LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A4BP6

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: BG061625.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.470	27	31	36	rVB2	22100	29856	1.27%	0.110%
2	3.734	73	76	85	rBV	52650	82775	3.51%	0.304%
3	3.893	99	103	111	rBV2	55432	86661	3.67%	0.319%
4	4.004	118	122	126	rBV3	24571	34771	1.47%	0.128%
5	4.069	131	133	138	rVB5	5998	8208	0.35%	0.030%
6	4.386	184	187	189	rBV4	4514	6055	0.26%	0.022%
7	4.604	220	224	226	rBV5	3360	3801	0.16%	0.014%
8	4.739	242	247	251	rBV4	8779	16160	0.69%	0.059%
9	4.792	251	256	265	rVB3	36687	61817	2.62%	0.227%
10	4.938	277	281	284	rBV5	4816	6557	0.28%	0.024%
11	4.985	286	289	293	rVB4	3444	4191	0.18%	0.015%
12	5.038	295	298	302	rBV5	5138	7937	0.34%	0.029%
13	5.150	313	317	322	rVB	38745	58166	2.47%	0.214%
14	5.238	327	332	337	rBV2	16694	27540	1.17%	0.101%
15	6.043	464	469	471	rBV5	2933	4085	0.17%	0.015%
16	6.137	478	485	490	rBV5	13255	25730	1.09%	0.095%
17	6.730	582	586	590	rVB3	2639	3687	0.16%	0.014%
18	7.012	631	634	639	rBV7	6849	12015	0.51%	0.044%
19	7.212	661	668	678	rVB	346581	606146	25.70%	2.228%
20	7.400	692	700	706	rBV	257617	428871	18.18%	1.576%
21	7.600	727	734	741	rBV	337843	571168	24.21%	2.100%
22	7.665	741	745	748	rVV2	13945	20582	0.87%	0.076%
23	7.929	788	790	793	rVB2	4611	4776	0.20%	0.018%
24	7.970	793	797	798	rBV2	3112	4712	0.20%	0.017%
25	8.076	808	815	821	rBV	247179	420757	17.84%	1.547%
26	8.129	821	824	830	rVB5	8114	13932	0.59%	0.051%
27	8.305	848	854	857	rBV4	5942	11221	0.48%	0.041%
28	8.763	925	932	939	rBV	361713	614601	26.05%	2.259%
29	8.828	939	943	947	rVV5	12287	19939	0.85%	0.073%
30	8.899	950	955	962	rVB3	38429	66675	2.83%	0.245%
31	9.239	1005	1013	1019	rBV	334559	583237	24.73%	2.144%
32	9.392	1037	1039	1046	rVB6	5637	9690	0.41%	0.036%
33	9.627	1073	1079	1082	rBV4	5005	8650	0.37%	0.032%
34	9.792	1100	1107	1114	rBV3	30398	53265	2.26%	0.196%
35	9.891	1121	1124	1128	rBV3	3198	5297	0.22%	0.019%
36	9.962	1128	1136	1143	rVV	279762	486578	20.63%	1.789%

LSC Area Percent Report

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Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

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	10.068	1146	1154	1159	rBV2	16932	35202	1.49%	0.129%
38	10.150	1166	1168	1170	rBV3	6303	7601	0.32%	0.028%
39	10.267	1185	1188	1191	rBV3	4111	5929	0.25%	0.022%
40	10.491	1219	1226	1233	rBV	458653	809683	34.33%	2.976%
41	10.655	1251	1254	1256	rVB4	4764	4218	0.18%	0.016%
42	10.808	1277	1280	1284	rBV5	3947	5759	0.24%	0.021%
43	10.884	1286	1293	1306	rBV	376888	722496	30.63%	2.656%
44	11.014	1308	1315	1323	rBV2	91693	199311	8.45%	0.733%
45	11.413	1379	1383	1390	rVB6	20222	33556	1.42%	0.123%
46	11.525	1399	1402	1405	rBV3	4534	6059	0.26%	0.022%
47	11.619	1411	1418	1427	rBV	74882	146714	6.22%	0.539%
48	11.995	1479	1482	1485	rBV3	3187	4947	0.21%	0.018%
49	12.465	1557	1562	1568	rVB3	11578	19536	0.83%	0.072%
50	12.535	1570	1574	1577	rBV3	7415	10000	0.42%	0.037%
51	12.718	1601	1605	1606	rBV2	3608	4085	0.17%	0.015%
52	12.747	1608	1610	1615	rVV4	4714	7805	0.33%	0.029%
53	13.076	1661	1666	1668	rBV5	7732	13549	0.57%	0.050%
54	13.158	1678	1680	1683	rVB3	4444	4693	0.20%	0.017%
55	13.246	1691	1695	1696	rVB4	3806	4608	0.20%	0.017%
56	13.305	1700	1705	1708	rBV4	7386	11304	0.48%	0.042%
57	13.417	1721	1724	1728	rVB4	2886	3809	0.16%	0.014%
58	13.452	1728	1730	1734	rBV3	3657	3818	0.16%	0.014%
59	13.669	1762	1767	1771	rVB5	29372	42926	1.82%	0.158%
60	13.816	1789	1792	1797	rBV4	7592	12363	0.52%	0.045%
61	13.875	1798	1802	1809	rVB7	15205	28082	1.19%	0.103%
62	13.963	1816	1817	1823	rBV4	3127	4146	0.18%	0.015%
63	14.028	1823	1828	1831	rBV5	9431	13711	0.58%	0.050%
64	14.104	1834	1841	1848	rBV	844504	1243760	52.73%	4.572%
65	14.186	1853	1855	1859	rVB3	6185	5900	0.25%	0.022%
66	14.233	1859	1863	1864	rBV2	4624	5824	0.25%	0.021%
67	14.339	1877	1881	1884	rBV6	14841	18869	0.80%	0.069%
68	14.398	1884	1891	1901	rVB	931568	1483068	62.87%	5.451%
69	14.557	1913	1918	1921	rBV6	5757	7931	0.34%	0.029%
70	14.698	1935	1942	1951	rBV	574318	992712	42.08%	3.649%
71	14.815	1960	1962	1964	rBV3	6517	7526	0.32%	0.028%
72	14.868	1964	1971	1977	rBV	418289	665148	28.20%	2.445%
73	14.956	1983	1986	1993	rVB7	14302	21261	0.90%	0.078%
74	15.027	1993	1998	2002	rBV7	26974	45453	1.93%	0.167%
75	15.097	2006	2010	2014	rBV3	33257	53475	2.27%	0.197%
76	15.156	2019	2020	2023	rBV3	5316	6021	0.26%	0.022%

LSC Area Percent Report

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Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

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

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Peak separation: 5

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

77	15.244	2032	2035	2038	rBV5	9924	14626	0.62%	0.054%
78	15.691	2104	2111	2117	rBV	1239645	1878472	79.63%	6.905%
79	15.743	2117	2120	2123	rVV4	29767	46506	1.97%	0.171%
80	15.790	2123	2128	2135	rVB	348268	503742	21.36%	1.852%
81	16.037	2167	2170	2178	rVB10	11718	18719	0.79%	0.069%
82	16.184	2193	2195	2197	rBV2	9310	6583	0.28%	0.024%
83	16.407	2230	2233	2236	rBV4	13961	17059	0.72%	0.063%
84	16.754	2290	2292	2295	rVB4	8805	4744	0.20%	0.017%
85	17.095	2345	2350	2356	rVB4	28318	44066	1.87%	0.162%
86	17.253	2375	2377	2383	rVB3	26552	36480	1.55%	0.134%
87	17.441	2403	2409	2413	rBV	740804	1170711	49.63%	4.303%
88	17.483	2413	2416	2421	rVV	439658	626748	26.57%	2.304%
89	17.541	2421	2426	2436	rVB	1303713	2035586	86.29%	7.482%
90	17.841	2473	2477	2480	rBV	41277	52225	2.21%	0.192%
91	18.335	2555	2561	2571	rBV2	601440	986465	41.82%	3.626%
92	18.511	2586	2591	2595	rBV2	110472	192865	8.18%	0.709%
93	18.846	2646	2648	2654	rVB2	84107	108925	4.62%	0.400%
94	19.486	2753	2757	2764	rVB	1062411	1475966	62.57%	5.425%
95	19.604	2773	2777	2785	rVB	342408	446807	18.94%	1.642%
96	19.821	2808	2814	2817	rBV	1548938	2358870	100.00%	8.671%
97	21.366	3073	3077	3083	rBV3	443402	696805	29.54%	2.561%
98	21.613	3116	3119	3124	rVB	297515	388980	16.49%	1.430%
99	21.707	3127	3135	3139	rBV2	803920	1952375	82.77%	7.177%
100	24.709	3642	3646	3654	rVB2	450727	1007614	42.72%	3.704%

Sum of corrected areas: 27204906

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
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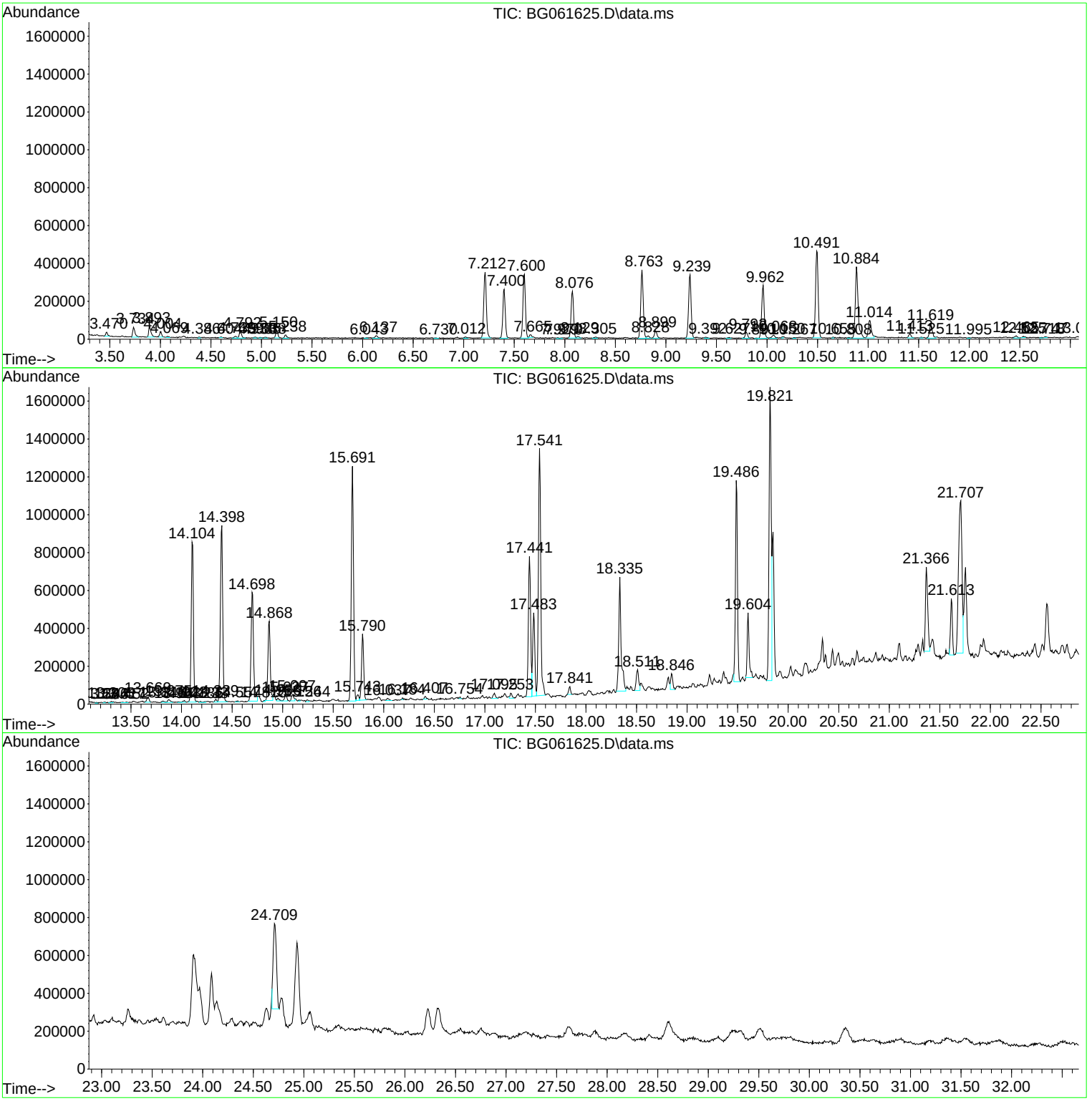
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

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\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

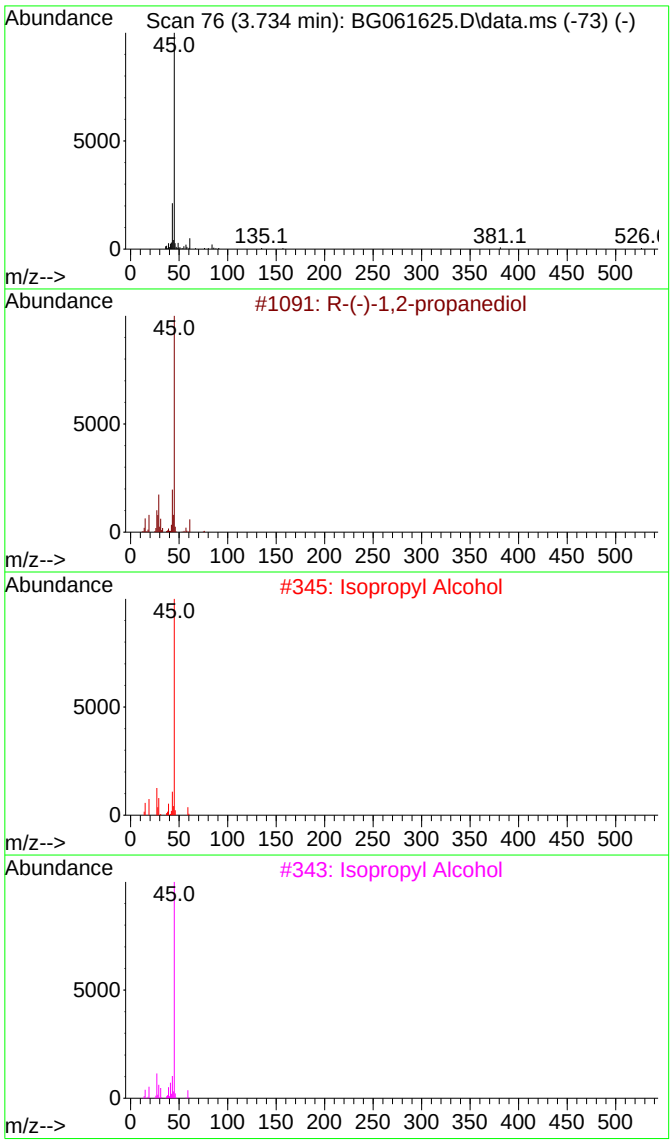
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

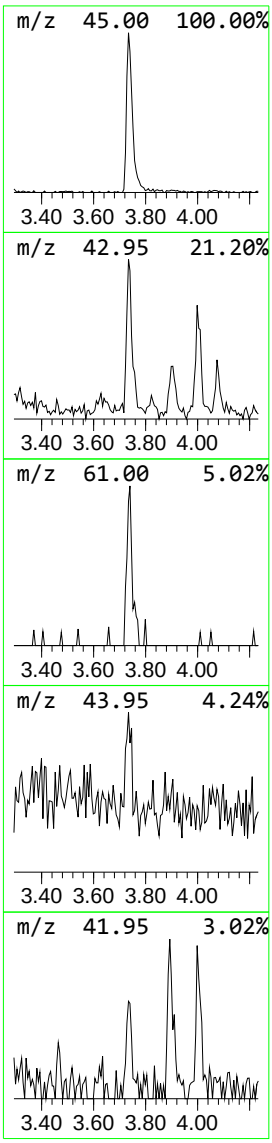
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.734	3.93 ng/ul	82775	1,4-Dichlorobenzene-d4	8.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
5	2-Hexanol	102	C6H14O	000626-93-7	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

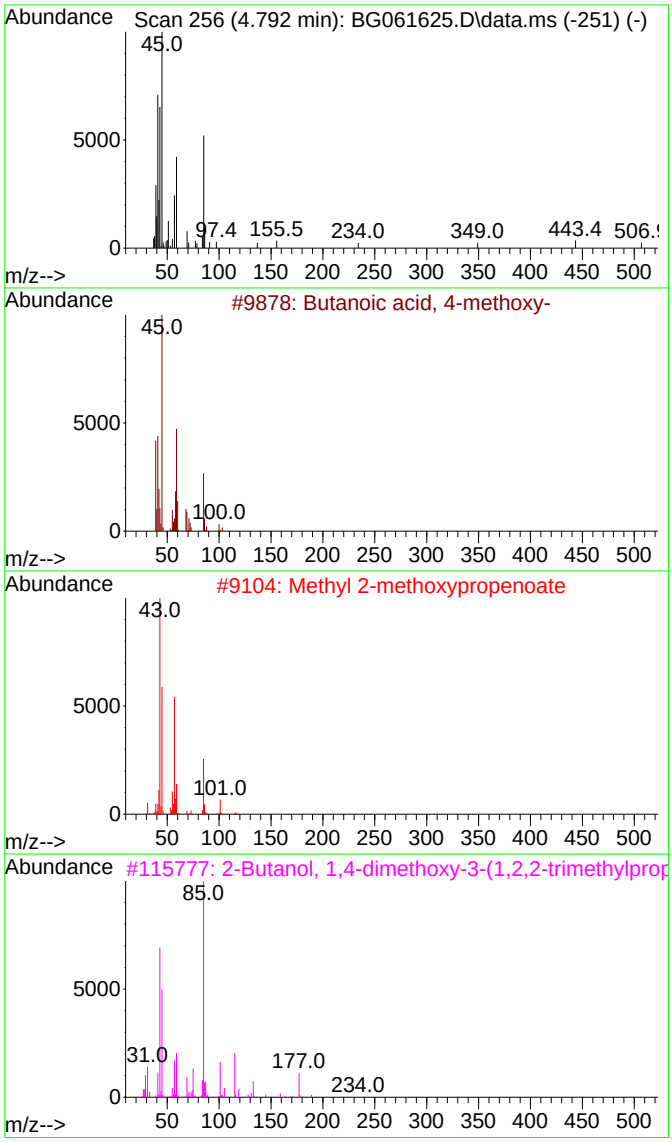
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

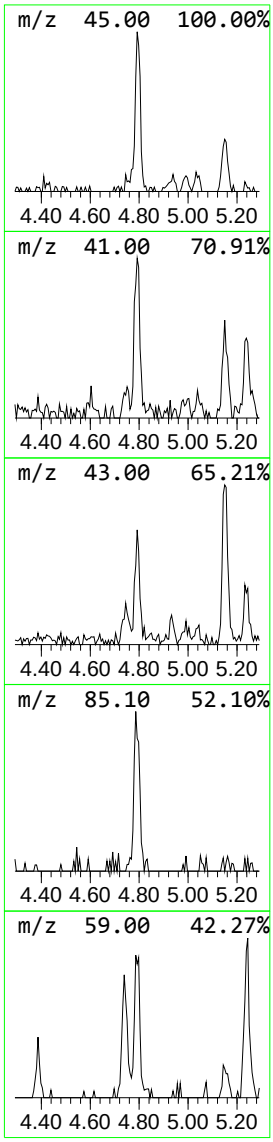
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.792	2.94 ng/ul	61817	1,4-Dichlorobenzene-d4	8.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	40
2	Methyl 2-methoxypropenoate	116	C5H8O3	007001-18-5	39
3	2-Butanol, 1,4-dimethoxy-3-(1,2,...	234	C12H26O4	079449-92-6	33
4	4-Methylpentan-2-yl propyl carbo...	188	C10H20O3	1000372-81-8	25
5	2-Hexanol, 3,4-dimethyl-	130	C8H18O	019550-05-1	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

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

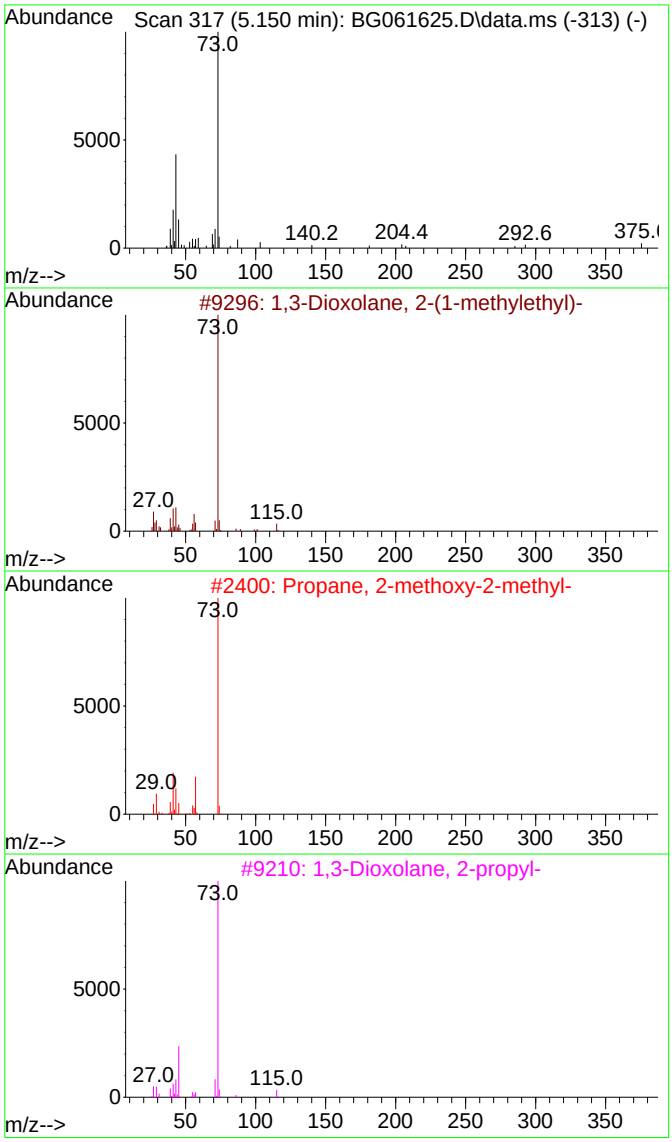
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

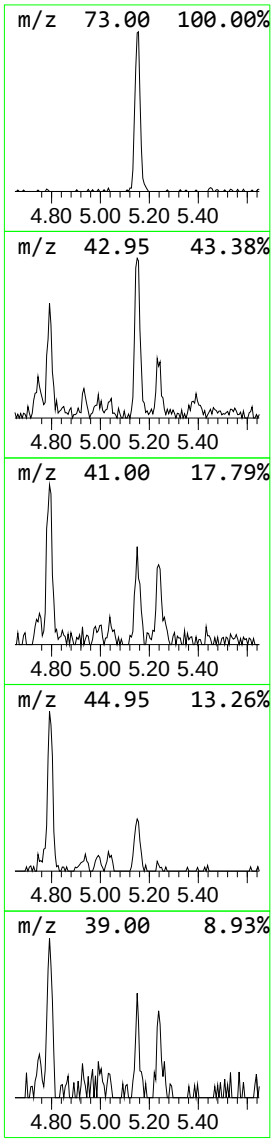
****

Peak Number 3 unknown-02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.150	2.76 ng/ul	58166	1,4-Dichlorobenzene-d4	8.076

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
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Acq On : 21 Jun 2024 18:14
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Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

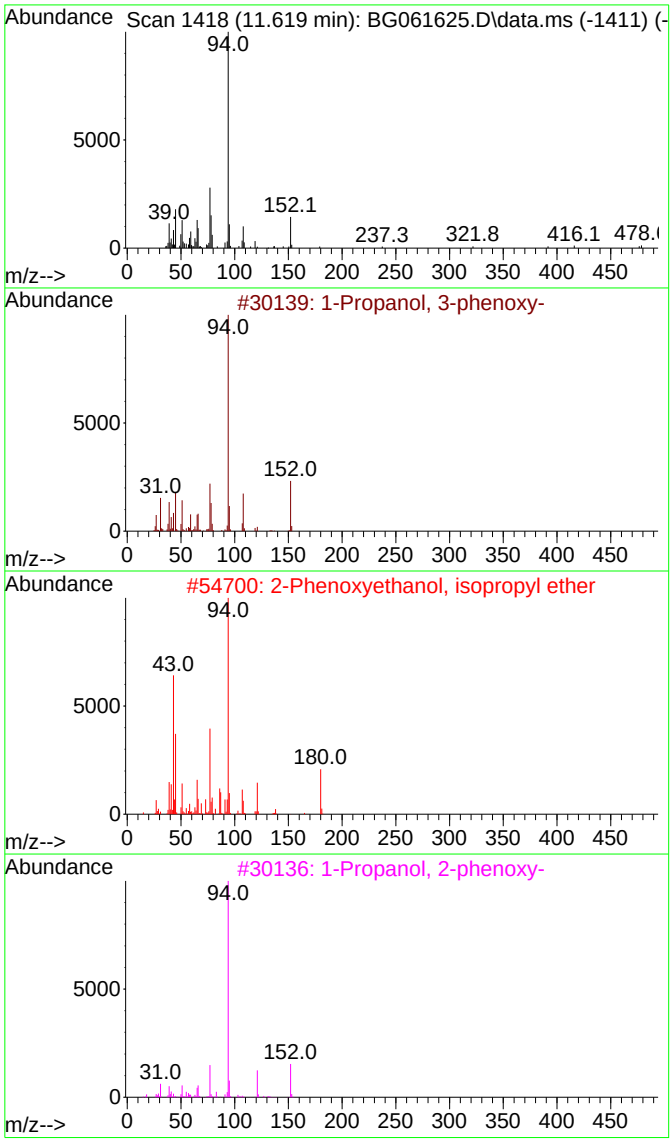
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

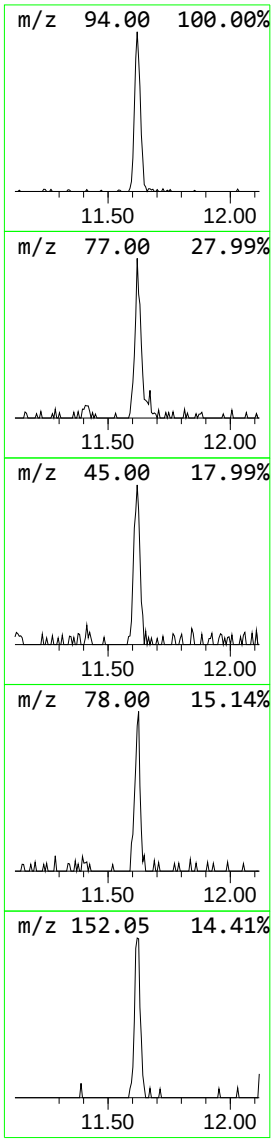
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.619	4.06 ng/ul	146714	Naphthalene-d8	10.884

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
2	2-Phenoxyethanol, isopropyl ether	180	C11H16O2	1000394-79-3	72
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

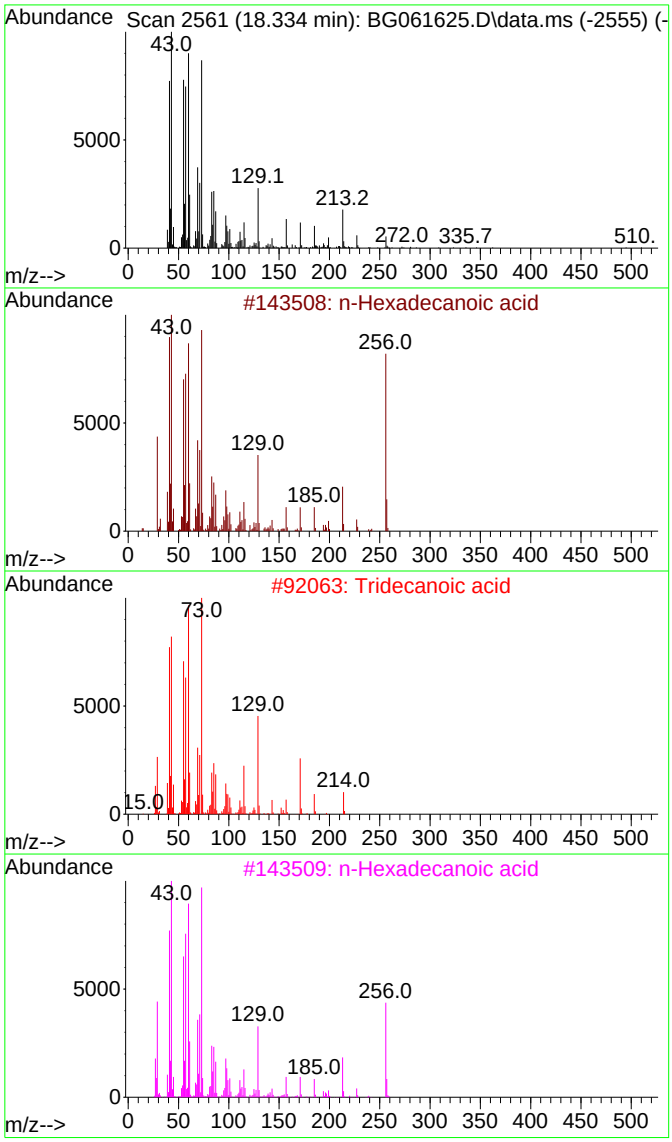
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

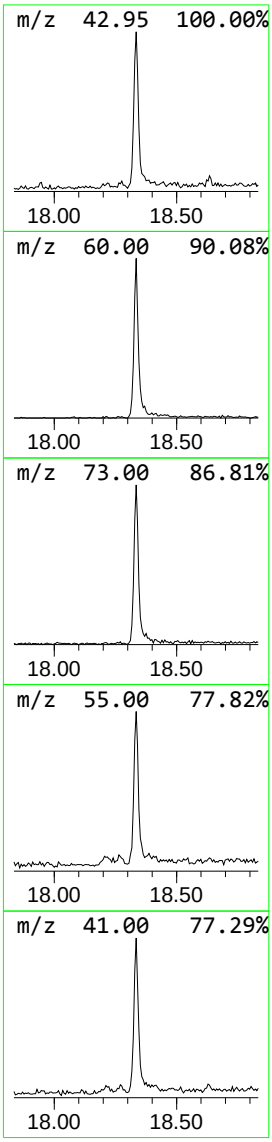
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.334	16.85 ng/ul	986465	Phenanthrene-d10	17.441

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

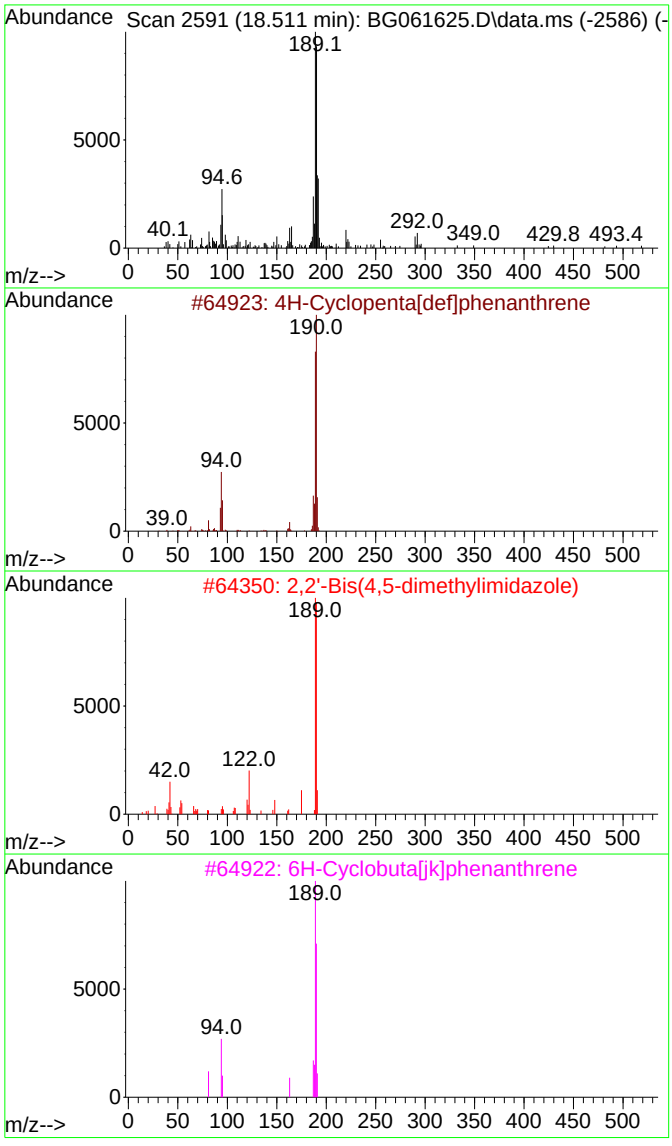
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

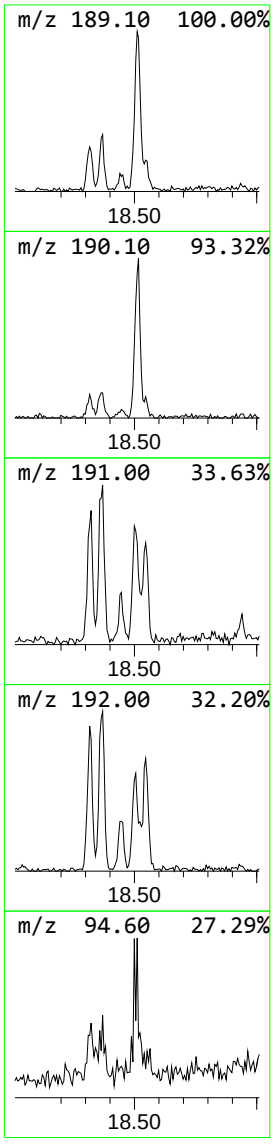
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	3.29 ng/ul	192865	Phenanthrene-d10	17.441

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	74
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

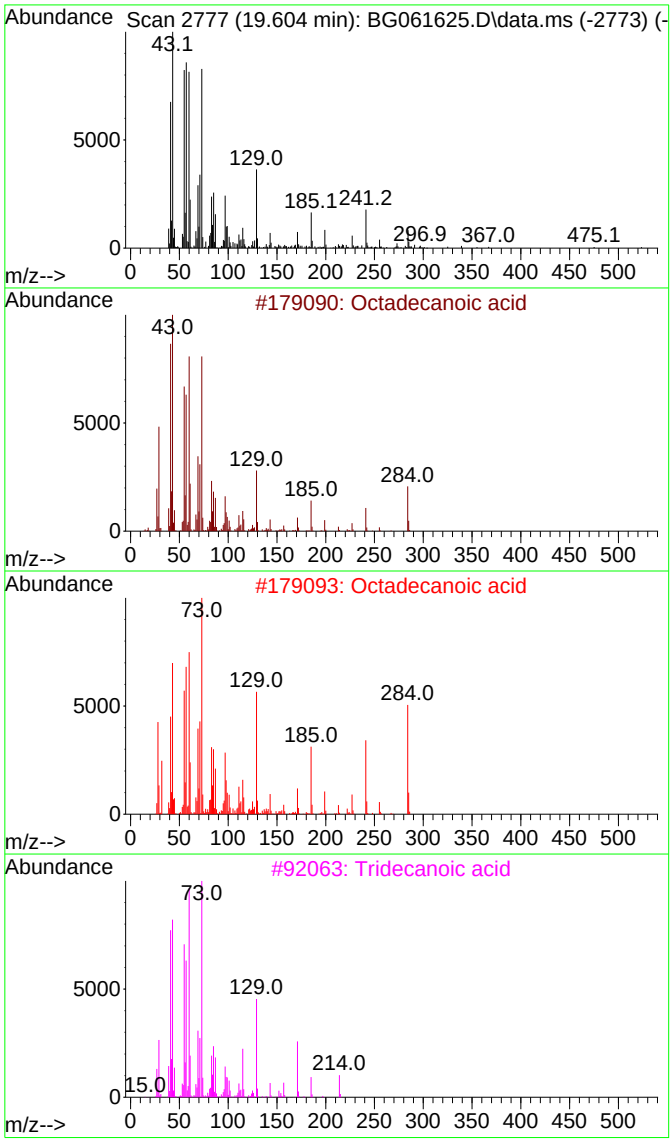
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

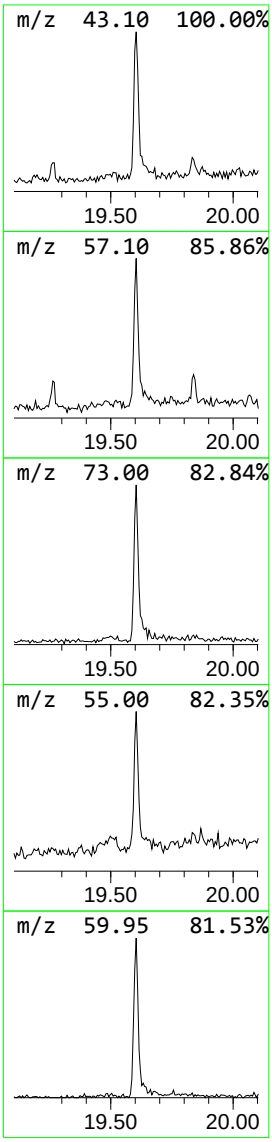
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.604	4.58 ng/ul	446807	Chrysene-d12	21.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

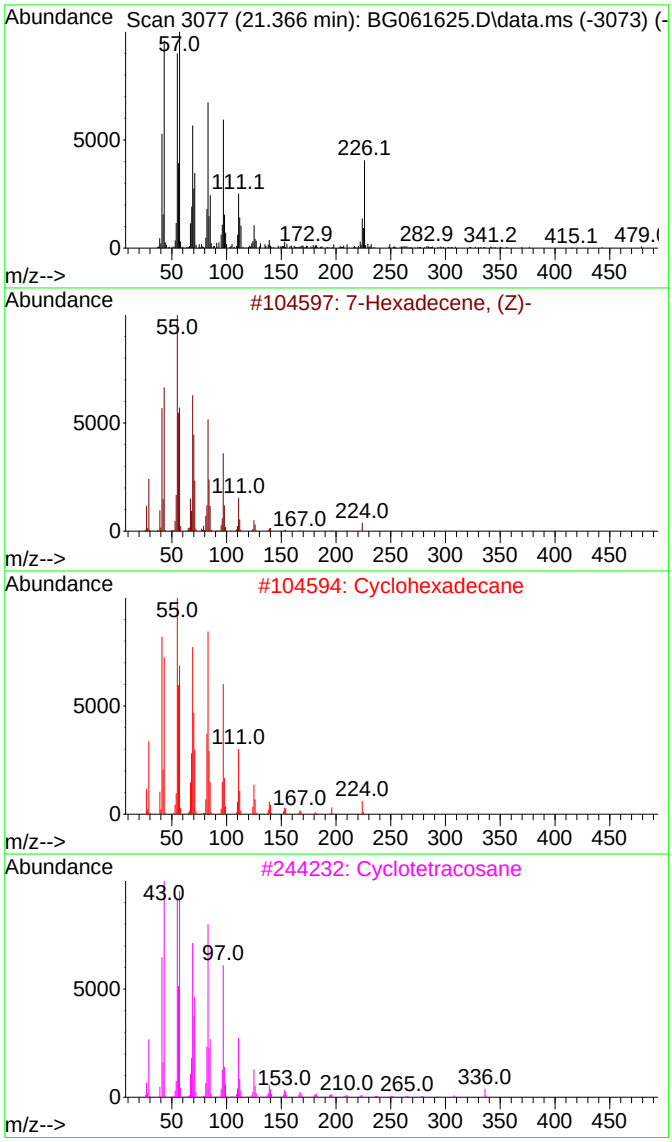
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

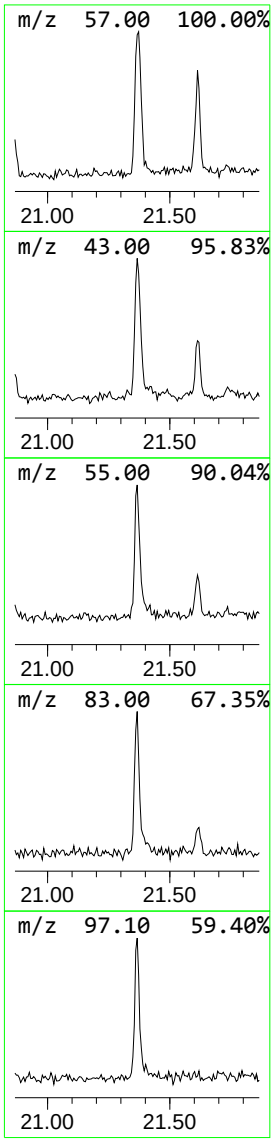
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.366	7.14 ng/ul	696805	Chrysene-d12	21.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	86
2	Cyclohexadecane	224	C16H32	000295-65-8	78
3	Cyclotetracosane	336	C24H48	000297-03-0	70
4	Cetene	224	C16H32	000629-73-2	70
5	1-Docosene	308	C22H44	001599-67-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061625.D
Acq On : 21 Jun 2024 18:14
Operator : MA/JU
Sample : P2754-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP6

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
R-(-)-1,2-propa...	3.734	3.9	ng/ul	82775	1	8.076	420757	20.0
unknown-01	4.792	2.9	ng/ul	61817	1	8.076	420757	20.0
unknown-02	5.150	2.8	ng/ul	58166	1	8.076	420757	20.0
1-Propanol, 3-p...	11.619	4.1	ng/ul	146714	2	10.884	722496	20.0
n-Hexadecanoic ...	18.334	16.9	ng/ul	986465	4	17.441	1170710	20.0
4H-Cyclopenta[d...	18.511	3.3	ng/ul	192865	4	17.441	1170710	20.0
Octadecanoic acid	19.604	4.6	ng/ul	446807	5	21.707	1952380	20.0
(DEL) Alkane: S...	21.366	7.1	ng/ul	696805	5	21.707	1952380	20.0