LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017551.D
Acq On : 05 Oct 2023 05:04
Operator : MA/JU
Sample : 04679-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

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-BP100423.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP017557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.287	31	34	42	rVB	26641	36976	0.50%	0.078%
2	3.728	106	109	124	rBV	160950	256901	3.46%	0.545%
3	4.034	157	161	166	rBV7	6443	11789	0.16%	0.025%
4	6.910	647	650	654	rVB6	7099	10121	0.14%	0.021%
5	7.099	675	682	692	rBV	135968	233631	3.15%	0.495%
6	7.281	707	713	723	rBV	542153	838495	11.29%	1.777%
7	7.458	737	743	754	rBV	535808	843580	11.36%	1.788%
8	7.546	754	758	766	rVB3	13292	25809	0.35%	0.055%
9	7.940	818	825	839	rBV	384421	615697	8.29%	1.305%
10	8.663	939	948	959	rBV	398844	671273	9.04%	1.423%
11	9.146	1023	1030	1045	rBV	678136	1106730	14.90%	2.346%
12	9.263	1046	1050	1053	rVB6	7805	10341	0.14%	0.022%
13	9.340	1059	1063	1068	rVV5	10037	17437	0.23%	0.037%
14	9.863	1144	1152	1163	rBV	546043	898313	12.10%	1.904%
15	10.069	1184	1187	1194	rVB7	6181	9858	0.13%	0.021%
16	10.393	1235	1242	1256	rBV	791620	1317121	17.74%	2.792%
17	10.622	1276	1281	1289	rVB	35868	63716	0.86%	0.135%
18	10.775	1299	1307	1314	rBV	529461	865592	11.66%	1.835%
19	10.946	1328	1336	1350	rBV	696550	1195928	16.11%	2.535%
20	11.151	1365	1371	1376	rVB4	10994	17973	0.24%	0.038%
21	11.551	1433	1439	1446	rBV10	11534	18966	0.26%	0.040%
22	11.793	1473	1480	1493	rBV	101851	226728	3.05%	0.481%
23	12.369	1572	1578	1583	rBV	13840	24934	0.34%	0.053%
24	12.875	1661	1664	1671	rVB8	4985	7466	0.10%	0.016%
25	13.375	1742	1749	1752	rBV9	6148	8383	0.11%	0.018%
26	13.469	1758	1765	1771	rBV	32055	53457	0.72%	0.113%
27	14.051	1857	1864	1873	rBV	1789175	2473340	33.31%	5.242%
28	14.245	1891	1897	1904	rBV	5466	9114	0.12%	0.019%
29	14.334	1904	1912	1921	rBV	1827369	2685821	36.17%	5.693%
30	14.634	1956	1963	1973	rVB	840732	1203988	16.21%	2.552%
31	14.881	2000	2005	2021	rBV	115655	247544	3.33%	0.525%
32	15.016	2024	2028	2037	rVV6	21935	40587	0.55%	0.086%
33	15.381	2086	2090	2096	rVB	43443	55920	0.75%	0.119%
34	15.634	2125	2133	2144	rBV	2546243	3703768	49.88%	7.850%
35	15.775	2151	2157	2170	rBV	891788	1217244	16.39%	2.580%
36	15.875	2170	2174	2180	rVB6	12496	21399	0.29%	0.045%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017551.D
Acq On : 05 Oct 2023 05:04
Operator : MA/JU
Sample : 04679-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

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-BP100423.MA.M
Title : SVOA CALIBRATION

37	16.304	2243	2247	2249	rBV5	6311	10137	0.14%	0.021%
38	16.769	2322	2326	2330	rBV5	12839	19060	0.26%	0.040%
39	17.081	2376	2379	2385	rBV8	7636	14879	0.20%	0.032%
40	17.422	2431	2437	2445	rVV	1126300	1554333	20.93%	3.295%
41	17.522	2448	2454	2470	rVV	3430087	4807312	64.74%	10.190%
42	17.769	2493	2496	2499	rBV4	6284	9344	0.13%	0.020%
43	18.045	2539	2543	2547	rVB3	16103	21929	0.30%	0.046%
44	18.151	2558	2561	2566	rBV7	7302	13293	0.18%	0.028%
45	18.269	2576	2581	2592	rBV	297575	461148	6.21%	0.977%
46	18.357	2594	2596	2601	rVB	17951	26445	0.36%	0.056%
47	19.345	2760	2764	2768	rBV3	49233	67874	0.91%	0.144%
48	19.404	2770	2774	2781	rVV2	79383	159349	2.15%	0.338%
49	19.516	2789	2793	2802	rBV	152363	225804	3.04%	0.479%
50	19.780	2832	2838	2844	rBV	5031844	6398053	86.17%	13.561%
51	20.763	3002	3005	3009	rVB	88503	93951	1.27%	0.199%
52	21.210	3077	3081	3091	rBV2	253360	412931	5.56%	0.875%
53	21.557	3135	3140	3147	rBV2	1499043	1966176	26.48%	4.167%
54	22.816	3350	3354	3359	rVB	202130	285128	3.84%	0.604%
55	23.974	3542	3551	3560	rVB	3628100	7425276	100.00%	15.739%
56	24.139	3573	3579	3589	rVB	1024948	2160522	29.10%	4.579%

Sum of corrected areas: 47178884

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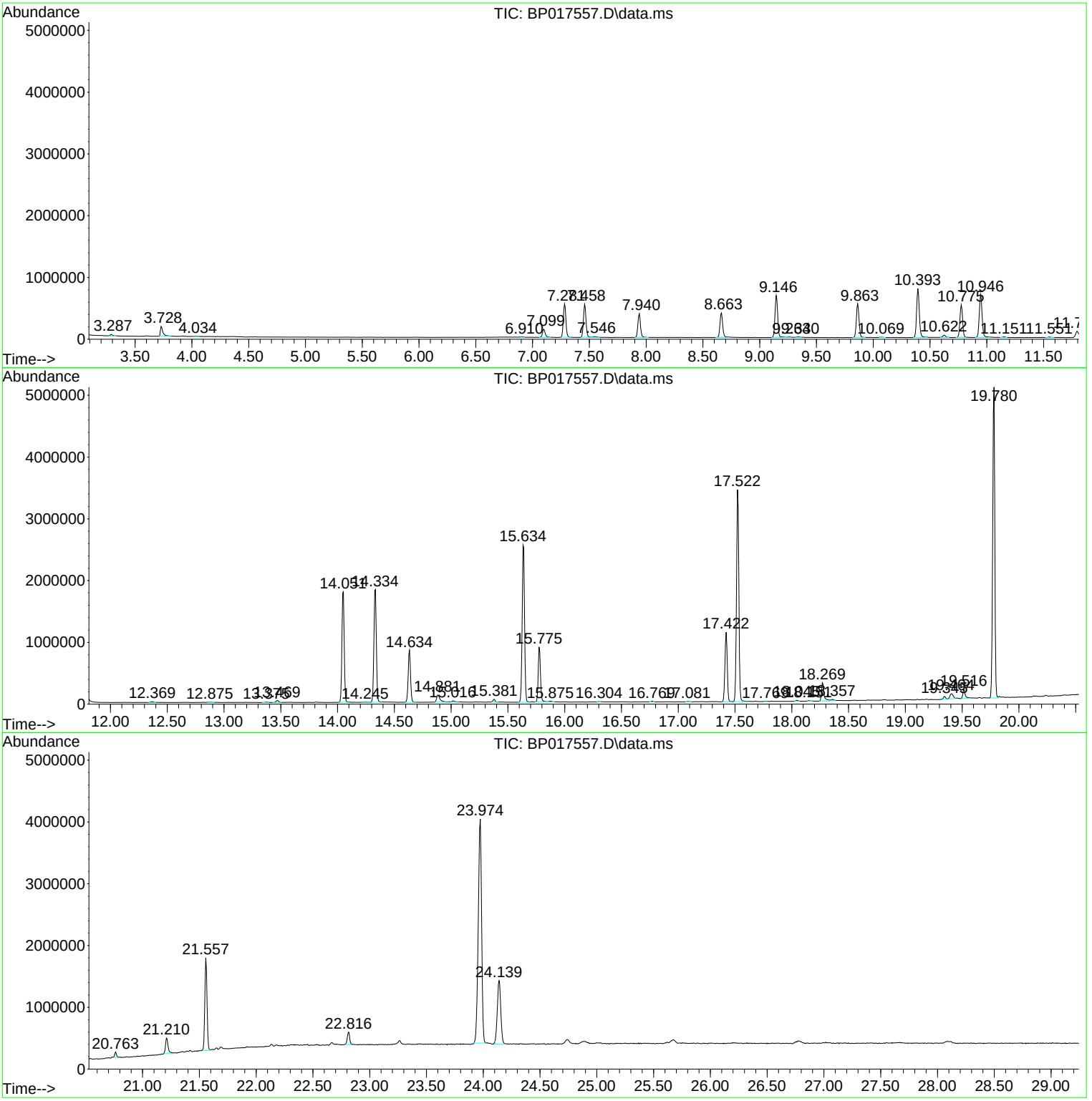
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.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\BP100423\
Data File : BP017551.D
Acq On : 05 Oct 2023 05:04
Operator : MA/JU
Sample : 04679-13
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Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

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Quant Title : SVOA CALIBRATION

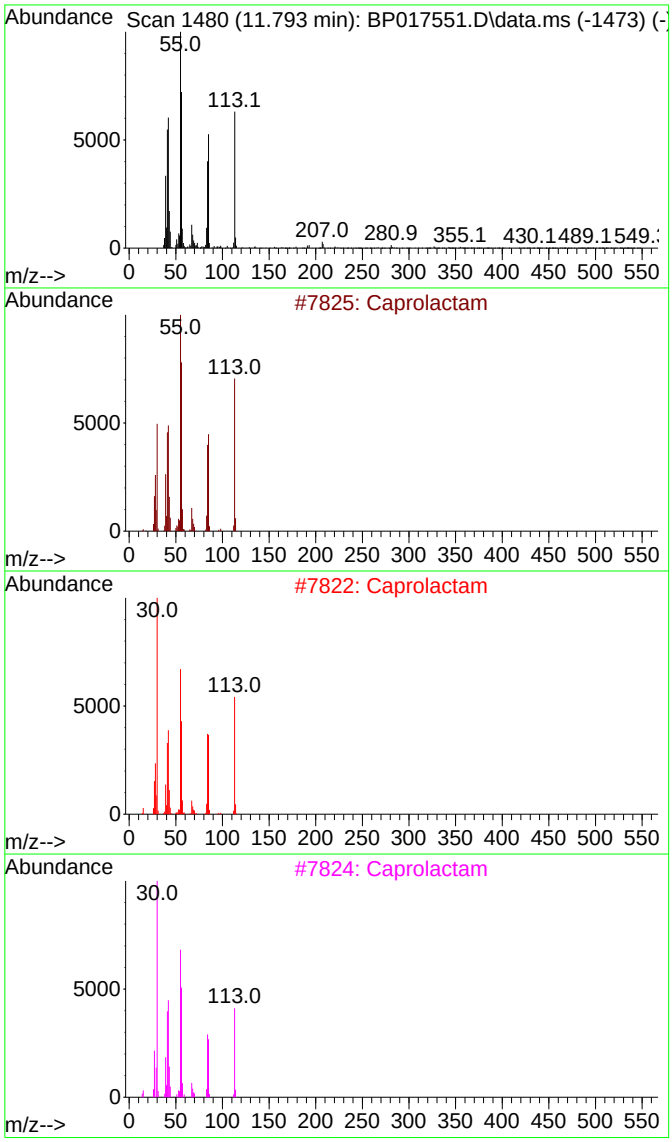
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

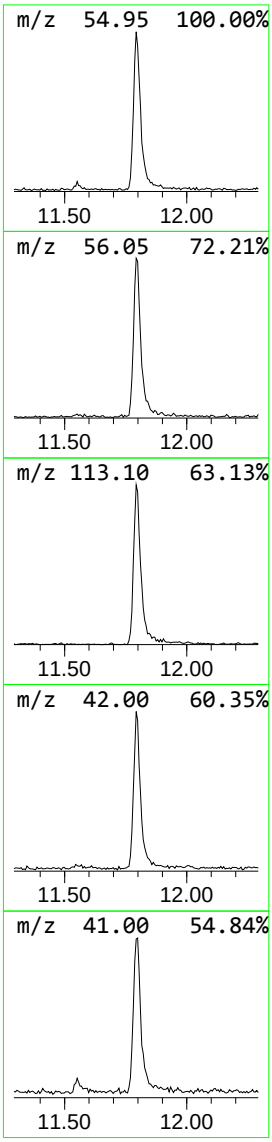
****

Peak Number 1 Capro lactam Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.793	5.24 ng/ul	226728	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caprolactam	113	C6H11NO	000105-60-2	95
2	Caprolactam	113	C6H11NO	000105-60-2	94
3	Caprolactam	113	C6H11NO	000105-60-2	94
4	Caprolactam	113	C6H11NO	000105-60-2	91
5	Caprolactam	113	C6H11NO	000105-60-2	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017551.D
Acq On : 05 Oct 2023 05:04
Operator : MA/JU
Sample : 04679-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

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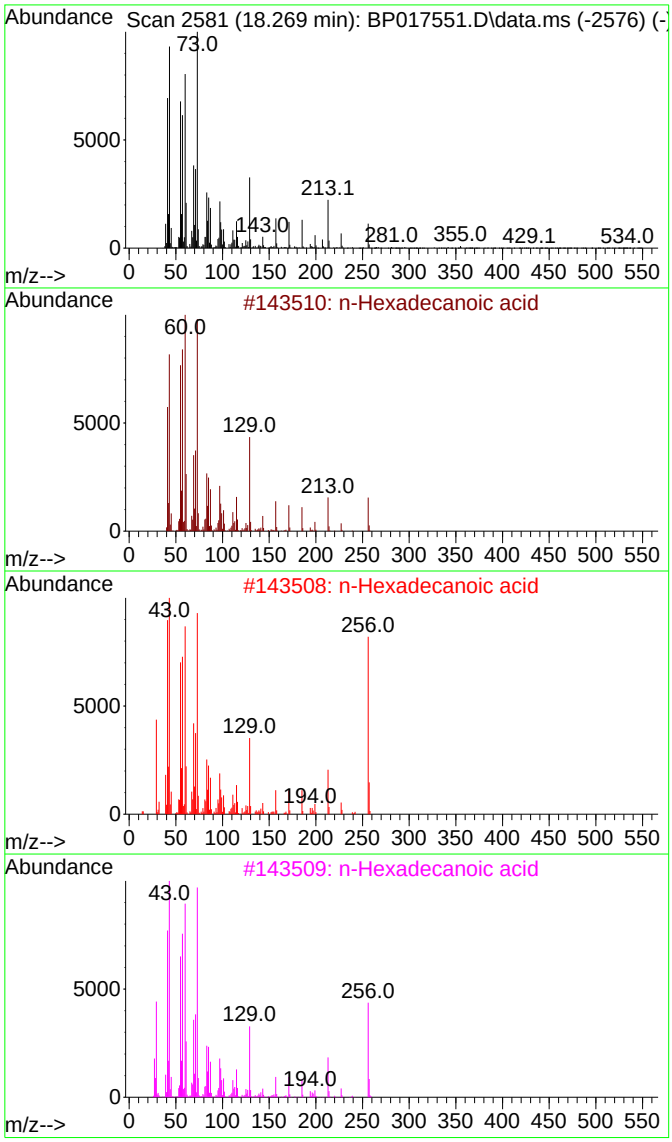
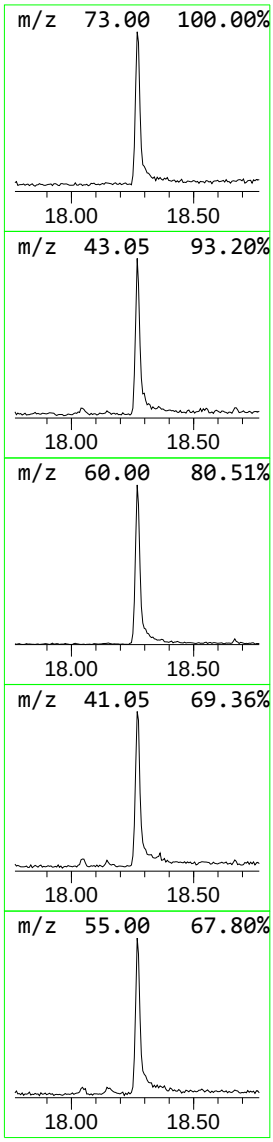
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.269	5.93 ng/ul	461148	Phenanthrene-d10	17.422

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	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017551.D
Acq On : 05 Oct 2023 05:04
Operator : MA/JU
Sample : 04679-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

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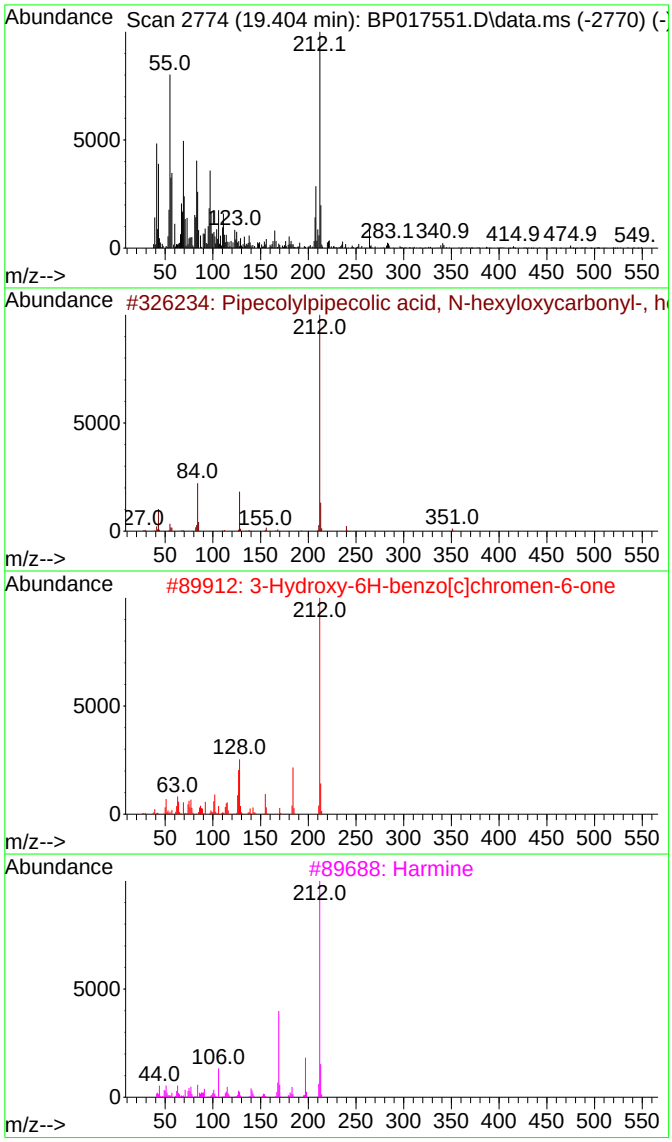
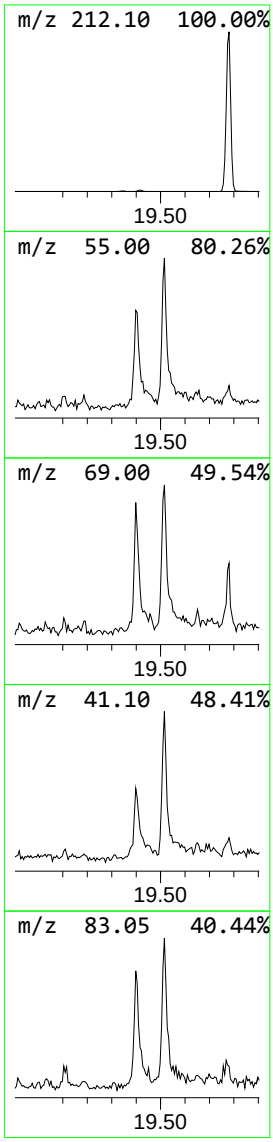
Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	2.05 ng/ul	159349	Phenanthrene-d10	17.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pipecolylpipecolic acid, N-hexyl...	452	C25H44N2O5	1010393-12-3	43
2	3-Hydroxy-6H-benzo[c]chromen-6-one	212	C13H8O3	001139-83-9	41
3	Harmine	212	C13H12N2O	000442-51-3	38
4	9H-Xanthen-9-one, 4-hydroxy-	212	C13H8O3	014686-63-6	38
5	4-Amino-1,8-naphthalimide	212	C12H8N2O2	001742-95-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
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Acq On : 05 Oct 2023 05:04
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Sample : 04679-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

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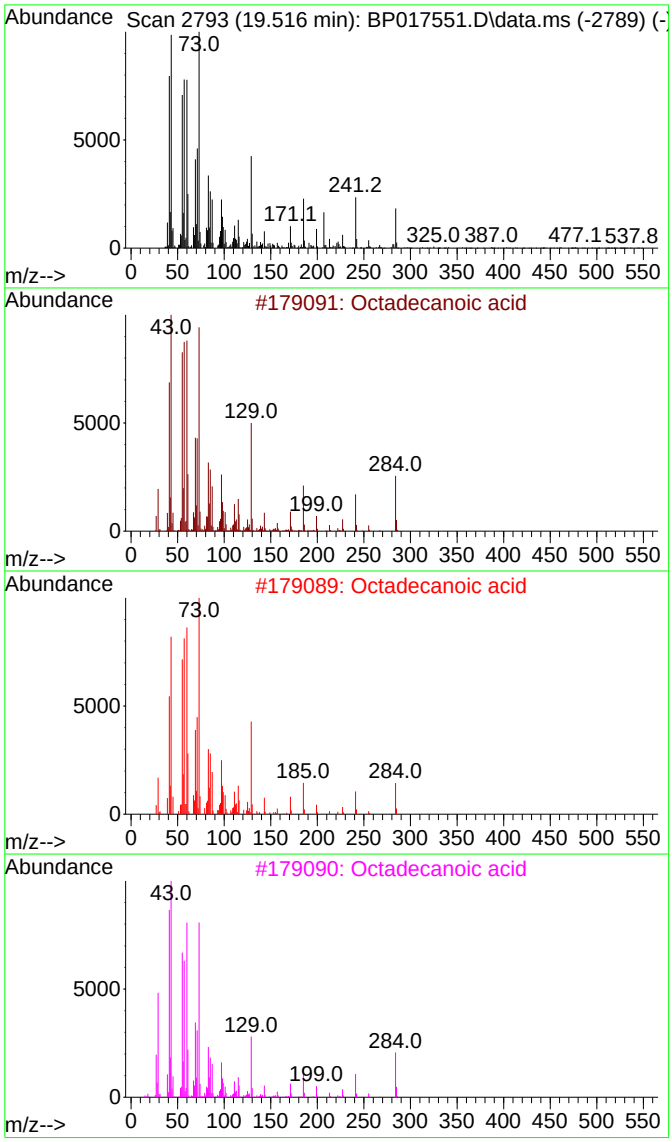
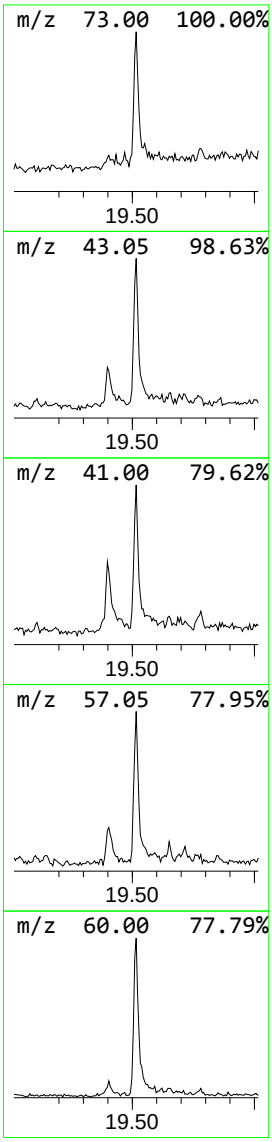
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.516	2.30 ng/ul	225804	Chrysene-d12	21.557

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





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Operator : MA/JU
Sample : 04679-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

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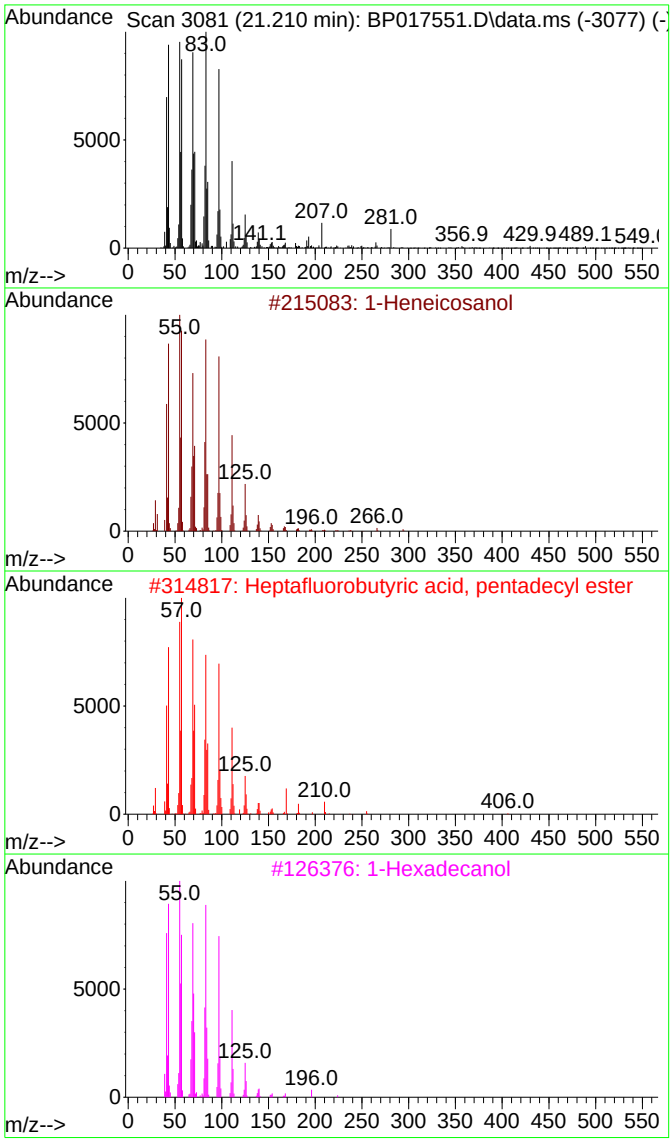
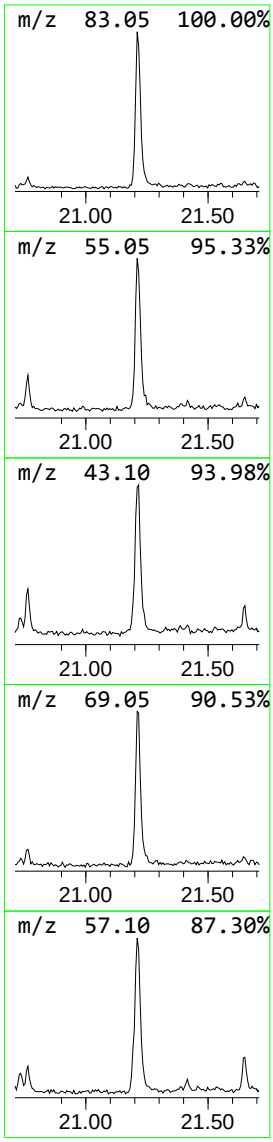
Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.210	4.20 ng/ul	412931	Chrysene-d12	21.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	1-Hexadecanol	242	C16H34O	036653-82-4	93
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





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Operator : MA/JU
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-1(20230927)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
Quant Title : SVOA CALIBRATION

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

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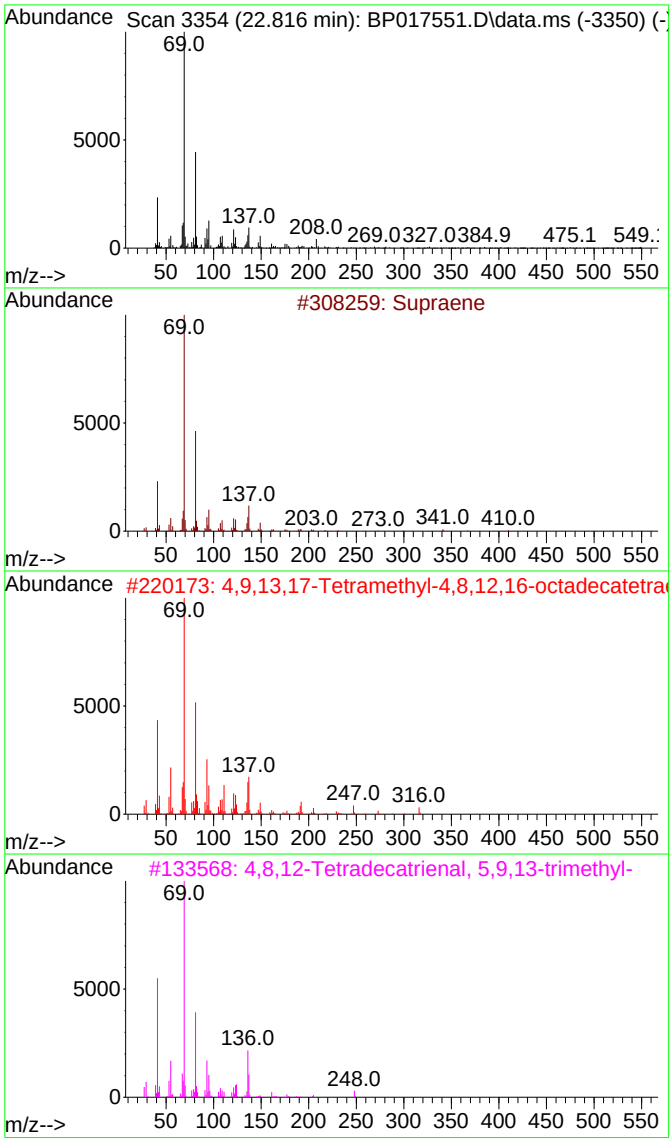
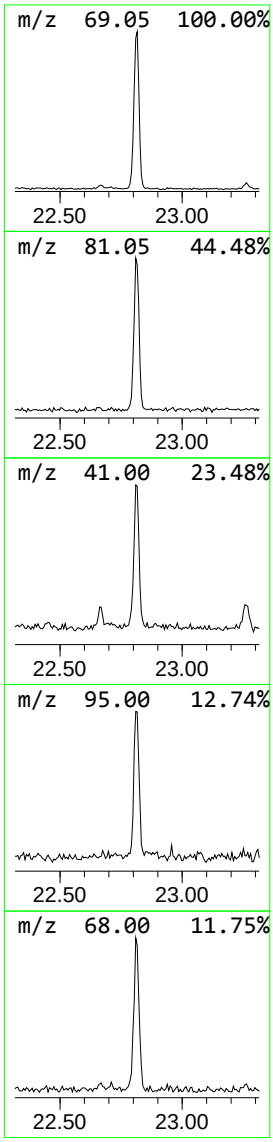
Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.816	2.90 ng/ul	285128	Chrysene-d12	21.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	53
5	3-Ethyl-1,5-octadiene	138	C10H18	1000114-87-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
Data File : BP017551.D
Acq On : 05 Oct 2023 05:04
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.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
Capro lactam	11.793	5.2	ng/ul	226728	2	10.775	865592	20.0
n-Hexadecanoic ...	18.269	5.9	ng/ul	461148	4	17.422	1554330	20.0
unknown-01	19.404	2.0	ng/ul	159349	4	17.422	1554330	20.0
Octadecanoic acid	19.516	2.3	ng/ul	225804	5	21.557	1966180	20.0
1-Heneicosanol	21.210	4.2	ng/ul	412931	5	21.557	1966180	20.0
Supraene	22.816	2.9	ng/ul	285128	5	21.557	1966180	20.0