LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101122\
Data File : BP012059.D
Acq On : 12 Oct 2022 02:01
Operator : CG/JU
Sample : N4991-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : C0BP3

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-BP101122.M
Title : SVOA CALIBRATION

Signal : TIC: BP012059.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.275	46	49	55	rBV	35362	46906	1.13%	0.107%
2	3.569	97	99	106	rVB	12075	15989	0.38%	0.037%
3	3.716	123	124	136	rBV	71995	129654	3.11%	0.297%
4	3.928	154	160	165	rVB	52864	76024	1.83%	0.174%
5	4.022	172	176	180	rVB	21213	28226	0.68%	0.065%
6	4.246	211	214	221	rVB2	17938	28798	0.69%	0.066%
7	4.399	237	240	245	rVB7	8963	14476	0.35%	0.033%
8	4.663	277	285	289	rBV2	14626	26462	0.64%	0.061%
9	4.716	291	294	298	rVV	12264	15121	0.36%	0.035%
10	4.963	329	336	344	rVV2	40853	85617	2.06%	0.196%
11	5.034	344	348	354	rVB8	2967	7256	0.17%	0.017%
12	5.163	366	370	386	rVB3	20935	42658	1.02%	0.098%
13	5.351	399	402	406	rVB4	4814	7024	0.17%	0.016%
14	5.416	409	413	419	rVB8	3558	7349	0.18%	0.017%
15	5.487	419	425	432	rBV2	11287	23674	0.57%	0.054%
16	5.851	481	487	492	rBV2	16925	28962	0.70%	0.066%
17	6.251	546	555	560	rVB5	8349	15857	0.38%	0.036%
18	6.381	573	577	581	rVB5	5040	9070	0.22%	0.021%
19	6.469	586	592	594	rBV7	4430	7728	0.19%	0.018%
20	6.728	629	636	643	rBV8	7251	20032	0.48%	0.046%
21	6.828	649	653	658	rVB5	7179	11393	0.27%	0.026%
22	6.887	658	663	668	rBV6	6274	11522	0.28%	0.026%
23	7.022	676	686	698	rBV	491561	812552	19.51%	1.859%
24	7.187	707	714	730	rVB	466877	766666	18.41%	1.754%
25	7.387	741	748	755	rBV	542807	883064	21.20%	2.020%
26	7.498	764	767	771	rVV2	7155	10918	0.26%	0.025%
27	7.534	771	773	778	rVB5	5762	7143	0.17%	0.016%
28	7.857	818	828	836	rBV	716441	1184350	28.44%	2.710%
29	7.916	836	838	843	rVB5	5658	7515	0.18%	0.017%
30	8.040	855	859	865	rVB8	4316	6697	0.16%	0.015%
31	8.498	929	937	938	rBV5	6245	11934	0.29%	0.027%
32	8.569	943	949	964	rVV	256079	453828	10.90%	1.038%
33	8.687	965	969	976	rVB	18929	35259	0.85%	0.081%
34	9.022	1019	1026	1033	rBV	487144	814032	19.55%	1.862%
35	9.187	1050	1054	1060	rVB9	5084	10577	0.25%	0.024%
36	9.334	1075	1079	1089	rVB10	5131	12029	0.29%	0.028%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_P
ClientSampleId :
C0BP3

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-BP101122.M
Title : SVOA CALIBRATION

37	9.422	1089	1094	1099	rBV3	6576	10070	0.24%	0.023%
38	9.745	1141	1149	1163	rBV	365740	653799	15.70%	1.496%
39	10.063	1198	1203	1208	rBV	21466	36469	0.88%	0.083%
40	10.286	1233	1241	1258	rBV	551548	999371	24.00%	2.287%
41	10.445	1262	1268	1283	rBV	165844	333168	8.00%	0.762%
42	10.663	1296	1305	1312	rBV	987517	1692367	40.64%	3.872%
43	10.710	1312	1313	1319	rVB	29055	31536	0.76%	0.072%
44	10.804	1323	1329	1345	rBV	333553	670117	16.09%	1.533%
45	11.569	1456	1459	1465	rVB8	6536	10782	0.26%	0.025%
46	11.686	1473	1479	1482	rBV5	7265	14040	0.34%	0.032%
47	11.839	1499	1505	1506	rBV5	5104	7204	0.17%	0.016%
48	12.081	1541	1546	1554	rVB	33214	53466	1.28%	0.122%
49	12.157	1554	1559	1562	rBV7	4921	9731	0.23%	0.022%
50	12.251	1571	1575	1580	rBV	17212	23966	0.58%	0.055%
51	12.328	1583	1588	1594	rVB	25419	41619	1.00%	0.095%
52	12.545	1619	1625	1631	rBV	24614	40954	0.98%	0.094%
53	12.751	1657	1660	1664	rBV6	4126	6666	0.16%	0.015%
54	13.033	1703	1708	1712	rVB4	10624	13330	0.32%	0.030%
55	13.233	1738	1742	1746	rBV7	8672	16649	0.40%	0.038%
56	13.322	1752	1757	1765	rVB3	34046	54474	1.31%	0.125%
57	13.392	1766	1769	1774	rVB3	11818	17349	0.42%	0.040%
58	13.545	1789	1795	1803	rVB4	28507	60615	1.46%	0.139%
59	13.639	1808	1811	1814	rBV5	4787	7291	0.18%	0.017%
60	13.822	1838	1842	1847	rBV3	15829	23183	0.56%	0.053%
61	13.916	1852	1858	1864	rVV	1056086	1454848	34.93%	3.329%
62	14.022	1873	1876	1880	rBV6	9557	14013	0.34%	0.032%
63	14.057	1880	1882	1885	rVB2	8703	8879	0.21%	0.020%
64	14.198	1899	1906	1915	rBV	1271152	1941149	46.61%	4.441%
65	14.398	1935	1940	1944	rVB	45065	63346	1.52%	0.145%
66	14.445	1944	1948	1951	rBV2	25426	37843	0.91%	0.087%
67	14.504	1951	1958	1965	rVV	1452782	2102195	50.48%	4.810%
68	14.663	1983	1985	1988	rBV2	17648	20118	0.48%	0.046%
69	14.710	1988	1993	2013	rVV	329965	664164	15.95%	1.520%
70	15.351	2098	2102	2106	rVB	46987	58609	1.41%	0.134%
71	15.498	2121	2127	2139	rBV	1860313	2717450	65.25%	6.218%
72	15.622	2143	2148	2157	rVV	286758	438350	10.53%	1.003%
73	15.751	2166	2170	2177	rVB3	43443	78389	1.88%	0.179%
74	16.216	2245	2249	2251	rBV	59857	84568	2.03%	0.193%
75	16.639	2317	2321	2328	rVB	145840	203205	4.88%	0.465%
76	16.710	2329	2333	2337	rVV	63536	81753	1.96%	0.187%

LSC Area Percent Report

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Operator : CG/JU
Sample : N4991-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BP3

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

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Title : SVOA CALIBRATION

77	17.016	2382	2385	2389	rVB3	60330	71867	1.73%	0.164%
78	17.263	2421	2427	2432	rBV	1692730	2433111	58.43%	5.567%
79	17.321	2435	2437	2439	rVV	118094	142383	3.42%	0.326%
80	17.357	2439	2443	2454	rVB2	1832616	2767994	66.47%	6.333%
81	17.757	2508	2511	2513	rBV2	37905	39783	0.96%	0.091%
82	18.033	2554	2558	2565	rBV3	85380	135547	3.25%	0.310%
83	18.145	2573	2577	2581	rBV	243846	304883	7.32%	0.698%
84	18.604	2652	2655	2664	rVB3	85100	200829	4.82%	0.459%
85	18.963	2712	2716	2721	rBV	240713	298443	7.17%	0.683%
86	19.027	2724	2727	2734	rVB3	127463	191824	4.61%	0.439%
87	19.239	2760	2763	2764	rBV2	74339	80424	1.93%	0.184%
88	19.268	2765	2768	2778	rVB2	188920	352651	8.47%	0.807%
89	19.380	2783	2787	2794	rBV3	156627	255397	6.13%	0.584%
90	19.492	2802	2806	2812	rBV	191088	257847	6.19%	0.590%
91	19.598	2818	2824	2835	rVB	2767764	4042401	97.07%	9.249%
92	20.727	3013	3016	3020	rBV	283356	280024	6.72%	0.641%
93	21.051	3068	3071	3081	rVB	373619	480725	11.54%	1.100%
94	21.162	3087	3090	3097	rBV	246890	313466	7.53%	0.717%
95	21.345	3117	3121	3127	rBV	2430660	3102153	74.49%	7.098%
96	23.603	3499	3505	3520	rVB2	1934495	4164498	100.00%	9.528%
97	23.762	3527	3532	3548	rVB2	1592117	3316713	79.64%	7.589%

Sum of corrected areas: 43706420

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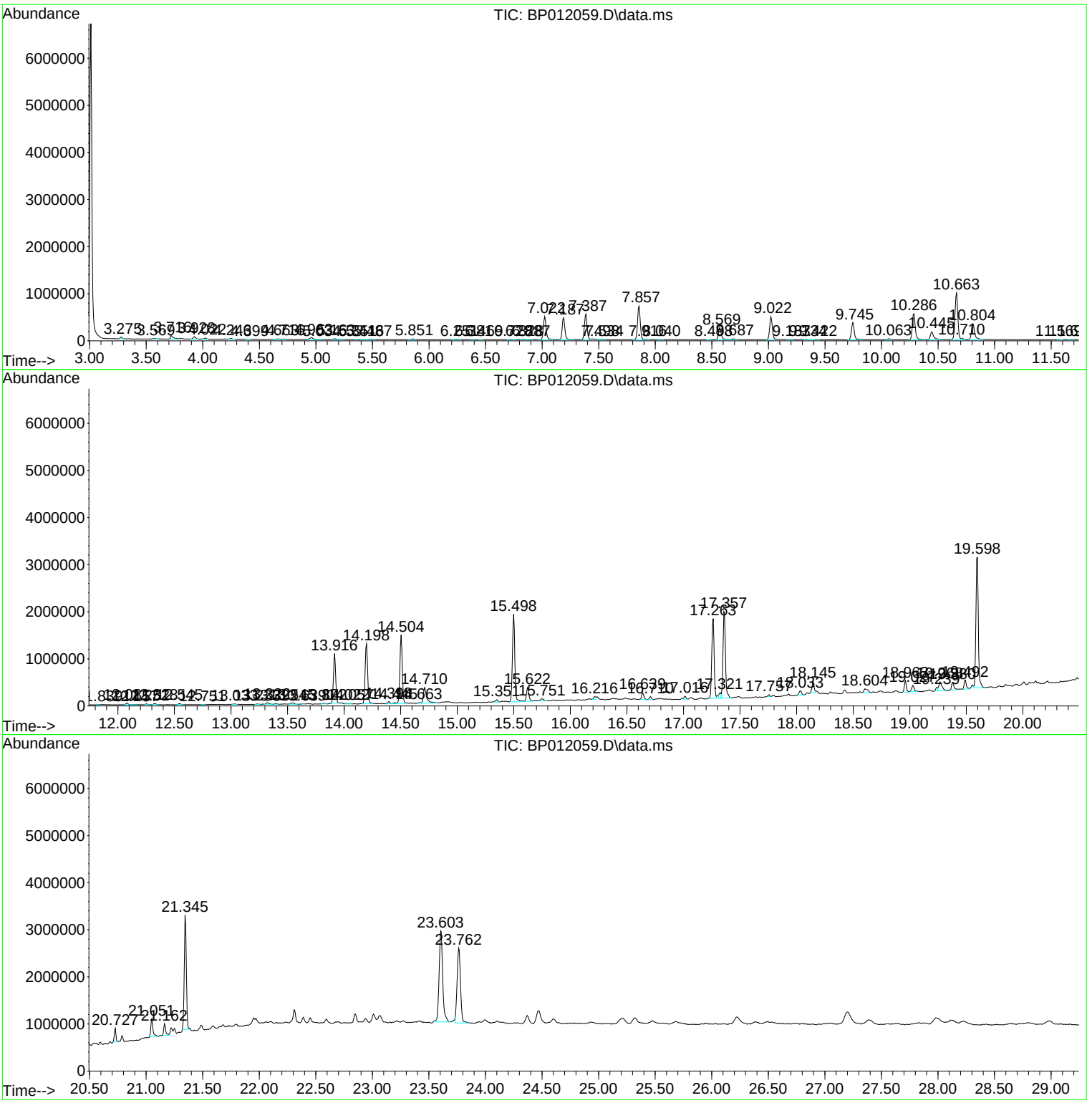
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101122\
Data File : BP012059.D
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Operator : CG/JU
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ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId :
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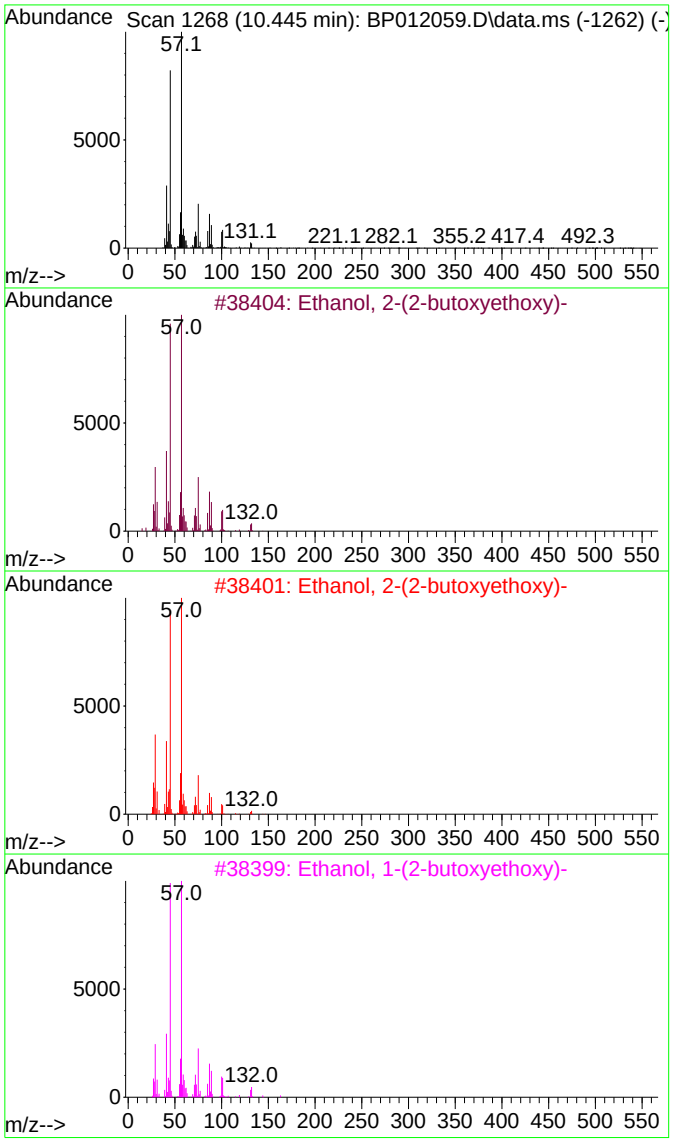
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

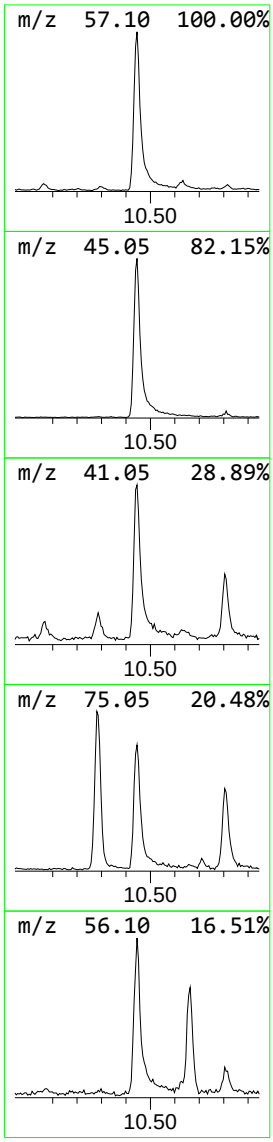
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	3.94 ng/ul	333168	Naphthalene-d8	10.663

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	90
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
4	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
5	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101122\
Data File : BP012059.D
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Sample : N4991-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

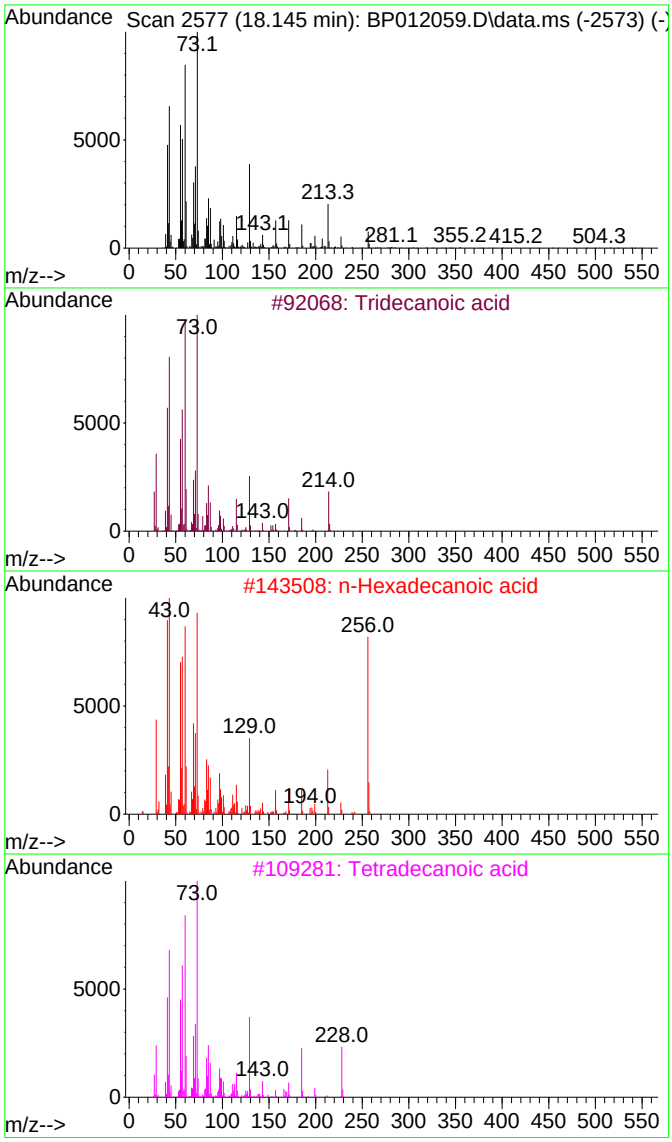
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

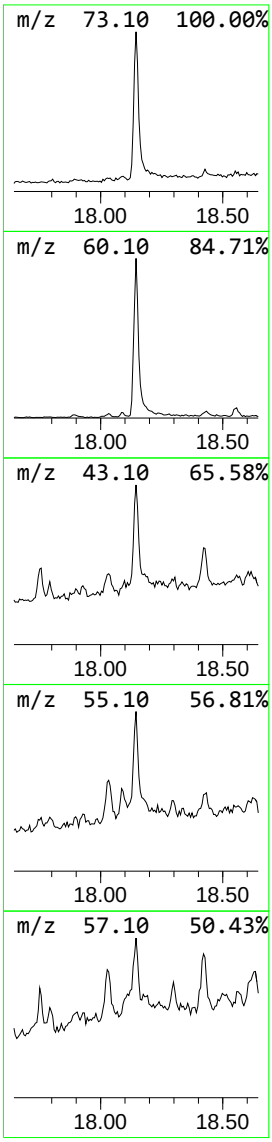
****

Peak Number 2 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	2.51 ng/ul	304883	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81





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Acq On : 12 Oct 2022 02:01
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BP3

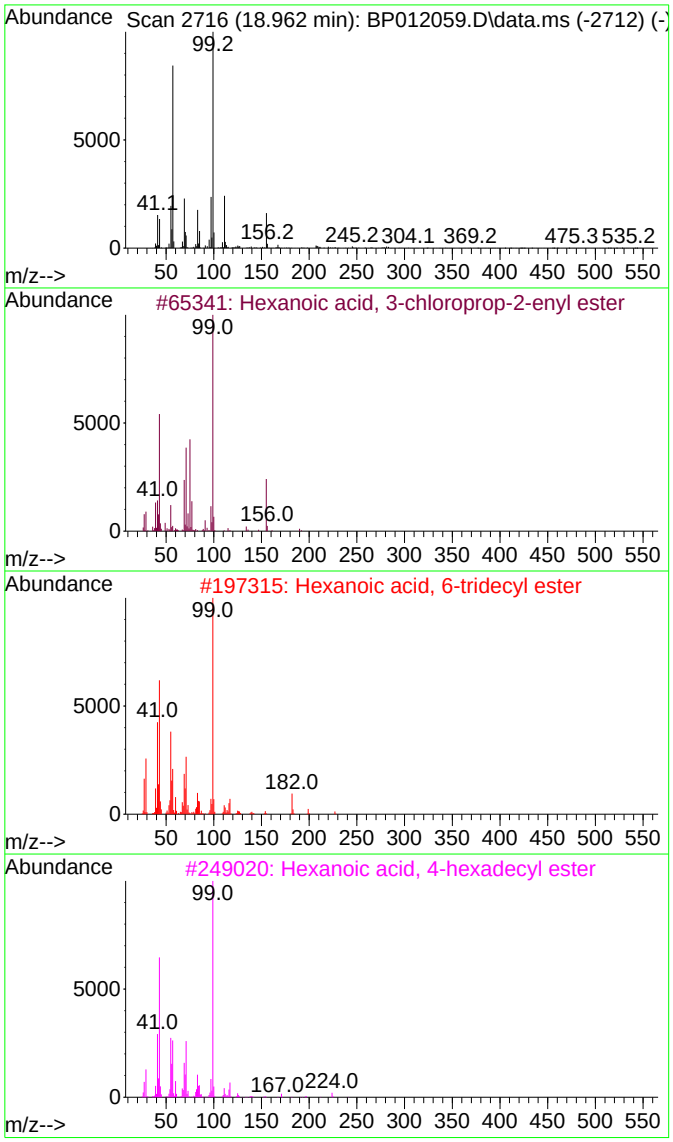
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

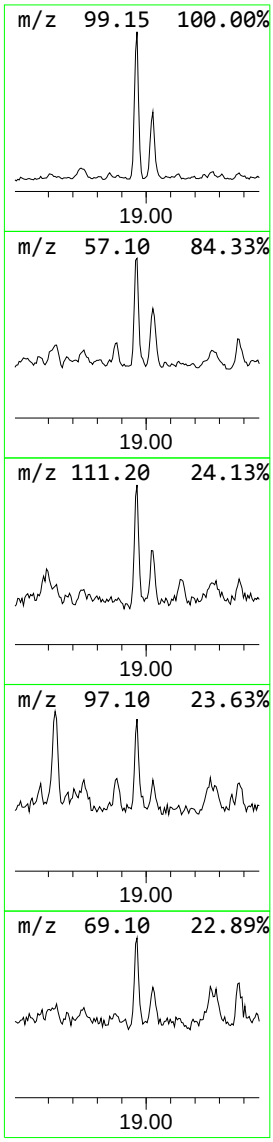
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexanoic acid, 3-chloroprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.962	2.45 ng/ul	298443	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	50
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	47
3	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	47
4	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	47
5	Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	47





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Instrument :
BNA_P
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C0BP3

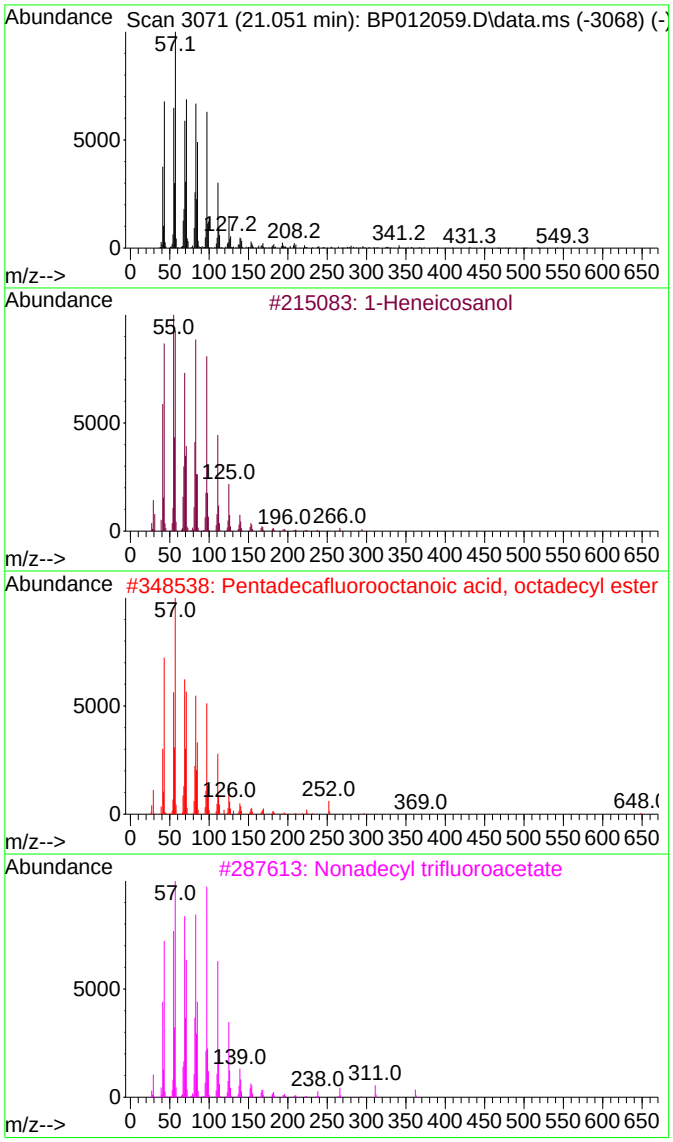
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

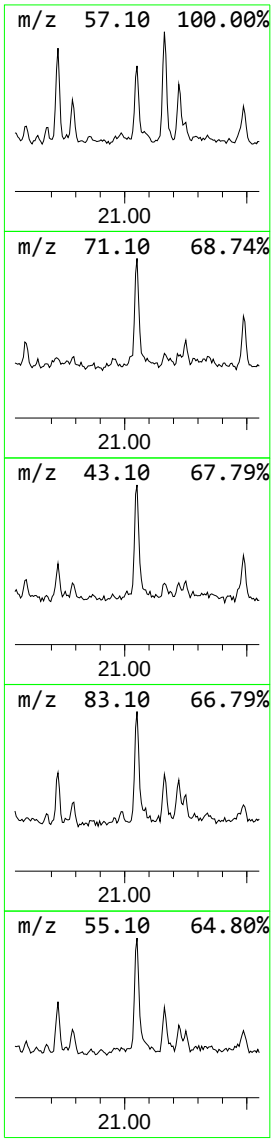
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	3.10 ng/ul	480725	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	89





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Data File : BP012059.D
Acq On : 12 Oct 2022 02:01
Operator : CG/JU
Sample : N4991-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

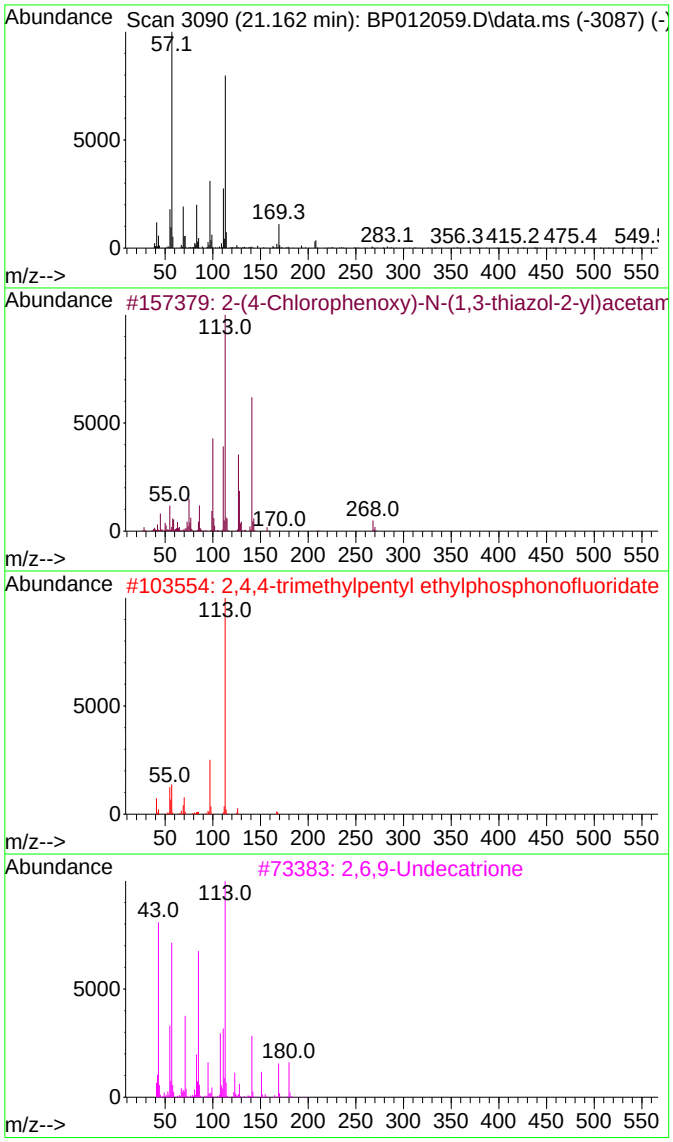
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

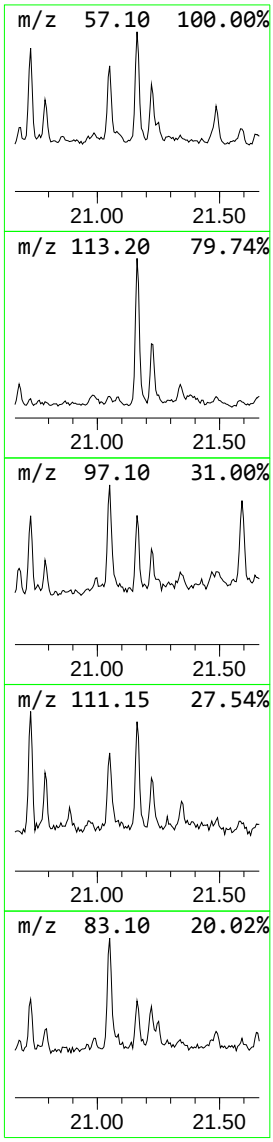
****

Peak Number 6 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	2.02 ng/ul	313466	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Chlorophenoxy)-N-(1,3-thiaz...	268	C11H9ClN2O2S	037666-22-1	43
2	2,4,4-trimethylpentyl ethylphosp...	224	C10H22FO2P	333416-13-0	43
3	2,6,9-Undecatrione	198	C11H18O3	078975-91-4	42
4	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	40
5	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101122\
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Sample : N4991-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.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
Ethanol, 2-(2-b...	10.445	3.9	ng/ul	333168	2	10.663	1692370	20.0
Tridecanoic acid	18.145	2.5	ng/ul	304883	4	17.263	2433110	20.0
Hexanoic acid, ...	18.962	2.5	ng/ul	298443	4	17.263	2433110	20.0
1-Heneicosanol	21.051	3.1	ng/ul	480725	5	21.345	3102150	20.0
unknown-01	21.162	2.0	ng/ul	313466	5	21.345	3102150	20.0