LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : E08N0

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_N\Methods\SFAM-EPA-BN041924.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN031245.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	22	26	36	rVB	64744	85103	1.17%	0.094%
2	3.411	69	72	81	rBV	50648	76981	1.06%	0.085%
3	3.546	92	95	114	rBV	620308	958876	13.22%	1.061%
4	3.858	144	148	153	rVB2	15590	21875	0.30%	0.024%
5	4.216	206	209	216	rVB2	19499	28849	0.40%	0.032%
6	4.534	257	263	269	rVB5	9193	16785	0.23%	0.019%
7	5.722	462	465	472	rVB2	13465	20646	0.28%	0.023%
8	6.240	549	553	556	rBV4	6844	11867	0.16%	0.013%
9	6.634	615	620	626	rVB	17394	30164	0.42%	0.033%
10	6.805	641	649	664	rBV	1259278	2041703	28.14%	2.259%
11	6.969	668	677	688	rBV	1041217	1612043	22.22%	1.783%
12	7.158	698	709	719	rBV	1310157	2046384	28.21%	2.264%
13	7.246	719	724	731	rVB8	8400	18564	0.26%	0.021%
14	7.622	781	788	796	rBV	1137710	1750261	24.13%	1.936%
15	7.699	796	801	808	rVB3	15535	33716	0.46%	0.037%
16	8.187	877	884	887	rBV5	6659	11575	0.16%	0.013%
17	8.334	902	909	919	rBV	1681606	2677910	36.91%	2.963%
18	8.781	977	985	998	rBV	1289761	2101078	28.96%	2.324%
19	8.940	1007	1012	1019	rVB5	12932	23379	0.32%	0.026%
20	9.169	1045	1051	1057	rVB2	34511	51830	0.71%	0.057%
21	9.346	1075	1081	1091	rBV	58792	95133	1.31%	0.105%
22	9.493	1099	1106	1120	rBV	1063799	1783323	24.58%	1.973%
23	9.728	1141	1146	1151	rBV2	15813	24490	0.34%	0.027%
24	9.816	1157	1161	1165	rBV4	8013	14805	0.20%	0.016%
25	9.922	1169	1179	1184	rBV3	25147	47130	0.65%	0.052%
26	10.028	1189	1197	1212	rVV	1715993	2786131	38.40%	3.082%
27	10.193	1218	1225	1235	rBV	127519	249951	3.45%	0.277%
28	10.404	1252	1261	1271	rBV	1676036	2727389	37.59%	3.017%
29	10.546	1278	1285	1309	rBV	1335399	2391261	32.96%	2.645%
30	10.810	1324	1330	1334	rVB7	5864	11973	0.17%	0.013%
31	10.951	1345	1354	1362	rVB6	15797	39810	0.55%	0.044%
32	11.151	1381	1388	1393	rBV3	53203	107576	1.48%	0.119%
33	11.198	1393	1396	1405	rVV5	20849	38400	0.53%	0.042%
34	11.351	1418	1422	1428	rVB4	20765	32088	0.44%	0.035%
35	11.828	1498	1503	1507	rBV4	13131	21586	0.30%	0.024%
36	11.910	1513	1517	1523	rVB2	9800	15867	0.22%	0.018%

LSC Area Percent Report

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Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

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_N\Methods\SFAM-EPA-BN041924.MA.M
Title : SVOA CALIBRATION

37	11.998	1523	1532	1538	rVB3	34431	56453	0.78%	0.062%
38	12.163	1555	1560	1565	rBV3	11580	21512	0.30%	0.024%
39	12.722	1650	1655	1661	rBV3	14623	26489	0.37%	0.029%
40	12.828	1669	1673	1677	rVB6	6496	11341	0.16%	0.013%
41	12.916	1683	1688	1692	rBV5	5349	9577	0.13%	0.011%
42	13.087	1707	1717	1725	rVV4	22003	44357	0.61%	0.049%
43	13.163	1725	1730	1735	rVV	25187	44661	0.62%	0.049%
44	13.234	1738	1742	1748	rVV7	8895	18896	0.26%	0.021%
45	13.310	1752	1755	1761	rVB5	10443	14291	0.20%	0.016%
46	13.687	1812	1819	1829	rBV	3045400	4277158	58.96%	4.732%
47	13.792	1834	1837	1843	rVB8	9787	16060	0.22%	0.018%
48	13.963	1855	1866	1874	rBV	3565351	5319675	73.33%	5.885%
49	14.169	1898	1901	1905	rVB3	14097	17852	0.25%	0.020%
50	14.210	1905	1908	1911	rBV	12256	18044	0.25%	0.020%
51	14.269	1912	1918	1929	rVB	2475819	3697892	50.97%	4.091%
52	14.492	1949	1956	1971	rBV	1459371	2400341	33.09%	2.655%
53	14.698	1987	1991	1999	rVB5	26824	48695	0.67%	0.054%
54	15.128	2061	2064	2068	rVB4	9522	13459	0.19%	0.015%
55	15.181	2068	2073	2074	rBV3	10064	14749	0.20%	0.016%
56	15.198	2074	2076	2081	rVB2	13416	15254	0.21%	0.017%
57	15.269	2081	2088	2098	rBV	4512928	6363847	87.72%	7.040%
58	15.392	2103	2109	2122	rVV	1352433	1911896	26.35%	2.115%
59	15.516	2125	2130	2138	rVB5	28780	61434	0.85%	0.068%
60	15.881	2188	2192	2195	rBV3	18482	30603	0.42%	0.034%
61	16.110	2227	2231	2234	rBV	19389	28572	0.39%	0.032%
62	16.233	2248	2252	2255	rBV3	19283	32347	0.45%	0.036%
63	16.404	2278	2281	2284	rBV	59864	79486	1.10%	0.088%
64	16.433	2284	2286	2290	rVB2	45141	48216	0.66%	0.053%
65	16.475	2290	2293	2295	rBV2	19357	24903	0.34%	0.028%
66	16.569	2307	2309	2314	rVB2	15888	18398	0.25%	0.020%
67	16.733	2335	2337	2343	rVB3	11454	15837	0.22%	0.018%
68	16.928	2364	2370	2377	rVB9	14518	39688	0.55%	0.044%
69	17.022	2377	2386	2393	rBV	3089601	4316008	59.49%	4.775%
70	17.122	2393	2403	2414	rVV2	4714333	6787193	93.55%	7.509%
71	17.204	2414	2417	2418	rVV2	17110	21620	0.30%	0.024%
72	17.222	2418	2420	2431	rVB9	28294	70040	0.97%	0.077%
73	17.698	2498	2501	2505	rVB5	29398	38408	0.53%	0.042%
74	17.804	2513	2519	2525	rBV2	63440	121793	1.68%	0.135%
75	17.863	2526	2529	2534	rVV4	35941	63708	0.88%	0.070%
76	17.928	2535	2540	2563	rVV	1302956	2000778	27.58%	2.213%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

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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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Title : SVOA CALIBRATION

77	18.357	2610	2613	2617	rVB6	24508	33532	0.46%	0.037%
78	18.404	2617	2621	2623	rBV	55248	79671	1.10%	0.088%
79	18.463	2629	2631	2640	rVB3	18949	31270	0.43%	0.035%
80	18.769	2679	2683	2691	rBV	93778	129578	1.79%	0.143%
81	18.839	2692	2695	2701	rVB3	30547	55945	0.77%	0.062%
82	18.986	2715	2720	2726	rBV2	75651	117911	1.63%	0.130%
83	19.069	2728	2734	2736	rVV2	296583	464740	6.41%	0.514%
84	19.098	2736	2739	2752	rVV2	1260200	2285181	31.50%	2.528%
85	19.216	2755	2759	2772	rVV	806632	1318479	18.17%	1.459%
86	19.322	2774	2777	2781	rVV	101801	162748	2.24%	0.180%
87	19.363	2781	2784	2787	rVV3	54569	96000	1.32%	0.106%
88	19.427	2789	2795	2801	rVV	5357921	7254842	100.00%	8.026%
89	19.480	2801	2804	2808	rVB	76834	88407	1.22%	0.098%
90	19.980	2885	2889	2894	rVB	109028	143662	1.98%	0.159%
91	20.310	2941	2945	2949	rBV	521356	715370	9.86%	0.791%
92	20.474	2970	2973	2977	rBV	156856	180534	2.49%	0.200%
93	20.598	2991	2994	2997	rBV2	99158	114625	1.58%	0.127%
94	20.957	3050	3055	3066	rBV	706316	1380574	19.03%	1.527%
95	21.257	3101	3106	3121	rBV	2561991	3781694	52.13%	4.184%
96	21.451	3135	3139	3144	rVB2	125935	167955	2.32%	0.186%
97	21.998	3229	3232	3236	rVB	100983	129270	1.78%	0.143%
98	22.610	3331	3336	3344	rVB2	240621	460176	6.34%	0.509%
99	23.957	3557	3565	3580	rVB2	2291486	5587228	77.01%	6.181%
100	24.157	3591	3599	3611	rVB	1416323	3444894	47.48%	3.811%

Sum of corrected areas: 90392319

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
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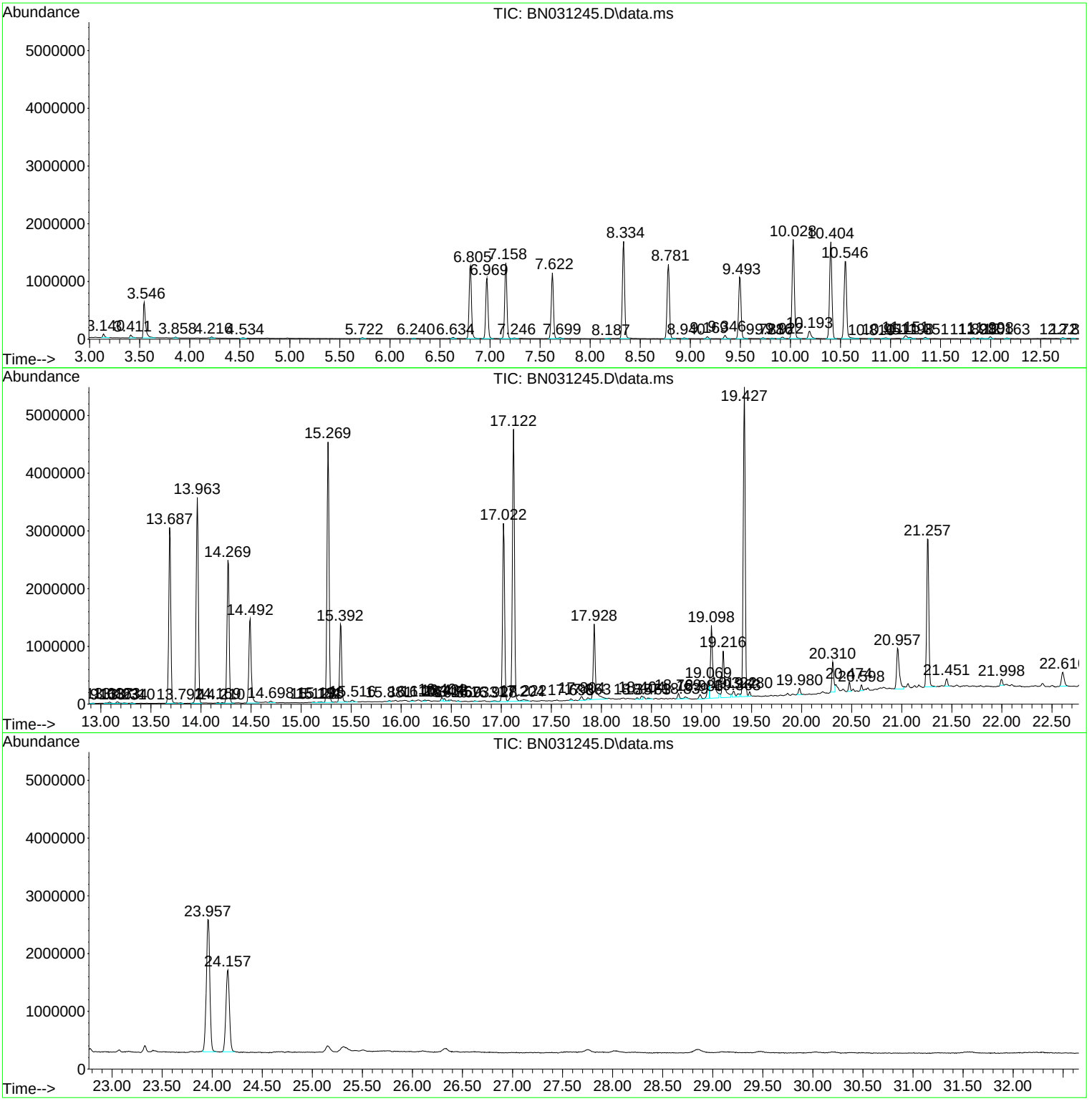
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

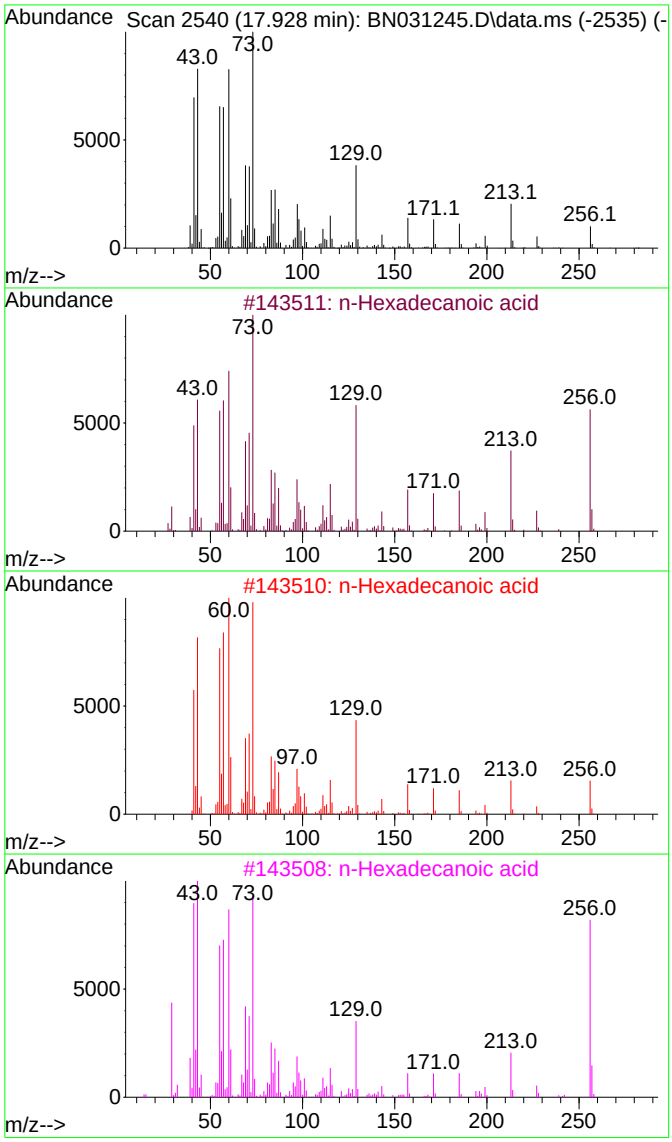
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

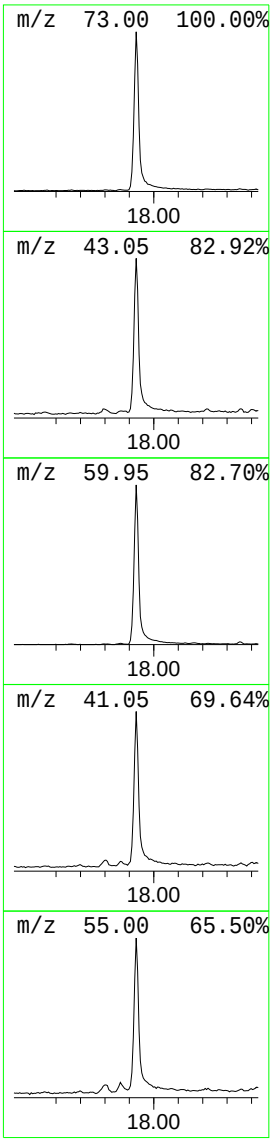
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.927	9.27 ng/ul	2000780	Phenanthrene-d10	17.022

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	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

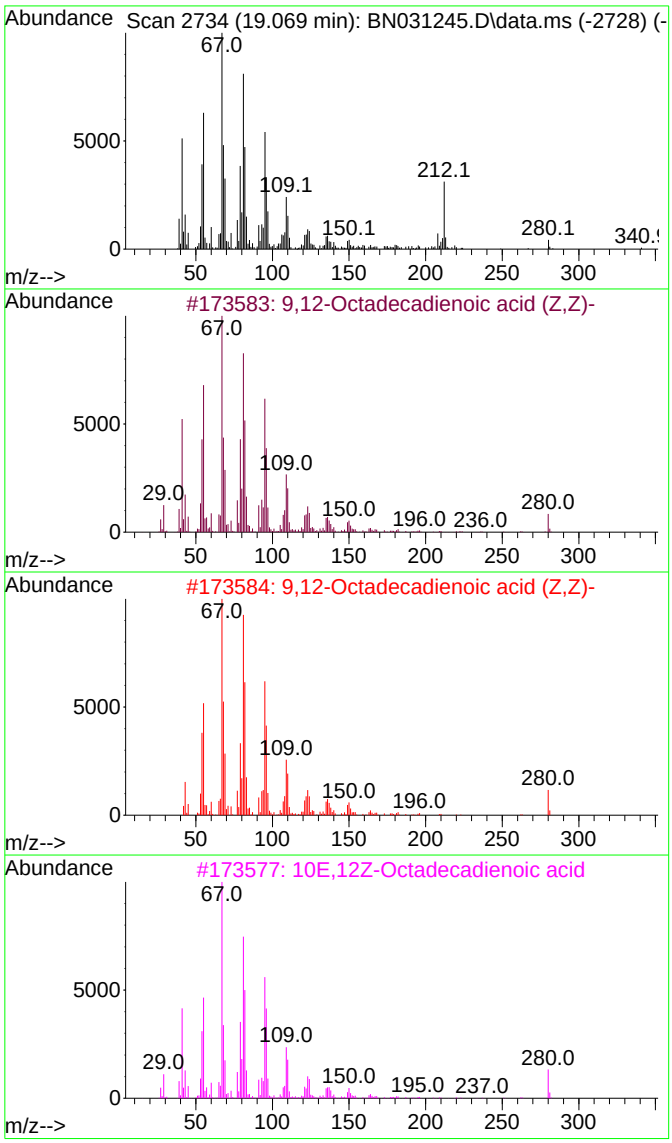
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

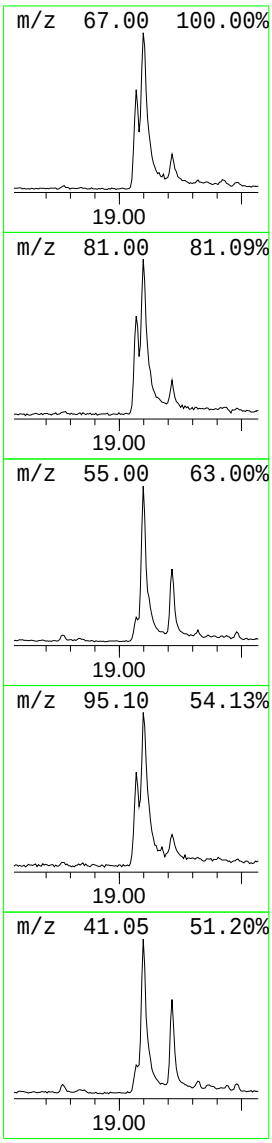
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 9,12-Octadecadienoic acid (... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.069	2.15 ng/ul	464740	Phenanthrene-d10	17.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
3	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
5	Linoelaidic acid	280	C18H32O2	000506-21-8	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

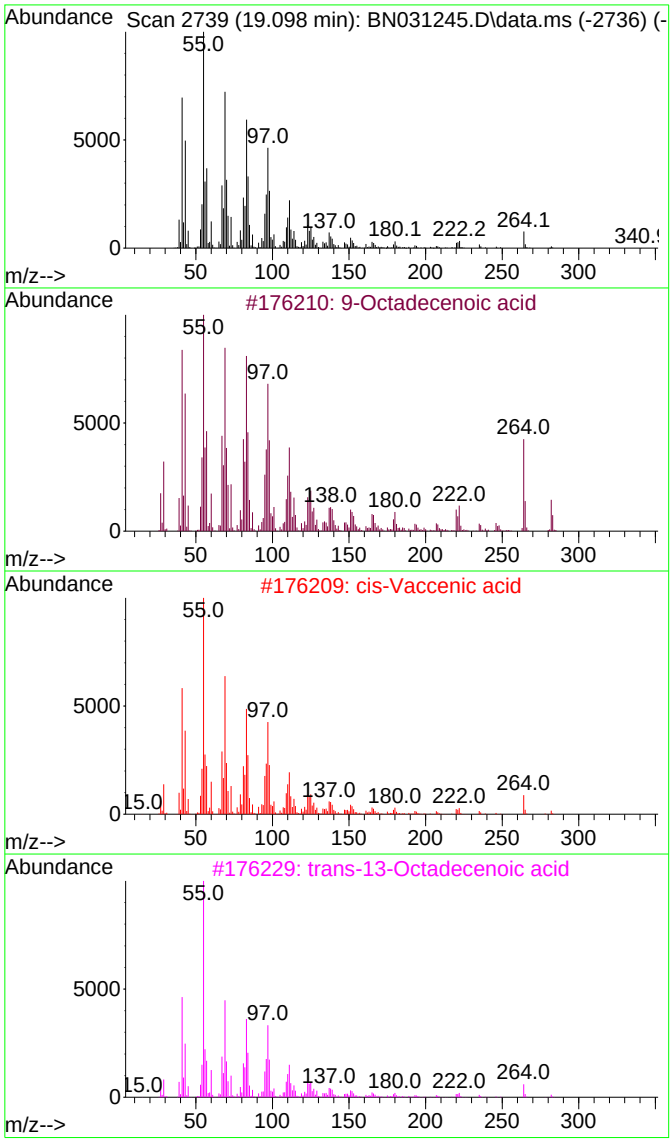
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

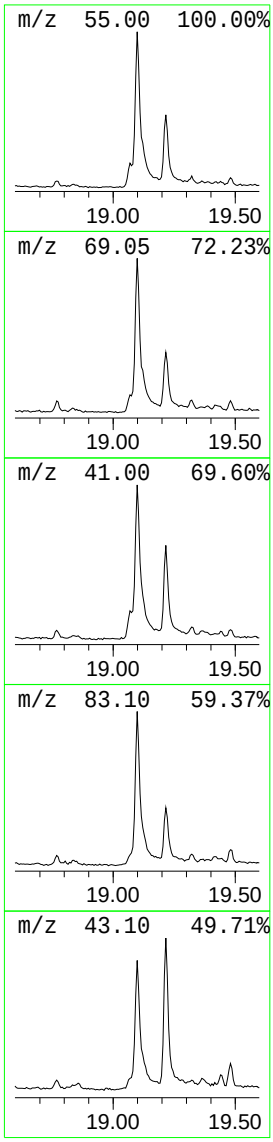
****

Peak Number 3 9-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.098	10.59 ng/ul	2285180	Phenanthrene-d10	17.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid	282	C18H34O2	002027-47-6	99
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	98
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	98
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97





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Data File : BN031245.D
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Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

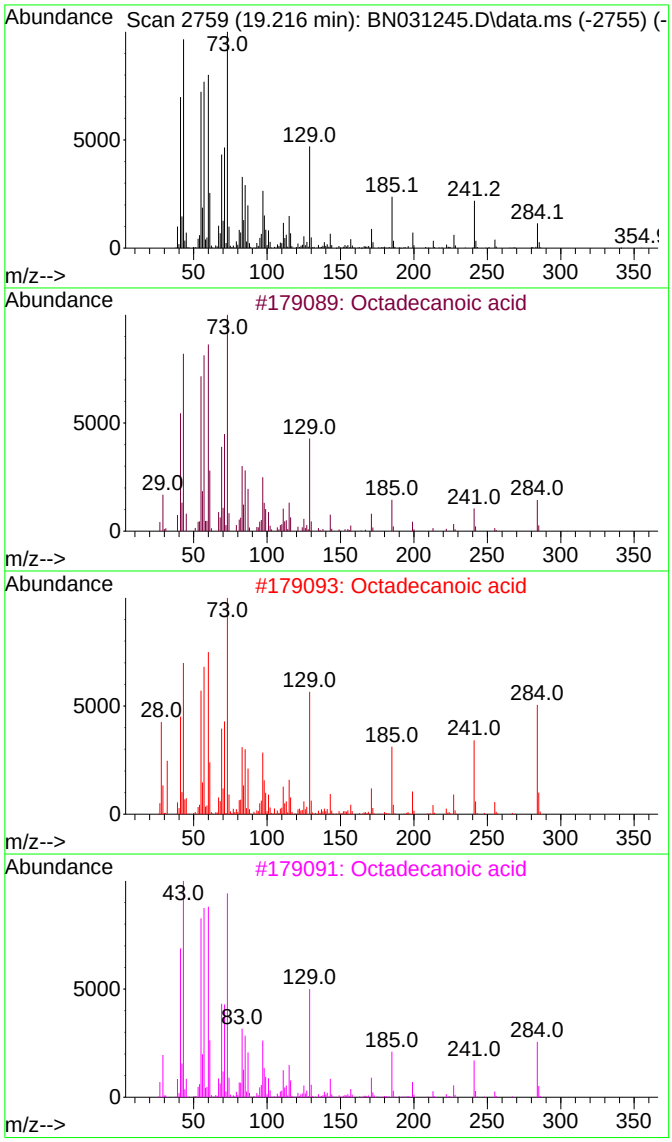
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

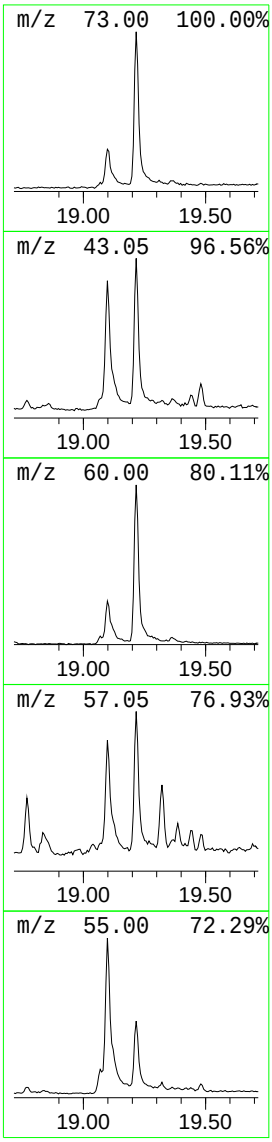
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.216	6.97 ng/ul	1318480	Chrysene-d12	21.263

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	99
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

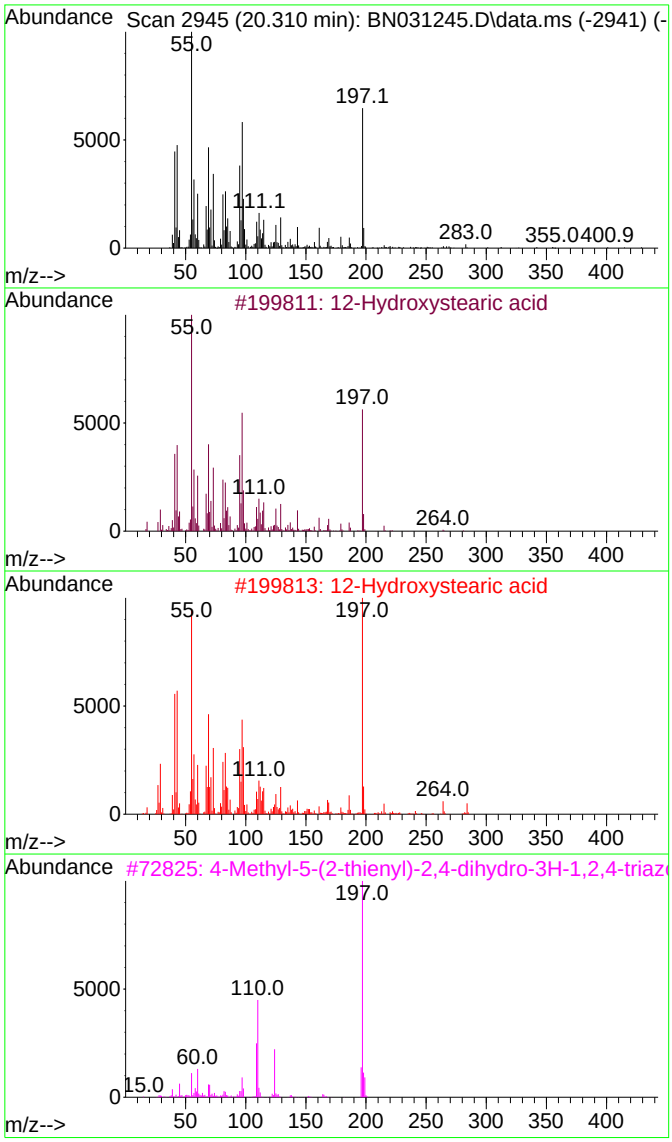
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

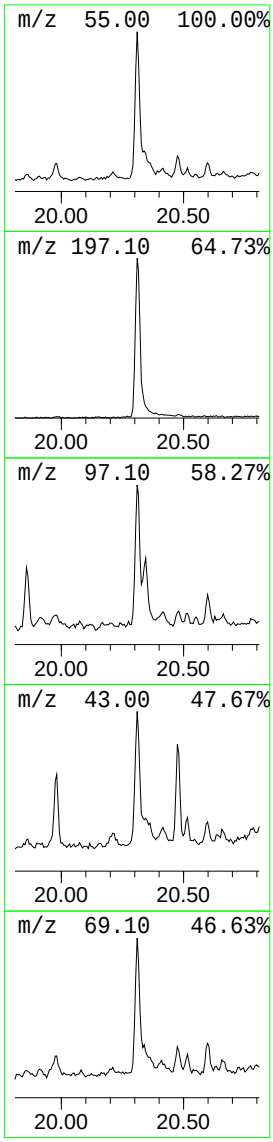
****

Peak Number 5 12-Hydroxystearic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.310	3.78 ng/ul	715370	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	94
2	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	49
3	4-Methyl-5-(2-thienyl)-2,4-dihyd...	197	C7H7N3S2	068744-66-1	22
4	Cyclopropanemethanol, 2,2,3,3-te...	128	C8H16O	002415-96-5	18
5	4-Methylcyclohexaneacetic acid (...	156	C9H16O2	1000453-59-2	14





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Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

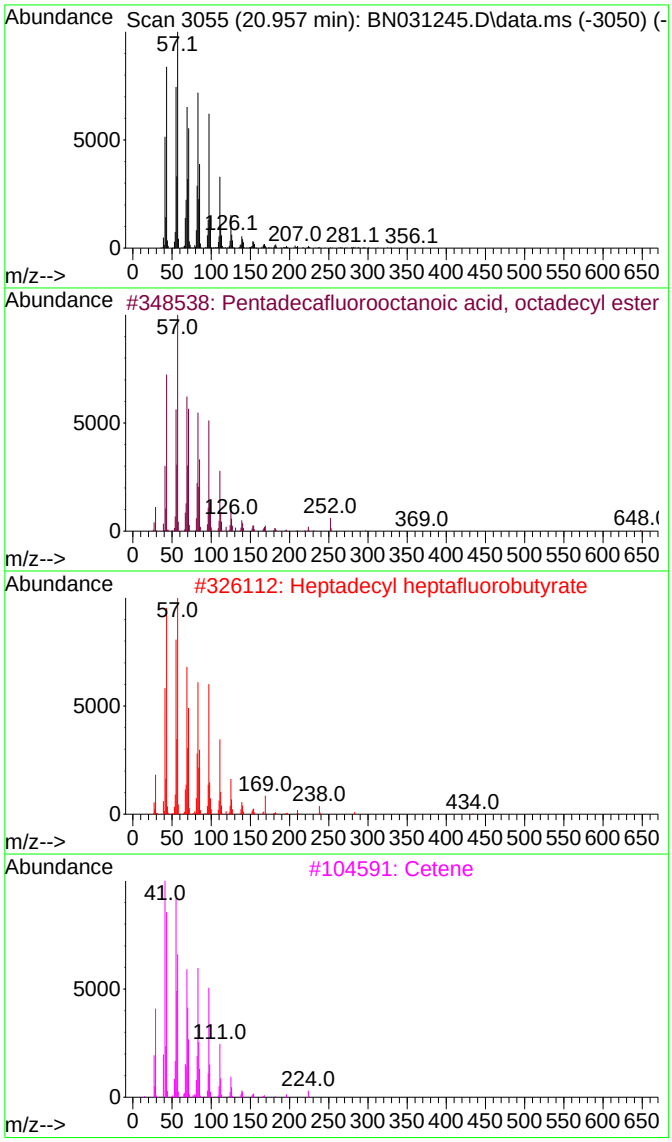
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

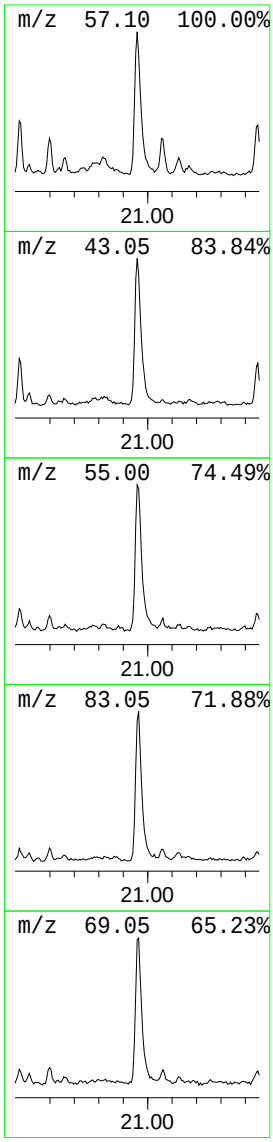
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	7.30 ng/ul	1380570	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Cetene	224	C16H32	000629-73-2	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

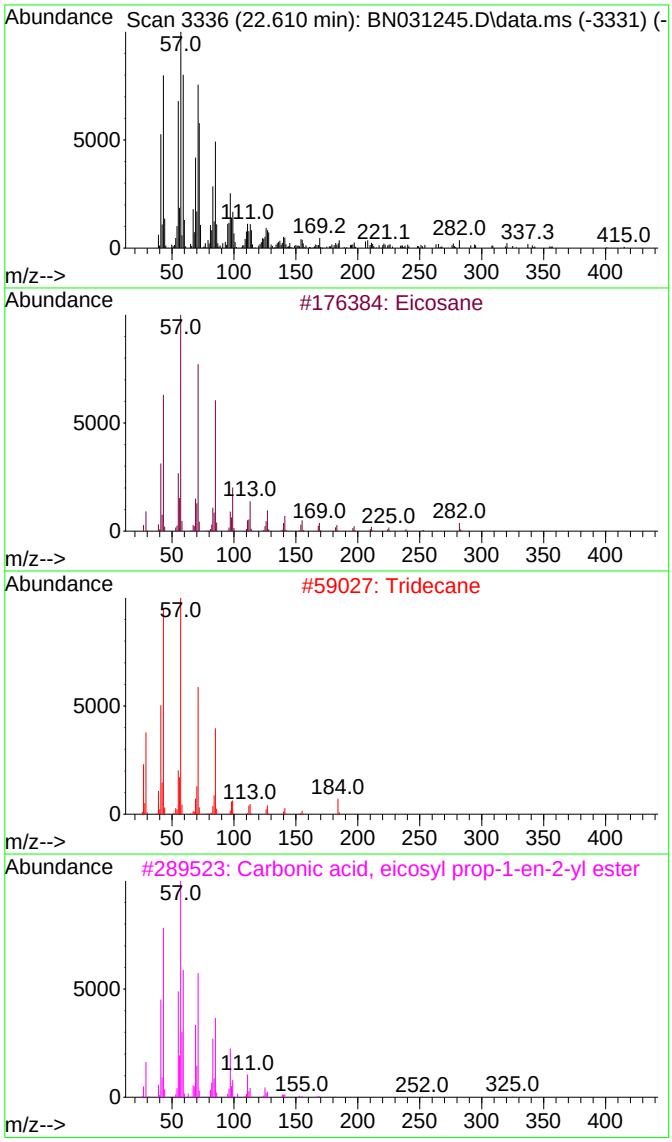
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.MA.M
Quant Title : SVOA CALIBRATION

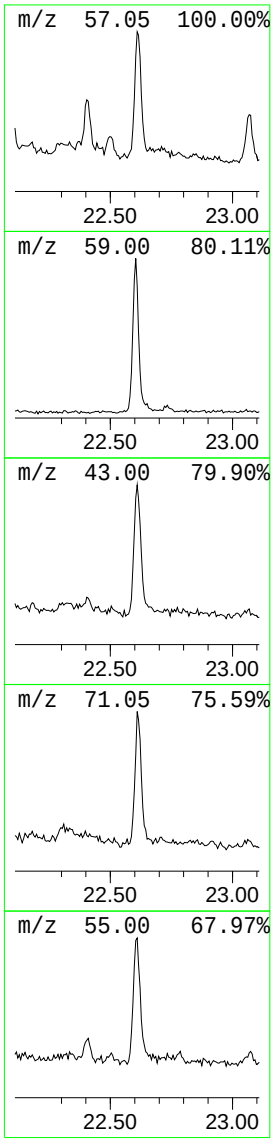
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.610	2.43 ng/ul	460176	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Tridecane	184	C13H28	000629-50-5	84
3	Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	76
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	66
5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN042624\
Data File : BN031245.D
Acq On : 26 Apr 2024 14:28
Operator : MA/JU
Sample : P2249-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E08N0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041924.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
n-Hexadecanoic ...	17.927	9.3	ng/ul	2000780	4	17.022	4316010	20.0
9,12-Octadecadi...	19.069	2.1	ng/ul	464740	4	17.022	4316010	20.0
9-Octadecenoic ...	19.098	10.6	ng/ul	2285180	4	17.022	4316010	20.0
Octadecanoic acid	19.216	7.0	ng/ul	1318480	5	21.263	3781690	20.0
12-Hydroxystear...	20.310	3.8	ng/ul	715370	5	21.263	3781690	20.0
Pentadecafluoro...	20.957	7.3	ng/ul	1380570	5	21.263	3781690	20.0
(DEL) Alkane: S...	22.610	2.4	ng/ul	460176	5	21.263	3781690	20.0