LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
Data File : BG052085.D
Acq On : 19 Jan 2022 22:58
Operator : CG/JU
Sample : N1179-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

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_G\Methods\SFAM-EPA-BG010622.M
Title : SVOA CALIBRATION

Signal : TIC: BG052085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.546	8	10	11	rBV2	2328	1899	0.17%	0.018%
2	3.569	11	14	20	rVB2	7823	11226	1.01%	0.108%
3	4.004	84	88	98	rBV	20177	35587	3.20%	0.343%
4	4.251	124	130	135	rVB	3713	5947	0.54%	0.057%
5	4.351	143	147	151	rBV	1943	2725	0.25%	0.026%
6	4.450	161	164	167	rVB2	1735	2063	0.19%	0.020%
7	4.903	238	241	245	rVB2	2659	2479	0.22%	0.024%
8	5.285	302	306	311	rVB	2166	3714	0.33%	0.036%
9	7.223	631	636	639	rBV2	1304	1993	0.18%	0.019%
10	7.382	655	663	674	rBB	38752	70703	6.37%	0.682%
11	7.546	685	691	705	rVB	106788	180724	16.27%	1.744%
12	7.770	723	729	737	rVB	118081	200398	18.04%	1.933%
13	8.245	803	810	817	rBV	102914	174100	15.67%	1.680%
14	8.944	920	929	937	rBV2	103809	183411	16.51%	1.769%
15	9.414	1000	1009	1019	rBB	154126	272154	24.50%	2.626%
16	9.567	1026	1035	1049	rBV2	82464	217195	19.55%	2.095%
17	10.149	1127	1134	1141	rBV	128001	232952	20.97%	2.247%
18	10.695	1219	1227	1235	rBV2	182426	332164	29.91%	3.205%
19	11.083	1286	1293	1302	rBB	144789	264566	23.82%	2.552%
20	11.206	1307	1314	1322	rBV	145355	267406	24.08%	2.580%
21	11.347	1331	1338	1343	rBV3	15322	33152	2.98%	0.320%
22	11.506	1357	1365	1375	rBV4	20783	54362	4.89%	0.524%
23	11.606	1378	1382	1384	rBV2	2709	2937	0.26%	0.028%
24	11.658	1384	1391	1399	rVB6	9222	24052	2.17%	0.232%
25	11.846	1417	1423	1427	rBV5	5789	11852	1.07%	0.114%
26	11.899	1427	1432	1433	rBV3	18385	25485	2.29%	0.246%
27	12.046	1454	1457	1458	rBV	4125	3980	0.36%	0.038%
28	12.240	1489	1490	1495	rVB4	2140	1913	0.17%	0.018%
29	12.475	1527	1530	1536	rVB2	1796	2676	0.24%	0.026%
30	12.645	1557	1559	1560	rBV2	1956	1961	0.18%	0.019%
31	12.657	1560	1561	1566	rVB2	3328	2933	0.26%	0.028%
32	13.697	1734	1738	1745	rVB2	4852	7451	0.67%	0.072%
33	13.855	1762	1765	1770	rVB2	1115	1587	0.14%	0.015%
34	14.278	1830	1837	1844	rBV	397816	561023	50.51%	5.413%
35	14.584	1881	1889	1896	rBV	429196	665035	59.88%	6.416%
36	14.766	1916	1920	1923	rBV	2576	3194	0.29%	0.031%

LSC Area Percent Report

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Data File : BG052085.D
Acq On : 19 Jan 2022 22:58
Operator : CG/JU
Sample : N1179-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

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_G\Methods\SFAM-EPA-BG010622.M
Title : SVOA CALIBRATION

37	14.836	1926	1932	1935	rVV2	2563	4646	0.42%	0.045%
38	14.889	1935	1941	1948	rVB	255860	392310	35.32%	3.785%
39	15.071	1965	1972	1981	rBV2	34300	65262	5.88%	0.630%
40	15.512	2041	2047	2051	rBV2	2314	3151	0.28%	0.030%
41	15.665	2068	2073	2077	rBV3	2509	3874	0.35%	0.037%
42	15.712	2077	2081	2085	rVB3	1973	2393	0.22%	0.023%
43	15.882	2101	2110	2118	rVB	534643	845814	76.15%	8.160%
44	15.988	2122	2128	2138	rVB	164643	254679	22.93%	2.457%
45	16.123	2147	2151	2155	rVB	3037	3705	0.33%	0.036%
46	16.546	2219	2223	2225	rBV2	1847	2041	0.18%	0.020%
47	16.751	2256	2258	2262	rVB2	2026	1786	0.16%	0.017%
48	17.368	2359	2363	2367	rVB2	3688	3785	0.34%	0.037%
49	17.421	2369	2372	2376	rVB3	1909	2471	0.22%	0.024%
50	17.527	2387	2390	2392	rBV2	3243	3391	0.31%	0.033%
51	17.639	2402	2409	2416	rBV	325632	485464	43.71%	4.684%
52	17.738	2416	2426	2436	rVB	641752	973091	87.61%	9.388%
53	18.238	2507	2511	2514	rBV2	985	1789	0.16%	0.017%
54	18.285	2516	2519	2522	rVB4	1514	2097	0.19%	0.020%
55	18.508	2552	2557	2561	rBV4	6210	10130	0.91%	0.098%
56	18.573	2565	2568	2575	rVB	2581	4593	0.41%	0.044%
57	18.884	2619	2621	2624	rVB3	1949	1987	0.18%	0.019%
58	18.925	2624	2628	2630	rBV4	3528	4756	0.43%	0.046%
59	19.254	2679	2684	2685	rBV2	1645	2488	0.22%	0.024%
60	19.371	2700	2704	2706	rBV4	2741	3049	0.27%	0.029%
61	19.418	2709	2712	2713	rBV3	2249	2231	0.20%	0.022%
62	19.577	2736	2739	2746	rVB4	9617	15667	1.41%	0.151%
63	19.653	2748	2752	2755	rBV3	8079	10280	0.93%	0.099%
64	19.806	2776	2778	2780	rBV	2803	2160	0.19%	0.021%
65	19.906	2791	2795	2797	rBV3	5054	5997	0.54%	0.058%
66	20.018	2807	2814	2822	rVB	791127	1110704	100.00%	10.716%
67	20.523	2896	2900	2902	rBV4	6002	6299	0.57%	0.061%
68	21.028	2982	2986	2989	rVB4	9285	11683	1.05%	0.113%
69	21.563	3072	3077	3082	rBV2	29979	58086	5.23%	0.560%
70	21.956	3138	3144	3155	rVB2	274804	488674	44.00%	4.715%
71	22.144	3172	3176	3180	rVB2	15104	19928	1.79%	0.192%
72	22.796	3285	3287	3295	rVB2	15805	25047	2.26%	0.242%
73	23.548	3407	3415	3422	rVB9	17886	46547	4.19%	0.449%
74	24.441	3562	3567	3573	rVB5	16843	35336	3.18%	0.341%
75	24.893	3642	3644	3645	rBV2	3963	2189	0.20%	0.021%
76	25.211	3687	3698	3712	rVB3	351469	1049348	94.48%	10.124%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
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Acq On : 19 Jan 2022 22:58
Operator : CG/JU
Sample : N1179-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

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_G\Methods\SFAM-EPA-BG010622.M
Title : SVOA CALIBRATION

77	25.451	3729	3739	3753	rVB2	167594	529281	47.65%	5.106%

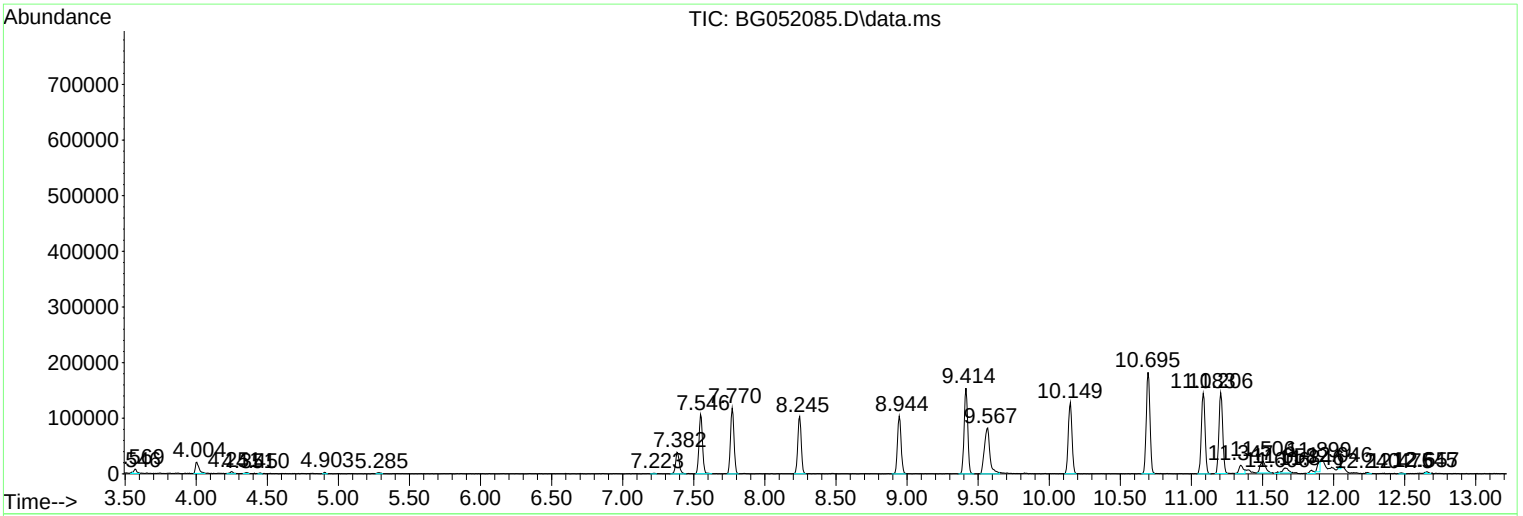
Sum of corrected areas: 10365208

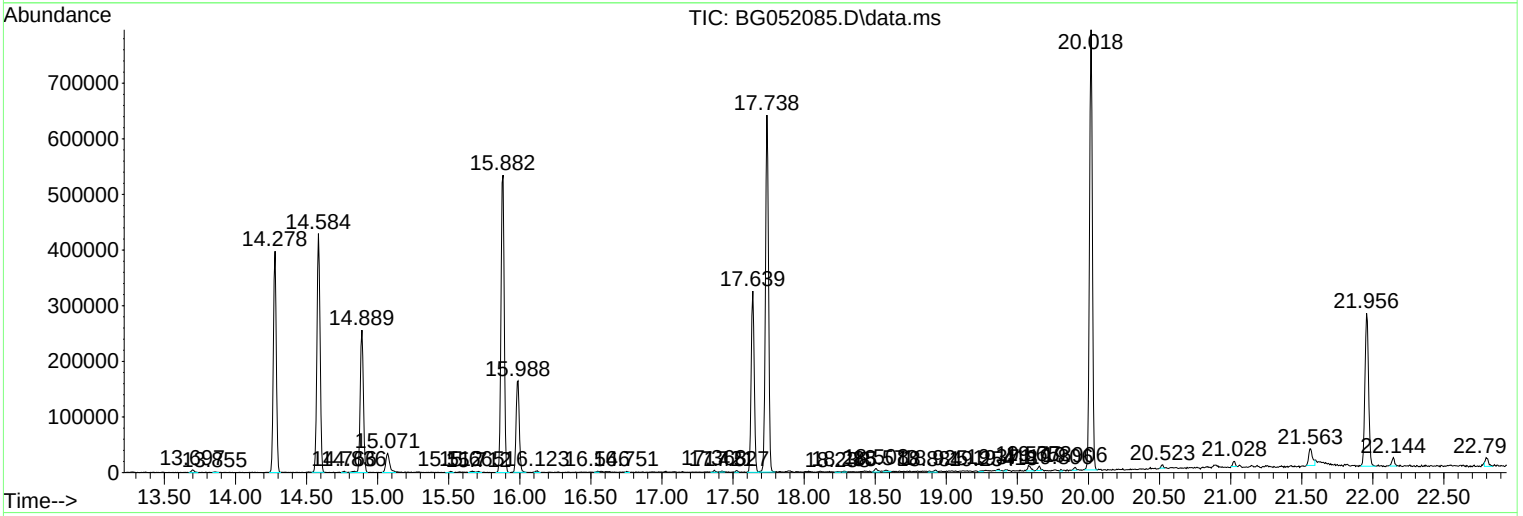
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
Data File : BG052085.D
Acq On : 19 Jan 2022 22:58
Operator : CG/JU
Sample : N1179-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

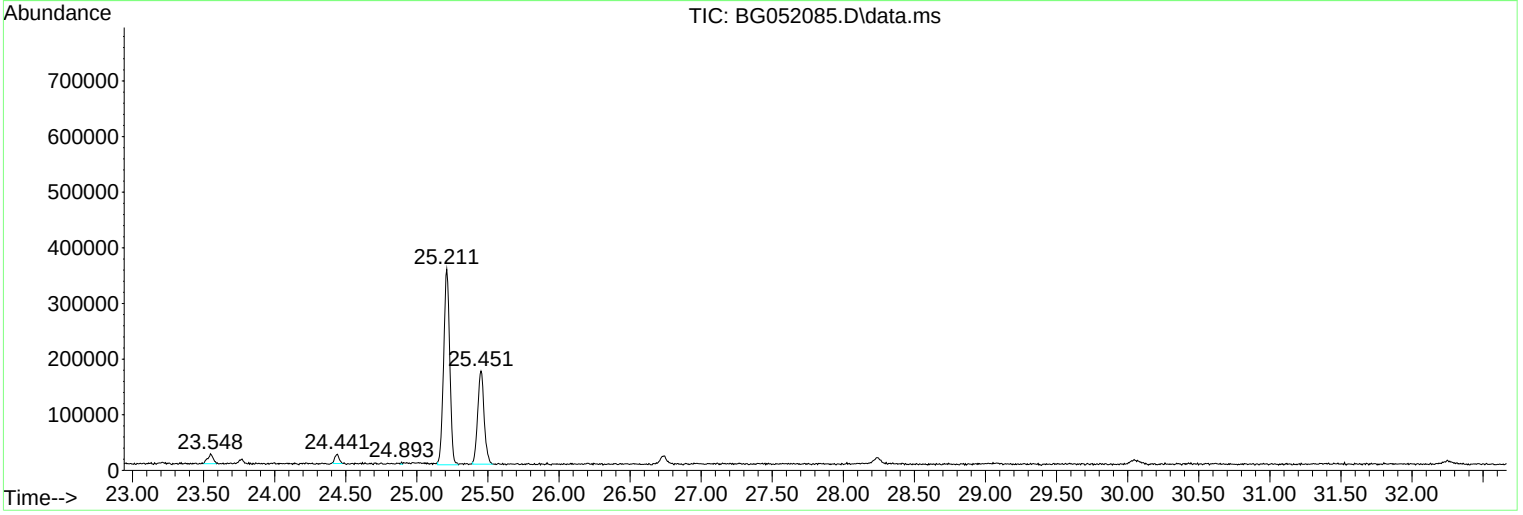
Instrument :
BNA_G
ClientSampleId :
C0HJ5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
Data File : BG052085.D
Acq On : 19 Jan 2022 22:58
Operator : CG/JU
Sample : N1179-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

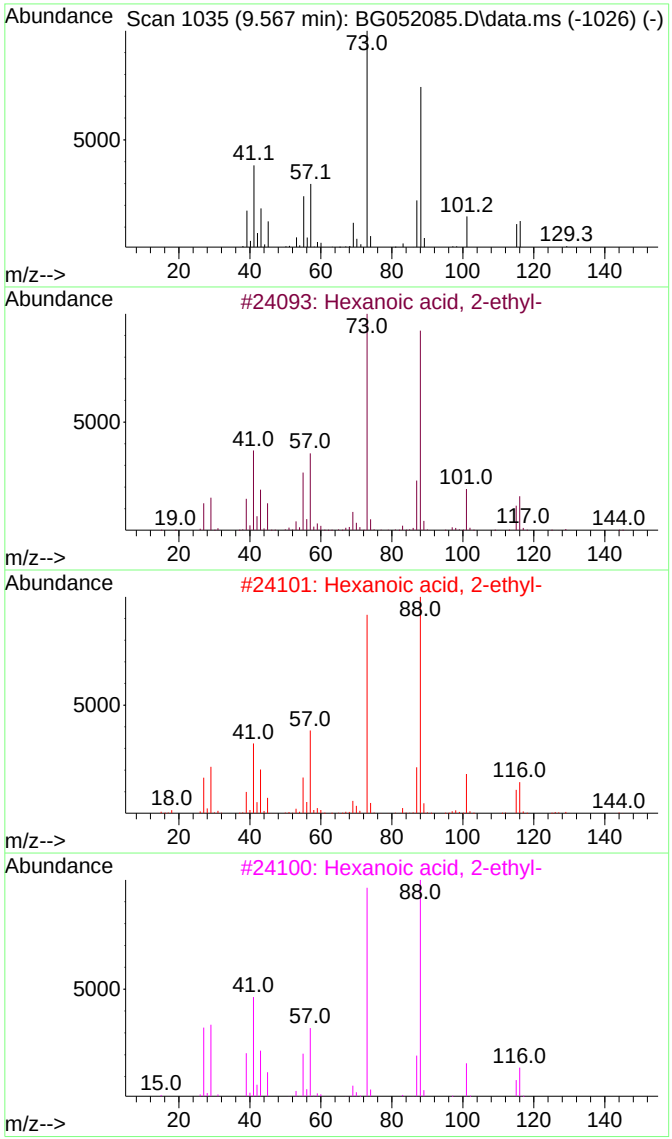
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

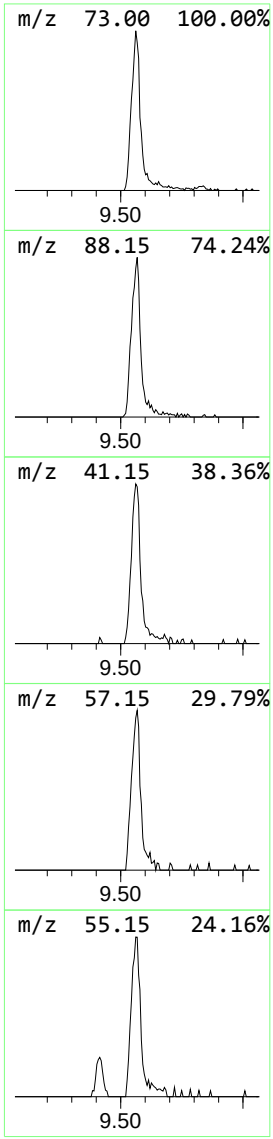
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	24.95 ng/ul	217195	1,4-Dichlorobenzene-d4	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
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Operator : CG/JU
Sample : N1179-03
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

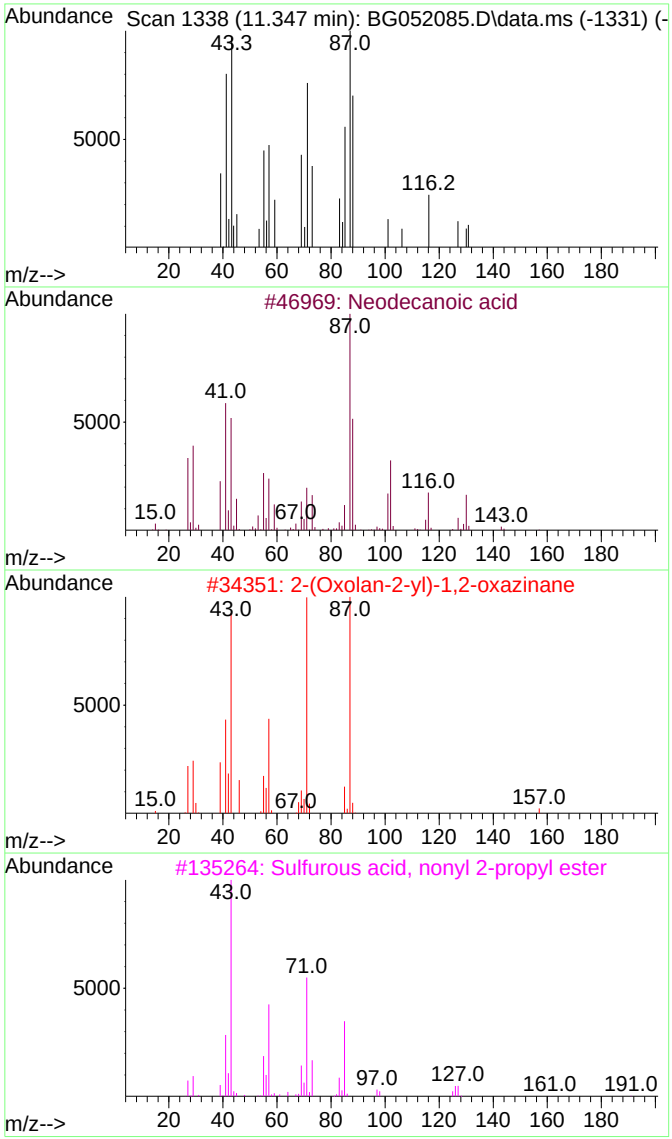
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

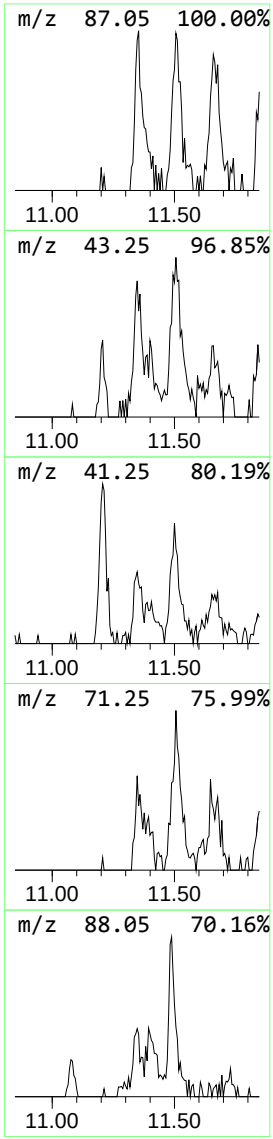
****

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.347	2.51 ng/ul	33152	Naphthalene-d8	11.083

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neodecanoic acid	172	C10H20O2	026896-20-8	38
2	2-(Oxolan-2-yl)-1,2-oxazinane	157	C8H15NO2	1000445-08-1	38
3	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	35
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	30
5	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

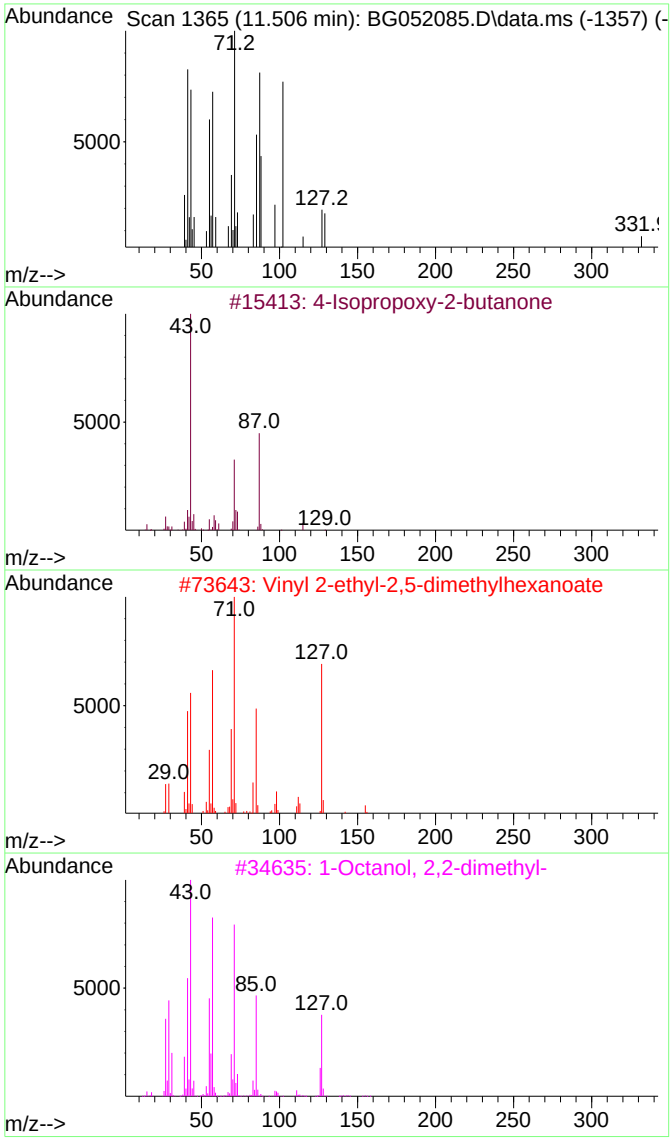
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

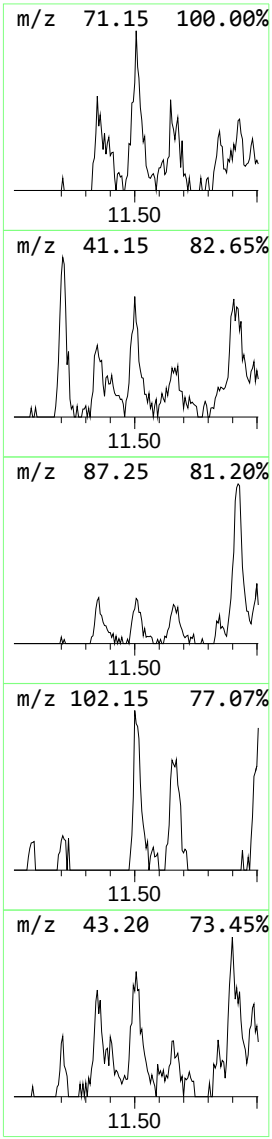
****

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.506	4.11 ng/ul	54362	Naphthalene-d8	11.083

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	35
2	Vinyl 2-ethyl-2,5-dimethylhexanoate	198	C12H22O2	1000498-24-9	22
3	1-Octanol, 2,2-dimethyl-	158	C10H22O	002370-14-1	22
4	Phytanic acid	312	C20H40O2	014721-66-5	16
5	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	14





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0HJ5

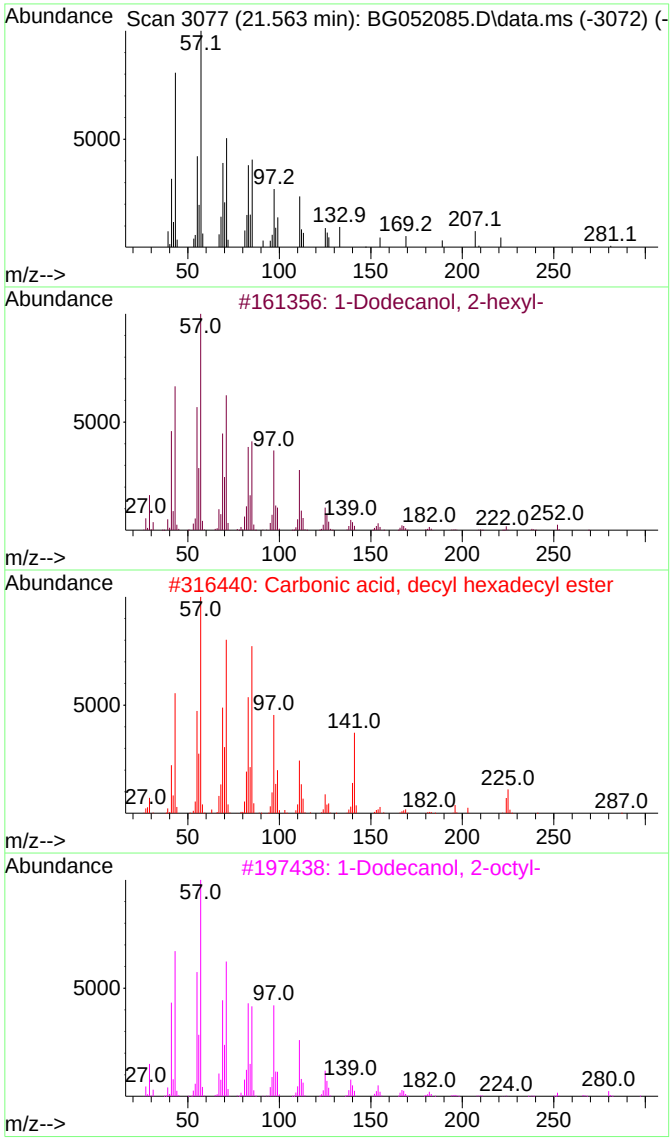
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

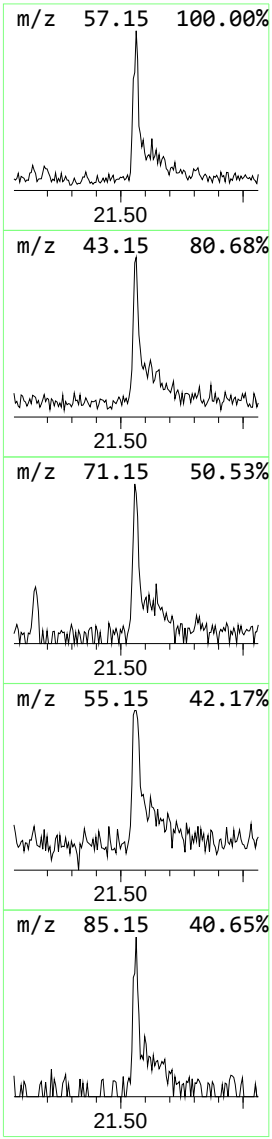
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Dodecanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	2.38 ng/ul	58086	Chrysene-d12	21.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
2	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	90
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83
5	Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011922\
Data File : BG052085.D
Acq On : 19 Jan 2022 22:58
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.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
Hexanoic acid, ...	9.567	24.9	ng/ul	217195	1	8.245	174100	20.0
unknown-01	11.347	2.5	ng/ul	33152	2	11.083	264566	20.0
unknown-02	11.506	4.1	ng/ul	54362	2	11.083	264566	20.0
1-Dodecanol, 2-...	21.563	2.4	ng/ul	58086	5	21.956	488674	20.0