LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

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_P\Methods\SFAM-EPA-BP120123.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP018763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	26	30	37	rVB	37384	47355	0.49%	0.079%
2	3.681	98	101	119	rBV	195139	309759	3.22%	0.516%
3	3.917	137	141	146	rVB2	11910	18306	0.19%	0.031%
4	4.011	154	157	164	rVB	9982	12994	0.14%	0.022%
5	4.540	243	247	253	rVV2	17931	25638	0.27%	0.043%
6	6.846	631	639	642	rBV9	5606	12550	0.13%	0.021%
7	7.011	660	667	678	rVB	132149	217763	2.27%	0.363%
8	7.175	689	695	707	rVB	540953	832218	8.66%	1.388%
9	7.369	721	728	736	rBV	527386	816054	8.49%	1.361%
10	7.840	800	808	816	rVB	616017	965846	10.05%	1.610%
11	8.552	922	929	940	rBV	381142	623645	6.49%	1.040%
12	8.999	998	1005	1016	rBV	644306	1029561	10.72%	1.717%
13	9.310	1021	1058	1062	rBV	1581134	9607409	100.00%	16.018%
14	9.722	1119	1128	1142	rBV	499907	829919	8.64%	1.384%
15	9.946	1154	1166	1182	rBV	225196	542699	5.65%	0.905%
16	10.257	1209	1219	1228	rBV	777120	1302812	13.56%	2.172%
17	10.634	1274	1283	1295	rBV	788051	1317818	13.72%	2.197%
18	10.775	1299	1307	1315	rBV	736859	1235889	12.86%	2.061%
19	10.834	1315	1317	1324	rVV4	10951	20504	0.21%	0.034%
20	10.916	1324	1331	1335	rVV	73806	133900	1.39%	0.223%
21	10.957	1335	1338	1344	rVV3	22464	42932	0.45%	0.072%
22	11.016	1344	1348	1349	rVV4	8403	11537	0.12%	0.019%
23	11.075	1349	1358	1366	rVV3	111262	251026	2.61%	0.419%
24	11.169	1369	1374	1377	rBV5	14881	24183	0.25%	0.040%
25	11.234	1377	1385	1389	rVV2	55620	140477	1.46%	0.234%
26	11.275	1389	1392	1398	rVB4	11268	18961	0.20%	0.032%
27	11.404	1408	1414	1418	rBV4	13876	25148	0.26%	0.042%
28	11.493	1427	1429	1436	rVB	126122	205398	2.14%	0.342%
29	11.569	1436	1442	1446	rVV2	175630	294024	3.06%	0.490%
30	11.616	1446	1450	1461	rVB	94555	192641	2.01%	0.321%
31	11.793	1477	1480	1486	rVB5	7002	10128	0.11%	0.017%
32	12.057	1518	1525	1529	rBV8	6172	11810	0.12%	0.020%
33	12.222	1547	1553	1558	rBV2	16376	29279	0.30%	0.049%
34	12.375	1574	1579	1592	rBV2	34160	68384	0.71%	0.114%
35	13.298	1733	1736	1742	rVB5	7347	10238	0.11%	0.017%
36	13.375	1742	1749	1753	rBV5	9877	19014	0.20%	0.032%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

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_P\Methods\SFAM-EPA-BP120123.MA.M
Title : SVOA CALIBRATION

37	13.887	1829	1836	1849	rBV	1633063	2246897	23.39%	3.746%
38	14.163	1876	1883	1892	rBV	1655800	2500003	26.02%	4.168%
39	14.281	1895	1903	1916	rVV	355612	623971	6.49%	1.040%
40	14.375	1917	1919	1926	rVV8	8025	10699	0.11%	0.018%
41	14.469	1928	1935	1943	rVB	1255143	1820934	18.95%	3.036%
42	14.675	1964	1970	1978	rBV	132165	232769	2.42%	0.388%
43	14.751	1979	1983	1989	rVB	39125	59624	0.62%	0.099%
44	14.887	2001	2006	2013	rVB9	13447	22511	0.23%	0.038%
45	15.175	2050	2055	2066	rBV	78588	135049	1.41%	0.225%
46	15.463	2096	2104	2118	rBV	2363714	3431663	35.72%	5.721%
47	15.581	2118	2124	2139	rVV	731335	1036502	10.79%	1.728%
48	15.704	2139	2145	2148	rVV4	10274	17614	0.18%	0.029%
49	16.034	2195	2201	2206	rBV9	6383	10914	0.11%	0.018%
50	16.187	2223	2227	2230	rVV5	6099	9846	0.10%	0.016%
51	16.239	2231	2236	2242	rVB7	7746	16119	0.17%	0.027%
52	16.616	2297	2300	2307	rBV8	9335	14668	0.15%	0.024%
53	16.763	2321	2325	2330	rBV8	8919	12626	0.13%	0.021%
54	16.981	2358	2362	2364	rBV3	8349	10979	0.11%	0.018%
55	17.028	2365	2370	2376	rVB4	17038	31007	0.32%	0.052%
56	17.216	2395	2402	2411	rBV	1672855	2364334	24.61%	3.942%
57	17.316	2412	2419	2430	rVV	2870794	4048839	42.14%	6.750%
58	17.810	2499	2503	2508	rBV	24705	32147	0.33%	0.054%
59	17.886	2514	2516	2522	rVB6	10149	12169	0.13%	0.020%
60	18.110	2548	2554	2562	rBV	227541	334572	3.48%	0.558%
61	18.575	2630	2633	2638	rVB3	14363	17496	0.18%	0.029%
62	19.128	2723	2727	2731	rBV2	51722	69733	0.73%	0.116%
63	19.198	2735	2739	2742	rBV	61229	82251	0.86%	0.137%
64	19.339	2759	2763	2769	rBV	171595	221565	2.31%	0.369%
65	19.551	2793	2799	2805	rBV	4156650	5489657	57.14%	9.153%
66	21.304	3092	3097	3106	rBV	2585663	3186956	33.17%	5.313%
67	23.516	3466	3473	3490	rVB	3564255	6948525	72.32%	11.585%
68	23.669	3492	3499	3509	rVB	1905464	3669178	38.19%	6.117%

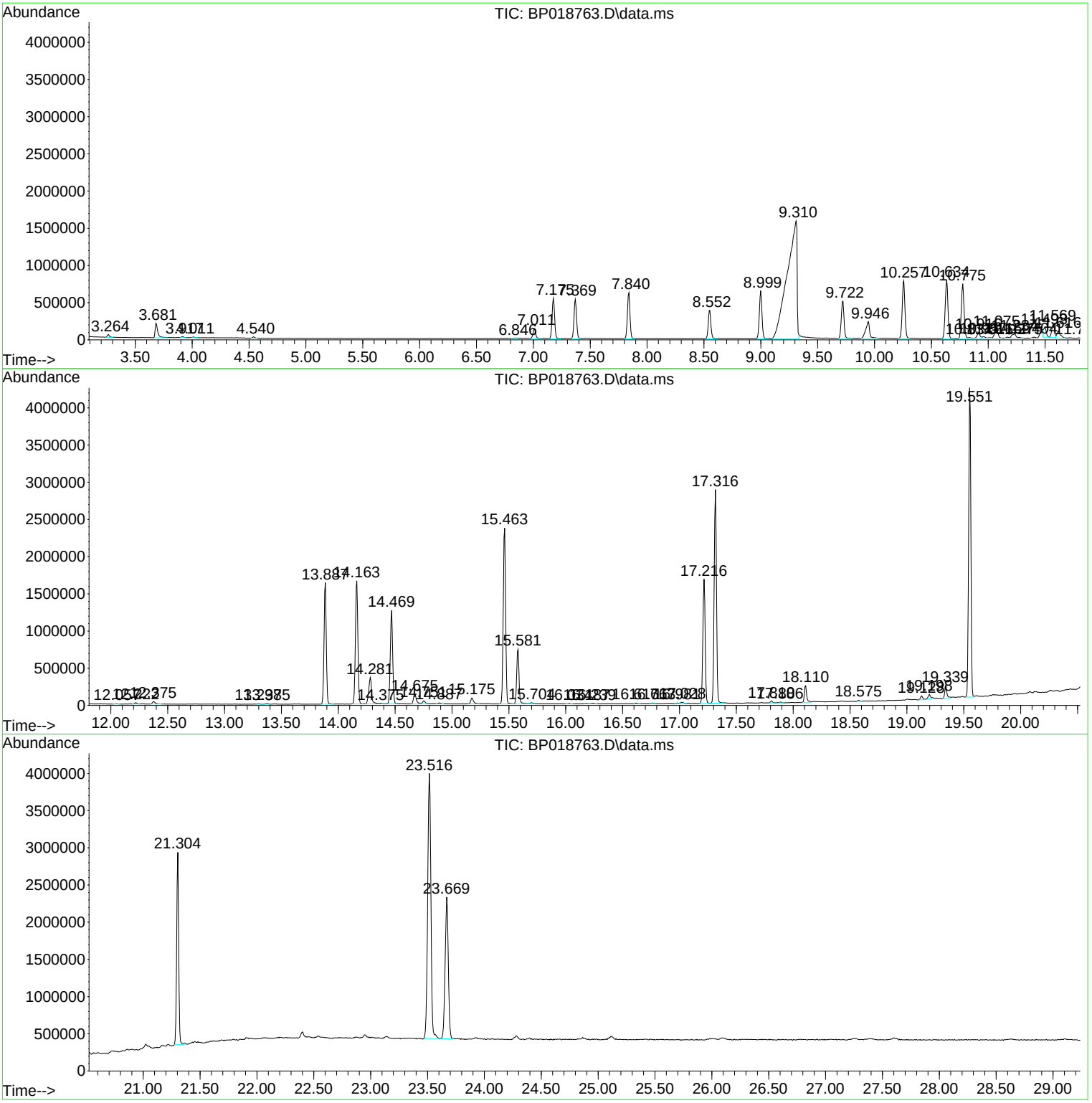
Sum of corrected areas: 59979636

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
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Instrument :
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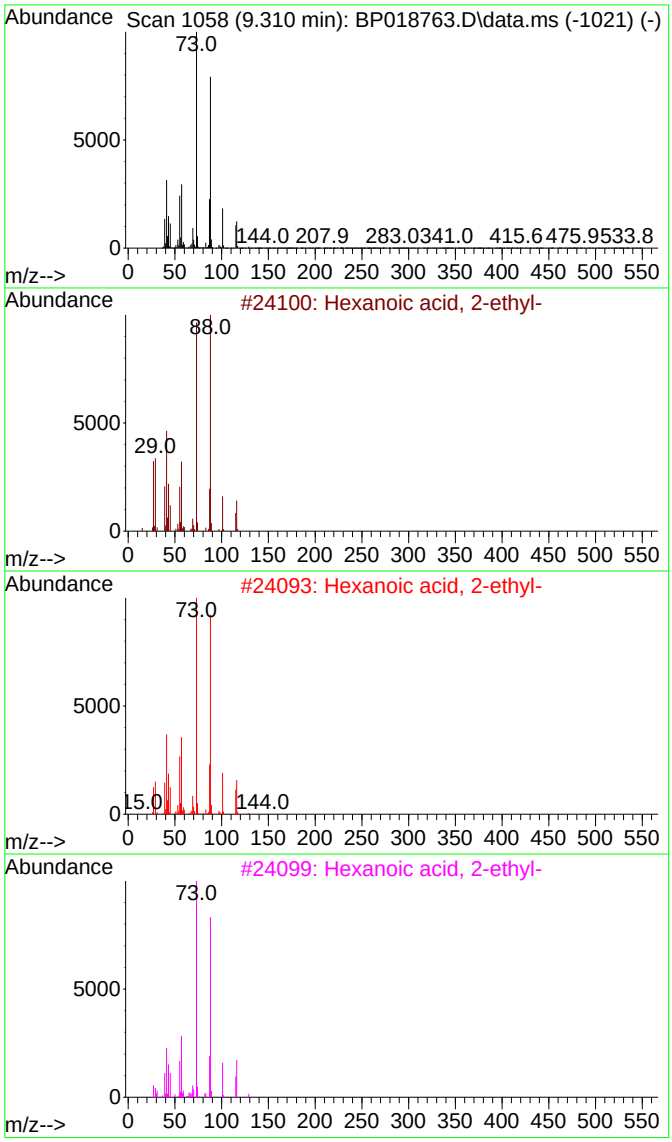
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

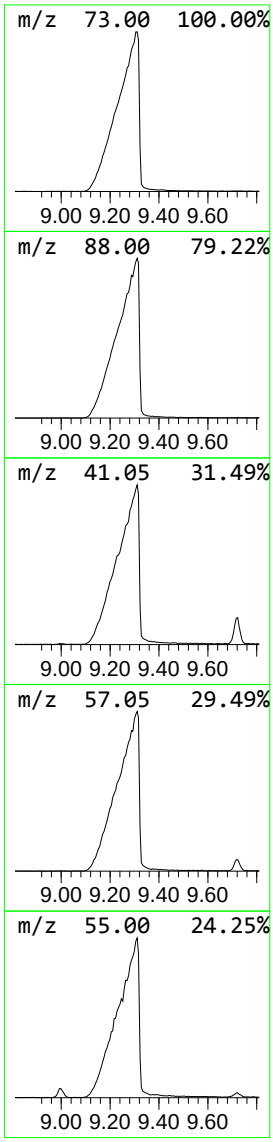
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.310	145.81 ng/ul	9607410	Naphthalene-d8	10.634

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

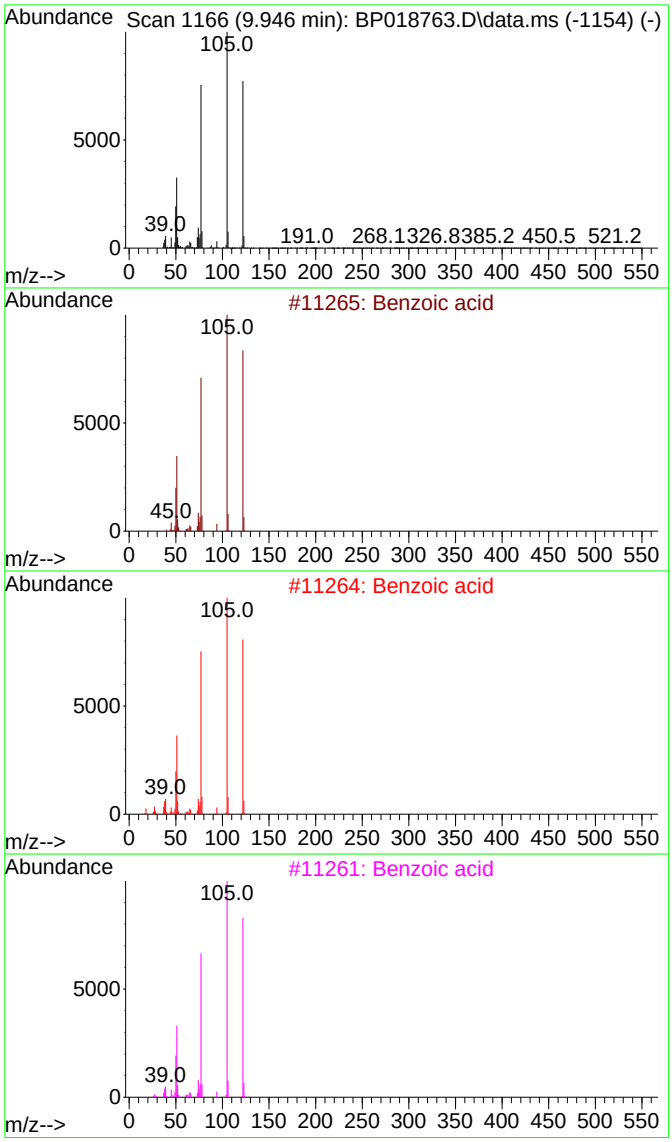
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

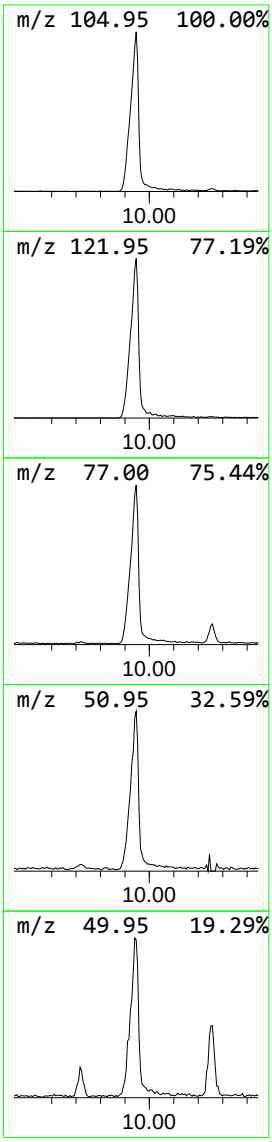
****

Peak Number 2 Benzoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.946	8.24 ng/ul	542699	Naphthalene-d8	10.634

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	94
3	Benzoic acid	122	C7H6O2	000065-85-0	94
4	Benzoic acid	122	C7H6O2	000065-85-0	93
5	Benzoic acid, silver(1+) salt	228	C7H5AgO2	000532-31-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

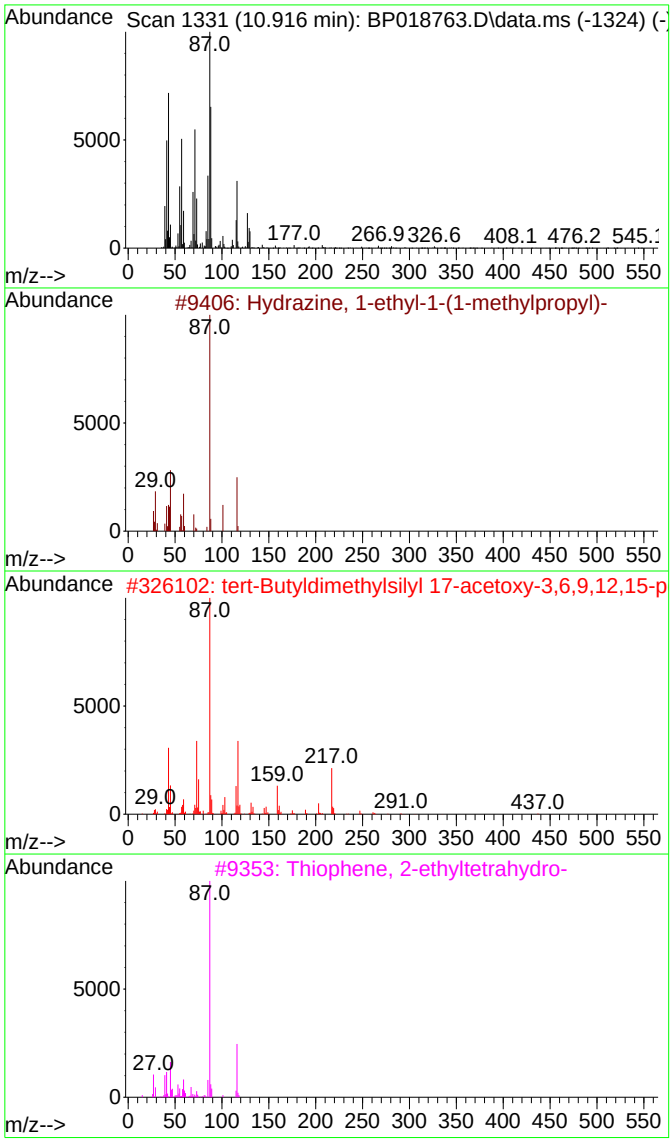
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

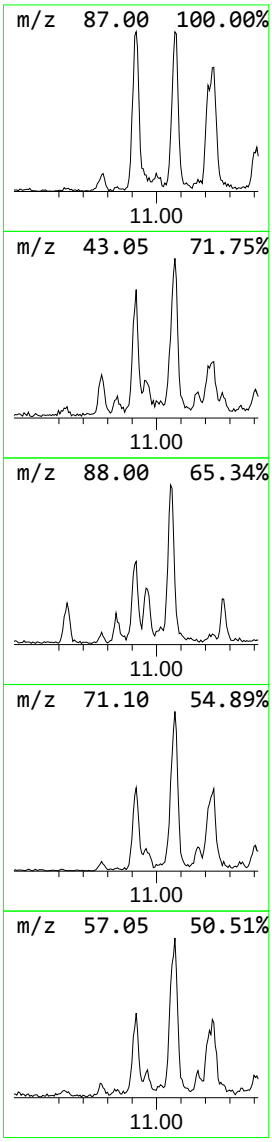
****

Peak Number 3 unknown-01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.916	2.03 ng/ul	133900	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	38
2	tert-Butyldimethylsilyl 17-aceto...	452	C20H40O9Si	1010366-90-4	35
3	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	35
4	Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	27
5	Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

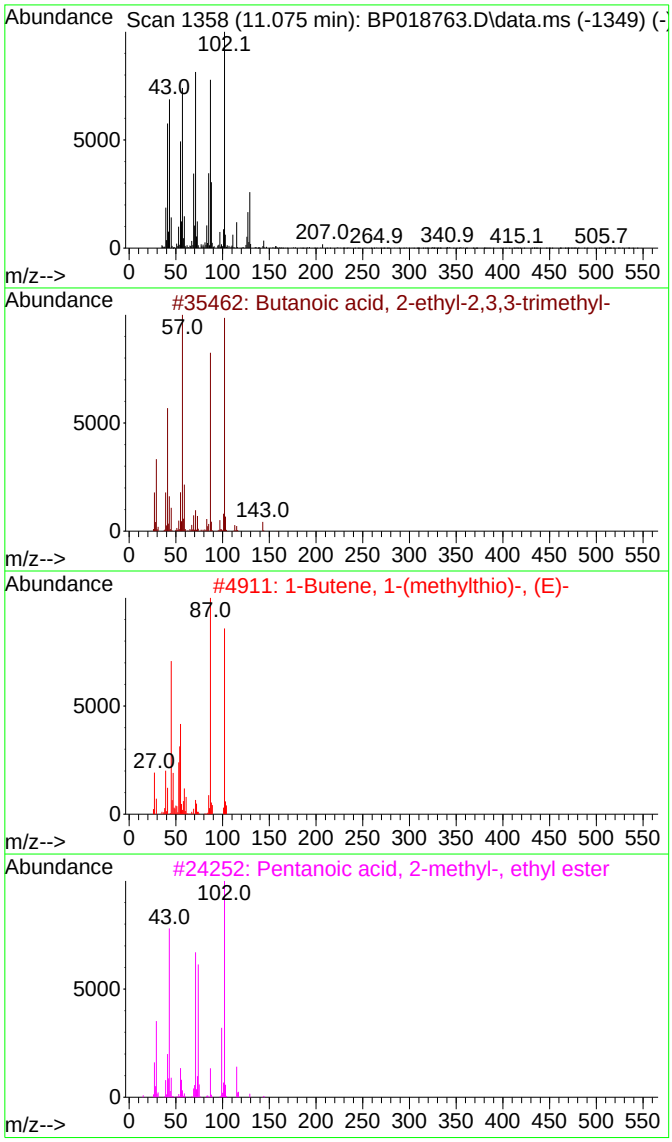
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

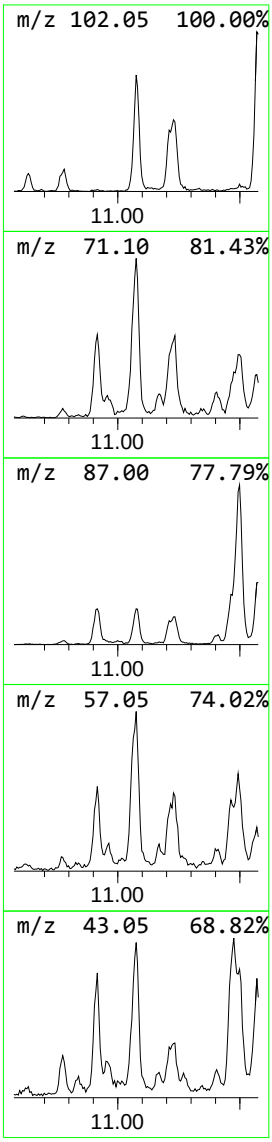
****

Peak Number 4 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.075	3.81 ng/ul	251026	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-2,3,3-tri...	158	C9H18O2	038541-67-2	43
2	1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	38
3	Pentanoic acid, 2-methyl-, ethyl...	144	C8H16O2	039255-32-8	38
4	Nonanoic acid, 4,6-dimethyl-, me...	200	C12H24O2	055955-66-3	35
5	3,4,6-Tri-O-methyl-d-glucose	222	C9H18O6	1000127-03-2	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

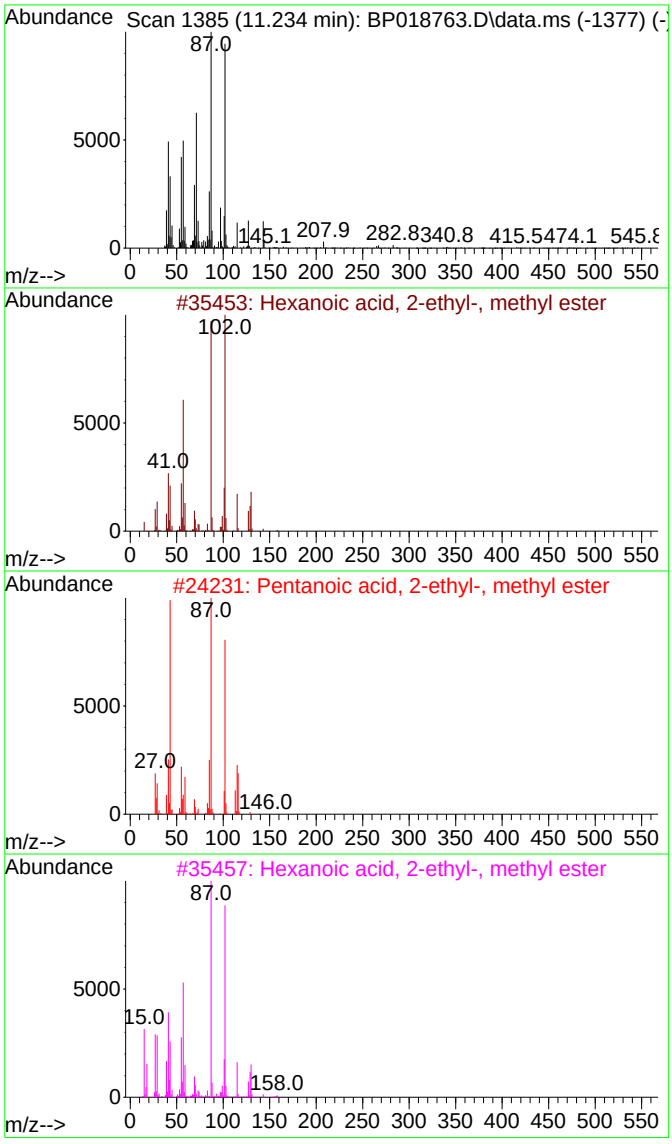
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

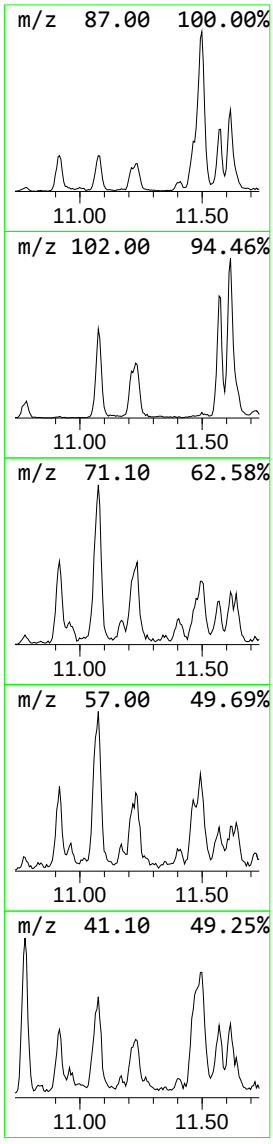
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexanoic acid, 2-ethyl-, me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.234	2.13 ng/ul	140477	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	50
2	Pentanoic acid, 2-ethyl-, methyl...	144	C8H16O2	000816-16-0	42
3	Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	40
4	1-Hepten-4-ol, 4-methyl-	128	C8H16O	001186-31-8	27
5	3-Methylundecanoic acid	200	C12H24O2	065781-38-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

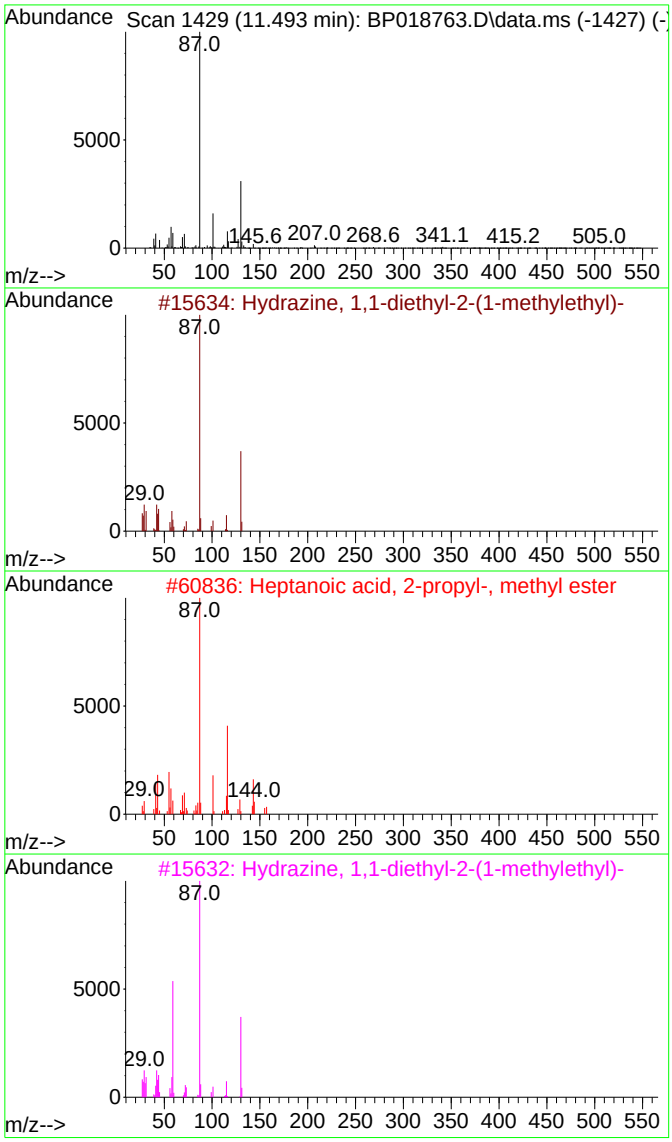
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

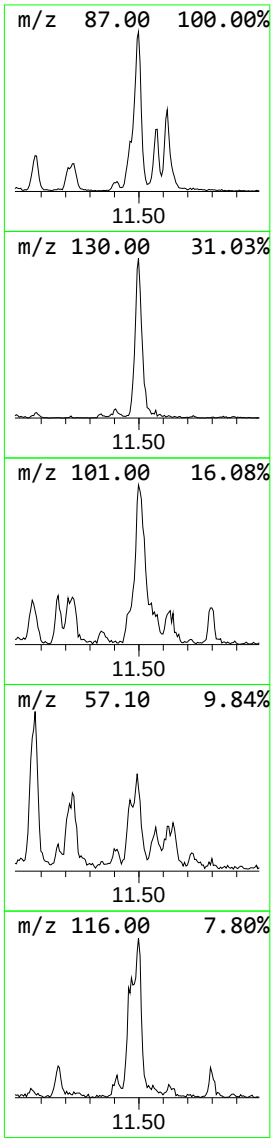
****

Peak Number 6 unknown-03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.493	3.12 ng/ul	205398	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	45
2	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	38
3	Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	9
4	4-Heptanol, 4-methyl-	130	C8H18O	000598-01-6	9
5	1,3-Dioxane, 2-pentadecyl-	298	C19H38O2	017352-27-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

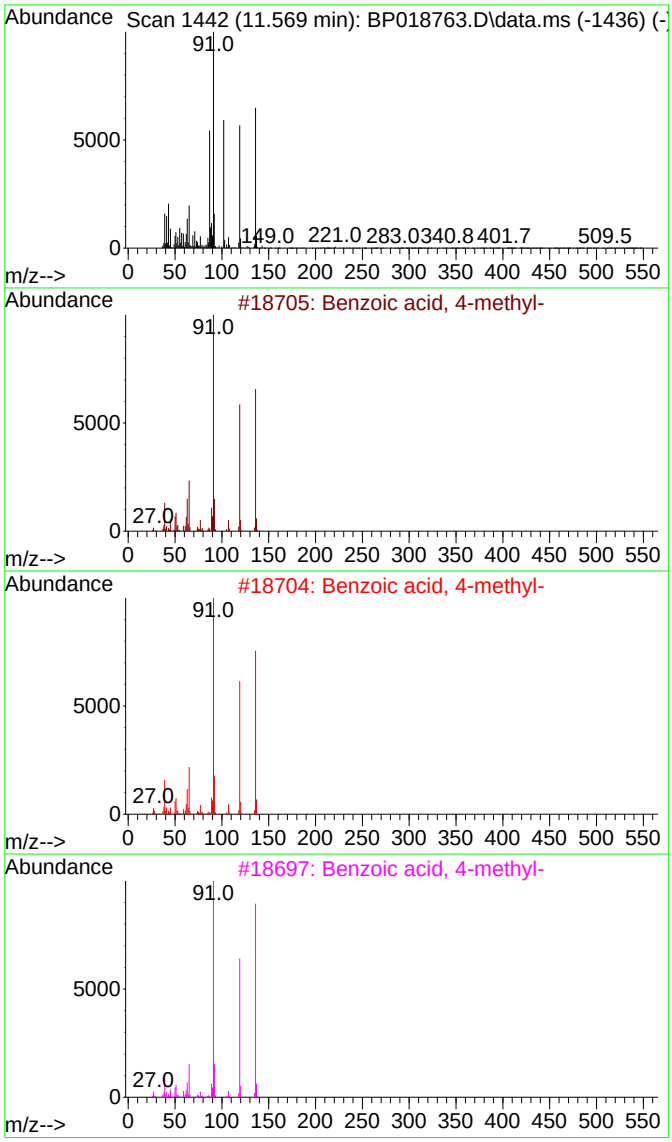
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

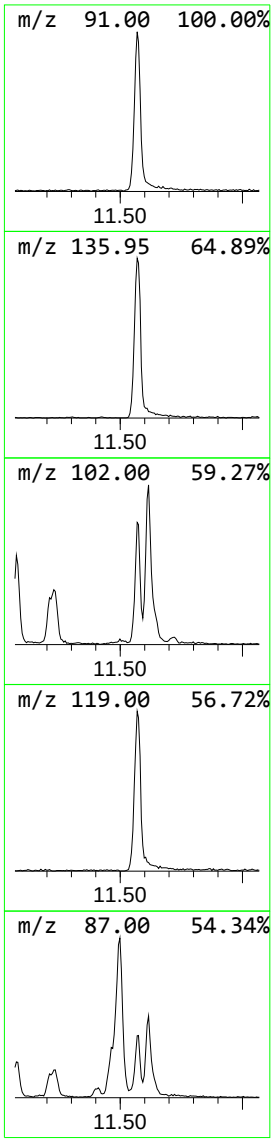
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzoic acid, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.569	4.46 ng/ul	294024	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	95
2	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	95
3	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	91
4	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	90
5	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	90





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Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

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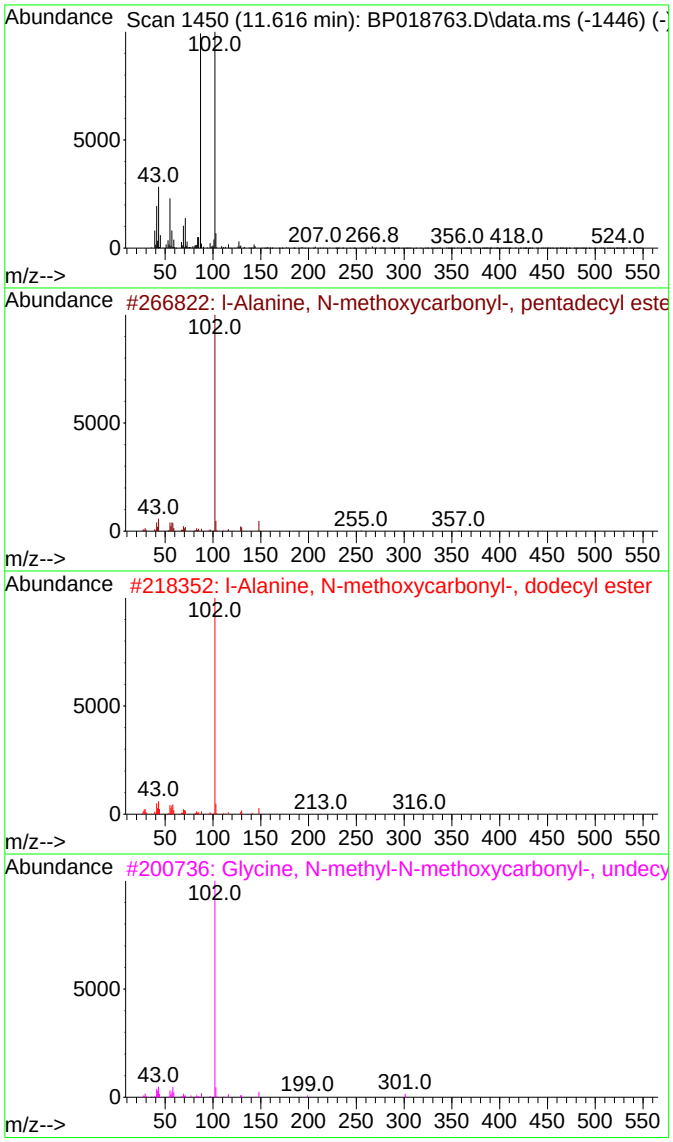
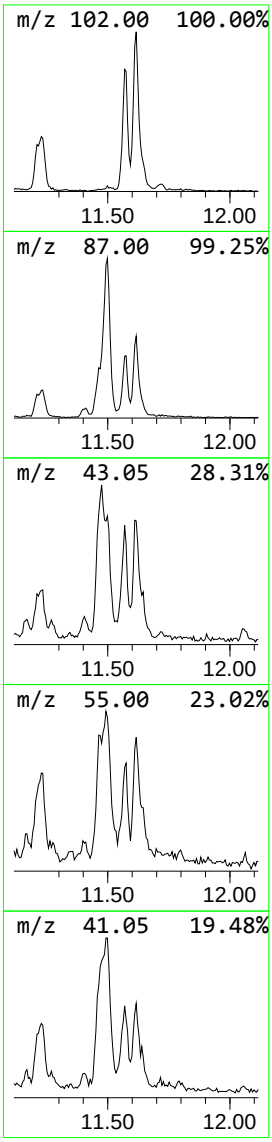
Peak Number 8 unknown-04 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	2.92 ng/ul	192641	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	l-Alanine, N-methoxycarbonyl-, p...	357	C20H39NO4	1000313-38-3	35
2	l-Alanine, N-methoxycarbonyl-, d...	315	C17H33NO4	1000313-38-0	35
3	Glycine, N-methyl-N-methoxycarbo...	301	C16H31NO4	1000320-61-2	35
4	Methyl 2-ethyldecanoate	214	C13H26O2	020483-47-0	33
5	.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

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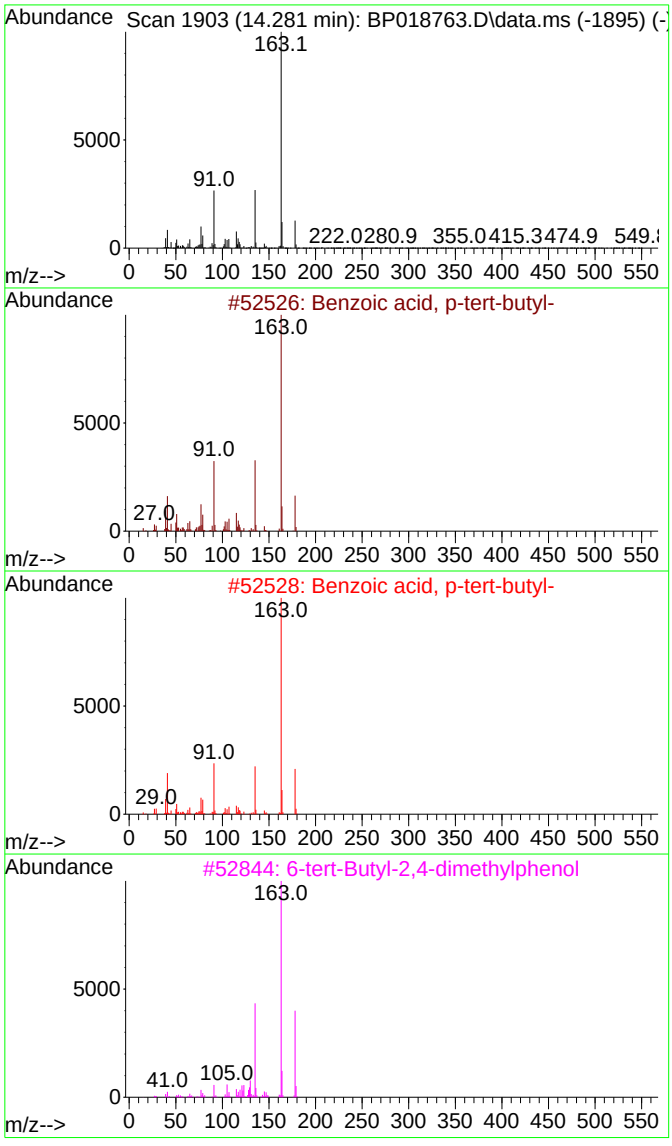
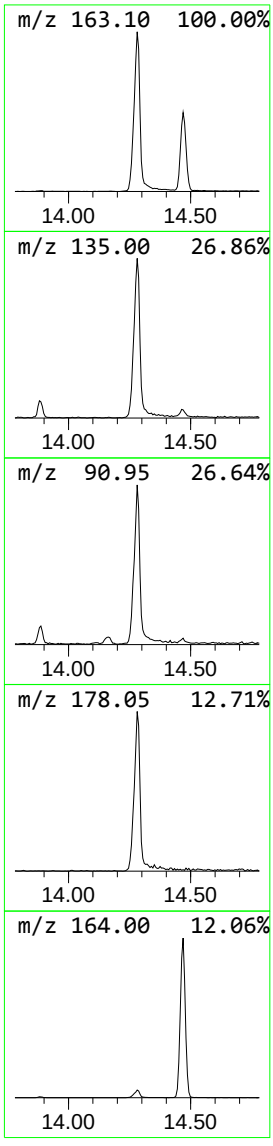
Peak Number 9 Benzoic acid, p-tert-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.281	6.85 ng/ul	623971	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
3	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	74
4	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
5	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

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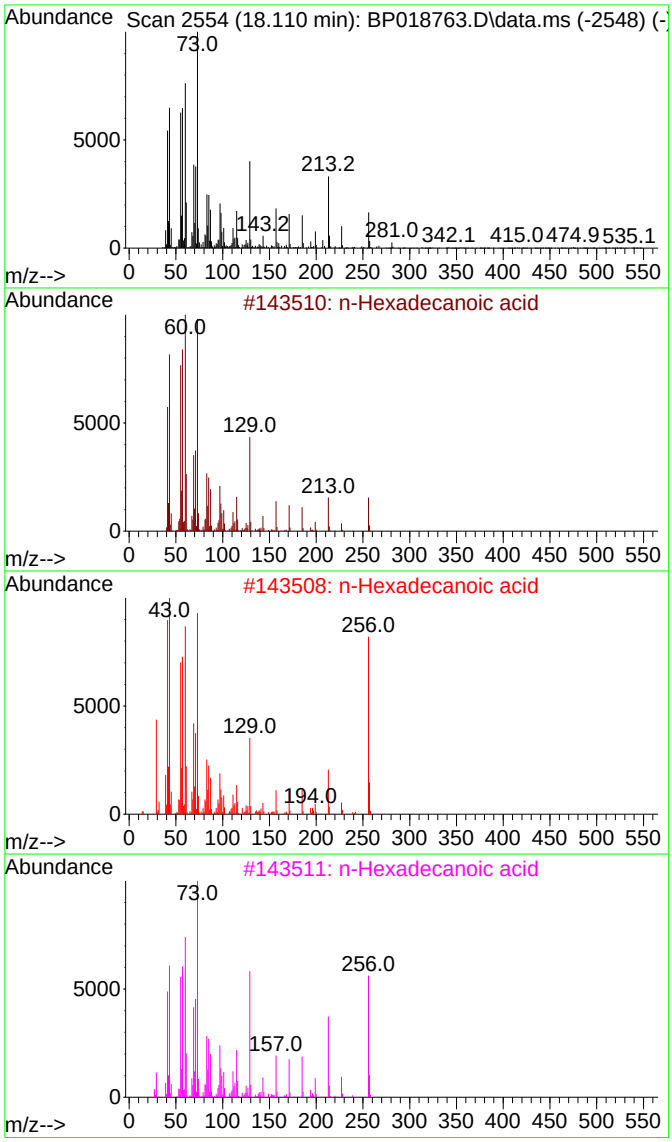
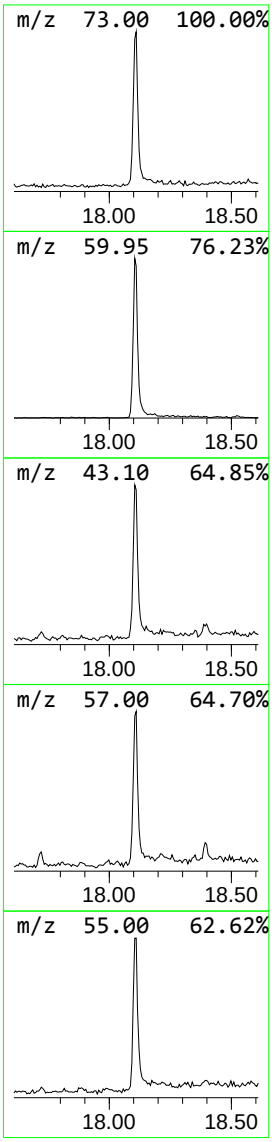
Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.110	2.83 ng/ul	334572	Phenanthrene-d10	17.216

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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018763.D
Acq On : 12 Dec 2023 12:21
Operator : MA/JU
Sample : 05675-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
H0AB6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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
Hexanoic acid, ...	9.310	145.8	ng/ul	9607410	2	10.634	1317820	20.0
Benzoic acid	9.946	8.2	ng/ul	542699	2	10.634	1317820	20.0
unknown-01	10.916	2.0	ng/ul	133900	2	10.634	1317820	20.0
unknown-02	11.075	3.8	ng/ul	251026	2	10.634	1317820	20.0
Hexanoic acid, ...	11.234	2.1	ng/ul	140477	2	10.634	1317820	20.0
unknown-03	11.493	3.1	ng/ul	205398	2	10.634	1317820	20.0
Benzoic acid, 4...	11.569	4.5	ng/ul	294024	2	10.634	1317820	20.0
unknown-04	11.616	2.9	ng/ul	192641	2	10.634	1317820	20.0
Benzoic acid, p...	14.281	6.8	ng/ul	623971	3	14.469	1820930	20.0
n-Hexadecanoic ...	18.110	2.8	ng/ul	334572	4	17.216	2364330	20.0