LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

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: BG062551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	17	19	25	rVB3	11559	15263	1.01%	0.078%
2	3.664	60	64	72	rBV	61679	89645	5.92%	0.461%
3	3.811	84	89	99	rBV	97580	155738	10.28%	0.801%
4	4.145	142	146	152	rVB4	4322	6618	0.44%	0.034%
5	5.044	296	299	306	rVB6	3841	5543	0.37%	0.028%
6	6.019	459	465	473	rBV2	9086	15343	1.01%	0.079%
7	6.636	564	570	575	rVB	28188	44654	2.95%	0.230%
8	6.924	614	619	621	rBV5	4312	6260	0.41%	0.032%
9	7.100	643	649	661	rVB	190155	332164	21.93%	1.708%
10	7.265	668	677	687	rBV	151444	247373	16.33%	1.272%
11	7.470	705	712	717	rBV	182568	315136	20.80%	1.620%
12	7.523	717	721	728	rVB	25512	43497	2.87%	0.224%
13	7.934	784	791	799	rVV	283437	472390	31.19%	2.429%
14	7.993	799	801	807	rVB4	6083	8806	0.58%	0.045%
15	8.633	902	910	920	rBV	168161	282998	18.68%	1.455%
16	9.086	979	987	999	rBV	187643	328944	21.72%	1.691%
17	9.197	1004	1006	1010	rVV4	2458	3221	0.21%	0.017%
18	9.526	1058	1062	1069	rVB5	3246	5390	0.36%	0.028%
19	9.644	1076	1082	1089	rBV3	29000	44188	2.92%	0.227%
20	9.808	1100	1110	1118	rBV	150844	266753	17.61%	1.372%
21	10.031	1143	1148	1156	rVB5	2956	4900	0.32%	0.025%
22	10.349	1195	1202	1211	rBV	246368	440716	29.10%	2.266%
23	10.725	1259	1266	1274	rBV	413731	740673	48.90%	3.808%
24	10.854	1279	1288	1301	rBV	180384	331334	21.87%	1.704%
25	11.259	1351	1357	1363	rBV3	12780	20028	1.32%	0.103%
26	11.465	1384	1392	1398	rBV	68634	129383	8.54%	0.665%
27	12.305	1532	1535	1541	rVV2	4932	7539	0.50%	0.039%
28	13.386	1715	1719	1725	rVV3	4281	7129	0.47%	0.037%
29	13.462	1730	1732	1739	rVB4	2316	4463	0.29%	0.023%
30	13.961	1811	1817	1824	rVB	457731	658283	43.46%	3.385%
31	14.249	1853	1866	1874	rBV	543952	864652	57.08%	4.446%
32	14.461	1897	1902	1909	rVB4	3077	5232	0.35%	0.027%
33	14.555	1911	1918	1926	rVV	746066	1159597	76.56%	5.962%
34	14.755	1944	1952	1955	rBV5	289355	607377	40.10%	3.123%
35	14.972	1985	1989	1995	rBV4	4315	7446	0.49%	0.038%
36	15.348	2049	2053	2058	rVB4	3228	5253	0.35%	0.027%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

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	15.412	2060	2064	2067	rBV2	3703	4485	0.30%	0.023%
38	15.548	2080	2087	2094	rBV	717852	1083719	71.55%	5.572%
39	15.659	2099	2106	2112	rBV	196377	288854	19.07%	1.485%
40	15.712	2112	2115	2119	rVB3	3343	4930	0.33%	0.025%
41	15.788	2124	2128	2133	rBV3	2839	4062	0.27%	0.021%
42	16.035	2166	2170	2174	rVB3	2719	4102	0.27%	0.021%
43	16.100	2174	2181	2189	rBV5	7927	19025	1.26%	0.098%
44	16.270	2204	2210	2214	rVV4	5299	6849	0.45%	0.035%
45	16.699	2279	2283	2287	rBV2	8919	12307	0.81%	0.063%
46	16.852	2304	2309	2314	rBV6	5287	8751	0.58%	0.045%
47	17.016	2333	2337	2340	rBV4	2907	3078	0.20%	0.016%
48	17.063	2340	2345	2348	rBV3	5575	8376	0.55%	0.043%
49	17.198	2364	2368	2372	rBV	18541	26786	1.77%	0.138%
50	17.298	2375	2385	2395	rVV	935552	1427058	94.21%	7.337%
51	17.398	2395	2402	2409	rVB	758989	1135115	74.94%	5.836%
52	17.474	2411	2415	2419	rVB4	5980	6718	0.44%	0.035%
53	17.586	2430	2434	2436	rBV4	3249	4762	0.31%	0.024%
54	17.645	2441	2444	2447	rBV5	4022	5686	0.38%	0.029%
55	17.692	2449	2452	2461	rVB5	4972	10261	0.68%	0.053%
56	17.933	2489	2493	2497	rBV6	5866	9867	0.65%	0.051%
57	17.974	2497	2500	2506	rVB	18607	24772	1.64%	0.127%
58	18.074	2511	2517	2520	rBV6	10951	18170	1.20%	0.093%
59	18.132	2525	2527	2531	rVB4	2921	3489	0.23%	0.018%
60	18.197	2532	2538	2547	rBV	149338	262771	17.35%	1.351%
61	18.309	2556	2557	2562	rVB5	7867	9603	0.63%	0.049%
62	18.497	2584	2589	2592	rBV5	9404	15020	0.99%	0.077%
63	18.538	2592	2596	2602	rVB7	11028	16882	1.11%	0.087%
64	18.626	2607	2611	2612	rBV4	3855	3933	0.26%	0.020%
65	18.825	2642	2645	2649	rBV6	3775	6077	0.40%	0.031%
66	19.055	2681	2684	2689	rBV6	5499	10062	0.66%	0.052%
67	19.113	2690	2694	2696	rVV4	11923	16832	1.11%	0.087%
68	19.143	2696	2699	2706	rVB6	26226	38213	2.52%	0.196%
69	19.248	2714	2717	2725	rVB6	12042	18407	1.22%	0.095%
70	19.319	2725	2729	2732	rBV2	20355	27852	1.84%	0.143%
71	19.348	2732	2734	2735	rVV2	4856	4498	0.30%	0.023%
72	19.372	2736	2738	2742	rVB5	5797	6096	0.40%	0.031%
73	19.466	2749	2754	2759	rBV	49753	76533	5.05%	0.393%
74	19.536	2762	2766	2775	rVV2	23062	42966	2.84%	0.221%
75	19.619	2777	2780	2784	rVV4	18505	23014	1.52%	0.118%
76	19.683	2785	2791	2797	rVV	874216	1276546	84.28%	6.563%

LSC Area Percent Report

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Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

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	19.730	2797	2799	2807	rVB7	10016	17605	1.16%	0.091%
78	20.071	2854	2857	2860	rVB5	7634	7848	0.52%	0.040%
79	20.135	2863	2868	2875	rBV7	26851	49711	3.28%	0.256%
80	20.200	2877	2879	2882	rVV3	11997	16580	1.09%	0.085%
81	20.229	2882	2884	2888	rVV3	22972	24657	1.63%	0.127%
82	20.288	2891	2894	2898	rVB6	7567	9925	0.66%	0.051%
83	20.347	2902	2904	2907	rBV4	5480	6978	0.46%	0.036%
84	20.453	2919	2922	2923	rBV3	7010	7499	0.50%	0.039%
85	20.523	2929	2934	2937	rBV7	16867	29270	1.93%	0.150%
86	20.558	2937	2940	2944	rVB4	33999	43146	2.85%	0.222%
87	20.664	2953	2958	2962	rBV	60195	74942	4.95%	0.385%
88	20.946	3004	3006	3009	rVB4	9881	8657	0.57%	0.045%
89	21.216	3047	3052	3062	rBV2	161726	272311	17.98%	1.400%
90	21.545	3101	3108	3116	rBV	885191	1383030	91.31%	7.111%
91	22.362	3239	3247	3257	rBV4	79384	232908	15.38%	1.198%
92	22.996	3353	3355	3360	rVB	20875	27235	1.80%	0.140%
93	23.178	3381	3386	3397	rVB	58318	117670	7.77%	0.605%
94	23.772	3480	3487	3493	rBV	106118	219308	14.48%	1.128%
95	23.836	3494	3498	3508	rVB9	29057	72093	4.76%	0.371%
96	24.412	3586	3596	3610	rBV	457297	1209113	79.82%	6.217%
97	24.629	3622	3633	3647	rBV	515143	1514717	100.00%	7.788%
98	25.746	3816	3823	3834	rVB4	64937	183178	12.09%	0.942%
99	25.875	3838	3845	3861	rVB6	49384	191624	12.65%	0.985%
100	29.687	4488	4494	4496	rBV6	35445	69012	4.56%	0.355%

Sum of corrected areas: 19449473

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
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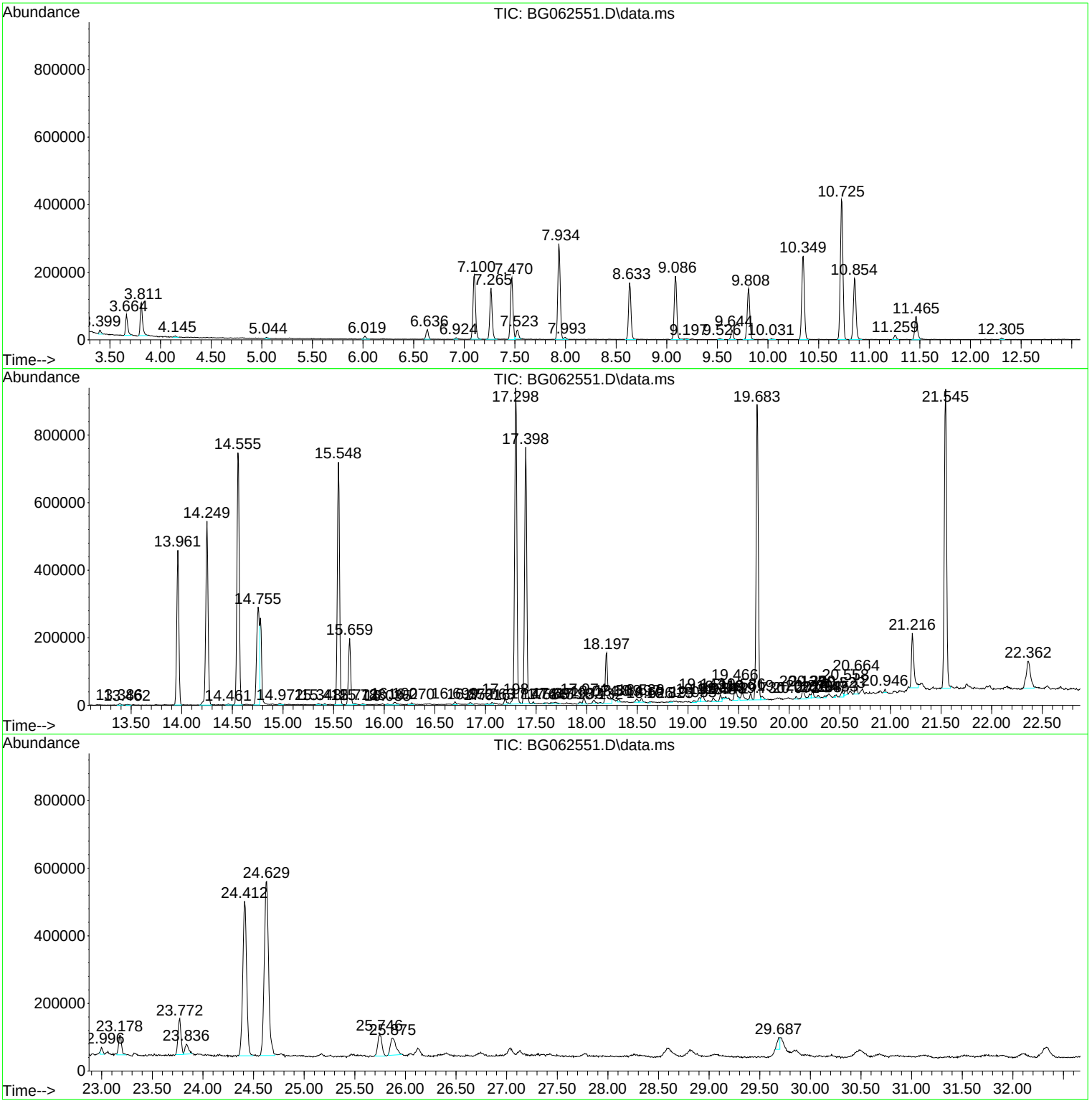
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

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\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

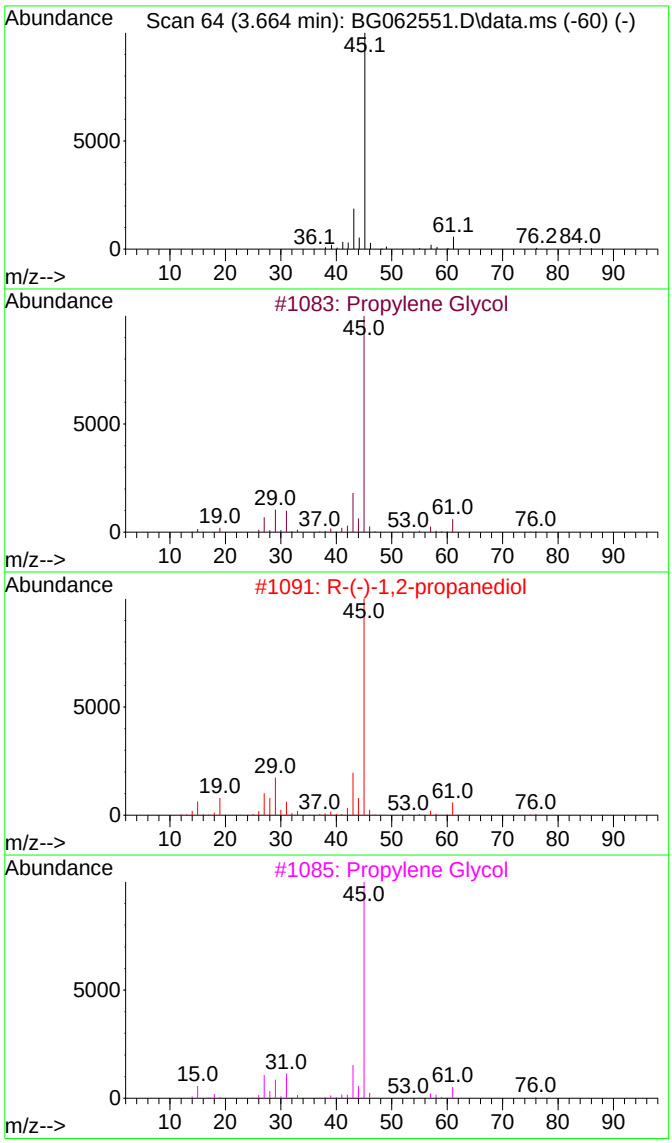
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

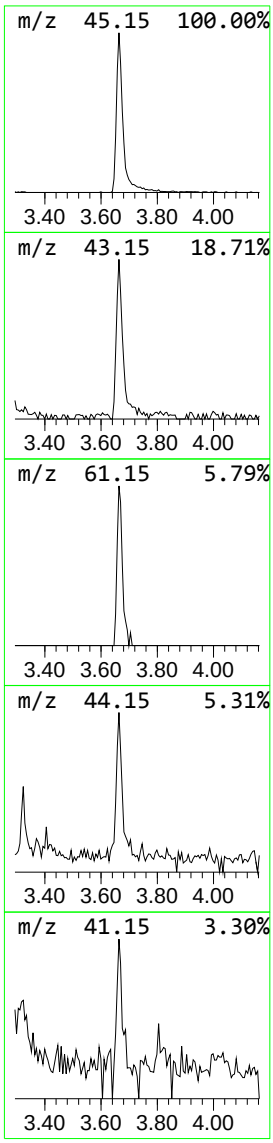
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.664	3.80 ng/ul	89645	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Propylene Glycol	76	C3H8O2	000057-55-6	56
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

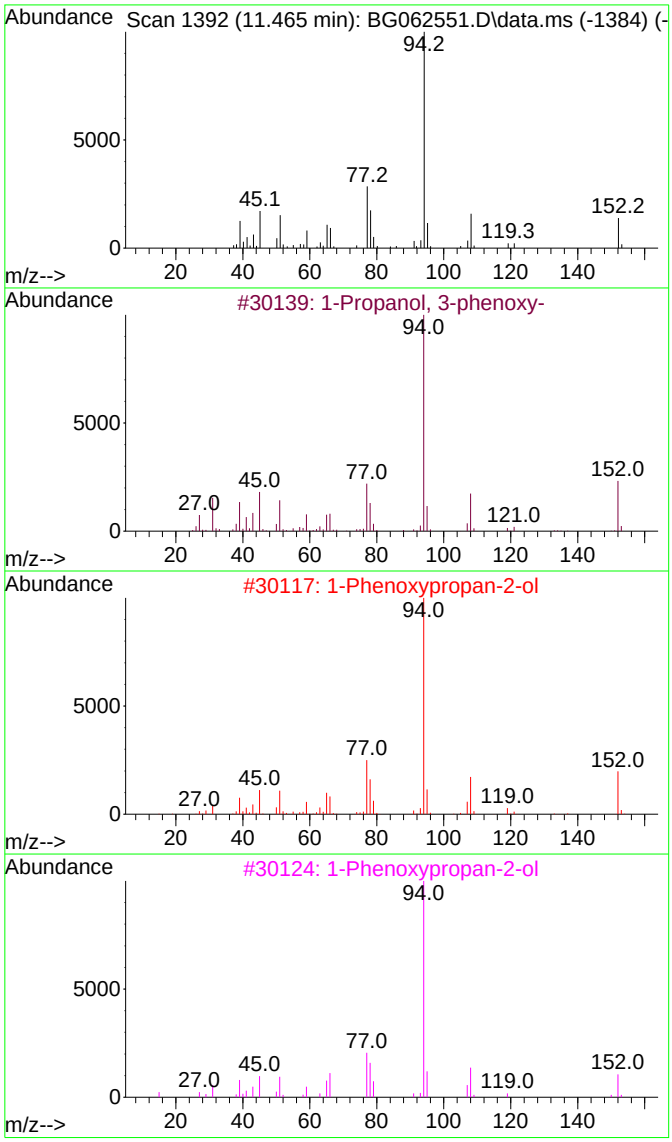
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

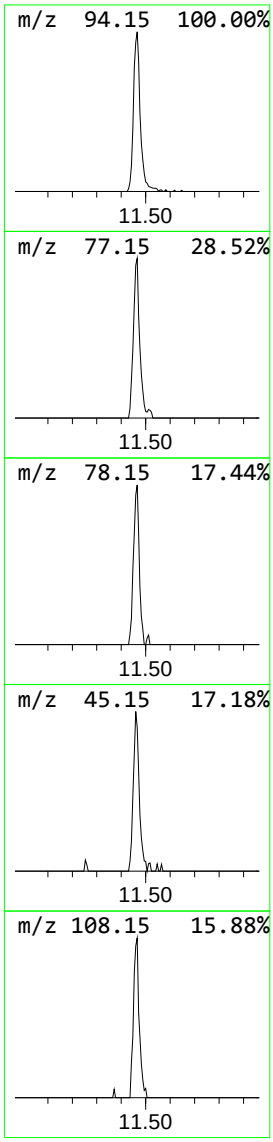
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanol, 3-phenoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.465	3.49 ng/ul	129383	Naphthalene-d8	10.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	94
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
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Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

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

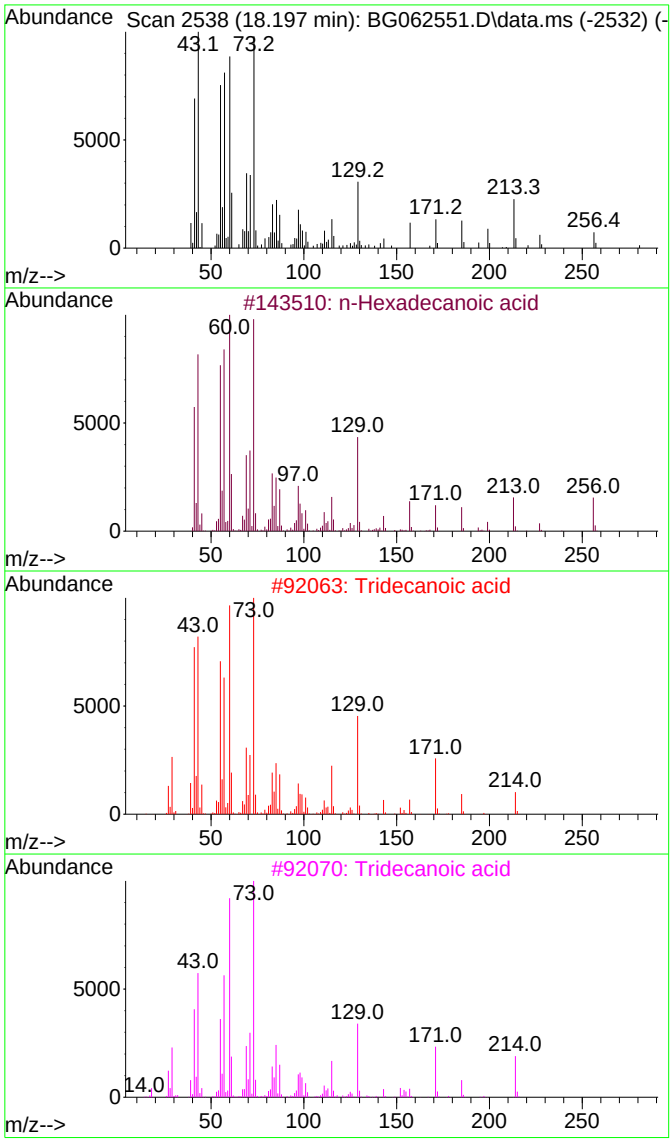
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

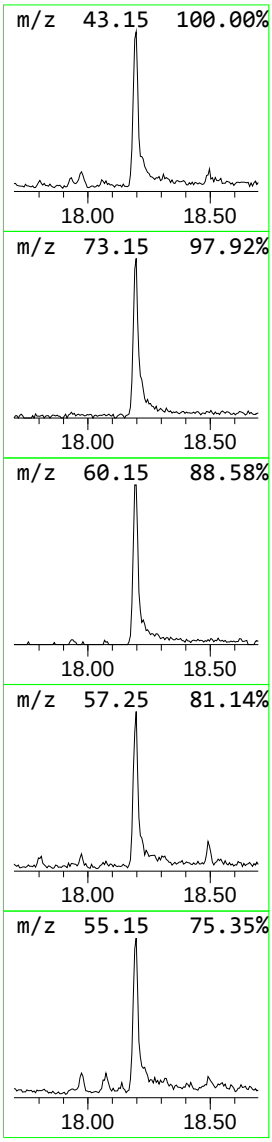
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.197	3.68 ng/ul	262771	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83





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Data File : BG062551.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

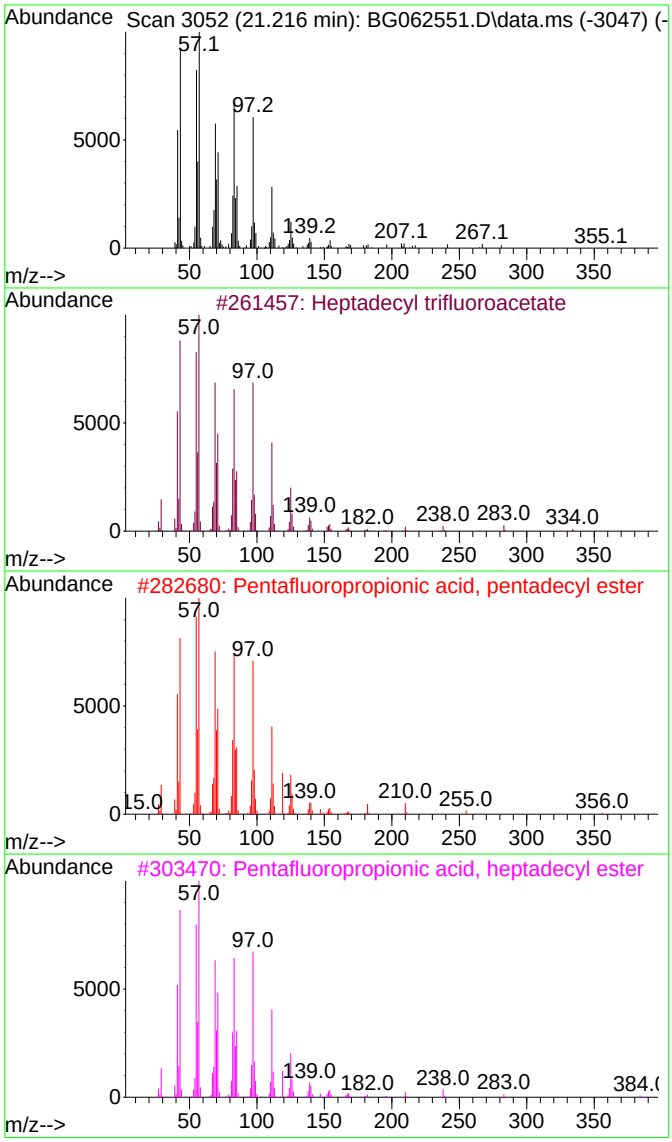
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

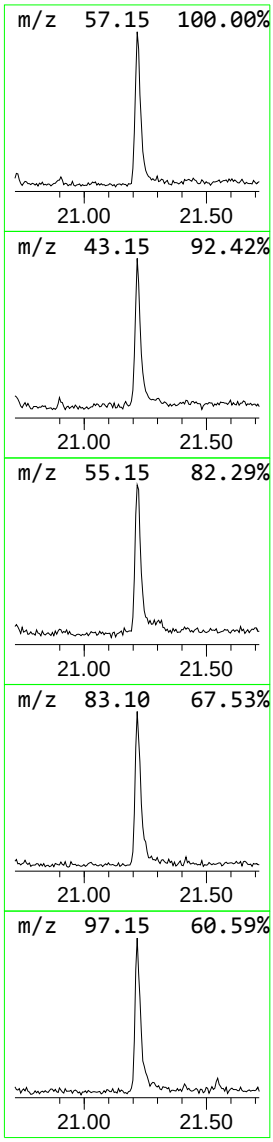
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.216	3.94 ng/ul	272311	Chrysene-d12	21.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

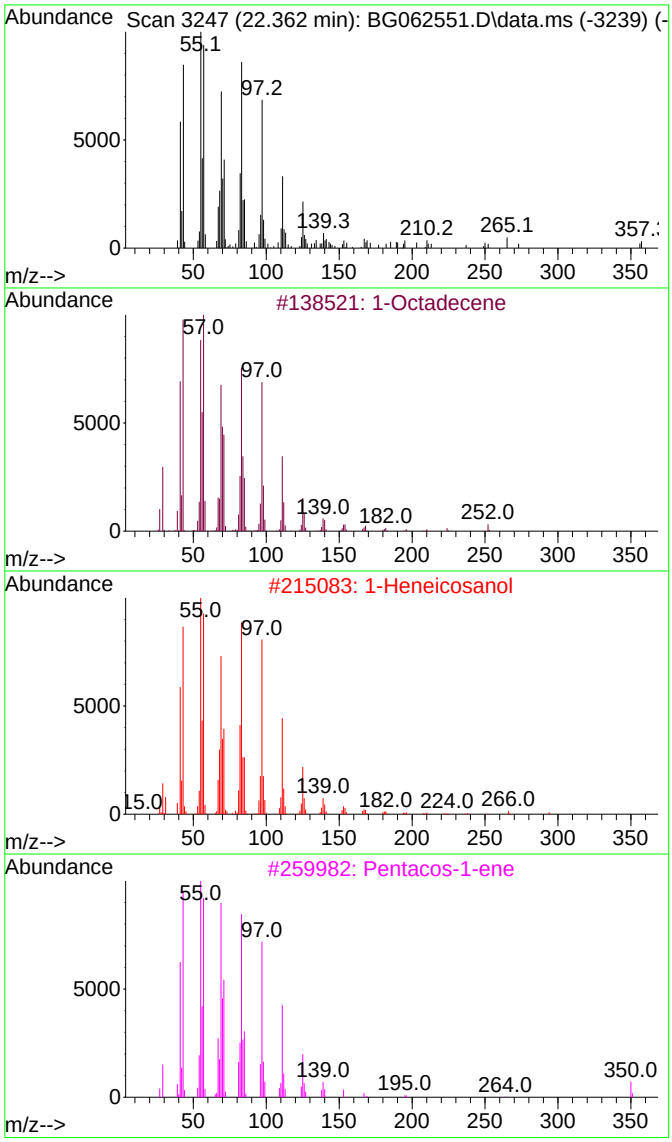
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

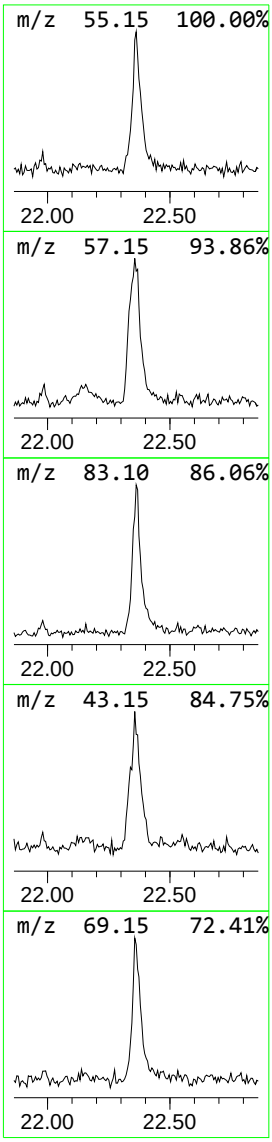
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.362	3.37 ng/ul	232908	Chrysene-d12	21.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Pentacos-1-ene	350	C25H50	016980-85-1	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	1-Octadecanol	270	C18H38O	000112-92-5	93





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Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

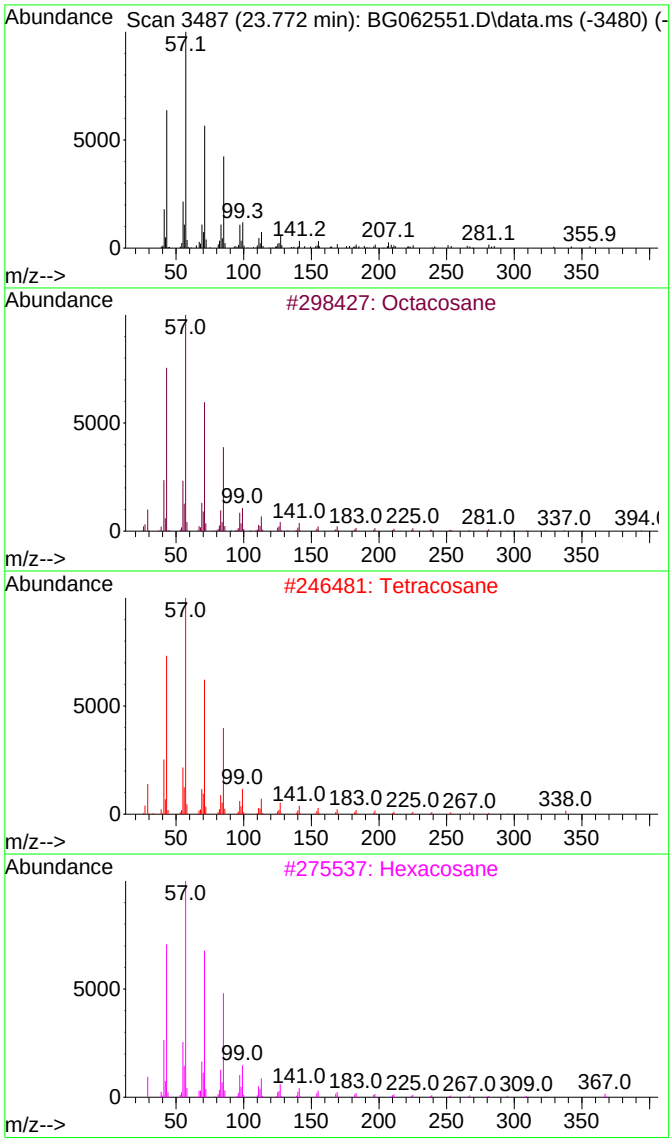
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

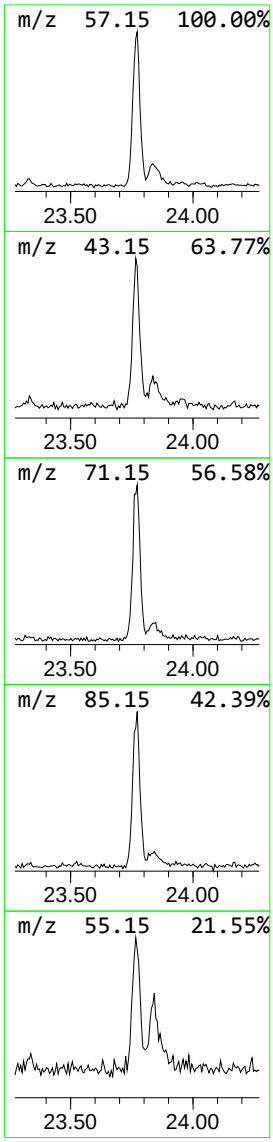
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.772	2.90 ng/ul	219308	Perylene-d12	24.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Heptacosane	380	C27H56	000593-49-7	87





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Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

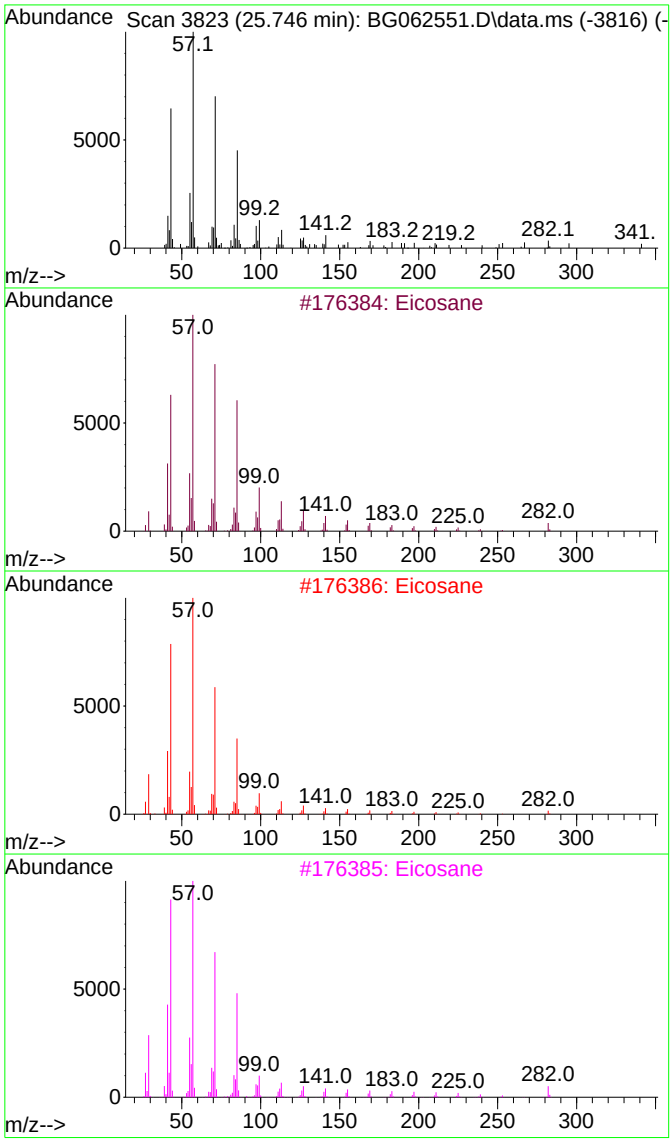
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

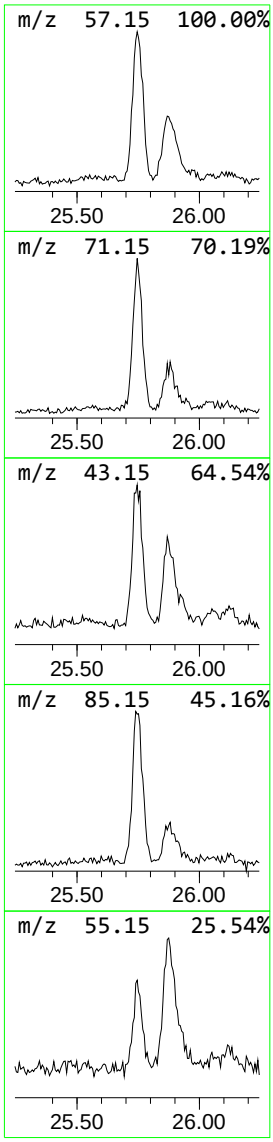
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.746	2.42 ng/ul	183178	Perylene-d12	24.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Eicosane	282	C20H42	000112-95-8	91
3	Eicosane	282	C20H42	000112-95-8	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

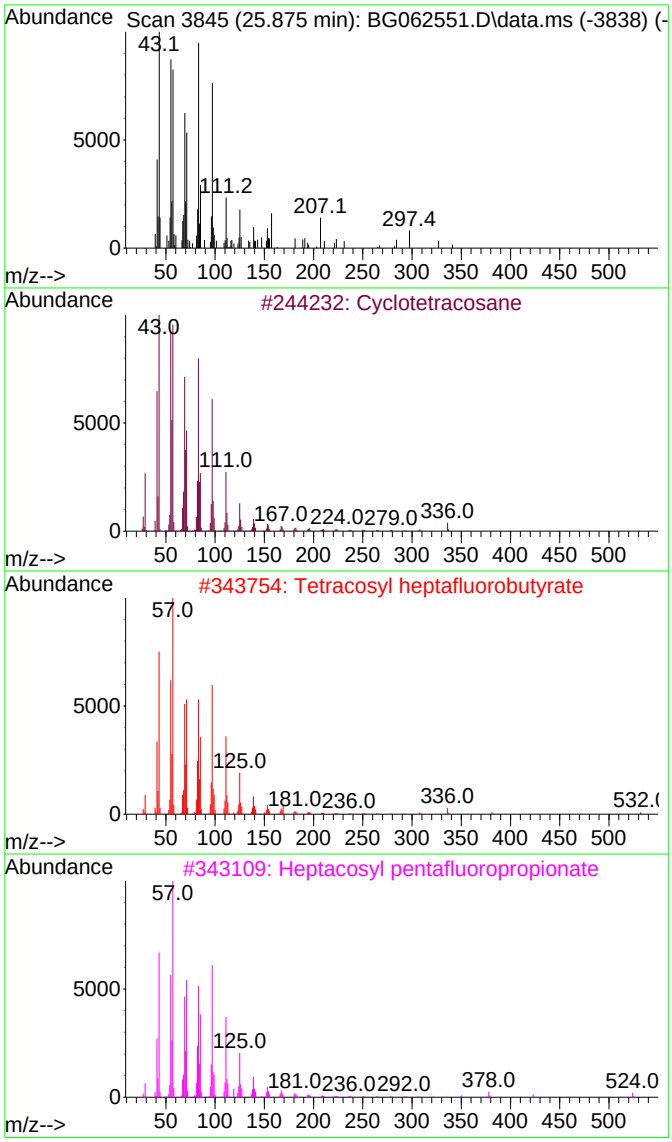
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

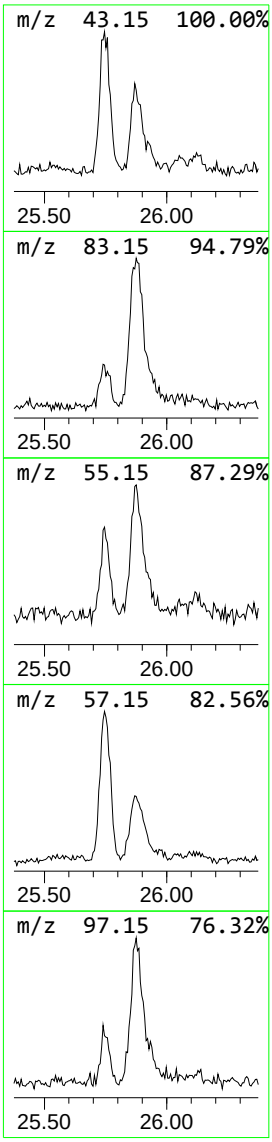
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Cyclic25.875 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.875	2.53 ng/ul	191624	Perylene-d12	24.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	80
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	38
3	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	30
4	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	30
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062551.D
Acq On : 22 Aug 2024 22:50
Operator : MA/JU
Sample : P3673-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD9

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
Propylene Glycol	3.664	3.8	ng/ul	89645	1	7.934	472390	20.0
1-Propanol, 3-p...	11.465	3.5	ng/ul	129383	2	10.725	740673	20.0
n-Hexadecanoic ...	18.197	3.7	ng/ul	262771	4	17.298	1427060	20.0
Heptadecyl trif...	21.216	3.9	ng/ul	272311	5	21.545	1383030	20.0
(DEL) Alkane: S...	22.362	3.4	ng/ul	232908	5	21.545	1383030	20.0
(DEL) Alkane: S...	23.772	2.9	ng/ul	219308	6	24.624	1514720	20.0
(DEL) Alkane: S...	25.746	2.4	ng/ul	183178	6	24.624	1514720	20.0
(DEL) Alkane: C...	25.875	2.5	ng/ul	191624	6	24.624	1514720	20.0