LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

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: BM037709.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.434	4	8	13	rBV	48305	69312	0.13%	0.054%
2	3.728	55	58	67	rBV	33753	57850	0.11%	0.045%
3	3.875	80	83	99	rBV	218250	426064	0.81%	0.330%
4	5.175	298	304	316	rVB	57770	88114	0.17%	0.068%
5	7.257	651	658	669	rVB	367253	585132	1.11%	0.454%
6	7.434	679	688	696	rBV	905414	1385594	2.62%	1.075%
7	7.634	716	722	733	rBV	890359	1423689	2.69%	1.104%
8	8.110	796	803	810	rBV	792321	1253104	2.37%	0.972%
9	8.816	916	923	934	rBV	858488	1344203	2.54%	1.042%
10	9.281	994	1002	1011	rBV	1136781	1849697	3.50%	1.434%
11	9.704	1014	1074	1103	rBV	5701988	52918841	100.00%	41.038%
12	10.010	1119	1126	1140	rVB	952220	1569118	2.97%	1.217%
13	10.298	1159	1175	1196	rBV	859605	2639908	4.99%	2.047%
14	10.545	1210	1217	1226	rVB	1398318	2255924	4.26%	1.749%
15	10.710	1240	1245	1258	rVB	134710	224978	0.43%	0.174%
16	10.933	1274	1283	1291	rBV	1291116	2117255	4.00%	1.642%
17	11.069	1298	1306	1321	rBV	925801	1642939	3.10%	1.274%
18	11.198	1323	1328	1333	rVV2	62181	113050	0.21%	0.088%
19	11.363	1348	1356	1368	rVB4	106560	252749	0.48%	0.196%
20	11.516	1376	1382	1388	rVB5	39221	96115	0.18%	0.075%
21	11.745	1414	1421	1423	rVV	111261	192790	0.36%	0.150%
22	11.775	1423	1426	1433	rVV2	136791	262280	0.50%	0.203%
23	11.845	1433	1438	1442	rVV2	122257	230505	0.44%	0.179%
24	11.892	1442	1446	1461	rVV	84719	201688	0.38%	0.156%
25	12.639	1568	1573	1584	rBV	208967	317061	0.60%	0.246%
26	13.580	1723	1733	1738	rBV	49166	78370	0.15%	0.061%
27	14.145	1821	1829	1835	rBV	2936075	3959588	7.48%	3.071%
28	14.368	1862	1867	1872	rBV2	39247	66634	0.13%	0.052%
29	14.433	1872	1878	1886	rVV	3070839	4369417	8.26%	3.388%
30	14.521	1888	1893	1901	rVV	135178	217836	0.41%	0.169%
31	14.739	1923	1930	1938	rBV	1976353	2899525	5.48%	2.249%
32	14.910	1953	1959	1970	rBV	506490	788314	1.49%	0.611%
33	15.004	1970	1975	1983	rVV	120684	186086	0.35%	0.144%
34	15.427	2042	2047	2057	rVV	94552	184765	0.35%	0.143%
35	15.721	2089	2097	2104	rBV	4011454	5682426	10.74%	4.407%
36	15.827	2109	2115	2128	rBV	1484864	2049881	3.87%	1.590%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

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	17.262	2355	2359	2366	rVB2	42956	66882	0.13%	0.052%
38	17.474	2388	2395	2401	rBV	2516740	3434479	6.49%	2.663%
39	17.574	2405	2412	2419	rBV	4489237	6299311	11.90%	4.885%
40	18.127	2502	2506	2511	rBV2	46170	58826	0.11%	0.046%
41	18.351	2538	2544	2559	rBV	546089	885409	1.67%	0.687%
42	19.415	2722	2725	2729	rBV2	59072	73246	0.14%	0.057%
43	19.480	2731	2736	2742	rBV3	90535	205596	0.39%	0.159%
44	19.615	2754	2759	2769	rBV	423026	630306	1.19%	0.489%
45	19.850	2793	2799	2809	rBV	5785533	7526826	14.22%	5.837%
46	20.821	2962	2964	2968	rVB	94322	91244	0.17%	0.071%
47	21.321	3046	3049	3059	rBV	351419	442383	0.84%	0.343%
48	21.639	3097	3103	3108	rBV	2859230	3813633	7.21%	2.957%
49	22.915	3317	3320	3326	rVB	215858	283163	0.54%	0.220%
50	23.339	3389	3392	3399	rVB	180668	257239	0.49%	0.199%
51	23.968	3491	3499	3510	rVB2	3471821	7376108	13.94%	5.720%
52	24.127	3520	3526	3537	rVB2	1739519	3506184	6.63%	2.719%

Sum of corrected areas: 128951637

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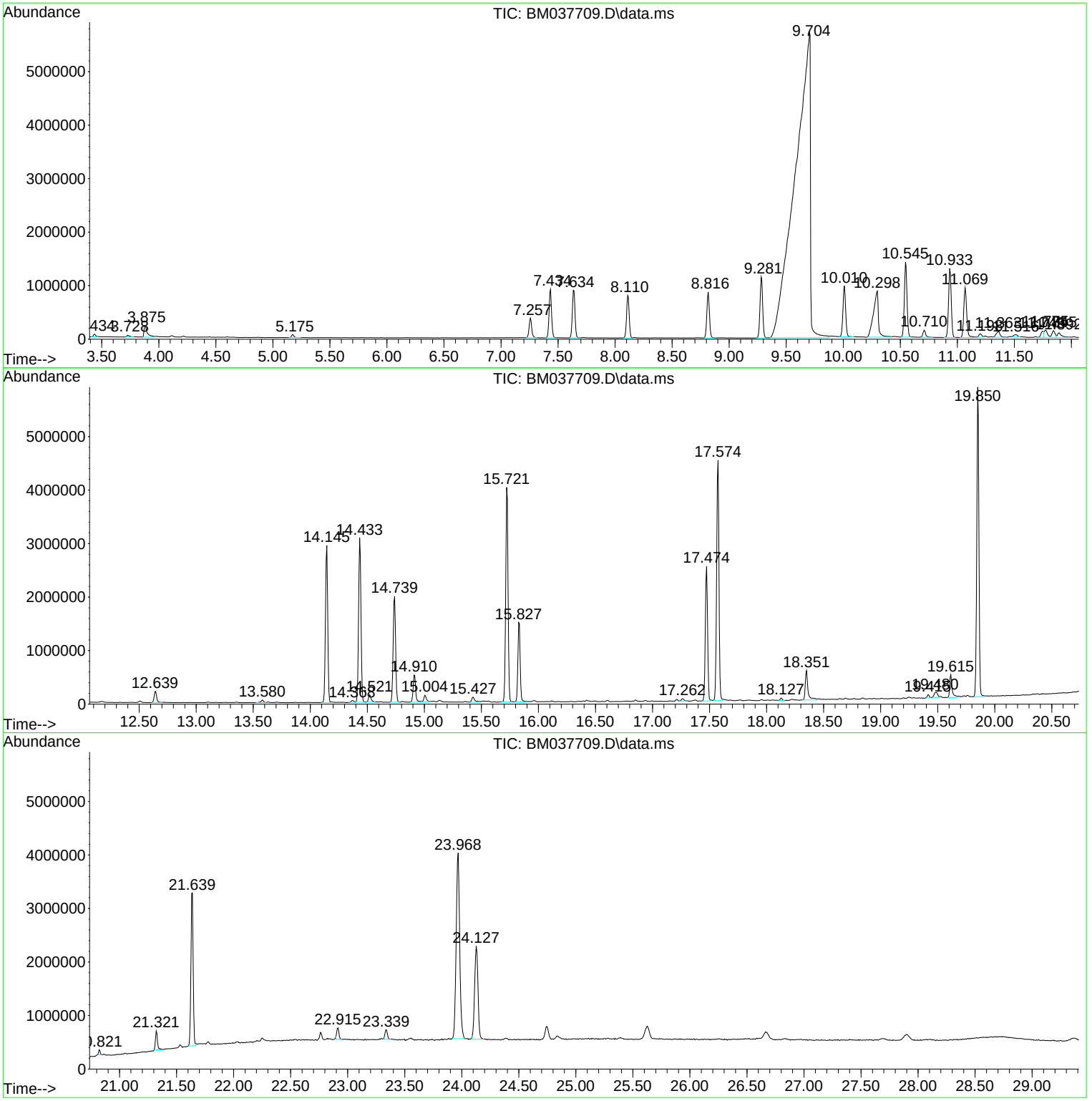
Instrument :
BNA_M
ClientSampleId :
C9810

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 : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

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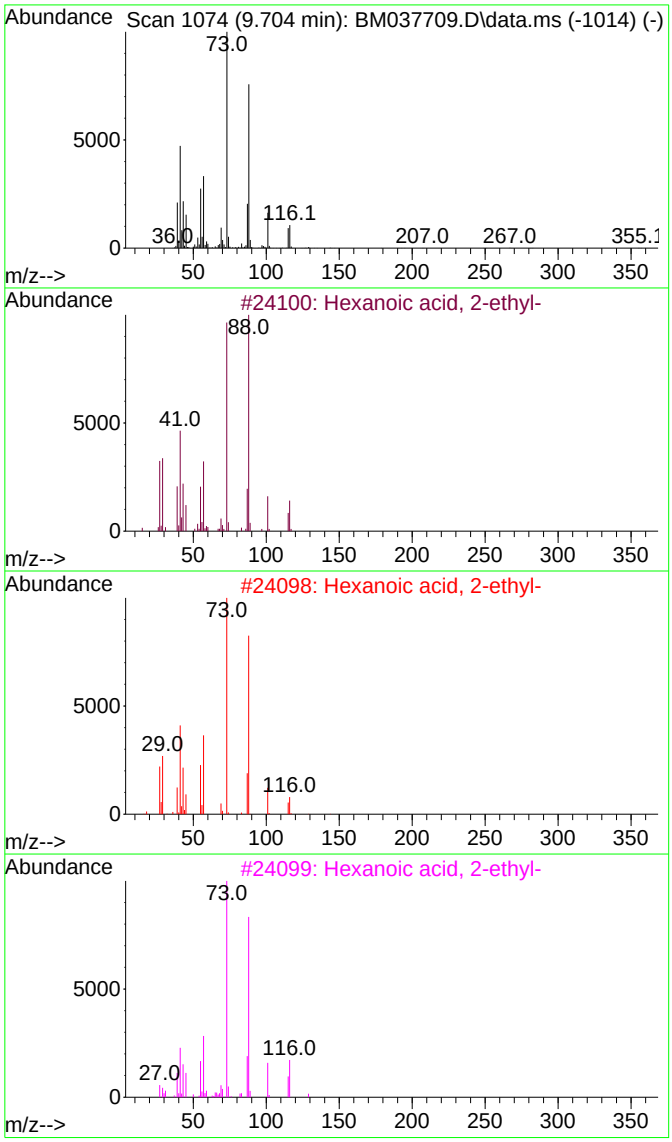
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

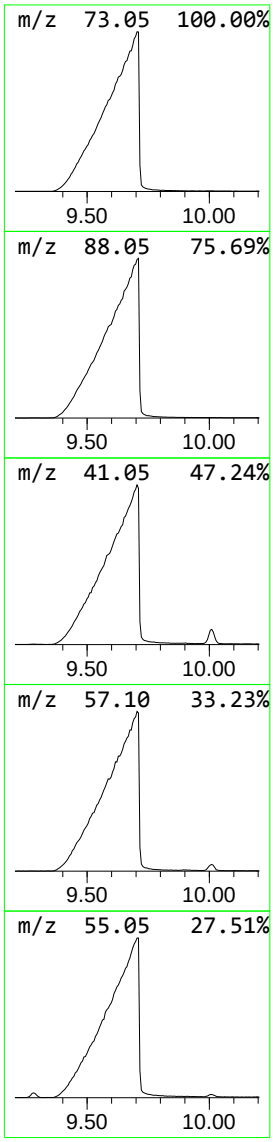
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	499.88 ng/ul	52918800	Naphthalene-d8	10.933

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	83
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72





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Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

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

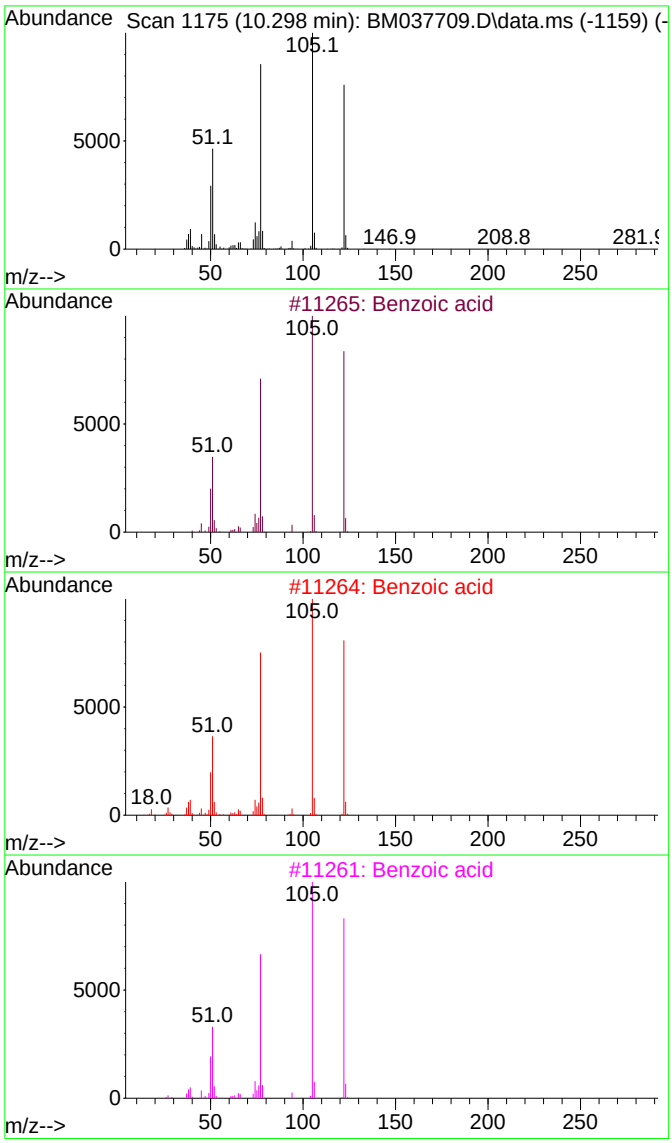
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

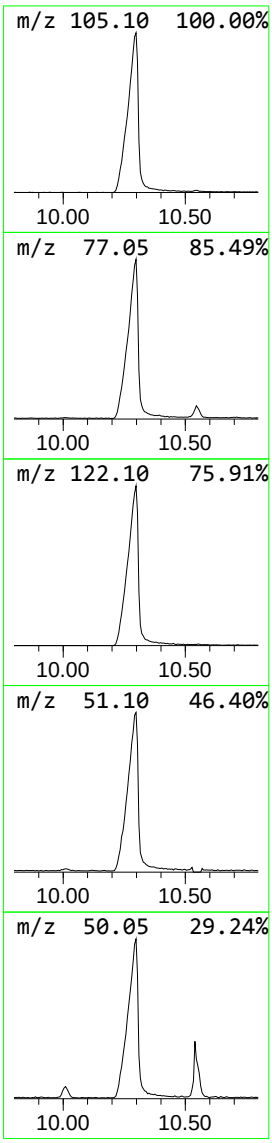
****

Peak Number 2 Benzoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.298	24.94 ng/ul	2639910	Naphthalene-d8	10.933

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	Benzoic acid	122	C7H6O2	000065-85-0	91
5	Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

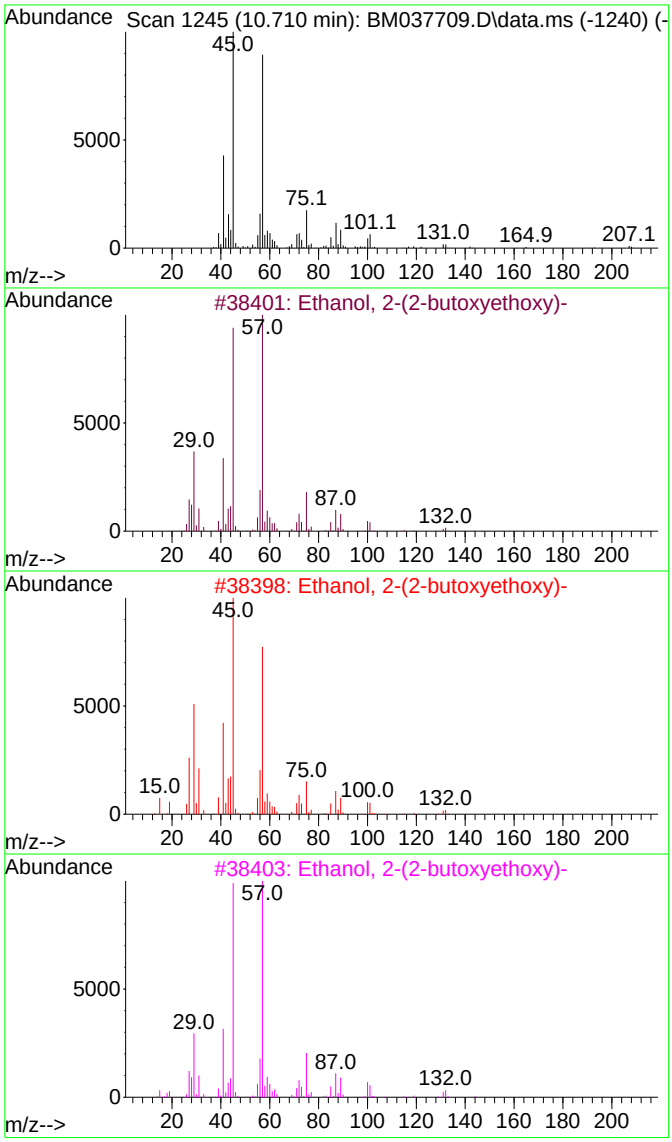
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

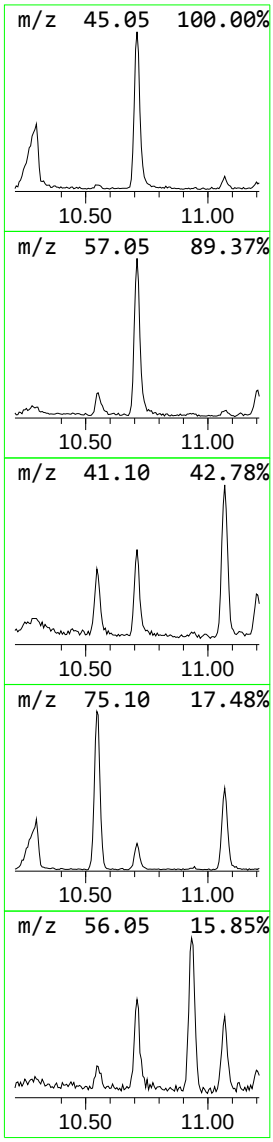
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	2.13 ng/ul	224978	Naphthalene-d8	10.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
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Acq On : 25 Nov 2022 23:33
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Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

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

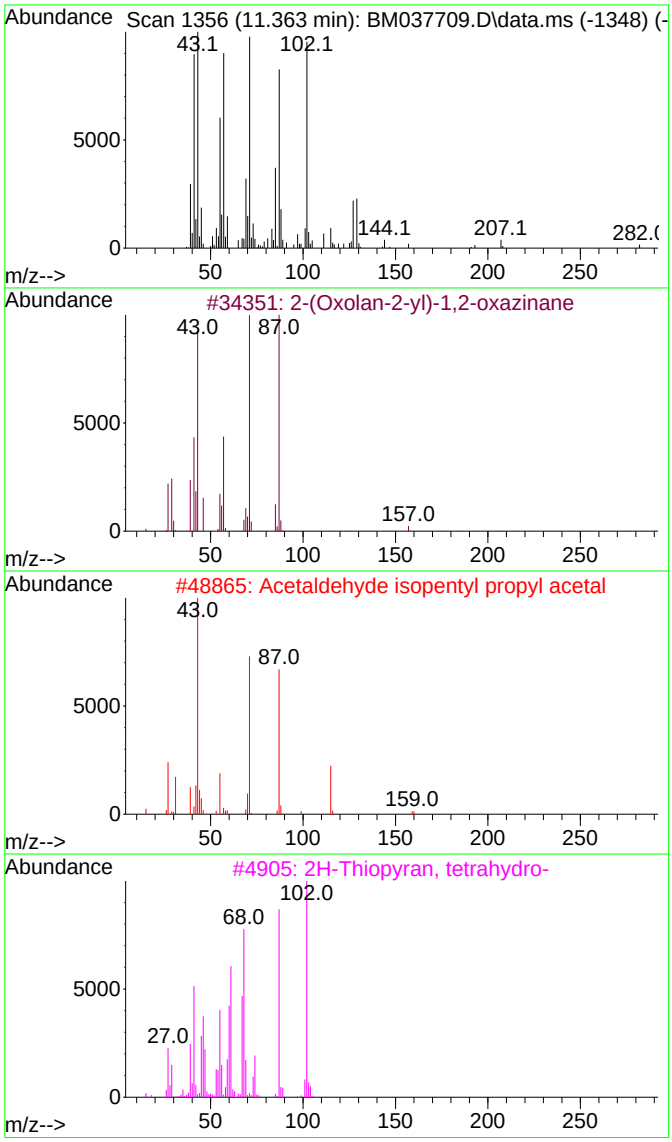
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

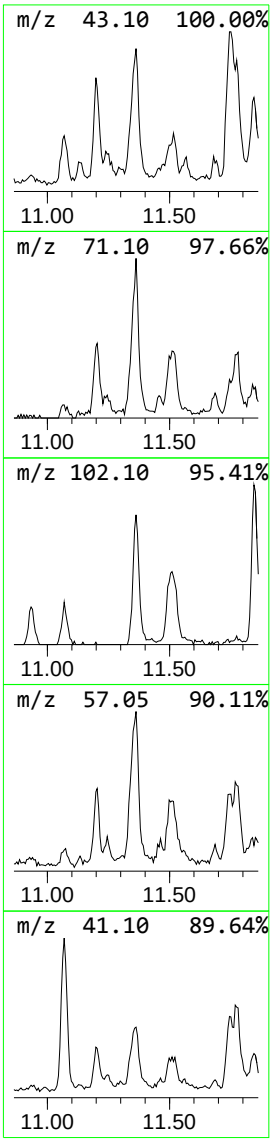
****

Peak Number 4 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.363	2.39 ng/ul	252749	Naphthalene-d8	10.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Oxolan-2-yl)-1,2-oxazinane	157	C8H15NO2	1000445-08-1	43
2	Acetaldehyde isopentyl propyl ac...	174	C10H22O2	1000431-62-2	38
3	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	38
4	Dodecane, 4-methyl-	184	C13H28	006117-97-1	14
5	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	14





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Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 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

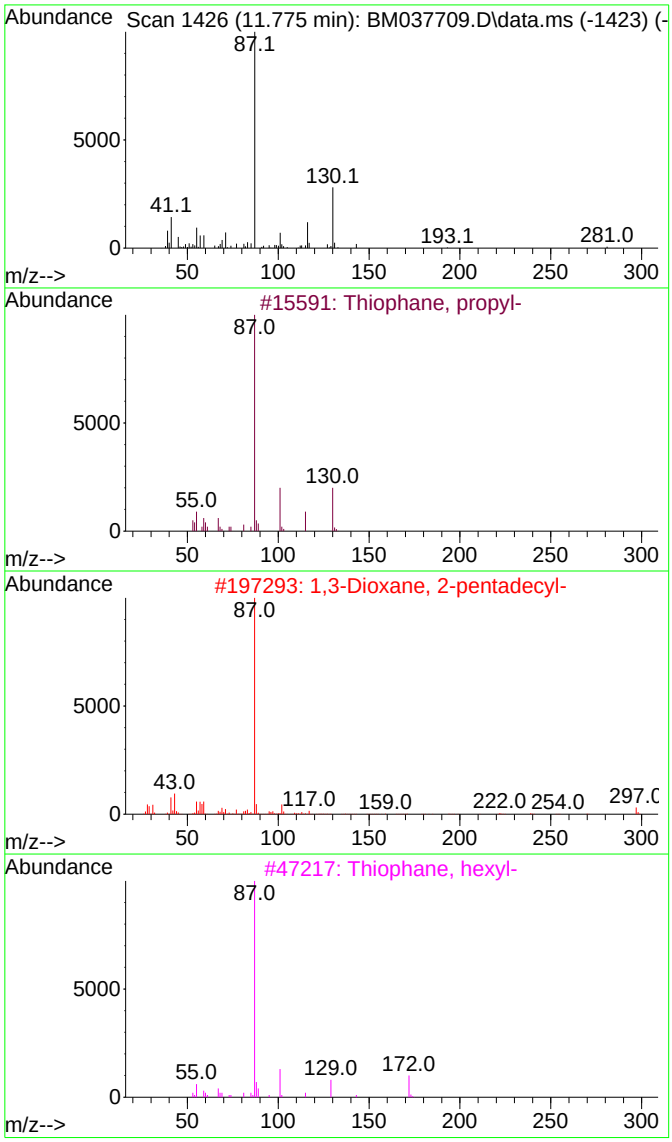
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

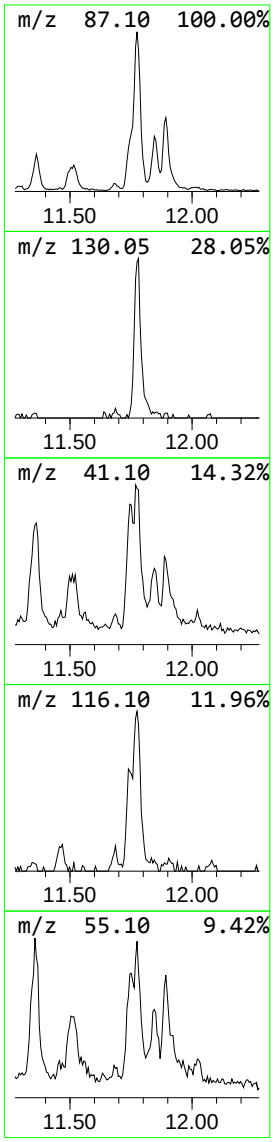
****

Peak Number 5 Thiophane, propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	2.48 ng/ul	262280	Naphthalene-d8	10.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophane, propyl-	130	C7H14S	001551-34-4	72
2	1,3-Dioxane, 2-pentadecyl-	298	C19H38O2	017352-27-1	50
3	Thiophane, hexyl-	172	C10H20S	000876-37-9	36
4	Ethyl acetoacetate ethylene acetal	174	C8H14O4	006413-10-1	33
5	Arachidamide, N-ethyl-	339	C22H45NO	1000420-44-1	33





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Data File : BM037709.D
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Operator : CG/JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

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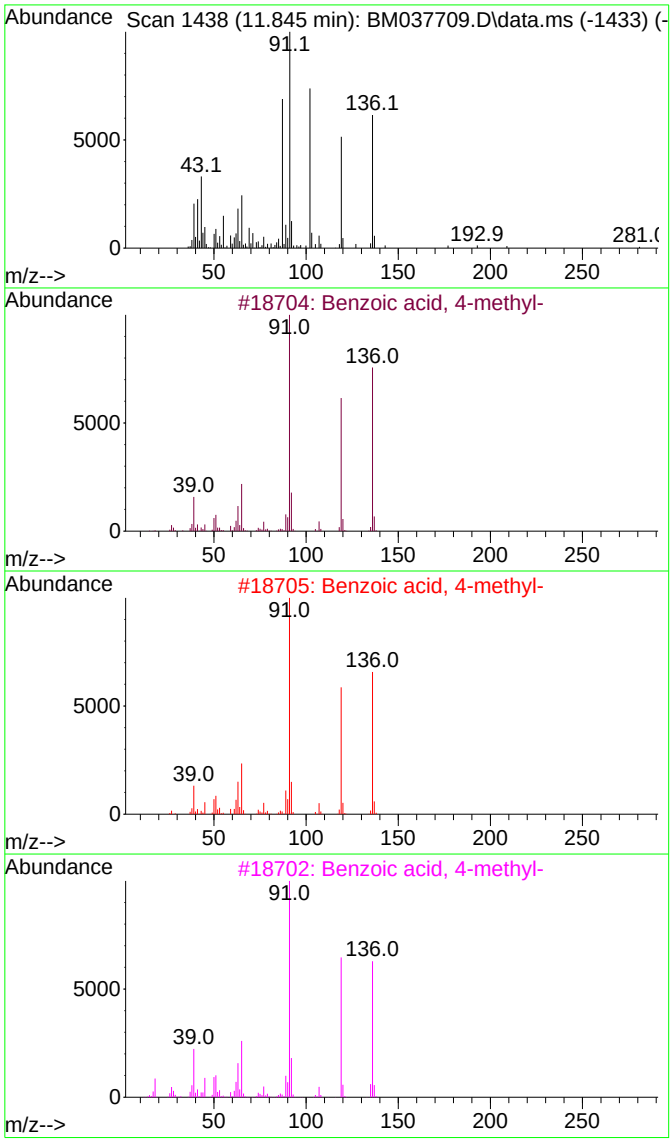
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

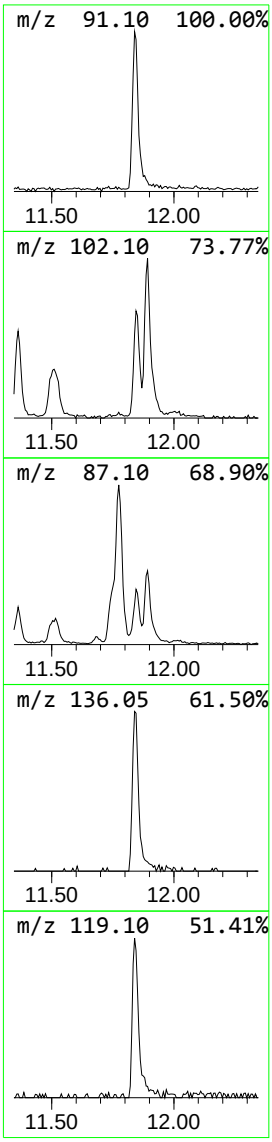
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzoic acid, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	2.18 ng/ul	230505	Naphthalene-d8	10.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	89
2	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	86
3	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	70
4	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	70
5	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	70





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Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

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

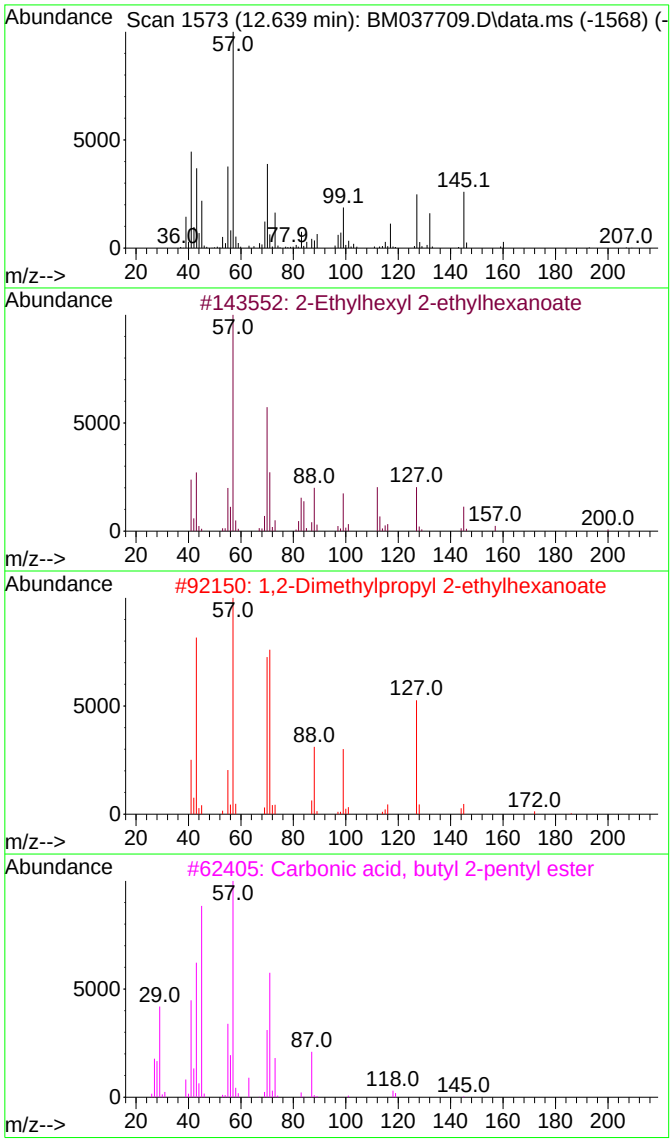
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

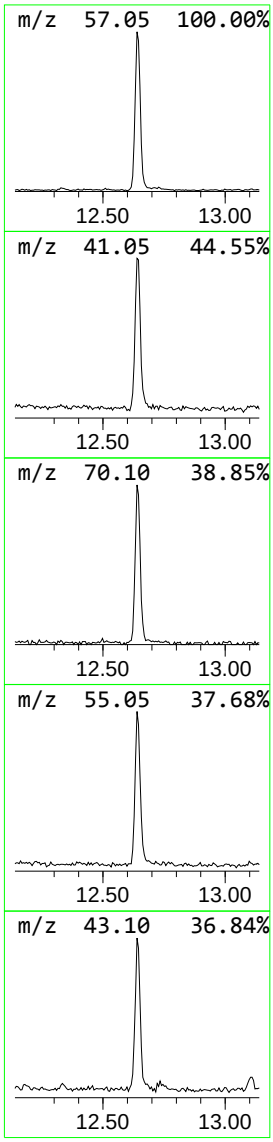
****

Peak Number 7 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	3.00 ng/ul	317061	Naphthalene-d8	10.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl 2-ethylhexanoate	256	C16H32O2	007425-14-1	40
2	1,2-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-1	32
3	Carbonic acid, butyl 2-pentyl ester	188	C10H20O3	1000357-84-0	27
4	1-Ethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-98-7	25
5	Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

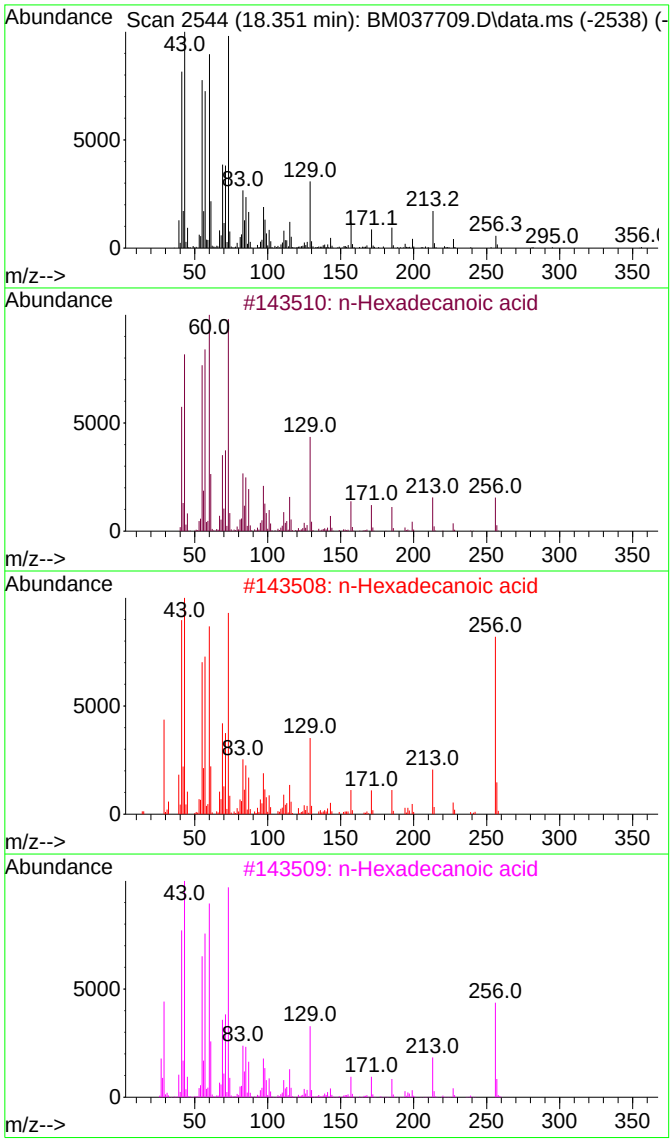
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

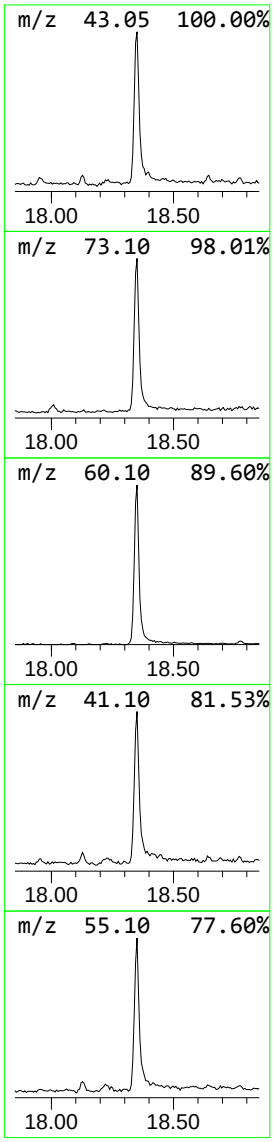
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	5.16 ng/ul	885409	Phenanthrene-d10	17.474

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	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90





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Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

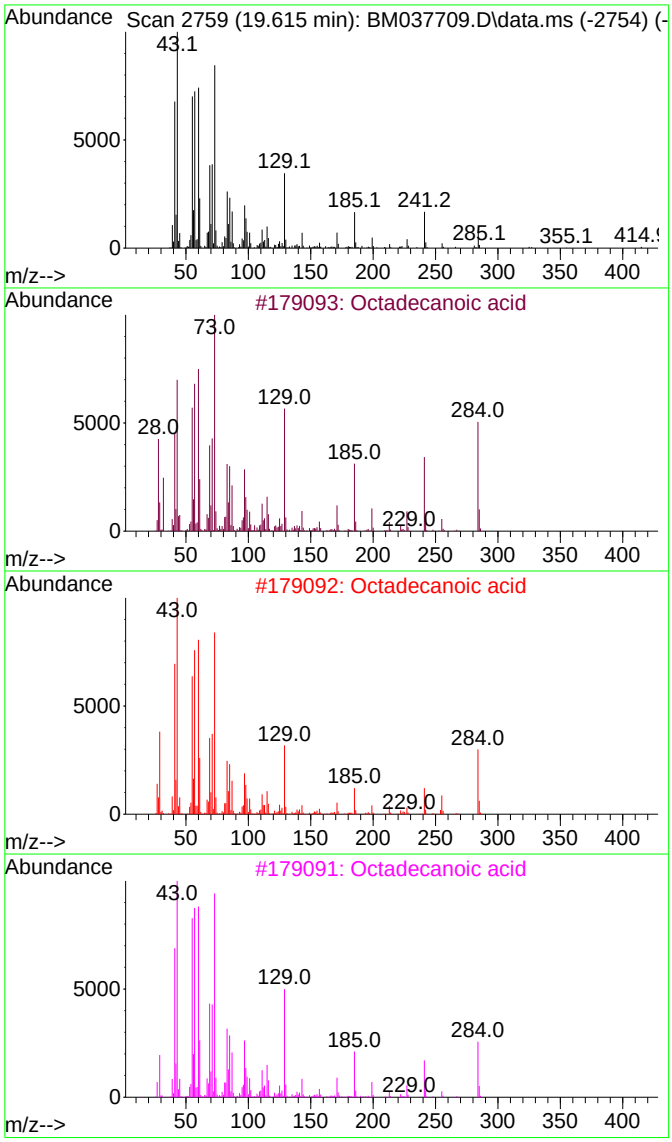
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

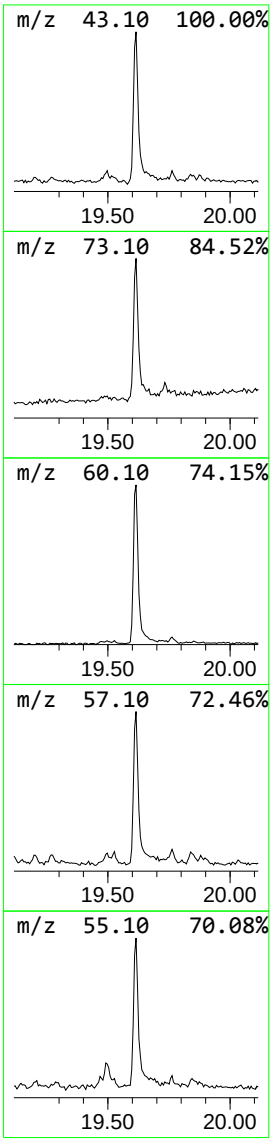
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.615	3.31 ng/ul	630306	Chrysene-d12	21.639

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	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

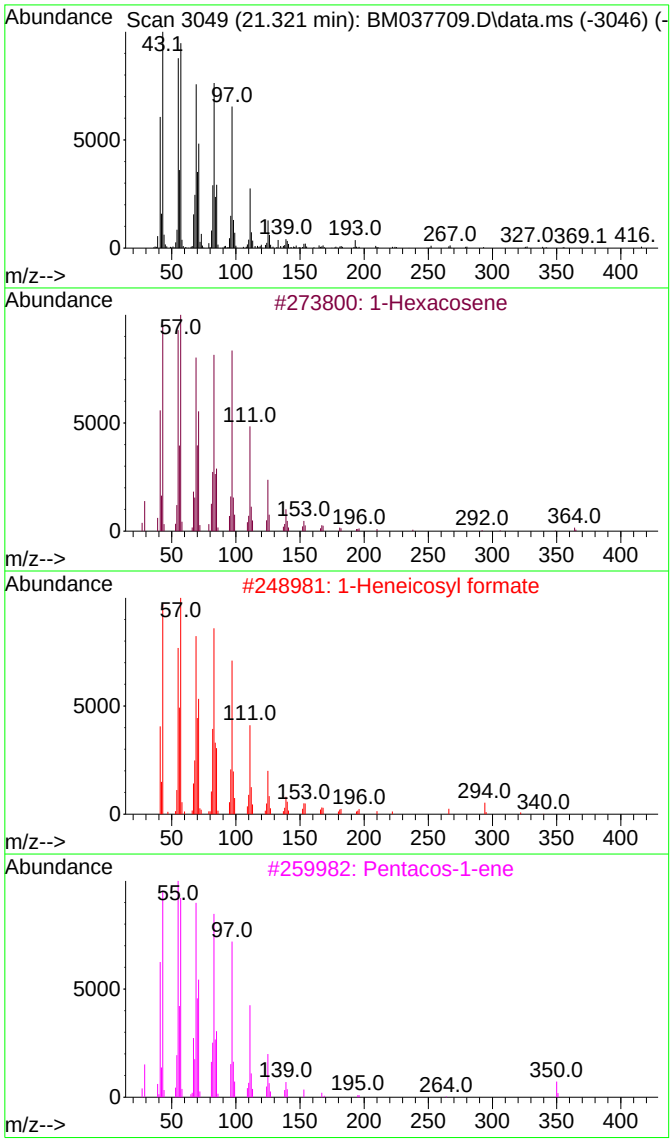
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

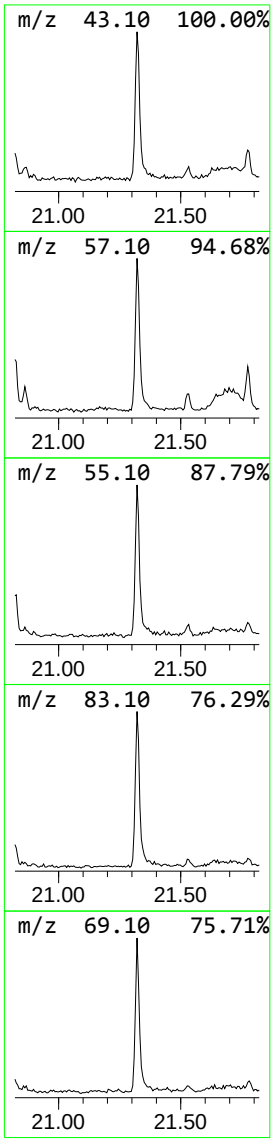
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.321	2.32 ng/ul	442383	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3	Pentacos-1-ene	350	C25H50	016980-85-1	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037709.D
Acq On : 25 Nov 2022 23:33
Operator : CG/JU
Sample : N5591-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C9810

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
Hexanoic acid, ...	9.704	499.9	ng/ul	52918800	2	10.933	2117260	20.0
Benzoic acid	10.298	24.9	ng/ul	2639910	2	10.933	2117260	20.0
Ethanol, 2-(2-b...	10.710	2.1	ng/ul	224978	2	10.933	2117260	20.0
unknown-01	11.363	2.4	ng/ul	252749	2	10.933	2117260	20.0
Thiophane, propyl-	11.775	2.5	ng/ul	262280	2	10.933	2117260	20.0
Benzoic acid, 4...	11.845	2.2	ng/ul	230505	2	10.933	2117260	20.0
unknown-02	12.639	3.0	ng/ul	317061	2	10.933	2117260	20.0
n-Hexadecanoic ...	18.351	5.2	ng/ul	885409	4	17.474	3434480	20.0
Octadecanoic acid	19.615	3.3	ng/ul	630306	5	21.639	3813630	20.0
(DEL) Alkane: S...	21.321	2.3	ng/ul	442383	5	21.639	3813630	20.0