LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DDC14MEDL

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-BG091724.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.740	109	111	116	rVB4	12430	16266	1.21%	0.198%
2	3.881	132	135	138	rBV4	3794	4829	0.36%	0.059%
3	4.327	209	211	214	rBV3	4961	4081	0.30%	0.050%
4	5.114	343	345	349	rVB2	3443	3826	0.28%	0.047%
5	5.455	401	403	408	rVB3	4218	4581	0.34%	0.056%
6	5.502	408	411	414	rBV3	3391	4849	0.36%	0.059%
7	5.884	472	476	482	rVB4	15026	22248	1.65%	0.271%
8	6.172	517	525	531	rVB4	12513	24056	1.78%	0.293%
9	6.425	563	568	572	rBV2	8679	14993	1.11%	0.182%
10	6.683	606	612	616	rBV5	7425	13486	1.00%	0.164%
11	6.736	616	621	622	rBV2	4820	6267	0.46%	0.076%
12	6.818	632	635	638	rBV4	6968	8388	0.62%	0.102%
13	6.854	638	641	645	rVB4	11415	15375	1.14%	0.187%
14	6.907	645	650	655	rBV2	12020	21028	1.56%	0.256%
15	7.024	662	670	678	rBV2	42817	86123	6.39%	1.048%
16	7.189	693	698	702	rBV2	21089	36288	2.69%	0.442%
17	7.241	705	707	712	rVV4	7419	11734	0.87%	0.143%
18	7.283	712	714	718	rVB3	10100	12159	0.90%	0.148%
19	7.382	723	731	738	rBV5	36549	82644	6.13%	1.006%
20	7.482	743	748	758	rVB4	67170	130039	9.64%	1.583%
21	7.588	764	766	768	rVB3	4239	3409	0.25%	0.041%
22	7.747	792	793	796	rBV	3383	3865	0.29%	0.047%
23	7.770	796	797	801	rVV4	5084	6225	0.46%	0.076%
24	7.852	804	811	818	rVV	179239	317943	23.57%	3.870%
25	7.923	818	823	828	rVB3	38302	70291	5.21%	0.855%
26	8.076	845	849	854	rVB2	22461	32197	2.39%	0.392%
27	8.140	859	860	866	rVB5	8757	11236	0.83%	0.137%
28	8.275	879	883	888	rBV5	11338	21812	1.62%	0.265%
29	8.446	908	912	916	rBV4	8412	11585	0.86%	0.141%
30	8.516	916	924	927	rBV7	18460	44292	3.28%	0.539%
31	8.558	927	931	938	rVB2	34229	58502	4.34%	0.712%
32	8.652	945	947	952	rVB3	8605	9496	0.70%	0.116%
33	8.810	970	974	976	rBV3	8718	11070	0.82%	0.135%
34	8.928	991	994	995	rBV3	3661	4134	0.31%	0.050%
35	8.963	995	1000	1003	rVV4	8946	16119	1.20%	0.196%
36	9.080	1016	1020	1027	rVB2	66181	104807	7.77%	1.276%

LSC Area Percent Report

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Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

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-BG091724.MA.M
Title : SVOA CALIBRATION

37	9.333	1061	1063	1064	rBV	6624	3489	0.26%	0.042%
38	9.727	1122	1130	1136	rBV7	29771	66443	4.93%	0.809%
39	9.897	1156	1159	1160	rBV2	4602	5047	0.37%	0.061%
40	9.997	1171	1176	1177	rBV4	7658	9672	0.72%	0.118%
41	10.185	1204	1208	1212	rVB5	5466	9375	0.70%	0.114%
42	10.267	1218	1222	1228	rVB3	35675	63299	4.69%	0.770%
43	10.338	1231	1234	1239	rVB4	7462	13678	1.01%	0.166%
44	10.502	1258	1262	1263	rBV2	7111	7318	0.54%	0.089%
45	10.514	1263	1264	1269	rVB4	8561	9633	0.71%	0.117%
46	10.643	1277	1286	1292	rBV	238636	465258	34.49%	5.662%
47	10.778	1301	1309	1314	rBV6	38744	89817	6.66%	1.093%
48	11.019	1346	1350	1357	rBV3	35305	61038	4.53%	0.743%
49	11.149	1369	1372	1379	rVB3	18506	29249	2.17%	0.356%
50	11.260	1388	1391	1395	rBV4	6873	10584	0.78%	0.129%
51	11.478	1426	1428	1434	rVB5	5643	6848	0.51%	0.083%
52	11.536	1434	1438	1440	rBV4	4913	7588	0.56%	0.092%
53	11.672	1457	1461	1465	rBV3	17056	27741	2.06%	0.338%
54	11.907	1497	1501	1504	rBV2	26704	36486	2.71%	0.444%
55	12.065	1524	1528	1532	rBV2	23761	40599	3.01%	0.494%
56	12.171	1544	1546	1549	rBV2	4365	4829	0.36%	0.059%
57	12.318	1566	1571	1578	rVB3	51283	74907	5.55%	0.912%
58	12.482	1592	1599	1602	rBV7	12627	21748	1.61%	0.265%
59	13.205	1720	1722	1723	rBV2	4773	3565	0.26%	0.043%
60	13.317	1736	1741	1747	rBV2	31131	50970	3.78%	0.620%
61	13.440	1760	1762	1766	rBV5	13125	14947	1.11%	0.182%
62	13.746	1811	1814	1818	rVB4	18979	27361	2.03%	0.333%
63	13.892	1835	1839	1844	rVB	70393	103744	7.69%	1.263%
64	14.180	1884	1888	1897	rVB2	62842	97047	7.20%	1.181%
65	14.392	1920	1924	1929	rVB	51725	63995	4.74%	0.779%
66	14.486	1934	1940	1947	rVB	396017	611326	45.32%	7.440%
67	14.697	1971	1976	1978	rBV6	24736	36014	2.67%	0.438%
68	15.003	2027	2028	2029	rBV	9584	6421	0.48%	0.078%
69	15.244	2067	2069	2073	rBV5	15837	16866	1.25%	0.205%
70	15.314	2077	2081	2083	rBV5	13591	19389	1.44%	0.236%
71	15.479	2105	2109	2116	rVB	95025	141327	10.48%	1.720%
72	15.849	2168	2172	2178	rVB3	28386	49885	3.70%	0.607%
73	16.207	2230	2233	2236	rBV2	37837	54807	4.06%	0.667%
74	16.889	2343	2349	2357	rBV	874922	1348803	100.00%	16.416%
75	17.236	2403	2408	2415	rVB	551944	781252	57.92%	9.508%
76	17.335	2421	2425	2430	rVB	111780	159895	11.85%	1.946%

LSC Area Percent Report

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Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

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-BG091724.MA.M
Title : SVOA CALIBRATION

77	17.735	2490	2493	2497	rBV2	29656	39986	2.96%	0.487%
78	17.911	2520	2523	2527	rVB3	22910	26336	1.95%	0.321%
79	19.633	2811	2816	2821	rBV	144946	219721	16.29%	2.674%
80	21.489	3126	3132	3138	rBV2	594403	944730	70.04%	11.498%
81	24.527	3640	3649	3659	rBV2	411338	1083247	80.31%	13.184%

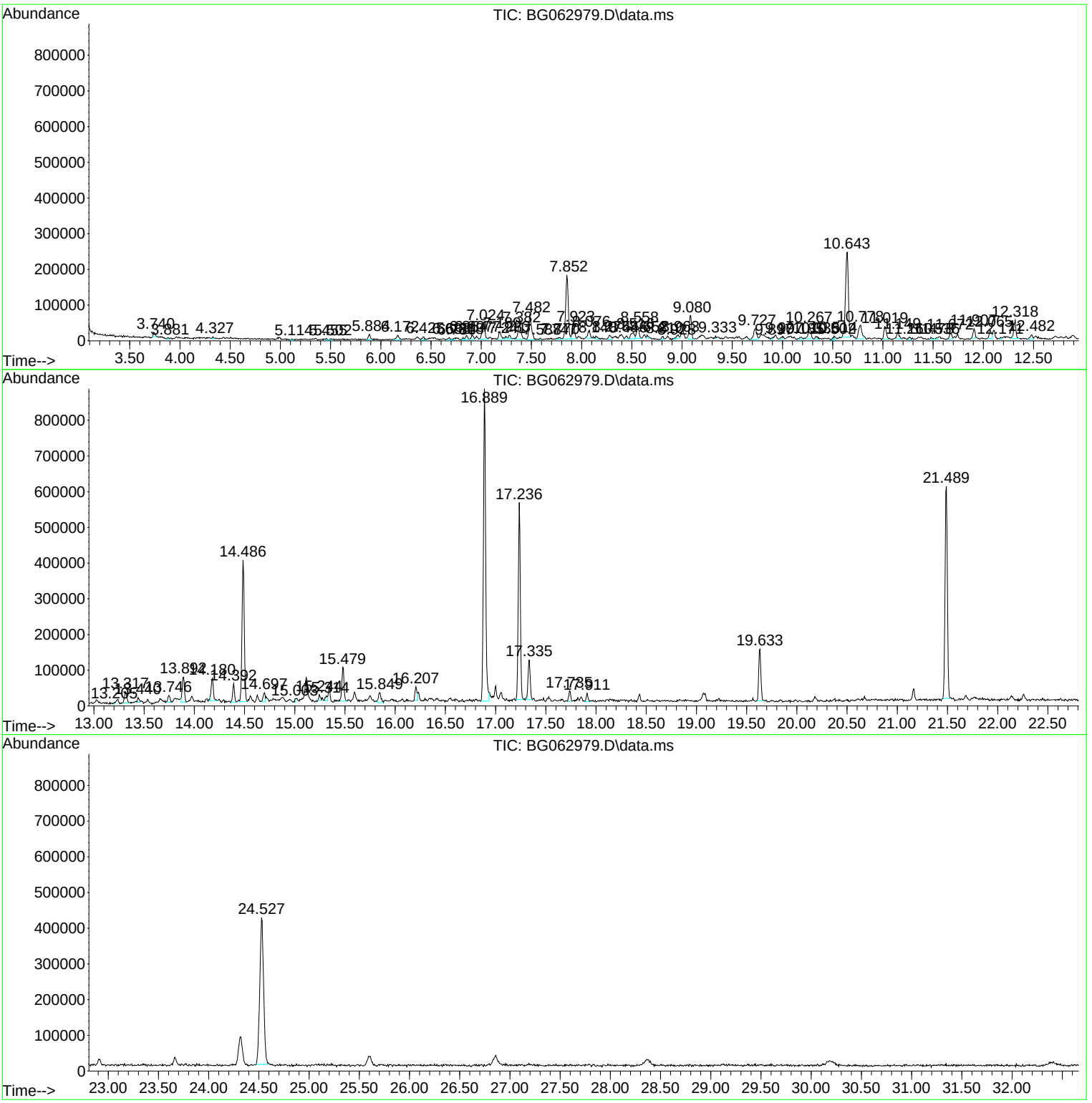
Sum of corrected areas: 8216523

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.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\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

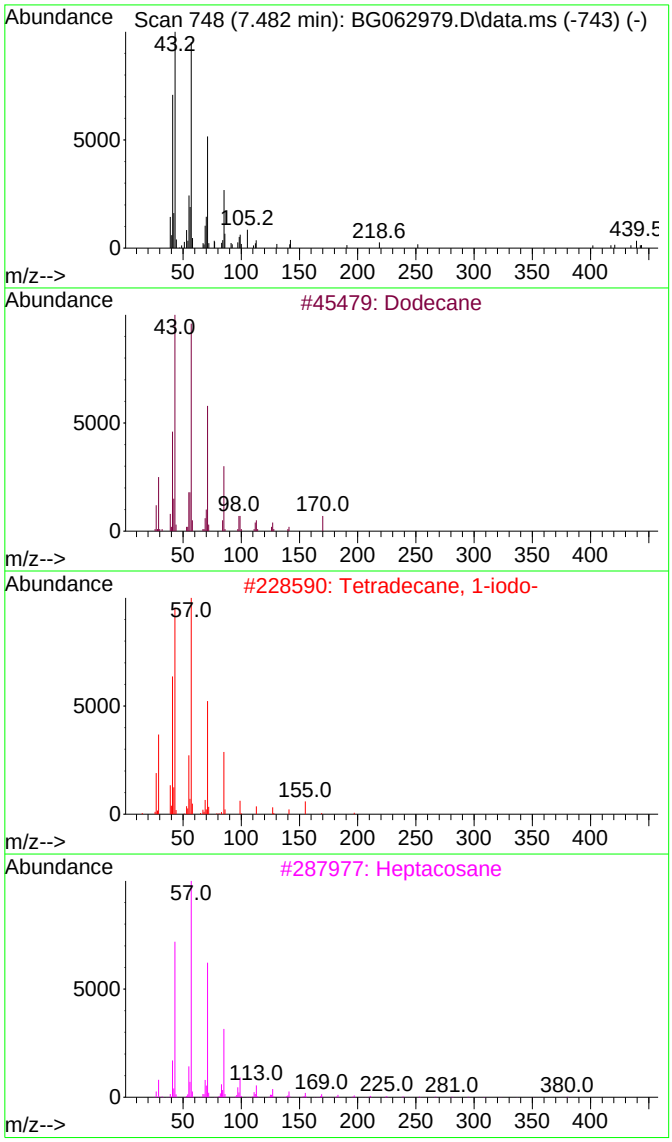
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

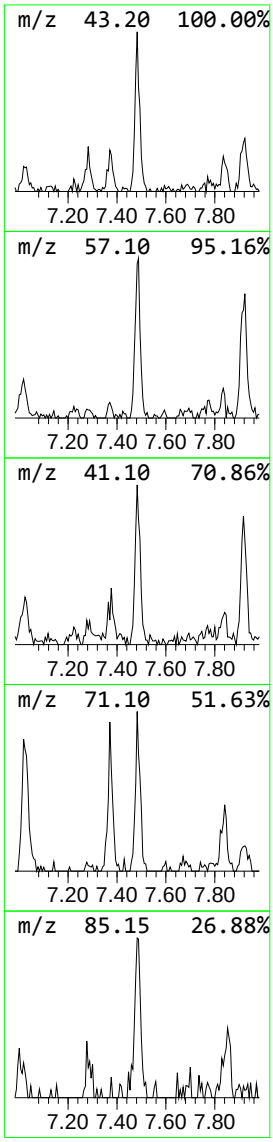
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.482	8.18 ng/ul	130039	1,4-Dichlorobenzene-d4	7.852

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	72
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
3	Heptacosane	380	C27H56	000593-49-7	64
4	Decane, 1-iodo-	268	C10H21I	002050-77-3	64
5	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

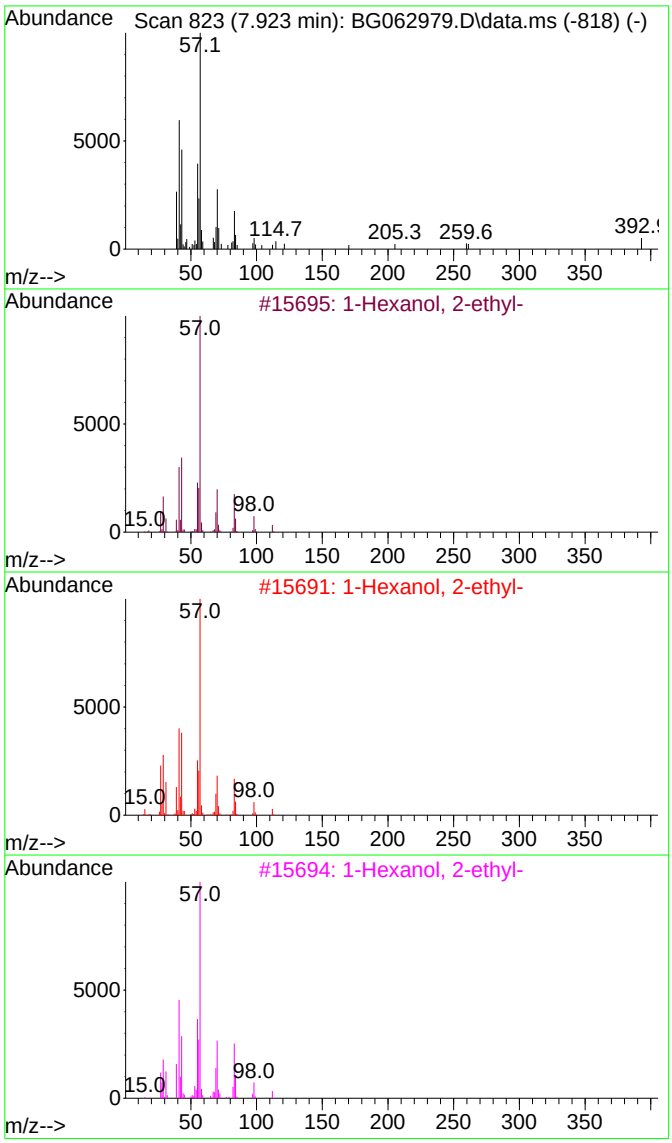
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

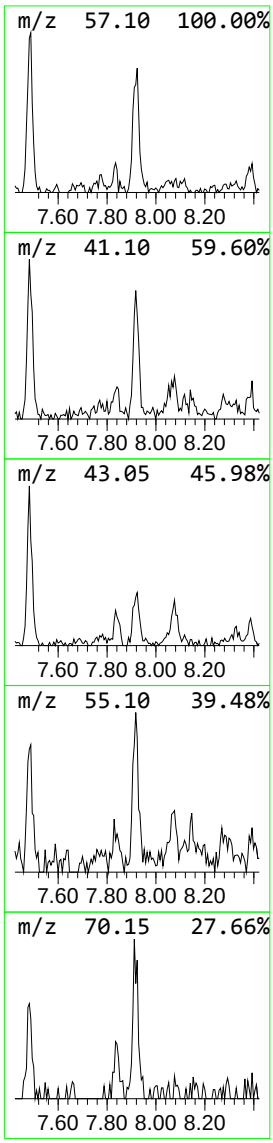
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.923	4.42 ng/ul	70291	1,4-Dichlorobenzene-d4	7.852

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	50
5	2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

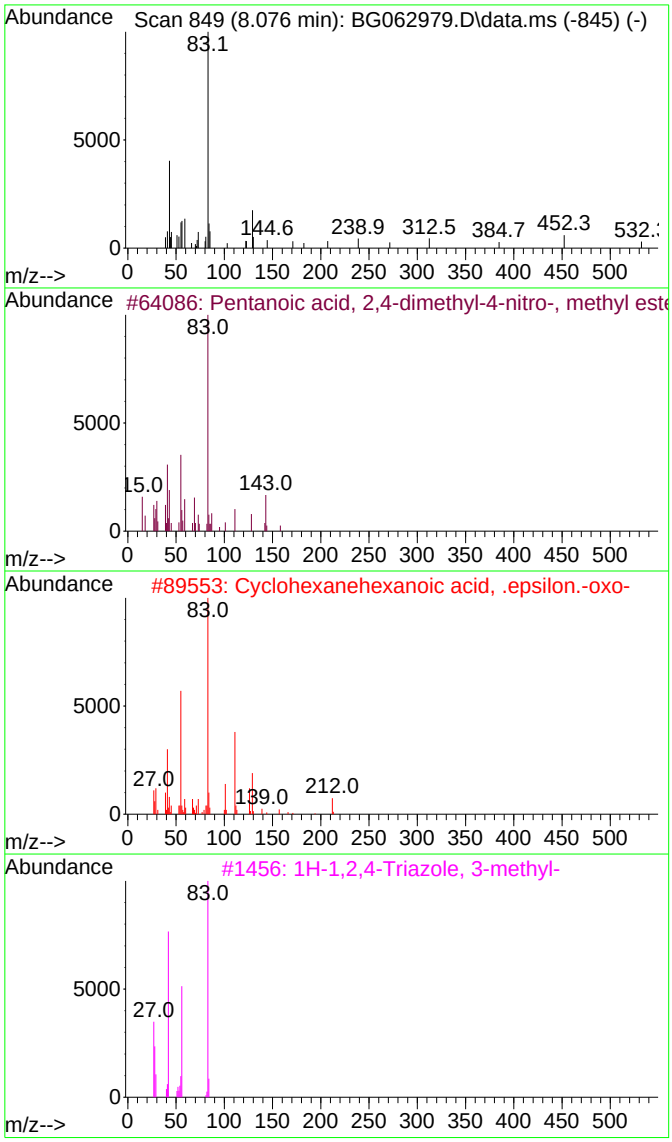
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

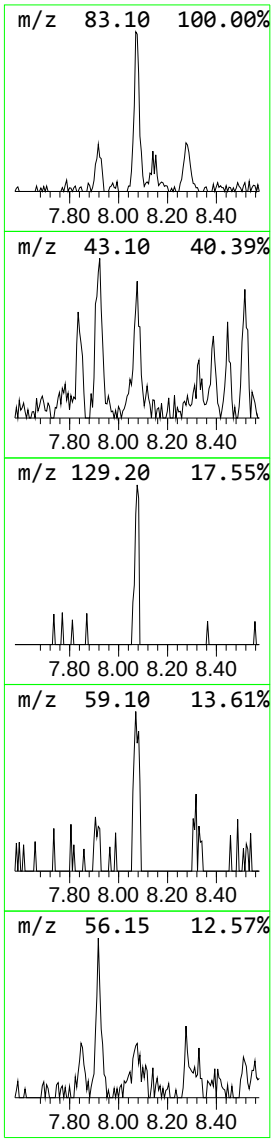
****

Peak Number 3 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.076	2.03 ng/ul	32197	1,4-Dichlorobenzene-d4	7.852

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2,4-dimethyl-4-n...	189	C8H15NO4	005762-40-3	45
2	Cyclohexanehexanoic acid, .epsil...	212	C12H20O3	020606-25-1	39
3	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	33
4	5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	28
5	N-Nitro-1H-1,2,4-triazol-3-amine	129	C2H3N5O2	034815-01-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
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Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

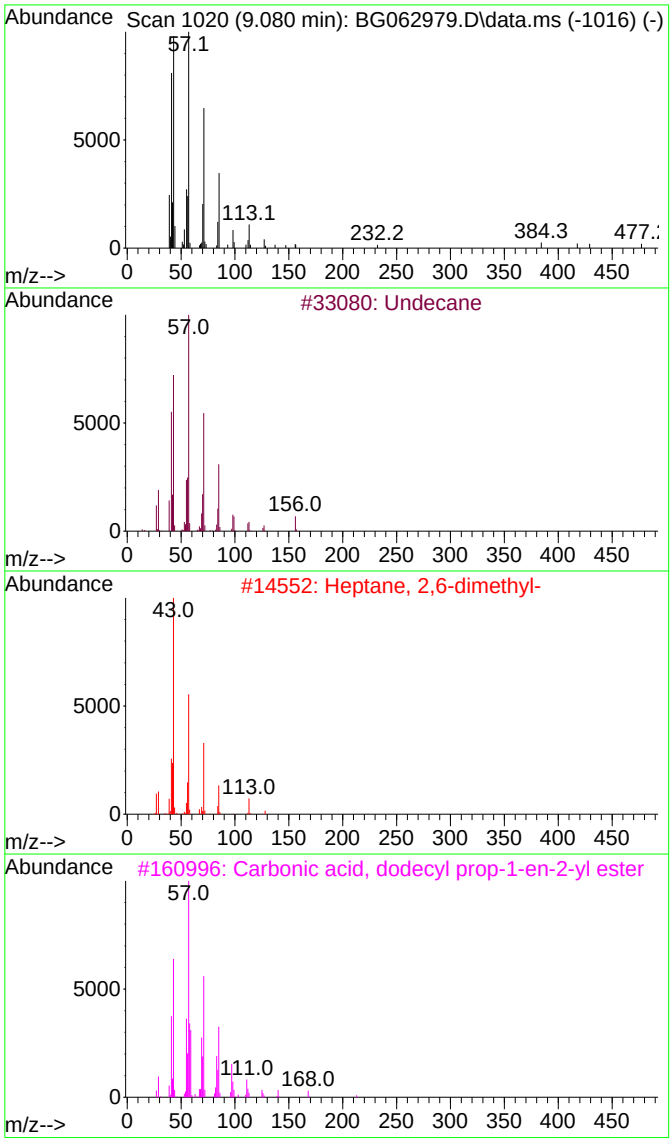
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

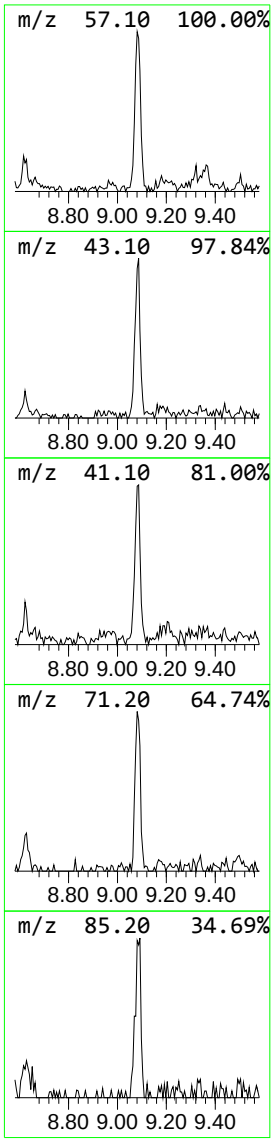
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.080	6.59 ng/ul	104807	1,4-Dichlorobenzene-d4	7.852

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	87
2	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	81
3	Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	78
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	72
5	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

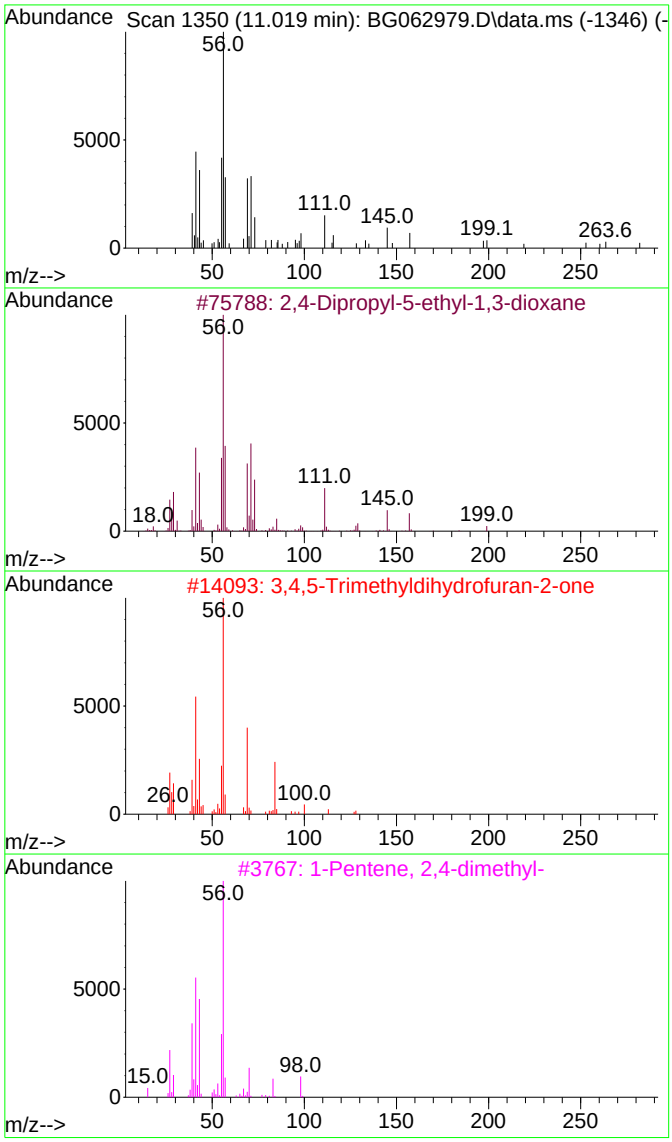
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

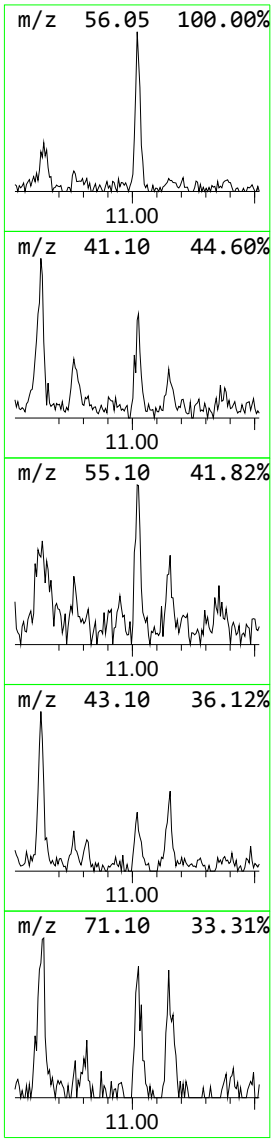
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.019	2.62 ng/ul	61038	Naphthalene-d8	10.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	56
2	3,4,5-Trimethyldihydrofuran-2-one	128	C7H12O2	1000194-05-2	43
3	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	43
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	43
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

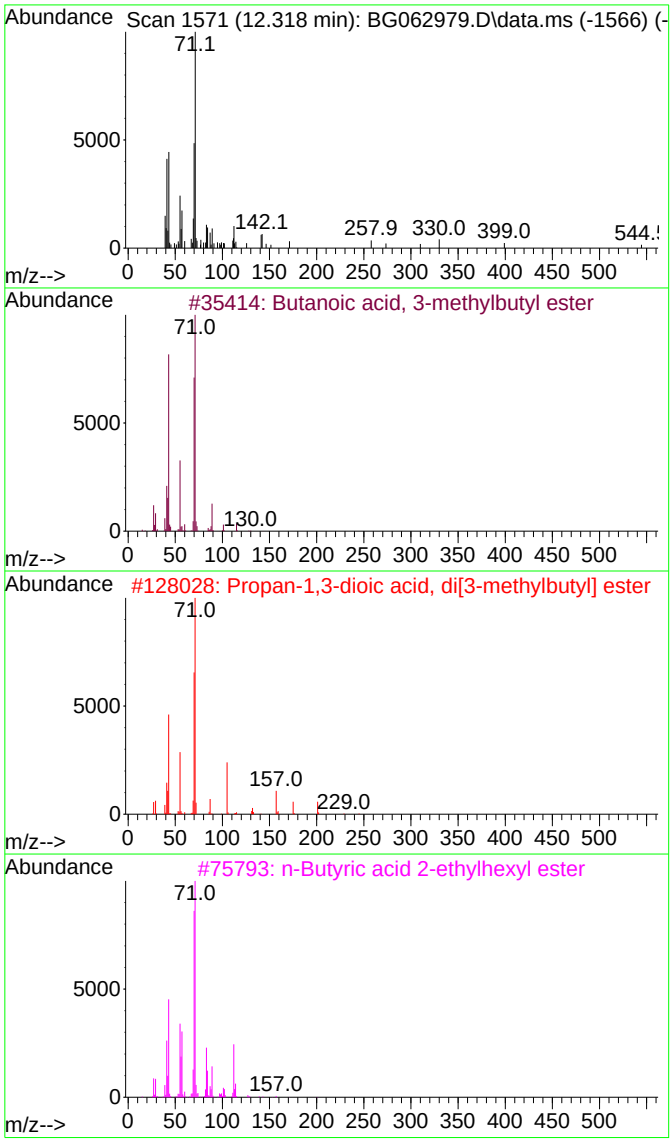
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

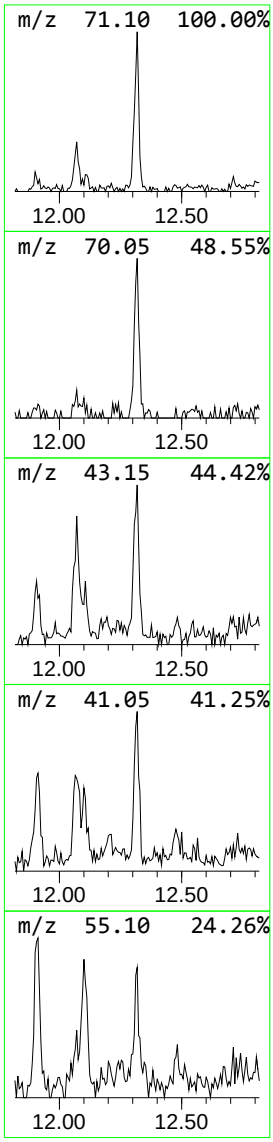
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, 3-methylbuty... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.318	3.22 ng/ul	74907	Naphthalene-d8	10.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	59
2	Propan-1,3-dioic acid, di[3-meth...	244	C13H24O4	064617-96-5	53
3	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	52
4	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	50
5	6-Methyl-2-heptanol, 2-methylpro...	200	C12H24O2	1000447-36-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

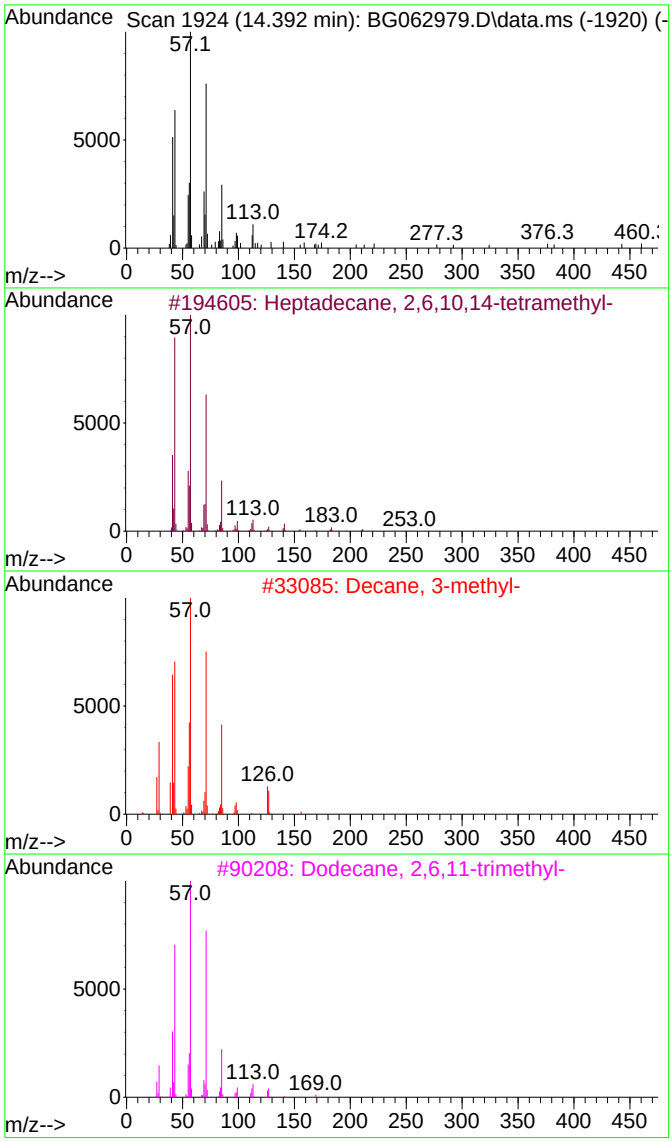
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

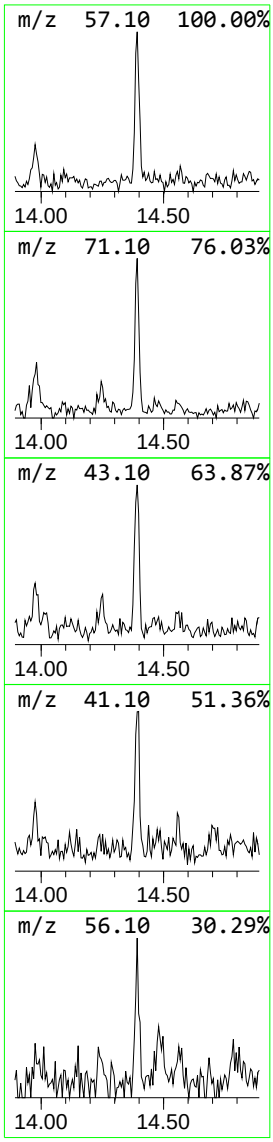
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	2.09 ng/ul	63995	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	78
2	Decane, 3-methyl-	156	C11H24	013151-34-3	72
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
4	Undecane, 2-methyl-	170	C12H26	007045-71-8	64
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062979.D
Acq On : 20 Sep 2024 15:26
Operator : JU/RC
Sample : P3898-03MEDL 5X
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC14MEDL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.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
(DEL) Alkane: S...	7.482	8.2	ng/ul	130039	1	7.852	317943	20.0
1-Hexanol, 2-et...	7.923	4.4	ng/ul	70291	1	7.852	317943	20.0
unknown-01	8.076	2.0	ng/ul	32197	1	7.852	317943	20.0
(DEL) Alkane: S...	9.080	6.6	ng/ul	104807	1	7.852	317943	20.0
2,4-Dipropyl-5-...	11.019	2.6	ng/ul	61038	2	10.643	465258	20.0
Butanoic acid, ...	12.318	3.2	ng/ul	74907	2	10.643	465258	20.0
(DEL) Alkane: S...	14.392	2.1	ng/ul	63995	3	14.486	611326	20.0