LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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: BG061810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.455	22	28	36	rVB7	15708	33960	2.07%	0.166%
2	3.731	70	75	80	rBV	23105	42327	2.58%	0.207%
3	3.889	97	102	109	rBV4	30478	70236	4.28%	0.343%
4	3.989	114	119	127	rVV	66150	107303	6.54%	0.524%
5	4.066	127	132	137	rVV4	8945	18248	1.11%	0.089%
6	4.101	137	138	142	rVB4	4348	4456	0.27%	0.022%
7	4.212	153	157	161	rBV4	5348	8108	0.49%	0.040%
8	4.289	167	170	175	rVB4	4210	6840	0.42%	0.033%
9	4.371	181	184	186	rBV4	4228	6326	0.39%	0.031%
10	4.729	239	245	247	rBV5	6215	10251	0.62%	0.050%
11	4.782	249	254	256	rVV3	18750	28984	1.77%	0.142%
12	4.812	257	259	266	rVB2	15651	21861	1.33%	0.107%
13	4.918	273	277	278	rBV3	6417	6569	0.40%	0.032%
14	5.029	291	296	298	rBV5	5133	7476	0.46%	0.037%
15	5.135	306	314	320	rBV	73873	116929	7.13%	0.571%
16	5.223	325	329	335	rVV2	16573	24001	1.46%	0.117%
17	6.116	476	481	486	rVV2	12333	21702	1.32%	0.106%
18	7.203	659	666	679	rVB	306201	536986	32.74%	2.622%
19	7.379	690	696	706	rVB	214637	353500	21.55%	1.726%
20	7.585	722	731	737	rBV	275955	478304	29.16%	2.336%
21	7.638	737	740	743	rVB2	12108	14350	0.87%	0.070%
22	8.055	804	811	817	rBV	269922	457037	27.86%	2.232%
23	8.120	817	822	828	rVB5	13044	31582	1.93%	0.154%
24	8.560	895	897	902	rVB4	6920	8428	0.51%	0.041%
25	8.695	917	920	922	rVB2	4965	5834	0.36%	0.028%
26	8.754	922	930	938	rBV	274506	479111	29.21%	2.340%
27	8.872	946	950	951	rBV	9665	9816	0.60%	0.048%
28	9.218	1002	1009	1016	rBV	291762	504906	30.78%	2.466%
29	9.377	1032	1036	1039	rVB4	6480	7869	0.48%	0.038%
30	9.771	1095	1103	1111	rVB3	35826	58196	3.55%	0.284%
31	9.941	1125	1132	1139	rBV2	252038	436073	26.58%	2.130%
32	10.482	1217	1224	1232	rBV	356583	627356	38.24%	3.064%
33	10.623	1245	1248	1251	rBV4	10342	12179	0.74%	0.059%
34	10.869	1279	1290	1297	rBV	403125	730625	44.54%	3.568%
35	10.916	1297	1298	1304	rVB4	13714	17029	1.04%	0.083%
36	10.999	1305	1312	1322	rBV2	168587	308696	18.82%	1.507%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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	11.210	1344	1348	1351	rVB2	2963	4342	0.26%	0.021%
38	11.392	1373	1379	1384	rVB6	19566	34328	2.09%	0.168%
39	11.598	1409	1414	1421	rBV3	47701	93544	5.70%	0.457%
40	11.862	1454	1459	1464	rBV7	10682	19157	1.17%	0.094%
41	12.444	1555	1558	1563	rVB3	5933	7944	0.48%	0.039%
42	12.514	1568	1570	1576	rVB6	9183	12441	0.76%	0.061%
43	12.632	1585	1590	1591	rVB4	3585	5082	0.31%	0.025%
44	12.661	1591	1595	1600	rBV3	5471	9745	0.59%	0.048%
45	12.738	1604	1608	1612	rVB4	7534	10683	0.65%	0.052%
46	13.043	1657	1660	1664	rVB4	4594	6181	0.38%	0.030%
47	13.496	1735	1737	1742	rBV5	6556	10545	0.64%	0.051%
48	13.596	1752	1754	1758	rVV2	4999	5435	0.33%	0.027%
49	13.631	1758	1760	1766	rVB5	5213	6940	0.42%	0.034%
50	13.860	1794	1799	1805	rVB6	5253	13106	0.80%	0.064%
51	13.948	1811	1814	1815	rBV3	4269	4385	0.27%	0.021%
52	14.007	1821	1824	1829	rVB5	7802	11505	0.70%	0.056%
53	14.089	1829	1838	1844	rBV	616514	890225	54.27%	4.347%
54	14.242	1860	1864	1869	rBV5	4953	9043	0.55%	0.044%
55	14.324	1874	1878	1881	rBV6	9792	14956	0.91%	0.073%
56	14.383	1881	1888	1898	rVB	672370	1049992	64.01%	5.128%
57	14.495	1904	1907	1909	rBV3	4632	6800	0.41%	0.033%
58	14.571	1919	1920	1924	rVV2	9988	9328	0.57%	0.046%
59	14.624	1927	1929	1931	rVV3	5616	4334	0.26%	0.021%
60	14.688	1932	1940	1946	rVV	586828	928459	56.60%	4.534%
61	14.747	1946	1950	1955	rVV3	23536	40233	2.45%	0.196%
62	14.800	1958	1959	1962	rBV3	5803	6001	0.37%	0.029%
63	14.865	1965	1970	1981	rVV	281959	492775	30.04%	2.406%
64	15.023	1991	1997	2002	rBV5	22425	39704	2.42%	0.194%
65	15.088	2002	2008	2012	rVV3	27872	48250	2.94%	0.236%
66	15.153	2016	2019	2022	rVB5	7608	9069	0.55%	0.044%
67	15.470	2069	2073	2078	rVB7	9862	15829	0.96%	0.077%
68	15.675	2101	2108	2114	rBV	855753	1267923	77.30%	6.192%
69	15.728	2114	2117	2122	rVV2	37408	48288	2.94%	0.236%
70	15.781	2122	2126	2131	rVV2	163443	238361	14.53%	1.164%
71	15.899	2141	2146	2147	rBV3	10087	14651	0.89%	0.072%
72	15.934	2150	2152	2156	rVV4	23556	26926	1.64%	0.131%
73	15.987	2158	2161	2162	rVV3	7459	7371	0.45%	0.036%
74	16.022	2164	2167	2173	rVB5	14197	24859	1.52%	0.121%
75	16.386	2225	2229	2231	rBV6	16150	24818	1.51%	0.121%
76	16.457	2240	2241	2244	rVB3	8388	6046	0.37%	0.030%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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

77	16.533	2251	2254	2257	rBV5	9564	11402	0.70%	0.056%
78	16.651	2272	2274	2277	rBV4	13933	16747	1.02%	0.082%
79	16.710	2280	2284	2285	rBV4	8400	9393	0.57%	0.046%
80	16.874	2310	2312	2314	rBV3	7334	7758	0.47%	0.038%
81	16.956	2323	2326	2330	rVB6	19858	21232	1.29%	0.104%
82	17.074	2344	2346	2352	rVB3	21580	29951	1.83%	0.146%
83	17.250	2372	2376	2381	rVB	20861	31510	1.92%	0.154%
84	17.332	2388	2390	2395	rVB6	19177	25105	1.53%	0.123%
85	17.426	2400	2406	2410	rBV	718572	1132416	69.03%	5.530%
86	17.473	2410	2414	2418	rVV	408792	612431	37.34%	2.991%
87	17.526	2418	2423	2434	rVB	890680	1420655	86.61%	6.938%
88	17.785	2465	2467	2468	rBV2	15105	10739	0.65%	0.052%
89	17.826	2472	2474	2478	rVB3	40480	48130	2.93%	0.235%
90	18.020	2502	2507	2514	rVB6	47995	101597	6.19%	0.496%
91	18.308	2552	2556	2560	rBV4	138216	205415	12.52%	1.003%
92	18.349	2561	2563	2567	rVB	71478	84822	5.17%	0.414%
93	18.496	2583	2588	2592	rBV3	117115	206118	12.57%	1.007%
94	18.601	2602	2606	2611	rVB8	34473	54149	3.30%	0.264%
95	18.772	2632	2635	2638	rBV5	46792	74744	4.56%	0.365%
96	19.477	2750	2755	2761	rVB	856520	1161827	70.83%	5.674%
97	19.812	2806	2812	2815	rBV	994300	1640366	100.00%	8.011%
98	21.339	3069	3072	3081	rVB5	275935	496186	30.25%	2.423%
99	21.686	3125	3131	3136	rBV3	668326	1419653	86.54%	6.933%
100	24.013	3523	3527	3533	rVB2	311711	562177	34.27%	2.745%

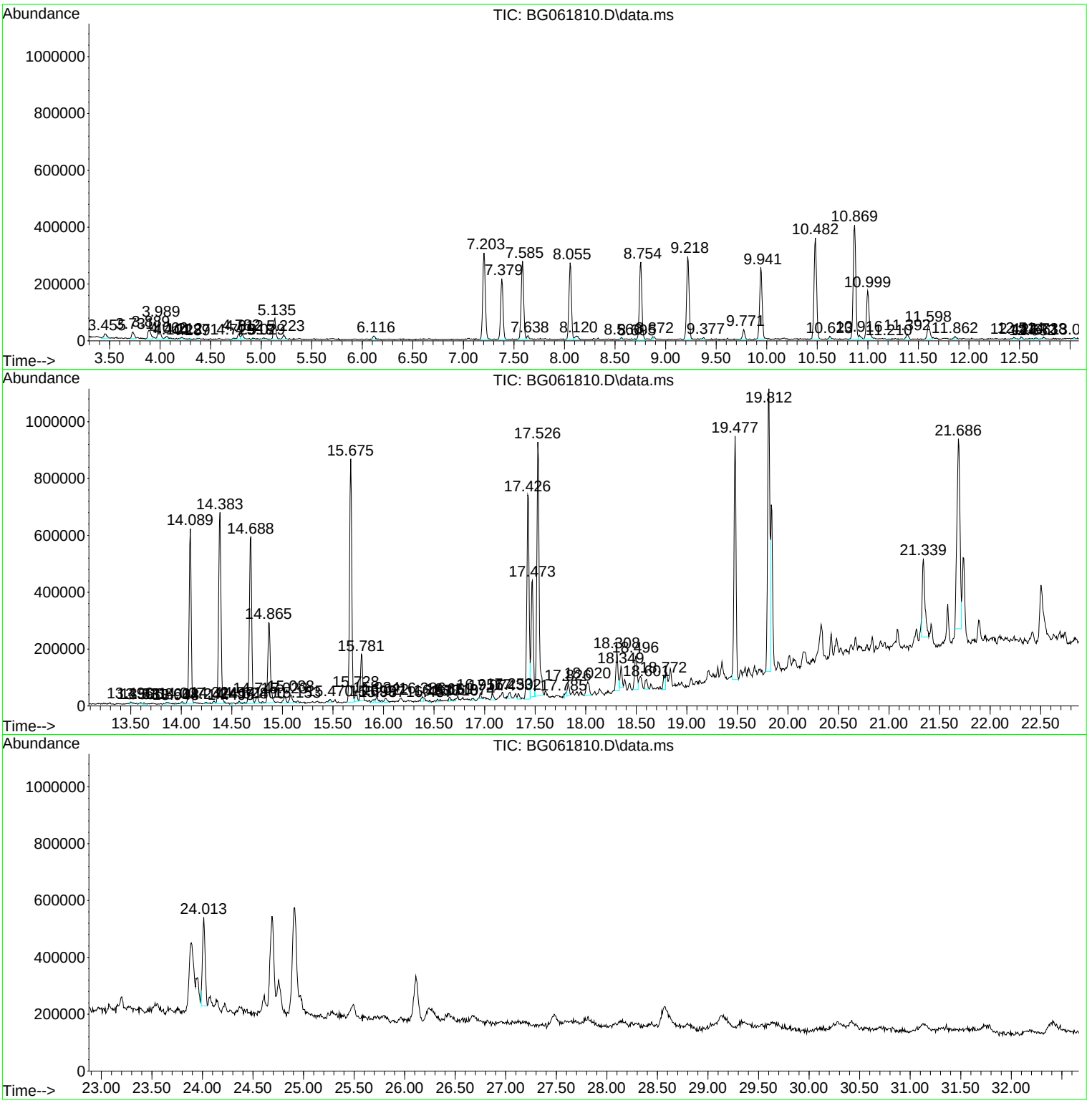
Sum of corrected areas: 20477581

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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

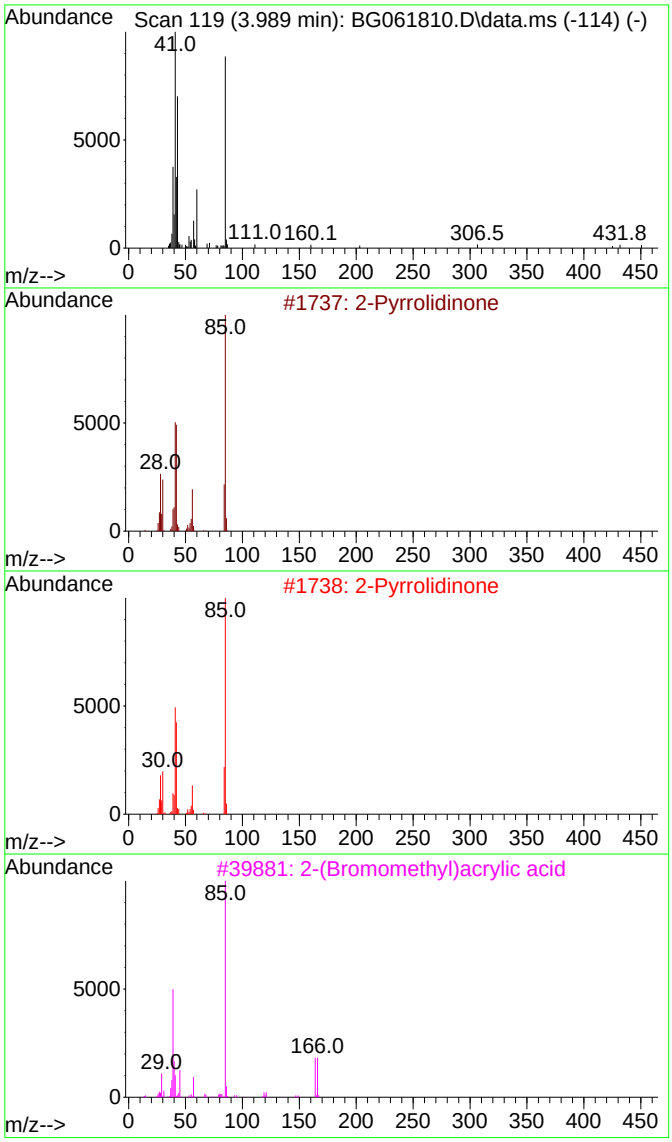
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

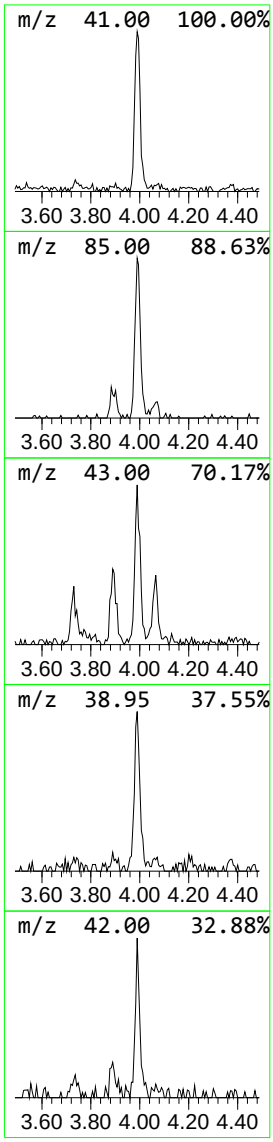
****

Peak Number 1 2-Pyrrolidinone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.989	4.70 ng/ul	107303	1,4-Dichlorobenzene-d4	8.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone	85	C4H7NO	000616-45-5	53
2	2-Pyrrolidinone	85	C4H7NO	000616-45-5	53
3	2-(Bromomethyl)acrylic acid	164	C4H5BrO2	072707-66-5	50
4	Butanoyl chloride, 3-methyl-	120	C5H9ClO	000108-12-3	45
5	Thiazole	85	C3H3NS	000288-47-1	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

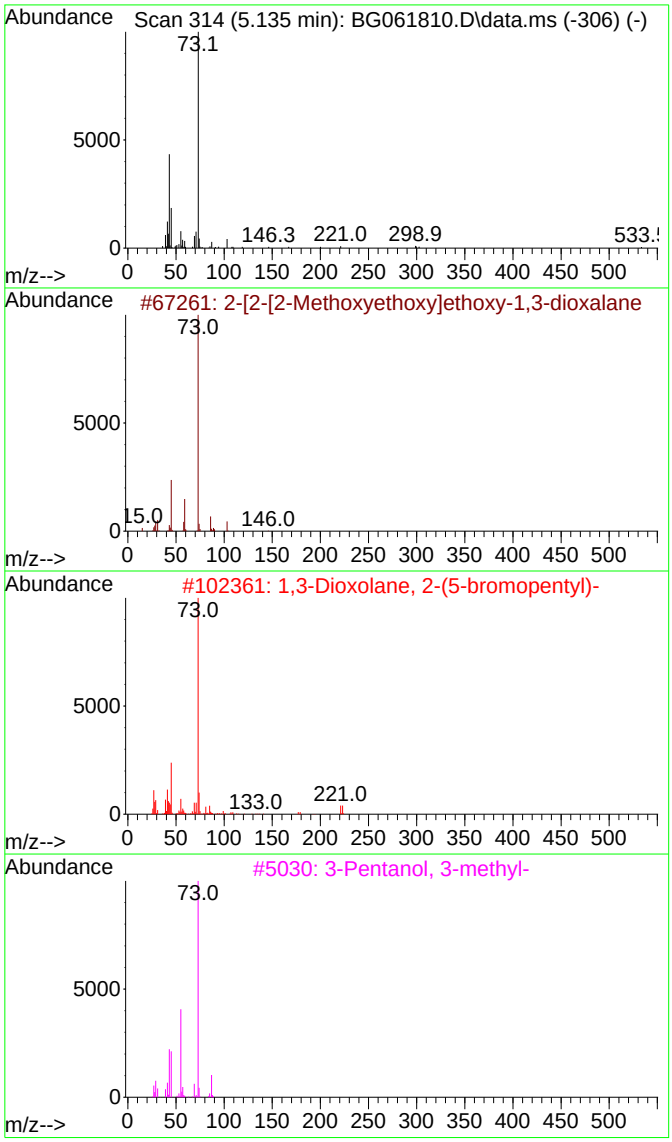
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

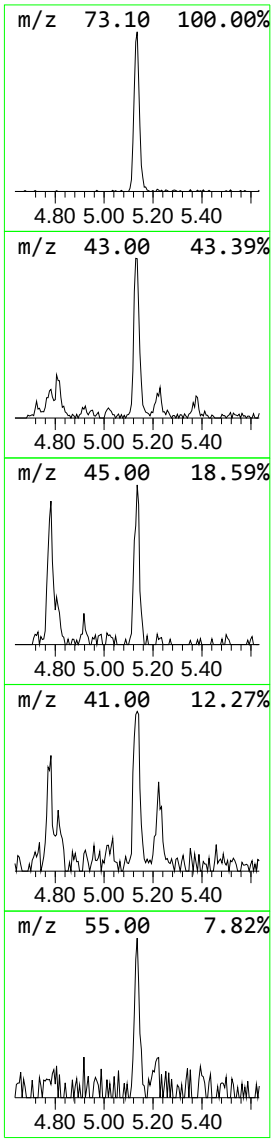
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.135	5.12 ng/ul	116929	1,4-Dichlorobenzene-d4	8.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-Methoxyethoxy]ethoxy-1,3...	192	C8H16O5	074733-99-6	36
2	1,3-Dioxolane, 2-(5-bromopentyl)-	222	C8H15BrO2	056741-68-5	33
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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

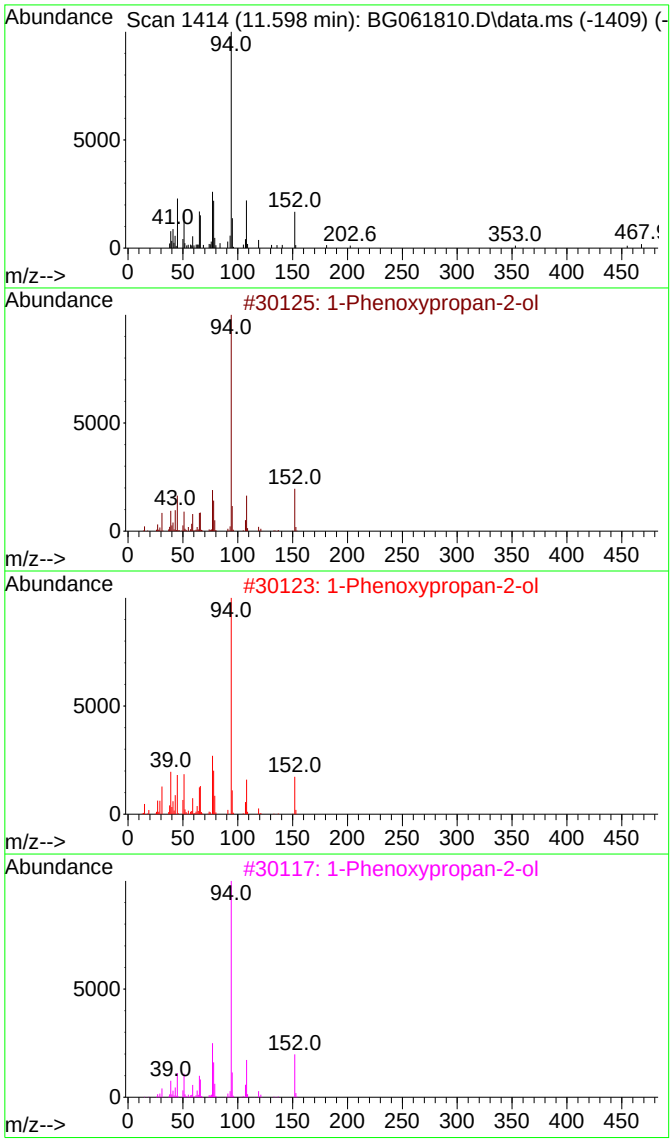
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

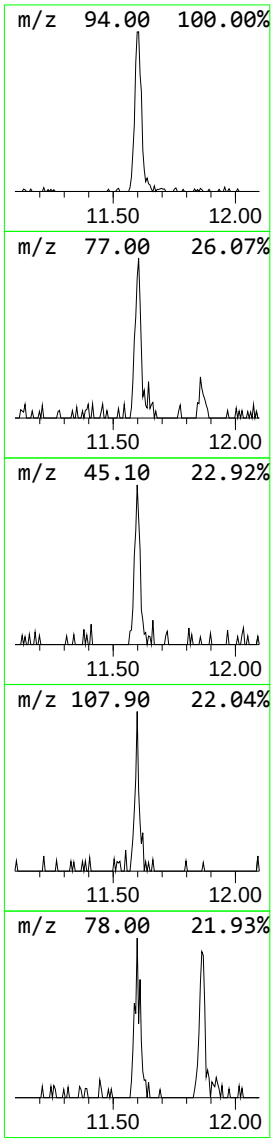
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.598	2.56 ng/ul	93544	Naphthalene-d8	10.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	83
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	81
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	68
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	50
5	butanedioic acid, monophenyl ester	194	C10H10O4	1000400-29-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

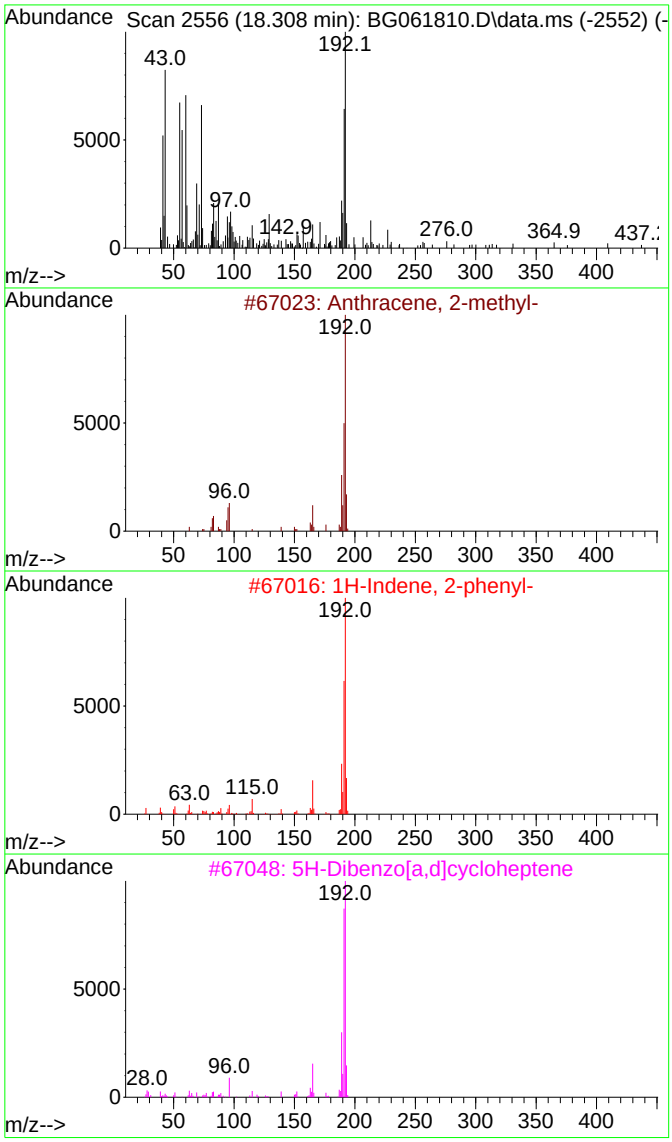
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

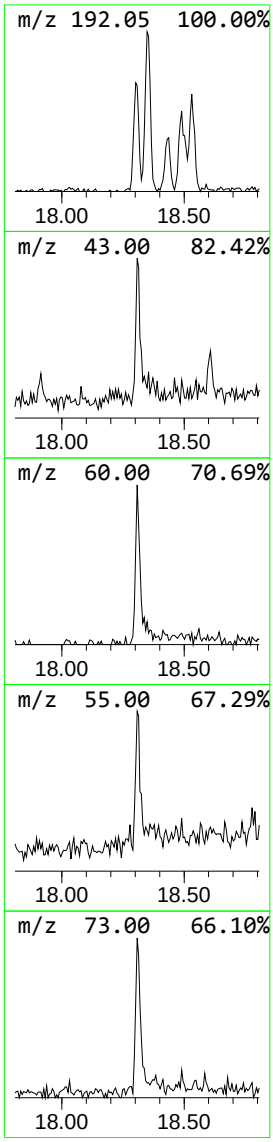
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.308	3.63 ng/ul	205415	Phenanthrene-d10	17.432

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	50
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	50
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

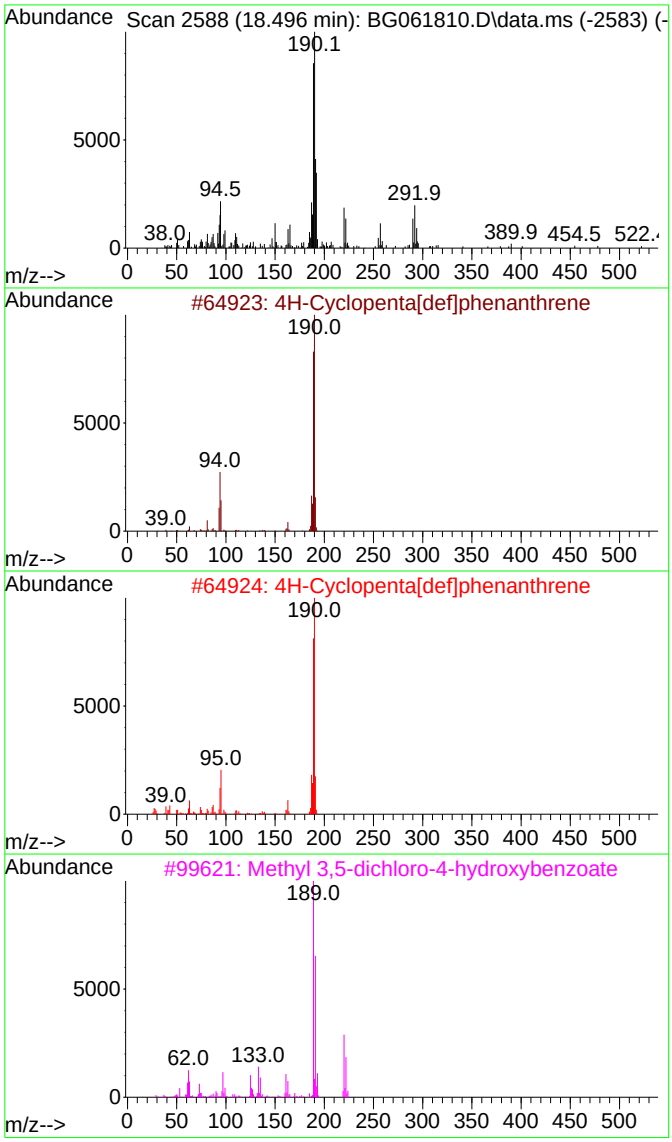
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

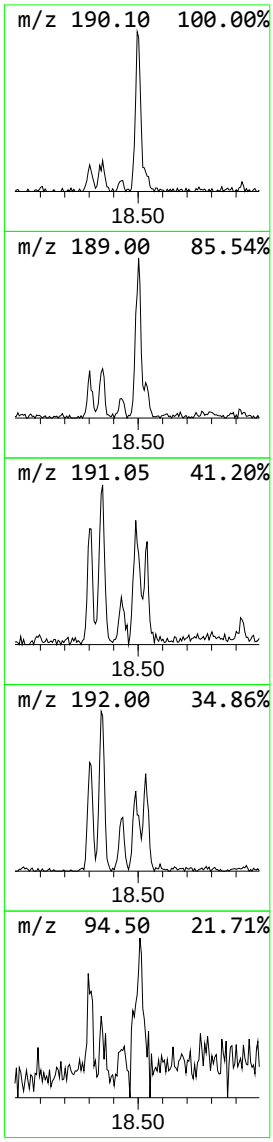
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.496	3.64 ng/ul	206118	Phenanthrene-d10	17.432

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	Methyl 3,5-dichloro-4-hydroxyben...	220	C8H6Cl2O3	003337-59-5	43
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	38
5	4-(4-Methyl-piperidin-1-yl)-phen...	190	C12H18N2	342013-25-6	37





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Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

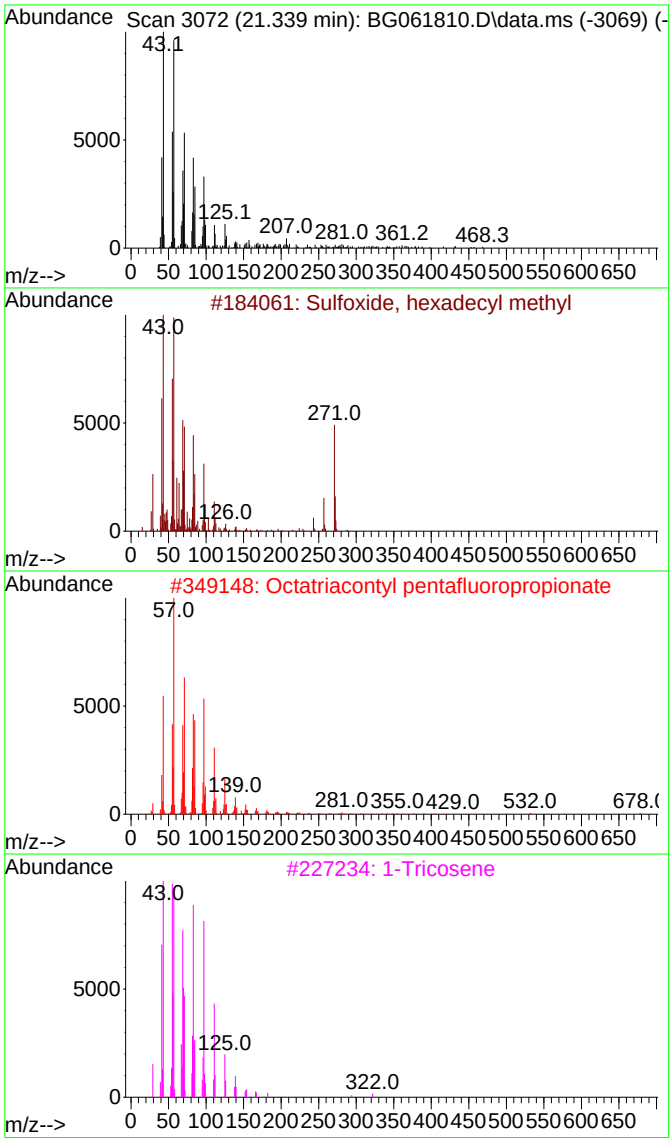
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

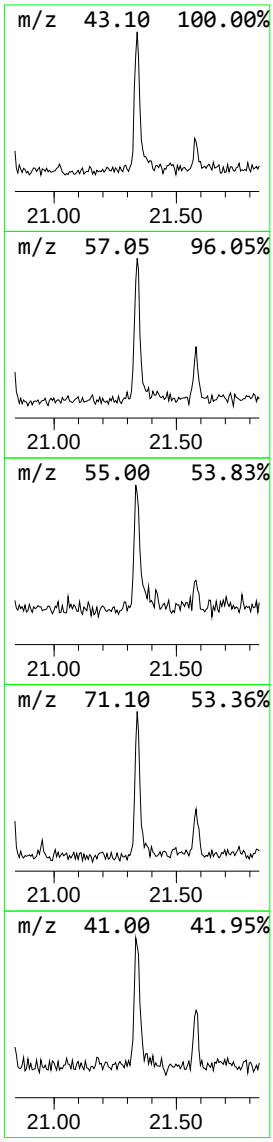
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Sulfoxide, hexadecyl methyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.339	6.99 ng/ul	496186	Chrysene-d12	21.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfoxide, hexadecyl methyl	288	C17H36OS	003079-32-1	95
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
3	1-Tricosene	322	C23H46	018835-32-0	78
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	74
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

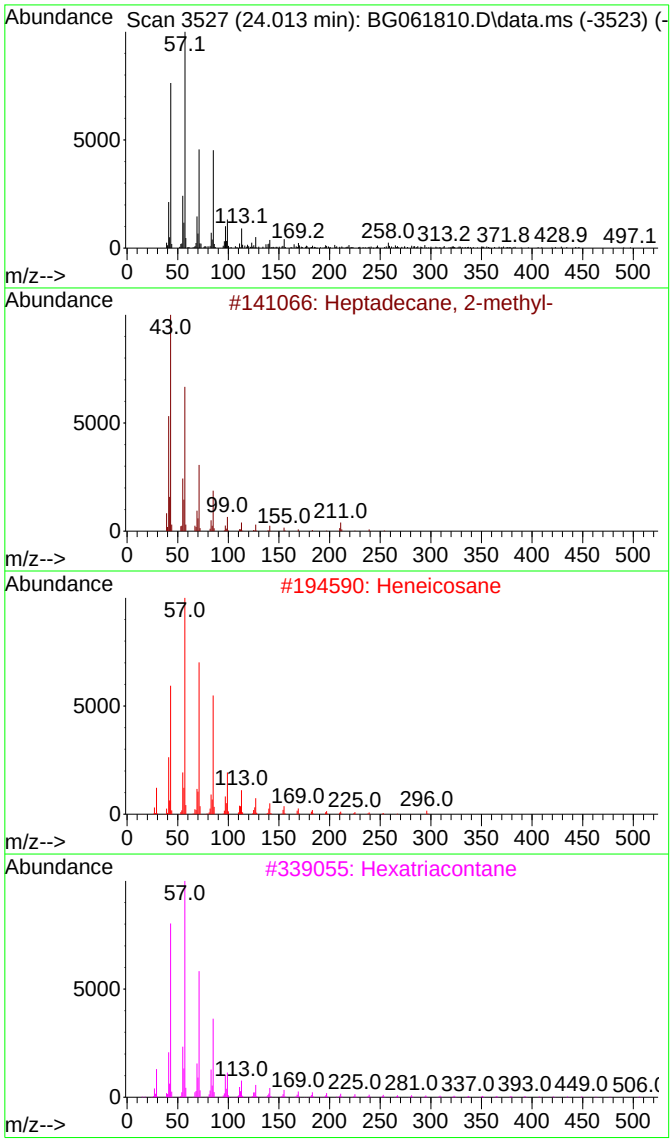
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

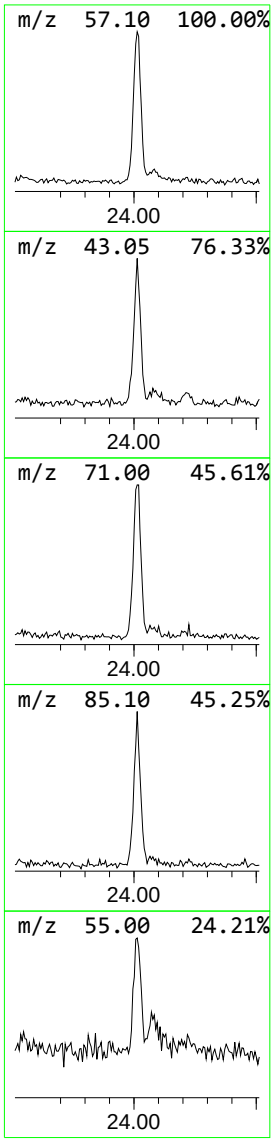
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.013	20.00 ng/ul	562177	Perylene-d12	24.912

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	76
2	Heneicosane	296	C21H44	000629-94-7	72
3	Hexatriacontane	507	C36H74	000630-06-8	64
4	Octacosane	394	C28H58	000630-02-4	62
5	Eicosane	282	C20H42	000112-95-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061810.D
Acq On : 1 Jul 2024 13:25
Operator : MA/JU
Sample : P2871-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4C54

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
2-Pyrrolidinone	3.989	4.7	ng/ul	107303	1	8.055	457037	20.0
unknown-01	5.135	5.1	ng/ul	116929	1	8.055	457037	20.0
1-Phenoxypropan...	11.598	2.6	ng/ul	93544	2	10.869	730625	20.0
Anthracene, 2-m...	18.308	3.6	ng/ul	205415	4	17.432	1132420	20.0
4H-Cyclopenta[d...	18.496	3.6	ng/ul	206118	4	17.432	1132420	20.0
Sulfoxide, hexa...	21.339	7.0	ng/ul	496186	5	21.692	1419650	20.0
(DEL) Alkane: S...	24.013	20.0	ng/ul	562177	6	24.912	562177	20.0