LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DDC73DL

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: BG062926.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.743	107	111	119	rBV	31641	54810	3.79%	0.474%
2	4.982	317	322	329	rBV2	58763	86518	5.98%	0.748%
3	5.347	382	384	389	rVB4	3730	4205	0.29%	0.036%
4	5.887	472	476	480	rBV2	17279	21960	1.52%	0.190%
5	6.122	513	516	517	rBV	4832	4498	0.31%	0.039%
6	6.175	520	525	530	rVB2	42715	71948	4.98%	0.622%
7	6.351	552	555	560	rBV3	4967	8845	0.61%	0.076%
8	6.422	564	567	572	rVB3	9472	14308	0.99%	0.124%
9	6.745	619	622	623	rBV2	4046	4131	0.29%	0.036%
10	6.909	646	650	654	rBV3	14798	22301	1.54%	0.193%
11	6.956	654	658	662	rVB4	13768	21390	1.48%	0.185%
12	7.027	662	670	676	rBV	97720	182482	12.62%	1.577%
13	7.186	691	697	703	rBV	54578	91153	6.30%	0.788%
14	7.244	705	707	711	rVV3	8736	13173	0.91%	0.114%
15	7.280	711	713	719	rVB3	15410	22601	1.56%	0.195%
16	7.391	727	732	740	rVB2	73356	123881	8.57%	1.071%
17	7.485	742	748	756	rBV3	67216	124454	8.61%	1.076%
18	7.661	775	778	781	rBV4	5341	6938	0.48%	0.060%
19	7.691	781	783	788	rVB4	4387	6271	0.43%	0.054%
20	7.855	805	811	818	rBV2	182616	312742	21.63%	2.703%
21	7.973	827	831	835	rBV6	7211	12129	0.84%	0.105%
22	8.120	852	856	858	rBV4	5958	8262	0.57%	0.071%
23	8.278	877	883	889	rBV2	74132	120404	8.33%	1.041%
24	8.390	899	902	908	rVB3	10571	18036	1.25%	0.156%
25	8.443	908	911	915	rBV3	7864	12779	0.88%	0.110%
26	8.560	926	931	937	rVB2	92620	156004	10.79%	1.348%
27	8.813	969	974	975	rBV5	6580	10083	0.70%	0.087%
28	8.854	977	981	986	rVB4	10221	18893	1.31%	0.163%
29	8.972	995	1001	1002	rBV3	9171	17160	1.19%	0.148%
30	9.007	1002	1007	1014	rVV3	67672	123275	8.53%	1.066%
31	9.083	1014	1020	1025	rVB2	55974	89456	6.19%	0.773%
32	9.160	1028	1033	1035	rBV4	8233	13717	0.95%	0.119%
33	9.283	1052	1054	1056	rBV2	4720	4913	0.34%	0.042%
34	9.618	1109	1111	1112	rBV2	3631	3807	0.26%	0.033%
35	9.724	1123	1129	1135	rBV3	70140	129652	8.97%	1.121%
36	10.006	1170	1177	1180	rBV7	5871	12812	0.89%	0.111%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

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	10.182	1204	1207	1213	rVB6	5986	9633	0.67%	0.083%
38	10.270	1216	1222	1228	rVB	101602	183464	12.69%	1.586%
39	10.329	1230	1232	1234	rBV2	4844	4857	0.34%	0.042%
40	10.640	1276	1285	1293	rBV	290783	570063	39.43%	4.927%
41	10.775	1302	1308	1319	rVB4	86831	194483	13.45%	1.681%
42	10.869	1322	1324	1328	rVB5	4924	5654	0.39%	0.049%
43	10.916	1328	1332	1335	rBV6	4894	8796	0.61%	0.076%
44	11.016	1347	1349	1358	rVB5	15103	27411	1.90%	0.237%
45	11.116	1363	1366	1367	rBV2	3961	4092	0.28%	0.035%
46	11.375	1402	1410	1412	rBV4	5448	9215	0.64%	0.080%
47	11.669	1456	1460	1468	rBV4	13411	27153	1.88%	0.235%
48	11.727	1468	1470	1474	rVB5	3770	4708	0.33%	0.041%
49	11.763	1474	1476	1479	rBV2	3683	4997	0.35%	0.043%
50	11.845	1485	1490	1492	rBV4	3295	5552	0.38%	0.048%
51	12.068	1523	1528	1531	rBV3	17499	29595	2.05%	0.256%
52	12.485	1593	1599	1603	rBV5	18068	34939	2.42%	0.302%
53	13.320	1735	1741	1747	rVB4	20757	37204	2.57%	0.322%
54	13.531	1773	1777	1783	rVB8	14096	25559	1.77%	0.221%
55	13.607	1787	1790	1792	rBV3	7109	6220	0.43%	0.054%
56	13.672	1792	1801	1804	rBV5	16369	36218	2.51%	0.313%
57	13.889	1833	1838	1845	rVB	182636	280438	19.40%	2.424%
58	13.972	1850	1852	1858	rVB4	8673	11232	0.78%	0.097%
59	14.177	1882	1887	1893	rBV	189865	289277	20.01%	2.500%
60	14.389	1920	1923	1927	rBV2	21206	24812	1.72%	0.214%
61	14.489	1934	1940	1948	rVB	445843	667269	46.15%	5.768%
62	14.624	1961	1963	1965	rVB3	6633	4705	0.33%	0.041%
63	14.689	1969	1974	1988	rBV4	64805	149511	10.34%	1.292%
64	15.012	2027	2029	2030	rBV2	5364	3705	0.26%	0.032%
65	15.117	2042	2047	2052	rBV2	117664	169061	11.69%	1.461%
66	15.347	2084	2086	2090	rVB2	25922	26202	1.81%	0.226%
67	15.482	2103	2109	2116	rVB	262559	398052	27.53%	3.441%
68	15.599	2125	2129	2134	rBV2	66880	94182	6.51%	0.814%
69	15.852	2167	2172	2178	rVB3	33172	51239	3.54%	0.443%
70	16.210	2228	2233	2242	rBV4	25340	56296	3.89%	0.487%
71	16.704	2314	2317	2318	rBV2	4333	4029	0.28%	0.035%
72	16.892	2343	2349	2363	rBV	928459	1445828	100.00%	12.497%
73	16.998	2365	2367	2372	rVB3	24230	28857	2.00%	0.249%
74	17.238	2402	2408	2419	rBV	607423	880440	60.90%	7.610%
75	17.338	2419	2425	2430	rVV	297149	442260	30.59%	3.823%
76	17.744	2491	2494	2501	rVB3	24994	28067	1.94%	0.243%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

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	17.855	2510	2513	2519	rVB8	26233	38430	2.66%	0.332%
78	17.914	2519	2523	2528	rBV2	37625	48218	3.33%	0.417%
79	18.437	2608	2612	2615	rBV2	20727	27026	1.87%	0.234%
80	19.324	2761	2763	2764	rBV	6929	3782	0.26%	0.033%
81	19.636	2810	2816	2823	rBV	378552	557603	38.57%	4.820%
82	21.492	3126	3132	3138	rBV2	633252	996760	68.94%	8.616%
83	24.318	3607	3613	3624	rVB	223940	538147	37.22%	4.652%
84	24.536	3641	3650	3662	rVB2	397457	1123897	77.73%	9.715%

Sum of corrected areas: 11569129

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
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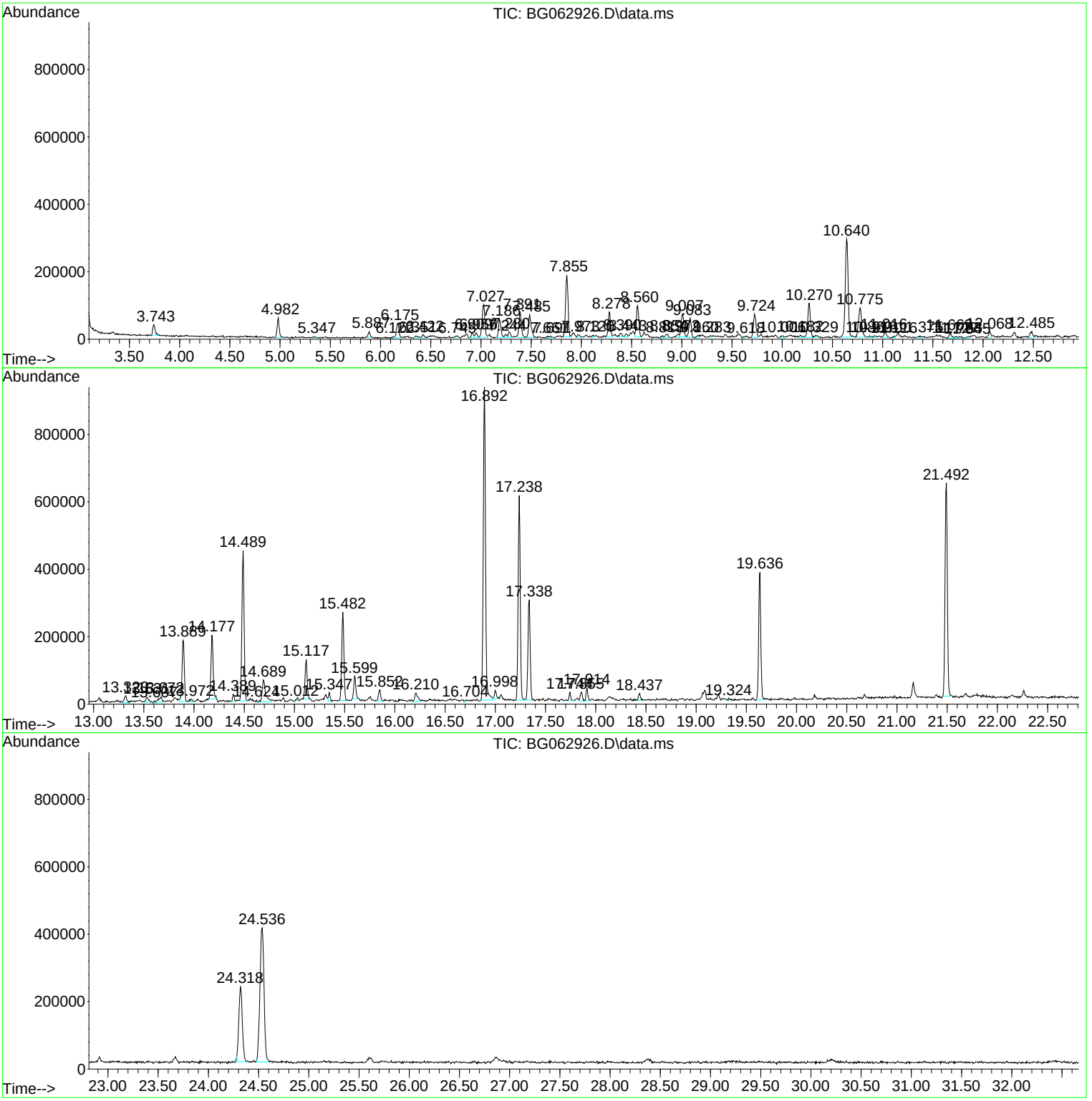
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

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 : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

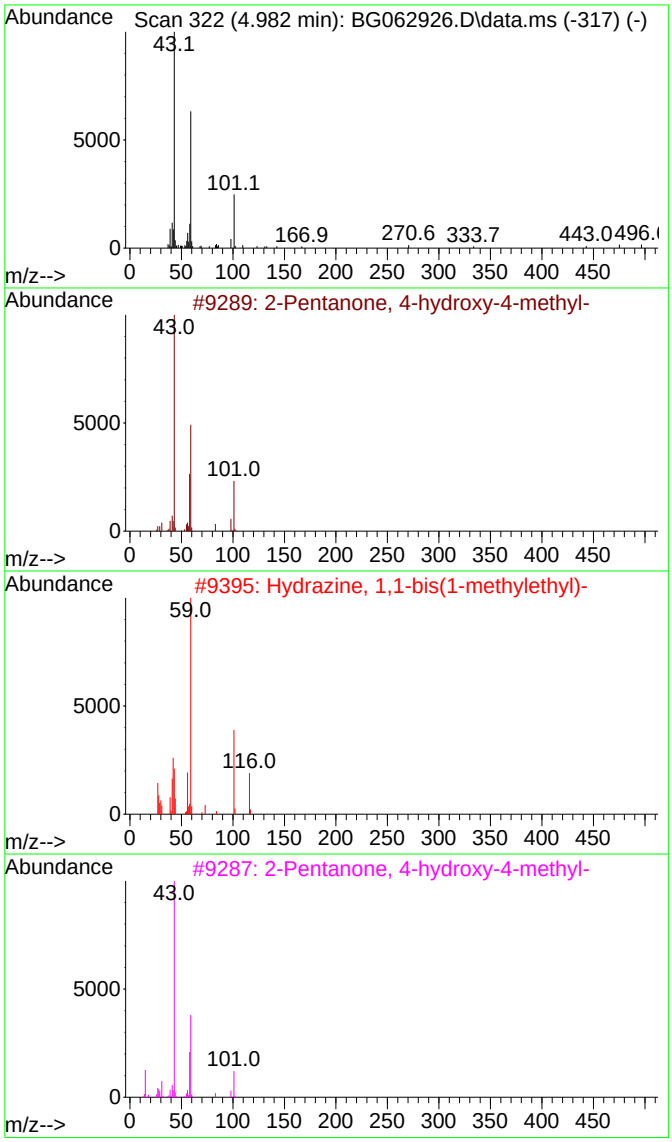
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

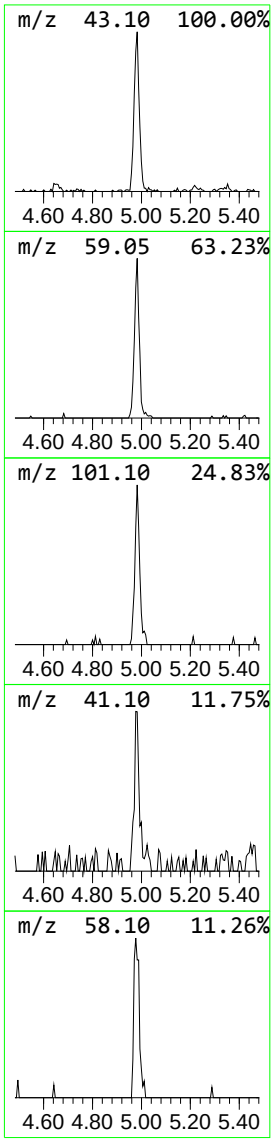
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.982	5.53 ng/ul	86518	1,4-Dichlorobenzene-d4	7.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	43
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

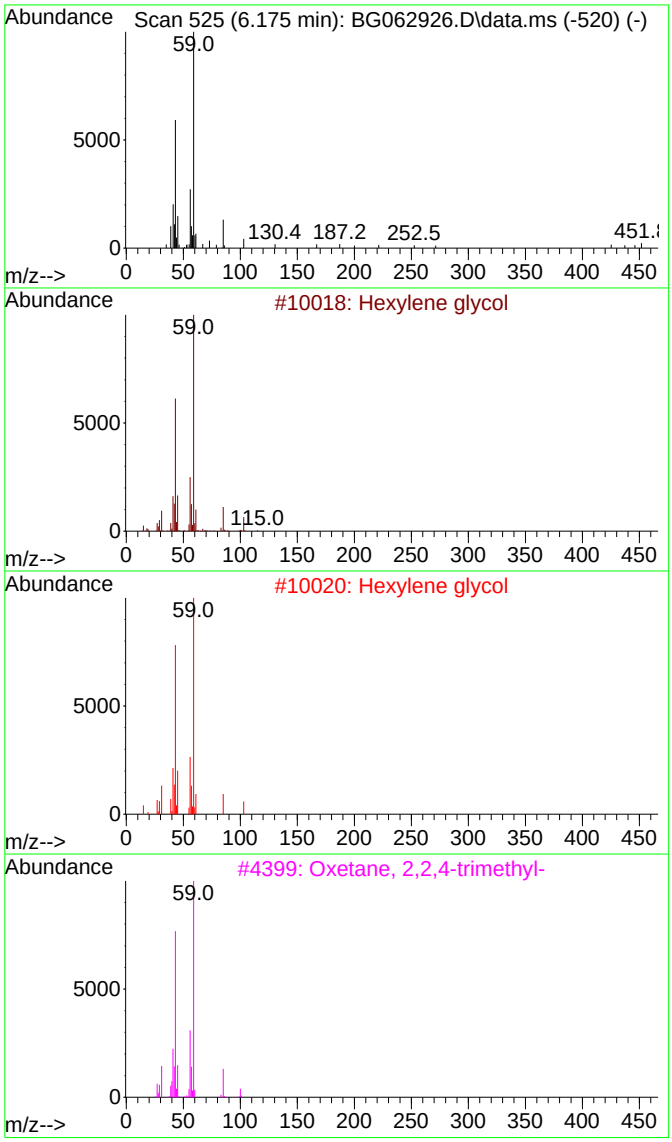
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

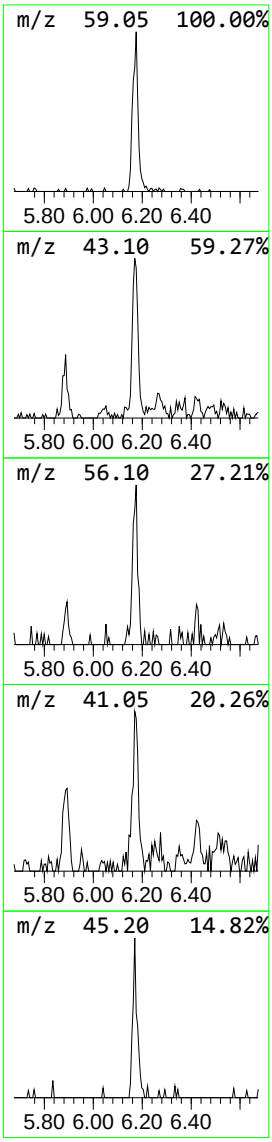
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.175	4.60 ng/ul	71948	1,4-Dichlorobenzene-d4	7.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	72
2	Hexylene glycol	118	C6H14O2	000107-41-5	72
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	72
4	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	56
5	Hexane, 1-ethoxy-	130	C8H18O	005756-43-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

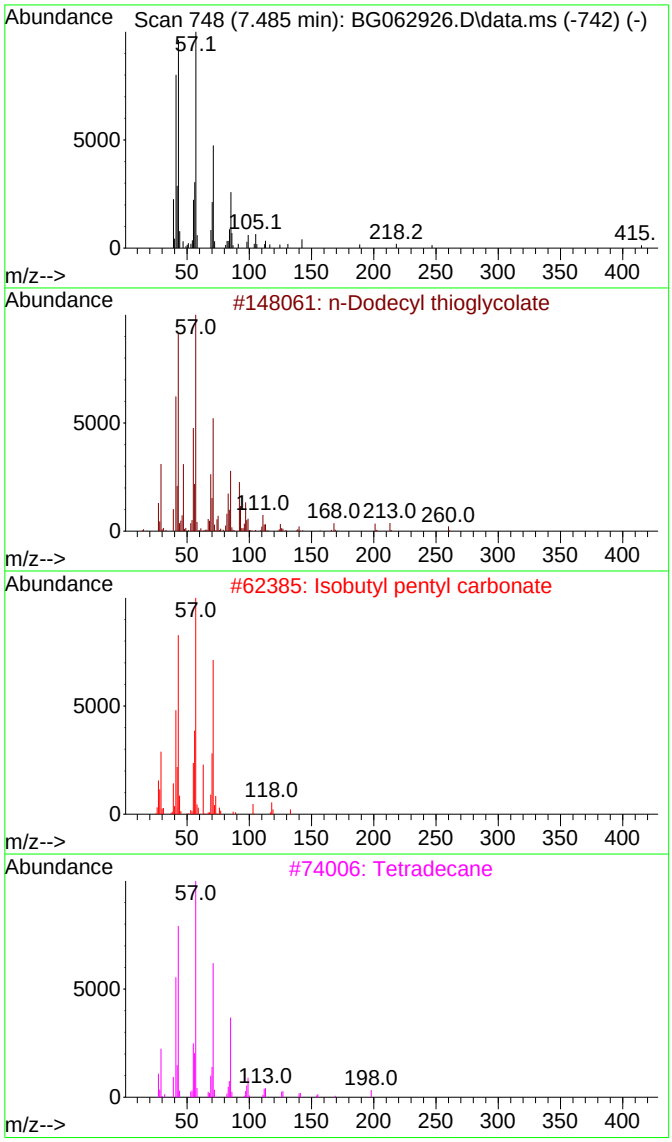
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

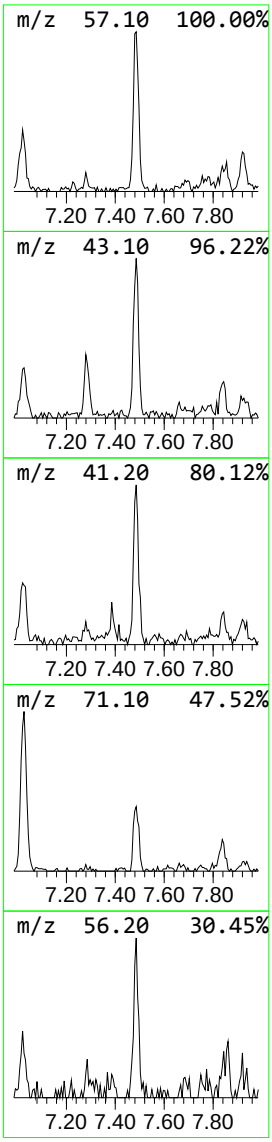
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Dodecyl thioglycolate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.485	7.96 ng/ul	124454	1,4-Dichlorobenzene-d4	7.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl thioglycolate	260	C14H28O2S	003746-39-2	64
2	Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	59
3	Tetradecane	198	C14H30	000629-59-4	59
4	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	58
5	Hexadecane	226	C16H34	000544-76-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

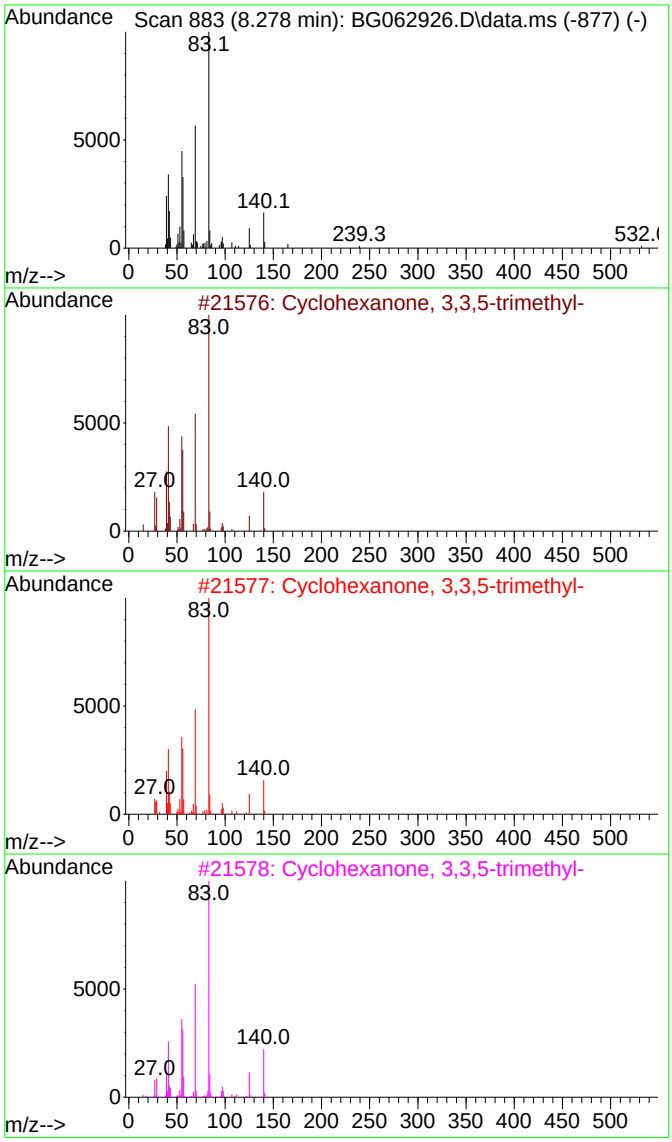
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

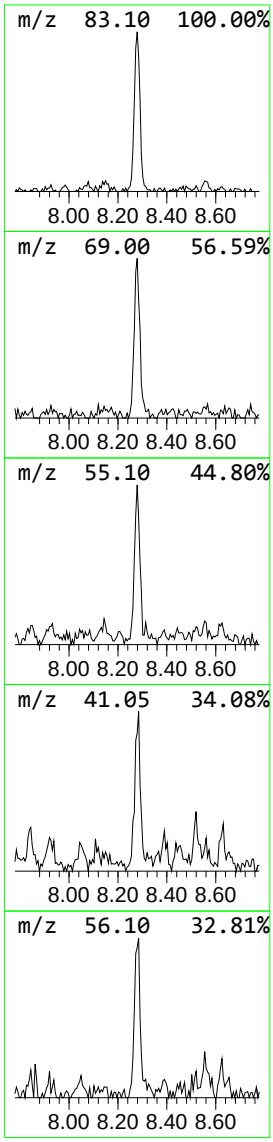
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.278	7.70 ng/ul	120404	1,4-Dichlorobenzene-d4	7.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
2	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
3	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	83
5	3,3-Dimethylcyclohexanone	126	C8H14O	002979-19-3	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

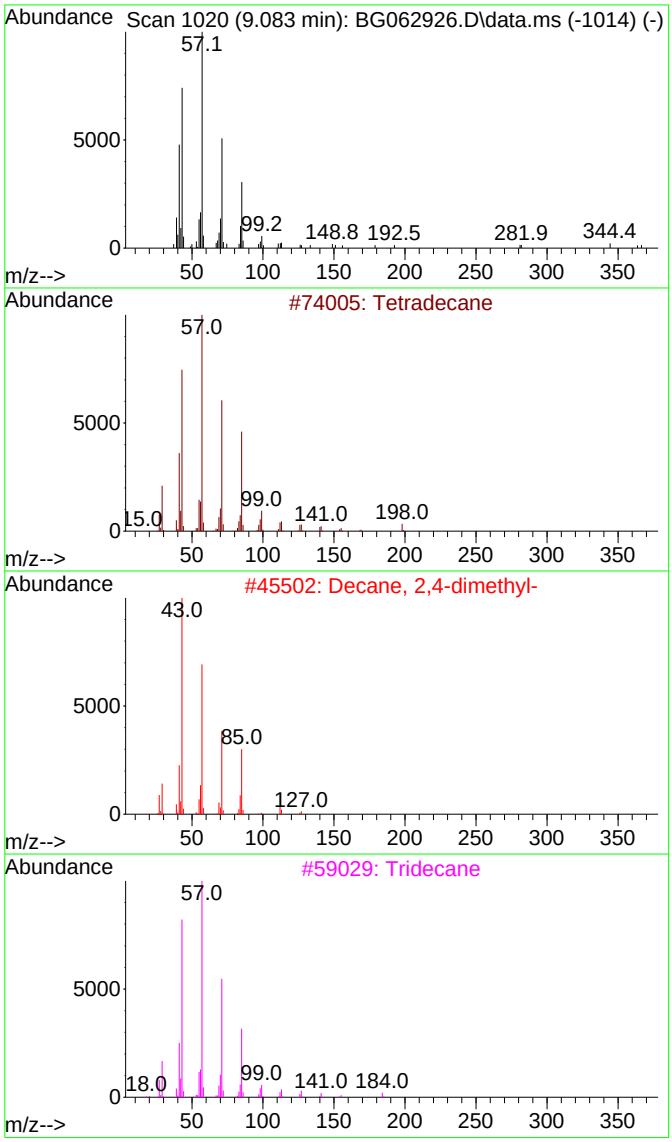
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091724.MA.M
Quant Title : SVOA CALIBRATION

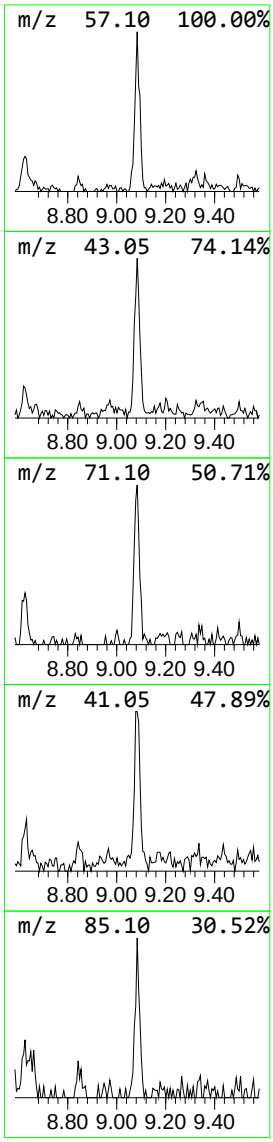
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.083	5.72 ng/ul	89456	1,4-Dichlorobenzene-d4	7.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	80
2	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	80
3	Tridecane	184	C13H28	000629-50-5	72
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
5	Tridecane	184	C13H28	000629-50-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091824\
Data File : BG062926.D
Acq On : 19 Sep 2024 3:00
Operator : JU/RC
Sample : P3899-22DL 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DDC73DL

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
2-Pentanone, 4-...	4.982	5.5	ng/ul	86518	1	7.855	312742	20.0
Hexylene glycol	6.175	4.6	ng/ul	71948	1	7.855	312742	20.0
n-Dodecyl thiog...	7.485	8.0	ng/ul	124454	1	7.855	312742	20.0
Cyclohexanone, ...	8.278	7.7	ng/ul	120404	1	7.855	312742	20.0
(DEL) Alkane: S...	9.083	5.7	ng/ul	89456	1	7.855	312742	20.0