LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019031.D
Acq On : 22 Dec 2023 09:45
Operator : MA/JU
Sample : 05808-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B08

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: BP019031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	24	28	35	rVB	39502	49469	0.85%	0.092%
2	3.528	72	75	89	rVB	139887	199282	3.41%	0.372%
3	3.675	96	100	119	rVB	159157	248886	4.25%	0.465%
4	3.993	150	154	160	rVB	18434	25362	0.43%	0.047%
5	4.922	307	312	316	rVB4	4696	8193	0.14%	0.015%
6	5.905	475	479	486	rVB3	6423	10533	0.18%	0.020%
7	6.999	654	665	673	rBV	641665	1064462	18.19%	1.989%
8	7.158	685	692	701	rVB	521711	797585	13.63%	1.491%
9	7.352	718	725	733	rBV	641998	1011133	17.28%	1.890%
10	7.434	734	739	750	rVB	26150	51030	0.87%	0.095%
11	7.816	796	804	812	rBV	521798	811935	13.88%	1.517%
12	7.899	812	818	826	rVB3	12573	25416	0.43%	0.048%
13	8.534	917	926	937	rBV	851693	1395237	23.84%	2.608%
14	8.981	993	1002	1011	rBV	626880	1010827	17.27%	1.889%
15	9.105	1018	1023	1028	rBV9	3257	6792	0.12%	0.013%
16	9.387	1066	1071	1078	rVB6	5670	7777	0.13%	0.015%
17	9.552	1091	1099	1108	rBV2	50789	78680	1.34%	0.147%
18	9.699	1116	1124	1137	rBV	522782	874847	14.95%	1.635%
19	10.240	1206	1216	1231	rBV	876768	1493876	25.53%	2.792%
20	10.610	1271	1279	1287	rBV	670644	1142006	19.52%	2.134%
21	10.757	1296	1304	1316	rBV	805694	1363069	23.29%	2.547%
22	11.163	1367	1373	1376	rBV5	16570	30485	0.52%	0.057%
23	11.193	1376	1378	1383	rVV2	18187	26087	0.45%	0.049%
24	11.252	1383	1388	1394	rVB4	19944	31921	0.55%	0.060%
25	11.363	1401	1407	1419	rBV	75418	155714	2.66%	0.291%
26	11.928	1500	1503	1509	rVB7	4259	7050	0.12%	0.013%
27	12.034	1515	1521	1527	rBV5	5873	9829	0.17%	0.018%
28	12.199	1545	1549	1558	rVB2	15817	27893	0.48%	0.052%
29	12.940	1670	1675	1680	rBV9	5947	8149	0.14%	0.015%
30	13.081	1694	1699	1700	rBV5	5869	6766	0.12%	0.013%
31	13.128	1704	1707	1711	rVB6	5422	7003	0.12%	0.013%
32	13.281	1728	1733	1737	rBV3	9893	14676	0.25%	0.027%
33	13.357	1740	1746	1750	rBV	22293	35591	0.61%	0.067%
34	13.428	1753	1758	1764	rVB9	3665	8535	0.15%	0.016%
35	13.675	1796	1800	1807	rVB	13308	19201	0.33%	0.036%
36	13.869	1825	1833	1848	rBV	1671128	2318084	39.61%	4.332%

LSC Area Percent Report

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Operator : MA/JU
Sample : 05808-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0B08

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	14.145	1869	1880	1891	rBV	1943539	2820986	48.21%	5.272%
38	14.451	1924	1932	1940	rBV	1113237	1615602	27.61%	3.019%
39	14.563	1946	1951	1958	rVB10	3980	8811	0.15%	0.016%
40	14.675	1958	1970	1989	rBV2	1780263	3996377	68.30%	7.469%
41	14.875	2000	2004	2016	rVB4	39218	62686	1.07%	0.117%
42	15.445	2094	2101	2114	rBV	2564610	3633532	62.09%	6.791%
43	15.575	2116	2123	2134	rBV	725331	1024943	17.52%	1.916%
44	15.687	2139	2142	2147	rVB2	10327	15193	0.26%	0.028%
45	16.010	2189	2197	2205	rBV9	16851	35145	0.60%	0.066%
46	16.234	2231	2235	2239	rVB4	11238	16747	0.29%	0.031%
47	16.522	2279	2284	2285	rBV5	4512	5904	0.10%	0.011%
48	16.610	2294	2299	2305	rBV3	27585	36589	0.63%	0.068%
49	16.887	2341	2346	2349	rBV7	4157	6164	0.11%	0.012%
50	16.969	2355	2360	2361	rBV5	6138	7884	0.13%	0.015%
51	17.204	2391	2400	2409	rBV	1467296	2054661	35.11%	3.840%
52	17.304	2410	2417	2427	rBV	2896200	4057285	69.34%	7.583%
53	17.381	2427	2430	2432	rBV4	9477	9326	0.16%	0.017%
54	17.492	2447	2449	2455	rVB4	6096	8608	0.15%	0.016%
55	17.604	2463	2468	2473	rBV8	7933	11643	0.20%	0.022%
56	17.704	2483	2485	2489	rBV5	6231	6084	0.10%	0.011%
57	17.881	2510	2515	2523	rVB	86270	99865	1.71%	0.187%
58	17.975	2528	2531	2537	rVB8	8248	14482	0.25%	0.027%
59	18.104	2547	2553	2569	rBV	946643	1446983	24.73%	2.704%
60	18.739	2659	2661	2669	rVB8	10621	14330	0.24%	0.027%
61	18.986	2700	2703	2705	rBV4	18160	26175	0.45%	0.049%
62	19.016	2705	2708	2712	rVB	95990	108713	1.86%	0.203%
63	19.116	2721	2725	2733	rVB4	49417	80340	1.37%	0.150%
64	19.192	2734	2738	2740	rBV	79552	109521	1.87%	0.205%
65	19.216	2740	2742	2753	rVB2	90852	134729	2.30%	0.252%
66	19.333	2757	2762	2775	rBV	494050	727221	12.43%	1.359%
67	19.545	2792	2798	2804	rBV	3923301	5140706	87.85%	9.608%
68	21.010	3043	3047	3056	rBV	417941	659961	11.28%	1.233%
69	21.298	3091	3096	3102	rBV	1980176	2535911	43.34%	4.739%
70	23.504	3464	3471	3483	rVB2	2913002	5851626	100.00%	10.936%
71	23.657	3490	3497	3507	rVB	1351566	2738268	46.79%	5.118%

Sum of corrected areas: 53506382

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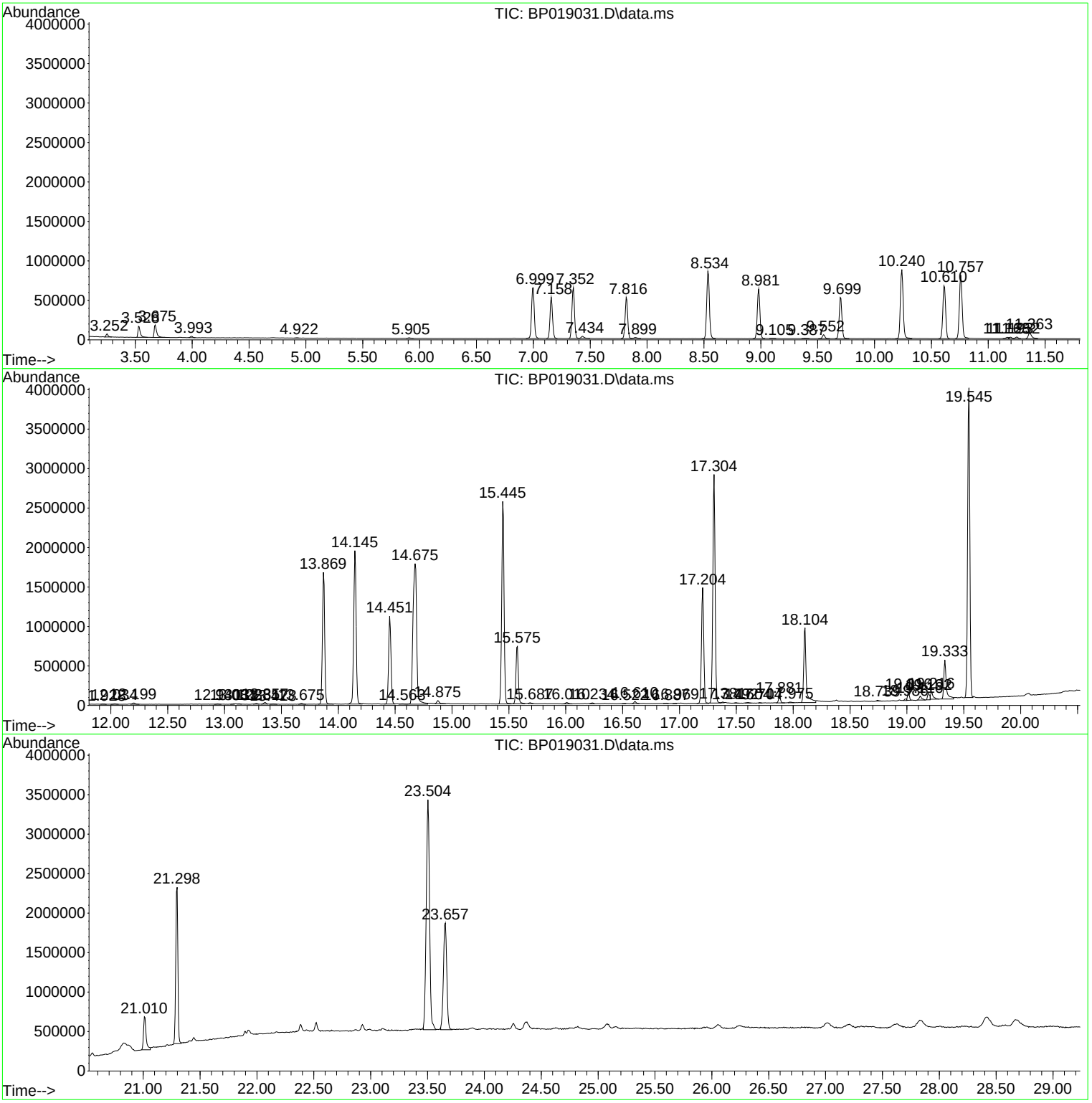
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B08

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\BP122123\
Data File : BP019031.D
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Operator : MA/JU
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Quant Title : SVOA CALIBRATION

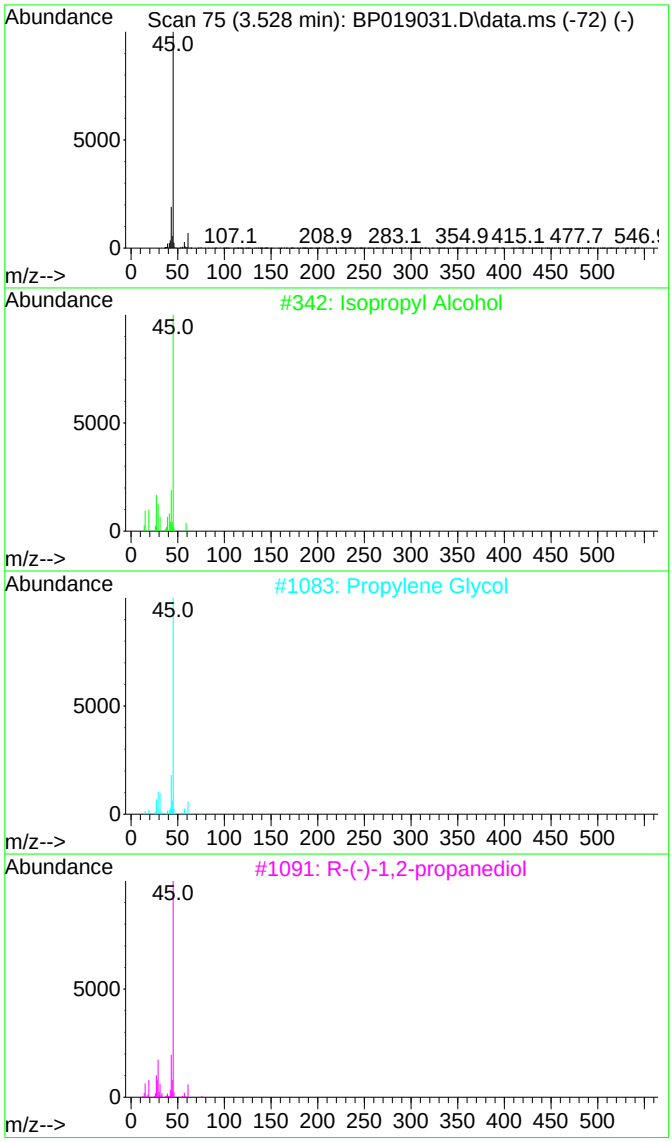
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

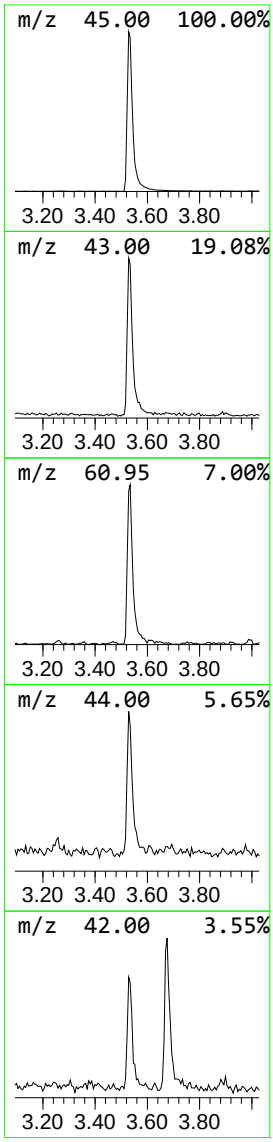
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.528	4.91 ng/ul	199282	1,4-Dichlorobenzene-d4	7.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2	Propylene Glycol	76	C3H8O2	000057-55-6	47
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019031.D
Acq On : 22 Dec 2023 09:45
Operator : MA/JU
Sample : 05808-14
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B08

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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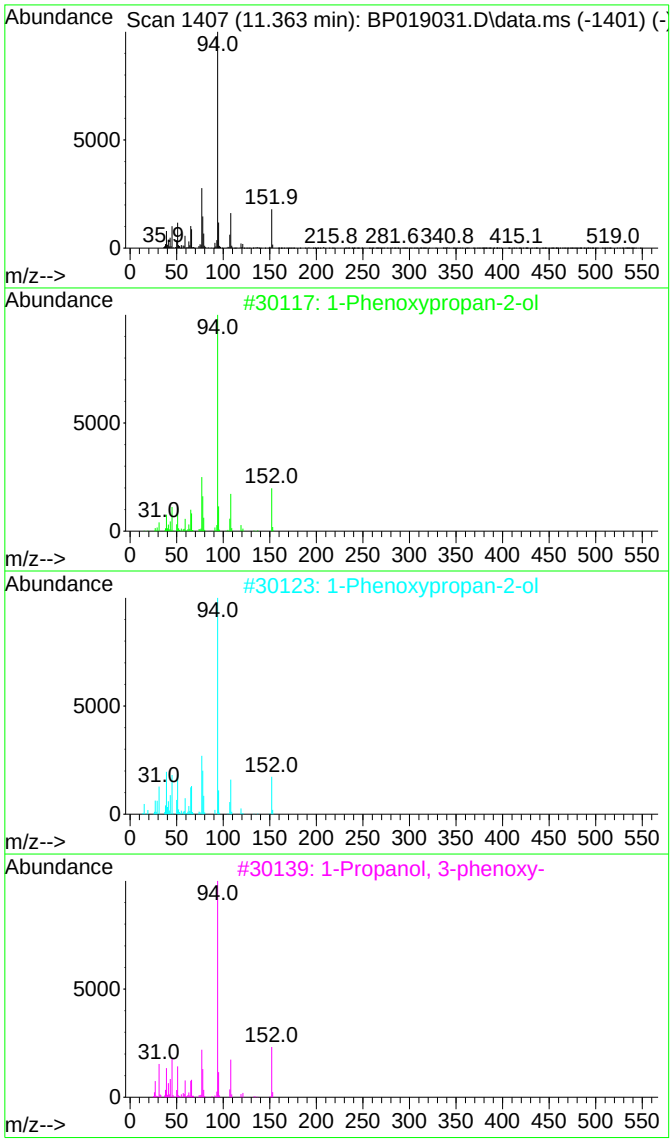
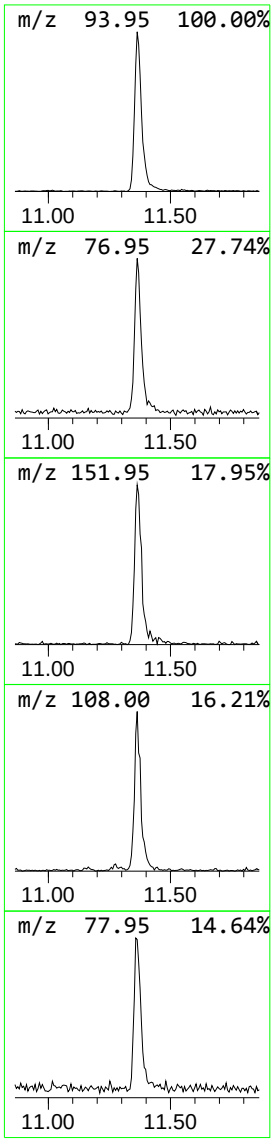
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.363	2.73 ng/ul	155714	Naphthalene-d8	10.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
3	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019031.D
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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B08

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

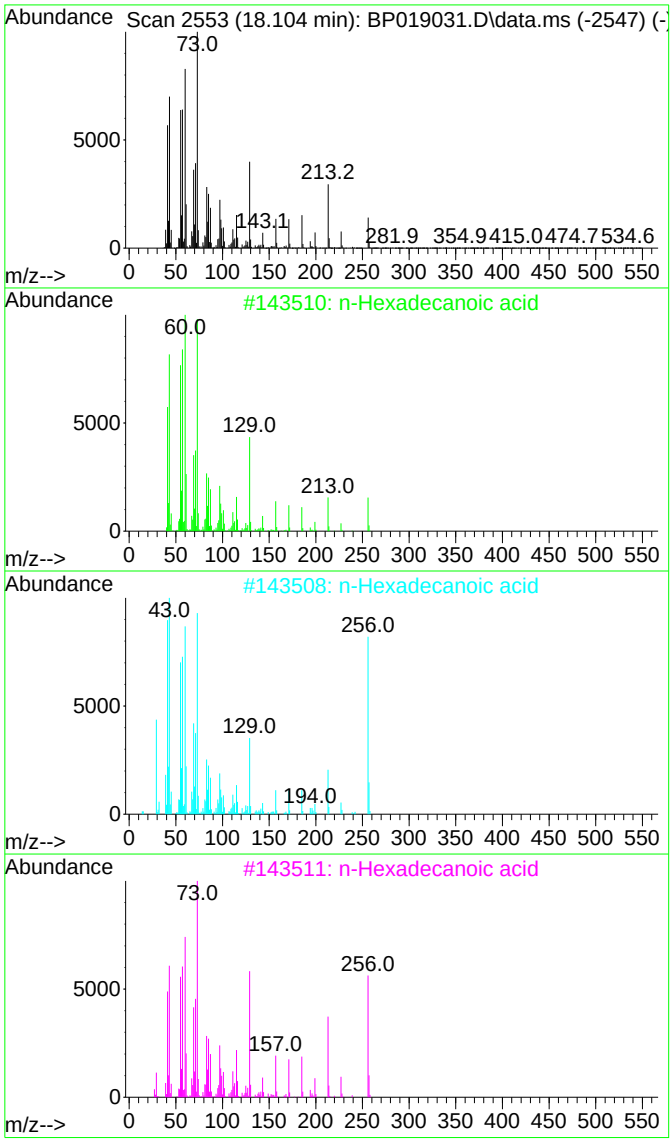
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

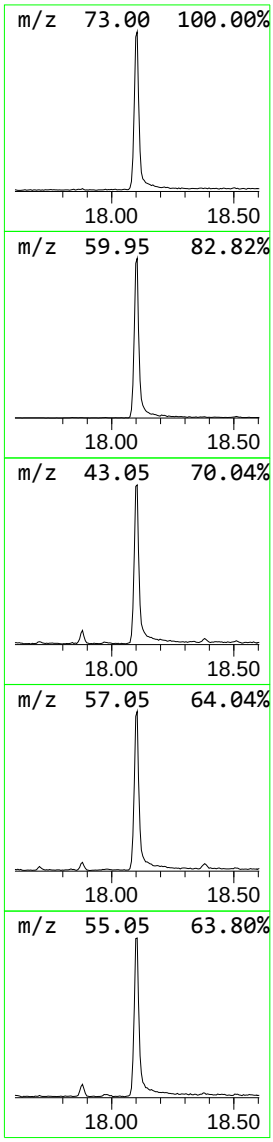
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	14.08 ng/ul	1446980	Phenanthrene-d10	17.204

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	99
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	94





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ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B08

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

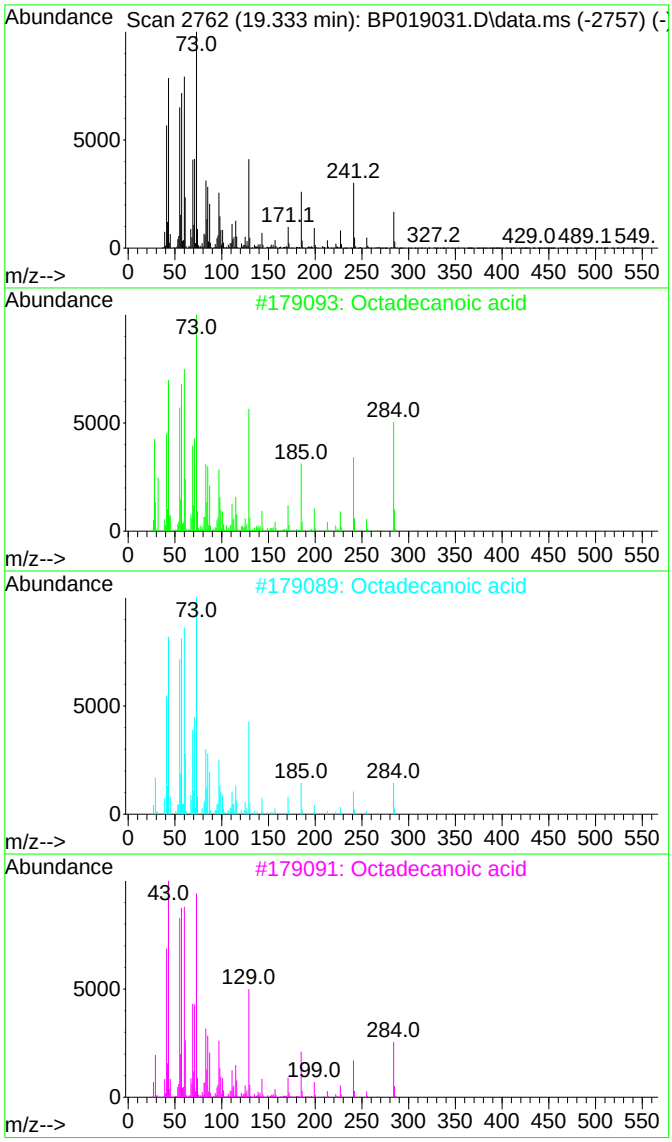
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

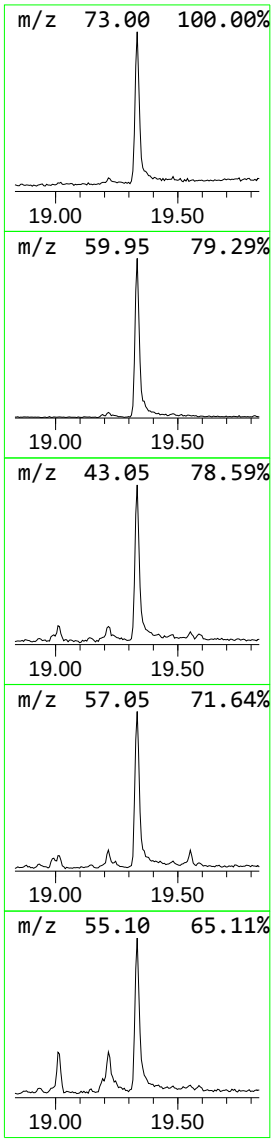
****

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.333	5.74 ng/ul	727221	Chrysene-d12	21.298

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	94
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0B08

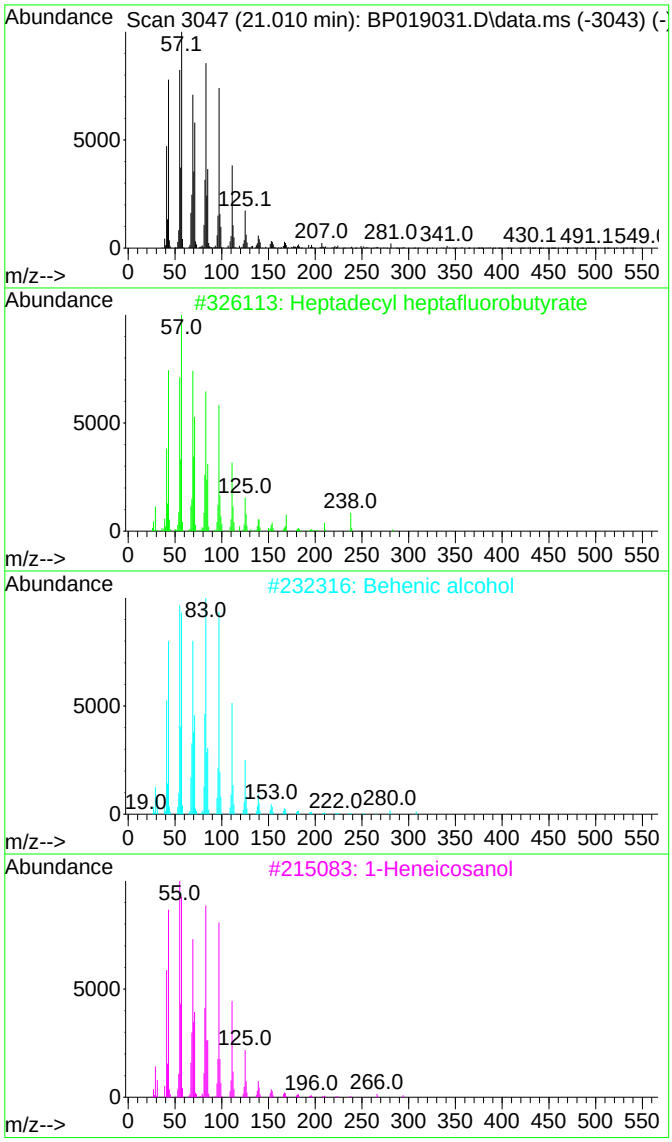
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

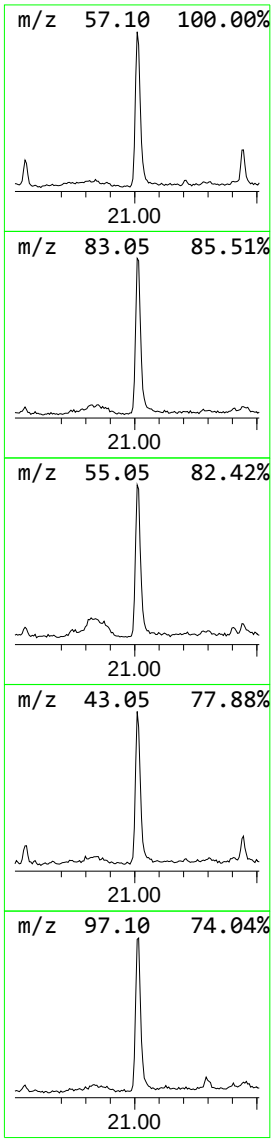
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	5.20 ng/ul	659961	Chrysene-d12	21.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl Alcohol	3.528	4.9	ng/ul	199282	1	7.816	811935	20.0
1-Phenoxypropan...	11.363	2.7	ng/ul	155714	2	10.610	1142010	20.0
n-Hexadecanoic ...	18.104	14.1	ng/ul	1446980	4	17.204	2054660	20.0
Octadecanoic acid	19.333	5.7	ng/ul	727221	5	21.298	2535910	20.0
Heptadecyl hept...	21.010	5.2	ng/ul	659961	5	21.298	2535910	20.0