LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN102621\
Data File : BN017111.D
Acq On : 27 Oct 2021 03:58
Operator : CG/JU
Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW-1

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-BN102621.M
Title : SVOA CALIBRATION

Signal : TIC: BN017111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.069	10	14	21	rVB	70065	93757	0.78%	0.108%
2	3.464	77	81	102	rVB	351843	572847	4.79%	0.660%
3	3.693	116	120	125	rVB	42514	63741	0.53%	0.073%
4	3.787	132	136	141	rVB3	13762	22819	0.19%	0.026%
5	3.887	150	153	158	rVB3	15609	19312	0.16%	0.022%
6	5.952	500	504	509	rVB	16612	20825	0.17%	0.024%
7	6.722	628	635	647	rVB	278323	441471	3.69%	0.509%
8	6.887	656	663	673	rBV	1009271	1618937	13.53%	1.865%
9	7.069	688	694	707	rBV	1055632	1604072	13.41%	1.848%
10	7.163	707	710	716	rVB5	8678	15231	0.13%	0.018%
11	7.534	767	773	782	rBV	627901	959465	8.02%	1.105%
12	7.763	808	812	818	rVB4	8620	13522	0.11%	0.016%
13	8.246	888	894	907	rVB	830343	1311172	10.96%	1.511%
14	8.687	961	969	979	rBV	1256800	1993176	16.66%	2.296%
15	9.404	1084	1091	1101	rBV	1001733	1622787	13.56%	1.869%
16	9.934	1174	1181	1192	rBV	1442840	2374251	19.85%	2.735%
17	10.104	1204	1210	1228	rBV	470596	759812	6.35%	0.875%
18	10.310	1237	1245	1252	rBV	935313	1555176	13.00%	1.792%
19	10.451	1262	1269	1284	rBV	1426890	2437910	20.38%	2.809%
20	11.910	1511	1517	1525	rBV	29659	46601	0.39%	0.054%
21	12.534	1616	1623	1627	rBV5	7662	12231	0.10%	0.014%
22	12.792	1663	1667	1672	rVB2	10353	14787	0.12%	0.017%
23	13.098	1712	1719	1725	rBV	100653	150379	1.26%	0.173%
24	13.610	1800	1806	1819	rBV	3392809	4686757	39.18%	5.399%
25	13.875	1844	1851	1870	rBV	3704996	5446619	45.53%	6.275%
26	14.186	1898	1904	1913	rBV	1590098	2268790	18.96%	2.614%
27	14.410	1936	1942	1957	rBV	287051	461511	3.86%	0.532%
28	14.628	1973	1979	1987	rVB6	12788	15698	0.13%	0.018%
29	15.186	2068	2074	2087	rBV	5011919	7385189	61.73%	8.508%
30	15.316	2090	2096	2111	rVV	1969138	2577525	21.55%	2.969%
31	15.428	2111	2115	2120	rVB2	32782	43941	0.37%	0.051%
32	15.645	2147	2152	2156	rBV5	14472	20057	0.17%	0.023%
33	16.104	2225	2230	2236	rBV5	10661	21036	0.18%	0.024%
34	16.733	2331	2337	2344	rBV3	17263	25375	0.21%	0.029%
35	16.945	2367	2373	2382	rVB	1972347	2814417	23.53%	3.242%
36	17.045	2383	2390	2404	rVV	6189922	8975682	75.03%	10.340%

LSC Area Percent Report

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Data File : BN017111.D
Acq On : 27 Oct 2021 03:58
Operator : CG/JU
Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW-1

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-BN102621.M
Title : SVOA CALIBRATION

37	17.157	2404	2409	2415	rVB3	42971	57287	0.48%	0.066%
38	17.475	2459	2463	2469	rBV3	12351	19204	0.16%	0.022%
39	17.651	2488	2493	2498	rBV	178643	213019	1.78%	0.245%
40	17.869	2525	2530	2537	rBV	79468	115691	0.97%	0.133%
41	17.933	2539	2541	2546	rVB	10112	14034	0.12%	0.016%
42	18.169	2577	2581	2586	rBV4	11124	14929	0.12%	0.017%
43	18.798	2684	2688	2690	rBV	49282	58110	0.49%	0.067%
44	18.833	2690	2694	2698	rVB	555134	603312	5.04%	0.695%
45	18.910	2703	2707	2713	rVB2	87492	117134	0.98%	0.135%
46	18.974	2713	2718	2724	rBV2	201497	300761	2.51%	0.346%
47	19.163	2747	2750	2753	rBV2	16440	20743	0.17%	0.024%
48	19.351	2773	2782	2795	rBV	8082484	10759677	89.94%	12.395%
49	19.998	2889	2892	2898	rVB6	23456	31158	0.26%	0.036%
50	20.074	2902	2905	2909	rBV3	17043	19540	0.16%	0.023%
51	20.239	2930	2933	2938	rVB6	10657	15315	0.13%	0.018%
52	20.316	2941	2946	2949	rBV7	10021	18523	0.15%	0.021%
53	20.369	2952	2955	2961	rVB5	18506	28459	0.24%	0.033%
54	20.439	2964	2967	2971	rVB4	16929	20276	0.17%	0.023%
55	20.898	3041	3045	3053	rBV	109507	231526	1.94%	0.267%
56	21.098	3076	3079	3083	rVB	17863	19041	0.16%	0.022%
57	21.151	3083	3088	3101	rBV	2564060	3299962	27.58%	3.802%
58	21.339	3117	3120	3123	rBV2	32604	37916	0.32%	0.044%
59	21.768	3190	3193	3200	rBV	43564	59288	0.50%	0.068%
60	22.233	3268	3272	3275	rBV	76147	96029	0.80%	0.111%
61	22.357	3287	3293	3298	rBV	596167	777942	6.50%	0.896%
62	22.733	3353	3357	3364	rBV	131527	194571	1.63%	0.224%
63	23.227	3432	3441	3449	rBV2	6418049	11963080	100.00%	13.782%
64	23.304	3450	3454	3458	rVV	210131	375336	3.14%	0.432%
65	23.362	3458	3464	3482	rVB2	1965133	3699998	30.93%	4.262%
66	23.945	3558	3563	3572	rVB	173107	335200	2.80%	0.386%
67	24.698	3685	3691	3699	rVB2	160199	320906	2.68%	0.370%
68	25.574	3834	3840	3854	rVB3	109417	287531	2.40%	0.331%
69	26.603	4009	4015	4026	rVB4	71706	211198	1.77%	0.243%

Sum of corrected areas: 86803574

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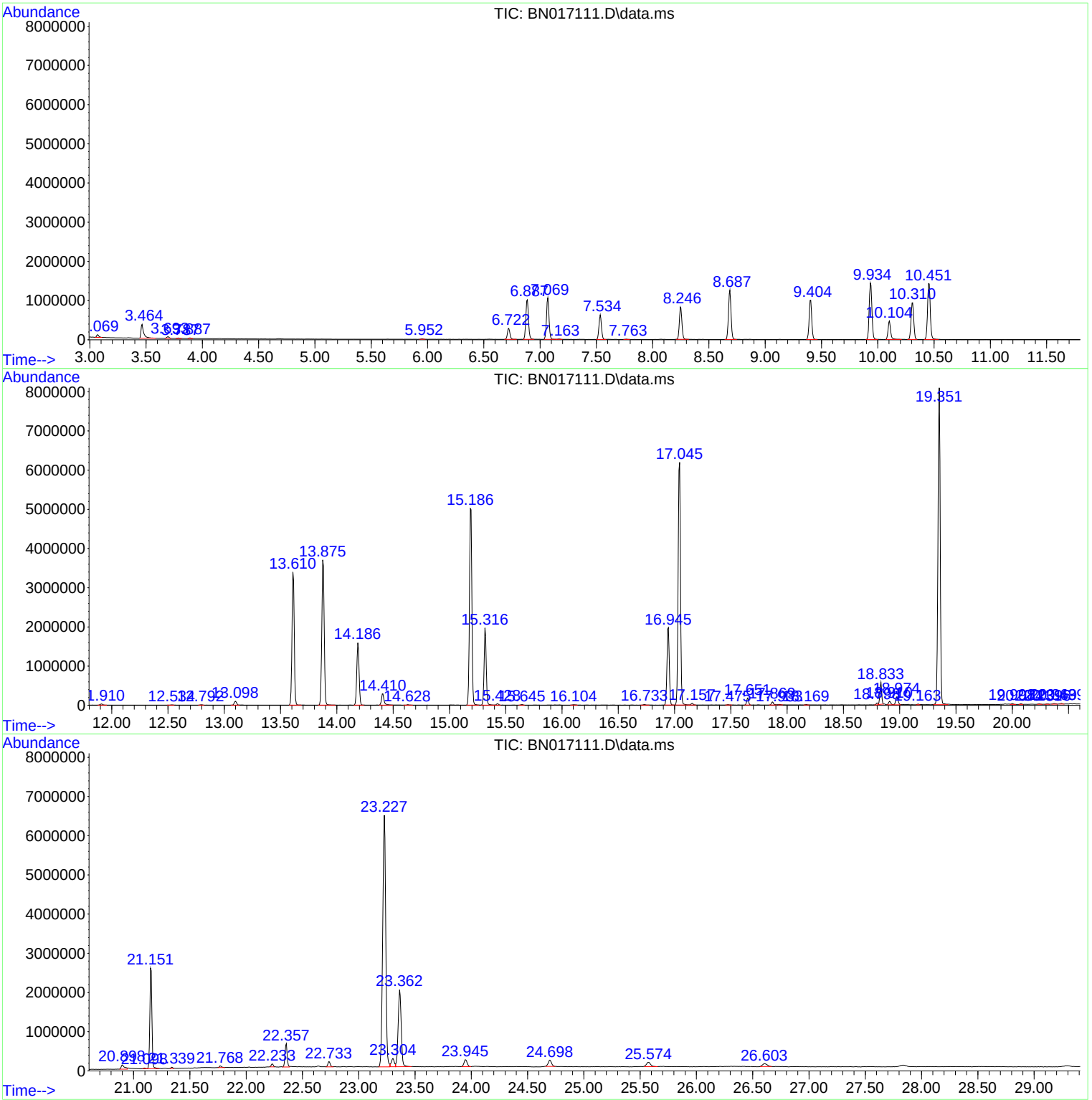
Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN102621.M
Quant Title : SVOA CALIBRATION

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



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Data File : BN017111.D
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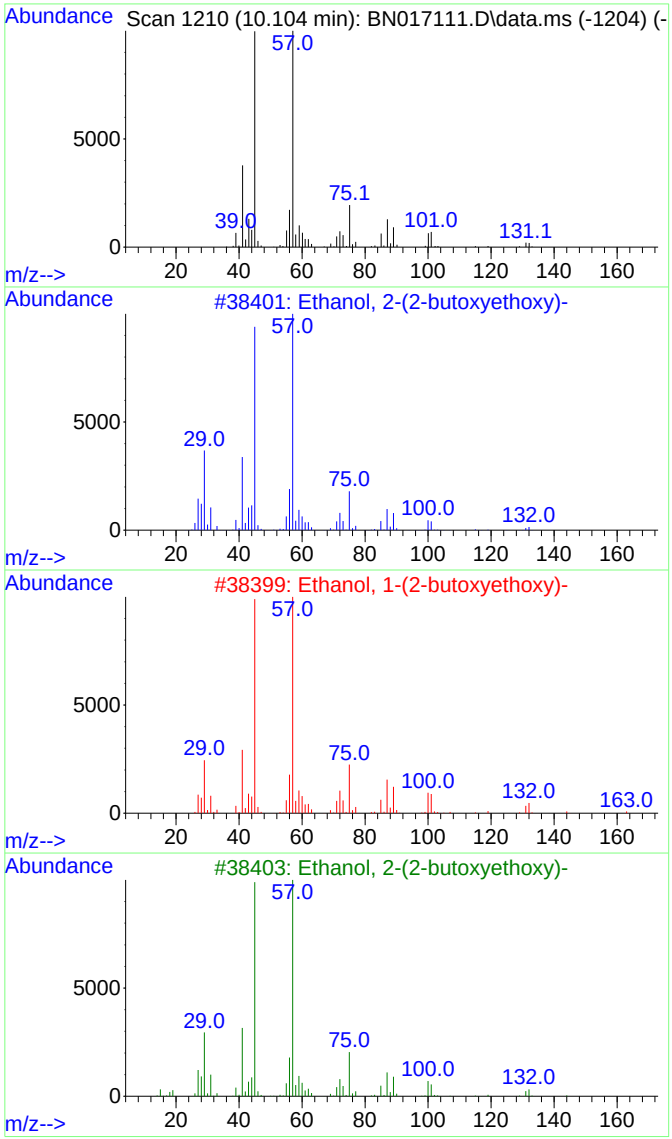
Quant Title : SVOA CALIBRATION

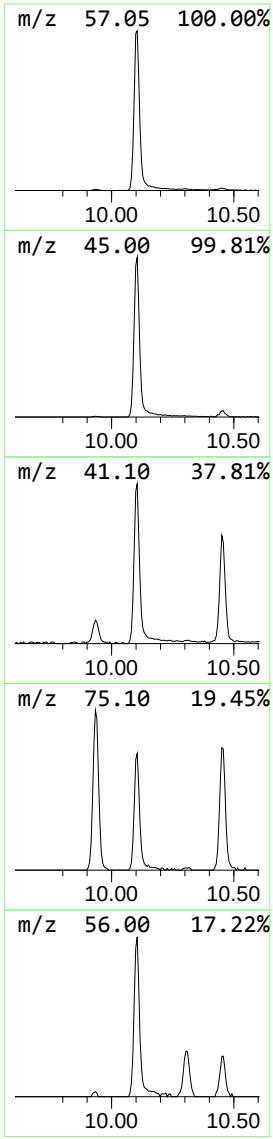
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.104	9.77 ng/ul	759812	Naphthalene-d8	10.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59





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Data File : BN017111.D
Acq On : 27 Oct 2021 03:58
Operator : CG/JU
Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW-1

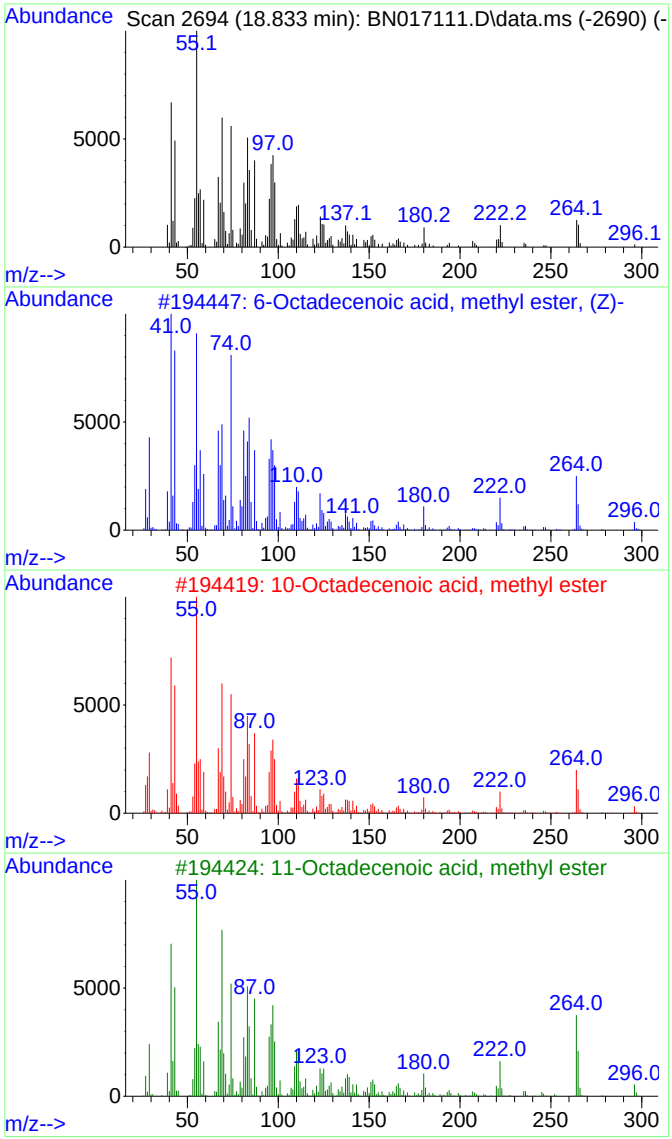
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN102621.M
Quant Title : SVOA CALIBRATION

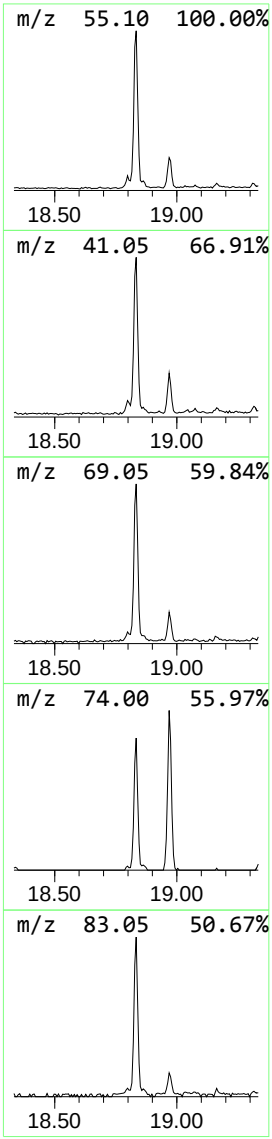
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 6-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.833	4.29 ng/ul	603312	Phenanthrene-d10	16.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN102621\
Data File : BN017111.D
Acq On : 27 Oct 2021 03:58
Operator : CG/JU
Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN102621.M
Quant Title : SVOA CALIBRATION

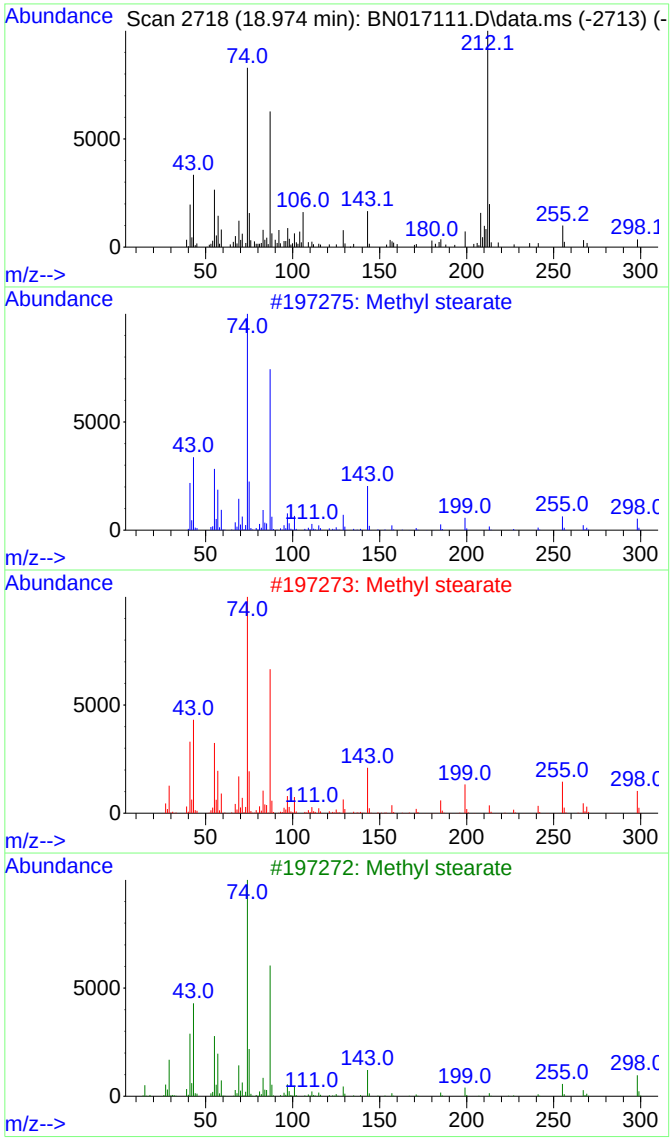
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

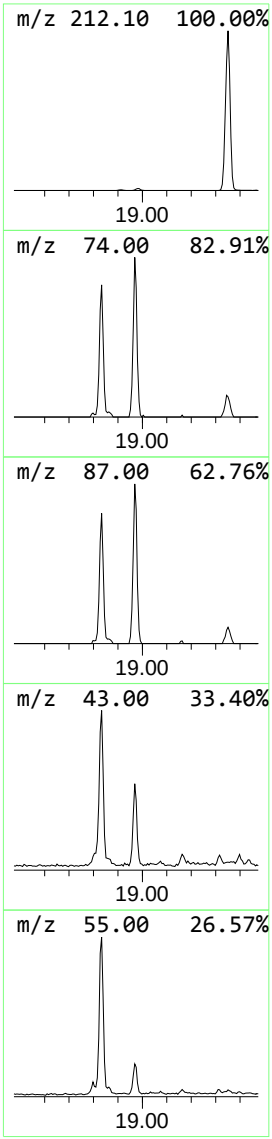
****

Peak Number 3 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	2.14 ng/ul	300761	Phenanthrene-d10	16.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	96
2	Methyl stearate	298	C19H38O2	000112-61-8	95
3	Methyl stearate	298	C19H38O2	000112-61-8	90
4	Methyl stearate	298	C19H38O2	000112-61-8	74
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN102621\
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Operator : CG/JU
Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN102621.M
Quant Title : SVOA CALIBRATION

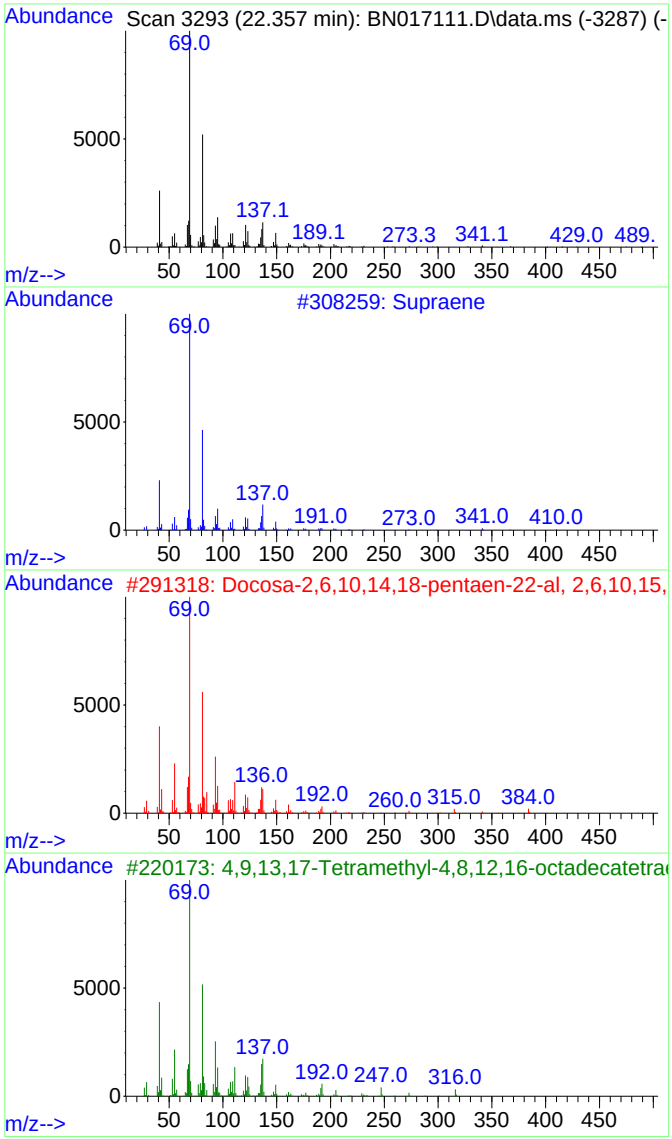
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

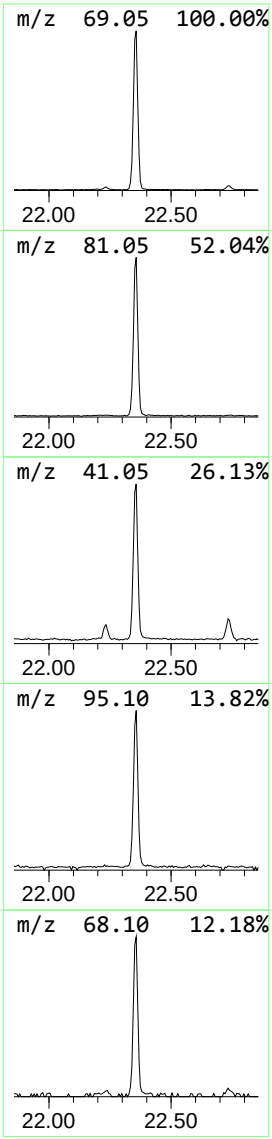
****

Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.357	4.21 ng/ul	777942	Perylene-d12	23.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	(2E,6E)-Farnesyl pentanoate	306	C20H34O2	126182-13-6	59





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Sample : M4307-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW-1

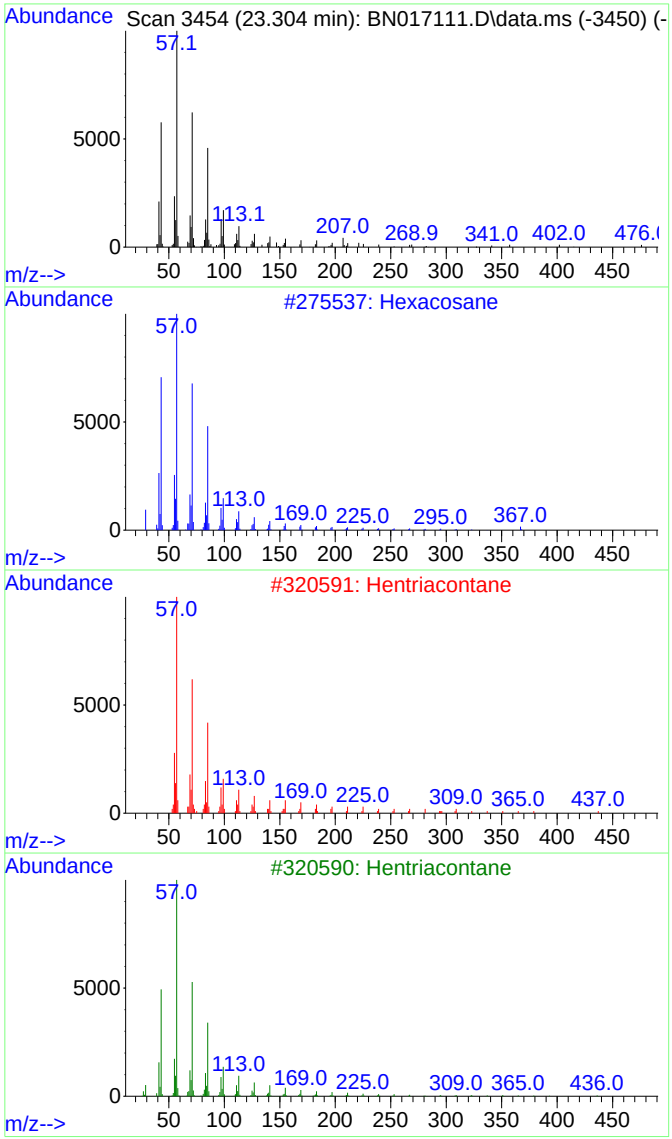
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN102621.M
Quant Title : SVOA CALIBRATION

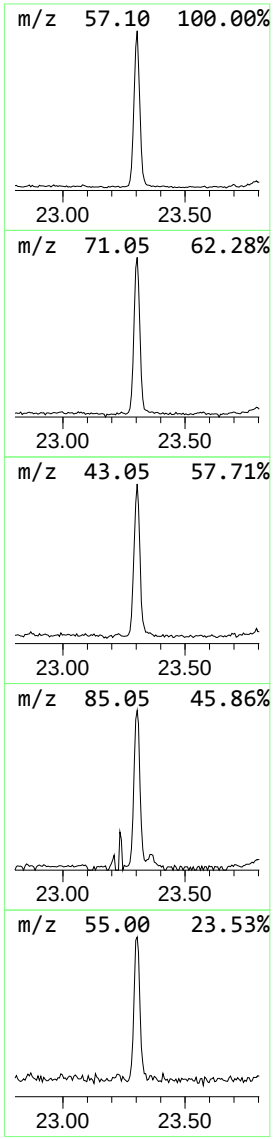
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.304	2.03 ng/ul	375336	Perylene-d12	23.362

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Hentriacontane	437	C31H64	000630-04-6	93
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN102621.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...	10.104	9.8	ng/ul	759812	2	10.310	1555180	20.0
6-Octadecenoic ...	18.833	4.3	ng/ul	603312	4	16.945	2814420	20.0
Methyl stearate	18.974	2.1	ng/ul	300761	4	16.945	2814420	20.0
Supraene	22.357	4.2	ng/ul	777942	6	23.362	3700000	20.0
(DEL) Alkane: S...	23.304	2.0	ng/ul	375336	6	23.362	3700000	20.0