LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

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-BG081424.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062533.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.406	16	20	26	rVB3	12520	20530	0.91%	0.071%
2	3.665	60	64	74	rBV	76667	118760	5.28%	0.409%
3	3.812	84	89	98	rBV	184380	298666	13.28%	1.029%
4	6.020	459	465	471	rBV3	7163	12835	0.57%	0.044%
5	6.367	520	524	529	rVB5	6057	7480	0.33%	0.026%
6	6.637	564	570	577	rVV	30937	47804	2.13%	0.165%
7	6.925	615	619	621	rBV4	4020	6585	0.29%	0.023%
8	7.101	642	649	659	rVV	293406	508387	22.61%	1.751%
9	7.266	671	677	692	rVB	206911	345099	15.35%	1.189%
10	7.471	705	712	718	rBV	283247	474815	21.12%	1.636%
11	7.524	718	721	731	rVB	26075	43697	1.94%	0.151%
12	7.941	784	792	798	rBV	249720	418951	18.63%	1.443%
13	8.000	798	802	809	rVB3	5067	8337	0.37%	0.029%
14	8.634	903	910	918	rBV	289191	493959	21.97%	1.702%
15	9.087	979	987	998	rBV	265306	470317	20.92%	1.620%
16	9.251	1011	1015	1020	rBV3	4164	6116	0.27%	0.021%
17	9.645	1075	1082	1089	rBV2	28596	46578	2.07%	0.160%
18	9.809	1103	1110	1120	rBV	229612	398384	17.72%	1.372%
19	10.038	1145	1149	1156	rVB6	4383	7575	0.34%	0.026%
20	10.350	1194	1202	1215	rBV	367927	652793	29.03%	2.249%
21	10.732	1259	1267	1280	rVB	381787	667000	29.66%	2.298%
22	10.861	1280	1289	1297	rBV	240835	447224	19.89%	1.541%
23	11.260	1352	1357	1362	rBV2	14760	23130	1.03%	0.080%
24	11.460	1385	1391	1409	rBV	68545	142744	6.35%	0.492%
25	11.613	1411	1417	1423	rBV3	6623	12587	0.56%	0.043%
26	11.877	1458	1462	1466	rBV3	3702	6521	0.29%	0.022%
27	12.312	1531	1536	1540	rVV2	5720	8800	0.39%	0.030%
28	13.463	1726	1732	1738	rVB7	6595	15360	0.68%	0.053%
29	13.892	1798	1805	1811	rVV5	6486	11304	0.50%	0.039%
30	13.962	1811	1817	1824	rBV	634365	901515	40.09%	3.106%
31	14.250	1855	1866	1876	rBV	727557	1164074	51.77%	4.010%
32	14.333	1876	1880	1886	rVB6	7164	10014	0.45%	0.034%
33	14.556	1908	1918	1926	rBV	629014	973854	43.31%	3.355%
34	14.632	1926	1931	1937	rBV6	8009	12554	0.56%	0.043%
35	14.744	1944	1950	1967	rVV2	272348	527954	23.48%	1.819%
36	14.897	1971	1976	1983	rVB4	14658	23343	1.04%	0.080%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
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Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

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-BG081424.MA.M
Title : SVOA CALIBRATION

37	14.967	1985	1988	1992	rBV3	7332	8649	0.38%	0.030%
38	15.361	2051	2055	2059	rVB3	6598	9011	0.40%	0.031%
39	15.413	2061	2064	2068	rBV4	3500	6486	0.29%	0.022%
40	15.472	2068	2074	2080	rVB4	20257	27094	1.20%	0.093%
41	15.549	2080	2087	2096	rBV	970198	1455284	64.72%	5.013%
42	15.660	2098	2106	2112	rBV	256962	388997	17.30%	1.340%
43	15.789	2123	2128	2134	rVV7	4247	8028	0.36%	0.028%
44	16.024	2166	2168	2176	rVV6	4924	6207	0.28%	0.021%
45	16.107	2178	2182	2183	rVV3	5067	6317	0.28%	0.022%
46	16.124	2183	2185	2192	rVB7	5505	8303	0.37%	0.029%
47	16.277	2206	2211	2214	rBV4	7072	11145	0.50%	0.038%
48	16.436	2229	2238	2244	rVB9	13881	24821	1.10%	0.086%
49	16.700	2281	2283	2288	rVV5	6400	11669	0.52%	0.040%
50	16.806	2294	2301	2305	rVB5	3727	7129	0.32%	0.025%
51	16.853	2305	2309	2313	rBV5	5163	9142	0.41%	0.031%
52	17.064	2342	2345	2347	rBV3	4815	5734	0.26%	0.020%
53	17.193	2361	2367	2371	rBV5	12860	20084	0.89%	0.069%
54	17.299	2375	2385	2392	rVV	751168	1123161	49.95%	3.869%
55	17.399	2395	2402	2411	rVB	911968	1375720	61.18%	4.739%
56	17.675	2446	2449	2456	rBV7	3950	8604	0.38%	0.030%
57	17.804	2467	2471	2475	rBV4	7545	10415	0.46%	0.036%
58	17.969	2495	2499	2506	rVB6	11787	16470	0.73%	0.057%
59	18.075	2509	2517	2521	rBV7	10843	23817	1.06%	0.082%
60	18.127	2524	2526	2531	rBV6	3906	5801	0.26%	0.020%
61	18.192	2532	2537	2549	rBV	195603	308154	13.70%	1.062%
62	18.456	2578	2582	2583	rBV4	5212	6339	0.28%	0.022%
63	18.486	2585	2587	2591	rVV5	13571	24420	1.09%	0.084%
64	18.515	2591	2592	2602	rVB6	15788	30465	1.35%	0.105%
65	18.638	2607	2613	2614	rBV5	9577	13512	0.60%	0.047%
66	18.668	2614	2618	2623	rVB8	10533	20626	0.92%	0.071%
67	19.079	2684	2688	2692	rBV6	8533	14632	0.65%	0.050%
68	19.114	2692	2694	2701	rVB6	14899	24088	1.07%	0.083%
69	19.244	2713	2716	2720	rBV2	12188	18162	0.81%	0.063%
70	19.320	2723	2729	2731	rBV3	52680	79768	3.55%	0.275%
71	19.461	2749	2753	2763	rBV2	62783	108618	4.83%	0.374%
72	19.614	2773	2779	2783	rBV8	15600	29596	1.32%	0.102%
73	19.678	2784	2790	2796	rBV	1209423	1770063	78.72%	6.098%
74	19.960	2834	2838	2844	rBV9	8527	21434	0.95%	0.074%
75	20.131	2863	2867	2872	rBV8	13901	22522	1.00%	0.078%
76	20.201	2875	2879	2880	rBV2	25527	29944	1.33%	0.103%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

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-BG081424.MA.M
Title : SVOA CALIBRATION

77	20.225	2880	2883	2887	rVB	58682	68308	3.04%	0.235%
78	20.554	2928	2939	2942	rBV	24756	76347	3.40%	0.263%
79	20.653	2953	2956	2960	rBV	47634	54088	2.41%	0.186%
80	20.718	2961	2967	2969	rBV6	52155	91993	4.09%	0.317%
81	20.765	2971	2975	2977	rBV5	28445	47951	2.13%	0.165%
82	21.023	3015	3019	3026	rBV3	33637	64007	2.85%	0.221%
83	21.176	3040	3045	3047	rBV3	67596	105541	4.69%	0.364%
84	21.211	3047	3051	3057	rVV	299179	492007	21.88%	1.695%
85	21.405	3079	3084	3088	rBV7	23671	48987	2.18%	0.169%
86	21.535	3100	3106	3119	rVB2	765805	1262749	56.16%	4.350%
87	21.752	3139	3143	3148	rBV3	32263	53937	2.40%	0.186%
88	21.969	3177	3180	3185	rVB3	44186	59391	2.64%	0.205%
89	22.345	3236	3244	3259	rBV	743566	1690865	75.20%	5.825%
90	23.320	3406	3410	3421	rVB3	64192	118431	5.27%	0.408%
91	23.755	3478	3484	3490	rBV	208200	439889	19.56%	1.515%
92	23.820	3490	3495	3510	rVB4	122227	328518	14.61%	1.132%
93	24.401	3584	3594	3605	rVB	682558	1759322	78.24%	6.061%
94	24.613	3620	3630	3647	rVB	482828	1370059	60.93%	4.720%
95	25.147	3715	3721	3729	rVB3	68147	165263	7.35%	0.569%
96	25.735	3814	3821	3831	rVB2	100917	282244	12.55%	0.972%
97	25.852	3833	3841	3858	rVB3	163589	572639	25.47%	1.973%
98	29.682	4480	4493	4509	rBV9	124210	612244	27.23%	2.109%
99	31.697	4823	4836	4867	rVB9	358004	2248516	100.00%	7.746%
100	32.314	4931	4941	4970	rVB9	95221	578252	25.72%	1.992%

Sum of corrected areas: 29027625

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
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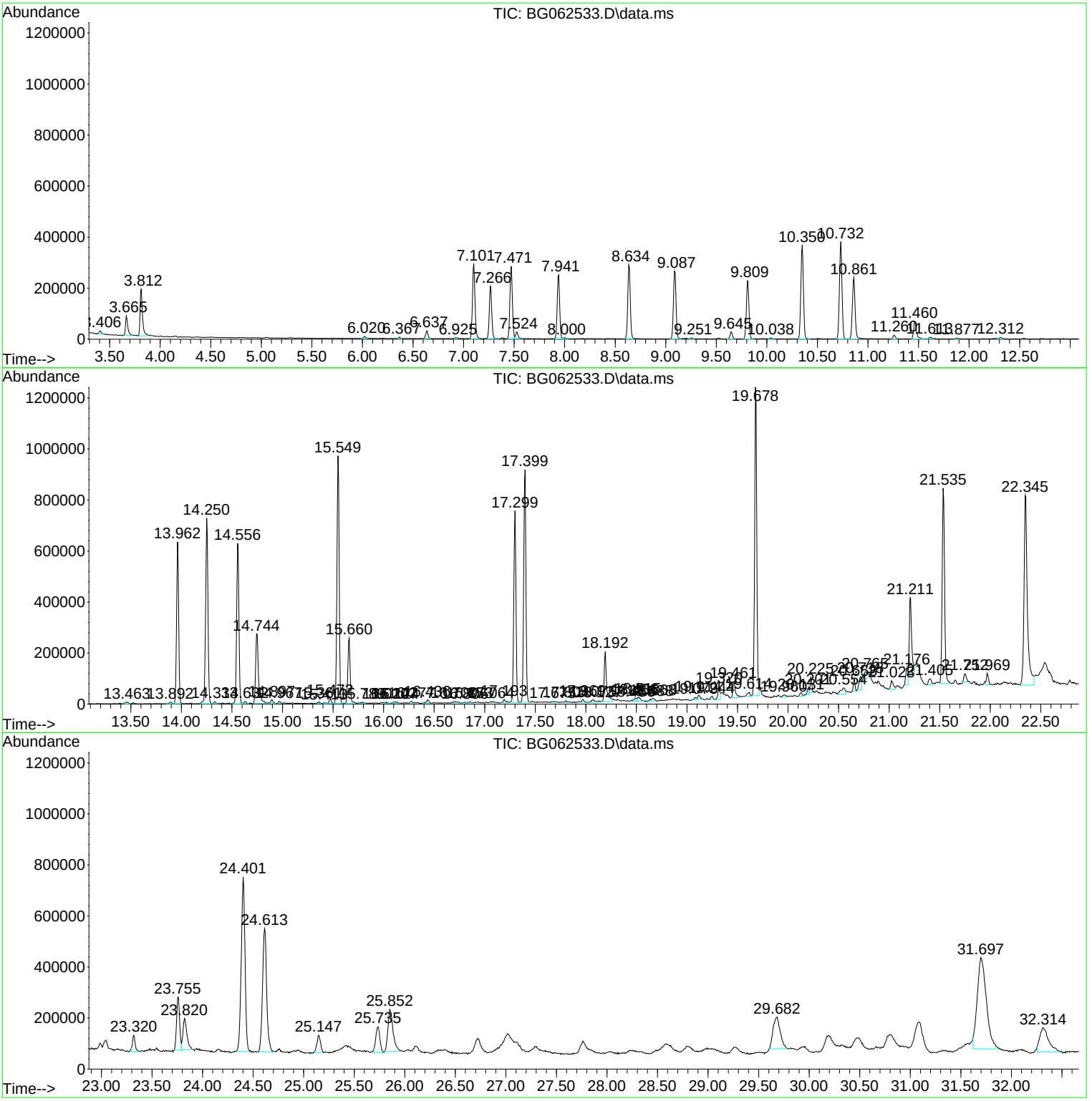
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

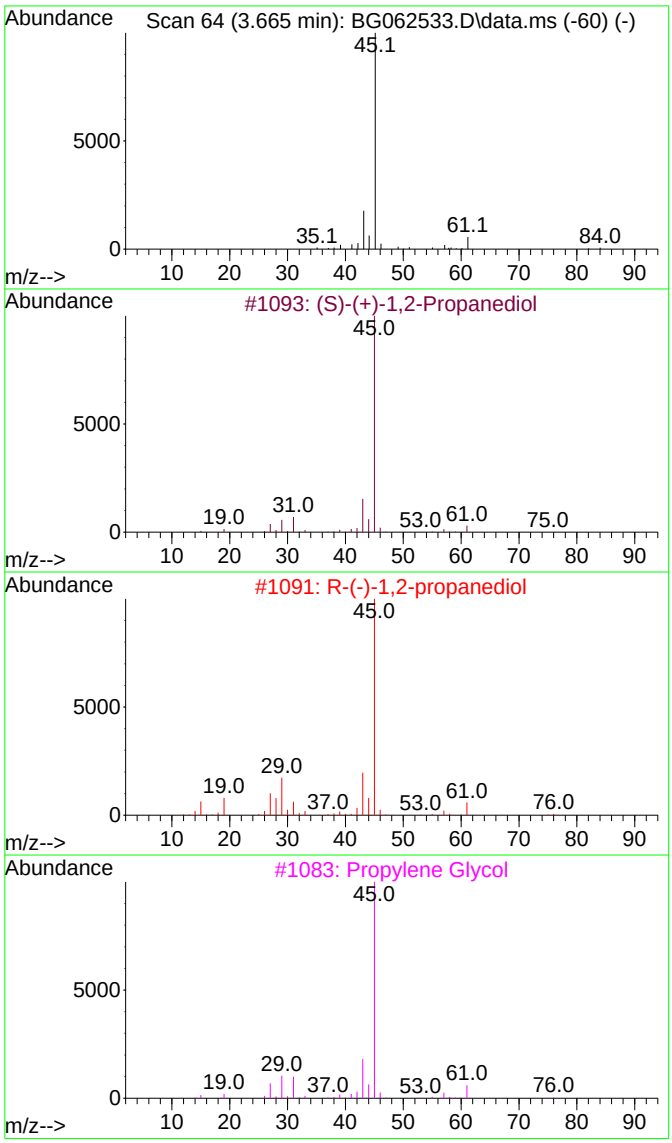
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

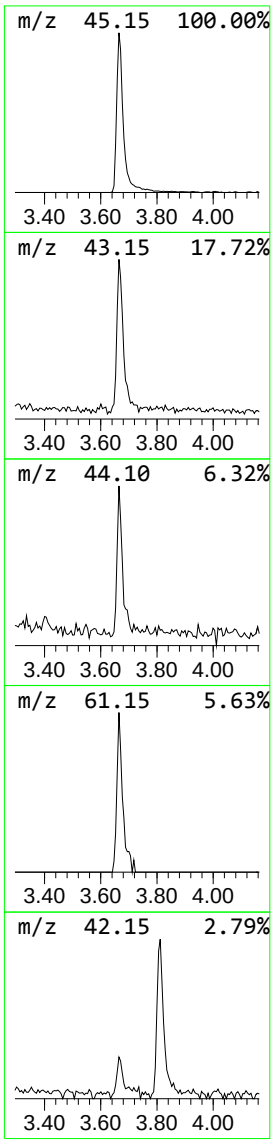
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.665	5.67 ng/ul	118760	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3	Propylene Glycol	76	C3H8O2	000057-55-6	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Butanol, 3-chloro-, (R*,S*)-	108	C4H9ClO	010325-41-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

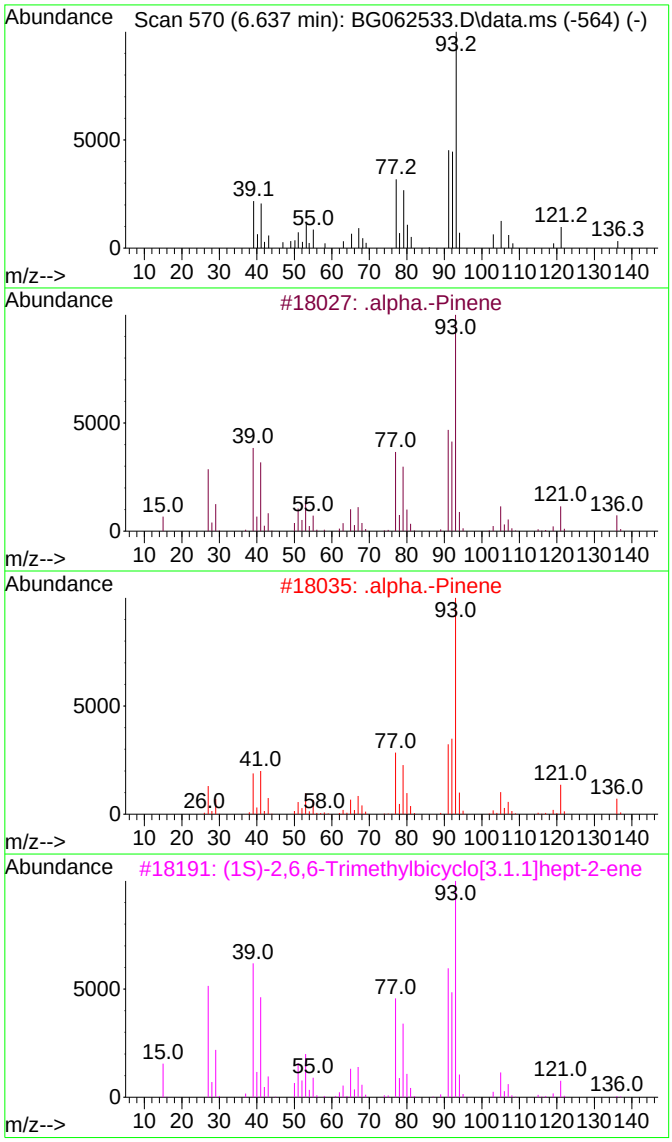
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

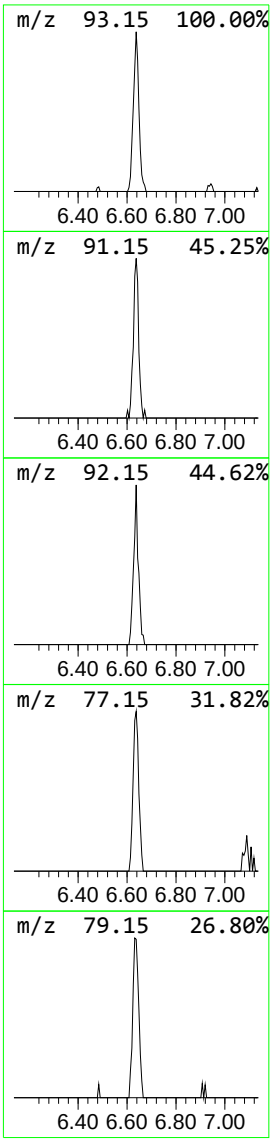
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 .alpha.-Pinene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.637	2.28 ng/ul	47804	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	91
3	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	83
4	.alpha.-Pinene	136	C10H16	000080-56-8	78
5	trans-.beta.-Ocimene	136	C10H16	003779-61-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

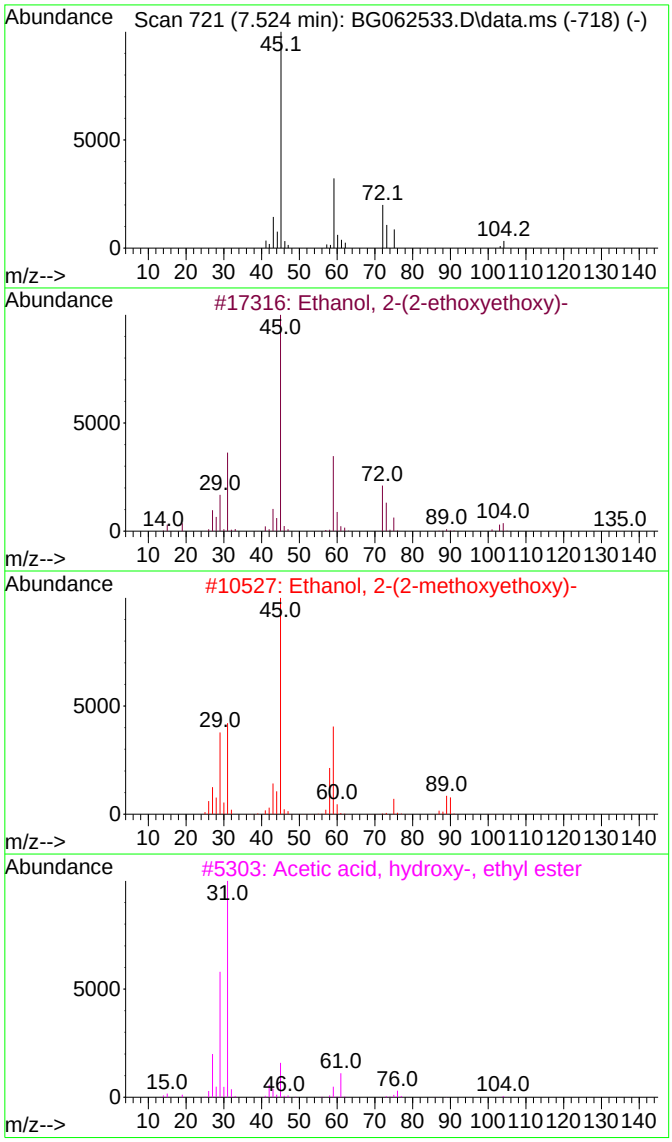
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

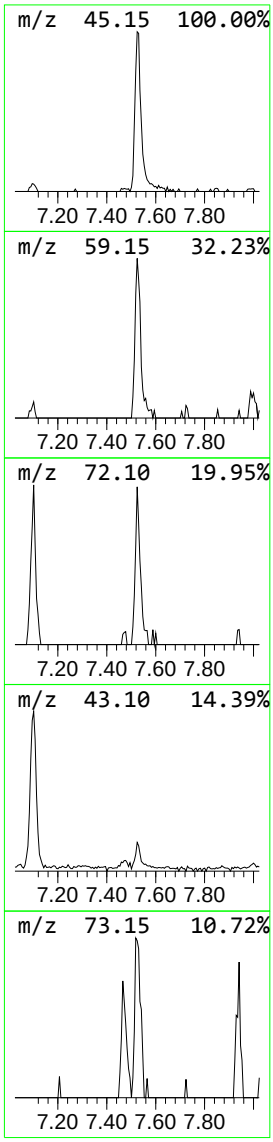
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.524	2.09 ng/ul	43697	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	59
3	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	42
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
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Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

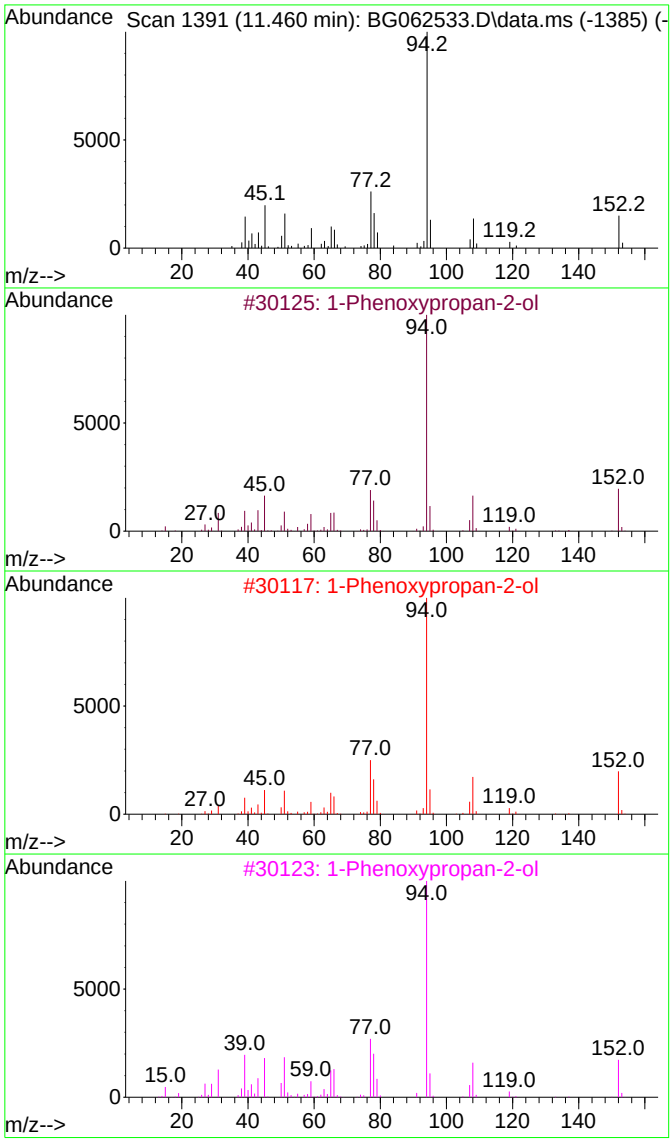
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

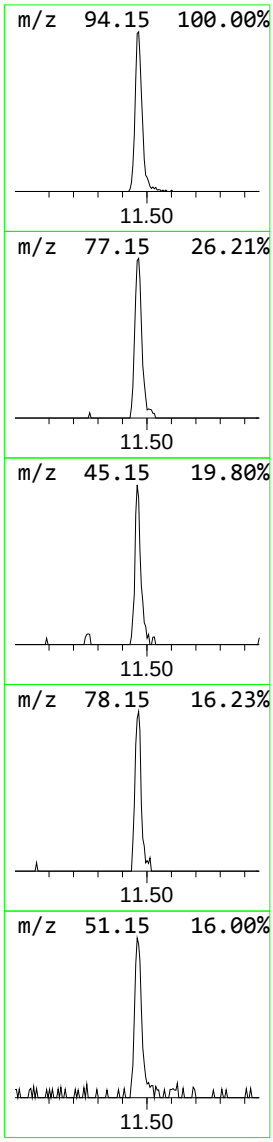
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.460	4.28 ng/ul	142744	Naphthalene-d8	10.732

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	92
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

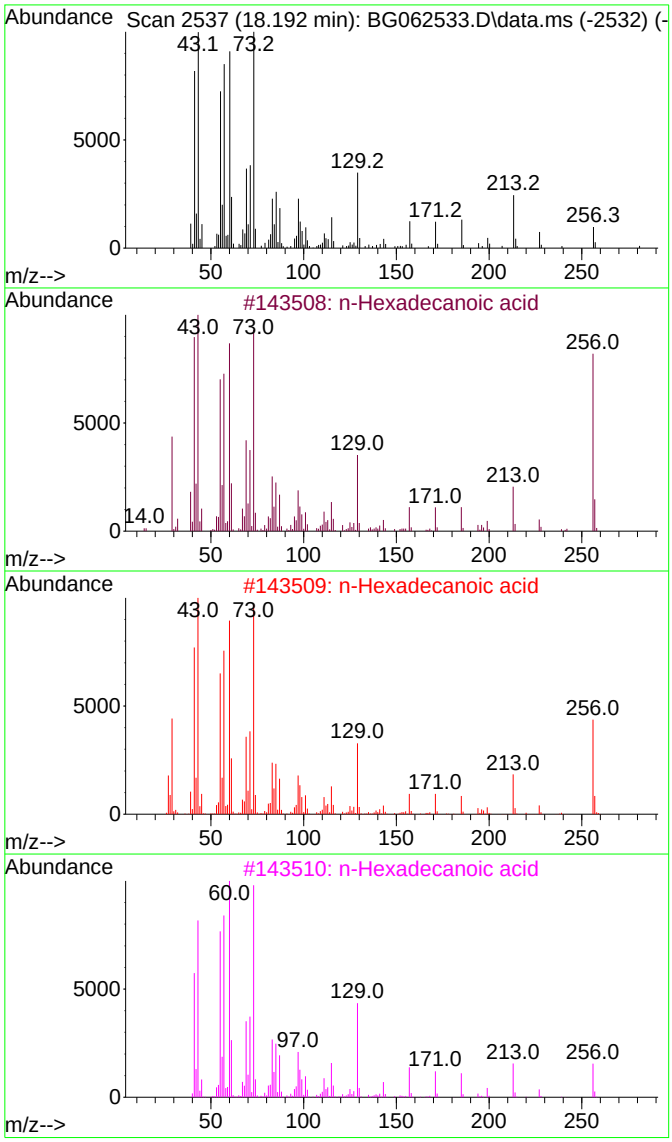
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

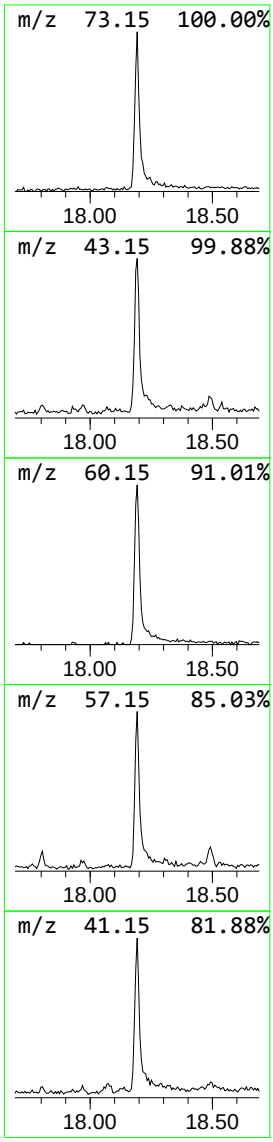
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	5.49 ng/ul	308154	Phenanthrene-d10	17.299

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87





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Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

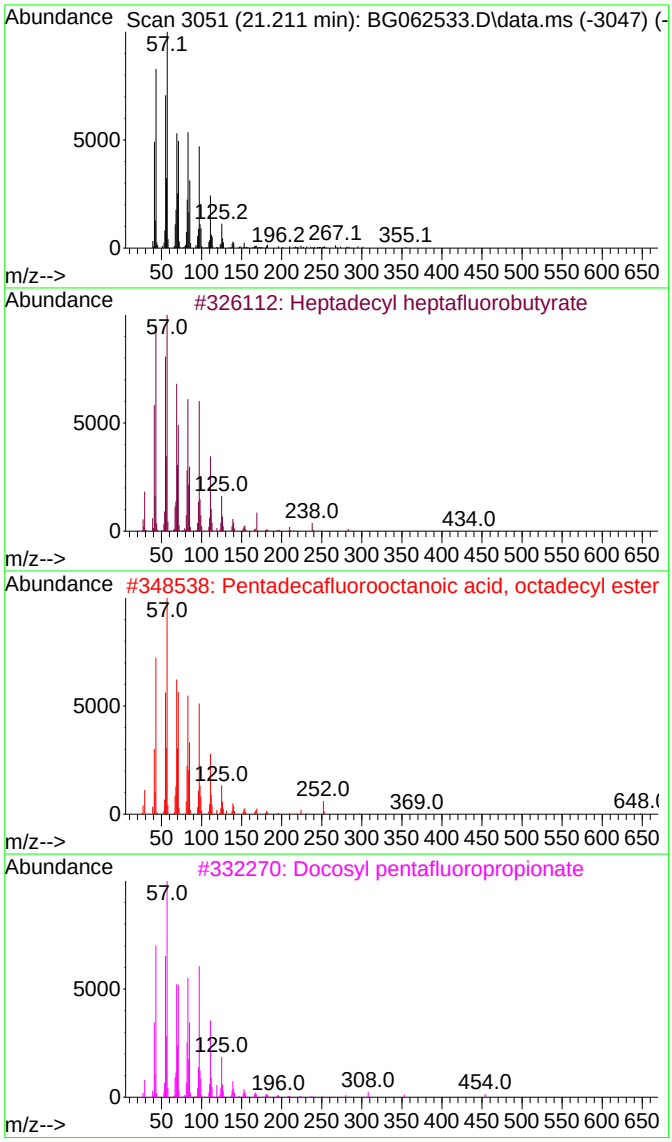
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

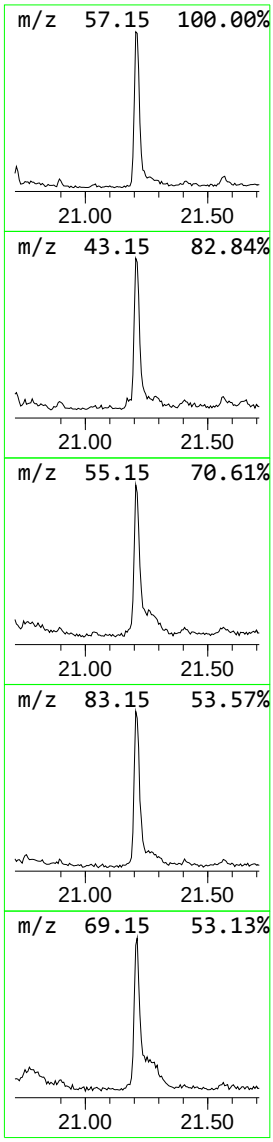
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.212	7.79 ng/ul	492007	Chrysene-d12	21.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





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Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

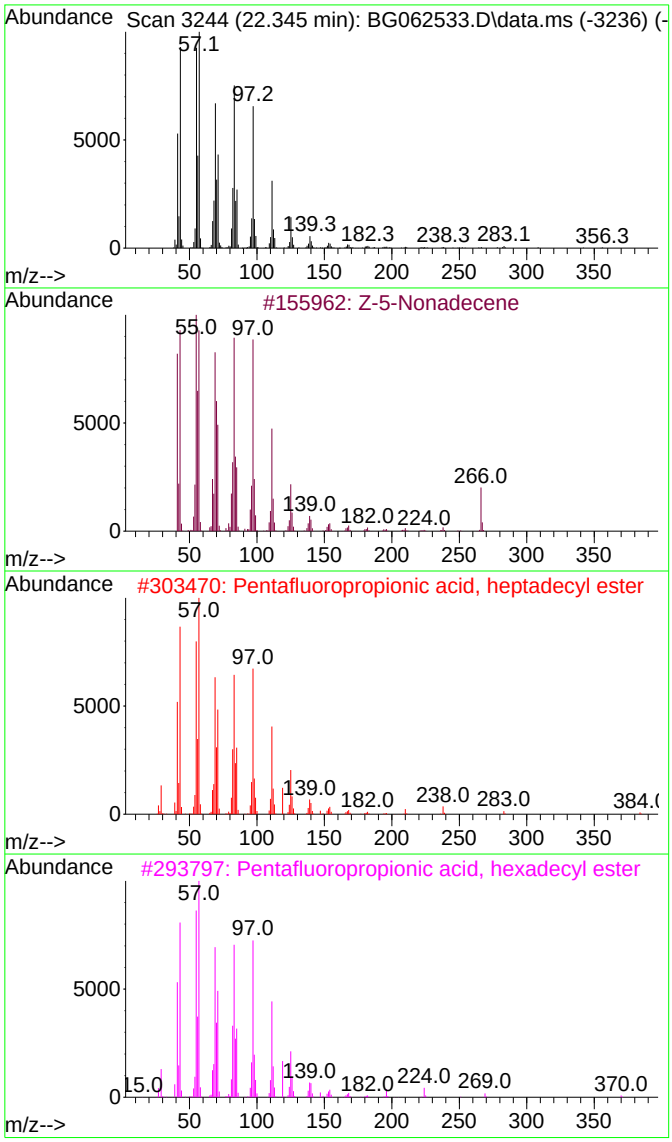
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

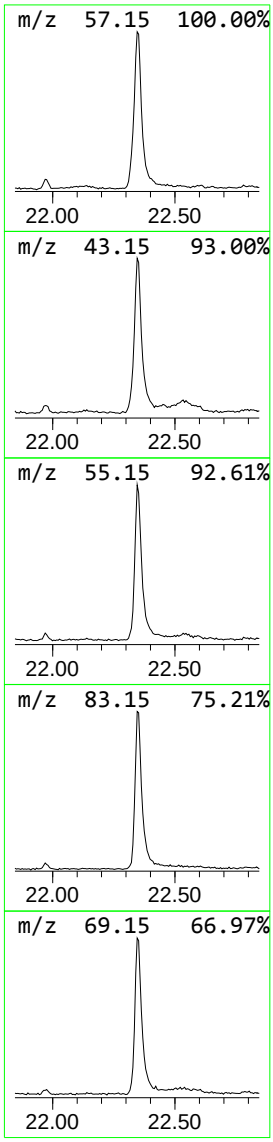
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.345	26.78 ng/ul	1690870	Chrysene-d12	21.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	94
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5	1-Docosene	308	C22H44	001599-67-3	94





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Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

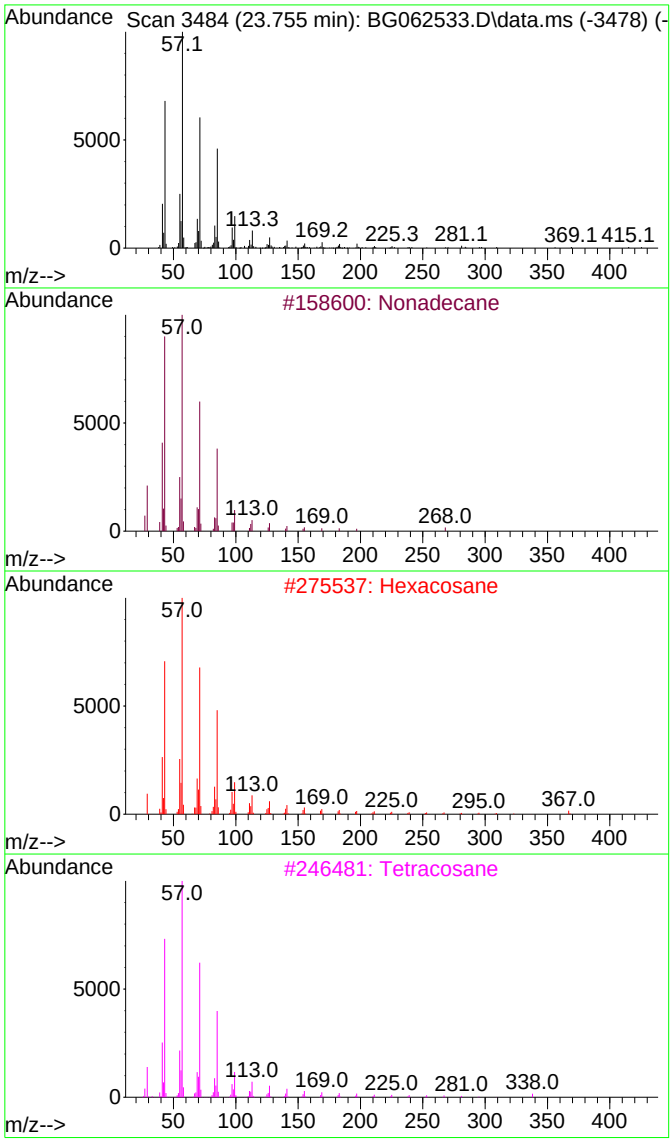
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

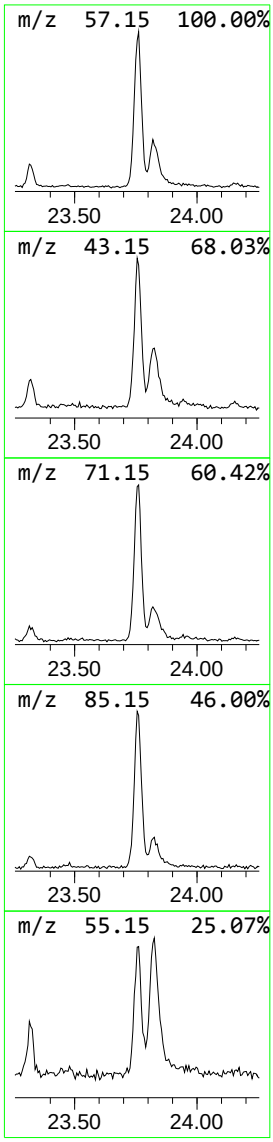
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.755	6.42 ng/ul	439889	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

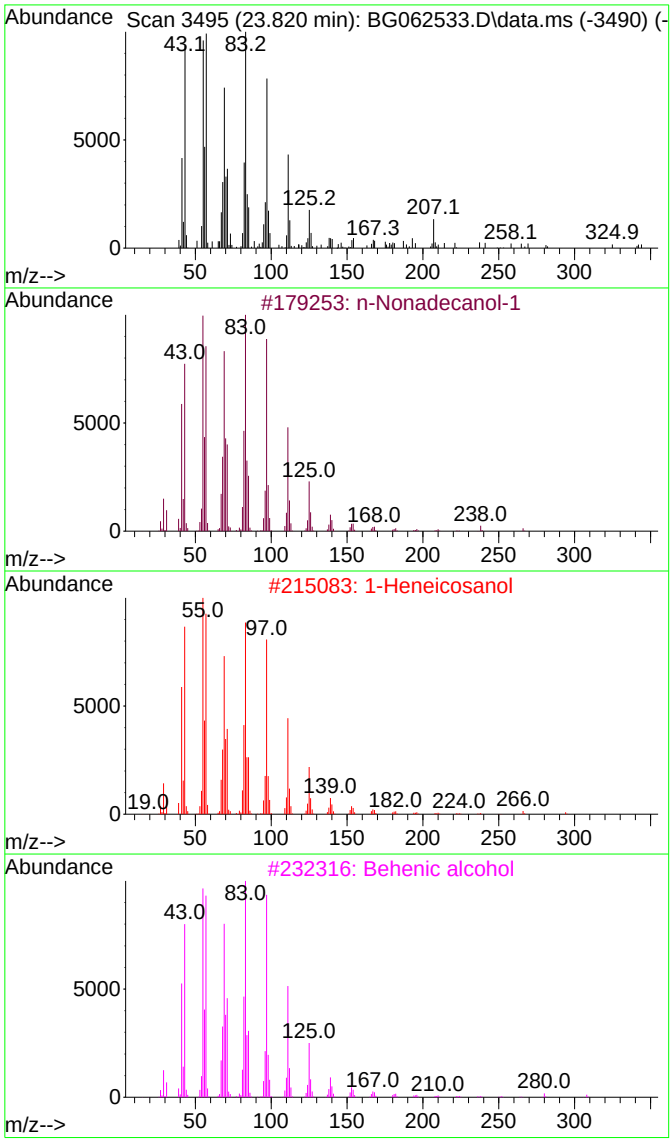
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

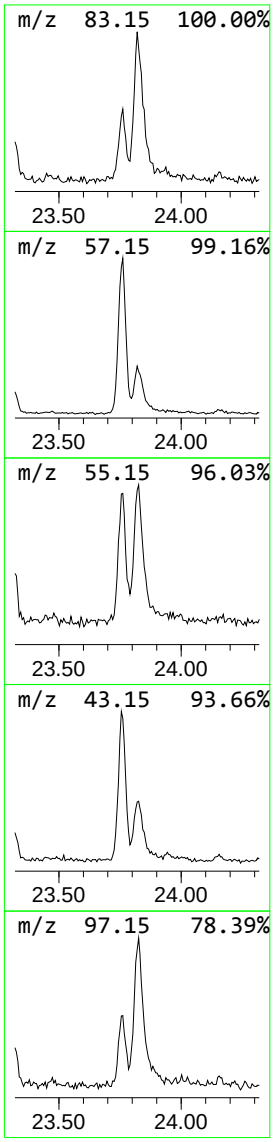
****

Peak Number 9 n-Nonadecanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.820	4.80 ng/ul	328518	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Eicosyl methyl ether	312	C21H44O	1000406-29-4	90
5	1-Octadecanol	270	C18H38O	000112-92-5	87





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Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

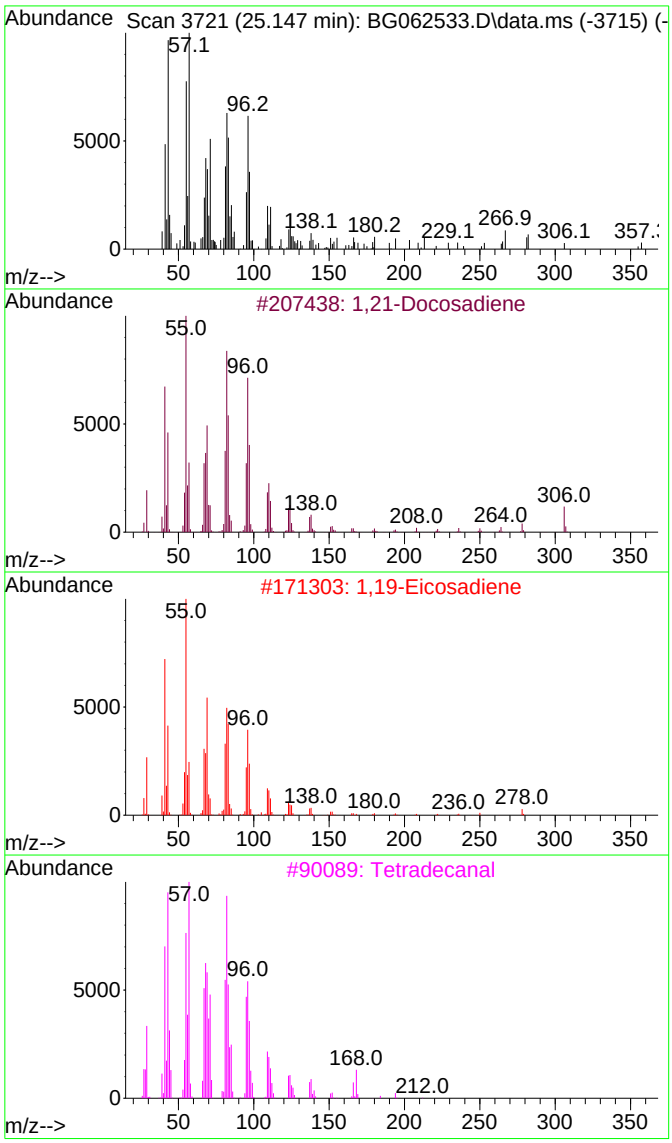
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

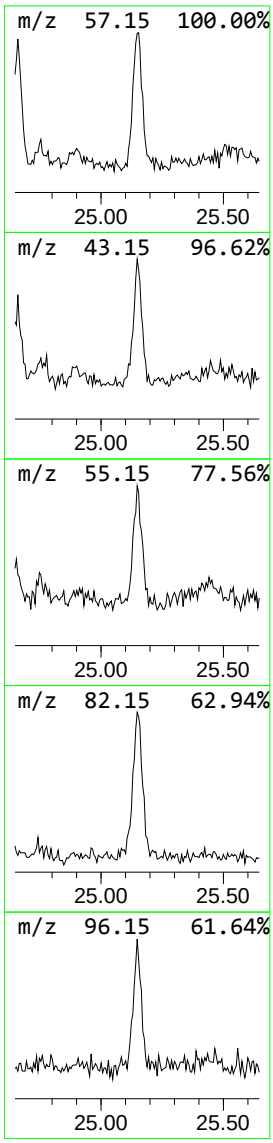
****

Peak Number 10 1,21-Docosadiene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.147	2.41 ng/ul	165263	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene	306	C22H42	053057-53-7	70
2	1,19-Eicosadiene	278	C20H38	014811-95-1	64
3	Tetradecanal	212	C14H28O	000124-25-4	47
4	1-Cyclohexylheptene	180	C13H24	114614-83-4	46
5	E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	45





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Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

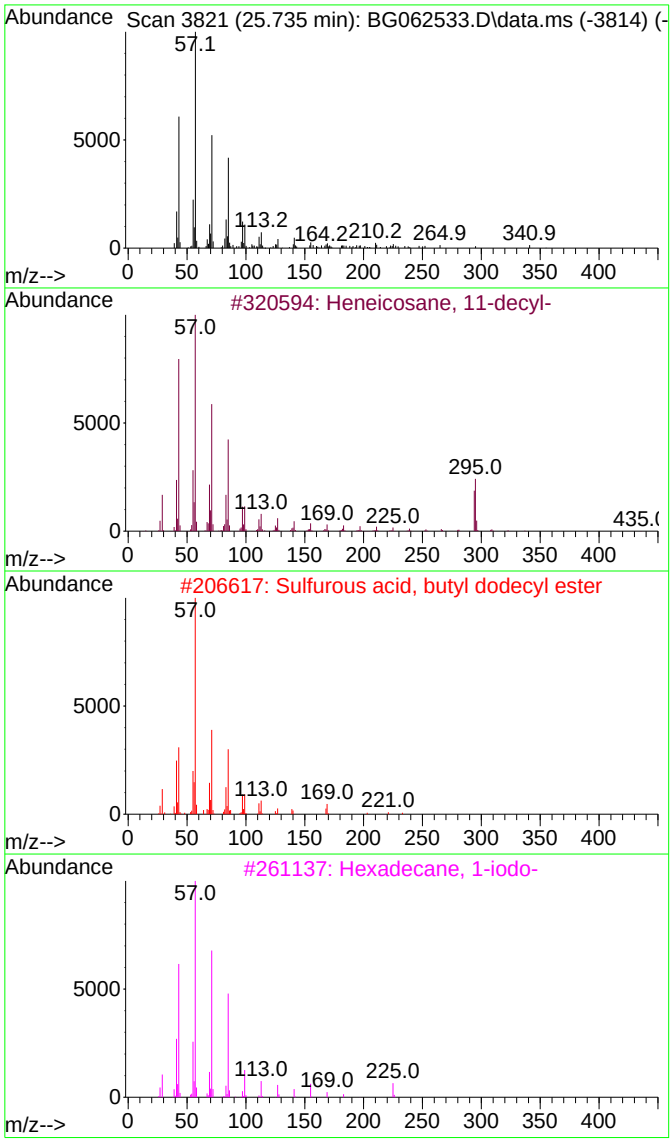
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

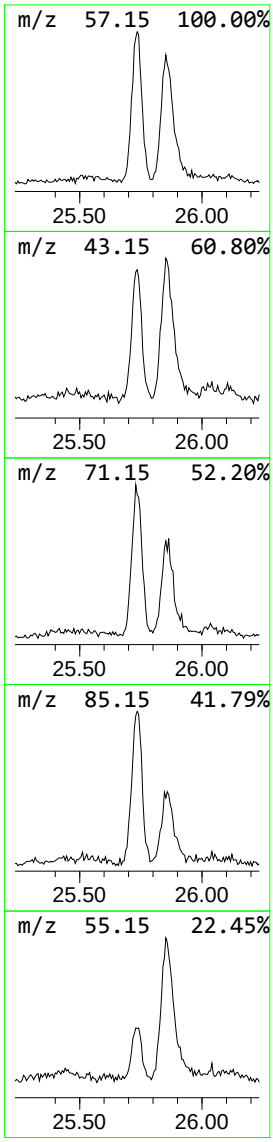
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.735	4.12 ng/ul	282244	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





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Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

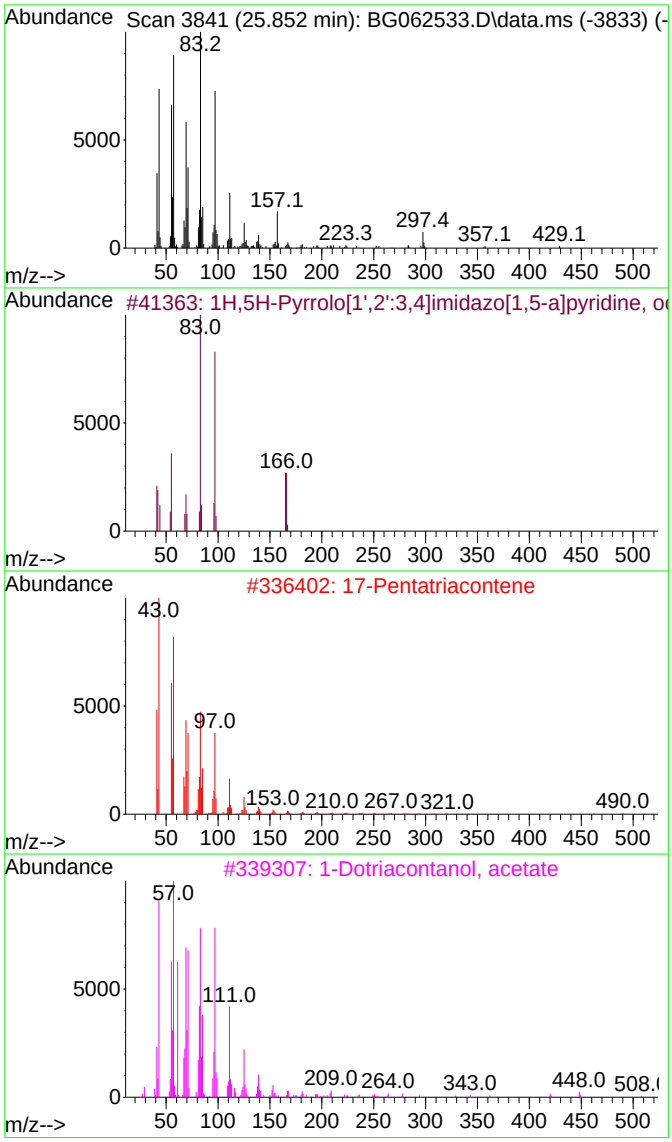
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

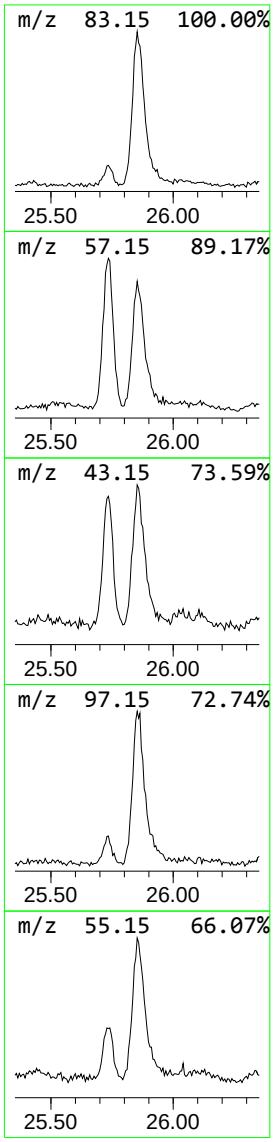
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1H,5H-Pyrrolo[1',2':3,4]imi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.852	8.36 ng/ul	572639	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H,5H-Pyrrolo[1',2':3,4]imidazo[...	166	C10H18N2	054966-11-9	58
2	17-Pentatriacontene	491	C35H70	006971-40-0	46
3	1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	43
4	Octacosyl acetate	452	C30H60O2	018206-97-8	43
5	Octacosanol	410	C28H58O	000557-61-9	43





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Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

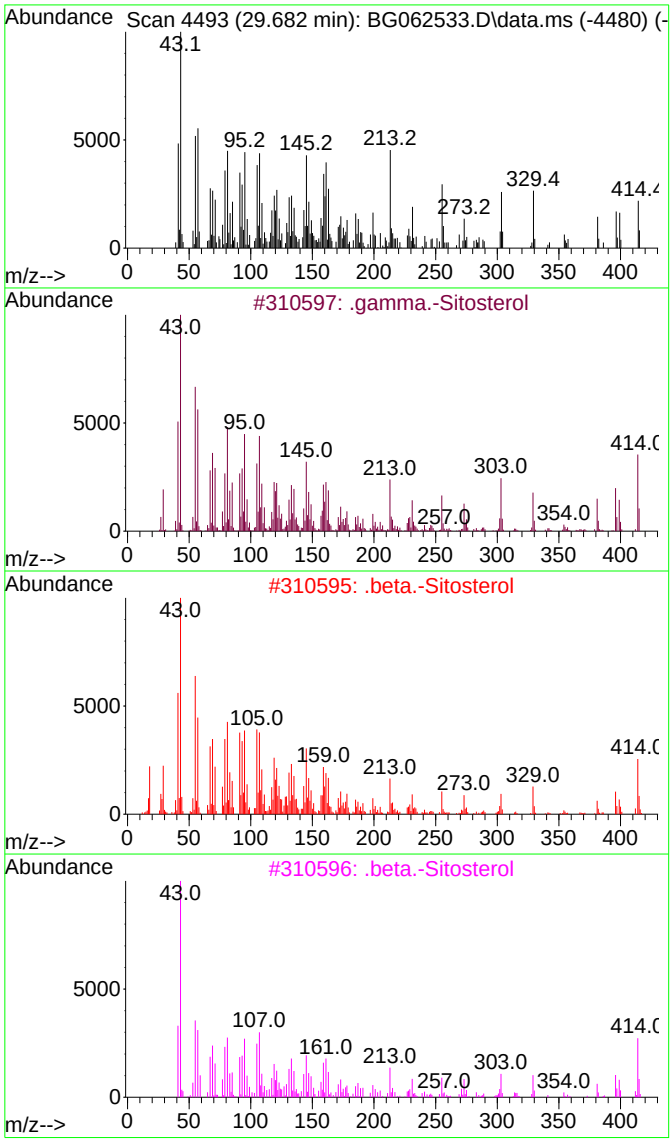
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

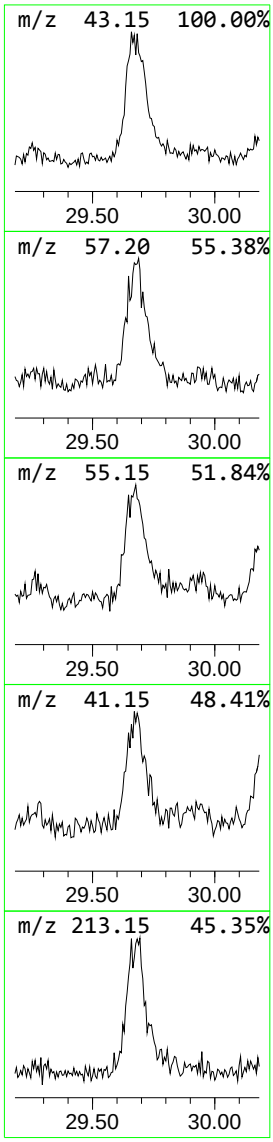
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.682	8.94 ng/ul	612244	Perylene-d12	24.613

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	60
4	Campesterol	400	C28H48O	000474-62-4	46
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	43





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Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

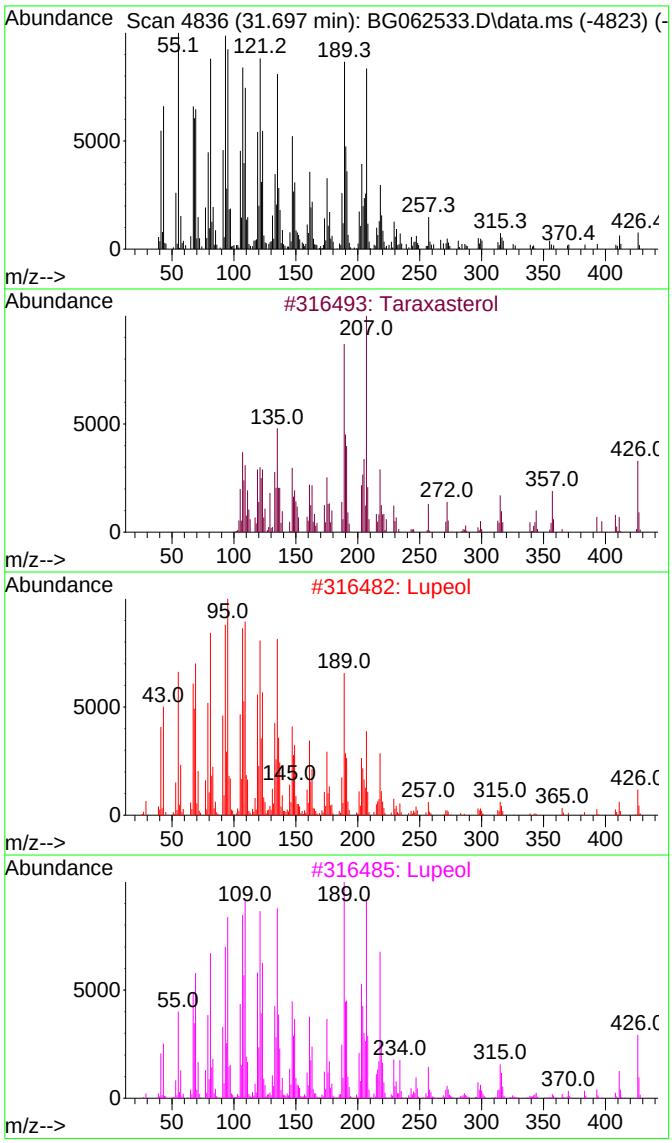
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

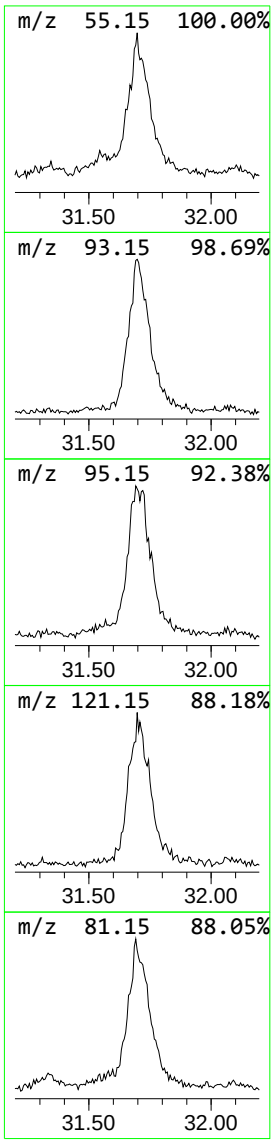
****

Peak Number 14 Taraxasterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.697	32.82 ng/ul	2248520	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Taraxasterol	426	C30H50O	001059-14-9	94
2	Lupeol	426	C30H50O	000545-47-1	90
3	Lupeol	426	C30H50O	000545-47-1	87
4	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	83
5	Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	53





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Acq On : 22 Aug 2024 8:13
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Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

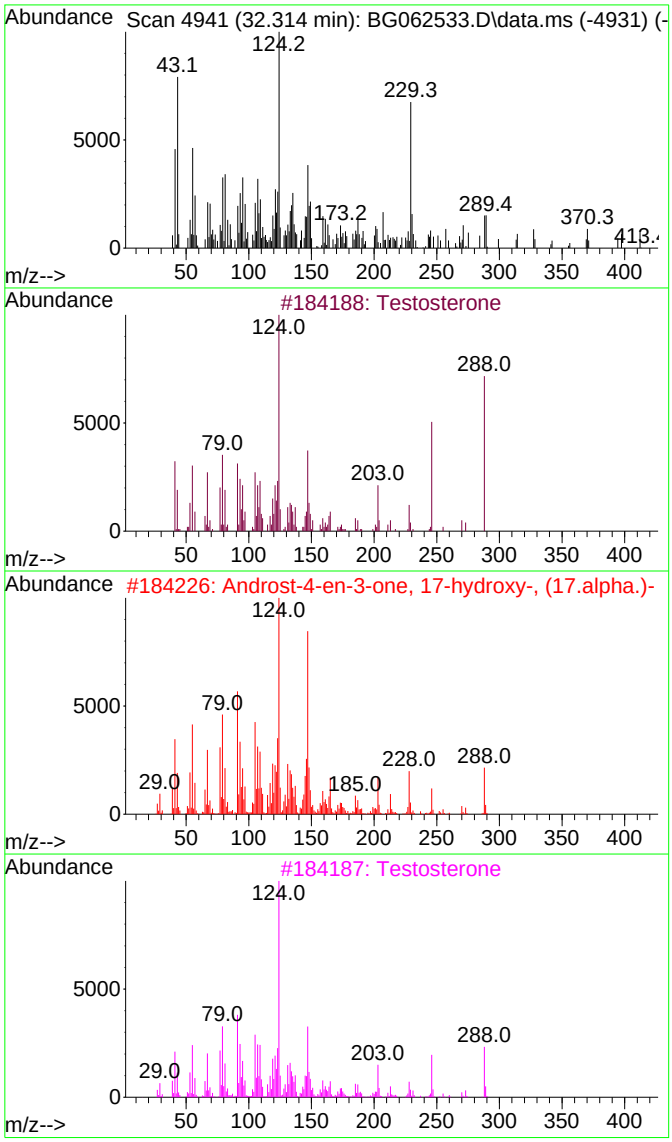
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

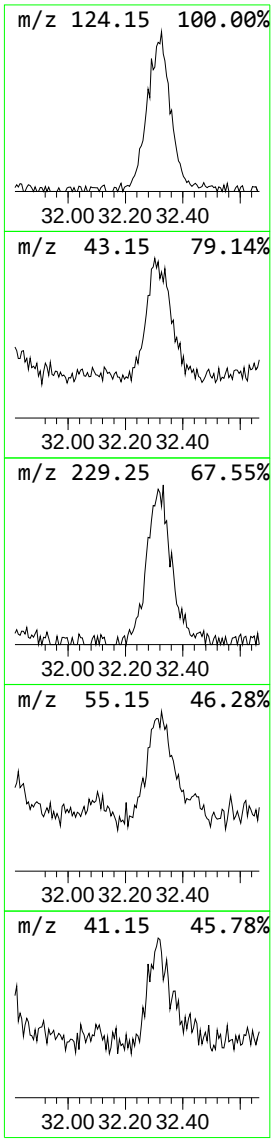
****

Peak Number 15 Testosterone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.314	8.44 ng/ul	578252	Perylene-d12	24.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Testosterone	288	C19H28O2	000058-22-0	70
2	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	41
3	Testosterone	288	C19H28O2	000058-22-0	41
4	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	30
5	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062533.D
Acq On : 22 Aug 2024 8:13
Operator : MA/JU
Sample : P3626-22
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.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
(S)-(+)-1,2-Pro...	3.665	5.7	ng/ul	118760	1	7.941	418951	20.0
.alpha.-Pinene	6.637	2.3	ng/ul	47804	1	7.941	418951	20.0
Ethanol, 2-(2-e...	7.524	2.1	ng/ul	43697	1	7.941	418951	20.0
1-Phenoxypropan...	11.460	4.3	ng/ul	142744	2	10.732	667000	20.0
n-Hexadecanoic ...	18.192	5.5	ng/ul	308154	4	17.299	1123160	20.0
Heptadecyl hept...	21.212	7.8	ng/ul	492007	5	21.535	1262750	20.0
(DEL) Alkane: S...	22.345	26.8	ng/ul	1690870	5	21.535	1262750	20.0
(DEL) Alkane: S...	23.755	6.4	ng/ul	439889	6	24.613	1370060	20.0
n-Nonadecanol-1	23.820	4.8	ng/ul	328518	6	24.613	1370060	20.0
1,21-Docosadiene	25.147	2.4	ng/ul	165263	6	24.613	1370060	20.0
(DEL) Alkane: S...	25.735	4.1	ng/ul	282244	6	24.613	1370060	20.0
1H,5H-Pyrrolo[1...	25.852	8.4	ng/ul	572639	6	24.613	1370060	20.0
.gamma.-Sitosterol	29.682	8.9	ng/ul	612244	6	24.613	1370060	20.0
Taraxasterol	31.697	32.8	ng/ul	2248520	6	24.613	1370060	20.0
Testosterone	32.314	8.4	ng/ul	578252	6	24.613	1370060	20.0