LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101422\
Data File : BN022113.D
Acq On : 14 Oct 2022 07:23
Operator : CG/JU
Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : C0BJ6

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-BN101222.M
Title : SVOA CALIBRATION

Signal : TIC: BN022113.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	41	45	55	rVB	32798	48724	1.27%	0.077%
2	3.722	123	125	131	rVV	12031	18425	0.48%	0.029%
3	3.811	136	140	147	rVB	20396	29775	0.77%	0.047%
4	3.934	155	161	167	rVB	39003	67504	1.76%	0.107%
5	4.034	172	178	184	rVB	16666	25556	0.67%	0.040%
6	4.422	240	244	251	rVB2	13441	20659	0.54%	0.033%
7	4.987	336	340	352	rVB	29384	51457	1.34%	0.081%
8	5.540	429	434	441	rBV3	7338	15121	0.39%	0.024%
9	5.922	492	499	503	rBV2	10952	16495	0.43%	0.026%
10	6.916	663	668	676	rBV8	10533	23912	0.62%	0.038%
11	7.110	689	701	713	rBV	640041	1080975	28.13%	1.711%
12	7.281	723	730	741	rVB	511354	823877	21.44%	1.304%
13	7.475	756	763	771	rBV	622233	991820	25.81%	1.570%
14	7.952	835	844	852	rBV	783934	1245140	32.40%	1.971%
15	8.669	959	966	977	rBV	706647	1170017	30.45%	1.852%
16	8.793	982	987	994	rVB	33916	56342	1.47%	0.089%
17	9.134	1038	1045	1052	rBV	605954	991194	25.79%	1.569%
18	9.293	1067	1072	1080	rVB7	10637	22363	0.58%	0.035%
19	9.528	1105	1112	1116	rBV	14020	23666	0.62%	0.037%
20	9.857	1162	1168	1181	rBV	490408	824840	21.46%	1.306%
21	10.199	1220	1226	1236	rVB6	9372	21012	0.55%	0.033%
22	10.399	1253	1260	1270	rBV	753446	1266527	32.96%	2.005%
23	10.557	1281	1287	1298	rBV	67383	123764	3.22%	0.196%
24	10.781	1314	1325	1332	rBV	1167738	2013398	52.39%	3.187%
25	10.834	1332	1334	1343	rVB2	19710	36725	0.96%	0.058%
26	10.928	1343	1350	1363	rBV	335341	596018	15.51%	0.944%
27	11.804	1494	1499	1508	rVB5	7063	17706	0.46%	0.028%
28	12.204	1562	1567	1569	rBV	12892	18571	0.48%	0.029%
29	12.251	1569	1575	1583	rVV	2268573	3439782	89.51%	5.446%
30	12.316	1583	1586	1592	rVV	7529	14783	0.38%	0.023%
31	12.375	1592	1596	1601	rVB2	15067	23791	0.62%	0.038%
32	12.451	1601	1609	1615	rVB	26351	39350	1.02%	0.062%
33	12.669	1641	1646	1652	rVB	21009	31510	0.82%	0.050%
34	13.440	1769	1777	1780	rVV2	17503	27973	0.73%	0.044%
35	13.475	1780	1783	1786	rVV3	17582	27296	0.71%	0.043%
36	13.516	1786	1790	1795	rVV	30921	51792	1.35%	0.082%

LSC Area Percent Report

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Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

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-BN101222.M
Title : SVOA CALIBRATION

37	13.569	1795	1799	1810	rVB9	6627	20514	0.53%	0.032%
38	13.951	1858	1864	1869	rVV3	23850	43679	1.14%	0.069%
39	14.039	1869	1879	1886	rVV	1299194	1841866	47.93%	2.916%
40	14.104	1886	1890	1895	rVV5	12655	24769	0.64%	0.039%
41	14.322	1920	1927	1939	rVB	1546325	2280040	59.33%	3.610%
42	14.516	1957	1960	1966	rVB	16469	21851	0.57%	0.035%
43	14.628	1969	1979	1986	rBV	1848232	2733034	71.12%	4.327%
44	14.828	2002	2013	2027	rBV	585022	920025	23.94%	1.457%
45	14.987	2035	2040	2044	rBV3	18301	32480	0.85%	0.051%
46	15.051	2044	2051	2057	rVV4	51254	108757	2.83%	0.172%
47	15.416	2106	2113	2116	rBV3	12110	21176	0.55%	0.034%
48	15.463	2116	2121	2127	rVB2	18522	29528	0.77%	0.047%
49	15.622	2141	2148	2154	rBV	1970932	2800144	72.87%	4.433%
50	15.739	2162	2168	2177	rBV	561786	750577	19.53%	1.188%
51	15.863	2185	2189	2194	rBV2	9879	15264	0.40%	0.024%
52	15.969	2201	2207	2213	rVB8	12966	29248	0.76%	0.046%
53	16.351	2265	2272	2278	rVV4	28856	66111	1.72%	0.105%
54	16.675	2323	2327	2334	rVB10	7835	15911	0.41%	0.025%
55	16.916	2364	2368	2372	rBV6	12034	18702	0.49%	0.030%
56	17.128	2397	2404	2408	rBV4	19153	34260	0.89%	0.054%
57	17.269	2423	2428	2435	rBV3	31548	53828	1.40%	0.085%
58	17.333	2435	2439	2441	rVV2	23361	29854	0.78%	0.047%
59	17.380	2441	2447	2453	rVV	2182090	3242335	84.37%	5.133%
60	17.422	2453	2454	2458	rVV	80353	86993	2.26%	0.138%
61	17.480	2458	2464	2476	rVV2	2011671	2940399	76.52%	4.655%
62	17.575	2476	2480	2490	rVB8	28631	52964	1.38%	0.084%
63	17.869	2526	2530	2534	rBV3	22608	27740	0.72%	0.044%
64	18.010	2552	2554	2557	rVV4	13140	16964	0.44%	0.027%
65	18.051	2557	2561	2568	rVB2	29118	41125	1.07%	0.065%
66	18.157	2574	2579	2583	rBV4	25679	38885	1.01%	0.062%
67	18.216	2584	2589	2594	rBV	152586	222260	5.78%	0.352%
68	18.280	2594	2600	2610	rVV	837014	1181647	30.75%	1.871%
69	18.451	2626	2629	2634	rVB3	19718	29876	0.78%	0.047%
70	18.492	2634	2636	2644	rVB2	15953	20850	0.54%	0.033%
71	18.569	2645	2649	2654	rBV2	43342	64505	1.68%	0.102%
72	18.704	2669	2672	2676	rVB4	14223	17267	0.45%	0.027%
73	18.769	2679	2683	2686	rVV2	24731	36340	0.95%	0.058%
74	18.804	2687	2689	2694	rVV6	17877	29586	0.77%	0.047%
75	18.857	2696	2698	2706	rVB5	14768	25084	0.65%	0.040%
76	19.133	2742	2745	2749	rBV6	14307	22381	0.58%	0.035%

LSC Area Percent Report

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Operator : CG/JU
Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

Integration Parameters: LSCINT.P
Integrator: RTE
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Sampling : 1 Min Area: 0.1 % of largest Peak
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Title : SVOA CALIBRATION

77	19.198	2749	2756	2759	rBV4	45646	85546	2.23%	0.135%
78	19.339	2778	2780	2787	rVB4	41747	64330	1.67%	0.102%
79	19.410	2788	2792	2794	rBV2	105303	143859	3.74%	0.228%
80	19.439	2794	2797	2807	rVB2	350370	648347	16.87%	1.026%
81	19.557	2812	2817	2826	rBV	280347	430906	11.21%	0.682%
82	19.780	2849	2855	2869	rVB	2558229	3725640	96.95%	5.898%
83	20.316	2939	2946	2953	rVB4	79865	153698	4.00%	0.243%
84	20.810	3027	3030	3034	rBV	75011	94981	2.47%	0.150%
85	20.980	3057	3059	3063	rVB2	51302	57979	1.51%	0.092%
86	21.280	3106	3110	3120	rBV	569427	860177	22.38%	1.362%
87	21.580	3155	3161	3166	rBV	2730215	3676699	95.68%	5.821%
88	21.727	3183	3186	3189	rBV2	109541	147021	3.83%	0.233%
89	22.080	3243	3246	3248	rBV4	84634	118637	3.09%	0.188%
90	22.198	3262	3266	3267	rBV2	180561	209338	5.45%	0.331%
91	22.704	3349	3352	3357	rVB2	173265	244526	6.36%	0.387%
92	22.968	3393	3397	3402	rVB3	168143	255744	6.66%	0.405%
93	23.280	3444	3450	3455	rBV2	767497	1351332	35.17%	2.139%
94	23.339	3455	3460	3473	rVB2	500626	1182267	30.77%	1.872%
95	23.886	3546	3553	3558	rBV2	1494668	3111105	80.96%	4.925%
96	24.051	3573	3581	3600	rVB	1568535	3573982	93.00%	5.658%
97	24.686	3682	3689	3699	rVB	890673	2011143	52.34%	3.184%
98	24.792	3701	3707	3719	rVB2	241832	713957	18.58%	1.130%
99	26.598	4009	4014	4033	rVB2	358441	1175203	30.58%	1.861%
100	27.603	4174	4185	4207	rBV3	900397	3842789	100.00%	6.084%

Sum of corrected areas: 63165885

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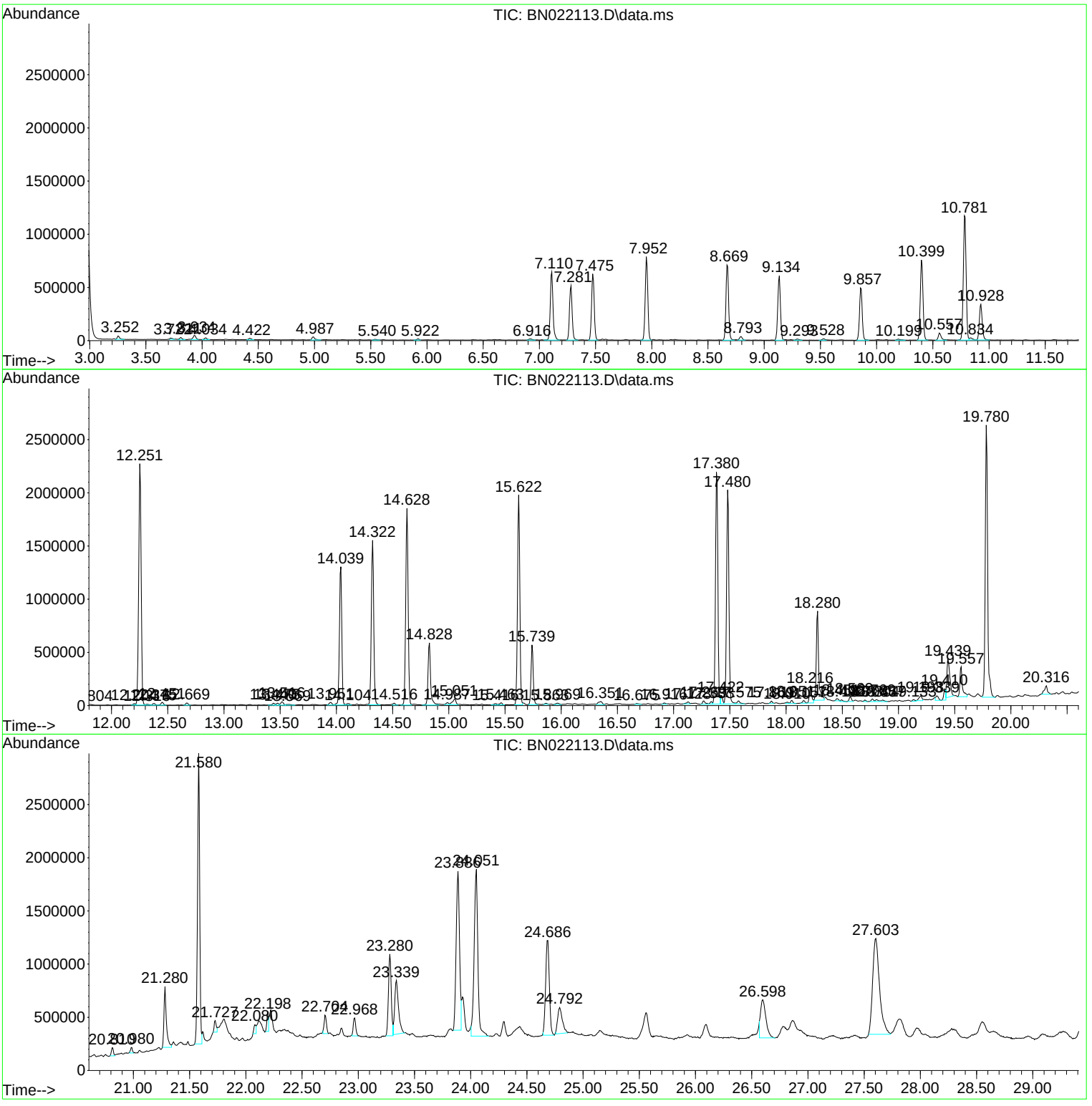
Instrument :
BNA_N
ClientSampleId :
C0BJ6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

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



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Data File : BN022113.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

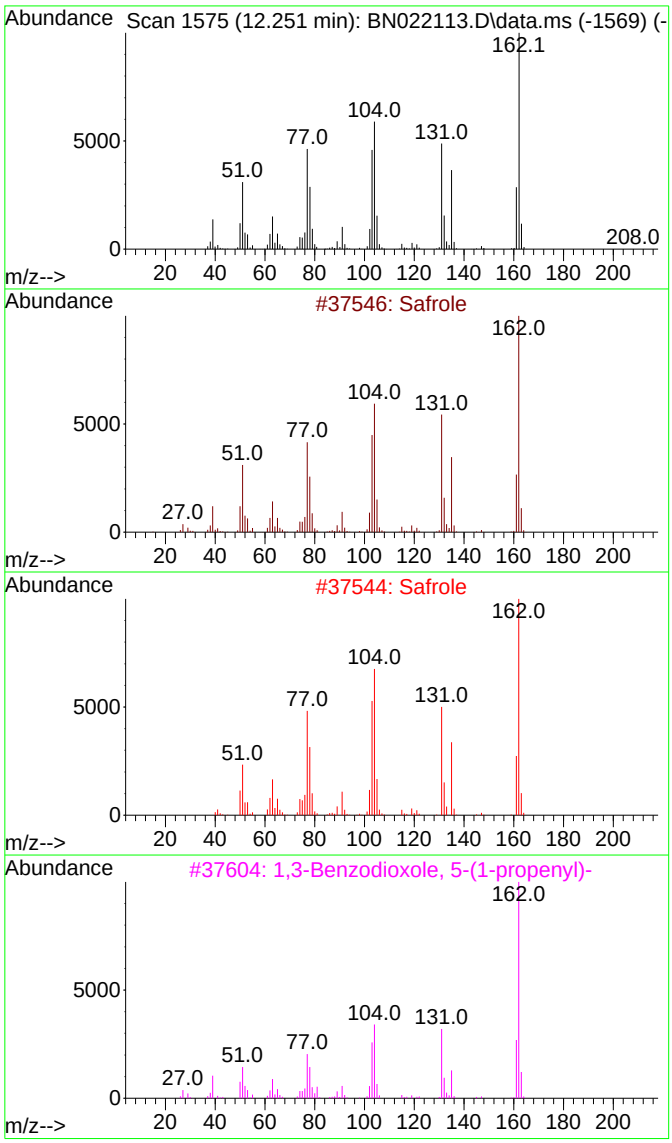
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

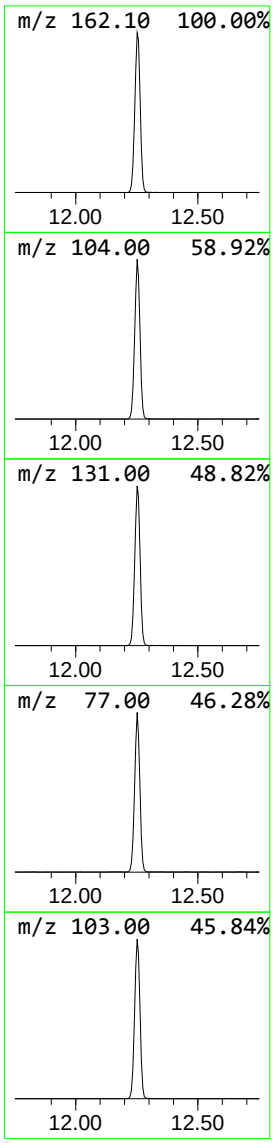
****

Peak Number 1 Safrole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.251	34.17 ng/ul	3439780	Naphthalene-d8	10.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	98
2	Safrole	162	C10H10O2	000094-59-7	98
3	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
4	Safrole	162	C10H10O2	000094-59-7	97
5	Safrole	162	C10H10O2	000094-59-7	97





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101422\
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Sample : N5049-06
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ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

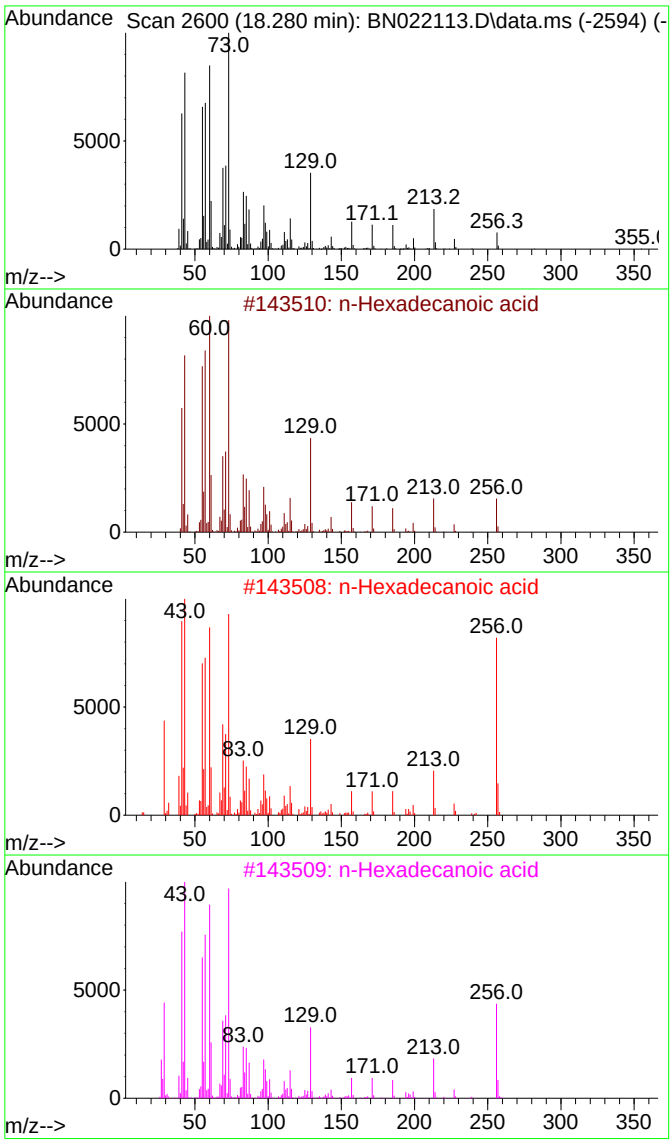
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

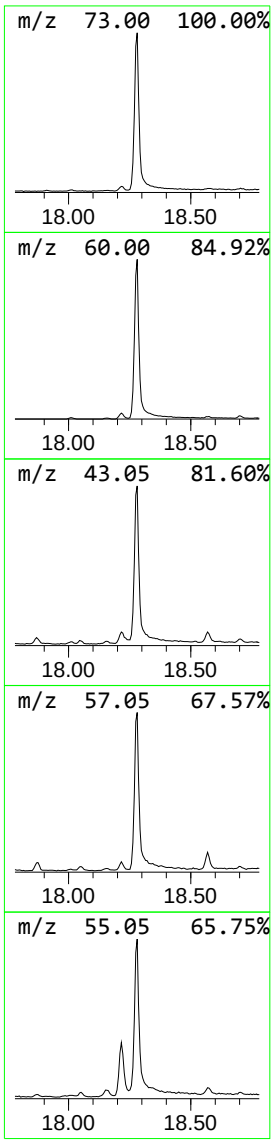
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.280	7.29 ng/ul	1181650	Phenanthrene-d10	17.381

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	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97





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ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

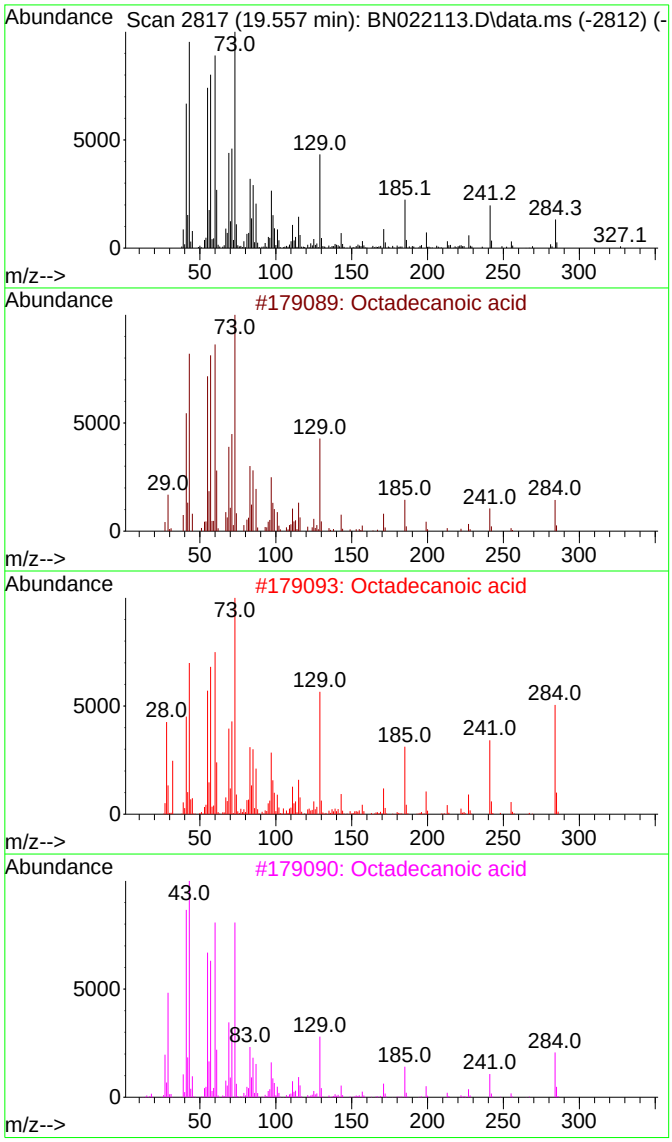
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

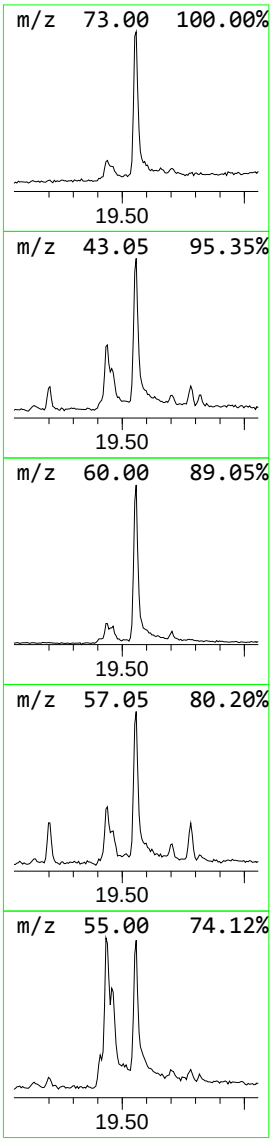
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.557	2.34 ng/ul	430906	Chrysene-d12	21.580

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	95





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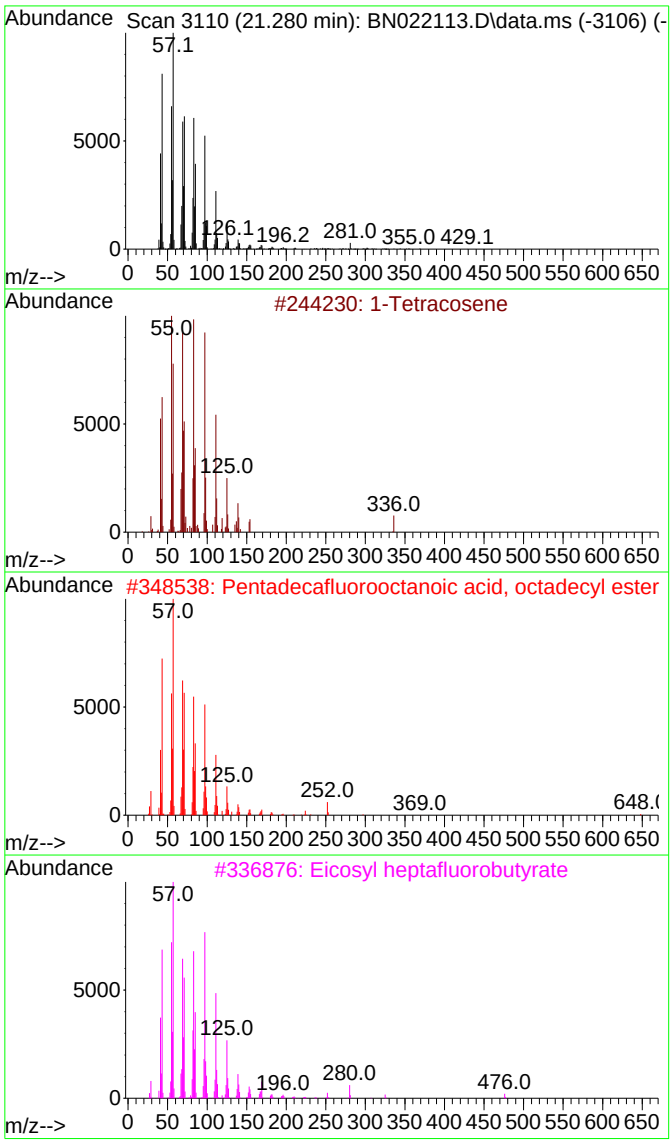
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

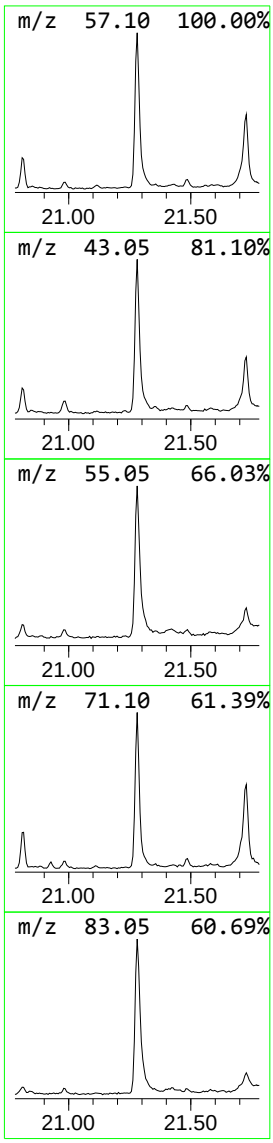
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.280	4.68 ng/ul	860177	Chrysene-d12	21.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91





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Data File : BN022113.D
Acq On : 14 Oct 2022 07:23
Operator : CG/JU
Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

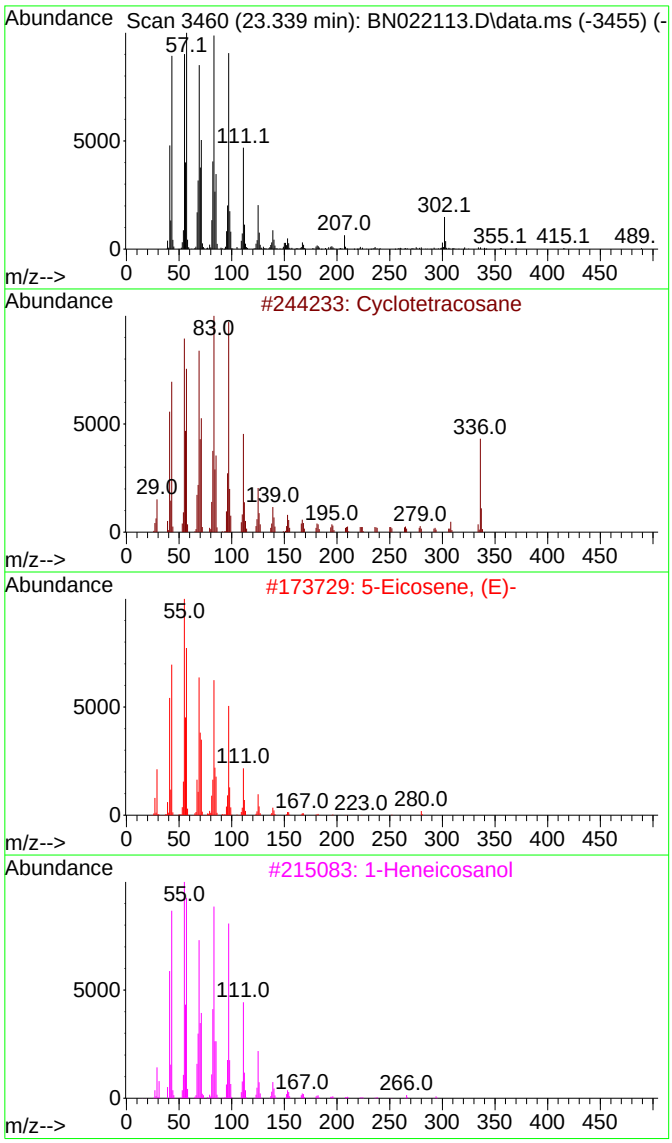
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

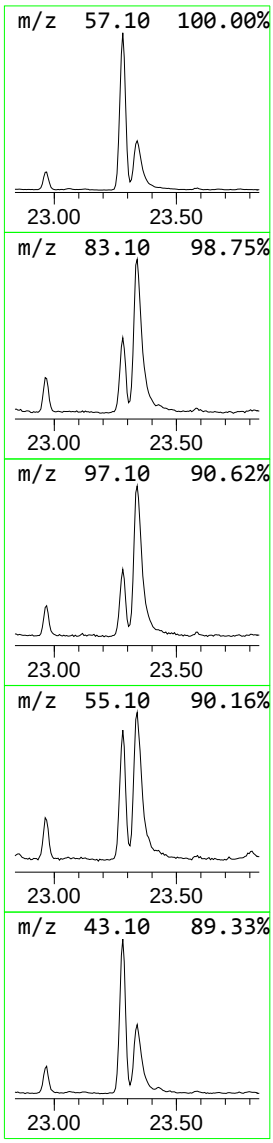
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic23.339 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.339	6.62 ng/ul	1182270	Perylene-d12	24.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN101422\
Data File : BN022113.D
Acq On : 14 Oct 2022 07:23
Operator : CG/JU
Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

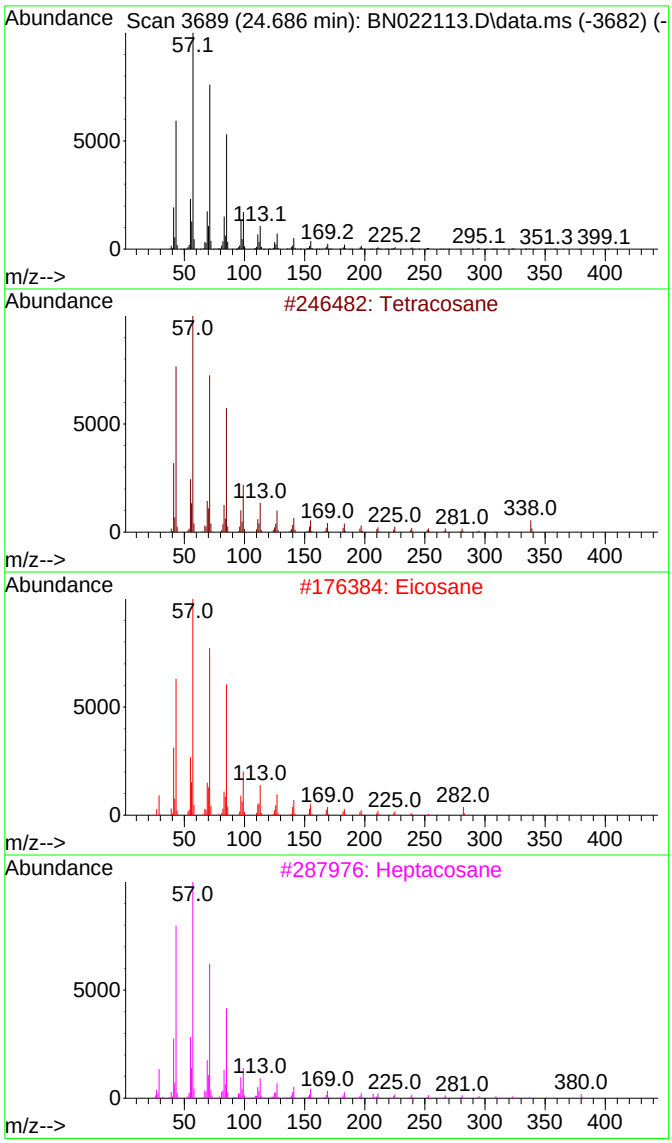
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

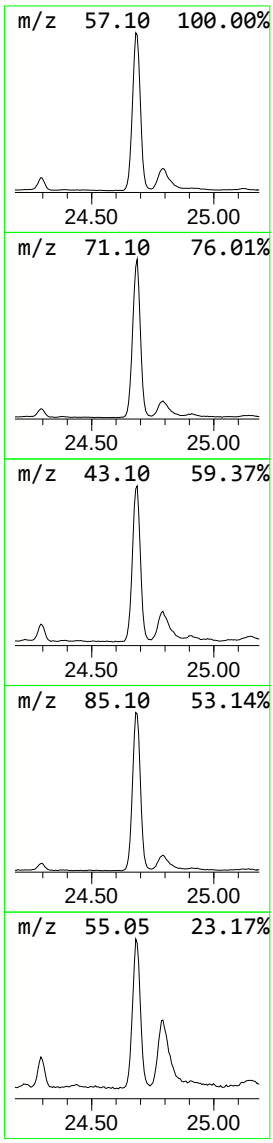
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.686	11.25 ng/ul	2011140	Perylene-d12	24.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	96
2	Eicosane	282	C20H42	000112-95-8	92
3	Heptacosane	380	C27H56	000593-49-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91





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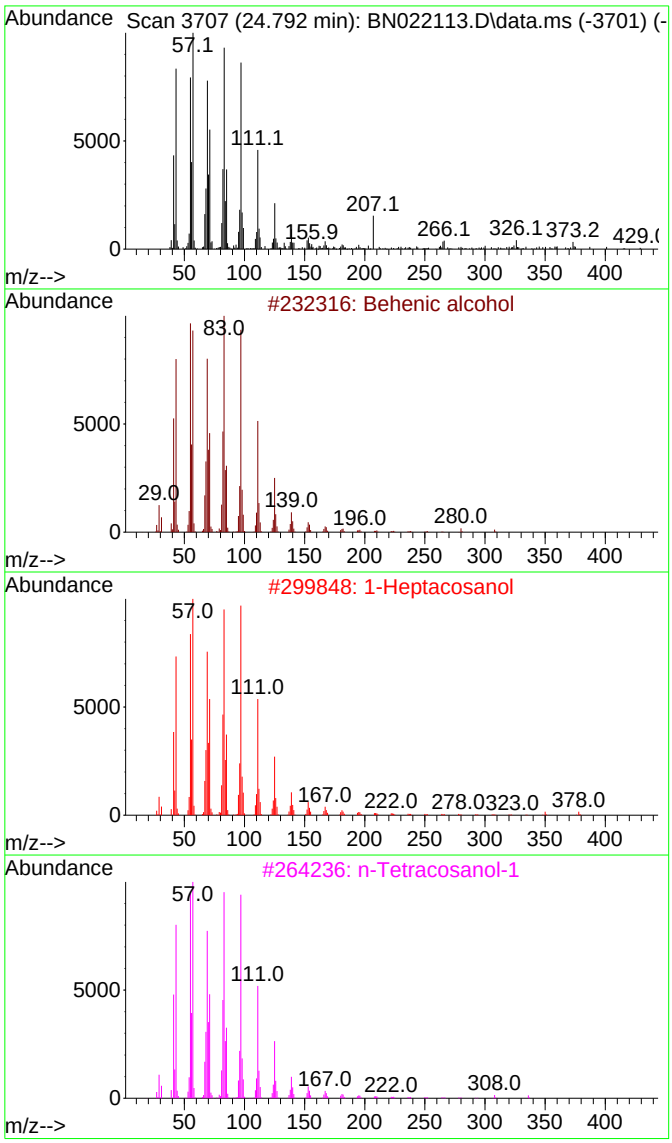
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

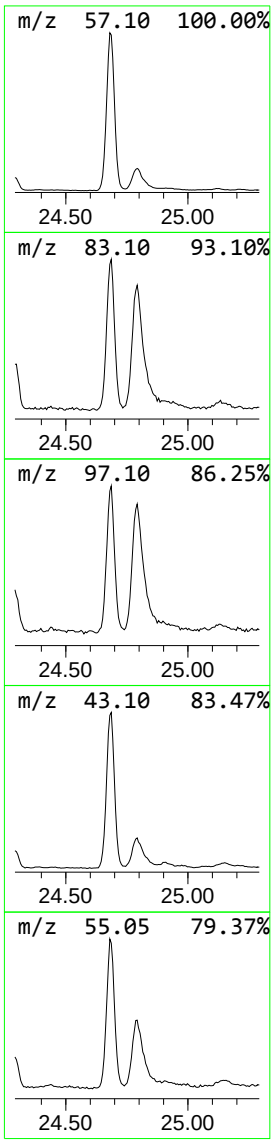
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.792	4.00 ng/ul	713957	Perylene-d12	24.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Data File : BN022113.D
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Operator : CG/JU
Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

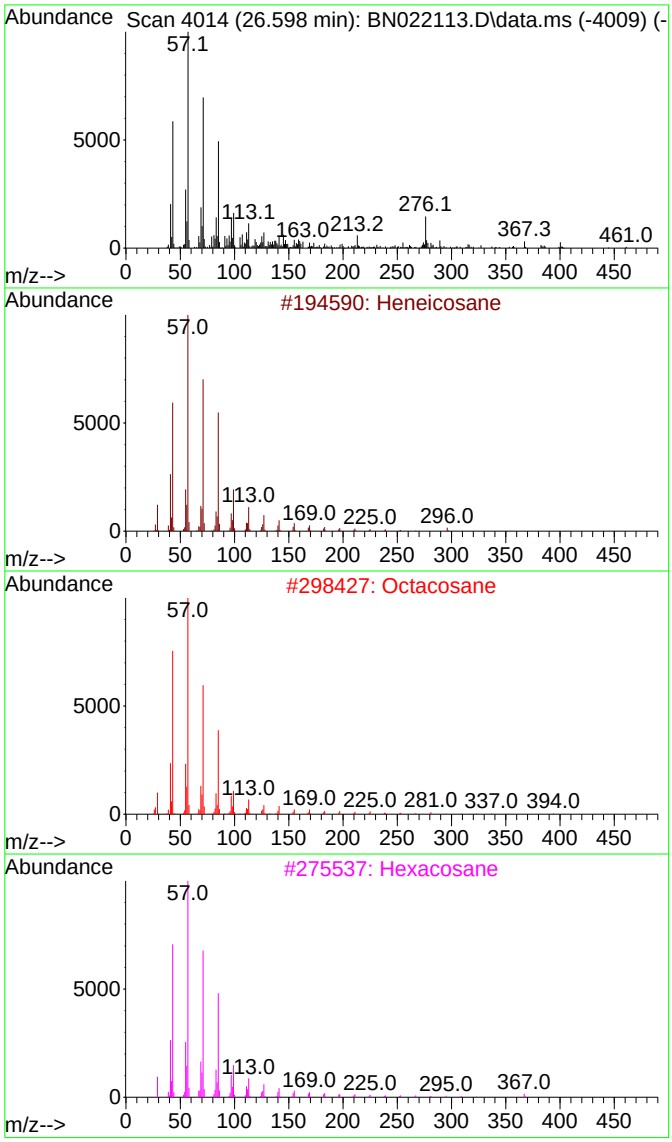
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

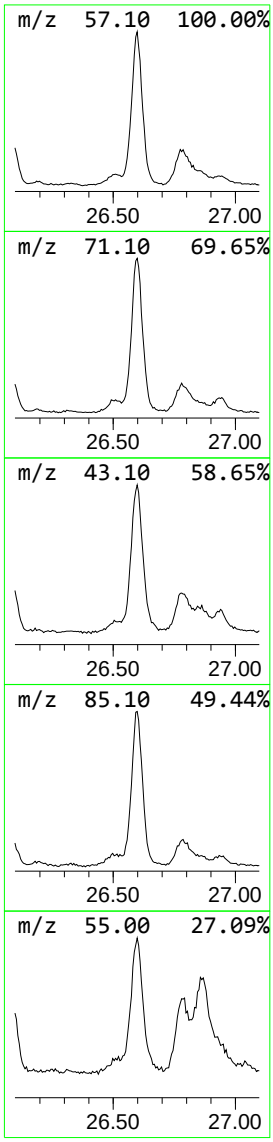
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.598	6.58 ng/ul	1175200	Perylene-d12	24.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Tetracosane	338	C24H50	000646-31-1	87





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Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

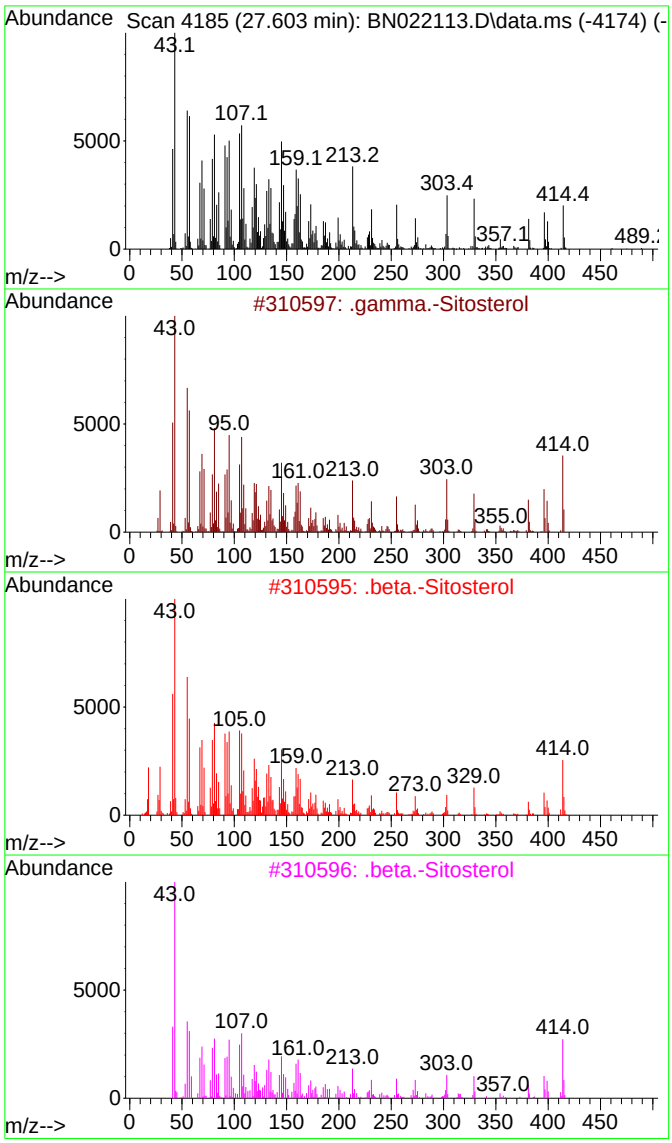
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.M
Quant Title : SVOA CALIBRATION

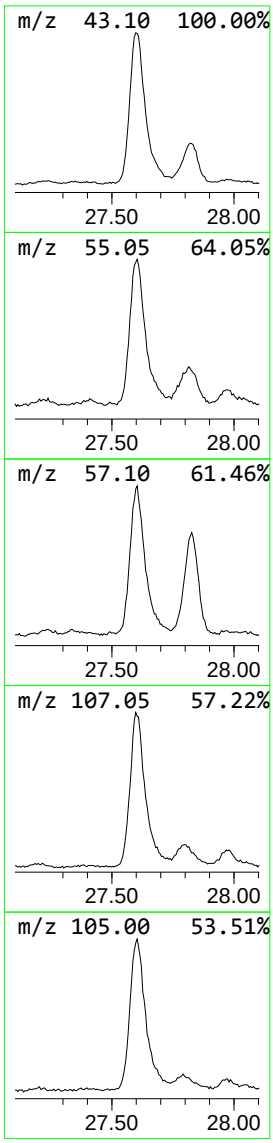
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.604	21.50 ng/ul	3842790	Perylene-d12	24.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	91
4	.gamma.-Sitosterol	414	C29H50O	000083-47-6	90
5	Campesterol	400	C28H48O	000474-62-4	64





Tentatively Identified Compound (LSC) summary

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Data File : BN022113.D
Acq On : 14 Oct 2022 07:23
Operator : CG/JU
Sample : N5049-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0BJ6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN101222.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
Safrole	12.251	34.2	ng/ul	3439780	2	10.781	2013400	20.0
n-Hexadecanoic ...	18.280	7.3	ng/ul	1181650	4	17.381	3242340	20.0
Octadecanoic acid	19.557	2.3	ng/ul	430906	5	21.580	3676700	20.0
(DEL) Alkane: S...	21.280	4.7	ng/ul	860177	5	21.580	3676700	20.0
(DEL) Alkane: C...	23.339	6.6	ng/ul	1182270	6	24.051	3573980	20.0
(DEL) Alkane: S...	24.686	11.3	ng/ul	2011140	6	24.051	3573980	20.0
Behenic alcohol	24.792	4.0	ng/ul	713957	6	24.051	3573980	20.0
(DEL) Alkane: S...	26.598	6.6	ng/ul	1175200	6	24.051	3573980	20.0
.gamma.-Sitosterol	27.604	21.5	ng/ul	3842790	6	24.051	3573980	20.0