LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061722\
Data File : BN020242.D
Acq On : 17 Jun 2022 16:46
Operator : CG/JU
Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : YB7L1

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-BN060622.M
Title : SVOA CALIBRATION

Signal : TIC: BN020242.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	9	11	19	rVV6	6321	11611	0.25%	0.027%
2	3.228	19	24	43	rVB2	399955	721911	15.33%	1.673%
3	3.664	95	98	111	rBV	168060	295912	6.28%	0.686%
4	3.905	134	139	144	rBV2	14099	22734	0.48%	0.053%
5	3.999	152	155	162	rVB2	7749	12528	0.27%	0.029%
6	4.528	239	245	255	rVB	79064	138488	2.94%	0.321%
7	4.793	287	290	294	rBV5	3557	5067	0.11%	0.012%
8	4.905	306	309	318	rVB4	8742	16768	0.36%	0.039%
9	5.093	335	341	349	rVB	135543	228095	4.84%	0.529%
10	6.399	556	563	570	rBV2	20486	35101	0.75%	0.081%
11	6.987	655	663	675	rBV	128019	223351	4.74%	0.518%
12	7.122	679	686	696	rBV	535088	880887	18.70%	2.041%
13	7.199	696	699	710	rVB	5990	12676	0.27%	0.029%
14	7.334	715	722	734	rBV	516700	950017	20.17%	2.201%
15	7.793	793	800	808	rBV	363119	611896	12.99%	1.418%
16	8.516	916	923	932	rBV	389219	668184	14.19%	1.548%
17	8.587	932	935	944	rVB4	13886	26784	0.57%	0.062%
18	8.940	988	995	1007	rBV	697784	1199827	25.48%	2.780%
19	9.110	1022	1024	1032	rVB6	3229	5420	0.12%	0.013%
20	9.399	1070	1073	1081	rVB2	6162	10356	0.22%	0.024%
21	9.663	1110	1118	1127	rBV	587217	982578	20.86%	2.277%
22	10.216	1205	1212	1226	rBV	819911	1449516	30.78%	3.359%
23	10.504	1256	1261	1267	rBV6	4778	11377	0.24%	0.026%
24	10.581	1267	1274	1283	rVB	618520	1069368	22.71%	2.478%
25	10.716	1290	1297	1310	rBV	281349	532481	11.31%	1.234%
26	11.399	1407	1413	1427	rBV2	37394	71873	1.53%	0.167%
27	12.075	1524	1528	1538	rBV4	2864	5726	0.12%	0.013%
28	12.169	1538	1544	1550	rBV	16063	27438	0.58%	0.064%
29	13.281	1727	1733	1738	rBV	19764	32845	0.70%	0.076%
30	13.834	1820	1827	1840	rBV	1799716	2557629	54.31%	5.927%
31	14.110	1867	1874	1893	rBV	1877020	2875930	61.07%	6.664%
32	14.281	1899	1903	1907	rVB4	4840	7228	0.15%	0.017%
33	14.422	1916	1927	1937	rBV	1021075	1545459	32.82%	3.581%
34	14.675	1960	1970	1979	rBV	81197	169045	3.59%	0.392%
35	14.781	1986	1988	1993	rVB4	5227	7556	0.16%	0.018%
36	14.851	1994	2000	2002	rVV7	12196	19076	0.41%	0.044%

LSC Area Percent Report

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Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
YB7L1

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-BN060622.M
Title : SVOA CALIBRATION

37	14.887	2002	2006	2013	rVB2	27078	42984	0.91%	0.100%
38	15.004	2020	2026	2030	rBV4	7213	11199	0.24%	0.026%
39	15.410	2085	2095	2108	rBV	2543258	3839486	81.52%	8.897%
40	15.534	2109	2116	2127	rVV	916696	1308578	27.79%	3.032%
41	15.651	2129	2136	2141	rVB	34048	52489	1.11%	0.122%
42	16.051	2200	2204	2209	rBV6	2713	5098	0.11%	0.012%
43	16.104	2209	2213	2217	rBV6	3150	4797	0.10%	0.011%
44	16.198	2224	2229	2237	rVB4	9910	16372	0.35%	0.038%
45	16.845	2334	2339	2341	rBV5	4482	5074	0.11%	0.012%
46	16.934	2350	2354	2358	rBV4	9111	16854	0.36%	0.039%
47	17.039	2367	2372	2376	rVB2	21452	30018	0.64%	0.070%
48	17.163	2386	2393	2402	rBV	1238448	1841224	39.10%	4.267%
49	17.263	2402	2410	2423	rBV	2659553	3944412	83.75%	9.140%
50	17.451	2438	2442	2448	rBV2	7043	10981	0.23%	0.025%
51	17.757	2490	2494	2497	rBV6	2987	5056	0.11%	0.012%
52	17.839	2504	2508	2515	rVB4	12765	20516	0.44%	0.048%
53	18.069	2541	2547	2555	rBV	220266	340730	7.23%	0.790%
54	18.134	2555	2558	2562	rVB	15825	23157	0.49%	0.054%
55	18.392	2600	2602	2607	rVB4	7679	10669	0.23%	0.025%
56	18.545	2623	2628	2633	rBV4	19297	31192	0.66%	0.072%
57	19.122	2720	2726	2731	rBV4	37942	59561	1.26%	0.138%
58	19.198	2733	2739	2742	rBV	43772	72158	1.53%	0.167%
59	19.351	2760	2765	2777	rBV	186027	297216	6.31%	0.689%
60	19.498	2787	2790	2793	rBV3	17478	20245	0.43%	0.047%
61	19.557	2794	2800	2808	rVV	3369061	4709583	100.00%	10.914%
62	19.804	2839	2842	2847	rVB3	15989	18229	0.39%	0.042%
63	20.116	2892	2895	2900	rBV2	16313	19807	0.42%	0.046%
64	20.569	2966	2972	2975	rBV2	40001	63776	1.35%	0.148%
65	20.616	2977	2980	2984	rVB2	24174	28403	0.60%	0.066%
66	21.080	3056	3059	3068	rBV6	56038	157745	3.35%	0.366%
67	21.351	3100	3105	3112	rBV	1492698	1910026	40.56%	4.426%
68	21.516	3130	3133	3137	rBV	54894	62034	1.32%	0.144%
69	21.963	3206	3209	3214	rBV	78733	98600	2.09%	0.228%
70	22.445	3287	3291	3298	rBV	126081	186352	3.96%	0.432%
71	22.974	3377	3381	3387	rVB	160062	237107	5.03%	0.549%
72	23.521	3466	3474	3480	rBV	1852998	3656824	77.65%	8.474%
73	23.574	3480	3483	3491	rVV	198169	339779	7.21%	0.787%
74	23.663	3492	3498	3510	rVB2	792133	1606116	34.10%	3.722%
75	24.257	3594	3599	3609	rVB	156936	332174	7.05%	0.770%
76	25.057	3730	3735	3744	rVB	123997	274164	5.82%	0.635%

LSC Area Percent Report

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Operator : CG/JU
Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
YB7L1

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_N\Methods\SFAM-EPA-BN060622.M
Title : SVOA CALIBRATION

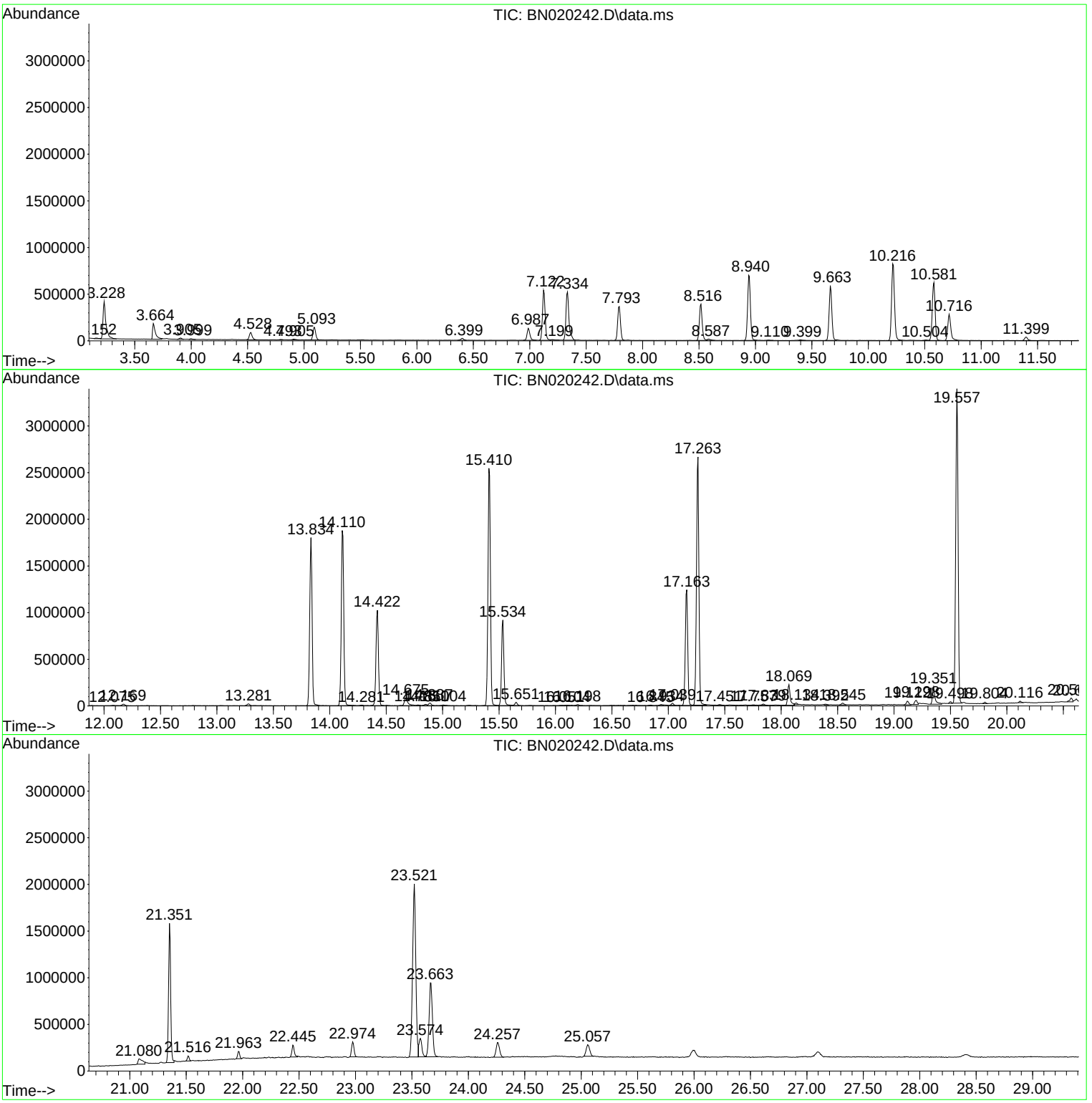
Sum of corrected areas: 43153523

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061722\
Data File : BN020242.D
Acq On : 17 Jun 2022 16:46
Operator : CG/JU
Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061722\
Data File : BN020242.D
Acq On : 17 Jun 2022 16:46
Operator : CG/JU
Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

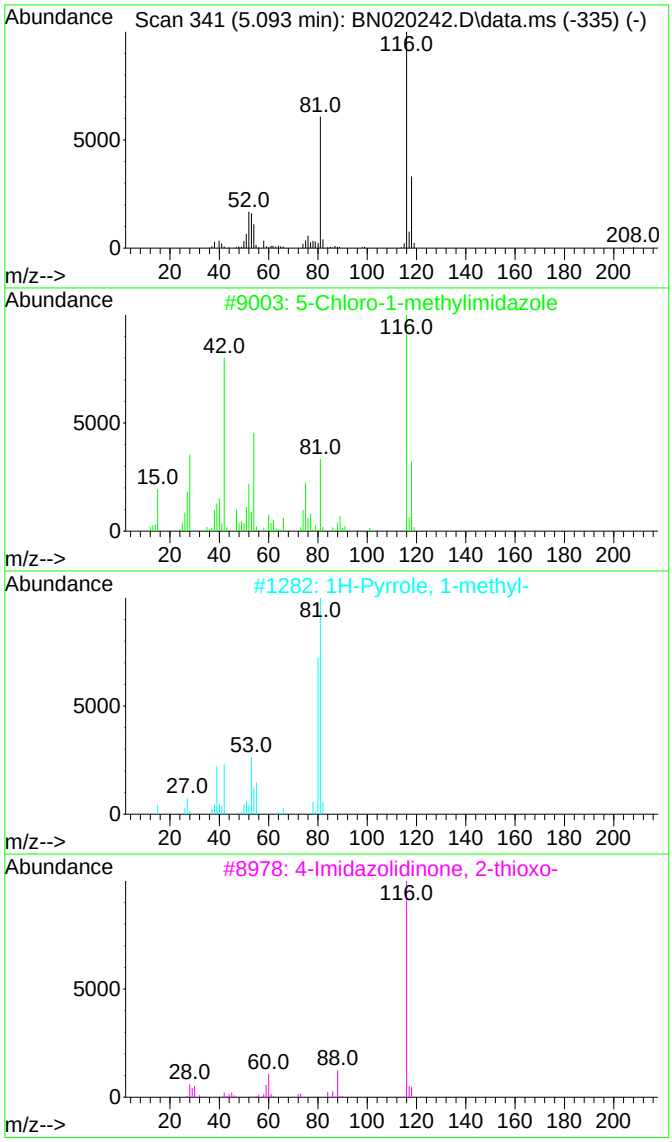
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

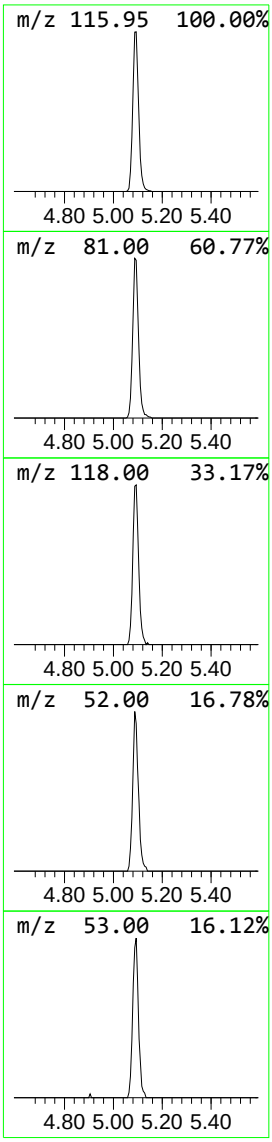
****

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	7.46 ng/ul	228095	1,4-Dichlorobenzene-d4	7.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Chloro-1-methylimidazole	116	C4H5ClN2	000872-49-1	45
2	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	10
3	4-Imidazolidinone, 2-thioxo-	116	C3H4N2OS	000503-87-7	9
4	Pyrimidine,4,6-difluoro-	116	C4H2F2N2	002802-62-2	9
5	Pyrimidine,2,4-difluoro-	116	C4H2F2N2	002802-61-1	9





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Data File : BN020242.D
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Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

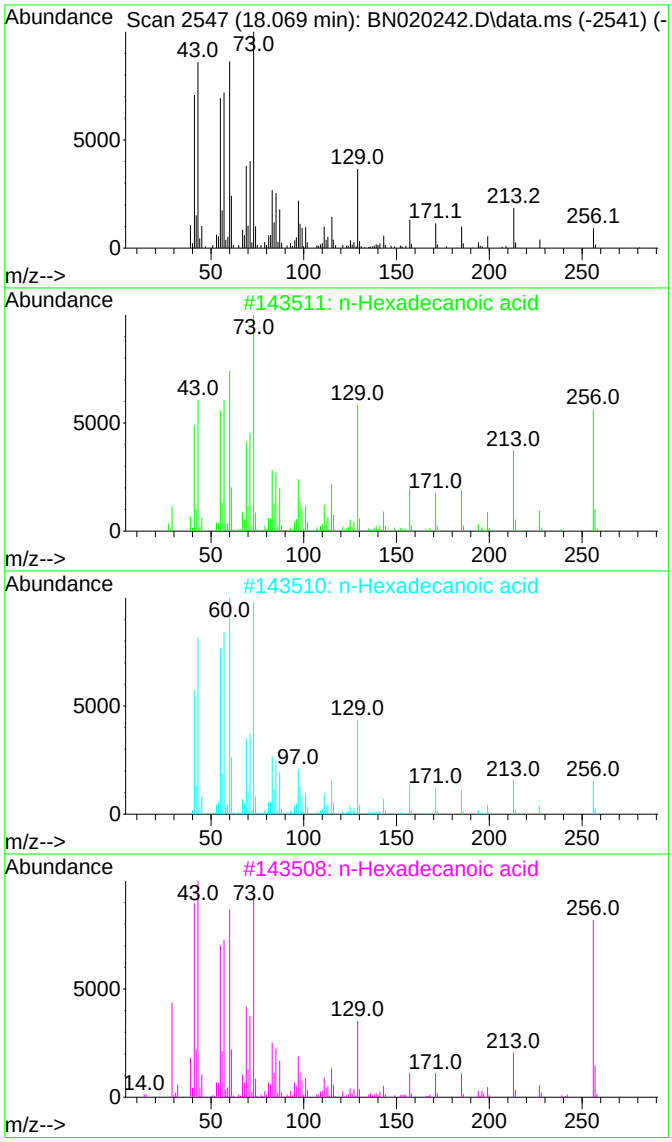
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

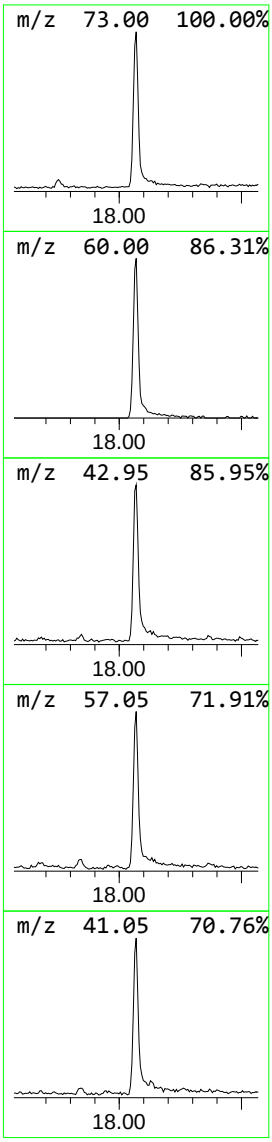
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	3.70 ng/ul	340730	Phenanthrene-d10	17.163

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	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061722\
Data File : BN020242.D
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Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

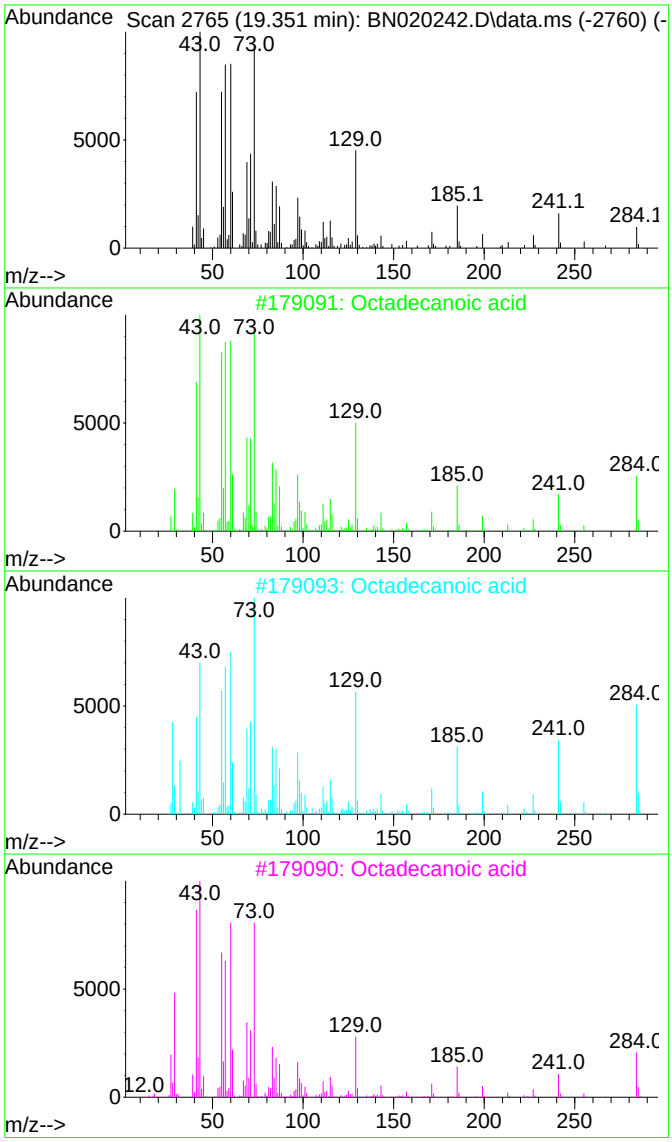
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

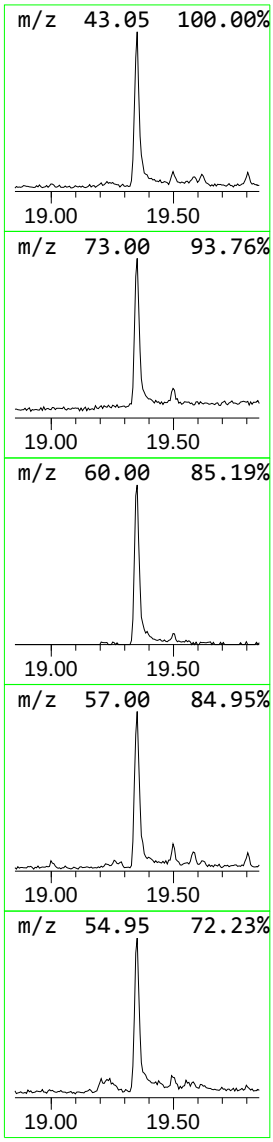
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	3.11 ng/ul	297216	Chrysene-d12	21.351

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	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061722\
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ALS Vial : 13 Sample Multiplier: 1

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BNA_N
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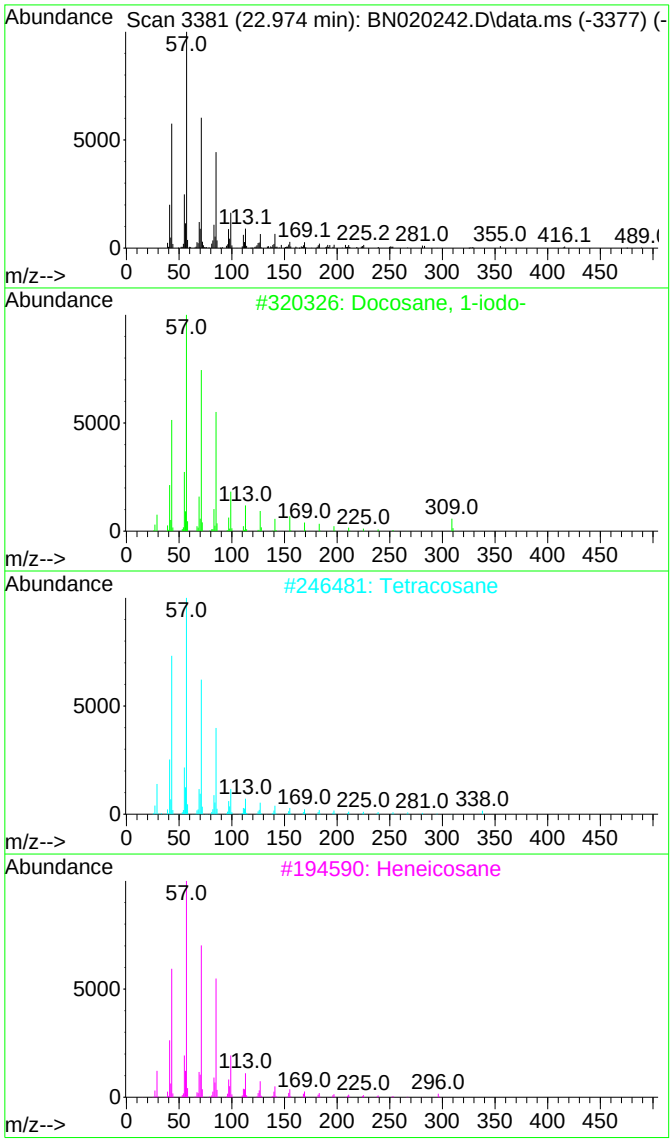
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

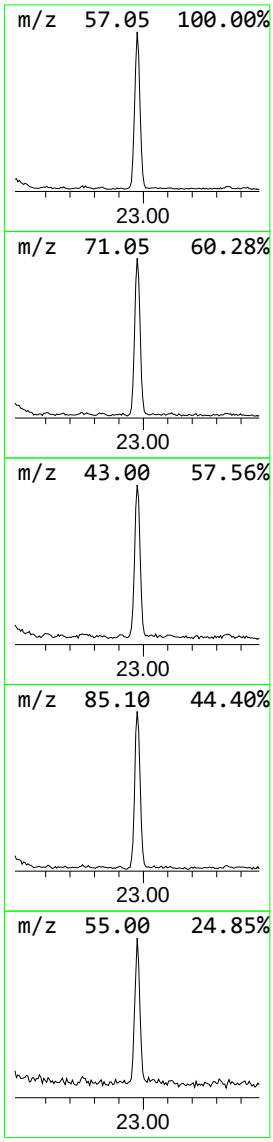
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Docosane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.974	2.95 ng/ul	237107	Perylene-d12	23.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	90





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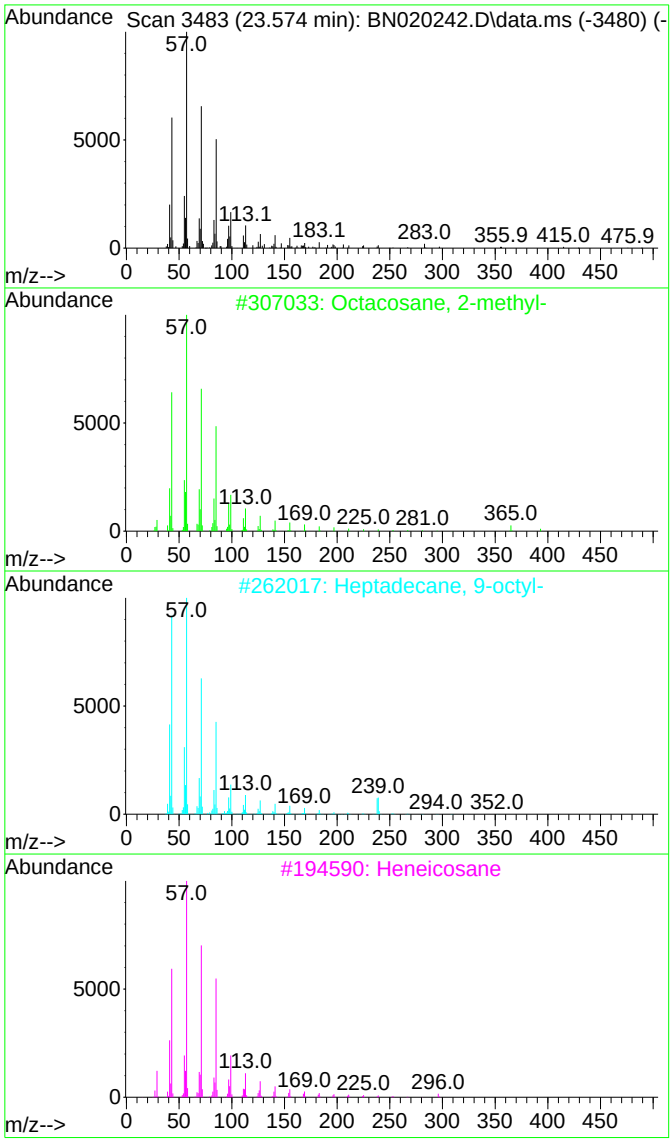
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

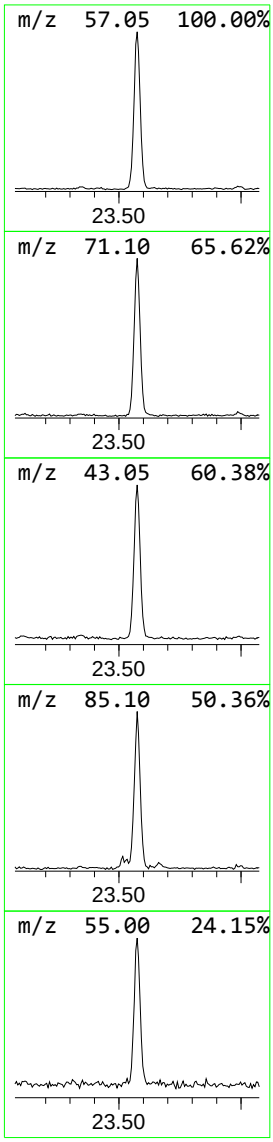
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.574	4.23 ng/ul	339779	Perylene-d12	23.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





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Data File : BN020242.D
Acq On : 17 Jun 2022 16:46
Operator : CG/JU
Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

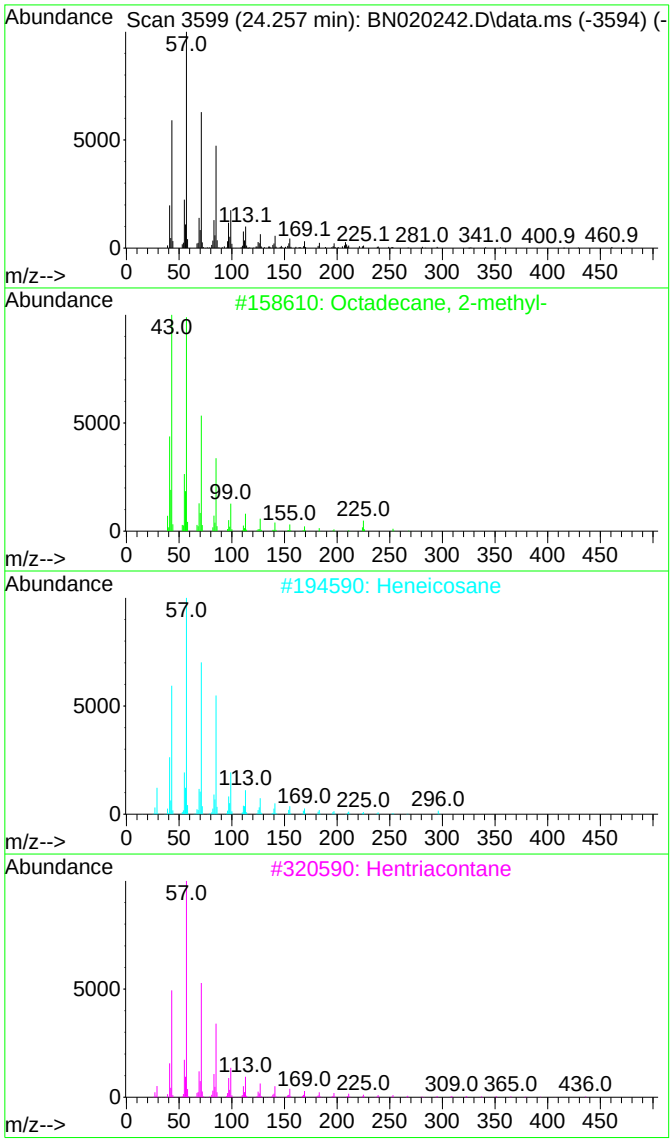
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

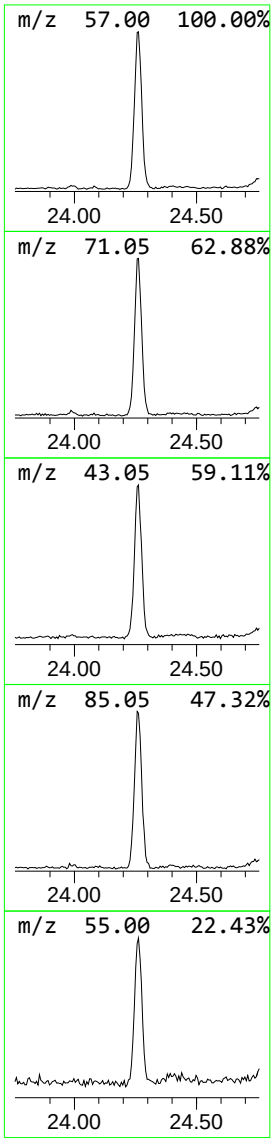
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.257	4.14 ng/ul	332174	Perylene-d12	23.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Tetracosane	338	C24H50	000646-31-1	90





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Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

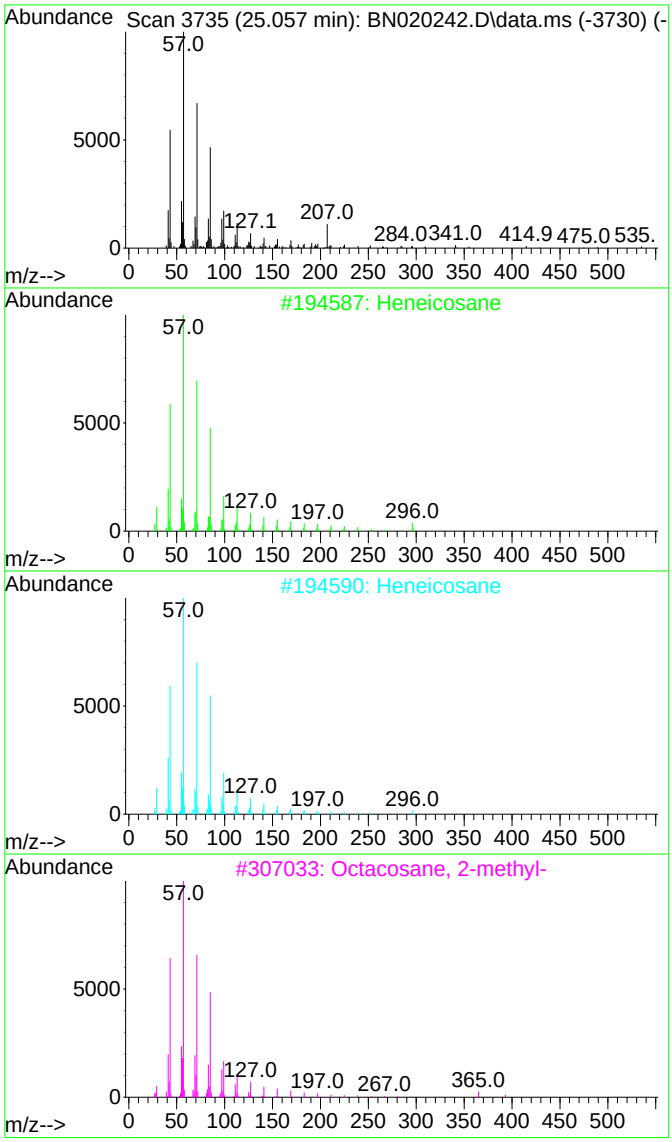
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.M
Quant Title : SVOA CALIBRATION

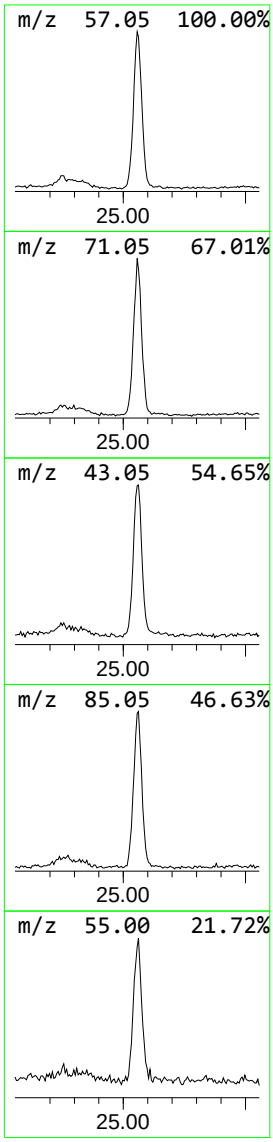
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.057	3.41 ng/ul	274164	Perylene-d12	23.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Heneicosane	296	C21H44	000629-94-7	93
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Hexacosane	366	C26H54	000630-01-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN061722\
Data File : BN020242.D
Acq On : 17 Jun 2022 16:46
Operator : CG/JU
Sample : N3313-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YB7L1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN060622.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
unknown-01	5.093	7.5	ng/ul	228095	1	7.793	611896	20.0
n-Hexadecanoic ...	18.069	3.7	ng/ul	340730	4	17.163	1841220	20.0
Octadecanoic acid	19.351	3.1	ng/ul	297216	5	21.351	1910030	20.0
Docosane, 1-iodo-	22.974	3.0	ng/ul	237107	6	23.663	1606120	20.0
(DEL) Alkane: S...	23.574	4.2	ng/ul	339779	6	23.663	1606120	20.0
(DEL) Alkane: S...	24.257	4.1	ng/ul	332174	6	23.663	1606120	20.0
(DEL) Alkane: S...	25.057	3.4	ng/ul	274164	6	23.663	1606120	20.0