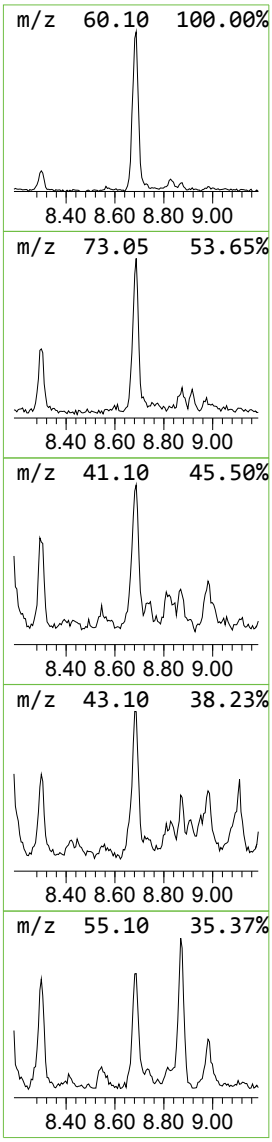
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Heptanoic acid Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.687	2.65 ng/ul	215395	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	80
2	Heptanoic acid	130	C7H14O2	000111-14-8	80
3	Heptanoic acid	130	C7H14O2	000111-14-8	72
4	Heptanoic acid	130	C7H14O2	000111-14-8	72
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64





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Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
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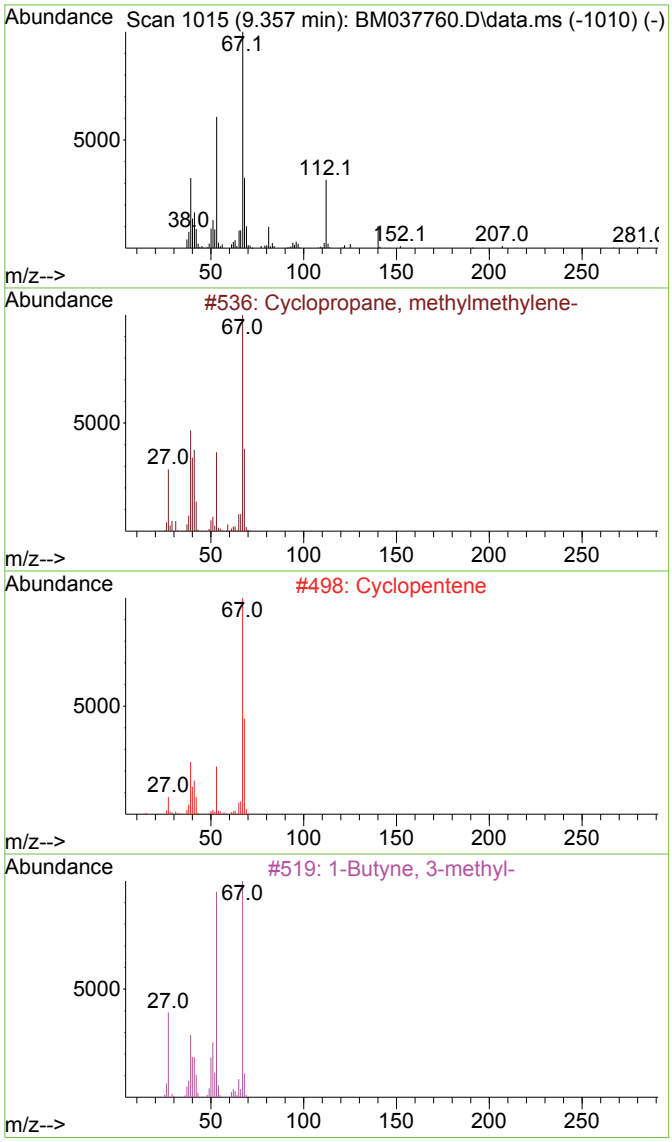
Quant Title : SVOA CALIBRATION

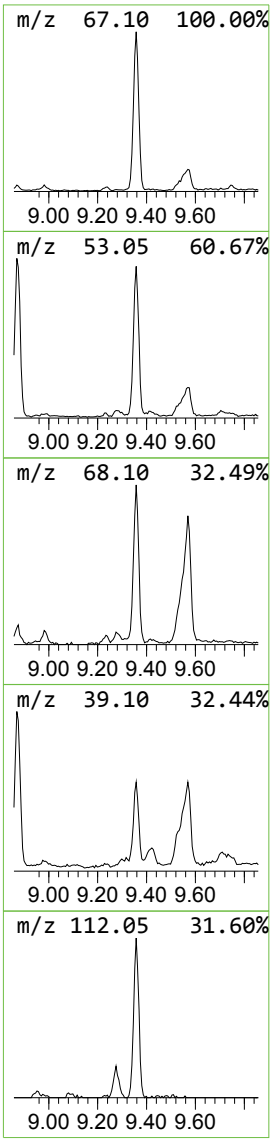
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopropane, methylmethylene- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.357	5.26 ng/ul	427250	1,4-Dichlorobenzene-d4	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	80
2	Cyclopentene	68	C5H8	000142-29-0	72
3	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	72
4	Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	46
5	Spiropentane	68	C5H8	000157-40-4	38





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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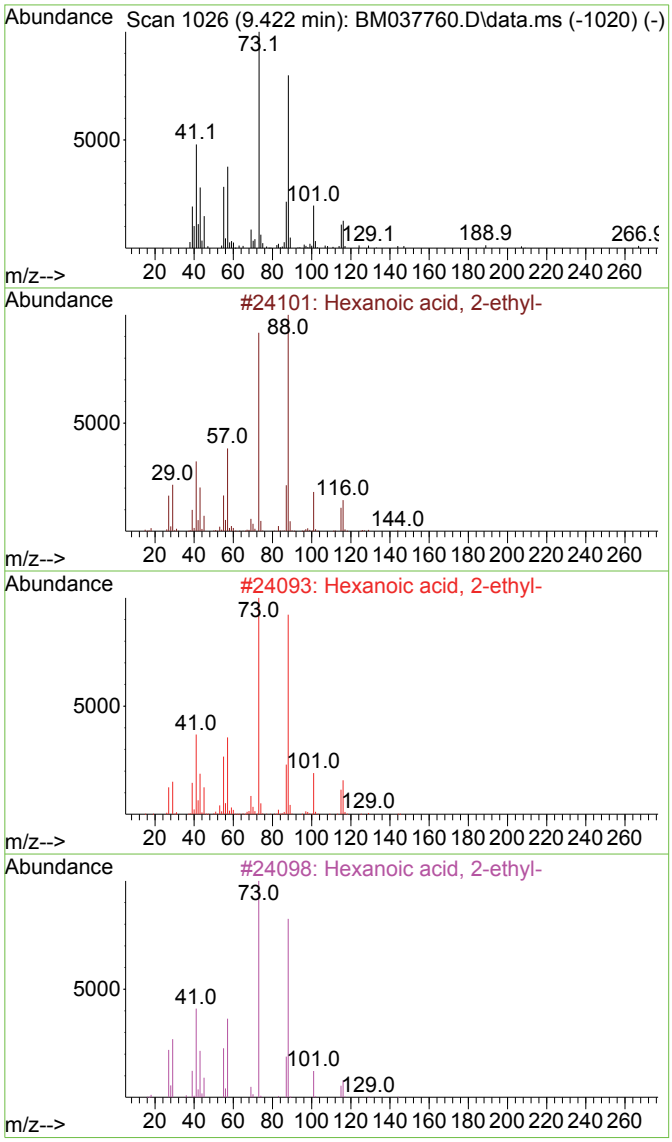
Quant Title : SVOA CALIBRATION

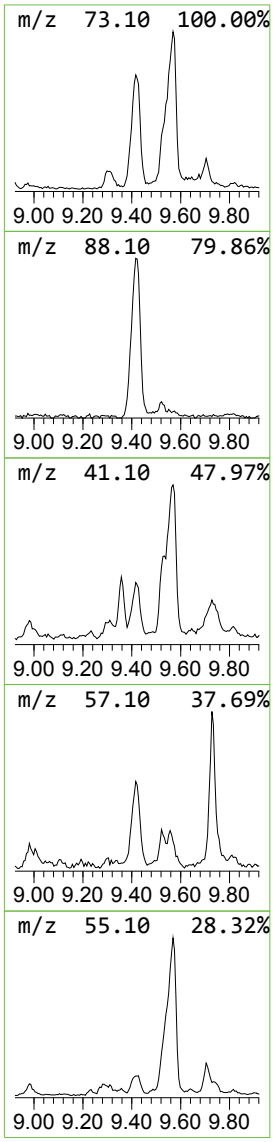
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Hexanoic acid, 2-ethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.422	2.78 ng/ul	225899	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	80
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

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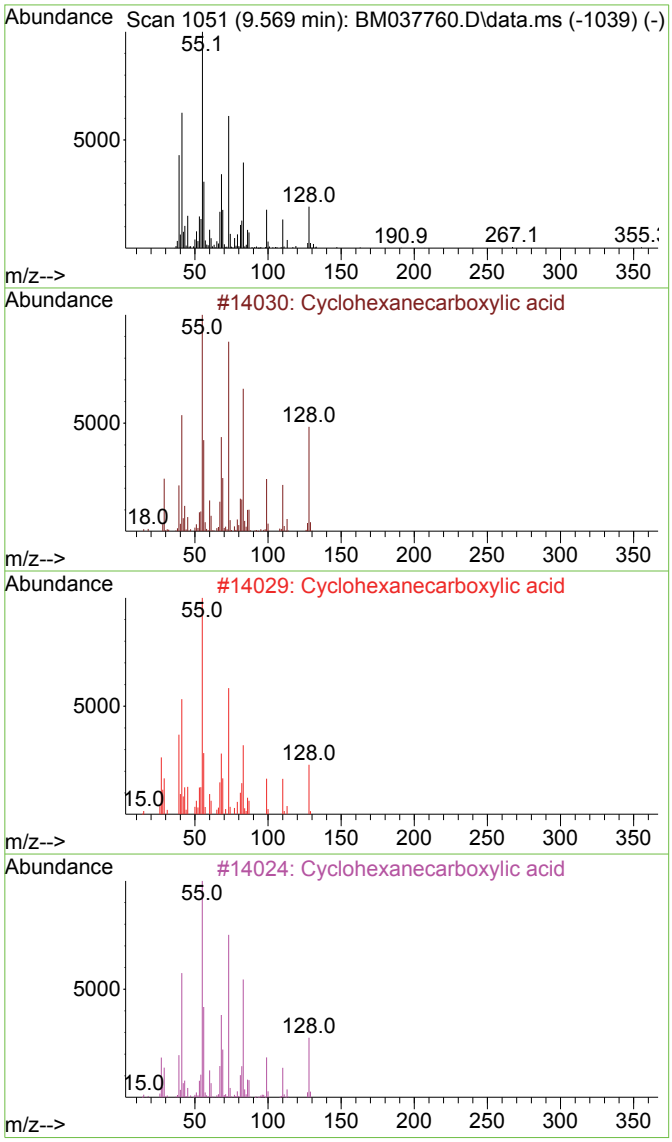
Quant Title : SVOA CALIBRATION

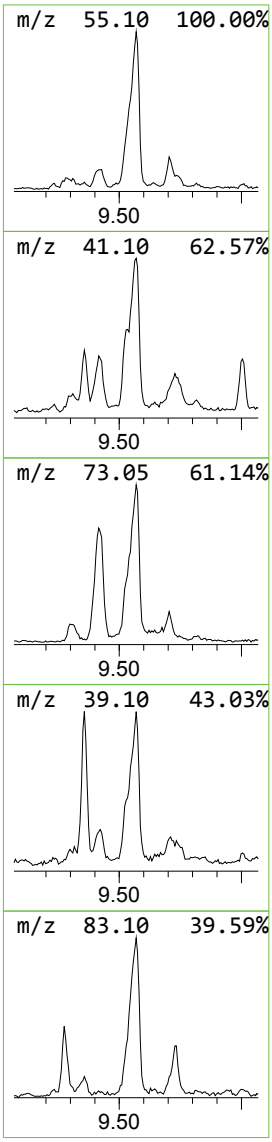
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Cyclohexanecarboxylic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.569	7.72 ng/ul	924234	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	94
2	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	93
3	Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	93
4	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	32
5	3-Penten-1-ol, (E)-	86	C5H10O	000764-37-4	14





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ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : SVOA CALIBRATION

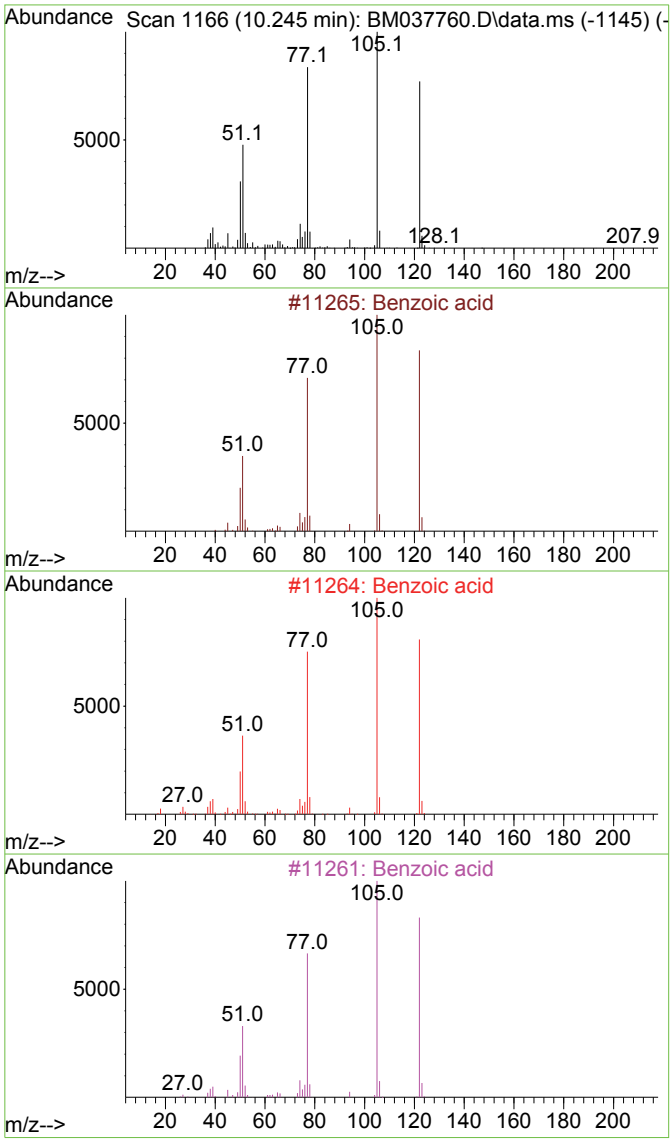
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

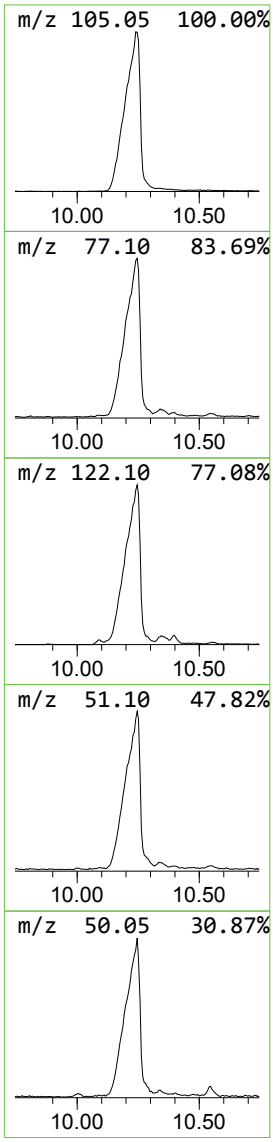
****

Peak Number 13 Benzoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.245	24.90 ng/ul	2981690	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid	122	C7H6O2	000065-85-0	95
2	Benzoic acid	122	C7H6O2	000065-85-0	94
3	Benzoic acid	122	C7H6O2	000065-85-0	94
4	Heptanediamide, N,N'-di-benzoyloxy-	398	C21H22N2O6	1000253-26-4	91
5	Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	91





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Instrument :
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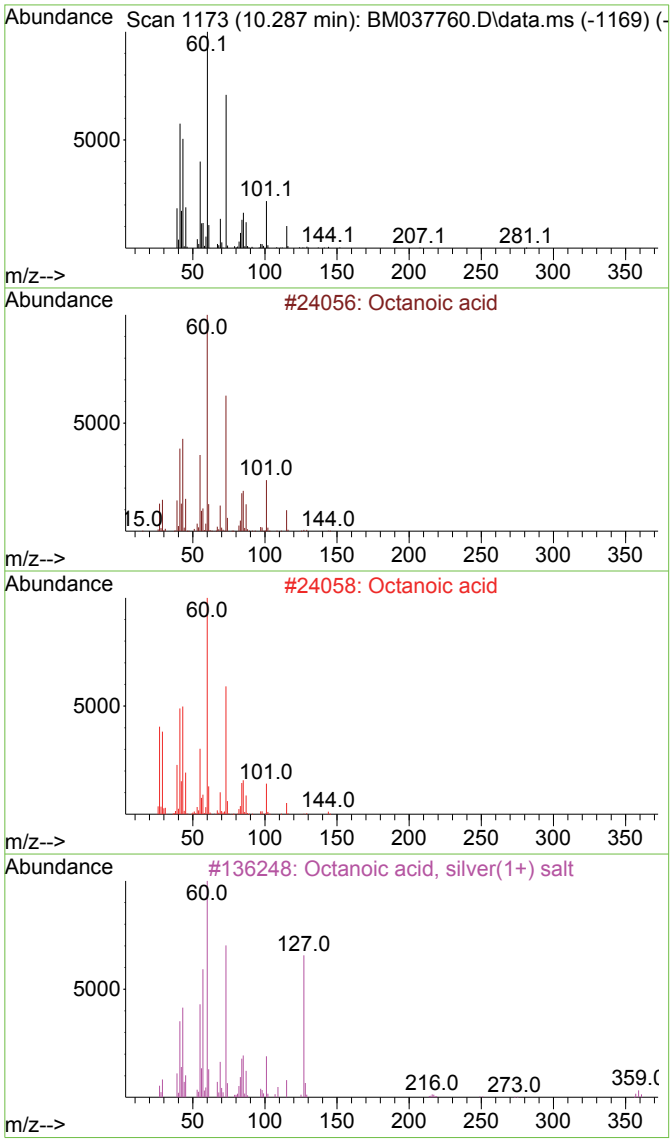
Quant Title : SVOA CALIBRATION

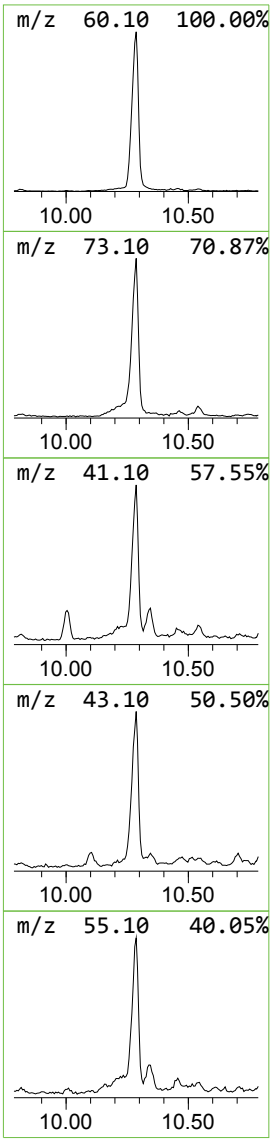
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Octanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.287	7.79 ng/ul	932303	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	90
2	Octanoic acid	144	C8H16O2	000124-07-2	87
3	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	80
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
5	Octanoic acid	144	C8H16O2	000124-07-2	53





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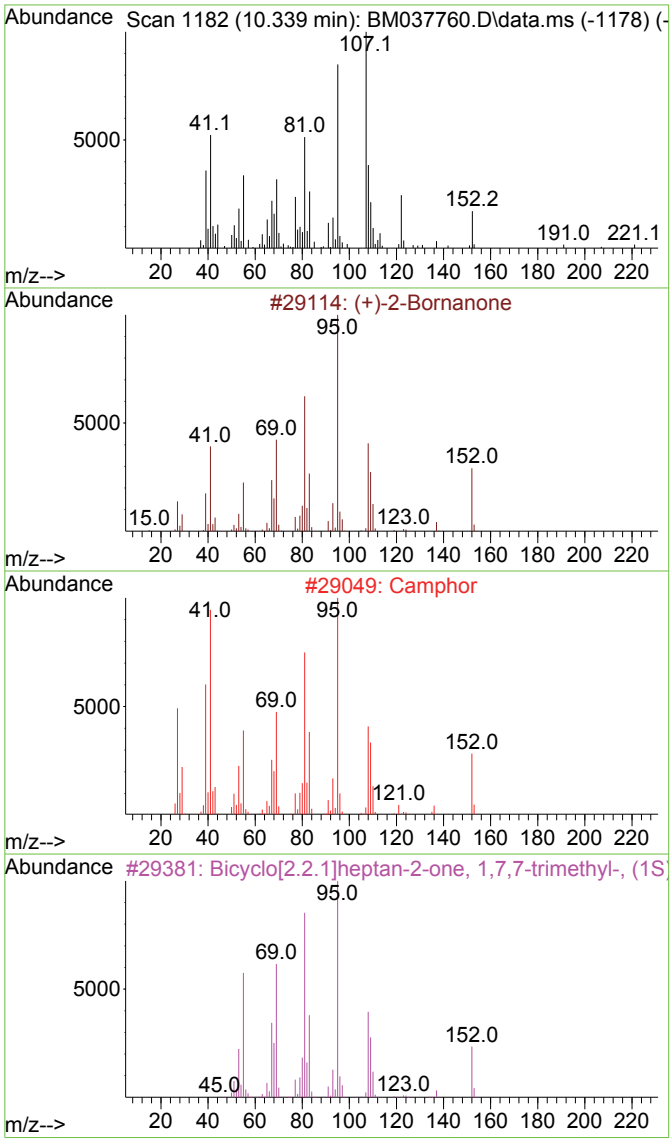
Quant Title : SVOA CALIBRATION

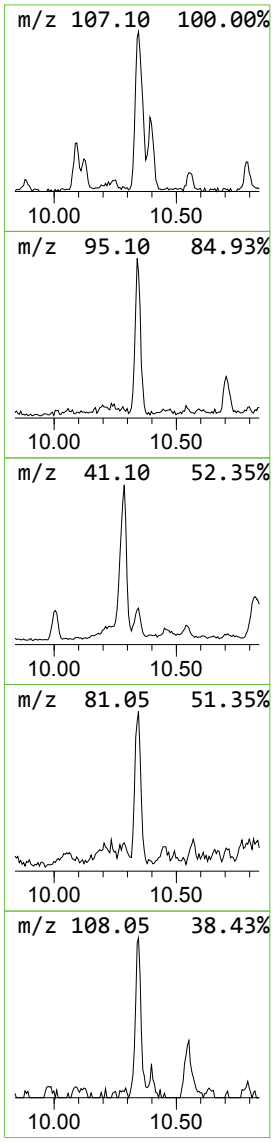
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 (+)-2-Bornanone Concentration Rank 27

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.339	2.11 ng/ul	252166	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	78
2	Camphor	152	C10H16O	000076-22-2	70
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	49
4	Camphor	152	C10H16O	000076-22-2	49
5	(+)-2-Bornanone	152	C10H16O	000464-49-3	38





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ALS Vial : 10 Sample Multiplier: 1

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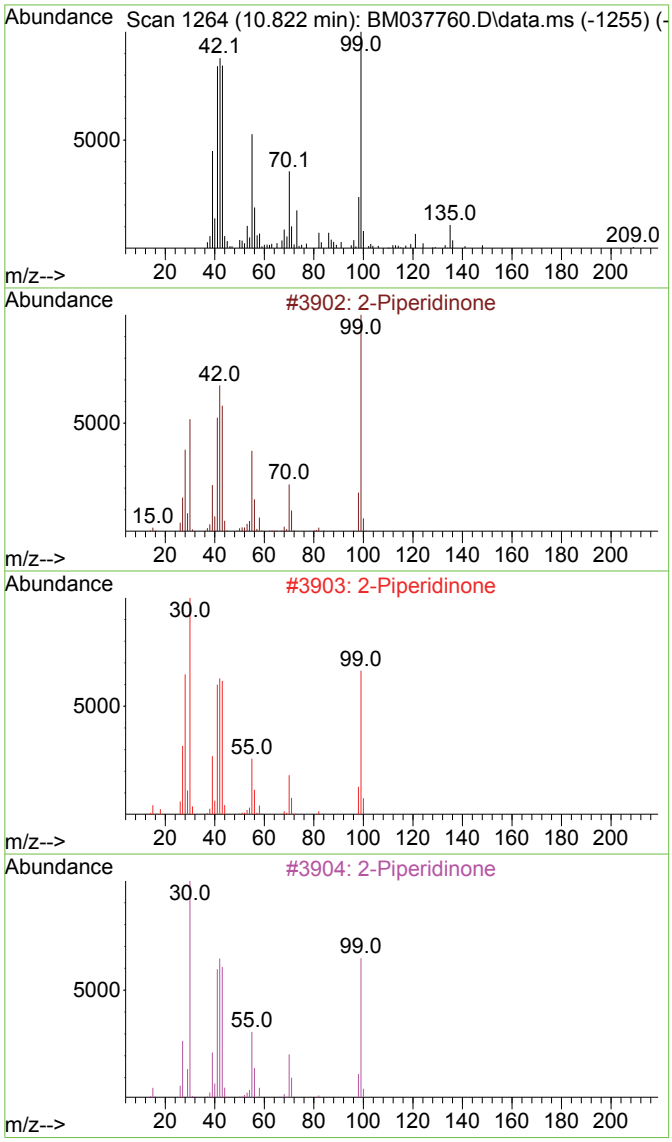
Quant Title : SVOA CALIBRATION

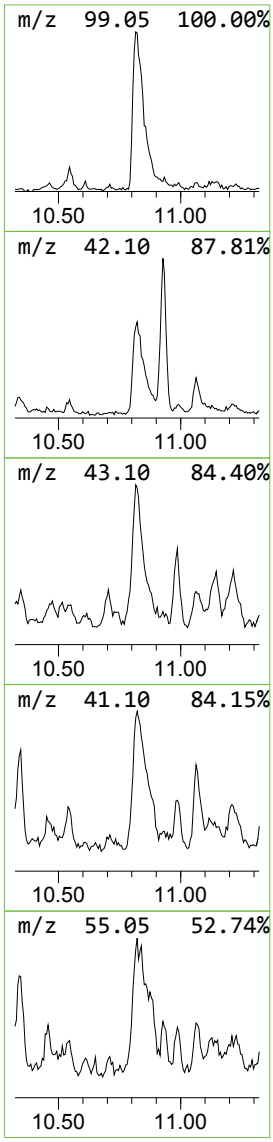
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 2-Piperidinone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	4.33 ng/ul	518614	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone	99	C5H9NO	000675-20-7	70
2	2-Piperidinone	99	C5H9NO	000675-20-7	62
3	2-Piperidinone	99	C5H9NO	000675-20-7	62
4	5-Aminopentanamide	116	C5H12N2O	013023-70-6	53
5	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	49





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Misc :
ALS Vial : 10 Sample Multiplier: 1

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Quant Title : SVOA CALIBRATION

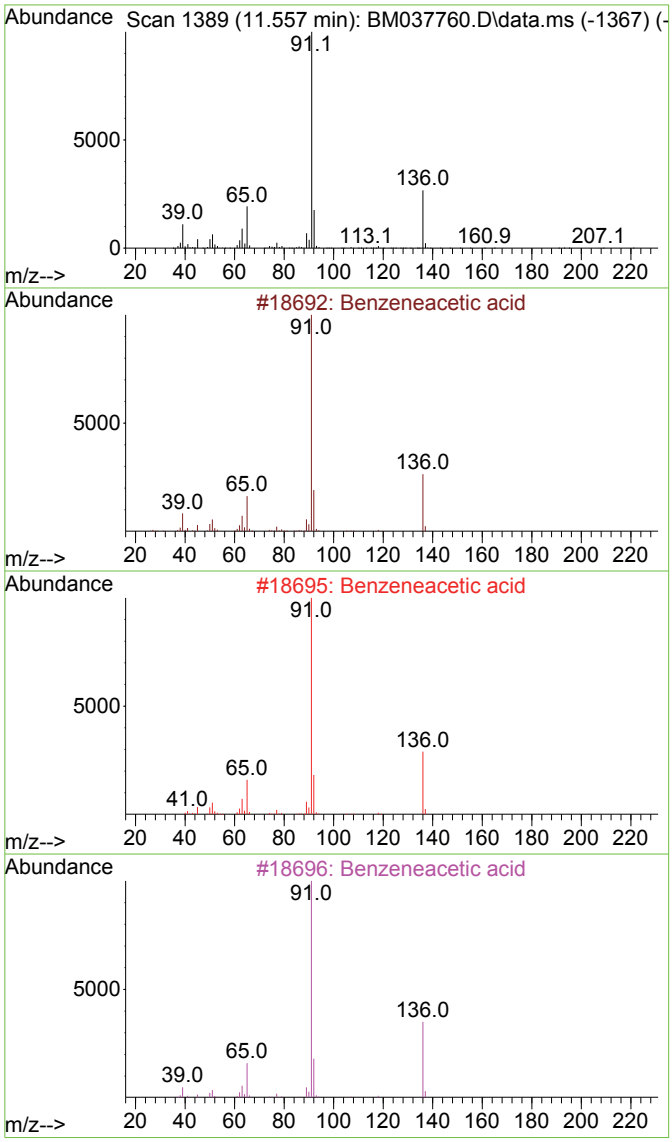
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

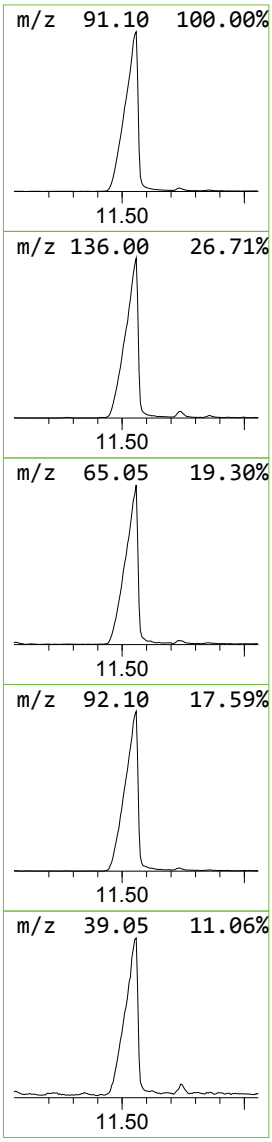
****

Peak Number 17 Benzeneacetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.557	76.65 ng/ul	9177380	Naphthalene-d8	10.928

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	90
5	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	64





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Acq On : 28 Nov 2022 15:24
Operator : CG/JU
Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AH0DL

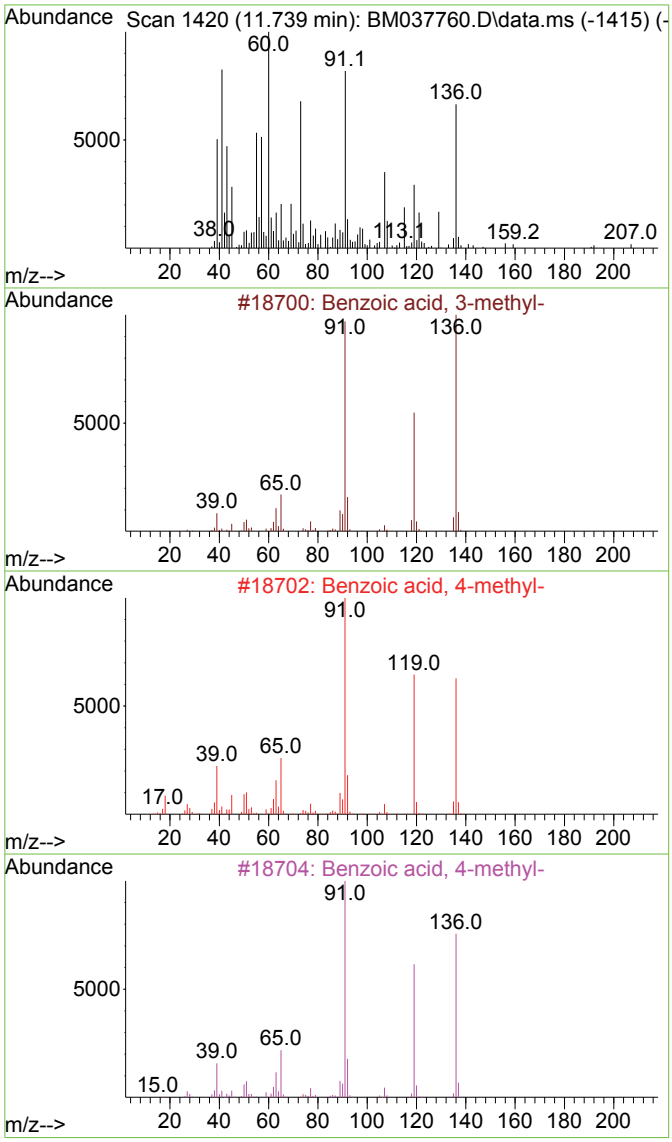
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

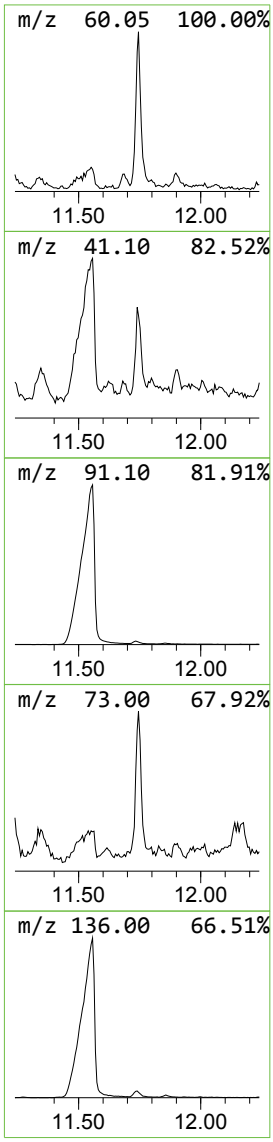
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzoic acid, 3-methyl- Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	2.51 ng/ul	300729	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	62
2	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	41
3	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	35
4	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	35
5	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	35





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

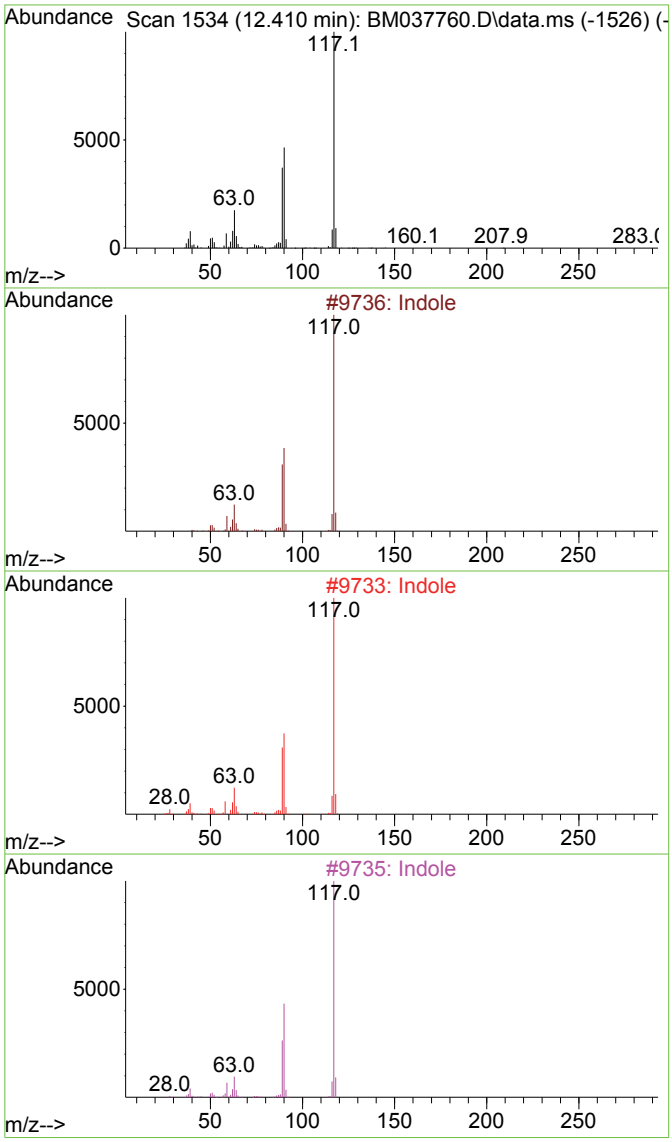
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

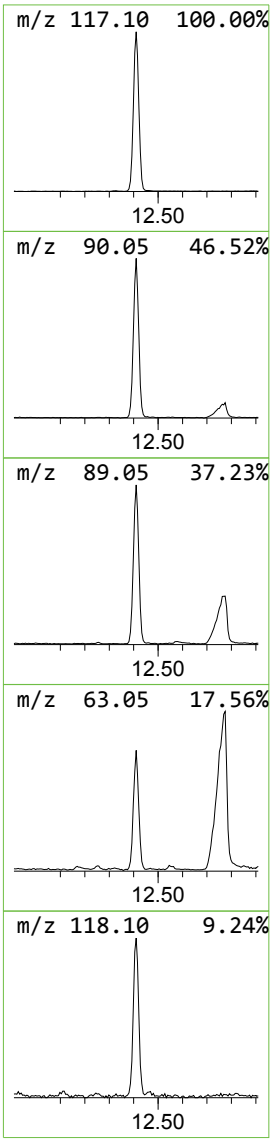
****

Peak Number 19 Indole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	8.38 ng/ul	1003900	Naphthalene-d8	10.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	97
2	Indole	117	C8H7N	000120-72-9	96
3	Indole	117	C8H7N	000120-72-9	91
4	Indole	117	C8H7N	000120-72-9	91
5	Indolizine	117	C8H7N	000274-40-8	91





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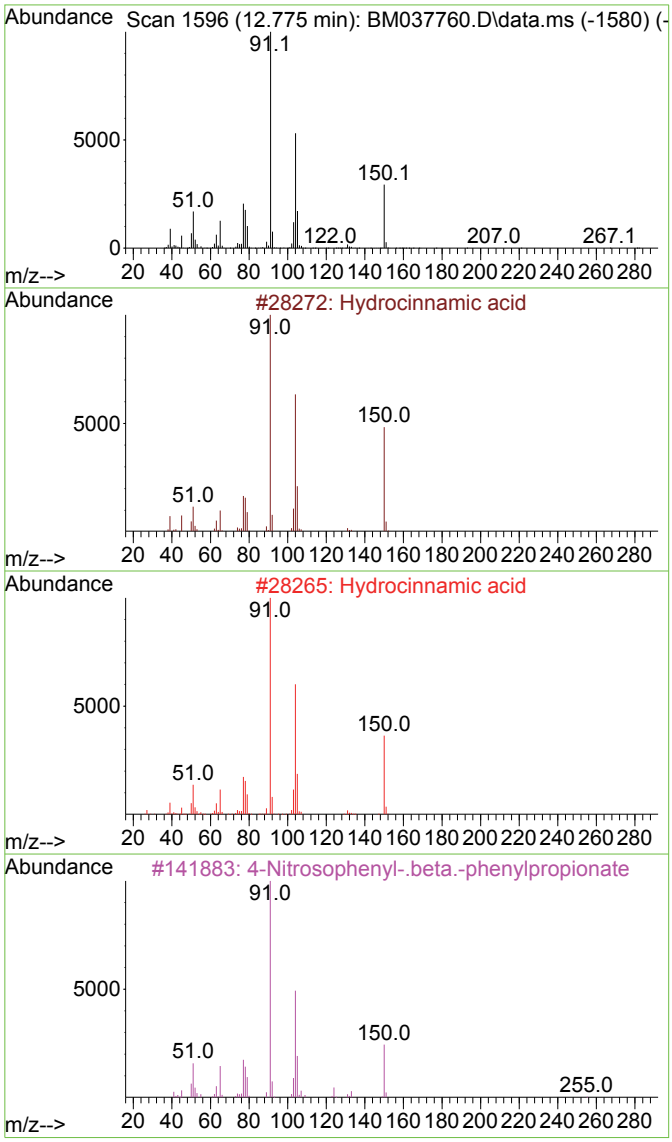
Quant Title : SVOA CALIBRATION

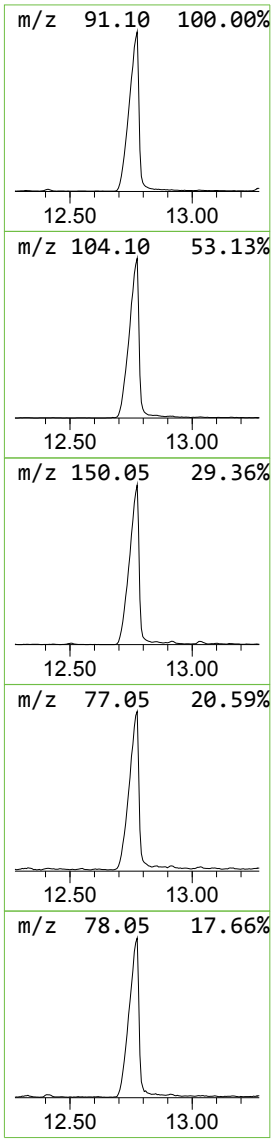
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Hydrocinnamic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	65.71 ng/ul	7868040	Naphthalene-d8	10.928

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 : 10 Sample Multiplier: 1

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ClientSampleId :
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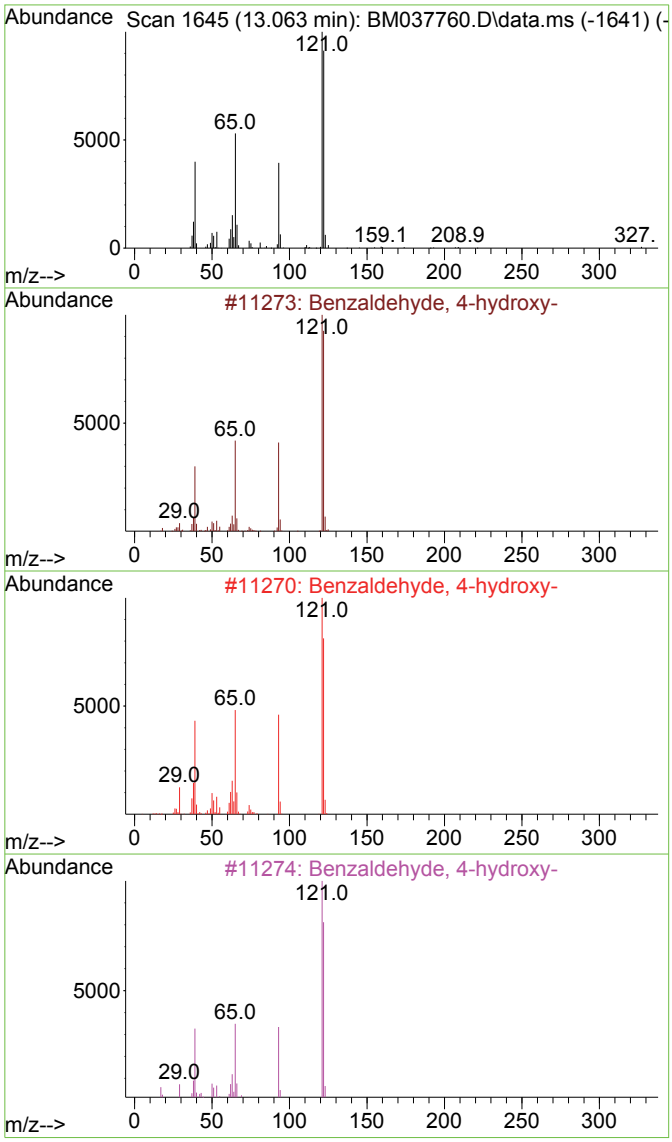
Quant Title : SVOA CALIBRATION

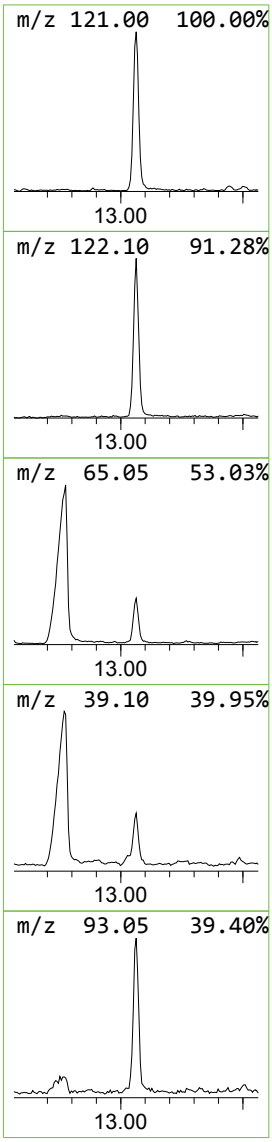
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 21 Benzaldehyde, 4-hydroxy- Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.063	2.52 ng/ul	446636	Acenaphthene-d10	14.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	94
2	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	93
3	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	91
4	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	87
5	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	81





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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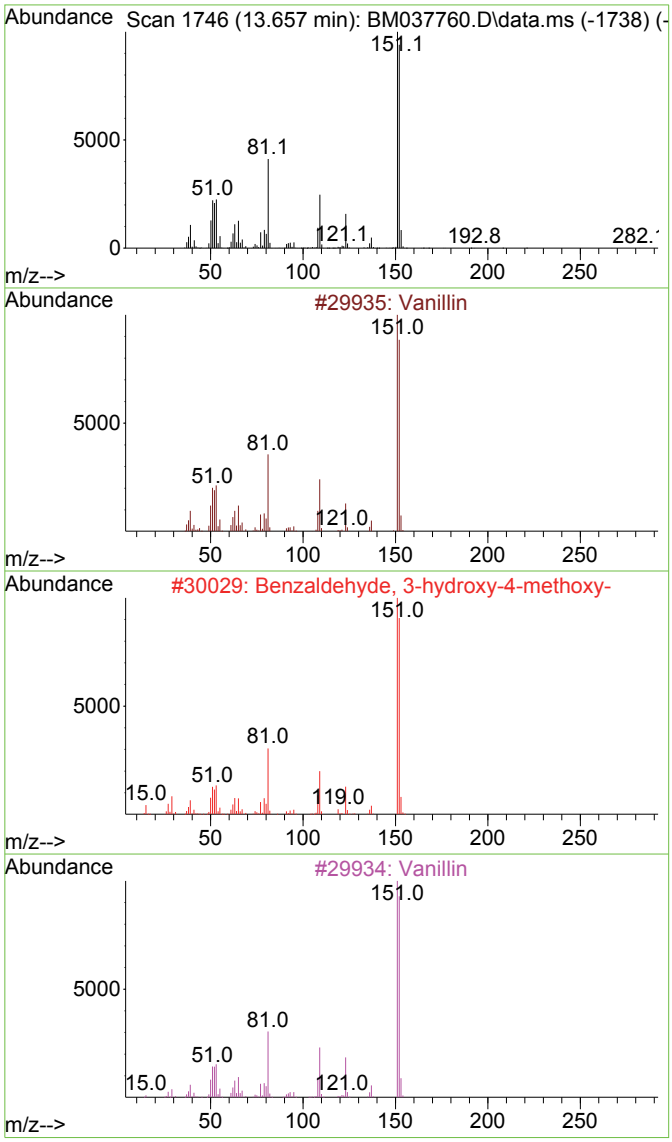
Quant Title : SVOA CALIBRATION

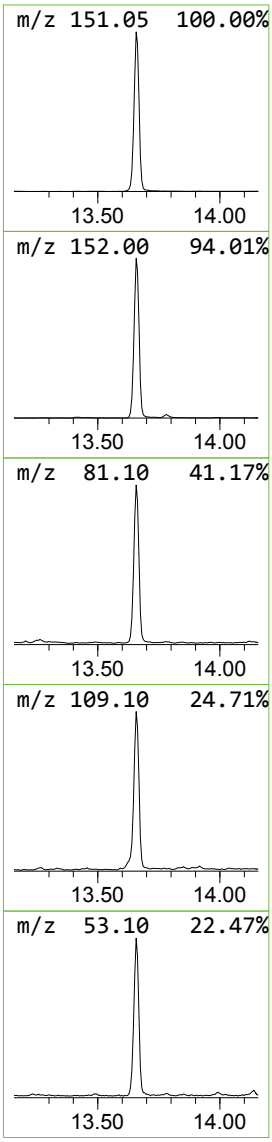
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 22 Vanillin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.657	20.45 ng/ul	3617260	Acenaphthene-d10	14.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	98
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3	Vanillin	152	C8H8O3	000121-33-5	97
4	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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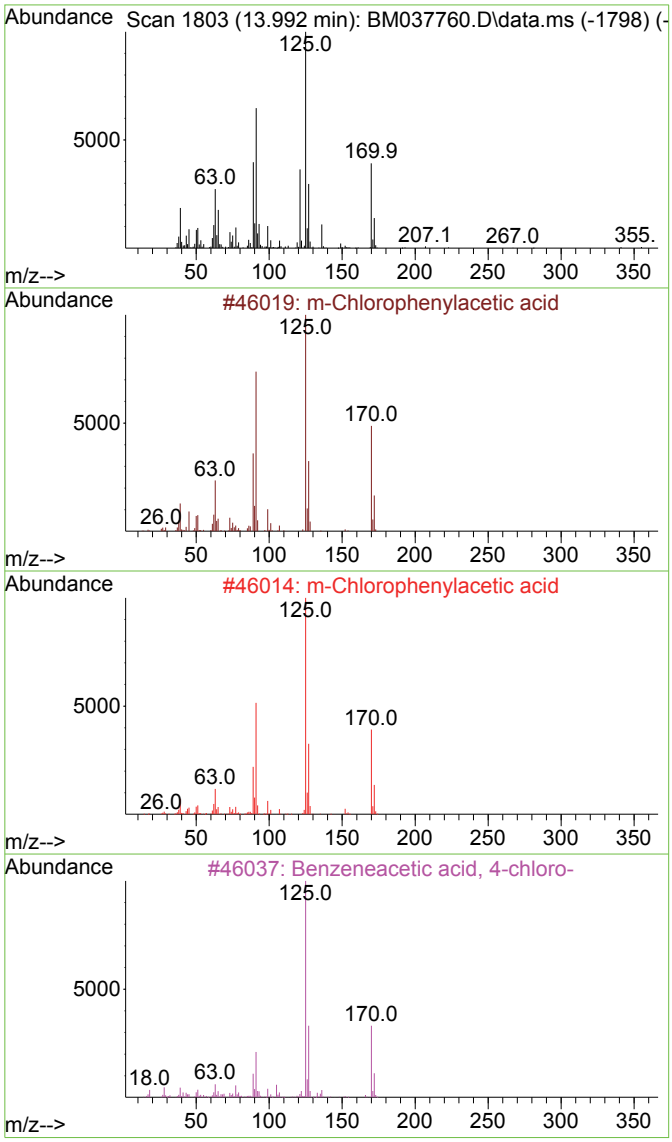
Quant Title : SVOA CALIBRATION

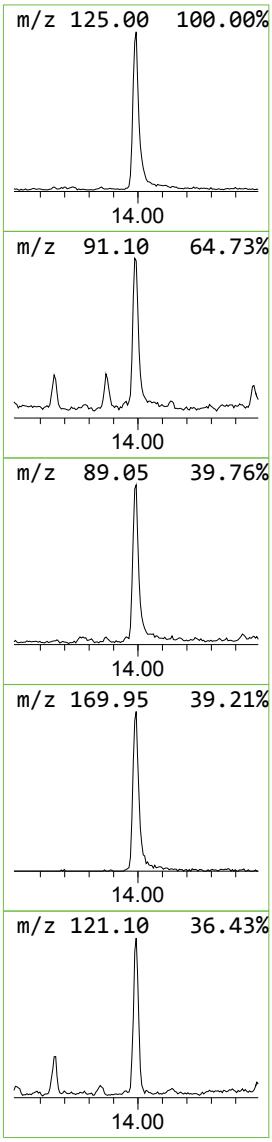
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 23 m-Chlorophenylacetic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	3.61 ng/ul	639153	Acenaphthene-d10	14.733

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	95
3	Benzeneacetic acid, 4-chloro-	170	C8H7ClO2	001878-66-6	94
4	Benzeneacetic acid, 4-chloro-	170	C8H7ClO2	001878-66-6	94
5	m-Chlorophenylacetic acid	170	C8H7ClO2	001878-65-5	93





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Sample : N5602-18DL 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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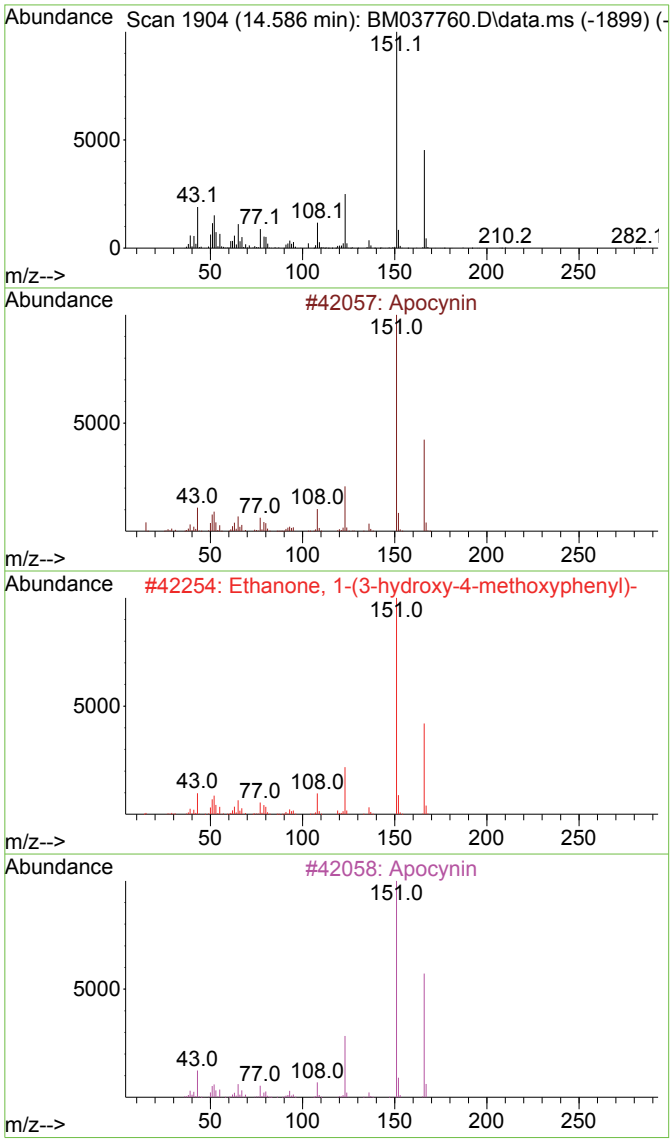
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

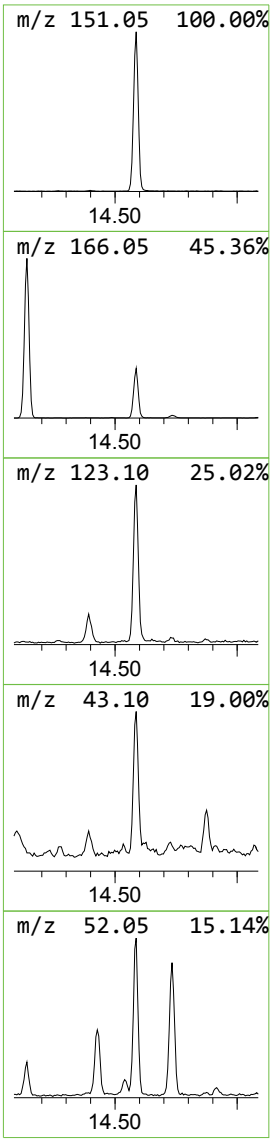
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 24 Apocynin Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	6.48 ng/ul	1146280	Acenaphthene-d10	14.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	97
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	95
3	Apocynin	166	C9H10O3	000498-02-2	94
4	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	94
5	Apocynin	166	C9H10O3	000498-02-2	93





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Quant Title : SVOA CALIBRATION

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

****
Peak Number 25 3,4-Dichlorophenylacetic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	4.68 ng/ul	828659	Acenaphthene-d10	14.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	005807-30-7	98
2	3,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	005807-30-7	98
3	3,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	005807-30-7	97
4	2,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	019719-28-9	96
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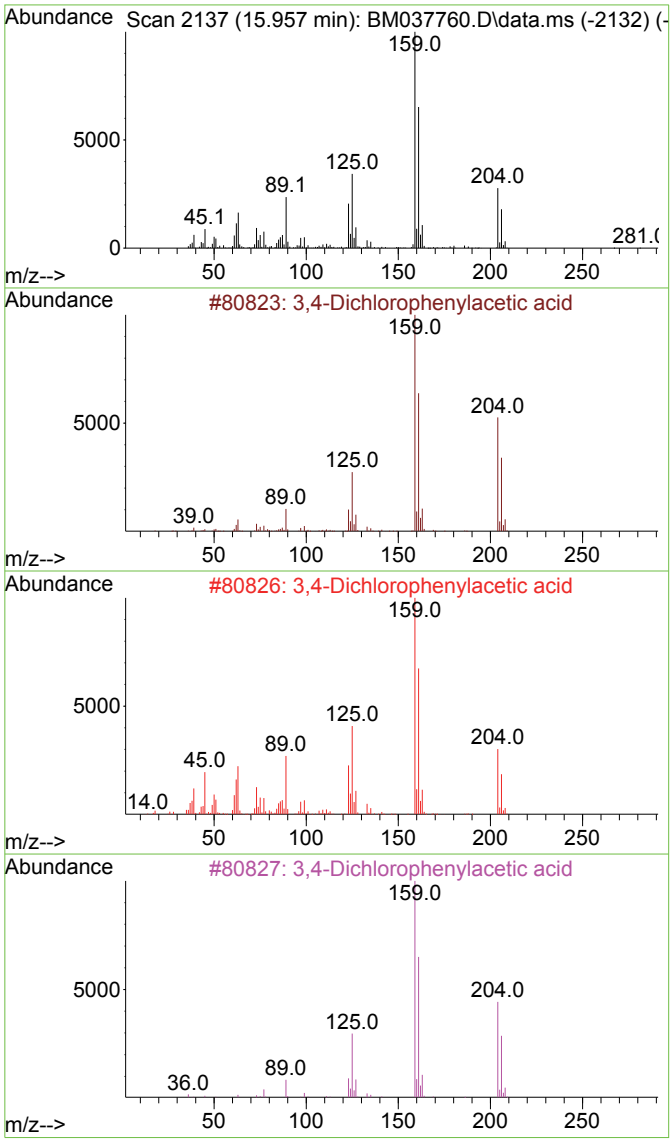

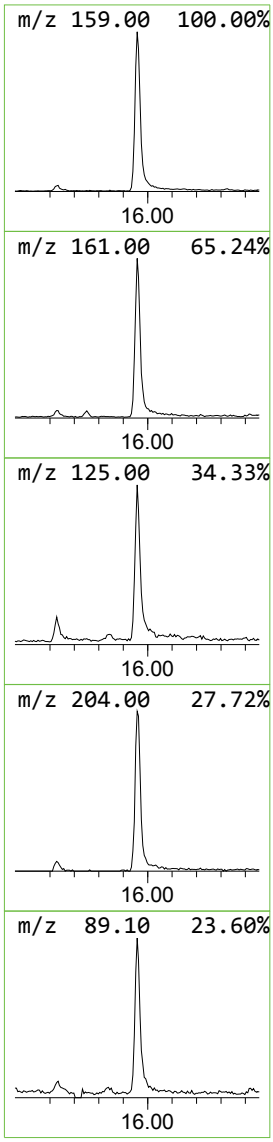

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ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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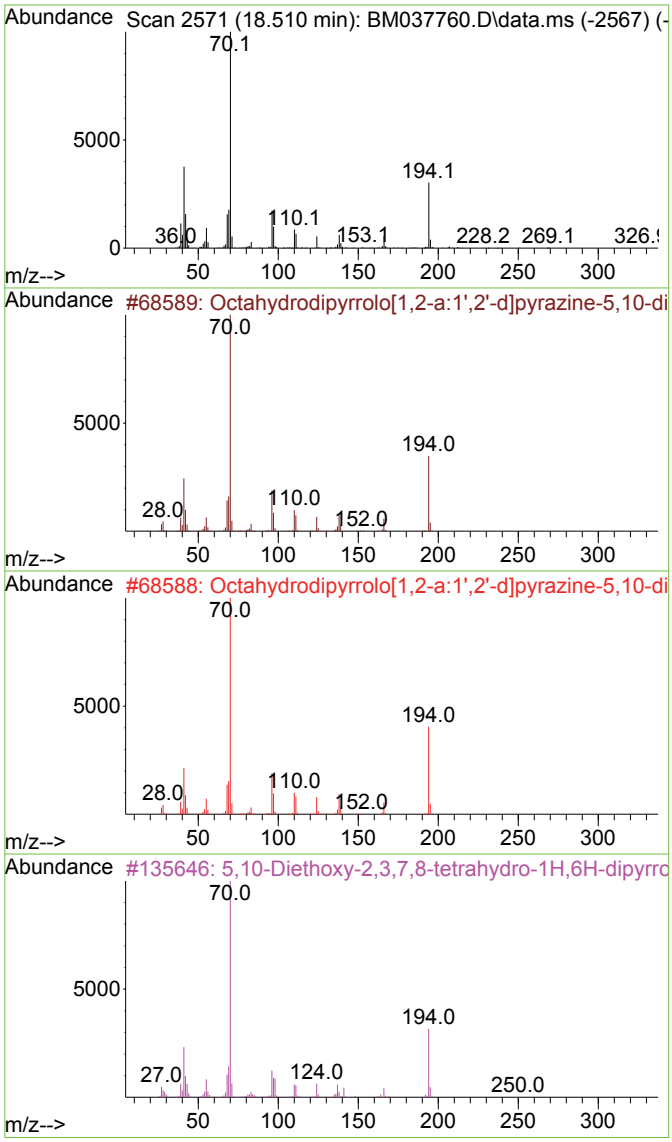
Quant Title : SVOA CALIBRATION

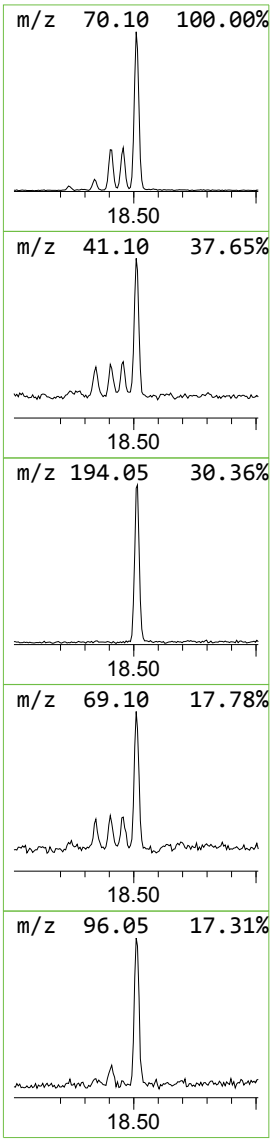
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 26 Octahydrodipyrrolo[1,2-a:1'... Concentration Rank 26

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.509	2.36 ng/ul	509031	Phenanthrene-d10	17.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octahydrodipyrrolo[1,2-a:1',2'-d...	194	C10H14N2O2	1000497-90-3	95
2	Octahydrodipyrrolo[1,2-a:1',2'-d...	194	C10H14N2O2	1000497-90-2	95
3	5,10-Diethoxy-2,3,7,8-tetrahydro...	250	C14H22N2O2	1000190-75-5	74
4	L-Proline, N-(3-cyclopentylpropi...	337	C20H35NO3	1000346-41-3	42
5	6,6-Dimethyl-cyclohex-2-en-1-ol	126	C8H14O	038313-10-9	37





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ClientSampleId :
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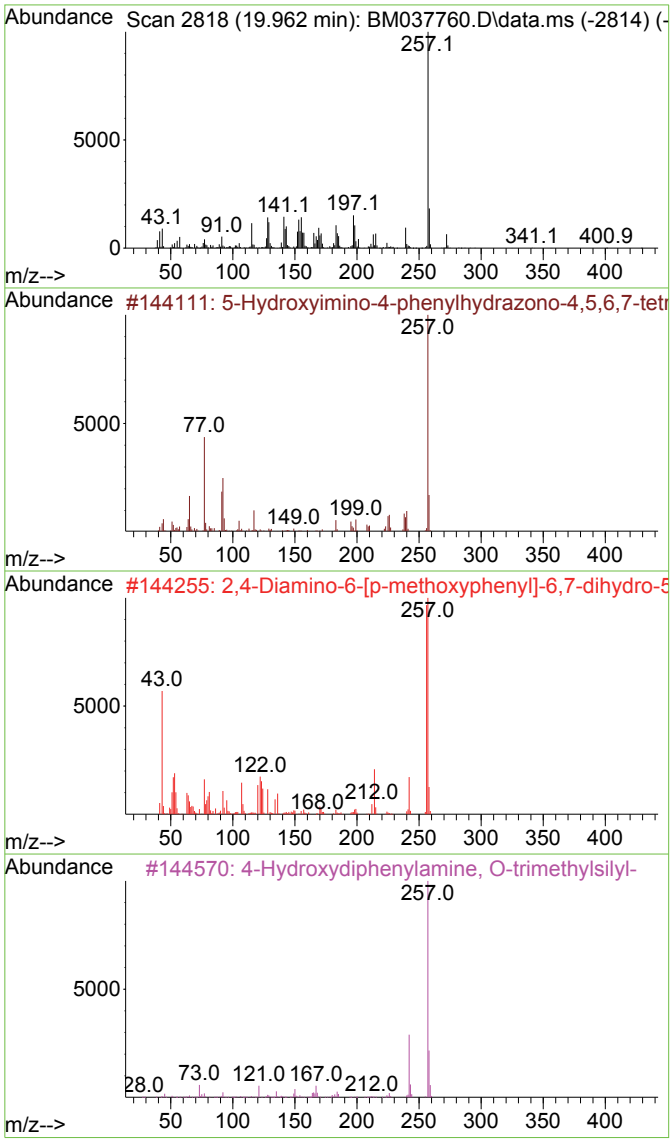
Quant Title : SVOA CALIBRATION

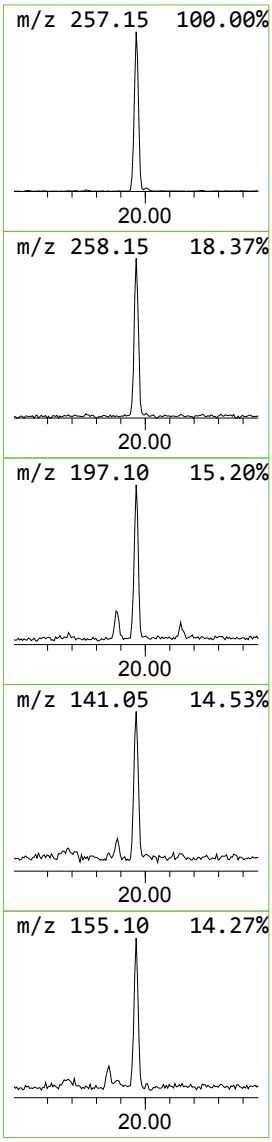
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 27 5-Hydroxyimino-4-phenylhydr... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.962	3.22 ng/ul	641155	Chrysene-d12	21.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxyimino-4-phenylhydrazono...	257	C12H11N5O2	1000110-69-8	50
2	2,4-Diamino-6-[p-methoxyphenyl]-...	257	C13H15N5O	1000251-46-9	49
3	4-Hydroxydiphenylamine, O-trimet...	257	C15H19NOSi	1000417-42-0	49
4	4-Methoxy-2,2'-dimethyl-4'-nitro...	257	C15H15NO3	031458-16-9	47
5	Ethyl 2-amino-3-cyano-4-oxo-4H-q...	257	C13H11N3O3	022353-70-4	47





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---			
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Propanoic acid,...	3.793	13.5	ng/ul	1091870	1	8.110	1623010	20.0
Butanoic acid	4.122	5.7	ng/ul	464694	1	8.110	1623010	20.0
Butanoic acid, ...	5.052	60.7	ng/ul	4924880	1	8.110	1623010	20.0
Butanoic acid, ...	5.199	25.8	ng/ul	2095330	1	8.110	1623010	20.0
Pentanoic acid	5.575	5.5	ng/ul	447324	1	8.110	1623010	20.0
Pentanoic acid,...	6.599	2.6	ng/ul	208378	1	8.110	1623010	20.0
Hexanoic acid	7.128	10.2	ng/ul	823455	1	8.110	1623010	20.0
1-Hexanol, 2-et...	8.169	2.6	ng/ul	211287	1	8.110	1623010	20.0
Heptanoic acid	8.687	2.6	ng/ul	215395	1	8.110	1623010	20.0
Cyclopropane, m...	9.357	5.3	ng/ul	427250	1	8.110	1623010	20.0
Hexanoic acid, ...	9.422	2.8	ng/ul	225899	1	8.110	1623010	20.0
Cyclohexanecarb...	9.569	7.7	ng/ul	924234	2	10.928	2394600	20.0
Benzoic acid	10.245	24.9	ng/ul	2981690	2	10.928	2394600	20.0
Octanoic acid	10.287	7.8	ng/ul	932303	2	10.928	2394600	20.0
(+)-2-Bornanone	10.339	2.1	ng/ul	252166	2	10.928	2394600	20.0
2-Piperidinone	10.822	4.3	ng/ul	518614	2	10.928	2394600	20.0
Benzeneacetic acid	11.557	76.7	ng/ul	9177380	2	10.928	2394600	20.0
Benzoic acid, 3...	11.739	2.5	ng/ul	300729	2	10.928	2394600	20.0
Indole	12.410	8.4	ng/ul	1003900	2	10.928	2394600	20.0
Hydrocinnamic acid	12.775	65.7	ng/ul	7868040	2	10.928	2394600	20.0
Benzaldehyde, 4...	13.063	2.5	ng/ul	446636	3	14.733	3538170	20.0
Vanillin	13.657	20.4	ng/ul	3617260	3	14.733	3538170	20.0
m-Chlorophenyla...	13.992	3.6	ng/ul	639153	3	14.733	3538170	20.0
Apocynin	14.586	6.5	ng/ul	1146280	3	14.733	3538170	20.0
3,4-Dichlorophe...	15.957	4.7	ng/ul	828659	3	14.733	3538170	20.0
Octahydrodipyrr...	18.509	2.4	ng/ul	509031	4	17.468	4308960	20.0
5-Hydroxyimino-...	19.962	3.2	ng/ul	641155	5	21.633	3976270	20.0