LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A4C51

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-BG062024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG061706.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.467	26	30	37	rVB3	16654	28664	0.74%	0.105%
2	3.731	71	75	87	rBV	112829	181888	4.71%	0.665%
3	3.890	98	102	111	rBV	98167	160586	4.16%	0.587%
4	4.043	125	128	131	rBV5	5450	7342	0.19%	0.027%
5	4.184	148	152	155	rVB4	5199	7961	0.21%	0.029%
6	4.219	155	158	164	rBV6	8205	15514	0.40%	0.057%
7	5.141	311	315	317	rBV3	7323	8380	0.22%	0.031%
8	6.134	479	484	492	rVB2	14781	30359	0.79%	0.111%
9	6.751	584	589	594	rVB4	15049	22964	0.59%	0.084%
10	7.027	629	636	637	rBV7	5508	8301	0.21%	0.030%
11	7.063	639	642	645	rVB4	13775	18015	0.47%	0.066%
12	7.215	661	668	675	rBV	269694	450533	11.66%	1.647%
13	7.398	693	699	707	rVB2	177761	298086	7.72%	1.089%
14	7.515	716	719	726	rVB5	7391	13672	0.35%	0.050%
15	7.597	726	733	739	rBV	220965	392746	10.17%	1.435%
16	7.656	739	743	749	rVB	54108	84184	2.18%	0.308%
17	8.073	806	814	821	rBV	236661	394365	10.21%	1.441%
18	8.132	821	824	828	rVB5	8847	11618	0.30%	0.042%
19	8.296	846	852	857	rBV7	8577	17788	0.46%	0.065%
20	8.385	862	867	871	rVB4	6228	9012	0.23%	0.033%
21	8.614	902	906	910	rBV4	6313	9495	0.25%	0.035%
22	8.767	924	932	943	rBV2	321746	553701	14.34%	2.024%
23	9.237	1005	1012	1019	rVV	244411	442235	11.45%	1.616%
24	9.319	1023	1026	1029	rVV5	8085	10582	0.27%	0.039%
25	9.795	1101	1107	1111	rBV3	32552	52426	1.36%	0.192%
26	9.959	1128	1135	1146	rVB2	216294	374928	9.71%	1.370%
27	10.083	1149	1156	1159	rVV3	9041	14312	0.37%	0.052%
28	10.165	1166	1170	1174	rVV5	5566	8184	0.21%	0.030%
29	10.300	1187	1193	1200	rVB2	82736	145007	3.75%	0.530%
30	10.494	1219	1226	1235	rVV	331911	590093	15.28%	2.157%
31	10.888	1284	1293	1300	rBV	400829	677083	17.53%	2.474%
32	10.946	1300	1303	1305	rVV3	11998	14466	0.37%	0.053%
33	11.017	1307	1315	1322	rVB	303141	566542	14.67%	2.070%
34	11.410	1378	1382	1386	rVB4	18788	25192	0.65%	0.092%
35	11.616	1410	1417	1427	rBV2	98884	188416	4.88%	0.689%
36	11.798	1444	1448	1451	rBV2	3772	6353	0.16%	0.023%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A4C51

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-BG062024.MA.M
Title : SVOA CALIBRATION

37	12.339	1532	1540	1547	rBV	2497875	3862460	100.00%	14.116%
38	12.462	1558	1561	1566	rBV4	6123	9959	0.26%	0.036%
39	12.550	1571	1576	1583	rVB5	37355	64644	1.67%	0.236%
40	13.067	1661	1664	1668	rVB4	14428	19532	0.51%	0.071%
41	13.543	1742	1745	1750	rBV4	17242	25398	0.66%	0.093%
42	13.884	1800	1803	1807	rBV3	4523	7554	0.20%	0.028%
43	14.107	1834	1841	1849	rBV	610455	905380	23.44%	3.309%
44	14.336	1877	1880	1884	rVV2	20978	29685	0.77%	0.108%
45	14.395	1884	1890	1899	rVB2	704560	1104237	28.59%	4.036%
46	14.583	1919	1922	1927	rVB4	3748	7203	0.19%	0.026%
47	14.642	1927	1932	1935	rBV6	5156	10052	0.26%	0.037%
48	14.701	1935	1942	1949	rBV	687490	1049907	27.18%	3.837%
49	14.871	1963	1971	1986	rBV	368466	690898	17.89%	2.525%
50	15.059	1997	2003	2006	rVV5	19320	32686	0.85%	0.119%
51	15.100	2006	2010	2017	rVB8	12130	27932	0.72%	0.102%
52	15.194	2021	2026	2028	rBV3	5220	8603	0.22%	0.031%
53	15.570	2087	2090	2093	rVB5	7879	9203	0.24%	0.034%
54	15.688	2103	2110	2119	rVB	963576	1463386	37.89%	5.348%
55	15.794	2121	2128	2135	rVV	306462	459139	11.89%	1.678%
56	15.841	2135	2136	2141	rVV3	12256	11517	0.30%	0.042%
57	15.935	2149	2152	2157	rVB6	6901	11824	0.31%	0.043%
58	16.029	2164	2168	2169	rBV3	5964	6374	0.17%	0.023%
59	16.228	2198	2202	2206	rBV4	16930	27877	0.72%	0.102%
60	16.316	2213	2217	2221	rBV7	15494	28125	0.73%	0.103%
61	16.440	2237	2238	2246	rVB4	12101	11897	0.31%	0.043%
62	16.552	2252	2257	2258	rBV4	6021	6245	0.16%	0.023%
63	16.563	2258	2259	2265	rVB6	6828	11130	0.29%	0.041%
64	16.828	2300	2304	2308	rBV3	8957	10341	0.27%	0.038%
65	16.910	2314	2318	2319	rBV3	4157	6416	0.17%	0.023%
66	16.986	2328	2331	2336	rVB5	8268	12235	0.32%	0.045%
67	17.151	2355	2359	2363	rVB7	4571	7501	0.19%	0.027%
68	17.198	2363	2367	2368	rBV2	6160	7771	0.20%	0.028%
69	17.333	2386	2390	2391	rVV3	6958	9475	0.25%	0.035%
70	17.351	2391	2393	2396	rVV3	6657	9065	0.23%	0.033%
71	17.445	2402	2409	2416	rVV	960534	1467584	38.00%	5.363%
72	17.544	2419	2426	2432	rVV2	1076036	1650435	42.73%	6.032%
73	17.615	2435	2438	2441	rVV5	8564	11641	0.30%	0.043%
74	17.680	2447	2449	2456	rVV5	7879	10890	0.28%	0.040%
75	17.809	2469	2471	2476	rBV5	5255	9758	0.25%	0.036%
76	18.108	2518	2522	2527	rVB2	27714	32667	0.85%	0.119%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Title : SVOA CALIBRATION

77	18.197	2533	2537	2538	rBV4	6519	7798	0.20%	0.028%
78	18.267	2546	2549	2552	rBV4	11288	12495	0.32%	0.046%
79	18.326	2554	2559	2568	rBV2	236769	344119	8.91%	1.258%
80	18.549	2594	2597	2600	rVB5	5664	7270	0.19%	0.027%
81	18.655	2613	2615	2617	rBV2	9981	11196	0.29%	0.041%
82	19.060	2680	2684	2686	rVB5	6836	8076	0.21%	0.030%
83	19.178	2700	2704	2711	rBV5	34490	49367	1.28%	0.180%
84	19.389	2734	2740	2743	rBV6	18141	29584	0.77%	0.108%
85	19.454	2746	2751	2753	rBV4	40935	60020	1.55%	0.219%
86	19.595	2771	2775	2779	rBV5	71559	95831	2.48%	0.350%
87	19.824	2806	2814	2819	rBV	1238614	1834833	47.50%	6.706%
88	20.318	2896	2898	2901	rBV4	9994	15630	0.40%	0.057%
89	20.359	2901	2905	2909	rVB5	56708	78730	2.04%	0.288%
90	20.858	2985	2990	2993	rBV3	38071	50341	1.30%	0.184%
91	21.358	3070	3075	3086	rBV	233884	391693	10.14%	1.431%
92	21.704	3127	3134	3141	rBV2	911467	1499098	38.81%	5.479%
93	21.916	3168	3170	3174	rVB2	40808	50530	1.31%	0.185%
94	22.539	3271	3276	3284	rBV6	59744	148812	3.85%	0.544%
95	23.244	3391	3396	3399	rBV5	42814	69576	1.80%	0.254%
96	24.060	3530	3535	3541	rVB4	66811	130914	3.39%	0.478%
97	24.713	3636	3646	3656	rBV	618033	1768082	45.78%	6.462%
98	24.930	3674	3683	3695	rBV	544689	1530040	39.61%	5.592%
99	26.181	3891	3896	3903	rVB3	79049	169077	4.38%	0.618%
100	27.774	4165	4167	4169	rBV3	12853	9875	0.26%	0.036%

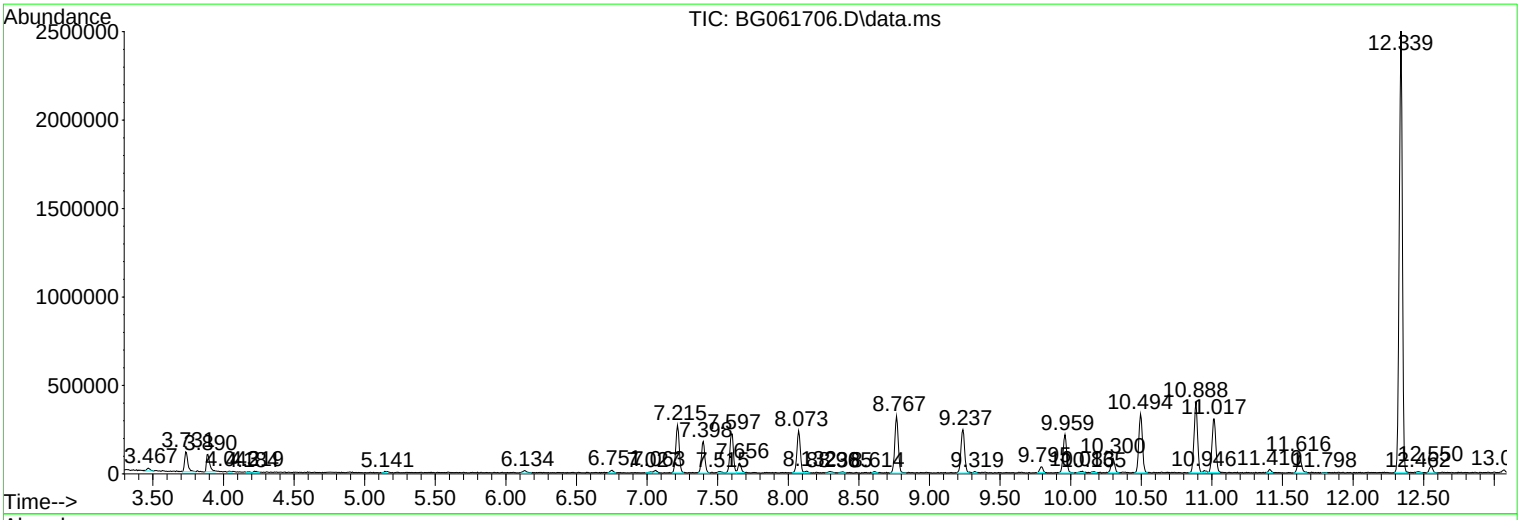
Sum of corrected areas: 27362606

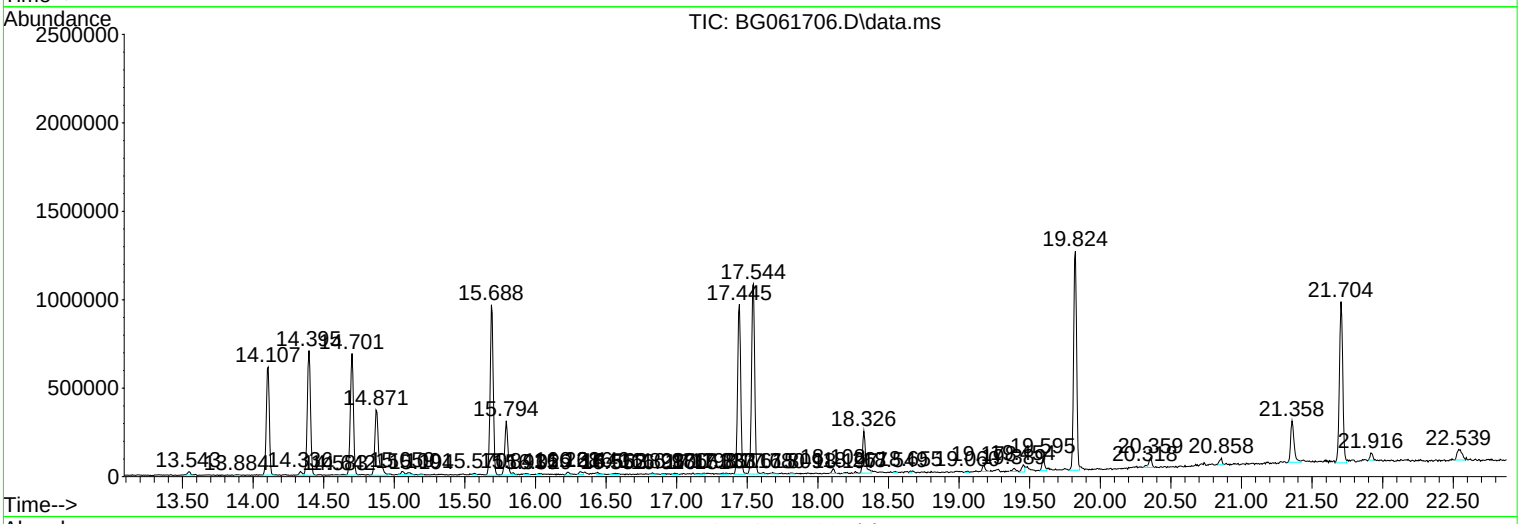
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

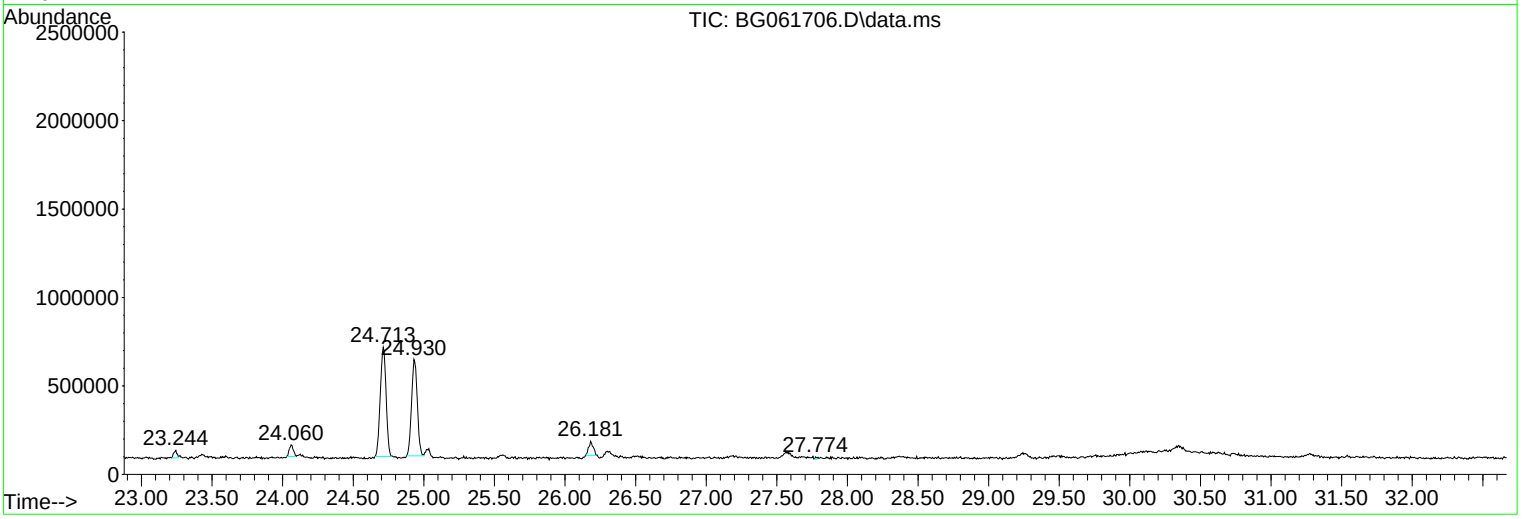
Instrument :
BNA_G
ClientSampleId :
A4C51

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.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\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

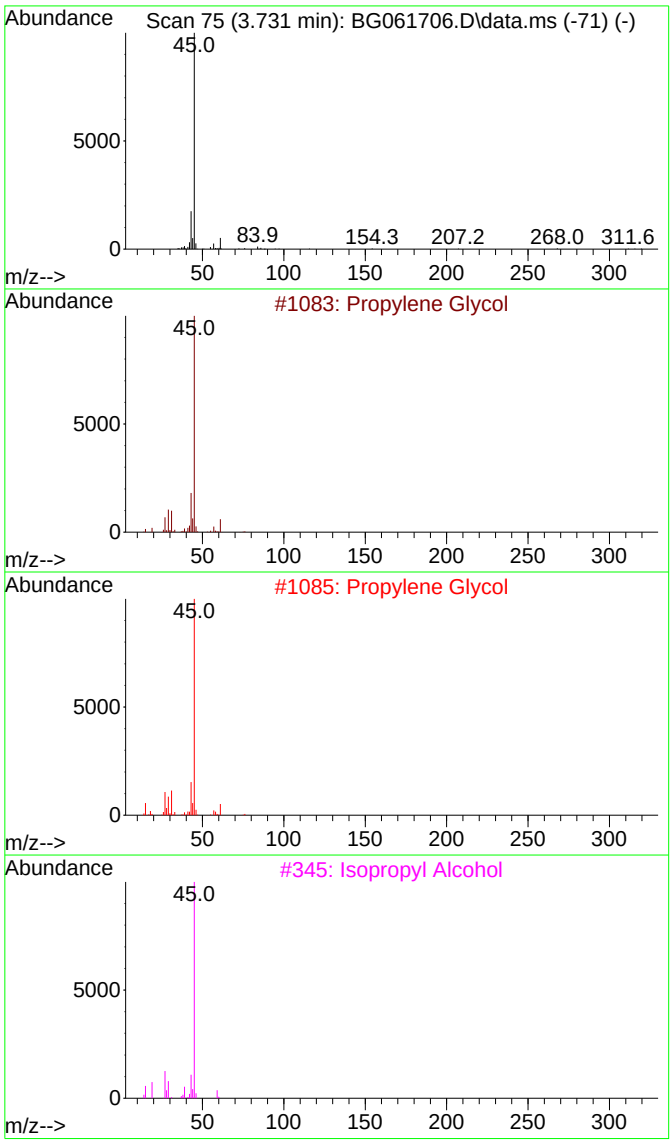
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

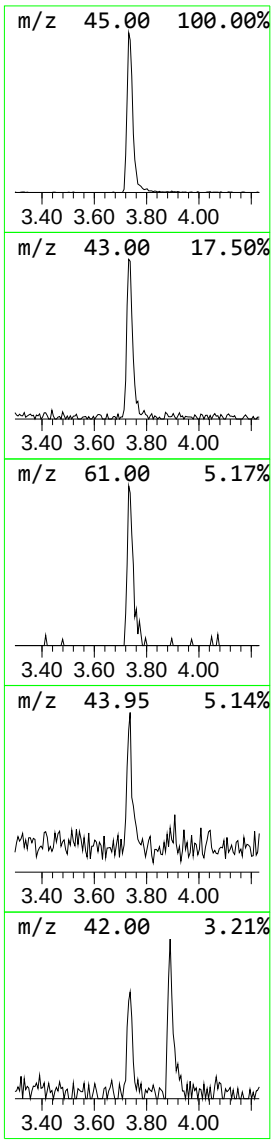
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.731	9.22 ng/ul	181888	1,4-Dichlorobenzene-d4	8.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	72
2	Propylene Glycol	76	C3H8O2	000057-55-6	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

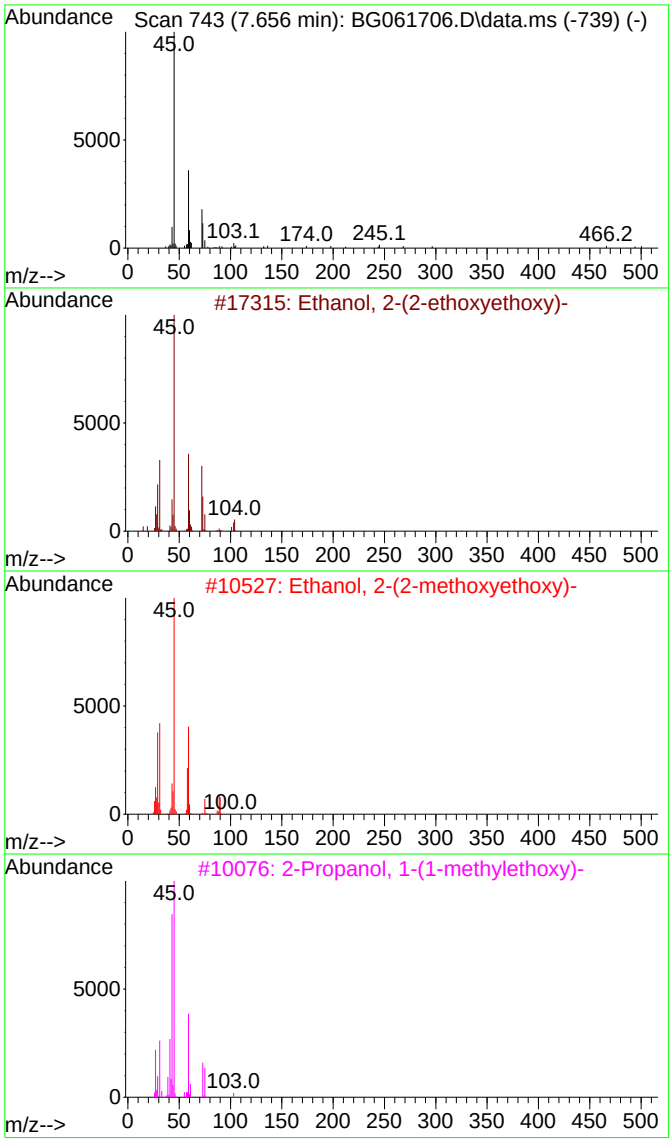
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

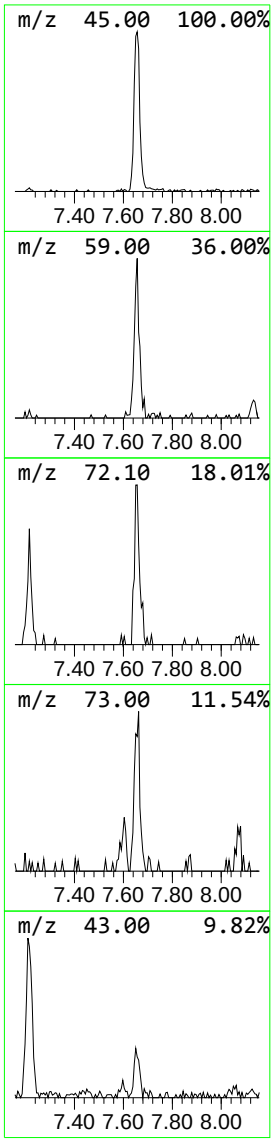
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.656	4.27 ng/ul	84184	1,4-Dichlorobenzene-d4	8.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	47
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
4	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	38
5	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

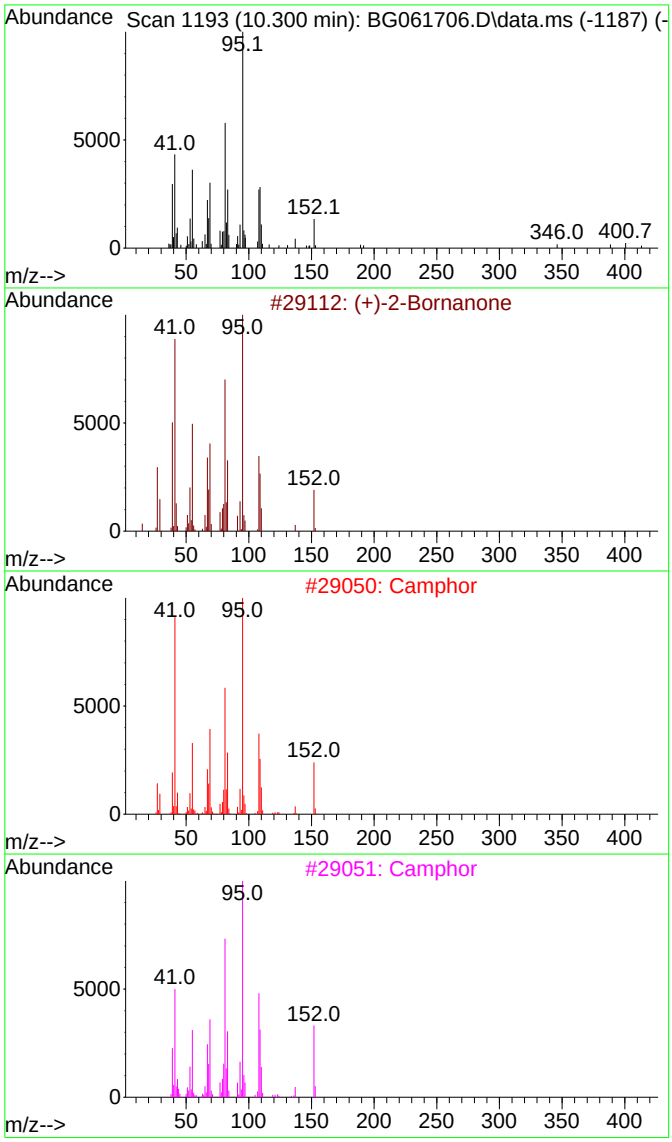
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

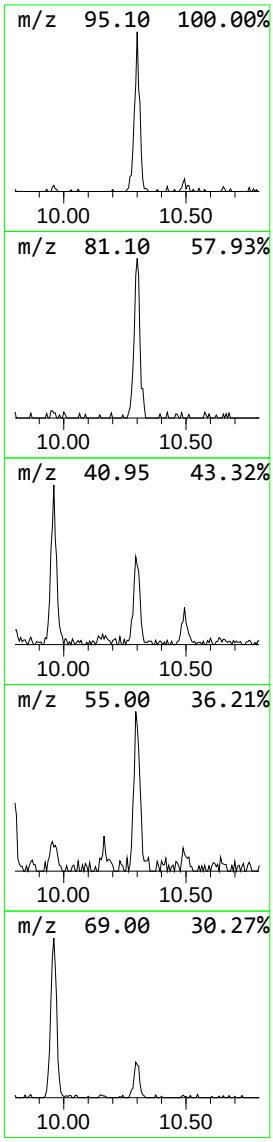
****

Peak Number 3 (+)-2-Bornanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.300	4.28 ng/ul	145007	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	91
2	Camphor	152	C10H16O	000076-22-2	87
3	Camphor	152	C10H16O	000076-22-2	80
4	(+)-2-Bornanone	152	C10H16O	000464-49-3	74
5	(+)-2-Bornanone	152	C10H16O	000464-49-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

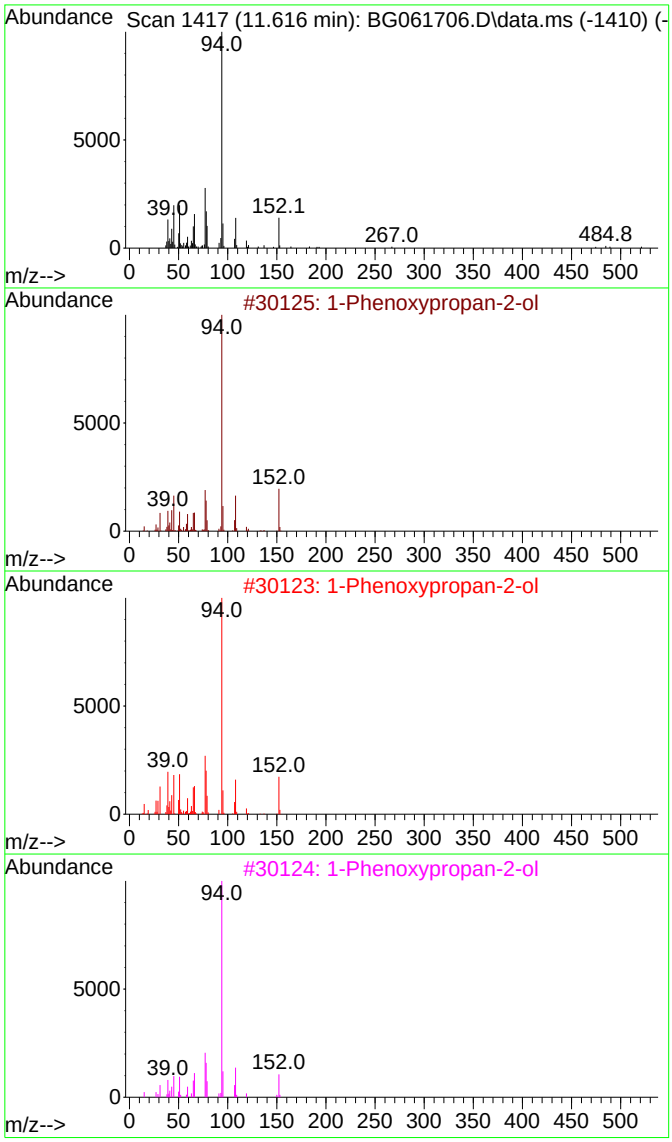
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

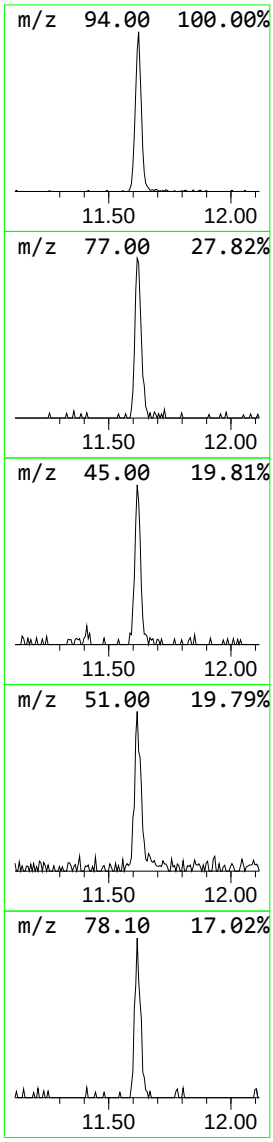
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	5.57 ng/ul	188416	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	81
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	80
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

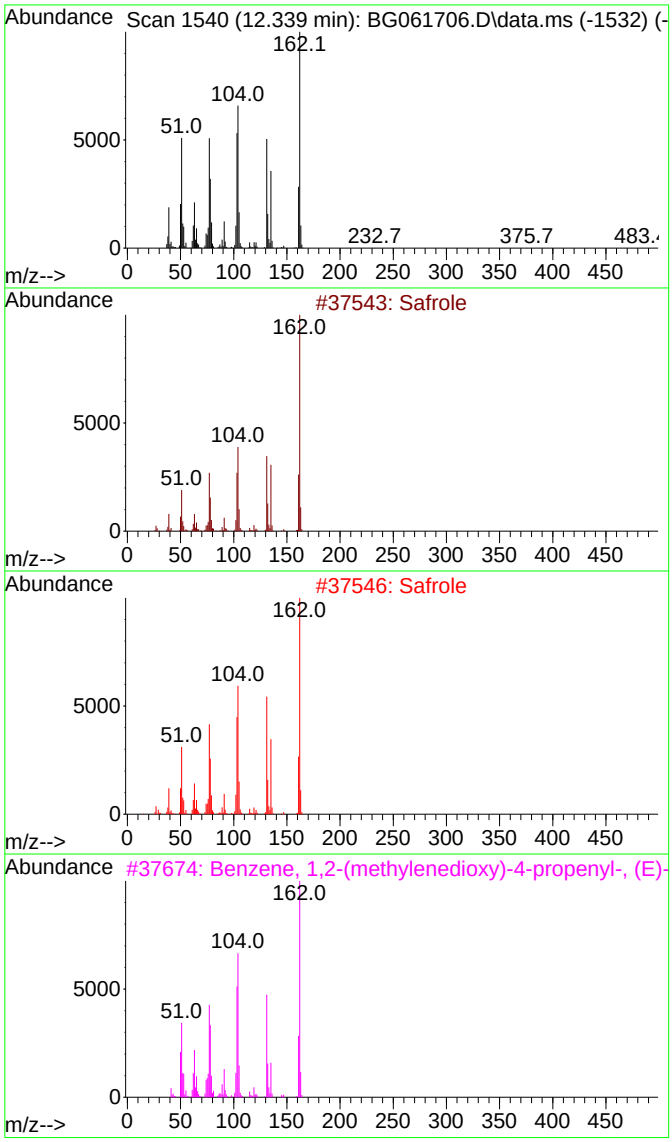
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

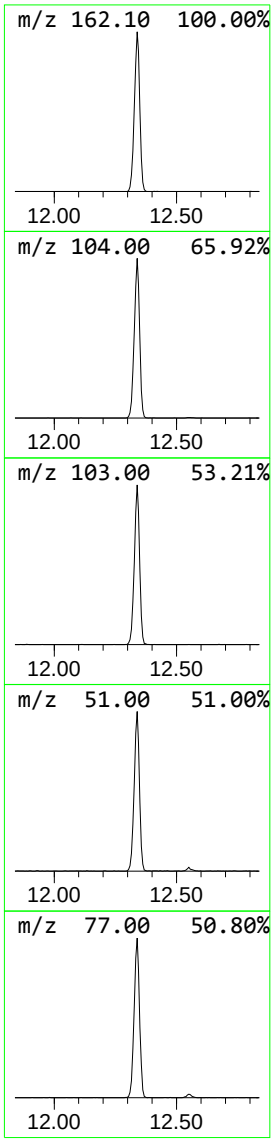
****

Peak Number 5 Safrole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.339	114.09 ng/ul	3862460	Naphthalene-d8	10.887

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	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	98
4	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	98
5	Safrole	162	C10H10O2	000094-59-7	98





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Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

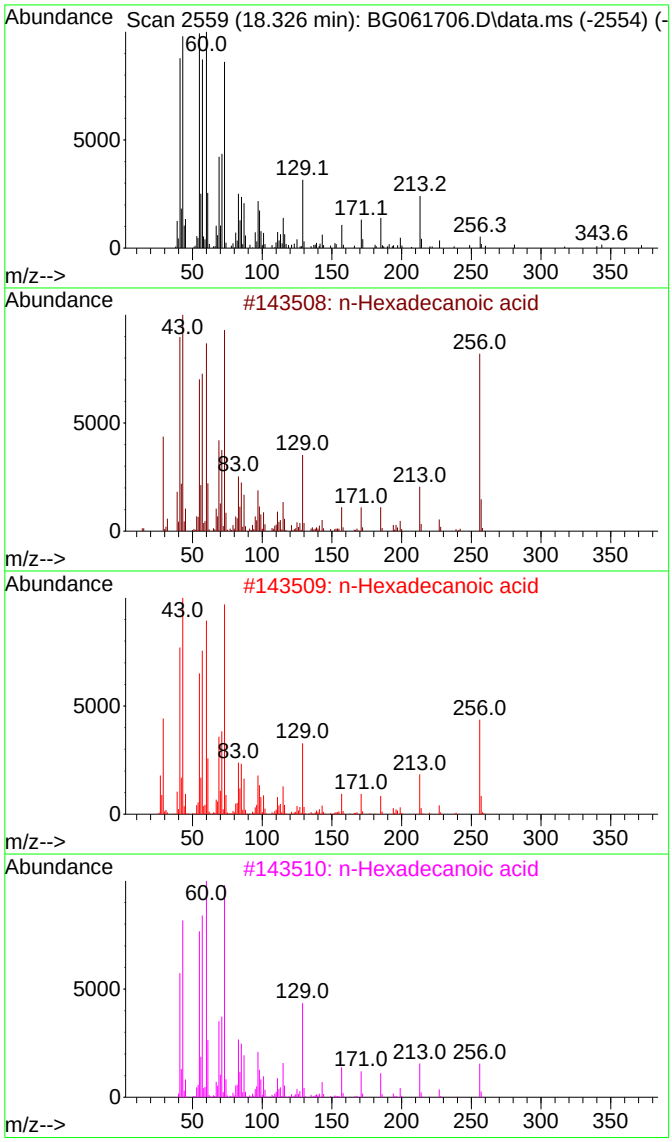
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

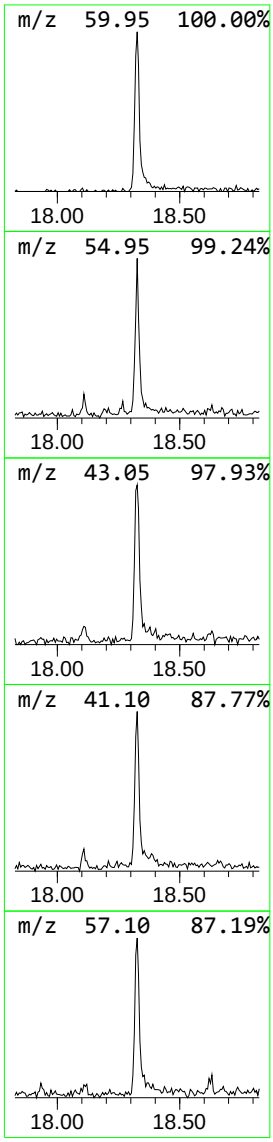
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.326	4.69 ng/ul	344119	Phenanthrene-d10	17.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

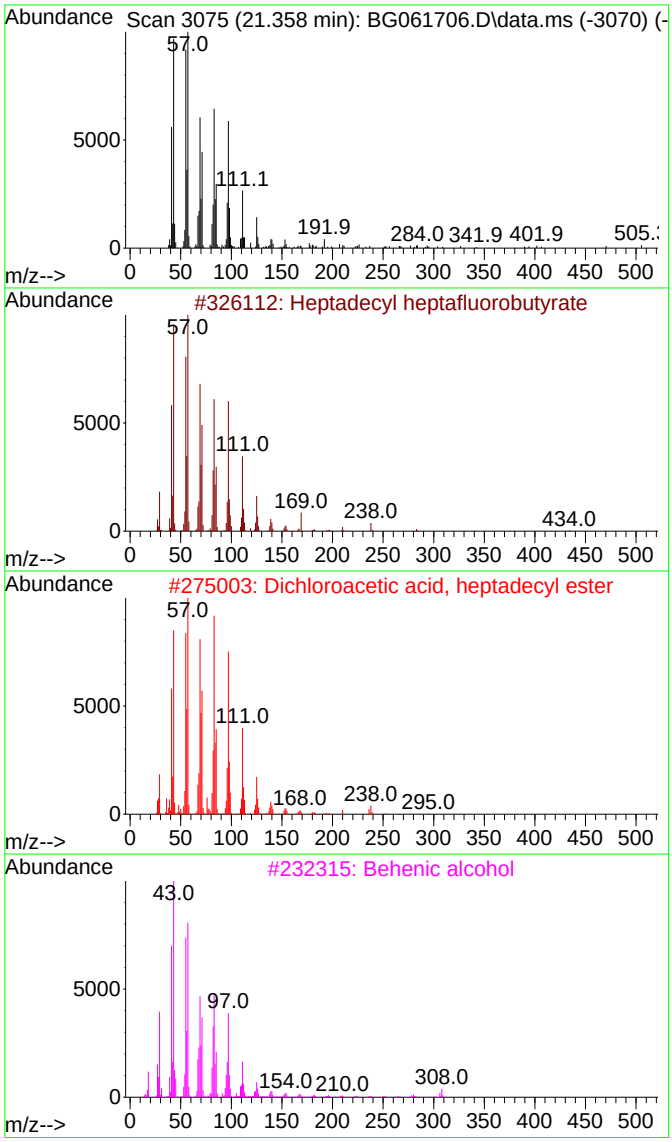
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

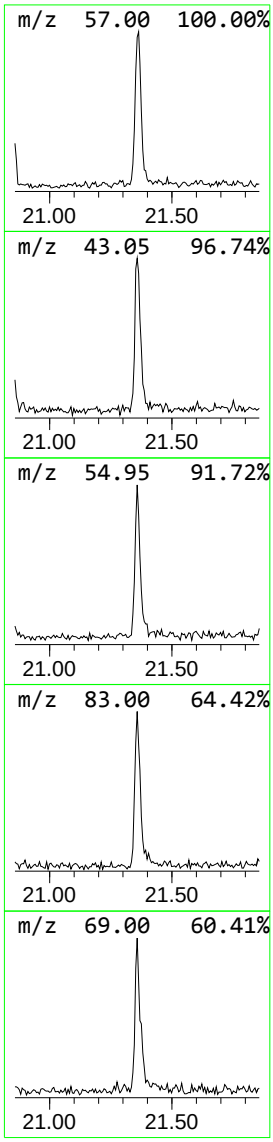
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.358	5.23 ng/ul	391693	Chrysene-d12	21.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	1-Nonadecene	266	C19H38	018435-45-5	87
5	Z-5-Nonadecene	266	C19H38	1000131-11-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

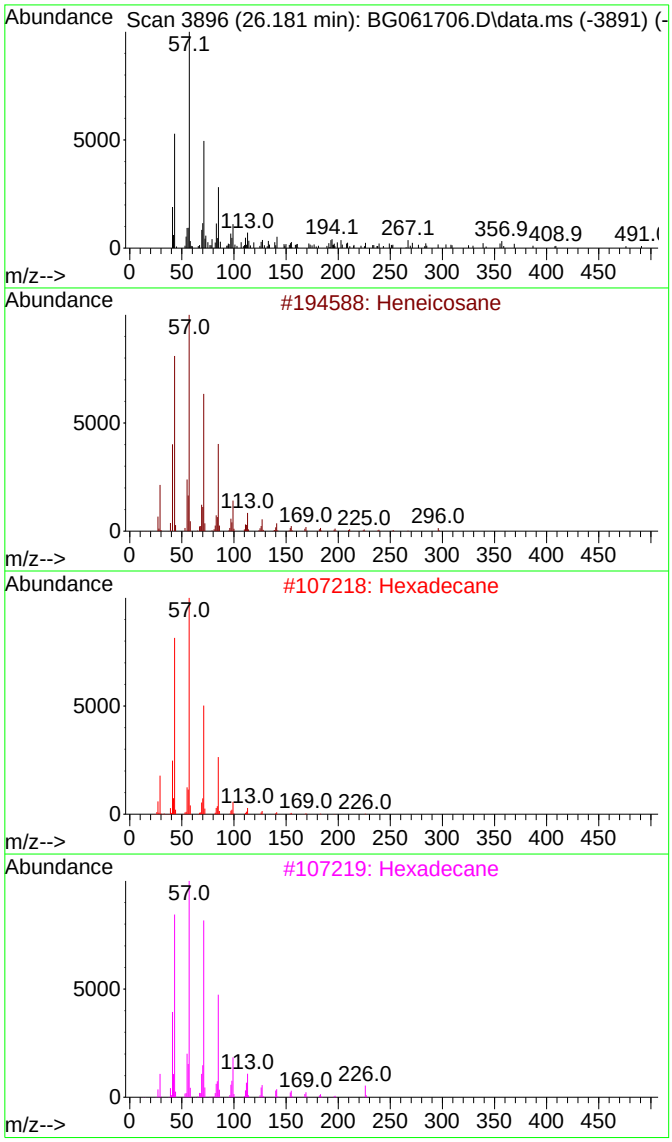
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

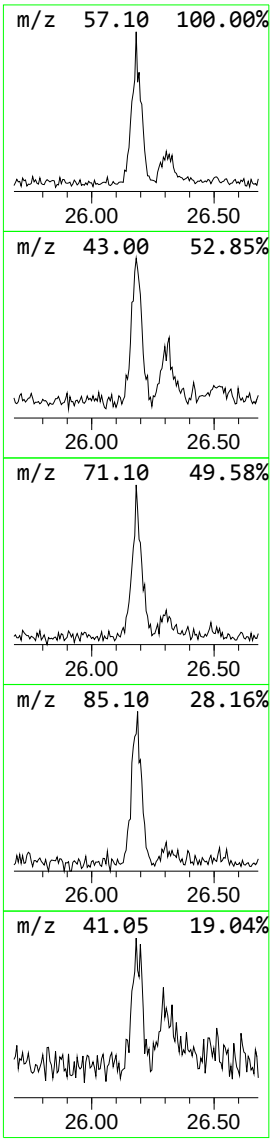
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.181	2.21 ng/ul	169077	Perylene-d12	24.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Hexadecane	226	C16H34	000544-76-3	81
3	Hexadecane	226	C16H34	000544-76-3	76
4	Octacosane	394	C28H58	000630-02-4	76
5	Undecane	156	C11H24	001120-21-4	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061706.D
Acq On : 25 Jun 2024 17:15
Operator : MA/JU
Sample : P2844-26
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C51

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.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
Propylene Glycol	3.731	9.2	ng/ul	181888	1	8.073	394365	20.0
unknown-01	7.656	4.3	ng/ul	84184	1	8.073	394365	20.0
(+)-2-Bornanone	10.300	4.3	ng/ul	145007	2	10.887	677083	20.0
1-Phenoxypropan...	11.616	5.6	ng/ul	188416	2	10.887	677083	20.0
Safrole	12.339	114.1	ng/ul	3862460	2	10.887	677083	20.0
n-Hexadecanoic ...	18.326	4.7	ng/ul	344119	4	17.445	1467580	20.0
Heptadecyl hept...	21.358	5.2	ng/ul	391693	5	21.704	1499100	20.0
(DEL) Alkane: S...	26.181	2.2	ng/ul	169077	6	24.930	1530040	20.0