LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

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-BP010824.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP019347.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.217	19	22	29	rVB	26699	32691	0.61%	0.067%
2	3.640	90	94	106	rBV	169003	279052	5.18%	0.571%
3	3.958	144	148	152	rVB3	11243	15713	0.29%	0.032%
4	6.810	628	633	640	rBV2	13259	25750	0.48%	0.053%
5	6.969	653	660	670	rVB	145489	241831	4.49%	0.495%
6	7.122	678	686	698	rBV	487814	768036	14.25%	1.571%
7	7.310	711	718	729	rBV	471995	763920	14.17%	1.563%
8	7.405	729	734	740	rBV	21079	36226	0.67%	0.074%
9	7.775	790	797	808	rBV	457199	733171	13.60%	1.500%
10	8.399	898	903	913	rVB5	8047	17449	0.32%	0.036%
11	8.504	913	921	935	rBV	420965	688383	12.77%	1.408%
12	8.946	988	996	1008	rBV	639435	1029666	19.10%	2.107%
13	9.193	1014	1038	1050	rBV	744843	3014130	55.91%	6.167%
14	9.293	1052	1055	1059	rVV5	9855	17064	0.32%	0.035%
15	9.340	1060	1063	1067	rVB6	5859	8746	0.16%	0.018%
16	9.434	1075	1079	1085	rVB7	7059	11511	0.21%	0.024%
17	9.663	1110	1118	1131	rBV	534728	878418	16.29%	1.797%
18	9.887	1144	1156	1160	rBV	124239	273997	5.08%	0.561%
19	9.934	1160	1164	1178	rVB	45826	90531	1.68%	0.185%
20	10.204	1200	1210	1226	rBV	754935	1300823	24.13%	2.661%
21	10.569	1265	1272	1280	rBV	628468	1051710	19.51%	2.152%
22	10.722	1290	1298	1314	rBV	662363	1203265	22.32%	2.462%
23	10.863	1316	1322	1326	rVV	53436	95222	1.77%	0.195%
24	10.910	1326	1330	1335	rVB	19894	31783	0.59%	0.065%
25	11.016	1340	1348	1359	rVB4	71281	171715	3.19%	0.351%
26	11.116	1360	1365	1368	rBV5	8750	14735	0.27%	0.030%
27	11.175	1368	1375	1379	rBV4	31043	70622	1.31%	0.144%
28	11.351	1398	1405	1409	rBV4	17356	31278	0.58%	0.064%
29	11.410	1409	1415	1418	rBV	106765	196490	3.64%	0.402%
30	11.440	1418	1420	1427	rVB3	89010	130797	2.43%	0.268%
31	11.528	1427	1435	1438	rBV3	76007	175269	3.25%	0.359%
32	11.557	1438	1440	1444	rVB	33943	42214	0.78%	0.086%
33	11.663	1455	1458	1468	rVB9	6034	12392	0.23%	0.025%
34	11.745	1468	1472	1478	rBV2	12334	18094	0.34%	0.037%
35	12.163	1538	1543	1549	rBV3	15299	27931	0.52%	0.057%
36	12.322	1566	1570	1576	rBV7	6564	10511	0.19%	0.022%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

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-BP010824.MA.M
Title : SVOA CALIBRATION

37	13.022	1685	1689	1697	rVB10	2664	5955	0.11%	0.012%
38	13.240	1721	1726	1732	rBV9	3643	6137	0.11%	0.013%
39	13.322	1732	1740	1745	rBV2	17823	29657	0.55%	0.061%
40	13.839	1821	1828	1842	rBV	1631936	2295737	42.58%	4.697%
41	14.116	1866	1875	1883	rBV	1741257	2520597	46.75%	5.157%
42	14.251	1889	1898	1913	rBV	360678	607154	11.26%	1.242%
43	14.422	1920	1927	1936	rVB	1147021	1654993	30.70%	3.386%
44	14.669	1963	1969	1978	rBV	137430	272454	5.05%	0.557%
45	14.739	1978	1981	1992	rVV4	20163	43522	0.81%	0.089%
46	14.851	1996	2000	2009	rVB10	9235	22219	0.41%	0.045%
47	15.169	2049	2054	2061	rBV	27861	63557	1.18%	0.130%
48	15.257	2066	2069	2078	rVB5	8353	17028	0.32%	0.035%
49	15.416	2086	2096	2109	rBV	2322733	3391697	62.91%	6.939%
50	15.557	2113	2120	2131	rBV	969773	1319597	24.48%	2.700%
51	15.663	2133	2138	2143	rVB3	12382	19671	0.36%	0.040%
52	15.933	2177	2184	2189	rBV5	19353	29764	0.55%	0.061%
53	15.998	2189	2195	2199	rVV8	3358	5517	0.10%	0.011%
54	16.133	2216	2218	2225	rVB8	4483	7687	0.14%	0.016%
55	16.204	2227	2230	2234	rVB3	10617	13186	0.24%	0.027%
56	16.592	2289	2296	2299	rBV7	6955	10714	0.20%	0.022%
57	16.775	2322	2327	2333	rBV	54369	75435	1.40%	0.154%
58	16.851	2337	2340	2345	rVV6	4920	6449	0.12%	0.013%
59	16.969	2357	2360	2365	rVB6	4388	7867	0.15%	0.016%
60	17.180	2389	2396	2405	rBV	1584695	2183689	40.50%	4.468%
61	17.280	2406	2413	2424	rVV	3032452	4129710	76.60%	8.449%
62	17.357	2424	2426	2433	rVB8	4108	6693	0.12%	0.014%
63	17.469	2442	2445	2450	rVB3	3957	7057	0.13%	0.014%
64	17.575	2460	2463	2471	rVB10	4802	9732	0.18%	0.020%
65	17.675	2476	2480	2484	rBV7	2879	5519	0.10%	0.011%
66	17.780	2495	2498	2503	rVB	7594	10914	0.20%	0.022%
67	17.851	2506	2510	2515	rVB7	13253	17963	0.33%	0.037%
68	18.075	2542	2548	2557	rBV	180932	264530	4.91%	0.541%
69	18.145	2557	2560	2563	rVB2	9728	13729	0.25%	0.028%
70	19.098	2718	2722	2728	rBV2	44566	60098	1.11%	0.123%
71	19.174	2730	2735	2738	rBV	44589	67083	1.24%	0.137%
72	19.310	2754	2758	2767	rBV	106033	152466	2.83%	0.312%
73	19.451	2780	2782	2788	rVB7	12775	14606	0.27%	0.030%
74	19.527	2789	2795	2801	rBV	3999859	5387042	99.92%	11.022%
75	19.704	2821	2825	2830	rBV5	26982	40114	0.74%	0.082%
76	20.992	3041	3044	3053	rBV3	76713	117654	2.18%	0.241%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

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-BP010824.MA.M
Title : SVOA CALIBRATION

77	21.286	3088	3094	3100	rBV	2026760	2588743	48.02%	5.297%
78	23.486	3461	3468	3481	rVB2	2755059	5391323	100.00%	11.031%
79	23.639	3487	3494	3502	rVB	1302840	2469508	45.81%	5.053%

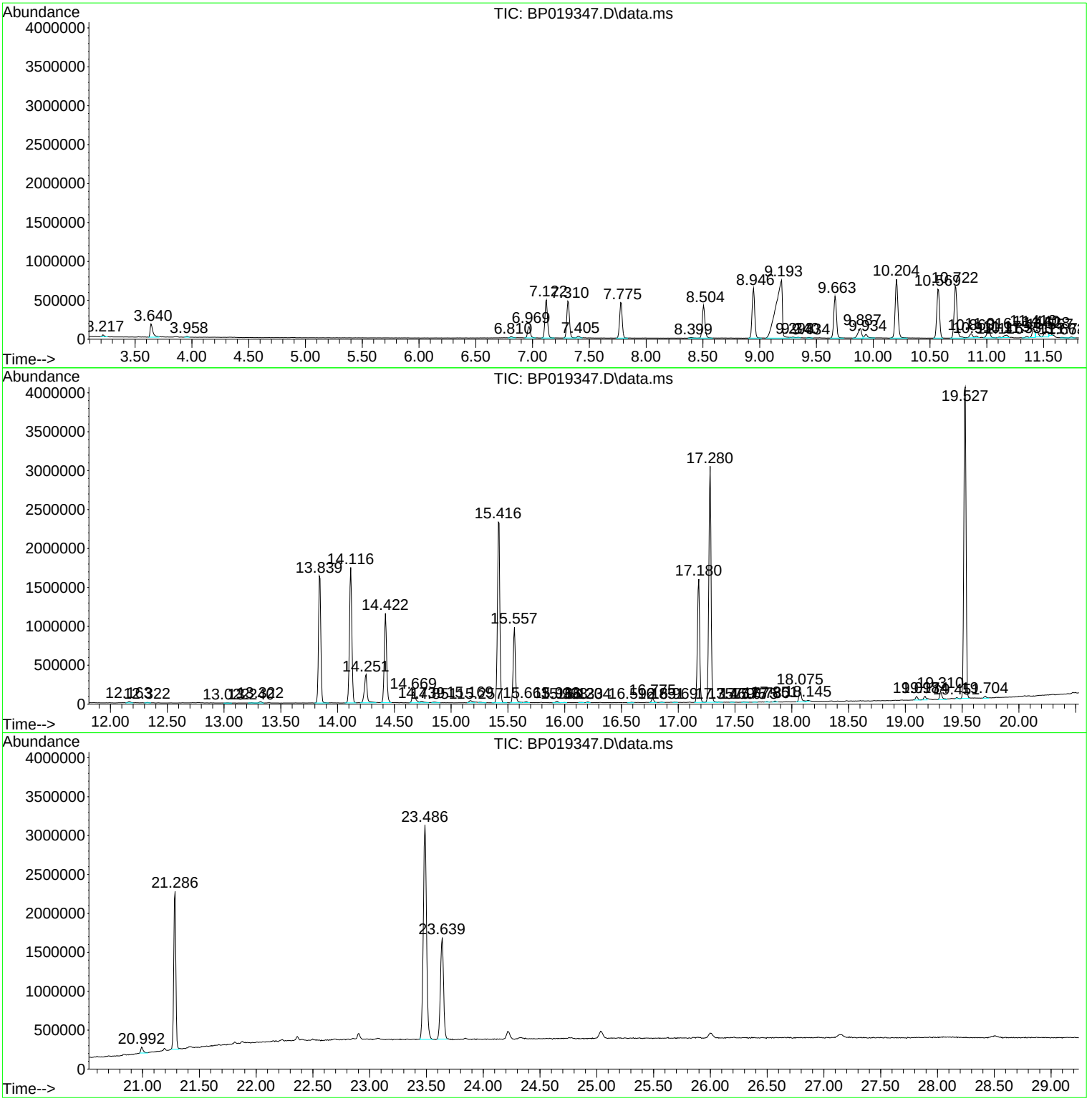
Sum of corrected areas: 48875903

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.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\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

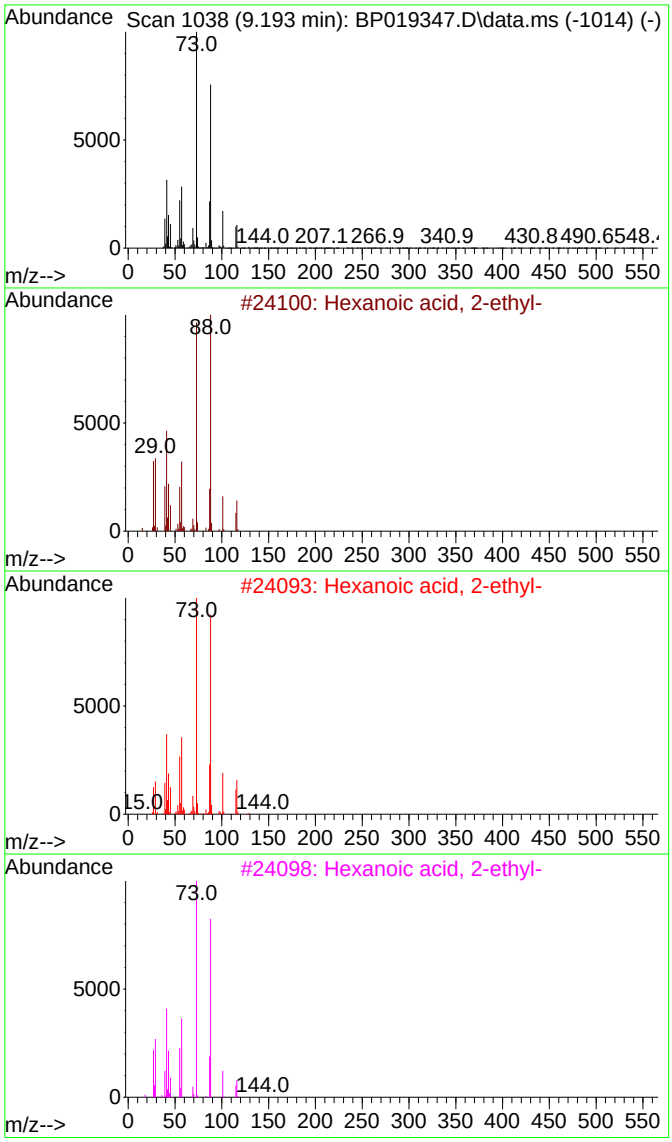
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

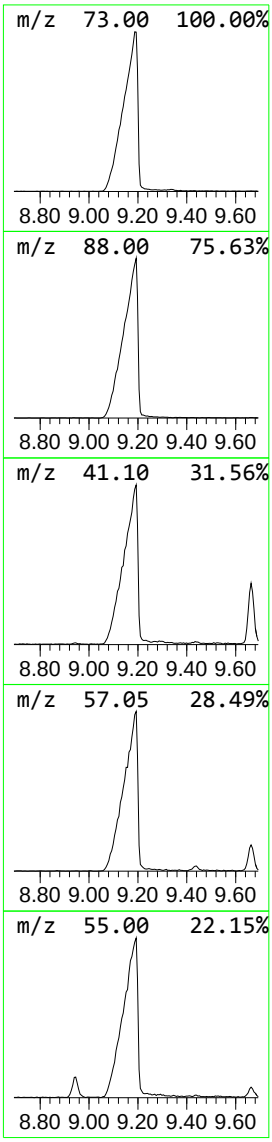
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.193	57.32 ng/ul	3014130	Naphthalene-d8	10.569

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	80
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	59
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

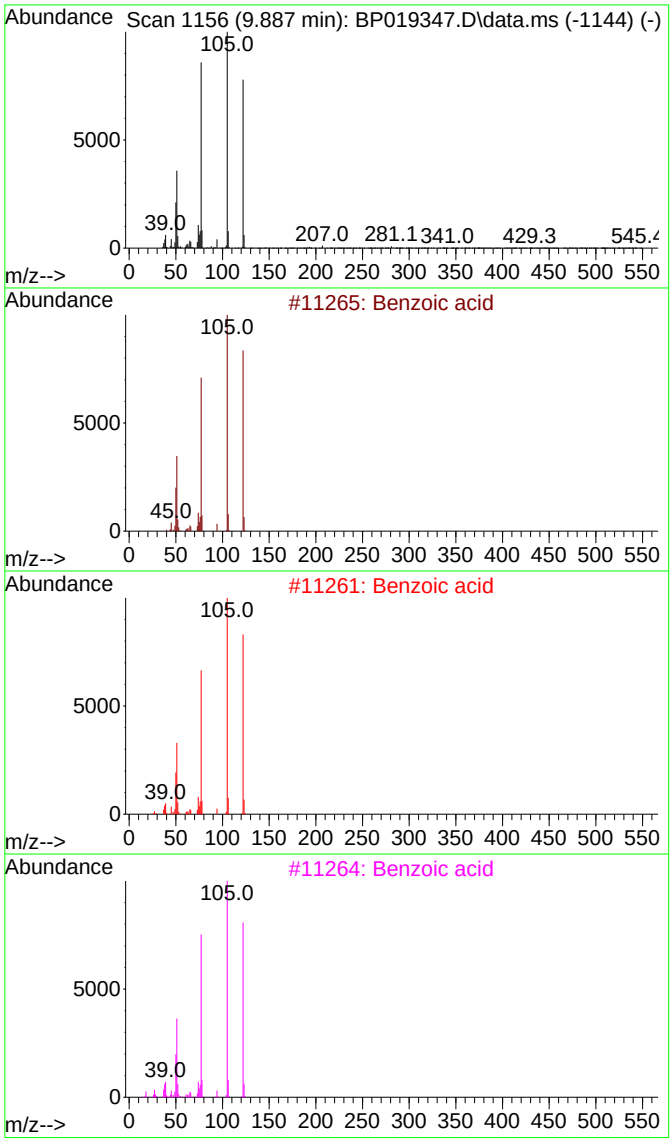
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

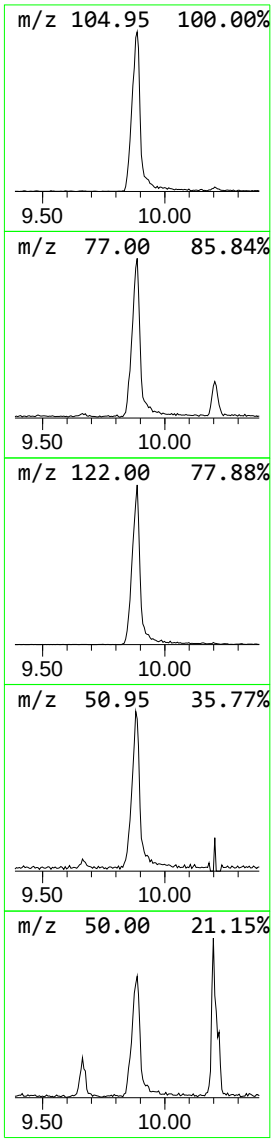
****

Peak Number 2 Benzoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.887	5.21 ng/ul	273997	Naphthalene-d8	10.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid	122	C7H6O2	000065-85-0	96
2	Benzoic acid	122	C7H6O2	000065-85-0	94
3	Benzoic acid	122	C7H6O2	000065-85-0	94
4	Benzoic acid, silver(1+) salt	228	C7H5AgO2	000532-31-0	90
5	Benzoic acid	122	C7H6O2	000065-85-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

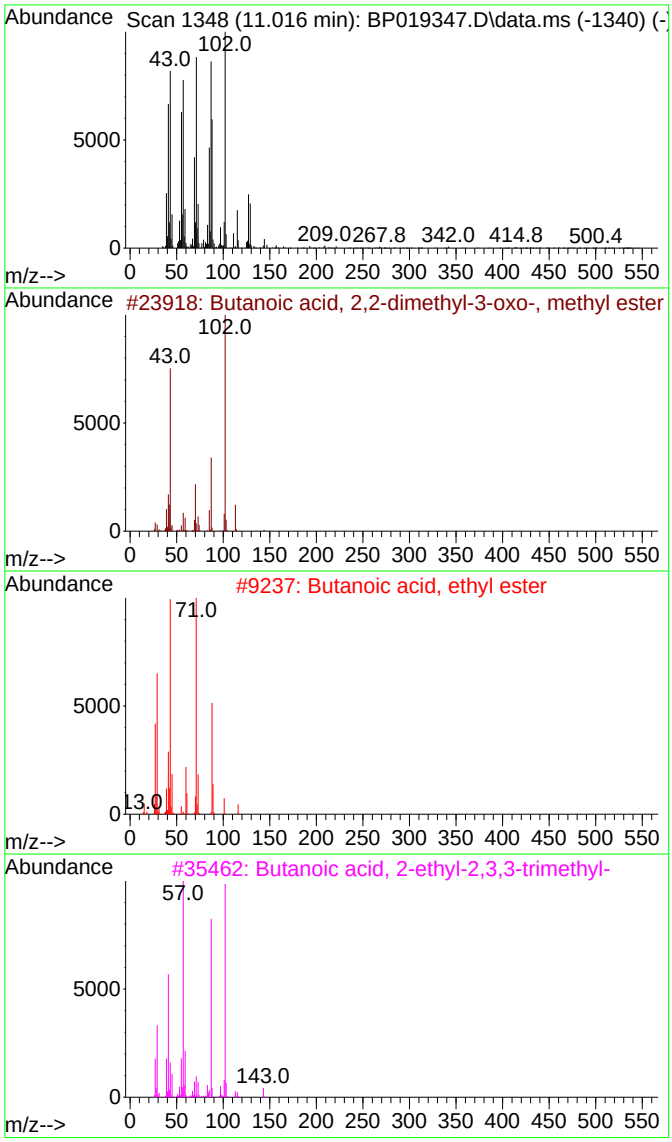
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

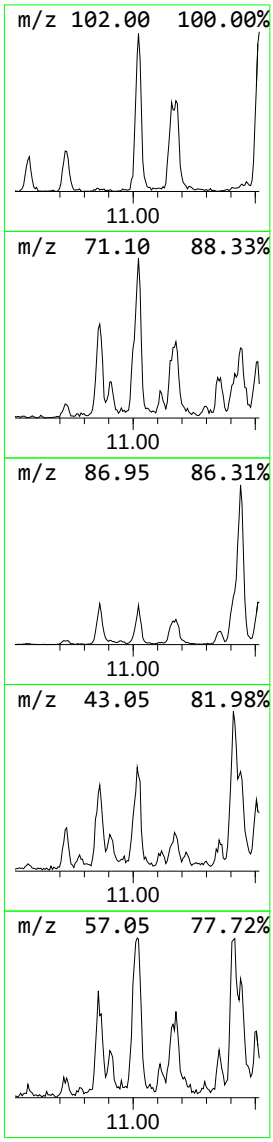
****

Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.016	3.27 ng/ul	171715	Naphthalene-d8	10.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2,2-dimethyl-3-ox...	144	C7H12O3	038923-57-8	43
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	38
3	Butanoic acid, 2-ethyl-2,3,3-tri...	158	C9H18O2	038541-67-2	38
4	Pentanoic acid, 2-methyl-, ethyl...	144	C8H16O2	039255-32-8	35
5	Heptanoic acid, 2-ethyl-, methyl...	172	C10H20O2	000816-63-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

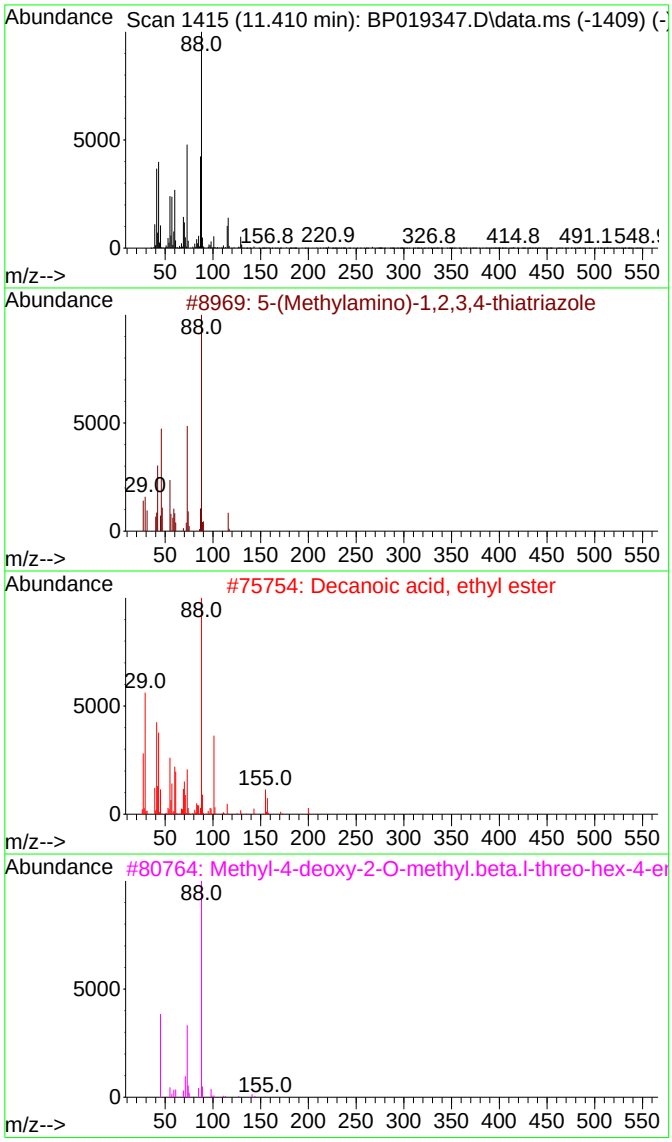
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

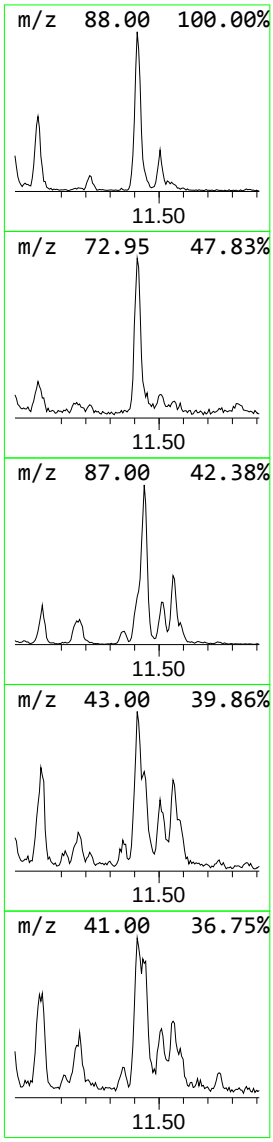
****

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.410	3.74 ng/ul	196490	Naphthalene-d8	10.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(Methylamino)-1,2,3,4-thiatria...	116	C2H4N4S	052098-72-3	47
2	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	38
3	Methyl-4-deoxy-2-O-methyl.beta.l...	204	C8H12O6	1000312-10-0	38
4	Methyl(methyl-4-deoxy-2-O-methyl...	218	C9H14O6	052545-23-0	37
5	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

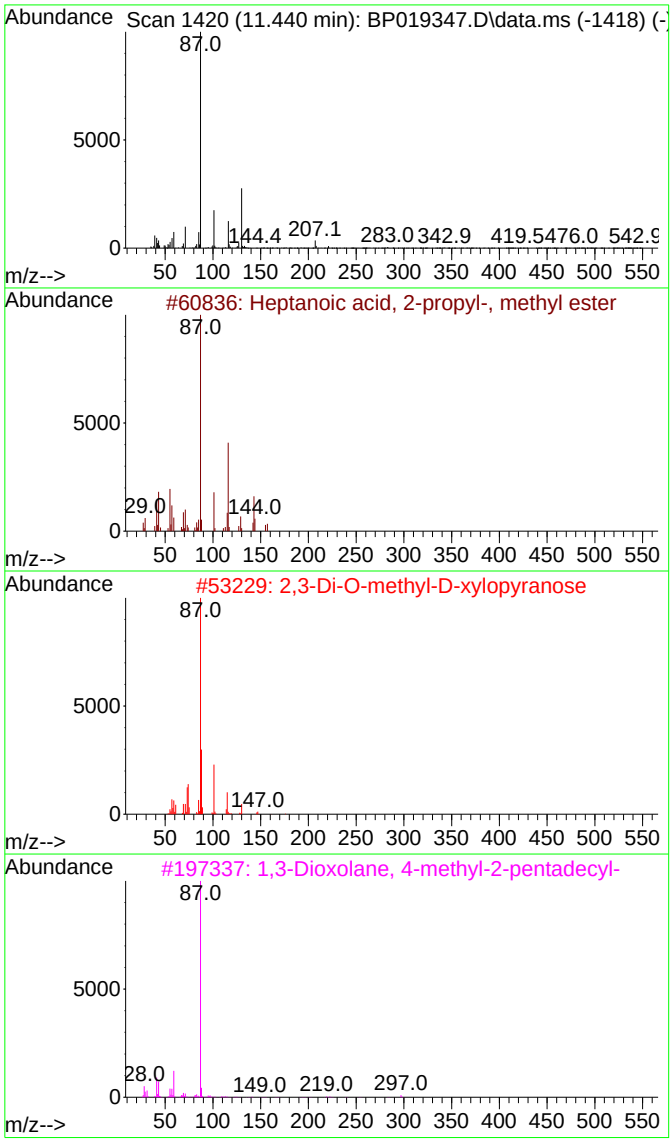
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

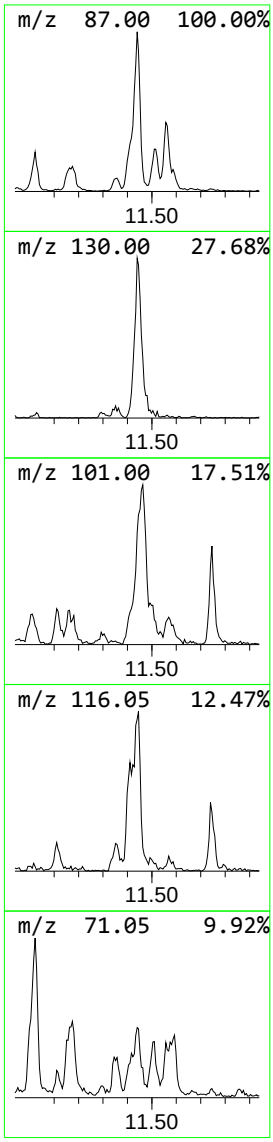
****

Peak Number 5 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.440	2.49 ng/ul	130797	Naphthalene-d8	10.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	45
2	2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	42
3	1,3-Dioxolane, 4-methyl-2-pentad...	298	C19H38O2	054950-56-0	37
4	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	33
5	2-[(2-Cyano-3,3-di-methylcyclopr...	195	C11H17NO2	129549-91-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

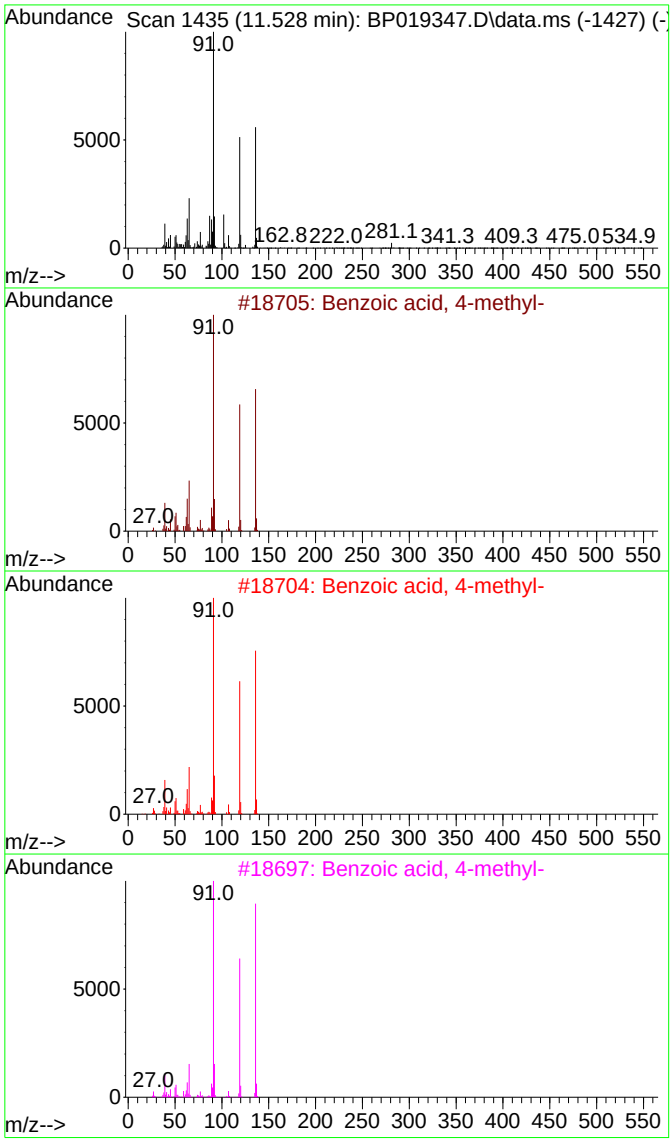
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

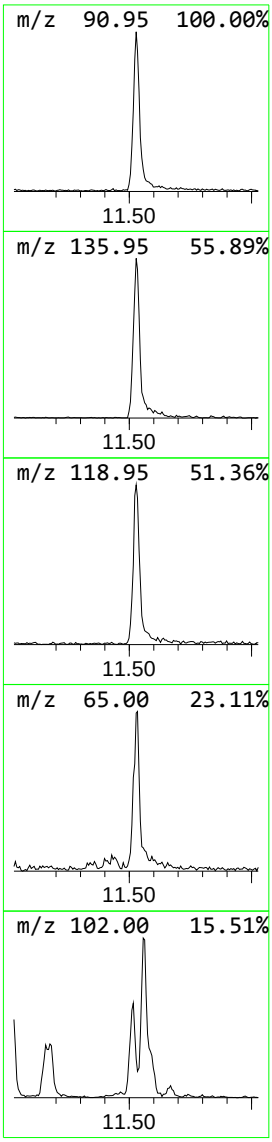
****

Peak Number 6 Benzoic acid, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.528	3.33 ng/ul	175269	Naphthalene-d8	10.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
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	87
5	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	87





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Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

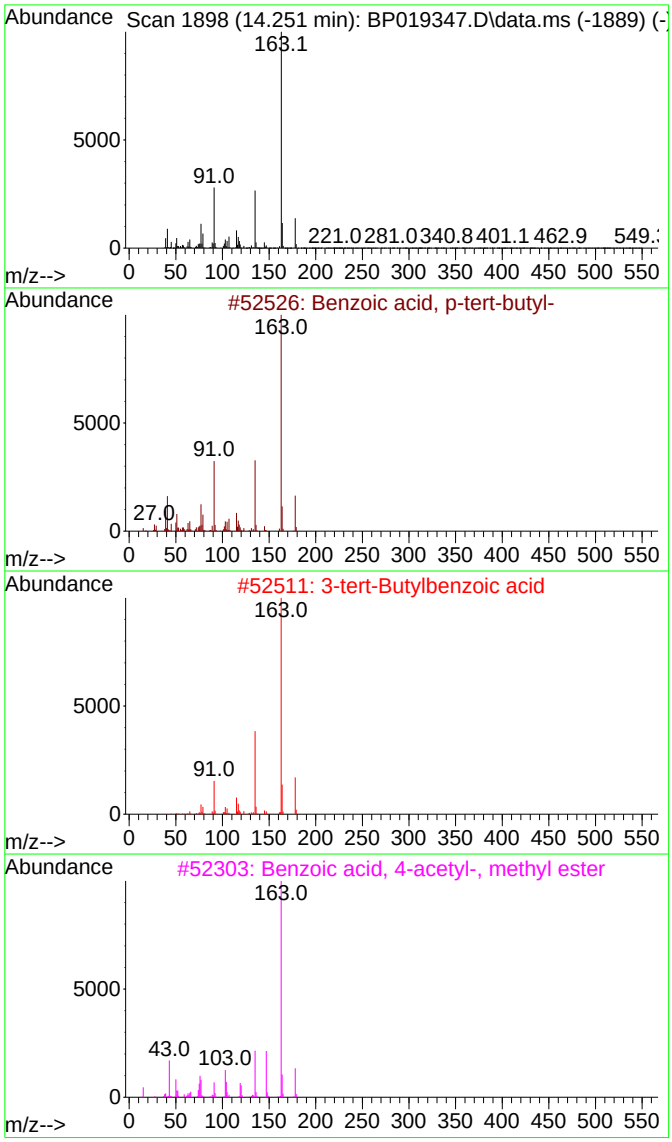
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

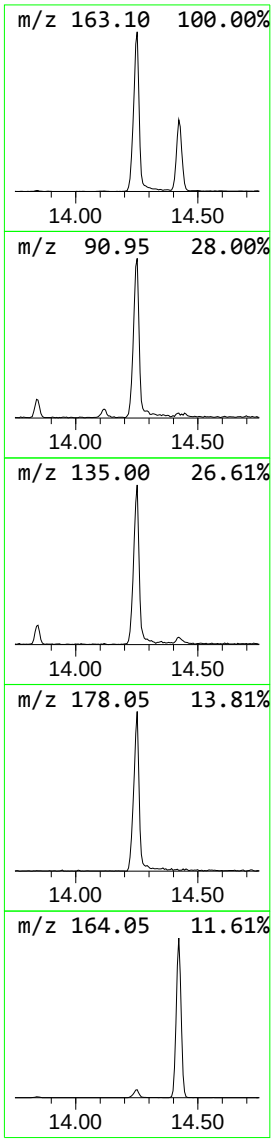
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzoic acid, p-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	7.34 ng/ul	607154	Acenaphthene-d10	14.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	93
3	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
4	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
5	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

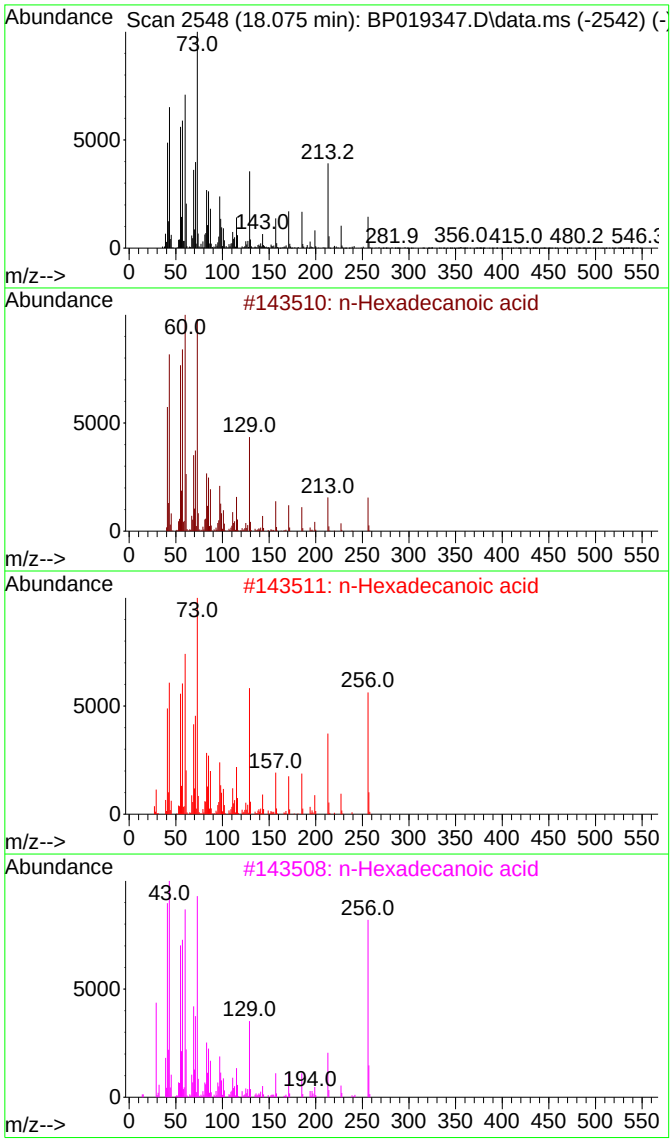
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.MA.M
Quant Title : SVOA CALIBRATION

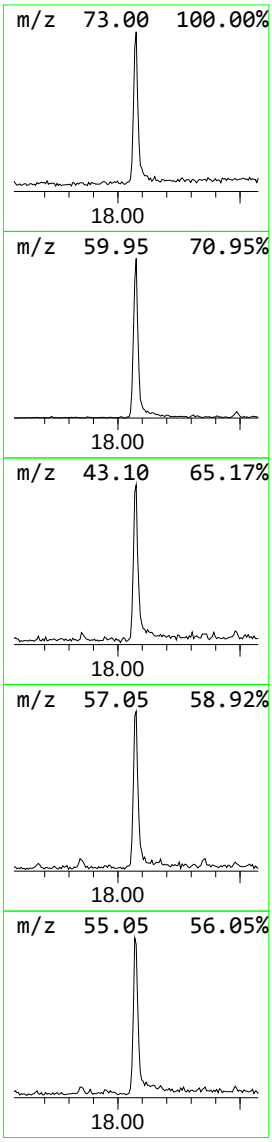
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.075	2.42 ng/ul	264530	Phenanthrene-d10	17.180

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
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	97
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011224\
Data File : BP019347.D
Acq On : 13 Jan 2024 00:55
Operator : MA/JU
Sample : P1091-16
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP010824.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, ...	9.193	57.3	ng/ul	3014130	2	10.569	1051710	20.0
Benzoic acid	9.887	5.2	ng/ul	273997	2	10.569	1051710	20.0
unknown-01	11.016	3.3	ng/ul	171715	2	10.569	1051710	20.0
unknown-02	11.410	3.7	ng/ul	196490	2	10.569	1051710	20.0
unknown-03	11.440	2.5	ng/ul	130797	2	10.569	1051710	20.0
Benzoic acid, 4...	11.528	3.3	ng/ul	175269	2	10.569	1051710	20.0
Benzoic acid, p...	14.251	7.3	ng/ul	607154	3	14.422	1654990	20.0
n-Hexadecanoic ...	18.075	2.4	ng/ul	264530	4	17.180	2183690	20.0