LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039531.D
Acq On : 20 Apr 2023 19:01
Operator : CG/JU
Sample : 02378-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK4

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-BM041823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM039531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.213	26	30	35	rVB	45482	57633	1.16%	0.099%
2	3.525	80	83	88	rBV2	8899	15882	0.32%	0.027%
3	3.643	101	103	118	rBV	162730	288962	5.83%	0.497%
4	3.749	118	121	128	rVB3	24592	41326	0.83%	0.071%
5	3.966	154	158	164	rVB	16445	25923	0.52%	0.045%
6	4.202	194	198	204	rVB	25414	33354	0.67%	0.057%
7	4.919	317	320	326	rVB	18443	26366	0.53%	0.045%
8	5.019	333	337	342	rVB5	6940	10641	0.21%	0.018%
9	5.113	350	353	360	rVB8	5152	8806	0.18%	0.015%
10	7.013	669	676	689	rBV	139730	326638	6.59%	0.562%
11	7.154	694	700	720	rVV	626062	1093252	22.06%	1.880%
12	7.354	728	734	751	rBV	646418	1159108	23.39%	1.993%
13	7.707	789	794	800	rVB	30290	49194	0.99%	0.085%
14	7.825	807	814	836	rBV	672358	1209537	24.40%	2.080%
15	8.178	869	874	884	rVB2	21370	43720	0.88%	0.075%
16	8.554	931	938	965	rBV	484512	1025404	20.69%	1.764%
17	8.995	1006	1013	1034	rBV	751502	1364040	27.52%	2.346%
18	9.148	1037	1039	1048	rVB10	8466	17038	0.34%	0.029%
19	9.384	1074	1079	1085	rVB2	16023	26262	0.53%	0.045%
20	9.719	1128	1136	1151	rBV	619583	1149948	23.20%	1.978%
21	9.878	1160	1163	1167	rVB6	3355	5095	0.10%	0.009%
22	10.266	1222	1229	1251	rBV	785269	1730221	34.91%	2.976%
23	10.631	1283	1291	1307	rBV	1027259	1824336	36.81%	3.138%
24	10.783	1310	1317	1339	rBV	452208	1074770	21.68%	1.848%
25	11.483	1431	1436	1437	rBV5	3104	5502	0.11%	0.009%
26	11.883	1501	1504	1512	rVB4	7931	12602	0.25%	0.022%
27	11.983	1514	1521	1522	rBV4	4018	7297	0.15%	0.013%
28	12.054	1527	1533	1537	rBV9	5296	9110	0.18%	0.016%
29	12.154	1545	1550	1556	rBV4	5918	13605	0.27%	0.023%
30	12.230	1559	1563	1572	rVB3	11464	23313	0.47%	0.040%
31	13.030	1697	1699	1704	rVB6	3465	5665	0.11%	0.010%
32	13.295	1740	1744	1749	rBV3	11578	14689	0.30%	0.025%
33	13.348	1749	1753	1755	rVV3	13024	21363	0.43%	0.037%
34	13.372	1755	1757	1765	rVB	18484	28948	0.58%	0.050%
35	13.460	1769	1772	1777	rVB7	4043	5720	0.12%	0.010%
36	13.895	1837	1846	1858	rBV	2138313	3150439	63.56%	5.418%

LSC Area Percent Report

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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Title : SVOA CALIBRATION

37	14.171	1886	1893	1911	rBV	2257968	3501569	70.65%	6.022%
38	14.295	1911	1914	1922	rVB9	13029	24291	0.49%	0.042%
39	14.371	1922	1927	1933	rVB4	10975	17924	0.36%	0.031%
40	14.477	1937	1945	1959	rBV	1654164	2540475	51.26%	4.369%
41	14.754	1986	1992	1993	rBV2	25457	42175	0.85%	0.073%
42	15.024	2034	2038	2042	rBV6	11544	17605	0.36%	0.030%
43	15.224	2066	2072	2084	rBV	634658	900566	18.17%	1.549%
44	15.318	2086	2088	2091	rVB2	7020	8020	0.16%	0.014%
45	15.477	2108	2115	2132	rBV	2926364	4429857	89.38%	7.619%
46	15.607	2132	2137	2152	rVV	753196	1187409	23.96%	2.042%
47	15.713	2152	2155	2162	rVB4	15185	29497	0.60%	0.051%
48	15.842	2171	2177	2191	rBV	1664539	2351639	47.45%	4.044%
49	16.042	2207	2211	2216	rVB6	6728	11870	0.24%	0.020%
50	16.165	2224	2232	2246	rBV	138226	420355	8.48%	0.723%
51	16.407	2268	2273	2279	rBV	45611	71376	1.44%	0.123%
52	16.642	2310	2313	2319	rBV8	10668	17326	0.35%	0.030%
53	16.865	2349	2351	2355	rBV4	4921	6023	0.12%	0.010%
54	16.912	2355	2359	2361	rBV4	7596	9842	0.20%	0.017%
55	16.983	2368	2371	2373	rBV3	11115	14533	0.29%	0.025%
56	17.107	2390	2392	2395	rBV4	5250	6551	0.13%	0.011%
57	17.230	2407	2413	2423	rBV	1934200	2856191	57.63%	4.912%
58	17.330	2424	2430	2442	rVV2	3055386	4475971	90.31%	7.698%
59	17.554	2463	2468	2479	rBV	312495	515941	10.41%	0.887%
60	18.136	2561	2567	2576	rBV	996383	1515982	30.59%	2.607%
61	18.418	2613	2615	2622	rBV7	14680	26299	0.53%	0.045%
62	19.195	2743	2747	2755	rBV4	38497	66777	1.35%	0.115%
63	19.265	2756	2759	2762	rBV2	44711	66353	1.34%	0.114%
64	19.412	2779	2784	2804	rBV	1326548	2094883	42.27%	3.603%
65	19.630	2815	2821	2834	rBV	3692761	4956444	100.00%	8.524%
66	21.059	3062	3064	3070	rVB2	71310	91494	1.85%	0.157%
67	21.136	3073	3077	3089	rVV	573236	1106135	22.32%	1.902%
68	21.424	3121	3126	3138	rBV	1972535	2653934	53.55%	4.564%
69	23.636	3495	3502	3516	rBV2	1927411	4046873	81.65%	6.960%
70	23.789	3522	3528	3539	rVB2	1059508	2156716	43.51%	3.709%

Sum of corrected areas: 58144605

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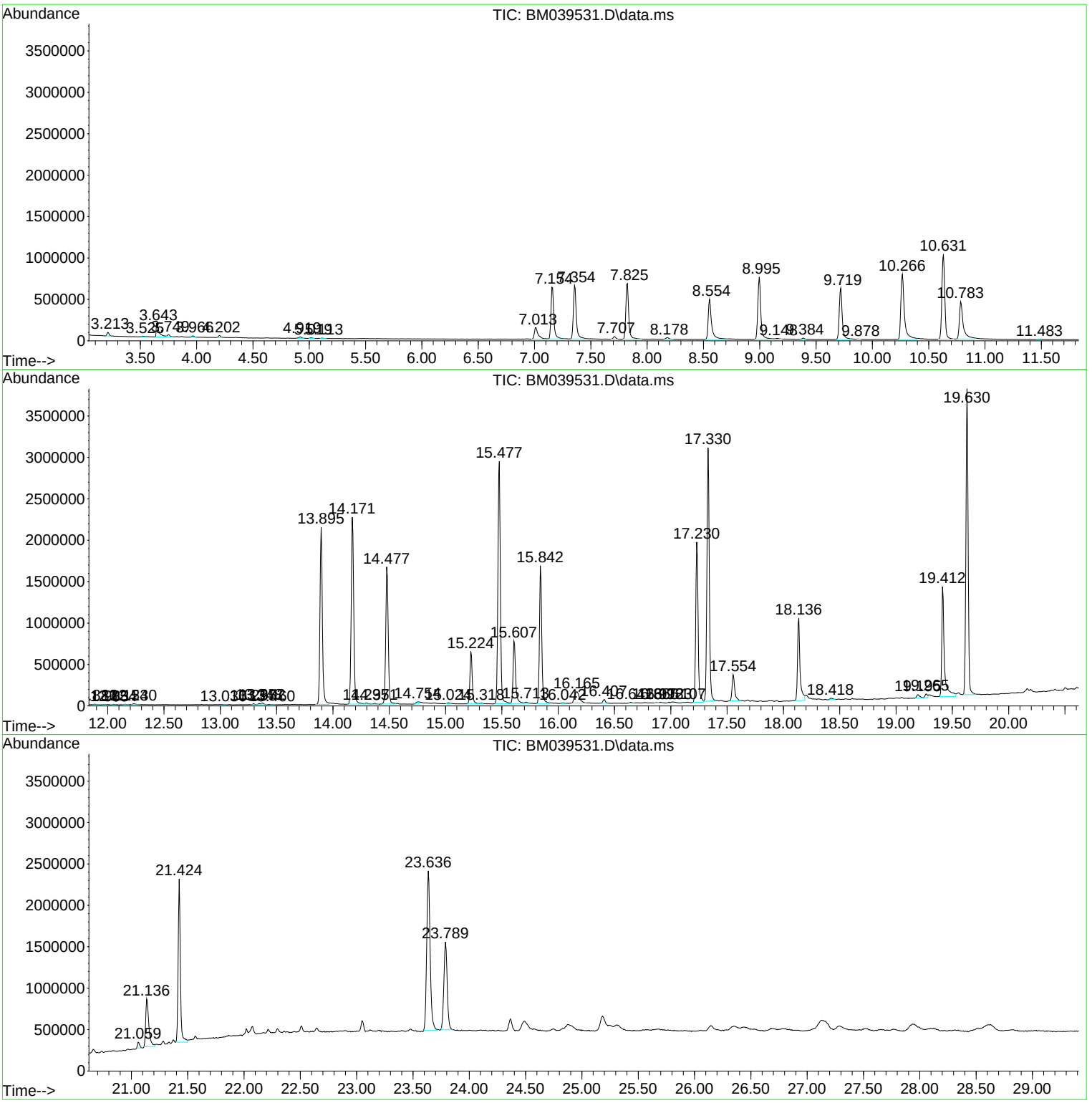
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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



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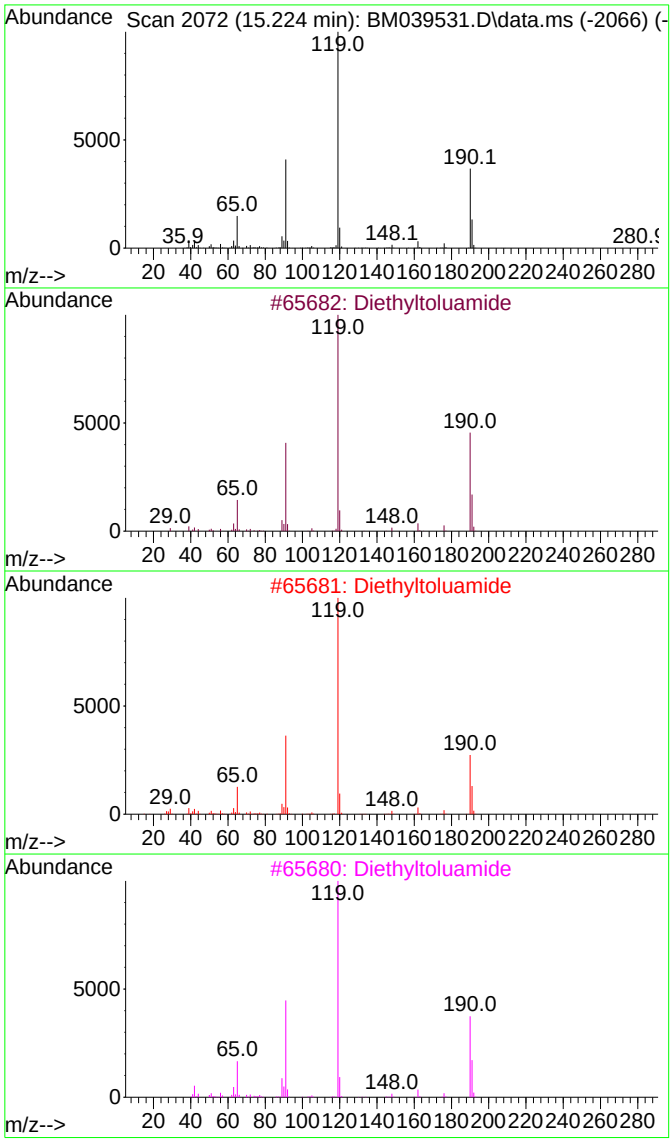
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

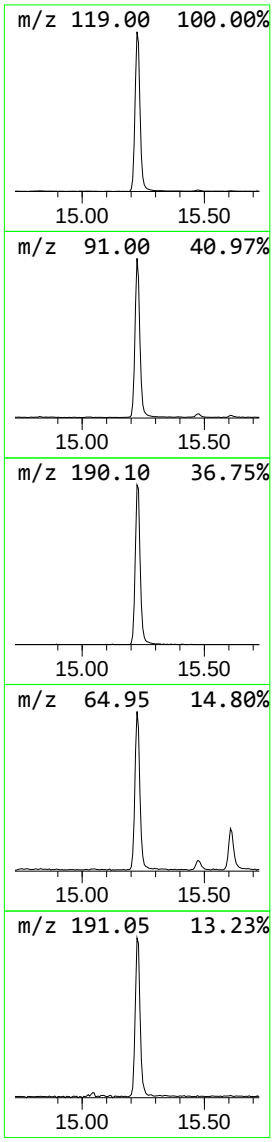
****

Peak Number 1 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	7.09 ng/ul	900566	Acenaphthene-d10	14.477

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	97
2	Diethyltoluamide	191	C12H17NO	000134-62-3	97
3	Diethyltoluamide	191	C12H17NO	000134-62-3	94
4	Benzamide, 2-methyl-N-methyl-N-p...	191	C12H17NO	1000421-44-4	87
5	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	87





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Operator : CG/JU
Sample : 02378-11
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

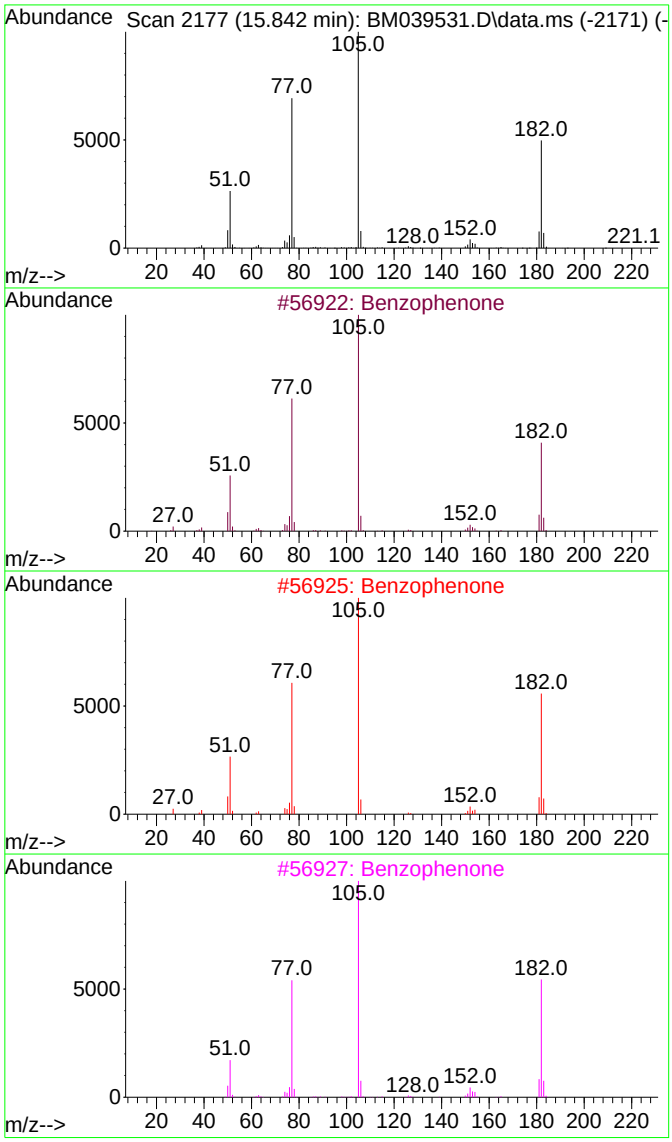
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

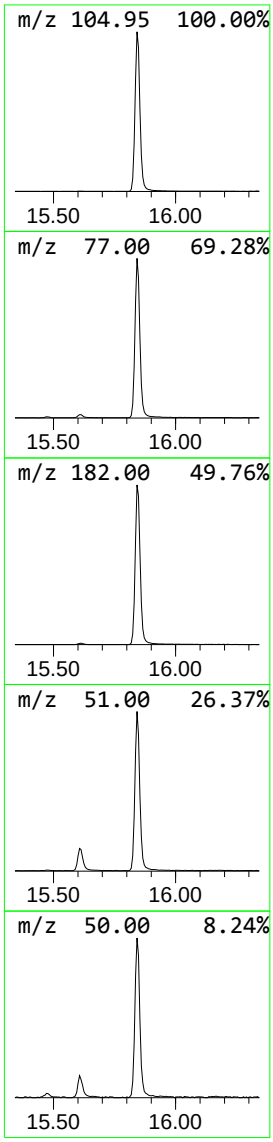
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.842	18.51 ng/ul	2351640	Acenaphthene-d10	14.477

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52





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Sample : 02378-11
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Instrument :
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ClientSampleId :
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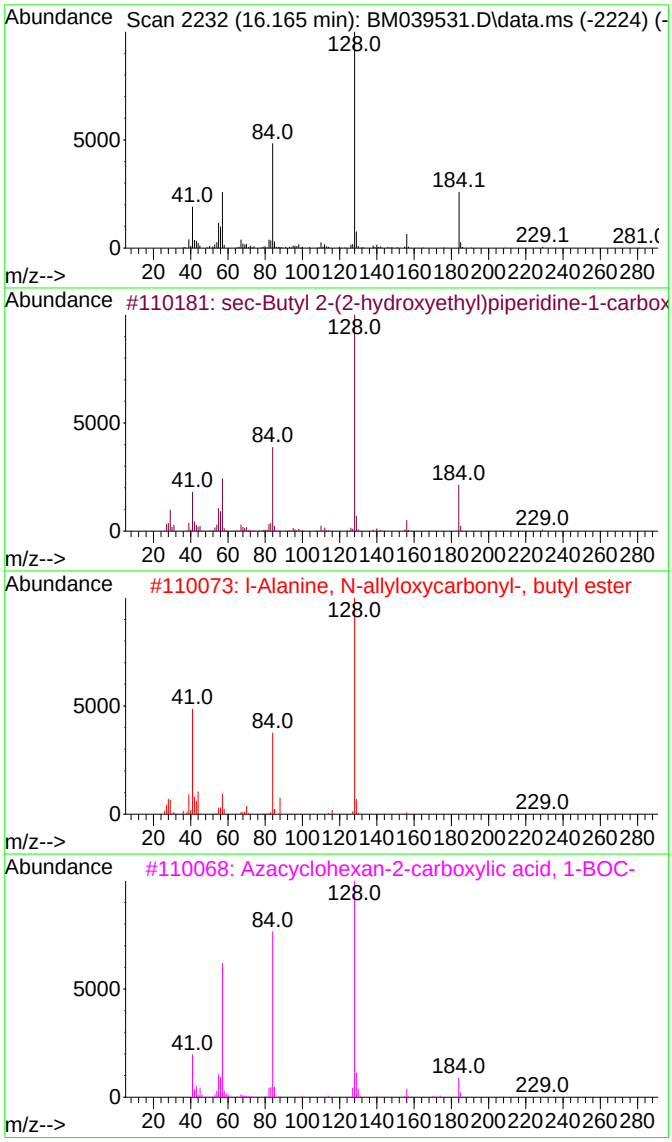
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

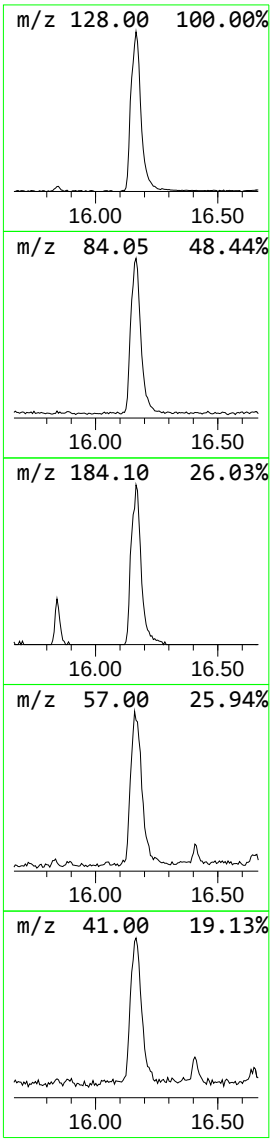
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 sec-Butyl 2-(2-hydroxyethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.166	2.94 ng/ul	420355	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	sec-Butyl 2-(2-hydroxyethyl)pipe...	229	C12H23NO3	119515-38-7	94
2	l-Alanine, N-allyloxycarbonyl-, ...	229	C11H19NO4	1000313-42-4	64
3	Azacyclohexan-2-carboxylic acid,...	229	C11H19NO4	1010126-80-6	64
4	l-Alanine, N-allyloxycarbonyl-, ...	341	C19H35NO4	1000313-43-3	59
5	l-Alanine, N-allyloxycarbonyl-, ...	213	C10H15NO4	1010313-43-8	59





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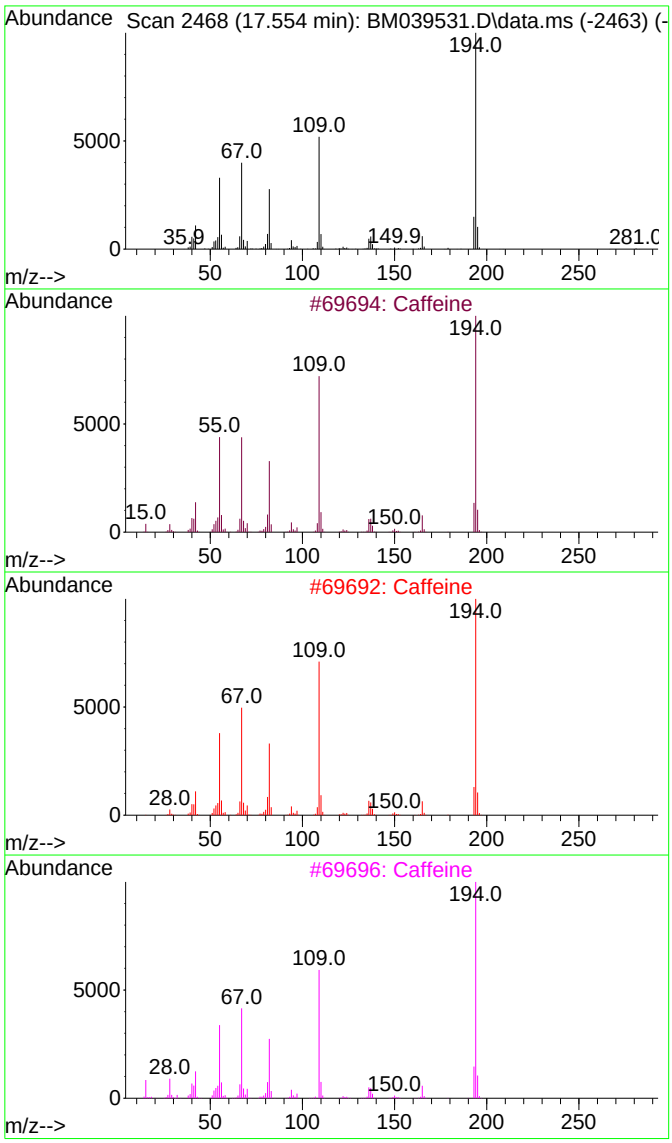
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

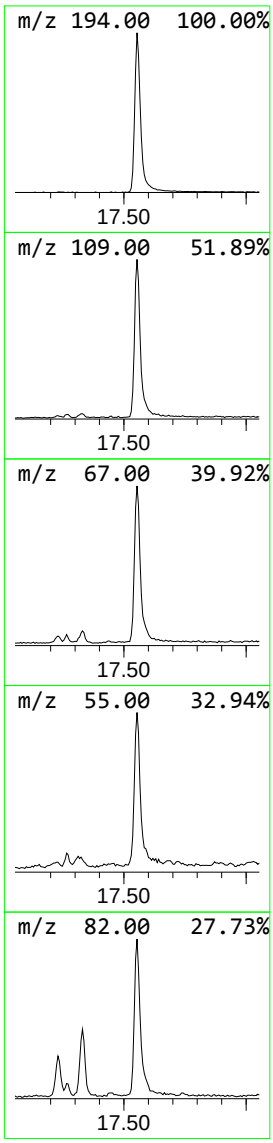
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Caffeine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.554	3.61 ng/ul	515941	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	97
2	Caffeine	194	C8H10N4O2	000058-08-2	96
3	Caffeine	194	C8H10N4O2	000058-08-2	95
4	Caffeine	194	C8H10N4O2	000058-08-2	94
5	Caffeine	194	C8H10N4O2	000058-08-2	94





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

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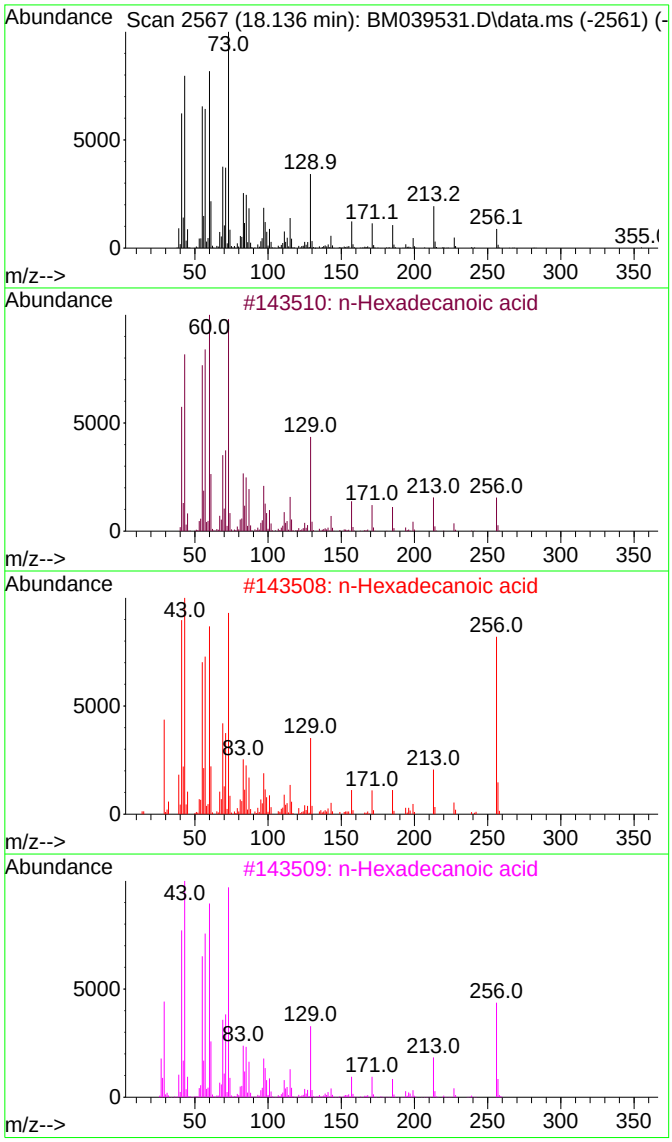
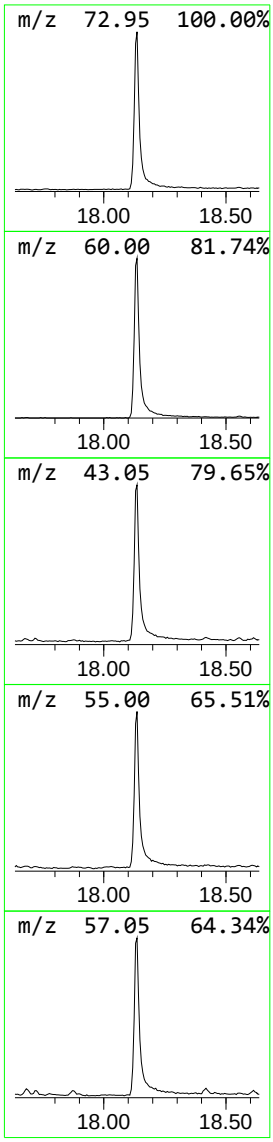
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.136	10.62 ng/ul	1515980	Phenanthrene-d10	17.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	94





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Quant Title : SVOA CALIBRATION

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

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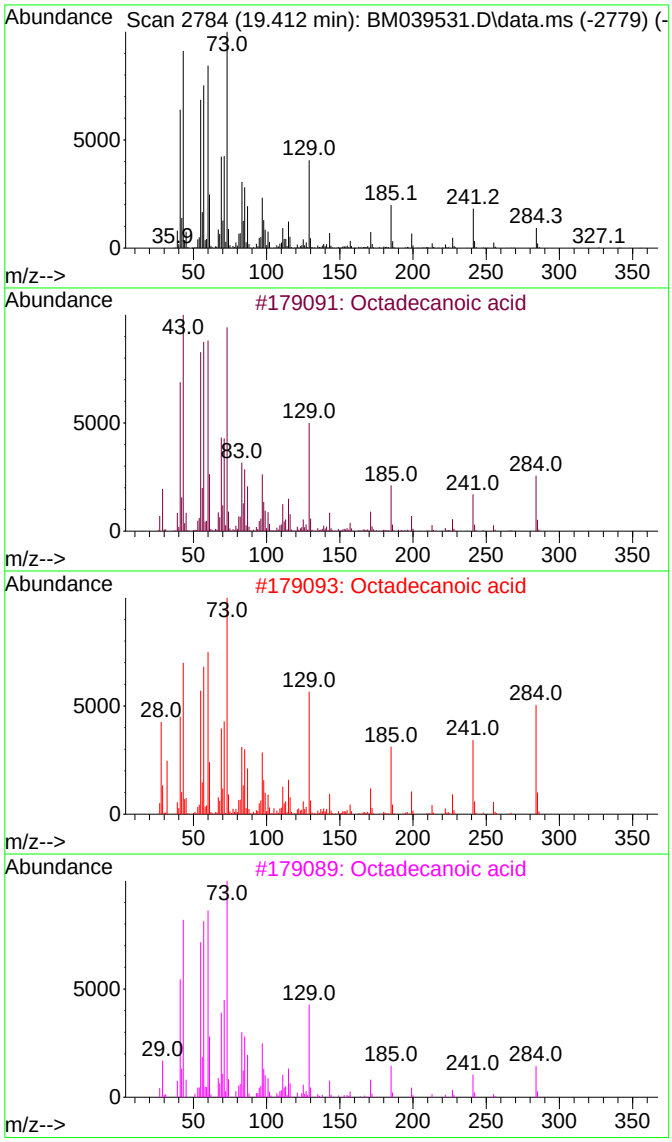
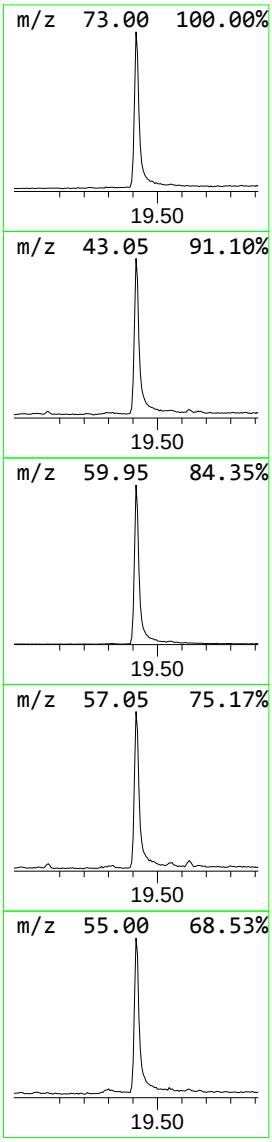
Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.412	15.79 ng/ul	2094880	Chrysene-d12	21.424

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	97
5	Octadecanoic acid	284	C18H36O2	000057-11-4	95





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Data File : BM039531.D
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Operator : CG/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0MK4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

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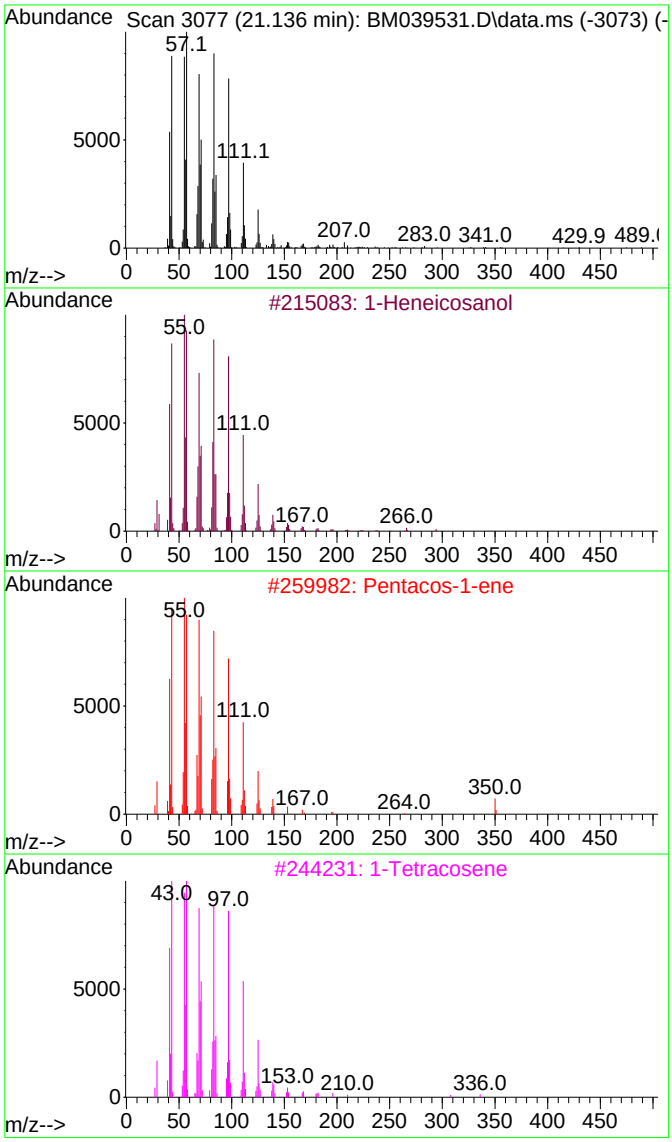
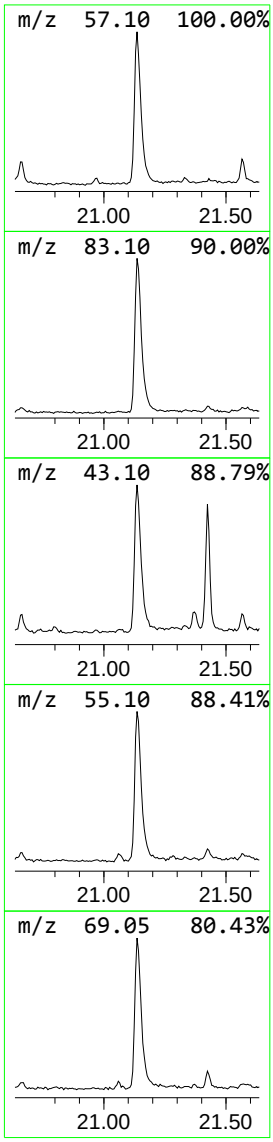
Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.136	8.34 ng/ul	1106140	Chrysene-d12	21.424

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	1-Tetracosene	336	C24H48	010192-32-2	93
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	1-Hexacosene	364	C26H52	018835-33-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039531.D
Acq On : 20 Apr 2023 19:01
Operator : CG/JU
Sample : 02378-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.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
Diethyltoluamide	15.224	7.1	ng/ul	900566	3	14.477	2540480	20.0
Benzophenone	15.842	18.5	ng/ul	2351640	3	14.477	2540480	20.0
sec-Butyl 2-(2-...	16.166	2.9	ng/ul	420355	4	17.230	2856190	20.0
Caffeine	17.554	3.6	ng/ul	515941	4	17.230	2856190	20.0
n-Hexadecanoic ...	18.136	10.6	ng/ul	1515980	4	17.230	2856190	20.0
Octadecanoic acid	19.412	15.8	ng/ul	2094880	5	21.424	2653930	20.0
1-Heneicosanol	21.136	8.3	ng/ul	1106140	5	21.424	2653930	20.0